

FINAL REPORT

Validation of Advanced Molecular Biological Tools to Monitor Chlorinated Solvent Bioremediation and Estimate cVOC Degradation Rates

ER 201726

March 24, 2020

Prepared by:

Mandy Michalsen U.S. Army Engineer Research Development Center

> Kate Kucharzyk, Craig Bartling, Jayda Meisel Battelle Memorial Institute

> > Paul Hatzinger Aptim Federal Services, LLC

John Wilson Scissortail Environmental Solutions, LLC

> Jonathan Istok Oregon State University

> Fadime Kara Murdoch University of Tennessee

Frank Löffler University of Tennessee and Oak Ridge National Laboratory

REPORT DOCUMENTATION PAGE					Form Approved OMB No. 0704-0188			
The public reporting sources, gathering aspect of this colled Operations and Re provision of law, no PLEASE DO NOT	g burden for this colle and maintaining the ction of information, ir ports (0704-0188), 1 person shall be subje RETURN YOUR FOR	ection of information data needed, and o noluding suggestion 215 Jefferson Davi ect to any penalty fo RM TO THE ABOVE	n is estimated to average 1 completing and reviewing th s for reducing the burden, t is Highway, Suite 1204, A or failing to comply with a co E ADDRESS.	hour per respons ne collection of infr o Department of D rlington, VA 22202 Illection of informat	e, including the ormation. Send lefense, Washin 2-4302. Respon cion if it does no	e time for reviewing instructions, searching existing data l comments regarding this burden estimate or any other ngton Headquarters Services, Directorate for Information ndents should be aware that notwithstanding any other ot display a currently valid OMB control number.		
1. REPORT DATE (DD-MM-YYYY) 2. REPORT TYPE					3. DATES COVERED (From - To)			
03/24/2020		ESTCP F	inal Report					
4. TITLE AND S	SUBTITLE				5a. C	ONTRACT NUMBER		
Validation of	Advanced Mole	ecular Biologio	cal Tools to Monitor	Chlorinated				
Solvent Biore	mediation and	Estimate cVC	C Degradation Rat	es	5b. G	5b. GRANT NUMBER		
					5c. Pl	ROGRAM ELEMENT NUMBER		
					5.1 D			
6. AUTHOR(S)			aaarah Davalanna	ant Contor	5d. P	ROJECT NUMBER		
Kata Kuahar	lisen, U.S. Arm	iy Engineer Re	esearch Developme	ent Center	ER-2	01726		
Rate Rucharz	cyk, Craig Barli or Antim Eodo	ral Sonvices I		mai mstitute	5e. T/	ASK NUMBER		
Iohn Wilson	Scissortail Env	vironmental Sci	olutions LLC Frank	Löffler,				
Ionathan Isto	k Oregon Stat	l Iniversity	Unive	ersity of Tenne	ssee 5f. W			
Fadime Kara	Murdoch, Univ	ersity of Tenn	and C	Dak Ridge Nati	onal			
				ratory				
US Army C	orps of Engine	ers	ADDRESS(ES)			REPORT NUMBER		
4735 E. Marc	ainal Way S.	010				ER-201726		
Seattle, WA	98134							
9. SPONSORIN	G/MONITORING	AGENCY NAME	S) AND ADDRESS(ES))		10. SPONSOR/MONITOR'S ACRONYM(S)		
Environmenta	al Security Tecl	hnology Certif	ication Program			ESTCP		
4800 Mark Center Drive, Suite 17D03								
Alexandria, VA 22350-3605				11. SPONSOR/MONITOR'S REPORT				
					NUMBER(S)			
					ER-201726			
12. DISTRIBUT								
DISTRIBUTION STATEMENT A. Approved for public release: distribution unlimited.								
13. SUPPLEME	NTARY NOTES							
14. ABSTRACT								
This demons	tration had thre	e specific obj	ectives. The first ob	jective was to	o demonsti	rate the utility of quantitative proteomics		
(qProt) to me	asure the abso	olute abundan	ce of Dhc reductive	dechlorinatio	on biomark	er proteins in laboratory-controlled		
microcosms v	with various Dr	ic cell titers. C	ontaminant concern	itration and e	inene mea	surements over time were used to		
rates with Dh	s-DCE and VC	reductive deci	niorination rates. Tr		jective was	of objectives 1 and 2 lead to a go/no go		
decision poin	t before condu	cting demonst	ration/validation off	orts of the de	Prot appros	of objectives 1 and 2 lead to a go/no-go		
						ethenes.		
15. SUBJECT TERMS								
validation, Advanced Molecular Biological Tools, Monitor Chlorinated Solvent Bioremediation, cVOC Degradation Rates								
16. SECURITY	CLASSIFICATION	OF:	17. LIMITATION OF	18. NUMBER	19a. NAME	OF RESPONSIBLE PERSON		
a. REPORT	b. ABSTRACT	c. THIS PAGE	ABSTRACT	OF	Mandy Mi	chalsen		
_ ·				PAGES				
				13/	206 764 C			
UNCLASS	UNCLASS	UNCLASS	UNCLASS		206-764-3324			

٦

TABLE OF CONTENTS

EXEC	CUTIVE SUMMARY	vi
1.0 IN	TRODUCTION	1
1.	1 BACKGROUND	1
1.	2 OBJECTIVES OF THE LABORATORY DEMONSTRATION	2
1.	3 REGULATORY DRIVERS	2
2.0 TI	ECHNOLOGY	3
2.	1 TECHNOLOGY DESCRIPTION	3
2.	2 TECHNOLOGY DEVELOPMENT	5
2.	3 ADVANTAGES AND LIMITATIONS OF THE TECHNOLOGY	9
3.0 PH	ERFORMANCE OBJECTIVES	11
4.0 SI	TE DESCRIPTION	14
4.	1 NBK Keyport Area 1, Bremerton, WASHINGTON	14
4.	2 VAFB SITE SA 288, VANDENBERG, CALIFORNIA	16
4.	3 JBLM LANDFILL 2, TACOMA, WASHINGTON	19
5.0 TI	EST DESIGN	21
5.	1 CONCEPTUAL EXPERIMENTAL DESIGN	21
5.	2 BASELINE CHARACTERIZATION ACTIVITIES	22
5.	3 DEVELOPMENT OF RDASE PEPTIDE TARGETS	22
5.	4 ESTABLISHING MDL AND IDL FOR TARGET PEPTIDES	23
5.	5 VALIDATION OF QPROT ASSAY QUANTITATION LIMITS	25
5.	6 LABORATORY MICROCOSM TESTING	26
5.	6.1 Growth of the SDC-9 Inoculum	26
5.	6.2 Microcosm Preparation and Treatments	26
5.	6.3 Microcosm Sampling Procedure	27
5.	7 SAMPLING & ANALYSIS METHODS	30
5.	7.1 Analytical Methods: Standard Geochemical cVOC Analyses	30
5.	7.2 Analytical Methods: Proteomics	31
5.	7.3 Analytical Methods: Quantitative PCR	32
5.	8 DATA ANALYSIS	34
6.0 PI	ERFORMANCE ASSESSMENT	36
6.	1 DETERMINATION OF RDASE TARGETS WITH SHOTGUN PROTEOMICS	36
6.	2 METHOD DETECTION AND INSTRUMENT DETECTION LIMIT RESULTS	37
6.	2 VALIDATION OF MRM ASSAY QUANTITATION LIMITS RESULTS	38
6.	3 MICROCOSM STUDY RESULTS	40
6.	4 BIOMARKERS AS PREDICTORS OF DECHLORINATION RATES	43
6.	5 APPLICABILITY OF LABORATORY STUDY RESULTS TO FIELD SITES	45
7.0 CC	OST ASSESSMENT	48
7.	I COST MODEL	48
7.	2 CUST DRIVERS	50
	5 CUST ANALYSIS	50
8.0 IN	1 PECHLATORY ACCEPTANCE	52
8.	1 KEGULAIUKY ACCEPIANCE	52
8.	LIMITED AVAILABILITY	52
8. • • • •	5 UUST UUMPAKED TU UTHEK MUNITUKING TUULS	33
9.0 KI	LFEKENUES	34

LIST OF TABLES

TABLE 1-1. SAFE DRINKING WATER ACT MAXIMUM CONTAMINANT LEVELS (MCLS) FOR KEY CVOCS	2
TABLE 2-1. RDASE GENES IDENTIFIED IN SDC-9 METAGENOME	7
TABLE 3-1. DEMONSTRATION PERFORMANCE OBJECTIVES FOR THE MICROCOSM STUDY	11
TABLE 5-1. PARAMETERS OF WATERS XEVO CE EQUATION	24
TABLE 5-2. NUMBER OF MICROCOSM TEST SAMPLES BY ANALYSIS	30
TABLE 5-3. SUMMARY OF STANDARD ANALYTICAL AND RDASE BIOMARKER METHODS	30
TABLE 5-4. SUMMARY OF SPECIFIC QPCR ASSAYS RUN FOR MICROCOSM SAMPLES	33
TABLE 6-1. PRM TRANSITIONS OF SELECTED RDASE SDC-9 ENDOGENOUS PEPTIDES	36
TABLE 6-2. MDL FOR PEPTIDES ANALYZED FOR SDC-9 CULTURE	38
TABLE 6-3. RESULTS OF QPROT ASSAY QUANTITATION LIMIT VALIDATION STUDY	39
TABLE 6-4. SUMMARY OF FITTED KCISDCE AND KVC BY MICROCOSM TEST	42
TABLE 6-5. RATE COEFFICIENTS AND BIOMARKER CORRELATIONS	43
TABLE 7-1. COST MODEL FOR PROTEOMICS	49
TABLE 7-2. COST COMPARISON OF CONVENTIONAL MBTS (E.G., QPCR) TO THE ADVANCED MBTS	51

LIST OF FIGURES

FIGURE 2-1. SCHEMATIC OF PROTEOMICS WORKFLOW	4
FIGURE 2-2. RDASE PEPTIDE CONCENTRATIONS VERSUS DEGRADATION RATE CONSTANTS	8
FIGURE 4-1. NBK KEYPORT AREA 1, SITE MAP	15
FIGURE 4-2. VAFB SA288 SITE MAP SHOWING GROUNDWATER CVOC CONCENTRATIONS	18
FIGURE 4-3. JBLM LANDFILL 2 TCE CONCENTRATIONS	20
FIGURE 5-1. MICROCOSM STUDY CONCEPTUAL DESIGN	21
FIGURE 5-2. PHOTOGRAPH OF MICROCOSMS	28
FIGURE 5-3. STEPS INVOLVED IN PROTEOMIC ANALYSIS OF MICROCOSM TEST SAMPLES	31
FIGURE 6-1. CONCENTRATIONS OF VOCS, VFAS AND BROMIDE IN MICROCOSMS.	40
FIGURE 6-2. MEASURED AND MODEL-FITTED CVOC CONCENTRATIONS IN MICROCOSMS	41
FIGURE 6-3. RATE COEFFICIENTS VS. BIOMARKER REGRESSION RESULTS	44
FIGURE 6-4. BIOMARKER-BASED RATE PREDICTIONS VS. MEASURED RATE COEFFICIENTS	45
FIGURE 6-5. RATE COEFFICIENTS VS. BIOMARKER ABUNDANCES WITH TREATMENTS DISTINGUISHED	46
FIGURE 6-6. PROTEIN/DHC CELL RATIOS VS. RATE COEFFICIENTS FOR MICROCOSM TESTS	47

LIST OF APPENDICES

APPENDIX A – MDL/IDL STUDY RESULTS FOR PROTEOMICS APPENDIX B – DILUTION STUDY APPENDIX C – ANALYTICAL SOPS APPENDIX D – MICROCOSM ANALYTICAL AND BIOMARKER ABUNDANCE DATA APPENDIX E – KEY POINTS OF CONTACT

LIST OF ACRONYMS

CE	collision energies
CID MS/MS	collision induced dissociation tandem mass spectrometry
<i>cis</i> -DCE	<i>cis</i> -1,2-dichloroethene
CO ₂	carbon dioxide
CTC	cost to complete
cVOC	chlorinated volatile organic compound
Dhc	<i>Dehalococcoides mccartyi</i>
DoD	Department of Defense
EISB	enhanced <i>in situ</i> bioremediation
EPA	Environmental Protection Agency
ESTCP	Environmental Security and Technology Certification Program
IDA IDL	information dependent acquisitions instrument detection limit
JBLM	Joint Base Lewis-McChord
LC	liquid chromatography
LC-MS/MS	liquid chromatography tandem mass spectrometry
LOD	level of detection
LOQ	level of quantitation
MBT	molecular biological tool
MCL	maximum contaminant level
MDL	method detection limit
MNA	monitored natural attenuation
MRM	multiple reaction monitoring
MS	mass spectrometry
NBK	Naval Base Kitsap
O&M	operation and maintenance
PRM	parallel reaction monitoring
PCE	tetrachloroethene
PI	Principle Investigator
QA	quality assurance
QC	quality control
qPCR	quantitative polymerase chain reaction
qProt	quantitative proteomics
QTOF-MS	quadrupole time-of-flight tandem mass spectrometer
RDase	reductive dehalogenase
ROD	Record of Decision
RPD	relative percent difference
RPM	remediation project manager

LIST OF ACRONYMS (continued)

RT-qPCR	reverse transcriptase qPCR
TCE	trichloroethene
<i>trans</i> -DCE	trans-1,2-dichloroethene
USACE	United States Army Corps of Engineers
VAFB	Vandenberg Air Force Base
VC	vinyl chloride

ACKNOWLEDGEMENTS

This report represents the results and conclusions of a collaborative effort between scientists and engineers at U.S. Army Engineer Research Development Center, Battelle Memorial Institute, Aptim Federal Services, LLC (Aptim), Scissortail Environmental Solutions, LLC, Oregon State University and University of Tennessee, Knoxville. This laboratory phase of the demonstration project was funded by the Environmental Security Technology Certification Program (ESTCP), with the goal of defining and validating correlations between *in situ* degradation rates of chlorinated volatile organic compounds (cVOCs) and quantities of biomarker genes and key reductive dehalogenase proteins (RDase).

Researchers for this project included Dr. Mandy Michalsen (Principal Investigator, U.S. Army Engineer Research Development Center), Dr. Kate Kucharzyk, Dr. Craig Bartling and Dr. Jayda Meisel (Battelle Memorial Institute), Dr. Paul Hatzinger (Aptim), Dr. John Wilson (Scissortail Environmental Solutions, LLC), Dr. Jonathan Istok (Oregon State University), Fadime Kara Murdoch (University of Tennessee, Knoxville) and Dr. Frank Löffler (University of Tennessee, Knoxville and Oak Ridge National Laboratory, Oak Ridge, TN). Several personnel at Battelle Memorial Institute, including Larry Mullins, Amy Hill and Angela Minard-Smith, were instrumental in assisting with metagenomic and metaproteomic data analysis and interpretation. Dr. Fadime Kara Murdoch from the University of Tennessee, Knoxville participated in analysis and interpretation of qPCR and transcript-related data. Other site personnel that provided significant project support included Charles Condee, Anthony Soto, Sheryl Streger, and Simon Vainberg from Aptim.

Finally, the project team wishes to thank Dr. Andrea Leeson and the support staff from the ESTCP program office for their help and guidance throughout this demonstration.

EXECUTIVE SUMMARY

Introduction. Knowledge about the rates of *in situ* contaminant degradation is crucial for optimizing remedial design and supporting site management decisions. Despite progress understanding the factors influencing microbial degradation of chlorinated ethenes, determining rates of microbial contaminant degradation at field sites remains challenging. Molecular biological tool (MBTs) for quantifying *Dehalococcoides mccartyi* (*Dhc*) nucleic biomarkers are available and guide site management decision making; however, these measurements have not been useful to generate good estimates of contaminant degradation rates. Quantification of reductive dehalogenases (RDases) may provide a more direct measure of activity (as these are the actual enzymes/proteins that catalyze biodegradation of chlorinated ethenes), and technological advances in mass spectrometry instrumentation allow the sensitive, quantitative determination of RDase proteins of interest in groundwater. This project explores if RDase gene and protein biomarker abundances, alone or in combination, may be used to estimate degradation rates.

Objectives. This demonstration had three specific objectives. The first objective was to demonstrate the utility of quantitative proteomics (qProt) to measure the absolute abundance of *Dhc* reductive dechlorination biomarker proteins in laboratory-controlled microcosms with various *Dhc* cell titers. Contaminant concentration and ethene measurements over time were used to determine *cis*-DCE and VC reductive dechlorination rates. The second objective was to correlate observed degradation rates with *Dhc* biomarker gene and protein abundances. The successful completion of objectives 1 and 2 lead to a go/no-go decision point before conducting demonstration/validation efforts of the qProt approach at military sites impacted with chlorinated ethenes.

Technology Description. The sensitive and quantitative measurement of proteins in environmental matrices is now possible, and process-specific biomarker proteins such as the *Dhc* RDases TceA, BvcA and VcrA can be measured in groundwater samples. Since the abundances of the catalysts (i.e., the specific RDase enzymes) control the rate of *cis*-DCE and VC reductive dechlorination, the quantitative measurement of these catalysts may be useful for estimating *in situ* degradation rates. Accurate assessment of *in situ* degradation rates often requires *in situ* test design, execution and appropriate data interpretation, which can be costly and time consuming to complete. Demonstration/validation of this qProt tool has significant potential to establish (1) the predictive link between *in situ* RDase enzyme abundances and corresponding *in situ* reductive dechlorination rates at multiple DoD field sites, (2) a framework remediation project managers (RPMs) may use to convert RDase enzyme abundances directly into a rate estimates, and (3) enhanced/expedited site management decisions that can result in substantial cost savings to the DoD and even early site closure.

Performance Assessment. The quantitative and qualitative performance metrics were met through demonstration in defined laboratory microcosm systems prepared using DoD site aquifer materials and the development of a model that predicts cVOC degradation rates based on RDase biomarker abundances. Bioaugmentation with the SDC-9 consortium was used to obtain the desired range of *Dhc* cell abundances and reductive dechlorination rates. Correlation and regression analyses results confirmed that RDase biomarker abundances were significantly and positively correlated with rate coefficients. Regression analysis results were used to test the rate-

predictive power of the RDase biomarker abundances. RDase proteins predicted rate constants k_{cisDCE} and k_{VC} values within one order of magnitude; using RDase proteins and genes combined further improved predictions.

Cost Assessment. Implementation of advanced molecular biological tools (MBTs) such as metagenome sequencing or proteomics, during the long-term monitoring and assessment phase of the project are impacted by multitude of factors such as: the size of the site, proximity of the site to nearby receptors, regulatory requirements, and nature and diversity of contaminant of concern. Although there are currently no regulatory requirements that specifically mandate advanced MBTs be used to assess a site, the data provided by the MBTs are meant to supplement and possibly replace other forms of data that provide lines of evidence that monitored natural attenuation (MNA) is occurring and to estimate a removal rate. Hence, the total sampling and analytical cost is driven by number of sample locations at a site and total number of samples collected (i.e., a greater number of samples equates to a higher cost). It should be noted however that the individual cost per sample may decrease based on a greater number of total samples requiring analyses since the lab work is highly specialized and cost efficiencies generally can be realized for a larger quantity of analyses.

Many of the advanced MBTs such as qProt have only limited commercial availability and/or are available through a university or other research laboratory. As such, application costs remain relatively high. It is expected as these techniques mature, they will become more widely available and the analytical cost per sample will decrease substantially. For comparison purposes, the cost of the metagenomics and metaproteomic analyses based on cost data collected during the commencement of ER-201726 in 2017 were \$300 and \$1,500 per sample, respectively, assuming analysis of a batch of 10 samples. These costs decreased to \$150 and \$1,000 (for cVOCs) when evaluated in 2019. These costs are anticipated to decrease further as the technologies mature.

Implementation Issues. The primary end users of qProt are expected to be DoD site managers, consultants and their contractors. The general concerns of these end users are likely to include the following: (1) regulatory acceptance; (2) insufficient confidence in results and access to specialized laboratories; and (3) technology cost compared to other more conventional monitoring options. Proteomics is a new tool in environmental assessment and one which requires further validation. It is anticipated that, as for many technologies such as qPCR, regulatory acceptance will occur as the technology is field-validated, its benefits over existing approaches (e.g., ability to predict cVOC degradation rates) are realized, and the regulatory community is educated regarding its field application. As noted in the previous section, the issues of limited commercial availability of the technique and relatively high cost are also likely to be improve over time (i.e., more availability and lower cost) as the qProt technology matures.

1.0 INTRODUCTION

1.1 BACKGROUND

The Department of Defense (DoD) is responsible for over 26,000 contaminated groundwater sites with cost to complete (CTC) values estimated at \$12.8 billion (in 2010 dollars) [1]. A majority of these sites are contaminated with chlorinated volatile organic compounds (cVOCs). With over 25% of the remedies in place using enhanced *in situ* bioremediation (EISB) and over 50% of remedies using monitored natural attenuation (MNA) either as a sole remedy or as a final phase after EISB and/or other treatment approaches, a significant portion of the CTC dollars will be spent on EISB and MNA remedy monitoring. For both EISB and MNA, monitoring of a wide range of chemical, geochemical, and microbial parameters is required to demonstrate that biodegradation of cVOCs is occurring and/or progressing as expected. What is currently missing is a monitoring technology that could directly confirm active contaminant degradation and provide *in situ* degradation rate estimates. A direct measure of reductive dechlorination activity and information about degradation rates would be marked improvements for supporting both EISB and MNA approaches for site remediation. Such advances in monitoring strategies are needed to optimize remedy implementation and monitoring, and to develop predictive understanding about the trajectory of a contaminant plume, which will ultimately accelerate site closures.

In groundwater contaminated with chlorinated ethenes, the dominant and productive biodegradation mechanism is typically reductive dechlorination, whereby the parent tetrachloroethene (PCE) and/or trichloroethene (TCE) are sequentially dehalogenated to cis-1,2dichloroethene (cis-DCE), vinyl chloride (VC) and finally ethene and/or ethane, which are considered environmentally benign [2]. A number of different dehalogenating bacteria catalyze one or more steps of this process, with Dehalococcoides mccartyi (Dhc) being the only microbial group known to complete the entire pathway [3]. Assessment of dehalogenating populations at a site is usually based on the enumeration of 16S rRNA genes using quantitative polymerase chain reaction (qPCR) [4]. A number of qPCR assays have been designed to enumerate specific reductive dehalogenase (RDase) genes such as the Dhc TCE RDase gene tceA and the VC RDase genes bvcA and vcrA [5-8]. In addition, specific qPCR assays are available to enumerate the 16S rRNA genes of Dhc and other dechlorinators. While the number of copies of 16S rRNA genes and RDases can provide useful abundance information, these measures do not necessarily correlate with dechlorination activity. In light of this limitation and in an effort to provide a more robust and specific measurement that directly correlates to degradation rates, a proteomic approach that quantifies specific RDase proteins has been developed. In general, the rate of an enzymatic reaction depends on the concentration of the substrate(s) and enzyme(s) involved; thus, the abundance of an RDase is directly proportional to the rate of dechlorination of the enzyme's substrate (e.g., VC). Such targeted measurements of specific proteins are made possible through technological advances in mass spectrometry and knowledge about keystone RDases involved in the detoxification of chlorinated ethenes. The overarching goal of this project was to validate the utility of quantitative proteomics (qProt), and to demonstrate that the integrated, quantitative analysis of biomarker genes and proteins provides estimates of cVOC degradation rates.

1.2 OBJECTIVES OF THE LABORATORY DEMONSTRATION

The value of molecular biological tools (MBTs) has been demonstrated; however, current tools fall short of providing information about contaminant degradation rates. The overarching goal of this demonstration was to validate a platform combining mature qPCR technology with targeted qProt measurements to generate rate estimates and enhance site-specific bioremediation decision making. The specific objectives were to: (1) demonstrate that proteomics can substantially increase the value of currently accepted MBTs for cVOC biodegradation monitoring, and (2) demonstrate the utility of integrated quantitative nucleic acid- and protein-based biomarker analysis applications to estimate cVOC degradation rates. The ultimate demonstration/validation approach for this technology will be to quantify the predictive relationship between RDase proteins and reductive dechlorination rates at multiple field sites. However, because this qProt technology has not yet been demonstrated for this purpose, the initial demonstration was performed in defined laboratory microcosms established with aquifer materials collected from military sites. A validated approach to assess in situ contaminant degradation rates that provides predictive understanding of the longevity of a contaminant plume would be a major advance over the current state-of-the art. The extrapolation of meaningful rate information from MBT data promises more efficient (i.e., lower costs and reduced environmental impact) implementation of EISB, as well as the more frequent implementation of MNA, which will accelerate site closures with substantial cost-savings realized for the DoD.

1.3 REGULATORY DRIVERS

Federal Safe Drinking Water Act Maximum Contaminant Levels (MCLs) for common cVOCs are summarized in Table 1-1. Persistence of cVOCs in groundwater, their prevalence at DoD hazardous waste sites, and their concentrations far in excess of health-based levels drive the need for cost-effective remediation technologies. DoD field sites featured in this demonstration (Section 4.0) all have MCL-based groundwater cleanup objectives.

Compound	MCLs, µg/L*
Tetraloroethene (PCE)	5
Trichlorethene (TCE)	5
<i>cis</i> -Dichloroethene (<i>cis</i> -DCE)	70
<i>trans</i> -Dichloroethene (<i>trans</i> -DCE)	100
Vinyl Chloride (VC)	2
*40 CFR 141.61	

 Table 1-1. Safe Drinking Water Act Maximum Contaminant Levels (MCLs) for Key cVOCs

2.0 TECHNOLOGY

2.1 TECHNOLOGY DESCRIPTION

Conventional Molecular Biological Tools (MBTs). The use of MBTs for detection and quantification of biomarkers, especially genes and transcripts, in environmental samples has been rapidly increasing over the last decade. MBTs are used by remediation professionals to aid remedial design, assess remedial performance, and perform long-term monitoring of biodegradation. The goal of MBT application is to measure the abundance of microorganisms of interest and their activities over temporal and spatial scales.

The most widely used MBT for environmental applications is qPCR, which allows absolute abundance measurements of genes or transcripts of interest within a sample. In the case of reductive dechlorination, qPCR assays that specifically quantify 16S rRNA and RDase genes are employed. The nucleic acid-based biomarkers for detoxification at sites impacted with chlorinated ethenes are the *vcrA* and the *bvcA* genes, which both encode VC RDases, as well as *pceA* and *tceA*, which encode PCE RDases, and TCE/DCE RDases, respectively.

The key organisms (i.e., *Dhc*) that aid in detoxification of chlorinated solvents as well as their relevant RDase genes involved in the reductive dechlorination of chlorinated ethenes have been identified, [6, 7, 9] and sensitive qPCR assays for detection and quantification of key biomarker genes have been developed and tested in multiple laboratories [3, 10, 11]. Further, refined protocols for extraction of nucleic acids from groundwater samples are available [8, 12-15]. Thus, qPCR tools that enumerate *Dhc* 16S rRNA genes and RDase genes can provide information about specific cVOC dechlorination steps [3, 6, 10, 16].

To date, efforts have been made to correlate cVOC degradation rates to *Dhc* and/or RDase gene or transcript abundance. The application of Monod-based equations showed that cVOC degradation kinetics can be roughly correlated to *Dhc* cell abundances, as determined with qPCR; however, there were large differences in activity per cell based on qPCR data collected from batch versus column studies [17]. Importantly, these correlations are based on qPCR assays that quantify all *Dhc*-like sequences, not just those responsible for cVOC degradation (i.e., those encoding and expressing RDase genes). In other words, the gene-centric qPCR approach also measures *Dhc* cells that are not contributing to the dechlorination of the target contaminant(s).

Advanced MBTs – Quantitative Proteomics (qProt). In contrast to nucleic acid based MBTs, quantitative proteomics (qProt) involves the identification and quantification of proteins (i.e., enzymes) within a sample. That is, nucleic acid-based tools generate information about potential activity, whereas protein-based measurements generate information about *actual* (i.e., functional) activity.

In general, a shotgun proteomic workflow for protein identification includes protein extraction, digestion with a protease (typically trypsin) to create tryptic peptides, and liquid chromatography tandem mass spectrometry (LC-MS/MS) for peptide separation and generation of mass-resolved spectra (Figure 2-1). Peptide identification involves querying the resulting spectra against a representative protein sequence database using search engines such as Mascot or ProteinPilot [18]. Ideally, these sequence databases are specific to the analyzed samples such that the highest

numbers of proteins can be accurately identified. Once identified using shotgun proteomics, peptides from proteins of interest (e.g., RDases) can be confirmed and quantified through the use of commercially available isotopically labeled peptides of the same sequence using multiple reaction monitoring (MRM) mass spectrometry.



Figure 2-1. Schematic of proteomics workflow

The MRM proteomic analysis allows multiplexing of protein assay and generation of highly accurate results with near absolute specificity. This proteomic strategy is a proven and widely accepted technique for quantification of proteins [18] and has been used for decades in various matrices such as serum [19] and recently in environmental samples of groundwater and sediments [20-23]. Quantitative MRM proteomic techniques rely on targeting specific precursor peptide ions and the resulting fragment ions produced from these precursors during the analysis. Moreover, the LC-MS/MS settings can be optimized to maximize the number of precursor ions that are fragmented and scanned. Thus, in the MRM assay, specific transitions (precursor \rightarrow fragment ions) for individual peptides are targeted and monitored as a function of LC retention time, which provides a highly selective, sensitive and reliable approach for quantitative analysis through integration of reproducible chromatographic peaks (Figure 2-1). With MRM, a suitable instrument such as triple-quadrupole mass spectrometer can be a priori configured to scan for a defined set of target peptides, and a selected subset of fragment ions.

Specific to this demonstration, MRM proteomic techniques have been recently used in microbial cultures to identify and quantify RDases from dechlorinators [24]. Thus, proteomics shows high potential for absolute quantification of RDases within a sample that contains mixed microbial communities. However, proteomics has not yet been exploited for the purpose of correlating cVOC

degradation rate to RDase absolute abundance. To this end, optimized protocols exist to extract proteins from biomass associated with aquifer solids or groundwater and detect and quantify key cVOC RDases with LC-MS/MS approaches [21-23].

MBTs in Assessment of cVOC Degradation Rates. Conventional nucleic-acid based MBTs can provide evidence for biodegradation, but do not aid site remediation project managers (RPMs) in prediction of contaminant longevity due to the lack of linkage to actual degradation rates. While models that include a microbial biomass, based on qPCR or total protein measurements exist [2, 17, 25, 26], their predictive power is limited. For example, batch culture/microcosm studies used biomass measurements to model cVOC degradation rates, but such models have a number of limitations and their application in support of *in situ* remediation decision making remains challenging. This limitation is due to the fact that the specific components of the microbial biomass responsible for the cVOC degradation (i.e., the RDase proteins) are not currently measured. Thus, while nucleic acid based MBTs or total biomass measurements are widely used and represent mature technologies, they may have limited value for inferring degradation rates unless combined with a more direct measure of activity (i.e., that provided by qProt). More specifically, nucleic acid-based MTBs provide a sensitive and routine means to detect and quantify DNA and transcripts of RDases, but without proteomic-based measurements, a defined correlation to cVOC degradation rate is difficult to achieve with environmental samples.

2.2 TECHNOLOGY DEVELOPMENT

At sites contaminated with chlorinated ethenes, biostimulation of indigenous dechlorinating bacteria or bioaugmentation with dechlorinating microbial consortia can achieve detoxification and environmental restoration. Contemporary bioremediation performance monitoring tools rely on nucleic acid biomarkers targeting key organohalide-respiring bacteria such as Dhc. Liquid chromatography coupled with tandem mass spectrometry (LC-MS/MS) allows the selective quantification of Dhc reductive dehalogenase (RDase) proteins that catalyze reductive dechlorination of chlorinated ethenes. This work applied LC-MS/MS to detect and quantify RDase peptides in the commercial bioaugmentation consortium SDC-9 comprising Dhc strains capable of reductive dechlorination of chlorinated ethenes and vinyl chloride to non-toxic ethene. Metagenome sequencing of the SDC-9 consortium provided a reference database for the accurate identification of target RDase peptide sequences. Shotgun proteomics workflow identified 143 RDase peptides and proteome characterization resulted in 36 distinct peptides corresponding to PceA, TceA and VcrA proteins that covered 99-100% of the annotated protein-coding sequences. From the 14 annotated RDase genes, two distinct pceA genes, one vcrA and one tceA gene were identified. Twelve of the 14 RDase genes were associated with RDase B. Quantification using parallel reaction monitoring (PRM) assays with ¹³C-labeled peptides determined 1.8x10³ for TceA, and 1.2×10^2 VcrA molecules per *Dhc* cell. This approach allowed for sensitive detection and accurate quantification of relevant Dhc RDases and has potential utility in bioremediation monitoring regimes.

qProt has now reached a maturity level that justifies its inclusion in environmental monitoring regimes. The combined gene-, transcript-, and protein-centric approach could reveal gene presence (functional potential), transcript abundance (gene activity), and protein abundance (actual catalytic activity). The integrated analysis of these biomarkers, together with geochemical parameters, can

be used to estimate degradation rates of specific contaminants of interest (e.g., cVOCs). In an effort to move this approach into field practice, the project team completed the following tasks to generate initial qProt data and to illustrate the reductive dechlorination rate-predictive potential in the ER-201726 project proposal.

- 1. Metagenomic sequencing and bioinformatics analysis enabled identification of a total of 14 RDase gene sequences in the SDC-9 consortium (Table 2-1).
- 2. The proteomic analysis revealed more than 14 unique RDase peptides as well as peptides from accessory proteins potentially involved in transferring electrons during the reductive dechlorination process (Table 2-1).
- 3. RDase peptides were identified and quantified in microcosm experiments using qProt procedures.
- 4. Utility of the MRM proteomics approach for quantifying RDase proteins was demonstrated in microcosm studies with the commercially available cVOC biodegradation consortium SDC-9 [27].

Results of the SDC-9 metagenomic sequencing suggested that the RDase peptides were derived from three RDase proteins (highlighted in grey, Table 2-1). Results also demonstrated that only three of the 14 RDases were identified to be expressed and presumably active, even though all 14 corresponding genes would probably be detected and enumerated with qPCR.

RDaseA gene locus ^a	RDaseB gene locus	Number of transmembrane helices in RDaseB	Putative taxonomy	TAT signal ^b	Percent amino acid identity	Accession number of best NCBI alignment	Predicted gene
scaffold-6337_195	scaffold-6337_193	3	Dehalococcoides	Yes	99%	WP_081042195.1	ND
scaffold-6337_194	scaffold-6337_193	3	Dehalococcoides	Yes	100%	WP_081042194.1	ND
scaffold-352_158	ND	3	Dehalococcoides	Yes	100%	BAZ97963.1	ND
scaffold-6337_252	scaffold-6337_251	3	Dehalococcoides	Yes	100%	WP_010935983.1	ND
scaffold-352_212	scaffold-352_213	3	Dehalococcoides	Yes	99%	AEI59454.1	vcrA
scaffold-178_59	scaffold-178_58	3	Dehalococcoides	Yes	99%	WP_062900263.1	tceA
scaffold-3176_24	scaffold-3176_25	3	Dehalobacter	Yes	94%	CAD28790.2	pceA
scaffold-6337_160	ND	3	Dehalococcoides	Yes	100%	BAZ97963.1	ND
scaffold- 133_66	scaffold-133_67	3	Dehalobacter	Yes	40%	WP_015043198.1	ND
scaffold-2271_52	scaffold-2271_51	3	Dehalococcoides	Yes	100%	WP_010935983.1	ND
scaffold-352_192	scaffold-352_191	3	Dehalococcoides	Yes	100%	WP_081042194.1	ND
scaffold-3175_18	scaffold-3175_19	3	Desulfitobacterium	Yes	100%	CDX01551.1	ND
scaffold-3176_29	scaffold-3176_30	3	Dehalobacter/ Desulfitobacterium	Yes	82%	WP_025206074.1/CDX02974.1	pceA
scaffold-352_193	scaffold-352_191	3	Dehalococcoides	Yes	99%	WP_081042195.1	ND

Table 2-1. RDase genes identified in SDC-9 metagenome

^aThe amino acid sequence encoded by scaffold-133_66 possessed a query coverage of 99% against reference sequence WP_015043198.1. All other amino acid sequences from RDase loci reported had query coverages of 100%. ^bNo SEC signal peptides were detected in any RDase amino acid sequences examined.

ND – not determined

To date, several RDase peptides have shown good calibration linearity ($R^2 = 0.9$) and a broad dynamic range, allowing quantification of RDases from sample extracts and a comparison of their absolute abundances to dechlorination activity. In fact, quantitative analysis of two RDase peptides (TceA and PceA) in the initial proof-of-concept microcosm experiments performed using SDC-9 cell suspensions yielded good correlations between dechlorination rate and RDase concentrations (Figure 2-2). In addition to these initial proof-of-concept microcosm studies, other similar experiments have shown that RDase peptides can be identified from environmental samples [21-23]. Specifically, BvcA, VcrA and TceA peptides were identified in samples from a cVOCcontaminated site.



Figure 2-2. RDase peptide concentrations versus degradation rate constants RDase peptide abundance vs. first order for TCE and cisDCE in SDC-9 microcosms.

The utility of qProt as an advanced MBT for environmental monitoring has been demonstrated. However, a quantitative link between RDase peptide abundance in environmental samples and reductive dechlorination rates has yet to be established in microcosm experiments. This demonstration (1) validated the qProt method for measuring RDase peptide abundances in environmental samples, and (2) established a quantitative link between biomarker abundance (RDase peptides and genes) and rates of *cis*-DCE and VC reductive dechlorination. This was accomplished through a series of microcosm studies performed using aquifer material from a cVOC-contaminated DoD site. A detailed description of the microcosm study design is provided in Section 5.0. Briefly, *Dhc* cell abundances were varied in each set of incubation vessels over six orders of magnitude $(10^3 - 10^9 \text{ cells/mL})$ and the rate of *cis*-DCE and VC reductive dechlorination was measured in each microcosm replicate. Live and killed controls were included and all biomarker and cVOC measurements were made in triplicate. This well-controlled and replicated microcosm study used real-world aquifer materials and provided data required to establish the quantitative link between abundances of peptides and nucleic acid biomarkers with reductive dechlorination rates. The results presented herein can now be applied in the field to validate the link between biomarker abundances and *in situ* reductive dechlorination rates at one or more cVOC-contaminated DoD sites.

2.3 ADVANTAGES AND LIMITATIONS OF THE TECHNOLOGY

The main advantage of proteomic techniques for the determination of *in situ* degradation rates is that the absolute amount of the reaction catalysts (e.g., RDase enzymes) are measured. Proteomicsbased techniques are limited by the amount of biomass (more specifically, the amount of proteins of interest) collected in the sample. This limitation is due to the fact that in contrast to nucleic acids, proteins cannot be amplified, so their quantification is inherently limited by the instrument detection limit (IDL) and overall method detection limit (MDL). The IDL is a function of the LC-MS/MS instrumentation and the concentration of specific peptides to be quantified. These detection limits can approach the low attomol (10^{-18}) range for quadrupole time-of-flight tandem mass spectrometers (QTOF-MS) [28]. The MDL considers the sensitivity of the overall method, including any loss associated with extraction and purification from interfering substances (e.g., detergents that can suppress MS signals), which can reduce sensitivity to high fmol to attomol (10⁻¹⁵ - 10⁻¹⁸) levels for environmental samples. Prior work at Battelle [21-23] and under SERDP ER-2312 [13] demonstrated that the overall MDL for the quantification of *Dhc* RDases approaches 3,000 fmol (3 pmol) RDase per liter of groundwater, which corresponds to an approximate Dhc biomass of 10⁶ total cells. Although *Dhc* abundances are generally low at MNA sites, the qProt assay may still be reliably used at these locations by collecting suitably large sample volumes, which will ensure the sample contains sufficient RDase mass to be above the quantitation limit. Because quantitation of RDases is paramount to the proteomics method being demonstrated, additional IDL and MDL studies were completed as part of this demonstration as described in Section 5.0.

The targeted nature of qProt is both an advantage and a limitation. The main limitation is that RDases (and other proteins of interest) from indigenous (native) dechlorinating organisms may respond to biostimulation and contribute to the observed degradation activity. These native RDases may have slightly different RDase sequences and may thus not be detected in the MRM proteomic assay (i.e., false-negative results). While this is a legitimate concern, the issue can be addressed by metagenome sequencing of DNA extracted from biomass collected from site groundwater. Metagenome sequencing has become a routine procedure and can be accomplished at reasonable cost (e.g., <\$1,000). Bioinformatics pipelines to extract RDase gene fragments from metagenome datasets are available and this information can then be used to determine the exact sequences of native RDase genes of interest. With this information, the peptides of native RDases can be predicted and therefore detected and quantified with the qProt approach.

Environmental distribution of the trichloroethene reductive dehalogenase gene (*tceA*) suggests lateral gene transfer among *Dehalococcoides* [29]. Therefore, a suite of qProt assays can be developed that will be applicable to the majority of sites. Prior studies have also demonstrated allelic sequence variations of RDases genes such as *tceA*; however, we expect that the sequence variability of *tceA* gene sequences will be limited at contaminated sites and we will not find new *tceA* sequences at every site investigated. Thus, as our study demonstrates that the development of

site-specific qProt assay will be cost feasible at most sites, our knowledge of RDase gene sequence variations suggests it may be possible to design a multiplexed RDase qProt assay which will encompass several target peptides that will be useful at the majority of sites.

3.0 PERFORMANCE OBJECTIVES

This project demonstrated the utility of advanced MBTs for prediction of cVOC degradation rates in laboratory microcosms. Demonstration results highlighted the utility of this approach for estimating *in situ* reductive dechlorination rates at field sites. The following section describes quantitative and qualitative performance objectives (Table 3.1) specific to the laboratory microcosm phase of the demonstration.

Performance Objective	Data Requirements	Success Criteria				
Quantitative Performance Objectives						
Quantify rate coefficients for <i>cis</i> - DCE and VC degradation in aquifer microcosms bioaugmented with reductive dechlorinating consortium SDC-9 at varied initial cell densities. Rates of production of VC from <i>cis</i> -DCE and ethene and ethane from VC will also be quantified.	Concentrations of <i>cis</i> -DCE, VC, ethene and ethane over a minimum of six time periods in triplicate microcosms. Data will be used to estimate rate coefficients and corresponding uncertainties for each test.	Initial cell densities in the bioaugmented microcosms will be varied by 4 orders of magnitude (10 ⁵ , 10 ⁶ , 10 ⁷ and 10 ⁸ cells/mL) to ensure we obtain a range of rate coefficients and reductive dechlorination activity levels. Rate coefficients estimated using the microcosm data will be of sufficient quality if the global R ² of the kinetic model is \geq 0.75, and if the average ratio of the 95% confidence interval to the rate coefficient value for both k_{cisDCE} and k_{VC} (i.e. the average of ratios in brackets $\left[\frac{95\% CI k_{cisDCE}}{k_{cisDCE}}, \frac{95\% CI k_{VC}}{k_{VC}}\right]$) is \leq 125%				
RDase biomarkers (RDase peptides, genes, and RNA transcripts) are quantifiable at microcosm-required and environmentally-relevant concentration levels.	Quantify initial and final RDase biomarker abundance and corresponding uncertainty for each treatment within each microcosm test.	RDase biomarker abundance measurments meet the Data Quality Objectives for this analysis. Ability to measure one or more of these RDase biomarkers at environmentally relevant <i>Dhc</i> concentrations (i.e., 10 ⁵ to 10 ⁶ cells/mL).				
One or more of the RDase biomarkers exhibits a quantifiable, predictive association with <i>cis</i> -DCE (and/or VC) degradation rates in the microcosms.	Rate constants for each microcosm that meet objectives described above. RDase biomarker abundance (peptides, genes, and RNA transcripts) measurements that meet objectives described above.	The association between RDase biomarker abundance (RDase peptides, genes, and RNA transcripts) and the rate constants is positive and significantly different from zero at the 95% confidence level.				
	Qualitative Performance Obje	ectives				
RDase biomarker abundance input to multivariate regression (or other suitable) model predicts reductive dechlorination rates with equal or better confidence than using conventional DNA-based MBTs alone.	Rate constants for each microcosm that meet objectives described above. RDase biomarker abundance (peptides, genes, and RNA transcripts) measurements that meet objectives described above.	Utility of RDase biomarkers (RDase peptides, genes, and RNA transcripts) – alone and in combination – will be quantified and documented.				
Effectively communicate benefits of advance MBTs to end users – particularly managers of cVOC- contaminated DoD groundwater sites – through multiple technology transfer platforms.	Rate constants for each microcosm that meet objectives described above. RDase biomarker abundance (peptides, genes, and RNA transcripts) measurements that meet objectives described above.	At the conclusion of the 2-year microcosm test, at least one manuscript will have been submitted to a top-quality, peer-reviewed journal.				

Table 3-1. Demonstration	performance ob	jectives for	the microcosm	study
--------------------------	----------------	--------------	---------------	-------

3.1 Quantify rate constants for *cis*-DCE and VC degradation in aquifer microcosms.

Rate constants were calculated for *cis*-DCE and VC degradation in each of the different microcosm treatments (Section 5.5.2). The procedure for calculating rate constants is provided in Section 5.7.

Data Required: The data required included concentrations of *cis*-DCE and VC as a function of incubation time in the microcosms. Concentrations of *cis*-DCE and VC were measured at a minimum of 8 time points in each microcosm treatment, which were prepared in triplicate. Analysis was conducted by EPA Method 8260 (Gas-Chromatography – Mass Spectrometry; GC-MS) using liquid 2-mL samples as described in Section 5.6.1.

<u>Success Criteria</u>: The first order rate constants were fit to the microcosm data and were considered to be of acceptable quality if the global R² of the kinetic model was ≥ 0.75 , and if the average ratio of the 95% confidence interval on the rate constant to the rate constant value itself for both k_{cisDCE} and k_{VC} (i.e. the average of ratios in brackets $\left[\frac{95\% CI k_{cisDCE}}{k_{cisDCE}}, \frac{95\% CI k_{VC}}{k_{VC}}\right]$) was $\le 125\%$.

3.2 Measure target RDase biomarkers (RDase genes and proteins) at environmentally relevant abundance levels.

Abundance of RDase proteins was linked to abundance of the reductive dechlorinating microbes expressing them. The microcosm test was designed to quantify RDase biomarkers associated with *Dhc* cell densities in the $< 10^6$ cells/mL range, which is relevant to MNA sites, and up to $> 10^8$ cells/mL range, which is relevant to biostimulated and bioaugmented sites.

Data Required: Required data include abundances of RDase biomarkers (genes and proteins) in each microcosm at the time corresponding to the beginning, middle and end of the incubation used to determine the rate constants for *cis*-DCE and VC degradation. The RDase biomarkers were quantified using methods described in Section 5.6.2 and 5.6.3.

<u>Success Criteria</u>: Abundance of RDase biomarkers met the method detection limits and other data quality objectives summarized in Section 5. Microcosm study results were utilized to establish a lower limit of detection for quantifying peptides of interest. Results showed that single RDase protein biomarkers in the $2x10^6$ *Dhc* cells/mL or more range corresponded to k_{cis} and k_{VC} rates in the range of 0.0001 day⁻¹ (0.04 year⁻¹), which is relevant to sites pursuing or managing MNA remedies.

3.3 Quantify relationship between target RDase biomarker abundances and reductive dechlorination (RD) activity in aquifer materials

Abundance of RDase biomarkers (genes and proteins) were compared with the rate constants for biodegradation of *cis*-DCE and VC collected from the microcosms.

<u>Data Required</u>: Rate constants for *cis*-DCE and VC degradation (Objective 3.1) and concentrations of RDase peptides and genes in each microcosm at the time corresponding the beginning of the incubation used to extract the rate constants (Objective 3.2).

<u>Success Criteria</u>: The association between abundance of individual RDase peptides and genes, and the rate constants was tested by first performing correlation analysis. RDase biomarkers and rate constants with correlation factors that were positive and significantly different from zero at the 95% confidence interval were considered acceptable, then were carried forward into a power law least squares regression analysis where the predictive relationship was established.

3.4 Develop a multivariate regression (or other suitable) model, which predicts the *cis*-DCE and VC rate constants using RDase biomarkers as input

A simple power regression model was developed to allow an end user to predict the *cis*-DCE and VC degradation rate constant using qPCR and qProt data as model input parameters.

Data Required: Rate constants from microcosms and corresponding abundance of RDase proteins and functional genes so that the quantitative relationship between these measures can be modeled and the predictive tool can be developed.

<u>Success Criteria</u>: Quantify the rate-predictive power of the regression model using RDase protein abundance only, RDase functional gene abundance only, and a combination of the two together to establish the relative contribution of each measure to the predictive power of the model. This performance objective was established as a *qualitative* objective for this laboratory microcosm phase of the demonstration.

3.5 Effectively transfer the new technology to end users

Results of the microcosm study are the first to demonstrate use of qProt for predictions of reductive dechlorination rates under environmentally relevant conditions.

Data Required: Rate constants from microcosms and corresponding abundance of RDase biomarkers and functional genes so that the quantitative relationship between these measures can be modeled and the predictive tool can be developed.

<u>Success Criteria</u>: Distribute microcosm study findings using effective technology transfer platforms. Submit at least one manuscript describing the results and benefits of the approach to a top-quality, peer-reviewed journal. Present results at multiple national remediation conferences.

4.0 SITE DESCRIPTION

Three cVOC-contaminated DoD sites were selected for potential inclusion in this project: Naval Base Kitsap (NBK) Keyport Area 1, Joint Base Lewis-McChord (JBLM) Landfill 2, and Vandenberg Air Force Base (VAFB) Site SA288. These sites were selected because (1) collection of aquifer material and groundwater was possible with minimal cost to the project through leveraging pre-planned site characterization activities, and (2) each site is potentially suitable for a future field demonstration. The following subsections provide an overview of each DoD field site – and basis for inclusion or exclusion from this laboratory project.

4.1 NBK KEYPORT AREA 1, BREMERTON, WASHINGTON

Site Location and History. Keyport Area 1 is a former solid waste landfill at NBK Keyport, located 45 miles north of Tacoma, Washington on the Kitsap Peninsula. It comprises approximately 9 acres in the western portion of the base, next to a wetlands area and the tidal flats that flow into Dogfish Bay (Figure 4-1). The Area 1 landfill was the primary disposal area for domestic and industrial wastes generated by the base from the 1930s until 1973, when the landfill was closed. NBK Keyport became a Superfund site in 1989. The remedial investigation and feasibility study [30] identified cVOCs as contaminants of concern in site soil, sediment, tissue, groundwater, and surface water. The Record of Decision [31] for the Area 1 landfill specified cVOC hotspot treatment using phytoremediation by poplar trees in concert with natural attenuation, as well as landfill liner upgrades, monitoring and other best management practices. The landfill liner upgrade was completed in 2003 and phytoremediation was implemented in 1999 by planting two poplar plantations (Figure 4-1).

Site Geology/Hydrogeology. There are two aquifers at the site. The sandy unconfined upper aquifer is present throughout the landfill area and is 4 to 15 feet thick, with depth to water between 4 to 10 feet below ground surface (bgs) [30]. Approximately 5 feet of landfill material lies above the groundwater surface in the unsaturated zone; up to 10 feet of landfill material lies within the saturated upper aquifer. Upper aquifer groundwater generally flows west and discharges into the marsh pond (Figure 4-1). The upper aquifer is underlain by an aquitard consisting of sandy silt to clean silt, which is 4 to 15 feet thick where present. The underlying intermediate aquifer is 5 to 25 feet thick, with groundwater flow direction generally toward the tide flats (Figure 4-1). The intermediate aquifer is underlain at 25 to 40 feet bgs by a thick nonglacial silt and clay aquitard known as the Clover Park Silt, which is approximately 100 feet thick and separates the contaminated aquifers from the deeper regional water-bearing units [30].



Figure 4-1. NBK Keyport Area 1, site map

Contaminant Distribution. In spite of a high degree of biodegradation and reductions in cVOC mass over time, groundwater concentrations of cVOCs beneath the south poplar plantation in the upper aquifer remain high and cVOC concentrations in surface water adjacent to the south plantation consistently exceed the surface water remediation goals. The maximum concentrations of cVOCs measured in upper aquifer monitoring wells in the south plantation were: TCE > 33,000 μ g/L, *cis*-DCE > 55,000 μ g/L, and VC > 6,000 μ g/L (Figure 4-1). Aquifer material and groundwater for this project will be collected from the upper aquifer, south plantation.

Project Inclusion Decision. Aquifer solids and groundwater were collected by NBK Keyport Area 1 contractors (Battelle Memorial Institute) in July and September 2017 and shipped on ice overnight to the Aptim laboratory in Lawrenceville, NJ. The quantity of aquifer material collected in July 2017 via direct-push drilling was limited but screening results were favorable so a larger quantity of aquifer material was collected in September 2017 via hollow stem auger. Unfortunately, the larger material sample exhibited a strong odor (suspected naphthalene, not confirmed). High/potentially inhibitory levels of contaminants, resulted in a decision to exclude the NBK Keyport Area 1 material during the laboratory project phase. However, results of the recent expanded site characterization make NBK Keyport Area 1 a good candidate for a future field demonstration.

4.2 VAFB SITE SA 288, VANDENBERG, CALIFORNIA

Site Location and History. The site is located 4.1 miles east of the Pacific Ocean and 2.8 miles north of the Santa Ynez River within the Cantonment Area on the Burton Mesa portion of VAFB. The site consists of three buildings that were used for various industrial processes since the 1960s. Investigation activities initiated in 2008 involved installation of soil borings and temporary wells, which identified the former chemical storage shed and the former freon processing shed as potential cVOC source areas to groundwater (Figure 4-2). Additional soil borings and monitoring wells were installed and sampled in 2016, the results of which are summarized in the contaminant distribution section below. Additional site characterization is planned to support a "remedy in place" scheduled goal of second quarter 2018.

Site Geology/Hydrogeology. The site is underlain primarily by Quaternary Orcutt Sand [32] with bedrock occurring at approximately 45 ft below ground surface. Surface water that does not infiltrate into the subsurface at the unpaved areas of the site enters a storm drain system and ultimately discharges into the Santa Ynez River to the south. Groundwater can be detected near ground surface following significant rainfall events but is typically observed within a saturated sandy silt layer, which is 2 to 5 ft thick across the site. Depth to this saturated sandy silt layer varies across the site but is typically encountered around 10 ft below ground surface. Groundwater flows in a southeast direction from the presumed source area toward New Mexico Avenue (Figure 4-2).

Contaminant Distribution. Maximum cVOC concentrations in groundwater were encountered during the 2016 monitoring event in well SA288-MW-01, which is located approximately 150 ft downgradient of the former freon processing shed [33]. Groundwater concentrations of TCE and *cis-DCE* were 2,200 μ g/L and VC was 76 μ g/L (Figure 4-2). Aquifer material and groundwater use during this project will be collected from the saturated sandy silt perched aquifer.

Project Inclusion Decision. Aquifer solids and groundwater were collected by VAFB SA288 contractors (Geosyntec Consultants) and shipped on ice overnight to the Aptim laboratory in Lawrenceville, NJ. Unfortunately, the groundwater and aquifer solids collected from SA288 were naturally acidic (pH \sim 3.5), which is inhibitory for *Dhc* cells, and was therefore deemed not acceptable for inclusion in the laboratory portion of the project. However, other portions of the SA288 site or even other cVOC-contaminated aquifers present at VAFB could be candidates for a future field demonstration.



Figure 4-2. VAFB SA288 site map showing groundwater cVOC concentrations [33]

4.3 JBLM LANDFILL 2, TACOMA, WASHINGTON

Site Location and History. JBLM is a major military installation located approximately 15 miles southwest of Tacoma, Washington. Landfill 2 (LF2) was used to dispose of petroleum products and solvents generated by the Logistics Center between the 1940s to 1970s (Figure 4-3). Soils under the LF2 area are highly transmissive and the groundwater table is shallow; consequently, LF2 contributed to a very large TCE groundwater plume. The Logistics Center, which includes LF2, was listed as a Superfund site in 1989. The Record of Decision (ROD) [34] specified a pump and treat groundwater remedy for LF2. The ROD was subsequently modified to include multiple source area removal actions and enhancements to the pump and treat remedy.

Site Geology/Hydrogeology. LF2 is located within the unconfined Vashon Aquifer, which is comprised of interlayered outwash and glacial till to an approximate depth of 100 ft below ground surface. In the vicinity of the LF2 source area, the Vashon Aquifer is divided into the Upper Vashon and the Lower Vashon, which are separated by a discontinuous low permeability till layer. The Vashon Aquifer is separated from the underlying confined Sea Level Aquifer by a 10 to 20 feet thick non-glacial aquitard unit. A "window" in the aquitard unit downgradient of the LF2 source area resulted in formation of a large cVOC plume in the underlying Sea Level Aquifer.

Contaminant Distribution. Multiple source area removal actions (excavation, thermal treatment) and pump and treat remedy implementation since the 1990s have significantly reduced cVOC concentrations present in the LF2 source area wells (Figure 4-3, inset). However, only select groundwater wells are sampled during compliance monitoring events and those low concentrations (see contours, Figure 4-3) do not explain the ~ 200 μ g/L sustained TCE concentrations routinely encountered in extraction well PW-1. Groundwater TCE concentrations in the ~ 1,000 μ g/L range are expected in the source area vicinity. New investigation wells are being installed and a comprehensive groundwater monitoring event is being conducted to refine the LF2 conceptual site model and confirm remaining TCE concentrations in source area groundwater. These investigation activities in the LF2 source area will be leveraged to provide aquifer material and groundwater for use during this ESTCP project.

Project Inclusion Decision. Aquifer solids and groundwater were collected by U.S. Army Engineer Research Development Center (ERDC) and Seattle District U.S. Army Corps of Engineers (USACE) and shipped on ice overnight to the Aptim laboratory in Lawrenceville, NJ in May 2017. Aquifer solids and groundwater samples were stored at 4°C until use. Initial screening of the groundwater samples showed cVOC concentrations and pH were within acceptable ranges. Next, the LF2 groundwater was screened for potential reductive dechlorination inhibitory substances by conducting a simple microcosm study. SDC-9 cells (10⁸ cells/mL), *cis*-DCE (10 mg/L) and lactate (500 mg/L) were added to LF2 groundwater followed by measurements of *cis*-DCE, VC and ethane/ethene concentration and pH over time. Rapid reductive dechlorination was observed in the screening microcosm, which supported a "go" decision to include LF2 materials in the laboratory project. pH reduction observed during the screening microcosm prompted inclusion of calcium carbonate buffer during subsequent microcosm experiments.



Figure 4-3. JBLM Landfill 2 TCE concentrations in Upper Vashon Aquifer source area wells (see inset)

5.0 TEST DESIGN

This section provides an overview of the experimental approach and field material collection (Sections 5.1 - 5.2), refinement and validation of the qProt assay specific to this project (Sections 5.3 - 5.5), as well as detailed experimental procedures, analytical methods and data analysis requirements for the project (Sections 5.6 - 5.8).

5.1 CONCEPTUAL EXPERIMENTAL DESIGN

The goal of this project was to demonstrate the utility of measuring RDase biomarkers (RDase genes, peptides) via qPCR and qProt to estimate in situ cVOC degradation rates. First, the RDase protein targets were identified to finalize the qProt assay for use during this project (Section 5.3) then MDL and IDL studies were performed to establish the quantitative framework for the qProt assay (Section 5.4). Next, we performed a study using diluted SDC-9 culture to validate quantitation limits of the qProt assay (Section 5.5). Finally, a series of microcosm studies were performed using DoD site aquifer materials where cis-DCE and VC degradation rates were quantified as a function of RDase biomarker gene and protein abundances (Section 5.6). Microcosms were prepared by amending JBLM LF2 aquifer material with cis-DCE, lactate as a growth substrate, and calcium carbonate buffer. Varied quantities of the dehalogenating consortium SDC-9, which contains Dhc strains carrying RDase genes including vcrA and tceA, were added to the microcosms as illustrated in Figure 5-1. Samples were collected from the microcosms over time and analyzed for cVOCs so that degradation rates of *cis*-DCE and VC could be calculated. Samples also were collected from the microcosms at multiple points for analysis of selected RDase biomarkers. As described in Section 6.0 below, results of this laboratory project illustrated that RDase biomarkers can be reliably quantified over ranges of *Dhc* cell abundances relevant to cVOC site management - from low abundance/low activity relevant to MNA to high abundance/high activity relevant to enhanced bioremediation. Furthermore, the positive and significant correlations established between the biomarker abundances and reductive dechlorination rate coefficients in this laboratory study lay the foundation for a follow-on field study where the quantitative link between RDase biomarkers and *in situ* rates can be validated.



Figure 5-1. Microcosm study conceptual design

5.2 **BASELINE CHARACTERIZATION ACTIVITIES**

Aquifer material was collected from the saturated zone of the JBLM LF2 cVOC-contaminated aquifer the week of May 29, 2017. The aquifer materials were sieved in the field to remove gravel, collected in large Zip-Loc-type freezer bags, labeled, and then stored on ice pending overnight shipment to the Aptim laboratory (Aptim). Wet solids were shipped on ice in Zip-Loc type bags labeled "JBLM-L236 8-50' BGS". The solids (wet sand and some small pebbles) were homogenized under a nitrogen atmosphere at Aptim and placed in sterile 4-L glass jars. The jars were stored at 15 °C. The wet soil was allowed to settle for a week, and the water was decanted to lower the moisture content of the solids. This was repeated several times over 10 weeks until the soil moisture content was 15% (wt/wt). Groundwater was collected from the extraction well PW-1 sampling port the week of May 29, 2017, and then again the week of March 5, 2018, into 18-L stainless steel kegs that had been bleached (2,500 mg/L chlorine), rinsed with Nano-Pure water, and autoclaved (15 psi, 121 °C, 45 minutes). Groundwater samples were placed on ice and shipped overnight to Aptim. Site groundwater was analyzed for cVOCs using methods described below prior to use in microcosms. The cVOCs present in the groundwater were removed by purging with N₂ prior to groundwater use in microcosm preparation to prevent any potential impacts of the native cVOCs on the growth and activity of dechlorinators in the SDC-9 consortium. In order to ensure reductive dechlorination was not affected by inhibitors associated with the aquifer materials, a single microcosm was prepared and sampled as described in Section 5.3 below for screening purposes. This microcosm was bioaugmented to achieve a *Dhc* cell density of 10^8 cells/mL with lactate as the electron donor, then screened for cis-DCE and VC degradation rates and pH changes only. If reductive dechlorination activity fell within the expected range (based upon historical data with the SDC-9 consortium), the aquifer material was considered acceptable and carried forward in the microcosm study. As described in Section 4.0, only aquifer material from JBLM LF2 was deemed acceptable to carry forward.

5.3 DEVELOPMENT OF RDASE PEPTIDE TARGETS

SDC-9 biomass was harvested during growth in a 4,000-L bioreactor maintained at Aptim at three time points and subjected to proteomic analysis. Targeted proteomic analysis was conducted using the same instrumentation and chromatographic method as used for shotgun proteomics except that the mass spectrometer was operated in parallel reaction monitoring (PRM) mode. A full scan spectrum was acquired (100 ms accumulation time) followed by product ion spectra of each target peptide (75 ms accumulation time), for a total cycle time of 1.9 seconds. The product ion scans were not time scheduled. Proteins were identified from MS/MS fragmentation data by searching the MS/MS data of the top n peaks against a custom FASTA library protein sequences acquired from the metagenome of consortium SDC-9. Searches were performed with the Paragon algorithm in Applied Biosystems ProteinPilot 4.5, with the following parameters: ID with 95% confidence, fixed modifications (carbamidomethyl), variable modifications (methionine oxidation).

ProtScore values for an identified protein were calculated by summing the ProtScore of each identified peptide after log transformation:

$$ProtScore = -log(1-Cn) \qquad equation 1$$

where n peptides with a confidence of Cn each contributes to the ProtScore of the identified protein. For example, a protein that has four peptides with 99% confidence match has a 99.9999999% chance (1 - 0.014) of being a true identification. In this case, each peptide contributes 2 units to the ProtScore for every peptide identified with a 99% confidence ID. High-confidence, non-tryptic peptides were subjected to analysis using a suite of open-source software to provide explanation for the observed cleavage site as follows:

- PRED-TAT (http://www.compgen.org/tools/PRED-TAT4), which is used to predict signal peptide domains; and
- PROSPER (https://prosper.erc.monash.edu.au/5), PeptideCutter (http://web.expasy.org/peptide_cutter/5), and the MEROPS peptidase database (https://www.ebi.ac.uk/merops/search.shtml6), all of which are used to predict protease specificity for a given protein sequence.

5.4 ESTABLISHING MDL AND IDL FOR TARGET PEPTIDES

The SDC-9 culture-specific RDase peptides were identified for quantification. These specific RDases were then used in a MRM targeted proteomic assay to establish quantitative biomarker rate correlations, which are needed to generate degradation rate estimates for chlorinated ethenes. MDL/IDL study methods are summarized below; details are included in Appendix A.

For determination of the MDL, the 12.5 pmol/µL stock solution of isotopically labeled (IS) peptides was diluted in 50 mM ammonium bicarbonate to prepare the following concentrations (final in 25 µL): 250, 83, 27, 9, 3, 1, 0.34, and 0.11 fmol/µL. Each sample was digested with trypsin overnight and desalted using C18 spin columns. To confirm instrument functionality and detectability of each IS peptide, infusion and injection steps were performed. Each IS peptide was prepared as 12.5 pmol/µL in dimethyl sulfoxide (DMSO)/Milli-Q water (50/50), aliquoted, and frozen at -80°C until use. Concentrated solutions for each peptide were provided to the analyst for subsequent dilution and infusion directly into the mass spectrometer (Waters Xevo TQ-XS) for confirmation of precursor (parent) ion, charge state, product ions (daughters), and optimization of collision energies (CE) (Table 2, Appendix A). This optimization step is performed to confirm that a peptide of a given sequence is detectable in the mass spectrometer and to optimize signal intensity for product ions. Each peptide was diluted to 0.5 pmol/µL or 1.25 pmol/µL in HPLC-grade water +0.1% formic acid and was directly infused into the mass spectrometer at a flow rate of 10 μ L/min. For each peptide, a mass spectrum of the precursor ion was obtained. For each precursor ion, a mass spectrum was obtained for the product ions after fragmentation with CE of ≥ 20 V. Using Waters Intellistart software, the CE for each peptide was optimized to maximize a signal from product ions. This was performed by infusing a single peptide into the mass spectrometer while Intellistart software varied cone voltage and CE to maximize a signal for each product ion. Skyline software was also used to output optimal CE for each peptide using equation 2 with parameters (slope, intercept) that are specific to Waters Xevo mass spectrometers (Table 5-1).

$$CE = slope *(precursor charge state) + intercept$$
 equation 2

Precursor Charge State	Slope	Intercept
+2	0.037	-1.066
+3	0.036	-1.328

 Table 5-1. Parameters of Waters Xevo CE Equation

After optimization of CE per each IS peptide further development of multiple reaction monitoring assay was performed, including optimization of dwell time, CE, and solvent program. During this phase, peptides with relatively poor response were dropped from the MRM method file. The Skyline-optimized CEs were used in initial MRM method development. Comparison to Intellistart-optimized CEs was performed later in MRM development, however improvements in signal intensity were insignificant.

For MRM method development, peptides were prepared as a mixture at 1.25 pmol/ μ L in HPLCgrade water + 0.1% formic acid from a 12.5 pmol/ μ L mixture in DMSO/Milli-Q water. The solvent program and modified versions thereof were used (see Appendix A, Table 3). The chromatographic system used was the Waters M-Class equipped with a trap column (Acquity UPLC M-Class Trap Symmetry® C18; 5 μ m particle size, 100Å pore size; 0.3 mm x 50 mm) and an analytical column (Acquity UPLC M-Class HSS T3 C18; 1.8 μ m particle size, 0.3 mm x 50 mm). Based on the observed maximum peak heights of each peptide at 1.25 pmol/ μ L prepared in HPLC-grade water + 0.1% formic acid (MS Parameters from September 5, 2017: 123 transitions; 30 ms dwell time; 3.7 s cycle time), some peptides were removed from the transition list based on poor response (peak height or peak area) relative to other peptides. Only those peptides with the largest responses were retained on the transition list.

Using the modified transition list and a 1.25 pmol/ μ L standard prepared in HPLC-grade water + 0.1% formic acid, three dwell times (20 ms, 50 ms, and 70 ms) were examined to assess the sensitivity of the signal to variation in dwell time. Based on the quality of the output data (peak height, peak shape, and points across a peak), the 50 ms dwell time was pursued for MDL experiments. The dwell time parameter was adjusted to 30 ms after further method development was prompted by failure of the first MDL set.

To establish IDL, IS peptides were prepared as a mixture at 12.5 pmol/ μ L in DMSO/Milli-Q water (50/50), aliquoted, and frozen at -80°C until use. A mixed, concentrated solution (12.5 pmol/ μ L) was provided fresh to the analyst during each day of analysis. The analyst diluted the sample to 250 fmol/ μ L in in HPLC-grade water + 0.1% formic acid and serially diluted this solution three-fold to prepare the following concentrations: 83, 27, 9, 3, 1, 0.34, and 0.11 fmol/ μ L. The lowest measurable concentration for each peptide, defined as S/N ≥ 3 (as measured by MassLynx) for the primary and secondary ion, represents the IDL for each peptide.

To determine the MDL of peptide targets, IS peptides were prepared as a mixture at 12.5 pmol/ μ L in DMSO/Milli-Q water (50/50), aliquoted, and frozen at -80°C until use. A mixed, concentrated solution (12.5 pmol/ μ L) was provided fresh to the analyst during each day of analysis. The analyst diluted the sample to 1.25 fmol/ μ L in HPLC-grade water + 0.1% formic acid to use as a control during the analysis sequence. The 12.5 pmol/ μ L stock solution was diluted in ammonium bicarbonate to prepare the following concentrations (final in 25 μ L): 250, 83, 27, 9, 3, 1, 0.3, and

0.1 fmol/ μ L. Each sample was digested with trypsin overnight and desalted using C18 spin columns. The lowest measurable concentration for each peptide, defined as S/N \geq 3 (as measured by MassLynx) for the primary and secondary ion, represents the MDL for each peptide.

A detailed report characterizes each step of system and IS peptide optimization (Appendix A). Data pertaining to system resolution check, calibration, and chromatograms of peptide detections are grouped per sample set.

5.5 VALIDATION OF QPROT ASSAY QUANTITATION LIMITS

After the development of the MRM assay and after the IDL and MDL values had been established for each RDase peptide, a study was performed with the SDC-9 consortium to identify the lowest *Dhc* cell titer that generated detectable and quantifiable concentrations of the RDase peptides selected for quantification. Validation study methods are summarized below; details are included in Appendix B.

To correlate the number of RDase proteins to *Dhc* cell abundances, qPCR was performed with the same samples. Briefly, to determine initial *Dhc* cell density, culture suspension (1 mL) of freshly grown SDC-9 consortium was filtered through 0.22 µm Durapore membrane filters (25 mm, Millipore, Billerica, MA) in triplicate to collect biomass, and then DNA was extracted by using a DNeasy PowerLyzer PowerSoil Kit (Qiagen, Valencia, CA) according to the manufacturer's instructions except for application of bead-beating method for enhanced cell lysis (OMNI Bead Rupter Homogenizer, OMNI International, GA) at 5 m/s for 3 min. Total DNA concentrations were determined using the Qubit dsDNA BR Assay (Invitrogen, Carlsbad, CA). TaqMan qPCR analysis of DNA was performed to determine the *Dhc* cell abundances using a *Dhc* 16S rRNA gene-targeted primer-probe set and qPCR conditions given in Section 5.6.3.

Based on initial *Dhc* cell density/mL determined by TaqMan qPCR assay, the SDC-9 culture was diluted to *Dhc* cell densities of 10^5 , 10^6 and 10^7 cells/mL using reduced mineral salt medium [35] inside an anoxic chamber. Sample preparations were performed in triplicate in sterile 50-mL Falcon plastic tubes. Samples (15 mL) were taken from each dilution and filtered through a 0.2 µm filter (0.22 µm, Millipore, Billerica, MA) at low flow speed for qPCR and qProt analyses. Each filter was placed in a sterile 50-mL Falcon tube and stored at -80°C immediately.

For qProt analysis, the filters were sent to Battelle on dry ice with an overnight carrier. Proteins were extracted with the Protein Extraction Kit (MoBio) and protein concentration was calculated using published methods [36]. An aliquot corresponding to 100 μ g of protein was mixed with 100 mM ammonium bicarbonate, 10 μ g bovine serum albumin (BSA) and isotopic peptide mix, reduced with dithiothreitol (10 mM), and incubated for 30 minutes at 57°C. Proteins were then alkylated with iodoacetamide (50 mM) for 30 min at room temperature in the dark. Excess iodoacetamide was quenched with dithiothreitol (16 mM final concentration). Peptides were digested with trypsin added in a 1:50 trypsin/protein ratio for 10 hours at 37°C. Samples were then acidified with an equal volume of 3% trifluoroacetic acid (TFA), dried via SpeedVac, then suspended in 270 μ L of 0.1% TFA. Samples were loaded on a C18 XTerra column (1 × 100 mm, 5 μ m pore size, 100 Å; Waters Corporation, Milford, MA, USA), desalted using 0.1% TFA, and peptides were eluted with 70% acetonitrile. Samples were dried via SpeedVac, then suspended in

a 2% indexed Retention Time (iRT) solution (Waters) prior to injection onto a Xevo TQ-XS Triple Quadrupole Mass Spectrometer.

5.6 LABORATORY MICROCOSM TESTING

The microcosms utilized for this project consisted of 500 mL (groundwater only) or 1000 mL (groundwater + soil) amber, narrow mouth glass bottles. Each bottle was fitted with a Teflon[®]-lined screw-cap. Microcosm tests were performed using materials from the JBLM LF2 field site (Section 4). One of the microcosm tests was performed using a mixture of groundwater and aquifer solids. Two of the microcosm tests were performed using a mixture of groundwater and aquifer solids. In order to most effectively simulate a groundwater aquifer, a high ratio of aquifer solids/groundwater was used in the solids-containing microcosms. All microcosms were placed on a bottle roller to ensure adequate mixing during incubation. Subsamples were collected as described in Section 5.6.3 and were subject to chemical, geochemical and molecular parameter analysis described in Section 5.7.

5.6.1 Growth of the SDC-9 Inoculum

The SDC-9 culture was inoculated in microcosms at varying densities to quantify and correlate rates of cVOC degradation with quantities of key RDase biomarkers. The SDC-9 inoculum was grown in reduced basal salts medium [37] in a 4,000-L fermenter using lactate as a source of carbon and electrons, PCE as a sole electron acceptor, and yeast extract as a source of nutrients. Further details concerning the fermentation and growth of SDC-9 are provided elsewhere [38]. For the current study, a volume of the culture was removed from the fermenter (or from a keg of culture previously grown and stored at 4°C for < 1 month), centrifuged, and suspended in medium to a *Dhc* density of ~ 1×10^{10} cells/mL based upon optical density (OD), $\alpha = 600$ nm [38]. The culture was then diluted for addition to microcosms as described below. Initial studies were conducted to estimate biodegradation rates of *cis*-DCE by SDC-9 prior to microcosm preparation.

5.6.2 Microcosm Preparation and Treatments

Microcosm #1, Groundwater Only Treatments. Six treatments (1-6) were tested in triplicate (a,b,c) microcosms. Microcosm construction and sampling was performed in a Coy anoxic chamber with a pure N_2 headspace. No H_2 gas was used in the chamber, which was thoroughly purged with N_2 prior to use to minimize any residual O_2 . Microcosms were constructed in 500 mL amber Boston Round analytical bottles with Teflon®-lined septa caps. Microcosm bottles were bleached, rinsed with deionized water (DI) and autoclaved prior to use. Due to the relatively low alkalinity and pH of the site water, 1.0 g calcium carbonate (CaCO₃) was added to each microcosm as a slow release buffer to maintain a neutral pH during incubation. Site water (475 mL) was added to each of the bottles. Bottles then received the following amendments to bring the final aqueous concentration in each to ~ 490 mL:

- 1. Lactic acid sodium salt (LASS) to 500 mg/L final concentration of lactate (4.1 mL of 6% LASS).
- 2. NaBr to a final Br⁻ concentration of 10 mg/L: (0.49 mL of 10,000 mg/L Br⁻ stock).
- 3. To individual bottles, washed SDC-9 culture was added in medium to achieve nominal *Dhc* titers listed below:

- 1a,b,cAdd 4.9 mL of 10^{10} Dhc /mL (final = 10^8 /cells Dhc per mL)2a,b,cAdd 4.9 mL of 10^9 Dhc /mL (final = 10^7 /cells Dhc per mL)3a,b,cAdd 4.9 mL of 10^8 Dhc /mL (final = 10^6 /cells Dhc per mL)
- 4a,b,c Add 4.9 mL of 10^7 *Dhc* /mL (final = 10^5 /cells *Dhc* per mL)
- 5a,b,c Add 4.9 mL of site water
- 6a,b,c Add 4.9 mL of site water and 0.333 g HgCl₂
- 4. A 5 mg/L final concentration of *cis*-DCE was added to each bottle (2.45 mL of 1,000 mg/L *cis*-DCE in DI water).
- 5. Small amounts of additional site water were added to achieve a final volume of 490 mL in each incubation vessel.

After all amendments were added, the microcosms were "topped off" with groundwater so that < 1 mL headspace was present in each bottle. The bottles were then tightly sealed with Teflon[®]-lined caps and removed from the anoxic chamber. Each bottle was then placed at 15 °C on a bottle roller operating at ~0.5 rotations per minute for incubation for an appropriate period of time depending on the treatment prior to sampling again for analysis of *cis*-DCE. The sampling procedure and analytes measured are provided in Section 5.6.3 and 5.7, respectively.

Microcosm #2, Groundwater Only and Groundwater + Solids Treatments. Ten treatments were established in the JBLM 2 microcosms, which were prepared in 1000 mL clean, sterile Boston Round Bottles. All microcosms were amended with 500 mg/L LASS, 10 mg/L cis-DCE, and 10 mg/L Br⁻ (NaBr) prepared as previously described. Microcosms received SDC-9 at four expected *Dhc* cell titers; 10^7 *Dhc*/mL (1a, b, c and 1d, e, f), 10^6 *Dhc*/mL (2a, b, c and 2d, e, f), 10^5 *Dhc*/mL (3a, b, c) and 10⁴ *Dhc*/mL (4a, b, c) as previously described except that dilutions were prepared in site groundwater rather than medium. Live (5a, b; 5 c, d) and killed (6 a, b; 6c, d) controls were also prepared. For replicates a,b,c in treatments 1-4 and a,b in treatments 5-6, only groundwater was added to the bottles. The remaining bottles (replicates d,e,f in treatments 1 and 2 and replicates c, d in treatments 5 and 6) received 353 g of aquifer solids at 15% moisture content (300 g dry weight). After all amendments had been added, the microcosms were completely filled with site groundwater, sealed and placed on a bottle roller (1 rpm) at 15 °C. After 10 days of incubation, 2 g of CaCO₃ (solid) was added to all microcosms due to an observed decline in pH in some bottles with SDC-9 added. Treatment 1, with the highest Dhc concentration, was set up a second time with an initial 2 g of CaCO₃ added to ensure that the declining pH did not affect degradation kinetics. A photograph of the JBLM 2 microcosm bottles with and without sediments is provided in Figure 5-2.

5.6.3 Microcosm Sampling Procedure

Water samples were collected from microcosms in order to measure contaminant degradation and RDase biomarkers as described below.

Microcosm #1 Sampling. All sampling was performed in a Coy anoxic chamber with a N₂ headspace. Liquid samples for chemical analysis were removed from the microcosms with gastight syringes to appropriate sample containers. Samples volumes consisted of the following: 2 mL for cVOCs (EPA Method 8260); 4 mL for methane, ethane and ethene (EPA 3810/RSK-175); 1 mL for anions (EPA Method 300.0) and volatile fatty acids (EPA 300m); and 5 mL for pH determination. The methods of analysis are provided in Section 5.7 and Appendix C.
Duplicate 15-mL aqueous samples, one for qPCR and the other for proteomic analysis, were removed using a glass pipette and transferred to sterile screw-cap 50-mL conical tubes. Cells were collected by centrifugation for 40 min at 11,000 rpm using a refrigerated Sorvall Lynx 6000 Centrifuge and a F21-8x50y rotor (Thermo Scientific). Immediately after centrifugation, the supernatant was aspirated from the cell pellets and the samples frozen at -80 °C. Microcosms were refilled with site water removed during sampling, punctured septa were replaced, and bottles were returned to rollers operating at 1 rpm and 15 °C.

Samples from the microcosm treatments were collected at different intervals based upon the initial concentration of *Dhc* added. See summary of cVOC sampling times bulleted below. Samples for qPCR and proteomic analysis were not collected and/or analyzed at each of these time points, but generally at the beginning, middle, and end of the incubating periods. Specific times for sample collection from each microcosm bottle are provided in Appendix E.

- Set 1: 0, 1, 2, 4, 6, 8, and 24 hours
- Set 2: 0, 8, 24, 48, 72, 96, 120 hours
- Set 3: 0, 6, 9, 13, 16, 20, 23, 27, 36, 55, and 83 days
- Set 4: 0, 6, 13, 20, 27, 36, 55, and 83 days
- Set 5 and Set 6: 0, 6, 9, 13, 16, 20, 23, 27, 55, and 83 days



Figure 5-2. Photograph of microcosms with and without sediments on the bottle roller (left) and settling for sample collection (right).

Microcosm #2 Sampling. Microcosm sampling was conducted as described for Microcosm #1, except that bottles with solids were removed from the rollers for 30 minutes to allow solids to settle prior to liquid sampling. See summary of cVOC sampling times bulleted below. Samples for qPCR and proteomic analysis were not collected and/or analyzed at each of these time points, but generally at the beginning, middle, and end of the incubating periods.

- Set 1: 0, 3, 7, 10, 14, 17, 21, 24, and 28 days
- Set 1 (duplicate): 0, 0.3, 1, 1.3, 2, 2.3, 3, 3.3, and 7 days
- Set 2: 0, 3, 7, 10, 14, 17, 21, 24, 28, 31, 35, 38, and 42 days
- Set 3 and Set 4: 0, 7, 14, 21, 28, 35, and 42 days
- Set 5 and Set 6: 0, 3, 7, 9, 14, 17, 21, 24, 28, 31, 35, 38, and 42 days

5.7 SAMPLING & ANALYSIS METHODS

This section provides a summary of all samples collected during the laboratory project (Table 5-2), as well as a summary of the analysis methods used (Table 5-3). Method SOPs and detailed QC procedures are included in Appendices C and D, respectively.

Component	Matrix	Number of Samples	Analyte	Location ^a
Screen aquifer	Groundwater	3	cVOCs, pH	JBLM LF2, VAFB SA288,
material from 3				NBK Keyport Area 1
candidate cVOC-	Groundwater/Aquifer	3	cVOCs, pH	JBLM LF2, VAFB SA288,
contaminated	Material Slurries			NBK Keyport Area 1
aquifer sites	<i>Dhc</i> activity inhibitor screening microcosm	3	cVOCs, pH	JBLM LF2 only
JBLM	Groundwater	24	peptides	JBLM LF2
Microcosm#1,	"	24	genes	"
Groundwater only	"	159	anions	"
	"	159	cVOCs	"
	"	159	VFAs	"
	"	159	dissolved gasses	**
JBLM	Groundwater	18	peptides	JBLM LF2
Microcosm#2,	"	18	genes	"
Groundwater only	"	182	anions	**
treatments	"	182	cVOCs	"
	"	182	VFAs	**
	"	182	dissolved gasses	**
JBLM	Groundwater ^b	18	peptides	JBLM LF2
Microcosm#2,	"	18	genes	**
Groundwater+	"	145	anions	**
aquifer solids	"	145	cVOCs	"
treatments	"	145	VFAs	"
	"	145	dissolved gasses	"

Table 5-2. Number of microcosm test samples by analysis

a. Field materials were collected from candidate sites described in Section 4.0.

b. Groundwater collected after allowing solids to settle per Section 5.6.3.

Table 5-3.	Summary of	standard :	analytical	and RDase	biomarker	methods
------------	------------	------------	------------	-----------	-----------	---------

Sample Type	Analyte	Method	Container	Preservative	Hold Time
	peptides	Proteomics (Section 5.4.2, Appendix B)	Sterile 15 mL plastic Falcon tube	-80°C	N/A
	genes qPCR (Section 5.4.3, Appendix B)		Sterile 15 mL plastic Falcon tube	-80°C	N/A
Microcosm	Anions	EPA 300.0	1 mL	4°C	7 days
Samples	cVOCs	EPA Method 8260B	2 mL	HC1	28 days
1	VFAs	EPA 300 m	< 100 µL (aliquot from anion sample)	4°C	7 days
	Dissolved gasses	EPA Method 3810, RSK-175	5 mL w/1 mL headspace	HC1	28 days

N/A reflects direct injection analysis for cVOCs and dissolved gasses upon sample collection

5.7.1 Analytical Methods: Standard Geochemical cVOC Analyses

Microcosm samples (groundwater/sediment mixture) were analyzed using the following standard EPA procedures or modifications of these procedures for the analytes of interest at Aptim. Detailed

method procedures are included in Appendix C. Inorganic anions were determined according to EPA Method 300.0, which uses ion chromatography. cVOCs were determined by EPA Method 8260B using gas chromatography and mass spectrometry. cVOCs were introduced into the gas chromatograph by the purge-and-trap method 5030B. Dissolved gases including methane, ethane and ethene were analyzed according to EPA Method 3810, RSK-175 [39]. For this method, a 4-mL volume of water from the microcosm was added to a 5 mL serum vial, and the vial was then sealed and shaken to equilibrate the headspace with the aqueous phase. The headspace was then analyzed for dissolved gases by GC using direct injection. The Henry's law coefficient for each gas was then used to calculate the aqueous concentration. Volatile fatty acids (VFAs) including acetate, lactate, formate, and propionate were measured using ion chromatography via modification of EPA method 300 (EPA 300m). pH was measured using a pH meter and microprobe.

5.7.2 Analytical Methods: Proteomics

Samples collected during the microcosm study were frozen at -80 °C then shipped on dry ice overnight to Battelle Memorial Institute for proteomic analyses. Proteins were extracted from lyophilized groundwater/sediment slurry samples, reduced, alkylated, trypsin digested, and subjected to LC-MS/MS using a Nano 415 LC system in line with an ABI Sciex Triple TOF 5600 high resolution MS instrument (Sciex, Concord, Canada) (Figure 5-3). During processing, the entire sample was subjected to protein extraction since protein and peptide concentration determination is a prerequisite for optimal protein digestion and optimal sample loading amount in bottom-up proteomics. The protein and peptide concentrations were calculated with a tryptophan assay [36]. For qProt, samples were spiked with selected isotopically labeled peptides at the digestion step for quantification of native peptide equivalents.



Figure 5-3. Steps involved in proteomic analysis of microcosm test samples

Sample MS and MS/MS data were acquired using an Eksigent Nano 415 liquid chromatograph system (Sciex, Concord, Canada) directly connected to a quadrupole time-of-flight (QqTOF) TripleTOF 5600 mass spectrometer (Sciex, Concord, Canada). The instrumentation is controlled using Analyst TF 1.6 and Eksigent software. A total of 25 μ L of sample was injected onto a 0.3 mm x 150 mm Eksigent C18-CL-120 analytical column (3 μ m particle size, 120 Å pore size,) using a trap-and-elute method. Peptide separation was achieved using a linear gradient of acetonitrile containing 0.1% (v/v) formic acid of different lengths depending on the acquisition

mode. Solvents used included 0.1% formic acid (v/v) (solvent A) and 0.1% formic acid (v/v) in acetonitrile (solvent B). Peptides were trapped on the loading column using 100% solvent A at a flow rate 5 μ L/min for 5 min. Trapped peptides were then separated at a predetermined flow rate using the following conditions: (1) 5% solvent B in A (from 0-5 min), (2) 5-35% solvent B in A (from 5-65 min), (3) 35-90% solvent B in A (from 65-66 minutes), and (4) 90% solvent B in A (from 66-70 minutes), with a total runtime of 90 min, including mobile phase equilibration.

Continuing mass calibration of the TOF MS and TOF MS/MS was performed throughout the analysis sequence by analyzing a digested β -galactosidase standard (Sciex, Concord, Canada). Mass spectrometric analysis was performed using data dependent acquisition (referred to as information dependent acquisitions, or IDA). Full scan spectra were acquired for specific *m/z* with a 250-millisecond acquisition time. For collision induced dissociation tandem mass spectrometry (CID MS/MS) in IDA mode, the mass window for precursor ion selection of the quadrupole mass analyzer was set to unit resolution ($\pm 0.5 m/z$). For MS/MS analysis, precursor ions were fragmented in a collision cell using nitrogen as the collision gas. For IDA analysis, the instrument was set to trigger product ion scans (from 100 to 1500 *m/z*) only after specific criteria were met by the precursor ions. These criteria were defined during the IDL and MDL analyses. The Rolling CE algorithm was used to determine the appropriate collision energy for each precursor mass.

For quantification, labeled RDase conserved peptides selected based on multiple sequence alignment of known RDase protein sequences and an internal bovine serum albumin control were spiked into sample extracts immediately prior to the protease digestion step. Native peptide concentrations were determined by comparing peak ratios of native and isotopically labeled peptides. Proteins were identified from LC-MS/MS spectra by searching against a database of protein sequences constructed from the metagenome sequences of the SDC-9 microbial community. In addition, sequences of protein contaminants typical for proteomic experiments (e.g., keratin and trypsin) were added to the database. The proteomic LC-MS/MS data were queried against this database and searched against the library of known selected enzymes involved in cVOC degradation. Only peptides with the "Protscore" for a particular protein higher than 1.3 were considered true positives. Statistical analyses of proteomic data were performed using Protein Pilot (confidence score and false discovery rate).

5.7.3 Analytical Methods: Quantitative PCR

Reductive dechlorination biomarker genes were enumerated in aqueous samples with qPCR following established procedures [7, 14]. Frozen cell pellets collected from the microcosms (details in Section 5.6.3) incubated in the Aptim laboratory were shipped overnight in a cooler with dry ice to the University of Tennessee. The samples were stored frozen at -80°C until analysis.

DNA extraction. The cell suspensions were thawed, and DNA was isolated from cell pellets with DNeasy PowerLyzer PowerSoil Kit (Qiagen, Valencia, CA) according to the manufacturer's instructions except for using a bead-beating method (OMNI Bead Rupter Homogenizer, 5 m/s for 3 min) (OMNI International, GA) for enhanced cell lysis. DNA was eluted into nuclease-free water and DNA concentration and quality were determined with a NanoDrop spectrophotometer (NanoDrop Technologies, Wilmington, DE, USA) and a Qubit fluorometer (Invitrogen) using

double stranded DNA (dsDNA) Broad-Range assay kit according to the manufacturer's manual. DNA was stored at -80°C until analysis.

qPCR. Primers and probes to enumerate total bacterial 16S rRNA, *Dhc* 16S rRNA, *tceA* and *vcrA* genes have been reported [3, 7, 10, 40]. In addition, new primer and probe combinations have been designed for SDC9_24_*pceA* and *fdhA* (Table 5-4).

Assay ID	Organism(s)	Target Gene
Bac_16S	Total Bacteria	16S rRNA
Dhc_16S	Dhc-specific	16S rRNA
SDC9_24_pceA	Dehalobacter restrictus/ Desulfitobacterium hafniense	PCE reductive dehalogenase
SDC9_59_tceA	Dhc	TCE reductive dehalogenase
SDC9_212_vcrA	Dhc	VC reductive dehalogenase
fdhA (omeA)	Dhc-specific	Molybdoenzyme involved in electron transfer to the RDase

Table 5-4. Summary of specific qPCR assays run for microcosm samples

Specific primers and TaqMan probe sequences targeting SDC9_24 *pceA* and *fdhA* were designed using Geneious R11.0.2 (http://www.geneious.com, [41]) and primers were synthesized by IDT (Integrated DNA Technologies). In order to ensure specific hybridization at a uniform temperature, probes with Minor Groove Binder (MGB) modification were synthesized by Thermo Fisher Scientific. Design parameters for the target assays included primer and probe annealing temperature close to 60°C, primer and probe lengths ranged between 14-30 and 16-25 base pairs (bp), respectively and parameters were set to ensure that it was thermodynamically unlikely to form hairpin structures, self-dimers and heterodimers for primers and TaqMan probes. The specificity of the primers and probes was also verified using primer-BLAST analysis [42].

(i) For regular qPCR, every 20- μ L reaction had 10 μ L of 2×TaqMan Universal PCR Master Mix (Applied Biosystems, Carlsbad, CA), 2 μ L of diluted (1:10 and 1:100) DNA template, and forward and reverse primers and probe at final concentrations of 300 nM each. Reactions were initially held for 2 min at 50°C and 10 min at 95°C following 40 cycles of denaturation at 95°C for 15 seconds and annealing and extension at 60°C for 1 min. The qPCR assay results were analyzed using the ViiA7 Software (Applied Biosystems, Carlsbad, CA). All qPCR assays were performed in triplicate.

(ii) For high-throughput qPCR in 384-well microtiter plates, all qPCR reactions were performed with the QuantStudio 12K Flex Real-Time PCR System (Applied Biosystems, Carlsbad, CA), a flexible platform enabling the instrument to accommodate one 384-well plate. Every 10- μ l reaction contained 5 μ L of 2×TaqMan Universal PCR Master Mix (Applied Biosystems, Carlsbad, CA), 2 μ L of diluted (1:10 and 1:100) DNA template, and forward and reverse primers and probe at final concentrations of 300 nM each. Reactions were initially held for 2 min at 50°C and 10 min at 95°C following 40 cycles of denaturation at 95°C for 15 seconds and annealing and extension at 60°C for 1 min. The qPCR assay results were analyzed using the QuantStudio 12K Flex Real-Time PCR System Software (Applied BiosystemsTM, Carlsbad, CA).

Plasmid DNA containing each of the cloned target gene was used as templates for standard curves. Standard curves were included with every qPCR plate using 10-fold serial dilutions of plasmid DNA over a 7 orders of magnitude range beginning at a 1 ng μL^{-1} concentration (~8 log gene copies) and decreasing to 10^{-7} ng μL^{-1} . All standard curves had a total of eight calibration points and were run in triplicate. To calculate the number of gene copies in a known amount of DNA and gene copies per sample, previously published equations were applied [7].

From this original dilution series, Level of Detection (LOD) and Level of Quantitation (LOQ) were determined experimentally as 1-10 copies/ μ L and 10-50 copies/ μ L, respectively based on targeted assay. Examples of qPCR standard curves are given in Appendix C.

To further understand RDase expression and regulation as well as potentially correlate degradation rate to gene expression, transcript (mRNA) measurements were planned. Using transcript measurements, some correlation between dechlorination activity and RDase gene expression has been demonstrated, but the correlation is highly inconsistent and currently unpredictable [5]. This inconsistency is due to the fact that RDase gene expression is regulated by various environmental factors (e.g., growth phase, contaminant concentrations, etc.) through poorly understood accessory proteins. Further, reproducible and quantitative RNA extraction remains challenging due to the inherent susceptibility of RNA to degradation (i.e., unintended loss of biomarker) [43]. Thus, while informative, assays that use ribonucleic acid provide no reliable correlation to degradation rate and no direct information about the catalysts (i.e., the enzymes) that actually perform the biodegradation reaction, and measurements of transcripts to determine gene activity were not applied to samples in this study.

5.8 DATA ANALYSIS

Estimating Reductive Dechlorination Rates. First-order rate coefficients for biological reductive dechlorination of *cis*-DCE and VC (k_{cDCE} and k_{VC}) in the microcosms were estimated by fitting a numerical approximation of the first order reaction equations for sequential degradation of *cis*-DCE to VC and then to ethene to the change in molar concentrations of *cis*-DCE, VC, and ethene (target compounds) over time in the microcosms. Microsoft Excel Solver was used to minimize the sum of squares error between the measured and model-estimated values to obtain the best fit. Measured values were corrected for dilution by applying a dilution factor equal to the total moles of target compounds present in the microcosm when the sample was collected divided by the total moles of target compounds present at time zero. Dilution correction using bromide concentrations yielded similar results. The number of moles in individual target compounds in microcosms that contained aquifer solids were corrected for sorption to the solids by assuming linear partitioning and using equation 3 below,

$$M_{tot,sorption\ corrected} = C_w V_w + C_w M_s (0.63 K_{ow} f_{oc})$$
 equation 3

where C_w is the dilution-corrected molar concentration in water, V_w is the volume of water present in the microcosm, M_s is the mass of solids in the microcosm, K_{ow} is the VOC-specific octanolwater partitioning coefficient, and f_{oc} is the fraction of organic carbon present in the solids, which was assumed to be 0.001. The constant 0.63 converts units of the product of K_{ow} and f_{oc} into L/kg. K_{ow} values used for *cis*-DCE, VC, and ethane were 72.4, 28.8, and 13.5, respectively [44]. Rate coefficients for each test replicate microcosm were determined separately using this approach; rate coefficients for live and killed controls were not determined. The 95% confidence interval associated with each fitted rate constant was determined using the approach described in Smith et al. 1998 [45].

Correlating Reductive Dechlorination Rates and Biomarker Abundances. Log-transformed rate coefficients and biomarker abundances were subject to the Shapiro-Wilk normality test. The Spearman Rank Order Correlation analysis followed by power law least squares regression analysis was used to quantify the relationship between biomarker abundances and rate coefficients. Rate coefficients represent an integrated measure of activity in each microcosm over time, whereas biomarker abundances provide a single measure at various time points during the incubation. Correlation analysis was performed twice: once using the global data, which included biomarker abundances collected at early, mid and late time points from each microcosm with the corresponding integrated rate coefficients measured for that microcosm, and again using only midpoint biomarker abundances and the corresponding rate coefficients.

Assessing Predictive Power of Biomarker Abundances. The microcosm experiments were divided into a "training set" and an "evaluation set." Rate coefficients and biomarker abundances from the "training set" microcosms were subject to power law least squares regression analysis of rate constants on abundance. Only data from microcosms where non-zero rate coefficients were obtained were included in the analysis. Measured biomarker abundances in the "evaluation set" of microcosms were entered as "x" variable in the regression equations to obtain a predicted rate coefficient. The predicted rate coefficient was then compared to the measured rate coefficient for that "evaluation set" microcosm. Two types of training sets were established. The first training set featured randomly selected microcosms that contained either 10^6 , 10^7 or 10^8 Dhc cells/mL. The second training set featured the global average of biomarker abundances and rate coefficients for all microcosms that contained either 10^6 , 10^7 or 10^8 Dhc cells/mL. The predictive power of the biomarkers were evaluated by comparing (1) the measured vs. predicted rate constants for each individual biomarker, (2) the measured vs. the average of the predicted rate constants for the various gene biomarkers, (3) the measured vs. the average of the predicted rate constants for the various peptide biomarkers, and (4) the measured vs. the average of the predicted rate constants for all of the biomarkers.

6.0 PERFORMANCE ASSESSMENT

6.1 DETERMINATION OF RDASE TARGETS WITH SHOTGUN PROTEOMICS

Shotgun proteomic analyses of SDC-9 extracts identified 35 RDase peptides. The tryptic peptides included the most abundant peptides of TceA, PceA and VcrA, which were detected with 99-100% peptide coverage. Five non-tryptic peptides (i.e., truncated from one end [either N-terminal or C-terminal] of the tryptic peptide), were observed with confidence levels exceeding 90% (three corresponding to PceA and two corresponding to TceA). A single peptide corresponding to VcrA was observed with low confidence (<50%). Sixteen peptides corresponding to PceA and fourteen peptides corresponding to TceA were identified with maximum confidence (100% sequence identity). The final list of SDC-9 unique RDase peptide targets and their transitions downselected for the MRM work are listed in Table 6-1.

Protein	Peptide Sequence	Precursor m/z	RT ^d	Product <i>m/z^c</i>	Ion	CVa	R ²	IDL ^b	Accession Number
		705 4		1225.7	y11	4.3			CAD28700 2
	IATQIPLLQDAAR	103.4 [M+2H] ²⁺	45.3	996.6	y9	3.5	0.98	5	WD 025206074 1
				883.5	y8	5.1	-		w1_023200074.1
		624 2		1025.5	y9	2.2			CAD28790.2
PceA	LESGYVQNMVK	034.3 [M+2H] ²⁺	33.2	938.5	y8	0.8	0.98	5	CDX02974.1
				718.4	y6	3.2	-		WP_025206074.1
		506.3		925.5	y8	7.3	_		CAD28790.2
	VYTDLELAPDKPR	500.5 [M+3H] ³⁺	33.2	683.4	y6	5.1	0.97	1	CDX02974.1
				612.3	y5	5.9			CDX02974.1
		701.2		1188.6	y11	4.9	_		
	VNNEPWWVTTR	[M+2H] ²⁺	43.6	945.5	у7	1.7	0.97	5	WP_062900263.1
				848.4	y6	4.1	-		
	YFGASSVGAIK	550.3 [M+2H] ²⁺		936.5	y10	2.9	_		WP_062900263.1
TceA			34.5	789.4	у9	3.4	0.98	0.5	
				661.4	у7	1.3			
	VSGWNNOGAVEI	033.8	54.5	978.4	b9	4.5	_		WP_062900263.1
	Y SGWNNQGA Y FL	933.8 [M+3H] ³⁺		1172.6	y10	1.6	NA	100	
	TEDTESTITIOR			1057.5	y9	3.4			
				1104.4	у9	2.6	_		See peptide BLAST
	VVTDLPIAPTPPID	806.7	567	989.4	y8	3.2	NA	100	results in SI; no match
	AGMFEFCK	[M+3H] ³⁺	30.7	918.4	y7	3.2	1111	100	with sequences from metagenomic hits
				1067.5	y8	3.1	_		See peptide BLAST
VerA	SUNNFPWYVK	634.3	48 1	839.4	y6	6.8	0.98	50	results in SI; no match
v crA		[M+2H] ²⁺	10.1	692.4	y5	6.6	0.90	20	with sequences from metagenomic hits
	GLGLAGAGIGAVA			1211.1	y23	_			
	ASAP-	1086.9	ND	1161.5	y22	- ND			AEI59454.1
	VFHDIDEFVSSEA NSTK	[M+3H] ³⁺		1126.0	y21	1.12			

Table 6-1. PRM transitions of selected RDase SDC-9 endogenous peptides

a. CV calculated from n=3 replicates from a 25, 50, 250 or 500 fmol/ μ L isotopically-labeled standard; b. units are in fmol/ μ L and values represent IDL for the isotopically-labled standards; c. bolded product m/z represent those used for quantitation; d. retention time, minutes

6.2 METHOD DETECTION AND INSTRUMENT DETECTION LIMIT RESULTS

RDase peptide hits identified from shotgun mass spectrometry experiments (Table 6-1) and additional FdhA peptides were selected for targeted quantification based on the following selection criteria: confidence score >90%, no missed cleavages, non-tryptic, no methionine oxidation, and no carbamidomethylation. Peptides were then searched against the National Center for Biotechnology Information (NCBI) protein database to assess specificity to RDase targets. Three peptides per protein were monitored, and the three most sensitive transitions per peptide were reported. Isotopically labeled peptide standards were used to verify transitions, quantify selected peptides and determine retention time on the liquid chromatography system for all peptides. Instrument detection limits were reported as the lowest isotopically labeled standard that satisfied a signal-to-noise ratio \geq 3 across three separate analyses. The most sensitive transition per peptide was used for quantification, and the remaining transitions were used as qualifiers. More specifically, several transitions for a given peptide ion were measured to validate the identification of a peptide, otherwise known as qualifiers. Only subsets of the transitions, typically the transition(s) with the highest intensities, were used for quantification of the peptide, also known as the quantifier. For example, the y9 ion of YFGASSVGAIK was the most sensitive ion for that peptide and was used for quantification, while detection of y7 and y10 ions were requisite to increase confidence in protein quantifications.

To determine the limit of detection, triplicate measurements of standard peptides at eight different concentrations in 0.1% formic acid were performed. The signal to noise ratio per each peptide was measured, and the standard deviations of the response at each concentration were calculated. CEs were optimized for initial 28 isotopically-labeled peptides to maximize the resulting signal from product ions. Following the optimization step, dwell time and solvent program were optimized and peptides that demonstrated poor signal response were discarded from the list. In total, 10 peptides were discarded from the list after optimization steps were completed and IDLs and MDLs were developed for the remaining peptides. Most peptides were observed in experimental samples during the IDL and MDL analysis, however VcrA peptides were observed exclusively in MDL experiments and not in IDL experiments (not observed is denoted as <250 fmol/µL), suggesting that sample digest and cleanup enhance the peptide signals for VcrA peptides. Two VcrA peptides (DQPWYVK and VPDHAVPINFK) were detectable in all MDL experiments while they were not detected in IDL experiments. Performance variation between IDL and MDL experiments are likely due to matrix effects. Some peptides performed similarly between MDL replicates (e.g., DQPWYVK) while others did not. Within the MDL set, inconsistencies were observed for sensitive peptides (e.g., TSPSLISSATVGK, VSSIIEPR, YFGASSVGAIK). This variation represents the variation present in the preparatory methods and instrumental analysis; it is unlikely that instrumental variation resulted in decreased sensitivity as control samples did not reveal loss of chromatographic quality or loss in mass spectrometer signal during the MDL runs.

Overall, the experiments performed allowed for identification of the most sensitive RDase and FdhA peptides for targeted quantification. MDL experiments resulted in detection of up to three of the most sensitive peptides per protein with up to three of the most intensive transition ions per peptide (Table 6-2).

						Established
Protein	ID	Peptide ¹	MDL 1	MDL 2	MDL 3	MDL
	FdhA2	SGSEIAFTGGLIK ¹	3	3	3	3
FdhA	FdhA5	ALGIVYLDSQA R	3	3	1	3
	FdhA8	NQAVSAPGEA K	3	3	3	3
	PceA4	IATQIPLLQDAA R	9	9	9	9
Deck	PceA5	LESGYVQNMV K	3	3	3	3
rceA	PceA7	DFWNNPEPI K	1	1	1	1
	PceA8	TSPSLISSATVG K	0.3	0.3	1	1
	TceA2	DVDDLLSAG K	0.3	3	3	3
TasA	TceA3	VSSIIEPR	0.3	0.3	1	1
IceA	TceA4	VNNEPWWVTT R	9	9	9	9
	TceA5	YFGASSVGAIK	0.3	0.3	1	1
	VcrA1	WGLYGPPHDSAPPDGSVP K	9	9	3	9
	VcrA2	YFGAGDVGALNLADP K	27	27	27	27
VcrA	VcrA3	VPDHAVPINFK	0.3	0.3	1	1
	VcrA4	GVYEGPPDAPFTSWGNR	83	27	27	83
	VcrA6	DQPWYVK	1	1	1	1
Units are	fmol-pept	ide. A 1.0 mL sample was extracted	l to determi	ne the MDI	Ĺs.	
¹ Bolded	letter den	ote heavy ¹³ C and ¹⁵ N labeled ami	no acid; th	e maximum	of three MI	DL test
replicates	was estab	blished as the MDL				

Table 6-2. MDL for peptides analyzed for SDC-9 culture

The data generated during the optimization and calibration experiments were built into the MRM method (i.e. the "qProt assay") used for quantification of RDase peptides in the microcosm experiment samples obtained during this laboratory study.

6.2 VALIDATION OF MRM ASSAY QUANTITATION LIMITS RESULTS

Quantitation limits of the qProt MRM assay for FdhA, PceA, TceA and VcrA proteins were validated by analyzing triplicate samples of SDC-9 culture diluted to 10⁵, 10⁶, or 10⁷ Dhc cells/mL.

Only two out of three FdhA peptides, namely FdhA2 and FdhA5, were observed in the analyzed samples. The FdhA8 peptide was not detected. FdhA2 and FdhA5 peptides were detected in all SDC-9 cell dilutions (10^5 to 10^7 *Dhc* cells). However, only 10^7 *Dhc* cells concentrations rendered quantifiable concentrations above the lower limit of MDL for these two peptides. FdhA2 peptide was selected as a quantifier based on the detection of the fragment ions showing the lowest LOQ. Table 6-3 shows FdhA peptide concentrations per total *Dhc* cell number. Peptides PceA4, PceA7 and PceA8 showed lower sensitivity than the PceA5 peptide, which was detected in samples with 10⁵ Dhc cells/mL. The lowest abundance of Dhc cells that generated detectable and quantifiable concentrations of PceA4, PceA7 and PceA8 was 10^6 , while 10^5 Dhc cells was needed to quantify the PceA5 peptide. The, PceA5 and PceA4 peptides were selected as quantifiers for the proceeding studies. The TceA2, TceA3 and TceA5 peptides had highest sensitivity and were detected and quantified in samples containing 10^5 Dhc cells (Table 6-3). However, the TceA5 peptide had a relatively inconsistent retention time variation and the peptides TceA2 and TceA3 were selected as quantifiers for the proceeding studies. The TceA4 peptide was detected in samples with $10^7 Dhc$ cells/mL. The VcrA peptides were least sensitive, with VcrA1, VcrA2, VcrA3 and VcrA6 peptides detected in the 10^6 and 10^7 Dhc cells and with small number of transition ions passing the accuracy

criteria. The VcrA4 peptide was detected but below the quantification limit in this study and most likely requires higher number of *Dhc* cells for quantification. Of all VcrA peptides, the VcrA3 was selected as a quantifier due to its highest sensitivity, detection of the highest number of transitions and its low MDL of 1 fmol/mL.

The analysis of the compiled data shows that the most sensitive peptides for quantification were FdhA2, PceA4 and PceA5, TceA2 and TceA3 and VcrA3 and required abundances of 2.2×10^6 Dhc cells/mL or more in the 15 mL sample that was extracted (corresponding to 10^7 Dhc cells or more extracted) to be detected (Table 6-3). These peptides served as quantifiers in the next set of experiments. The remainder of qualifier peptides was used to confirm accuracy of the detection method and were analyzed in all subsequent experiments. Additionally, four to six transition ions were analyzed per peptide ion to confirm accuracy and sensitivity of the method and to confirm peptide sequence. In this study, up to six transitions for a given peptide ion were measured to validate the identification of a peptide.

The required lowest concentration of *Dhc* cells for detection of the remainder of peptides varied per protein, for example, to detect other TceA peptides a minimum of 10^5 *Dhc* cells are required, but to detect VcrA specific peptides the cell concentrations need to be an order of magnitude higher. Thus, the total recommended *Dhc* cells in a sample for targeted proteomics is 10^7 cells, regardless of sample volume.

			<i>Dhc</i> ab	D					
		1.3x10 ⁵	2.2x10 ⁶	3.1x10 ⁷	1.3x10 ⁵	2.2x10 ⁶	3.1x10 ⁷	protein concentrations in	
Ductoin	Peptide	Peptid	Peptide concentration in			oncentration	in culture,	culture, fmol/mL	
Protein	ID	cu	iture, imoi/i		111101	me (protein)		(protein/ceii)	
	FdhA2 ^a	$<3.0x10^{0}$	$<3.0x10^{0}$	8.5×10^{0}				$^{[46]}$ KBI, D2 culture (TCE):	
FdhA	FdhA5	<3.0x10 ⁰	<3.0x10 ⁰	1.1x10 ¹	$<3.0 \text{ x}10^{\circ}$	$<3.0 \text{ x}10^{\circ}$	$(3.8 \times 10^{\circ})$	$9.0x10^{4} - 1.0x10^{2}$ $(2.3x10^{3} - 3.5x10^{3})$	
	PceA4 ^a	<9.0x10 ⁰	<9.0x10 ⁰	2.1x10 ¹					
Dut	PceA5 ^a	6.3x10 ²	1.9x10 ²	6.8x10 ¹	(2-102	1.9x10 ² 4.4x10 ¹	4.4.101		
PceA	PceA7	<1.0x10 ⁰	2.2x10 ¹	1.9x10 ¹	0.3X10 ²		4.4x10 ⁴		
	PceA8	<1.0x10 ⁰	$1.7 x 10^{1}$	$1.2x10^{1}$					
	TceA2 ^a	<3.0x10 ⁰	1.9x10 ¹	1.3x10 ¹					
Tert	TceA3 ^a	<1.0x10 ⁰	3.1x10 ¹	2.1x10 ¹	<1.0x10 ⁰	2.5x10 ¹	$1.7 x 10^{1}$ (7.7 x 10 ³)		
IceA	TceA4	<9.0x10 ⁰	<9.0x10 ⁰	2.3x10 ¹		$(1.1x10^4)$		$(^{[47]}2.3x10^{3})$	
	TceA5	<1.0x10 ⁰	2.4x10 ¹	$1.7 x 10^{1}$					
	VcrA1	<9.0x10 ⁰	1.7x10 ²	1.8x10 ¹					
	VcrA2	$<2.7x10^{1}$	7.6x10 ¹	4.9x10 ¹					
VerA	VcrA3 ^a	$< 1.0 \times 10^{0}$	5.7x10 ¹	9.3x10 ¹	$<1.0x10^{0}$	5.7×10^{1} (2.6 × 10 ⁴)	9.3x10 ⁰ (4.2x10 ³)	Difficult to quantify due to	
	VcrA4	<8.3x10 ¹	<8.3x10 ¹	<8.3x10 ¹		(2.0110)	(4.2310°)	low pepude sensitivity	
	VcrA6	<1.0x10 ⁰	5.8x10 ¹	1.1x10 ¹					

Table 6-3. Results of qProt assay quantitation limit validation study

^aQuantifier peptides used to estimate protein abundance, in cases where multiple quantifier proteins exist those abundances are averaged to obtain protein abundance, a 1:1 peptide to protein ratio is assumed; ^b15mL of each cell density were extracted, corresponding to $2x10^6$ to $5x10^8$ *Dhc* cells extracted; ^cDetected proteins were expressed in both fmol/mL and protein/cell concentration units

6.3 MICROCOSM STUDY RESULTS

Reductive dechlorination of *cis*-DCE and VC and subsequent production of ethene were observed in the microcosm experiments as a general function of the SDC-9 inoculum concentration; Figure 6-1 provides an example of relevant microcosm data. Losses in uninoculated-live and killedcontrol microcosms were comparatively small and similar in magnitude, presumably due to volatilization during sample collection (see panel C in Figure 6-1 for data from an uninoculatedlive microcosm). The data indicate that indigenous dechlorinating organisms did not contribute significantly to the observed rates of *cis*-DCE or VC degradation. In microcosms inoculated with SDC-9, lactate was generally fermented to acetate and propionate (Figure 6-1, panel B), which then declined slowly over time. Bromide was used as a conservative tracer to document losses of VOCs and fatty acids due to dilution as all water in the bottles was replaced with VOC- and VFAfree site water after sample collection (Figure 6-1, panel D).



Figure 6-1. Concentrations of VOCs, VFAs and bromide in select JBLM #1 microcosms. Panel A and panel B show VOC and VFA concentrations, respectively, in microcosms receiving the highest SDC-9 inoculum (~ 10⁸ cells/ml). Panel C shows VOC concentrations in the live microcosms that were not inoculated with SDC-9, and Panel D shows bromide concentrations in these same microcosms (uninoculated) over time as a measure of dilution during sampling.

Example measured and model-fitted time-series *cis*-DCE, VC and ethene concentrations from selected microcosm sets are shown in Figure 6-2. Initial acceptance criteria for fitted rate constants required that the 95% confidence interval on the fitted rate constant be \leq the rate coefficient value itself. However, because best fit k_{cisDCE} , k_{vc} and global model R² are not independent, (i.e. reflect tradeoff between goodness of fit to parent and daughter product time-series concentrations subject to mass balance constraints), a more appropriate acceptance criterion was established to require (1) a global R² value of \geq 0.75, and (2) an average ratio of the 95% confidence interval on the k_{cisDCE} and k_{vc} rate constants of \geq 125%. Of the 40 microcosm tests performed (excluding live and killed controls), 26 and 15 tests respectively yielded acceptable quality k_{cisDCE} and k_{VC} rate coefficient data for further evaluation during this study (Table 6-4). A summary of all microcosm analytical data, as well as gene and protein abundance average and standard deviation values (triplicate analyses of single samples) obtained for each microcosm set at each time point sampled, is included in Appendix E.



Figure 6-2. Measured and model-fitted cVOC concentrations in microcosms Measured (symbols) and fitted (dashed line) time series cVOC and ethene mass values measured in selected microcosms inoculated with 10⁹ (i), 10⁷(ii), 10⁶ (iii), 10⁷ (iv) *Dhc* cells/mL. Symbols for chlorinated ethenes are red circles (*cis*-DCE), yellow squares (VC), and ethene (green triangles).

Microcosm Test			R ²	Average Ratio of 95% Confidence Interval to Rate				
Replicate	^a kcisDCE, day ⁻¹	^a kvc, day ⁻¹	model	Constant for k_{cisDCE} , and k_{VC}				
		JBLM1						
JBLM1 Set1A	62.6 ± 73.1	10.2 ± 3.9	0.85	77%				
JBLM1 Set1B	57.0 ± 53.7	10.2 ± 3.6	0.86	65%				
^a JBLM1 Set1C	73.6 ± 146.0	11.3 ± 5.9	0.77	125%				
JBLM1 Set2A	1.48 ± 0.50	0.31 ± 0.073	0.88	29%				
JBLM1_Set2B	$1.49 \pm \ 0.48$	$0.34 ~\pm~ 0.078$	0.89	28%				
JBLM1 Set2C	1.68 ± 0.53	0.34 ± 0.070	0.91	26%				
JBLM1 Set3A	0.024 ± 0.0026	0.0015 ± 0.0018	0.90	65%				
JBLM1 Set3B	$0.016 \pm 1.20 \mathrm{x10^{-8}}$	$0.00058 \pm 6.6 \mathrm{x10^{-8}}$	0.88	0.0%				
JBLM1_Set3C	$0.026 \pm 2.20 \mathrm{x10^{-7}}$	$0.0037 \pm 6.6 \mathrm{x10^{-7}}$	0.89	0.0%				
JBLM1 Set4A								
JBLM1_Set4B	$0.0013 \ \pm \ 0.00013$	^b	0.91					
JBLM1_Set4C	0.0014 ± 0.0014	0.000001 ± 0.026	0.91					
		JBLM2	-					
JBLM2 Set1A	1.05 ± 0.94	0.11 ± 0.018	0.94	53%				
JBLM2 Set1B	1.05 ± 1.14	0.13 ± 0.028	0.92	65%				
JBLM2 Set1C	1.13 ± 1.28	0.17 ± 0.041	0.83	68%				
JBLM2 Set1A Dup	0.28 ± 0.038	0.013 ± 0.031	0.99	128%				
JBLM2 Set1B Dup	0.30 ± 0.031	0.000027 ± 0.023	0.99	43591%				
JBLM2 Set1C Dup	0.22 ± 0.017	0.0067 ± 0.021	1.00	161%				
JBLM2 Set2A	0.0028 ± 0.00040	0.0031 ± 0.0086	0.49	145%				
JBLM2 Set2B	0.0018 ± 0.00024	0.0026 ± 0.0083	0.53	168%				
JBLM2_Set2C	$0.00244~\pm~0.00039$	0.0042 ± 0.0099	0.34	125%				
JBLM2_Set3A	0.0010 ± 0.00026	0.0028 ± 0.013	0.05	255%				
JBLM2_Set3B	$0.00088~\pm~0.00022$	0.0033 ± 0.013	0.13	210%				
JBLM2_Set3C	0.00096 ± 0.00025	0.0017 ± 0.013	0.06	401%				
JBLM2_Set4A	0.0011 ± 0.00030	0.0037 ± 0.014	0.03	197%				
JBLM2_Set4B	$0.00082 \pm \ 0.00021$	$0.0037 \pm \ 0.013$	0.12	189%				
JBLM2_Set4C								
JBLM2_Set5A		Live con	trols					
JBLM2_Set5B		Live con	uois					
JBLM2_Set6A		Killed cor	ntrols					
JBLM2_Set6B		0.010		27 0 /				
*JBLM2_Set1D	0.14 ± 0.016	0.019 ± 0.0081	0.97	27%				
*JBLM2_Set1E	0.088 ± 0.013	0.018 ± 0.015	0.92	51%				
*JBLM2_Set1F	0.096 ± 0.015	0.021 ± 0.015	0.92	44% 810070/				
"JBLM2_SetID_Dup	$0.0/8 \pm 0.0046$	0.00001 ± 0.010	0.97	81907%				
*JBLM2_Set1E_Dup	0.059 ± 0.0038	0.018 ± 0.020	0.96	57%				
*JBLM2_Set1F_Dup	0.057 ± 0.0035	0.0027 ± 0.018	0.96	343%				
*JBLM2_Set2D	0.001 ± 0.00026	0.00009 ± 0.015	-0.26	8447%				
*JBLM2_Set2E	0.001 ± 0.00029	0.00001 ± 0.017	-0.15	83025%				
*JBLM2_Set2F	0.00001 ± 0.00048	0.0001 ± 2.88	-0.22	1439925%				
*IDLM2_SetSU		Live con	trols					
JDLM2_Set3D								
*JBLM2_Set6C		Killed cor	ntrols					
*JBLM2_Set6D	Kined controls							

Table 6-4. Summary of fitted k_{cisDCE} and k_{vc} by microcosm test

'-" indicates no rate was computed; "Best fit rate constants ± the 95% confidence interval on the rate constant; grey-highlighted values did not meet acceptance criteria and were excluded from further analysis; "*" indicates microcosm included groundwater and aquifer solids

6.4 BIOMARKERS AS PREDICTORS OF REDUCTIVE DECHLORINATION RATES

Gene and protein abundances collected from early, middle and late time points from each microcosm were positively and significantly correlated with the k_{cisDCE} and k_{vc} rate coefficients extracted from those microcosms (Table 6-5). The correlation coefficients between biomarker abundances and rate coefficients were generally highest when only the middle time point biomarker abundances were included in the correlation analysis. For example, the correlation coefficient for VcrA protein and the k_{cisDCE} rate coefficient increased from 0.374 to 0.725 when only the midpoint protein abundances were considered (Table 6-5). This may reflect the general metabolic status of the dechlorinating organisms in the batch system (i.e., organisms had time to assimilate to the groundwater environment after inoculation and were actively biodegrading cis-DCE). This status may most effectively simulate that found in a flow-through aquifer system, where electron acceptor (e.g., cis-DCE) and nutrients are resupplied by groundwater flow. Accordingly, the rate coefficient vs. biomarker abundances regression analyses were performed using the midpoint biomarker abundances only. Note that while the pceA gene is carried by reductive dechlorinators present in the SDC-9 consortium, and both pceA gene and PceA protein abundances were found to be positively correlated with reductive dechlorination rates, these RDase biomarkers are not present in Dhc cells and are not reflective of complete dechlorination to ethene. Therefore, pceA gene and PceA protein abundances were not carried forward during rate and biomarker abundance regression analysis.

Biomarker abundance correlations with rate coefficients (biomarker abundance, all microcosm time points)										
	FdhA	PceA	TceA	VcrA	DHC_16S gene	tceA	vcrA	fdhA	pceA	
Log kcis	0.737	0.571	0.575	0.374	0.844	0.859	0.856	0.801	0.804	
p value	2x10 ⁻⁷	6x10 ⁻⁶	1x10 ⁻⁶	6x10 ⁻³	2x10 ⁻⁷	2x10 ⁻⁷	2x10 ⁻⁷	2x10 ⁻⁷	2x10 ⁻⁷	
n	57	55	62	54	64	64	64	64	62	
Log k _{VC}	0.774	0.797	0.652	0.678	0.932	0.934	0.93	0.905	0.91	
p value	2x10 ⁻⁷	2x10 ⁻⁷	3x10 ⁻⁵	3x10 ⁻⁵	2x10 ⁻⁷	2x10 ⁻⁷	2x10 ⁻⁷	2x10 ⁻⁷	2x10 ⁻⁷	
n	35	33	34	30	36	36	36	36	36	
Biomarker abundance correlations with rate coefficients (biomarker abundance, microcosm mid-points only)										
Biomarl	ker abunda	ince correlat	tions with rat	te coefficients	s (biomarker abund	lance, mi	crocosm n	id-points	only)	
Biomarl	ker abunda FdhA	nce correla PceA	tions with rat TceA	te coefficients VcrA	s (biomarker abund DHC_16S gene	lance, mie <i>tceA</i>	crocosm n vcrA	nid-points fdhA	only) pceA	
Biomarl Log k _{cis}	ker abunda FdhA 0.852	nce correlat PceA 0.793	tions with rat TceA 0.755	te coefficients VcrA 0.725	s (biomarker abund DHC_16S gene 0.863	lance, mic <i>tceA</i> 0.905	crocosm m <i>vcrA</i> 0.918	id-points <i>fdhA</i> 0.881	only) <i>pceA</i> 0.854	
Biomarl Log k _{cis} p value	ker abunda FdhA 0.852 2x10 ⁻⁷	PceA 0.793 2x10 ⁻⁷	tions with rat <u>TceA</u> 0.755 2x10 ⁻⁷	vcrA 0.725 7x10 ⁻⁴	biomarker abund DHC_16S gene 0.863 2x10 ⁻⁷	lance, mid tceA 0.905 2x10 ⁻⁷	vcrA 0.918 2x10 ⁻⁷	<i>id-points</i> <i>fdhA</i> 0.881 2x10 ⁻⁷	only) pceA 0.854 2x10 ⁻⁷	
Biomarl Log k _{cis} p value n	ker abunda FdhA 0.852 2x10 ⁻⁷ 21	nce correlat PceA 0.793 2x10 ⁻⁷ 21	tions with rat TceA 0.755 2x10 ⁻⁷ 23	vcrA 0.725 7x10 ⁻⁴ 17	biomarker abund DHC_16S gene 0.863 2x10 ⁻⁷ 23	tceA 0.905 2x10 ⁻⁷ 23	vcrA 0.918 2x10 ⁻⁷ 23	fdhA 0.881 2x10 ⁻⁷ 23	only) pceA 0.854 2x10 ⁻⁷ 23	
Biomarl Log k _{cis} p value n Log kvc	ker abunda FdhA 0.852 2x10 ⁻⁷ 21 0.925	PceA 0.793 2x10 ⁻⁷ 21 0.836	tions with rat <u>TceA</u> 0.755 2x10 ⁻⁷ 23 0.765	c coefficients VcrA 0.725 7x10 ⁻⁴ 17 0.916	biomarker abund DHC_16S gene 0.863 2x10 ⁻⁷ 23 0.934	lance, mie <i>tceA</i> 0.905 2x10 ⁻⁷ 23 0.953	vcrA 0.918 2x10 ⁻⁷ 23 0.962	fdhA 0.881 2x10-7 23 0.966	only) pceA 0.854 2x10-7 23 0.943	
Biomarl Log k _{cis} p value n Log kvc p value	ker abunda FdhA 0.852 2x10 ⁻⁷ 21 0.925 2x10 ⁻⁷	PceA 0.793 2x10 ⁻⁷ 21 0.836 2x10 ⁻⁷	tions with rat TceA 0.755 2x10 ⁻⁷ 23 0.765 4x10 ⁻⁴	vcrA 0.725 7x10 ⁻⁴ 17 0.916 2x10 ⁻⁷	biomarker abunc DHC_16S gene 0.863 2x10 ⁻⁷ 23 0.934 2x10 ⁻⁷	lance, mie tceA 0.905 2x10 ⁻⁷ 23 0.953 2x10 ⁻⁷	vcrA 0.918 2x10 ⁻⁷ 23 0.962 2x10 ⁻⁷	fdhA 6 1 0.881 2x10-7 23 0.966 2x10-7	only) pceA 0.854 2x10 ⁻⁷ 23 0.943 2x10 ⁻⁷	

Table 6-5. Rate coefficients and biomarker correlations

Results of the power law least squares regression analysis of *cis*-DCE and VC rate coefficients versus gene and protein abundances are presented in Figure 6-3. Following the regression trends of target proteins down to the highest of the method detection limit for targeted proteins in this study of 3 fmol (e.g. TceA2, Table 6-1), which is equivalent to a typical 1-L groundwater sample containing $2x10^6$ proteins/mL, would translate to *kcisDCE* and *kvc* rate constants both in the range of 0.0001 day⁻¹ (~ 0.04 yr⁻¹), which is suitably low to be relevant to MNA sites¹. Thus, the proteomics

¹ For example, an apparent first order degradation rate coefficient of 0.04 yr⁻¹ means 500 μ g/L VC would decrease to the 2 μ g/L VC maximum contaminant level in 138 years.

assay is sensitive enough to quantify proteins over a wide range of *Dhc* abundances and activities relevant to both biostimulated or bioaugmented sites where biomarker abundances and rates of reductive dechlorination are high, as well as to MNA sites where biomarker abundances and reductive dechlorination rates are quite low.



Figure 6-3. Rate coefficients vs. biomarker regression results

Microcosms that yielded acceptable rate coefficients (Table 6-4) and their corresponding midpoint RDase gene and biomarker abundances were used to complete regression results shown above.

The predictive power of gene and protein biomarkers was tested using regression equations featured in Figure 6-3 and biomarker abundances from microcosm tests that met the data quality acceptance screening criteria (Table 6-4) but that were not included in the regression analysis. The test was performed in two ways (1) using randomly selected biomarker abundances corresponding to a range of *Dhc* cell abundances, and (2) using global averages of all biomarker abundances that corresponded to *Dhc* cell abundances at 10⁶, 10⁷, 10⁸ cells/mL. The randomly-selected biomarker abundances corresponded to the time zero sampling from microcosm sets JBLM1_Set1B, JBLM1_Set2C, and JBLM2_Set1F. As shown in Figure 6-4, protein-based rate predictions (white bars with black dots) were within an order of magnitude of measured rate coefficients (green boxes) for all tests. Rates predicted using a combination of genes and proteins (green bars, Figure 6-4) were generally better than those predicted using proteins alone.



Figure 6-4. Biomarker-based rate predictions vs. measured rate coefficients Green boxes reflect the error range associated with the measured rate coefficients during the study. Rates predicted using a combination of RDase genes and proteins (green bars) generally yielded an improved rate prediction compared to RDase proteins alone.

6.5 CONSIDERING APPLICABILITY OF THE LABORATORY STUDY RESULTS TO FIELD SITES

The simple laboratory microcosm systems were appropriate for confirming a quantitative relationship between biomarker abundances and reductive dechlorination rates mediated by *Dhc* cells from the SDC-9 consortia. However, conditions in the laboratory microcosms do not perfectly emulate conditions in aquifers at cVOC-contaminated field sites, which is where the qProt tool must be useful to provide maximal benefit. Here we consider how the quantitative link established between the biomarker abundances in the laboratory might be different than the link established in the field.

First, the majority of the bioaugmented microcosm test completed under this project featured only groundwater; relatively few microcosms featured groundwater with aquifers solids. Results of the rate coefficient vs. protein biomarker abundance regressions are reproduced in Figure 6-5 below, here with the groundwater-only (blue symbols) and groundwater with soil (orange symbols) differentiated for each biomarker. Microcosms that featured groundwater with soil generally clustered at the low end of the biomarker abundances and activity rates. Although the plus soil treatments tended to have lower biomarker abundances and activities, the results were generally consistent with the entirety of the data set, suggesting no significant difference in the presence of aquifer solids. It should be noted that all microcosm tests with soil were performed relatively quickly, under continuously mixed conditions, and were not designed to assess or account for *Dhc* cell attachment that may occur overtime; attachment was assumed to be negligible during these

tests. The contribution of attached vs. planktonic *Dhc* cells was beyond the scope of this laboratory study but will be addressed in the pending follow-on field demonstration.



Figure 6-5. Rate coefficients vs. biomarker abundances with treatments distinguished. Blue and orange symbols represent biomarker and rate coefficient results from groundwater-only microcosms and groundwater with aquifer solids microcosms, respectively.

Second, in a natural aquifer system, the abundance of bacteria will adjust to a level where growth sustained by the supply of the limiting electron acceptor (e.g., *cis*-DCE) is balanced by maintenance and cell death (e.g., predation). Indeed, viable microbes present in a natural system may consume dead cells as a nutrient source [48] and thereby "turn over" the dead cells. This cell "turn over" in natural systems will, in theory, minimize the chance of detecting "carcass proteins" (i.e., in this case RDases associated with dead cells). While the presence of such RDases in nonviable cells would be difficult to quantify, we did evaluate whether the protein levels detected were reasonable based upon the density of *Dhc* cells measured. If protein to *Dhc* cell abundances were greater than physiologically expected, or if ratios were much larger than have been previously published for RDase proteins in Dhc, the presence of RDases not associated with viable cells could be a confounding factor in RDase biomarker vs. rate coefficient regressions established in this study. Observed ratios were generally between 10^3 and 10^5 proteins/cell (Figure 6-6), which is in the range of previously published values of 7.6×10^3 and 2.60×10^4 for TceA reported for KB-1 and D2 cultures, respectively [46]. Further, the theoretical maximum number of proteins that could "fit" in the periplasmic space of a Dhc cell was estimated using the computational approach of Milo 2013 [52] to be 10⁵ proteins. If we assume 10% of the proteins in a *Dhc* cell are RDases, the maximum RDases per Dhc cell would be 10⁴. Therefore, the observed range of RDase proteins per *Dhc* cell during this study do not exceed the realm of physiological possibility.



Figure 6-6. Protein/*Dhc* cell ratios vs. rate coefficients for microcosm tests Blue and orange symbols represent biomarker and rate coefficient results from groundwater-only microcosms and groundwater with aquifer solids microcosms, respectively.

Finally, because first order-based kinetics often describe reductive dechlorination at field scales reasonably well, our first order-based regressions (Figures 6-3 and 6-5) will be directly applicable for supporting qProt assay interpretation at many field sites. In a natural system – in this case a cVOC-contaminated aquifer undergoing monitored natural attenuation – *Dhc* abundance will adjust to a level where growth sustained by the supply of chlorinated ethenes is balanced by self-consumption to sustain metabolism, and predation. In this case the abundance of *Dhc* and concentration of chlorinated ethenes remain relatively constant at any one position along the flow path. In such cases cVOC degradation kinetics can be described by a pseudo first-order kinetic model; i.e. at any one location along the flow path, the overall rate of degradation of the substrate in the groundwater ($\mu g/L$ per day) divided by the concentration of the substrate ($\mu g/L$) is a fixed ratio. If an end user of the qProt assay wishes to use an alternative kinetic model to interpret test-or field site-specific results, published kinetic constants in the literature could be used to do so.

7.0 COST ASSESSMENT

7.1 COST MODEL

Standard analytical costs to obtain RDase activity rate estimates during the microcosm studies, as well as costs to obtain RDase biomarker abundance, were tracked as part of this laboratory project (Table 7-1). Costs to perform the microcosm study, analyze the data, and prepare a memorandum were tracked and recorded as well. Capital and operation and maintenance (O&M) costs were *not* tracked or reported. A field demonstration is necessary to a complete cost assessment with sufficient detail that a future "end user" of proteomics technology could compare costs between proteomics and existing MBTs and develop a reasonable cost estimate for conducting proteomic analysis at a cVOC-contaminated site. It should be noted that the microcosm testing conducted during this phase of the ESTCP Project would not be required during a field application of proteomic technology, so the associated costs are not relevant.

Cost Element	Details	Tracked Demonstration Data	Discounted Costs
Capital Costs			
System Design	Labor		
	Labor		
Well Installation and Development	Materials	These data were	not tracked as part of
	Subcontracts	the laboratory pro	oject but would be
	Labor	tracked during su	bsequent field
System Installation	Equipment & Materials	demonstration	
	Subcontracts		
Travel			
		Subtotal	
Operation and Maintenance (O&M	M) Costs		
Groundwater Sampling	Labor		
Groundwater Sampring	Materials		
Analytical	In-house Labor	These data were	not tracked as part of
- Anarytical	Laboratory	the laboratory pro	oject but would be
System O&M	Labor	bsequent field	
System O&M	Materials	demonstration	
Reporting & Data Management	Labor		
Travel			
		Subtotal	
Other Technology-Specific Costs			
Site Selection	Labor & Travel		
	Labor		
Site Characterization	Materials		
	Subcontractor	The cost to set up	and run all the
	Labor	microcosm tests,	including all the cVOC
Treatability Testing	Materials	analysis and prep	earing the concentration
	Subcontractor	data for analysis,	was \$215K. Cost per
Meetings & Reporting	Labor & Travel	sample for RDas	e blomarker analysis is
Technology Transfer	Labor & Travel	below	ery in Section 7.5
Demonstration Plan/Work Plan	Labor	Delow.	
Final Report	Labor	_	
Cost and Performance Report	Labor		Г
		Subtotal	
		TOTAL COSTS	
ES	FIMATED TREATMENT	VOLUME (CY)	
ESTI	MATED TREATMENT V	<u>OLUME (GAL)</u>	
APPRO	XIMATE TREATMENT	COST (PER CY)	
APPROX	IMATE TREATMENT CO	OST (PER GAL)	

Table 7-1. Cost model for proteomics

7.2 COST DRIVERS

Implementation of advanced MBTs during the assessment phase, remedy implementation and monitoring of the project are impacted by the factors as described above. Although there are currently no regulatory requirements that specifically mandate advanced MBTs be used to assess a site, the data provided by the MBTs are meant to supplement and possibly replace other forms of data that provide lines of evidence that MNA is occurring and to estimate a degradation rate. Hence, the total sampling and analytical cost is driven by number of sample locations at a site and total number of samples collected (i.e., a greater number of samples equates to a higher cost). It should be noted however that the individual cost per sample for analyses with advanced MBTs may decrease based on a greater number of total samples requiring analyses since the lab work is highly specialized and cost efficiencies generally can be realized for a larger quantity of analyses.

7.3 COST ANALYSIS

The microcosm studies conducted for this project to correlate rates of cVOC biodegradation with RDase abundance were extensive and would not be required for field implementation. The cost for the microcosm work including analytical (cVOCs, VFAs, dissolved gases, anions, pH) for all studies, collection and shipping of samples for qPCR and proteomic analysis, as well as preparation of the treatability study workplan and keeping a project database was \$215K. This included \$209K in labor and \$6K in materials, supplies, equipment, and shipping costs. No subcontracts were issued as all work including analytical was conducted at Aptim's laboratory in Lawrenceville, NJ. Collection of site materials for the microcosm studies is not included in these costs.

With the exception of metagenomics and metaproteomics, the techniques used to assess the contaminant degradation and continued potential for natural attenuation are common and costs to apply these techniques are well documented in the literature [49-51]. As discussed in Section 7.2, costs are highly dependent on the number of samples collected, frequency of sampling, and number/types of analytes, which are primarily dictated by the nature/diversity of the contaminants of concern (COCs), size of the site, proximity of receptors, and regulatory requirements. Hence, it is not the intent of this demonstration report to generate a life-cycle cost estimate for a hypothetical site at which these techniques are applied to evaluate remedial performance and subsequent natural attenuation of the remaining COCs to achieve site remedial action objectives (RAOs).

Table 7-2 provides a general cost comparison of conventional MBTs (e.g., qPCR) to the advanced MBTs, including proteomics. As indicated in the last column of the table, many of these techniques have only limited commercial availability and/or are available through a university or other research laboratory. As such, application costs remain relatively high. It is expected as these techniques mature, they will become more widely available and the analytical cost per sample will decrease substantially. For comparison purpose, the cost of shotgun and quantitative metaproteomic analyses based on cost data collected during this demonstration were \$1,200 and \$800 per sample, respectively, assuming analysis of a batch of 12 samples. The cost of the metaproteomic analyses included use of an existing metaproteomic platform but assumed development of a workflow specific for cVOCs.

Molecular Tool	Identity/ Potential Activity/ Expressed Activity ^a	Quantitative, Qualitative (QA/QL)	Cost Range (\$) ^b	Availability ^c
	Conven	tional MBTs		
Compound specific isotope analysis	Е	QA	100 to 2,500	C/R
Quantitative polymerase chain reaction	I/P/E	QA	275 to 425	WC
Microarrays	I/P/E	QL	1,250 to 5,000	C/R
Stable isotope probing	I/P/E	QA/QL	1,500 and up	C/R
Enzyme activity probes	Е	QA	250 to 2,500	C/R
	Advanced	(omic) MBTs ^d		
Metagenomics (16S Sequencing)	Ι	QL	150 to 500	WC/R
Shotgun Metaproteomics	Е	QL	800 to 1,500	C/R
MRM Metaproteomics	E	QA	500 and up	C/R

Table 7-2. Cost comparison of conventional MBTs (e.g., qPCR) to the advanced MBTs.

Adapted from ITRC (2011). ^aI - identity of microorganisms (i.e., genus or species), P - potential activity (i.e., genetically capable of completing the activity), E - expressed activity (i.e., actually completing the activity at a given time). ^b Estimated price per sample. Low end represents compound specific restricted analysis. ^c WC - widely commercially available, C- minimally commercially available, R - available through university or other research laboratory. ^dThe cost of advanced omic MBTs represents cost from two commercial laboratories and Battelle metagenomic and proteomic lab. These costs are based on current costs from 2017 and higher number of batches (20 samples). These costs elements are reduced since the methods are maturing and proteomic analyses becomes more routinely used.

8.0 IMPLEMENTATION ISSUES

This section focuses on proteomic analysis and the potential of this technology to facilitate assessment of MNA. The primary end users of qProt are expected to be DoD site managers, consultants and their contractors. The general concerns of these end users are likely to include the following: (1) regulatory acceptance; (2) insufficient confidence in results and access to specialized laboratories; and (3) technology cost compared to other more conventional monitoring options. These implementation issues are addressed in the following sections.

8.1 **REGULATORY ACCEPTANCE**

Proteomics is a new tool in environmental assessment and one which requires validation. The relationship between specific proteins and protein levels and degradation rates of various cVOCs is now being established, with the work reported herein providing key data in this regard. At present, proteomics can be used to provide a direct line of evidence that biodegradation is actively occurring based on the detection of proteins that are produced during the degradation process. However, in the future, it is conceivable that proteomics could provide a direct measure of degradation rates based on the concentrations of proteins that are measured in a sample, which could eliminate or reduce the need to measure concentrations of cVOCs. It is therefore expected that regulatory acceptance of this technology will in part be based on the application and end use of the resulting data.

As with any new technology, detailed demonstration and validation are required to ensure accuracy and precision of results for both techniques before widespread regulatory acceptance can be obtained. Standardized methods and procedures for sample collection and shipping, analytical methods, QA/QC and data evaluation must be further developed and validated to help ensure regulatory acceptance. In addition, technology transfer through SERDP/ESTCP, peer reviewed journal articles, webinars, conferences, and other meetings will play an important role to facilitate understanding and acceptance of these powerful tools.

8.2 LIMITED AVAILABILITY

Proteomic analysis of enzymes involved in the reductive dehalogenation of cVOCs in field samples is a relatively new endeavor. The results provided in this report provide a strong basis for moving forward with this MBT for site assessment purposes. However, as with any new technology, availability and data quality are important concerns. Due to the young state of the practice, QA/QC guidelines for environmental applications of proteomic analysis are not yet available. In addition, only few analytical environmental laboratories offer advanced MBTs, and qProt is not yet commercially available. As with other important MBTs (e.g., qPCR) it is anticipated that these issues will be resolved over time as the method becomes more widely accepted and commercially applied.

8.3 COST COMPARED TO OTHER MONITORING TOOLS

The costs for qProt analysis are high compared to conventional technologies but are expected to decrease substantially as the technology continues to advance. Although costs per sample currently range from several hundred dollars to about \$1,000 for these types of analyses, MBTs help to answer a variety of management questions and facilitate decision making that can result in a reduction of the life-cycle cost of a remedy. For instance, MBTs such as metagenomics and metaproteomics, may be used instead of laborious microcosm studies to definitively state if microorganisms of interest are performing required activities and are actively degrading specific contaminants. These new MBTs characterize the contaminant-degrading *in situ* microbiome with unprecedented resolution. Information provided by these new MBTs, together with data from conventional MBTs, provides a comprehensive assessment and enables site management decisions to be made with greater confidence. Not only will this likely result in a direct cost savings to the project since microcosm studies can be more costly than the MBT analyses, but it also reduces the time required for assessment because microcosm studies generally take 60 to 90 days to perform.

During remediation efforts, MBT data help to design the remedy, to optimize remedial strategies, and to troubleshoot unsuccessful treatment approaches. Results can be used to determine when to reapply amendments to optimize growth and distribution of the target organisms, which can help to minimize the time required for the active portion of the remedy. Conceivably, in the near future, proteomics may provide the necessary means to directly calculate degradation rates, which then can be augmented during the active portion of the remedy to facilitate removal of cVOCs, thereby reducing application time and life-cycle cost.

Proteomics can facilitate long-term monitoring efforts by confirming that active degradation is occurring across the site, and eventually may aid to estimate the rate of degradation to decide if site-specific cleanup goals can be achieved within a desired timeframe. This could result in less frequent monitoring events and or a reduced number of analytes, which may reduce the life-cycle long-term monitoring cost and may support more rapid site closure. As metagenomics and proteomics are increasingly used in environmental applications, and as more laboratories begin to offer these analyses, competition increases, and techniques are refined, which will bring down the costs.

9.0 REFERENCES

- 1. Council, N.R., *Alternative for Managing the Nation's Complex Contaminated Groundwater Sites*. 2013: Washington, DC.
- 2. Yu, S., M.E. Dolan, and L. Semprini, *Kinetics and inhibition of reductive dechlorination of chlorinated ethylenes by two different mixed cultures*. Environmental science & technology, 2005. **39**(1): p. 195-205.
- 3. Hatt, J.K. and F.E. Löffler, *Quantitative real-time PCR (qPCR) detection chemistries affect enumeration of the Dehalococcoides 16S rRNA gene in groundwater.* Journal of microbiological methods, 2012. **88**(2): p. 263-270.
- 4. Izbicki, J.A., et al., *Groundwater movement, recharge, and perchlorate occurrence in a faulted alluvial aquifer in California (USA).* Hydrogeology Journal, 2014: p. 1-25.
- 5. Kruse, T., H. Smidt, and U. Lechner, *Comparative Genomics and Transcriptomics of Organohalide-Respiring Bacteria and Regulation of rdh Gene Transcription*, in *Organohalide-Respiring Bacteria*. 2016, Springer. p. 345-376.
- 6. Löffler, F.E., et al., *Isolated reductive dehalogenase genes*. 2014, Google Patents.
- 7. Ritalahti, K.M., et al., *Quantitative PCR targeting 16S rRNA and reductive dehalogenase genes simultaneously monitors multiple Dehalococcoides strains*. Applied and Environmental Microbiology, 2006. **72**(4): p. 2765-2774.
- 8. Ritalahti, K.M., et al., *Comparing on-site to off-site biomass collection for Dehalococcoides biomarker gene quantification to predict in situ chlorinated ethene detoxification potential.* Environmental science & technology, 2010. **44**(13): p. 5127-5133.
- 9. Krajmalnik-Brown, R., et al., *Genetic identification of a putative vinyl chloride reductase in Dehalococcoides sp. strain BAV1*. Applied and Environmental Microbiology, 2004. **70**(10): p. 6347-6351.
- 10. Hatt, J.K., et al., *Design and application of an internal amplification control to improve Dehalococcoides mccartyi 16S rRNA gene enumeration by qPCR*. Environmental science & technology, 2013. 47(19): p. 11131-11138.
- 11. Thompson, M.R., et al., *Experimental approach for deep proteome measurements from small-scale microbial biomass samples*. Analytical chemistry, 2008. **80**(24): p. 9517-9525.
- 12. Chourey, K., et al., *Direct cellular lysis/protein extraction protocol for soil metaproteomics*. Journal of proteome research, 2010. **9**(12): p. 6615-6622.
- 13. Hettich, R.L., et al., *Metaproteomics: harnessing the power of high performance mass spectrometry to identify the suite of proteins that control metabolic activities in microbial communities.* Analytical chemistry, 2013. **85**(9): p. 4203-4214.
- 14. Ritalahti, K.M., et al., *RNA extraction and cDNA analysis for quantitative assessment of biomarker transcripts in groundwater*, in *Handbook of Hydrocarbon and Lipid Microbiology*. 2010, Springer. p. 3671-3685.
- Stedtfeld, R.D., et al., DNA Extraction-Free Quantification of Dehalococcoides spp. in Groundwater Using a Hand-Held Device. Environmental science & technology, 2014.
 48(23): p. 13855-13863.
- 16. Löffler, F.E., et al., *Dehalococcoides mccartyi gen. nov., sp. nov., obligately* organohalide-respiring anaerobic bacteria relevant to halogen cycling and

bioremediation, belong to a novel bacterial class, Dehalococcoidia classis nov., order Dehalococcoidales ord. nov. and family Dehalococcoidaceae fam. nov., within the phylum Chloroflexi. International Journal of Systematic and Evolutionary Microbiology, 2013. **63**(2): p. 625-635.

- 17. Schaefer, C.E., et al., *Bioaugmentation for chlorinated ethenes using Dehalococcoides sp.: Comparison between batch and column experiments.* Chemosphere, 2009. **75**(2): p. 141-148.
- 18. Zhang, Y., et al., *Protein analysis by shotgun/bottom-up proteomics*. Chemical reviews, 2013. **113**(4): p. 2343-2394.
- 19. Keller, M. and R.L. Hettich, *Environmental proteomics: a paradigm shift in characterizing microbial activities at the molecular level.* Microbiology and Molecular Biology Reviews, 2009. **73**(1): p. 62-70.
- 20. Abraham, P.E., et al., *Metaproteomics: extracting and mining proteome information to characterize metabolic activities in microbial communities.* Current Protocols in Bioinformatics, 2014: p. 13.26. 1-13.26. 14.
- 21. Kucharzyk, K.H., C. Bartling, and L. Mullins, *Multiple Reaction Monitoring (MRM)* Assay for Detection of Peptides Expressed During Degradation of Enviornmental Pollutants. (in preparation to submission), 2016.
- 22. Kucharzyk, K.H., C. Bartling, and D. Stoeckel. *Omic Technologies in Assessing* Degradation Markers of Chlorinated Contaminants. . in Third International Symposium on Bioremediation and Sustainable Environmental Technologies. 2015. Miami, FL.
- 23. Kucharzyk, K.H., C. Bartling, and D. Stoeckel, *Omic Technologies in Assessing Degradation Markers of Chlorinated Contaminants.*, in *National Environmental Monitoring Conference*. 2015: Chicago, IL.
- 24. Schiffmann, C., et al., *Comparison of targeted peptide quantification assays for reductive dehalogenases by selective reaction monitoring (SRM) and precursor reaction monitoring (PRM)*. Analytical and bioanalytical chemistry, 2014. **406**(1): p. 283-291.
- 25. Becker, J.G., *A modeling study and implications of competition between Dehalococcoides ethenogenes and other tetrachloroethene-respiring bacteria*. Environmental science & technology, 2006. **40**(14): p. 4473-4480.
- 26. Lai, Y. and J.G. Becker, *Compounded effects of chlorinated ethene inhibition on ecological interactions and population abundance in a Dehalococcoides-Dehalobacter coculture*. Environmental science & technology, 2013. **47**(3): p. 1518-1525.
- 27. CB&I, Dehalococcoides-containing microbial consortium (SDC-9TM) for anaerobicbioremediation - technical summary. 2013.
- 28. Andrews, G.L., et al., *Performance characteristics of a new hybrid triple quadrupole time-of-flight tandem mass spectrometer*. Analytical chemistry, 2011. **83**(13): p. 5442.
- 29. Krajmalnik-Brown, R., et al., *Environmental distribution of the trichloroethene reductive dehalogenase gene (tceA) suggests lateral gene transfer among Dehalococcoides*. Fems Microbiology Ecology, 2007. **59**(1): p. 206-214.
- 30. U.S. Navy, Remedial Investigation Report, NUWC Keyport. Prepared by URS Consultants and Science Applications International Corporation for EFA NW under CLEAN Contract No. N62474-89-D-9295, CTO 10. 1993a.
- 31. U.S. Navy, U.S.E.P.A.U., and Washington State Department of Ecology (Ecology)., 1998. Record of Decision for Operable Unit 1, Naval Undersea Warfare Center Division, Keyport, Washington. Prepared by URS Greiner and Science Applications International

Corporation for EFA NW under CLEAN Contract No. N62474-89-D-9295, CTO 10. September 30, 1998.

- 32. Dibblee, T.W., Jr., Geologic map of the Ventura and Pitas Point quadrangles, Ventura County, California: Dibblee Geological Foundation, Map DF-21 (Ehrenspeck, H.E., ed.), scale 1:24,000. 1988.
- 33. Arcadis, Final Pre-Design Investigation Work Plan SA288. Performance-Based Remediation, Vandenberg Air Force Base, California. 2015.
- 34. U.S.EPA, a.F.L., Record of Decision for the Department of the Army, Logistics Center, Fort Lewis, Washington. September 1990. 1990
- 35. Yan, J., et al., *The corrinoid cofactor of reductive dehalogenases affects dechlorination rates and extents in organohalide-respiring Dehalococcoides mccartyi.* Isme Journal, 2016. **10**(5): p. 1092-1101.
- 36. Wiśniewski, J.R. and F.Z. Gaugaz, *Fast and sensitive total protein and Peptide assays for proteomic analysis*. Analytical chemistry, 2015. **87**(8): p. 4110-4116.
- Shelton, D.R. and J.M. Tiedje, *General method for determining anaerobic biodegradation potential*. Applied and Environmental Microbiology, 1984. 47(4): p. 850-857.
- Steffan, R.J. and S. Vainberg, Production and handling of Dehalococcoides bioaugmentation cultures, in Bioaugmentation for Groundwater Remediation. 2013, Springer. p. 89-115.
- 39. Kampbell, D.H. and S.A. Vandegrift, *Analysis of Dissolved Methane, Ethane, and Ethylene in Ground Water by a Standard Gas Chromatography Technique*. Journal of Chromatographic Science, 1998. **36**: p. 253-256.
- 40. Johnson, D.R., et al., *An internal reference technique for accurately quantifying specific mRNAs by real-time PCR with application to the tceA reductive dehalogenase gene.* Applied and Environmental Microbiology, 2005. **71**(7): p. 3866-3871.
- 41. Kearse, M., et al., *Geneious Basic: An integrated and extendable desktop software platform for the organization and analysis of sequence data.* Bioinformatics, 2012. **28**(12): p. 1647-1649.
- 42. Ye, J., et al., *Primer-BLAST: A tool to design target-specific primers for polymerase chain reaction.* Bmc Bioinformatics, 2012. **13**.
- 43. Amos, B.K., et al., *Oxygen Effect on Dehalococcoides Viability and Biomarker Quantification*. Environmental science & technology, 2008. **42**(15): p. 5718-5726.
- 44. NCBI, PubChem Database, available online: https://www.ncbi.nlm.nih.gov/pccompound.
- 45. Smith, L.H., P.L. McCarty, and P.K. Kitanidis, *Spreadsheet method for evaluation of biochemical reaction rate coefficients and their uncertainties by weighted nonlinear least-squares analysis of the integrated Monod equation*. Applied and Environmental Microbiology, 1998. **64**(6): p. 2044-2050.
- 46. Werner, J.J., et al., *Absolute quantification of Dehalococcoides proteins: enzyme bioindicators of chlorinated ethene dehalorespiration*. Environmental Microbiology, 2009. **11**(10): p. 2687-2697.
- 47. Rowe, A.R., et al., *Relating Chloroethene Respiration Rates in Dehalococcoides to Protein and mRNA Biomarkers.* Environmental Science & Technology, 2012. **46**(17): p. 9388-9397.
- 48. Roszak, D.B. and R.R. Colwell, *Survival strategies of bacteria in the natural environment*. Microbiological Reviews, 1987. **51**(3): p. 365–379.

- 49. Lo, I., et al., *Strain-resolved community proteomics reveals recombining genomes of acidophilic bacteria.* Nature, 2007. **446**(7135): p. 537-541.
- 50. Wohlbrand, L., K. Trautwein, and R. Rabus, *Proteomic tools for environmental microbiology-A roadmap from sample preparation to protein identification and quantification*. Proteomics, 2013. **13**(18-19): p. 2700-2730.
- 51. Fouhy, F., et al., 16S rRNA gene sequencing of mock microbial populations- impact of DNA extraction method, primer choice and sequencing platform. Bmc Microbiology, 2016. 16.
- 52. Milo, R. *What is the total number of protein molecules per cell volume? A call to rethink some published values.* 2013. Insights & Perspectives, **35** (12), 1050-1055.

APPENDIX A *QUANTITATIVE PROTEOMICS METHOD DETECTION LIMIT AND INSTRUMENTATION DETECTION LIMIT STUDY RESULTS*

Assessment of Instrument Detection Limit and Method Detection Limit for Reductive Dehalogenase Isotopic Peptides

REPORT

Battelle Memorial Institute 505 King Avenue Columbus, OH 43201

Mandy Michalsen, Ph.D., P.E. Research Engineer U.S. Army Engineer Research Development Center Environmental Lab

This report is a work prepared for the U.S. Army Engineer Research Development Center Environmental by Battelle. In no event shall either U.S. Army Engineer Research Development Center Environmental or Battelle have any responsibility or liability for any consequences of any use, misuse, inability to use, or reliance on any product, information, designs, or other data contained herein, nor does either warrant or otherwise represent in any way the utility, safety, accuracy, adequacy, efficacy, or applicability of the contents hereof.

Table of Contents

List of Acronyms	ii
1. Introduction	
2. RDase Peptide Selection, Protein Extraction and Quantification	
2.1 RDase Peptide Selection	
2.2 Protein Extraction and Quantification	5
3. Infusion and Injection of Isotopic Peptides	6
4. Multiple Reaction Monitoring (MRM) Method Development	7
5. Calibration and System Suitability	
6. Instrument Detection Limit (IDL).	
7. Method Detection Limit (MDL)	
8. <u>Summary</u>	

List of Tables

Table 1. List of SDC-9 Peptides Selected for Quantification	6
Table 2. Parameters of Waters Xevo CE Equation	7
Table 3. Solvent Program for M-Class Chromatographic System	7
Table 4. List of SDC-9 Peptides Used in Optimization Experiments	9
Table 5. Selected Peptides Used in IDL/MDL Experiments	10
Table 6. IDL Replicate Experiment Results	12
Table 7. MDL Replicate Experiment Results	13

List of Figures

r!
4
5
<u>r</u>
6

List of Appendices

APPENDIX A: Protein Extraction, Quantification and Cleanup	A
APPENDIX B: List of all Isotopic Peptides and Their Transitions	B
APPENDIX C: IDL Data Set 1	C
APPENDIX D: IDL Data Set 2	D
APPENDIX E: IDL Data Set 3	Е
APPENDIX F: MDL Data Set 1	F
APPENDIX G: MDL Data Set 2	G

APPENDIX H: MDL	, Data Set 3	.H

List of Acronyms

CEs	collision energies
DHC	Dehalococcoides
IDL IS	instrument detection limit internal standards
LOD LOQ LLOQ	limit of detection limit of quantification Lower level of quantification
MRM m/z	multiple reaction monitoring-based mass-to-charge ratios
PCE	tetrachloroethene
RDase	reductive dehalogenase
S/N	Signal-to-noise
TCE	trichloroethene
VC	vinyl chloride

Introduction

In preparation for microcosm experiments planned for this project, the Battelle proteomics team, in collaboration with the University of Tennessee, has identified SDC-9 culture-specific reductive dehalogenase (RDase) peptides for quantification. These specific RDases are used in a multiple reaction monitoring-based (MRM) targeted proteomic assay to establish quantitative biomarker rate correlations, which are needed to generate in situ degradation rate estimates of chlorinated ethenes.

During the development phase, the MRM assay was thoroughly evaluated for limit of detection (LOD) and limit of quantification (LOQ). To maximize precision, stable isotope labeled internal standards (IS) are frequently used to account for errors and losses that can occur during sample handling and variability in peptide ionization in the analysis of peptides. Because of the rigors of establishing these assays and successfully performing them in complex matrices, they tend to be implemented on only a selected number of analytes in parallel. With only a small number of analytes measured, it is common to expend considerable time optimizing tune parameters and collision energies (CEs) of each analyte individually to attain the highest sensitivity possible.

Prior to the use of IS peptides for MRM proteomics, general MS instrument parameters that work well with the broad diversity of peptides to be targeted needed to be determined (**Figure 1**). Peptide standards are directly infused to optimize these parameters empirically. CE is an instrument parameter that is frequently optimized to maximize fragment ion intensities. Multiple instrument manufacturers offer automated routines for CE optimization by peptide infusion as part of the instrument tuning software.

Once the system is optimized (resolution and calibration) and optimal CEs are determined, instrument detection limits and method detection limits are established for each IS peptide. Most analytical instruments produce a signal even when a blank (matrix without analyte) is analyzed. This signal is referred to as the instrument background level. Noise is a measure of the magnitude of the background signal. It is generally measured by calculating the standard deviation of a number of consecutive point measurements of the background signal or by measuring the magnitude of a defined region of background. Signal-to-noise (S/N) is obtained by calculating the ratio between the magnitude of the signal and the magnitude of the noise. Thus, the instrument detection limit (IDL), also known as LOD, is the analyte concentration required to produce a signal that is distinguishable from the noise level.

For most applications, required sample preparation methods may result in alteration of clean analyte prepared in solvent. It may be necessary to remove unwanted matrix components, digest, extract and concentrate the analyte, or even derivatize the analyte for improved chromatography or detection. The analyte may also be further diluted or concentrated prior to analysis on an instrument. Additional steps in a sample preparation method add additional opportunities for error (losses). Determination of the detection limit when sample preparation/manipulation steps are incorporated into the preparatory and analysis scheme results in an identified method detection limit (MDL), also known as LOQ. An MDL or LOQ accounts for additional losses that occur during the course of sample manipulation/preparation. Theoretically, the IDL is lower than the MDL for a given target analyte.

In this report, each step of system and IS peptide optimization is characterized in the sections below. Data pertaining to system resolution check, calibration, and chromatograms of peptide detections are grouped per sample set in **Appendices C** through **H**.


Figure 1. Optimization of Instrument Parameters and Isotopic Standards Characteristics

RDase Peptide Selection, Protein Extraction and Quantification

RDase Peptide Selection

Dehalococcoides (DHC) comprise a genus-level group of bacteria within the phylum *Chloroflexi*, notable for their ability to respire halogenated compounds including recalcitrant groundwater contaminants. Their obligate use of halogenated organic compounds as an energy source has allowed successful development of DHC-containing enrichment cultures for bioaugmentation of chlorinated ethene-contaminated sites, such as SDC-9 consortium. Each DHC strain contains a unique complement of genes that are homologs of known RDases, the genes required for respiration of halogenated organic compounds. The SDC-9 consortium is a well-defined enrichment culture with a variety of robust tetrachloroethene (PCE) – vinyl chloride (VC) dechlorinators. A metagenome sequencing project for the SDC-9 consortium was completed by Battelle Memorial Institute and the University of Tennessee to determine specific RDase genes that could serve as targets in proteomic analyses.

Overall, 14 genes encoding RDases were identified, 10 of which best matched previously identified RDases from members of the genus *Dehalococcoides*. Of these 14 sequences, one *vcrA* and one *tceA* gene were identified, as well as two separate *pceA* genes. Of these 14 RDases, 12 were associated with small, protein coding RDase B genes that are predicted to have three membrane-spanning helices. Peptide sequences of RDases and several sequences of FdhA protein that encodes for formate dehydrogenase were selected for targeted proteomic analysis. The detailed list of peptide sequences is presented in **Table 1**.

Protein Extraction and Quantification

For determination of the MDL, the 12.5 pmol/ μ L stock solution was diluted in ammonium bicarbonate to prepare the following concentrations (final in 25 μ L): 250, 83, 27, 9, 3, 1, 0.34, and 0.11 fmol/ μ L. Each sample was digested with trypsin overnight and desalted using C18 spin columns. Protein extraction protocol, including protein detection with tryptophan assay and sample cleanup, has been developed for work with environmental samples and is located in **Appendix A** of this report. Copies of laboratory pages of sample extraction for MDL are also in **Appendix A**.

Protein	Peptide	Precursor
Trotem		(m/z)
	SELEVISSLLSR	671.9
	SGSEIAFTGGLIK	644.4
	SWDWALGEIANK	699.4
	AAGASDWEEK	536.2
FdhA	ALGIVYLDSQAR	658.4
	VSSLQQLESPEEL R	812.9
	LSWTYSTNPSAADVA K	859.9
	NQAVSAPGEAK	540.3
	TDTNTDYSYVNAIK	806.9
	VETWNHDVA R	412.9
	FDEWFGYSGPVNPEE R	969.9
	LLPWDLP K	495.3
DesA	IATQIPLLQDAAR	710.4
PCEA	LESGYVQNMV K	638.3
	VYTDLELAPDKP R	509.6
	DFWNNPEPI K	634.3
	TSPSLISSATVGK	628.4
	FLGADLVGIAPYDE R	823.4
	DVDDLLSAGK	520.8
TceA	VSSIIEP R	455.8
	VNNEPWWVTT R	706.4
	YFGASSVGAI K	554.3
	WGLYGPPHDSAPPDGSVPK	662.3
	YFGAGDVGALNLADP K	808.4
X 7 · A	VPDHAVPINF K	415.6
vcrA	GVYEGPPDAPFTSWGNR	930.4
	TGAAIHWK	446.2
	DQPWYVK	472.2
	LVNELTEFAK	582.3
DCA*	AEFVEVTK	461.7
DSA "	EYEATLEECCAK	751.8
	QTALVELLK	507.8
*BSA pep	tides were added to the method as in	nternal standard
for peptid	le recovery based on discovery data	run previously

Table 1. List of SDC-9 Peptides Selected for Quantification

Infusion and Injection of Isotopic Peptides

To confirm instrument functionality and detectability of each IS, infusion and injection steps were performed. Each isotopically labeled (IS) peptide was prepared as 12.5 pmol/ μ L in dimethyl sulfoxide (DMSO)/Milli-Q water (50/50), aliquoted, and frozen at -80°C until use. Concentrated solutions for each peptide were provided to the analyst for subsequent dilution and infusion directly into the mass spectrometer (Waters Xevo TQ-XS) for confirmation of precursor (parent) ion, charge state, product ions (daughters),

and optimization of CE (**Table 2**). This optimization step is performed to confirm that a peptide of a given sequence is detectable in the mass spectrometer and to optimize signal intensity for product ions. Each peptide was diluted to 0.5 pmol/ μ L or 1.25 pmol/ μ L in HPLC-grade water + 0.1% formic acid and was directly infused into the mass spectrometer at a flow rate of 10 μ L/min. For each peptide, a mass spectrum of the precursor ion was obtained (**Appendix B**). For each precursor ion, a mass spectrum was obtained for the product ions after fragmentation with CE of \geq 20 V.

Using Waters Intellistart software, the CE for each peptide was optimized to maximize a signal from product ions. This was performed by infusing a single peptide into the mass spectrometer while Intellistart software varied cone voltage and CE to maximize a signal for each product ion. Skyline software was also used to output optimal CE for each peptide using the following equation with parameters (slope, intercept) that are specific to Waters Xevo mass spectrometers (**Table 2**).

CE = slope *(precursor charge state) + intercept

Precursor Charge State	Slope	Intercept
+2	0.037	-1.066
+3	0.036	-1.328

Table 2. Parameters of Waters Xevo CE Equation

Multiple Reaction Monitoring (MRM) Method Development

After optimization of CE per each IS peptide further development of multiple reaction monitoring assay was performed, including optimization of dwell time, CE, and solvent program. During this phase, peptides with relatively poor response were dropped from the MRM method file. The Skyline-optimized CEs were used in initial MRM method development. Comparison to Intellistart-optimized CEs was performed later in MRM development, however improvements in signal intensity were insignificant.

For MRM method development, peptides were prepared as a mixture at 1.25 pmol/ μ L in HPLC-grade water + 0.1% formic acid from a 12.5 pmol/ μ L mixture in DMSO/Milli-Q water. The solvent program and modified versions thereof listed in **Table 2** were used. The chromatographic system used was the Waters M-Class equipped with a trap column (Acquity UPLC M-Class Trap Symmetry® C18; 5 μ m particle size, 100Å pore size; 0.3 mm x 50 mm) and an analytical column (Acquity UPLC M-Class HSS T3 C18; 1.8 μ m particle size, 0.3 mm x 50 mm). **Table 3** displays the solvent program used where A = HPLC-grade water + 0.1% formic acid and B = HPLC-grade acetonitrile + 0.1% formic acid.

Time (min)	Flow Rate (µL/min)	% A	% B
-	10	95	5
5	10	95	5
65	10	35	65
66	10	10	90
70	10	10	90
80	10	95	5
85	10	95	5

Fable	3.	Solvent	Program	for	M-Class	Chromate	ographic	System
	•••	~~~~				0		~,~~~

Based on the observed maximum peak heights of each peptide at 1.25 pmol/ μ L prepared in HPLC-grade water + 0.1% formic acid (MS Parameters from September 5, 2017: 123 transitions; 30 ms dwell time; 3.7 s cycle time), some peptides were removed from the transition list based on poor response (peak height or peak area) relative to other peptides. Only those peptides with the largest responses were retained on the transition list as specified in **Table 4** and **Table 5**.

Using the modified transition list and a 1.25 pmol/ μ L standard prepared in HPLC-grade water + 0.1% formic acid, three dwell times (20 ms, 50 ms, and 70 ms) were examined to assess the sensitivity of the signal to variation in dwell time. Based on the quality of the output data (peak height, peak shape, and points across a peak), the 50 ms dwell time was pursued for MDL experiments. The dwell time parameter was adjusted to 30 ms after further method development was prompted by failure of the first MDL set.

Calibration and System Suitability

Prior to each analytical run for IDL and MDL samples, the instrument was calibrated using a commercially available tuning solution (NAIRB) and a resolution check was performed. Instrument calibration ensures that the proper mass-to-charge ratios (m/z) have been assigned. The instrument is tuned in both MS1 and MS2 modes. Source and lens parameters are adjusted to optimize peak intensity and shape and the resolution and ion energy parameters are set for unit mass resolution on MS1 and MS2. This is performed by infusing a calibrant solution of NAIRB into the mass spectrometer and allowing the software to calibrate across the specified mass range (100-2000 m/z). Although triple quadrupole instruments are known to hold their calibrations for weeks to months, calibrations are performed or verified prior to each analysis sequence for sample sets. For infusion and optimization experiments, the instrument may or may not be calibrated prior to use each day. After instrument calibration, the mass accuracy (residuals) should be ± 0.2 Da.

System suitability was determined by injecting a commercially available retention time synthetic peptide mixture (Pierce[™] Peptide Retention Time Calibration Mixture, Thermo Fisher Scientific) and a solvent spike (1.25 pmol/uL peptide mixture in HPLC-grade water + 0.1% formic acid) followed by solvent blank(s) (HPLC-grade water) before each sample set. Experimental samples were bracketed by injections of the retention time peptide mixture and the solvent spike to ensure the instrument functioned as anticipated and to track any loss of sensitivity or signal if observed during the course of the run. Checks for sensitivity, peak width, retention time, and carryover were performed qualitatively by inspection of the chromatograms of retention time peptide injections, solvent spike injections, and solvent blanks. While instrument sensitivity can vary day to day, no significant losses in instrument performance were observed during the course of IDL and MDL runs.

Protein	Peptide	Precursor (m/z)	Observed (Y/N)	Retained (Y/N)
FdhA	SELEVISSLLSR	671.9	Ν	Ν
	SGSEIAFTGGLIK	644.4	Y	Y
	SWDWALGEIANK	699.4	Ν	Ν
	AAGASDWEEK	536.2	Y	Y*
	ALGIVYLDSQAR	658.4	Y	Y
	VSSLQQLESPEEL R	812.9	Y	Ν
	LSWTYSTNPSAADVA K	859.9	Y	Ν
	NQAVSAPGEAK	540.3	Y	Y
	TDTNTDYSYVNAIK	806.9	Y	Ν
PceA	VETWNHDVA R	412.9	Ν	Ν
	FDEWFGYSGPVNPEE R	969.9	Ν	Ν
	LLPWDLPK	495.3	Y	Ν
	IATQIPLLQDAAR	710.4	Y	Y
	LESGYVQNMVK	638.3	Y	Y
	VYTDLELAPDKPR	509.6	Ν	Ν
	DFWNNPEPIK	634.3	Y	Y
	TSPSLISSATVGK	628.4	Y	Y
	FLGADLVGIAPYDE R	823.4	Y	Y
	DVDDLLSAGK	520.8	Y	Y
TceA	VSSIIEPR	455.8	Y	Y
	VNNEPWWVTT R	706.4	Y	Y
	YFGASSVGAIK	554.3	Y	Y
	WGLYGPPHDSAPPDGSVPK	662.3	Ν	Y
	YFGAGDVGALNLADP K	808.4	Ν	Y
VorA	VPDHAVPINFK	415.6	Ν	Y
VCIA	GVYEGPPDAPFTSWGN R	930.4	Ν	Y
	TGAAIHWK	446.2	Ν	Ν
	DQPWYVK	472.2	Y	Y
	LVNELTEFAK	582.3	Ν	Y
RS A¥	AEFVEVTK	461.7	Ν	Y
DOA	EYEATLEECCAK	751.8	N	Y
	QTALVELLK	507.8	Ν	Y

Table 4. List of SDC-9 Peptides Used in Optimization Experiments

Bolded letters represent isotopically labeled amino acids

*Peptide was added to the transition list at a later date

⁴BSA peptides were added to the method based on discovery data run previously

ID	Peptide	Precursor <i>m/z</i>	Product <i>m/z</i>	Ion	Charge
			1056.6	y10	+1
		644 4	927.6	y9	+1
FdhA2	SGSEIAFTGGLIK	$[M+2H]^{2+}$	814.5	y8	+1
			743.5	у7	+1
			1133.6	b12	+1
		526.2	929.4	y8	+1
FdhA4			872.4	у7	+1
FdhA4	AAGASDWEE K	$[M+2H]^{2+}$	801.4	y6	+1
		[]	714.3	y5	+1
			599.3	y4	+1
			1131.6	y10	+1
		658.4 [M+2H] ²⁺	961.5	y8	+1
FdhA5	ALGIVYLDSQAR		862.4	у7	+1
			699.4	уб	+1
			730.4	b7	+1
		540.3 [M+2H] ²⁺	837.5	y9	+1
			766.4	y8	+1
FdhA8	NQAVSAPGEAK		667.4	у7	+1
			580.3	y6	+1
			571.3	b6	+1
	IATQIPLLQDAA R	710.4 [M+2H] ²⁺	1235.7	y11	+1
			1134.7	y10	+1
PceA4			1006.6	y9	+1
PceA4			893.5	y8	+1
			796.5	у7	+1
		638.3 [M+2H] ²⁺	1162.6	y10	+1
			1033.5	y9	+1
PceA5	LESGYVQNMVK		946.5	y8	+1
			889.5	у7	+1
			726.4	y6	+1
		(24.2	1005.5	y8	+1
		634.3	819.4	у7	+1
PceA7	DFWNNPEPI K	[M+2H]	705.4	y6	+1
			591.4	y5	+1
			677.3	b5	+1
			1067.6	y11	+1
		(20.2	970.6	y10	+1
PceA8	TSPSLISSATVG K	628.3	883.5	y9	+1
		$[M+2H]^{2}$	770.4	y8	+1
			657.4	у7	+1
TceA1	FLGADLVGIAPYDE R	823.4	1385.7	y13	+1

		$[M+2H]^{2+}$	1029.5	y9	+1
			930.5	y8	+1
			873.4	y7	+1
			886.5	b9	+1
			826.4	y8	+1
Teo 12	DVDDLISAGK	520.8 [M+2H] ²⁺	711.4	y7	+1
I CCA2	DVDDELSAGK		596.4	y6	+1
			483.3	y5	+1
			811.5	y7	+1
		155 0	724.4	y6	+1
TceA3	VSSIIEPR	$(M+2H)^{2+}$	637.4	y5	+1
			524.3	y4	+1
			411.2	y3	+1
			1198.6	y9	+1
		706 4	1084.5	y8	+1
TceA4	VNNEPWWVTT R	[M+2H] ²⁺	955.5	y7	+1
			858.4	y6	+1
			1025.5	b8	+1
TceA5		554.3 [M+2H] ²⁺	944.5	y10	+1
			797.5	y9	+1
	YFGASSVGAIK		740.4	y8	+1
			669.4	y7	+1
			582.4	y6	+1
		662.3 [M+3H] ³⁺	899.9	y18	+2
			871.4	y17	+2
VcrA1	WGLYGPPHDSAPPDGSVP		814.9	y16	+2
	К		733.4	y15	+2
			704.9	y14	+2
			1305.7	y14	+1
		000.4	1177.6	y12	+1
VcrA2	YFGAGDVGALNLADP K	808.4	1005.6	y10	+1
		[M+2H] ²	906.5	y9	+1
			1364.6	b14	+1
			725.4	6	+1
			626.4	5	+1
VcrA3	VPDHAVPINFK	415.6	573.3	10	+2
		[M+3H]	467.3	8	+2
			520.3	5	+1
			1411.7	y13	+1
			1354.6	v12	+1
VcrA4	GVYEGPPDAPFTSWGN R	930.4	1254.6	y11	+1
		[M+2H] ²⁺	1045.5	y9	+1
			974.5	y8	+1
VcrA6	DQPWYVK	472.2	700.4	y5	+1

$[M+2H]^{2+}$	603.3	y4	+1
	417.3	y3	+1
	811.4	y6	+1

Instrument Detection Limit (IDL)

To establish IDL, IS peptides were prepared as a mixture at 12.5 pmol/ μ L in DMSO/Milli-Q water (50/50), aliquoted, and frozen at -80°C until use. A mixed, concentrated solution (12.5 pmol/ μ L) was provided fresh to the analyst during each day of analysis. The analyst diluted the sample to 250 fmol/ μ L in in HPLC-grade water + 0.1% formic acid and serially diluted this solution three-fold to prepare the following concentrations: 83, 27, 9, 3, 1, 0.34, and 0.11 fmol/ μ L. The lowest measurable concentration for each peptide, defined as S/N \geq 3 (as measured by MassLynx) for the primary and secondary ion, represents the IDL for each peptide. Three trials were performed with the same dilution scheme; results generated are displayed in **Table 6** below.

IDL 1 IDL 2 IDL 3 Protein Peptide (fmol/µL) (fmol/µL) (fmol/µL) 83² 83 27 **SGSEIAFTGGLIK** AAGASDWEEK >250 >250 >250 FdhA 83 250 83 ALGIVYLDSOAR 27^{f} NQAVSAPGEAK 27 27 IATOIPLLODAAR 83² 250² 83² 250^{2} **LESGYVQNMVK** 250 250 PceA **DFWNNPEPIK** >250 >250 >250 $27^{\text{¥}}$ 27^{f} **TSPSLISSATVGK** 27 **FLGADLVGIAPYDER** >250 >250 250 **DVDDLLSAGK** 250^A 83 250 9 3 9 TceA **VSSIIEPR VNNEPWWVTTR** >250 >250 >250 **YFGASSVGAIK** 250 >250 250 **WGLYGPPHDSAPPDGSVPK** >250 >250 >250 >250 **YFGAGDVGALNLADPK** >250 >250 VcrA **VPDHAVPINFK** >250 >250 >250 **GVYEGPPDAPFTSWGNR** >250 >250 >250 **DQPWYVK** >250 >250 >250

Table 6. IDL Replicate Experiment Results

IDL units are fmol/µL

>250 fmol/µL denotes peptide was "not observed"

[¥]Primary and secondary ion pass at 3 fmol/µL with failure at 9 fmol/µL

^A Primary ion meets criteria at 3 fmol/µL

[£] Primary ion meets criteria at 9 fmol/µL

^a Primary ion meets criteria at 27 fmol/µL

³Secondary ion fails to meet criteria at 9 fmol/µL

Method Detection Limit (MDL)

To determine the MDL of peptide targets, IS peptides were prepared as a mixture at 12.5 pmol/µL in DMSO/Milli-Q water (50/50), aliquoted, and frozen at -80°C until use. A mixed, concentrated solution (12.5 pmol/µL) was provided fresh to the analyst during each day of analysis. The analyst diluted the sample to 1.25 fmol/µL in HPLC-grade water + 0.1% formic acid to use as a control during the analysis sequence. The 12.5 pmol/µL stock solution was diluted in ammonium bicarbonate to prepare the following concentrations (final in 25 µL): 250, 83, 27, 9, 3, 1, 0.3, and 0.1 fmol/µL. Each sample was digested with trypsin overnight and desalted using C18 spin columns. The lowest measurable concentration for each peptide, defined as S/N \geq 3 (as measured by MassLynx) for the primary and secondary ion, represents the MDL for each peptide. Three trials were performed with the same dilution scheme; results generated are displayed in **Table 7**. An example total ion chromatogram displaying RDase peptides detected in the IS mix during the MDL study is shown in **Figure 2**.

Protein	Peptide	MDL 1	MDL 2	MDL 3
		(fmol/ µL)	(fmol/ µL)	(fmol/ µL)
FdhA	SGSEIAFTGGLIK	27	83	83
	AAGASDWEEK	>250	>250	>250
	ALGIVYLDSQAR	3	83	83
	NQAVSAPGEAK	>250	>250	>250
PceA	IATQIPLLQDAAR	27 ^F	250 ^G	250
	LESGYVQNMVK	27 ^D	250 ^C	>250
	DFWNNPEPIK	27 ^D	250	250 ^C
	TSPSLISSATVG K	9	83	27
TceA	FLGADLVGIAPYDE R	27	250 ^C	250 ^C
	DVDDLLSAGK	1	83	250 ^B
	VSSIIEPR	3	27	83
	VNNEPWWVTT R	83	>250	>250
	YFGASSVGAIK	9	83 ^A	250 ^G
VcrA	WGLYGPPHDSAPPDGSVPK	83	>250	>250
	YFGAGDVGALNLADPK	83	>250	>250
	VPDHAVPINFK	3	9	9
	GVYEGPPDAPFTSWGN R	250	>250	>250
	DQPWYVK	27	27	27

Table 7. MDL Replicate Experiment Results

MDL units are fmol/µL

>250 fmol/µL denotes peptide was "not observed"

^A Primary and secondary ion pass at 3 fmol/µL with failure at 9 and 27 fmol/µL

^B Primary and secondary ion pass at 9 fmol/µL with failure at 27 and 83 fmol/µL

^C Primary ion meets criteria at 83 fmol/µL

^D Primary ion meets criteria at 9 fmol/µL

^F Primary ion meets criteria at 3 fmol/µL

^G Primary ion meets criteria at 27 fmol/µL



Figure 2. Representative Total Ion Chromatogram Displaying Detected RDase peptides; BSA peptides not shown as detection signals are significantly larger than for RDase peptides; the two panels to the right are more detailed chromatograms displaying the signal from each product ion for the VcrA peptide VPDHAVPINFK.

All BSA peptides were observed during MDL analysis. An example chromatogram of BSA peptides (10 μ g of BSA was added prior to each MDL sample prior to digestion) is displayed in **Figure 3** (from the MDL dataset 9/18/2017).



Figure 3. BSA Peptides Detected in MDL Samples

Two VcrA peptides (DQPWYVK and VPDHAVPINFK) were detectable in all MDL experiments while they were not detected in IDL experiments (**Figure 4**). The causes of performance variation between IDL and MDL experiments are likely due to matrix effects. Some peptides performed similarly between MDL replicates (e.g., DQPWYVK) while others did not. Within the MDL set, inconsistencies were observed for sensitive peptides (e.g., TSPSLISSATVGK, VSSIIEPR, YFGASSVGAIK). This variation represents the variation present in the preparatory methods and instrumental analysis; it is unlikely that instrumental variation resulted in decreased sensitivity as control samples of 1.25 pmol/uL mixed peptide prepared in HPLC-grade water + 0.1% formic acid and a Thermo Retention Time Peptide Mixture that bracketed samples did not reveal loss of chromatographic quality or loss in mass spectrometer signal during the course of the MDL runs. For peptides that have poor secondary ion responses (e.g., YFGASSVGAIK), a more restrictive quality control scheme (that is, requiring two product ions to be present at $S/N \ge 3$) will result in higher detection limits. It is proposed that during sample analysis, the S/N of all analytes be calculated using MassLynx to satisfy the following acceptance criteria: those samples with $S/N \le 3$ would be categorized as not detected, and those that meet $S/N \ge 3$ would be accepted as true detections and would be reported with quantitative values.



Figure 4. Representative detailed chromatogram, peak area contributions, and retention time variation for 0.11-250 fmol/µL VcrA peptide VPDHAVPINFK standard from MDL experiment 1 (9/11/2017).

Summary

In groundwater contaminated with chlorinated ethenes, the dominant and most productive biodegradation mechanism is typically reductive dechlorination. This is a process whereby the parent compound(s) PCE and/or TCE are sequentially dehalogenated to *cis*-1,2-dichloroethene (cis-DCE), vinyl chloride (VC) and finally ethene and/or ethane, which are considered environmentally benign. A number of different dehalogenating bacteria catalyze one or more steps throughout this process, with DHC being the only organismal group known to complete the entire pathway. In an effort to provide a robust and specific measurement that directly correlates to degradation rates, our team has developed a proteomics approach to quantify RDase proteins using a targeted MRM assay.

Prior to development of the MRM assay for targeted quantification, SDC-9 culture-specific RDase peptides were identified. Overall, a total of 28 peptide sequences, including those encoding for FdhA protein, were selected for quantification. During the initial steps of MRM assay development confirmation of instrument functionality and detection of peptide targets were performed. For that purpose, isotopically labeled peptide standards were injected into the mass spectrometer and their CE were optimized. Instrument and MDLs were subsequently established for each respective peptide.

In this study, CEs were optimized for initial 28 IS peptides to maximize the resulting signal from product ions. Following the optimization step, dwell time and solvent program were optimized and peptides that demonstrated poor signal response were discarded from the list. In total, 10 peptides were discarded from the list after optimization steps were completed and IDLs and MDLs were developed for the remaining peptides. Most peptides were observed in experimental samples during the IDL and MDL analysis, however VcrA peptides were observed exclusively in MDL experiments and not in IDL experiments (not observed is denoted as >250 fmol/µL), suggesting that sample digest and cleanup enhance the peptide signals for VcrA peptides. Two VcrA peptides (DQPWYVK and VPDHAVPINFK) were detectable in all MDL experiments while they were not detected in IDL experiments. Performance variation between IDL and MDL experiments (e.g., DQPWYVK) while others did not. Within the MDL set, inconsistencies were observed for sensitive peptides (e.g., TSPSLISSATVGK, VSSIIEPR, YFGASSVGAIK). This variation represents the variation present in the preparatory methods and instrumental analysis; it is unlikely that instrumental variation resulted in decreased sensitivity as control samples did not reveal loss of chromatographic quality or loss in mass spectrometer signal during the MDL runs.

Overall, the experiments performed during this study allowed for identification of the most sensitive RDase and FdhA peptides for targeted quantification. MDL experiments resulted in detection of up to three most sensitive peptides per protein with up to three most intensive transition ions per peptide. The data generated during the optimization and calibration experiments will be built into the MRM method used for quantification of native RDase peptides in microcosm experiment samples planned to be tested in the next phase of this project.

Re-Assessment of Instrument Detection Limit and Method Detection Limit for Reductive Dehalogenase Isotopic Peptides

REPORT

Battelle Memorial Institute 505 King Avenue Columbus, OH 43201

Mandy Michalsen, Ph.D., P.E. Research Engineer U.S. Army Engineer Research Development Center Environmental Lab

This report is a work prepared for the U.S. Army Engineer Research Development Center Environmental by Battelle. In no event shall either U.S. Army Engineer Research Development Center Environmental or Battelle have any responsibility or liability for any consequences of any use, misuse, inability to use, or reliance on any product, information, designs, or other data contained herein, nor does either warrant or otherwise represent in any way the utility, safety, accuracy, adequacy, efficacy, or applicability of the contents hereof.

Introduction

A suite of SDC-9 culture-specific reductive dehalogenase (RDase) peptides have been previously identified for quantification. These specific RDases are used in a multiple reaction monitoring-based (MRM) targeted proteomic assay to determine their quantities. During the initial development phase, the MRM assay was evaluated for empirical limits of detection (LOD) and limit of quantification (LOQ). While LOD and LOQ data were obtained during initial method development, the data was poorly reproducible among replicates (see Table 1 and 2 below) with some peptides not being observed even at the highest calibration level. Preparation and analysis of a second batch of samples was initiated to improve the reproducibility of the data. Changes to instrumental methods and updated tables are discussed below.

Protein	Peptide	IDL I	IDL 2	IDL 3
	SGSEIAFTGGLI K	83 ²	83	27
FdhA SGSEIAFTGGLIK 83 ² FdhA AAGASDWEEK >250 > AAGASDWEEK >250 > > MQAVSAPGEAK 27 [£] > > PceA IATQIPLLQDAAR 83 ⁸ > > ILESGYVQNMVK 250 > > > PceA DFWNNPEPIK >250 > > FLGADLVGIAPYDER >250 > > > TceA VSSIIEPR 9 > > > VcrA VSIEPR 9 > > > > VcrA VPDHAVPINFK >250 > > > > > VcrA QPWYVK >250 > > > > >	>250	>250		
	ALGIVYLDSQA R	83	250	83
	NQAVSAPGEAK	27^{f}	27	27
FdhA PceA TceA	IATQIPLLQDAAR	83 ²	250 ²	83 ²
	LESGYVQNMVK	250	250	250 ²
	DFWNNPEPIK	>250	>250	>250
	TSPSLISSATVG K	27	$27^{\text{¥}}$	27^{f}
FdhA SGSEIAFTGGLIK 83 ^e 83 AAGASDWEEK >250 >250 ALGIVYLDSQAR 83 250 NQAVSAPGEAK 27 ^t 27 IATQIPLLQDAAR 83 ^e 250 ^e PceA LESGYVQNMVK 250 >250 TSPSLISSATVGK 27 27 ^t 27 FLGADLVGIAPYDER >250 >250 TceA DFWNNPEPIK >250 >250 TCeA VSSIIEPR 9 3 ^h VNNEPWWVTTR >250 >250 YFGASSVGAIK 250 >250 VCrA VPDHAVPINFK >250 >250 GVYEGPPDAPFTSWGNR >250 >250 DQPWYVK >250 >250	FLGADLVGIAPYDE R	>250	>250	250
	DVDDLLSAG K	250	250 ^A	83
	3 Ϡ	9		
	VNNEPWWVTT R	>250	>250	>250
	YFGASSVGAIK	250	>250	250
	WGLYGPPHDSAPPDGSVPK	>250	>250	>250
	YFGAGDVGALNLADP K	>250	>250	>250
FdhA SGSEIAFTGGLIK 83 ² 83 AAGASDWEEK >250 >250 ALGIVYLDSQAR 83 250 NQAVSAPGEAK 27 [£] 27 IATQIPLLQDAAR 83 ⁸ 250 ⁸ LESGYVQNMVK 250 >250 DFWNNPEPIK >250 >250 TSPSLISSATVGK 27 27 [¥] FLGADLVGIAPYDER >250 >250 DVDDLLSAGK 250 >250 VNNEPWWVTTR >250 >250 YFGASSVGAIK 250 >250 VCrA VPDHAVPINFK >250 >250 VCrA VPDHAVPINFK >250 >250 DQPWYVK >250 >250	>250	>250		
	GVYEGPPDAPFTSWGN R	>250	>250	>250
	DQPWYVK	>250	>250	>250

Table 1. Previously Determined Limits of Detection for RDase peptides

Units are fmol/mL

>250 fmol/ mL denotes peptide was "not observed"

[¥]Primary and secondary ion pass at 3 fmol/µL with failure at 9 fmol/mL

^A Primary ion meets criteria at 3 fmol/mL

[£] Primary ion meets criteria at 9 fmol/mL

² Primary ion meets criteria at 27 fmol/mL

³Secondary ion fails to meet criteria at 9 fmol/mL

Table 2. Previously Determined Limits of Quantification for RDase peptides

Protein	ID	Peptide	MDL 1	MDL 2	MDL 3	MDL 4	MDL 5
FdhA	FdhA2	SGSEIAFTGGLIK	27	83	83	83	250 ^{A,G}
	FdhA5	ALGIVYLDSQA R	3	83	83	83	27
	FdhA8	NQAVSAPGEAK	>250	>250	>250	>2250	>2250
PceA	PceA4	IATQIPLLQDAAR	27 ^F	250 ^G	250	83 ^G	750 ^G
	PceA5	LESGYVQNMV K	27 ^D	250 ^C	>250	250 [°]	750^{H}
	PceA7	DFWNNPEPI K	27 ^D	250	250 ^C	83	250
	PceA8	TSPSLISSATVG K	9	83	27	27	27
	TceA1	FLGADLVGIAPYDE R	27	250 ^C	250 ^C	750 ^H	750^{H}
	TceA2	DVDDLLSAG K	1	83	250 ^B	83 ^D	83 ^G
TceA	TceA3	VSSIIEP R	3	27	83	9	9
	TceA4	VNNEPWWVTT R	83	>250	>250	750	1000^{I}
	TceA5	YFGASSVGAIK	9	83 ^A	250 ^G	83 ^G	83 ^F
	VcrA1	WGLYGPPHDSAPPDGSVPK	83	>250	>250	750	750
VcrA	VcrA2	YFGAGDVGALNLADP K	83	>250	>250	750 ^H	1000
	VcrA3	VPDHAVPINFK	3	9	9	27	27
	VcrA4	GVYEGPPDAPFTSWGN R	250	>250	>250	2250 ^I	2250
	VcrA6	DQPWYVK	27	27	27	250 ^G	750 ^D

Units are fmol/mL

>250 fmol/ µL denotes peptide was "not observed"

^A Primary and secondary ion pass at 3 fmol/µL with failure at 9 and 27 fmol/mL

 B Primary and secondary ion pass at 9 fmol/µL with failure at 27 and 83 fmol/mL

^C Primary ion meets criteria at 83 fmol/mL

^D Primary ion meets criteria at 9 fmol/mL

^F Primary ion meets criteria at 3 fmol/mL

^G Primary ion meets criteria at 27 fmol/mL

^HPrimary ion meets criteria at 250 fmol/mL

¹Primary ion meets criteria at 750 fmol/mL

Calibration and System Suitability

Prior to sample analysis, the instrument was tuned in both MS1 and MS2 modes to maximize transmission of ions using a commercially available tuning solution (NAIRB). Using the instrument's automated tuning program, source and lens parameters were auto-adjusted to optimize peak intensity and shape, and the resolution and ion energy parameters were set for unit mass resolution on MS1 and MS2. A resolution check was also performed by the analyst to confirm the instrument met unit mass resolution. The instrument was also calibrated prior to each run using NAIRB. This was performed by infusing a calibrant solution of NAIRB into the mass spectrometer and allowing the software to auto-calibrate across the specified mass range (100-2000 m/z).

System suitability was determined by injecting a commercially available retention time synthetic peptide mixture (PierceTM Peptide Retention Time Calibration Mixture, Thermo Fisher Scientific) and a solvent spike (31 fmol/mL peptide mixture in HPLC-grade water + 0.1% formic acid) followed by solvent blank(s) (HPLC-grade water) before each sample set. Experimental samples were bracketed by injections of the retention time peptide mixture and the solvent spike to ensure the instrument functioned as anticipated and to track changes in sensitivity during the analytical run.

Multiple Reaction Monitoring (MRM) Method Updates

A new column was purchased for use on the program. It was observed that peptide FdhA8 displayed poor retention on the trap and analytical columns. The solvent program (Table 3) was modified by increased the percentage of starting acetonitrile (organic phase), which improved retention of peptide FdhA8.

Time (min)	Flow Rate (µL/min)	% A	% B*
-	10	95	1
5	10	95	1
65	10	35	65
66	10	10	90
70	10	10	90
80	10	95	1
85	10	95	1

Table 8. Solvent Program for M-Class Chromatographic System

*Starting acetonitrile (organic phase) changed from 5% to 1%

The peptides monitored were updated to reflect most recent practices (Table 4).

Table 4. Mass Transitions Used for Updated IDL/MDL Experiments

ID	Peptide	Precursor <i>m/z</i>	Product <i>m/z</i>	Ion	Charge
Edh A 2	SCSELVETCCLIK	644.4	814.5	y8	+1
runA2	SUSEIAFTUULI K	[M+2H] ²⁺	743.5	у7	+1
Edh 4.5		658.4	961.5	y8	+1
FuiAS	ALOIVILDSQAK	[M+2H] ²⁺	862.4	у7	+1
EdhAQ	NOAVSADGEAK	540.3	837.5	y9	+1
гипло	NQAVSAFOLAK	[M+2H] ²⁺	667.4	y7	+1
Deckd		710.4	1006.6	y9	+1
r ceA4	IATQII LLQDAAK	[M+2H] ²⁺	893.5	y8	+1
D 4.5	LECONMONIMUL	638.3	1033.5	y9	+1
PceA5	LESGYVQNMVK	[M+2H] ²	726.4	y6	+1
Peo A 7	DEWNINIPEPIK	634.3 [M+2H] ²⁺	819.4	у7	+1
I CEA /	DI WINN LI IK		591.4	y5	+1
PceA8	TSPSI ISSATVG K	628.3 [M+2H] ²⁺	770.4	y8	+1
1 00/10			657.4	y7	+1
TceA2	DVDDLLSAGK	520.8 [M+2H] ²⁺	826.4	y8	+1
	2 . 2 2 2 2		711.4	у7	+1
TceA3	VSSIIEPR	455.8	724.4	y6	+1
	V SSILL R	[M+2H] ²⁺	524.3	y4	+1
TceA4	VNNFPWWVTT R	706.4	1198.6	y9	+1
100/14		[M+2H] ²⁺	955.5	y7	+1
Tee 15	VEGASSVGAIK	554.3	797.5	y9	+1
ПСАЗ	II GASS VOAI K	[M+2H] ²⁺	669.4	у7	+1
Vor A 1	WGI VGPPHDSAPPDCSVPK	662.3	814.9	y16	+2
VUAI	WOLTOITIDSAITDOSVI K	[M+3H] ³⁺	733.4	y15	+2
VcrA2	YFGAGDVGALNLADP K	808.4	1177.6	y12	+1

		[M+2H] ²⁺	906.5	y9	+1
VcrA3	VDDUAVDINEV	415.6	573.3	y10	+2
	VPDHAVPINF K	[M+3H] ³⁺	626.4	y5	+1
VcrA4	GVYEGPPDAPFTSWGN R	930.4 [M+2H] ²⁺	1411.7	y13	+1
			974.5	y8	+1
VcrA6	DODWVVVK	472.2	700.4	y5	+1
	DQPWIVK	[M+2H] ²⁺	417.3	y3	+1

Bovine serum albumin (Table 5) was used to monitor digestion efficiency for MDL sample preparation. This was performed by spiking in 10 μ g of BSA into ammonium bicarbonate alongside the IS peptides prior to digestion and C18 desalting.

Table 5. Mass Transitions Used to Monitor Digestion Efficiency

ID	Peptide	Precursor <i>m/z</i>	Product <i>m/z</i>	Ion	Charge
BSA1	I VNELTEEA V	582.3	951.5	y8	+1
	LVNELIEFA N	[M+2H] ²⁺	708.4	y6	+1
DCA1	AEFVEVTK R	461.7 [M+2H] ²⁺	722.4	y6	+1
BSA2			575.3	y5	+1
BSA3	EYEATLEECCAK	751.8	909.4	y7	+1
		[M+2H] ²⁺	796.3	y6	+1
DCAA		507.8	785.5	y7	+1
DSA4	QIALVELLK	[M+2H] ²⁺	604.4	y5	+1

Digestion Efficiency

Digestion efficiencies for each BSA peptide were calculated by taking the ratio between the peak areas for the peptide in the MDL standard (containing IS peptides and BSA) and the digestion control (reference containing BSA only) (Table 6).

			Digest	Efficien	cy (%)	Avg Digest	Standard	RSD
Protein ¹	ID	Peptide	MDL 1	MDL 2	MDL 3	Efficiency (%)	deviation (%)	(%)
BSA1	BSA1	LVNELTEFAK	111	112	ND	111.5	0.7	0.6
	BSA2	AEFVEVTK	112	116	119	115.7	3.5	3.0
	BSA3	EYEATLEECCAK	ND	161	157	159.0	2.8	1.8
	BSA4	QTALVELLK	113	108	ND	110.5	3.5	3.2

Table 6. Mass Transitions Used to Monitor Digestion Efficiency

¹ Level of BSA spiked was 10 µg

ND Peptide was not detected in the reference digest sample; calculation of efficiency could not be calculated RSD (relative standard deviation)

Depending on the peptide, the digestion efficiency ranged from 111-159%. While BSA peptides 3 and 4 are diagnostic of efficiency, however these peptides should not be used as they are prone to cyclizing because of their N-terminal glutamine and glutamate amino acids. The replicates (n = 7 standards) were

precise with relative standard deviations \leq 3%. While this data indicates that the digestion efficiency is well controlled, it is recommended that the level of BSA spiked be reduced by half to mitigate any detector saturation that could occur. While no saturation was observed in these sample sets, the intensities of BSA peptide in the samples (>10e6) are close to the level of detector saturation (10e7 - 10e8).

Instrument Detection Limit (IDL)

Isotopically labeled peptides were prepared as a mixture at 12.5 pmol/µL in DMSO/Milli-Q water (50/50), aliquoted, and frozen at -80°C until use. Mixed IS peptide solution (12.5 pmol/ μ L) was provided fresh to the analyst during each day of analysis. The analyst diluted the sample to 250 fmol/ μ L in in HPLC-grade water + 0.1% formic acid and serially diluted this solution 3-fold in water + 0.1% formic acid to prepare the following concentrations: 83, 27, 9, 3, 1, and 0.34 fmol/ μ L. The lowest measurable concentration for each peptide, defined as signal-to-noise $(S/N) \ge 3$ (as measured by MassLynx) for the primary and secondary ion, was assigned as the IDL for each peptide. Three trials were performed with the same dilution scheme; results generated are displayed in Table 7 below.

Protein	ID	Peptide	IDL 1	IDL 2	IDL 3	Revised Average IDL
	FdhA2	SGSEIAFTGGLI K	0.3	0.3	0.3	0.3
FdhA	FdhA5	ALGIVYLDSQA R	0.3	0.3	0.3	0.3
	FdhA8	NQAVSAPGEAK	9	1	1	9
	PceA4	IATQIPLLQDAA R	3	1	0.3	3
DooA	PceA5	LESGYVQNMV K	1	0.3	0.3	1
ICEA	PceA7	DFWNNPEPI K	3	1	0.3	3
	PceA8	TSPSLISSATVG K	0.3	0.3	0.3	0.3
	TceA2	DVDDLLSAG K	0.3	0.3	0.3	0.3
TeeA	TceA3	VSSIIEP R	0.3	0.3	0.3	0.3
ICCA	TceA4	VNNEPWWVTT R	9	3	3	9
	TceA5	YFGASSVGAIK	0.3	0.3	0.3	0.3
	VcrA1	WGLYGPPHDSAPPDGSVPK	27	83	27	83
	VcrA2	YFGAGDVGALNLADP K	27	9	3	27
VcrA	VcrA3	VPDHAVPINFK	0.3	0.3	0.3	0.3
	VcrA4	GVYEGPPDAPFTSWGNR	83	83	27	83
	VcrA6	DQPWYVK	1	0.3	0.3	1
Units are fr	nol/mL of sa	ample				

Table 7. IDL Replicate Experiment Results

¹ Bolded letters denote heavy ¹³C and ¹⁵N labeled amino acid

The revised IDL was assigned as the largest IDL observed between the three replicate measurements. The revised IDL represents the lowest standard in diluent (water + 0.1% formic acid) that was observed on the instrument with signal to noise ≥ 3 .

Method Detection Limit (MDL)

To determine the MDL of peptide targets, the 12.5 pmol/ μ L stock solution of IS peptides was diluted in ammonium bicarbonate to prepare the following final concentrations: 250, 83, 27, 9, 3, 1, and 0.3 fmol/µL. Each sample was digested with trypsin overnight and desalted using C18 spin columns. This procedure mimics the matrix that is used during digestion and cleanup of field samples. The lowest measurable concentration for each peptide, defined as $S/N \ge 3$ (as measured by MassLynx) for the primary and secondary ion, was assigned as the MDL for each peptide. Three trials were performed with the same dilution scheme; results generated are displayed in Table 8.

Protein	ID	Peptide ¹	MDL 1	MDL 2	MDL 3	Revised Average MDL	
	FdhA2	SGSEIAFTGGLI K	3	3	3	3	
FdhA	FdhA5	ALGIVYLDSQA R	3	3	1	3	
	FdhA8	NQAVSAPGEAK	3	3	3	3	
	PceA4	IATQIPLLQDAA R	9	9	9	9	
Deck	PceA5	LESGYVQNMV K	3	3	3	3	
PceA	PceA7	DFWNNPEPI K	1	1	1	1	
	PceA8	TSPSLISSATVG K	0.3	0.3	1	1	
	TceA2	DVDDLLSAG K	0.3	3	3	3	
TeeA	TceA3	VSSIIEP R	0.3	0.3	1	1	
IceA	TceA4	VNNEPWWVTT R	9	9	9	9	
	TceA5	YFGASSVGAIK	0.3	0.3	1	1	
	VcrA1	WGLYGPPHDSAPPDGSVP K	9	9	3	9	
	VcrA2	YFGAGDVGALNLADP K	27	27	27	27	
VcrA	VcrA3	VPDHAVPINFK	0.3	0.3	1	1	
	VcrA4	GVYEGPPDAPFTSWGN R	83	27	27	83	
	VcrA6	DQPWYVK	1	1	1	1	
Units are fmol/mL of extract							

Table 8. MDL Replicate Experiment Results

¹ Bolded letters denote heavy ¹³C and ¹⁵N labeled amino acid

The revised MDL was assigned as the largest MDL observed between the three replicate measurements. The revised MDL represents the lowest standard in matrix (ammonium bicarbonate with subsequent C18 desalting) that was observed on the instrument with signal to noise ≥ 3 .

Comparison of Revised IDL and MDL Levels

The Battelle proteomics team expected the measured MDL to be larger than the measured IDL for two reasons: (1) matrix effects can result in suppression or enhancement of an analyte's response and, (2) sample handling and cleanup can result in signal losses. Note that for the majority of peptides, this expectation holds true: the measured MDL > measured IDL. For 3 peptides (FdhA8, PceA7, VcrA1, highlighted in red in Table 9), the relationship was reversed: measured MDL < measured IDL. This indicates that the analyte's response enhanced by addition of matrix (ammonium bicarbonate with C18 cleanup). For 4 peptides (TceA4, VcrA2, VcrA4, and VcrA6), the measured MDL = measured IDL. This suggests that the peptide response was not affected by the addition of matrix (ammonium bicarbonate with C18 cleanup).

While the measured IDL is useful for method development, the measured MDL is the more important in quantitative experiments as it represents the minimum quantifiable value for a given method. For subsequent quantitative experiments with microcosm samples, the MDL for each peptide will be used as the minimum quantifiable level. Samples with quantified peptide levels that are below the MDL are not reportable values but can be important for diagnostic purposes and for subsequent method development (Table 9).

Protein	ID	Peptide ¹	Experimental IDL	Experimental MDL		
	FdhA2	SGSEIAFTGGLI K	0.3	3		
FdhA	FdhA5	ALGIVYLDSQA R	0.3	3		
	FdhA8	NQAVSAPGEA K	9	3		
PceA	PceA4	IATQIPLLQDAA R	3	9		
	PceA5	LESGYVQNMV K	1	3		
	PceA7	DFWNNPEPI K	3	1		
	PceA8	TSPSLISSATVG K	0.3	1		
	TceA2	DVDDLLSAG K	0.3	3		
TeeA	TceA3	VSSIIEP R	0.3	1		
IceA	TceA4	VNNEPWWVTT R	9	9		
	TceA5	YFGASSVGAIK	0.3	1		
	VcrA1	WGLYGPPHDSAPPDGSVP K	83	9		
	VcrA2	YFGAGDVGALNLADP K	27	27		
VcrA	VcrA3	VPDHAVPINFK	0.3	1		
	VcrA4	GVYEGPPDAPFTSWGN R	83	83		
	VcrA6	DQPWYVK	1	1		
Units are fmol/mL of extract ¹ Bolded letters denote heavy ¹³ C and ¹⁵ N labeled amino acid						

Table 9. Comparison of Experimental Instrument and Method Detection Limits

Comparison of Theoretical Detection Limits with IDL/MDL Results

A theoretical IDL for each peptide was also determined with existing IDL data (Table 10). Calculated (theoretical) IDL values are typically the IDL levels reported for publication. The theoretical IDLs were determined by measuring signal to noise for the secondary ions for each peptide at a concentration yielding signal to noise between 10 and 20. The proportionality between concentration and signal to noise was used to calculate the concentration of peptide that would theoretically yield a signal to noise = 3. This calculation assumes a linear relationship between concentration and signal to noise.

Protein	ID	Peptide ¹	Theoretical IDL	Experimental IDL	Experimental MDL
	FdhA2	SGSEIAFTGGLIK	0.08	0.3	3
FdhA	FdhA5	ALGIVYLDSQA R	0.02	0.3	3
	FdhA8	NQAVSAPGEAK	0.84	9	3
	PceA4	IATQIPLLQDAA R	0.58	3	9
DerA	PceA5	LESGYVQNMV K	0.59	1	3
PceA	PceA7	DFWNNPEPIK	0.21	3	1
	PceA8	TSPSLISSATVG K	0.09	0.3	1
	TceA2	DVDDLLSAG K	0.04	0.3	3
Tra A	TceA3	VSSIIEPR	0.02	0.3	1
IceA	TceA4	VNNEPWWVTT R	2.17	9	9
	TceA5	YFGASSVGAIK	0.03	0.3	1
	VcrA1	WGLYGPPHDSAPPDGSVP K	19.15	83	9
	VcrA2	YFGAGDVGALNLADP K	9.68	27	27
VcrA	VcrA3	VPDHAVPINFK	0.33	0.3	1
	VcrA4	GVYEGPPDAPFTSWGN R	28.89	83	83
	VcrA6	DQPWYVK	0.25	1	1
Units are f	fmol/mL of	extract			

Table 10. Comparison of Detection Limits

¹ Bolded letters denote heavy ¹³C and ¹⁵N labeled amino acid

APPENDIX B VALIDATION STUDY OF QPROT ASSAY QUANTITATION LIMITS

Determination of RDase Peptide Concentrations in the Validation Study

REPORT

Battelle Memorial Institute 505 King Avenue Columbus, OH 43201

Mandy Michalsen, Ph.D., P.E. Research Engineer U.S. Army Engineer Research Development Center Environmental Lab

This report is a work prepared for the U.S. Army Engineer Research Development Center Environmental by Battelle. In no event shall either U.S. Army Engineer Research Development Center Environmental or Battelle have any responsibility or liability for any consequences of any use, misuse, inability to use, or reliance on any product, information, designs, or other data contained herein, nor does either warrant or otherwise represent in any way the utility, safety, accuracy, adequacy, efficacy, or applicability of the contents hereof.

Table of Contents

List of Acronyms	ii
1. Introduction	3
2. Dilution Study Setup, Protein Extraction and Quantification	1
2.1 Dilution Study Set up	1
2.2 RDase Isotopic Peptides	1
2.3 Protein Extraction and Quantification	2
2.4 Protein Concentrations in Dilution Study Samples	2
3. Summary	3

List of Tables

Table 1. Gene specific qPCR analysis of SDC-9 sample	1
Table 2. RDase peptides used in MRM assay	2

List of Appendices

APPENDIX A: Protein Extraction, Quantification and Cleanup	A
APPENDIX B: List of all Isotopic Peptides and Their Transitions	B
APPENDIX C: Dilution Study I	C
APPENDIX D: Dilution Study II	D
•	

List of Acronyms

CEs	collision energies
DHC	Dehalococcoides
IDL IS	instrument detection limit internal standards
LOD LOQ	limit of detection limit of quantification
MDL MRM	method detection limit multiple reaction monitoring-based
PCE	tetrachloroethene
RDase	reductive dehalogenase
VC	vinyl chloride

Introduction

In preparation for microcosm experiments planned for this project, the Battelle proteomics team, in collaboration with the University of Tennessee, has identified SDC-9 culture-specific reductive dehalogenase (RDase) peptides for quantification. These specific RDases are used in a multiple reaction monitoring-based (MRM) targeted proteomic assay to establish quantitative biomarker rate correlations, which are needed to generate in situ degradation rate estimates of chlorinated ethenes.

After the development of the MRM assay and determination of instrument detection limit (IDL) and method detection limit (MDL) for each RDase, dilution study was performed. The dilution study severed to identify the lowest concentration of DHC cells that generate detectable and quantifiable concentrations of reductive dehalogenases (RDases) selected for quantification.

To maximize precision, stable isotope labeled internal standards (IS) were used to account for errors and losses that can occur during sample handling and variability in peptide ionization in the analysis of peptides. Because of the rigors of establishing these assays and successfully performing them in complex matrices, they tend to be implemented on only a selected number of analytes in parallel. With only a small number of analytes measured, it is common to expend considerable time optimizing tune parameters and collision energies (CEs) of each analyte individually to attain the highest sensitivity possible.

This report discusses set up of the dilution study and generated results. Data pertaining to system resolution check, calibration, and chromatograms of peptide detections are grouped per sample set in **Appendices C** and **D**.

Validation Study Setup, Protein Extraction and Quantification

Validation Study Set up

SDC-9 dechlorinating consortium was shipped to Battelle from Aptim in September 2017. The culture was aliquoted into 50 mL tubes and kept frozen in -80 °C until use. For the purposed of the dilution study, one 50 mL tube was shipped to the University of Tennessee for determination of DHC cell concentration and RDase genes (**Table 1**). Another tube was used for proteomic analysis. Starting SDC-9 culture of 2 x 10^7 DHC cells was diluted in triplicate to concentrations: 10^4 , 10^5 , 10^6 and 10^7 , and subject to protein extraction, tryptic digestion and quantification.

Sample ID:	SDC-9 Culture		
Analysis: qPCR			
Volume of sample filtered (mL)	30		
Isolated DNA concentration (ng/µL)	67.5		
Volume of purified DNA (µL)	50		
qPCR Assays (gene copies/mL)			
General Bacteria 16S rRNA gene	3.18E+8		
Dehalococcoides 16S rRNA gene	2.26E+7		
<i>Dehalococcoides vcrA</i> gene (cDCE→Ethene)	2.70E+7		
<i>Dehalococcoides bvcA</i> gene (cDCE→Ethene)	ND		
Dehalococcoides tceA gene (TCE→VC)	2.23E+7		

Fable 1. Gen	e specific	aPCR	analysis	of SDC-9	sample
	e speeme	yı civ	anarysis		sampre

RDase Isotopic Peptides

Dehalococcoides (DHC) comprise a genus-level group of bacteria within the phylum *Chloroflexi*, notable for their ability to respire halogenated compounds including recalcitrant groundwater contaminants. Their obligate use of halogenated organic compounds as an energy source has allowed successful development of DHC-containing enrichment cultures for bioaugmentation of chlorinated ethene-contaminated sites, such as SDC-9 consortium. Each DHC strain contains a unique complement of genes that are homologs of known RDases, the genes required for respiration of halogenated organic compounds. The SDC-9 consortium is a well-defined enrichment culture with a variety of robust tetrachloroethene (PCE) – vinyl chloride (VC) dechlorinators. A metagenome sequencing project for the SDC-9 consortium was completed by Battelle Memorial Institute and the University of Tennessee to determine specific RDase genes that could serve as targets in proteomic analyses.

Overall, 14 genes encoding RDases were identified, 10 of which best matched previously identified RDases from members of the genus *Dehalococcoides*. Of these 14 sequences, one *vcrA* and one *tceA* gene were identified, as well as two separate *pceA* genes. Peptide sequences of RDases and several sequences of FdhA protein that encodes for formate dehydrogenase were selected for targeted proteomic analysis. The detailed list of peptide sequences is presented in **Table 2**.

Protein	Peptide ID	Peptide	MDL 1 (fmol/ μL)	MDL 2 (fmol/ μL)	MDL 3 (fmol/ µL)	
FdhA	FdhA2	SGSEIAFTGGLIK	27	83	83	
	FdhA5	ALGIVYLDSQA R	3	83	83	
	FdhA8	NQAVSAPGEAK	>250	>250	>250	
PceA	PceA4	IATQIPLLQDAAR	27 ^F	250 ^G	250	
	PceA5	LESGYVQNMVK	27 ^D	250 ^C	>250	
	PceA7	DFWNNPEPIK	27 ^D	250	250 ^C	
	PceA8	TSPSLISSATVG K	9	83	27	
	TceA2	DVDDLLSAGK	1	83	250 ^B	
TceA	TceA3	VSSIIEP R	3	27	83	
	TceA4	VNNEPWWVTT R	83	>250	>250	
	TceA5	YFGASSVGAIK	9	83 ^A	250 ^G	
	VcrA1	WGLYGPPHDSAPPDGSVPK	83	>250	>250	
VcrA	VcrA2	YFGAGDVGALNLADP K	83	>250	>250	
	VcrA3	VPDHAVPINF K	3	9	9	
	VcrA4	GVYEGPPDAPFTSWGN R	250	>250	>250	
	VcrA6	DQPWYVK	27	27	27	
MDL units are fmol/µL >250 fmol/µL denotes peptide was "not observed" ^A Primary and secondary ion pass at 3 fmol/µL with failure at 9 and 27 fmol/µL ^B Primary and secondary ion pass at 9 fmol/µL with failure at 27 and 83 fmol/µL ^C Primary ion meets criteria at 83 fmol/µL ^D Primary ion meets criteria at 9 fmol/µL ^F Primary ion meets criteria at 3 fmol/µL ^G Primary ion meets criteria at 27 fmol/µL						

Table 2. RDase peptides used in MRM assay

Protein Extraction and Quantification

For protein quantification, each sample was digested with trypsin and desalted using C18 spin columns. Protein extraction protocol, including protein detection with tryptophan assay and sample cleanup, has been developed for work with environmental samples and is located in **Appendix A** of this report.

Protein Concentrations in Dilution Study Samples

On average, 1 mg/mL protein was extracted in each sample. Peptide concentration data is tabulated in Excel file entitled "USACE ESTCP Dilution Study 11.15.17" attached to this report.

Only two out of three FdhA peptides, namely FdhA2 and FdhA 5, were observed in the dilution study. The FdhA8 peptide was not detected. FdhA 2 and FdhA 5 peptides were detected above method detection limit in **all** SDC-9 cell dilutions (10^4 to 10^7 DHC cells). However, their per cell concentrations were higher than reported in the literature. **Figure 1A** shows FdhA peptide concentrations per total cell number.



Figure 1. Concentration of (A) FdhA, (B) PceA, (C) TceA and (D) VcrA peptide in Dilution Study Samples

Figure 1B shows PceA peptide concentrations per total cell number. PceA5, PceA7 and PceA8 showed lower sensitivity than PceA4 peptide which was detected in 10^4 starting DHC cells. The lowest concentration of DHC cells that generated detectable and quantifiable concentrations of PceA5 and PceA7 was 10^5 , while 10^6 cells was needed to quantify PceA8 peptide. Thus, PceA4 peptide will be selected as a quantifier for the proceeding studies.

The TceA2 peptide, had highest sensitivity and was detected and quantified in samples containing 10^4 DHC cells (**Figure 1C**). This peptide will be selected as a quantifier for the proceeding studies. TceA3 peptide was detected in 10^5 DHC cell concentration and TceA4 and TceA5 were the least sensitive. These two peptides required 10^6 and 10^7 starting cell concentrations for quantification.

VcrA peptides were the least sensitive, with only VcrA3 peptide detected in 10^5 and 10^6 DHC cells (**Figure 1D**). The other two peptides, VcrA1 and VcrA4, were detected within their corresponding MDLs in 10^7 DHC cell concentration.

The analysis of the compiled data shows that the lowest concentration of DHC cells for quantification of FdhA, PceA and TceA peptides is 10^5 . However, quantification of VcrA peptides is possible when DHC concentrations of 10^6 or 10^7 are used.

Summary

Dilution study was set up to establish the minimum concentration of DHC cells required to detect FdhA, PceA, TceA and VcrA peptides using a targeted MRM assay. Prior to sample analysis, SDC-9 culture-specific RDase peptides were down selected and IDL and MDL were established for each peptide.

In this study, sample of SDC-9 culture was diluted in triplicate to 10^7 , 10^6 , 10^5 , 10^4 DHC cells and concentration of RDase and FdhA protein was analyzed using MRM proteomics.

Overall, the most sensitive peptides for quantification were FdhA5, PceA4, TceA2 and VcrA3 and required between 10^4 and 10^5 DHC cells to be detected. These peptides will serve as quantifiers in the next set of experiments. The required lowest concentration of DHC cells for detection of the reminder of peptides varied per protein, for example, to detect other TceA peptides a minimum of 10^5 cells need to be provided, but to detect VcrA specific peptides the cell concentrations need to be couple orders of magnitude higher. Thus, the total recommended DHC concentration for targeted proteomics is 10^6 cells, regardless of sample volume.

APPENDIX C

METHOD STANDARD OPERATING PROCEDURES AND CALIBRATION OF ANALYTICAL EQUIPMENT

Primer and probe design

The amino acid sequences of RDases determined in SDC-9TM metagenomic analysis were compared to other published sequences in NCBI using BLASTP (http://www.ncbi.nlm.nih.gov/BLAST), and sequences were aligned with Geneious R11.0.2 (<u>http://www.geneious.com</u>, Kearse et al., 2012). The specificity of primers and probes targeting regions of the target genes met the criteria of the Geneious R11.0.2 and the specificity of the primers and probes was also verified using BLAST analysis.

To validate each assay, primers were tested first with SYBR Green chemistry using QuantStudio 12K Flex Real-Time PCR System (Life Technologies, Grand Island, NY). The 10 μ L qPCR mixture was composed of 5 μ L of Power SYBR Green PCR Master Mix (Applied Biosystems, Foster City, CA), 300 nM of each primer, 2.0 μ L of template DNA and the remaining volume sterile nuclease-free water. The PCR cycle parameters applied were as follows: 2 min at 50°C and 10 min at 95°C, followed by 40 cycles of 15 s at 95°C and 1 min at 60°C. After amplification, a melting curve analysis was carried out to confirm that the signal obtained in SYBR Green qPCR originated from specific target PCR products, not from primer dimers or non-specific amplifications. SYBR-Green qPCR assay criteria were used to validate each assay (i.e., the efficiency of the reaction should be 90-110%; the slope of standard curve should be between -3.1 to -3.6, and R² should >0.99, respectively). Amplification efficiencies were calculated by the method of Pfaffl (2001).

Following validation and optimization of each assay with SYBR Green qPCR, the primers and probe specific to each target assay were used for TaqMan qPCR. Each 10 μ L mixture contained 5 μ L of TaqMan Universal PCR Master Mix No AmpErase UNG (Applied Biosystems, Foster City, CA), 300 nM of each primer, 300 nM of probe and 2.0 μ L of template DNA. TaqMan qPCR assays were run using QuantStudio 12K Flex Real-Time PCR System under the same PCR cycle conditions as described for SYBR Green qPCR. The target assays had amplification efficiencies between 90-110%, a standard curve slope between -3.3 to -3.6 and a standard curve with R²> 0.99. These values met the parameters suggested in literature (Holmes et al., 2006; Karlen et al., 2007; Ritalahti et al., 2009). The default instrument settings were used and LOD and LOQ values were determined as 1-10 and 10-50 copies per μ L for each assay.

Standard curve preparation: Plasmid DNA was served as templates for standard curve preparation. Template plasmid DNA (pDNA) was synthesized utilizing the pMK-RQ vector and incorporated into *E. coli* by Life Technologies (Grand Island, NY) or the target gene fragment was inserted into the pCRTM 2.1 Vector using the Invitrogen TA CloningTM kit (Life Technologies, Grand Island, NY) according to maufacturer's instructions. The *E. coli* transformant was grown in Luria Broth with ampicillin (100 mg/L) or kanamycin (50 mg/L) at 37°C overnight. pDNA was isolated using the Zymo Research ZyppyTM Plasmid Miniprep Kit (Zymo Research Corp., Irvine, CA) and quantified using a NanoDrop and the Qubit 2.0 Fluorometer.

Standard curves were included with every qPCR plate using 10-fold serial dilutions of plasmid DNA over a 7 orders of magnitude range beginning at a 1 ng μ L⁻¹ concentration (~8 log gene copies) and decreasing to 10⁻⁷ ng μ L⁻¹. All standard curves had a total of eight calibration points

and were run in triplicate. To calculate the number of gene copies in a known amount of DNA and gene copies per sample, the equations given in Ritalahti et al. (2006) were applied.



Figure 1. Example of standard curve for DHC_16S assay



Figure 2. Example of standard curve for *tceA* assay


Figure 3. Example of standard curve for *vcrA* assay



Figure 4. Example of standard curve for SDC9_24 pceA assay



Figure 5. Example of standard curve for *fdhA* assay

SHOTGUN AND TARGETED PROTEOMICS

The procedure described below has been developed and used by the Battelle Memorial Proteomics lab and is protected under the provisional patent.

Initial Discovery - Shotgun (bottom-up) Proteomics

- 1. Samples are analyzed by reverse-phase microflow HPLC-ESI-MS/MS using an Eksigent Nano 415 liquid chromatograph system (Sciex, Concord, CAN) which is directly connected to a quadrupole time-of-flight (QqTOF) TripleTOF 5600 mass spectrometer (Sciex, Concord, CAN).
- 2. The instrumentation is controlled using Analyst TF 1.6 and the Eksigent control software.
- 3. A total of 100 μ L of sample is injected onto the analytical column (Eksigent 3C18-CL-120, 3 μ m particle size, 120 Å pore size, 0.3 x 150 mm) using a trap-and-elute method. In order to achieve 100 μ L on column, 10 full loop volumes (10 μ L loop) are injected and trapped onto a Pepmap 300 cartridge (C18, 5 μ m particle size, 0.3 x 5 mm, Thermo Scientific, Rockwood, TN). Each loop injection is washed with mobile phase A.
- 4. Once fully loaded, the samples are eluted from the trap and separated. All solvent concentration changes are linear with respect to time. Mobile phase solutions are purchased from Burdick and Jackson and are as follows: mobile phase A: 0.1% formic acid (v/v) in water (LC-MS grade); and mobile phase B: 0.1% formic acid (v/v) in acetonitrile (LC-MS grade).
- 5. Continuing mass calibration of the TOF MS and TOF MS/MS is performed throughout the analysis sequence by analyzing a digested beta-galactosidase standard (Sciex, Concord, CAN). Mass spectrometric analysis is performed using data dependent acquisition (referred to as information dependent acquisitions, or IDA). Full scan spectra are acquired from 400 to 1250 m/z with a 250 millisecond acquisition time.
- 6. For collision induced dissociation tandem mass spectrometry (CID MS/MS) in IDA mode, the mass window for precursor ion selection of the quadrupole mass analyzer is set to unit resolution (\pm 0.5 m/z). For MS/MS analysis, precursor ions were fragmented in a collision cell using nitrogen as the collision gas. For IDA analysis, the instrument is set to trigger product ion scans (from 100 1500 m/z) only after specific criteria are met by the precursor ions. The Rolling Collision Energy algorithm is used to determine the appropriate collision energy for each precursor mass.

Additional Discovery plus Select Targets - Shotgun (bottom-up) Proteomics

Based on the results of the initial shotgun analysis, specific targets are identified for further investigation. These targets are divided into two groups and samples are analyzed in two separate analyses. The instrument is set up with an inclusion list of these specific targets that would automatically trigger a product ion scan if the specified precursor was detected. The instrumentation, mobile phase, LC method, and injection volume were the same as the initial discovery analysis.

Labeled Peptide Analysis

- 1. Isotopically labeled peptides are purchased from Thermo Fisher Scientific based on the results of the targeted analysis.
- 2. Individual stocks of each peptide are prepared in 0.1% formic acid. From these stocks, multiple mixed solutions are prepared at 0.1, 1.0, 10, 100, and 1000 Xmol/ μ L in order to determine the approximate detection limit of each peptide and also the instrumental linearity.
- 3. Two test samples that were previously analyzed are split and spiked at a final on-column concentration of 200 fmol. Using these samples, 90 minute is udes for all further analysis. All instrumentation, mobile phase, and injection volumes were the same as the initial discovery analysis

Shotgun with Peptide Targets

Test samples are split and spiked with each labeled peptide. These samples are analyzed using the 90 minute gradient for specific CVOC targets plus any additional discovery data that may have been missed on the first initial analyses. The instrumentation, mobile phase, LC method, and injection volume were the same as the labeled peptide analysis.

MRMHR for MTBE Quantification

- 1. A mass spectrometric method will be built to perform product ion scans of the specific targets plus associated labeled peptides that were previously purchased. The analysis is performed using a 15 minute gradient, with a total runtime of 16 minutes, including mobile phase equilibration. The samples will be spiked with both labeled peptides for a final concentration of X mol on column. The instrumentation, mobile phase, and LC method are the same as the labeled peptide analysis.
- Integrated reconstructed ion chromatograms of precursor-product ion transitions of both the labeled and un-labeled peptide targets are produced using MultiQuant software version 2.1 (Sciex, Concord, CAN). Multiple precursor-product ion transitions are plotted to add confidence to the tentative target detections.

3. Using the response of each labeled peptide and its spiked concentration, a response factor is calculated. These calculated response factors are used for quantification of the unlabeled peptide targets.

CALLIBRATION OF AB SCIEX TripleTOF® 5600/5600+ INSTRUMENT

For tuning the system, use the following solutions that come with the installation kit:

For positive mode:

• For optimizing TOF MS - MSMS high resolution or MSMS High Sensitivity, use the Tuning Solution.

• For Q1calibration, use the PPG POS solution.

In negative mode:

• For optimizing TOF MS - MSMS High Resolution or MSMS High Sensitivity, use Taurocholic acid.

• For Q1calibration, use the PPG 3000 solution.

Required material

• Tuning solutions that are supplied in the Standards Chemical Kit shipped with the system. If needed, a new Kit can be ordered from AB SCIEX.

• Gas-tight syringes (1.0 ml is recommended)

• PEEK (red) sample tubing

Prerequisites

- Make sure that a printer is configured.
- Make sure that the spray is stable and that the proper tuning solution is being used.

Optimize the Instrument

The following procedure shows how to verify the performance of the instrument.

1. In the Navigation bar, under Tune and Calibrate, double-click Manual Tuning.

2. Run a TOF MS or Product ion scan type and confirm that there is a stable TIC and that the peaks of interest are present in the spectrum.

3. In the Navigation bar, under Tune and Calibrate, double-click Instrument

Optimization.

Note: AB SCIEX recommends that after using the Taurocholic acid, repeat the channel alignment using the PPG 3000 solution.

4. Select a tuning solution. Make sure that the tuning solution matches the reference table.

5. The Verify Performance Only check box is preselected. Click Next.

For this example, leave this option selected. If the report indicates that the instrument needs tuning, then run Instrument Optimization again and select one or more scan modes to optimize. Make sure that the ion source and syringe parameters are suitable.

7. Click GO.

The Verifying Performance screen appears. After the process has completed, the Results Summary appears showing the resolution and intensity for each scan mode.

Example of continuing calibration method with beta galactosidase is detailed in Table A1. Figures A1 and A2 show reference table editor for the opening calibration with tuning solution. And beta-galactosidase. The editor references the compounds and masses used during calibration.

_

HPLC	
Mass Spectrometer	Eksigent Nano 415
	AB Sciex 5600+ Triple ToF
Mass Spec Source	Electrospray, positive ion mode
Mass Spec Parameters	Experiment 1: Scan Type: ToF MS ToF Mass Range: 400 - 1500 Da Accumulation Time: 0.250 seconds
	Experiment 2: Scan Type: Product Ion Products of: 729.37 Da ToF Mass Range: 100-1500 Da Accumulation Time: 0.500 seconds
HPLC Column	Eksigent 3C18-CL-120, 3 µm, 120 A, 0.3 x 150 mm
Column Temperature	30° c
Mobile Phase Components	A=0.1% formic acid inwater B= 0.;% formic acid in methanol
Gradient Profile	All changes are linear with respect to time: $1.$ T $\%8$ Flow rate,ime. $$ 0 5 5 1 5 $0.$ 5 $$ 8 35 $3.$ 5 $$ 9 90 $6.$ 5 $$ 11 90 $9.$ 5 $$ 12 5 $2.$ 5 5
Injection Volume	1μ L (Trap and Elute, 5 minute wash with Mobile Phase A at 5μ L/min)
Run Time	16 min

Table H1. Continuing calibration method with beta-galactosidase.

Referen	nce Tabl	le Editor											X
<u>N</u> ame: Refere	APCI Pos	iitive Calibration Solution i for TOF MS Calibrati	ion:	▼ Ne	w Copy	y Deleta	e Positive	CN	legative Refere (Produc	Calibra ence Ions t of 609.28	ation Valve Position: for MS/MS Calibrat 3066 Da)	4 💌	
	Use	Compound Name	Precursor m/z (Da)	Use for MS/MS	CE for MS/MS	DP for MS/MS	Retention Time (min)			Use	Fragment Name	Fragment m/z (Da)	
1	N	aminoheptanoic acid	146.11756		30.000	80.000	0.00	-	1	V	C11H12NO	174.09130	
2	2	amino-dPEG 4-acid	266.15981		30.000	80.000	0.00		2	V	C10H11O4	195.06520	1
3	V	clomipramine	315.16225		27.000	80.000	0.00		3	V	C13H18NO3	236.12810	1
4	N	amino-dPEG 6-acid	354.21224		30.000	80.000	0.00		4	V	C22H25N2O3	365.18600	1
5	N	amino-dPEG 8-acid	442.26467		30.000	80.000	0.00		5	N	C23H29N2O4	397.21220	1
6	N	reserpine	609.28066	N	45.000	80.000	0.00		6	N	C23H30NO8	448.19660	1
7	N	amino-dPEG 12-acid	618.36953		30.000	80.000	0.00		7	N	C33H40N2O9	609.28066	
8	V V	Hexakis(2,2,3,3-tetra	922.00980		30.000	80.000	0.00		8				
9	Г	Hexakis(1,1,5-octafl	1521.97148		30.000	80.000	0.00		9				
10	Г								10				
11			1						11				
12			1						12				
13								1000	13				1000
14		1							114		1		
Retenti	on time is d	only used for non-CDS o	onfiguration.	Retentio	on Time Tole	rance: +/-	0.000 se	:c Help					

Figure H1. Reference table editor for the opening calibration with tuning solution. The editor references the compounds and masses used during calibration. Not all compounds are used and have a check mark if the mass is used for calibration.

Refere	nce Tabl	e Editor											×
<u>N</u> ame: Refere	Beta Gala	actosidase Digest	ion:	▼ Ne	w Cop	y Delete	e 🛛 📀 Positive	C	legative Refer	Calibra	ation Valve Position:	a 🗸	
									(Produ	ct of 729.3	6520 Da)		
	Use	Compound Name	Precursor m/z (Da)	Use for MS/MS	CE for MS/MS	DP for MS/MS	Retention Time (min)	^		Use	Fragment Name	Fragment m/z (Da)	
1		WLPAMSER	495.24730		24.000	100.000	6.75	-	1		y1	175.11900	
2	Г	YSQQQLMETSHR	503.23680		27.000	100.000	9.11		2	N	y3	347.20370	
3		RDWENPGVTQLNR	528.93410		25.000	100.000	13.40		3	V V	y5	563.27840	
4	Г	WVGYGQDSR	534.24890		23.000	100.000	9.65		4			729.36520	
5	V	GDFQFNISR	542.26450		26.000	100.000	8.00		5	V	y8	832.45230	
6	V	IDPNAVWER	550.28020		27.000	100.000	7.67		6	N	y10	1061.52220	
7	Г	DVSLLHKPTTQISDF	567.05510		30.000	100.000	13.31		7	V	y12	1289.63320	
8	V	VDEDQPFPAVPK	671.33790		33.000	100.000	7.50		8			1	
9	V V	WENPGVTQLNR	714.84690		32.000	100.000	7.50		9				
10	V	APLDNDIGVSEATR	729.36520	v	48.000	100.000	6.99		10				
11									11				
12									12				
13								122	13				1000
14		1		F					14		1		
Retenti	on time is o	only used for non-CDS o	onfiguration.	Retenti	on Time Tole	rance: +/- Cancel	180.000 se	e Help					

Figure H2. Reference table editor for the opening calibration with betagalactosidase. The editor references the compounds and masses used during calibration. Not all compounds are used and have a check mark if the mass is used for calibration.

APPENDIX D *MICROCOSM ANALYTICAL AND BIOMARKER ABUNDANCE DATA*

SET 1	Fo	rt Lewis JB!	лL.	Start 7/18/2	017 9:30 A	M																							
108 DHC/	nL																												
								VOC's ug/	Ĺ				Meth	nane/Ethene	ug/L			A	nions mg/L						VFA mg/L				
DATE	TIME (hrs)	Bottle	pH	mean/SD	ATL ID	VC	Q	mean	cDCE	Q	mean	Methane	Q	mean	Ethene	Q	mean	Bromide	Q	mean	Lactic	Q	mean	Acetic	Q	mean	Proprionic	Q	mean
		1A	6.87			1060	D		3100	D		9.45			19.8			9.84			243	D		77.7	D		3.7	U	
7/18/17 9:30	0	1B	6.76	6.88	9721	938	D	1093	3090	D	2787	9.35		9.87	21.16		26.82	9.25		9.70	276	D	250.33	77.1	D	51.91	3.7	U	3.70
		1C	7.01	0.13		1280	D	173.32	2170	D	534.07	10.8		0.81	39.5		11.00	10.0		0.40	232.0	D	22.90	0.93	U	44.15	3.7	U	0.00
		1A	7.23			2230	D		301	D		32.7			133			9.05			252	D		0.93	U		3.7	U	
7/18/17 10:30	1	1B	7.26	7.26	9721	2320	D	2183	465	D	269	30.5		37.27	130		164.00	8.58		8.66	250	D	249.67	65.6	D	51.91	24.9	D	10.77
		1C	7.28	0.03		2000	D	165.03	41	U	213.80	48.6		9.88	229		56.31	8.35		0.36	247	D	2.52	89.2	D	45.70	3.7	U	12.24
		1A	7.19			1450	D	_	41	U		156		_	430			7.86		_	160	D	_	20.3	D		3.7	U	
7/18/17 11:30	2	1B	7.45	7.38	9721	1620	D	1447	41	U	41.00	158		167.00	456		472.00	7.56		7.65	198	D	166.33	0.93	U	27.38	3.7	U	12.43
		1C	7.49	0.16		1270	D	175.02	41	U	0.00	187		17.35	530		51.88	7.53		0.18	141	D	29.02	60.9	D	30.60	29.9	D	15.13
		1A	7.16			163	J	_	41	U		594		-	896			7.77		-	188	D		28.9	D		3.7	U	
7/18/17 13:30	4	1B	7.4	7.36	9721	182	J	145	41	U	41.00	504		559.00	844		867.67	7.51		7.73	230	D	196.67	84.6	D	49.13	3.7	U	9.00
		1C	7.52	0.18		88.6	J	49.36	41	U	0.00	579		48.22	863		26.31	7.91		0.20	172	D	29.96	33.9	D	30.82	19.6	JD	9.18
		1A	7.18			53	U		41	U		1130			1000			8.16		-	175	D		25.3	D		27.7	D	
7/18/17 15:30	6	1B	7.47	7.39	9721	53	U	53.00	41	U	41.00	940		1026.67	937		931.33	7.29		7.72	185	D	186.67	69.0	D	39.10	3.7	U	11.70
		1C	7.52	0.18		53	U	0.00	41	U	0.00	1010		96.09	857		71.67	7.71		0.44	200	D	12.58	23	D	25.92	3.7	U	13.86
		1A	7.38			53	U		41	U		1340			823			7.56		_	149	D		38.6	D		25.3	D	
7/18/17 17:30	8	1B	7.46	7.43	9721	53	U	53.00	41	U	41.00	1290		1343.33	855		830.67	7.12		7.40	106	D	128.67	56.8	D	44.20	24.5	D	26.60
		1C	7.46	0.05		53	U	0.00	41	U	0.00	1400		55.08	814		21.55	7.53		0.25	131	D	21.59	37.2	D	10.93	30.0	D	2.97
		1A	6.90			53	U	_	41	U	-	5200			912			7.79		-	34.6	D		75.9	D		63.2	D	
7/19/17 9:30	24	1B	6.98	6.94	9721	53	U	53.00	41	U	41.00	5180		5153.33	901		863.00	7.88		7.80	2.23	U	14.62	62.9	D	99.93	51.1	D	67.00
		1C	6.95	0.04		53	U	0.00	41	U	0.00	5080		64.29	776		75.54	7.74		0.07	7.02	JD	17.47	161	D	53.28	86.7	D	18.10

SET 2	Fo	rt Lewis JBN	۹L.	Start 7/18/2	017 9:45 A	М																							
107 DHC/r	ıL																												
								VOC's ug/					Meth	ane/Ethene	ug/L			A	Anions mg/	L					VFA mg/L				
DATE	TIME (hrs)	Bottle	pН	mean	ATL ID	VC	Q	mean	cDCE	Q	mean	Methane	Q	mean	Ethene	Q	mean	Bromide	Q	mean	Lactic	Q	mean	Acetic	Q	mean	Proprionic	Q	mean
		2A	7.51			22.7	J		4730	D		3.41			0.44	U		9.28			261	D		0.93	U		3.7	U	
7/18/17 9:45	0	2B	7.67	7.62	9721	52.1	J	46	4470	D	4473	3.15		3.29	0.44	U	0.44	9.35		9.32	197	D	210.00	0.93	U	0.93	3.7	U	3.70
		2C	7.67	0.09		62.6	J	21	4220	D	255	3.31		0.13	0.44	U	0.00	9.32		0.04	172	D	45.90	0.93		0.00	4		0.00
		2A	7.89	_		828	D	_	2450	D		28.9			15.2		_	8.25			160	D	_	0.93	U	-	3.7	U	
7/18/17 17:45	8	2B	8.04	7.99	9721	851	D	879	2540	D	2467	28.7		28.87	15.2		15.07	7.99		8.32	159	D	171.33	0.93	U	0.93	3.7	U	3.70
		2C	8.04	0.09		958	D	69	2410	D	67	29.0		0.15	14.8		0.23	8.73		0.38	195	D	20.50	0.93	U	0.00	3.7	U	0.00
		2A	7.50	_		1930	D	_	1030	D	_	115			76.7		_	7.97			197	D	_	0.93	U	-	3.7	U	
7/19/17 9:45	24	2B	7.61	7.56	9721	1720	D	1867	902	D	873	114		113.33	77.9		78.17	8.46		8.20	159	D	181.67	0.93	U	0.93	3.7	U	3.70
		2C	7.58	0.06		1950	D	127	686	D	174	111		2.08	79.9		1.62	8.17		0.25	189	D	20.03	0.93	U	0.00	3.7	U	0.00
		2A	7.33			2550	D	_	41	U		182			228		_	8.07			265	D	_	24.8	D	_	3.7	U	
7/20/17 9:45	48	2B	7.58	7.50	9724	2270	D	2163	41	U	41	186		178.67	242		233.00	8.07		8.11	465	D	341.67	22.4	D	28.30	11.9	JD	7.33
		2C	7.60	0.15		1670	D	450	41	U	0	168		9.45	229		7.81	8.18		0.06	295	D	107.86	37.7	D	8.23	6.38	JD	4.18
		2A	7.58			1510	D	_	41	U		285			431		_	7.95			271	D	_	26.9	D	_	7.21	JD	
7/21/17 9:45	72	2B	7.60	7.60	9724	1230	D	1320	41	U	41	274		278.33	426		428.00	8.12		8.02	278	D	282.33	26.6	D	30.73	9.83	JD	8.68
		2C	7.63	0.03		1220	D	165	41	U	0	276		5.86	427		2.65	7.99		0.09	298	D	14.01	38.7	D	6.90	8.99	JD	1.34
		2A	7.21			721	D	_	41	U		462			581		_	7.46			212	D	_	41.8	D	_	38.9	D	
7/22/17 9:45	96	2B	7.24	7.23	9724	573	D	597	41	U	41	549		503.00	678		617.00	7.97		7.84	229	D	209.67	66.2	D	60.67	48.9	D	49.50
		2C	7.23	0.02		496	D	114	41	U	0	498		43.71	592		53.11	8.1		0.34	188	D	20.60	74.0	D	16.80	60.7	D	10.91
		2A	6.93			81.5	JD	_	41	U		1010			779		_	7.62			2.23	U	_	79.6	D	_	166	D	
7/23/17 9:45	120	2B	6.98	6.97	9724	53	U	63	41	U	41	927		959.33	708		716.33	7.99		8.02	2.23	U	2.23	110	D	98.87	145	D	154.00
		2C	7.01	0.04		53	U	16	41	U	0	941		44.43	662		58.94	8.45		0.42	2.23	U	0.00	107	D	16.75	151	D	10.82

SET 3	Fo	rt Lewis JB!	ML	START		7/18/17 10:55																							
10 ⁶ DHC/m	L							VOC's ug/I					Metha	ne/Ethe ne	ug/L			1	Anions mg/l	Ĺ					VFA mg/L				
								VOC's ug/I	_				Metha	ne/Ethe ne	ug/L			1	Anions mg/l	Ĺ					VFA mg/L				
DATE	TIME (days)	Bottle	pH	mean	ATL ID	VC	Q	mean	cDCE	Q	mean	Methane	Q	mean	Ethene	Q	mean	Bromide	Q	mean	Lactic	Q	mean	Acetic	Q	mean	Proprionic	Q	mean
		3A	7.62			53	U		4560	D		3.03			0.44	U		9.08			152	D		0.93	U		3.7	U	
7/18/17 10:55	0	3B	7.77	7.74	9721	53	U	53.00	4680	D	4427	3.45		2.97	0.44	U	0.44	8.98		9.17	180	D	180.67	0.93	U	0.93	3.7	U	3.70
		3C	7.84	0.11		53	U	0	4040	D	340	2.44		0.51	0.44	U	0.00	9.44		0.24	210	D	29.01	0.93	U	0.00	3.7	U	0.00
		3A	7.17			159	JD		4040	D		13.3			0.44	U		9.47			196	D		45.4	D		100	D	
7/24/17 9:00	5.9	3B	7.50	7.31	9742	67.6	JD	124.87	4020	D	3963.33	10.8		12.20	0.44	U	0.44	8.77		8.94	296	D	219.00	22.9	D	33.07	13.7	JD	57.80
		3C	7.25	0.17		148	D	49.89843	3830		115.9023	12.5		1.28	0.44	U	0.00	8.57		0.47	165	D	68.46	30.9	D	11.41	59.7	D	43.18
		3A	6.97			64.8	JD		2700	D		63.3			0.44	U		8.07			2.23	U		114	D		220	D	
7/27/17 9:00	8.9	3B	6.92	7.00	9726	61.2	JD	84.67	3050	D	2956.67	63.6		64.93	0.44	U	0.44	8.69		8.48	2.23	U	2.23	121	D	119.67	226	D	225.00
		3C	7.10	0.09		128	JD	37.57091	3120	D	225.0185	67.9		2.57	0.44	U	0.00	8.69		0.36	2.23	U	0.00	124	D	5.13	229	D	4.58
		3A	7.00			577	D		3180	D		145			2.42			9.46			2.23	U		187	D		170	D	
7/31/17 9:00	12.9	3B	7.06	7.04	9727	323	D	474.33	3430	D	3260.00	271		200.00	1.08	J	1.99	9.34		9.25	1.16	U	1.52	109	D	129.67	120	D	158.33
		3C	7.07	0.04		523	D	133.8108	3170	D	147.3092	184		64.51	2.47		0.79	8.96		0.26	1.16	U	0.62	93	D	50.29	185	D	34.03
		3A	6.97			695	D		3050	D		227			4.61		_	8.60			1.16	U		108	D		195	D	
8/3/17 9:00	15.9	3B	6.98	6.99	9728	433	D	595.67	3320	D	3073.33	300		262.00	1.73	J	3.39	8.33		8.35	1.16	U	1.16	101	D	101.60	186	D	188.67
		3C	7.02	0.03		659	D	142.0188	2850	D	235.8672	259		36.59	3.84		1.49	8.12		0.24	1.16	U	0.00	95.8	D	6.12	185	D	5.51
		3A	7.12			932	D	_	2810	D		273			9.9			8.50			1.12	U		76	D		138	D	
8/7/17 9:00	19.9	3B	7.10	7.13	9730	529	D	774.00	3120	D	2793.33	334		297.00	2.97	J	6.78	8.23		8.30	1.12	U	1.12	100	D	91.00	184	D	166.67
		3C	7.16	0.03		861	D	215.1255	2450	D	335.3108	284		32.51	7.46		3.52	8.18		0.17	1.12	U	0.00	97	D	13.08	178	D	25.01
		3A	7.05	_		977	D		2410	D		225			11.1		_	7.52			1.12	U		90.6	D	_	164	D	
8/10/17 9:00	22.9	3B	7.05	7.06	9734	586	D	849.00	2840	D	2490.00	268		234.33	3.30		7.90	7.97		7.76	1.12	U	1.12	102	D	93.60	187	D	176.00
		3C	7.07	0.01		984	D	227.7916	2220	D	317.6476	210		30.11	9.29		4.08	7.78		0.23	1.12	U	0.00	88.2	D	7.37	177	D	11.53
		3A	7.06	_		1110	D	_	2210	D		228			17.5		_	6.94			1.12	U	_	91.5	D	_	164	D	
8/14/17 9:40	26.9	3B	7.12	7.12	9735	740	D	1000.00	2750	D	2290.00	154		201.00	2.88	J	12.49	6.98		6.99	1.12	U	1.12	101	D	97.50	183	D	175.67
		3C	7.18	0.06		1150	D	226.0531	1910	D	425.6759	221		40.85	17.1		8.33	7.04		0.05	1.12	U	0.00	100	D	5.22	180	D	10.21
		3A	7.06	_		1820	D	_	1760	D	_	199			0.37	U	_	7.25			1.12	U	_	108	D	_	208	D	
8/23/17 9:00	35.9	3B	7.08	7.08	9738	1250	D	1566.67	2250	D	1733.33	210		199.33	0.37	U	0.37	7.42		7.44	1.12	U	1.12	115	D	113.33	221	D	219.00
		3C	7.09	0.02		1630	D	290.2298	1190	D	530.5029	189	(10.50	0.37	U	0.00	7.66		0.21	1.12	U	0.00	117	D	4.73	228	D	10.15
		3A	7.09	_		1770	D	_	600	D	_	146			75.5		_	7.04			1.12	U	_	78	D	_	170	D	
9/11/17 9:00	54.9	3B	7.00	7.05	9739	1390	D	1576.67	1250	D	776.00	248		209.67	33.1		92.53	7.13		7.05	1.12	U	1.12	74.1	D	98.03	177	D	221.00
		3C	7.06	0.05		1570	D	190.0877	478	D	415.0036	235		55.52	169		69.53	6.99		0.07	1.12	U	0.00	142	D	38.13	316	D	82.35
		3A	7.48			1820	D		41	U		241			168			5.35		_	1.16	U		103	D	_	213	D	
10/9/17 10:00	83.0	3B	7.44	7.46	9752	1690	D	1663.33	340	D	140.67	188		195.33	100		160.00	5.25		5.34	1.16	U	1.16	96.7	D	102.23	208	D	214.33
		3C	7.46	0.02		1480	D	171.5615	41	U	172.6277	157		42.48	212		56.43	5.42		0.09	1.16	U	0.00	107	D	5.19	222	D	7.09

SET 4	Fo	rt Lewis JBM	/IL	START		7/18/17 11:50																							
10 ⁵ DHC/mL								VOC's ug/I					Met	hane/Ethen	e ug/L			Α	nions mg/I	L					VFA mg/L				
								VOC's ug/I	_				Met	hane/Ethen	e ug/L			A	nions mg/I	L					VFA mg/L				
DATE	TIME(days)	Bottle	pН	mean	ATL ID	VC	Q	mean	cDCE	Q	mean	Methane	Q	mean	Ethene	Q	mean	Bromide	Q	mean	Lactic	Q	mean	Acetic	Q	mean	Proprionic	Q	mean
		4A	7.80	_		53	U		4380	D		5.43			2.89		_	9.13			298	D		39.4	D		3.7	U	_
7/18/17 10:55	0	4B	7.81	7.80	9721	53	U	53.00	4470	D	4480	3.29		3.74	0.44	U	1.26	9.06		9.20	194	D	238.00	29.4	D	40.50	3.7	U	3.70
		4C	7.78	0.02		53	U	0.00	4590	D	105.36	2.51		1.51	0.44	U	1.41	9.40		0.18	222	D	53.81	52.7	D	11.69	3.7	U	0.00
		4A	7.70			53	U		4500	D		2.07			0.44	U		8.77			337	D		10.2	JD		3.7	U	
7/24/17 10:00	5.9	4B	7.94	7.88	9742	53	U	53.00	5110	D	4580.00	1.88		1.95	0.44	U	0.44	8.74		8.71	311	D	333.00	11.8	JD	13.97	3.7		3.70
		4C	7.99	0.16		55	U	0.00	4130	D	494.87	1.9		0.10	0.44	U	0.00	8.62		0.08	351	D	20.30	19.9	JD	5.20	5.7		0.00
7/21/17 10:00	12.0	4A 4P	6.95	6.00	0727	52.9	TT.	52.80	4560	D	4200.00	2.51		2.07	0.44	II	0.44	9.61		0.02	1.16	T	1.70	150	D	142.50	147	D	170.50
//31/17 10:00	12.9	4B 4C	6.04	0.90	9121	52.8	U	0.00	4040	D	367.70	2.62		0.63	0.44	U	0.00	0.01		9.03	2.23	U	0.76	130	D	10.61	212		45.96
		44	0.74	0.00		52.0	0	0.00	1010	D	507.70	2.02		0.05	0.44	0	0.00	7.45		0.57	2.23	0	0.70	155	D	10.01	212		45.70
8/7/17 10:00	19.9	4B	6.97	6.99	9730	52.8	U	52.80	4420	D	4190.00	33.4		32.45	0.44	U	0.44	8.40		8.40	1.12	U	1.12	108	D	104.50	194	D	188.50
		4C	7.01	0.03		52.8	U	0.00	3960	D	325.27	31.5		1.34	0.44	U	0.00	8.39		0.01	1.12	U	0.00	101	D	4.95	183	D	7.78
		4A																											
8/14/17 10:40	27.0	4B	6.98	7.02	9735	52.8	U	52.80	4310	D	4065.00	57.5		63.75	0.44	U	0.44	7.54		7.54	1.12	U	1.12	110	D	119.50	196	D	208.00
		4C	7.06	0.06		52.8	U	0.00	3820	D	346.48	70.0		8.84	0.44	U	0.00	7.54		0.00	1.12	U	0.00	129	D	13.44	220	D	16.97
		4A																											
8/23/17 11:00	36.0	4B	7.03	7.04	9738	90.7	J	102.85	2930	D	3235.00	62.3		68.80	0.44	U	0.44	6.86		7.47	1.12	U	1.12	104	D	119.00	188	D	219.50
		4C	7.05	0.01		115	J	17.18	3540	D	431.34	75.3		9.19	0.44	U	0.00	8.07		0.86	1.12	U	0.00	134	D	21.21	251	D	44.55
		4A																						1.40					
9/11/17 10:00	54.9	4B	7.08	7.09	9739	177	J	164.50	3940	D	3645.00	86.5		95.75	0.44	U	0.44	7.52		7.50	1.12	U	1.12	169	D	131.00	369	D	292.50
-		4C	7.09	0.01		152	J	1/.68	5550	D	417.19	105		13.08	0.44	U	0.00	/.4/		0.04	1.12	U	0.00	93	D	53.74	216	0	108.19
10/0/17 10:20	82.0	4A 4D	7.26	7.22	0752	220	D	220.00	2020	D	2705.00	76.1		80.05	0.44	II	0.44	5.08		6.08	1.16	T	1.16	99.1	D	100.05	174	D	205.00
10/9/17 10:30	04.9	40 4C	7.20	0.09	9/32	239	I I	220.00	2560	D	332.34	102		18 31	0.44	U U	0.44	6.18		0.08	1.10	U	0.00	130	D	20.63	236		43.84
		4L	1.39	0.09		201	J	20.87	2000	D	552.34	102		18.31	0.44	U	0.00	0.18		0.14	1.10	U	0.00	130	D	29.03	230	D	43.84

SET 5	Fo	ort Lewis JB!	ML	START		7/18/17 12:30																				í.			
Live Control								VOC's ug/	L				Met	hane/Ethene	e ug/L			1	nions mg/	L					VFA mg/L	-			
								VOC's ug/	L				Met	hane/Ethene	e ug/L			A	nions mg/	L					VFA mg/L				
DATE	TIME (days)	Bottle	pH	mean	ATL ID	VC	Q	mean	cDCE	Q	mean	Methane	Q	mean	Ethene	Q	mean	Bromide	Q	mean	Lactic	Q	mean	Acetic	Q	mean	Proprionic	Q	mean
		5A	7.79			53	U		4010	D		3.12			0.44	U		8.97			254	D		76.6	D		3.7	U	
7/18/17 12:30	0	5B	7.88	7.86	9721	53	U	53.00	4630	D	4030	2.82		2.98	0.44	U	0.44	9.56		9.18	292	D	294.33	0.93	U	40.48	3.7	U	3.70
		5C	7.92	0.07		53	U	0	3450	D	590	2.99		0.150	0.44	U	0	9.02		0.33	337	D	41.55	43.9	D	37.95	3.7	U	0.00
		5A	7.60			53	U		4220	D		1.97			0.44	U		8.76			388	D		21.2	D		3.7	U	
7/24/17 11:00	5.9	5B	7.99	7.88	9742	53	U	53.00	4310	D	4197	0.95	U	1.67	0.44	U	0.44	8.74		8.76	336	D	340.67	17.4	D	17.83	3.7	U	3.70
		5C	8.06	0.25		53	U	0	4060	D	127	2.09		0.626	0.44	U	0	8.79		0.03	298	D	45.18	14.9	JD	3.17	3.7	U	0.00
		5A	7.65			75.5	U		2590	D		3.11			0.44	U		8.78			288	D		19.7	JD		3.7	U	
7/27/17 11:00	8.9	5B	8.05	7.93	9726	75.5	U	75.50	1540	D	2507	1.93		· 223	0.44	U	0.44	8.72		8.72	341	D	305.67	15.7	JD	16.60	3.7	U	3.70
		5C	8.08	0.24		75.5	U	0	3390	D	928	1.65		0.775	0.44	U	0	8.67		0.06	288	D	30.60	14.4	JD	2.76	3.7	U	0.00
		5A	7.75	1		52.8	U		4070	D		1.73		1	0.44	U	1	8.45			358	D	1	0.47	U		1.85	U	
7/31/17 11:00	12.9	5B	7.88	7.88	9727	52.8	U	52.80	4120	D	3987	1.15		1.52	0.44	U	0.44	8.47		8.45	256	D	313.33	0.93	U	0.78	3.70	U	3.08
		5C	8.02	0.14		52.8	U	0.00	3770	D	189	1.68		0.321	0.44	U	0	8.42		0.03	326	D	52.17	0.93	U	0.27	3.70	U	1.07
		5A	7.41			52.8	U		5000	D		1.95			0.44	U		8.62			332	D		0.47	U		1.85	U	
8/3/17 11:00	15.9	5B	7.82	7.71	9728	52.8	U	52.80	4210	D	4360	2.07		2.04	0.44	U	0.44	8.59		8.57	349	D	339.33	0.47	U	0.47	1.85	U	1.85
		5C	7.91	0.27		52.8	U	0.00	3870	D	580	2.1		0.079	0.44	U	0	8.49		0.07	337	D	8.74	0.47	U	0.00	1.85	U	0.00
		5A	7.33			52.8	U		4030	D		1.79			0.44	U		8.55			322	D		0.47	U		1.85	U	
8/7/17 11:00	19.9	5B	7.68	7.65	9730	52.8	U	52.80	4020	D	3953	1.68		1.63	0.44	U	0.44	7.96		8.16	342	D	324.67	0.47	U	0.47	1.85	U	1.85
		5C	7.95	0.31		52.8	U	0.00	3810	D	124	1.42		0.19	0.44	U	0	7.96		0.340637	310	D	16.17	0.47	U	0.00	1.85	U	0.00
		5A	7.47			52.8	U		3890	D		1.98			0.44	U		8.14			320	D		0.47	U		1.85	U	
8/10/17 11:00	22.9	5B	7.88	7.75	9734	52.8	U	52.80	4020	D	3867	1.31		1.54	0.44	U	0.44	8.86		8.27	342	D	329.00	0.47	U	0.47	1.85	u	1.85
		5C	7.89	0.24		52.8	U	0.00	3690	D	166	1.34		0.378462	0.44	U	0	7.80		0.541233	325	D	11.53	0.47	U	0.00	1.85	U	0.00
		5A	7.05			52.8	U		3730	D		1.89			0.44	U		7.34			329	D		0.47	U		1.85	U	
8/14/17 13:00	27.0	5B	7.77	7.57	9735	52.8	U	52.80	3870	D	3673	1.66		1.87	0.44	U	0.44	7.47		7.41	301	D	326.67	0.47	U	0.47	1.85	U	1.85
		5C	7.88	0.45		52.8	U	0.00	3420	D	230	2.05		0.196044	0.44	U	0	7.43		0.066583	350	D	24.58	0.47	U	0.00	1.85	U	0.00
		5A	7.35			52.8	U		3510	D		3.01			0.44	U		7.82			418	D		0.47	U		1.85	U	
9/11/17 11:00	54.9	5B	7.73	7.60	9739	52.8	U	52.80	4020	D	3657	2.94		2.83	0.44	U	0.44	7.86		7.75	379	D	392.33	0.47	U	0.47	1.85	U	1.85
		5C	7.72	0.22		52.8	U	0.00	3440	D	317	2.53		0.259294	0.44	U	0	7.57		0.157162	380	D	22.23	0.47	U	0.00	1.85	U	0.00
		5A	7.77			52.8	U		3160	D		2.77			0.44	U		6.32			329	D		84.3	D		1.85	U	
10/9/17 12:00	83.0	5B	7.94	7.88	9752	52.8	U	52.80	3130	D	3047	1.69		2.14	0.44	U	0.44	5.90		6.15	485	D	391.33	0.47	U	28.41	1.85	U	1.85
		5C	7.94	0.10		52.8	U	8.7E-15	2850	D	171	1.95		0.563678	0.44	U	0	6.22		0.219393	360	D	82.59	0.47	U	48.40	1.85	U	0.00

SET 6	Fo	rt Lewis JB!	ML	START		7/18/17 14:00																							
Killed Cont	rol							VOC's ug/l	L				Met	hane/Ethe n	e ug/L			A	Anions mg/	L					VFA mg/L				
								VOC's ug/l	L				Met	hane/Ethe n	e ug/L			A	Anions mg/	L					VFA mg/L				
DATE	TIME (days)	Bottle	pH	mean	ATL ID	VC	Q	mean	cDCE	Q	mean	Methane	Q	mean	Ethene	Q	mean	Bromide	Q	mean	Lactic	Q	mean	Acetic	Q	mean	Proprionic	Q	mean
		6A	6.60			53	U		3450	D		2.95			0.44	U		8.13			331	D		33.4	D		3.7	U	
7/18/17 14:00	0	6B	6.59	6.59	9721	53	U	53.00	2810	D	3293.33	3.23		3.28	0.44	U	0.44	6.61		7.85	317	D	334.00	63.1	D	38.13	3.7	U	3.70
		6C	6.58	0.01		53	U	0.00	3620	D	427.12	3.66		0.36	0.44	U	0.00	8.81		1.13	354	D	18.68	17.9	D	22.97	3.7	U	0.00
		6A	6.93			53	U		4570	D		1.74			0.44			7.84			298	D		14.9	JD		3.7	U	
7/24/17 12:00	5.9	6B	6.94	6.93	9742	53	U	53.00	4250	D	4433.33	1.69		1.66	0.44		0.44	8.22		8.09	359	D	343.00	0.93	U	5.59	3.7	U	3.70
		6C	6.93	0.01		53	U	0.00	4480	D	165.03	1.55		0.10	0.44		0.00	8.20		0.21	372	D	39.51	0.93	U	8.07	3.7	U	0.00
		6A	6.92			× 75.5	×		3700	D		1.73		1	0.44	U		8.43		1	384	D		0.93	U		3.7	U	
7/27/17 12:00	8.9	6B	6.94	6.94	9726	75.5	U	75.50	1520	D	2633.33	1.09		1.49	0.44	U	0.44	8.97		8.70	357	D	343.67	0.47	U	0.78	1.85	U	3.08
		6C	6.96	0.02		75.5	ι.	0.00	2680	D	1090.75	1.66		0.35	0.44	U	0.00	8.70		0.27	290	D	48.40	0.93	U	0.27	3.7	U	1.07
		6A	6.98			52.8	U		4230	D		1.71		1	0.44	U		9.87			357	D		130	D		1.85	U	
7/31/17 12:00	12.9	6B	6.96	6.97	9727	52.8	U	52.80	4080	D	4113.33	1.34		1.49	0.44	U	0.44	9.17		9.26	321	D	346.67	27.9	D	56.90	3.7	U	3.08
		6C	6.98	0.01		52.8	U	0.00	4030	D	104.08	1.43		0.19	0.44	U	0.00	8.73		0.57	362	D	22.37	12.8	D	63.76	3.7	U	1.07
		6A	6.96			52.8	U		4290	D		2.21		1	0.44	U		8.92			317	D		103	D		1.85	U	
8/3/17 12:00	15.9	6B	6.98	6.97	9728	52.8	U	52.80	4170	D	4066.67	0.19	U	1.30	0.44	U	0.44	8.31		8.47	356	D	344.33	24.1	D	48.87	1.85	U	1.85
		6C	6.98	0.01		52.8	U	0.00	3740	D	289.19	1.51		1.03	0.44	U	0.00	8.18		0.40	360	D	23.76	19.5	D	46.94	1.85	U	0.00
		6A	6.99			52.8	U		4200	D		1.59		1	0.44	U		7.29			338	D		0.47	U		1.85	U	
8/7/17 12:00	19.9	6B	7.01	7.01	9730	52.8	U	52.80	4130	D	4010.00	1.64		1.49	0.44	U	0.44	7.64		7.55	342	D	330.00	0.47	U	0.47	1.85	U	1.85
		6C	7.02	0.02		52.8	U	0.00	3700	D	270.74	1.24		0.22	0.44	U	0.00	7.71		0.23	310	D	17.44	0.47	U	0.00	1.85	U	0.00
		6A	7.00			52.8	U		4160	D		1.68			0.44	U		7.22			341	D		0.47	U		1.85	U	
8/10/17 12:00	22.9	6B	7.05	7.04	9734	52.8	U	52.80	3950	D	3963.33	1.37		1.47	0.44	U	0.44	7.45		7.38	345	D	347.67	0.47	U	0.47	1.85	U	1.85
		6C	7.06	0.03		52.8	U	0.00	3780	D	190.35	1.36		0.18	0.44	U	0.00	7.46		0.14	357	D	8.33	0.47	U	0.00	1.85	U	0.00
		6A	6.88			52.8	U		3940	D		1.35			0.44	U		7.82			343	D		0.47	U		1.85	U	
8/14/17 13:45	27.0	6B	6.97	6.95	9735	52.8	U	52.80	3800	D	3920.00	1.70		1.49	0.44	U	0.44	6.97		7.29	356	D	355.33	0.47	U	0.47	1.85	U	1.85
		6C	7.00	0.06		52.8	U	0.00	4020	D	111.36	1.43		0.18	0.44	U	0.00	7.09		0.46	367	D	12.01	0.47	U	0.00	1.85	U	0.00
		6A	6.98			52.8	U		3640	D		2.37			0.44	U		6.05			380	D		0.47	U		1.85	U	-
9/11/17 12:00	54.9	6B	6.99	6.99	9739	52.8	U	52.80	3620	D	3600.00	2.72		2.49	0.44	U	0.44	7.09		6.84	376	D	387.67	0.47	U	0.47	1.85	U	1.85
		6C	7.00	0.01		52.8	U	0.00	3540	D	52.92	2.39		0.20	0.44	U	0.00	7.38		0.70	407	D	16.86	0.47	U	0.00	1.85	U	0.00
<u> </u>		6A	7.23			52.8	U		2980	D	1	1.48		1	0.44	U		5.48			529	D		0.47	U		1.85	U	1
10/9/17 11:30	82.9	6B	7.10	7.17	9752	52.8	U	52.80	3160	D	2936.67	1.62		1.58	0.44	U	0.44	5.97		5.81	538	D	510.00	0.47	U	0.47	1.85	U	1.85
		6C	7.19	0.07		52.8	U	0.00	2670	D	247.86	1.64		0.09	0.44	U	0.00	5.97		0.28	463	D	40.95	0.47	U	0.00	1.85	U	0.00

SET 1 (A,B,C=	water only)	Fc	rt Lewis JB!	ML	Start	3/12/18 8:00																			
10 ⁷ DHC/mL																									
To Diferine								VOCI/I			1	Made					A	/T		-		V	A	-	
DATE		D ut		(CD)	177.10	NG	0	VOC S ug/L	DOD O		N	Meth	iane/Ednene	ug/L	0		Amor	ns mg/L	×	0		V P	A mg/L		
DATE	TIME (hrs)	Bottle	рн	mean/SD	AILID	vc	Q	mean	CDCE Q	mean	Methane	Q	mean	Etnene	Q	mean	Bromide	Q mean	Lactic	Q	mean	Acetic	Q mean	Proprionic Q	mean
		IA	/.41		0.000	148	U		8820		2.41			0.44	0		11.70		632	, ,		0.9	0	3.7 U	
3/12/18 8:00	0.0	IB	7.45	7.45	9789	148	U	148	11580	10047	3.07		2.64	0.44	U	0.44	11.70	12.07	593		584.67	393.0	131.60	3.7 U	3.70
		1C	7.5	0.05		148	U	0.00	9740	1405.32	2.44		0.37	0.44	U	0.00	12.80	0.64	529		52.00	0.9	U 226.38	3.7 U	0.00
		1D	7.30			148	U		7540		2.19			0.44	U	-	12.10		606		-	0.9	U	3.7 U	·
3/12/18 8:00	0.0	1E	7.46	7.42	9789	148	U	148	12400	9953	2.00		1.97	0.44	U	0.44	11.00	11.70	500		549.00	0.9	U 0.90	3.7 U	3.70
		1F	7.50	0.11		148	U	0.00	9920	2430.17	1.72		0.24	0.44	U	0.00	12.00	0.61	541		53.45	0.9	U 0.00	3.7 U	0.00
		1A	7.08			4270			76 U		26.1			237			10.10		400			66.0		56.1	
3/15/18 8:00	3.0	1B	7.09	7.09	9790	5441		4634	76 U	76	26.90		24.93	235		240.00	10.60	10.47	359		355.67	58.4	57.87	45.7	46.03
		1C	7.11	0.02		4192		699.68	76 U	0.00	21.8		2.74	248		7.00	10.70	0.32	308		46.09	49.2	8.41	36.3	9.90
		1D	7.58			1669			4860		1.87			37.9			10.50		426			66.8		6.1 J	
3/15/18.8:00	3.0	1E	7.61	7.62	9790	1689		1671	7160	5973	1.78		1.84	29.7		34.10	9.42	10.14	342		366.00	56.3	56.83	4.3 J	4.68
		1E	7.67	0.05		1656		16.62	5900	1151.75	1.87		0.05	34.7		4.13	10.50	0.62	330		52.31	47.4	9.71	3.7 1	1 24
		14	6.54	0.00		1587		10.02	76 II	1151.15	75.80		0.05	512	-	1.1.0	10.10	0.02	4.1	-	52:51	04.0	2.11	101	
2/10/10 0 00	7.0	10	(52	6.54	0701	2220		1592	76 U	76	94.40	-	05 72	((2)		(5) (7	10.10	10.12	7.1	-	11.75	120.0	106.62	220	210.22
3/19/18 8:00	7.0	16	0.55	0.04	9/91	2359		1585	76 U	/0	127.00	-	95.75	705		030.07	10.20	10.15	21.4	T 2	0.02	120.0	100.05	229	210.55
		IC	0.34	0.01		823		/ 38.01	76 U	0.00	127.00		27.42	/95		141.01	10.10	0.06	9.8		8.83	105.0	12.03	211	19.01
		ID	7.08		0.004	3193			2380		2.87			141			10.30		2.2	0		152.0		256	-
3/19/18 8:00	7.0	IE	7.25	7.22	9791	2938		2914	4090	3263	2.37		2.43	119	-	127.33	10.20	10.20	2.2	U	2.20	109.0	125.33	186	213.40
		1F	7.34	0.13		2612		291.22	3320	856.41	2.05		0.41	122		11.93	10.10	0.10	2.2	U	0.00	115.0	23.29	198	37.39
		1A	6.05			1044			76 U		97.8			530			9.69		2.2	U		97.6		202	_
3/22/18 7:25	10.0	1B	6.04	6.06	9792	622		605	76 U	76	195	[150.93	1180		890.00	10.00	9.85	2.2	U	2.20	97.4	93.53	226	210.67
		1C	6.09	0.03		148	U	448.25	76 U	0.00	160		49.23	960		330.61	9.86	0.16	2.2	U	0.00	85.6	6.87	204	13.32
		1D	6.81			2844			1750		2.26			123			10.00		2.2	U		125.0		219	
3/22/18 7:25	10.0	1E	6.87	6.85	9792	3000		2844	4000	3023	4.45		3.00	103		113.00	9.90	9.96	2.2	U	2.20	130.0	127.33	227	225.00
		1F	6.87	0.03		2689		155.50	3320	1153.96	2.29		1.26	113		10.00	9.98	0.05	2.2	U	0.00	127.0	2.52	229	5.29
		1A	7.60			223	J		76 U		278			1140			9.65		2.2	U		136.0		274	
3/26/18.8:00	14.0	1B	7.66	7.65	9793	148	U	173	76 U	76	307	-	303.33	1540		1300.00	9.88	9.80	2.2	U	2.20	121.0	130.00	245	262.33
		10	7.70	0.05		148	Ū	43.30	76 U	0.00	325		23.71	1220		211.66	9.88	0.13	2.2	U	0.00	133.0	7.94	268	15.31
		10	7.25	0.05		3113		19190	1720		3 51	••••••		210		211.00	9.67		2.2	II	0.00	135.0		238	
2/26/18 8:00	14.0	115	7.25	7.20	0702	2020		2016	2850	2962	2.72	-	2.07	124		165.67	0.58	0.64	2.2	T 7	2.20	108.0	125.22	105	224.22
5/20/18 8:00	14.0	1E	7.20	7.50	9195	3020		2910	3850	1072.61	2.73	-	0.40	1.54	-	20.55	9.58	9.04	2.2	11	2.20	100.0	125.55	240	224.33
		١٢	7.38	0.07		2014	**	203.30	3020	10/3.01	2.91		0.40	155		39.33	9.08	0.00	2.2	U	0.00	155.0	15.04	240	23.42
	18.0	IA	7.68		0804	148	U		76 U		246			987	-		9.48		2.2	0		116		248	
3/29/18 8:00	17.0	IB	7.72	7.74	9794	148	U	148	76 U	76	2/3		2/1.6/	1220	-	1066.00	9.64	9.60	2.2	U	2.20	125	119.33	264	250.33
		1C	7.81	0.07		148	U	0.00	76 U	0.00	296		25.03	991		133.38	9.68	0.11	2.2	U	0.00	117	4.93	239	12.66
		1D	7.50			2087		-	1390	_	3.12			179			9.79	-	2.2	U		122	-	233	_
3/29/18 8:00	17.0	1E	7.38	7.45	9794	2010		1953	3190	2377	2.19		2.66	93.6		132.20	9.59	9.68	2.2	U	2.20	111	116.33	217	223.67
		1F	7.46	0.06		1761		170.39	2550	912.43	2.68	[0.47	124		43.29	9.65	0.10	2.2	U	0.00	116	5.51	221.0	8.33
		1A	7.70			148	U		76 U		325			1100			9.09		2.2	U		91.7		200	
4/2/18 8:00	21.0	1B	7.74	7.73	9795	148	U	148	76 U	76	239		297.00	961		1009.00	9.05	9.08	2.2	U	2.20	108	99.57	180	187.33
		1C	7.76	0.03		148	U	0.00	76 U	0.00	327		50.24	966		78.85	9.1	0.03	2.2	U	0.00	99	8	182	11.02
		1D	7.33			2009			1240		3.51			171			8.98		2.2	U		108		196	
4/2/18 8:00	21.0	1E	7.32	7.34	9795	1609		1863	2760	2287	2.88		3.19	125		148.00	8.79	8.86	2.2	U	2.20	102	104.33	187	195.67
		1F	7.36	0.02		1970		220.55	2860	907.82	3.17		0.32	148		23.00	8.8	0.11	2.2	U	0.00	103	3.21	204.0	8.50
		14	7.75			148	U		76 U		291			1050			8 32		2.2	U		84		185	
4/5/18 8:00	24.0	18	7.75	7.75	9796	148	U	148	76 U	76	309.00	-	307.33	990		1013 33	8 70	8.65	2.2	U,	2 20	80.3	78.40	206	197.00
40.018 8.00	24.0	10	7.74	0.02	7170	140	U	0.00	76 U	0.00	307.00	-	15 57	1000		22.15	8.77	0.00	2.2	п,	0.00	61.0	14.52	200.0	10.82
		10	7.17	0.02		2472		0.00	1240	0.00	2.02		15.57	1000		52.15	0.04	0.29	2.2		0.00	112	14.55	200.0	10.62
		ID ID	7.42			2472			1340		5.02			100			8.74		2.2			115		210	-
4/5/18 8:00	24.0	IE	7.36	7.41	9796	937		1818	1900	2037	2.92		2.87	139	-	139.33	8.49	8.56	2.2	0	2.20	101	99.57	199	194.67
	-	1F	7.44	0.04		2045		792.28	2870	774.10	2.67		0.18	113		26.50	8.46	0.15	2.2	U	0.00	84.7	14.20	169.0	23.80
		1A	7.69	-		148	U	-	76 U	-	311			1070		-	8.53	-	2.2	U	_	98.2	-	221	
4/9/18 8:00	28.0	1B	7.73	7.72	9797	148	U	148	76 U	76	214		282.33	854	+	960.33	8.70	8.70	2.2	U	2.20	97.2	96.83	210	212.67
		1C	7.74	0.03		148	U	0.00	76 U	0.00	322		59.43	957		108.04	8.88	0.18	2.2	U	0.00	95.1	1.58	207	7.37
		1D	7.38			1966			1500		3.04			156			8.6		2.2	U		103		190	
4/9/18 8:00	28.0	1E	7.39	7.39	9797	1989		1812	3390	2460	2.11		2.56	86		113.67	8.37	8.47	2.2	U	2.20	98	99.93	192	192.67
		1F	7.39	0.01		1480		287.46	2490	945.36	2.53		0.47	99		37.22	8.4	0.12	2.2	U	0.00	99	2.77	196	3.06

JBLM2, #1 DUP

SET 1 DUP (A	B,C= water	only)			Start	4/16/18 8:00																						S
10 ⁷ DHC/mL		For	t Lewis J	BML																								
							١	OC's ug/	L			N	Methane	/Ethen	e ug/L			Anions	mg/L		-		V	FA mg	/L		-	
DATE	TIME (hrs)	Bottle	pН	mean/SD	ATL ID	VC	Q	mean	cDCE	Q	mean	Methane	Q r	mean	Ethene	Q	mean	Bromide Q	mean	Lactic	Q	mean	Acetic	Q	mean	Proprionic	Q	mean
		1A	7.58			148	U		10120			3.33			0.44	U		10.5		572			0.93	U		3.7	U	
4/16/18 8:00	0.0	1B	7.96	7.84	9802	148	U	148	8710		9490	3.51	1	3.46	0.44	U	0.44	10.7	10.60	587		556.67	0.93	U	0.93	3.7	U	3.70
		1C	7.97	0.22		148	U	0.00	9640		716.87	3.54	(0.11	0.44	U	0.00	10.6	0.10	511		40.25	0.93	U	0.00	3.7	U	0.00
		1D	7.75			148	U		10110			3.89			0.44	U		11.8		650			0.93	U		3.7	U	
4/16/18 8:00	0.0	1E	7.82	7.78	9802	148	U	148	11650		10587	3.37	1	3.50	0.44	U	0.44	12.40	12.00	677		663.67	0.93	U	0.93	3.7	U	3.70
		1F	7.78	0.04		148	U	0.00	10000		922.51	3.24	(0.34	0.44	U	0.00	11.8	0.35	664		13.50	0.93	U	0.00	3.7	U	0.00
		1A	7.97			148	U	_	9150		_	3.32			0.44	U		9.52		607			0.93	U		3.7	U	_
4/16/18 14:00	6	1B	8.12	7.73	9803	148	U	148	8640		9300	3.36		3.31	0.44	U	0.44	9.66	9.73	565		573.67	0.93	U	0.93	3.7	U	3.70
		1C	7.11	0.55		148	U	0.00	10110		746.39	3.24	(0.06	0.44	U	0.00	10.0	0.25	549		29.96	0.93	U	0.00	3.7	U	0.00
		1D	7.74			148	U		7790			3.21			0.44	U		9.37		524			0.93	U		3.7	U	
4/16/18 14:00	6	1E	7.79	7.79	9803	148	U	148	9350		8710	3.04		3.16	0.44	U	0.44	9.45	9.45	529		530.00	0.93	U	0.93	3.7	U	3.70
		1F	7.83	0.05		148	U	0.00	8990		816.82	3.24	(0.11	0.44	U	0.00	9.53	0.08	537		6.56	0.93	U	0.00	3.7	U	0.00
		1A	8.06			148	U		8850			2.12	-		0.44	U	-	9.23		542			0.93	U		3.7	U	
4/17/18 8:00	24	1B	8.05	8.06	9804	148	U	148	7850		8517	2.64		2.54	0.44	U	0.44	9.92	9.61	551		544.67	0.93	U	0.93	3.7	U	3.70
		1C	8.06	0.01		148	U	0.00	8850		577.35	2.87	(0.38	0.44	U	0.00	9.67	0.35	541		5.51	0.93	U	0.00	3.7	U	0.00
		1D	7.78			187	J		6600			2.75	· ·		0.74	J		9.42		518			0.93	U		3.7	U	
4/17/18 8:00	24	IE	7.80	7.81	9804	198	J	190	8190		7773	2.16		2.36	0.60	J	0.59	9.57	9.53	529		523.67	0.93	U	0.93	3.7	0	3.70
		IF	7.85	0.04		186	J	6.66	8530		1030.26	2.17	(0.34	0.44	U	0.15	9.61	0.10	524		5.51	0.93	U	0.00	3.7	U	0.00
		1A	7.96			148	U		8650			2.05			0.44	U		9.11		497	_		0.93	U		3.7	U	
4/17/18 14:00	30	1B	8.07	8.05	9804	148	U	148	7350		7970	2.06		2.31	0.44	U	0.44	9.40	9.31	518		512.00	0.93	U	0.93	3.7	U	3.70
		IC	8.12	0.08		148	U	0.00	7910		652.07	2.85		0.45	0.44	U	0.00	9.41	0.17	521		13.08	0.93	U	0.00	5.7	<u>U</u>	0.00
	20	ID	7.77		0004	274			6000		(700	3.09		2.00	1.80	J		8.98	0.02	489		101.00	0.93	U	0.02	3.7	0	2.70
4/17/18 14:00	30	IE 1E	7.80	7.81	9804	322		2/5	6/10		6793	2.95		2.89	1.40	J	1.34	9.06	9.03	494	_	491.33	0.93	U	0.93	3.7	U	3.70
	-	IF	7.85	0.04		228	J	47.00	7670	-	838.11	2.64	(0.23	0.82	J	0.49	9.05	0.04	491	-	2.52	0.93	U	0.00	3.7	U	0.00
	40	IA	8.04	0.14	0005	22	J	117	7810		7407	1.8/	· · .	2.22	0.44	U	0.44	8./3	0.05	492		404 (7	0.93	U 11	0.02	3.7	U	2.70
4/18/18 8:00	48	18	8.18	8.14	9805	148	U	117	7110		7427	2.13		2.22	0.44	U	0.44	9.10	8.95	531		484.67	0.90	0	0.92	3.7	U	3.70
		IC	8.20	0.09		148	U	53.69	7360		354.73	2.65		0.40	0.44	<u> </u>	0.00	9.02	0.19	431		50.40	0.93	U	0.02	3.7	<u>U</u>	0.00
	40	ID 1E	7.86	7.00	0005	512		474	5130		52(0	2.35	· · .	0.07	4.65		2.69	8.65	0.01	436		420 (7	0.93	0	0.02	3.7	U 11	2.70
4/18/18 8:00	48	IE	7.92	7.92	9805	501		4/4	4560		5260	2.49		2.37	3.00		3.68	8.77	8.81	443	-	439.67	0.93	U	0.93	3.7	U 11	3.70
		14	7.97	0.06		410	T	55.99	8000	-	113.24	2.28		0.11	2.75	TT	0.96	9.00	0.18	440	-	3.51	0.93	U	0.00	3.7	U	0.00
4/10/10 14 00	5.4	1A 1D	/.82	8.02	0905	149	J	115	8000		7767	2.65	· · .	2.44	0.44	U	0.44	9.06	8.06	408		500.00	0.93	U 11	0.02	3.7	U	2 70
4/18/18 14:00	54	16	8.1	8.02	9805	148	U	57.16	/010		//6/	2.12		2.44	0.44	U	0.44	8.89	8.96	498		10.15	0.93	U U	0.93	3.7	U	3.70
		10	8.15	0.17		148	0	57.10	8290		0/1.14	2.34	······	0.28	0.44		0.00	8.94	0.09	491		10.15	0.93	<u>U</u>	0.00	3.7		0.00
4/19/19 14:00	54	1D	7.80	7.97	0205	502		500	6120		5060	2.15		2 21	3.28		4.32	8.05	0.60	409		445.22	0.95	U U	0.02	3.7	U 11	2 70
4/18/18 14:00	54	115	7.00	0.07	9805	422		20.15	6140		204.62	2.32		0.17	4.10		4.32	0.04	0.00	411		20.44	0.93	U I	0.95	3.7	U	3.70
		14	7.94	0.07		423		69.15	8210	-	294.02	2.47	· · · ·	0.17	0.66	T	0.90	0.10	0.08	409		30.44	0.93	U	0.00	3.7	U	0.00
4/19/18 8-00	72	1A 1B	8.12	8.07	9806	156	I	207	6720		7460	2.43		2 56	0.00	J	0.51	9.10	9.16	505		476 33	0.93	U V	0.93	3.7	U	3 70
4/19/18 8.00	12	10	8.16	0.12	2800	150	J	91.24	7350		800.69	2.71		0.14	0.44	U	0.13	9.20	0.06	426		43 73	0.93	U 1	0.95	3.7	U	0.00
		10	7 03	0.12		806		91.24	4250		000.09	2.34		0.14	7 15		0.15	9.20 8 77	0.00	400		43.75	0.93	<u> </u>	0.00	3.7	<u> </u>	0.00
4/10/19 9:00	72	15	7.95	7.00	0806	638		710	5170		4010	2.11		2 2 2	6.44		6.22	8.07	8.01	474		472 33	0.93	U I	0.03	3.7	U	3 70
4/17/18 8.00	12	1E	8.06	0.07	2800	712		84.20	5310		575.85	2.00		0.25	5.08		1.05	8.99	0.12	444		27.54	0.93	U I	0.00	3.7	U	0.00
		14	7.89	0.07		290	-	04.20	6640	-	515.05	3.04	· · · ·	0.25	1.26	I	1.05	8.07	0.12	443	-	21.54	0.93	U	0.00	3.7	U	0.00
4/19/18 14:00	78	1R	8.06	8.01	9806	201	I	228	6010		6310	3 38		3.08	3.00	5	1.63	8.50	8 35	434		441 33	0.93	U U	0.93	3.7	U	3 70
417/1014.00	70	10	8.09	0.01	2000	194	I	53.52	6280		316.07	2.82		0.28	0.64	T	1.05	8.49	0.25	447		6.66	0.93	U	0.00	3.7	U	0.00
	••••••	10	7.81			946			4840			2.02		0.20	9.92			7 74	0.25	403		0.00	0.93	TI I	0.00	37	- U	
4/19/18 14:00	78	1E	7.89	7.89	9806	971		893	6450		5613	2.37	· ·	2.26	6.94		7.23	7.89	7.85	395		388 33	0.93	U	0.93	3.7	U	3,70
010101400	70	1E	7.97	0.08	2000	763		113.56	5550		806.87	1.98		0.24	4.84		2.55	7.93	0.10	367		18.90	0.93	U	0.00	3.7	U	0.00
		1A	7.86	0.00		2390		110.00	1860		500.07	31.55			33.58		2.00	8.57	0.10	2.23	U	10.70	109.14		0.00	223.51	Ŭ	0.00
4/23/18 8:00	168	1B	7.94	7.91	9807	2160		2202	1430		1860	21.08	2	22.73	23.48		24.18	8.64	8.62	2.23	U	2.23	94.96		100.16	195.94		205.84
		10	7.94	0.05	2.507	2055		171.34	2290		430.00	15.55	1 1	8.13	15.47		9.08	8.64	0.04	2.23	U	0.00	96.38		7.81	198.1		15.34
		1D	7.53			1286			2720			2.65	`		41.27			8.11		2.23	Ū		98.53			203.44	******	
4/23/18 8:00	168	1E	7.62	7.60	9807	1140		1292	4080		3803	2.55		2.53	27.88		29.22	8.21	8.17	2.23	U	2.23	92.71		94.50	168.15		186.42
		1F	7.66	0.07		1449		154.58	4610		974.90	2.39		0.13	18.52		11.43	8.2	0.05	2.23	U	0.00	92.25		3.50	187.7		17.68

SET 2 (A,B,C= 10 ⁶ DHC/mL	water only)	Fo	rt Lewis JI	3ML	Start	3/12/18 9:00		10.01																		
DATE	TIME (days)	Bottle	рН	mean	ATL ID	VC	Q	mean	cDCE	Q	mean	Methane	Q mean	e ug/L Ethene	Q	mean	Bromide	Q mean	Lactic	Q	mean	Acetic	Q Q	mean	Proprionic	Q mean
3/12/18 9:00	0.0	2A 2B 2C	7.85 7.90 7.90	7.88 0.03	9789	148 148 148	U U U	148 0	8500 10150 8840		9163 871	1.06 1.25 1.16	1.16 0.10	0.44 0.44 0.44	U U U	0.44	12.9 11.1 11.6	11.87 0.93	522 551 545		539.33 15.31	0.93 0.93 0.93	U U U	0.93 0.00	3.7 3.7 3.7	U U 3.70 U 0.00
3/12/18 9:00	0.0	2D 2E 2F	7.35 7.58 7.60	7.51 0.14	9789	148 148 148	U U U	148 0	9720 8280 10590		9530 1167	1.04 1.12 0.97	1.04 0.08	0.44 0.44 0.44	U U U	0.44	11.1 11.2 11.0	11.10 0.10	552 665 720		645.67 85.65	0.93 0.93 0.93	U U U	0.93 0.00	3.7 3.7 3.7	U U 3.70 U 0.00
3/15/18 9:00	3.0	2A 2B 2C	7.99 8.02 8.01	8.01 0.02	9790	148 148 148		148 0	7830 10060 8760		8883 1120	1.11 1.06 0.99	1.05	0.44 0.44 0.44	U U U	0.44	11.2 10.6 10.6	10.80 0.35	650 667 556		624.33 59.79	0.93 0.93 0.93	U U U	0.93 0.00	3.7 3.7 3.7	U U 3.70 U 0.00
3/15/18 9:00	3.0	2D 2E 2F	7.88 7.89 7.9	7.89 0.01	9790	148 148 148		148	8000 7460 10090		8517 1389	1.18 1.20 1.20	1.19	0.44 0.44 0.44	U U U	0.44	10.0 10.8 10.9	10.57 0.49	512 402 628		514.00 113.01	0.93 0.93 0.93	U U U	0.93	3.7 3.7 3.7	U 3.70 U 0.00
3/19/18 9:00	7.0	2A 2B 2C	6.89 6.81 6.77	6.82 0.06	9791	223 181 230	J J J	211	8270 9790 8200		8753 898	3.99 3.34 4.65	3.99	0.44 0.44 0.44	U U U	0.44	11.2 10.5 10.4	10.70	160 334 243		245.67 87.03	47.6 102 72.6	-	74.07 27.23	65.1 141 101	102.37
3/19/18 9:00	7.0	2D 2E 2F	6.54 7.66 7.76	7.32 0.68	9791	148 148 148	U U U	148 0	8520 6890 8960		8123 1091	1.58 1.50 1.33	1.47	0.46 0.44 0.44	J U U	0.45	10.2 10.0 9.9	10.03 0.15	405 561 359		441.67 105.87	43.5 49.0 29.4		40.63 10.11	16.1 7.0 4	J J 8.93 U 6.42
3/22/18 8:35	10.0	2A 2B 2C	6.37 6.29 6.30	6.32 0.04	9792	311 237 290	J J J	279 38	7390 9870 7440		8233 1418	4.35 3.64 4.07	4.02 0.36	0.6 0.44 0.44	J U U	0.49	10.7 10.3 10.2	10.40	65.6 43.4 72.5		60.50 15.21	110 73.3 104		95.77 19.69	198 138 189	175.00 32.36
3/22/18 8:35	10.0	2D 2E 2F	6.87 7.07 7.18	7.04 0.16	9792	179 148 148	J U U	158 18	8160 6590 8610		7787 1060	1.41 1.78 1.80	1.66 0.22	0.45 0.5 0.78	J J J	0.58 0.18	9.7 9.8 9.9	9.81 0.10	2.2 105 2	U	36.47 59.35	139 84 64		95.83 38.74	238 130 98	155.17 73.55
3/26/18 9:00	14.0	2A 2B 2C	7.71 7.71 7.73	7.72	9793	380 259 318	J J	319 61	7370 9320 7650		8113 1054	10.70 9.21 9.48	9.80 0.79	0.47 0.44 0.44	J U U	0.45	10.6 10.1 10.0	10.23	2.2 2.2 2.5	U U J	2.30	114 112 136		120.67 13.32	245 244 278	255.67 19.35
3/26/18 9:00	14.0	2D 2E 2F	7.35 7.42 7.41	7.39 0.04	9793	169 181 260	J J J	203 49	7250 6950 11090		8430 2309	3.64 2.79 3.22	3.22 0.43	1.13 1.25 0.99	J J	1.12 0.13	10.0 9.7 9.7	9.79 0.15	2.2 2.2 2.6	U U J	2.33 0.23	155 154 161		156.67 3.79	262 273 280	271.67
3/29/18 9:30	17.0	2A 2B 2C	7.64 7.66 7.65	7.65	9794	314 193 279	J J J	262 62	7130 8570 7130		7610 831	14.10 14.00 14.00	14.03	0.44 0.44 0.44	U U U	0.44	10.4 9.7 9.9	9.99	2.2 2.2 2	U U U	2.20	116 118 122		118.67 3.06	221 255 262	246.00 21.93
3/29/18 9:30	17.0	2D 2E 2F	7.35 7.36 7.39	7.37	9794	148 148 420	U U J	239 157	7300 5990 8170		7153 1097	3.62 3.18 3.23	3.34 0.24	1.26 1.05 1.67	J J J	1.33 0.32	9.57 9.63 9.66	9.62	2.2 2.2 2.2	U U U	2.20	127 120 111		119.33 8.02	232 216 208	218.67
4/2/18 9:00	21.0	2A 2B 2C	7.71 7.71 7.7	7.71	9795	239 234 289	J J J	254 30	5680 8300 7420		7133 1333	2.39 33.1 21.8	19.10 15.53	0.44 0.44 0.44	U U U	0.44	10.1 9.62 9.67	9.80 0.26	2.2 2.2 2.2	U U U	2.20	119 117 104	-	113.33 8	250 251 223	241.33 15.89
4/2/18 9:00	21.0	2D 2E 2F	7.41 7.4 7.43	7.41	9795	148 148 148	U U U	148 0	6300 5950 8300		6850 1268	3.83 3.06 3.39	3.43 0.39	1.30 1.06 1.61	J J J	1.32 0.28	9.28 9.15 9.28	9.24 0.08	2.2 2.2 2.2	U U U	2.20 0.00	118 114 120		117.33 3.06	195 203 216	204.67
4/5/18 9:00	24.0	2A 2B 2C	7.71 7.74 7.75	7.73	9796	358 269 314	J J J	314 45	7290 7830 7940		7687 348	34.8 37.1 36.9	36.27	0.44 0.44 0.44	U U U	0.44	9.53 8.99 8.95	9.16	2.2 2.2 2.2	U U U	2.20	102 110 105		105.67	214 234 222	223.33 10.07
4/5/18 9:00	24.0	2D 2E 2F	7.41 7.47 7.48	7.45	9796	127 134 132	J J J	131	7360 7050 7630		7347 290	3.75 3.16 3.3	3.40 0.31	1.37 1.13 1.89	J J J	1.46 0.39	8.48 8.53 8.53	8.51 0.03	2.2 2.2 2.2	U U U	2.20 0.00	115 109 106.00		110.00 4.58	202 194 191	195.67 5.69
4/9/18 9:00	28.0	2A 2B 2C	7.74 7.7 7.76	7.73	9797	336 276 311	J J J	308 30	6790 8580 7580		7650 897	61.1 73.1 54.7	62.97 9.34	0.44 0.44 0.44	U U U	0.44	9.51 9.1 9.17	9.26	2.2 2.2 2.2	U U U	2.20	111 103 105		106.33 4.16	231 201 211	214.33 15.28
4/9/18 9:00	28.0	2D 2E 2F	7.49 7.49 7.49	7.49 0.00	9797	105 105 130	J J J	113 14	6660 5440 7850		6650 1205	3.44 2.23 1.77	2.48 0.86	1.15 1.58 1.00	J J J	1.24 0.30	8.54 8.48 8.41	8.48 0.07	2.2 2.2 2	U U U	2.20 0.00	111 114 90.70		105.23 12.68	188 199 164	183.67 17.90
4/12/18 9:00	31.0	2A 2B 2C	7.60 7.65 7.65	7.63	9800	311 263 270	J J J	281 26	6700 8130 6750		7193 812	74.6 54.3 68.5	65.80 10.42	0.44 0.44 0.44	U U U	0.44	9.28 8.80 8.86	8.98 0.26	2.2 2.2 2.2	U U U	2.20	91.5 100 110		100.50 9.26	195 217 224	212.00 15.13
4/12/18 9:00	31.0	2D 2E 2F	7.45 7.45 7.65	7.52	9800	131 109 149	J J J	130 20	6990 5460 9630		7360 2109	2.43 3.12 2.7	2.75	0.83 1.05 1.55	J J J	1.14	8.41 8.40 8.37	8.39 0.02	2.2 2.2 2.2	U U U	2.20 0.00	97.4 109 111		105.80 7.34	153 182 193	176.00 20.66
4/16/18 9:00	35.0	2A 2B 2C	7.78 7.85 7.81	7.81	9802	268 203 229	J J J	233 33	6024 7420 6729		6724 698	107 105 82.6	98.20 13.55	0.44 0.44 0.44	U U U	0.44	9.33 8.73 8.87	8.98	2.23 2.23 2.32	U U U	2.26	107 122 105		111.33 9.29	212 264 224	233.33 27.23
4/16/18 9:00	35.0	2D 2E 2F	7.65 7.66 7.80	7.70	9802	96 88 116	J J	100	6219 5509 7421		6383 966	2.89 3.20 3.60	3.23	0.96 1.17 2.34	J	1.49	8.44 8.46 8.23	8.38 0.13	2.23 2.23 2.23	U U U	2.23 0.00	111 118 113		114.00 3.61	173 191 187	183.67 9.45
4/19/18 9:00	38.0	2A 2B 2C	7.71 7.79 7.78	7.76	9806	282 215 295	J	264 43	5930 7220 7850		7000 979	93.3 99.0 80.2	90.83 9.64	0.44 0.44 0.44	U U U	0.44	8.86 8.60 8.55	8.67	2.23 2.23 2.32	U U U	2.26	91 104 109		101.33 9.29	181 218 234	211.00
4/19/18 9:00	38.0	2D 2E 2F	7.52 7.54 7.58	7.55	9806	91 108 111	J J J	103	5910 5610 7640		6387 1096	2.75 3.55 2.37	2.89	0.97 1.33 1.50	J J	1.27	8.39 8.30 8.32	8.34	2.23 2.23 2.23	U U U	2.23	116 125 115		118.67	183 194 181	186.00
4/23/18 9:00	42.0	2A 2B 2C	7.83 7.89 7.91	7.88	9807	357 267 239		288	7270 7960 6550	Π	7260	83.02 89.16 74.23	82.14	0.44 0.44 0.44	U U U	0.44	9.35 8.74 8.62	8.90	2.23 2.23 2.23	U U U	2.23	102.74 94.05 94.94		97.24 4.78	224.44 207.26 210.63	214.11
4/23/18 9:00	42.0	2D 2E	7.66	7.71	9807	95 107	J	103	6270 5300		6210	2.86 3.22	3.13	1.06	J	1.55	8.30 8.42	8.34	2.23 2.23	UUU	2.23	94.02 92.00		93.44	143.19 148.76	149.29

SET 3	For	Lewis JB	ML		Start	3/12/18 11:00																						
10 ⁵ DHC/mL																												
							1	OCs ug/	L			N	Aetha	ane/Ether	e ug/L			Anions	mg/L				VI	A mg	/L			
DATE	TIME (days)	Bottle	pН	mean	ATL ID	VC	Q	mean	cDCE	Q	mean	Methane	Q	mean	Ethene	Q	mean	Bromide Q	mean	Lactic	Q	mean	Acetic	Q	mean	Proprionic	Q	mean
		3A	7.71			148	U		9050			0.81	J		0.44	U		11.90		555			0.93	U		3.7	U	
3/12/18 11:00	0.0	3B	7.76	7.75	9789	148	U	148.0	12960		10360	1.11		1.04	0.44	U	0.44	12.00	11.73	607		572.33	0.93	U	0.93	3.7	U	3.70
		3C	7.78	0.04		148	U	0.00	9070		2251.69	1.20		0.20	0.44	U	0.00	11.30	0.38	555		30.02	0.93	U	0.00	3.7	U	0.00
		3A	8.02			148	U		9040			0.90	J		0.44	U		10.40		559			0.93	U		3.7	U	
3/19/18 10:00	7.0	3B	8.04	8.03	9791	148	U	148.00	8730		8980	0.95		0.93	0.44	U	0.44	10.50	10.30	470		502.67	0.93	U	0.93	3.7	U	2.78
		3C	8.02	0.01		148	U	0.00	9170		226.05	0.93	J	0.03	0.44	U	0.00	10.00	0.26	479		48.99	0.93	U	0.00	0.93	U	1.60
		3A	8.02			148	U		8400			1.13			0.44	U		10.30		439			0.93	U		3.7	U	
3/26/18 11:00	14.0	3B	8.03	8.03	9793	148	U	148.00	9680		9040	1.22		1.18	0.44	U	0.44	10.30	10.30	352		395.50	66.8	ľ	33.87	74.0		38.85
		3C	8.03	0.01		148	U	0.00	8870		905.10	1.23		0.06	0.44	U	0.00	10.30	0.00	339		61.52	74.4		46.58	96.5		49.71
		3A	7.96			148	U		7340			1.09			0.44	U		9.83		259			71.4			99.5		
4/2/18 11:00	21.0	3B	7.83	7.82	9795	148	U	148.00	9370		8355	1.36		1.23	0.44	U	0.44	10.10	9.97	195		227.00	90.60		81.00	153		126.25
		3C	7.66	0.15		148	U	0.00	8110		1435.43	1.1		0.19	0.44	U	0.00	9.94	0.19	110		45.25	100		13.58	117		37.83
		3A	7.84			148	U		8320			0.99			0.44	U		9.43		213			87.90			138		
4/9/18 11:00	28.0	3B	7.68	7.69	9797	148	U	148.00	9060		8690	1.31		1.15	0.44	U	0.44	9.64	9.54	106		159.50	109		98.45	204		171.00
		3C	7.54	0.15		148	U	0.00	9770		523.26	1.0		0.23	0.44	U	0.00	9.48	0.15	13.2		75.66	123		14.92	258		46.67
		3A	7.75			148	U		9259			1.11			0.44	U		9.56		154			101			173		
4/16/18 11:00	35.0	3B	7.62	7.66	9802	148	U	148.00	9733		9496	1.48		1.30	0.44	U	0.44	9.60	9.58	26.2		90.10	115		108.00	245		209.00
		3C	7.61	0.08		148	U	0.00	7548		335.17	1.50		0.26	0.44	U	0.00	9.28	0.03	2.23	U	90.37	115		9.90	267		50.91
		3A	7.73	_		148	U	_	8540			0.93	J		0.44	U		9.65		68.54			98			184		
4/23/18 11:30	42.0	3B	7.73	7.74	9807	148	U	148.00	9280		8910	1.42		1.18	0.44	U	0.44	9.58	9.62	5.94	J	37.24	176		137.11	401		292.69
		3C	7.75	0.01		148	U	0.00	8990		523.26	1.70		0.35	0.44	U	0.00	9.56	0.05	34.94		44.26	101.5		55.01	205.76		153.71

SET 4	H	ort Lewis JBMI	L		Start	3/12/18 11:00)																				
10 ⁴ DHC/mL																											
								VOC's ug/L				Met	hane/Ethene	e ug/L			Anion	s mg/L				V	FA mş	g/L			
DATE	TIME(days)	Bottle	pH	mean	ATL ID	VC	Q	mean	cDCE	Q mean	Methane	Q	mean	Ethene	Q	mean	Bromide	Q mea	Lac	ic (Q mean	Acetic	Q	mean	Proprionic	Q	mean
		4A	7.58			148	U		7950		1.05			0.44	U		11.7		459			0.93	U		3.7	U	
3/12/18 11:00	0.0	4B	7.76	7.71	9789	148	U	148.00	11700	9726.67	1.06		0.94	0.44	U	0.44	11.7	11.6	63		565.33	0.93	U	0.93	3.7	U	3.70
		4C	7.80	0.12		148	U	0.00	9530	1882.72	0.71	J	0.20	0.44	U	0.00	11.6	0.06	60		92.80	0.93	U	0.00	3.7	U	0.00
		4A	8.00			148	U		7260		0.89	J		0.44	U		10.4		50			0.93	U		3.7	U	
3/19/18 10:00	7.0	4B	7.97	7.96	9791	148	U	148.00	10590	8623.33	1.02		0.94	0.44	U	0.44	10.20	10.2	464		533.33	0.93	U	0.93	3.7	U	3.70
		4C	7.95	0.01		148	U	0.00	8020	1745.06	0.91	J	0.07	0.44	J	0.00	10.2	0.12	63:		89.97	0.93	U	0.00	3.7	U	0.00
		4A	8.40			148	U		8420		0.79	J		0.44	U		9.92		383			0.93	U		3.7	U	
3/26/18 11:00	14.0	4B	8.42	8.41	9793	148	U	148.00	9800	9110.00	1.05		0.92	0.44	U	0.44	10.2	10.0	56		472.50	0.93	U	0.93	3.7	U	3.70
BROKEN		4C		0.01				0.00		975.81			0.18			0.00		0.20			126.57			0.00			0.00
		4A	8.35			148	U		7500		1.12			0.44	U		9.46		49:			0.93	U		3.7	U	
4/2/18 11:00	21.0	4B	8.26	8.31	9795	148	U	148.00	9450	8475.00	1.06		1.09	0.44	U	0.44	10.3	9.88	50		501.00	0.93	U	0.93	4.89	J	4.30
		4C		0.06				0.00		1378.86			0.04			0.00		0.59			8.49			0.00			0.84
		4A	8.13			148	U		7100		0.82	J		0.44	U		4.35		49			0.93	U		16.7	J	
4/9/18 11:00	28.0	4B	8.12	8.13	9797	148	U	148.00	9290	8195.00	0.91	J	0.87	0.44	U	0.44	9.81	7.08	52		509.50	1	U	0.93	22.8	J	19.75
		4C		0.01				0.00		1548.56			0.06			0.00		3.80			16.26			0.00			4.31
		4A	7.98			148	U		7197		0.93	J		0.44	U		8.91		34			60.6			71.3		
4/16/18 11:00	35.0	4B	8.01	8.00	9802	148	U	148.00	9791	8494.00	0.97		0.95	0.44	U	0.44	9.57	9.24	357		349.00	73.8		67.20	63.5		67.40
		4C		0.02				0.00		1834.23			0.03			0.00		0.47			11.31			9.33			5.52
		4A	7.78			148	U		7610		0.87	J		0.44	U		9.57		196.	4		78.46			114.65		
4/23/18 11:30	42.0	4B	7.97	7.88	9807	148	U	148.00	9660	8635.00	1.31		1.09	0.44	U	0.44	9.46	9.52	230	3	213.47	71.61		75.04	93.7		104.18
		4C		0.13				0.00		1449.57			0.31			0.00		0.08			23.80			4.84			14.81

SET 5 Live	For	t Lewis JB	ML		Start	3/12/18 11:30)																					
Live Control																												
								VOC's ug/	L			1	Metha	ne/Ethen	e ug/L			Anion	s mg/L				VI	A n	g/L			
DATE	TIME (days)	Bottle	pН	mean	ATL ID	VC	Q	mean	cDCE	Q	mean	Methane	Q	mean	Ethene	Q	mean	Bromide	Q mean	Lactic	Q	mean	Acetic	Q	mean	Proprionic	Q	mean
3/12/18 11:30	0.0	5A	7.66	7.68	9789	148	U	148.00	10850		10965	1.07		1.03	0.44	U	0.44	11.7	11.70	600		616.00	0.93	U	0.93	3.7	U	3.70
		5B	7.69	0.02		148	U	0	11080		163	0.98	J	0.064	0.44	U	0	11.7	0.00	632		22.63	0.93	U	0.00	3.7	U	0.00
3/12/18 11:30	0.0	5C	7.60	7.61	9789	148	U	148.00	9030		9360	0.51	J	0.81	0.44	U	0.44	11.3	11.65	567		578.00	0.93	U	0.93	3.7	U	3.70
		5D	7.61	0.01		148	U	0	9690		467	1.11		0.424	0.44	U	0	12.0	0.49	589	_	15.56	0.93	U	0.00	3.7	U	0.00
3/15/18 11:30	3.0	5A	8.01	8.01	9790	148	U	148.00	10400		10000	0.99		0.99	0.44	U	0.44	10.9	10.42	537		518.00	0.93	U	0.93	3.7	U	3.70
		28	8.01	0.00	0700	148	U	0	9600		566	0.98		0.007	0.44	U	0	9.9	0.68	499		26.87	0.93		0.00	3.7	U	0.00
3/15/18 11:30	3.0	50	7.8	/.81	9790	148	U	148.00	8900		8825	1.17		1.18	0.44	U	0.44	10.9	10.75	230		4/6.50	0.93	U	0.93	3.7	U	3.70
2/10/18 11:00	7.0	50	7.82	7.07	0701	148	U	148.00	0270		0465	0.06		0.014	0.44	U	0.44	10.0	10.20	41/		507.50	0.95	U	0.00	3.7	U	3.70
3/19/18 11:00	7.0	5R	7.97	0.00	9/91	148	U	148.00	9660		276	0.90		0.97	0.44	U	0.44	10.3	0.14	589	-	115.26	0.93	U	0.93	3.7	U	0.00
3/19/18 11:00	7.0	50	7 78	7 78	9791	148	U U	148.00	7490		7910	14	,	1 44	0.44	U U	0.55	9.9	9.60	383		335.50	0.93	U	0.00	3.7	U,	3 70
5/15/10/11:00	/10	5D	7.77	0.01		148	U	0	8330		594	1.47		0.049	0.65	J	0	9.3	0.42	288		67.18	0.93	U	0.00	3.7	U	0.00
3/22/18 9:50	9,9	5A	7.83	7.82	9792	148	U	148.00	10130		10035	0.94	J	0.97	0.44	U	0.44	10.1	10.05	516		443.00	0.93	U	0.93	3.7	U	3.70
		5B	7.81	0.01		148	U	0	9940		134	1.00		0.042	0.44	U	0	10.0	0.07	370		103.24	0.9	U	0.00	3.7	U	0.00
3/22/18 9:50	9.9	5C	7.11	7.16	9792	148	U	148.00	7960		8265	1.66		1.50	0.79	J	0.81	9.7	9.70	28		101.30	84.6		80.65	132		116.50
		5D	7.21	0.07		148	U	0	8570		431	1.33		0.233	0.83	J	0.03	9.7	0.04	175		104.23	76.7		5.59	101		21.92
3/26/18 11:30	14.0	5A	8.40	8.41	9793	148	U	148.00	10450		10285	1.07		1.07	0.44	U	0.44	10.0	9.96	545		551.50	0.93	U	0.93	3.7	U	3.70
		5B	8.42	0.01		148	U	0	10120		233	1.06		0.007	0.44	U	0	10.0	0.01	558		9.19	0.9	U	0.00	3.7	U	0.00
3/26/18 11:30	14.0	5C	7.36	7.35	9793	148	U	148.00	8330		8190	1.60		1.91	1.14	J	1.14	9.6	9.42	64		33.00	151		121.35	239		196.00
		5D	7.33	0.02		148	U	0	8050		198	2.22		0.438	1.13	J	0	9.3	0.24	2	U	43.56	91.7		41.93	153		60.81
3/29/18 11:30	17.0	5A	8.36	8.34	9794	148	U	148.00	8930		8915	1.00		0.99	0.44	U	0.44	9.6	9.80	497		487.00	0.93	U	0.93	3.7	U	3.70
		5B	8.32	0.03		148	U	0	8900		21	0.98		0.014	0.44	U	0	10.0	0.29	477		14.14	0.93	U	0.00	3.7	U	0.00
3/29/18 11:30	17.0	5C	7.33	7.34	9794	148	U	148.00	6800		6865	2.09		1.78	1.15	J	1.11	9.6	9.60	12	J	7.10	128		117.50	214	[200.50
		5D	7.34	0.01		148	U	0	6930		92	1.47		0.438	1.07	J	0	9.6	0.04	2	U	6.93	107		14.85	187		19.09
4/2/18 11:30	21.0	5A	8.22	8.30	9795	148	U	148.00	9040		9205	0.88	J	0.95	0.44	U	0.44	9.6	9.55	448		450.00	0.93	U	0.93	12.6	J	8.15
	21.0	28	8.38	0.11	0705	148	U	0	9370		233	1.02	,	0.099	0.44	U	0	9.5	0.07	452		2.83	0.9	U	0.00	3.7	U	6.29
4/2/18 11:30	21.0	50	7.83	7.59	9795	148	U	148.00	9030		8255	2.9		2.94	2.13	J	2.32	9.0	8.99	10	J	6.20	116		116.00	196		197.00
4/5/10 11 20	24.0	50	7.54 9.16	0.35	0706	148	U	148.00	/480		1096	2.98	T	0.057	2.51	TI	0.44	9.0	0.05	442	0	5.00	110	II	0.00	198.0	,	1.41
4/5/18 11:50	24.0	5R	8.10	0.02	9790	140	U	148.00	0160		148	0.91	J	0.92	0.44	U	0.44	9.5	9.20	443		20.51	0.93	U	0.93	4.58	T	12.39
4/5/18 11:30	24.0	50	7 47	7 42	9796	148		148.00	7550		7065	2.63		2 51	1.86	T	1.58	8.8	8 79	11	Ť	6 70	111		110 50	181		183.00
4.0/1011.00	24.0	5D	7.36	0.08	7170	148	U	0	6580		686	2.39		0.170	1.29	J	0	8.8	0.02	2	U	6.36	110.0		0.71	185.0	-	2.83
4/9/18 11:30	28.0	5A	8.13	8.15	9797	148	U	148.00	8770		9030	0.96		0.98	0.44	U	0.44	9.1	9.21	454	-	458.50	0.93	U	0.93	28.1	J	20.85
		5B	8.16	0.02		148	U	0	9290		368	0.99	-	0.021	0.44	U	0	9.3	0.19	463		6.36	0.9	U	0.00	13.6	J	10.25
4/9/18 11:30	28.0	5C	7.42	7.80	9797	148	Ū	148.00	7180		7240	2.69		2.76	1.83	J	1.64	8.8	8.85	15	J	8.45	125		124.00	199		202.00
		5D	8.18	0.54		148	U	0	7300		85	2.82	-	0.092	1.44	J	0	8.9	0.08	2	U	8.84	123		1.41	205.0	-	4.24
4/12/18 11:30	31.0	5A	8.09	8.11	9800	148	U	148.00	8740		9355	0.85	J	0.82	0.44	U	0.44	9.0	9.06	432		418.50	0.93	U	0.93	26.3		21.85
		5B	8.13	0.03		148	U	0	9970		870	0.79	J	0.042	0.44	U	0	9.1	0.05	405		19.09	0.9	U	0.00	17.4	J	6.29
4/12/18 11:30	31.0	5C	7.34	7.35	9800	148	U	148.00	7200		7240	2.41		2.45	1.69	J	1.49	8.7	8.78	15	J	8.75	120		120.50	193		193.50
		5D	7.36	0.01		148	U	0	7280		57	2.48		0.049	1.29	J	0	8.8	0.09	2	U	9.26	121.0		0.71	194.0		0.71
4/16/18 11:30	35.0	5A	8.12	8.14	9802	148	U	148.00	8229		8353	0.97		0.95	0.44	U	0.44	8.8	8.94	375		380.00	55.3		57.30	29.9		27.45
		5B	8.15	0.02		148	U	0	8476		175	0.93	J	0.028	0.44	U	0	9.0	0.14	385		7.07	59.3		2.83	25.0		3.46
4/16/18 11:30	35.0	5C	7.53	7.50	9802	148	U	148.00	7364		7175	2.91		2.83	2.81		2.20	8.7	8.75	12	J	6.87	128		118.00	192		184.50
		5D	7.46	0.05		148	U	0	6985		268	2.75	Ļ	0.113	1.58	J	0.87	8.8	0.03	2	U	6.55	108	_	14.14	177	[10.61
4/19/18 11:30	38.0	5A	8.09	8.10	9806	148	U	148.00	8490		8565	0.74	J	0.82	0.44	U	0.44	9.0	9.33	365		375.00	56.0		53.90	34.4		32.05
		5B	8.1	0.01	+	148	U	0	8640		106	0.90	J	0.113	0.44	U	0	9.6	0.44	385		14.14	51.8		2.97	29.7	,	3.32
4/19/18 11:30	38.0	5C	7.49	7.46	9806	148	U	148.00	6530		6345	1.97	-	2.37	1.35	×	1.48	8.7	8.70	9	J	5.68	125		124.00	187		186.50
100110-11	12.0	50	7.43	0.04	0007	148	U	U 140.00	6160		262	2.76	┝─,	0.559	1.60	J	0 11	8.7	0.02	2	U	4.88	125		1.41	186.00		0.71
4/23/18 11:30	42.0	5P	8.07	8.08	9807	148		148.00	8610		8595	1.15	T	0.99	0.44	U	0.44	9.0	8.93	288		290.87	59.94		58.62	37.15	-	36.27
4/22/18 11/20	42.0	о С	0.00	7.50	0807	140		149.00	6060		6740	0.82	J	2.51	0.44		2.60	0.7	0.06	294		5.95	102.40		1.8/	33.4		1.24
4/25/18 11:30	42.0	5D	7.55	0.05	9807	148	11	148.00	6520		311	2.08	-	3.31	4.02		3.00	8.0	0.02	2	J	3.00	06.2		5.17	101.28	-	3 72
1		50	1.55	0.03	1	140		U	0520		511	4.34		1.1/4	4.72		4	0.0	0.02	4	10	3.77	70.2		5.17	150.0		3.14

SET 6 Killed	I	ort Lewis JBN	ſL.		Start	3/12/18 12:00																			
Live Control																									
							VOC's ug/	L				Methane/Ethene	ug/L			Anio	ons mg/L				VI	A mg/L			
DATE	TIME(days)	Bottle	pH	mean	ATL ID	VC	Q mean	cDCE	Q	mean	Methane	Q mean	Ethene	Q	mean	Bromide	Q mean	Lactic	Q	mean	Acetic	Q mean	Proprionic	Q	mean
3/12/18 12:00	0.0	6A	6.10	6.12	9789	148	U 148.00	9920		9245	1.12	1.09	0.44	U	0.44	9.4	9.95	615		612.50	0.93	U 0.93	3.7	U	3.70
		6B	6.13	0.02		148	U 0	8570		955	1.06	0.042	0.44	U	0	10.5	0.78	610		3.54	0.93	U 0.00	3.7	U	0.00
3/12/18 12:00	0.0	6C	6.30	6.34	9789	148	U 148.00	10860	_	9775	0.59	J 0.89	0.44	U	0.44	8.84	9.77	501		519.50	0.93	U 0.93	3.7	U	3.70
		<u>5D</u>	6.38	0.06		148	U 0	8690	_	1534	1.19	0.424	0.44	U	0	10.7	1.32	538	_	26.16	0.93	U 0.00	3.7	U	0.00
3/15/18 12:15	3.0	6A	6.17	6.17	9790	148	U 148.00	8820	_	8330	0.98	0.99	0.44	U	0.44	9.48	10.04	421		420.50	0.93	U 0.93	3.7	U	3.70
		6B	6.17	0.00		148	0 0	7840		693	0.99	0.007	0.44	U .	0	10.6	0.79	420	,	0.71	0.93	U 0.00	3.7	U	0.00
3/15/18 12:15	3.0	6C	6.57	6.61	9790	148	U 148.00	9980		9080	2.39	2.11	0.44	0	0.44	9.68	9.12	367		358.50	0.93	0.93	3.7	U	3.70
		6D	6.65	0.06	0701	148	U U	8180	_	1273	1.82	0.403	0.44	<u> </u>	0	8.56	0.79	350		12.02	0.93	0.00	3.7	<u> </u>	0.00
3/19/18 12:00	7.0	6A	6.19	0.17	9791	148	U 148.00	7520		8095	1.05	0.042	0.44	U U	0.44	9.62	8.94	625	-	018.50	0.93	U 0.93	3.7	U	3.70
2/10/19 12:00	7.0	0B	6.52	6.50	0701	140	U 148.00	0500		013	2.12	2.68	0.44		0.44	7.24	6.37	464		9.19	0.93	U 0.00	3.7	1	2.70
3/19/18 12:00	7.0	6D	6.65	0.09	9791	140	U 148.00	7920	_	1181	2.13	0.643	0.44	U .	0.44	5.10	1.45	515		36.06	0.93	U 0.95	3.7	11	0.00
2/22/18 10:50	10.0	64	6.23	6.22	0702	148	U 148.00	8730		8140	0.81	L 0.75	0.44	U,	0.44	7.78	8.59	520		519.50	0.93	U 0.93	3.7	U	3.70
3/22/18/10:50	10.0	6B	6.20	0.02	7172	148	U 0	7550	-	834	0.69	J 0.085	0.44	U U	0.44	939	1 14	519		0.71	0.93	U 0.00	3.7	U	0.00
3/22/18 10:50	10.0	6C	6.56	6.61	9792	148	U 148.00	9100		8370	3.6	2.68	0.53	I	0.49	6.80	6.03	504		511.00	0.93	U 0.93	3.7	U.	3 70
3/22/10/10:50	10.0	6D	6.65	0.06	7172	148	U 0	7640	_	1032	1.76	1.301	0.44	U	0	5.25	1.10	518		9.90	0.93	U 0.00	3.7	U	0.00
3/26/18 12:00	14.0	6A	7.39	7.39	9793	148	U 148.00	9140		8460	1.05	0.98	0.44	U	0.44	7.38	8.36	443		487.00	0.93	U 0.93	3.7	U	3.70
		6B	7.39	0.00		148	U 0	7780		962	0.90	J 0.106	0.44	U	0	9.34	1.39	531		62.23	0.93	U 0.00	3.7	U	0.00
3/26/18 12:00	14.0	6C	7.12	7.14	9793	148	U 148.00	10140		8940	3.96	3.35	0.44	U	0.44	7.09	5.92	520		478.00	0.93	U 0.93	3.7	U	3.70
		6D	7.15	0.02		148	U 0	7740		1697	2.73	0.870	0.44		0	4.74	1.66	436		59.40	0.93	U 0.00	3.7	U	0.00
3/29/18 12:00	17.0	6A	7.35	7.36	9794	148	U 148.00	8320	1	7785	0.93	J 0.93	0.44	U	0.44	7.13	8.03	518		512.50	0.93	U 0.93	3.7	U	3.70
		6B	7.36	0.01		148	U 0	7250		757	0.93	J 0.000	0.44	U	0	8.92	1.27	507		7.78	0.93	U 0.00	3.7	U	0.00
3/29/18 12:00	17.0	6C	7.12	7.15	9794	148	U 148.00	8150		7295	3.54	3.07	0.44	U	0.44	7.24	5.65	508		490.50	0.93	U 0.93	3.7	U	3.70
		6D	7.17	0.04		148	U 0	6440		1209	2.59	0.672	0.44	U	0	4.05	2.26	473		24.75	0.93	U 0.00	3.7	U	0.00
4/2/18 12:00	21.0	6A	7.4	7.40	9795	148	U 148.00	7380		7520	1.03	1.03	0.44	U	0.44	6.83	7.80	470		491.50	0.93	U 0.93	3.7	U	3.70
		6B	7.39	0.01		148	U 0	7660		198	1.02	0.007	0.44	U	0	8.77	1.37	513		30.41	0.93	U 0.00	3.7	U	0.00
4/2/18 12:00	21.0	6C	7.18	7.21	9795	148	U 148.00	9520	_	8765	4.28	3.62	0.44	U	0.44	6.66	5.33	466		481.50	0.93	U 0.93	3.7	U	3.70
		6D	7.23	0.04		148	U 0	8010	_	1068	2.96	0.933	0.44		0	4.00	1.88	497	_	21.92	0.93	U 0.00	3.7	U	0.00
4/5/18 12:00	24.0	6A	7.38	7.38	9796	148	U 148.00	7960	_	7710	0.86	J 0.88	0.44	U	0.44	6.98	7.47	513		481.50	0.93	U 0.93	3.7	U	3.70
		6B	7.38	0.00		148	0 0	7460		354	0.9	J 0.028	0.44	,	0	7.96	0.69	450		44.55	0.93	U 0.00	3.7		0.00
4/5/18 12:00	24.0	6C	7.19	7.21	9796	148	U 148.00	8640		8210	3.88	3.20	0.44	0	0.44	6.18	4.97	534		508.50	0.93	0 0.93	3.7	U	3.70
	20.0	6D	7.23	0.03	0707	148	U U	//80	_	608	2.52	0.962	0.44	<u> </u>	0	3.76	1.71	483		36.06	0.93	0 0.00	3.7	<u> </u>	0.00
4/9/18 12:00	28.0	6A	7.39	7.40	9/9/	148	U 148.00	8070	_	//40	1.15	1.0/	0.98	1.1	0.71	6.88	7.63	490		496.50	0.93	U 0.93	3.7	0	3.70
40/10 12:00	28.0	0B	7.4	7.24	0707	148	U 148.00	/410		467	0.98	0.120	0.44	- U	0.44	6.44	1.05	503		9.19	0.93	U 0.00	3.7		2.70
4/9/18/12:00	20.0	6D	7.22	0.03	9191	140	U 148.00	7730	-	785	2.80	0.679	0.44	I	0.44	3.80	1.87	4/1		485.00	0.93	U 0.00	3.7	U	0.00
4/12/18 12:00	31.0	64	7.31	7.32	9800	148	U 148.00	8800	_	8455	0.80	I 0.83	0.44	U	0.44	7.01	7.78	492		491.50	0.93	U 0.93	61	I I	4.92
412101230	51.0	6B	7.32	0.01	,,,,,,	148	U 0	8110	_	488	0.85	J 0.035	0.44	U	0	8.55	1.09	491		0.71	0.93	U 0.00	3.7	U	1.73
4/12/18 12:00	31.0	6C	7.1	7.15	9800	148	U 148.00	9730		8840	3.63	3.00	0.44	U	0.44	6.36	5.07	485		477.00	0.93	U 0.93	3.7	U	3.70
		6D	7.2	0.07		148	U 0	7950		1259	2.37	0.891	0.44	U	0	3.77	1.83	469		11.31	0.93	U 0.00	3.7	U	0.00
4/16/18 12:00	35.0	6A	7.39	7.40	9802	148	U 148.00	8156	1	7779	0.95	0.95	0.44	U	0.44	7.25	8.03	488		483.00	0.93	U 0.93	3.7	U	3.70
		6B	7.4	0.01		148	U 0	7402		533	0.95	0.000	0.44	U	0	8.81	1.10	478		7.07	0.93	U 0.00	3.7	U	0.00
4/16/18 12:00	35.0	6C	7.23	7.28	9802	148	U 148.00	8543		7823	4.17	3.64	0.44	U	0.44	6.08	4.75	400		427.50	0.93	U 0.93	3.7	U	3.70
		6D	7.33	0.07		148	U 0	7102		1019	3.10	0.757	0.44	U	0	3.41	1.89	455		38.89	0.93	U 0.00	3.7	U	0.00
4/19/18 12:00	38.0	6A	7.35	7.36	9806	148	U 148.00	8020		7275	0.77	J 0.84	0.44	U	0.44	9.31	8.71	615		579.50	0.93	U 0.93	3.7	U	3.70
		6B	7.36	0.01		148	U 0	6530		1054	0.90	J 0.092	0.44	U	0	8.11	0.85	544		50.20	0.93	U 0.00	3.7	U	0.00
4/19/18 12:00	38.0	6C	7.17	7.22	9806	148	U 148.00	9590		8055	3.10	3.08	0.44	U	0.48	5.83	4.24	473		468.00	0.93	U 0.93	3.7	U	3.70
		6D	7.26	0.06		148	U 0	6520	_	2171	3.05	0.035	0.51	J	0	2.64	2.26	463		7.07	0.93	U 0.00	3.7	U	0.00
4/23/18 12:00	42.0	6A	7.38	7.39	9807	148	U 148.00	7930	_	7520	0.82	J 0.83	0.44	U	0.44	7.69	8.11	425	+	430.27	0.93	U 0.93	3.7	U	3.70
		6B	7.39	0.01	ļ	148	U 0	7110		580	0.84	J 0.014	0.44	U	0	8.52	0.59	435		7.23	0.93	U 0.00	3.7	U	0.00
4/23/18 12:00	42.0	6C	7.22	7.29	9807	148	U 148.00	8410	_	7560	3.49	3.00	0.44	U	0.44	5.76	4.32	421	+	420.35	0.93	U 0.93	3.7	U	3.70
		6D	7.36	0.10		148	U 0	6710		1202	2.5	0.700	0.44	I U ſ	0	2.87	2.04	420		0.31	0.93	U 0.00	3.7	U	0.00

JBLM1, Compiled rate coefficients and biomarker abundances

																					LOG + 0							
																					Transformed							
																					for Analysis							
						Genes	Functiona		DHC gene								Peptides				Rates					UG18.xls	om RATES_07A	Fro
A pceA std	pceA	fdhA std	fdhA	vcrA std	vcrA	tceA std	tceA	DHC std	DHC_16S gene	VcrA std	VcrA	TceA std	TceA	PceA std	PceA	FdhA std	FdhA	LogKvcSD	Log Kvc	KcisSD	Log Kcis	Kvc 95%CI	Kvc	Kcis 95%CI	Kcis) n	TIME ZERO	
234 6.513652	7.4423	7.727589	8.641358	8.361673	9.014401	8.262871	9.040522	8.07	8.88	11.92		12.97		12.35		13.54		9.53E-01	1.01E+00	2.22E+00	1.80E+00	3.91E+00	1.02E+01	7.31E+01	6.26E+01	21	Set1A	JBLM1 TIMEZERO
558 6.513652	7.3265	7.727589	8.534854	8.361673	8.785642	8.262871	8.883965	8.07	8.72	11.92	13.10	12.97	13.31	12.35	12.80	13.54	13.76	9.18E-01	1.01E+00	2.09E+00	1.76E+00	3.61E+00	1.02E+01	5.37E+01	5.70E+01	21	Set1B	JBLM1 TIMEZERO
075 6.513652	7.4000	7.727589	8.542048	8.361673	8.823625	8.262871	8.902009	8.07	8.80	11.92	13.14	12.97	13.17	12.35	12.82	13.54	13.23	1.13E+00	1.05E+00	2.52E+00	1.87E+00	5.87E+00	1.13E+01	1.46E+02	7.36E+01	21	Set1C	JBLM1 TIMEZERO
198 4.905415	5.8431	6.264624	7.136456	6.647669	7.448951	6.679881	7.469212	6.53	7.30	11.27	11.42	11.50	11.64	11.52	11.82	11.45	11.28	-7.80E-01	-5.13E-01	5.84E-02	1.70E-01	7.25E-02	3.07E-01	4.99E-01	1.48E+00	21	Set2A	JBLM1 TIMEZERO
.007 4.905415	5.7490	6.264624	7.054482	6.647669	7.311446	6.679881	7.373395	6.53	7.14	11.27	11.54	11.50	11.72	11.52	11.89	11.45	11.80	-7.49E-01	-4.66E-01	4.53E-02	1.72E-01	7.78E-02	3.42E-01	4.84E-01	1.49E+00	21	Set2B	JBLM1 TIMEZERO
296 4.905415	5.8472	6.264624	7.174965	6.647669	7.45093	6.679881	7.520002	6.53	7.28	11.27	11.79	11.50	11.91	11.52	11.94	11.45	11.83	-7.92E-01	-4.73E-01	8.24E-02	2.26E-01	7.04E-02	3.37E-01	5.28E-01	1.68E+00	21	Set2C	JBLM1 TIMEZERO
.067 4.167062	3.8420	5.377145	5.045074	5.55058	5.166447	5.621864	5.252395	5.49	5.05	10.28	10.71	10.95	11.24	9.84	10.51	10.16	10.58	-2.28E+00	-2.81E+00	-2.13E+00	-1.62E+00	1.84E-03	1.54E-03	2.60E-03	2.41E-02	33	Set3A	JBLM1 TIMEZERO
122 4.167062	3.0231	5.377145	4.303506	5.55058	4.56745	5.621864	4.607223	5.49	4.36	10.28	10.38	10.95	10.84	9.84	10.49	10.16	10.48	-6.72E+00	-3.24E+00	-7.47E+00	-1.81E+00	6.57E-08	5.81E-04	1.18E-08	1.57E-02	33	Set3B	JBLM1 TIMEZERO
.371 4.167062	4.4613	5.377145	5.672771	5.55058	5.84498	5.621864	5.916362	5.49	5.78	10.28	10.19	10.95	10.90	9.84	#DIV/0!	10.16	10.23	-5.72E+00	-2.44E+00	-6.20E+00	-1.58E+00	6.64E-07	3.66E-03	2.18E-07	2.60E-02	33	Set3C	JBLM1 TIMEZERO
.909 1.692881	1.6839	3.487099	3.344207	3.554586	3.686425	3.592633	3.670815	3.21	3.58	9.39	9.48	9.43	9.91			9.95	10.23									24	Set4A	JBLM1 TIMEZERO
.097 1.692881	2.1210	3.487099	3.841064	3.554586	3.978503	3.592633	3.998031	3.21	3.69	9.39	9.89	9.43	10.07			9.95	10.47			-3.49E+00	-2.87E+00			1.32E-04	1.34E-03	24	Set4B	JBLM1 TIMEZERO
167 1.692881	1.6561/	3.487099	3.071343	3.554586	3.391993	3.592633	3.362912	3.21	3.24	9.39	9.78	9.43	9.84			9.95	#DIV/0!			-2.48E+00	-2.87E+00			1.36E-03	1.36E-03	24	Set4C	JBLM1 TIMEZERO
																										30	Set5A	
																										30	Set5B	
																										30	Set5C	
																					LOG + 0							
																					Transformed							
																					for Analysis							
						Genes	Functiona		DHC gene								Peptides				Rates							
A pceA std	pceA	fdhA std	fdhA	vcrA std	vcrA	tceA std	tceA	DHC std	DHC_16S gene	VcrA std	VcrA	TceA std	TceA	PceA std	PceA	FdhA std	FdhA	LogKvcSD	Log Kvc	KcisSD	Log Kcis	Kvc 95%CI	Kvc	Kcis 95%CI	Kcis	[n	TIME MIDPOINT	T
.479 6.5273	7.2554	7.2764	8.474142	7.078091	8.841375	7.992841	8.781646	7.626064285	8.709371652	12.55	12.13	12.88	12.73	12.36	12.41	12.65	12.44	9.53E-01	1.01E+00	2.22E+00	1.80E+00	3.91E+00	1.02E+01	7.31E+01	6.26E+01	21	Set1A	JBLM1 TIMETWO
236 6.5273	7.3382	7.2764	8.525947	7.078091	8.855585	7.992841	8.887602	7.626064285	8.742700785	12.55	11.94	12.88	13.11	12.36	12.43	12.65	12.22	9.18E-01	1.01E+00	2.09E+00	1.76E+00	3.61E+00	1.02E+01	5.37E+01	5.70E+01	21	Set1B	JBLM1 TIMETWO
151 6.5273	7.3931	7.2764	8.498583	7.078091	8.845142	7.992841	8.891143	7.626064285	8.670652654	12.55	12.86	12.88	12.78	12.36	12.73	12.65	12.95	1.13E+00	1.05E+00	2.52E+00	1.87E+00	5.87E+00	1.13E+01	1.46E+02	7.36E+01	21	Set1C	JBLM1 TIMETWO
.457 4.669666	5.9144	4.943032	7.045005	6.232483	7.260628	5.74561	7.371944	5.418067973	7.179655172	11.02	10.26	11.57	11.39	11.63	11.37	11.27	11.08	-7.80E-01	-5.13E-01	5.84E-02	1.70E-01	7.25E-02	3.07E-01	4.99E-01	1.48E+00	21	Set2A	JBLM1 TIMETWO
.457 4.669666	5.9144	4.943032	7.051332	6.232483	7.321486	5.74561	7.388871	5.418067973	7.166144123	11.02	11.32	11.57	11.81	11.63	11.94	11.27	11.46	-7.49E-01	-4.66E-01	4.53E-02	1.72E-01	7.78E-02	3.42E-01	4.84E-01	1.49E+00	21	Set2B	JBLM1 TIMETWO
386 4.669666	5.8693	4.943032	7.045974	6.232483	7.329584	5.74561	7.389834	5.418067973	7.179078359	11.02	10.57	11.57	11.71	11.63	11.59	11.27	11.37	-7.92E-01	-4.73E-01	8.24E-02	2.26E-01	7.04E-02	3.37E-01	5.28E-01	1.68E+00	21	Set2C	JBLM1 TIMETWO
716 4.22574	4.4897	5.67668	5.930635	5.883705	6.140923	5.896323	6.154825	5.698525843	5.956243093	#DIV/0!	#VALUE!	10.21	10.23	10.40	10.01	9.97	9.56	-2.28E+00	-2.81E+00	-2.13E+00	-1.62E+00	1.84E-03	1.54E-03	2.60E-03	2.41E-02	33	Set3A	JBLM1 TIMETWO
365 4.22574	2.9453	5.67668	4.353225	5.883705	4.587023	5.896323	4.635994	5.698525843	4.452861088	#DIV/0!	#VALUE!	10.21	10.58	10.40	9.93	9.97	9.82	-6.72E+00	-3.24E+00	-7.47E+00	-1.81E+00	6.57E-08	5.81E-04	1.18E-08	1.57E-02	33	Set3B	JBLM1 TIMETWO
388 4.22574	3.4338	5.67668	4.568244	5.883705	4.895441	5.896323	4.934293	5.698525843	4.699565761	#DIV/0!	#VALUE!	10.21	10.57	10.40	10.72	9.97	10.32	-5.72E+00	-2.44E+00	-6.20E+00	-1.58E+00	6.64E-07	3.66E-03	2.18E-07	2.60E-02	33	Set3C	JBLM1 TIMETWO
UE! #DIV/0!	#VALU	2.046297	#VALUE!	2.874253	#VALUE!	2.493885	#VALUE!	2.75119299		#DIV/0!	#VALUE!	9.58	#DIV/0!	#DIV/0!	#DIV/0!	#DIV/0!	#DIV/0!									24	Set4A	JBLM1 TIMETWO
UE! #DIV/0!	#VALU	2.046297	3.346434	2.874253	3.449032	2.493885	3.386912	2.75119299	3.240529006	#DIV/0!	#VALUE!	9.58	9.93	#DIV/0!	#DIV/0!	#DIV/0!	10.30			-3.49E+00	-2.87E+00			1.32E-04	1.34E-03	24	Set4B	JBLM1 TIMETWO
UE! #DIV/0!	#VALU	2.046297	3.314517	2.874253	3.243887	2.493885	3.300238	2.75119299	2.974263199	#DIV/0!	#VALUE!	9.58	9.91	#DIV/0!	#DIV/0!	#DIV/0!	#DIV/0!			-2.48E+00	-2.87E+00			1.36E-03	1.36E-03	24	Set4C	JBLM1 TIMETWO
																								1		30	Set5A	
																										30	Set5B	
					issing	not sent/m	sampling				NA/ND															30	Set5C	
198 007 296 067 122 371 909 097 167 167 407 236 151 1457 1386 1716 388 1457 1386 1457 1386 1457 1386 1457 14	5.84313 5.74300 3.0231 1.6339 2.12100 1.65610 1.65610 1.65610 1.65610 1.65610 1.65610 1.65610 1.65610 1.65610 1.65610 1.65610 1.65610 1.65610 1.65610 1.65610 1.65610 1.655100 1.655100 1.655100 1.65510000000000000000000000000000000000	6.264524 6.264524 6.264524 5.377145 5.377145 5.377145 3.487099 3.487099 3.487099 3.487099 3.487099 3.487099 2.487099 2.487099 2.487099 2.487099 2.48709 2.2764 4.943032 2.567668 5.67668 5.67668 5.67668	7.136455 7.054482 7.054482 5.045074 3.03306 5.672711 3.841064 3.071343 3.04107 3.841064 3.071343 3.041042 8.825947 8.825947 8.849858 7.065352 7.045374 4.355225 7.045374 4.355225 7.045374 3.34634 3.34517	6.647669 6.647669 5.5005 5.5005 3.55058 3.554586 3.554586 3.554586 3.554586 3.554586 3.554586 3.554586 3.554586 3.554586 3.554586 4.7076091 7.076091 4.7076091 6.232483 6.232483 6.232483 2.883705 5.883705 2.883705 2.883705 2.883705 2.883705 2.883705 2.883705	7,448951 7,311446 7,311446 4,56745 5,16647 3,456745 5,8498 8,868452 3,978503 3,391993 3,391943 3,391943 3,391943 3,291564 2,391943 3,291564 2,391943 3,291564 2,391943 3,291564 2,391943 3,291564 2,391943 3,291564 2,391943 3,291564 2,391943 3,291946 3,291945 3,29194 3,291945 3,291955 3,2919555 3,291955555555555555555555555555555555555	6, 679881 6, 679881 6, 679881 5, 621864 5, 621864 3, 592633 3, 592633 5, 792841 5, 792841 5, 74561 5, 74561 5, 74561 5, 74562 5, 74563 2, 493885 2, 493885 2, 493885	7,469212 7,373395 7,52000 5,252395 5,916362 3,998031 3,3670815 3,998031 3,3670815 3,998031 3,3670815 3,998031 3,3670815 3,998031 3,3670815 3,998031 3,3670815 3,398031 4,378284,37828 4,37848 4,37848 4,37848 4,37848 4,37848 4,37848 4,378484,37848 4,37848 4,37848	6.53 6.53 5.49 5.49 3.21 3.21 3.21 3.21 7.62064285 7.75119299	7.30 7.14 7.28 5.05 4.36 5.78 3.58 3.69 3.24 DHC gene DHC L55 gene 8.70937162 8.70937162 8.870937162 7.71097182 9.595624303 8.4595655761 3.340529006 2.574263199	11.27 11.27 11.27 10.28 10.28 9.39 9.39 9.39 9.39 9.39 9.39 9.39 9.3	11-12 11-54 11-79 10.71 10.38 10.19 9.78 9.78 9.78 9.78 9.78 9.78 9.78 9.7	11:50 11:50 11:50 11:50 10:55 9:43 9:43 9:43 9:43 9:43 9:43 9:43 9:43	11.64 11.72 11.72 11.72 11.71 11.24 10.90 9.91 10.07 9.84 10.07 9.84 10.07 9.84 10.07 10.73 10.11 12.73 10.11 12.73 13.11 12.78 13.11 13.1	11.52 11.52 9.84 9.84 9.84 9.84 9.84 9.84 9.84 12.36 1	11.82 11.89 11.94 10.51 10.49 7004/00 7004/00 7004/00 10.40 10.410	11.45 11.45 10.16 10.16 10.16 10.16 10.16 10.16 10.16 10.16 10.95 9.95 9.95 9.95 9.95 9.95 9.95 9.95	11.28 11.80 11.83 10.58 10.23 10.23 10.47 #DIV/01 Peptides FdhA 12.44 12.22 12.95 11.08 11.46 11.37 9.56 9.82 10.32 #DIV/01	- 7-986-01 7-926-01 7-926-01 7-926-01 7-926-01 5-726-00 5-726-00 9-936-01 9	5,138-00,466-01,466-00-000-000-000-000-000-000-000-000-0	5.84E-02 4.53E-02 8.24E-02 -2.13E+00 -7.47E=00 -6.20E+00 -3.49E+00 -2.48E+00 2.22E+00 2.22E+00 2.22E+00 2.52E+00 5.84E+02 -2.48E+00 -6.20E+00 -3.49E+00 -2.48E+00	1.70E-01 1.77E-01 2.26E-01 -1.62E+00 -1.58E+00 -2.87E+00 -2.87E+00 -2.87E+00 -2.87E+00 -2.87E+00 -2.87E+00 -1.86E+00 -1.86E+00 -1.58E+00 -2.87E+00 -2.	7.25E-02 7.78E-02 7.04E-02 1.84E-03 6.54E-03 6.64E-07 8.54E-07 8.595KC1 3.91E-00 3.51E+00 3.51E+00 5.87E+00 7.72E-02 7.72E-02 7.72E-02 7.74E-02 7.74E-02 6.57E-08 6.57E-08 6.57E-08 6.57E-08 6.57E-08	3.07E-01 3.47E-01 3.47E-01 1.54E-03 5.81E-04 3.66E-03 1.02E+01 1.02E+01 1.02E+01 1.02E+01 1.02E+01 1.02E+01 3.47E-01 3.47E-01 3.47E-01 5.81E-04 3.66E-03	4 996 (1) 4 846 (1) 5 286 (1) 5 286 (1) 1 326 (4) 1 326 (4) 1 326 (4) 1 326 (4) 1 466 (2) 1 466 (2) 1 466 (2) 1 466 (2) 1 486 (2) 1 136 (3) 1 136 (3)	1.488-00 1.688-00 2.411-02 1.576-02 2.606-02 1.346-03 1.366-03 1.366-03 1.366-03 1.366-03 1.366-03 1.488-00 1.488+00000000000000000000000000000000000	21 21 33 33 33 24 24 24 24 24 30 30 30 30 30 7 7 7 1 21 21 21 21 21 21 21 21 21 21 33 33 30 30 30 30 30 30 30 30 30 30 30	Set2A Set2B Set2C Set3A Set3B Set3C Set4A Set4B Set4C Set5A Set5A Set5C Set5A Set5C Set5A Set5C Set5A Set5C Set5A Set2C Set2A Set2B Set2C Set2A Set3B Set3C Set3A Set3B Set3C Set5A Set3B Set3C Set5A Set3B Set3C Set5A Set5B Set5C	JBLMI TIMEZERO JBLMI TIMETWO JBLMI TIMETWO

JBLM2, Compiled rate coefficients and biomarker abundances

| |

 | | |
 | | | LOG + 0 Transfor
 | rmed for Ana | lysis | | | | | |
 | | | | | | | | | | | | | |
--
--
---	--	--	--
--	--	---	--
--	--	--	--

 | | |
 | | | Rates
 | | | | Peptides | | | |
 | | | | DHC gene | | Functional | Genes | | | | | | |
| |

 | TIME ZERO | Kcis | Kcis 95%CI
 | Kvc | Kvc 95%Cl | Log Kcis
 | KcisSD | Log Kvc | LogKvcSD | FdhA | FdhA std | PceA | PceA std | TceA
 | TceA std | VcrA | VcrA std | DHC 16S gene | DHC std | tceA 1 | tce A std | vcrA | vcrA std | fdhA | fdhA std | pceA | pceA std |
| IL | BLM2 TZERO

 | Set1A | 1.05E+00 | 9.37E-01
 | 1.13E-01 | 1.82E-02 | 0.021
 | 0.386 | -0.946 | -1.326 | 10.38 | 9.96 | 10.77 | 10.67 | 10.55
 | 10.58 | #VALUE! | 9.58 | 7.13 | 7.06 | 7.24 | 6.38 | 7.17 | 6.74 | 7.24 | 6.78 | 6.06 | 4.64 |
| JI | BLM2 TZERO

 | Set1B | 1.05E+00 | 1.14E+00
 | 1.32E-01 | 2.78E-02 | 0.021
 | 0.472 | -0.880 | -1.141 | 10.16 | 9.96 | 10.35 | 10.67 | 10.07
 | 10.58 | 10.05 | 9.58 | 7.19 | 7.06 | 7.16 | 6.38 | 7.04 | 6.74 | 7.15 | 6.78 | 6.03 | 4.64 |
| JI | BLM2 TZERO

 | Set1C | 1.13E+00 | 1.28E+00
 | 1.74E-01 | 4.06E-02 | 0.051
 | 0.522 | -0.759 | -0.977 | 10.52 | 9.96 | 10.74 | 10.67 | 10.75
 | 10.58 | 9.76 | 9.58 | 7.54 | 7.06 | 7.29 | 6.38 | 7.34 | 6.74 | 7.41 | 6.78 | 6.03 | 4.64 |
| 1 | BLM2 TZERO

 | Set1A_Dup | 2.82E-01 | 3.76E-02
 | 1.26E-02 | 3.07E-02 | -0.550
 | -1.249 | -1.898 | -1.337 | 10.64 | 10.14 | 10.76 | 10.73 | 10.63
 | 10.55 | #VALUE! | 9.70 | 7.16 | 6.76 | 7.06 | 6.48 | 7.03 | 6.49 | 7.04 | 6.58 | 5.85 | 5.38 |
| 1 | BLWIZ TZERO

 | Set1C Dup | 2.97E-01
2.21E-01 | 3.14E-02
1 71E-02
 | 2.01E-05 | 2.28E-02
2.11E-02 | -0.527
 | -1.328 | -4.583 | -1.467 | 10.51 | 10.14 | 10.56 | 10.73 | 10.41
 | 10.55 | 9.95 | 9.70 | 6.02 | 6.76 | 6.84 | 6.48 | 6.91 | 6.49 | 6.84 | 6.58 | 5.05 | 5.38 |
| ≥ ji | BLM2 TZERO

 | Set2A | 2.77E-03 | 4.03E-04
 | 3.10E-03 | 8.56E-03 | -2.557
 | -2.901 | -2.509 | -1.573 | 10.05 | 10.14 | 11.77 | 11.52 | 11.64
 | 11.55 | 12.03 | 11.27 | 4.51 | 4.38 | 4.32 | 4.02 | 4.32 | 4.22 | 4.65 | 4.35 | 2.95 | 2.38 |
| Š I | BLM2 TZERO

 | Set2B | 1.76E-03 | 2.44E-04
 | 2.57E-03 | 8.29E-03 | -2.755
 | -3.118 | -2.590 | -1.587 | | | 11.84 | 11.52 | 11.72
 | 11.55 | 12.00 | 11.27 | 3.79 | 4.38 | 3.66 | 4.02 | 3.66 | 4.22 | 3.75 | 4.35 | 2.63 | 2.38 |
| Ş 1 | BLM2 TZERO

 | Set2C | 2.40E-03 | 3.91E-04
 | 4.22E-03 | 9.89E-03 | -2.620
 | -2.913 | -2.374 | -1.510 | | | 11.85 | 11.52 | 11.91
 | 11.55 | 11.92 | 11.27 | 3.30 | 4.38 | 3.06 | 4.02 | 3.06 | 4.22 | 2.99 | 4.35 | 2.91 | 2.38 |
| JI | BLM2 TZERO

 | Set3A | 1.00E-03 | 2.62E-04
 | 2.79E-03 | 1.35E-02 | | | | | | | | | | | |
 | | | | | | | |
 | | | | | | | | | | | | | |
| 11 | BLM2 TZERO

 | Set3B | 8.75E-04 | 2.18E-04
 | 3.31E-03 | 1.31E-02 | | | | | | | | | | | |
 | | | | | | | |
 | | | | | | | | | | | | | |
| 1 | BLM2 TZERO

 | Set3C | 9.61E-04 | 2.52E-04
 | 1.71E-03 | 1.33E-02 | | | | | | | | | | | |
 | | | | | | | |
 | | | | | | | | | | | | | |
| 1 | BLWIZ TZERO

 | Set4A
Set4B | 8 25E-04 | 2.95E-04
2.09E-04
 | 3.72E-03 | 1.37E-02 | | | | | | | | | | | |
 | | | | | | | |
 | | | | | | | | | | | | | |
| , ii | BLM2 TZERO

 | Set4C | not sample | not sample
 | not sample | not sampled | | | | | | | | | | | |
 | | | | | | | |
 | | | | | | | | | | | | | |
| JI | BLM2 TZERO

 | Set5A | rate not co | rate not co
 | rate not co | rate not compu | ted
 | | | | | | | |
 | | | | | | | | | | | | | |
| JI | BLM2 TZERO

 | Set5B | rate not co | rate not co
 | rate not co | rate not compu | ted
 | | | | | | | |
 | | | | | | | | | | | | | |
| 11 | BLM2 TZERO

 | Set6A
Set6B | rate not co | rate not co
 | rate not co | rate not compu | ted
 | | | | | | | |
 | | | | | | | | | | | | | |
| 1 | BLIVIZ TZERO

 | Set0b
Set1D | 1.42F-01 | 1.57E-02
 | 1.89F-02 | 8.12F-03 | -8.48F-01
 | -1.52E+00 | -1.72F+00 | -1.80F+00 | 9.55 | 9.20 | 9.33 | 9.46 | 9.13
 | 9.25 | 8.56 | 8.41 | 5.98 | 6.29 | 6.01 | 6.31 | 6.10 | 6.38 | 6.14 | 6.56 | 4.85 | 4.94 |
| , | BLM2 TZERO

 | Set1E | 8.75E-02 | 1.33E-02
 | 1.76E-02 | 1.52E-02 | -1.06E+00
 | -1.59E+00 | -1.75E+00 | -1.53E+00 | 8.92 | 9.20 | #N/A | 9.46 | #N/A
 | 9.25 | 8.78 | 8.41 | 5.85 | 6.29 | 6.00 | 6.31 | 6.12 | 6.38 | 6.11 | 6.56 | 4.79 | 4.94 |
| JI | BLM2 TZERO

 | Set1F | 9.62E-02 | 1.50E-02
 | 2.07E-02 | 1.51E-02 | -1.02E+00
 | -1.54E+00 | -1.68E+00 | -1.53E+00 | 9.61 | 9.20 | 9.78 | 9.46 | 9.60
 | 9.25 | 7.96 | 8.41 | 6.62 | 6.29 | 6.66 | 6.31 | 6.74 | 6.38 | 6.88 | 6.56 | 5.33 | 4.94 |
| J | 3LM2 TZERO

 | Set1D_Dup | 7.83E-02 | 4.63E-03
 | 1.00E-05 | 1.64E-02 | -1.11E+00
 | -1.92E+00 | -5.00E+00 | -1.37E+00 | 9.86 | 9.55 | 9.84 | 10.19 | 9.86
 | 10.08 | 9.39 | 9.35 | 7.01 | 6.08 | 6.91 | 6.32 | 7.09 | 6.30 | 7.12 | 5.92 | 5.93 | 5.06 |
| S - | BLM2 TZERO

 | Set1E_Dup | 5.92E-02 | 3.78E-03
 | 1.83E-02 | 1.98E-02 | -1.23E+00
 | -2.01E+00 | -1.74E+00 | -1.29E+00 | 9.99 | 9.55 | 10.29 | 10.19 | 10.21
 | 10.08 | 9.39 | 9.35 | 6.92 | 6.08 | 6.95 | 6.32 | 6.92 | 6.30 | 7.07 | 5.92 | 5.85 | 5.06 |
| S | BLM2 TZERO

 | Set1F_Dup
Set2D | 5.67E-02
1.00E-03 | 3.50E-03
 | 2.69E-03 | 1.83E-02
1.52E-02 | -1.25E+00
 | -2.04E+00 | -2.57E+00 | -1.32E+00 | 9.99 | 9.55 | #DIV/01 | 8 15 | 8 10
 | 8 13 | 9.80 | 9.35 | 5.20 | 4.60 | 5.28 | 0.32
4.46 | 5.41 | 4.85 | 5.59 | 4.89 | 4.01 | 3.58 |
| ÷ ji | BLM2 TZERO

 | Set2E | 1.00E-03 | 2.86E-04
 | 1.00E-05 | 1.66E-02 | -3.00E+00
 | -3.05E+00 | -5.00E+00 | -1.29E+00 | 8.60 | 8.29 | #DIV/0! | 8.15 | 8.34
 | 8.13 | #VALUE! | 8.73 | 5.36 | 4.60 | 5.39 | 4.46 | 5.60 | 4.85 | 5.41 | 4.89 | 3.96 | 3.58 |
| ار ق | BLM2 TZERO

 | Set2F | 1.00E-05 | 4.84E-04
 | 1.00E-04 | 2.88E+00 | -5.00E+00
 | -2.82E+00 | -4.00E+00 | 9.53E-01 | 8.85 | 8.29 | 8.68 | 8.15 | 8.51
 | 8.13 | 8.01 | 8.73 | 5.35 | 4.60 | 5.36 | 4.46 | 5.54 | 4.85 | 5.58 | 4.89 | 4.21 | 3.58 |
| J | 3LM2 TZERO

 | Set5C | rate not co | rate not co
 | rate not co | rate not compu | ted
 | | | | | | | |
 | | | | | | | | | | | | | |
| 1 | BLM2 TZERO

 | Set5D | rate not co | rate not co
 | rate not co | rate not compu | ted
 | | | | | | | |
 | | | | | | | | | | | | | |
| 1 | BLIVIZ TZERO

 | Set6D | rate not co | rate not co
 | rate not co | rate not compu | ted
 | | | | | | | |
 | | | | | | | | | | | | | |
| |

 | | | | | | | | | | | | | |
 | | |
 | | | | | | | |
 | | | | | | | | | | | | | |
| |

 | | | | | | | | | | | | | |
 | | |
 | | | | | | | |
 | | | | | | | | | | | | | |
| |

 | | |
 | | | LOG + 0 Transfor
 | med for Ana | lysis | | | | | |
 | | | | | | | | | | | | | |
| |

 | | |
 | | | LOG + 0 Transfor
Rates
 | med for Ana | lysis | | Peptides | | | |
 | | | | DHC gene | 1 | Functional | Genes | | | | | | |
| |

 | | |
 | | | LOG + 0 Transfor
Rates
 | rmed for Ana | lysis | | Peptides | | | |
 | | | 1 | DHC gene | | Functional | Genes | | | | | | |
| |

 | TIMETWO | Kcis | Kcis 95%CI
 | Kvc | Kvc 95%Cl | LOG + 0 Transfor
Rates
Log Kcis
 | rmed for Ana
KcisSD | Log Kvc | LogKvcSD | Peptides
FdhA | FdhA std | PceA | PceA std | TceA
 | TceA std | VcrA | VcrA std | DHC gene
DHC_16S gene | DHC std | Functional
tceA 1 | Genes
tceA std | vcrA | vcrA std | fdhA | fdhA std | pceA | pceA std |
| | BLM2 TTWO

 | TIME TWO
Set1A | Kcis
1.0486058 | Kcis 95%CI
0.937007
 | Kvc
0.1131681 | Kvc 95%Cl
0.018179135 | LOG + 0 Transfor
Rates
Log Kcis
0.021
 | KcisSD | Log Kvc
-0.946 | LogKvcSD
-1.326 | Peptides
FdhA
10.40 | FdhA std | PceA
10.72 | PceA std
10.26 | TceA
10.65
 | TceA std
10.22 | VcrA
#VALUE! | VcrA std
9.00 | DHC gene
DHC_16S gene
6.73 | DHC std
5.97 | Functional
tceA 1
6.79 | Genes
tceA std
6.14 | vcrA
6.86 | vcrA std
6.21 | fdhA
6.81 | fdhA std
6.16 | pceA
5.73 | pceA std
5.01 |
|]] | BLM2 TTWO
BLM2 TTWO
BLM2 TTWO

 | TIME TWO
Set1A
Set1B
Set1C | Kcis
1.0486058
1.0497445
1.1256485 | Kcis 95%Cl
0.937007
1.141049
1.279709
 | Kvc
0.1131681
0.1317895
0.1741944 | Kvc 95%Cl
0.018179135
0.027812426
0.040566336 | LOG + 0 Transfor
Rates
Log Kcis
0.021
0.021
0.051
 | KcisSD
0.386
0.472
0.522 | Log Kvc
-0.946
-0.880
-0.759 | LogKvcSD
-1.326
-1.141
-0.977 | Peptides
FdhA
10.40
10.14
10.38 | FdhA std
9.84
9.84
9.84 | PceA
10.72
10.34
10.43 | PceA std
10.26
10.26 | TceA
10.65
10.25
10.37
 | TceA std
10.22
10.22
10.22 | VcrA
#VALUE!
9.60
9.41 | VcrA std
9.00
9.00 | DHC gene
DHC_16S gene
6.73
6.68
6.82 | DHC std
5.97
5.97
5.97 | Functional
tceA 1
6.79
6.60
6.82 | Genes
tceA std
6.14
6.14 | vcrA
6.86
6.71
6.92 | vcrA std
6.21
6.21
6.21 | fdhA
6.81
6.62
6.83 | fdhA std
6.16
6.16 | pceA
5.73
5.54
5.71 | pceA std
5.01
5.01 |
|]] | 3LM2 TTWO
3LM2 TTWO
3LM2 TTWO
3LM2 TTWO

 | TIME TWO
Set1A
Set1B
Set1C
Set1A_Dup | Kcis
1.0486058
1.0497445
1.1256485
0.2817833 | Kcis 95%Cl
0.937007
1.141049
1.279709
0.037581
 | Kvc
0.1131681
0.1317895
0.1741944
0.012635 | Kvc 95%Cl
0.018179135
0.027812426
0.040566336
0.03067384 | LOG + 0 Transfor
Rates
Log Kcis
0.021
0.021
0.051
-0.550
 | KcisSD
0.386
0.472
0.522
-1.249 | Log Kvc
-0.946
-0.880
-0.759
-1.898 | LogKvcSD
-1.326
-1.141
-0.977
-1.337 | Peptides
FdhA
10.40
10.14
10.38
10.57 | FdhA std
9.84
9.84
9.84
9.84
9.75 | PceA
10.72
10.34
10.43
10.75 | PceA std
10.26
10.26
10.26
10.14 | TceA
10.65
10.25
10.37
10.41
 | TceA std
10.22
10.22
10.22
9.98 | VcrA
#VALUE!
9.60
9.41
9.46 | VcrA std
9.00
9.00
9.00
9.82 | DHC_16S gene
6.73
6.68
6.82
6.94 | DHC std
5.97
5.97
5.97
6.37 | Functional
tceA 1
6.79
6.60
6.82
6.91 | Genes
tceA std
6.14
6.14
6.14
6.54 | vcrA
6.86
6.71
6.92
6.89 | vcrA std
6.21
6.21
6.21
6.21 | fdhA
6.81
6.62
6.83
6.92 | fdhA std
6.16
6.16
6.16
6.28 | pceA
5.73
5.54
5.71
5.78 | pceA std
5.01
5.01
5.01
5.01
5.41 |
| | 3LM2 TTWO
3LM2 TTWO
3LM2 TTWO
3LM2 TTWO
3LM2 TTWO
3LM2 TTWO

 | TIME TWO
Set1A
Set1B
Set1C
Set1A_Dup
Set1B_Dup | Kcis
1.0486058
1.0497445
1.1256485
0.2817833
0.2973343 | Kcis 95%Cl
0.937007
1.141049
1.279709
0.037581
0.031359
 | Kvc
0.1131681
0.1317895
0.1741944
0.012635
2.61E-05 | Kvc 95%Cl
0.018179135
0.027812426
0.040556336
0.03067384
0.022750745 | LOG + 0 Transfor
Rates
Log Kcis
0.021
0.021
0.051
-0.550
-0.527
 | KcisSD
0.386
0.472
0.522
-1.249
-1.328 | Log Kvc
-0.946
-0.880
-0.759
-1.898
-4.583 | LogKvcSD
-1.326
-1.141
-0.977
-1.337
-1.467 | Peptides
FdhA
10.40
10.14
10.38
10.57
10.63 | FdhA std
9.84
9.84
9.84
9.84
9.75
9.75 | PceA
10.72
10.34
10.43
10.75
10.66 | PceA std
10.26
10.26
10.26
10.14
10.14 | TceA
10.65
10.25
10.37
10.41
10.33
 | TceA std
10.22
10.22
10.22
9.98
9.98 | VcrA
#VALUE!
9.60
9.41
9.46
10.17 | VcrA std
9.00
9.00
9.82
9.82 | DHC_165 gene
6.73
6.68
6.82
6.94
6.94 | DHC std
5.97
5.97
5.97
6.37
6.37 | Functional
tceA 1
6.79
6.60
6.82
6.91
6.58 | Genes
tceA std
6.14
6.14
6.54
6.54 | vcrA
6.86
6.71
6.92
6.89
6.59 | vcrA std
6.21
6.21
6.21
6.55
6.55 | fdhA
6.81
6.62
6.83
6.92
6.83 | fdhA std
6.16
6.16
6.28
6.28 | pceA
5.73
5.54
5.71
5.78
5.62 | pceA std
5.01
5.01
5.01
5.41
5.41 |
| | 3LM2 TTWO
3LM2 TTWO
3LM2 TTWO
3LM2 TTWO
3LM2 TTWO
3LM2 TTWO
3LM2 TTWO

 | TIME TWO
Set1A
Set1B
Set1C
Set1A_Dup
Set1B_Dup
Set1C_Dup | Kcis
1.0486058
1.0497445
1.1256485
0.2817833
0.2973343
0.2206698 | Kcis 95%Cl
0.937007
1.141049
1.279709
0.037581
0.031359
0.017099
 | Kvc
0.1131681
0.1317895
0.1741944
0.012635
2.61E-05
0.006713 | Kvc 95%Cl
0.018179135
0.027812426
0.040566336
0.03067384
0.022750745
0.02105224 | LOG + 0 Transfor
Rates
Log Kcis
0.021
0.021
0.051
-0.550
-0.527
-0.656
 | KcisSD
0.386
0.472
0.522
-1.249
-1.328
-1.591 | Log Kvc
-0.946
-0.880
-0.759
-1.898
-4.583
-2.173 | LogKvcSD
-1.326
-1.141
-0.977
-1.337
-1.467
-1.501 | Peptides
FdhA
10.40
10.14
10.38
10.57
10.63
10.61 | FdhA std
9.84
9.84
9.84
9.84
9.75
9.75
9.75 | PceA
10.72
10.34
10.43
10.75
10.66
10.64 | PceA std
10.26
10.26
10.26
10.14
10.14
10.14 | TceA
10.65
10.25
10.37
10.41
10.33
10.19
 | TceA std
10.22
10.22
9.98
9.98
9.98 | VcrA
#VALUE!
9.60
9.41
9.46
10.17
10.14 | VcrA std
9.00
9.00
9.82
9.82
9.82
9.82 | DHC gene
DHC_165 gene
6.73
6.68
6.82
6.94
6.94
6.94
7.11 | DHC std
5.97
5.97
6.37
6.37
6.37 | Functional
tceA 1
6.79
6.60
6.82
6.91
6.58
7.03 | Genes
tceA std
6.14
6.14
6.54
6.54
6.54 | vcrA
6.86
6.71
6.92
6.89
6.59
7.04 | vcrA std
6.21
6.21
6.21
6.55
6.55
6.55 | fdhA
6.81
6.62
6.83
6.92
6.83
7.02 | fdhA std
6.16
6.16
6.28
6.28
6.28
6.28 | pceA
5.73
5.54
5.71
5.78
5.62
5.97 | pceA std
5.01
5.01
5.41
5.41
5.41 |
| | 3LM2 TTWO
3LM2 TTWO
3LM2 TTWO
3LM2 TTWO
3LM2 TTWO
3LM2 TTWO
3LM2 TTWO

 | TIME TWO
Set1A
Set1B
Set1C
Set1A_Dup
Set1B_Dup
Set1C_Dup
Set2A | Kcis
1.0486058
1.0497445
1.1256485
0.2817833
0.2973343
0.2206698
0.0027742 | Kcis 95%Cl
0.937007
1.141049
1.279709
0.037581
0.031359
0.017099
0.000403
 | Kvc
0.1131681
0.1317895
0.1741944
0.012635
2.61E-05
0.006713
0.0030997 | Kvc 95%Cl
0.018179135
0.027812426
0.040566336
0.03067384
0.022750745
0.022105224
0.008559355 | LOG + 0 Transfor
Rates
Log Kcis
0.021
0.051
-0.550
-0.527
-0.656
-2.557
 | KcisSD
0.386
0.472
0.522
-1.249
-1.328
-1.591
-2.901 | Log Kvc
-0.946
-0.880
-0.759
-1.898
-4.583
-2.173
-2.509 | LogKvcSD
-1.326
-1.141
-0.977
-1.337
-1.467
-1.501
-1.573 | Peptides
FdhA
10.40
10.14
10.38
10.57
10.63
10.61 | FdhA std
9.84
9.84
9.84
9.84
9.75
9.75
9.75 | PceA
10.72
10.34
10.43
10.75
10.66
10.64 | PceA std
10.26
10.26
10.26
10.14
10.14
10.14 | TceA
10.65
10.25
10.37
10.41
10.33
10.19
 | TceA std
10.22
10.22
9.98
9.98
9.98 | VcrA
#VALUE!
9.60
9.41
9.46
10.17
10.14 | VcrA std
9.00
9.00
9.82
9.82
9.82 | DHC gene
DHC_165 gene
6.73
6.68
6.82
6.94
6.94
7.11 | DHC std
5.97
5.97
6.37
6.37
6.37 | Functional
tceA 1
6.79
6.60
6.82
6.91
6.58
7.03 | Genes
tceA std
6.14
6.14
6.54
6.54
6.54 | vcrA
6.86
6.71
6.92
6.89
6.59
7.04 | vcrA std
6.21
6.21
6.55
6.55
6.55 | fdhA
6.81
6.62
6.83
6.92
6.83
7.02 | fdhA std
6.16
6.16
6.28
6.28
6.28 | pceA
5.73
5.54
5.71
5.78
5.62
5.97 | pceA std
5.01
5.01
5.41
5.41
5.41 |
| w only | BLM2 TTWO
BLM2 TTWO
BLM2 TTWO
BLM2 TTWO
BLM2 TTWO
BLM2 TTWO
BLM2 TTWO
BLM2 TTWO

 | TIME TWO
Set1A
Set1B
Set1C
Set1A_Dup
Set1B_Dup
Set1B_Dup
Set2A
Set2A
Set2B
Set2A | Kcis
1.0486058
1.0497445
1.1256485
0.2817833
0.2973343
0.2206698
0.0027742
0.0017588 | Kcis 95%Cl
0.937007
1.141049
1.279709
0.037581
0.031359
0.017099
0.000403
0.000244
 | Kvc
0.1131681
0.1317895
0.1741944
0.012639
2.61E-05
0.006713
0.0030997
0.0025722 | Kvc 95%Cl
0.018179135
0.027812426
0.040566336
0.0207844
0.022750745
0.02105224
0.008559355
0.008290165 | LOG + 0 Transfor
Rates
Log Kcis
0.021
0.021
0.021
0.051
-0.550
-0.550
-0.557
-2.755
2.755
 | KcisSD
0.386
0.472
0.522
-1.249
-1.328
-1.591
-2.901
-3.118 | Log Kvc
-0.946
-0.880
-0.759
-1.898
-4.583
-2.173
-2.509
-2.590
-2.590 | LogKvcSD
-1.326
-1.141
-0.977
-1.337
-1.467
-1.501
-1.573
-1.587
-1.587 | Peptides
FdhA
10.40
10.14
10.58
10.57
10.63
10.61 | FdhA std
9.84
9.84
9.75
9.75
9.75 | PceA
10.72
10.34
10.43
10.75
10.66
10.64 | PceA std
10.26
10.26
10.14
10.14
10.14 | TceA
10.65
10.25
10.37
10.41
10.33
10.19
 | TceA std
10.22
10.22
9.98
9.98
9.98 | VcrA
#VALUE!
9.60
9.41
9.46
10.17
10.14 | VcrA std
9.00
9.00
9.82
9.82
9.82 | DHC gene
DHC_165 gene
6.73
6.68
6.82
6.94
7.11 | DHC std
5.97
5.97
6.37
6.37
6.37 | Functional tceA 1 6.79 6.60 6.82 6.91 6.58 7.03 | Genes
tceA std
6.14
6.14
6.54
6.54
6.54 | vcrA
6.86
6.71
6.92
6.89
6.59
7.04 | vcrA std
6.21
6.21
6.21
6.55
6.55
6.55 | fdhA
6.81
6.62
6.83
6.92
6.83
7.02 | fdhA std
6.16
6.16
6.28
6.28
6.28 | pceA
5.73
5.54
5.71
5.78
5.62
5.97 | pceA std
5.01
5.01
5.01
5.41
5.41
5.41 |
| | BLM2 TTWO
BLM2 TTWO
BLM2 TTWO
BLM2 TTWO
BLM2 TTWO
BLM2 TTWO
BLM2 TTWO
BLM2 TTWO
BLM2 TTWO

 | TIME TWO
Set1A
Set1B
Set1C
Set1A_Dup
Set1B_Dup
Set1C_Dup
Set2A
Set2A
Set2B
Set2C
Set3A | Kcis
1.0486058
1.0497445
1.1256485
0.2817833
0.297343
0.2206698
0.0027742
0.0017588
0.002399
0.002099 | Kcis 95%Cl
0.937007
1.141049
1.279709
0.037581
0.031359
0.007099
0.000403
0.000244
0.000245
 | Kvc
0.1131683
0.1317895
0.1741944
0.012635
2.61E-05
0.006712
0.0030997
0.0025725
0.0025725
0.0025725 | Kvc 95%Cl
0.018179135
0.027812426
0.040566336
0.0207384
0.022750745
0.0205224
0.0008559355
0.008290165
0.009893947
0.0013478322 | LOG + 0 Transfor
Rates
Log Kcis
0.021
0.021
0.051
-0.550
-0.527
-0.656
-2.557
-2.755
-2.620
 | KcisSD
0.386
0.472
0.522
-1.249
-1.328
-1.591
-2.901
-3.118
-2.913 | Log Kvc
-0.946
-0.880
-0.759
-1.898
-4.583
-2.173
-2.509
-2.590
-2.374 | LogKvcSD
-1.326
-1.141
-0.977
-1.337
-1.467
-1.501
-1.573
-1.587
-1.510 | Peptides
FdhA
10.40
10.14
10.58
10.57
10.63
10.61 | FdhA std
9.84
9.84
9.75
9.75
9.75 | PceA
10.72
10.34
10.43
10.75
10.66
10.64 | PceA std
10.26
10.26
10.26
10.14
10.14
10.14 | TceA
10.65
10.25
10.37
10.41
10.33
10.19
 | TceA std
10.22
10.22
9.98
9.98
9.98 | VcrA
#VALUE!
9.60
9.41
9.46
10.17
10.14 | VcrA std
9.00
9.00'
9.82
9.82'
9.82' | DHC gene
DHC_165 gene
6.73
6.68
6.82
6.94
7.11 | DHC std
5.97
5.97
6.37
6.37
6.37 | tceA 1 6.79 6.60 6.82 6.91 6.58 7.03 | Genes
tceA std
6.14
6.14
6.54
6.54
6.54 | vcrA
6.86
6.71
6.92
6.89
6.59
7.04 | vcrA std
6.21
6.21
6.21
6.55
6.55
6.55 | fdhA
6.81
6.62
6.83
6.92
6.83
7.02 | fdhA std
6.16
6.16
6.28
6.28
6.28 | pceA
5.73
5.54
5.71
5.78
5.62
5.97 | pceA std
5.01
5.01
5.01
5.41
5.41
5.41 |
| GW ONLY
C T T T T T T T T T T T T T T T T T T T | BLM2 TTWO
BLM2 TTWO

 | TIME TWO
Set1A
Set1B
Set1C
Set1A_Dup
Set1A_Dup
Set1B_Dup
Set2A
Set2A
Set2A
Set2A
Set3A
Set3A | Kcis
1.0486058
1.0497445
1.1256485
0.2817833
0.297343
0.2206698
0.0027742
0.0017588
0.002399
0.0010045
0.000045 | Kcis 95%Cl
0.937007
1.141049
1.279709
0.037581
0.031359
0.017099
0.000403
0.000022
0.000244
0.000222
0.000218
 | Kvc
0.1131681
0.1317895
0.1741944
0.012632
2.61E-05
0.006713
0.00025725
0.0042237
0.00225725
0.0042237
0.0027905 | Kvc 95%Cl
0.018179135
0.027812426
0.04056336
0.0207384
0.022750745
0.02105224
0.00859355
0.008290165
0.008893947
0.013478322
0.013478322 | LOG + 0 Transfor
Rates
Log Kcis
0.021
0.051
-0.550
-0.527
-0.656
-2.557
-2.755
-2.620
 | KcisSD
0.386
0.472
0.522
-1.249
-1.328
-1.591
-2.901
-3.118
-2.913 | Log Kvc
-0.946
-0.880
-0.759
-1.898
-4.583
-2.173
-2.509
-2.590
-2.374 | LogKvcSD
-1.326
-1.141
-0.977
-1.337
-1.467
-1.501
-1.573
-1.587
-1.510 | Peptides
FdhA
10.40
10.14
10.38
10.57
10.63
10.61 | FdhA std
9.84
9.84
9.84
9.75
9.75
9.75 | PceA
10.72
10.34
10.43
10.75
10.66
10.64 | PceA std
10.26
10.26
10.26
10.14
10.14
10.14 | TceA
10.65
10.25
10.37
10.41
10.33
10.19
 | TceA std
10.22
10.22
9.98
9.98
9.98 | VcrA
#VALUE!
9.60
9.41
9.46
10.17
10.14 | VcrA std
9.00
9.00
9.82
9.82
9.82 | DHC gene
DHC_165 gene
6.73
6.68
6.82
6.94
7.11 | DHC std
5.97
5.97
6.37
6.37
6.37 | tceA 1 6.79 6.60 6.82 6.91 6.58 7.03 | Genes
tceA std
6.14
6.14
6.14
6.54
6.54
6.54 | vcrA
6.86
6.71
6.92
6.89
6.59
7.04 | vcrA std
6.21
6.21
6.55
6.55
6.55 | fdhA
6.81
6.62
6.83
6.92
6.83
7.02 | fdhA std
6.16
6.16
6.28
6.28
6.28 | pceA
5.73
5.54
5.78
5.62
5.97 | pceA std
5.01
5.01
5.41
5.41
5.41 |
| | BLM2 TTWO
BLM2 TTWO

 | TIME TWO
Set1A
Set1B
Set1C
Set1A_Dup
Set1A_Dup
Set2A
Set2A
Set2A
Set2Z
Set3A
Set3B
Set3C | Kcis
1.0486058
1.0497445
1.1256485
0.2817833
0.2207343
0.202742
0.0027742
0.0027742
0.002758
0.002399
0.001045
0.0008609
0.000853
0.0008609 | Kcis 95%Cl
0.937007
1.141049
1.279709
0.037581
0.037581
0.017099
0.000403
0.000244
0.000391
0.000248
0.000252
 | Kvc
0.1131681
0.1317895
0.1741944
0.012632
2.616-05
0.006713
0.0003725
0.0025725
0.0042237
0.00227905
0.00227905
0.0032133
0.003133 | Kvc 95%Cl
0.018179135
0.027812426
0.040556336
0.03067384
0.022750745
0.02105224
0.00859355
0.008290165
0.008893947
0.013478322
0.013478322 | LOG + 0 Transfor
Rates
Log Kcis
0.021
0.021
-0.550
-0.550
-0.557
-2.557
-2.755
-2.620
 | KcisSD
0.386
0.472
0.522
-1.249
-1.328
-1.591
-2.901
-3.118
-2.913 | Log Kvc
-0.946
-0.880
-0.759
-1.898
-4.583
-2.599
-2.590
-2.374 | LogKvcSD
-1.326
-1.141
-0.977
-1.337
-1.501
-1.573
-1.587
-1.510 | Peptides
FdhA
10.40
10.14
10.38
10.57
10.63
10.61 | FdhA std
9.84
9.84
9.75
9.75
9.75 | PceA
10.72
10.34
10.43
10.75
10.66
10.64 | PceA std
10.26
10.26
10.14
10.14
10.14 | TceA
10.65
10.25
10.37
10.41
10.33
10.19
 | TceA std
10.22
10.22
9.98
9.98
9.98 | VcrA
#VALUE!
9.60
9.41
9.46
10.17
10.14 | VcrA std
9.00
9.00'
9.82
9.82'
9.82' | DHC gene
DHC_16S gene
6.73
6.68
6.82
6.94
7.11 | DHC std
5.97
5.97
6.37
6.37
6.37 | Functional tceA 1 6.79 6.60 6.82 6.91 6.58 7.03 | Genes
tceA std
6.14
6.14
6.14
6.54
6.54
6.54 | vcrA
6.86
6.71
6.92
6.89
6.59
7.04 | vcrA std
6.21
6.21
6.25
6.55
6.55 | fdhA
6.81
6.62
6.83
6.92
6.83
7.02 | fdhA std
6.16
6.16
6.28
6.28
6.28 | pceA
5.73
5.54
5.71
5.78
5.62
5.97 | pceA std
5.01
5.01
5.41
5.41
5.41 |
| | BLM2 TTWO
BLM2 TTWO

 | TIME TWO
Set1A
Set1B
Set1A_Dup
Set1B_Dup
Set1B_Dup
Set2A
Set2A
Set2A
Set2A
Set3A
Set3A
Set3A
Set3A
Set3A
Set3A | Kcis
1.0486058
1.0497445
1.1256485
0.2817833
0.297343
0.202742
0.0027742
0.0027742
0.002758
0.002399
0.0010045
0.0008753
0.0009600 | Kcis 95%Cl
0.937007
1.141049
1.279709
0.037581
0.013359
0.017099
0.00044
0.00042
0.000262
0.000252
0.000252
 | Kvc
0.1131681
0.1317892
0.1741944
0.012635
2.61E-05
0.006713
0.0025725
0.0042237
0.0025705
0.0042237
0.0027905
0.003138
0.0027905 | Kvc 95%Cl
0.018179135
0.027812426
0.040566336
0.03067384
0.022750745
0.0028290165
0.008290165
0.008893947
0.013478322
0.013063268
0.013659581 | LOG + 0 Transfor
Rates
Log Kcis
0.021
0.021
0.051
-0.550
-0.550
-0.557
-0.656
-2.557
-2.755
-2.620
 | KcisSD
0.386
0.472
0.522
-1.249
-1.328
-1.591
-2.901
-3.118
-2.913 | Log Kvc
-0.946
-0.880
-0.759
-1.898
-4.583
-2.599
-2.590
-2.374 | LogKvcSD
-1.326
-1.141
-0.977
-1.337
-1.467
-1.573
-1.551
-1.573 | Peptides
FdhA
10.40
10.14
10.38
10.57
10.63
10.61 | FdhA std
9.84
9.84
9.85
9.75
9.75 | PceA
10.72
10.34
10.43
10.75
10.66
10.64 | PceA std
10.26
10.26
10.26
10.14
10.14
10.14 | TceA
10.65
10.25
10.37
10.41
10.33
10.19
 | TceA std
10.22
10.22
9.98
9.98
9.98 | VcrA
#VALUEI
9.60
9.41
9.46
10.17
10.14 | VcrA std
9.00
9.00
9.82
9.82
9.82 | DHC gene
DHC_16S gene
6.73
6.68
6.82
6.94
7.11 | DHC std
5.97
5.97
6.37
6.37
6.37 | tceA 1 6.79 6.60 6.82 6.91 6.58 7.03 | Genes
tceA std
6.14
6.14
6.54
6.54
6.54 | vcrA
6.86
6.71
6.92
6.89
6.59
7.04 | vcrA std
6.21
6.21
6.55
6.55
6.55 | fdhA
6.81
6.62
6.83
6.92
6.83
7.02 | fdhA std
6.16
6.16
6.28
6.28
6.28 | pceA
5.73
5.54
5.71
5.78
5.62
5.97 | pceA std
5.01
5.01
5.41
5.41
5.41 |
| | SLM2 TTWO
SLM2 TTWO

 | TIME TWO
Set1A
Set1B
Set1C_Dup
Set1B_Dup
Set1B_Dup
Set2A
Set2A
Set2A
Set2A
Set3B
Set3A
Set3B
Set3A
Set4B | Kcis
1.0486058
1.0497445
1.1256485
0.287743
0.2206698
0.027742
0.0017588
0.002399
0.0010045
0.0008753
0.00008753
0.00008753 | Kcis 95%Cl
0.937007
1.141049
1.279709
0.037581
0.017099
0.000403
0.000242
0.000262
0.000262
0.000225
0.000225
0.000295
 | Kvc
0.1131681
0.1121894
0.012635
2.61E-05
0.006713
0.0030997
0.0025725
0.0042237
0.0022905
0.003135
0.0007131
0.0037185
0.0037426 | Kvc 95%Cl
0.018179135
0.027812426
0.03067384
0.022750745
0.022105224
0.00859355
0.008290165
0.008290165
0.00839347
0.013478322
0.013063268
0.013283913
0.013659581
0.013224546 | LOG + 0 Transfor
Rates
Log Kcis
0.021
0.051
-0.550
-0.527
-0.656
-2.557
-2.620
 | KcisSD
0.386
0.472
0.522
-1.249
-1.328
-1.591
-2.901
-3.118
-2.913 | Log Kvc
-0.946
-0.880
-0.759
-1.898
-4.583
-2.173
-2.509
-2.590
-2.374 | LogKvcSD
-1.326
-1.141
-0.977
-1.337
-1.467
-1.501
-1.573
-1.587
-1.510 | Peptides
FdhA
10.40
10.38
10.57
10.63
10.61 | FdhA std
9.84
9.84
9.75
9.75
9.75 | PceA
10.72
10.34
10.43
10.75
10.66
10.64 | PccA std
10.26
10.26
10.26
10.14
10.14
10.14 | TceA
10.65
10.25
10.37
10.41
10.33
10.19
 | TceA std
10.22
10.22
9.98
9.98
9.98 | VcrA
#VALUE!
9.600
9.41
9.46
10.17
10.14 | VcrA std
9.00'
9.00'
9.82
9.82'
9.82' | DHC gene
DHC_165 gene
6.73
6.68
6.82
6.94
7.11 | DHC std
5.97
5.97
6.37
6.37
6.37 | tceA 1 6.79 6.60 6.82 6.91 6.58 7.03 | Genes
tceA std
6.14
6.14
6.54
6.54
6.54 | vcrA
6.86
6.71
6.92
6.89
6.59
7.04 | vcrA std
6.21
6.21
6.55
6.55
6.55 | fdhA
6.81
6.83
6.92
6.83
7.02 | fdhA std
6.16
6.16
6.28
6.28
6.28 | pceA
5.73
5.54
5.71
5.78
5.62
5.97 | pceA std
5.01
5.01
5.01
5.41
5.41
5.41 |
| | SLM2 TTWO
SLM2 TTWO

 | TIME TWO
Set1A
Set1B
Set1C
Set1A,Dup
Set1B,Dup
Set1B,Dup
Set2B,Set1C,Dup
Set2A
Set2C
Set2A
Set2C
Set3A
Set3C
Set3A
Set3C
Set4A
Set4A
Set4A
Set4A | Kcis
1.0486058
1.0497445
1.1256485
0.2817833
0.2206698
0.027742
0.0017588
0.002399
0.0010045
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.00087 | Kcis 95%Cl
0.937007
1.141049
1.279709
0.031359
0.017099
0.000403
0.000244
0.000241
0.000252
0.000255
0.000255
0.000259
 | Kvc
0.1131681
0.1317895
0.1741944
0.01263
2.61E-00
0.006712
0.0030997
0.0025725
0.0025725
0.0025725
0.0023135
0.0027905
0.0033135
0.0027905
0.0033135
0.0027905
0.0033145
0.0037426
0.0037426 | Kvc 95%Cl
0.013179135
0.027812426
0.040566330
0.004056334
0.002750745
0.002750745
0.002879075
0.002893947
0.01382436
0.01362458
0.01362458
0.0132659581
0.0132659581 | LOG + 0 Transfor
Rates
Log Kcis
0.021
0.021
0.050
-0.550
-0.550
-0.557
-2.557
-2.755
-2.755
-2.755
 | KcisSD
0.386
0.472
0.522
-1.249
-1.328
-1.591
-2.901
-3.118
-2.913 | Log Kvc
-0.946
-0.880
-0.759
-1.898
-4.583
-2.173
-2.509
-2.590
-2.374 | LogKvcSD
-1.326
-1.141
-0.977
-1.367
-1.501
-1.573
-1.587
-1.510 | Peptides
FdhA
10.40
10.14
10.57
10.63
10.61 | FdhA std
9.84
9.84
9.75
9.75
9.75 | PceA
10.72
10.34
10.43
10.75
10.66
10.64 | PccA std
10.26
10.26
10.26
10.14
10.14 | TceA
10.65
10.25
10.37
10.41
10.33
10.19
 | TceA std
10.22
10.22
9.98
9.98
9.98 | VcrA
#VALUE!
9.60
9.41
9.46
10.17
10.14 | VcrA std
9.00
9.00'
9.82
9.82'
9.82' | DHC gene
DHC_165 gene
6.73
6.68
6.94
6.94
7.11 | DHC std
5.97
5.97
6.37
6.37
6.37 | Functional
tceA 1
6.79
6.60
6.82
6.91
6.58
7.03 | Genes
tceA std
6.14
6.14
6.14
6.54
6.54
6.54 | vcrA
6.86
6.71
6.92
6.89
6.59
7.04 | vcrA std
6.21
6.21
6.55
6.55
6.55 | fdhA
6.81
6.62
6.83
6.92
6.83
7.02 | fdhA std
6.16
6.16
6.28
6.28
6.28 | pceA
5.73
5.54
5.71
5.78
5.62
5.97 | pceA std
5.01
5.01
5.41
5.41
5.41 |
| GW ONLY
C C C C C C C C C C C C C C C C C C C | SLM2 TTWO
SLM2 TTWO

 | TIME TWO
Set1A
Set1B
Set1C
Set1A_Dup
Set1C_Dup
Set2A
Set28
Set2A
Set28
Set23
Set3A
Set33
Set33
Set34
Set44
Set48
Set44
Set48
Set44
Set45
Set44 | Kcis
1.0486058
1.0497445
1.1256485
0.2973343
0.207742
0.0027742
0.0027942
0.001758
0.002399
0.001045
0.0008609
0.001121
0.0008245
not sample
rate not co | Kcis 95%Cl
0.937007
1.141049
1.279709
0.037581
0.017099
0.000403
0.000244
0.000252
0.000218
0.000252
0.000252
0.000295
0.000299
not sample
rate not co
 | Kvc
0.1131681
0.1317895
0.1741944
0.012633
2.61E-05
0.006713
0.003977
0.0025725
0.0042233
0.0027905
0.0042233
0.0027905
0.0033135
0.0037185
0.0037185
0.0037185
0.0037185 | Kvc 95%Cl
0.018179135
0.027812426
0.027812426
0.027812426
0.02757047
0.02757047
0.02757047
0.008593957
0.008893947
0.013478325
0.01363268
0.01363268
0.01363268
0.01363268
0.01363268
0.01363268
0.01324546
0.01324546
0.0134695981 | LOG + 0 Transfor
Rates
Log Kcis
0.021
0.021
0.051
0.0550
0.0550
0.0557
-0.2557
-2.2755
-2.2755
-2.620
ted
 | KcisSD
0.386
0.472
0.522
-1.249
-1.591
-2.901
-3.118
-2.913 | Log Kvc
-0.946
-0.880
-0.759
-1.898
-4.583
-2.173
-2.509
-2.500
-2.374 | LogKvcSD
-1.326
-1.141
-0.977
-1.337
-1.467
-1.573
-1.587
-1.587
-1.510 | Peptides
FdhA
10.40
10.14
10.38
10.57
10.63
10.61 | FdhA std
9.84
9.84
9.75
9.75
9.75
9.75 | PceA
10.72
10.34
10.43
10.75
10.66
10.64 | PceA std
10.26
10.26
10.26
10.14
10.14
10.14 | TceA
10.65
10.25
10.37
10.41
10.33
10.19
 | TceA std
10.22
10.22
9.98
9.98
9.98 | VcrA
#VALUE!
9.60
9.41
9.46
10.17
10.14 | VcrA std
9.00
9.00
9.82
9.82
9.82 | DHC gene
DHC_165 gene
6.73
6.68
6.82
6.94
7.11 | DHC std
5.97
5.97
6.37
6.37 | Functional
tceA 1
6.79
6.60
6.82
6.91
6.58
7.03 | Genes
tceA std
6.14
6.14
6.54
6.54
6.54 | vcrA
6.86
6.71
6.92
6.89
6.59
7.04 | vcrA std
6.21
6.21
6.55
6.55
6.55 | fdhA
6.81
6.62
6.83
6.92
6.83
7.02 | fdhA std
6.16
6.16
6.28
6.28
6.28 | pceA
5.73
5.54
5.71
5.78
5.62
5.97 | pceA std
5.01
5.01
5.41
5.41
5.41 |
| GW ONLY
T T T T T T T T T T T T T T T T T T T | BLM2 TTWO
SLM2 TTWO

 | TIME TWO
Set1A
Set1B
Set1C
Set1B, Dup
Set1B, Dup
Set12, Dup
Set2A
Set2A
Set2A
Set2A
Set2A
Set3B
Set3C
Set3B
Set3A
Set4A
Set4B
Set4A
Set4B
Set4A
Set5B
Set5A
Set5B | Kcis
1.0486058
1.0497445
1.1256485
0.2973343
0.2973343
0.2027742
0.0027742
0.002758
0.00299
0.0010045
0.0009609
0.001121
0.0008245
not sample
rate not co
rate not co
rate not co | Kcis 95%Cl
0.937007
1.141049
1.279709
0.037581
0.031359
0.000244
0.000252
0.000245
0.000252
0.000252
0.000255
0.000259
0.000209
not sampli
rate not co
rate not co
 | Kvc
0.1131681
0.1317895
0.1741944
0.012633
2.61E-05
0.0005712
0.00025725
0.00027905
0.00027905
0.00033138
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.00037185
0.000037185
0.000037185
0.000037185
0.000375
0.00005000000000000000000 | Kvc 95%Cl
0.018179135
0.027812426
0.04056336
0.0207879745
0.03067244
0.0008539355
0.008290165
0.01362384
0.013283913
0.013829315
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.013283913
0.01328391000000000000000000000000000000000000 | LOG + 0 Transfor
Rates
Log Kcis
0.021
0.051
0.055
-0.557
-2.557
-2.557
-2.557
-2.620
-2.557
-2.620
-2.620
 | KcisSD
0.386
0.472
0.522
-1.249
-1.591
-2.901
-3.118
-2.913 | Log Kvc
-0.946
-0.880
-0.759
-1.898
-4.583
-2.173
-2.509
-2.509
-2.500
-2.374 | LogKvcSD
-1.326
-1.141
-0.977
-1.337
-1.467
-1.501
-1.573
-1.587
-1.510 | Peptides
FdhA
10.40
10.14
10.38
10.57
10.63
10.61 | FdhA std
9.84
9.84
9.75
9.75
9.75 | PceA
10.72
10.34
10.43
10.75
10.66
10.64 | PceA std
10.26
10.26
10.14
10.14
10.14 | TceA
10.65
10.25
10.37
10.41
10.33
10.19
 | TceA std
10.22
10.22
9.98
9.98
9.98 | VcrA
#VALUEI
9.60
9.41
9.46
10.17
10.14 | VcrA std
9.00
9.00'
9.82
9.82' | DHC gene
DHC_165 gene
6.73
6.68
6.82
6.94
7.11 | DHC std
5.97
5.97
6.37
6.37
6.37 | Functional
6.79
6.60
6.82
6.91
6.58
7.03 | Genes
tceA std
6.14
6.14
6.14
6.54
6.54
6.54 | vcrA
6.86
6.71
6.92
6.89
6.59
7.04 | vcrA std
6.21
6.21
6.55
6.55
6.55 | fdhA
6.81
6.62
6.83
6.92
6.83
7.02 | fdhA std
6.16
6.16
6.28
6.28
6.28 | pceA
5.73
5.54
5.71
5.78
5.62
5.97 | pceA std
5.01
5.01
5.41
5.41 |
| | SLM2 TTWO
SLM2 TTWO

 | TIME TWO
Set1A
Set1B
Set1C
Set1C Dup
Set1B_Dup
Set1A_Dup
Set2A
Set2A
Set2A
Set2A
Set3A
Set3A
Set3A
Set3A
Set4B
Set4A
Set4A
Set4A
Set5A
Set5A
Set5A
Set6B | Kcis
1.0486058
1.0497445
1.1256485
0.2817833
0.2206698
0.0027742
0.0017588
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0008753
0.0007748
0.0008753
0.0008753
0.0008753
0.0007748
0.0007748
0.0007748
0.0007748
0.0007758
0.0007748
0.0007758
0.0007758
0.0007758
0.0007748
0.0007758
0.0007758
0.0007758
0.0007758
0.0007758
0.0007758
0.0007758
0.0007758
0.0007758
0.0007758
0.0007758
0.0007758
0.0007758
0.0007758
0.0007758
0.0007758
0.0007758
0.0007758
0.0007758
0.0007758
0.0007758
0.0007758
0.0007758
0.0007758
0.0007758
0.0007758
0.0007758
0.0007758
0.0007758
0.0007758
0.0007758
0.0007758
0.0007758
0.0007758
0.0007758
0.0007758
0.0007758
0.0007758
0.0007758
0.0007758
0.0007758
0.0007758
0.0007758
0.0007758
0.0007758
0.0007758
0.0007758
0.0007758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.000758
0.0007 | Kcis 95%Cl
0.937007
1.141049
1.279709
0.037581
0.031359
0.000244
0.000262
0.000218
0.000252
0.000255
0.000255
0.000255
0.000209
not sampli
rate not cc
rate not cc
rate not cc
 | Kvc
0.1131681
0.1317895
0.1741944
0.012633
2.61E-05
0.0025725
0.0025725
0.0025725
0.0025725
0.0025725
0.003133
0.0017131
0.0037188
0.0037426
rot sampla
rate not co
rate not co
rate not co | Kvc 95%CI
0.018179135
0.027812426
0.027812426
0.020765236
0.022750745
0.0026290165
0.000859381
0.0013478322
0.013663981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.013263981
0.01363981
0.01363981
0.01363981
0.01363981
0.01363981
0.013639810 | LOG + 0 Transfor
Rates
Log Kcis
0.021
0.021
0.0521
-0.550
-0.527
-2.557
-2.2755
-2.2755
-2.620
ted
ted
ted
 | KcisSD
0.386
0.472
0.522
-1.249
-1.328
-1.591
-2.901
-3.118
-2.913 | Log Kvc
-0.946
-0.880
-0.759
-1.898
-4.583
-2.579
-2.590
-2.374 | LogKvcSD
-1.326
-1.141
-0.977
-1.337
-1.467
-1.501
-1.573
-1.587
-1.510 | Peptides
FdhA
10.40
10.14
10.38
10.57
10.65
10.61 | FdhA std
9.84
9.84
9.75
9.75
9.75
9.75 | PceA
10.72
10.34
10.43
10.75
10.66
10.64 | PceA std
10.26
10.26
10.26
10.14
10.14 | TceA
10.65
10.25
10.37
10.41
10.33
10.19
 | TceA std
10.22
10.22
9.98
9.98
9.98 | VcrA
#VALUE1
9.60
9.41
9.46
10.17
10.14 | VcrA std
9.00
9.00'
9.82'
9.82' | DHC gene
DHC_165 gene
6.73
6.682
6.94
7.11 | DHC std
5.97
5.97
6.37
6.37 | Functional
tceA 1
6.79
6.60
6.82
6.91
6.58
7.03 | Genes
tceA std
6.14
6.14
6.54
6.54
6.54 | vcrA
6.86
6.71
6.92
6.89
6.59
7.04 | vcrA std
6.21
6.22
6.55
6.55
6.55 | fdhA
6.81
6.62
6.83
6.92
6.83
7.02 | fdhA std
6.16
6.16
6.16
6.28
6.28
6.28 | pceA
5.73
5.54
5.71
5.78
5.62
5.97 | pceA std
5.01
5.01
5.41
5.41
5.41 |
| | SLM2 TTWO
SLM2 TTWO

 | TIME TWO
Set1A
Set1B
Set1C
Set1A_Dup
Set12_Dup
Set2C_Dup
Set2A
Set28
Set28
Set28
Set24
Set38
Set33
Set34
Set44
Set48
Set44
Set48
Set44
Set48
Set45
Set58
Set58
Set58
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set50
Set | Kcis
1.0486058
1.0497445
1.1256485
0.821783
0.297343
0.020698
0.0027742
0.001758
0.0002753
0.0009609
0.001121
0.0008625
not sample
rate not co
rate not co
rate not co
rate not co | Kcis
95%Cl
0.937007
1.141049
1.279709
0.037581
0.031359
0.000244
0.000244
0.000252
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.0000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.00055
0.00055
0.00055
0.00055
0.00055
0.00055
0.00055
0.00055
0.00055
0.00055
0.00055
0.00055
0.00055
0.00055
0.00055
0.00055
0.00055
0.00055
0.00055
0.00055
0.00055
0.00055
0.00055
0.00055
0.00055
0.00055
0.00055
0.00055
0.00055
0.00055
0.00055
0.00055
0.00055
0.00055
0.00055
0.00055
0.00055
0.00055
0.00055
0.00055
0.00055
0.00055
0.00055
0.00055
0.00055
0.00055
0.00055
0.00055
0.00055
0.00055
0.00055
0.00055
0.00055
0.00055
0.00055
0.00055
0.00055
0.00055
0.00055
0.00055
0.00055
0.00055
0.00055
0.00055
0.00055
0.00055
0.00055
0.00055
0.00055
0.00055
0.00055
0.00055
0.00055
0.00055
0.00055
0.00055
0.00055
0.00055
0.00055
0.00055
0.00055
0.00055
0.00055
0.00055
0.00055
0.00055
0.00055
0.000555
0.000555
0.0005 | Kvc
0.1131681
0.117892
0.1741944
0.012633
2.616-05
0.0005712
0.00025725
0.0042237
0.0022905
0.0023905
0.0023905
0.0023905
0.0023905
0.0023905
0.0023905
0.0023905
0.0023905
0.0023905
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0023915
0.0025915
0.0025915
0.0025915
0.0025915
0.0025915
0.00 | Kvc 95%Cl
0.018179135
0.027812426
0.040566336
0.020570246
0.0215224
0.002693045
0.002893047
0.003893947
0.003893947
0.01387382
0.0138635881
0.013859581
0.013859581
0.013859581
0.013859581
0.013824546
0.013824546
0.013824546
0.013824546
0.013824546
0.013824546
0.013824546
0.013824546
0.013824546
0.013824546
0.013824546
0.013824546
0.013824546
0.013824546
0.013824546
0.013824546
0.013824546
0.013824546
0.013824546
0.013824546
0.013824546
0.013824546
0.013824546
0.013824546
0.013824546
0.013824546
0.013824546
0.013824546
0.013824546
0.013824546
0.013824546
0.013824546
0.013824546
0.013824546
0.013824546
0.013824546
0.013824546
0.013824546
0.013824546
0.013824546
0.013824546
0.013824546
0.013824546
0.013824546
0.013824546
0.013824546
0.013824546
0.013824546
0.013824546
0.013824546
0.013824546
0.013824546
0.013824546
0.013824546
0.013824546
0.013824546
0.013824546
0.013824546
0.013824546
0.013824546
0.013824546
0.013824546
0.013824546
0.013824546
0.01487454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454
0.001477454 | LOG + 0 Transfor
Rates
Log Kcis
0.021
0.021
0.051
-0.550
-0.550
-0.555
-2.575
-2.755
-2.755
-2.755
-2.620
ted
ted
ted
ted
.8.48E-01
 | KcisSD 0.386 0.422 0.522 -1.249 -1.328 -1.591 -2.901 -3.118 -2.913 | Log Kvc
-0.946
-0.880
-0.789
-1.888
-4.583
-2.173
-2.509
-2.509
-2.509
-2.374
-2.374
-2.374 | LogKvcSD
-1.326
-1.141
-0.977
-1.337
-1.4501
-1.573
-1.570
-1.510
-1.510 | Peptides
FdhA
10.40
10.14
10.38
10.57
10.63
10.61 | FdhA std
9.84
9.84
9.84
9.75
9.75
9.75 | PceA
10.72
10.34
10.43
10.75
10.66
10.64 | PccA std
10.26
10.26
10.26
10.14
10.14 | TceA
10.65
10.25
10.37
10.41
10.19
 | TceA std
10.22
10.22
9.98
9.98
9.98 | VcrA
#VALUE!
9.60
9.41
9.46
10.17
10.14 | VcrA std
9.00
9.00'
9.82'
9.82'
9.82'
9.82'
9.82' | DHC gene
DHC_165 gene
6.73
6.68
6.94
6.94
7.11
7.11 | DHC std
5.97
5.97
6.37
6.37
6.37 | Functional
tceA 1
6.79
6.60
6.82
6.91
6.58
7.03 | Genes
tceA std
6.14
6.14
6.54
6.54
6.54 | vcrA
6.86
6.71
6.92
6.89
6.59
7.04 | vcrA std
6.21
6.23
6.55
6.55
6.55 | fdhA
6.81
6.62
6.83
6.92
6.83
7.02 | fdhA std
6.16
6.16
6.28
6.28
6.28 | pceA
5.73
5.54
5.57
5.62
5.97 | pceA std
5.01
5.01
5.41
5.41
5.41 |
| | BLM2 TTWO
SLM2 TTWO

 | TIME TWO
Set1A
Set1B
Set1C
Set1B Dup
Set1B Dup
Set2A
Set2A
Set2A
Set2A
Set2A
Set3B
Set3C
Set3A
Set3B
Set3A
Set4A
Set4B
Set4A
Set5B
Set4A
Set5B
Set4A
Set5B
Set4A
Set5B
Set4A
Set5B
Set4A
Set5B
Set4A
Set5B
Set4A
Set5B
Set4A
Set5B
Set4A
Set5B
Set4A
Set5B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
S | Kcis
1.0486058
1.0497445
1.1256485
0.2817833
0.297343
0.200628
0.0023742
0.0017588
0.002399
0.001045
0.0008753
0.0008609
0.00121
0.0008245
not sample
rate not co
rate not co | Kcis
95%Cl
0.937007
1.141049
1.279709
0.037581
0.031359
0.000403
0.000262
0.000218
0.000252
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0.000255
0 | Kvc
0.1131681
0.1317899
0.01741944
0.012632
2.61E-05
0.006712
0.00027905
0.00227905
0.00227905
0.0023732
0.00227905
0.0033135
0.0027905
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0038711
0.0176385 | Kvc 95%Cl
0.018179135
0.027812426
0.04056336
0.027879745
0.03067324
0.0008539355
0.008290165
0.01362380
0.013823913
0.013823913
0.013823913
0.013823913
0.013823913
0.013823913
0.013823913
0.013823913
0.013823913
0.013823913
0.013823913
0.013823913
0.01382192
748 not compup
rate not compup
rate not compup
rate not compup
rate not compup
rate not compup | LOG + 0 Transfor
Rates
Log
Kcis
0.021
0.051
0.055
0.0557
-0.656
-0.527
-2.620
-2.557
-2.620
-2.557
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.6200
-2.6200
-2.6200
-2.6200
-2.6200
-2.6200
-2.6200
- | • Med for Ana KcisSD 0.386 0.472 0.522 -1.249 -1.328 -1.591 -3.118 -2.913 -1.52E+00 -1.52E+00 -1.55E+00 | lysis
Log Kvc
-0.946
-0.880
-0.759
-1.898
-4.1838
-2.173
-2.509
-2.590
-2.590
-2.374
-1.72E+00
-1.72E+00
-1.75E+00 | LogKvcSD
-1.326
-1.141
-0.977
-1.367
-1.573
-1.573
-1.587
-1.510
-1.575
-1.510
-1.587
-1.510
-1.587+00
-1.538+00 | Peptides
FdhA
10.40
10.14
10.57
10.63
10.61
9.60
9.60
9.91 | FdhA std
9.84
9.84
9.75
9.75
9.75
9.75 | PceA
10.72
10.34
10.75
10.66
10.64 | PccA std
10.26
10.26
10.26
10.14
10.14
10.14 | TceA
10.65
10.25
10.37
10.41
10.33
10.19
 | TceA std
10.22
10.22
9.98
9.98
9.98 | VcrA
#VALUE!
9.60
9.41
9.46
10.17
10.14 | VcrA std
9.00
9.00
9.82
9.82
9.82
9.82 | DHC gene
DHC_165 gene
6.73
6.68
6.82
6.94
7.11
7.11
5.55
5.55
5.70 | DHC std
5.97
5.97
6.37
6.37
6.37
6.37
5.35
5.35 | Functional
tceA 1
6.79
6.60
6.82
6.91
6.58
7.03 | Genes
tceA std
6.14
6.54
6.54
6.54
6.54
5.53
5.53 | vcrA
6.86
6.71
6.92
6.89
6.59
7.04
5.84
6.04 | vcrA std
6.21
6.22
6.55
6.55
6.55 | fdhA
6.81
6.62
6.83
7.02
7.02
5.74
5.93 | fdhA std
6.16
6.16
6.28
6.28
6.28
5.28 | pceA
5.73
5.54
5.62
5.97 | pceA std
5.01
5.01
5.41
5.41
5.41
5.41
9.41
9.41
9.41
9.41
9.41
9.41
9.41
9 |
| | SLM2 TTWO
SLM2 TTWO | TIME TWO
Set1A
Set1B
Set1C
Set1C
Set2A
Set2B
Set2A
Set2A
Set2A
Set2A
Set2A
Set2A
Set2A
Set2A
Set3A
Set3C
Set4A
Set4A
Set4A
Set4A
Set5A
Set5B
Set5A
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set5B
Set | Kcis
1.0486058
1.0497445
1.1256485
0.2817833
0.2206698
0.0027742
0.0017588
0.002399
0.001045
0.001045
0.0008045
0.0008245
not sample
rate not co
rate not co
rate not co
rate not co
rate not co
rate not co | Kcis 95%Cl
0.937007
1.141049
1.279709
0.037581
0.031359
0.000403
0.000240
0.000240
0.000252
0.000255
0.000295
0.000295
0.000295
0.000295
0.000295
0.000295
0.000295
0.000295
0.000295
0.000295
0.000295
0.000295
0.000295
0.000295
0.000295
0.000295
0.000295
0.000295
0.000295
0.000295
0.000295
0.000295
0.000295
0.000295
0.000295
0.000295
0.000295
0.000295
0.000295
0.000295
0.000295
0.000295
0.000295
0.000295
0.000295
0.000295
0.000295
0.000295
0.000295
0.000295
0.000295
0.000295
0.000295
0.000295
0.000295
0.000295
0.000295
0.000295
0.000295
0.000295
0.000295
0.000295
0.000295
0.000295
0.000295
0.000295
0.000295
0.000295
0.000295
0.000295
0.000295
0.000295
0.000295
0.000295
0.000295
0.000295
0.000295
0.000295
0.000295
0.000295
0.000295
0.000295
0.000295
0.000295
0.000295
0.000295
0.000295
0.000295
0.000295
0.000295
0.000295
0.000295
0.000295
0.000295
0.000295
0.000295
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.0000000000 | Kvc
0.1131681
0.1317892
0.1317892
0.1371992
0.0025722
0.0042233
0.0027905
0.0023722
0.0042233
0.0017133
0.0017133
0.0017133
0.0037182
0.0037426
rots ampli-
rate not cc
rate n | Kvc 95%CI
0.018179135
0.027812426
0.027812426
0.020765236
0.0022750745
0.0022750745
0.00262920165
0.000829305
0.000829305
0.000829305
0.01322430
0.013655981
0.01322450
0.01322450
0.01322450
0.01322450
0.01322450
0.01322450
0.01322450
0.01322450
0.01322450
0.01322450
0.01322450
0.01322450
0.01322450
0.01322450
0.01322450
0.013225551 | LOG + 0 Transfor
Rates
Log Kcis
0.021
0.021
0.051
-0.550
-0.527
-0.656
-2.557
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
- | KcisSD 0.386 0.472 0.522 1.249 -1.328 -1.591 -2.901 -3.118 -2.913 -1.591 -1.592 -1.592 -1.594 -1.594 -1.594 -1.594 -1.548 | Log Kvc
-0.946
-0.896
-0.759
-1.898
-4.583
-2.173
-2.509
-2.509
-2.570
-2.374
-1.72E+00
-1.75E+00
-1.68E+00 | LogKvcSD
-1.326
-1.141
-0.977
-1.337
-1.467
-1.501
-1.573
-1.573
-1.510
-1.537
-1.510
-1.538+00
-1.538+00
-1.538+00 | Peptides
FdhA
10.40
10.14
10.38
10.67
10.63
10.61 | FdhA std
9.84
9.84
9.75
9.75
9.75
9.75
9.75 | PceA
10.72
10.34
10.43
10.75
10.66
10.64
9.42
9.42
9.42
9.74 | PccA std
10.26
10.26
10.14
10.14
10.14
10.14
9.24 | TceA
10.65
10.25
10.37
10.41
10.33
10.19 | TceA std
10.22
10.22
9.98
9.98
9.98
9.98
9.98 | VcrA
#VALUE!
9.46
10.17
10.14
9.46
9.41
10.14 | VcrA std
9.00
9.00'
9.82
9.82'
9.82'
9.82'
9.82'
9.82' | DHC gene
DHC_165 gene
6.73
6.682
6.94
7.11
7.11
7.11 | DHC std
5.97
5.97
6.37
6.37
6.37 | Functional
tceA 1
6.79
6.60
6.82
7.03
7.03
5.74
5.74
5.93
6.09 | Genes
tee A std
6.14
6.54
6.54
6.54
6.54
6.54
5.53
5.53
5.53 | vcrA
6.86
6.71
6.92
6.89
7.04
5.84
4.6.94 | vcrA std
6.21
6.25
6.55
6.55
6.55 | fdhA
6.81
6.62
6.83
7.02
5.74
5.74
5.96 | fdhA std
6.16
6.16
6.28
6.28
6.28
6.28 | pceA
5.73
5.54
5.78
5.62
5.97
4.23
4.43
4.43 | pccA std
5.01
5.01
5.41
5.41
5.41
3.41
3.81
3.81
3.81 |
| | BLM2 TTWO
SLM2 TTWO
BLM2 TTWO

 | TIME TWO
Set1A
Set1B
Set1C
Set1A_Dup
Set1C_Dup
Set2C_Dup
Set2A
Set28
Set28
Set28
Set32
Set33
Set33
Set34
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set48
Set | Kcis
1.0486058
1.1256485
0.2817833
0.22056698
0.0027742
0.0017588
0.0008753
0.0008753
0.0008753
0.00086753
0.00086753
0.00086753
0.00086754
0.0008245
not sample
rate not co
rate not co | Kcis
95%Cl
0.937007
1.141049
1.279709
0.037581
0.017099
0.000403
0.000262
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.0000252
0.0000252
0.0000252
0.0000252
0.0000252
0.0000252
0.0000252
0.000000
0.0000000
0.0000000000 | Kvc
0.1131681
0.1317895
0.1317895
0.1317895
0.012632
2.61E-00
0.006713
0.0025722
0.0025722
0.0027905
0.0027905
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0037185
0.0025725
0.0037185
0.0037185
0.0025725
0.0037185
0.0037185
0.0037185
0.0025725
0.0037185
0.0037185
0.0025725
0.0037185
0.0037185
0.0025725
0.0037185
0.0037185
0.0037185
0.002577
0.0037185
0.002577
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.000575
0.0005755
0.0005755
0.0005755
0.0005755
0.00055 | Kvc 95%Cl
0.018179135
0.027812426
0.027812426
0.027812426
0.02781246
0.02750748
0.002859347
0.0038593947
0.013287312
0.0132859581
0.00132859581
0.00132859581
0.0132859581
0.0132859581
0.0132859581
0.0132859581
0.0132859581
0.0132859581
0.0132859581
0.0132859581
0.0132859581
0.0132859581
0.0132859581
0.01328581
0.01328581
0.008812199
0.015322088
0.008812199
0.015322088 | LOG + 0 Transfor
Rates
Log
Kcis
0.021
0.021
0.051
-0.550
-0.557
-0.550
-0.557
-2.755
-2.2755
-2.2755
-2.2755
-2.2620
-2.557
-2.2755
-2.2620
-2.557
-2.2755
-2.2620
-2.557
-2.2755
-2.2620
-2.557
-2.2755
-2.2755
-2.2755
-2.2620
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.2755
-2.27 | KcisSD 0.368 0.472 0.522 1.249 1.521 2.901 -3.118 -2.913 -1.521 -0.2913 -1.525+00 -1.525+00 -1.542+00 -1.542+00 -1.542+00 -1.922+00 | Log Kvc
-0.946
-0.880
-0.759
-1.898
-4.583
-2.599
-2.590
-2.374
-1.72E+00
-1.72E+00
-1.78E+00
-1.68E+00
-5.00E+00
-5.00E+00 | LogKvcSD
-1.326
-1.141
-0.977
-1.337
-1.467
-1.531
-1.573
-1.587
-1.510
-1.537
-1.510
-1.538+00
-1.538+00
-1.538+00
-1.538+00
-1.538+00
-1.538+00 | Peptides
FdhA
10.04
10.14
10.53
10.63
10.61
9.60
9.60
9.91
9.93
9.83
9.83
9.87
9.87 | FdhA std
9.84
9.84
9.75
9.75
9.75
9.75 | PceA
10.72
10.34
10.43
10.75
10.66
10.64
9.04
9.94
2
9.74
9.74
9.76 | PccA std
10.26
10.26
10.26
10.14
10.14
10.14
9.24
9.24
9.24
9.24
9.73
9.73 | TceA
10.65
10.25
10.37
10.41
10.33
10.19
10.19
 | TceA std
10.22
10.22
9.98
9.98
9.98
9.98
9.98
9.98
9.88
9.8 | VcrA
#VALUEI
9.60
9.40
10.17
10.14
9.68
9.68
9.68
9.51
9.51
9.53 | VcrA std
9.00
9.00'
9.82
9.82
9.82
9.82'
9.82'
9.82'
9.82'
9.82'
9.82'
9.82'
9.82'
9.82'
9.82'
9.82'
9.82' | DHC gene
DHC_165 gene
6.73
6.68
6.82
6.94
7.11
7.11
5.55
5.70
5.90
6.72
7.70
5.90
6.72
5.55
5.70 | DHC std
5.97
5.97
6.37
6.37
6.37
6.37 | Functional
tceA 1
6.79
6.60
6.82
6.91
6.58
7.03
7.03 | Genes
tceA std
6.14
6.54
6.54
6.54
6.54
6.54
6.54
6.54
5.53
5.53
5.53 | vcrA
6.86
6.71
6.92
6.89
6.59
7.04
5.59
7.04
5.58
4
6.04
6.19
6.33 | vcrA std
6.21
6.21
6.55
6.55
6.55
6.55
6.55 | fdhA
6.81
6.62
6.83
7.02
5.74
5.74
5.74
5.75
6.62
7.02 | fdhA std
6.16
6.16
6.28
6.28
6.28
6.28
5.30
5.30
5.30
6.44
6.44 | pceA
5.73
5.54
5.72
5.78
5.62
5.97 | pceA std
5.01
5.01
5.41
5.41
5.41
3.81
3.81
3.81
3.81
3.81
5.09
5.09 |
| LIDS GWONLY GWONLY | BLM2 TTWO
SLM2 TTWO

 | TIME TWO
Set1A
Set1B
Set1C
Set1B
Dup
Set1B_Dup
Set1C_Dup
Set1C_Dup
Set2C
Set3A
Set2C
Set3A
Set3B
Set3C
Set4A
Set4B
Set4A
Set5B
Set4A
Set5B
Set4A
Set5B
Set4A
Set5B
Set4A
Set5B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B | Kcis
1.0488058
1.0497445
1.1256485
0.2817833
0.2973343
0.202792
0.0017588
0.002399
0.001045
0.0008753
0.0009695
0.0008245
not complement
rate not co
rate not co
rate not co
rate not co
rate not co
rate not co
rate not co
0.1417804
0.097549
0.0963964
0.097549
0.0963964
0.097549
0.097549
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097549
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0.097548
0 | Kcis 95%Cl
0.937007
1.141049
1.279709
0.037581
0.000244
0.000244
0.000242
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000552
0.000552
0.0015542
0.0015542
0.004629
0.003784
0.004629
 | Kvc
0.1131681
0.131789
0.131789
0.131789
0.131789
0.01763
0.002790
0.0002792
0.002790
0.002790
0.002790
0.0037185
0.002790
0.0037185
0.0037426
0.0037426
0.0037426
0.0037426
0.0037426
0.0037426
0.0037426
0.0037426
0.0037426
0.0037426
0.0037426
0.0037426
0.0037426
0.0037426
0.003875
0.001638
0.0026977
1E-00
0.0183197
0.0026977 | Kvc 95%Cl
0.018179135
0.027812426
0.04256336
0.027879745
0.03067244
0.03067244
0.03067244
0.03067244
0.03065245
0.01362345
0.013262345
0.013262345
0.013262345
0.013262345
0.013262345
0.01322345
0.01322345
0.01322345
0.01322345
0.01322345
0.01322345
0.01322345
0.01322345
0.01322345
0.01322345
0.01322345
0.01322345
0.01322345
0.01322345
0.01322345
0.01323245
0.01323245
0.01323245
0.01323245
0.01323245
0.01323245
0.01323245
0.01323245
0.0132345
0.0132345
0.0132345
0.0132345
0.0132345
0.0132345
0.0132345
0.0132345
0.0132345
0.0132345
0.0132345
0.0132345
0.0132345
0.0132345
0.0132345
0.0132345
0.0132345
0.0132345
0.0132345
0.0132345
0.0132345
0.0132345
0.0132345
0.013245
0.013245
0.013245
0.013245
0.013245
0.013245
0.013245
0.013245
0.013245
0.013245
0.013245
0.013245
0.013245
0.013245
0.013245
0.013245
0.013245
0.013245
0.013245
0.013245
0.013245
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0.0135
0 | LOG + 0 Transfor
Rates
Log
Kcis
0.021
0.051
0.055
0.0557
0.0556
0.0557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.25577
2.25577
2.25577
2.25577
2.255777
2.255777
2.2557777777777 | ************************************ | Log Kvc
-0.946
-0.880
-0.759
-1.898
-4.583
-2.579
-2.590
-2.374
-1.72E+00
-1.75E+00
-1.75E+00
-1.68E+00
-5.50E+00
-1.74E+00
-2.57E+00
-2.57E+00
-2.57E+00
-2.57E+00
-2.57E+00
-2.57E+00
-2.57E+00
-2.57E+00
-2.57E+00
-2.57E+00
-2.57E+00
-2.57E+00
-2.57E+00
-2.57E+00
-2.57E+00
-2.57E+00
-2.57E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.58E+00
-2.5 | LogKvcSD
-1.326
-1.141
-0.977
-1.337
-1.567
-1.501
-1.573
-1.573
-1.587
-1.510
-1.538+00
-1.538+00
-1.378+00
-1.378+00
-1.379+00 | Peptides FdhA 10.40 10.14 10.38 10.67 10.61 9.60 9.60 9.51 9.83 9.87 10.12 10.12 | FdhA std
9.84
9.75
9.75
9.75
9.75
9.75
9.75
9.75
9.75 | PccA
10.72
10.34
10.43
10.75
10.66
10.66
10.64
9.42
9.42
9.42
9.42
9.42
9.42
9.42
10.21
10.22 | PccA std
10.26
10.26
10.26
10.14
10.14
10.14
9.24
9.24
9.24
9.24
9.23
9.23
9.23
9.23
9.24 |
TceA
10.65
10.25
10.37
10.41
10.33
10.19
10.02
10.02
10.02
10.02
10.11
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
10.21
1 | TceA std
10.22
9.98
9.98
9.98
9.98
9.98
9.98
9.98
9 | VcrA
#VALUEI
9.600
9.41
10.17
10.14 | VcrA std
9.00
9.00'
9.82'
9.82'
9.82'
9.82'
9.82'
9.82'
9.82'
9.82'
9.82'
9.82'
9.82'
9.82'
9.82'
9.82'
9.82'
9.82' | DHC gene
DHC_165 gene
6.73
6.68
6.82
6.94
7.11
7.11
5.55
5.55
5.70
5.70
5.70
6.72
7.70 | DHC std
5.97
5.97
6.37
6.37
6.37
6.37
6.37
6.37
5.35
5.35
5.35
5.35
5.35
5.35
6.67
6.47 | Functional
tceA 1
6.79
6.60
6.82
6.91
6.58
7.03
7.03
7.03
7.03
7.03
7.03
7.03
7.03 | Genes
tceA std
6.14
6.54
6.54
6.54
6.54
6.54
6.54
6.54
7
7
5.53
5.53
5.53
5.53 | vcrA
6.86
6.71
6.92
6.59
7.04
5.84
6.59
7.04
5.84
6.59
7.04
6.53
5.84
6.04
6.13
6.25
6.25
6.25
7.04 | vcrA std
6.21
6.23
6.55
6.55
6.55
6.55
5.63
5.63
5.63
5.6 | fdhA
6.81
6.62
6.83
7.02
7.02
5.74
5.93
5.96
7.99
6.99
6.99 | fdhA std
6.16
6.16
6.28
6.28
6.28
5.30
5.30
5.30
5.30
5.30
5.30 | pceA
5.73
5.74
5.771
5.78
5.62
5.97
4.23
4.43
4.47
5.58
5.58
5.58 | pceA std
5.01
5.01
5.41
5.41
5.41
3.81
3.81
3.81
3.81
3.81
3.89
5.09
5.09 |
| Sources GW ONLY GW ONLY | SLM2 TTWO
SLM2 TTWO

 | TIME TWO
Set1A
Set1B
Set1C
Set1B Dup
Set1B Dup
Set1A Dup
Set2A
Set2A
Set2A
Set2A
Set2A
Set3A
Set3C
Set4A
Set4A
Set4A
Set4A
Set4A
Set4A
Set4A
Set5A
Set5A
Set5B
Set6B
Set1D
Set15
Set16
Dup
Set11F
Set11 Dup
Set11F Dup
Set11F Dup | Kcis
1.049748
1.1256485
0.2817833
0.297343
0.207343
0.0027742
0.0017588
0.0028753
0.0008753
0.00086753
0.00086753
0.00086753
0.0008121
0.0008269
0.00121
0.0008269
0.00961964
0.0782689
0.0592448
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0.059248
0. | Kcis 95%Cl
0.937007
1.279709
0.03784
0.031359
0.00024
0.00024
0.00024
0.00025
0.000021
0.000025
0.000025
0.000025
0.000025
0.000025
0.000025
0.000025
0.000025
0.000324
0.00324
0.00324
0.00324
 | Kvc
0.1131681
0.1317895
0.1741944
0.012633
2.616-05
0.0030937
0.0025725
0.0022702
0.003733
0.0027905
0.0037482
0.0037482
0.0037482
0.0037485
0.0037485
0.0037485
0.0037485
0.0037485
0.0037485
0.0037485
0.0037485
0.0037485
0.0037485
0.0037485
0.0037485
0.0026977
1E-05
0.0183713
0.0026875
0.0026875
0.0026875
0.0026875
0.0026875
0.0026875
0.0026875
0.0026875
0.0026875
0.0026875
0.0026875
0.0026875
0.0026875
0.0026875
0.0026875
0.0026875
0.0026875
0.0026875
0.0026875
0.0026875
0.0026875
0.0026875
0.0026875
0.0026875
0.0026875
0.0026875
0.0026875
0.0026875
0.0026875
0.0026875
0.0026875
0.0026875
0.0026875
0.0026875
0.0026875
0.0026875
0.0026875
0.0026875
0.0026875
0.0026875
0.0026875
0.0026875
0.0026875
0.0026875
0.0026875
0.0026875
0.0026875
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378
0.00378 | Kvc 95%CI
0.018179135
0.027812426
0.027812426
0.027812426
0.02075244
0.022750745
0.0028290165
0.000829305
0.000829305
0.01322430
0.013659581
0.01322450
0.01322450
0.01322450
0.01322450
0.01322450
0.01322450
0.01322450
0.01322450
0.01322450
0.01322450
0.01322450
0.01322450
0.013821650
0.013821650
0.013821650
0.013821650
0.013821650
0.013821650
0.013821650
0.013821755
0.013821650
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013821755
0.013855
0.013855
0.0138555
0.01385555
0.013855555
0.013855555
0.0138 | LOG + 0 Transfor
Rates
Log
Kcis
0.021
0.021
0.051
0.055
-0.527
-0.656
-2.557
-2.620
-2.557
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.525
-2.620
-2.525
-2.620
-2.525
-2.620
-2.525
-2.620
-2.525
-2.525
-2.620
-2.525
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2 | KcisSD 0.386 0.472 0.522 1.249 -1.328 -1.591 -2.901 -3.118 -2.913 -1.59E+00 -1.54E+00 -1.92E+00 -2.01E+00 -2.01E+00 -3.09E+00 -3.09E+00 | Log Kvc
-0.946
-0.880
-0.759
-1.898
-4.583
-2.509
-2.590
-2.590
-2.374
-2.590
-2.374
-2.590
-2.374
-2.590
-2.590
-2.374
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.590
-2.59 | LogKvcSD
-1.326
-1.141
-0.977
-1.501
-1.531
-1.537
-1.537
-1.537
-1.537
-1.538+00
-1.538+00
-1.358+00
-1.358+00
-1.328+00
-1.328+00
-1.328+00 | Peptides
FdhA
10.40
10.14
10.38
10.67
10.63
10.61
9.95
9.60
9.95
9.83
9.87
10.12 | FdhA std
9,84
9,75
9,75
9,75
9,75
9,75
9,75
9,75
9,75 | PceA
10.72
10.34
10.43
10.75
10.66
10.64
9.42
9.42
9.42
9.42
9.74
9.66 | PccA std
10.26
10.26
10.26
10.14
10.14
10.14
9.24
9.24
9.24
9.73
9.73 | TceA
10.65
10.25
10.37
10.41
10.33
10.19
10.02
10.31
10.02
10.31
10.23
 | TceA std
10.22
10.27
9.98
9.98
9.98
9.98
9.98
9.98
9.98
9.9 | VcrA
9.60
9.41
9.46
10.17
10.14
9.46
9.46
9.41
9.46
9.21
9.58
10.03
9.44
9.72 | VcrA std
9:00
9:82
9:82
9:82
9:82
9:82
9:82
9:82
9:82 | DHC gene
DHC_165 gene
6.73
6.68
6.94
7.11
7.11
7.11
7.11
7.11
7.11
7.11
7.1 | DHC std
5.97
5.97
6.37
6.37
6.37
6.37
5.35
5.35
5.35
5.35
5.35
5.35 | Functional tceA 6.79 6.60 6.82 6.58 7.03 5.74 5.74 5.93 6.09 6.29 6.70 6.31 | Genes
tceA std
6.14
6.14
6.14
6.54
6.54
6.54
6.54
6.54
7
5.53
5.53
5.53
5.53
5.53 | vcrA
6.868
6.771
6.92
6.89
7.04
5.84
6.59
7.04
5.84
6.59
7.04
6.59
7.04
6.53
6.71
6.33 | vcrA std
6.21
6.21
6.55
6.55
6.55
6.55
6.55
5.63
5.63
5.63 | fdhA
6.81
6.62
6.83
7.02
7.02
5.74
5.74
5.74
5.74
5.74
5.79
5.66
5.99
6.92
6.47 | fdhA std
6.16
6.16
6.28
6.28
6.28
5.30
5.30
5.30
6.44
6.44 | pccA
5.73
5.54
5.78
5.78
5.62
5.97
4.23
4.43
4.43
4.43
4.43
5.58
5.58
5.58 | pceA std
5.01
5.41
5.41
3.81
3.81
3.81
5.09
5.09 |
| W + SOLIDS
E E E E E E E E E E E E E E E E E E E | 3LM2 TTWO
3LM2 TTWO

 | TIME TWO
Set1A
Set1A
Set1B
Set1C Dup
Set2A
Set2B
Set2C
Set2A
Set2B
Set2C
Set3A
Set3B
Set4A
Set4B
Set4A
Set4B
Set4A
Set4B
Set4A
Set5B
Set4A
Set5B
Set4A
Set5B
Set4A
Set5B
Set4A
Set5B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
S
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set | Kcis
1.0486058
1.0497445
1.1256485
0.021742
0.0201742
0.00027742
0.00027742
0.00017588
0.00027742
0.0008245
0.0008245
0.0008245
0.0008245
0.0012
0.0008245
0.0012
0.00124
0.00782689
0.0566669
0.0566669
0.0566669
0.0566669
0.0566669
0.0566669
0.0566669
0.0566669
0.0566669
0.0566669
0.0566669
0.0566669
0.0566669
0.0566669
0.0566669
0.056669
0.056669
0.056669
0.056669
0.056669
0.056669
0.056669
0.056669
0.056669
0.056669
0.056669
0.056669
0.056669
0.056669
0.056669
0.056669
0.056669
0.056669
0.056669
0.056669
0.056669
0.056669
0.056669
0.056669
0.056669
0.056669
0.056669
0.056669
0.056669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.0569
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.05669
0.0569 | Kcis
95%Cl
0.937007
1.29700
0.037581
0.001359
0.000403
0.00024
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.001592
0.001592
0.001592
0.001592
0.001592
0.001592
0.001592
0.001592
0.001592
0.001592
0.001592
0.001592
0.001592
0.001592
0.001592
0.001592
0.001592
0.001592
0.001592
0.001592
0.001592
0.001592
0.001592
0.001592
0.001592
0.001592
0.001592
0.001592
0.001592
0.001592
0.001592
0.001592
0.001592
0.001592
0.001592
0.001592
0.001592
0.001592
0.001592
0.001592
0.001592
0.001592
0.001592
0.001592
0.0001592
0.0001592
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.000159
0.00000000000000000000000000000000000 | Kvc 0.113168;
0.131789;
0.131789;
0.131789;
0.001253;
0.002790;
0.003279;
0.003279;
0.003279;
0.003742;
0.003742;
0.003742;
0.003742;
0.003742;
0.003742;
0.003742;
0.003742;
0.003742;
0.003742;
0.003742;
0.003742;
0.003742;
0.003742;
0.003742;
0.003742;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.002687;
0.00267;
0.00267;
0.00267;
0.00267;
0.00267;
0.00267;
0.00267;
0.00267;
0.00 | Kvc 95%C1
0.018179135
0.027812426
0.04056336
0.0278750745
0.003573955
0.008539355
0.008539355
0.008539355
0.008539355
0.003823910
0.013607385
0.01362385
0.013224546
0.01362326
0.00136123208
0.00136123208
0.0016123208 | LOG + 0 Transfor
Rates
Log
Kcis
0.021
0.051
0.051
0.0550
-0.527
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2577
-2.2557
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.25777
-2.25777
-2.25777
-2.25777
-2.25777
-2.25777
-2.25777
-2.25777
-2.25777
-2.25777
-2.2 | Image Image KcisSD 0.386 0.472 0.522 1.249 1.328 -1.521 2.901 -2.901 -3.913 -2.913 -2.913 -1.52E+00 -1.552E+00 -1.52E+00 -1.52E+00 -1.52E+00 -1.52E+00 -1.52E+00 -1.52E+00 -1.52E+00 -1.52E+00 -1.52E+00 -1.52E+00 -1.52E+00 -1.92E+00 -2.04E+00 -2.04E+00 -3.05E+00 -3.05E+00 | Log Kvc
-0.946
-0.880
-0.759
-1.898
-4.737
-2.509
-2.509
-2.374
-1.72E+00
-1.75E+00
-1.65E+00
-1.75E+00
-1.74E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.50E+00
-2.5 | LogKvcSD
-1.326
-1.141
-0.977
-1.331
-1.573
-1.570
-1.510
-1.510
-1.531eV0
-1.531eV0
-1.37E+00
-1.37E+00
-1.32E+00
-1.32E+00
-1.32E+00
-1.32E+00 | Peptides
FdhA
10.44
10.58
10.57
10.63
10.61
9.61
9.90
9.91
9.93
9.87
10.12
10.12 | FdhA std
9.84
9.75
9.75
9.75
9.75
9.75
9.75
9.75
9.31
9.31
9.31
9.31
9.31
9.34
9.46 | PccA
10.72
10.34
10.34
10.75
10.64
10.64
9.942
9.74
9.74
9.74
9.74
9.72
10.22 | PceA std
10.26
10.26
10.26
10.14
10.14
10.14
10.14
9.24
9.24
9.24
9.24
9.27
9.27
9.27
9.27 | TccA
10.65
10.25
10.37
10.41
10.33
10.19
10.19
 | TceA std
10.22
9.88
9.98
9.98
9.98
9.98
9.98
9.89
9.89
9.89
9.89
9.89
9.89
9.81 | VcrA
#VALUE
9.60
9.44
10.17
10.14
9.46
9.94
9.95
9.68
9.921
9.58
9.928
9.928
9.929 | VcrA std
9.00
9.00
9.82
9.82
9.82
9.82
9.82
9.82
9.82
9.82 | DHC gene
DHC_165 gene
6.73
6.68
6.82
6.94
7.11
7.11
5.55
5.55
5.70
5.50
6.73
7.00
6.67 | DHC std
5.97
5.97
6.37
6.37
6.37
6.37
5.35
5.35
5.35
5.35
5.35
6.47
6.47 | Functional
tccA
6.79
6.60
6.82
7.03
5.74
5.74
5.74
5.74
6.09
6.29
6.70
6.31 | Genes
tceA std
6.14
6.14
6.54
6.54
6.54
6.54
8.55
5.53
5.53
5.53
5.53 | vcrA
6.866
6.71
6.92
7.04
7.04
5.84
6.69
6.99
6.39
6.39 | verA std 1
6.21
6.52
6.55
6.55
6.55
5.63
5.63
5.63
5.63
5.63 | fdhA
6.61
6.62
6.83
7.02
7.02
5.74
5.74
5.93
5.96
6.67
9.92
6.47 | fdhA sid
6.16
6.16
6.28
6.28
6.28
5.30
5.30
5.30
6.44
6.44
6.44 | pceA
5.73
5.54
5.71
5.78
5.62
5.97
4.23
4.43
4.43
4.43
4.47
5.58
5.15 | pceA std
5.01
5.41
5.41
3.81
3.81
3.81
3.81
5.09
5.09
5.09 |
| GW + SOLIDS
E E E E E E E E E E E E E E E E E E E | BLM2 TTWO

 | TIME TWO
Set1A
Set1A
Set1B
Set1C
Dup
Set1B_Dup
Set1C_Dup
Set2A
Set2A
Set2C
Set3A
Set2C
Set3A
Set3B
Set4A
Set6B
Set4A
Set6B
Set6A
Set6B
Set6B
Set1C
Set1E
Set1F_Dup
Set1E_Dup
Set1E_Dup
Set1E_Dup
Set1E_Dup
Set1E_Dup
Set1E_Dup
Set2C
Set2A
Set2B
Set2A
Set3B
Set3B
Set4A
Set6B
Set4A
Set6B
Set6B
Set1D
Set1E_Dup
Set1E_Dup
Set1E_Dup
Set2B
Set2B
Set2B
Set2B
Set2B
Set2B
Set2B
Set2B
Set2B
Set2B
Set2B
Set2B
Set2B
Set2B
Set2B
Set2B
Set2B
Set2B
Set2B
Set2B
Set2B
Set2B
Set2B
Set2B
Set2B
Set2B
Set2B
Set2B
Set2B
Set2B
Set2B
Set2B
Set2B
Set2B
Set2B
Set2B
Set2B
Set2B
Set3B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
S
Set4B
S
Set4B
S
Set4B
S
Set4B
S
Set4B
S
Set4B
S
Set4B
S
Set4B
S
Set4B
S
Set4B
S
Set4B
S
Set4B
S
Set4B
S
Set4B
S
Set4B
S
Set4B
S
Set4B
S
Set4B
S
Set4B
S
Set4B
S
Set4B
S
Set4B
S
Set4B
S
Set4B
S
Set4B
S
Set4B
S
Set4B
S
Set4B
S
Set4B
S
Set4B
S
Set4B
S
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
S | Kcis
1.0486058
1.0497445
1.1256485
0.2817833
0.2006786
0.0027742
0.0017588
0.0029742
0.0008609
0.001045
0.0008609
0.000121
0.0008609
0.000121
0.0008609
0.001121
0.008248
0.087549
0.0956469
0.001
0.001
0.0001
0.001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001
0.0001 | Kcis 95%CC
0.937007
0.937007
1.29700
0.000403
0.00024
0.00028
0.00029
0.000028
0.00029
0.000028
0.00029
0.000028
0.00029
0.000028
0.000029
0.000028
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.00029
0.0000000000 | Kvc
0.1131683
0.174194
0.002637
0.000572
0.000572
0.000572
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.00073
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.00025
0.00025
0.00025
0.00025
0.00025
0.00025
0.00025
0.00025
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0005
0.0000 | Kvc 95%Cl
0.018179135
0.027812426
0.04056336
0.027879745
0.03067244
0.0008539355
0.006290165
0.01362346
0.01362346
0.01362346
0.01362346
0.01362346
0.01362346
0.01362346
0.01362346
0.01362346
0.01352346
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.01352345
0.0135235000000000000000000000000000000000 | LOG + 0 Transfor
Rates
Log
Kcis
0.021
0.051
0.055
0.0557
0.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.2557
2.25577
2.25577
2.25577
2.25577
2.25577
2.255777
2.255777
2.2557777777777 | ************************************ | Log Kvc
-0.94
-0.880
-0.759
-1.898
-4.583
-2.539
-2.590
-2.590
-2.590
-2.590
-2.374
-1.72E+00
-1.75E+00
-1.75E+00
-1.75E+00
-1.75E+00
-1.75E+00
-1.75E+00
-1.257E+00
-1.50E+00
-2.57E+00
-2.57E+00
-1.40E+00
-5.00E+00
-4.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00
-5.00E+00E+00
-5.00E+00E+00
-5.00 | LogKvcSD
-1.326
-1.141
-0.977
-1.337
-1.501
-1.573
-1.570
-1.510
-1.538+00
-1.538+00
-1.3378+00
-1.3378+00
-1.328+00
-1.328+00
-1.328+00
-1.328+00
-1.328+00 | Peptides
FdhA
10.40
10.53
10.63
10.61
9.60
9.60
9.91
9.83
9.87
10.12 | FdhA std
9.84
9.75
9.75
9.75
9.75
9.75
9.75
9.75
9.75 | PceA
10.72
10.34
10.43
10.75
10.66
10.64
9.42
9.42
9.42
9.42
9.42
10.22
10.24 | PeeA std
10.26
10.26
10.10
10.14
10.14
10.14
10.14
9.24
9.24
9.24
9.24
9.24
9.24
9.24
9.2 | TceA
10.65
10.27
10.41
10.33
10.19
10.02
10.02
10.31
10.19
 | TceA std
10.22
10.22
9.98
9.98
9.98
9.98
9.88
9.88
9.89
9.89
9.89
9.89
9.89
9.89
9.89
9.89
9.89
9.81 | VcrA
#VALUE!
9.60
9.46
10.17
10.14
10.14
9.68
9.21
9.58
9.21
9.58
9.21
9.58
9.21
9.58
9.21
9.58
9.21
9.58
9.21
9.58
9.21
9.58
9.58
9.58
9.58
9.58
9.58
9.58
9.58 | VerA std
9.00
9.00
9.82
9.82
9.82
9.82
9.82
9.82
9.82
9.82 | DHC gene
DHC_165 gene
6.73
6.68
6.82
6.94
7.11
7.11
5.55
5.70
5.90
6.73
7.00
6.67 | DHC std
5.97
5.97
6.37
6.37
6.37
6.37
6.37
6.37
5.35
5.35
5.35
5.35
5.35
6.67
6.47 | Eurotional
6.79
6.60
6.82
6.94
6.58
7.03
7.03
5.74
5.93
6.09
6.29
6.20
6.20
6.31 | Genes
tceA std
6.14
6.54
6.54
6.54
6.54
5.53
5.53
5.53
6.54
6.54 | vcrA
6.86
6.71
6.92
7.04
5.84
6.99
7.04
5.84
6.04
6.19
6.35
6.71
6.39 | verA std
621
621
635
655
655
655
655
655
655
655
655
655 | fdhA
6.81
6.62
6.83
7.02
5.74
5.93
5.96
6.79
6.92
6.47 | fdhA std
6.16
6.16
6.28
6.28
6.28
6.28
5.30
5.30
5.30
5.30
6.44
6.44 | pceA
5.73
5.54
5.62
5.97
4.23
4.43
4.43
5.58
5.58
5.58 | pceA std
5.01
5.41
5.41
5.41
3.81
3.81
3.81
3.81
3.81
3.81
3.81
3.8 |
| 6W+SOLDS
EEEEEEEEEEEEEEEEEEEEEEEEEEEEEEEEEEEE | SLM2 TTWO
SLM2 T | TIME TWO
Set1A
Set1B
Set1C
Set2C
Set2A
Set2B
Set2C
Set2A
Set2B
Set2C
Set3A
Set3C
Set3C
Set4B
Set4C
Set4B
Set4C
Set4B
Set4C
Set5A
Set5B
Set5B
Set5B
Set5B
Set5B
Set1D
Set1F
Set1D
Set1F
Set1D
Set1F
Set1F
Set1F
Set1F
Set1F
Set1F
Set1F
Set1F
Set1F
Set2F
Set2F
Set2F
Set2F
Set2F
Set2F
Set2F
Set2F
Set2F
Set2F
Set2F
Set2F
Set2F
Set2F
Set2F
Set2F
Set2F
Set2F
Set2F
Set2F
Set2F
Set2F
Set2F
Set2F
Set2F
Set2F
Set2F
Set2F
Set2F
Set2F
Set2F
Set2F
Set2F
Set2F
Set2F
Set2F
Set2F
Set2F
Set2F
Set2F
Set2F
Set2F
Set2F
Set2F
Set2F
Set2F
Set2F
Set2F
Set2F
Set2F
Set2F
Set2F
Set2F
Set2F
Set2F
Set2F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set3F
Set | Kcis
1.0497445
1.1256485
0.2817833
0.297343
0.2206698
0.0027742
0.0017588
0.0028753
0.0008753
0.0008753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00082753
0.00092753
0.00092753
0.00092753
0.00092753
0.00092753
0.00092753
0.00092753
0.00092753
0.00092753
0.00092753
0.00092753
0.00092753
0.00092755
0.00092755
0.00092755
0.00092755
0.00092755
0.00092755
0.00092755
0.00092755
0.00092755
0.00092755
0.00092755
0.00092755
0.00092755
0.00092755
0.00092755
0.00092755
0.00092755
0.00092755
0.00092755
0.00092755
0.00092755
0.00092755
0.00092755
0.00092755
0.00092755
0.00092755
0.00092755
0.00092755
0.00092755
0.00092755
0.00092755
0.00092755
0.00092755
0.00092755
0.00092755
0.00092755
0.00092755
0.00092755
0.00092755 | Kcis 95%CC
0.937007
1.247008
0.037581
0.037581
0.000403
0.00024
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.0000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.000252
0.00025
0.00025
0.00025
0.00025
0.00025
0.00025
0.00025
0.00025
0.00025
0.00025
0.00025
0.00025
0.00025
0.00025
0.00025
0.00025
0.00025
0.000025
0.000025
0.000025
0.000025
0.000025
0.000025
0.000025
0.000025
0.000025
0.000025
0.000025
0.000025
0.000025
0.000025
0.000025
0.000025
0.000025
0.000025
0.000025
0.000025
0.00005
0.00005
0.00005
0.00005
0.00005
0.00005
0.00005
0.00005
0.00005
0.00005
0.00005
0.00005
0.00005
0.00005
0.00005
0.00005
0.00005
0.00005
0.00005
0.00005
0.00005
0.00005
0.00005
0.00005
0.00005
0.00005
0.00005
0.00005
0.00005
0.00005
0.00005
0.00005
0.00005
0.00005
0.00005
0.00005
0.00005
0.00005
0.00005
0.00005
0.00005
0.00005
0.00005
0.00005
0.00005
0.00005
0.00005
0.00005
0.00005
0.00005
0.00005
0.00005
0.00005
0.00005
0.00005
0.00005
0.00005
0.00005
0.00005
0.00005
0.00005
0.00005
0.00005
0.00005
0.00005
0.00005
0.00005
0.00005
0.00005
0.00005
0.00005
0.00005
0.00005
0.00005
0.00005
0.00005
0.00005
0.00005
0.00005
0.00005
0.00005
0.00005
0.00005
0.00005
0.00005
0.00005
0.00005
0.00005
0.00000000 | Kvc 0.113168; 0.131769; 0.131769; 0.131769; 0.131769; 0.131769; 0.131769; 0.131769; 0.131769; 0.002372; 0.003762; 0.003313; 0.002763; 0.003762; 0.003312; 0.002763; 0.003762; 0.003312; 0.003762; 0.003312; 0.003762; 0.003762; 0.003762; 0.003762; 0.003762; 0.003762; 0.003762; 0.002677; 0.16339; 0.002677; 0.16339; 0.002677; 0.003762; 0.002677; 0.003762; 0.002677; 0.0025; 0. | Kvc 95%CI
0.018179135
0.027812426
0.027812426
0.0207812426
0.02078244
0.02078244
0.02078244
0.000853935
0.0008293015
0.000893947
0.013478322
0.013659581
0.01322456
0.01322456
0.01322456
0.01322456
0.01322456
0.01322456
0.01322456
0.01322456
0.01322456
0.01322456
0.01322456
0.013827851
0.013827851
0.013827851
0.013827851
0.013827851
0.013827851
0.013827851
0.013827851
0.013827851
0.013827851
0.013827851
0.013827851
0.013827851
0.013827851
0.013827851
0.013827851
0.013827851
0.013827851
0.013827851
0.013827851
0.013827851
0.013827851
0.013827851
0.013817852
0.013827851
0.013817852
0.013827851
0.013817852
0.013827851
0.013817852
0.013827851
0.013817852
0.013827851
0.013817852
0.013827851
0.013817852
0.013827851
0.013817852
0.013827851
0.013817852
0.013827851
0.013817852
0.013827851
0.013817852
0.013827851
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817852
0.013817 | LOG + 0 Transfor
Rates
Log Kcis
0.021
0.021
0.051
0.055
-0.527
-0.656
-2.557
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.620
-2.525
-2.620
-2.620
-2.520
-2.620
-2.520
-2.620
-2.520
-2.620
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2.520
-2 | KcisSD 0.386 0.422 0.522 1.249 -1.318 -2.901 -3.118 -2.913 -1.592 -1.592 -1.592 -2.913 -1.592 | Log Kvc
-0.946
-0.880
-0.759
-1.898
-4.583
-2.173
-2.590
-2.590
-2.374
-2.590
-2.374
-2.590
-2.374
-2.590
-2.374
-2.590
-2.374
-2.590
-1.72E+00
-1.78E+00
-1.78E+00
-1.78E+00
-5.00E+00
-2.57E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
-4.00E+00
- | LogkvcSD
-1.326
-1.141
-0.977
-1.501
-1.531
-1.537
-1.587
-1.510
-1.538+00
-1.538+00
-1.328+00
-1.328+00
-1.328+00
-1.328+00
-1.328+00
-1.328+00
-1.328+00
-1.328+00
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1.538+01
-1. | Peptides
FdhA
10.40
10.13
10.57
10.63
10.61
9.60
9.91
9.83
9.87
10.12 | FdhA std
9,84
9,75
9,75
9,75
9,75
9,75
9,75
9,75
9,75 | PceA
10.72
10.34
10.43
10.64
10.64
10.64
9.42
9.74
9.62
10.22
10.24 | PeeA std
10.26
10.26
10.12
10.14
10.14
10.14
10.14
9.24
9.24
9.24
9.24
9.24
9.24
9.24
9.2 | TceA
10.65
10.25
10.37
10.41
10.19
10.19 | TceA std 1
10.22
9.98
9.999
9.98
9.98
9.98
9.98
9.98 | VcrA
47ALUE1
9.60
9.46
10.17
10.14
10.14
10.14
9.94
9.921
9.58
10.03
9.44
9.72 | VerA std
9.00
9.00
9.82
9.82
9.82
9.82
9.82
9.82
9.82
9.82 | DHC gene
DHC_165 gene
6.73
6.68
6.82
6.94
7.11
7.11
7.11
7.11
7.11
7.11
7.11
7.1 | DHC std
5.97
5.97
6.37
6.37
6.37
6.37 | Functional tccA 6.79 6.60 6.82 7.03 5.74 5.73 6.89 6.91 6.92 6.93 6.93 6.94 7.03 | Genes
tccA std
6.14
6.14
6.54
6.54
6.54
5.53
5.53
5.53
5.53
5.53
6.24 | vcrA
6.86
6.71
6.92
6.89
6.89
7.04
5.84
6.64
6.04
6.93
6.71
6.39 | verA std
6.21
6.21
6.55
6.55
6.55
6.55
6.55
6.55
6.55
6.5 | fdhA
6.81
6.62
6.83
7.02
7.02
5.74
5.74
5.93
5.96
6.79
5.92
6.47 | fdhA std
6.16
6.16
6.28
6.28
6.28
5.30
5.30
5.30
5.30
5.30 | pceA
5.73
5.54
5.72
5.97
5.97
4.23
4.43
4.43
4.43
5.58
5.58
5.58 | pceA std
5.01
5.41
5.41
3.81
3.81
3.81
3.81
3.81
5.09
5.09 |
| GW+SOLIDS
EXTERTED FOR ENTRY GWONY | BLM2 TTWO BLM2 TTWO <td< td=""><td>TIME TWO
Set1A
Set1A
Set1B
Set1C Dup
Set2A
Set2B
Set2C
Set2A
Set2C
Set3A
Set3B
Set3C
Set3A
Set4A
Set4B
Set4A
Set4B
Set4A
Set4B
Set4A
Set4B
Set4A
Set4B
Set4A
Set5B
Set4A
Set5B
Set4A
Set5B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B</td><td>Kcis
1.0486058
1.0497445
1.1256485
0.027742
0.021788
0.0027742
0.0017588
0.0027742
0.0008245
not sample
rate not co
rate not co</td><td>Kcis
95%C(1)
937007
1.141049
1.279709
0.0037581
0.0037581
0.0037581
0.00026
0.000026
0.000026
0.000026
0.000026
0.000026
0.000026
0.000026
0.000026
0.000026
0.000026
0.000026
0.000026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.0000</td><td>Kvc
0.113168/80
0.13178990
0.002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.000257
0.000257
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.000000</td><td>Kvc 95%C1
0.018179135
0.027812426
0.04056336
0.027812426
0.000559355
0.000859355
0.0008593955
0.0008593955
0.000829391
0.013605385
0.013262381
0.013262381
0.013262381
0.013224546
enot sampled
rate not compu
rate not compu
rate not compu
rate not compu
rate not compu
o.000812798
0.0015226881
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.013855
0.0138555
0.01385555
0.0138555555555555555555555555555555555555</td><td>LOG + 0 Transfor
Rates
Log
Kcis
0.021
0.021
0.051
0.055
0.0557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.25777
-2.2577
-2.2577
-2.25777
-2.25777
-2.25777
-2.</td><td>Immed for Ana KcisSD 0.386 0.472 0.522 1.249 1.328 -1.521 -2.901 -3.118 -2.913 -2.913 -1.521+00 -1.525+00 -1.525+00 -1.525+00 -1.525+00 -1.927+00 -2.045+00 -3.055+00 -3.055+00 -3.055+00 -2.825+00</td><td>lysis
Log Kvc
-0.96
-0.880
-0.759
-1.898
-4.583
-2.173
-2.509
-2.374
-2.590
-2.374
-2.590
-2.374
-1.72E+00
-1.75E+00
-1.68E+00
-1.75E+00
-1.68E+00
-2.50E+00
-4.00E+00
-4.00E+00</td><td>LogKvcSD
-1.326
-1.141
-0.977
-1.331
-1.573
-1.570
-1.570
-1.570
-1.510
-1.534
-1.534
-1.534+00
-1.5334+00
-1.3774+00
-1.3274+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.344+00
-1.344+00
-1.344+00
-1.344+00
-1.344+00
-1.344+00
-1</td><td>Peptides
FdhA
10.40
10.53
10.63
10.61
10.61
9.60
9.91
9.83
9.87
10.12
10.12</td><td>FdhA std
9.84
9.75
9.75
9.75
9.75
9.75
9.75
9.75
9.75</td><td>PceA
10.72
10.34
10.75
10.66
10.64
9.42
9.42
9.42
9.42
9.42
9.42
9.42
9.4</td><td>PceA std
10.26
10.26
10.26
10.14
10.14
10.14
9.24
9.24
9.24
9.24
9.24
9.24
9.24
9.2</td><td>TceA
10.65
10.25
10.37
10.41
10.31
10.19</td><td>TceA std 1
10.22
9.98
9.98
9.98
9.98
9.88
9.89
9.89
9</td><td>VcrA
#VALUE1
9.60
9.46
10.17
10.14
9.68
9.10
9.21
9.58
9.21
10.03
9.44
9.72</td><td>VcrA std
9.00
9.02
9.82
9.82
9.82
9.82
9.82
9.82
9.82
9.8</td><td>DHC gene
DHC_165 gene
6.73
6.68
6.82
6.94
7.11
7.11
5.55
5.70
5.70
5.70
6.73
7.00
6.67</td><td>DHC std
5.97
6.37
6.37
6.37
6.37
5.35
5.35
5.35
5.35
5.35
6.47</td><td>LccA 1
6.79
6.60
6.82
7.03
5.74
5.93
6.09
6.58
7.03
7.03
6.09
6.29
6.70
6.31</td><td>Genes
tccA std
6.14
6.54
6.54
6.54
6.54
5.53
5.53
5.53
6.24</td><td>verA
6.86
6.71
6.92
6.89
7.04
5.84
6.59
7.04
5.84
6.64
6.04
6.39
6.39</td><td>vcr4 std
6.21
6.55
6.55
6.55
6.55
5.63
5.63
5.63
5.63</td><td>fdhA
6.81
6.62
6.83
7.02
5.74
5.74
5.93
5.93
6.92
6.92
6.47</td><td>fdhA std
6.16
6.16
6.28
6.28
6.28
6.28
5.30
5.30
5.30
5.30
5.30
5.30
5.30</td><td>pceA
5.73
5.54
5.71
5.72
5.62
5.97
4.23
4.43
4.43
4.43
4.447
5.548
5.15</td><td>pceA std
5.01
5.41
5.41
5.41
5.41
3.81
3.81
3.81
3.81
5.09
5.09</td></td<> | TIME TWO
Set1A
Set1A
Set1B
Set1C
Dup
Set2A
Set2B
Set2C
Set2A
Set2C
Set3A
Set3B
Set3C
Set3A
Set4A
Set4B
Set4A
Set4B
Set4A
Set4B
Set4A
Set4B
Set4A
Set4B
Set4A
Set5B
Set4A
Set5B
Set4A
Set5B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B | Kcis
1.0486058
1.0497445
1.1256485
0.027742
0.021788
0.0027742
0.0017588
0.0027742
0.0008245
not sample
rate not co
rate not co | Kcis 95%C(1)
937007
1.141049
1.279709
0.0037581
0.0037581
0.0037581
0.00026
0.000026
0.000026
0.000026
0.000026
0.000026
0.000026
0.000026
0.000026
0.000026
0.000026
0.000026
0.000026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.00026
0.0000 | Kvc
0.113168/80
0.13178990
0.002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.0002572
0.000257
0.000257
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.000000
 | Kvc 95%C1
0.018179135
0.027812426
0.04056336
0.027812426
0.000559355
0.000859355
0.0008593955
0.0008593955
0.000829391
0.013605385
0.013262381
0.013262381
0.013262381
0.013224546
enot sampled
rate not compu
rate not compu
rate not compu
rate not compu
rate not compu
o.000812798
0.0015226881
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.01382385
0.013855
0.0138555
0.01385555
0.0138555555555555555555555555555555555555 | LOG + 0 Transfor
Rates
Log Kcis
0.021
0.021
0.051
0.055
0.0557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2557
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.2577
-2.25777
-2.2577
-2.2577
-2.25777
-2.25777
-2.25777
-2. | Immed for Ana KcisSD 0.386 0.472 0.522 1.249 1.328 -1.521 -2.901 -3.118 -2.913 -2.913 -1.521+00 -1.525+00 -1.525+00 -1.525+00 -1.525+00 -1.927+00 -2.045+00 -3.055+00 -3.055+00 -3.055+00 -2.825+00 | lysis
Log Kvc
-0.96
-0.880
-0.759
-1.898
-4.583
-2.173
-2.509
-2.374
-2.590
-2.374
-2.590
-2.374
-1.72E+00
-1.75E+00
-1.68E+00
-1.75E+00
-1.68E+00
-2.50E+00
-4.00E+00
-4.00E+00 |
LogKvcSD
-1.326
-1.141
-0.977
-1.331
-1.573
-1.570
-1.570
-1.570
-1.510
-1.534
-1.534
-1.534+00
-1.5334+00
-1.3774+00
-1.3274+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.3224+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.324+00
-1.344+00
-1.344+00
-1.344+00
-1.344+00
-1.344+00
-1.344+00
-1 | Peptides
FdhA
10.40
10.53
10.63
10.61
10.61
9.60
9.91
9.83
9.87
10.12
10.12 | FdhA std
9.84
9.75
9.75
9.75
9.75
9.75
9.75
9.75
9.75 | PceA
10.72
10.34
10.75
10.66
10.64
9.42
9.42
9.42
9.42
9.42
9.42
9.42
9.4 | PceA std
10.26
10.26
10.26
10.14
10.14
10.14
9.24
9.24
9.24
9.24
9.24
9.24
9.24
9.2 | TceA
10.65
10.25
10.37
10.41
10.31
10.19 | TceA std 1
10.22
9.98
9.98
9.98
9.98
9.88
9.89
9.89
9 | VcrA
#VALUE1
9.60
9.46
10.17
10.14
9.68
9.10
9.21
9.58
9.21
10.03
9.44
9.72 | VcrA std
9.00
9.02
9.82
9.82
9.82
9.82
9.82
9.82
9.82
9.8 | DHC gene
DHC_165 gene
6.73
6.68
6.82
6.94
7.11
7.11
5.55
5.70
5.70
5.70
6.73
7.00
6.67 | DHC std
5.97
6.37
6.37
6.37
6.37
5.35
5.35
5.35
5.35
5.35
6.47 | LccA 1
6.79
6.60
6.82
7.03
5.74
5.93
6.09
6.58
7.03
7.03
6.09
6.29
6.70
6.31 | Genes
tccA std
6.14
6.54
6.54
6.54
6.54
5.53
5.53
5.53
6.24 | verA
6.86
6.71
6.92
6.89
7.04
5.84
6.59
7.04
5.84
6.64
6.04
6.39
6.39 | vcr4 std
6.21
6.55
6.55
6.55
6.55
5.63
5.63
5.63
5.63 | fdhA
6.81
6.62
6.83
7.02
5.74
5.74
5.93
5.93
6.92
6.92
6.47 | fdhA std
6.16
6.16
6.28
6.28
6.28
6.28
5.30
5.30
5.30
5.30
5.30
5.30
5.30 | pceA
5.73
5.54
5.71
5.72
5.62
5.97
4.23
4.43
4.43
4.43
4.447
5.548
5.15 | pceA std
5.01
5.41
5.41
5.41
5.41
3.81
3.81
3.81
3.81
5.09
5.09 |
| GW + SOLDS
GW + SOLDS
GW ONLY
GW ONL | BLM2 TTWO BLM2 TTWO <td< td=""><td>TIME TWO
Set1A
Set1A
Set1B
Set1C
Dup
Set1B_Dup
Set1C_Dup
Set2A
Set2A
Set2C
Set3A
Set3C
Set3A
Set3C
Set4B
Set3C
Set4B
Set4A
Set6B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set</td><td>Kcis
1.0486058
1.0497445
1.1256485
0.281783
0.2007742
0.0017588
0.00237742
0.0017588
0.0008675
0.0008675
0.0008675
0.0008675
0.0008121
0.0008248
0.00856669
0.00592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0</td><td>Kcis 95%C(0
0.937007
1.29700
0.037581
0.037581
0.000403
0.00024
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000000000</td><td>Kvc
0.113168/
0.124196
0.124196
0.005712
0.005725
0.005725
0.005725
0.005725
0.005725
0.005725
0.007235
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000724
0.000724
0.000724
0.000724
0.000724
0.000724
0.000724
0.000742
0.000742
0.000742
0.000742
0.000742
0.000742
0.000742
0.000742
0.000742
0.000742
0.000742
0.000742
0.000742
0.000742
0.000742
0.000742
0.000742
0.000742
0.000742
0.000742
0.000742
0.000742
0.000742
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.000000</td><td>Kvc 95%Cl
0.018179135
0.027812426
0.042566336
0.027812426
0.03057324
0.03057324
0.03057324
0.031278745
0.01326326
0.01326326
0.01326326
0.01326326
0.01326326
0.01326326
0.01326326
0.0132235
0.0132235
0.0132235
0.0132235
0.0132235
0.0132235
0.013235
0.013235
0.013235
0.013235
0.013235
0.013235
0.013235
0.013235
0.013235
0.013235
0.013235
0.013235
0.013235
0.013235
0.013235
0.013235
0.013235
0.013235
0.013235
0.013235
0.013235
0.013235
0.013235
0.013235
0.013235
0.013235
0.013235
0.013235
0.013235
0.013235
0.013235
0.013235
0.013235
0.013235
0.013235
0.013235
0.013235
0.013235
0.013235
0.013235
0.013235
0.013235
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.0132555
0.0132555
0.0132555
0.0132555
0.0132555
0.0132555
0.01355555
0.013555555
0.01355555555555555555555555555555555555</td><td>LOG + 0 Transfor
Rates
Log Kcis
0.021
0.051
0.055
0.0557
0.0557
0.0557
0.0557
0.2577
0.2577
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.25700
0.25700
0.25700
0.25700
0.25700000000000000000000000000000000000</td><td>**************************************</td><td>lysis
Log Kvc
-0.946
-0.880
-0.759
-1.898
-4.583
-2.509
-2.509
-2.590
-2.374
-2.590
-2.374
-1.72E+00
-1.75E+00
-1.74E+00
-2.57E+00
-4.05E+00
-4.05E+00
-4.05E+00</td><td>LogKvcSD
-1.326
-1.141
-0.977
-1.337
-1.501
-1.573
-1.573
-1.510
-1.538+00
-1.538+00
-1.538+00
-1.328+00
-1.328+00
-1.328+00
-1.328+00
-1.328+00
-1.328+00</td><td>Peptides
FdhA
10.40
10.14
10.53
10.63
10.61
9.60
9.60
9.91
9.83
9.87
10.12
10.12</td><td>FdhA std
9.84
9.75
9.75
9.75
9.75
9.75
9.75
9.75
9.75</td><td>PceA
10.72
10.34
10.43
10.66
10.64
10.64
9.42
9.42
9.42
9.42
9.42
9.10.21
10.22
10.24</td><td>PeeA std
10.26'
10.26'
10.10'
10.14'
10.14'
9.24
9.24
9.24'
9.24'
9.24'
9.24'
9.24'
9.24'
9.24'
9.24'
9.24'
9.24'</td><td>TceA
10.65
10.25
10.37
10.41
10.19
10.19</td><td>TceA std
10.22
9.98
9.98
9.98
9.98
9.98
9.98
9.98
9</td><td>VcrA
#VALUE!
9.60
9.46
10.17
10.14
10.14
9.46
9.46
9.46
9.42
9.51
9.52
9.44
9.72</td><td>VerA std
9.00
9.00
9.82
9.82
9.82
9.82
9.82
9.82
9.82
9.82</td><td>DHC gene
DHC_165 gene
6.73
6.68
6.82
6.94
7.11
7.11
7.11
7.11
7.11
7.11
7.11
7.1</td><td>DHC std
5.97
5.97
6.37
6.37
6.37
6.37
6.37
5.35
5.35
5.35
5.35
5.35
6.647
6.47</td><td>Functional
6.79
6.60
6.82
7.03
7.03
5.74
5.93
6.09
6.29
6.29
6.20
6.31</td><td>Genes
tccA std
6.14
6.14
6.54
6.54
6.54
5.53
5.53
5.53
5.53
5.53
6.24
6.24</td><td>vcrA
6.86
6.71
6.92
6.89
7.04
5.84
6.59
7.04
5.84
6.60
6.04
6.33
6.71
6.39</td><td>vcr4 std
6.21
6.21
6.55
6.55
6.55
6.55
6.55
6.55
6.55
6.5</td><td>fdhA
6.81
6.62
6.83
7.02
7.02
5.74
5.74
5.74
5.93
5.56
6.29
6.22
6.47</td><td>fdhA std
6.16
6.16
6.28
6.28
6.28
5.30
5.30
5.30
5.30
6.44
6.44</td><td>pceA
5.73
5.54
5.62
5.62
5.97
4.23
4.43
4.43
5.48
5.15</td><td>pceA std
5.01
5.41
5.41
5.41
3.81
3.81
3.81
3.81
3.81
5.09
5.09</td></td<> | TIME TWO
Set1A
Set1A
Set1B
Set1C
Dup
Set1B_Dup
Set1C_Dup
Set2A
Set2A
Set2C
Set3A
Set3C
Set3A
Set3C
Set4B
Set3C
Set4B
Set4A
Set6B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set4B
Set | Kcis
1.0486058
1.0497445
1.1256485
0.281783
0.2007742
0.0017588
0.00237742
0.0017588
0.0008675
0.0008675
0.0008675
0.0008675
0.0008121
0.0008248
0.00856669
0.00592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0592488
0.0 | Kcis 95%C(0
0.937007
1.29700
0.037581
0.037581
0.000403
0.00024
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000052
0.000000000 | Kvc
0.113168/
0.124196
0.124196
0.005712
0.005725
0.005725
0.005725
0.005725
0.005725
0.005725
0.007235
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000723
0.000724
0.000724
0.000724
0.000724
0.000724
0.000724
0.000724
0.000742
0.000742
0.000742
0.000742
0.000742
0.000742
0.000742
0.000742
0.000742
0.000742
0.000742
0.000742
0.000742
0.000742
0.000742
0.000742
0.000742
0.000742
0.000742
0.000742
0.000742
0.000742
0.000742
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.00000
0.000000 | Kvc 95%Cl
0.018179135
0.027812426
0.042566336
0.027812426
0.03057324
0.03057324
0.03057324
0.031278745
0.01326326
0.01326326
0.01326326
0.01326326
0.01326326
0.01326326
0.01326326
0.0132235
0.0132235
0.0132235
0.0132235
0.0132235
0.0132235
0.013235
0.013235
0.013235
0.013235
0.013235
0.013235
0.013235
0.013235
0.013235
0.013235
0.013235
0.013235
0.013235
0.013235
0.013235
0.013235
0.013235
0.013235
0.013235
0.013235
0.013235
0.013235
0.013235
0.013235
0.013235
0.013235
0.013235
0.013235
0.013235
0.013235
0.013235
0.013235
0.013235
0.013235
0.013235
0.013235
0.013235
0.013235
0.013235
0.013235
0.013235
0.013235
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.013255
0.0132555
0.0132555
0.0132555
0.0132555
0.0132555
0.0132555
0.01355555
0.013555555
0.01355555555555555555555555555555555555 | LOG + 0 Transfor
Rates
Log Kcis
0.021
0.051
0.055
0.0557
0.0557
0.0557
0.0557
0.2577
0.2577
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.257
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.2570
0.25700
0.25700
0.25700
0.25700
0.25700000000000000000000000000000000000 | ************************************** | lysis
Log Kvc
-0.946
-0.880
-0.759
-1.898
-4.583
-2.509
-2.509
-2.590
-2.374
-2.590
-2.374
-1.72E+00
-1.75E+00
-1.74E+00
-2.57E+00
-4.05E+00
-4.05E+00
-4.05E+00 | LogKvcSD
-1.326
-1.141
-0.977
-1.337
-1.501
-1.573
-1.573
-1.510
-1.538+00
-1.538+00
-1.538+00
-1.328+00
-1.328+00
-1.328+00
-1.328+00
-1.328+00
-1.328+00 | Peptides
FdhA
10.40
10.14
10.53
10.63
10.61
9.60
9.60
9.91
9.83
9.87
10.12
10.12 | FdhA std
9.84
9.75
9.75
9.75
9.75
9.75
9.75
9.75
9.75 | PceA
10.72
10.34
10.43
10.66
10.64
10.64
9.42
9.42
9.42
9.42
9.42
9.10.21
10.22
10.24 | PeeA std
10.26'
10.26'
10.10'
10.14'
10.14'
9.24
9.24
9.24'
9.24'
9.24'
9.24'
9.24'
9.24'
9.24'
9.24'
9.24'
9.24' | TceA
10.65
10.25
10.37
10.41
10.19
10.19 | TceA std
10.22
9.98
9.98
9.98
9.98
9.98
9.98
9.98
9 | VcrA
#VALUE!
9.60
9.46
10.17
10.14
10.14
9.46
9.46
9.46
9.42
9.51
9.52
9.44
9.72 | VerA std
9.00
9.00
9.82
9.82
9.82
9.82
9.82
9.82
9.82
9.82 | DHC gene
DHC_165 gene
6.73
6.68
6.82
6.94
7.11
7.11
7.11
7.11
7.11
7.11
7.11
7.1 | DHC std
5.97
5.97
6.37
6.37
6.37
6.37
6.37
5.35
5.35
5.35
5.35
5.35
6.647
6.47 | Functional
6.79
6.60
6.82
7.03
7.03
5.74
5.93
6.09
6.29
6.29
6.20
6.31 | Genes
tccA std
6.14
6.14
6.54
6.54
6.54
5.53
5.53
5.53
5.53
5.53
6.24
6.24 | vcrA
6.86
6.71
6.92
6.89
7.04
5.84
6.59
7.04
5.84
6.60
6.04
6.33
6.71
6.39 | vcr4 std
6.21
6.21
6.55
6.55
6.55
6.55
6.55
6.55
6.55
6.5 | fdhA
6.81
6.62
6.83
7.02
7.02
5.74
5.74
5.74
5.93
5.56
6.29
6.22
6.47 | fdhA std
6.16
6.16
6.28
6.28
6.28
5.30
5.30
5.30
5.30
6.44
6.44 | pceA
5.73
5.54
5.62
5.62
5.97
4.23
4.43
4.43
5.48
5.15 | pceA std
5.01
5.41
5.41
5.41
3.81
3.81
3.81
3.81
3.81
5.09
5.09 |

JBLM2, Compiled rate coefficients and biomarker abundances (continued)

							LOG + 0 Transfo	rmed for Ana	lysis																			
							Rates			F	Peptides								DHC gene		Functional	Genes						
		TIME THREE	Kcis	Kcis 95%CI	Kvc	Kvc 95%Cl	Log Kcis	KcisSD	Log Kvc	LogKycSD	FdhA	FdhA std	PceA	PceA std	TceA 1	rceA std	VcrA	VcrA std	DHC 165 gene	DHC std	tceA	ceA std	vcrA	vcrA std	fdhA fe	dhA std	pceA	pceA std
	JBLM2 TTHREE	Set1A	1.0486058	0.937007	0.1131681	0.018179135	0.021	0.386	-0.946	-1.326	10.54	9.87	10.76	10.25	10.82	10.37	8.34	9.47	6.62	5.63	6.61	4.55	6.66	5.11	6.71	5.97	5.36	4.55
	JBLM2 TTHREE	Set1B	1.0497445	1.141049	0.1317895	0.027812426	0.021	0.472	-0.880	-1.141	10.46	9.87	10.57	10.25	10.63	10.37	9.72	9.47	6.68	5.63	6.60	4.55	6.66	5.11	6.70	5.97	5.45	4.55
	JBLM2 TTHREE	Set1C	1.1256485	1.279709	0.1741944	0.040566336	0.051	0.522	-0.759	-0.977	10.38	9.87	10.35	10.25	10.49	10.37	9.72	9.47	6.70	5.63	6.60	4.55	6.64	5.11	6.54	5.97	5.33	4.55
	JBLM2 TTHREE	Set1A Dup	0.2817833	0.037581	0.012639	0.03067384	-0.550	-1.249	-1.898	-1.337	10.57	9.75	10.59	10.10	10.18	9.90	9.72	9.53	6.65	5.88	6.62	5.53	6.33	5.29	6.60	6.02	5.84	4.97
	JBLM2 TTHREE	Set1B Dup	0.2973343	0.031359	2.61E-05	0.022750745	-0.527	-1.328	-4.583	-1.467	10.58	9.75	10.70	10.10	10.35	9.90	10.02	9.53	6.77	5.88	6.67	5.53	6.26	5.29	6.74	6.02	5.84	4.97
	JBLM2 TTHREE	Set1C Dup	0.2206698	0.017099	0.006713	0.02105224	-0.656	-1.591	-2.173	-1.501	10.48	9.75	10.52	10.10	10.17	9.90	10.06	9.53	6.76	5.88	6.68	5.53	6.33	5.29	6.77	6.02	5.72	4.97
Ľ	JBLM2 TTHREE	Set2A	0.0027742	0.000403	0.0030997	0.008559355	-2.557	-2.901	-2.509	-1.573																		
ő	JBLM2 TTHREE	Set2B	0.0017588	0.000244	0.0025729	0.008290165	-2.755	-3.118	-2.590	-1.587																		
ŝ	JBLM2 TTHREE	Set2C	0.002399	0.000391	0.0042237	0.009893947	-2.620	-2.913	-2.374	-1.510																		
	JBLM2 TTHREE	Set3A	0.0010045	0.000262	0.0027909	0.013478322																		- I				
	JBLM2 TTHREE	Set3B	0.0008753	0.000218	0.0033135	0.013063268																						
	JBLM2 TTHREE	Set3C	0.0009609	0.000252	0.0017131	0.013283913																						
	JBLM2 TTHREE	Set4A	0.001121	0.000295	0.0037189	0.013659581																						
	JBLM2 TTHREE	Set4B	0.0008245	0.000209	0.0037426	0.013224546																						
	JBLM2 TTHREE	Set4C	not sample	not sample	not sample	not sampled																						
	JBLM2 TTHREE	Set5A	rate not cor	rate not co	rate not co	rate not compu	ited																					
	JBLM2 TTHREE	Set5B	rate not cor	rate not co	rate not co	rate not compu	ited																					
	JBLM2 TTHREE	Set6A	rate not cor	rate not co	rate not co	rate not compu	ited																					
	JBLM2 TTHREE	Set6B	rate not cor	rate not co	rate not co	rate not compu	ited																					
	JBLM2 TTHREE	Set1D	0.1417804	0.015692	0.0188711	0.008121799	-8.48E-01	-1.52E+00	-1.72E+00	-1.80E+00	9.55	9.23	9.08	8.96	10.05	9.93	9.79	9.36	5.87	5.49	5.81	5.47	5.81	5.48	5.84	5.49	4.86	4.48
	JBLM2 TTHREE	Set1E	0.087549	0.013327	0.0176388	0.015232098	-1.06E+00	-1.59E+00	-1.75E+00	-1.53E+00	9.81	9.23	9.36	8.96	10.31	9.93	9.26	9.36	5.74	5.49	5.63	5.47	5.70	5.48	5.69	5.49	4.71	4.48
	JBLM2 TTHREE	Set1F	0.0961964	0.015042	0.0206977	0.015125851	-1.02E+00	-1.54E+00	-1.68E+00	-1.53E+00	9.77	9.23	9.46	8.96	10.31	9.93	9.49	9.36	5.12	5.49	4.76	5.47	4.85	5.48	4.95	5.49	4.10	4.48
	JBLM2 TTHREE	Set1D_Dup	0.0782689	0.004629	1E-05	0.016380863	-1.11E+00	-1.92E+00	-5.00E+00	-1.37E+00	9.45	9.54	9.74	10.05	9.58	9.73	9.98	9.64	6.74	6.45	6.37	6.02	6.41	6.11	6.75	6.55	5.41	5.15
S	JBLM2 TTHREE	Set1E_Dup	0.0592448	0.003784	0.0183197	0.019813992	-1.23E+00	-2.01E+00	-1.74E+00	-1.29E+00	9.08	9.54	10.38	10.05	10.09	9.73	9.02	9.64	5.01	6.45	5.36	6.02	4.63	6.11	5.01	6.55	3.25	5.15
E	JBLM2 TTHREE	Set1F_Dup	0.0566669	0.003497	0.0026875	0.018287361	-1.25E+00	-2.04E+00	-2.57E+00	-1.32E+00	9.08	9.54	9.38	10.05	9.17	9.73	9.64	9.64	6.61	6.45	6.15	6.02	6.25	6.11	6.83	6.55	5.36	5.15
+ S(JBLM2 TTHREE	Set2D	0.001	0.000261	0.00009	0.015181954	-3.00E+00	-3.09E+00	-4.05E+00	-1.32E+00																		
Ś	JBLM2 TTHREE	Set2E	0.001	0.000286	0.00001	0.016602235	-3.00E+00	-3.05E+00	-5.00E+00	-1.29E+00																		
G	JBLM2 TTHREE	Set2F	0.00001	0.000484	0.0001	2.875014984	-5.00E+00	-2.82E+00	-4.00E+00	9.53E-01																		
	JBLM2 TTHREE	Set5C	rate not con	rate not co	rate not co	rate not compu	ited																					
	JBLM2 TTHREE	Set5D	rate not cor	rate not co	rate not co	rate not compu	ited																					
	JBLM2 TTHREE	Set6C	rate not cor	rate not co	rate not co	rate not compu	ited																					
	JBLM2 TTHREE	Set6D	rate not con	rate not co	rate not co	rate not compu	ited																					

APPENDIX E *KEY POINTS OF CONTACT*

KEY POINTS OF CONTACT

The key personnel involved in this project and their contact information is summarized in Table 8-1 below. The Principal Investigator (PI) and all co-PIs share responsibility for the overall execution and delivery of this project, including data quality, analysis, interpretation and preparation of deliverables. Mandy Michalsen, PI, is responsible for the overall execution of this project and identification/coordination with cVOC-contaminated DoD field sites. Ember Korver, USACE Project Manager, is responsible for contractual oversight and general project support. Paul Hatzinger, co-PI, is responsible for microcosm testing, SDC-9[™] culture growth and application, chemical analyses for microcosms, and data interpretation. Frank Löffler, co-PI, is responsible for qPCR, gene-transcript-protein correlation factors, data interpretation. Kate Kucharzyk, co-PI, is responsible for technical reviews and data interpretation.

POINT OF	ORGANIZATION	Phone	
CONTACT	Name	Fax	Role in Project
Name	Address	E-mail	
Mandy Michalsen	U.S. Army Corps of	(p) 206-764-3324	Principal Investigator,
	Engineers, Seattle	mandy.m.michalsen@usace.army.mil	Field Support
Ember Korver	U.S. Army Corps of	(p) 206-764-6792	Project Management,
	Engineers, Seattle	ember.e.korver@usace.army.mil	Contract Administration
Paul Hatzinger	CB&I	(p) 267-337-4003	Co-Principal
-		paul.hatzinger@cbifederalservices.com	Investigator
Frank Löffler	University of	(p) 865-974-4933	Co-Principal
	Tennessee	frank.loeffler@utk.edu	Investigator
Kate Kucharzyk	Battelle Memorial	(p) 614-424-5489	Co-Principal
-	Institute	kucharzyk@battelle.org	Investigator
John Wilson	Scissortail	(p) 580-421-3551	Co-Principal
	Environmental	john@sissortailenv.com	Investigator
	Solutions		_
Jack Istok	Oregon State	(p) 541-619-3996	Co-Principal
	University	jack.istok@oregonstate.edu	Investigator

 Table 8-1.
 Project points of contact