Supplementary Information

S.1 Detailed JUMP explanations

Name	P	R	N	O	C	T
6His SUMO ME MT	J23100	B0034	6 His TEV	SUMO :: GS	*M. edulis* MT	L2U2H09
6His SUMO MG MT	J23100	B0034	6 His TEV	SUMO :: GS	*M. galloprovincialis* MT	L2U2H09
6His SUMO CS MT	J23100	B0034	6 His TEV	SUMO :: GS	*C. sapidus* MT	L2U2H09
6His SUMO DR MT	J23100	B0034	6 His TEV	SUMO :: GS	*D. rerio* MT	L2U2H09
6His SUMO PF MT	J23100	B0034	6 His TEV	SUMO :: GS	*P. fluorescens* MT	L2U2H09
6His SUMO SC MT	J23100	B0034	6 His TEV	SUMO :: GS	*S. cerevisiae* MT	L2U2H09
6 His ME MT	J23100	B0034	6His TEV	O filler	*M. edulis* MT	L2U2H09

Due to the modularity of the JUMP assembly method, each desired level 1 sequence is composed of multiple level 0 parts to form a functional expression cassette. Each cassette must have a promoter (P) part for initiating transcription, a ribosome-binding site (R) part for allowing ribosomes to bind the RNA, a terminator (T) part for ending transcription and the insert (N, O and C) parts that are expressed by the transformed cell as a fusion protein. As each part creates unique overhangs when digested by BsaI, there is only one way the DNA can be assembled and ligated into the pJUMP29-1A(lacZ) backbone plasmid (Valenzuela-Ortega and French, 2021).

S.2. DNA sequences of all parts

S.2.1 Basic (level 0) Parts

J23100

ggagttgacggctagctcagtcctaggtacagtgctagcgtact

B0034

tactagagaaagaggagaaatactaaatg

6 His TEV

AATGcatcatcatcatcatgaaaacctgtattttcagggAGCC

SUMO :: GS

AGCCATGTCGGACAGCGAAGTAAACCAAGAAGCTAAACCCGAGGTCAAACCTGAGGTA
AAACCGGAGACACATATCAATTTGAAGGTATCAGACGGGTCCTCAGAAATCTTCTTCAA
GATTAAGAAAACAACGCCCCTTCGTCGTTTAATGGAAGCATTCGCTAAGCGTCAGGGAA
AGGAAATGGATAGTTTACGTTTTTTGTATGATGGCATCCGTATTCAAGCCGACCAAACTC
CAGAGGACCTGGATATGGAGGATAACGATATCATCGAAGCTCACCGCGAACAGATCGGA
GGAGGAGGTTCGGGCGGTTCG

L2U2H09

gctttcgaacggccctcgcaagggccgtttttttgtatgttcgct

M. edulis MT (ME MT)

TTCGATGCCTGCTCCTTGTAATTGCATCGAAACGAACGTGTGCATTTGTGACACAGGTTG
CTCCGGGGAAGGGTGTCGCTGCGGTGACGCCTGCAAGTGTTCGGGCGCTGACTGCAAAT
GTTCAGGCTGCAAGGTCGTCTGTAAATGTAGTGGCTCATGCGCTTGTGAGGGAGGTTGCA
CCGGGCCTTCGACTTGTAAGTGTGCACCCGGATGCTAGTAGGCTT

M. galloprovincialis MT (MG MT)

TTCGATGCCTGCACCTTGTAACTGTATCGAATCAAatgtgtgtatctgtggcactgggtgtagcggtgaaggttgtc
gctgtggtgacgcctgcaagtgctcgggcgccgactgtaaatgttccggttgtaaagtagtttgcaagtgttcaggtagctgtgcgtgtgaagcagg
gtgtacagggccttcaacgtgtagatgtgcacctggttgctcctgcaaatgatgatgaGCTT

C. sapidus MT (CS MT)

TTCGATGCCAGGACCCTGTTGTAACGACAAATGTGTATGCCAGGAAGGCGGATGCAAGG
CGGGCTGTCAATGCACCTCTTGCCGCTGCTCACCGTGCCAAAAATGCACGTCTGGCTGTA
AATGCGCAACAAAAGAGGAATGCTCGAAGACGTGTACCAAGCCCTGTTCATGTTGCCCT
AAAtgatgaGCTT

D. rerio MT (DR MT)

TTCGATGGACCCATGTGAATGCGCGAAAACAGGTGCCTGTAACTGTGGCGCTACATGTA
AGTGTACGAACTGCCAATGCACGACATGCAAGAAGTCATGTTGTAGTTGTTGTCCATCCG
GCTGCTCTAAATGTGCCTCAGGGTGCGTGTGTAAGGGCAATTCCTGCGGAACGTCATGCT
GCCAGtgatgaGCTT

P. fluorescens MT (PF MT)

TTCGATGAACGAGTTACGTTGTGGCTGCCCTGACTGTCACTGTAAAGTAGATCCTGAGCG
TGTATTTAACCACGATGGGGAGGCATATTGTTCGCAAGCGTGTGCAGAACAGCATCCAA
ATGGTGAGCCATGCCCTGCACCCGACTGCCACTGTGAACGCTCAGGCAAAGTGGGTGGA
CGCGACATCACTAATAACCAGTTAGACGAAGCTTTGGAAGAGACCTTTCCGGCCTCTGAT
CCTATTAGCCCGtgatgaGCTT

S. cerevisiae MT (SC MT)

TTCGatgtttagcgaactgattaactttcagaacgaaggccatgaatgccagtgccagtgcggcagctgcaaaaacaacgaacagtgccagaa
aagctgcagctgcccgaccggctgcaacagcgatgataaatgcccgtgcggcaacaaaagcgaagaaaccaaaaaaagctgctgcagcggca
aatgatgaGCTT

S2.2 Compound (level 1) parts

6His SUMO ME MT

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GAGGTAAAACCGGAGACACATATCAATTTGAAGGTATCAGACGGGTCCTCAGAAATCTT
CTTCAAGATTAAGAAAACAACGCCCCTTCGTCGTTTAATGGAAGCATTCGCTAAGCGTCA
GGGAAAGGAAATGGATAGTTTACGTTTTTTGTATGATGGCATCCGTATTCAAGCCGACCA
AACTCCAGAGGACCTGGATATGGAGGATAACGATATCATCGAAGCTCACCGCGAACAGA
TCGGAGGAGGAGGTTCGGGCGGTTCGATGCCTGCTCCTTGTAATTGCATCGAAACGAAC
GTGTGCATTTGTGACACAGGTTGCTCCGGGGAAGGGTGTCGCTGCGGTGACGCCTGCAA
GTGTTCGGGCGCTGACTGCAAATGTTCAGGCTGCAAGGTCGTCTGTAAATGTAGTGGCTC
ATGCGCTTGTGAGGGAGGTTGCACCGGGCCTTCGACTTGTAAGTGTGCACCCGGATGCTA
GTAGgctttcgaacggccctcgcaagggccgtttttttgtatgtt

6His SUMO MG MT

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cgaacggccctcgcaagggccgttttttgtatgtt

6His SUMO CS MT

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GAGGTAAAACCGGAGACACATATCAATTTGAAGGTATCAGACGGGTCCTCAGAAATCTT
CTTCAAGATTAAGAAAACAACGCCCCTTCGTCGTTTAATGGAAGCATTCGCTAAGCGTCA
GGGAAAGGAAATGGATAGTTTACGTTTTTTGTATGATGGCATCCGTATTCAAGCCGACCA
AACTCCAGAGGACCTGGATATGGAGGATAACGATATCATCGAAGCTCACCGCGAACAGA
TCGGAGGAGGAGGTTCGGGCGGTTCGATGCCAGGACCCTGTTGTAACGACAAATGTGTA
TGCCAGGAAGGCGGATGCAAGGCGGGCTGTCAATGCACCTCTTGCCGCTGCTCACCGTG
CCAAAAATGCACGTCTGGCTGTAAATGCGCAACAAAAGAGGAATGCTCGAAGACGTGTA
CCAAGCCCTGTTCATGTTGCCCTAAAtgatgagctttcgaacggccctcgcaagggccgttttttgtatgtt

6His SUMO DR MT

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gtattttcagggAGCCATGTCGGACAGCGAAGTAAACCAAGAAGCTAAACCCGAGGTCAAACCT
GAGGTAAAACCGGAGACACATATCAATTTGAAGGTATCAGACGGGTCCTCAGAAATCTT
CTTCAAGATTAAGAAAACAACGCCCCTTCGTCGTTTAATGGAAGCATTCGCTAAGCGTCA
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AACTCCAGAGGACCTGGATATGGAGGATAACGATATCATCGAAGCTCACCGCGAACAGA
TCGGAGGAGGAGGTTCGGGCGGTTCGATGGACCCATGTGAATGCGCGAAAACAGGTGCC
TGTAACTGTGGCGCTACATGTAAGTGTACGAACTGCCAATGCACGACATGCAAGAAGTC
ATGTTGTAGTTGTTGTCCATCCGGCTGCTCTAAATGTGCCTCAGGGTGCGTGTGTAAGGG
CAATTCCTGCGGAACGTCATGCTGCCAGtgatgagctttcgaacggccctcgcaagggccgttttttgtatgtt

6His SUMO PF MT

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GAGGTAAAACCGGAGACACATATCAATTTGAAGGTATCAGACGGGTCCTCAGAAATCTT
CTTCAAGATTAAGAAAACAACGCCCCTTCGTCGTTTAATGGAAGCATTCGCTAAGCGTCA
GGGAAAGGAAATGGATAGTTTACGTTTTTTGTATGATGGCATCCGTATTCAAGCCGACCA
AACTCCAGAGGACCTGGATATGGAGGATAACGATATCATCGAAGCTCACCGCGAACAGA

TCGGAGGAGGAGGTTCGGGCGGTTCGATGAACGAGTTACGTTGTGGCTGCCCTGACTGTC
ACTGTAAAGTAGATCCTGAGCGTGTATTTAACCACGATGGGGAGGCATATTGTTCGCAAG
CGTGTGCAGAACAGCATCCAAATGGTGAGCCATGCCCTGCACCCGACTGCCACTGTGAA
CGCTCAGGCAAAGTGGGTGGACGCGACATCACTAATAACCAGTTAGACGAAGCTTTGGA
AGAGACCTTTCCGGCCTCTGATCCTATTAGCCCGtgatgagctttcgaacggccctcgcaagggccgttttttttgtat
gtt

6His SUMO SC MT

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gtattttcagggAGCCATGTCGGACAGCGAAGTAAACCAAGAAGCTAAACCCGAGGTCAAACCT
GAGGTAAAACCGGAGACACATATCAATTTGAAGGTATCAGACGGGTCCTCAGAAATCTT
CTTCAAGATTAAGAAAACAACGCCCCTTCGTCGTTTAATGGAAGCATTCGCTAAGCGTCA
GGGAAAGGAAATGGATAGTTTACGTTTTTTGTATGATGGCATCCGTATTCAAGCCGACCA
AACTCCAGAGGACCTGGATATGGAGGATAACGATATCATCGAAGCTCACCGCGAACAGA
TCGGAGGAGGAGGTTCGGGCGGTTCGatgtttagcgaactgattaactttcagaacgaaggccatgaatgccagtgccagt
gcggcagctgcaaaaacaacgaacagtgccagaaaagctgcagctgcccgaccggctgcaacagcgatgataaatgcccgtgcggcaacaaa
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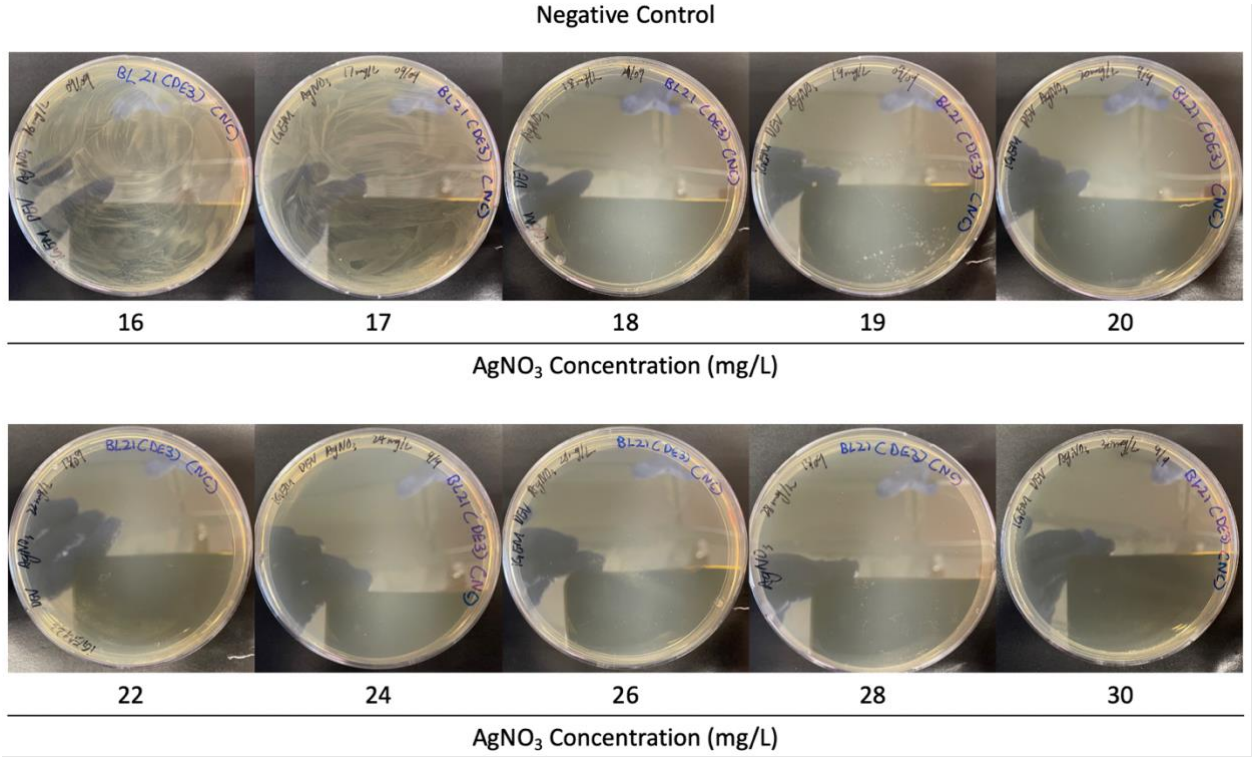
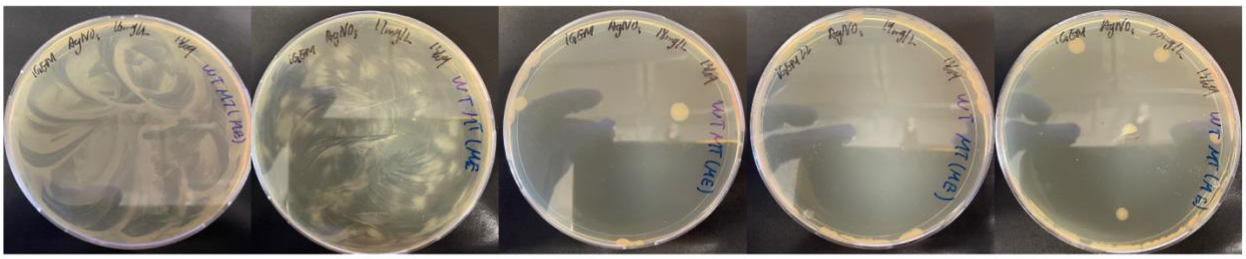
S.3 All Plates Labelled

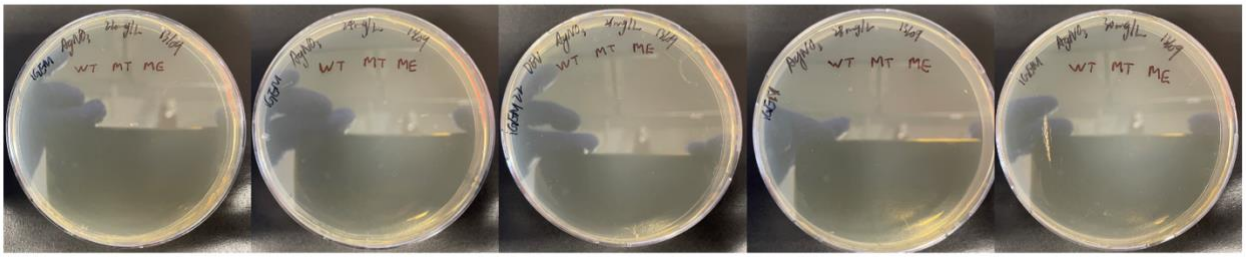


WT; *M. edulis*



16 17 18 19 20

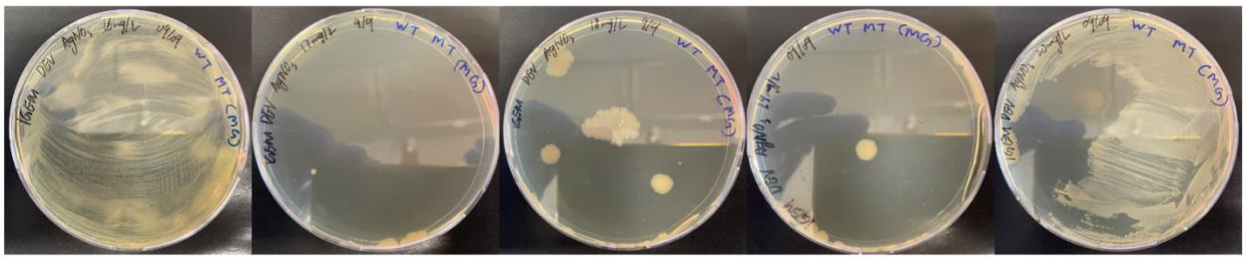
$AgNO_3$ Concentration (mg/L)



22 24 26 28 30

$AgNO_3$ Concentration (mg/L)

WT; *M. galloprovincialis*



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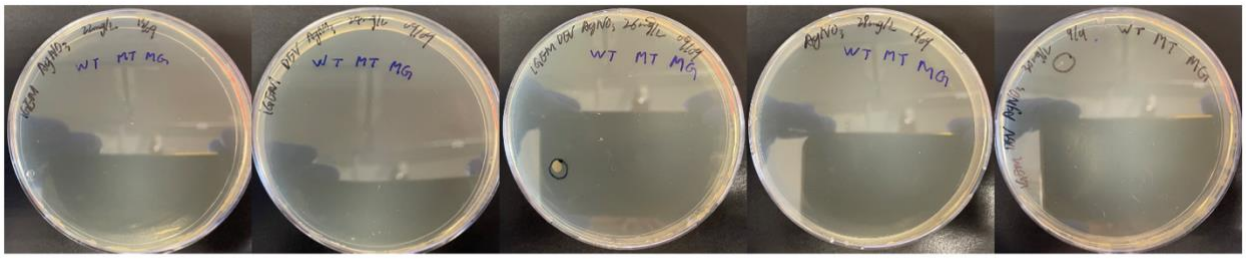
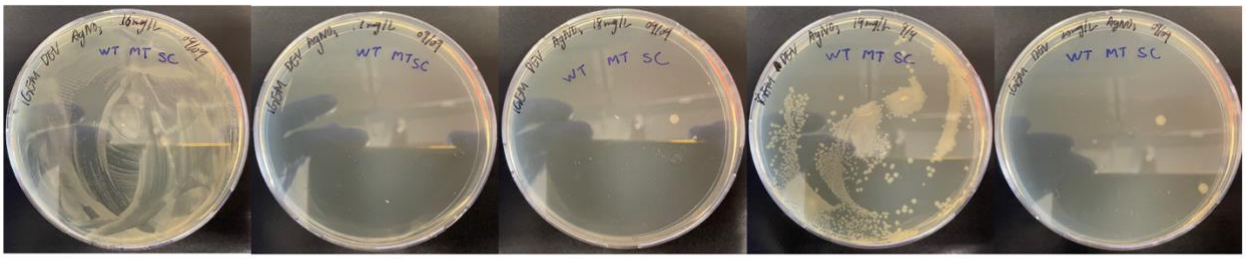
$AgNO_3$ Concentration (mg/L)



22 24 26 28 30

$AgNO_3$ Concentration (mg/L)

WT; *S. cerevisiae*



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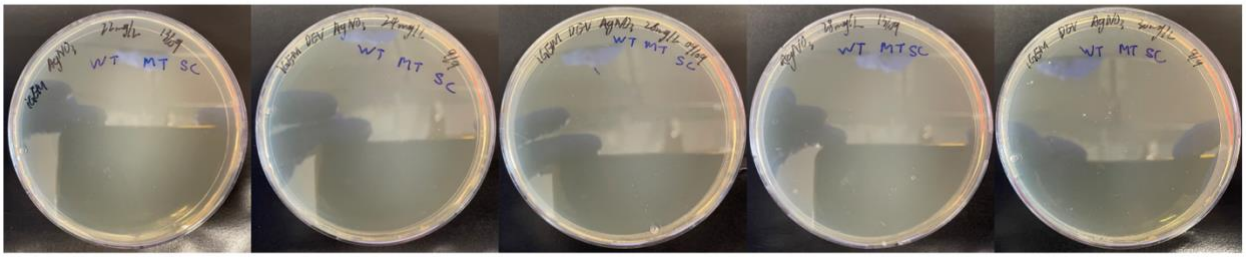
$AgNO_3$ Concentration (mg/L)



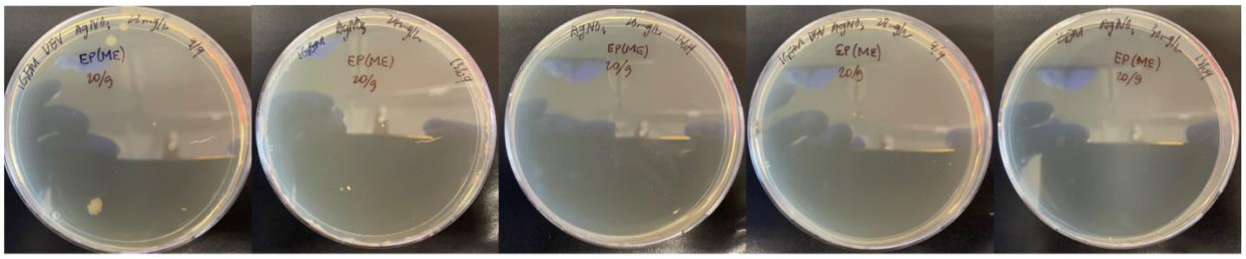
22 24 26 28 30

$AgNO_3$ Concentration (mg/L)

EP; *M. edulis*

16 17 18 19 20

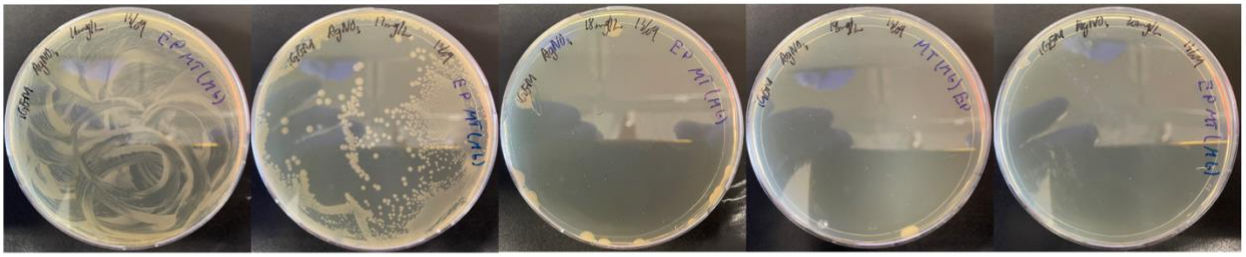
$AgNO_3$ Concentration (mg/L)



22 24 26 28 30

$AgNO_3$ Concentration (mg/L)

EP; *M. galloprovincialis*



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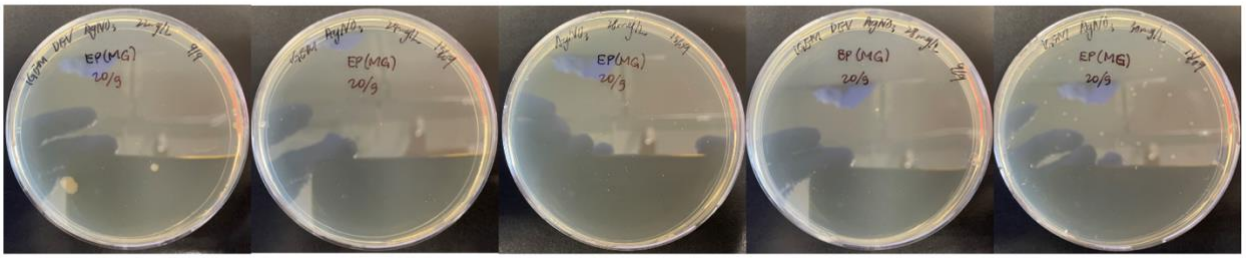
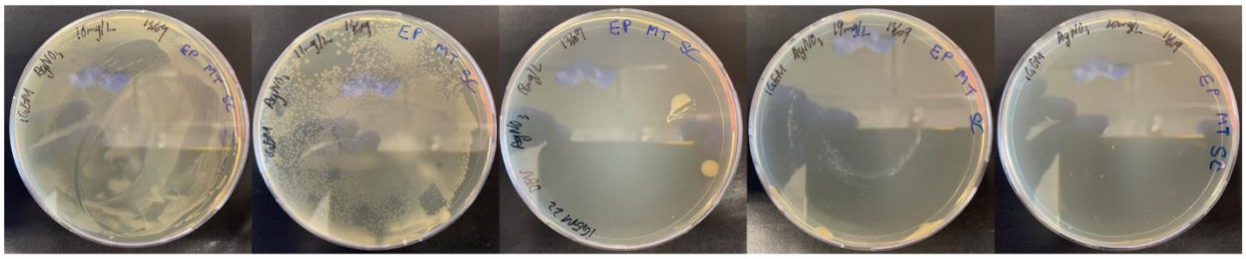
$AgNO_3$ Concentration (mg/L)



22 24 26 28 30

$AgNO_3$ Concentration (mg/L)

EP; S. cerevisiae



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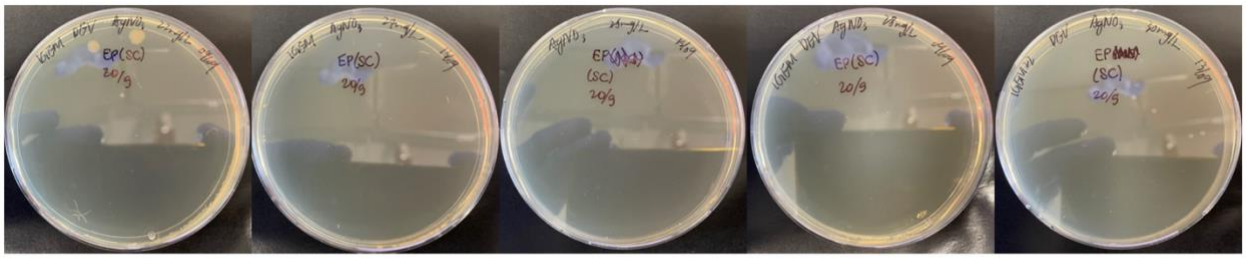
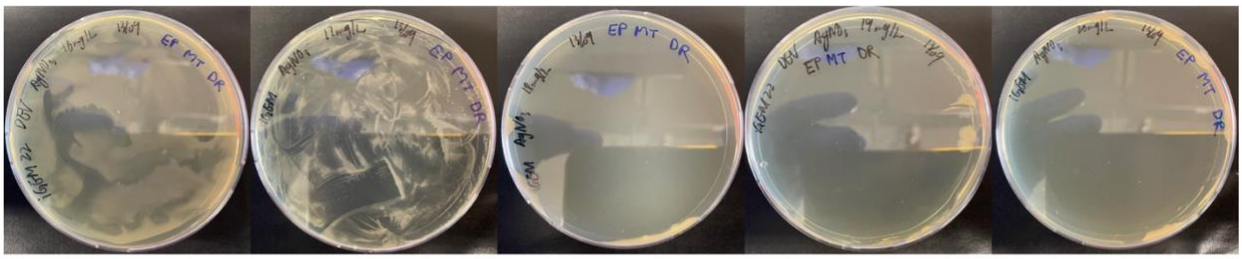
$AgNO_3$ Concentration (mg/L)

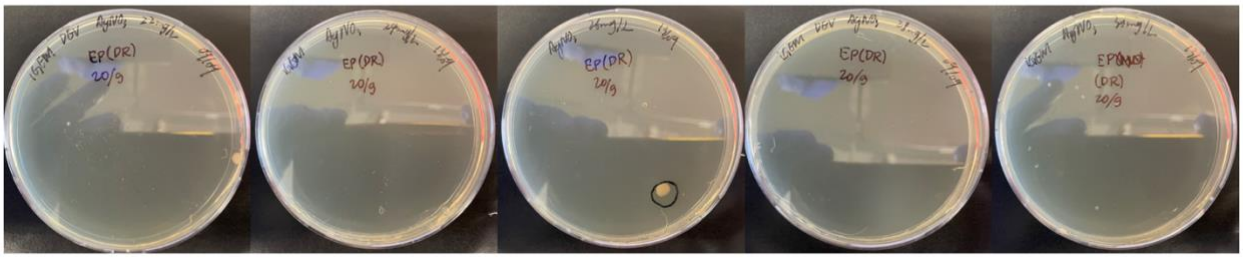


22 24 26 28 30

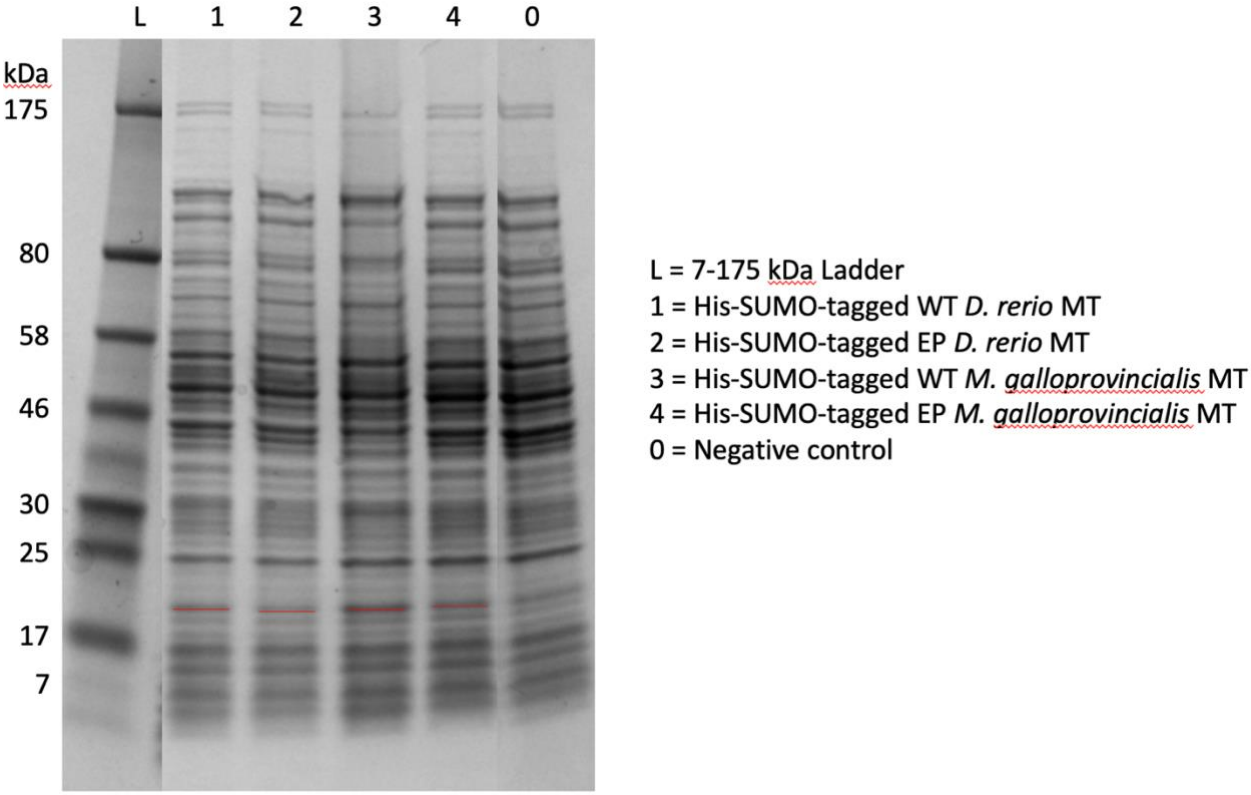
$AgNO_3$ Concentration (mg/L)

EP; *D. rerio*





S.4 SDS page labelled



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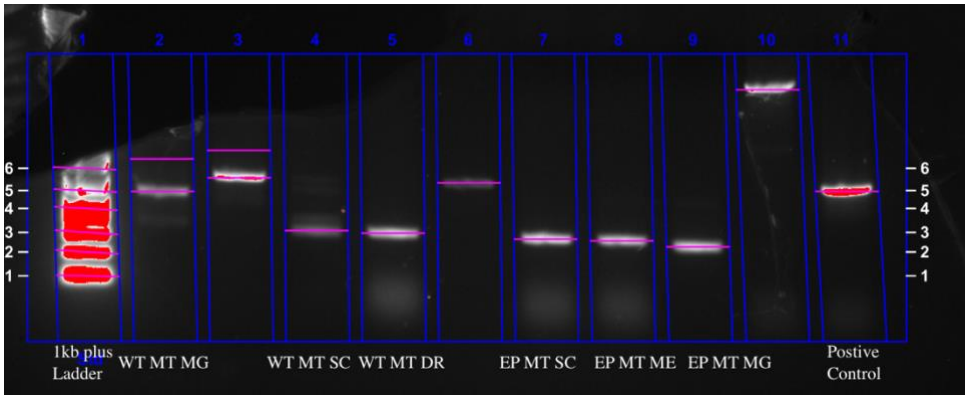

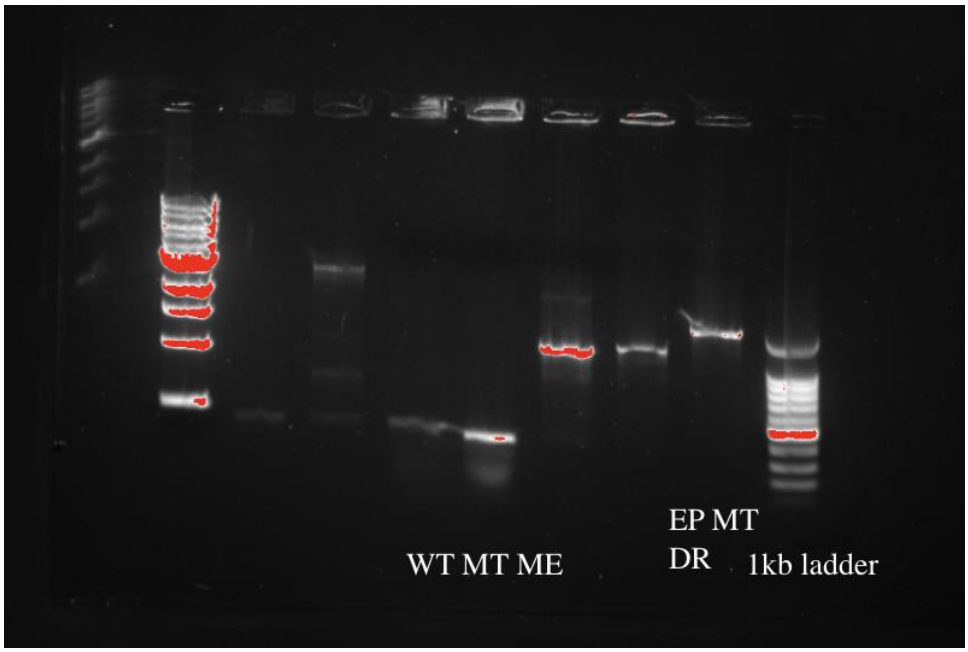

S.6 Mutation Sites:

The letters in red are sites we suggest for mutation to get functional metal binding motifs. Based on:

cys-x-cys, cys-x-x-cys, x-cys-cys-x and x-cys-cys-cys-x (Ziller and Fraissinet-Tachet, 2018)

C. sapidus

MPGPCCNDKCVCQEGGCKAGCQCTSCRCSPCQKCTSGCKCATKEECSKTCTKPCSCCPK

D. rerio

MDPCECAKTGACNCGATCKCTNCQCTTCKKSCCSCCPSGCSKCASGCVCKGNSCGTSCCQ

M. edulis

MPAPCNCIETNVCICDTGCSGEGCRCGDACKCSGADCKCSGCKVVCKCSGSCACEGGCTGPS
TCKCAPGC

M. galloprovincialis

MPAPCNCIESNVCICGTGCSGEGCRCGDACKCSGADCKCSGCKVVCKCSGSCACEAGCTGPS
TCRCAPGCSCK

P. fluorescens

MNELRCGCPDCHCKVDPERVFNHDGEAYCSQACAEQHPNGEPCPAPDCHCERSGKVGGRDI
TNNQLDEALEETFPASDPISP

S. cerevisiae

MFSELINFQNEGHECQCQCGSCKNNEQCQKSCSCPTGCNSDDKCPCGNKSEETKKSCCSGK

S.7 Site Specific Mutagenesis:

We introduced mutations using mutagenic primers, for both GeneORator and Targeted Mutagenesis. Primers were designed by first identifying regions where mutations would be introduced, usually 15bp long, and flanked with complementary DNA sequences, each with a melting temperature of 60°C. GeneORator primers replaced target codons with NNK, resulting in any possible amino acid with reduced stop codon frequency, whereas targeted mutagenesis primers replaced the mutation site with TGT, encoding cysteine. One round of asymmetric PCR using the mutagenic primer and a normal reverse primer produces the mutagenic megaprimer, which is used for the second round of symmetric PCR using the forward primer (Currin et al., 2019).

S7.1. GeneOrator primers:

S7.1.1. *M. edulis*

M. edulis forward: CGTCTCGGTCTCCTTCGATGCC

M. edulis Set 1 Primer 1:
ATGCCTGCTCCTTGTAATTGCNNKGAAACGAACGTGTGCATTTGTGAC

M. edulis Set 2 Primer 2:
GAAACGAACGTGTGCATTTGTGACACANNKTGCTCCGGGGAAGGG

M. edulis Set 2 Primer 1:
GAAACGAACGTGTGCATTTGTNNKACAGGTTGCTCCGGGGAAGGG

M. edulis Set 3 Primer 2: GGGTGTCGCTGCGGTGACNNKTGCAAGTGTTCGGGCGCT

M. edulis Set 3 Primer 1: GGGTGTCGCTGCGGTNNKGCCTGCAAGTGTTCGGGCGCT

M. edulis Set 4 Primer 1:
GTGACGCCTGCAAGTGTTCGNNKGCTGACTGCAAATGTTCAGGCTG

M. edulis Set 5 Primer 2:
CGCTGACTGCAAATGTTCAGGCTGCAAGNNKGTCTGTAAATGTAGTGGCTC

M. edulis Set 5 Primer 1:
CGCTGACTGCAAATGTTCANNKTGCAAGGTCGTCTGTAAATGTAGTGGCTC

M. edulis Set 6 Primer 2:
CGTCTGTAAATGTAGTGGCTCATGCGCTTGTGAGNNKGGTTGCACCGGG

M. edulis Set 6 Primer 1:
CGTCTGTAAATGTAGTGGCNNKTGCGCTTGTGAGGGAGGTTGCACCGGG

M. edulis Set 7 Primer 2:
GCACCGGGCCTTCGACTTGTAAGTGTNNKCCCGGATGCTAGTAGG

M. edulis Set 7 Primer 1:
GCACCGGGCCTNNKACTTGTAAGTGTGCACCCGGATGCTAGTAGG

M. edulis reverse: CGTCTCAGGTCTCGAAGCCTACTAGC

S.7.1.2. *M. galloprovincialis*

M. galloprovincialis forward: CGTCTCGGTCTCCTTCGATGCC

M. galloprovincialis Set 1 Primer 1:
GCCTGCACCTTGTAACTGTNNKGAATCAAatgtgtgtatctgtggcac

M. galloprovincialis Set 2 Primer 1:
CTGTATCGAATCAAatgtgtgtatctgtNNKactgggtgtagcggtgaaggttgt

M. galloprovincialis Set 2 Primer 2:
CTGTATCGAATCAAatgtgtgtatctgtggcactNNKtgtagcggtgaaggttgt

M. galloprovincialis Set 3 Primer 1: ctgggtgtagcggtgaaNNKtgtcgctgtggtgacgcctgc

M. galloprovincialis Set 4 Primer 2: gtgaaggttgtcgctgtggtgacNNKtgcaagtgctcgggcg

M. galloprovincialis Set 4 Primer 1: gtgaaggttgtcgctgtggtNNKgcctgcaagtgctcgggcg

M. galloprovincialis Set 5 Primer 1: gtgacgcctgcaagtgctcgNNKgccgactgtaaatgttccggttgtaaag

M. galloprovincialis Set 6 Primer 2: cgccgactgtaaatgttccggttgtaaaNNKgtttgcaagtgttcaggtag

M. galloprovincialis Set 6 Primer 1: cgccgactgtaaatgtNNKggttgtaaagtagtttgcaagtgttcaggtag

M. galloprovincialis Set 7 Primer 2: gtttgcaagtgttcaggtagctgtgcgtgtgaaNNKgggtgtacagggcc

M. galloprovincialis Set 7 Primer 1: gtttgcaagtgttcaggtNNKtgtgcgtgtgaagcagggtgtacagggcc

M. galloprovincialis Set 8 Primer 1: ggtgtacagggcctNNKacgtgtagatgtgcacctggttgctcctg

M. galloprovincialis Set 8 Primer 2: ggtgtacagggccttcaacgtgtagatgtNNKcctggttgctcctg

M. galloprovincialis reverse: CGTCTCAGGTCTCGAAGCtcatcatca

S.7.1.3. *C. sapidus*

C. sapidus forward: CGTCTCGGTCTCCTTCGATGCC

Set 1 Primer 2:
GTAACGACAAATGTGTATGCCAGGAAGGCNNKTGCAAGGCGGGCTGTCAATGCAC

Set 1 Primer 1:
GTAACGACAAATGTGTATGCNNKGAAGGCGGATGCAAGGCGGGCTGTCAATGCAC

Set 2 Primer 1: GTCAATGCACCTCTTGCCGCTGCNNKCCGTGCCAAAAATGCACGTCTGG

Set 3 Primer 2: CCGTGCCAAAAATGCACGTCTNNKTGTAAATGCGCAACAAAAGAGG

Set 3 Primer 1: CCGTGCCAAAAATGCACGNNKGGCTGTAAATGCGCAACAAAAGAGG

Set 4 Primer 1: GCACGTCTGGCTGTAAATGCNNKACAAAAGAGGAATGCTCGAAGACGTG

Set 5 Primer 1:
GCAACAAAAGAGGAATGCNNKAAGACGTGTACCAAGCCCTGTTCATGTTG

Set 5 Primer 2:
GCAACAAAAGAGGAATGCTCGAAGACGTGTNNKAAGCCCTGTTCATGTTG

Set 6 Primer 1: GTGTACCAAGCCCTGTTCATGTTGCCCTNNKtgatgaGCTTCGAGACC

C. sapidus reverse: CGTCTCAGGTCTCGAAGCtcatcaTTTAGG

S.7.1.4 *D. rerio*

D. rerio forward: CGTCTCGGTCTCCTTCGATGGACC

D. rerio Set 1 Primer 1:
GGTCTCCTTCGATGGACCCATGTNNKTGCGCGAAAACAGGTGCCTGTAAC

D. rerio Set 2 Primer 1:
GCGCGAAAACAGGTNNKTGTAACTGTGGCGCTACATGTAAGTGTACGAACTG

D. rerio Set 2 Primer 2:
GCGCGAAAACAGGTGCCTGTAACTGTGGCNNKACATGTAAGTGTACGAACTG

D. rerio Set 3 Primer 1:
TGTGGCGCTACATGTAAGTGTNNKAACTGCCAATGCACGACATGCA

D. rerio Set 4 Primer 1:
GAAGTCATGTTGTAGTTGTTGTCCATCCNNKTGCTCTAAATGTGCCTCAGGGT

D. rerio Set 5 Primer 2: AGGGTGCGTGTGTAAGNNKAATTCCTGCGGAACGTCATGCTGC

D. rerio Set 5 Primer 1: AGGGTGCGTGTGTNNKGGCAATTCCTGCGGAACGTCATGCTGC

D. rerio Set 5 Primer 3: AGGGTGCGTGTGTAAGGGCNNKTCCTGCGGAACGTCATGCTGC

D. rerio Set 5 Primer 4: AGGGTGCGTGTGTAAGGGCAATNNKTGCGGAACGTCATGCTGC

D. rerio reverse:CGTCTCAGGTCTCGAAGCtcatcaCT

S.7.1.5 *P. fluorescens*

P. fluorescens forward: CGTCTCGGTCTCCTTCGATGAACGA

P. fluorescens Set 1 Primer 3:
TCGGTCTCCTTCGATGAACGAGTTANNKTGTGGCTGCCCTGACT

P. fluorescens Set 1 Primer 1:
TCGGTCTCCTTCGATGAACNNKTTACGTTGTGGCTGCCCTGACT

P. fluorescens Set 1 Primer 2:
TCGGTCTCCTTCGATGAACGAGNNKCGTTGTGGCTGCCCTGACT

P. fluorescens Set 2 Primer 1:
CGAGTTACGTTGTGGCTGCCCTNNKTGTCACTGTAAAGTAGATCCTGAGCG

P. fluorescens Set 3 Primer 1:
CCCTGACTGTCACTGTAAAGTANNKCCTGAGCGTGTATTTAACCACGATGG

P. fluorescens Set 4 Primer 2:
TAACCACGATGGGGAGGCATATTGTTCGNNKGCGTGTGCAGAACAG

P. fluorescens Set 4 Primer 1:
TAACCACGATGGGGAGNNKTATTGTTCGCAAGCGTGTGCAGAACAG

P. fluorescens Set 5 Primer 1:
AAATGGTGAGCCATGCCCTGCANNKGACTGCCACTGTGAACGCTCAG

P. fluorescens Set 6 Primer 2:
CCGACTGCCACTGTGAACGCTCAGGCNNKGTGGGTGGACGC

P. fluorescens Set 6 Primer 1:
CCGACTGCCACTGTGAANNKTCAGGCAAAGTGGGTGGACGC

P. fluorescens Set 7 Primer 2:
CGCTCAGGCAAAGTGGGTNNKCGCGACATCACTAATAACCAGTTAGACGAAGC

P. fluorescens Set 7 Primer 3:
CGCTCAGGCAAAGTGGGTGGACGCNNKATCACTAATAACCAGTTAGACGAAGC

P. fluorescens Set 7 Primer 1:
CGCTCAGGCAAAGTGNNKGGACGCGACATCACTAATAACCAGTTAGACGAAGC

P. fluorescens Set 8 Primer 1:
GTGGACGCGACATCACTAATNNKCAGTTAGACGAAGCTTTGGAAGAG

P. fluorescens reverse: CGTCTCAGGTCTCGAAGCtcatcaCG

S.7.1.6 *S. cerevisiae*

S. cerevisiae forward: CGTCTCGGTCTCCTTCGatgtttagcg

S. cerevisiae Set 1 Primer 2: GTCTCCTTCGatgtttagcgNNKtgattaactttcagaacgaaggccatg

S. cerevisiae Set 1 Primer 1: GTCTCCTTCGatgtttagcgaaNNKattaactttcagaacgaaggccatg

S. cerevisiae Set 2 Primer 1: gcgaactgattaactttcagaacgaaggccatNNKtgccagtgccagtgcg

S. cerevisiae Set 3 Primer 1: gcggcagctgcaaaNNKaacgaacagtgccagaaaagctgc

S. cerevisiae Set 3 Primer 2: gcggcagctgcaaaaacaacNNKcagtgccagaaaagctgc

S. cerevisiae Set 4 Primer 2: gcagctgcccgaccggctgcNNKagcgatgataaatgcccgtgc

S. cerevisiae Set 4 Primer 1: gcagctgcccgNNKggctgcaacagcgatgataaatgcccgtgc

S. cerevisiae Set 5 Primer 1: cccgtgcggcNNKaaaagcgaagaaaccaaaaaaagctgctgc

S. cerevisiae Set 5 Primer 2: cccgtgcggcaacaaaagcgaaNNKaccaaaaaaagctgctgc

S. cerevisiae Set 6 Primer 1: caaaagcgaagaaaccaaaaaaagctgctgcagcNNKaaatgatgaGCTTCGAGAC

S. cerevisiae reverse: CGTCTCAGGTCTCGAAGCtcatcatttgc

S.8 Targeted Mutagenesis primers

S.8.1 M. edulis

M. edulis TM1: ATGCCTGCTCCTTGTAATTGCTGTGAAACGAACGTGTGCATTTGTGAC

M. edulis TM2: GAAACGAACGTGTGCATTTGTGACACATGTTGCTCCGGGGAAGGG

M. edulis TM3: GAAACGAACGTGTGCATTTGTTGTACAGGTTGCTCCGGGGAAGGG

M. edulis TM4: GGGTGTCGCTGCGGTGACTGTTGCAAGTGTTCGGGCGCT

M. edulis TM5: GGGTGTCGCTGCGGTTGTGCCTGCAAGTGTTCGGGCGCT

M. edulis TM6: GTGACGCCTGCAAGTGTTCGTGTGCTGACTGCAAATGTTCAGGCTG

M. edulis TM7:
CGCTGACTGCAAATGTTCAGGCTGCAAGTGTGTCTGTAAATGTAGTGGCTC

M. edulis TM8:
CGCTGACTGCAAATGTTCATGTTGCAAGGTCGTCTGTAAATGTAGTGGCTC

M. edulis TM9: CGTCTGTAAATGTAGTGGCTCATGCGCTTGTGAGTGTGGTTGCACCGGG

M. edulis TM10:
CGTCTGTAAATGTAGTGGCTGTTGCGCTTGTGAGGGAGGTTGCACCGGG

M. edulis TM11: GCACCGGGCCTTCGACTTGTAAGTGTTGTCCCGGATGCTAGTAGG

M. edulis TM12: GCACCGGGCCTTGTACTTGTAAGTGTGCACCCGGATGCTAGTAGG

S.8.2 *M. galloprovincialis*

M. galloprovincialis TM1: GCCTGCACCTTGTAACTGTTGTGAATCAAatgtgtgtatctgtggcac

M. galloprovincialis TM2: CTGTATCGAATCAAatgtgtgtatctgtTGTactgggtgtagcggtgaaggttgt

M. galloprovincialis TM3: CTGTATCGAATCAAatgtgtgtatctgtggcactTGTtgtagcggtgaaggttgt

M. galloprovincialis TM4: ctgggtgtagcggtgaaTGTtgtcgctgtggtgacgcctgc

M. galloprovincialis TM5: gtgaaggttgtcgctgtggtgacTGTtgcaagtgctcgggcg

M. galloprovincialis TM6: gtgaaggttgtcgctgtggtTGTgcctgcaagtgctcgggcg

M. galloprovincialis TM7: gtgacgcctgcaagtgctcgTGTgccgactgtaaatgttccggttgtaaag

M. galloprovincialis TM8: cgccgactgtaaatgttccggttgtaaaTGTgtttgcaagtgttcaggtag

M. galloprovincialis TM9: cgccgactgtaaatgtTGTggttgtaaagtagtttgcaagtgttcaggtag

M. galloprovincialis TM10: gtttgcaagtgttcaggtagctgtgcgtgtgaaTGTgggtgtacagggcc

M. galloprovincialis TM11: gtttgcaagtgttcaggtTGTtgtgcgtgtgaagcagggtgtacagggcc

M. galloprovincialis TM12: ggtgtacagggcctTGTacgtgtagatgtgcacctggttgctcctg

M. galloprovincialis TM13: ggtgtacagggccttcaacgtgtagatgtTGTcctggttgctcctg

S.8.3 *C. sapidus*

C. sapidus TM1:
GTAACGACAAATGTGTATGCCAGGAAGGCTGTTGCAAGGCGGGCTGTCAATGCA
C

C. sapidus TM2:
GTAACGACAAATGTGTATGCTGTGAAGGCGGATGCAAGGCGGGCTGTCAATGCA
C

C. sapidus TM3:
GTCAATGCACCTCTTGCCGCTGCTGTCCGTGCCAAAAATGCACGTCTGG

C. sapidus TM4:
CCGTGCCAAAAATGCACGTCTTGTTGTAAATGCGCAACAAAAGAGG

C. sapidus TM5:
CCGTGCCAAAAATGCACGTGTGGCTGTAAATGCGCAACAAAAGAGG

C. sapidus TM6:
GCACGTCTGGCTGTAAATGCTGTACAAAAGAGGAATGCTCGAAGACGTG

C. sapidus TM7:
GCAACAAAAGAGGAATGCTGTAAGACGTGTACCAAGCCCTGTTCATGTTG

C. sapidus TM8:
GCAACAAAAGAGGAATGCTCGAAGACGTGTTGTAAGCCCTGTTCATGTTG

C. sapidus TM9: GTGTACCAAGCCCTGTTCATGTTGCCCTTGTtgatgaGCTTCGAGACC

S.8.4 *D. rerio*

D. rerio TM1: GGTCTCCTTCGATGGACCCATGTTGTTGCGCGAAAACAGGTGCCTGTAAC

D. rerio TM2:
GCGCGAAAACAGGTTGTTGTAACTGTGGCGCTACATGTAAGTGTACGAACTG

D. rerio TM3:
GCGCGAAAACAGGTGCCTGTAACTGTGGCTGTACATGTAAGTGTACGAACTG

D. rerio TM4: TGTGGCGCTACATGTAAGTGTTGTAACTGCCAATGCACGACATGCA

D. rerio TM5:
GAAGTCATGTTGTAGTTGTTGTCCATCCTGTTGCTCTAAATGTGCCTCAGGGT

D. rerio TM6: AGGGTGCGTGTGTAAGTGTAATTCCTGCGGAACGTCATGCTGC

D. rerio TM7: AGGGTGCGTGTGTTGTGGCAATTCCTGCGGAACGTCATGCTGC

D. rerio TM8: AGGGTGCGTGTGTAAGGGCTGTTCCTGCGGAACGTCATGCTGC

D. rerio TM9: AGGGTGCGTGTGTAAGGGCAATTGTTGCGGAACGTCATGCTGC

S.8.5 *P. fluorescens*

P. fluorescens TM1: TCGGTCTCCTTCGATGAACGAGTTATGTTGTGGCTGCCCTGACT

P. fluorescens TM2: TCGGTCTCCTTCGATGAACTGTTTACGTTGTGGCTGCCCTGACT

P. fluorescens TM3: TCGGTCTCCTTCGATGAACGAGTGTCGTTGTGGCTGCCCTGACT

P. fluorescens TM4:
CGAGTTACGTTGTGGCTGCCCTTGTTGTCACTGTAAAGTAGATCCTGAGCG

P. fluorescens TM5:
CCCTGACTGTCACTGTAAAGTATGTCCTGAGCGTGTATTTAACCACGATGG

P. fluorescens TM6:
TAACCACGATGGGGAGGCATATTGTTCGTGTGCGTGTGCAGAACAG

P. fluorescens TM7:
TAACCACGATGGGGAGTGTTATTGTTCGCAAGCGTGTGCAGAACAG

P. fluorescens TM8:
AAATGGTGAGCCATGCCCTGCATGTGACTGCCACTGTGAACGCTCAG

P. fluorescens TM9: CCGACTGCCACTGTGAACGCTCAGGCTGTGTGGGTGGACGC

P. fluorescens TM10: CCGACTGCCACTGTGAATGTTCAGGCAAAGTGGGTGGACGC

P. fluorescens TM11:
CGCTCAGGCAAAGTGGGTTGTCGCGACATCACTAATAACCAGTTAGACGAAGC

P. fluorescens TM12:
CGCTCAGGCAAAGTGGGTGGACGCTGTATCACTAATAACCAGTTAGACGAAGC

P. fluorescens TM13:
CGCTCAGGCAAAGTGTGTGGACGCGACATCACTAATAACCAGTTAGACGAAGC

P. fluorescens TM14:
GTGGACGCGACATCACTAATTGTCAGTTAGACGAAGCTTTGGAAGAG

S.8.6 *S. cerevisiae*

S. cerevisiae TM1: GTCTCCTTCGatgtttagcgTGTtgattaactttcagaacgaaggccatg

S. cerevisiae TM2: GTCTCCTTCGatgtttagcgaaTGTattaactttcagaacgaaggccatg

S. cerevisiae TM3: gcgaactgattaactttcagaacgaaggccatTGTtgccagtgccagtgcg

S. cerevisiae TM4: gcggcagctgcaaaTGTaacgaacagtgccagaaaagctgc

S. cerevisiae TM5: gcggcagctgcaaaaacaacTGTcagtgccagaaaagctgc

S. cerevisiae TM6: gcagctgcccgaccggctgcTGTagcgatgataaatgcccgtgc

S. cerevisiae TM7: gcagctgcccgTGTggctgcaacagcgatgataaatgcccgtgc

S. cerevisiae TM8: cccgtgcggcTGTaaaagcgaagaaaccaaaaaaagctgctgc

S. cerevisiae TM9: cccgtgcggcaacaaaagcgaaTGTaccaaaaaaagctgctgc

S. cerevisiae TM10: caaaagcgaagaaaccaaaaaaagctgctgcagcTGTaaatgatgaGCTTCGAGAC

S.9 Generalised PS1 and PS2 primers

PS1

AGGGCGGCGGATTTGTCC

PS2

GCGGCAACCGAGCGTTC

EP MT F 72

M. edulis Forward: CGTCTCGGTCTCCTTCGATGCC

EP MT R 72

M. edulis Reverse: GCTAGTAGGCTTCGAGACCTGAGACG

S.10 RT-DNA to ORF.py

```
#!/usr/bin/env python


def FastaToDict(fasta):
#with open(fasta) as f:
# lines = f.readlines()
sequences = []
sequences_dict = {}
fasta_dict = {}
for i in lines:
if i[0] == ">":
sequences.append(i)
for j in sequences:
index = lines.index(j)
sequences_dict[j] = index
for k in range(len(sequences_dict)):
if k == len(sequences_dict)-1:
key = list(sequences_dict.keys())[k]
fasta = lines[sequences_dict[key]+1::]
fasta = "".join(fasta)
fasta = fasta.replace('\r', '').replace('\n', '')
fasta = fasta.upper()
fasta_dict[key] = fasta
else:
key = list(sequences_dict.keys())[k]
next_key = list(sequences_dict.keys())[k+1]
```

```
fasta = lines[sequences_dict[key]+1:sequences_dict[next_key]]
fasta = "".join(fasta)
fasta = fasta.replace('\r', '').replace('\n', '')
fasta = fasta.upper()
fasta_dict[key] = fasta
return(fasta_dict)



def RT_ORF_finder(fasta):
fasta_dict = FastaToDict(fasta)
ORF_seq = ""
output = ""
for key in fasta_dict:
value = fasta_dict[key]
start_sites =[]
end_sites = []
for i in range(len(value)):
if value[i:i+3] == "ATG":
start_sites.append(i)
if value[i:i+3] == "TAA" or value[i:i+3] == "TAG" or value[i:i+3] == "TGA":
end_sites.append(i)
longest_orf = [0, 0]
for j in start_sites:
for k in end_sites:
if k - j > longest_orf[1] - longest_orf[0]:
if (k - j) % 3 == 0:
longest_orf[0] = j
longest_orf[1] = k
break
if longest_orf[1] == 0:
longest_orf[1] = len(value)
ORF_seq = value[longest_orf[0]:longest_orf[1]+3]
```

```
output += str(key) + str(ORF_seq) + "\n"
return(output)

import sys
inFile = sys.argv[1]
outFile = sys.argv[2]


with open(inFile,'r') as i:
lines = i.readlines()


processedLines = RT_ORF_finder(lines)


with open(outFile,'w') as o:
for line in processedLines:
o.write(line)
```

S.11 clean_automation.sh

```
### FULL AUTOMATION OF METALLOTHIONEIN DOCKING ###


#       Defining some paths
DOCKING=/Users/maartenvandenancker/Desktop/DEv/docking
MGLTools=~/MGLTools/MGLToolsPckgs/AutoDockTools/Utilities24/

#       This assumes you are starting in a directory where you want to work
#       This directory must have the MT you want to use (here D_rerio.pdb)
#       For preparing structures from alphafold structures you need to delete the first and second
#       last lines
#       This directory must also have the ligand file (Ag.pdb)
#       This directory must also have a modified AD4_parameters.dat file with the extra
```

```
#       Atom types you want to use


##CREATING LIST OF CYSTEINES AND MAKING A FOLDER FOR EACH##
grep -e "SG" D_rerio.pdb | awk '{ print $6 }' > cys_list.txt
LIST=$(cat cys_list.txt)
for i in $LIST; do mkdir cys${i}; done
for i in $LIST/; do cp Ag.pdb cys${i}/; cp D_rerio.pdb cys${i}/; done

#       All the preparation files need python2 to run
#       py27 is a conda environment running python 2.7.18 and numpy 1.12.0
source ~/opt/miniconda3/etc/profile.d/conda.sh
conda activate py27
export PYTHONPATH="${PYTHONPATH}:/usr/local/lib/python2.7/site-packages:/usr/lib/python2.7/site-packages"

##PREPARING COVALENT STRUCTURES##
for i in $LIST; do cd cys${i}; python ~/adcovalent/prepareCovalent.py --ligand Ag.pdb --ligindices 1,2 --receptor D_rerio.pdb --residue A:CYS${i} --outputfile ligcovalent.pdb; cd ..; done

##PREPARING THE RECEPTOR##
export PYTHONPATH=~/MGLTools/MGLToolsPckgs/:$PYTHONPATH
for i in $LIST; do cd cys${i}; $MGLTools/prepare_receptor4.py -r D_rerio.pdb -A Hydrogens; cd ..; done
#       The ligand also uses prepare_receptor4.py for flexible docking / covalent docking
for i in $LIST; do cd cys${i}; $MGLTools/prepare_receptor4.py -r ligcovalent.pdb; cd ..; done
#       Gasteiger charges are stripped from Ag+ because prepare_receptor4.py doesnt recognise
#       the atom type, so I'll just replace the 0.000 charge with 1.000 (because Ag+)
for i in $LIST; do cd cys${i}; cat ligcovalent.pdbqt | sed 's/0.000/1.000/g' > gasteiger_lig.pdbqt; cd ..; done

##GENERATING FLEXIBLE PDBQT FILES##
#       Receptor:
```

for i in $LIST; do cd cys${i}; $MGLTools/prepare_flexreceptor4.py -r D_rerio.pdbqt -s D_rerio:A:CYS${i}; cd ..; done

Ligand:

for i in $LIST; do cd cys${i}; $MGLTools/prepare_flexreceptor4.py -r gasteiger_lig.pdbqt -s gasteiger_lig:A:CYS${i}; cd ..; done

##GENERATING PARAMETER FILES##

Grid parameter files (GPFs) - for autogrid

for i in $LIST; do cd cys${i}; $MGLTools/prepare_gpf4.py -r D_rerio_rigid.pdbqt -x gasteiger_lig_flex.pdbqt -l gasteiger_lig_flex.pdbqt -y -I 20 -o D_rerio.gpf; cd ..; done

Docking parameter files (DPFs) - for autodock

for i in $LIST; do cd cys${i}; touch empty; $MGLTools/prepare_dpf4.py -r D_rerio_rigid.pdbqt -x gasteiger_lig_flex.pdbqt -l gasteiger_lig_flex.pdbqt -o dock_protein.dpf -p move='empty'; cd ..; done

Changing the unbound model parameter

for i in $LIST; do cd cys${i}; cat dock_protein.dpf | sed 's/unbound_model extended/unbound_energy 0.0/g' > new_dpf.dpf; cd ..; done

Telling autogrid and autodock to use new atom type parameter file

for i in $LIST; do cd cys${i}; echo -e "parameter_file AD4_parameters.dat\n$(cat new_dpf.dpf)" > new_dpf.dpf; echo -e "parameter_file AD4_parameters.dat\n$(cat D_rerio.gpf)" > D_rerio.gpf; cd ..; done

##AUTODOCK AND AUTOGRID##

conda deactivate

Autogrid:

for i in $LIST; do cd cys${i}; cp ../AD4_parameters.dat .; autogrid4 -p D_rerio.gpf -l D_rerio.glg; cd ..; done

Autodock:

for i in $LIST; do cd cys${i}; ~/autodock4 -p new_dpf.dpf -l cys${i}.dlg; cd ..; done

##THRESHOLD##

Maximum free energy is 0.60kcal/mol

This is because the free energy of rotation is always 0.60kcal/mol

This is because new atom types cannot be used while calculating RMSD

Finding the free energy of binding

This removes the surrounding text, and if there is a plus it removes it

```
touch docked_coords.pdb

touch docked_resids.txt


for i in $(cat cys_list.txt); do gibbs=$(grep -e "Estimated Free Energy of Binding" cys${i}/cys${i}.dlg | head -n 1 | sed 's/DOCKED\: USER    Estimated Free Energy of Binding    \= //g' | sed 's/kcal\/mol  \[\=(1)+(2)+(3)-(4)\]//g' | sed 's/+//g'); echo $gibbs; if (( $(echo "$gibbs < 0.60" | bc -l) )); then echo "$i passes" >> docked_resids.txt; grep -A2 'DOCKED: ATOM      3' cys${i}/cys${i}.dlg | head -2 | sed 's/ATOM      4/HETATM    4/g' | sed 's/DOCKED\: //g' >> docked_coords.pdb; else echo "$i fails" >> docked_resids.txt; fi; done


##STRUCTURE PREPARATION##

#       Make the model template

#       Getting the coords of all docked metals + gamma sulfur

#       Putting the coords into the model template and removing existing gamma sulfurs


echo -e "$(grep -v "SG" D_rerio.pdb | sed '$d' | sed '$d')\n$(cat docked_coords.pdb)\n$(tail -n 2 D_rerio.pdb)" > docked_model.pdb


for i in $(cat cys_list.txt); do gibbs=$(grep -e "Estimated Free Energy of Binding" cys${i}/cys${i}.dlg | head -n 1 | sed 's/DOCKED\: USER    Estimated Free Energy of Binding    \= //g' | sed 's/kcal\/mol  \[\=(1)+(2)+(3)-(4)\]//g' | sed 's/+//g'); if (( $(echo "$gibbs < 0.60" | bc -l) )); then echo "$i $gibbs pass" >> stats.txt; else echo "$i $gibbs fail" >> stats.txt; fi; done
```

S12. Summarised Docking statistics

S12.1 Overall

Metallothionein	**Total cysteines**	**Total number binding**	**Total free energy of binding (pass and corrected)**	**Free energy per binding cysteine**
M. edulis	20	4	-0.83	-0.2075
M. galloprovincialis	21	5	-0.85	-0.17
D. rerio	20	4	-0.58	-0.145
C. sapidus	18	5	-0.65	-0.13
P. fluorescens	9	6	-2.44	-0.406666667
S. cerevisiae	12	5	-1.87	-0.374

S12.2 *M. edulis*

	Free energy of binding	Corrected free energy	Pass/Fail
5	3.35	2.75	Fail

7	3.85	3.25	Fail
13	0.79	0.19	Fail
15	0.78	0.18	Fail
19	N/A	N/A	Fail
24	0.39	-0.21	Pass
26	0.91	0.31	Fail
30	1.84	1.24	Fail
32	0.68	0.08	Fail
37	0.42	-0.18	Pass
39	0.76	0.16	Fail
42	N/A	N/A	Fail
46	N/A	N/A	Fail
48	0.5	-0.1	Pass
52	1.37	0.77	Fail
54	0.67	0.07	Fail
58	0.26	-0.34	Pass
64	2.49	1.89	Fail
66	1.06	0.46	Fail
70	N/A	N/A	Fail

S12.3 *M. galloprovincialis*

Residue number	Free energy of binding	Corrected free energy	Pass/Fail
5	1.59	0.99	Fail
7	1.71	1.11	Fail
13	0.28	-0.32	Pass
15	N/A	N/A	Fail
19	0.97	0.37	Fail
24	0.41	-0.19	Pass
26	N/A	N/A	Fail
30	1.66	1.06	Fail
32	2.99	2.39	Fail
37	N/A	N/A	Fail
39	0.58	-0.02	Pass
42	0.77	0.17	Fail
46	0.41	-0.19	Pass
48	N/A	N/A	Fail
52	N/A	N/A	Fail
54	N/A	N/A	Fail
58	N/A	N/A	Fail
64	N/A	N/A	Fail
66	0.47	-0.13	Pass
70	2.7	2.1	Fail
72	0.98	0.38	Fail

S12.4 *D. rerio*

Residue number	Free energy of binding	Corrected free energy	Pass/Fail
4	0.41	-0.19	Pass
6	0.98	0.38	Fail
12	0.75	0.15	Fail
14	0.32	-0.28	Pass
18	N/A	N/A	Fail
20	N/A	N/A	Fail
23	1.29	0.69	Fail
25	0.52	-0.08	Pass
28	1.61	1.01	Fail
32	N/A	N/A	Fail
33	N/A	N/A	Fail
35	N/A	N/A	Fail
36	1.25	0.65	Fail
40	N/A	N/A	Fail
43	0.94	0.34	Fail
47	N/A	N/A	Fail
49	0.66	0.06	Fail
54	0.57	-0.03	Pass
58	0.86	0.26	Fail
59	1.59	0.99	Fail

S12.5 *C. sapidus*

Residue number	Free energy of binding	Corrected free energy	Pass/Fail
5	0.56	-0.04	Pass
6	N/A	N/A	Fail
10	0.45	-0.15	Pass
12	0.6	0	Fail
17	0.46	-0.14	Pass
21	N/A	N/A	Fail
23	3.1	2.5	Fail
26	4.71	4.11	Fail
28	N/A	N/A	Fail
31	0.74	0.14	Fail
34	0.36	-0.24	Pass
38	1.17	0.57	Fail
40	0.52	-0.08	Pass
46	2.74	2.14	Fail
50	0.96	0.36	Fail
54	67.28	66.68	Fail
56	N/A	N/A	Fail
57	0.64	0.04	Fail

S12.6 *P. fluorescens*

Residue number	Free energy of binding	Corrected free energy	Pass/Fail
6	0.99	0.39	Fail
8	0.04	-0.56	Pass
11	1.05	0.45	Fail
13	0.39	-0.21	Pass
29	0.32	-0.28	Pass
33	0.14	-0.46	Pass
43	0.26	-0.34	Pass
48	0.01	-0.59	Pass
50	1.3	0.7	Fail

S12.7 *S. cerevisiae*

Residue number	Free energy of binding	Corrected free energy	Pass/Fail
15	N/A	N/A	Fail
17	N/A	N/A	Fail
19	N/A	N/A	Fail
22	0.37	-0.23	Pass
28	0.48	-0.12	Pass
32	0.41	-0.19	Pass
34	1.09	0.49	Fail
38	-0.01	-0.61	Fail
44	0.27	-0.33	Pass
46	N/A	N/A	Fail
57	0.74	0.14	Fail
58	0.21	-0.39	Pass

S.13 Docking Log Summaries of the best model

S.13.1 *M. edulis*

CYS5

DOCKED: USER Estimated Free Energy of Binding = +3.35 kcal/mol [=(1)+(2)+(3)-(4)]

DOCKED: USER

DOCKED: USER (1) Final Intermolecular Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Fixed Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Moving Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER (2) Final Total Internal Energy = +2.76 kcal/mol
DOCKED: USER Internal Energy Ligand = +0.00 kcal/mol
DOCKED: USER Internal Moving-Fixed Receptor = +2.47 kcal/mol
DOCKED: USER Internal Moving-Moving Receptor = +0.28 kcal/mol
DOCKED: USER (3) Torsional Free Energy = +0.60 kcal/mol
DOCKED: USER (4) Unbound System's Energy = +0.00 kcal/mol

CYS7

DOCKED: USER Estimated Free Energy of Binding = +3.85 kcal/mol [=(1)+(2)+(3)-(4)]
DOCKED: USER
DOCKED: USER (1) Final Intermolecular Energy = +0.00 kcal/mol
DOCKED: USER Moving Ligand-Fixed Receptor = +0.00 kcal/mol
DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol
DOCKED: USER Electrostatic Energy = +0.00 kcal/mol
DOCKED: USER Moving Ligand-Moving Receptor = +0.00 kcal/mol
DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol
DOCKED: USER Electrostatic Energy = +0.00 kcal/mol
DOCKED: USER (2) Final Total Internal Energy = +3.25 kcal/mol
DOCKED: USER Internal Energy Ligand = +0.00 kcal/mol
DOCKED: USER Internal Moving-Fixed Receptor = +2.83 kcal/mol
DOCKED: USER Internal Moving-Moving Receptor = +0.43 kcal/mol
DOCKED: USER (3) Torsional Free Energy = +0.60 kcal/mol
DOCKED: USER (4) Unbound System's Energy = +0.00 kcal/mol

CYS13

DOCKED: USER Estimated Free Energy of Binding = +0.79 kcal/mol [=(1)+(2)+(3)-(4)]
DOCKED: USER
DOCKED: USER (1) Final Intermolecular Energy = +0.00 kcal/mol
DOCKED: USER Moving Ligand-Fixed Receptor = +0.00 kcal/mol
DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol
DOCKED: USER Electrostatic Energy = +0.00 kcal/mol
DOCKED: USER Moving Ligand-Moving Receptor = +0.00 kcal/mol
DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol
DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER (2) Final Total Internal Energy = +0.19 kcal/mol
DOCKED: USER Internal Energy Ligand = +0.00 kcal/mol
DOCKED: USER Internal Moving-Fixed Receptor = +0.01 kcal/mol
DOCKED: USER Internal Moving-Moving Receptor = +0.18 kcal/mol
DOCKED: USER (3) Torsional Free Energy = +0.60 kcal/mol
DOCKED: USER (4) Unbound System's Energy = +0.00 kcal/mol

CYS15

DOCKED: USER Estimated Free Energy of Binding = +0.78 kcal/mol [=(1)+(2)+(3)-(4)]
DOCKED: USER
DOCKED: USER (1) Final Intermolecular Energy = +0.00 kcal/mol
DOCKED: USER Moving Ligand-Fixed Receptor = +0.00 kcal/mol
DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol
DOCKED: USER Electrostatic Energy = +0.00 kcal/mol
DOCKED: USER Moving Ligand-Moving Receptor = +0.00 kcal/mol
DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol
DOCKED: USER Electrostatic Energy = +0.00 kcal/mol
DOCKED: USER (2) Final Total Internal Energy = +0.18 kcal/mol
DOCKED: USER Internal Energy Ligand = +0.00 kcal/mol
DOCKED: USER Internal Moving-Fixed Receptor = -0.00 kcal/mol
DOCKED: USER Internal Moving-Moving Receptor = +0.18 kcal/mol
DOCKED: USER (3) Torsional Free Energy = +0.60 kcal/mol
DOCKED: USER (4) Unbound System's Energy = +0.00 kcal/mol

CYS24

DOCKED: USER Estimated Free Energy of Binding = +0.39 kcal/mol [=(1)+(2)+(3)-(4)]
DOCKED: USER
DOCKED: USER (1) Final Intermolecular Energy = +0.00 kcal/mol
DOCKED: USER Moving Ligand-Fixed Receptor = +0.00 kcal/mol
DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol
DOCKED: USER Electrostatic Energy = +0.00 kcal/mol
DOCKED: USER Moving Ligand-Moving Receptor = +0.00 kcal/mol
DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol
DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER (2) Final Total Internal Energy = -0.20 kcal/mol
DOCKED: USER Internal Energy Ligand = +0.00 kcal/mol
DOCKED: USER Internal Moving-Fixed Receptor = -0.35 kcal/mol
DOCKED: USER Internal Moving-Moving Receptor = +0.15 kcal/mol
DOCKED: USER (3) Torsional Free Energy = +0.60 kcal/mol
DOCKED: USER (4) Unbound System's Energy = +0.00 kcal/mol

CYS26
DOCKED: USER Estimated Free Energy of Binding = +0.91 kcal/mol [=(1)+(2)+(3)-(4)]
DOCKED: USER
DOCKED: USER (1) Final Intermolecular Energy = +0.00 kcal/mol
DOCKED: USER Moving Ligand-Fixed Receptor = +0.00 kcal/mol
DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol
DOCKED: USER Electrostatic Energy = +0.00 kcal/mol
DOCKED: USER Moving Ligand-Moving Receptor = +0.00 kcal/mol
DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol
DOCKED: USER Electrostatic Energy = +0.00 kcal/mol
DOCKED: USER (2) Final Total Internal Energy = +0.31 kcal/mol
DOCKED: USER Internal Energy Ligand = +0.00 kcal/mol
DOCKED: USER Internal Moving-Fixed Receptor = -0.14 kcal/mol
DOCKED: USER Internal Moving-Moving Receptor = +0.45 kcal/mol
DOCKED: USER (3) Torsional Free Energy = +0.60 kcal/mol
DOCKED: USER (4) Unbound System's Energy = +0.00 kcal/mol

CYS30
DOCKED: USER Estimated Free Energy of Binding = +1.84 kcal/mol [=(1)+(2)+(3)-(4)]
DOCKED: USER
DOCKED: USER (1) Final Intermolecular Energy = +0.00 kcal/mol
DOCKED: USER Moving Ligand-Fixed Receptor = +0.00 kcal/mol
DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol
DOCKED: USER Electrostatic Energy = +0.00 kcal/mol
DOCKED: USER Moving Ligand-Moving Receptor = +0.00 kcal/mol
DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol
DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER (2) Final Total Internal Energy = +1.24 kcal/mol
DOCKED: USER Internal Energy Ligand = +0.00 kcal/mol
DOCKED: USER Internal Moving-Fixed Receptor = +0.99 kcal/mol
DOCKED: USER Internal Moving-Moving Receptor = +0.26 kcal/mol
DOCKED: USER (3) Torsional Free Energy = +0.60 kcal/mol
DOCKED: USER (4) Unbound System's Energy = +0.00 kcal/mol

CYS32

DOCKED: USER Estimated Free Energy of Binding = +0.68 kcal/mol [=(1)+(2)+(3)-(4)]
DOCKED: USER
DOCKED: USER (1) Final Intermolecular Energy = +0.00 kcal/mol
DOCKED: USER Moving Ligand-Fixed Receptor = +0.00 kcal/mol
DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol
DOCKED: USER Electrostatic Energy = +0.00 kcal/mol
DOCKED: USER Moving Ligand-Moving Receptor = +0.00 kcal/mol
DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol
DOCKED: USER Electrostatic Energy = +0.00 kcal/mol
DOCKED: USER (2) Final Total Internal Energy = +0.08 kcal/mol
DOCKED: USER Internal Energy Ligand = +0.00 kcal/mol
DOCKED: USER Internal Moving-Fixed Receptor = -0.19 kcal/mol
DOCKED: USER Internal Moving-Moving Receptor = +0.27 kcal/mol
DOCKED: USER (3) Torsional Free Energy = +0.60 kcal/mol
DOCKED: USER (4) Unbound System's Energy = +0.00 kcal/mol

CYS37

DOCKED: USER Estimated Free Energy of Binding = +0.42 kcal/mol [=(1)+(2)+(3)-(4)]
DOCKED: USER
DOCKED: USER (1) Final Intermolecular Energy = +0.00 kcal/mol
DOCKED: USER Moving Ligand-Fixed Receptor = +0.00 kcal/mol
DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol
DOCKED: USER Electrostatic Energy = +0.00 kcal/mol
DOCKED: USER Moving Ligand-Moving Receptor = +0.00 kcal/mol
DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol
DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER (2) Final Total Internal Energy = -0.18 kcal/mol
DOCKED: USER Internal Energy Ligand = +0.00 kcal/mol
DOCKED: USER Internal Moving-Fixed Receptor = -0.31 kcal/mol
DOCKED: USER Internal Moving-Moving Receptor = +0.14 kcal/mol
DOCKED: USER (3) Torsional Free Energy = +0.60 kcal/mol
DOCKED: USER (4) Unbound System's Energy = +0.00 kcal/mol

CYS39
DOCKED: USER Estimated Free Energy of Binding = +0.76 kcal/mol [=(1)+(2)+(3)-(4)]
DOCKED: USER
DOCKED: USER (1) Final Intermolecular Energy = +0.00 kcal/mol
DOCKED: USER Moving Ligand-Fixed Receptor = +0.00 kcal/mol
DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol
DOCKED: USER Electrostatic Energy = +0.00 kcal/mol
DOCKED: USER Moving Ligand-Moving Receptor = +0.00 kcal/mol
DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol
DOCKED: USER Electrostatic Energy = +0.00 kcal/mol
DOCKED: USER (2) Final Total Internal Energy = +0.16 kcal/mol
DOCKED: USER Internal Energy Ligand = +0.00 kcal/mol
DOCKED: USER Internal Moving-Fixed Receptor = -0.20 kcal/mol
DOCKED: USER Internal Moving-Moving Receptor = +0.36 kcal/mol
DOCKED: USER (3) Torsional Free Energy = +0.60 kcal/mol
DOCKED: USER (4) Unbound System's Energy = +0.00 kcal/mol

CYS48
DOCKED: USER Estimated Free Energy of Binding = +0.50 kcal/mol [=(1)+(2)+(3)-(4)]
DOCKED: USER
DOCKED: USER (1) Final Intermolecular Energy = +0.00 kcal/mol
DOCKED: USER Moving Ligand-Fixed Receptor = +0.00 kcal/mol
DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol
DOCKED: USER Electrostatic Energy = +0.00 kcal/mol
DOCKED: USER Moving Ligand-Moving Receptor = +0.00 kcal/mol
DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol
DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER (2) Final Total Internal Energy = -0.10 kcal/mol
DOCKED: USER Internal Energy Ligand = +0.00 kcal/mol
DOCKED: USER Internal Moving-Fixed Receptor = -0.27 kcal/mol
DOCKED: USER Internal Moving-Moving Receptor = +0.17 kcal/mol
DOCKED: USER (3) Torsional Free Energy = +0.60 kcal/mol
DOCKED: USER (4) Unbound System's Energy = +0.00 kcal/mol

CYS52

DOCKED: USER Estimated Free Energy of Binding = +1.37 kcal/mol [=(1)+(2)+(3)-(4)]
DOCKED: USER
DOCKED: USER (1) Final Intermolecular Energy = +0.00 kcal/mol
DOCKED: USER Moving Ligand-Fixed Receptor = +0.00 kcal/mol
DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol
DOCKED: USER Electrostatic Energy = +0.00 kcal/mol
DOCKED: USER Moving Ligand-Moving Receptor = +0.00 kcal/mol
DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol
DOCKED: USER Electrostatic Energy = +0.00 kcal/mol
DOCKED: USER (2) Final Total Internal Energy = +0.77 kcal/mol
DOCKED: USER Internal Energy Ligand = +0.00 kcal/mol
DOCKED: USER Internal Moving-Fixed Receptor = +0.57 kcal/mol
DOCKED: USER Internal Moving-Moving Receptor = +0.20 kcal/mol
DOCKED: USER (3) Torsional Free Energy = +0.60 kcal/mol
DOCKED: USER (4) Unbound System's Energy = +0.00 kcal/mol

CYS54

DOCKED: USER Estimated Free Energy of Binding = +0.67 kcal/mol [=(1)+(2)+(3)-(4)]
DOCKED: USER
DOCKED: USER (1) Final Intermolecular Energy = +0.00 kcal/mol
DOCKED: USER Moving Ligand-Fixed Receptor = +0.00 kcal/mol
DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol
DOCKED: USER Electrostatic Energy = +0.00 kcal/mol
DOCKED: USER Moving Ligand-Moving Receptor = +0.00 kcal/mol
DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol
DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER (2) Final Total Internal Energy = +0.07 kcal/mol
DOCKED: USER Internal Energy Ligand = +0.00 kcal/mol
DOCKED: USER Internal Moving-Fixed Receptor = -0.12 kcal/mol
DOCKED: USER Internal Moving-Moving Receptor = +0.19 kcal/mol
DOCKED: USER (3) Torsional Free Energy = +0.60 kcal/mol
DOCKED: USER (4) Unbound System's Energy = +0.00 kcal/mol

CYS58

DOCKED: USER Estimated Free Energy of Binding = +0.26 kcal/mol [=(1)+(2)+(3)-(4)]
DOCKED: USER
DOCKED: USER (1) Final Intermolecular Energy = +0.00 kcal/mol
DOCKED: USER Moving Ligand-Fixed Receptor = +0.00 kcal/mol
DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol
DOCKED: USER Electrostatic Energy = +0.00 kcal/mol
DOCKED: USER Moving Ligand-Moving Receptor = +0.00 kcal/mol
DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol
DOCKED: USER Electrostatic Energy = +0.00 kcal/mol
DOCKED: USER (2) Final Total Internal Energy = -0.33 kcal/mol
DOCKED: USER Internal Energy Ligand = +0.00 kcal/mol
DOCKED: USER Internal Moving-Fixed Receptor = -0.62 kcal/mol
DOCKED: USER Internal Moving-Moving Receptor = +0.29 kcal/mol
DOCKED: USER (3) Torsional Free Energy = +0.60 kcal/mol
DOCKED: USER (4) Unbound System's Energy = +0.00 kcal/mol

CYS64

DOCKED: USER Estimated Free Energy of Binding = +2.49 kcal/mol [=(1)+(2)+(3)-(4)]
DOCKED: USER
DOCKED: USER (1) Final Intermolecular Energy = +0.00 kcal/mol
DOCKED: USER Moving Ligand-Fixed Receptor = +0.00 kcal/mol
DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol
DOCKED: USER Electrostatic Energy = +0.00 kcal/mol
DOCKED: USER Moving Ligand-Moving Receptor = +0.00 kcal/mol
DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol
DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER (2) Final Total Internal Energy = +1.89 kcal/mol

DOCKED: USER Internal Energy Ligand = +0.00 kcal/mol

DOCKED: USER Internal Moving-Fixed Receptor = +1.47 kcal/mol

DOCKED: USER Internal Moving-Moving Receptor = +0.42 kcal/mol

DOCKED: USER (3) Torsional Free Energy = +0.60 kcal/mol

DOCKED: USER (4) Unbound System's Energy = +0.00 kcal/mol

CYS66

DOCKED: USER Estimated Free Energy of Binding = +1.06 kcal/mol [=(1)+(2)+(3)-(4)]

DOCKED: USER

DOCKED: USER (1) Final Intermolecular Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Fixed Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Moving Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER (2) Final Total Internal Energy = +0.47 kcal/mol

DOCKED: USER Internal Energy Ligand = +0.00 kcal/mol

DOCKED: USER Internal Moving-Fixed Receptor = +0.09 kcal/mol

DOCKED: USER Internal Moving-Moving Receptor = +0.38 kcal/mol

DOCKED: USER (3) Torsional Free Energy = +0.60 kcal/mol

DOCKED: USER (4) Unbound System's Energy = +0.00 kcal/mol

S.13.2 *M. galloprovincialis*

CYS5

DOCKED: USER Estimated Free Energy of Binding = +1.59 kcal/mol [=(1)+(2)+(3)-(4)]

DOCKED: USER

DOCKED: USER (1) Final Intermolecular Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Fixed Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Moving Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER (2) Final Total Internal Energy = +0.99 kcal/mol

DOCKED: USER Internal Energy Ligand = +0.00 kcal/mol

DOCKED: USER Internal Moving-Fixed Receptor = +0.77 kcal/mol

DOCKED: USER Internal Moving-Moving Receptor = +0.23 kcal/mol

DOCKED: USER (3) Torsional Free Energy = +0.60 kcal/mol

DOCKED: USER (4) Unbound System's Energy = +0.00 kcal/mol

CYS7

DOCKED: USER Estimated Free Energy of Binding = +1.81 kcal/mol [=(1)+(2)+(3)-(4)]

DOCKED: USER

DOCKED: USER (1) Final Intermolecular Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Fixed Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Moving Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER (2) Final Total Internal Energy = +1.22 kcal/mol

DOCKED: USER Internal Energy Ligand = +0.00 kcal/mol

DOCKED: USER Internal Moving-Fixed Receptor = +0.75 kcal/mol

DOCKED: USER Internal Moving-Moving Receptor = +0.46 kcal/mol

DOCKED: USER (3) Torsional Free Energy = +0.60 kcal/mol

DOCKED: USER (4) Unbound System's Energy = +0.00 kcal/mol

CYS13

DOCKED: USER Estimated Free Energy of Binding = +0.28 kcal/mol [=(1)+(2)+(3)-(4)]

DOCKED: USER

DOCKED: USER (1) Final Intermolecular Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Fixed Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Moving Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER (2) Final Total Internal Energy = -0.31 kcal/mol

DOCKED: USER Internal Energy Ligand = +0.00 kcal/mol

DOCKED: USER Internal Moving-Fixed Receptor = -0.51 kcal/mol

DOCKED: USER Internal Moving-Moving Receptor = +0.20 kcal/mol

DOCKED: USER (3) Torsional Free Energy = +0.60 kcal/mol

DOCKED: USER (4) Unbound System's Energy = +0.00 kcal/mol

CYS19

DOCKED: USER Estimated Free Energy of Binding = +0.97 kcal/mol [=(1)+(2)+(3)-(4)]

DOCKED: USER

DOCKED: USER (1) Final Intermolecular Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Fixed Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Moving Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER (2) Final Total Internal Energy = +0.37 kcal/mol

DOCKED: USER Internal Energy Ligand = +0.00 kcal/mol

DOCKED: USER Internal Moving-Fixed Receptor = +0.11 kcal/mol

DOCKED: USER Internal Moving-Moving Receptor = +0.26 kcal/mol

DOCKED: USER (3) Torsional Free Energy = +0.60 kcal/mol

DOCKED: USER (4) Unbound System's Energy = +0.00 kcal/mol

CYS24

DOCKED: USER Estimated Free Energy of Binding = +0.41 kcal/mol [=(1)+(2)+(3)-(4)]

DOCKED: USER

DOCKED: USER (1) Final Intermolecular Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Fixed Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Moving Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER (2) Final Total Internal Energy = -0.19 kcal/mol

DOCKED: USER Internal Energy Ligand = +0.00 kcal/mol

DOCKED: USER Internal Moving-Fixed Receptor = -0.46 kcal/mol

DOCKED: USER Internal Moving-Moving Receptor = +0.27 kcal/mol

DOCKED: USER (3) Torsional Free Energy = +0.60 kcal/mol

DOCKED: USER (4) Unbound System's Energy = +0.00 kcal/mol

CYS30

DOCKED: USER Estimated Free Energy of Binding = +1.66 kcal/mol [=(1)+(2)+(3)-(4)]

DOCKED: USER

DOCKED: USER (1) Final Intermolecular Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Fixed Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Moving Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER (2) Final Total Internal Energy = +1.06 kcal/mol

DOCKED: USER Internal Energy Ligand = +0.00 kcal/mol

DOCKED: USER Internal Moving-Fixed Receptor = +0.79 kcal/mol

DOCKED: USER Internal Moving-Moving Receptor = +0.27 kcal/mol

DOCKED: USER (3) Torsional Free Energy = +0.60 kcal/mol

DOCKED: USER (4) Unbound System's Energy = +0.00 kcal/mol

CYS32

DOCKED: USER Estimated Free Energy of Binding = +2.99 kcal/mol [=(1)+(2)+(3)-(4)]

DOCKED: USER

DOCKED: USER (1) Final Intermolecular Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Fixed Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Moving Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER (2) Final Total Internal Energy = +2.69 kcal/mol

DOCKED: USER Internal Energy Ligand = +0.00 kcal/mol

DOCKED: USER Internal Moving-Fixed Receptor = +2.69 kcal/mol

DOCKED: USER Internal Moving-Moving Receptor = +0.00 kcal/mol

DOCKED: USER (3) Torsional Free Energy = +0.30 kcal/mol

DOCKED: USER (4) Unbound System's Energy = +0.00 kcal/mol

CYS39

DOCKED: USER Estimated Free Energy of Binding = +0.58 kcal/mol [=(1)+(2)+(3)-(4)]

DOCKED: USER

DOCKED: USER (1) Final Intermolecular Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Fixed Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Moving Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER (2) Final Total Internal Energy = -0.02 kcal/mol

DOCKED: USER Internal Energy Ligand = +0.00 kcal/mol

DOCKED: USER Internal Moving-Fixed Receptor = -0.20 kcal/mol

DOCKED: USER Internal Moving-Moving Receptor = +0.18 kcal/mol

DOCKED: USER (3) Torsional Free Energy = +0.60 kcal/mol

DOCKED: USER (4) Unbound System's Energy = +0.00 kcal/mol

CYS42

DOCKED: USER Estimated Free Energy of Binding = +0.77 kcal/mol [=(1)+(2)+(3)-(4)]

DOCKED: USER

DOCKED: USER (1) Final Intermolecular Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Fixed Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Moving Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER (2) Final Total Internal Energy = +0.17 kcal/mol

DOCKED: USER Internal Energy Ligand = +0.00 kcal/mol

DOCKED: USER Internal Moving-Fixed Receptor = -0.11 kcal/mol

DOCKED: USER Internal Moving-Moving Receptor = +0.28 kcal/mol

DOCKED: USER (3) Torsional Free Energy = +0.60 kcal/mol

DOCKED: USER (4) Unbound System's Energy = +0.00 kcal/mol

CYS46

DOCKED: USER Estimated Free Energy of Binding = +0.41 kcal/mol [=(1)+(2)+(3)-(4)]

DOCKED: USER

DOCKED: USER (1) Final Intermolecular Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Fixed Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Moving Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER (2) Final Total Internal Energy = -0.19 kcal/mol

DOCKED: USER Internal Energy Ligand = +0.00 kcal/mol

DOCKED: USER Internal Moving-Fixed Receptor = -0.40 kcal/mol

DOCKED: USER Internal Moving-Moving Receptor = +0.21 kcal/mol

DOCKED: USER (3) Torsional Free Energy = +0.60 kcal/mol

DOCKED: USER (4) Unbound System's Energy = +0.00 kcal/mol

CYS66

DOCKED: USER Estimated Free Energy of Binding = +0.47 kcal/mol [=(1)+(2)+(3)-(4)]

DOCKED: USER

DOCKED: USER (1) Final Intermolecular Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Fixed Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Moving Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER (2) Final Total Internal Energy = -0.13 kcal/mol

DOCKED: USER Internal Energy Ligand = +0.00 kcal/mol

DOCKED: USER Internal Moving-Fixed Receptor = -0.36 kcal/mol

DOCKED: USER Internal Moving-Moving Receptor = +0.23 kcal/mol

DOCKED: USER (3) Torsional Free Energy = +0.60 kcal/mol

DOCKED: USER (4) Unbound System's Energy = +0.00 kcal/mol

CYS70

DOCKED: USER Estimated Free Energy of Binding = +2.70 kcal/mol [=(1)+(2)+(3)-(4)]

DOCKED: USER

DOCKED: USER (1) Final Intermolecular Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Fixed Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Moving Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER (2) Final Total Internal Energy = +2.11 kcal/mol

DOCKED: USER Internal Energy Ligand = +0.00 kcal/mol

DOCKED: USER Internal Moving-Fixed Receptor = +1.80 kcal/mol

DOCKED: USER Internal Moving-Moving Receptor = +0.31 kcal/mol

DOCKED: USER (3) Torsional Free Energy = +0.60 kcal/mol

DOCKED: USER (4) Unbound System's Energy = +0.00 kcal/mol

CYS72

DOCKED: USER Estimated Free Energy of Binding = +0.98 kcal/mol [=(1)+(2)+(3)-(4)]

DOCKED: USER

DOCKED: USER (1) Final Intermolecular Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Fixed Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Moving Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER (2) Final Total Internal Energy = +0.38 kcal/mol

DOCKED: USER Internal Energy Ligand = +0.00 kcal/mol

DOCKED: USER Internal Moving-Fixed Receptor = +0.21 kcal/mol

DOCKED: USER Internal Moving-Moving Receptor = +0.17 kcal/mol

DOCKED: USER (3) Torsional Free Energy = +0.60 kcal/mol

DOCKED: USER (4) Unbound System's Energy = +0.00 kcal/mol

S.13.3 *D. rerio*

CYS4

DOCKED: USER Estimated Free Energy of Binding = +0.41 kcal/mol [=(1)+(2)+(3)-(4)]

DOCKED: USER

DOCKED: USER (1) Final Intermolecular Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Fixed Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Moving Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER (2) Final Total Internal Energy = -0.18 kcal/mol

DOCKED: USER Internal Energy Ligand = +0.00 kcal/mol

DOCKED: USER Internal Moving-Fixed Receptor = -0.47 kcal/mol

DOCKED: USER Internal Moving-Moving Receptor = +0.29 kcal/mol

DOCKED: USER (3) Torsional Free Energy = +0.60 kcal/mol

DOCKED: USER (4) Unbound System's Energy = +0.00 kcal/mol

CYS6

DOCKED: USER Estimated Free Energy of Binding = +0.98 kcal/mol [=(1)+(2)+(3)-(4)]

DOCKED: USER

DOCKED: USER (1) Final Intermolecular Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Fixed Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Moving Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER (2) Final Total Internal Energy = +0.39 kcal/mol

DOCKED: USER Internal Energy Ligand = +0.00 kcal/mol

DOCKED: USER Internal Moving-Fixed Receptor = +0.08 kcal/mol

DOCKED: USER Internal Moving-Moving Receptor = +0.31 kcal/mol

DOCKED: USER (3) Torsional Free Energy = +0.60 kcal/mol

DOCKED: USER (4) Unbound System's Energy = +0.00 kcal/mol

CYS12

DOCKED: USER Estimated Free Energy of Binding = +0.75 kcal/mol [=(1)+(2)+(3)-(4)]

DOCKED: USER

DOCKED: USER (1) Final Intermolecular Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Fixed Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Moving Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER (2) Final Total Internal Energy = +0.15 kcal/mol

DOCKED: USER Internal Energy Ligand = +0.00 kcal/mol

DOCKED: USER Internal Moving-Fixed Receptor = -0.09 kcal/mol

DOCKED: USER Internal Moving-Moving Receptor = +0.24 kcal/mol

DOCKED: USER (3) Torsional Free Energy = +0.60 kcal/mol

DOCKED: USER (4) Unbound System's Energy = +0.00 kcal/mol

CYS14

DOCKED: USER Estimated Free Energy of Binding = +0.32 kcal/mol [=(1)+(2)+(3)-(4)]

DOCKED: USER

DOCKED: USER (1) Final Intermolecular Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Fixed Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Moving Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER (2) Final Total Internal Energy = -0.28 kcal/mol

DOCKED: USER Internal Energy Ligand = +0.00 kcal/mol

DOCKED: USER Internal Moving-Fixed Receptor = -0.47 kcal/mol

DOCKED: USER Internal Moving-Moving Receptor = +0.19 kcal/mol

DOCKED: USER (3) Torsional Free Energy = +0.60 kcal/mol

DOCKED: USER (4) Unbound System's Energy = +0.00 kcal/mol

CYS23

DOCKED: USER Estimated Free Energy of Binding = +1.29 kcal/mol [=(1)+(2)+(3)-(4)]

DOCKED: USER

DOCKED: USER (1) Final Intermolecular Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Fixed Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Moving Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER (2) Final Total Internal Energy = +0.99 kcal/mol

DOCKED: USER Internal Energy Ligand = +0.00 kcal/mol

DOCKED: USER Internal Moving-Fixed Receptor = +0.99 kcal/mol

DOCKED: USER Internal Moving-Moving Receptor = +0.00 kcal/mol

DOCKED: USER (3) Torsional Free Energy = +0.30 kcal/mol

DOCKED: USER (4) Unbound System's Energy = +0.00 kcal/mol

CYS25

DOCKED: USER Estimated Free Energy of Binding = +0.52 kcal/mol [=(1)+(2)+(3)-(4)]

DOCKED: USER

DOCKED: USER (1) Final Intermolecular Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Fixed Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Moving Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER (2) Final Total Internal Energy = -0.08 kcal/mol

DOCKED: USER Internal Energy Ligand = +0.00 kcal/mol

DOCKED: USER Internal Moving-Fixed Receptor = -0.57 kcal/mol

DOCKED: USER Internal Moving-Moving Receptor = +0.49 kcal/mol

DOCKED: USER (3) Torsional Free Energy = +0.60 kcal/mol

DOCKED: USER (4) Unbound System's Energy = +0.00 kcal/mol

CYS28

DOCKED: USER Estimated Free Energy of Binding = +1.61 kcal/mol [=(1)+(2)+(3)-(4)]

DOCKED: USER

DOCKED: USER (1) Final Intermolecular Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Fixed Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Moving Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER (2) Final Total Internal Energy = +1.01 kcal/mol

DOCKED: USER Internal Energy Ligand = +0.00 kcal/mol

DOCKED: USER Internal Moving-Fixed Receptor = +0.75 kcal/mol

DOCKED: USER Internal Moving-Moving Receptor = +0.27 kcal/mol

DOCKED: USER (3) Torsional Free Energy = +0.60 kcal/mol

DOCKED: USER (4) Unbound System's Energy = +0.00 kcal/mol

CYS36

DOCKED: USER Estimated Free Energy of Binding = +1.25 kcal/mol [=(1)+(2)+(3)-(4)]

DOCKED: USER

DOCKED: USER (1) Final Intermolecular Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Fixed Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Moving Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER (2) Final Total Internal Energy = +0.66 kcal/mol

DOCKED: USER Internal Energy Ligand = +0.00 kcal/mol

DOCKED: USER Internal Moving-Fixed Receptor = +0.48 kcal/mol

DOCKED: USER Internal Moving-Moving Receptor = +0.18 kcal/mol

DOCKED: USER (3) Torsional Free Energy = +0.60 kcal/mol

DOCKED: USER (4) Unbound System's Energy = +0.00 kcal/mol

CYS43

DOCKED: USER Estimated Free Energy of Binding = +0.94 kcal/mol [=(1)+(2)+(3)-(4)]

DOCKED: USER

DOCKED: USER (1) Final Intermolecular Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Fixed Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Moving Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER (2) Final Total Internal Energy = +0.34 kcal/mol

DOCKED: USER Internal Energy Ligand = +0.00 kcal/mol

DOCKED: USER Internal Moving-Fixed Receptor = +0.23 kcal/mol

DOCKED: USER Internal Moving-Moving Receptor = +0.12 kcal/mol

DOCKED: USER (3) Torsional Free Energy = +0.60 kcal/mol

DOCKED: USER (4) Unbound System's Energy = +0.00 kcal/mol

CYS49

DOCKED: USER Estimated Free Energy of Binding = +0.66 kcal/mol [=(1)+(2)+(3)-(4)]

DOCKED: USER

DOCKED: USER (1) Final Intermolecular Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Fixed Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Moving Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER (2) Final Total Internal Energy = +0.06 kcal/mol

DOCKED: USER Internal Energy Ligand = +0.00 kcal/mol

DOCKED: USER Internal Moving-Fixed Receptor = -0.15 kcal/mol

DOCKED: USER Internal Moving-Moving Receptor = +0.21 kcal/mol

DOCKED: USER (3) Torsional Free Energy = +0.60 kcal/mol

DOCKED: USER (4) Unbound System's Energy = +0.00 kcal/mol

CYS54

DOCKED: USER Estimated Free Energy of Binding = +0.57 kcal/mol [=(1)+(2)+(3)-(4)]

DOCKED: USER

DOCKED: USER (1) Final Intermolecular Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Fixed Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Moving Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER (2) Final Total Internal Energy = -0.02 kcal/mol

DOCKED: USER Internal Energy Ligand = +0.00 kcal/mol

DOCKED: USER Internal Moving-Fixed Receptor = -0.23 kcal/mol

DOCKED: USER Internal Moving-Moving Receptor = +0.20 kcal/mol

DOCKED: USER (3) Torsional Free Energy = +0.60 kcal/mol

DOCKED: USER (4) Unbound System's Energy = +0.00 kcal/mol

CYS58

DOCKED: USER Estimated Free Energy of Binding = +0.86 kcal/mol [=(1)+(2)+(3)-(4)]

DOCKED: USER

DOCKED: USER (1) Final Intermolecular Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Fixed Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Moving Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER (2) Final Total Internal Energy = +0.26 kcal/mol

DOCKED: USER Internal Energy Ligand = +0.00 kcal/mol

DOCKED: USER Internal Moving-Fixed Receptor = -0.09 kcal/mol

DOCKED: USER Internal Moving-Moving Receptor = +0.35 kcal/mol

DOCKED: USER (3) Torsional Free Energy = +0.60 kcal/mol

DOCKED: USER (4) Unbound System's Energy = +0.00 kcal/mol

CYS59

DOCKED: USER Estimated Free Energy of Binding = +1.59 kcal/mol [=(1)+(2)+(3)-(4)]

DOCKED: USER

DOCKED: USER (1) Final Intermolecular Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Fixed Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Moving Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER (2) Final Total Internal Energy = +0.99 kcal/mol

DOCKED: USER Internal Energy Ligand = +0.00 kcal/mol

DOCKED: USER Internal Moving-Fixed Receptor = +0.82 kcal/mol

DOCKED: USER Internal Moving-Moving Receptor = +0.17 kcal/mol

DOCKED: USER (3) Torsional Free Energy = +0.60 kcal/mol

DOCKED: USER (4) Unbound System's Energy = +0.00 kcal/mol

S.13.4 *C. sapidus*

CYS5

DOCKED: USER Estimated Free Energy of Binding = +0.56 kcal/mol [=(1)+(2)+(3)-(4)]

DOCKED: USER

DOCKED: USER (1) Final Intermolecular Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Fixed Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Moving Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER (2) Final Total Internal Energy = -0.04 kcal/mol

DOCKED: USER Internal Energy Ligand = +0.00 kcal/mol

DOCKED: USER Internal Moving-Fixed Receptor = -0.43 kcal/mol

DOCKED: USER Internal Moving-Moving Receptor = +0.39 kcal/mol

DOCKED: USER (3) Torsional Free Energy = +0.60 kcal/mol

DOCKED: USER (4) Unbound System's Energy = +0.00 kcal/mol

CYS10

DOCKED: USER Estimated Free Energy of Binding = +0.45 kcal/mol [=(1)+(2)+(3)-(4)]

DOCKED: USER

DOCKED: USER (1) Final Intermolecular Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Fixed Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Moving Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER (2) Final Total Internal Energy = -0.14 kcal/mol

DOCKED: USER Internal Energy Ligand = +0.00 kcal/mol

DOCKED: USER Internal Moving-Fixed Receptor = -0.35 kcal/mol

DOCKED: USER Internal Moving-Moving Receptor = +0.21 kcal/mol

DOCKED: USER (3) Torsional Free Energy = +0.60 kcal/mol

DOCKED: USER (4) Unbound System's Energy = +0.00 kcal/mol

CYS12

DOCKED: USER Estimated Free Energy of Binding = +0.60 kcal/mol [=(1)+(2)+(3)-(4)]

DOCKED: USER

DOCKED: USER (1) Final Intermolecular Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Fixed Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Moving Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER (2) Final Total Internal Energy = +0.01 kcal/mol

DOCKED: USER Internal Energy Ligand = +0.00 kcal/mol

DOCKED: USER Internal Moving-Fixed Receptor = -0.16 kcal/mol

DOCKED: USER Internal Moving-Moving Receptor = +0.17 kcal/mol

DOCKED: USER (3) Torsional Free Energy = +0.60 kcal/mol

DOCKED: USER (4) Unbound System's Energy = +0.00 kcal/mol

CYS17

DOCKED: USER Estimated Free Energy of Binding = +0.46 kcal/mol [=(1)+(2)+(3)-(4)]

DOCKED: USER

DOCKED: USER (1) Final Intermolecular Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Fixed Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Moving Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER (2) Final Total Internal Energy = -0.14 kcal/mol

DOCKED: USER Internal Energy Ligand = +0.00 kcal/mol

DOCKED: USER Internal Moving-Fixed Receptor = -0.35 kcal/mol

DOCKED: USER Internal Moving-Moving Receptor = +0.21 kcal/mol

DOCKED: USER (3) Torsional Free Energy = +0.60 kcal/mol

DOCKED: USER (4) Unbound System's Energy = +0.00 kcal/mol

CYS23

DOCKED: USER Estimated Free Energy of Binding = +3.10 kcal/mol [=(1)+(2)+(3)-(4)]

DOCKED: USER

DOCKED: USER (1) Final Intermolecular Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Fixed Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Moving Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER (2) Final Total Internal Energy = +2.50 kcal/mol

DOCKED: USER Internal Energy Ligand = +0.00 kcal/mol

DOCKED: USER Internal Moving-Fixed Receptor = +2.37 kcal/mol

DOCKED: USER Internal Moving-Moving Receptor = +0.13 kcal/mol

DOCKED: USER (3) Torsional Free Energy = +0.60 kcal/mol

DOCKED: USER (4) Unbound System's Energy = +0.00 kcal/mol

CYS26

DOCKED: USER Estimated Free Energy of Binding = +4.71 kcal/mol [=(1)+(2)+(3)-(4)]

DOCKED: USER

DOCKED: USER (1) Final Intermolecular Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Fixed Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Moving Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER (2) Final Total Internal Energy = +4.12 kcal/mol

DOCKED: USER Internal Energy Ligand = +0.00 kcal/mol

DOCKED: USER Internal Moving-Fixed Receptor = +3.90 kcal/mol

DOCKED: USER Internal Moving-Moving Receptor = +0.22 kcal/mol

DOCKED: USER (3) Torsional Free Energy = +0.60 kcal/mol

DOCKED: USER (4) Unbound System's Energy = +0.00 kcal/mol

CYS31

DOCKED: USER Estimated Free Energy of Binding = +0.74 kcal/mol [=(1)+(2)+(3)-(4)]

DOCKED: USER

DOCKED: USER (1) Final Intermolecular Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Fixed Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Moving Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER (2) Final Total Internal Energy = +0.14 kcal/mol

DOCKED: USER Internal Energy Ligand = +0.00 kcal/mol

DOCKED: USER Internal Moving-Fixed Receptor = -0.05 kcal/mol

DOCKED: USER Internal Moving-Moving Receptor = +0.20 kcal/mol

DOCKED: USER (3) Torsional Free Energy = +0.60 kcal/mol

DOCKED: USER (4) Unbound System's Energy = +0.00 kcal/mol

CYS34

DOCKED: USER Estimated Free Energy of Binding = +0.36 kcal/mol [=(1)+(2)+(3)-(4)]

DOCKED: USER

DOCKED: USER (1) Final Intermolecular Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Fixed Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Moving Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER (2) Final Total Internal Energy = -0.24 kcal/mol

DOCKED: USER Internal Energy Ligand = +0.00 kcal/mol

DOCKED: USER Internal Moving-Fixed Receptor = -0.46 kcal/mol

DOCKED: USER Internal Moving-Moving Receptor = +0.22 kcal/mol

DOCKED: USER (3) Torsional Free Energy = +0.60 kcal/mol

DOCKED: USER (4) Unbound System's Energy = +0.00 kcal/mol

CYS38

DOCKED: USER Estimated Free Energy of Binding = +1.17 kcal/mol [=(1)+(2)+(3)-(4)]

DOCKED: USER

DOCKED: USER (1) Final Intermolecular Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Fixed Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Moving Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER (2) Final Total Internal Energy = +0.57 kcal/mol

DOCKED: USER Internal Energy Ligand = +0.00 kcal/mol

DOCKED: USER Internal Moving-Fixed Receptor = +0.36 kcal/mol

DOCKED: USER Internal Moving-Moving Receptor = +0.21 kcal/mol

DOCKED: USER (3) Torsional Free Energy = +0.60 kcal/mol

DOCKED: USER (4) Unbound System's Energy = +0.00 kcal/mol

CYS40

DOCKED: USER Estimated Free Energy of Binding = +0.52 kcal/mol [=(1)+(2)+(3)-(4)]

DOCKED: USER

DOCKED: USER (1) Final Intermolecular Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Fixed Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Moving Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER (2) Final Total Internal Energy = -0.08 kcal/mol

DOCKED: USER Internal Energy Ligand = +0.00 kcal/mol

DOCKED: USER Internal Moving-Fixed Receptor = -0.39 kcal/mol

DOCKED: USER Internal Moving-Moving Receptor = +0.31 kcal/mol

DOCKED: USER (3) Torsional Free Energy = +0.60 kcal/mol

DOCKED: USER (4) Unbound System's Energy = +0.00 kcal/mol

CYS46

DOCKED: USER Estimated Free Energy of Binding = +2.74 kcal/mol [=(1)+(2)+(3)-(4)]

DOCKED: USER

DOCKED: USER (1) Final Intermolecular Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Fixed Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Moving Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER (2) Final Total Internal Energy = +2.14 kcal/mol

DOCKED: USER Internal Energy Ligand = +0.00 kcal/mol

DOCKED: USER Internal Moving-Fixed Receptor = +2.01 kcal/mol

DOCKED: USER Internal Moving-Moving Receptor = +0.13 kcal/mol

DOCKED: USER (3) Torsional Free Energy = +0.60 kcal/mol

DOCKED: USER (4) Unbound System's Energy = +0.00 kcal/mol

CYS50

DOCKED: USER Estimated Free Energy of Binding = +0.96 kcal/mol [=(1)+(2)+(3)-(4)]

DOCKED: USER

DOCKED: USER (1) Final Intermolecular Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Fixed Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Moving Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER (2) Final Total Internal Energy = +0.36 kcal/mol

DOCKED: USER Internal Energy Ligand = +0.00 kcal/mol

DOCKED: USER Internal Moving-Fixed Receptor = -0.01 kcal/mol

DOCKED: USER Internal Moving-Moving Receptor = +0.37 kcal/mol

DOCKED: USER (3) Torsional Free Energy = +0.60 kcal/mol

DOCKED: USER (4) Unbound System's Energy = +0.00 kcal/mol

CYS54

DOCKED: USER Estimated Free Energy of Binding = +67.28 kcal/mol [=(1)+(2)+(3)-(4)]

DOCKED: USER

DOCKED: USER (1) Final Intermolecular Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Fixed Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Moving Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER (2) Final Total Internal Energy = +66.99 kcal/mol

DOCKED: USER Internal Energy Ligand = +0.00 kcal/mol

DOCKED: USER Internal Moving-Fixed Receptor = +66.99 kcal/mol

DOCKED: USER Internal Moving-Moving Receptor = +0.00 kcal/mol

DOCKED: USER (3) Torsional Free Energy = +0.30 kcal/mol

DOCKED: USER (4) Unbound System's Energy = +0.00 kcal/mol

CYS57

DOCKED: USER Estimated Free Energy of Binding = +0.64 kcal/mol [=(1)+(2)+(3)-(4)]

DOCKED: USER

DOCKED: USER (1) Final Intermolecular Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Fixed Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Moving Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER (2) Final Total Internal Energy = +0.04 kcal/mol

DOCKED: USER Internal Energy Ligand = +0.00 kcal/mol

DOCKED: USER Internal Moving-Fixed Receptor = -0.13 kcal/mol

DOCKED: USER Internal Moving-Moving Receptor = +0.18 kcal/mol

DOCKED: USER (3) Torsional Free Energy = +0.60 kcal/mol

DOCKED: USER (4) Unbound System's Energy = +0.00 kcal/mol

S.13.5 *P. fluorescens*

CYS6

DOCKED: USER Estimated Free Energy of Binding = +0.99 kcal/mol [=(1)+(2)+(3)-(4)]

DOCKED: USER

DOCKED: USER (1) Final Intermolecular Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Fixed Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Moving Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER (2) Final Total Internal Energy = +0.39 kcal/mol

DOCKED: USER Internal Energy Ligand = +0.00 kcal/mol

DOCKED: USER Internal Moving-Fixed Receptor = +0.17 kcal/mol

DOCKED: USER Internal Moving-Moving Receptor = +0.22 kcal/mol

DOCKED: USER (3) Torsional Free Energy = +0.60 kcal/mol

DOCKED: USER (4) Unbound System's Energy = +0.00 kcal/mol

CYS8

DOCKED: USER Estimated Free Energy of Binding = +0.04 kcal/mol [=(1)+(2)+(3)-(4)]

DOCKED: USER

DOCKED: USER (1) Final Intermolecular Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Fixed Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Moving Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER (2) Final Total Internal Energy = -0.56 kcal/mol

DOCKED: USER Internal Energy Ligand = +0.00 kcal/mol

DOCKED: USER Internal Moving-Fixed Receptor = -0.93 kcal/mol

DOCKED: USER Internal Moving-Moving Receptor = +0.37 kcal/mol

DOCKED: USER (3) Torsional Free Energy = +0.60 kcal/mol

DOCKED: USER (4) Unbound System's Energy = +0.00 kcal/mol

CYS11

DOCKED: USER Estimated Free Energy of Binding = +1.05 kcal/mol [=(1)+(2)+(3)-(4)]

DOCKED: USER

DOCKED: USER (1) Final Intermolecular Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Fixed Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Moving Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER (2) Final Total Internal Energy = +0.46 kcal/mol

DOCKED: USER Internal Energy Ligand = +0.00 kcal/mol

DOCKED: USER Internal Moving-Fixed Receptor = +0.30 kcal/mol

DOCKED: USER Internal Moving-Moving Receptor = +0.16 kcal/mol

DOCKED: USER (3) Torsional Free Energy = +0.60 kcal/mol

DOCKED: USER (4) Unbound System's Energy = +0.00 kcal/mol

CYS13

DOCKED: USER Estimated Free Energy of Binding = +0.39 kcal/mol [=(1)+(2)+(3)-(4)]

DOCKED: USER

DOCKED: USER (1) Final Intermolecular Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Fixed Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Moving Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER (2) Final Total Internal Energy = -0.21 kcal/mol

DOCKED: USER Internal Energy Ligand = +0.00 kcal/mol

DOCKED: USER Internal Moving-Fixed Receptor = -0.52 kcal/mol

DOCKED: USER Internal Moving-Moving Receptor = +0.32 kcal/mol

DOCKED: USER (3) Torsional Free Energy = +0.60 kcal/mol

DOCKED: USER (4) Unbound System's Energy = +0.00 kcal/mol

CYS29

DOCKED: USER Estimated Free Energy of Binding = +0.32 kcal/mol [=(1)+(2)+(3)-(4)]

DOCKED: USER

DOCKED: USER (1) Final Intermolecular Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Fixed Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Moving Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER (2) Final Total Internal Energy = -0.28 kcal/mol

DOCKED: USER Internal Energy Ligand = +0.00 kcal/mol

DOCKED: USER Internal Moving-Fixed Receptor = -0.53 kcal/mol

DOCKED: USER Internal Moving-Moving Receptor = +0.25 kcal/mol

DOCKED: USER (3) Torsional Free Energy = +0.60 kcal/mol

DOCKED: USER (4) Unbound System's Energy = +0.00 kcal/mol

CYS33

DOCKED: USER Estimated Free Energy of Binding = +0.14 kcal/mol [=(1)+(2)+(3)-(4)]

DOCKED: USER

DOCKED: USER (1) Final Intermolecular Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Fixed Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Moving Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER (2) Final Total Internal Energy = -0.45 kcal/mol

DOCKED: USER Internal Energy Ligand = +0.00 kcal/mol

DOCKED: USER Internal Moving-Fixed Receptor = -0.68 kcal/mol

DOCKED: USER Internal Moving-Moving Receptor = +0.23 kcal/mol

DOCKED: USER (3) Torsional Free Energy = +0.60 kcal/mol

DOCKED: USER (4) Unbound System's Energy = +0.00 kcal/mol

CYS43

DOCKED: USER Estimated Free Energy of Binding = +0.26 kcal/mol [=(1)+(2)+(3)-(4)]

DOCKED: USER

DOCKED: USER (1) Final Intermolecular Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Fixed Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Moving Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER (2) Final Total Internal Energy = -0.33 kcal/mol

DOCKED: USER Internal Energy Ligand = +0.00 kcal/mol

DOCKED: USER Internal Moving-Fixed Receptor = -0.62 kcal/mol

DOCKED: USER Internal Moving-Moving Receptor = +0.28 kcal/mol

DOCKED: USER (3) Torsional Free Energy = +0.60 kcal/mol

DOCKED: USER (4) Unbound System's Energy = +0.00 kcal/mol

CYS48

DOCKED: USER Estimated Free Energy of Binding = +0.01 kcal/mol [=(1)+(2)+(3)-(4)]

DOCKED: USER

DOCKED: USER (1) Final Intermolecular Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Fixed Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Moving Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER (2) Final Total Internal Energy = -0.58 kcal/mol

DOCKED: USER Internal Energy Ligand = +0.00 kcal/mol

DOCKED: USER Internal Moving-Fixed Receptor = -0.86 kcal/mol

DOCKED: USER Internal Moving-Moving Receptor = +0.28 kcal/mol

DOCKED: USER (3) Torsional Free Energy = +0.60 kcal/mol

DOCKED: USER (4) Unbound System's Energy = +0.00 kcal/mol

CYS50

DOCKED: USER Estimated Free Energy of Binding = +1.30 kcal/mol [=(1)+(2)+(3)-(4)]

DOCKED: USER

DOCKED: USER (1) Final Intermolecular Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Fixed Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Moving Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER (2) Final Total Internal Energy = +0.71 kcal/mol

DOCKED: USER Internal Energy Ligand = +0.00 kcal/mol

DOCKED: USER Internal Moving-Fixed Receptor = +0.20 kcal/mol

DOCKED: USER Internal Moving-Moving Receptor = +0.51 kcal/mol

DOCKED: USER (3) Torsional Free Energy = +0.60 kcal/mol

DOCKED: USER (4) Unbound System's Energy = +0.00 kcal/mol

S.13.6 *S. cerevisiae*

CYS22

DOCKED: USER Estimated Free Energy of Binding = +0.37 kcal/mol [=(1)+(2)+(3)-(4)]

DOCKED: USER

DOCKED: USER (1) Final Intermolecular Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Fixed Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Moving Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER (2) Final Total Internal Energy = -0.22 kcal/mol

DOCKED: USER Internal Energy Ligand = +0.00 kcal/mol

DOCKED: USER Internal Moving-Fixed Receptor = -0.35 kcal/mol

DOCKED: USER Internal Moving-Moving Receptor = +0.13 kcal/mol

DOCKED: USER (3) Torsional Free Energy = +0.60 kcal/mol

DOCKED: USER (4) Unbound System's Energy = +0.00 kcal/mol

CYS28

DOCKED: USER Estimated Free Energy of Binding = +0.48 kcal/mol [=(1)+(2)+(3)-(4)]

DOCKED: USER

DOCKED: USER (1) Final Intermolecular Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Fixed Receptor = +0.00 kcal/mol
DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol
DOCKED: USER Electrostatic Energy = +0.00 kcal/mol
DOCKED: USER Moving Ligand-Moving Receptor = +0.00 kcal/mol
DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol
DOCKED: USER Electrostatic Energy = +0.00 kcal/mol
DOCKED: USER (2) Final Total Internal Energy = -0.12 kcal/mol
DOCKED: USER Internal Energy Ligand = +0.00 kcal/mol
DOCKED: USER Internal Moving-Fixed Receptor = -0.29 kcal/mol
DOCKED: USER Internal Moving-Moving Receptor = +0.17 kcal/mol
DOCKED: USER (3) Torsional Free Energy = +0.60 kcal/mol
DOCKED: USER (4) Unbound System's Energy = +0.00 kcal/mol

CYS32

DOCKED: USER Estimated Free Energy of Binding = +0.41 kcal/mol [=(1)+(2)+(3)-(4)]
DOCKED: USER
DOCKED: USER (1) Final Intermolecular Energy = +0.00 kcal/mol
DOCKED: USER Moving Ligand-Fixed Receptor = +0.00 kcal/mol
DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol
DOCKED: USER Electrostatic Energy = +0.00 kcal/mol
DOCKED: USER Moving Ligand-Moving Receptor = +0.00 kcal/mol
DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol
DOCKED: USER Electrostatic Energy = +0.00 kcal/mol
DOCKED: USER (2) Final Total Internal Energy = -0.19 kcal/mol
DOCKED: USER Internal Energy Ligand = +0.00 kcal/mol
DOCKED: USER Internal Moving-Fixed Receptor = -0.40 kcal/mol
DOCKED: USER Internal Moving-Moving Receptor = +0.21 kcal/mol
DOCKED: USER (3) Torsional Free Energy = +0.60 kcal/mol
DOCKED: USER (4) Unbound System's Energy = +0.00 kcal/mol

CYS34

DOCKED: USER Estimated Free Energy of Binding = +1.09 kcal/mol [=(1)+(2)+(3)-(4)]
DOCKED: USER
DOCKED: USER (1) Final Intermolecular Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Fixed Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Moving Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER (2) Final Total Internal Energy = +0.50 kcal/mol

DOCKED: USER Internal Energy Ligand = +0.00 kcal/mol

DOCKED: USER Internal Moving-Fixed Receptor = +0.28 kcal/mol

DOCKED: USER Internal Moving-Moving Receptor = +0.21 kcal/mol

DOCKED: USER (3) Torsional Free Energy = +0.60 kcal/mol

DOCKED: USER (4) Unbound System's Energy = +0.00 kcal/mol

CYS38

DOCKED: USER Estimated Free Energy of Binding = -0.01 kcal/mol [=(1)+(2)+(3)-(4)]

DOCKED: USER Estimated Inhibition Constant, Ki = 984.92 mM (millimolar) [Temperature = 298.15 K]

DOCKED: USER

DOCKED: USER (1) Final Intermolecular Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Fixed Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Moving Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER (2) Final Total Internal Energy = -0.61 kcal/mol

DOCKED: USER Internal Energy Ligand = +0.00 kcal/mol

DOCKED: USER Internal Moving-Fixed Receptor = -0.83 kcal/mol

DOCKED: USER Internal Moving-Moving Receptor = +0.22 kcal/mol

DOCKED: USER (3) Torsional Free Energy = +0.60 kcal/mol

CYS44

DOCKED: USER Estimated Free Energy of Binding = +0.27 kcal/mol [=(1)+(2)+(3)-(4)]

DOCKED: USER

DOCKED: USER (1) Final Intermolecular Energy = +0.00 kcal/mol
DOCKED: USER Moving Ligand-Fixed Receptor = +0.00 kcal/mol
DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol
DOCKED: USER Electrostatic Energy = +0.00 kcal/mol
DOCKED: USER Moving Ligand-Moving Receptor = +0.00 kcal/mol
DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol
DOCKED: USER Electrostatic Energy = +0.00 kcal/mol
DOCKED: USER (2) Final Total Internal Energy = -0.33 kcal/mol
DOCKED: USER Internal Energy Ligand = +0.00 kcal/mol
DOCKED: USER Internal Moving-Fixed Receptor = -0.45 kcal/mol
DOCKED: USER Internal Moving-Moving Receptor = +0.12 kcal/mol
DOCKED: USER (3) Torsional Free Energy = +0.60 kcal/mol
DOCKED: USER (4) Unbound System's Energy = +0.00 kcal/mol

CYS57

DOCKED: USER Estimated Free Energy of Binding = +0.74 kcal/mol [=(1)+(2)+(3)-(4)]
DOCKED: USER
DOCKED: USER (1) Final Intermolecular Energy = +0.00 kcal/mol
DOCKED: USER Moving Ligand-Fixed Receptor = +0.00 kcal/mol
DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol
DOCKED: USER Electrostatic Energy = +0.00 kcal/mol
DOCKED: USER Moving Ligand-Moving Receptor = +0.00 kcal/mol
DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol
DOCKED: USER Electrostatic Energy = +0.00 kcal/mol
DOCKED: USER (2) Final Total Internal Energy = +0.15 kcal/mol
DOCKED: USER Internal Energy Ligand = +0.00 kcal/mol
DOCKED: USER Internal Moving-Fixed Receptor = -0.15 kcal/mol
DOCKED: USER Internal Moving-Moving Receptor = +0.29 kcal/mol
DOCKED: USER (3) Torsional Free Energy = +0.60 kcal/mol
DOCKED: USER (4) Unbound System's Energy = +0.00 kcal/mol

CYS58

DOCKED: USER Estimated Free Energy of Binding = +0.21 kcal/mol [=(1)+(2)+(3)-(4)]
DOCKED: USER

DOCKED: USER (1) Final Intermolecular Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Fixed Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER Moving Ligand-Moving Receptor = +0.00 kcal/mol

DOCKED: USER vdW + Hbond + desolv Energy = +0.00 kcal/mol

DOCKED: USER Electrostatic Energy = +0.00 kcal/mol

DOCKED: USER (2) Final Total Internal Energy = -0.39 kcal/mol

DOCKED: USER Internal Energy Ligand = +0.00 kcal/mol

DOCKED: USER Internal Moving-Fixed Receptor = -0.68 kcal/mol

DOCKED: USER Internal Moving-Moving Receptor = +0.29 kcal/mol

DOCKED: USER (3) Torsional Free Energy = +0.60 kcal/mol

DOCKED: USER (4) Unbound System's Energy = +0.00 kcal/mol

S.14 Reagent List:

- dNTP mix (10 µM each) - QIAGEN

Enzymes:

- BsaI - NEB
- BsmBI - NEB
- T4 ligase - NEB
- EcoRI (Heat Inactivated)- NEB
- Gotaq polymerase - Promega
- Taq polymerase - NEB

Enzyme Buffers:

- Gotaq - Promega
- rCutSmart - NEB
- ThermoPol - NEB