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SUPPLEMENTARY TABLES

2 **Table S1.** Details of the open reading frames (ORFs) identified as metal uptake ABC transporter proteins from the transporter class 3.A.1
3 extracted from the TransportDB 2.0¹ and Structural-Biological Whole Cell Project (<http://www.thermus.org>) databases.

S. No.	ORF number	UniProt ID	⁺ Protein name	*(SP) Protein length	Cellular location	**ABC subunit
1.	TTHA0596	Q5SKP7	ABC transporter solute-binding protein	(1-21) 281	Periplasm	SBP
2.	TTHA0597	Q5SKP6	Uncharacterized protein	(-) 553	-	-
3.	TTHA0598	Q5SKP5	Putative transport integral membrane protein (chloride channel)	(-) 481	Membrane	TMD
4.	TTHA1628	Q5SHV2	Iron ABC transporter, periplasmic iron- binding protein	(-) 330	Periplasm	SBP
5.	TTHA1629	Q5SHV1	Iron ABC transporter, permease protein	(-) 516	Membrane	TMD
6.	TTHA1630	Q5SHV0	Iron ABC transporter, ATP-binding protein	(-) 350	Cytosol	NBD
7.	TTHB218	Q53VW1	ABC transporter, ATP-binding protein	(-) 258	Cytosol	NBD
8.	TTHB219	Q53VW0	Hemin ABC transporter, permease protein	(-) 341	Membrane	TMD
9.	TTHB220	Q53VV9	Hemin ABC transporter, periplasmic hemin- binding protein	(1-36) 301	Periplasm	SBP

10.	TTHA0723	Q5SKC0	Iron(III) ABC transporter, solute-binding protein	(1-18) 265	Periplasm	SBP
11.	TTHA0746	Q5SKA2	Iron ABC transporter, substrate-binding protein	(1-22) 284	Periplasm	SBP
12.	TTHA0747	Q5SKA1	Iron ABC transporter, permease protein	(-) 342	Membrane	TMD
13.	TTHA0748	Q5SKA0	Iron ABC transporter, ATP-binding protein	(-) 250	Cytosol	NBD
14.	TTHB175	Q53VZ4	ABC transporter, ATP-binding protein	(-) 368	Cytosol	NBD
15.	TTHB176	Q53VZ3	Putative iron ABC transporter, permease protein	(-) 565	Membrane	TMD
16.	TTHB177	Q53VZ2	Iron ABC transporter, periplasmic iron-binding protein	(1-18) 358	Periplasm	SBP
17.	TTHA0069	Q5SM74	ABC transporter, periplasmic binding protein	(1-46) 293	Periplasm	SBP
18.	TTHA0070	Q5SM73	ABC transporter permease protein	(-) 211	Membrane	TMD
19.	TTHA0071	Q5SM72	ABC-transporter, ATP-binding subunit	(-) 224	Cytosol	NBD
20.	TTHA0715	Q5SKC8	ABC transporter ATP-binding protein	(-) 339	Cytosol	NBD
21.	TTHA0716	Q5SKC7	Molybdenum ABC transporter, permease protein	(-) 224	Membrane	TMD

22.	TTHA0717	Q5SKC6	Molybdenum ABC transporter molybdate-binding protein	(1-19) 289	Periplasm	SBP
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4 ⁺ Protein names are according to UniProtKB database.

5 * SP: Signal peptide.

6 ** SBP: Solute (substrate)-binding protein; TMD: Transmembrane domain; NBD: Nucleotide-binding domain.

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8 **Table S2.** Protein annotation and UniProt ids of the ORFs interacting with the respective metal binding ABC transporter protein obtained
9 in the interactome map analysis.

ORF number	*ORF number of the interacting protein	UniProt ID of the interacting protein	⁺ Protein name
TTHA0723	TTHA0747	Q5SKA1	Iron ABC transporter permease
	TTHA0748	Q5SKA0	Iron ABC transporter ATP-binding protein
	TTHA0722	Q5SKC1	Histidinol dehydrogenase
	TTHA1534	Q5SI46	Ribonuclease II family protein
	TTHA0910	Q5SJU8	Ribonuclease R
	TTHA0724	Q5SKB9	Serine protease
	TTHA0721	Q5SKC2	Hypothetical protein

	TTHA0720	Q5SKC3	Hypothetical protein
	TTHA1628	Q5SHV2	Iron ABC transporter substrate-binding protein
	TTHA0683	Q5SKG0	TolR-type transport protein
TTHA0746	TTHA0748	Q5SKA0	Iron ABC transporter ATP-binding protein
	TTHA0747	Q5SKA1	Iron ABC transporter permease
	TTHA0749	Q5SK99	Hypothetical protein
	TTHA1534	Q5SI46	Ribonuclease II family protein
	TTHA0910	Q5SJU8	Ribonuclease R
	TTHA0750	Q5SK98	3-oxoacyl-ACP reductase
	TTHA1628	Q5SHV2	Iron ABC transporter substrate-binding protein
	TTHA0683	Q5SKG0	TolR-type transport protein
	TTHA0684	Q5SKF9	TolQ-type transport protein
TTHA0069 and TTHA0717	TTHA0716	Q5SKC7	Molybdenum ABC transporter, permease protein
	TTHA0070	Q5SM73	ABC transporter permease protein
	TTHA0071	Q5SM72	ABC-transporter, ATP-binding subunit
	TTHA0715	Q5SKC8	ABC transporter ATP-binding protein
	TTHA1159	Q5SJ55	Amino acid ABC transporter, ATP-binding protein

	TTHA1630	Q5SHV0	Iron ABC transporter, ATP-binding protein
	TTHA1424	Q5SIF0	ABC transporter ATP-binding protein
	TTHA0975	Q5SJN3	Sugar ABC transporter, ATP-binding protein
	TTHA0579	Q5SKR4	Sugar ABC transporter, ATP-binding protein
	TTHA0380	Q5SLB3	Aldehyde: ferredoxin oxidoreductase

10 * Only the top 10 interacting proteins sorted by the best confidence score in the decreasing order are provided.

11 + Protein names are according to UniProtKB database.

12

13 **Table S3.** Details of the template protein used for model building of each SBP.

ORF number	Template	PDB ID of template	Microorganism	Protein name	Bound Ligand
TTHB220	RhuT	5GJ3	<i>Roseiflexus sp.</i>	<i>RsRhuT</i>	Heme
TTHA0723	BhuT	5Y8A	<i>Burkholderia cenocepacia</i>	<i>BcBhuT</i>	Heme
TTHA0746	ShuT	2R7A	<i>Shigella dysenteriae</i>	<i>SdShuT</i>	Heme
TTHB177	Atu	3C9H	<i>Agrobacterium fabrum</i>	<i>AfAtu</i>	Mg ²⁺ -citrate
TTHA0069	TupA	3LR1	<i>Geobacter sulfurreducens</i>	<i>GsTupA</i>	Tungsten (W ⁶⁺) ion
TTHA0717	ModA	1ATG	<i>Azotobacter vinelandii</i>	<i>AvMoDA</i>	Tungstate (WoO ₄ ²⁻)

14

15 **Table S4.** Top 20 structural homologs (ranked by the Z-score) of the selected proteins obtained using the web server Dali.²

ORF number	PDB ID	UniProt ID	⁺ Protein name	Bound ligand	**Z- score	RMSD (Å)	LALI	NRES	SI (%)
TTHB220	5GJ3	A5UZ69	Periplasmic binding protein	Heme	42.0	0.5	260	270	49
	5Y8B			-	38.9	1.1	258	263	49
	5GIZ	B4EKB3	Putative hemin transport system, substrate-binding protein	-	33.0	1.8	260	271	37
	3MD9	Q56991	Hemin-binding periplasmic protein HmuT	-	32.9	1.5	252	253	34
	5Y8A	B4EKB3	Putative hemin transport system, substrate-binding protein	Heme	32.9	1.8	260	268	37
	3NU1	A0A0E1N WS3	Hemin-binding periplasmic protein	Heme	32.8	1.7	253	254	34
	5Y89	B4EKB3	Putative hemin transport system, substrate-binding protein	Heme	32.3	2.3	260	267	37
	2R7A	O70018	Uncharacterized protein	Heme	30.1	2.0	252	255	36
	2RG7			-	29.6	1.8	250	255	36

	5AZ3	Q8NTB8	ABC-type transporter, periplasmic component	Heme	28.5	2.3	254	309	35
	2R79	O68879	Periplasmic binding protein	Heme	28.2	2.0	253	279	30
	5KHL	A0A0H3A E70	Hemin ABC transporter, periplasmic hemin-binding protein HutB	-	28.0	2.1	251	257	30
	4M7O	A0A0H2V HB1	Iron binding protein	-	26.0	3.0	251	258	21
	1N2Z	P37028	Vitamin B12-binding protein	Co- cyanocobalamin	23.2	3.1	242	245	26
	1N4D			-	23.0	2.9	241	244	27
	2Q8Q	Q7A652	High-affinity heme uptake system protein IsdE	Heme	22.8	3.1	241	258	21
	5JOQ	Q7AP55	Lmo2184 protein	-	22.7	3.5	246	258	22
	4HN9	C4Z2B5	Iron complex transport system substrate-binding protein	-	22.2	2.5	245	323	20

	4N01	D1BNS2	Periplasmic binding protein	-	21.7	2.9	247	296	17
	3PSH	P44206	Uncharacterized protein HI_1472	Molybdate	22.7	3.3	261	326	24
TTHA0723	5Y8A	B4EKB3	Putative hemin transport system, substrate-binding protein	Heme	34.2	1.1	240	271	24
	5GIZ			-	33.7	1.2	240	271	23
	5Y89			Heme	32.3	1.8	241	267	23
	3MD9	Q56991	Hemin-binding periplasmic protein HmuT	-	30.5	1.7	239	253	22
	3NU1	A0A0E1N WS3	Hemin-binding periplasmic protein	Heme	30.2	2.1	240	254	22
	5Y8B	A5UZ69	Periplasmic binding protein	-	29.2	1.8	241	263	22
	5GJ3			Heme	29.1	1.8	241	270	23
	2R7A	O70018	Uncharacterized protein	Heme	26.9	2.0	233	255	21
	2RG7			-	26.4	2.1	233	255	21
	2R79	O68879	Periplasmic binding protein	Heme	24.3	2.3	233	279	21
	5KHL	A0A0H3A E70	Hemin ABC transporter, periplasmic hemin-binding	-	24.2	2.4	236	257	20

			protein HutB						
	1N4A	P37028	Vitamin B12-binding protein	Co-cyanocobalamin	23.9	2.6	234	244	25
	5AZ3	Q8NTB8	ABC-type transporter, periplasmic component	Heme	23.2	2.4	236	309	17
	4FI3	P06609	Vitamin B12 import system permease protein BtuC	-	23.1	2.7	233	245	24
	4M7O	A0A0H2V HB1	Iron binding protein	-	23.0	2.9	235	258	25
	5M29	P37028	Vitamin B12-binding protein	Cob(II)inamide	22.7	2.5	220	229	26
	2Q8Q	Q7A652	High-affinity heme uptake system protein IsdE	Heme	20.1	3.0	226	258	19
	5JOQ	Q7AP55	Lmo2184 protein	-	19.9	3.2	231	258	19
	4MLZ	C7R301	Periplasmic binding protein	-	19.7	2.7	236	299	19
	5AD1	Q0P8Q4	Enterochelin uptake periplasmic binding protein	Fe ³⁺	19.5	2.6	231	290	16
TTHA0746	2R7A	O70018	Uncharacterized protein	Heme	29.7	1.8	244	255	25

	2RG7			-	29.6	1.8	244	255	25
	4HN9	C4Z2B5	Iron complex transport system substrate-binding protein	-	29.1	2.1	258	323	21
	5Y8B	A5UZ69	Periplasmic binding protein	-	27.6	1.9	244	263	27
	4M7O	A0A0H2V HB1	Iron-binding protein	-	27.6	2.1	245	258	27
	5GJ3	A5UZ69	Periplasmic binding protein	Heme	27.2	1.9	244	270	27
	5Y8A	B4EKB3	Putative hemin transport system, substrate-binding protein	Heme	27.1	1.9	243	268	23
	2R79	O68879	Periplasmic binding protein	Heme	26.8	2.1	244	279	25
	5GIZ	B4EKB3	Putative hemin transport system, substrate-binding protein	-	26.7	2.1	246	271	22
	3NU1	A0A0E1N WS3	Hemin-binding periplasmic protein	Heme	26.3	2.5	240	254	26
	1N2Z	P37028	Vitamin B12-binding protein	Co- cyanocobalamin	26.2	2.4	238	245	26
	5Y89	B4EKB3	Putative hemin transport system,	Heme	26.1	2.7	243	267	23

			substrate-binding protein						
	3MD9	Q56991	Hemin-binding periplasmic protein HmuT	-	26.1	2.2	240	253	26
	5KHL	A0A0H3A E70	Hemin ABC transporter, periplasmic hemin-binding protein HutB	-	25.9	1.9	243	257	19
	3PSH	P44206	Uncharacterized protein HI_1472	Molybdate	25.3	2.8	258	326	20
	3PSA			Tungstate	25.2	2.8	258	326	20
	5AZ3	Q8NTB8	ABC-type transporter, periplasmic component	Heme	25.0	2.7	256	309	19
	4OVK	D1BR49	Periplasmic binding protein	-	25.0	3.3	259	329	22
	4N01	D1BNS2	Periplasmic binding protein	-	25.0	2.3	253	296	21
	5M29	P37028	Vitamin B12-binding protein	Cob(II)inamide	24.9	2.3	223	229	27
TTHB177	3C9H	Q7CWZ6	ABC transporter, substrate binding protein (Iron)	Mg ²⁺ citrate	53.1	0.7	336	339	35
	4R74	A3N294	ABC-type Fe ³⁺ transport system, periplasmic component	Fructose-6- phosphate	31.0	2.6	303	319	20

	1MRP	P35755	Iron-utilization periplasmic protein	Fe ³⁺ phosphate	27.5	3.0	292	309	14
	2OWT	Q7VXW9	Putative iron binding protein	Fe ³⁺ carbonate	27.5	3.1	290	315	17
	4R6Y	P96062	Putative 2-aminoethyl phosphonate-binding periplasmic protein	*Acetate	27.4	3.1	298	317	18
	1Q35	Q9Z4N6	Iron ABC transporter substrate-binding protein	*Formic acid	26.9	3.3	292	317	16
	2VP1	Q55835	Iron uptake protein A2	Fe ³⁺	26.9	3.2	286	313	19
	1XVY	P21408	Fe(3+)-binding periplasmic protein	*Citric acid	26.6	3.6	291	307	16
	2QRY	P31550	Thiamine-binding periplasmic protein	Thiamin phosphate	26.3	2.8	291	318	16
	3TTM	Q9I6J1	Putrescine-binding periplasmic protein SpuD	Putrescine	25.5	2.9	292	341	15
	1XC1	P17259	Major ferric iron-binding protein	Oxo-zirconium(IV)	25.4	3.6	293	309	16

				cluster					
	1O7T	Q50964	FbpA protein	Metal nanoclusters	25.3	3.7	292	309	16
TTHA0069	3LR1	Q749P2	Tungstate ABC transporter, periplasmic tungstate-binding protein	Tungsten ion	38.1	0.2	224	232	39
	5MY5	Q316W1	ABC transporter periplasmic substrate-binding protein	-	25.5	3.0	229	250	38
	3KN3	Q7M8V9	Putative periplasmic protein	*Citrate	24.9	3.3	225	238	35
	3CVG	J3KFC8	Uncharacterized protein	-	24.8	2.3	225	270	25
	3MUQ	Q87PK2	Uncharacterized protein	-	21.9	5.3	151	233	32
	1AMF	P37329	Molybdate-binding protein ModA	Molybdate	18.7	2.9	207	231	12
	1ATG	Q7SIH2	Binding protein	Tungstate	18.5	3.0	205	231	14
	1SBP	P02906	Sulfate-binding protein	Sulfate ion	17.4	2.9	216	309	11
	4Q8R	A0A0H2Y SI2	Phosphate ABC transporter, phosphate-binding protein	Phosphate ion	17.4	2.8	205	241	18

	5Y2W	P73862	Rubisco operon transcriptional regulator	*2-phosphoglycolic acid	17.3	3.0	198	208	15
	3CFZ	Q58586	Molybdate/tungstate-binding protein WtpA	Tungstate	17.2	3.2	210	289	11
	5UM2	Q8PNN7	ABC transporter sulfate binding protein	Sulfate ion	17.2	2.9	216	316	11
	2ONR	O30142	Molybdate/tungstate-binding protein WtpA	Molybdate	17.1	3.3	213	314	12
	5TED	Q8Y9N7	Lmo0488 protein	Shikimate	17.1	2.7	200	210	11
	4GD5	A0A0H2Y SI2	Phosphate ABC transporter, phosphate-binding protein	Phosphate ion	17.1	2.8	204	243	18
	3FJ7	Q0PBL7	Major antigenic peptide PEB3	L-phospholactate	17.1	3.3	207	231	14
	4JB7	Q9KTQ6	Accessory colonization factor AcfC	D-malate	16.7	3.3	206	233	9
	2FYI	Q47083	HTH-type transcriptional regulator cbl	-	16.7	2.6	195	223	13

	3GLB	P07774	HTH-type transcriptional regulator CatM	*Hexa-2,4-dienedioic acid	16.3	2.8	198	215	16
	2QL3	Q0SFM8	Probable transcriptional regulator, LysR family protein	-	16.3	3.1	194	205	14
TTHA0717	1ATG	Q7SIH2	Binding protein	Tungstate	33.2	1.2	228	231	29
	3GZG	Q8PHA1	Molybdate-binding protein ModA	Molybdate	29.1	1.9	221	232	29
	1WOD	P37329	Molybdate-binding protein ModA	Tungstate	28.8	1.8	224	231	26
	4RXL	Q9KLL7	Molybdenum ABC transporter, periplasmic molybdenum-binding protein	Tungstate	28.7	1.9	223	229	23
	3CFX	Q8TTZ5	Uncharacterized solute-binding protein MA_0280	Tungstate	26.3	2.1	238	293	18
	3CIJ	O30142	Molybdate/tungstate-binding protein WtpA	Tungstate	26.0	2.1	239	291	18
	3CFZ	Q58586	Molybdate/tungstate-binding	Tungstate	25.4	2.2	235	289	20

			protein WtpA						
	3CG1	Q8U4K5	Molybdate/tungstate-binding protein WtpA	Tungstate	25.3	2.1	238	293	16
	3CG3	O57890	Molybdate/tungstate-binding protein WtpA	Tungstate	24.6	2.3	241	315	17
	4KD5	Q18A64	ABC-type transport system, molybdenum-specific extracellular solute-binding protein	-	24.0	3.1	224	229	21
	1SBP	P02906	Sulfate-binding protein	Sulfate ion	22.5	2.7	228	309	14
	5UM2	Q8PNN7	ABC transporter sulfate binding protein	Sulfate ion	22.3	2.6	228	316	15
	3FJM	Q0PBL7	Major antigenic peptide PEB3	Phosphate ion	19.5	3.1	218	231	14
	4R73	A3N294	ABC-type Fe ³⁺ transport system, periplasmic component	Glucose-6- phosphate, Mannose-6- phosphate	19.4	3.3	225	319	14

	3CVG	J3KFC8	Uncharacterized protein	-	19.2	3.6	228	270	11
	3LR1	Q749P2	Tungstate ABC transporter, periplasmic tungstate-binding protein	Tungsten ion	18.8	2.8	210	232	14
	3C9H	Q7CWZ6	ABC transporter, substrate binding protein (Iron)	Mg ²⁺ citrate	18.7	2.9	226	339	12
	2QRY	P31550	Thiamine-binding periplasmic protein	Thiamin phosphate	18.5	3.4	224	309	13
	4JB7	Q9KTQ6	Accessory colonization factor AcfC	D-malate	18.4	3.2	218	233	14
	4Q8R	A0A0H2Y SI2	Phosphate ABC transporter, phosphate-binding protein	Phosphate ion	18.0	3.0	209	241	8

16 ⁺ Protein names are according to UniProtKB database.

17 * These molecules bound at the active site of the protein were present in the crystallization buffer.

18

19 ** Z-score = $[(S(A, B) - m(N)) / (\sigma(N))]$, where S(A, B) = similarity score between protein A and B; m(N) = mean score of average length

20 N; σ = average standard deviation.

21 Abbreviations: RMSD, root mean square deviation; LALI, length of the alignment; NRES, number of residues; SI: sequence identity.

22

23 **Table S5.** Details of the proteins used for generating the structure-based distance tree for SBP classification.

Cluster	PDB ID	UniProt ID	Protein name	Organism	Proposed ligand(s)
A-I	1PQ4	P73085	ZntC	<i>Synechocystis sp.</i>	Zinc
A-I	1TOA	P96116	TroA	<i>Treponema pallidum</i>	Zinc
A-I	1XVL	Q79EF9	MntC	<i>Synechocystis sp.</i>	Manganese
A-I	3MFQ	A4VY63	TroA	<i>Streptococcus suis</i>	Zinc
A-I	4K3V	D9RF12	MntC	<i>Staphylococcus aureus</i>	Manganese
A-II	2R7A	O70018	ShuT	<i>Shigella dysenteriae</i>	Heme
A-II	2R79	O68879	PhuT	<i>Pseudomonas aeruginosa</i>	Heme
A-II	3EIW	A0A0H3JM89	HtsA	<i>Staphylococcus aureus</i>	Staphyloferrin A
A-II	3NU1	A0A0E1NWS3	HmuT	<i>Yersinia pestis</i>	Heme
A-II	4HN9	C4Z2B5	N.D.	<i>Eubacterium eligens</i>	Iron complex
A-II	5AZ3	Q8NTB8	HmuT	<i>Corynebacterium glutamicum</i>	Heme
A-II	5Y8A	B4EKB3	BhuT	<i>Burkholderia cenocepacia</i>	Heme
B	4F11	O75899	GABBR2	<i>Homo sapiens</i>	GABA

B	4MQE	Q9UBS5	GABBR1	<i>Homo sapiens</i>	GABA
B-I	1TJY	Q8ZKQ1	IsrB	<i>Salmonella typhimurium</i>	Autoinducer2
B-I	3D02	A6THR5	N.D.	<i>Klebsiella pneumoniae</i>	Sugar
B-I	3T95	Q74PW2	IsrB	<i>Yersinia pestis</i>	Autoinducer 2
B-I	4WZZ	A9KIX1	N.D.	<i>Clostridium phytofermentans</i>	Sugar
B-II	3IP5	Q7CX36	Atu2422	<i>Agrobacterium fabrum</i>	Amino acids (GABA)
B-II	3TD9	Q9X0L9	LivK	<i>Thermotoga maritima</i>	Branched-chain amino acids
B-II	4GNR	J9PBT7	N.D.	<i>Streptococcus pneumoniae</i>	Branched-chain amino acids
B-II	4N0Q	Q8YEE8	N.D.	<i>Brucella melitensis</i>	Leucine/ Isoleucine/ Valine
B-II	4NQR	Q3MFZ5	N.D.	<i>Anabaena variabilis</i>	Amino acid, amide
B-III	3SG0	Q2IR47	N.D.	<i>Rhodopseudomonas palustris</i>	Aromatic compounds
B-III	3UK0	Q139W5	N.D.	<i>Rhodopseudomonas palustris</i>	Aromatic compounds
B-III	4EVS	Q6NB45	N.D.	<i>Rhodopseudomonas palustris</i>	Aromatic compounds
B-III	4EY3	Q13AR6	N.D.	<i>Rhodopseudomonas palustris</i>	N.D.

B-III	4F06	Q2IXT5	N.D.	<i>Rhodopseudomonas palustris</i>	N.D.
B-IV	1DP4	P18910	Npr1	<i>Rattus norvegicus</i>	Natiuretic peptides
B-IV	1JDN	P17342	NPR3	<i>Homo sapiens</i>	Natiuretic peptides
B-IV	1YK0	P01160	NPPA	<i>Homo sapiens</i>	Natiuretic peptides
B-V	1EWK	P23385	Grm1	<i>Rattus norvegicus</i>	Glutamate
B-V	2E4U	P31422	Grm3	<i>Rattus norvegicus</i>	Glutamate
B-V	2E4Z	P35400	Grm7	<i>Rattus norvegicus</i>	Glutamate
B-V	3LMK	P41594	GRM5	<i>Homo sapiens</i>	Glutamate
B-V	3MQ4	Q14831	GRM7	<i>Homo sapiens</i>	Glutamate
B-V	4XAQ	Q14416	GRM2	<i>Homo sapiens</i>	Glutamate
C	1DPP	P23847	DppA	<i>Escherichia coli</i>	Dipeptide
C	1XOC	P42061	AppA	<i>Bacillus subtilis</i>	Oligopeptide
C	2D5W	Q5SHU6	N.D.	<i>Thermus thermophilus</i>	Peptide
C	3M8U	B8F653	HbpA	<i>Haemophilus parasuis</i>	Heme
C	5F1Q	A0A0H2YM47	N.D.	<i>Yersinia pestis</i>	Dipeptide
D-I	2B3B	Q72KX2	GGBP	<i>Thermus thermophilus</i>	Glucose
D-I	3O06	Q27GR2	AcbH	<i>Actinoplanes sp.</i>	Galactose

D-I	3ZKK	A0A0J9X1B4	N.D.	<i>Bifidobacterium animalis</i>	Sugar
D-I	4G68	J9PBT4	N.D.	<i>Caldanaerobius</i>	N.D.
D-I	4R2B	A6X5L9	N.D.	<i>Ochrobactrum anthropi</i>	Sugar
D-II	1A99	P31133	PotF	<i>Escherichia coli</i>	Putrescine
D-II	1POT	P0AFK9	PotD	<i>Escherichia coli</i>	Spermidine, Putrescine
D-II	3RPW	Q6N0W2	N.D.	<i>Rhodopseudomonas palustris</i>	N.D.
D-II	3TTM	Q9I6J1	SpuD	<i>Pseudomonas aeruginosa</i>	Putrescine
D-II	4GL0	Q8Y8T4	N.D.	<i>Listeria monocytogenes</i>	Spermidine, Putrescine
D-III(A)	1ATG	Q7SIH2	ModA	<i>Azotobacter vinelandii</i>	Tungstate (VI)
D-III(A)	1WOD	P37329	ModA	<i>Escherichia coli</i>	Molybdate
D-III(A)	2H5Y	Q8PHA1	ModA	<i>Xanthomonas axonopodis</i>	Molybdate
D-III(A)	3C9H	Q7CWZ6	Atu	<i>Agrobacterium fabrum</i>	Iron
D-III(A)	3CVG	J3KFC8	N.D.	<i>Coccidioides immitis</i>	Metal
D-III(A)	3LR1	Q749P2	TupA	<i>Geobacter sulfurreducens</i>	Tungstate
D-III(A)	4RXL	Q9KLL7	N.D.	<i>Vibrio cholerae</i>	Molybdate
D-III(B)	2ONR	O30142	WtpA/ ModA	<i>Archaeoglobus fulgidus</i>	Molybdate/ Tungstate

D-III(B)	3CFX	Q8TTZ5	ModA	<i>Methanosarcina acetivorans</i>	Tungstate
D-III(B)	3CFZ	Q58586	WtpA	<i>Methanocaldococcus jannaschii</i>	Molybdate/ Tungstate
D-III(B)	3CG1	Q8U4K5	WtpA	<i>Pyrococcus furiosus</i>	Molybdate/ Tungstate
D-III(B)	3CG3	O57890	WtpA	<i>Pyrococcus horikoshii</i>	Molybdate/ Tungstate
D-IV	1MRP	P35755	FbpA	<i>Haemophilus influenzae</i>	Iron
D-IV	1SI0	Q9Z4N6	FbpA	<i>Mannheimia haemolytica</i>	Iron
D-IV	1XVX	A1JLH5	YfuA	<i>Yersinia enterocolitica</i>	Iron
D-IV	1Y4T	Q0PBW4	CfbpA	<i>Campylobacter jejuni</i>	Iron
D-IV	2PT2	P72827	FutA1	<i>Synechocystis sp.</i>	Iron
E-I	4MX6	Q8ECK4	DctP	<i>Shewanella oneidensis</i>	Succinate
E-I	4NF0	Q9HVVH5	N.D.	<i>Pseudomonas aeruginosa</i>	L-maltate
E-I	4O7M	A3QCW5	N.D.	<i>Shewanella loihica</i>	L-malate
E-I	4O94	Q2IUT5	N.D.	<i>Rhodopseudomonas palustris</i>	Succinate
E-I	4OVS	D1AZL7	N.D.	<i>Sulfurospirillum deleyianum</i>	Succinate
E-II	2DVZ	Q7W0A0	BugE	<i>Bordetella pertussis</i>	Glutamate
E-II	2F5X	Q7VTS1	BugD	<i>Bordetella pertussis</i>	Aspartate

E-II	2QPQ	Q7W019	Bug27	<i>Bordetella pertussis</i>	N.D.
F-I	2G29	P73452	NrtA	<i>Synechocystis sp.</i>	Nitrate
F-I	2I48	Q55460	CmpA	<i>Synechocystis sp.</i>	Bicarbonate
F-I	2X26	P75853	SsuA	<i>Escherichia coli</i>	Aliphatic sulfonate
F-I	3E4R	Q8PHQ1	SsuA	<i>Xanthomonas axonopodis</i>	Alkanesulfonate
F-I	3UN6	Q2G1I5	N.D.	<i>Staphylococcus aureus</i>	N.D.
F-II	3K2D	Q8DFC1	LlpA	<i>Vibrio vulnificus</i>	Methionine
F-II	3TQW	Q83F42	N.D.	<i>Coxiella burnetii</i>	Methionine
F-II	4K3F	Q9HT68	N.D.	<i>Pseudomonas aeruginosa</i>	N.D.
F-II	4QHQ	B4EA88	N.D.	<i>Burkholderia cenocepacia</i>	Methionine
F-II	4YAH	P28635	MetQ	<i>Escherichia coli</i>	Methionine
F-III	3O66	A0A0H3K0Z1	OpuCC	<i>Staphylococcus aureus</i>	Glycine Betaine/ Carnitine/ Choline
F-III	3PPN	O32243	OpuCC	<i>Bacillus subtilis</i>	Glycine Betaine/ Carnitine/ Choline
F-III	4ND9	A9CKK7	N.D.	<i>Agrobacterium fabrum</i>	Proline/ Glycine/ Betaine

F-III	4WEP	P33362	YehZ	<i>Escherichia coli</i>	Glycine/ Betaine
F-III	4Z7E	Q8Y775	N.D.	<i>Listeria monocytogenes</i>	N.D.
F-IV	2XHD	P42262	GRIA2	<i>Homo sapiens</i>	Glutamate
F-IV	3DLN	P19492	Gria3	<i>Rattus norvegicus</i>	Glutamate
F-IV	3FAT	P19493	Gria4	<i>Rattus norvegicus</i>	Glutamate
F-IV	3S9E	P42264	Grik3	<i>Rattus norvegicus</i>	Glutamate
F-IV	5FTH	P19491	Gria2	<i>Rattus norvegicus</i>	Glutamate

24 N.D.: Not defined.

25

26 **Table S6.** Details of the molecular docking results of various metal ions and/or their complexes with SBPs.

ORF number	Ligand	EFBE (kcal mol ⁻¹)	NHBOND	Interactions	
				Ligand atom	Protein residue atom
TTHB220	Heme	-9.83	4	O1D	Tyr161 O, Arg163 N ^{η2}
				O1A	Arg163 N ^{η2}
				O2A	Arg163 N ^{η2}
TTHA0723	Heme (conformation-A)	-8.19	4	O1A	Lys191 N ^ζ
				O2A	Lys191 N ^ζ

	Heme (conformation-B)	-8.02	8	O1D	Lys195 N ζ
				O2D	Lys195 N ζ
				Fe	Tyr44 O
				NA	Tyr44 O
				NB	Tyr44 O
				ND	Tyr44 O
				O1A	Thr45 O γ^1
				O2A	Thr45 O γ^1
				O1D	Lys191 N ζ
				O2D	Lys191 N ζ
TTHA0746	Cyanocobalamin	-4.16	5	O28	Asp238 O δ^2
				O34	Arg243 N ϵ
				O39	Thr99 O
				O44	Ser78 O γ
				N40	Glu100 O
	Heme	-8.39	6	O2A	Gly184 O, Phe186 N
				NB	Tyr158 O

				NC	Tyr158 O
				ND	Tyr158 O
				Fe	Tyr158 O
TTHB177	Mg ²⁺ -Citrate	-8.94	21	O1	Mg ²⁺
				O2	Mg ²⁺ , Ser198 O ^γ , Thr199 N
				O3	Ser26 O, Arg246 N ^{η1}
				O4	Mg ²⁺ , Ser26 O
				O5	Thr55 O ^{γ1} , Ser164 O ^γ
				O6	Thr55 N
				O7	Mg ²⁺
	Fe ²⁺ -Citrate	-10.02	20	O1	Fe ²⁺
				O2	Fe ²⁺ , Ser198 O ^γ , Thr199 N
				O3	Fe ²⁺ , Ser26 O
				O4	Ser26 O, Arg246 N ^{η1}
				O5	Thr55 O ^γ , Ser164 O ^γ
				O6	Thr55 N
				O7	Fe ²⁺

TTHA0069	WO ₄ ²⁻	-2.92	7	O1	His55 N
				O2	Thr37 O ^γ 1, His55 O, Gly120 N
				O3	Thr121 N & O ^γ 1
				O4	Arg115 N ^η 2
TTHA0717	WO ₄ ²⁻	-2.73	13	O1	Ser7 N & O ^γ , Asp8 N
				O2	Ala164 N
				O3	Ser7 O ^γ
				O4	Ser36 N
				W	Ser7 O ^γ
	MoO ₄ ²⁻	-2.89	13	O1	Ser7 N & O ^γ , Asp8 N
				O2	Ser7 O ^γ
				O3	Ala164 N
				O4	Ser36 N
				Mo	Ser7 O ^γ ,

27 Abbreviations: EFBE, estimated free energy of binding; NHBOND, number of hydrogen bonds.

28

29 **References**

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