

Table S3. Test Case

Source	PDB hit	gi	template (%id homology modeling template)	FOLD	Cys position	Active Site Similarity score	Cys Reactivity score	Combined score
<i>Pyrococcus horikoshii</i>	1J08			thioredoxin	149	1.5	1.75	3.25
<i>Mycoplasma pneumoniae</i>	1LQL			OsmC-like	252	1.5	1.25	2.75
<i>Escherichia coli</i>	1SK0			thioredoxin	12	2.5	1	3.5
<i>Bos taurus Mitochondrial</i>	1ZYE			thioredoxin	47	3.5	0.5	4
<i>Neisseria meningitidis</i>	2FY6			thioredoxin	67	2.5	1	3.5
<i>Neisseria gonorrhoeae</i>	2H30			thioredoxin	68	2.5	1	3.5
<i>Ectromelia virus</i>	2HZF			thioredoxin	23	2	1.25	3.25
<i>Saccharomyces cerevisiae</i>	2JAC			thioredoxin	30	1.5	1.5	3
<i>Pseudomonas aeruginosa</i>	2O4D			AhpD-like	51	3.5	2	5.5
<i>Silicibacter sp. TM1040</i>	2PFX			thioredoxin	88	3.5	2	5.5
<i>Aquifex aeolicus</i>	2YWM			thioredoxin	151	1.625	1.25	2.875
<i>Clostridium kluyveri</i>		gi 153955052	1XM0(62%)	Mss4-like	119	2.25	2	4.25
<i>Rattus norvegicus</i>		gi 16758004	1FVA (85%)	Ferredoxin-like	72	3.5	2	5.5
<i>Xenopus laevis</i>		gi 148235445	1FVA (70%)	Ferredoxin-like	51	3.5	2	5.5
<i>Bos taurus</i>	1GP1			thioredoxin	45	2.75	0.5	3.25
<i>Bacillus cereus</i>		gi 52143310	2P5Q(48%)	thioredoxin	35	2.25	1.75	4
<i>Drosophila melanogaster</i>		gi 24656772	2P5R(51%)	thioredoxin	49	2.25	0.75	3
<i>Escherichia coli</i>	1TRB			FAD/NAD-linked reductases	135	1.25	2	3.25
<i>Mus musculus</i>	1ZKQ			FAD/NAD-linked reductases	86	1.25	2	3.25
<i>Crithidia fasciculata</i>	2TPR			FAD/NAD-linked reductases	51	1	2	3
<i>Oryza Sativa</i>		gi 4106694	1FEC(44%)	FAD/NAD-linked reductases	70	1	2	3
<i>Saccharomyces cerevisiae</i>	1A6R			Papain-like	73	0	0.5	0.5
<i>Homo sapiens</i>	1CB5			Papain-like	73	0	0	0
<i>Homo sapiens</i>	1NL6			Cysteine proteinases	25	0.5	1.25	1.75
<i>Homo sapiens</i>	1XD3			Cysteine proteinases	95	0.5	1.75	2.25
<i>Cryptococcus neoformans</i>	2AAZ			Thymidylate synthase	187	0	1.25	1.25
<i>Selenomonas ruminantium</i>	2B4U			(Phosphotyrosine protein)	252	0	1.25	1.25
<i>Bos taurus</i>	2DCC			Cysteine proteinases	29	0	0.75	0.75
<i>Homo sapiens</i>	2ETL			Cysteine proteinases	90	0	1.75	1.75
<i>Campylobacter jejuni</i>	2GI4			(Phosphotyrosine protein)	8	0	1	1
<i>Fasciola hepatica</i>	2O6X			Cysteine proteinases	116	0	1	1
<i>Cryptosporidium hominis</i>	2OIP			Thymidylate synthase	402	0.5	1.5	2
<i>Mycobacterium tuberculosis</i>	2OZ5			(Phosphotyrosine protein)	160	0	2	2
<i>Lactobacillus casei</i>	2TDM			Thymidylate synthase	198	0.5	1.5	2
<i>Homo sapiens</i>	2D2Z			Glutathione S-transferase (GST), C-terminal Domain	234	1.25	1	2.25
<i>Rattus norvegicus</i>	1FLJ			Carbonic anhydrase	188	0	0	0
<i>Homo sapiens</i>	1HNL			Lysozyme-like	95	1.25	1	2.25
<i>Oryctolagus cuniculus</i>	1IJJ			Ribonuclease H-like motif	374	0.5	0.75	1.25
<i>Homo sapiens</i>	1KCG			C-type lectin-like	109	0.5	0.75	1.25
<i>Homo sapiens</i>	1EEM			Glutathione S-transferase (GST), thioredoxin-like domain	32	1.5	1	2.5
<i>Homo sapiens</i>	2O02			alpha-alpha superhelix	25	0.5	0.5	1
<i>Homo sapiens</i>	1W7B			Annexin	294	1.25	1	2.25
<i>Homo sapiens</i>		gi 1703322	1ANN(59%)	Annexin	133	0.5	1	1.5

<i>Ovis aries</i>	1UW3			Prion-like	148	1.5	0	1.5
<i>Homo sapiens</i>		<i>gi 23512328</i>	2OVR (34%)	Ferredoxin-like	245	0	0.5	0.5
<i>Homo sapiens</i>		<i>gi 119172</i>	1NOU(64%)	Reductase/isomerase/	567	0.5	0	0.5
<i>Homo sapiens</i>		<i>gi 55584035</i>	1F60(81%)	Reductase/isomerase/elongation factor common domain	234	0.25	1.5	1.75
<i>Homo sapiens</i>		<i>gi 21264428</i>	1YUW(55%)	Ribonuclease H-like motif	487	0	0	0
<i>Homo sapiens</i>		<i>gi 6166599</i>	2AKA(48%)	P-loop containing nucleoside triphosphate hydrolases	91	0.25	0.25	0.5
<i>Homo sapiens</i>	1CYN			Cyclophilin-like	202	0.25	0.75	1
<i>Homo sapiens</i>	2GF9			P-loop containing nucleoside triphosphate hydrolases	184	0.5	0.75	1.25
<i>Homo sapiens</i>		<i>gi 730922</i>	1Q3R(38%)	GroEL-intermediate domain like /Cystatin like domain	406	0.75	0	0.75
<i>Homo sapiens</i>		<i>gi 74762725</i>	1XTD(46%)	SH3-like barrel	73	0	1	1
<i>Homo sapiens</i>	1TR2			Four-helical up-and-down	85	0.25	0	0.25