Computational Structural Analysis and Interaction Network Profiling of Lipases: Implications for Biomedical and Therapeutic Applications

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Table S1. Structural features of organic solvent stable lipases

S. No	Source Organism	PDB ID	Resolution	Organic solvent	No. of Hydrophobic interactions	No. of Disulphide bridges	No. of Ionic interactions	No. of Aromatic-Aromatic interactions	No. of Aromatic-Sulphur interactions	Area (Å3)	Volume (Å2)	Solvation Energy (Kcal/mol)
Non polar												
1	Thermomyces lanuginosus	4FLF	2.15 Å	4-nitrobenzaldehyde	454	6	52	38	4	80647.22	34535.83	-7710.89
2	Thermomyces lanuginosus	4KJX	2.1 Å	LAURIC ACID	459	6	52	38	6	80828.56	34677.84	-7568.49
3	Thermomyces lanuginosus	4GI1	2.43 Å	16-hydroxyhexadecanoic acid	451	5	51	40	6	81086.42	34714.85	-7744.43
4	Thermomyces lanuginosus	4N8S	2.3 Å	4-nitrobenzaldehyde	449	6	52	38	7	80543.30	34456.66	-7408.29
5	Thermomyces lanuginosus	4GLB	2.69 Å	4-nitrobenzaldehyde	454	6	48	39	5	81069.25	34745.24	-7696.53
6	*Pseudomonasaeruginosa* LST-03 (PAL)	1EX9	2.54 Å	HEXYLENE GLYCOL	184	1	17	7	3	83116.21	35826.11	-2390.80
7	Thermomyces lanuginosus	4GHW	2.6 Å	DECANOIC ACID	456	6	50	41	6	80705.43	34597.49	-7343.64

Polar												
8	Bacillus sp. H-257	4KE7	1.7 Å	(4S)-2-METHYL-2,4-PENTANEDIOL	445	no	54	18	14	74149.18	32083.92	-6925.85
9	*Candida antarctica* Lipase A (CALA)	2VEO	2.2 Å	Tetraethylene glycol	842	4	51	47	2	128665.43	55717.50	-7458.08
10	Thermomyces lanuginosus	4S0X	2.1 Å	ETHYLENE GLYCOL	456	6	52	38	6	80504.50	34472.05	-7593.52
11	Malassezia globosa	3UUF	2.6 Å	N-ACETYL-D-GLUCOSAMINE	257	1	30	12	7	86008.13	36964.26	-2868.64
12	Malassezia globosa	4UU3	1.45 Å	PEG MONOMETHYL ETHER	262	no	37	19	2	52567.31	22480.03	-5136.17
13	*Serratia marcescens* ECU1010 (SML)	2QUA	1.95 Å	HEXYLENE GLYCOL	470	no	40	32	2	111083.05	48016.20	-14767.24
14	Bacteroides thetaiotaomicron	4HF7	1.77 Å	Bicine	172	no	16	14	no	61710.79	26580.54	-2452.40
15	*Bacillus* strain 42 (BL42)	4FKB	1.22 Å	Glycerol	659	no	100	65	20	119284.17	51350.58	-6764.71
16	Lactobacillus plantarum	4BZZ	3.0 Å	sodium acetate	269	no	11	9	1	84296.28	36468.55	-2584.03
17	Geobacillus sp. SBS-4S	3AUK	1.66 Å	Imidazole	323	no	48	32	8	119192.15	51217.57	-3284.95
18	Mus musculus | Homo sapiens	3OHM	2.7 Å	HEPES	967	no	117	59	23	103242.58	44469.33	-19282.60
19	Yarrowia lipolytica	3O0D	1.7 Å	HEXYLENE GLYCOL	-	-	-	-	-	92284.49	39893.02	-37938.65
20	*Bacillus subtilis* DS-9 (BSL)	1i6w	1.5Å	Ethanol amine	296	no	15	2	2	53082.29	22925.76	-3275.45

21	*Bacillus stearothermophilus* P1 (BSLP)	1JI3	2.2 Å	HEPES	640	no	81	62	15	120169.83	51632.41	-6894.15
22	*Candida Antarctica* Lipase B (CALB)	1TCA	1.55 Å	N-Acetyl-D-Glucosamine	266	3	7	10	5	91225.25	39583.84	-1831.96
23	*Bacillus thermocatenulatus* (BTL)	2W22	2.2 Å	Triton X 100	278	no	40	20	7	119048.64	51073.69	-3166.36
24	Saccharomyces cerevisiae	2Y6U	1.9 Å	GLYCEROL	296	no	43	14	6	115460.12	49972.06	-3759.55
25	Saccharomyces cerevisiae	2Y6V	2.83 Å	HEPES	870	no	115	42	23	111815.03	48587.02	-12204.26
26	Mycobacterium smegmatis	3AJA	2.9 Å	BisTris-propane	406	4	30	8	no	76272.35	32836.49	-8643.24
27	*Thermostable Bacillus subtilis* lipase (TBSL)	3D2C	2.18 Å	HEPES	-	-	-	-	-	53373.38	22986.53	-17793.92
28	Bacillus sp. H-257	3RLI	1.85 Å	HEXYLENE GLYCOL	222	no	26	10	7	73930.74	31983.89	-3248.75
29	Bacillus sp. H-257	3RM3	1.2 Å	HEXYLENE GLYCOL	224	no	25	11	7	74078.76	32006.31	-3238.47
30	Uncultured bacterium	3V9A	2.07 Å	TRIS	299	no	34	7	5	86809.81	37635.75	-2799.01
31	Moesziomyces antarcticus	3W9B	2.9 Å	3,6,9,12,15,18,21-HEPTAOXATRICOSANE-1,23- DIOL	1059	12	28	44	20	90742.68	39173.03	-7610.96
32	Proteus mirabilis	3W9U	2.0 Å	ETHYLENE GLYCOL	234	no	22	12	2	83583.16	35980.58	-3060.47
33	Lactobacillus plantarum	4BZW	2.15 Å	TRIS-HYDROXYMETHYL-METHYL-AMMONIUM	237	no	26	19	3	84149.18	36448.18	-4914.77
34	Thermomyces lanuginosus	4DYH	2.0 Å	N-ACETYL-D-GLUCOSAMINE	458	6	54	38	7	80140.42	34238.75	-7415.50
35	Thermomyces lanuginosus	4EA6	2.3 Å	HEPES	443	6	53	41	7	81725.85	35156.00	-7488.44

36	Unidentified	4FBL	1.99 Å	SPERMIDINE	989	no	77	18	30	73133.77	31932.18	-12726.85
37	Unidentified	4FBM	2.8 Å	TRIS	493	no	39	10	15	75324.32	32833.26	-5450.44
38	Bacillus sp. L2	4FDM	1.6 Å	PEG 6000	318	no	44	32	8	116921.91	50320.28	-3334.45
39	Geobacillus stearothermophilus	4FMP	2.3 Å	PEG 20000	632	no	82	66	15	118533.47	51064.83	-6171.75
40	Proteus mirabilis	4GW3	2.0 Å	2-PROPANOL	245	no	25	11	2	85891.92	36875.54	-3044.62
41	Thermomyces lanuginosus	4GWL	2.55 Å	N-ACETYL-D-GLUCOSAMINE	455	6	53	38	6	80574.09	34520.47	-7441.02
42	Streptomyces albidoflavus	4HYQ	1.75 Å	PEG400	187	3	13	13	2	65456.28	28075.19	-1846.03
43	Neisseria meningitidis	4K3U	2.16 Å	4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID	603	2	55	32	13	103987.67	44942.12	-6169.07
44	Moesziomyces antarcticus	4K6G	1.5 Å	ETHYLENE GLYCOL	533	6	15	20	12	89165.54	38461.05	-3999.99
45	Escherichia coli	4KRX	1.8 Å	TETRAETHYLENE GLYCOL	930	3	91	65	38	98607.65	42584.31	-14079.76
46	Pseudomonas cepacia(PCL)	3LIP	2.0 Å	CALCIUM ION	206	1	12	8	no	91443.24	39517.54	-2035.37
47	*Rhizopus chinensis* (RCL)	4L3W	2.0 Å	ethylene glycol	239	3	22	16	2	80549.61	34678.37	-2153.94
48	Bacillus sp. H-257	4LHE	1.96 Å	tartrate	453	no	52	20	10	75612.99	32727.55	-6974.40
49	Bacteroides uniformis	4M8K	1.9 Å	polyethylene glycol	319	no	39	32	4	-	-	-6541.43
50	Bacteroides ovatus	4NRD	2.1 Å	ETHYLENE GLYCOL	-	-	-	-	-	64233.24	27533.11	-16063.03
51	Uncultured bacterium	4Q05	2.05 Å	PEG 8000	624	no	60	22	2	96600.31	41649.53	-9579.39
52	unidentified	4Q3K	1.57 Å	TRIETHYLENE GLYCOL	528	no	37	32	10	-	-	-6398.21
53	Chitinophaga pinensis	4Q7Q	1.45 Å	TETRAETHYLENE GLYCOL	461	no	31	28	no	79450.79	34158.78	-5418.61

54	Pseudomonas aeruginosa	4R1D	1.75 Å	BIS TRIS	680	no	99	43	6	A(158147.609) B(93177.59288)	A(67837.46878) B(39861.20977)	-10322.88
55	Veillonella parvula	4RW0	2.0 Å	GLYCEROL	273	no	23	21	3	-	-	-8587.36
56	Thalassospira sp. GB04J01	4V2I	1.69 Å	TRIS-HCL	626	no	67	20	4	93421.14	40436.85	-9361.46
57	Moesziomyces antarcticus	4ZV7	2.0 Å	PEG	263	3	7	10	6	90198.92	38886.18	-1881.97
58	Bacillus subtilis	5CRI	1.63 Å	Ethanolamine	301	no	13	2	2	53063.02	22924.21	-3373.79
59	Bacillus subtilis	5CT4	1.49 Å	Ethanolamine	303	no	14	2	2	52888.78	22797.59	-3142.90
60	*Bacillus stearothermophilus* L1 (BSLL)	IKU0	2.0 Å	Zinc ion, Calcium ion	621	no	88	60	15	120296.98	51825.14	-6530.88
61	Bacillus subtilis	5CT6	1.9 Å	1-butyl-3-methylimidazolium	299	no	15	2	2	52905.16	22795.48	-3301.57
62	Bacillus subtilis	5CT5	1.75 Å	1-butyl-3-methylimidazolium	301	no	19	2	2	53015.79	22886.82	-3227.10
63	Escherichia coli	4KRY	2.3 Å	PENTAETHYLENE GLYCOL	-	-	-	-	-	99344.32	42881.85	-32874.16
64	unidentified	4Q3O	1.74 Å	2-(N-MORPHOLINO)-ETHANESULFONIC ACID	-	-	-	-	-	96777.39	41840.79	-21781.96
65	Acinetobacter baumannii	4OPM	1.7 Å	POLYETHYLENE GLYCOL PEG4000	584	no	55	14	no	-	-	-5126.23
66	Parabacteroides merdae	4Q9A	2.86 Å	polyethylene glycol	367	no	53	36	6	67344.63	28997.04	-4504.01
67	Neisseria meningitidis	4K40	2.63 Å	HEPES	587	2	58	33	14	104296.37	45013.17	-6013.75
68	Thermomyces lanuginosus	4ZGB	2.3 Å	HEPES	442	6	52	42	7	81000.63	34708.82	-7411.17

69	Uncultured bacterium	4J7A	1.49 Å	sodium malonate	-	-	-	-	-	102883.44	44454.90	-29251.44
70	Bacteroides fragilis	4PPY	2.0 Å	polyethylene glycol	490	no	35	39	no	61928.43	26625.85	-6897.63
71	Neisseria meningitidis	4K9S	2.33 Å	HEPES	510	no	58	33	no	100781.89	43450.62	-6193.58
72	Thermomyces lanuginosus	4GBG	2.9 Å	N-ACETYL-D-GLUCOSAMINE	447	6	56	38	7	80421.03	34377.66	-7479.69
73	Bacteroides thetaiotaomicron	4H08	1.8 Å	2-PROPANOL	189	no	22	3	no	-	-	-2563.62
74	Bacteroides uniformis	4IYJ	1.37 Å	2 Propanol	334	no	35	26	no	62416.90	26888.72	-5143.17
75	Proteus mirabilis	4GXN	2.2 Å	TRIETHYLENE GLYCOL	233	no	23	10	2	86476.86	37237.59	-3022.76
76	Diutina rugosa	3RAR	2.19 Å	N-ACETYL-D-GLUCOSAMINE	472	2	35	27	6	159300.00	69044.82	-6340.21
77	Mus musculus | Homo sapiens	4QJ3	3.0 Å	GUANOSINE-5'-DIPHOSPHATE	978	no	117	62	22	A (103154.342) B (241758.3848)	A (44545.13114) B (104963.648)	-13532.68
78	*Rhizomucor miehei* (RML)	4TGL	2.6 Å	Diethyl Phosphonate	211	3	20	11	3	80267.39	34476.74	-2907.93
79	Clostridium botulinum	5AH1	1.2 Å	TRIS	360	no	39	25	8	132267.44	56955.81	-6123.76
80	Moesziomyces antarcticus	5A6V	2.28 Å	2-PROPANOL	539	6	12	19	10	90551.12	39112.28	-3746.36
81	Lactobacillus plantarum	4C01	2.3 Å	phenyl acetate	-	-	-	-	-	83970.02	36266.05	-15554.12
82	Neisseria meningitidis	4K7J	1.97 Å	4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID	601	2	58	33	14	104288.87	45041.20	-6113.73