Cell-Free Supernatants (CFSs) from the Culture of *Bacillus subtilis* Inhibit *Pseudomonas* sp. Biofilm Formation

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Table S1: List of bacterial strains used for the antagonistic test

Sl. no.	Name of the used bacterial strains
01	*Klebsiella pneumoniae*
02	*Pseudomonas* sp.
03	*Escherichia coli*
04	*Staphylococcus aureus*

Table S2: Ligand No, PubChem CID of the molecules identified through GC-MS based and their docking score

Compounds	CID	R.T	Area Percentage	Docking Score
1. 1-Butanol, 3-methyl-	31260	1.965	0.06	-4.2
2. Disulfide, dimethyl	12232	4.327	6.06	-2.3
3. Butanoic acid, 2-methyl-	8314	6.933	0.19	-4.6
4. Oxime-, methoxy-phenyl-_	9602988	7.346	0.21	-5.0
5. 2-Heptanone	8051	7.531	0.67	-4.9
6. Anisole	7519	8.104	0.46	-4.9
7. Hexanoic acid, methyl ester	7824	8.25	0.08	-4.9
8. 2-Heptanone, 4-methyl-	94317	8.507	0.1	-4.0
9. 1-(9H-Fluoren-2-yl)-2-(1-phenyl-1H-tetrazol-5-ylsulfanyl)-ethanone	606333	8.755	0.15	-7.0
10. Dimethyl trisulfide	19310	8.821	0.86	-2.6
11. Benzaldehyde	240	9.045	0.18	-4.8
12. Pentasulfide, dimethyl	81772	9.184	8.51	-2.4
13. 3-Cyclopentyl-1-propyne	521007	9.411	14.45	-5.4
14. Phenol, 2-chloro-	7245	9.597	2.34	-4.4
15. Pyridine, 2,3,6-trimethyl-	15100	9.696	1.74	-5.8
16. Propanoic acid, 2,2-dimethyl-, propyl ester	138418	9.776	1.02	-4.2
17. Pyrazine, trimethyl-	26808	9.866	0.63	-5.2
18. Diethylene glycol tert-butyl ether methyl ether	104324	10.003	0.24	-4.3
19. Benzene, 1,4-dichloro-	4685	10.09	0.13	-5.0
20. Butane, 1-[(1-methylethyl)thio]-	522478	10.15	0.15	-3.4
21. 5-Hydroxy-hex-2-enoic acid, methyl ester	5369246	10.22	0.13	-5.0
22. 5-Chloropentanoic acid, 2-ethylcyclohexyl ester	544276	10.262	0.19	-4.7

23. 2-Ethyl-1-hexanol	7720	10.319	0.18	-4.8
24. D-Limonene	440917	10.355	0.21	-5.8
25. Propane, 2-(chloromethyl)-1,3-dimethoxy-2-methyl-	542360	10.527	0.21	-3.5
26. Oxirane, 2-[2-(benzyloxy)-1-(1-methoxy-1-methylethoxy)ethyl]	552649	10.626	0.23	-4.8
27. 2-Nonanone	13187	10.773	0.11	-5.0
28. Propionic acid, (3,6,7,8-tetrahydro-3,7-methano-2,4,6-trimethyl-2H-oxocin-7-yl)methyl ester	583617	10.848	0.11	-5.7
29. Pyrazine, 3-ethyl-2,5-dimethyl-	25916	11.203	0.56	-4.4
30. 1-Heptanol, 2,4-dimethyl-,	101564277	11.28	0.1	-5.4
31. o-Toluic acid, 2-ethylhexyl ester	577168	11.363	0.36	-5.5
32. 2-Nonanone	13187	11.43	0.92	-5.0
33. 2,5-Dihydroxybenzaldehyde, 2TMS derivative	622536	11.476	1.27	-4.0
34. 2,2'-Anhydro-1-arabinofuranosyluracil	569411	11.55	0.12	-6.0
35. 1-Heptanol, 2-propyl-	24847	11.617	0.23	-4.5
36. Nonanal	31289	11.675	0.1	-4.2
37. Succinic acid, 3,7-dimethyloct-6-en-1-yl pentyl ester	91702362	11.748	0.19	-4.1
38. Phorone	10438	11.79	0.16	-5.1
39. Phenylethyl Alcohol	6054	11.873	0.37	-5.1
40. Benzene, 1-chloro-4-methoxy-	12167	11.99	0.29	-4.2
41. Silane, dimethyl(dimethyl(dimethyl(2-isopropylphenoxy)silyloxy)silyloxy)(2-isopropylphenoxy)-	91743286	12.015	0.19	-3.3
42. Benzenemethanol, 4-methyl-	11505	12.264	0.22	-5.5
43. 2,6-Dodecadien-1-al	6430759	12.387	0.1	-5.2
44. (+)-3-Carene, 2-(acetylmethyl)-	576614	12.546	0.2	-5.4
45. Hexadecanal, 2-methyl-	546976	12.634	0.06	-5.1
46. 1-Methoxy-2-methyl-4-(methylthio)benzene	592820	12.724	0.22	-4.4

47. 1,3-Propanediol, 2-butyl-2-ethyl-	61038	12.83	0.14	-4.6
48. Neophytadiene	10446	12.943	1.36	-4.6
49. n-Decyl methylphosphonofluoridate	567104	13.104	0.35	-4.6
50. Azulene	9231	13.184	0.31	-5.8
51. Fumaric acid, 2,5-dimethylphenyl nonyl ester	91711256	13.28	0.22	-5.4
52. 16-Methyl-heptadecane-1,2-diol, trimethylsilyl ether	91742675	13.565	0.12	-3.4
53. Tetrasulfide, dimethyl	79828	13.677	2.24	-2.3
54. Benzothiazole	7222	13.834	1.51	-5.1
55. Benzene, 1,3-bis(1,1-dimethylethyl)-	71343282	14.086	0.75	-5.8
56. 1,7-Di(3-ethylphenyl)-2,2,4,4,6,6-hexamethyl-1,3,5,7-tetraoxa-2,4,6-trisilaheptane	91742720	14.203	0.05	-7.1
57. Bicyclo[3.2.0]hepta-3,6-diene-1-carbonitrile	575776	14.88	10.91	-4.5
58. o-Methoxymandelic acid, 2TMS derivative	530206	14.992	0.33	-4.1
59. Pyrazine, 2,5-dimethyl-3-(3-methylbutyl)-	519564	15.044	0.19	-5.3
60. Trichloroacetic acid, 6-ethyl-3-octyl ester	550155	15.105	0.05	-4.9
61. 3-tert-Butyl-2-pyrazolin-5-one	520421	15.169	0.21	-5.2
62. E-10,13,13-Trimethyl-11-tetradecen-1-ol acetate	5365074	15.565	0.05	-4.5
63. 3,5-Dibutoxy-1,1,1,7,7,7-hexamethyl-3,5-bis(trimethylsiloxy)tetrasiloxane	551995	15.885	0.71	-3.4
64. Dodecanedioic acid, 2TBDMS derivative	634058	15.745	0.08	-4.2
65. 3-(2-Hydroxy-cyclopentylidene)-2-methyl-propionic acid	5369050	15.824	0.13	-5.2
66. Ethane, 2-chloro-1-ethoxy-1-methoxy-	548381	15.94	0.08	-3.4
67. Dodecanedioic acid, 2TBDMS derivative	634058	15.968	0.09	-3.5
68. 16-Methyl-heptadecane-1,2-diol, trimethylsilyl ether	91742675	16.005	0.06	-4.3
69. 3,5-Dibutoxy-1,1,1,7,7,7-hexamethyl-3,5-bis(trimethylsiloxy)tetrasiloxane	551995	16.105	0.2	-4.2
70. 1-Heptacosanol	74822	16.175	0.05	-4.7

71. Tetradecane	12389	16.287	0.12	-5.0
72. Dodecanedioic acid, 2TBDMS derivative	634058	16.388	0.11	-4.1
73. Carbonic acid, 2-ethylhexyl heptadecyl ester	91693166	16.45	0.06	-5.0
74. 2-Piperidinone, N-[4-bromo-n-butyl]-	536377	16.58	0.05	-4.4
75. 2,5-di-tert-Butyl-1,4-benzoquinone	17161	17.337	0.19	-5.6
76. 2-Dodecen-1-yl(-)succinic anhydride	5362708	17.524	0.13	-5.2
77. 2-Tridecanone	11622	17.593	0.33	-4.3
78. Phenol, 3,5-bis(1,1-dimethylethyl)-	5614	17.777	4.66	-4.2
79. N1,N1,N4-Tris(tert-butyldimethylsilyl)succinamide	91744783	17.98	0.29	-4.3
80. Bis(pentamethylcyclotrisiloxy)tetramethyldisiloxane	553163	18.062	0.07	-6.2
81. 1,4-Methanobenzocyclodecene, 1,2,3,4,4a,5,8,9,12,12a-decahydro-	556414	19.992	0.04	-4.3
82. 1,1,1,3,5,7,9,11,11,11-Decamethyl-5-(trimethylsiloxy)hexasiloxane	6329082	20.093	0.18	-4.8
83. Oxalic acid, cyclohexylmethyl tridecyl ester	6421725	20.658	1.33	-6.4
84. 7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione	545303	24.3	0.25	-3.3
85. Tetracosamethyl-cyclododecasiloxane	167767	36.94	0.85	-3.6

Table S3: Protein-Ligand interactions of Caseinolytic proteases (Clp)) enzymes (PDB ID: 7M1M) with top 8 volatile compounds of *Bacillus subtilis*

Compound Name	**Hydrogen bond**		**Hydrophobic bond**	
	Residues	Distance (A°)	Residues	Distance (A°)
1-(9H-Fluoren-2-yl)-2-(1-phenyl-1H-tetrazol-5-ylsulfanyl)-ethanone			Met-41 Tyr-22	5.8 4.40

			Tyr-22	4.04
Oxalic acid, cyclohexylmethyl tridecyl ester	Thr-22 Thr-22	4.46 5.15		
Bis(pentamethylcyclotrisiloxy)tetramethyldisiloxane	Gln-48	5.27	Tyr-22 Tyr-22 Tyr-22 Tyr-22 Tyr-22 Val-5	4.19 4.48 4.57 5.36 4.78
2,2'-Anhydro-1-arabinofuranosyluracil	Val-34 Val-34	3.17 4.24	Met-41 Tyr-22	5.59 4.21