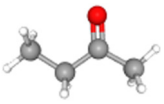
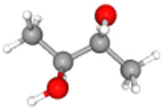
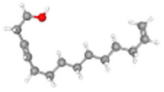
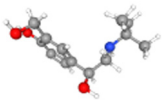
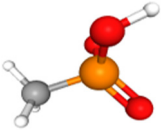
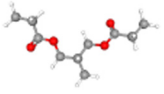
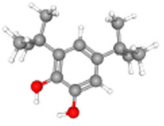
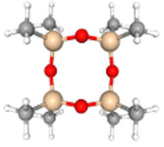
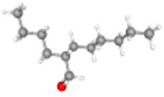
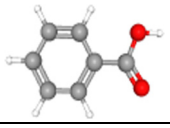
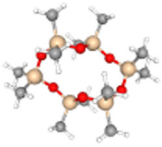
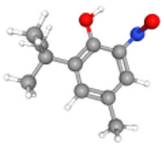
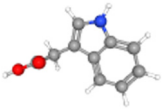
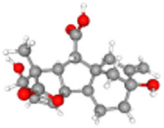
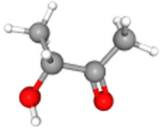
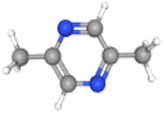
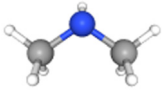
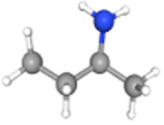
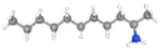
Supplementary material

Table S1: Predicting the physicochemical properties and toxicity potential of the studied volatile compounds

	Molecular Formula	Molecular Weight	H-Bond Donor	H-Bond Acceptor Count	3D structure
2-Butanone (6569)	C_4H_8O	72.11	0	1	
2 *R* ,3 *R* – Butanediol (262)	$C_4H_{10}O_2$	90.12	2	2	
13-Tetradecadien-1-ol (21770590)	$C_{14}H_{26}O$	210.36	1	1	
2-Methyl-n-1-tridecene 140334))	$C_{14}H_{28}$	196.37	0	0	
Albuterol (2083)	$C_{13}H_{21}NO_3$	239.31	4	4	
Methylphosphonic acid (13818)	CH_5O_3P	96.022	2	3	
1,3-Propanediol, 2-methyl- ,dipropanoate (345905)	$C_{10}H_{18}O_4$	202.25	0	4	
Silanediol, dimethyl 44151799	$C5H_{14}O_3Si$	150.25	2	3	—
1,2-Benzenediol,3,5-bis(1,1-dimethylethyl) 66099	$C_{14}H_{22}O_2$	222.32	2	2	
Cyclotetrasiloxane, octamethyl- 11169	$C8H_{24}O_4Si_4$	296.61	0	4	
1-Octanol,2-butyl 71344432	$C_{25}H_{54}O_5$	434.7	4	5	
Benzoic acid 243	$C7H_6O_2$	122.12	1	2	

(Continued)

Table S1: *Continued*

	Molecular Formula	Molecular Weight	H-Bond Donor	H-Bond Acceptor Count	3D structure
Cyclohexasiloxane, dodecamethyl-10911	$C_{12}H_{36}O_6Si6$	444.92	0	6	
Phenol,2-(1,1-dimethylethyl)-4-methyl 12273770	$C_{11}H_{15}NO_2$	193.24	1	3	
indole-3-acetic acid 802	$C_{10}H9NO_2$	175.18	2	2	
Gibberellic acid	$C_{19}H_{22}O_6$	346.4	3	6	
Hexadecane 11006	$C_{16}H_{34}$	226.44	0	0	
Acetoin 179	C_4H8O_2	88.11	1	2	
2,5-dimethylpyrazine 31252	$C_6H_8N_2$	108.14	0	2	
Dimethylamine 674	C_2H_7N	45.08	1	1	
2-butanamine 24874	$C4H_{11}N$	73.14			
1-decanol 8174	$C_{10}H_{22}O$	158.28	1	1	
1-dodecanol 8193	$C_{12}H_{26}O$	186.33	1	1	
2-undecanone 8163	$C_{11}H_{22}O$	170.29	0	1	
2-tridecanone 11622	$C_{13}H_{26}O$	198.34	0	1	
2-heptadecanone 18027	$C_{17}H_{34}O$	254.5	0	1	
1-methyldecylamine 114476	$C_{11}H_{25}N$	171.32	1	1	
Dodecane 8182	$C_{12}H_{26}$	170.33	0	0	

(Continued)

Table S1: *Continued*

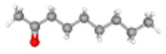
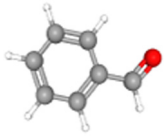
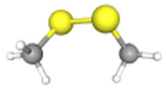
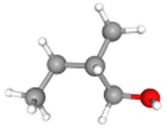
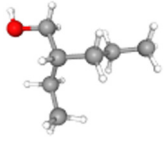
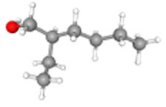
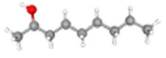
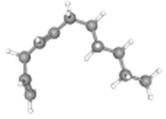
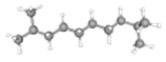
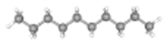
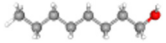
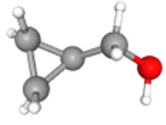
	Molecular Formula	Molecular Weight	H-Bond Donor	H-Bond Acceptor Count	3D structure
2-piperidinone 12665	C_5H_9NO	99.13	1	1	
2-nonanone 13187	$C_9H_{18}O$	142.24	0	1	
1-Undecene 13190	$C_{11}H_{22}$	154.29	0	0	
Benzaldehyde 240	C_7H_6O	106.12	0	1	
Dimethyl disulphide 12232	$C_2H_6S_2$	94.20	0	2	
2-methyl-1-butanol 8723	$C_5H_{12}O$	88.15	1	1	
2-ethyl-1-pentanol 123424	$C_7H_{16}O$	116.20	1	1	
2-Ethylhexanol 7720	C_8H18O	130.23	1	1	
2-nonanol 12367	$C_9H_{20}O$	144.25	1	1	
1,4-undecadiene 5358328	$C_{11}H_{20}$	152.28	0	0	
2,9-dimethyldecane 517733	$C_{12}H_{26}$	170.33	0	0	
Decane 15600	$C_{10}H_{22}$	142.28	0	0	
1-octanol 957	$C_8H_{18}O$	130.23	1	1	
1-heptadecanol 15076	$C_{17}H_{36}O$	256.5	1	1	
Cyclopropyl carbinol 75644	C_4H_8O	72.11	1	1	
1-tetradecanol 8209	$C_{14}H_{30}O$	214.39	1	1	

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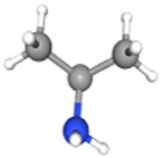
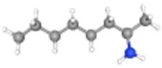
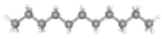
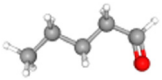
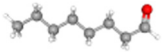
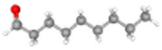
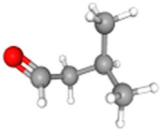
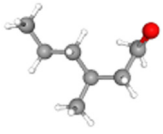
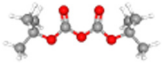
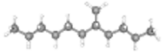
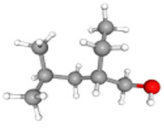
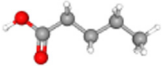
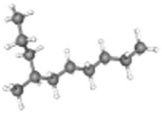
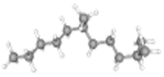
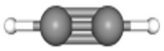
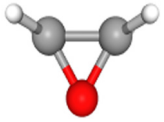
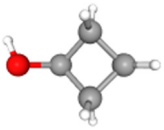
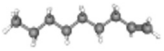
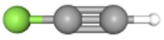
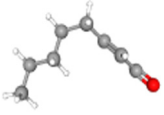
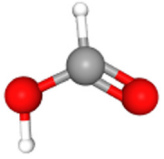
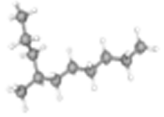
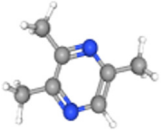
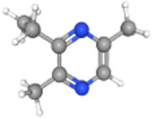
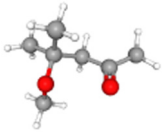
Table S1: *Continued*

	Molecular Formula	Molecular Weight	H-Bond Donor	H-Bond Acceptor Count	3D structure
2-propanamine 6363	C_3H_9N	59.11	1	1	
2-octanamine 12735	$C8H_{19}N$	129.24	1	1	
1-tridecanol 8207	$C_{13}H_{28}O$	200.36	1	1	
Undecane 14257	$C_{11}H_{24}$	156.31	0	0	
Pentanal 8063	$C5H_{10}O$	86.13	0	1	
Octanal 454	$C8H_{16}O$	128.21	0	1	
Nonanal 31289	$C9H_{18}O$	142.24	0	1	
Decanal 8175	$C_{10}H_{20}O$	156.26			
3-methylbutanal 11552	$C5H_{10}O$	86.13	0	1	
3-tridecanone 73751	$C_{13}H_{26}O$	198.34	0	1	
4-methyl-2-heptanone 94317	$C_8H_{16}O$	128.21	0	1	
Hexadecanal 984	$C_{16}H_{32}O$	240.42	0	1	
Di-tert-butyl-dicarbonate 90495	$C_{10}H_{18}O_5$	218.25	0	5	
5-methylundecane 94213	$C_{12}H_{26}$	170.33	0	0	
2-ethyl-4-methyl-1-pentanol 7821	$C8H_{18}O$	130.23	1	1	
Pentanoic Acid 7991	$C5H_{10}O_2$	102.13	1	2	
4-methyldecane 17835	$C_{11}H_{24}$	156.31	0	0	

(Continued)

Table S1: *Continued*

	Molecular Formula	Molecular Weight	H-Bond Donor	H-Bond Acceptor Count	3D structure
2,6-dimethylundecane 28453	$C_{13}H_{28}$	184.36	0	0	
Ethyne	C_2H_2	26.04	0	0	
Ethylene oxide 6354	C_2H_4O	44.05	0	1	
Cyclobutanol 76218	C_4H_8O	72.11	1	1	
1-nonene 31285	C_9H_{18}	126.24	0	0	
Fluoroethyne 32759	C_2HF	44.03	0	1	
2-octenal	$C8H_{14}O$	126.20	0	1	
Benzene ethanol 21965192	$C_8H_{12}O$	124.18	1	1	—
2-ethynyloxy-ethanol,	—	—	—	—	—
1,3-bis(1,1-dimethyl-ethyl)benzene	—	—	—	—	—
Formic acid 284	CH_2O_2	46.025	1	2	
4-methyldecane 17835	$C_{11}H_{24}$	156.31	0	0	
Trimethylpyrazine 26808	$C_7H_{10}N2$	122.17	0	2	
3-ethyl-2,5-dimethylpyrazine 25916	$C_8H_{12}N_2$	136.19	0	2	
4-methyl-2-pentanone 7884	$C_7H_{14}O_2$	130.18	0	2	

(Continued)

Table S1: *Continued*

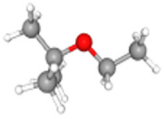
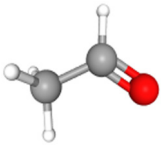
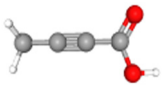
	Molecular Formula	Molecular Weight	H-Bond Donor	H-Bond Acceptor Count	3D structure
2-ethoxy-2-methylpropane	$C_6H_{14}O$	12512	0	1	
Acetaldehyde 177	C_2H_4O	44.05	0	1	
2-butynoic acid 68535	$C_4H_4O_2$	84.07	1	2	

Table S2: Physicochemical properties and cytotoxic and genetic potential calculated for compounds produced by bacteria

Name (Accession code)	Lipo-philicity	Water solubility		Pharmacokinetics					
	Log $P_{o/w}$ (iLogP)	Log *S* (ESOL)	Class [a]	CYP1A2 inhibitor	CYP2C19 inhibitor	CYP2C9 inhibitor	CYP2D6 inhibitor	CYP3A4 inhibitor	Log K_p (skin permeation)
2-Butanone (6569)	1.42	−0.40	Very soluble	No	No	No	No	No	−6.53 cm/s
2 *R* ,3 *R* – Butanediol (262)	1.26	−0.25	Highly soluble	No	No	No	No	No	−7.50 cm/s
13-Tetradecadien-1-ol (21770590)	3.59	−3.65	Soluble	Yes	No	No	No	No	−3.94 cm/s
2-Methyl-n-1-tridecene (140334)	4.02	−5.04	Moderately soluble	Yes	No	No	No	No	−2.27 cm/s
Albuterol (2083)	2.40	−1.45	Very soluble	No	No	No	No	No	−7.54 cm/s
Methylphosphonic acid (13818)	−0.20	0.57	Highly soluble	No	No	No	No	No	−8.02 cm/s
1,3-Propanediol, 2-methyl-, dipropanoate (345905)	2.82	−1.66	Very soluble	No	No	No	No	No	−6.30 cm/s
Silanediol, dimethyl 44151799	2.02	−0.80	Very soluble	No	No	No	No	No	−7.19 cm/s
1,2-Benzenediol,3,5-bis(1,1-dimethylethyl) 66099	2.91	−4.23	Moderately soluble	Yes	No	No	Yes	No	−4.43 cm/s
Cyclotetrasiloxane, octamethyl 11169	3.93	−4.21	Moderately soluble	No	No	No	No	No	−5.26 cm/s
1-Octanol,2-butyl 71344432	6.63	−7.36	Poorly soluble	Yes	Yes	Yes	No	No	−2.18 cm/s
Benzoic acid 243	1.11	−2.20	Soluble	No	No	No	No	No	−5.72 cm/s
Cyclohexasiloxane, dodecamethyl-10911	4.84	−6.40	Poorly soluble	No	No	No	No	No	−4.73 cm/s
Phenol,2-(1,1-dimethylethyl)-4-methyl	2.63	−3.45	Soluble	Yes	No	No	No	No	−4.97 cm/s
indole-3-acetic acid 802	1.01	−2.19	Soluble	No	No	No	No	No	−6.37 cm/s
Gibberellic acid 6466	1.50	−2.07	Soluble	No	No	No	No	No	−8.24 cm/s
Hexadecane 11006	4.67	−5.60	Moderately soluble	Yes	No	No	No	No	−1.80 cm/s
Acetoin	0.98	−0.13	Very soluble	No	No	No	No	No	−7.05 cm/s
2,5-dimethylpyrazine	1.57	−1.46	Very soluble	No	No	No	No	No	−6.51 cm/s

(Continued)

Table S2: *Continued*

Name (Accession code)	Lipo-philicity	Water solubility		Pharmacokinetics					
	Log $P_{o/w}$ (iLogP)	Log *S* (ESOL)	Class [a]	CYP1A2 inhibitor	CYP2C19 inhibitor	CYP2C9 inhibitor	CYP2D6 inhibitor	CYP3A4 inhibitor	Log K_p (skin permeation)
Dimethylamine 674	1.24	0.01	Highly soluble	No	No	No	No	No	−6.72 cm/s
2-butanamine	1.58	−0.69	Very soluble	No	No	No	No	No	−6.22 cm/s
1-decanol	2.99	−3.17	Soluble	No	No	No	No	No	−4.02 cm/s
1-dodecanol	3.37	−3.57	Soluble	Yes	No	No	No	No	−3.79 cm/s
2-undecanone	3.01	−2.94	Soluble	Yes	No	No	No	No	−4.43 cm/s
2-tridecanone	3.56	−3.67	Soluble	Yes	No	No	No	No	−3.84 cm/s
2-heptadecanone	4.44	−5.12	Moderately soluble	Yes	No	No	No	No	−2.64 cm/s
1-methyldecylamine	3.28	−3.06	Soluble	No	No	No	No	No	−4.31 cm/s
Dodecane	3.82	−4.15	Moderately soluble	Yes	No	No	No	No	−3.01 cm/s
2-piperidinone	1.28	−0.16	Very soluble	No	No	No	No	No	−7.23 cm/s
2-nonanone	2.56	−2.30	Soluble	No	No	No	No	No	−4.94 cm/s
1-Undecene	3.40	−4.20	Moderately soluble	Yes	No	No	No	No	−2.81 cm/s
Benzaldehyde	1.36	−1.92	Very soluble	Yes	No	No	No	No	−5.90 cm/s
Dimethyl disulfide	1.69	−1.47	Very soluble	No	No	No	No	No	−5.62 cm/s
2-methyl-1-butanol	1.80	−1.07	Very soluble	No	No	No	No	No	−5.92 cm/s
2-ethyl-1-pentanol	2.17	−1.64	Very soluble	No	No	No	No	No	−5.50 cm/s
2-Ethylhexanol	2.50	−2.26	Soluble	No	No	No	No	No	−4.91 cm/s
2-nonanol	2.76	−2.51	Soluble	No	No	No	No	No	−4.74 cm/s
1,4-undecadiene	3.43	−3.45	Soluble	Yes	No	No	No	No	−3.70 cm/s
2,9-dimethyldecane	3.69	−4.30	Moderately soluble	Yes	No	No	No	No	−2.98 cm/s
Decane	3.29	−3.42	Soluble	No	No	No	No	No	−3.61 cm/s
1-octanol	2.51	−2.14	Soluble	No	No	No	No	No	−4.96 cm/s

(Continued)

Table S2: *Continued*

Name (Accession code)	Lipo-philicity	Water solubility		Pharmacokinetics					
	Log $P_{o/w}$ (iLogP)	Log *S* (ESOL)	Class [a]	CYP1A2 inhibitor	CYP2C19 inhibitor	CYP2C9 inhibitor	CYP2D6 inhibitor	CYP3A4 inhibitor	Log K_p (skin permeation)
1-heptadecanol	4.70	−5.26	Moderately soluble	Yes	No	No	No	No	−2.43 cm/s
Cyclopropyl carbinol	1.42	−0.40	Very soluble	No	No	No	No	No	−6.53 cm/s
1-tetradecanol	3.90	−4.18	Moderately soluble	Yes	No	No	No	No	−3.33 cm/s
2-propanamine	1.38	−0.26	Very soluble	No	No	No	No	No	−6.60 cm/s
2-octanamine	2.59	−1.97	Very soluble	No	No	No	No	No	−5.21 cm/s
1-tridecanol	3.65	−3.81	Soluble	Yes	No	No	No	No	−3.62 cm/s
Undecane	3.59	−3.78	Soluble	Yes	No	No	No	No	−3.31 cm/s
Pentanal	1.52	−0.86	Very soluble	No	No	No	No	No	−6.05 cm/s
Octanal	2.29	−1.95	Very soluble	No	No	No	No	No	−5.15 cm/s
Nonanal	2.44	−2.31	Soluble	No	No	No	No	No	−4.85 cm/s
Decanal	2.72	−2.67	Soluble	No	No	No	No	No	−4.56 cm/s
3-methylbutanal	1.49	−0.87	Very soluble	No	No	No	No	No	−6.12 cm/s
3-tridecanone	3.58	−3.62	Soluble	Yes	No	No	No	No	−3.89 cm/s
4-methyl-2-heptanone	2.25	−1.81	Very soluble	No	No	No	No	No	−5.46 cm/s
Hexadecanal	4.15	−4.85	Moderately soluble	Yes	No	No	No	No	−2.76 cm/s
Di-tert-butyl-dicarbonate	2.73	−2.48	Soluble	No	No	No	No	No	−5.74 cm/s
5-methylundecane	3.72	−4.42	Moderately soluble	No	No	Yes	No	No	−2.77 cm/s
2-ethyl-4-methyl-1-pentanol	2.34	−1.88	Very soluble	No	No	No	No	No	−5.40 cm/s
Pentanoic Acid	1.32	−1.15	Very soluble	No	No	No	No	No	−5.94 cm/s
4-methyldecane	3.49	−4.05	Moderately soluble	No	No	No	No	No	−3.08 cm/s
2,6-dimethylundecane	3.89	−4.66		No	No	No	No	No	−2.68 cm/s

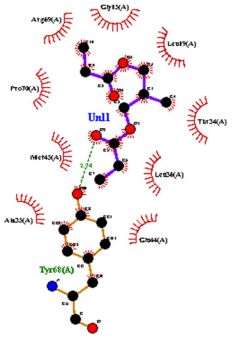
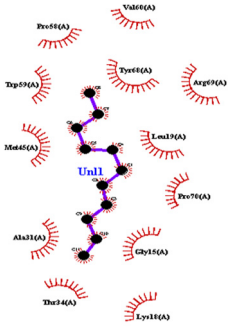
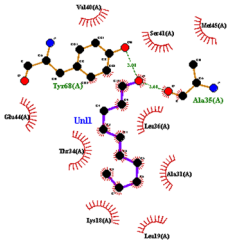
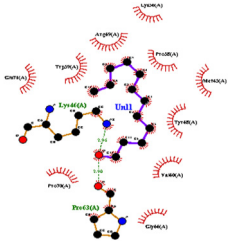
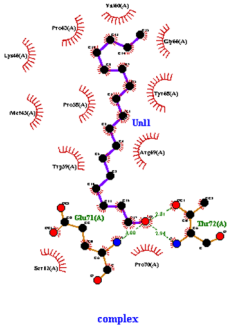
(Continued)

Table S2: *Continued*

Name (Accession code)	Lipo-philicity	Water solubility		Pharmacokinetics					
	Log $P_{o/w}$ (iLogP)	Log *S* (ESOL)	Class [a]	CYP1A2 inhibitor	CYP2C19 inhibitor	CYP2C9 inhibitor	CYP2D6 inhibitor	CYP3A4 inhibitor	Log K_p (skin permeation)
			Moderately soluble						
Ethyne	1.21	−0.25	Very soluble	No	No	No	No	No	−6.18 cm/s
Ethylene oxide	1.17	−0.02	Very soluble	No	No	No	No	No	−6.68 cm/s
Cyclobutanol	1.37	−0.57	Very soluble	No	No	No	No	No	−6.42 cm/s
1-nonene	2.96	−3.47	Soluble	No	No	No	No	No	−3.41 cm/s
Fluoroethyne	1.25	−0.64	Very soluble	No	No	No	No	No	−5.97 cm/s
2-octenal	2.21	−1.94	Very soluble	No	No	No	No	No	−5.22 cm/s
Benzene ethanol 21965192	2.07	−2.39	Soluble	Yes	No	No	No	No	−5.61 cm/s
2-ethynyloxy-ethanol	—	—	—	—	—	—	—	—	—
1,3-bis(1,1-dimethyl-ethyl)benzene	—	—	—	—	—	—	—	—	—
Formic acid	0.27	0.00	Highly soluble	No	No	No	No	No	−6.72 cm/s
4-methyldecane	3.49	−4.05	Moderately soluble	No	No	No	No	No	−3.08 cm/s
Trimethyl pyrazine	1.73	−1.69	Very soluble	No	No	No	No	No	−6.37 cm/s
3-ethyl-2,5-dimethylpyrazine	1.98	−2.02	Soluble	No	No	No	No	No	−6.05 cm/s
4-methyl-2-pentanone,	1.99	−0.67	Very soluble	No	No	No	No	No	−6.85 cm/s
2-ethoxy-2-methylpropane	2.28	−1.24	Very soluble	No	No	No	No	No	−5.91 cm/s
Acetaldehyde	0.80	0.06	Highly soluble	No	No	No	No	No	−6.76 cm/s
2-butynoic acid	0.98	−0.85	Very soluble	No	No	No	No	No	−6.26 cm/s

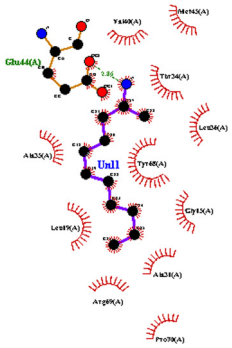
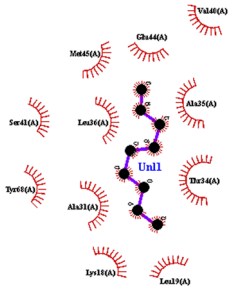
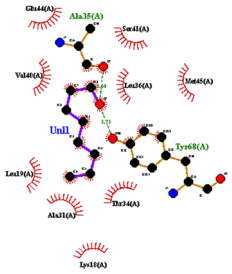
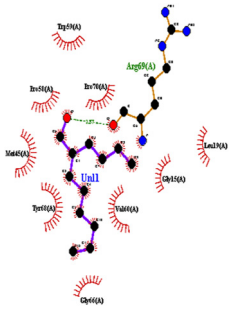
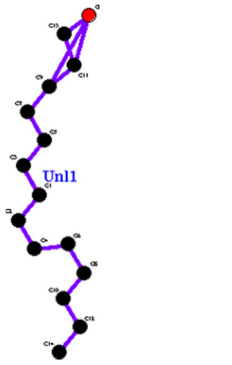
[a]S: Soluble; VS: Very soluble.

Table S3: The binding energy and the interactions between the active site of Lea protein and the compounds with the highest binding energy

ligand	Name	Binding energy	Inhibit constant	Amino acids involved in the reaction
1	1,3-Propanediol, 2-methyl-, dipropanoate	−4.26	759.46 μM	
2	1,4-Undecadiene	−4.52	484.6 μM	
3	1-Decanol	−4.51	495.34 μM	
4	1-Dodecanol	-4.43	565.45 μM	
5	1-Heptadecanol	−4.68	372.11 μM	

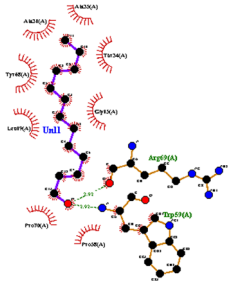
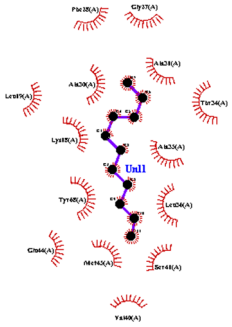
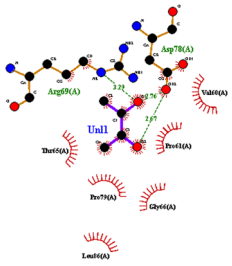
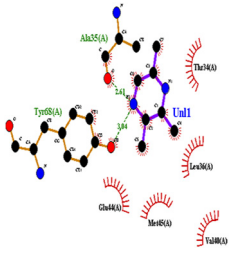
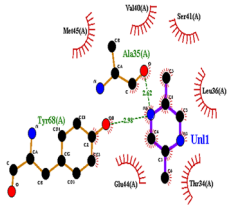
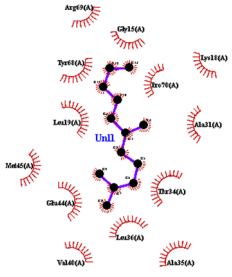
(Continued)

Table S3: *Continued*

ligand	Name	Binding energy	Inhibit constant	Amino acids involved in the reaction
6	1-methyldecylamine	−4.9	254.89 μM	
7	1-Nonene	−4.06	1.06 mM	
8	1-Octanol	−3.98	1.22 mM	
9	1-Octanol, 2-butyl-	−4.53	475.87 μM	
10	1-Tetradecanol	−4.84	282.7 μM	

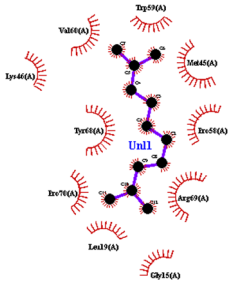
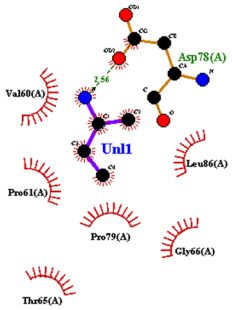
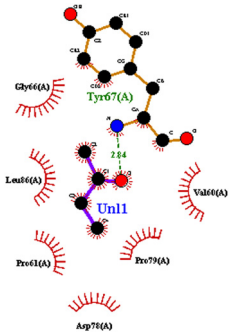
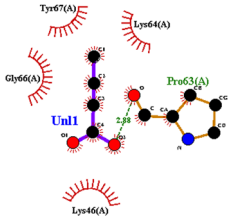
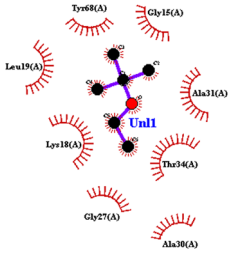
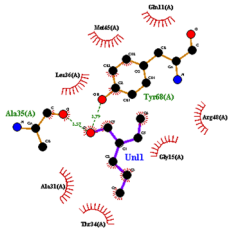
(Continued)

Table S3: *Continued*

ligand	Name	Binding energy	Inhibit constant	Amino acids involved in the reaction
11	1-Tridecanol	−4.57	444.69 μM	
12	1-Undecene	−4.49	511.52 μM	
13	2 R ,3 R - Butanediol	−3.04	5.9 mM	
14	2,3,5-Trimethylpyrazine	−4.11	979.28 μM	
15	2,5-Dimethylpyrazine	−3.71	1.9 mM	
16	2,6-Dimethylundecane	−5.08	188.13 μM	

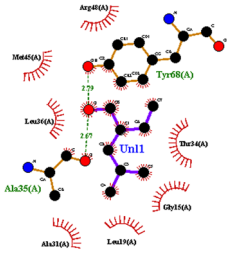
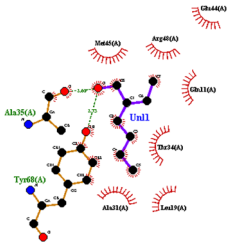
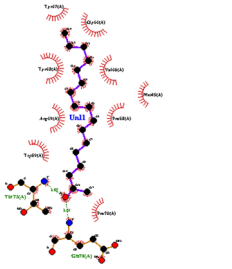
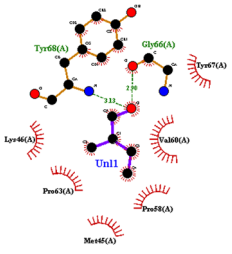
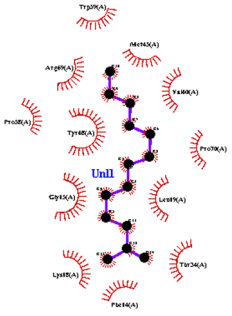
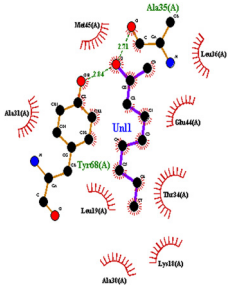
(Continued)

Table S3: *Continued*

ligand	Name	Binding energy	Inhibit constant	Amino acids involved in the reaction
17	2,9-Dimethyldecane	−4.79	310.33 µM	
18	2-butanamine	−3.95	1.28 mM	
19	2-Butanone	−3.09	5.43 mM	
20	2-Butynoic acid	−3.46	2.91 mM	
21	2-ethoxy-2-methylpropane	−3.24	4.23 mM	
22	2-Ethyl-1-pentanol	−3.54	2.55 mM	

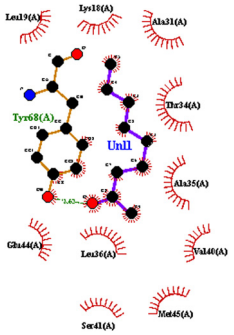
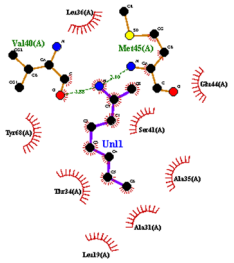
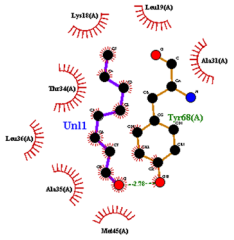
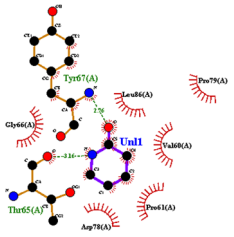
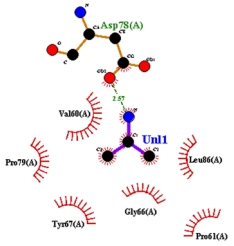
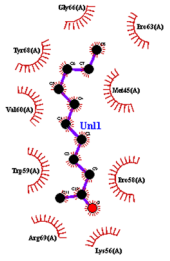
(Continued)

Table S3: *Continued*

ligand	Name	Binding energy	Inhibit constant	Amino acids involved in the reaction
23	2-Ethyl-4-methylpentan-1-ol	−4.17	873.6 μM	
24	2-Ethylhexanol	−4.02	1.12 mM	
25	2-Heptadecanone	−4.84	284.51 μM	
26	2-Methyl-1-butanol	−3.24	4.18 mM	
27	2-Methyl-1-tridecene	−4.88	266.79 μM	
28	2-Nonanol	−4.48	516.96 μM	

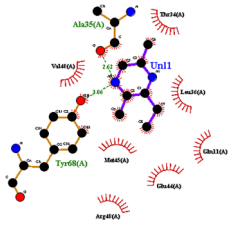
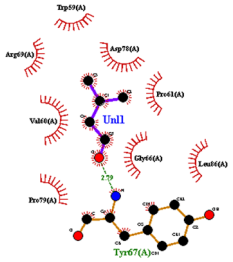
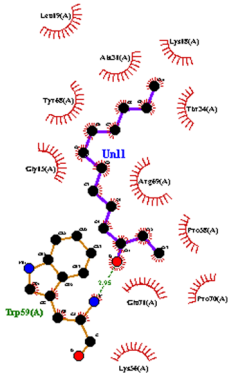
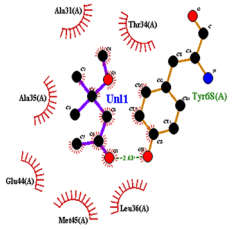
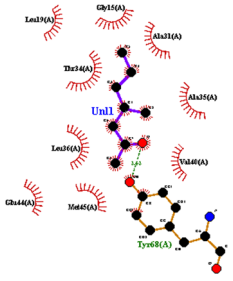
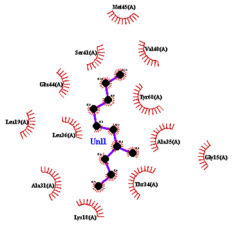
(Continued)

Table S3: *Continued*

ligand	Name	Binding energy	Inhibit constant	Amino acids involved in the reaction
29	2-Nonanone	−4.62	409.99 μM	
30	2-octanamine	−4.5	499.74 μM	
31	2-Octenal	−4.34	654.75 μM	
32	2-piperidinone	−4.16	900.01 μM	
33	2-propanamine	−3.76	1.77 mM	
34	2-undecanone	−4.67	377.37 μM	

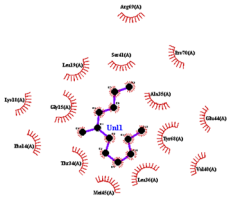
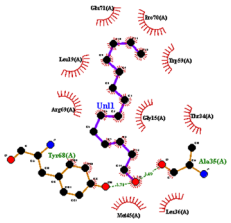
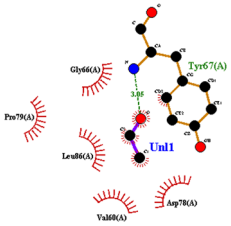
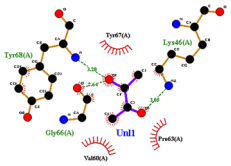
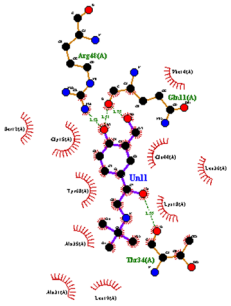
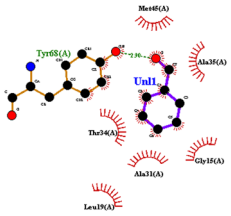
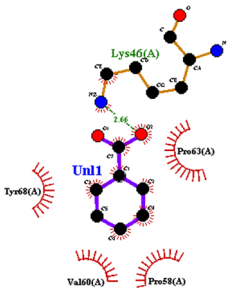
(Continued)

Table S3: *Continued*

ligand	Name	Binding energy	Inhibit constant	Amino acids involved in the reaction
35	3-Ethyl-2,5-dimethylpyrazine	−4.31	698.39 μM	
36	3-Methylbutanal	−3.21	4.44mM	
37	3-Tridecanone	−4.93	241.64 μM	
38	4-Methoxy-4-methyl-2-pentanone	−3.88	1.43 mM	
39	4-Methyl-2-heptanone	−4.46	536.89 μM	
40	4-Methyldecane	−4.62	409.99 μM	

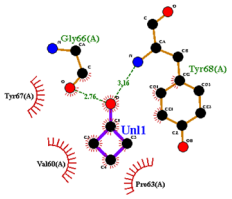
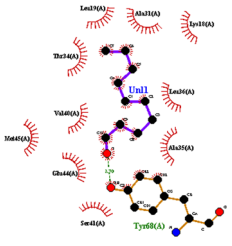
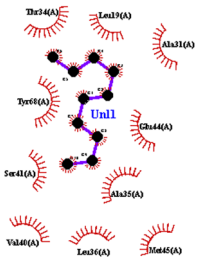
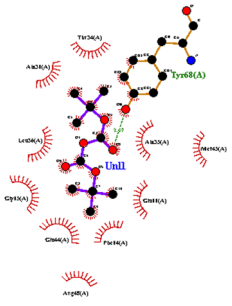
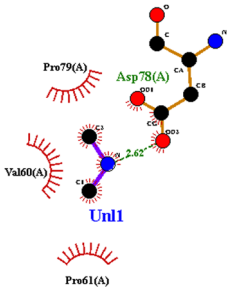
(Continued)

Table S3: *Continued*

ligand	Name	Binding energy	Inhibit constant	Amino acids involved in the reaction
41	5-Methylundecane	−4.65	389.76 μM	
42	13-Tetradecadien-1-ol	−5.07	191.81 μM	
43	Acetaldehyde	−2.27	21.82 mM	
44	Acetoin	−3.28	3.93 mM	
45	Albuterol	−6.01	39.0 μM	
46	Benzaldehyde	−4.05	1.07 mM	
47	Benzoic acid	−4.53	478.14 μM	

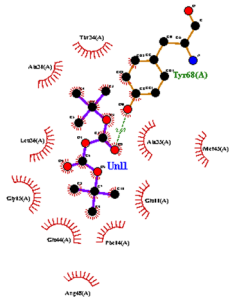
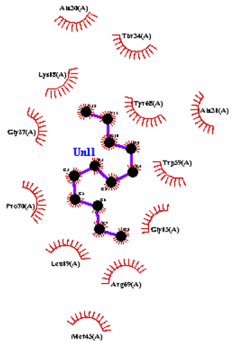
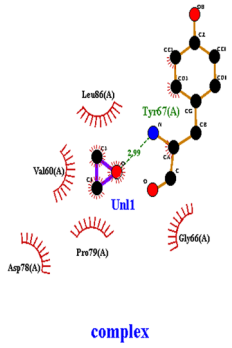
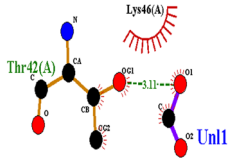
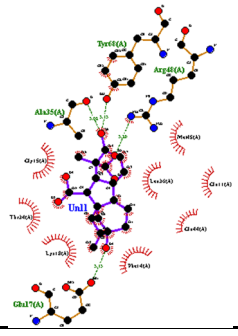
(Continued)

Table S3: *Continued*

ligand	Name	Binding energy	Inhibit constant	Amino acids involved in the reaction
48	Cyclobutanol	−3.27	4.03 mM	
49	Cyclohexasiloxane, dodecamethyl	—	—	—
50	Cyclopropylmethanol	−2.72	10.17 mM	—
51	Cyclotetrasiloxane, octamethyl-	—	—	—
52	Decanal	−4.18	863.45 μM	
53	Decane	−4.09	1.01 mM	
54	Dimethyl disulfide	−2.36	18.65 mM	
55	Dimethylamine	−2.6	12.53 mM	

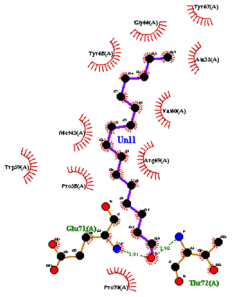
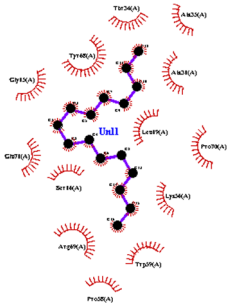
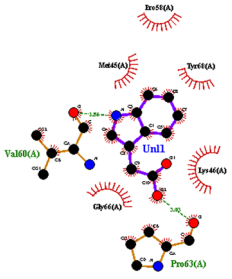
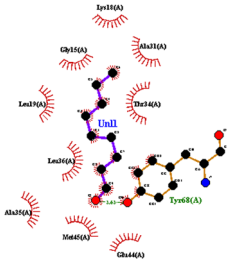
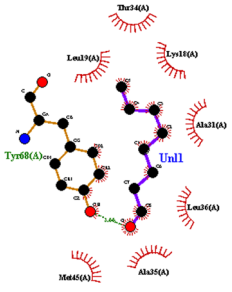
(Continued)

Table S3: *Continued*

ligand	Name	Binding energy	Inhibit constant	Amino acids involved in the reaction
56	Di-tert-butyl dicarbonate	−4.69	364.78 μM	
57	Dodecane	−4.34	663.98 μM	
58	Ethylene oxide	−1.94	38.1 mM	 complex
59	Ethyne	−1.79	48.83 mM	—
60	Fluoroethyne	—	—	
61	Formic acid	−2.8	8.9 mM	
62	Gibberellic acid	−7.78	1.99 μM	

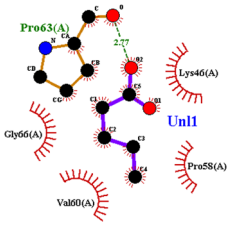
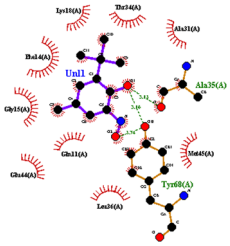
(Continued)

Table S3: *Continued*

ligand	Name	Binding energy	Inhibit constant	Amino acids involved in the reaction
63	Hexadecanal	−4.91	252.17 μM	
64	Hexadecane	−4.61	414.54 μM	
65	Indole-3-acetic acid	−6.09	34.47 μM	
66	Methylphosphonic acid	—	—	
67	Nonanal	−3.87	1.46 mM	
68	Octanal	−3.93	1.32 mM	

(Continued)

Table S3: *Continued*

ligand	Name	Binding energy	Inhibit constant	Amino acids involved in the reaction
69	Pentanoic Acid	−4.02	1.14 mM	
70	Phenol,2-(1,1-dimethylethyl)-4-methyl	−6.38	21.11 μM	
71	Undecane	−3.98	1.21 mM