Supplementary Materials

Efficacy of Phytochemicals Derived from *Avicennia officinalis* for the Management of COVID-19: A Combined In Silico and Biochemical Study

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Citation: Mahmud, S.; Paul, G.K.; Afroze, M.; Islam, S.; Gupt, S.B.R.; Razu, M.H.; Biswas, S.; Zaman, S.; Uddin, S.; Khan, M.; et al. Efficacy of Phytochemicals Derived from *Avicennia officinalis* for the Management of COVID-19: A Combined In Silico and Biochemical Study. *Molecules* **2021**, *26*, 2210. https://doi.org/10.3390/molecules26082210

Received: 12 March 2021
Accepted: 9 April 2021
Published: 12 April 2021

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Table S1. Free radical scavenging activity of methanolic extract of *Avicennia officinalis* with standard BHT concentrations.

Name of Samples	Conc. (µg/ml)	Absorbance (Mean ± SD)	% of Scavenging Activity	IC_{50} (µg/ml)
BHT	50	0.281 ± 0.007	61.56	11.24
	100	0.125 ± 0.059	82.85	
	150	0.036 ± 0.006	95.08	
Leaf	50	0.075 ± 0.010	89.73	41.17
	100	0.050 ± 0.007	93.17	
	150	0.029 ± 0.008	95.97	
Fruits	50	0.141 ± 0.021	80.56	47.22
	100	0.083 ± 0.010	88.54	
	150	0.055 ± 0.008	92.48	

Here, BHT: butylated hydroxytoluene.

Table S2. Cytotoxic mortality percentage of leaf and fruits extract of *Avicennia officinalis* against *Artemia salina.*

Concentration (µg/ml)	**No. of Artemia Taken**	**Mean± SD value of Live Artemia**		**Mortality Percentage**		**LC_{50} µg/mL**	
		Fruits	Leaf	Fruits	Leaf	Leaf	Fruits
25	15	14.00 ± 1.00	14.67 ± 0.58	6.67	2.22	217.77	179.78
50		11.00 ± 2.00	13.33 ± 0.58	26.67	11.11		
100		8.00 ± 1.00	9.67 ± 2.08	46.67	35.56		
200		5.67 ± 0.58	6.67 ± 2.08	62.22	55.56		
300		3.33 ± 1.53	4.67 ± 0.578	77.78	68.89		
400		1.33 ± 4.93	6.33 ± 0.578	91.11	88.89		
500		0.00 ± 0.00	0.33 ± 0.578	100	97.78		

Table S3. Phytochemical compounds identification from *Avicennia officinalis* plant leaves extract by GC-MS.

SL. No.	Compound Name	Retention Time	% Peak Area
1.	Name: (8*Z*,11*Z*,14*Z*)-icosa-8,11,14-trienoic acid Formula:$C_{20}H_{34}O_2$ MW: 306.5	3.519	1.423
2.	Name: 2-(3methoxyanilino)benzoic acid Formula: $C_{14}H_{13}NO_3$ MW: 243.26	3.796	1.675
3.	Name: 2,4-di-*tert*-butylphenol Formula: $C_{14}H_{22}O$ MW: 206.32	11.05	2.656
4.	Name: Methyl (*Z*)-hexadec-9-enoate Formula: $C_{17}H_{32}O_2$ MW: 268.4	15.775	1.160
5.	Name: Methyl hexadecanoate Formula: $C_{17}H_{34}O_2$ MW: 270.5	16.127	7.715
6.	Name: Methyl 3-(3,5-di*tert*-butyl-4-hydroxyphenyl)propanoate Formula: $C_{18}H_{28}O$ MW: 292.4	16.275	1.280
7.	Name: Methyl (9*Z*,12*Z*)-octadeca-9,12-dienoate Formula: $C_{19}H_{34}O_2$ MW: 294.5	18.84	1.543

8.	Name: Methyl (*E*)-11-hydroperoxyoctadec-9-enoate Formula: $C_{19}H_{36}O_4$ MW: 328.5	18.947	4.330
9.	Name: (*E*,7*R*,11*R*)-3,7,11,15-tetramethylhexadec-2-en-1-ol Formula: $C_{20}H_{40}O$ MW: 296.5	19.117	3.254
10.	Name: Methyl octadecanoate Formula: $C_{19}H_{38}O_2$ MW: 298.5	19.369	5.251
11.	Name: 1-iododotriacontane Formula: $C_{32}H_{65}I$ MW: 576.8	20.615	1.160
12.	Name: (*Z*)-5-methylhenicos-6-en-11-one Formula: $C_{22}H_{42}O$ MW: 322.6	22.135	1.208
13.	Name: 1,38-dibromooctatriacontane Formula: $C_{38}H_{76}Br_2$ MW: 692.8	22.252	1.651
14.	Name: 1,54-dibromotetrapentacontane Formula: $C_{54}H_{108}Br_2$ MW: 917.2	25.45	1.112

15.	Name: (*Z*)-*N*-(2-hydroxyethyl)octadec-9-enamide Formula: $C_{20}H_{39}NO_2$ MW: 325.5	23.257	21.818
16.	Name: 1,54-dibromotetrapentacontane Formula: $C_{54}H_{108}Br_2$ MW: 917.2	23.783	1.567
17.	Name: 2-methyltetracosane Formula: $C_{25}H_{52}$ MW: 352.7	23.905	2.679
18.	Name: 2-methylhexacosane Formula: $C_{27}H_{56}$ MW: 380.7	24.037	3.744
19.	Name: 6-(5-methylheptyl)oxan-2-one Formula: $C_{13}H_{24}O_2$ MW: 212.33	25.03	1.423
20.	Name: 2-methylpropyl 2-methylpentanoate Formula: $C_{10}H_{20}O_2$ MW:172.26	25.08	3.242
21.	Name: Heptadecane Formula: $C_{41}H_{62}FN_5O_{10}$ MW: 804	25.239	1.842
22.	Name: Tetrapentacontane Formula: $C_{54}H_{110}$ MW: 759.4	25.632	2.440

23.	Name: Dioctyl benzene-1,2-dicarboxylate Formula: $C_{24}H_{38}O_4$ MW: 390.6	26.026	2.512
24.	Name: 1-bromotriacontane Formula: $C_{30}H_{61}Br$ MW: 501.7	26.915	1.316
25.	Name: 3-octadecoxypropane-1,2-diol Formula: $C_{21}H_{44}O_3$ MW:344.6	27.015	2.368
26.	Name: 2-hexyldecan-1-ol Formula: $C_{17}H_{38}O_4S$ MW: 338.5	27.17	2.069
27.	Name: [(*E*)-non-1-enyl]cyclohexane Formula: $C_{15}H28$ MW: 208.38	29.07	1.172
28.	Name: (*E*)-pentatriacont-17-ene Formula: $C_{35}H_{70}$ MW: 490.9	29.091	1.220
29.	Name: 10-*tert*-butylperoxy-1,5,9-trimethyl-11,14,15,16-tetraoxatetracyclo[10.3.1.$0^{4,13}$.$0^{8,13}$]hexadecane Formula: $C_{15}H_{24}O_2$ MW: 356.5	29.475	1.220
30.	Name: 2-hydroxy-4*a*,5-dimethyl-3-prop-1-en-2-yl-2,3,4,5,6,7,8,8*a*-octahydronaphthalen-1-one Formula: $C_{15}H_{24}O_2$ MW: 236.35	30.1	1.280

31.	Name: (6*E*,10*E*,14*E*,18*E*)-2,6,10,15,19,23-hexamethyltetracosa-2,6,10,14,18,22-hexaene Formula: $C_{30}H_{50}$ MW: 410.7	30.294	3.038
32.	Name: [(*E*)-2-(8-methoxy-2,15-dimethyl-14-pentacyclo[8.7.0.0^{2,7}.0^{5,7}.0^{11,15}]heptadecanyl)-6-methylhept-4-en-3-yl] 2,2-dimethylpropanoate Formula: $C_{33}H_{54}O_3$ MW: 498.8	32.362	1.280
33.	Name: Ethane;propane;1-[(1E,3Z)-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)cycloocta-1,3-dien-6-yn-1-yl]cyclopropane-1-carboxylic acid Formula: $C_{25}H_{43}BO_4$ MW: 418	38.315	1.950
34.	Name: 2-hydroxy-4*a*,5-dimethyl-3-prop-1-en-2-yl-2,3,4,5,6,7,8,8*a*-octahydronaphthalen-1-one Formula: $C_{15}H_{24}0_2$ MW: 236.35	39.74	1.471

Table S4. Phytochemical compounds identification from *Avicennia officinalis* plant fruits extract by GC-MS.

SL. No.	Compound name	Retention Time	% Peak Area
1.	Name: 2,3,4,5,6,7,8-heptahydroxyoctanal Formula: $C_8H_{16}O_8$ MW: 240.21	3.519	0.84
2.	Name: 1-propan-2-yl-3,6-diazatricyclo[4.3.1.1^{3,8}]undecan-9-one Formula: $C_{12}H_{20}N_2O$ MW: 208.3	3.56	0.86
3.	Name: Butyl undec-10-enoate Formula: $C_{15}H_{28}O_2$ MW: 240.38	3.59	0.88
4.	Name: 2,3-dimethoxy-1,4-dioxane Formula: $C_6H_{12}O_4$ MW: 148.16	3.656	2.39
5.	Name: 3-ethoxypropane-1,2-diol Formula: $C_5H_{12}O_3$ MW: 120.15	3.735	1.81
6.	Name: 3-[2-hydroxy-3-[(9Z,11Z)-octadeca-9,11-dienoyl]oxypropoxy]carbonylbenzoic acid Formula: $C_3H_8O_3$ MW: 92.09	3.772	1.22
7.	Name: Cyclopent-2-en-1-one Formula: C_5H_6O MW: 82.1	3.829	1.00
8.	Name: 2-[2-(2-methoxyethoxy)ethoxy]ethyl 2-methylpropyl carbonate	3.915	0.55

	Formula: $C_{12}H_{24}O_6$ MW: 264.31		
9.	Name: (2*S*)-2-amino-3-methylbutan-1-ol Formula: $C_5H_{13}NO$ MW: 103.16	4.407	1.02
10.	Name: Cyclopentane-1,2-dione Formula: C_5H_6O2 MW: 98.1	4.817	3.39
11.	Name: Prop-2-enyl formate Formula: $C_4H_6O_2$ MW: 86.09	5.575	1.23
12.	Name: 5-methyl-1*H*-pyrimidine-2,4-dione Formula: $C_5H_6N_2O_2$ MW: 126.11	6.556	0.54
13.	Name: 2,4,6-trimethyloctane Formula: $C_{11}H_{24}$ MW: 156.31	6.868	0.37
14.	Name: 2,3-dihydro-1-benzofuran Formula: C_8H_8O MW: 120.15	8.174	0.86
15.	Name: 4-ethenyl-2-methoxyphenol Formula: $C_9H_{10}O_2$ MW: 150.17	9.227	0.38
16.	Name: Cyclohexylmethyl hexadecyl sulfite Formula: $C_{23}H_{46}O_3S$ MW: 402.7	9.611	0.96

17.	Name: 6-(1-hydroxy-3-methylcyclohex-3-en-1-yl)-3-methylcyclohex-2-en-1-one Formula: $C_{14}H_{20}O_2$ MW: 220.31	10.125	0.53
18.	Name: 2-(hydroxymethyl)-2-nitropropane-1,3-diol - Formula: $C_4H_6NO_6P$ MW: 195.07	10.324	3.59
19.	Name: Methyl 3-hydroxypropanoate Formula: $C_4H_8O_3$ MW: 104.1	10.465	0.42
20.	Name: 2,4-di*tert*-butylphenol Formula: $C_{14}H_{22}O$ MW:206.32	11.049	0.53
21.	Name: 2-methylundecan-5-ol Formula: $C12H_{26}O$ MW: 186.33	11.246	0.46
22.	Name: [(2*R*,3*R*,4*S*,5*R*,6*S*)-6-methoxy-3,4,5-tris(trimethylsilyloxy)oxan-2-yl]methanol Formula: $C_{16}H_{38}O_6Si_3$ MW: 410.72	11.688	1.02
23.	Name: (2R,3S,4S,5R,6S)-2-(hydroxymethyl)-6-methoxyoxane-3,4,5-triol Formula: $C_7H_{14}O_6$ MW: 194.18	11.852	55.24
24.	Name: Methyl hexadecanoate Formula: $C_{17}H_{34}O_2$ MW: 270.5	16.121	1.21

25.	Name: Methyl (*Z*)-octadec-9-enoate Formula: $C_{19}H_{36}O2$ MW: 296.5	18.947	0.39
26.	Name: Methyl octadecanoate Formula: $C_{19}H_{36}O_2$ MW: 296.5	19.363	0.68
27.	Name: (*Z*)-*N*-(2-hydroxyethyl)octadec-9-enamide Formula: $C_{38}H_{35}NO$ MW: 281.5	23.253	8.07
28.	Name: Ooctacosane Formula: $C_{28}H_{58}$ MW: 394.8	24.037	0.40
29.	Name: Hexacontane Formula: $C_{60}H_{122}$ MW: 843.6	25.092	0.35
30.	Name: 4-*O*-heptan-4-yl 1-*O*-tridec-2-ynyl butanedioate Formula: $C_{24}H_{42}O_4$ MW:394.6	25.215	0.36
31.	Name: 11-methyltricosane Formula: $C_{24}H50$ MW: 338.7	25.378	0.36
32.	Name: 1-nonoxyicosane Formula: $C_{29}H_{60}O$ MW: 424.8	25.492	0.73
33.	Name: 1-(6-methylheptan-2-yl)-4-(4-methylpentyl)cyclohexane Formula:$C_{20}H_{40}$	26.135	0.47

	MW: 280.5		
34.	Name: Undecan-5-ylcyclohexane Formula: $C_{17}H_{34}$ MW: 238.5	26.248	0.35
35.	Name: Methyl 3-[methyl-(3-methyl-5-nitroimidazol-4-yl)amino]propanoate Formula: $C_9H_{14}N_4O_4$ MW: 242.23	26.415	0.59
36.	Name: 1-propoxytetratriacontane Formula: $C_{37}H_{76}O$ MW: 537	26.59	0.39
37.	Name: Tetratriacontyl 2,2,3,3,4,4,4-heptafluorobutanoate Formula: $C_{38}H_{69}F_7O_2$ MW: 690.9	26.781	0.32
38.	Name: 11-methyltricosane Formula: $C_{24}H_{50}$ MW: 338.7	27.178	0.33
39.	Name: 4-hexadecoxy-3-nitrobenzenesulfonyl fluoride Formula: $C_{22}H_{36}FNO_2S$ MW: 445.6	28.145	0.52
40.	Name: 2-(3-ethyl-3,6,10,13,14-pentamethylpentadecyl)-1,1,3,6-tetramethylcyclohexane Formula: $C_{32}H_{64}$ MW: 448.8	29.072	0.58
41.	Name: (6*E*,10*E*,14*E*,18*E*)-2,6,10,15,19,23-hexamethyltetracosa-2,6,10,14,18,22-hexaene Formula: $C_{30}H_{50}$ MW:410.7	30.293	0.38

Table S5. Pharmacological assessment of all the compounds.

Parameter	(8*Z*,11*Z*,14*Z*)-icosa-8,11,14-trienoic acid	2-(3methoxyanilino)benzoic acid	2,6-di*tert*-butyl-4-[(3,5-di*tert*-butyl-4-hydroxyphenyl)methyl]phenol	Methyl (*Z*)-hexadec-9-enoate	Methyl hexadecanoate	Methyl 3-(3,5-di*tert*-butyl-4-hydroxyphenyl) propanoate	Methyl (9*Z*,12*Z*)-octadeca-9,12-dienoate	Methyl (*E*)-8-hydroperoxyoctadec-9-enoate
Molecular Weight	306.5	243.262	206.32	268.4	270.5	292.4	294.5	328.49
LogP	6.44	3.137	3.99	5.42	5.64	4.09	4.03	5.67
Surface Area	136.560	104.838	93.145	119.164	119.853	127.880	131.204	141.731
Blood Brain Barrier	0.9646 (+)	0.8603 (-)	0.9946 (+)	0.9958 (+)	1.0000 (+)	0.9102 (+)	0.9958 (+)	0.9675 (+)
Human Intestinal Absorption	0.9087 (+)	0.9149 (+)	0.9928 (+)	0.9567 (+)	0.6286 (-)	0.9918 (+)	0.9567 (+)	0.9419 (+)
P-Glycoprotein Inhibitor	0.6699 (-)	0.7873 (-)	0.9680 (-)	0.8083 (-)	0.8550 (-)	0.9272 (-)	0.7265 (-)	0.6029 (-)
AMES Toxicity	0.9674 (-)	0.8360 (-)	0.9494 (-)	0.9321 (-)	0.9765 (-)	0.8612 (-)	0.9296 (-)	0.8053 (-)
HERG Inhibition	0.9133 (WI)	0.9391 (WI)	0.9482 (WI)	0.8861 (WI)	0.9104 (WI)	0.9582 (WI)	0.9026 (WI)	0.8879 (WI)
Hepatotoxicity	No	No	No	No	No	No	No	No

Parameter	(*E*,7*R*,11*R*)-3,7,11,15-tetramethylhexadec-2-en-1-ol	Methyl octadecanoate	1-iododotriacontane	(*Z*)-5-methylhenicos-6-en-11-one	1,38-dibromooctatriacontane	1,54-dibromotetrapentacontane	(*Z*)-*N*-(2-hydroxyethyl)octadec-9-enamide	1,54-dibromotetrapentacontane
Molecular Weight	296.5	298.5	576.8	322.6	692.8	917.2	325.5	917.2
LogP		6.42	6.3611.14	7.64	15.82	22.06	5.13	22.06
Surface Area	133.778	132.583	225.314	145.875	271.977	373.816	143.489	373.816
Blood Brain Barrier	0.9375(+)	0.9848	1.000 (+)	0.9871 (+)	1.0000 (+)	1.0000(+) 1.0000(+)	0.9652 (+)	1.0000(+) 1.0000 (+)
Human Intestinal Absorption	0.9846(+)	0.9881 (+)	0.866 (+)	0.9797 (+)	0.9841 (+)	0.7509 (+)	0.8112 (+)	0.7509 (+)
P-Glycoprotein Inhibitor	0.8620 (-)	0.8222 (-)	0.7973 (-)	0.6918 (-)	0.7558 (-)	0.7558 (-)	0.7725 (-)	0.7558 (-)
AMES Toxicity	0.9132 (-)	0.9765 (-)	0.9550 (-)	0.9383 (-)	0.8988 (-)	0.8988 (-)	0.8778 (-)	0.8988 (-)
HERG Inhibition	0.7838 (WI)	0.9104 (WI)	0.8538 (WI)	0.7441 (WI)	0.7740 (WI)	0.7740 (WI)	0.9499 (WI)	0.7740 (WI)
Hepatotoxicity	No	No	No	No	No	No	No	No

Parameter	2-methyltetracosane	2-methylhexacosane	10-methyldodecan-5-olide	Heptadecane	Tetrapentacontane	Dioctyl benzene-1,2-dicarboxylate	1-bromotriacontane	3-octadecoxypropane-1,2-diol
Molecular Weight	352.7	3	172.26	240.475	759.4	390.6	501.7	344.6
LogP	9.85	10.63	2.62	6.88	21.31	5.67	12.32	6.94
Surface Area	161.498	174.228	75.299	110.578	346.081	170.550	207.190	150.740
Blood Brain Barrier	1.0000 (+)	1.0000 (+)	1.0000 (+)	1.0000 (+)	0.9821 (+)	0.9812 (+)	1.0000 (+)	0.9107 (+)
Human Intestinal Absorption	0.9588 (+)	0.9588 (+)	0.9838 (+)	0.8865 (+)	0.8865 (+)	1.0000 (+)	0.8662 (+)	0.8825 (+)
P-Glycoprotein Inhibitor	0.8321 (-)	0.7988 (-)	0.9603 (-)	0.9285 (-)	0.7233 (-)	0.6940 (+)	0.8219 (-)	0.8489 (-)
AMES Toxicity	0.9916 (-)	0.9916 (-)	0.9475 (-)	0.9965 (-)	0.9965 (-)	0.9504 (-)	0.9133 (-)	0.8907 (-)
HERG Inhibition	0.8929 (WI)	0.8929 (WI)	0.8033 (WI)	0.8620 (WI)	0.8620 (WI)	0.8980 (WI)	0.8800 (WI)	0.8696 (WI)
Hepatotoxicity	No	No	No	No	No	No	No	No

Parameter	2-hexyldecan-1-ol	1-cyclohexylnonene	[(*E*)-non-1-enyl]cyclohexane	10-*tert*-butylperoxy-1,5,9-trimethyl-11,14,15,16-tetraoxatetracyclo[10.3.1.0^{4,13}.0^{8,13}]hexadecane	(2-hydroxy-4*a*,5-dimethyl-3-prop-1-en-2-yl-2,3,4,5,6,7,8,8*a*-octahydronaphthalen-1-one	(6*E*,10*E*,14*E*,18*E*)-2,6,10,15,19,23-hexamethyltetracosa-2,6,10,14,18,22-hexaene	[(*E*)-2-(8-methoxy-2,15-dimethyl-14-pentacycloheptadecanyl)-6-methylhept-4-en-3-yl] 2,2-dimethylpropanoate	Ethane;propane;1-[(1E,3Z)-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)cycloocta-1,3-dien-6-yn-1-yl]cyclopropane-1-carboxylic acid
Molecular Weight	338.5	208.38	490.9	356.5	236.35	410.7	498.8	418.4
LogP	4.82	5.48	13.6755	3.9411	2.9549	2.9549	8.08	4.6807
Surface Area	138.007	96.153	224.458	149.825	104.103	189.185	221.087	185.193
Blood Brain Barrier	0.9723 (+)	1.0000 (+)	1.0000 (+)	0.9642 (+)	0.8256 (+)	0.9962 (+)	0.8729 (+)	0.9746 (+)
Human Intestinal Absorption	0.8484 (+)	0.9603 (+)	0.9148 (+)	0.8171 (+)	0.9918 (+)	0.9975 (+)	0.9856 (+)	0.9610 (+)
P-Glycoprotein Inhibitor	0.8356 (-)	0.9578 (-)	0.5954 (-)	0.7059 (-)	0.9046 (-)	0.9803 (-)	0.7129 (-)	0.9046 (-)
AMES Toxicity	0.9798 (-)	0.9911 (-)	0.9901 (-)	0.6536 (-)	0.9457 (-)	0.9518 (-)	0.8666 (-)	0.5294 (-)
HERG Inhibition	0.8899 (WI)	0.7461 (WI)	0.8273 (WI)	0.9563 (WI)	0.9314 (WI)	0.7689 (WI)	0.9653 (WI)	0.9833 (WI)
Hepatotoxicity	No	No	No	No	No	No	No	No

Parameter	2-hydroxy-4*a*,5-dimethyl-3-prop-1-en-2-yl-2,3,4,5,6,7,8,8*a*-octahydronaphthalen-1-one	2,3,4,5,6,7,8-heptahydroxyoctanal	1-propan-2-yl-3,6-diazatricyclo[4.3.1.1^{3,8}]undecan-9-one	Butyl undec-10-enoate	2,3-dimethoxy-1,4-dioxane	3-ethoxypropane-1,2-diol	3-[2-hydroxy-3-[(9Z,11Z)-octadeca-9,11-dienoyl]oxypropoxy]carbonylbenzoic acid	Cyclopent-2-en-1-one
Molecular Weight	236.35	240.21	208.3	240.38	148.16	120.15	92.09	82.102
LogP	2.95	-4.66	0.46			-1.662	-1.6681	0.9055
Surface Area	104.103	91.015	91.417	106.434	60.012	48.901	35.852	36.665
Blood Brain Barrier	0.8256 (+)	0.9028 (-)	0.9891 (+)	0.9974 (+)	0.9652 (+)	0.8485 (+)	0.6136 (+)	0.9845 (+)
Human Intestinal Absorption	0.9975 (+)	0.6807 (+)	0.9712 (+)	0.9962 (+)	0.8520 (+)	0.9907 (+)	0.923 (+)	0.9955 (+)
P-Glycoprotein Inhibitor	0.9046 (-)	0.9576 (-)	0.9575 (-)	0.8219(-)	0.9608 (-)	0.9855 (-)	0.9186 (-)-	0.8672 (-)
AMES Toxicity	0.9457 (-)	0.9132 (-)	0.7157 (-)	0.9406 (-)	0.6787 (-)	0.5335 (-)	0.8278 (-)	0.793 (-)
HERG Inhibition	0.9314 (WI)	0.9883 (WI)	0.8263(WI)	0.8776 (WI)	0.9400 (WI)	0.9403 (WI)	0.9670 (WI)	0.8463 (WI)
Hepatotoxicity	No	No	No	No	No	No	No	No

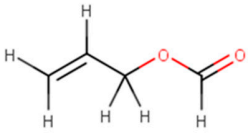
Parameter	2-[2-(2-methoxyethoxy) ethoxy]ethyl 2-methylpropyl carbonate	(2*S*)-2-amino-3-methylbutan-1-ol	Cyclopentane-1,2-dione	Prop-2-enyl formate	5-methyl-1*H*-pyrimidine-2,4-dione	2,4,6-trimethyloctane -	2,3-dihydro-1-benzofuran	4-ethenyl-2-methoxyphenol
Molecular Weight	264.31	103.16	98.1	86.09	126.11	156.31	120.15	150.17
LogP	1.4752	-5.0368	0.3085	0.3454	-0.62838	4.1048	1.6215	2.0438
Surface Area	108.483	103.779	41.516	36.420	50.559	72.389	54.269	65.744
Blood Brain Barrier	0.9353 (+)	0.7320 (-)	0.9819 (+)	0.9813 (+)	0.9790 (+)	0.9813 (+)	0.9868 (+)	0.8480 (+)
Human Intestinal Absorption	0.9887 (+)	0.7897 (-)	0.9898 (+)	0.9800 (+)	0.9742 (+)	0.9958 (+)	1.0000 (+)	0.9904 (+)
P-Glycoprotein Inhibitor	0.7541 (-)	0.5649 (-)	0.6700 (-)	0.9252 (-)	0.9303 (-)	0.8553 (-)	0.9353 (-)	0.6833 (-)
AMES Toxicity	0.6645 (-)	0.8389 (-)	0.5085 (+)	0.9133 (-)	0.9230 (-)	0.9947 (-)	0.6217 (-)	0.9132 (-)
HERG Inhibition	0.8835 (WI)	0.9936 (WI)	0.8807 (WI)	0.9604 (WI)	0.9562	0.9587	0.7106	0.8946
Hepatotoxicity	No	No	No	No	No	No	No	No

Parameter	Cyclohexylmethyl hexadecyl sulfite	6-(1-hydroxy-3-methylcyclohex-3-en-1-yl)-3-methylcyclohex-2-en-1-one	2-(hydroxymethyl)-2-nitropropane-1,3-diol -	Methyl 3-hydroxypropanoate	2,4-di*tert*-butylphenol	2-methylundecan-5-ol	[(2*R*,3*R*,4*S*,5*R*,6*S*)-6-methoxy-3,4,5-tris(trimethylsilyloxy)oxan-2-yl]methanol	(2R,3S,4S,5R,6S)-2-(hydroxymethyl)-6-methoxyoxane-3,4,5-triol
Molecular Weight	402.7	220.31	151.118	104.105	206.329	410.72	410.732	194.18
LogP	7.6599	2.7731	-2.0212	-0.4582	3.9872	3.0103	3.0103	-2.5673
Surface Area	171.781	97.048	56.870	41.903	93.145	156.082	156.082	75.327
Blood Brain Barrier	0.9564 (+)	0.9381(+)	0.5544 (+)	0.9660 (+)	0.9502(+)	0.8362 (+)	0.9868 (+)	0.6148 (-)
Human Intestinal Absorption	1.0000 (+)	1.0000 (+)	0.8455 (+)	0.9432 (+)	0.9941(+)	0.9404 (-)	1.0000 (+)	0.8373(-)
P-Glycoprotein Inhibitor	0.5805 (-)	0.5938 (-)	0.9072 (-)	0.9140 (-)	0.9160 (-)	0.5722 (-)	0.9353 (-)	0.8601 (-)
AMES Toxicity	0.5341 (-)	0.8317 (-)	0.8871 (-)	0.9320 (-)	0.9494 (-)	0.5613 (-)	0.6217 (-)	0.6078 (-)
HERG Inhibition	0.7276 (SI)	0.9297 (WI)	0.9200 (WI)	0.9641 (WI)	0.9482 (WI)	0.9463 (WI)	0.7106 (WI)	0.9535 (WI)
Hepatotoxicity	No	No	No	No	No	No	No	No

Parameter	Methyl hexadecanoate	Methyl (*Z*)-octadec-9-enoate	Methyl octadecanoate	(*Z*)-*N*-(2-hydroxyethyl) octadec-9-enamide	Octacosane	4-*O*-heptan-4-yl 1-*O*-tridec-2-ynyl butanedioate	Succinic acid, tridec-2-yn-1-yl 4-heptyl ester	11-methyltricosane
Molecular Weight	270.5	296.5	298.511	325.537	394.772	843.6	394.6	338.7
LogP	5.6407	6.1969	6.4209	5.1324	11.1688	23.652	6.356	9.4643
Surface Area	119.853	131.894	132.583	5.1324	180.593	384.271	172.682	155.133
Blood Brain Barrier	0.9848 (+)	0.9838 (+)	0.9848 (+)	0.9089 (+)	0.9821 (+)	0.9821 (+)	0.9578 (+)	0.9821 (-)
Human Intestinal Absorption	0.9881 (+)	0.9941 (+)	0.9881 (+)	0.9934 (+)	0.9921 (+)	0.9921 (+)	0.9310 (+)	0.9921 (-)
P-Glycoprotein Inhibitor	0.8951 (-)	0.8472 (-)	0.8951 (-)	0.8468 (-)	0.8985 (-)	0.8985(-)	0.7063 (-)	0.8985 (-)
AMES Toxicity	0.9765 (-)	0.9321 (-)	0.9765 (-)	0.8778 (-)	0.9965 (-)	0.9965(-)	0.9348 (-)	0.8109 (-)
HERG Inhibition	0.9104 (SI)	0.8861 (WI)	0.9104 (WI)	0.9499 (WI)	0.8620 (WI)	0.8620 (WI)	0.9324 (WI)	0.8620 (WI)
Hepatotoxicity	No	No	No	No	No	No	No	No

Parameter	1-nonoxyicosane	1-(6-methylheptan-2-yl)-4-(4-methylpentyl)cyclohexane	Undecan-5-ylcyclohexane	Methyl 3-[methyl-(3-methyl-5-nitroimidazol-4-yl)amino]propanoate	1-propoxytetratriacontane	Tetratriacontyl 2,2,3,3,4,4,4-heptafluorobutanoate	11-methyltricosane	4-hexadecoxy-3-nitrobenzenesulfonyl fluoride
Molecular Weight	424.8	280.5	238.5	242.23	537	690.9	338.7	445.6
LogP	10.7953	7.0815	6.3435	0.3276	13.9161	14.8656	9.4643	7.1131
Surface Area	192.071	128.667	109.572	97.948	242.991	282.676	155.133	180.123
Blood Brain Barrier	0.9870 (+)	0.9791 (+)	0.9825 (+)	0.8499 (+)	0.9870 (+)	0.9931 (+)	0.9813 (+)	0.8613 (+)
Human Intestinal Absorption	0.9958 (+)	0.9901 (+)	0.9950 (+)	0.9244 (+)	0.9958 (+)	1.0000 (+)	0.9914 (+)	1.0000 (+)
P-Glycoprotein Inhibitor	0.8414 (-)	0.9089 (-)	0.9100 (-)	0.6772 (-)	0.8414 (-)	0.8719 (-)	0.8729 (-)	0.6686(+)
AMES Toxicity	0.9102 (-)	0.9559 (-)	0.9957 (-)	0.7878 (-)	0.9102 (-)	0.9296 (-)	0.9934 (-)	0.5111(+)
HERG Inhibition	0.6690 (SI)	0.8517 (WI)	0.8373 (WI)	0.6104 (WI)	0.6690 (WI)	0.9546 (WI)	0.8522 (WI)	0.6502 (WI)
Hepatotoxicity	No	No	No	No	No	No	No	No

Parameter	2-(3-ethyl-3,6,10,13,14-pentamethylpentadecyl)-1,1,3,6-tetramethylcyclohexane	(6*E*,10*E*,14*E*,18*E*)-2,6,10,15,19,23-hexamethyltetracosa-2,6,10,14,18,22-hexaene
Molecular Weight	448.8	410.7
LogP	11.1863	10.605
Surface Area	205.047	189.185
Blood Brain Barrier	0.9876 (+)	0.9442 (+)
Human Intestinal Absorption	0.9956 (+)	0.9895 (+)
P-Glycoprotein Inhibitor	0.7808 (-)	0.7230 (-)
AMES Toxicity	0.9778 (-)	0.9518 (-)
HERG Inhibition	0.9177 (WI)	0.7689 (WI)
Hepatotoxicity	No	No



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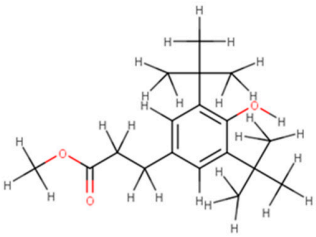

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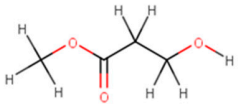

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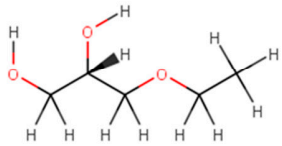

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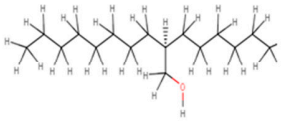

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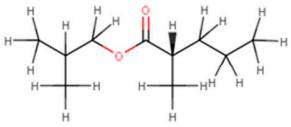

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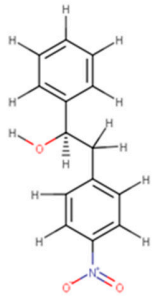

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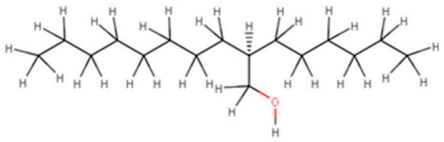

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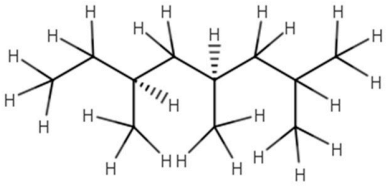

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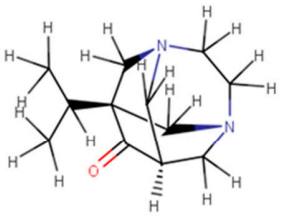

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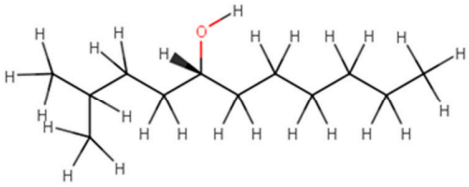

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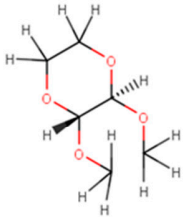

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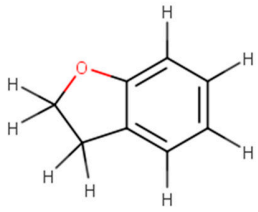

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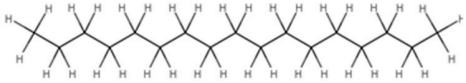

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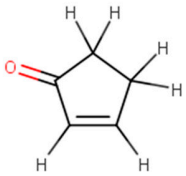

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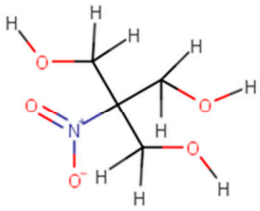

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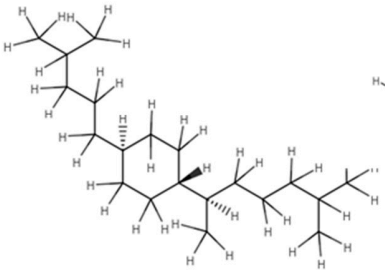

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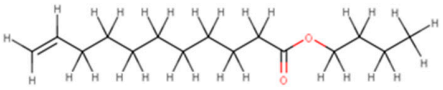

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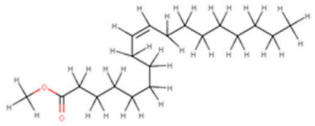

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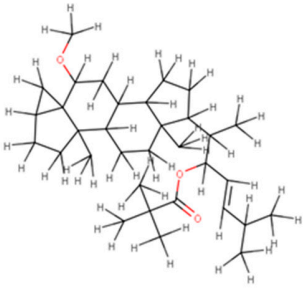

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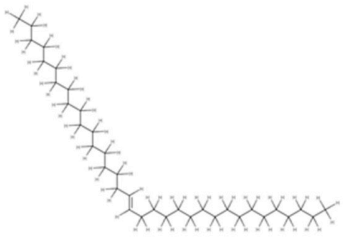

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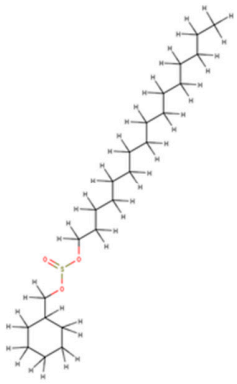

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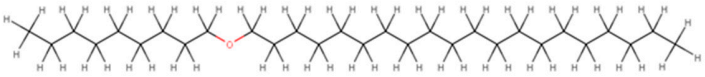

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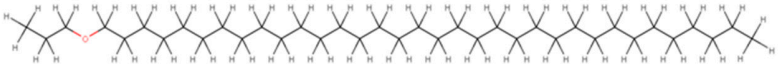

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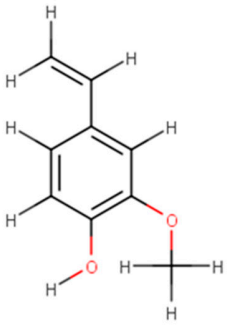

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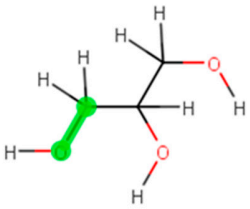

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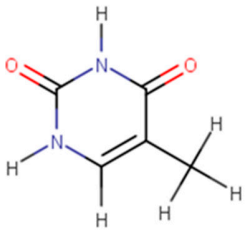

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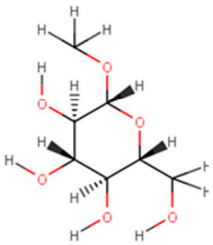

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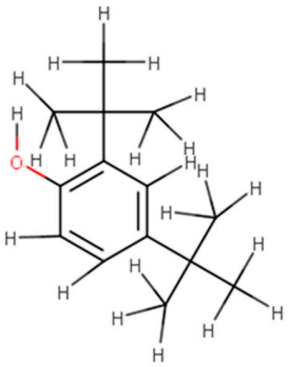

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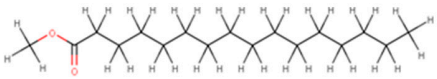

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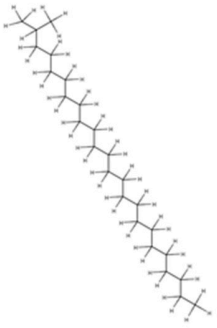

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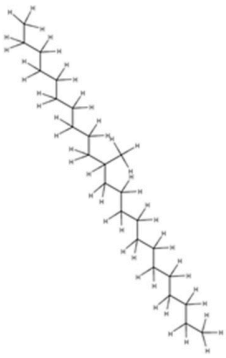

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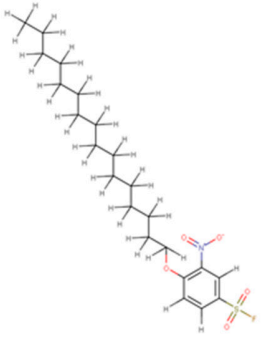

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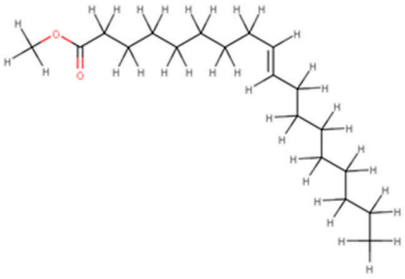

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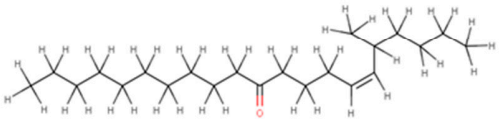

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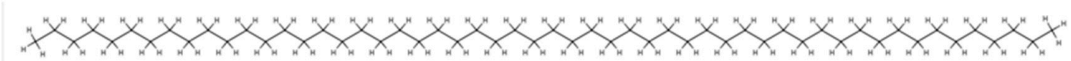

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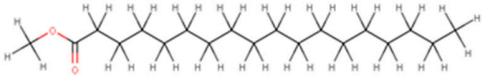

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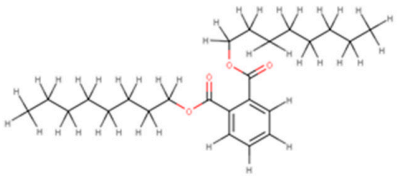

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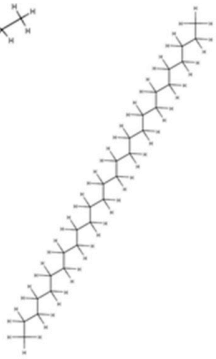

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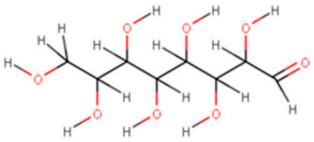

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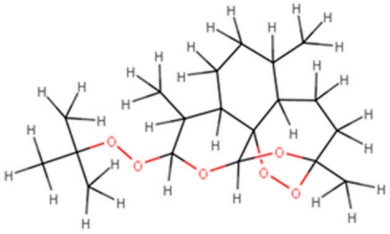

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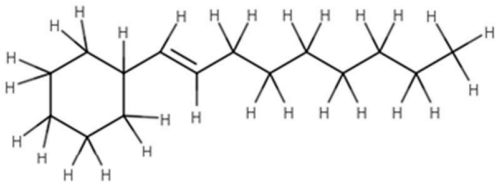

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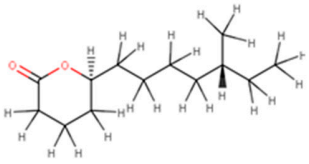

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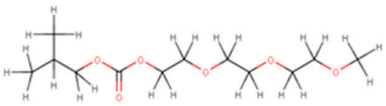

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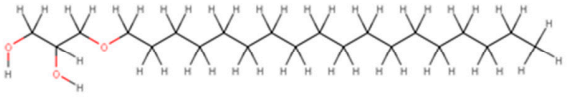

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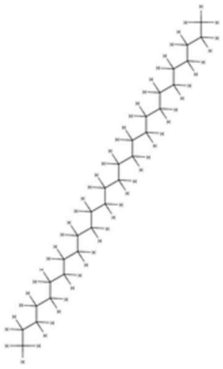

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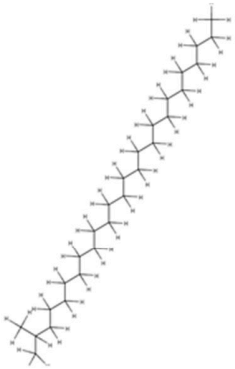

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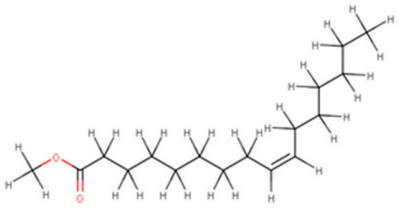

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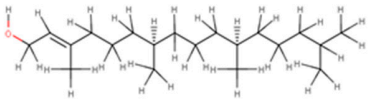

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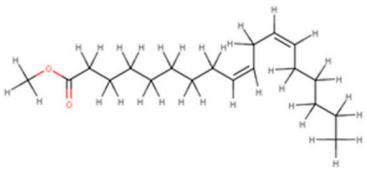

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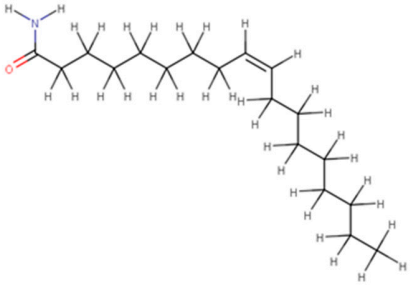

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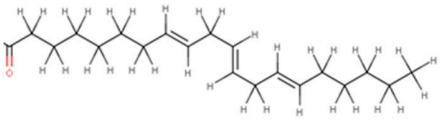

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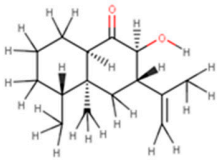

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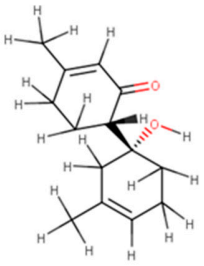

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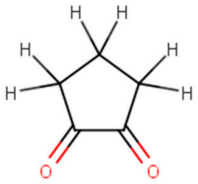

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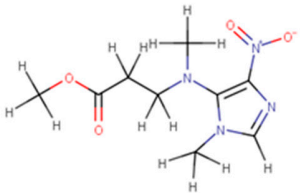

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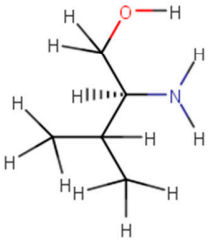

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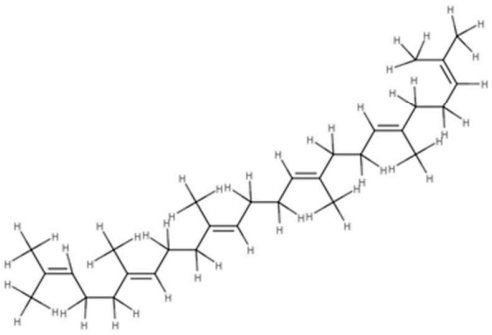

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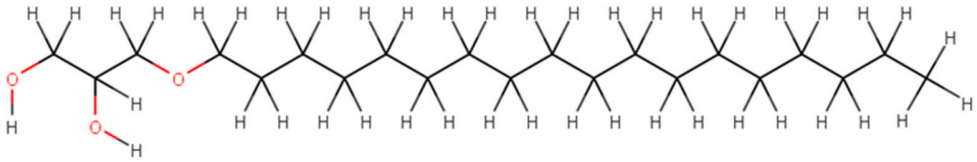

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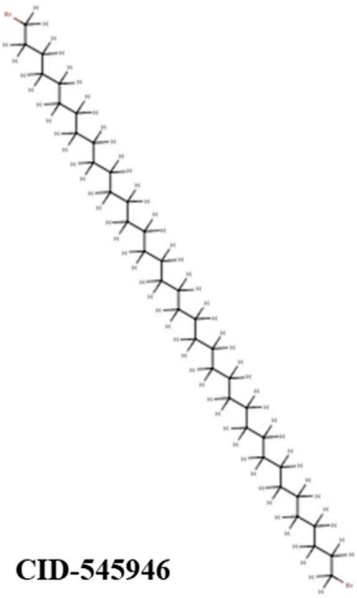

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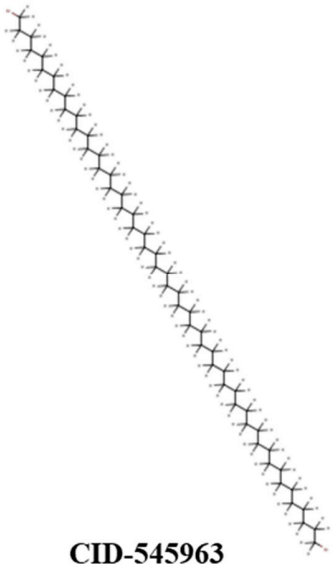

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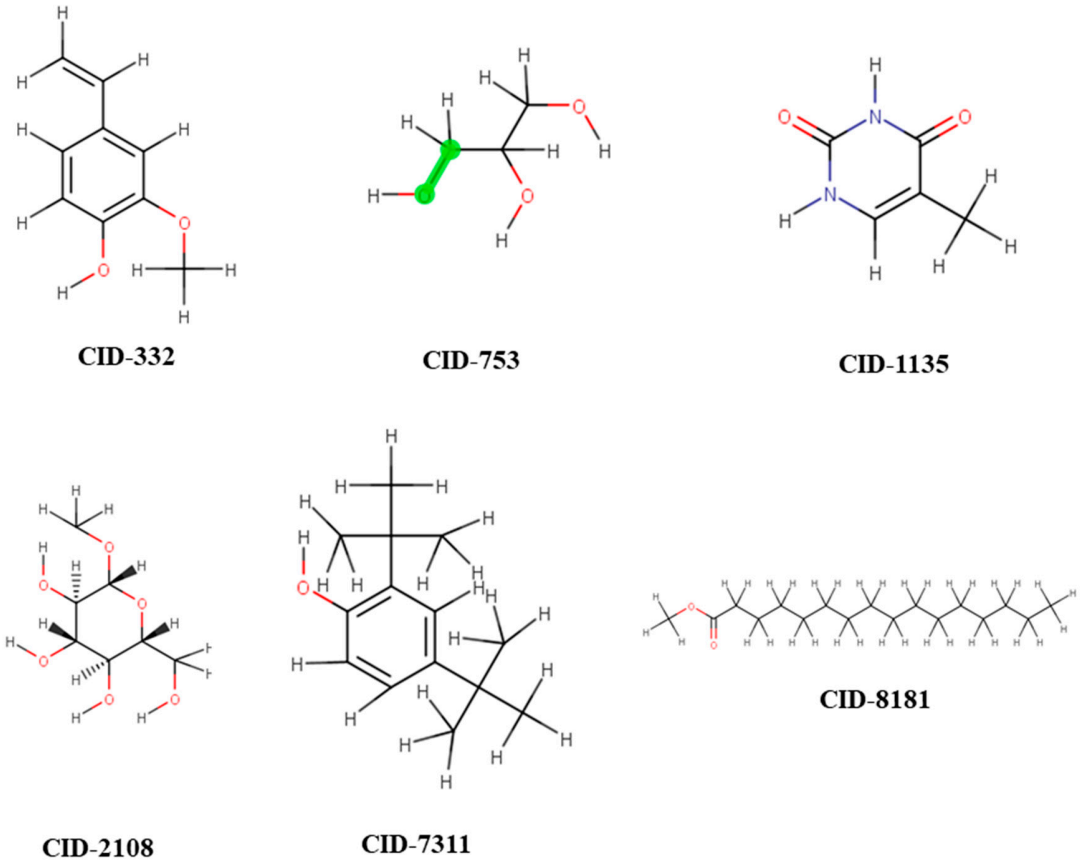

Figure S1: Two dimensional (SD)-structure of *Avicennia officinalis* plant leaf compounds.