Supplementary file on

Natural defense against multi-drug resistant *Pseudomonas aeruginosa*: *Cassia occidentalis* L. *in vitro* and *in silico* antibacterial activity

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Figure S1. Illustrates the morphological changes in *Cassia occidentalis* L. before and after flowering. The images showcase the distinct characteristics of the plant at two different stages, allowing for a visual comparison of its appearance during the pre-flowering and post-flowering phases.

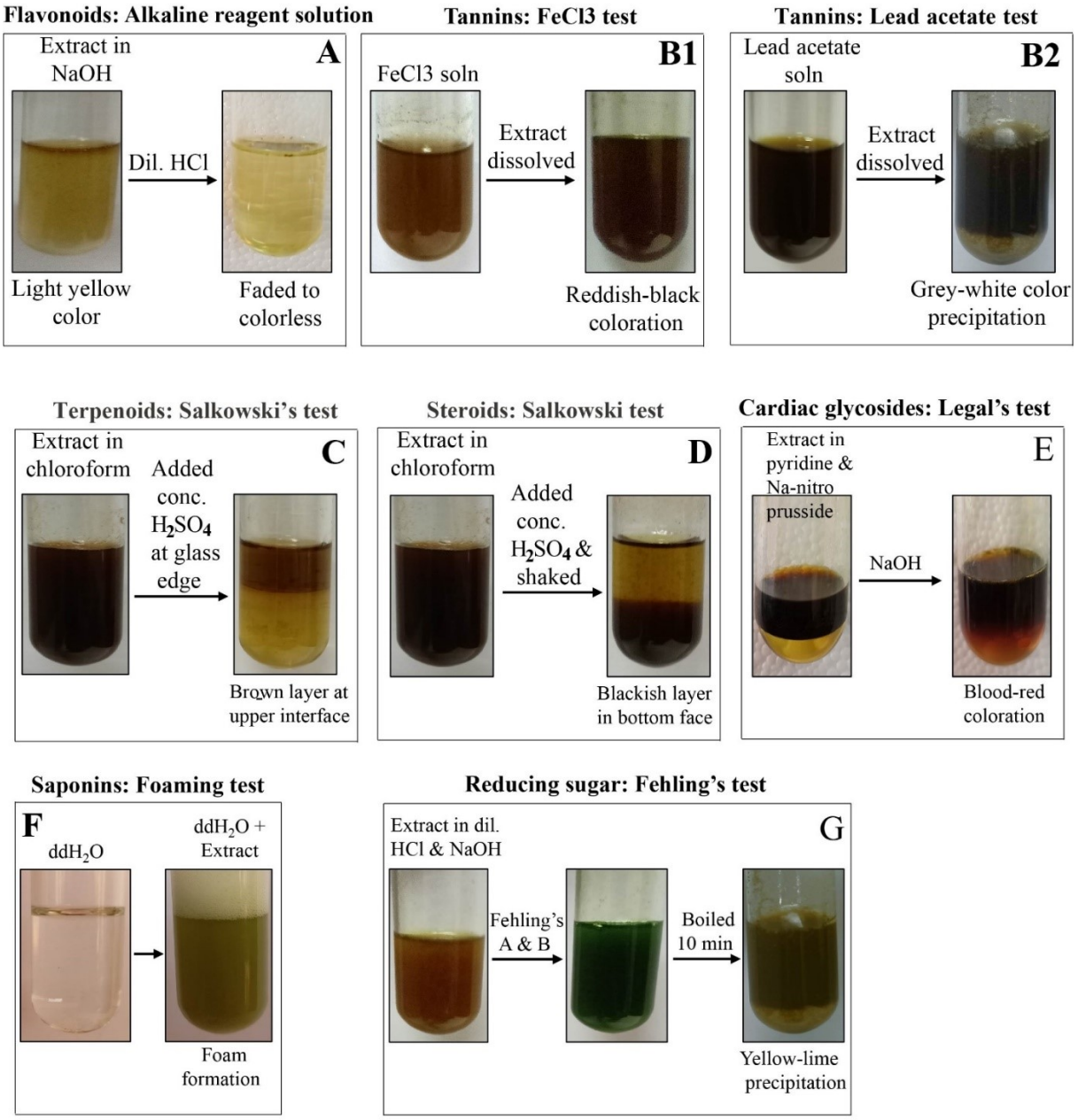


Figure S2. Displays the results of the preliminary phytochemical screening of *C. occidentalis* L. leaves extracts, achieved through color change experiments. The different panels represent the specific tests conducted to identify various phytochemical classes in the plant extract: (A) Alkaline reagent test for flavonoids, (B1) FeCl3 test for tannins, (B2) Lead acetate test for tannins, (C) Salkowski's test for terpenoids, (D) Salkowski's test for steroids, (E) Legal's test for cardiac glycosides, (F) Foaming test for saponins, and (G) Fehling's test for reducing sugar.

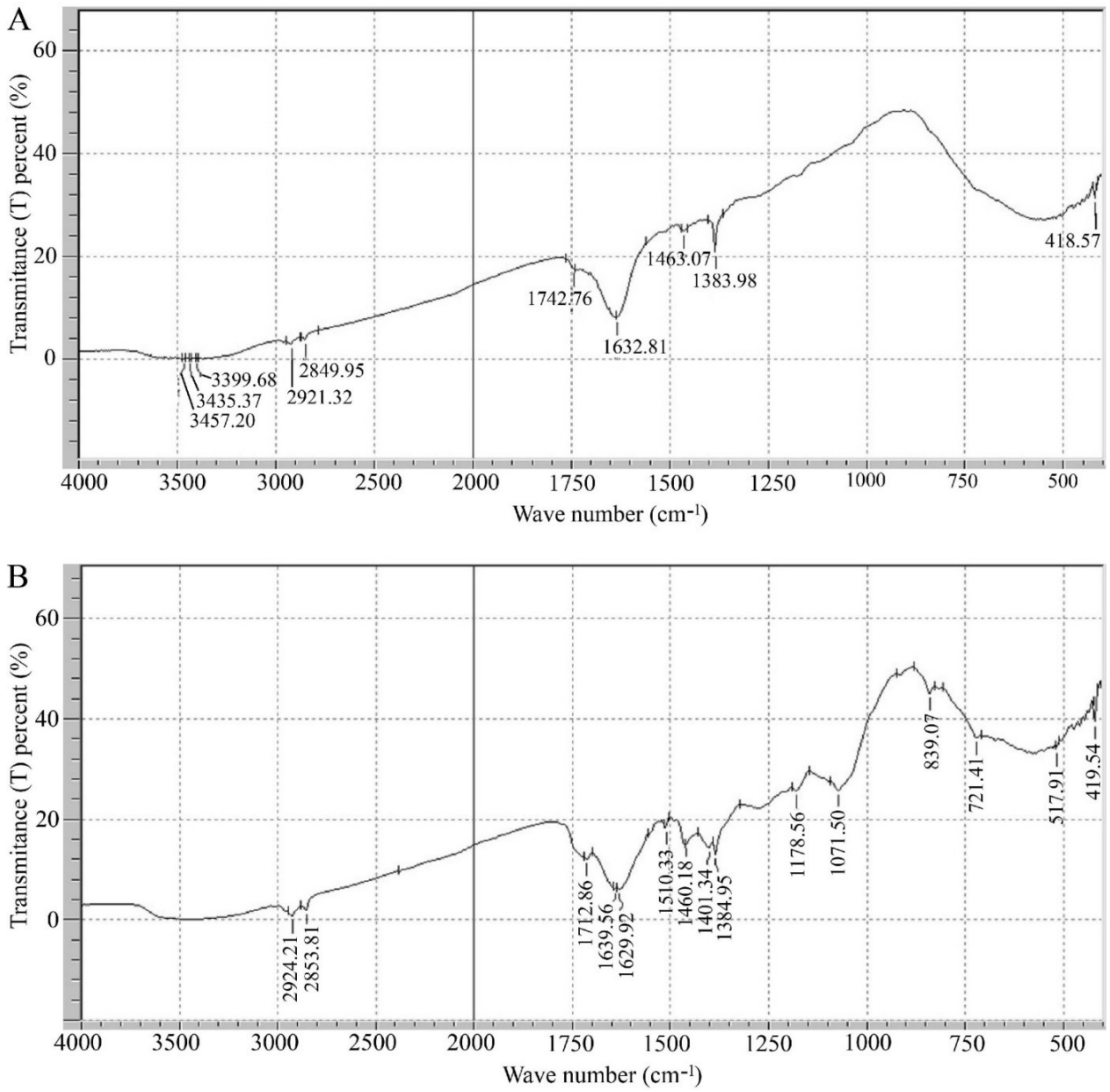


Figure S3. Fourier transform-infrared spectra (FT-IR) of MECOL and EAECOL. (A) Peaks at 3700-3000 and 1178.56, 2921.32, 2849.95, 1742.76, 1632.81, 1463.07-1383.96, and 418.57 cm^{-1} indicate the presence of corresponding functional groups in MECOL: carboxylic acids (O-H stretch), aliphatic hydrocarbons (C-H stretch), aldehydes (C-H stretch), aldehydes/esters (C=O stretch), alkenes (C=C stretch), alkanes ((-CH_3- bend), and alkyl halides (C-X). (B) Peaks at 3700-3000 and 1178.56, 2924.21, 2853.81, 1712.86, 1639.56, 1629.92, 1510.33, 1460.18, and 1384.95, 1401.34 and 839.07, 1071.50, 839.07, 721.41, 517.91-419.57 cm-1, denote the existence of respective functional groups in EAECOL: carboxylic acids (O-H stretch), aliphatic hydrocarbons (C-H stretch), aldehydes (C-H stretch), aldehyde/ketone (C=O stretch), alkene (C=C stretch), primary or secondary amine (N-H bend), nitro (N=O stretch),

alkane (-CH_3- bend), aldehyde/alkane (C-H bend), alcohol/phenol (O-H stretch), alkyl chloride (C-Cl) and alkyl halide (C-X).

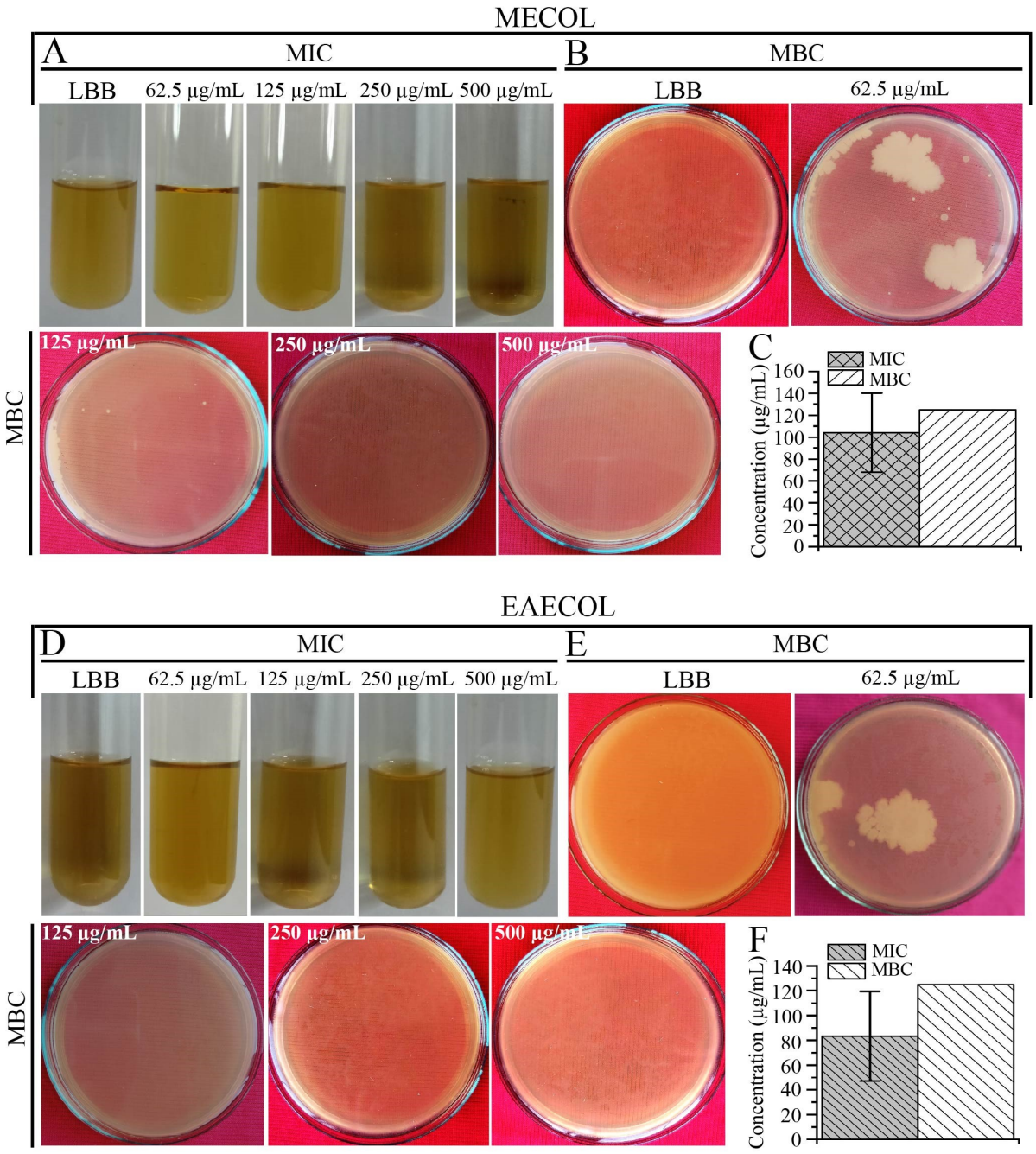
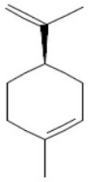
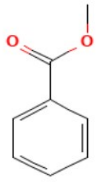
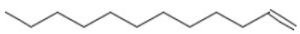
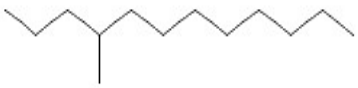
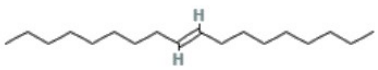
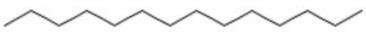
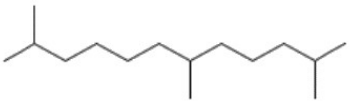
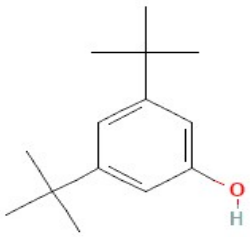
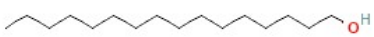
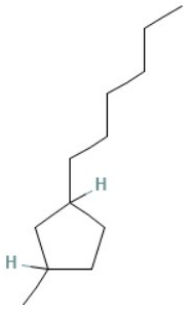
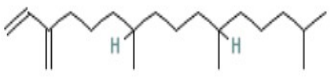
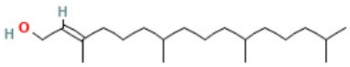
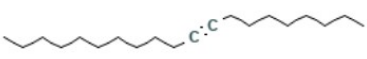


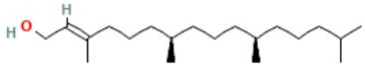
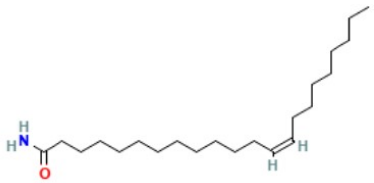
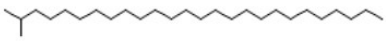
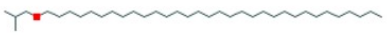
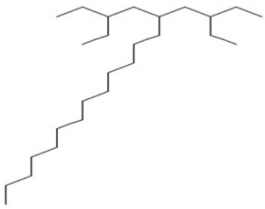
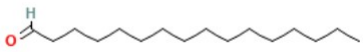
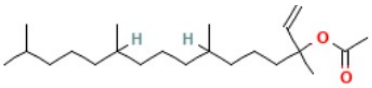
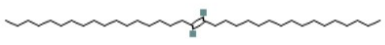
Figure S4. The MIC and MBC of MECOL and EAECOL against MDR Pseudomonas aeruginosa. The MIC in µg/mL (A) and the MBC in µg/mL (B) of MECOL. (C) MECOL demonstrated comparable MIC and MBC against MDR Pseudomonas aeruginosa. The MIC in µg/mL (D) and the MBC in µg/mL (E) of EAECOL. (F) EAECOL demonstrated comparable MIC and MBC against MDR Pseudomonas aeruginosa. The data are represented by the mean

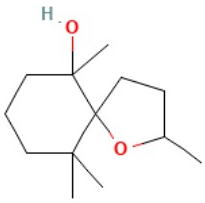
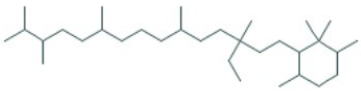
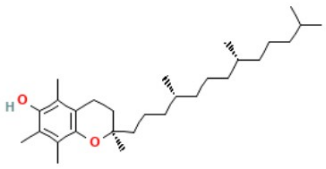
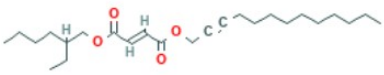
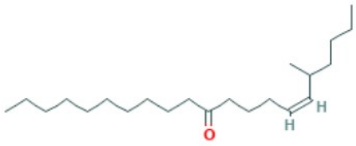
± STD (n = 3). LBB = LB broth; MIC = Minimum inhibitory concentration; MBC = Minimum bactericidal concentration.

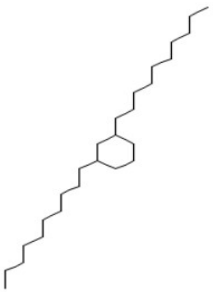
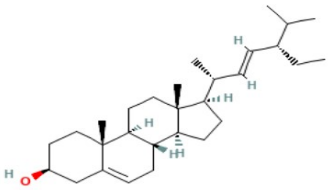
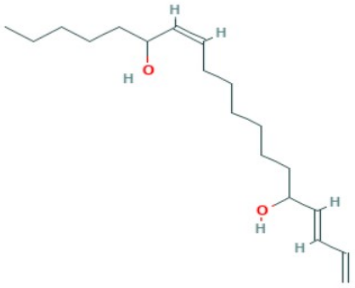
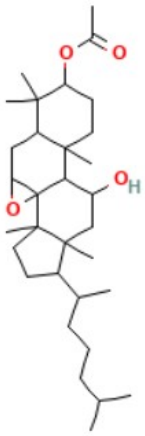
Table S1. The table presents the GC-MS identified phytochemicals in the MECOL along with their corresponding peak numbers, chemical structures, names, formulas, nature of phytochemicals, compound CID, retention time, and relative area percentage (area%).

Peak	Chemical Name	Nature	CID	Retention time	Area%
1	 1-Decene ($C_{10}H_{20}$)	Alkene	13381	5.467	1.01
2	 Decane ($C_{10}H_{22}$)	Alkane	15600	5.561	0.75
3	 D-Limonene ($C_{10}H_{16}$)	Terpenes	440917	5.965	1.51
4	 Hexane, 3,3-dimethyl- (C_8H_{18})	Alkane	11233	6.181	0.88
5	 Benzoic acid, methyl ester (Methyl benzoate) ($C_8H_8O_2$)	Ester	7150	6.775	2.60
6	 1-Dodecene ($C_{12}H_{24}$)	Alkene	8183	7.717	3.09
7	 Dodecane ($C_{12}H_{26}$)	Alkane	8182	7.806	1.09
8	 Dodecane, 4-methyl- ($C_{13}H_{28}$)	Alkane	521958	8.595	0.81
9	 9-Octadecene, (E) ($C_{18}H_{36}$)	Alkene	5364599	9.774	3.61
10	 Tetradecane ($C_{14}H_{30}$)	Alkane	12389	9.846	1.66

	 Dodecane, 2,6,11-trimethyl- ($C_{15}H_{32}$)	Branched alkane	35768	10.671	0.99
12	 Phenol, 3,5-bis(1,1-dimethylethyl)- ($C_{14}H_{22}O$)	Phenolics	70825	10.882	1.79
13	 1-Hexadecanol ($C_{16}H_{34}O$)	Alcohol	2682	11.636	3.74
14	 1,3-Propanediol, ethyl tetradecyl ether ($C_{19}H_{40}O_2$)	Alcohol	91693148	11.698	2.86
15	 Cyclopentane, 1-hexyl-3-methyl- ($C_{12}H_{24}$)	Alkane	544055	12.7	0.78
16	Eicosane ($C_{20}H_{42}$)	Alkane	8222	12.764	1.66
17	 1-Nonadecene ($C_{19}H_{38}$)	Alkene	29075	13.924	1.97
18	 N eophytadiene ($C_{20}H_{38}$)	Diterpene	10446	14.498	4.44
19	 3,7,11,15-Tetramethyl-2-hexadecen-1-ol ($C_{20}H_{40}O$)	Alcohol	5366244	14.835	0.73
20	 9-Eicosyne($C_{20}H_{38}$)		557019	15.109	1.18

21	Heneicosane($C_{21}H_{44}$)		12403	15.552	1.02
22	 n-Nonadecanol-1($C_{19}H_{40}O$)	Alcohol	80281	16.813	1.64
23	 Phytol($C_{20}H_{40}O$)	Diterpene alcohol	5280435	18.676	2.29
24	 Triacontane, 1-iodo- ($C_{15}H_9BrCl_2N_2O_3$)	-	12696145	28.077	1.02
25	 13-Docosenamide, (Z)- ($C_{22}H_{43}NO$)	Amide	5365371	29.313	7.53
26	 2-Methylhexacosane ($C_{27}H_{56}$)	Branched alkane	150931	30.078	1.10
27	 Dotriacontyl isobutyl ether ($C_{36}H_{74}O$)	Ether	91693114	30.467	2.91
28	 Octadecane, 3-ethyl-5-(2-ethylbutyl)- ($C_{26}H_{54}$)		292285	30.8	1.34
29	Tetrapentacontane ($C_{54}H_{110}$)	Alkane	521846	30.98	3.85
30	 Hexadecanal ($C_{16}H_{32}O$)	Aldehyde	984	31.035	0.65
31	 Isophytol, acetate ($C_{22}H_{42}O_2$)	Alcohol	94042	31.13	1.04
32	 17-Pentatriacontene ($C_{35}H_{70}$)	Alkene	5365022	31.284	0.81
33	 Octatriacontyl trifluoroacetate ($C_{40}H_{77}F_3O_2$)	Alkane	91693163	31.468	1.63

34	 2,6,10,10-Tetramethyl-1-oxaspiro [4.5] decan-6-ol ($C_{13}H_{24}O_2$)	Alkane	65428	31.635	0.65
35	 1,1,3,6-tetramethyl-2-(3,6,10,13,14-pentamethyl-3-ethyl-pentadecyl) cyclohexane ($C_{32}H_{64}$)	Aromatic Alkane	91693134	31.841	2.36
36	Hexacontane ($C_{60}H_{122}$)	Alkane	24318	32.344	1.44
37	 Vitamin E ($C_{29}H_{50}O_2$)	Tocopherols	14985	34.206	1.99
38	 Fumaric acid, 2-ethylhexyl tridec-2-yn-1-yl Ester ($C_{25}H_{42}O_4$)	Ester	91701131	35.63	2.96
39	Tetrapentacontane, 1,54-dibromo- ($C_{54}H_{108}Br_2$)	Alkane	545963	35.767	1.76
40	 Z-5-Methyl-6-heneicosen-11-one ($C_{22}H_{42}O$)	Carbonyl Ketone	5363254	36.37	2.78

41	 Cyclohexane, 1,3-didecyl- ($C_{26}H_{52}$)	Aromatic Alkene	276893	36.393	2.33
42	 Stigmasterol ($C_{29}H_{48}O$)	Steroid	5280794	37.479	10.28
43	 E, E, Z-1,3,12-Nonadecatriene-5,14-diol ($C_{19}H_{34}O_2$)	Alcohol	5364768	37.845	1.47
44	 7,8-Epoxylanostan-11-ol, 3-acetoxy-($C_{32}H_{54}O_4$)	Alcohol	541562	38.701	3.17

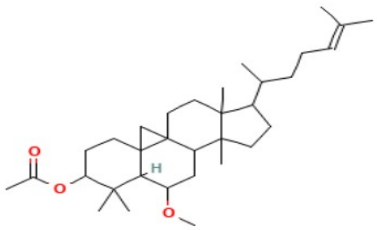
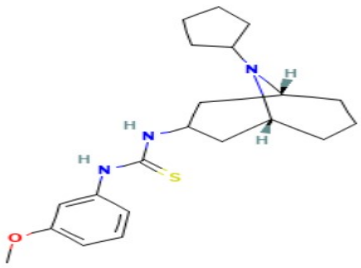
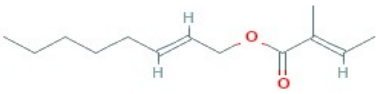
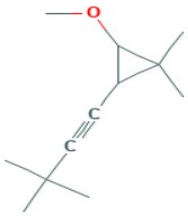
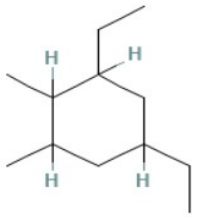
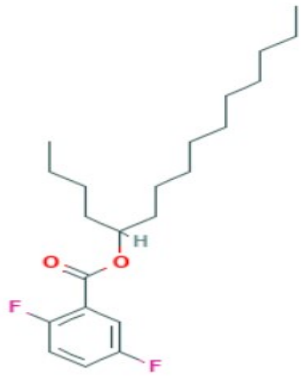
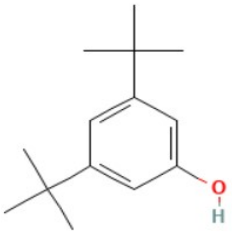
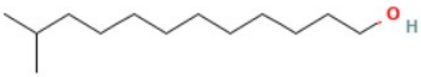
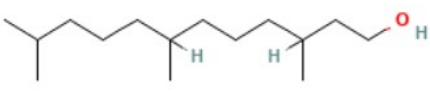
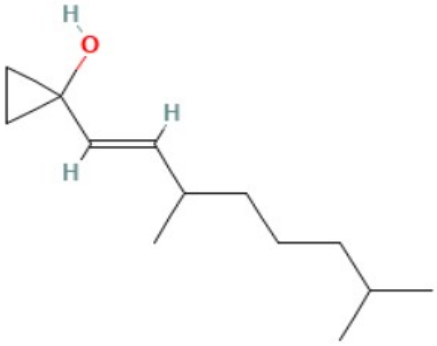
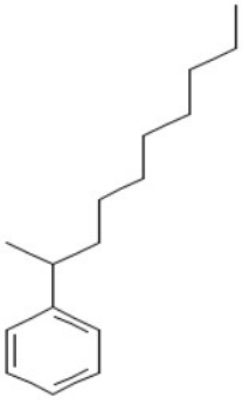
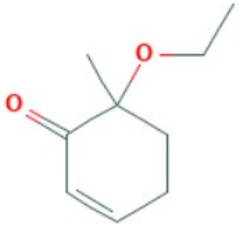
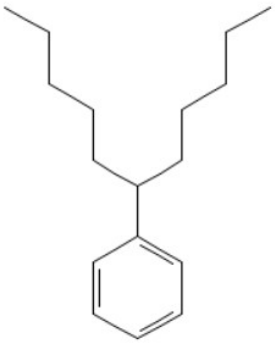
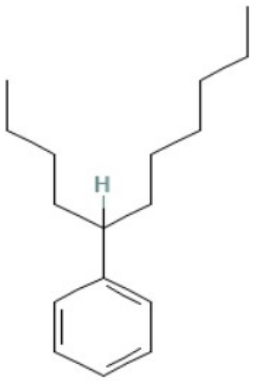
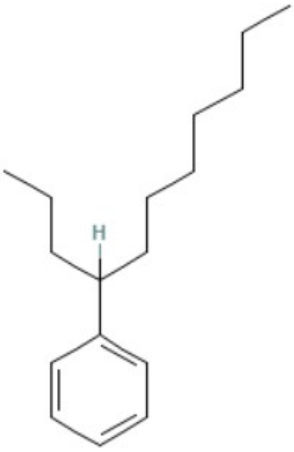
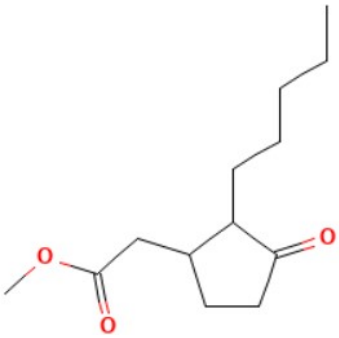
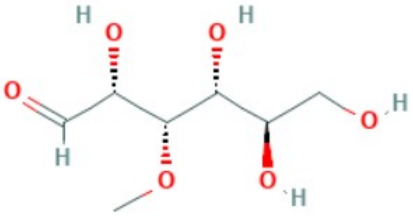
45	 3-O-Acetyl-6-methoxy-cycloartenol ($C_{33}H_{54}O_3$)	Alcohol	537607	39.217	3.31
46	 Isocalamenediol ($C_{21}H_{31}N_3OS$)	Alcohol	146158381	39.61	0.97

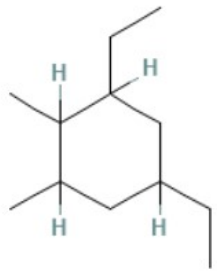
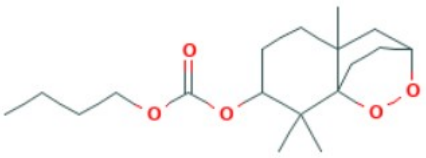
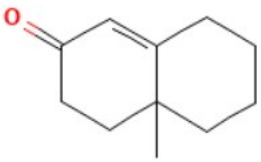
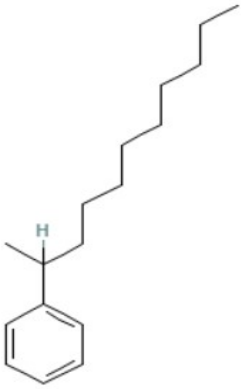
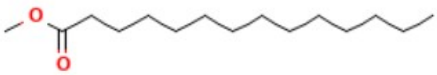
Table S2. The table presents the GC-MS identified phytochemicals in the EAECOL, along with their corresponding peak numbers, chemical structures, names, formulas, nature of phytochemicals, Compound CID, retention times, and relative area percentages (%).

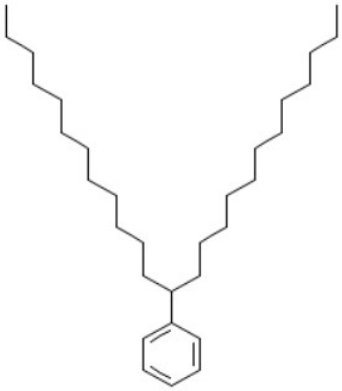
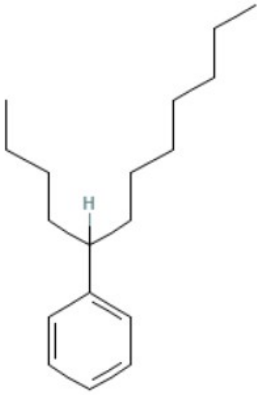
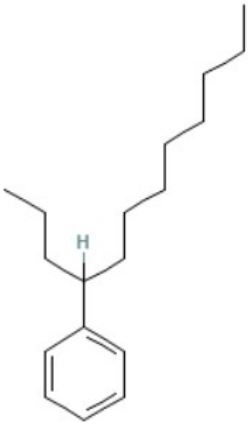
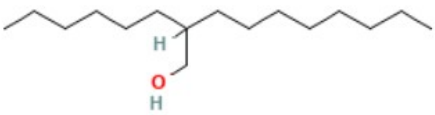
Peak	Name of the Compounds	Nature of phytochemicals	Compound CID	Retention time	Area %
1	 E-2-Octenyl tiglate ($C_{13}H_{22}O_2$)	Ester	5367738	8.535	0.34
2	 Hexane, 3,3-dimethyl- (C_8H_{18})	Alkane	11233	8.594	0.52
3	 n-Tridecan-1-ol ($C_{13}H_{28}O$)	Alcohol	8207	8.87	0.26
4	 Cyclopropane, 1-methoxy-2,2-dimethyl-3-(3,3-dimethyl-1-propynyl)- ($C_{12}H_{20}O$)	Aromatic Alkane	596548	10.445	0.22

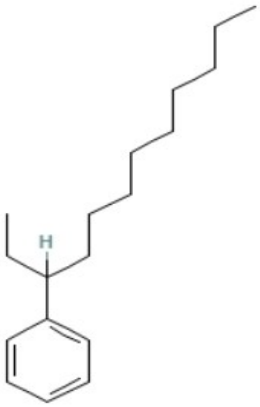
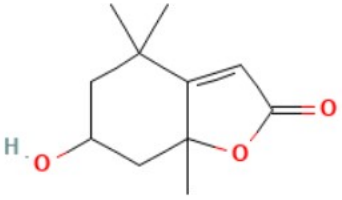
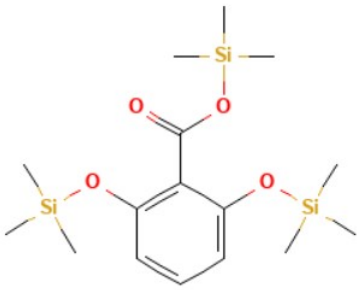
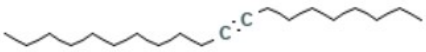
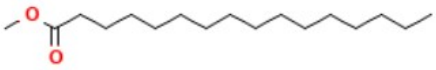
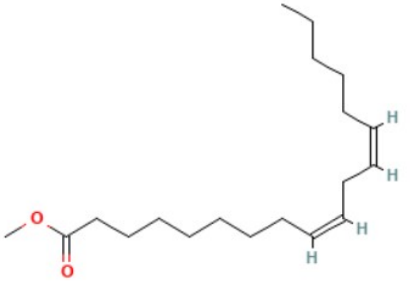
5	 Cyclohexane, 1,5-diethyl-2,3-dimethyl- ($C_{12}H_{24}$)	-	557905	10.615	0.52
6	 Hexadecane ($C_{16}H_{34}$)	Alkane	11006	10.667	0.74
7	 2,5-Difluorobenzoic acid, 5-pentadecyl ester ($C_{22}H_{34}F_2O_2$)	Ester	91716874	10.756	0.38
8	 Phenol, 3,5-bis(1,1-dimethylethyl) ($C_{14}H_{22}O$)	Phenolics	70825	10.875	0.84
9	 n-Nonadecanol-1 ($C_{19}H_{40}O$)	Alcohol	80281	10.934	1.03
10	 11-Methyldodecanol ($C_{13}H_{28}O$)	Alcohol	33865	11.011	0.34
11	 Eicosane ($C_{20}H_{42}$)	Alkane	8222	11.076	0.32
12	 1-Dodecanol, 3,7,11-trimethyl- ($C_{15}H_{32}O$)	Alcohol	138824	11.177	0.45

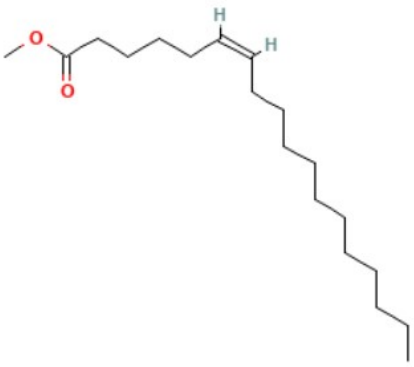
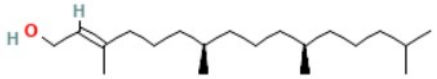
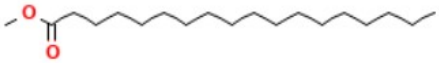
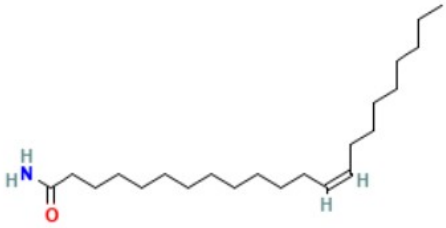
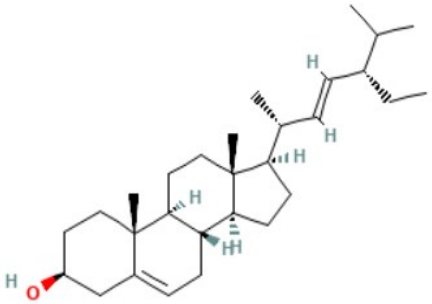
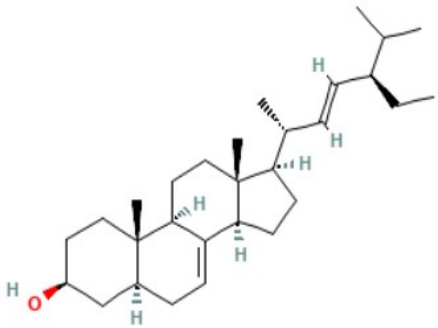
13	 Cyclopropanol, 1-(3,7-dimethyl-1-octenyl)- ($C_{13}H_{24}O$)	Alcohol	5367736	11.27	0.26
14	 Benzene, (1-methylnonyl)- ($C_{16}H_{26}$)	Carbonyl	20659	11.775	0.26
15	 6-Ethoxy-6-methyl-2-cyclohexenone ($C_9H_{14}O_2$)	Ketone	537457	11.975	1.12
16	 Benzene, (1-pentylhexyl)- ($C_{17}H_{28}$)	Carbonyl	20660	12.025	1.00

17	 Benzene, (1-butylheptyl)- ($C_{17}H_{28}$)	Carbonyl	20661	12.063	1.06
18	 Benzene, (1-propyloctyl)- ($C_{17}H_{28}$)	Carbonyl	20654	12.182	0.91
19	 Cyclopentaneacetic acid, 3-oxo-2-pentyl-, methyl ester (Methyl dihydrojasmonate) ($C_{13}H_{22}O_3$)	Ester	102861	12.278	0.29
20	 3-O-Methyl-d-glucose ($C_7H_{14}O_6$)	Carbohydrates	8973	12.532	9.43

21	 Cyclohexane,1,5-diethyl-2,3-dimethyl- ($C_{12}H_{24}$)	Alkane	557905	12.693	0.95
22	 2-Butyloxycarbonyloxy-1,1,10-trimethyl-6,9-epidioxydecalin ($C_{18}H_{30}O_5$)	-	384923	12.742	0.88
23	 2(3H)-Naphthalenone,4,4a,5,6,7,8-hexahydro-4a-methyl- (4a-Methyl-6-(3-oxobutyl)-4,4a,5,6,7,8-hexahydronaphthalen-2(3H)-one) ($C_{11}H_{16}O$)	Ketone	136654	12.818	0.55
24	 Benzene, (1-methyldecyl)- ($C_{17}H_{28}$)	Carbonyl	20656	12.876	0.68
25	 Ethanol, 2-(tetradecyloxy)- ($C_{16}H_{34}O_2$)	Alcohol	16491	12.99	1.06
26	 Methyl tetradecanoate ($C_{15}H_{30}O_2$)	Methyl ester	31284	13.024	1.04

27	 Pentacosane, 13-phenyl- ($C_{31}H_{56}$)	Fatty Alkane	138643	13.114	1.44
28	 Benzene, (1-butyloctyl)- ($C_{18}H_{30}$)	Carbonyl	17630	13.175	0.69
29	 Benzene, (1-propylnonyl)- ($C_{18}H_{30}$)	Carbonyl	17631	13.346	0.63
30	 1-Decanol, 2-hexyl- ($C_{16}H_{34}O$)	Alcohol	95337	13.465	0.54

31	 Benzene, (1-ethyldecyl)- ($C_{18}H_{30}$)	Carbonyl	16979	13.65	0.23
32	 6-Hydroxy-4,4,7a-trimethyl-5,6,7,7a-tetrahydrobenzofuran-2(4H)-one ($C_{11}H_{16}O_3$)	Ketone	14334	13.885	0.41
33	 2, 6-Dihydroxybenzoic acid, 3TMS derivative ($C_{16}H_{30}O_4Si_3$)	Natural phenol	520869	14.343	0.78
34	 9-Eicosyne ($C_{20}H_{38}$)	Aliphatic hydrocarbon	557019	14.483	0.60
35	 Hexadecanoic acid, methyl ester ($C_{17}H_{34}O_2$)	Carboxylic ester	8181	15.736	21.00
36	 9, 12-Octadecadienoic acid (Z, Z)-, methyl ester ($C_{19}H_{34}O_2$)	Carboxylic ester	5284421	18.385	7.05

37	 6-Octadecenoic acid, methyl ester, (Z)- ($C_{19}H_{36}O_2$)	Carboxylic ester	5362717	18.487	23.39
38	 Phytol ($C_{20}H_{40}O$)	Diterpene alcohol	5280435	18.653	4.61
39	 Methyl stearate ($C_{19}H_{38}O_2$)	Fatty acid methyl ester	8201	18.906	2.35
40	 13-Docosenamide, (Z)- ($C_{22}H_{43}NO$)	Amide	5365371	29.292	5.24
41	 Stigmasterol ($C_{29}H_{48}O$)	Steroid	5280794	36.365	1.60
42	 ChondrillasterolF ($C_{29}H_{48}O$)	Steroid	5283663	37.461	2.47

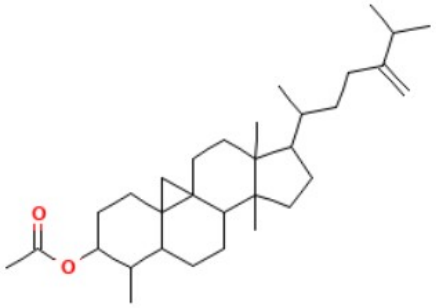
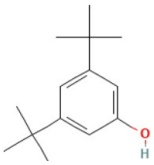
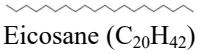
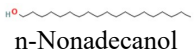
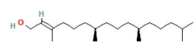
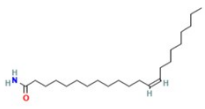
43	 9, 19-Cycloergost-24(28)-en-3-ol, 4, 14-dimethyl-, acetate, (3. beta. 4. alpha., 5. alpha.)- ($C_{32}H_{52}O_2$)		Ester	537081	39.189	1.51			

Table S3. The table presents the phytochemical compounds that have been identified by GC-MS analysis and found to be commonly present in both MECOL and EAECOL.

SN	Name	CID	Nature	MECOL			EAECOL		
				Peak	Retention time	Area %	Peak	Retention time	Area %
1	 Hexane, 3,3 dimethyl (C_8H_{18})	11233	Hydrocarbon	4	6.181	0.88	2	8.594	0.52
2	 Phenol, 3,5-bis(1,1-dimethylethyl)- ($C_{14}H_{22}O$)	70825	Phenolic	12	10.882	1.79	8	10.875	0.84
3	 Eicosane ($C_{20}H_{42}$)	8222	Alkane	16/21	12.764	1.66	11	11.076	0.32
4	 n-Nonadecanol ($C_{19}H_{40}O$)	80281	Long-chain fatty alcohol	22	16.813	1.64	9	10.934	1.03
5	 Phytol ($C_{20}H_{40}O$)	5280435	Acyclic diterpene alcohol	23/28	18.676	2.29	38	18.653	4.61
6	 13-Docosenamide, (Z)- ($C_{22}H_{43}NO$)	5365371	Amide	25	29.313	7.53	40	29.292	5.24

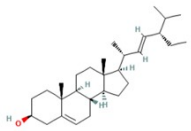
7	 Stigmasterol ($C_{29}H_{48}O$)	5280794	Unsaturated phytosterol	43	37.479	10.18	41	36.365	1.60

Table S4. The table displays the XP Glide docking results of various phytochemicals with the LasR receptor in *P. aeruginosa*. The docking analysis provides valuable insights into the potential interactions and binding affinities of the phytochemicals with the LasR receptor.

SN	PubChem Identifier	Compounds	Docking score	XPG Score
1	CID 5363254	Z-5-Methyl-6-heneicosen-11-one	-8.01	-8.01
2	CID 91716874	2,5-Difluorobenzoic acid, 5-pentadecyl	-7.553	-7.553
3	CID 8973	3-O-Methyl-d-glucose	-6.671	-6.672
4	CID 91701131	Fumaric acid, 2-ethylhexyl tridec-2-yn-1-yl ester	-6.288	-6.288
5	CID 102861	Methyl dihydrojasmonate	-5.923	-5.923
6	CID 7150	Methyl benzoate	-5.811	-5.811
7	CID 557905	1,5-Diethyl-2,3-dimethylcyclohexane	-5.513	-5.513
8	CID 136654	4a-Methyl-4,4a,5,6,7,8-hexahydro-2(3H)-	-5.472	-5.472
9	CID 5364768	E, E, Z-1,3,12-Nonadecatriene-5,14-diol	-5.459	-5.459
10	CID 5365371	13-Docosenamide, (Z)-	-5.421	-5.421
11	CID 94042	1,5,9,13-Tetramethyl-1-vinyltetradecyl	-5.417	-5.417
12	CID 138824	3,7,11-Trimethyl-1-dodecanol	-5.139	-5.139
13	CID16491	2-(Tetradecyloxy)ethanol	-5.136	-5.136
14	CID 3246941 (LasR Native)	N-3-Oxo-Dodecanoyl-L-Homoserine Lactone (redocking)	-5.375 -5.125 -5.475	-5.313 -5.11 -5.275

Table S5. Free energy of ligand binding to LasR obtained from post-docking MM-GBSA analysis

Phytochemical Identifier	MM-GBSA (kcal/mol)	MM-GBSA (kcal/mol) Bind Coulomb	ΔGBind H-bond	MMGBSA ΔG Bind Lipo	MMGBSA ΔG Bind vdW
CID 91701131	-40.23	-1.61	0	-30.31	-17.65
CID 5365371	-47.19	-0.19	0	-34.63	-16.29
CID 5363254	-39.52	1.37	0	-30.95	-13.13

CID 138824	-23.06	-0.24	0	-15.91	-8.31
CID 91716874	-12.71	-0.92	0	-28.65	-12.71
CID 94042	-18.05	-0.43	0	-27.42	-11.9
CID 16491	-31.77	-1.31	0	-24.56	-11.13
CID 5364768	-36.41	-0.09	0	-28.25	-13.16
CID 557905	-16.01	-0.03	0	-14.36	-8.06
CID 102861	-24.49	-2.18	-0.12	-18.67	-10.48
CID 7150	-14.2	-0.15	-0.14	-6.95	-9.28
CID 8973	-18.62	3.61	0	-9.19	-9.44
CID 136654	-20.78	-3.37	0	-15.86	-9.09
CID 3246941 (Native)	-13.9	-1.09	-0.08	-4.95	-8.05

Table S6. This table presents the pharmacokinetics (ADME) and toxicity (T) characteristics of the 12 most interactive phytochemicals. The symbols "+" and "-" represent the presence and absence of specific features, respectively. "NI" stands for Noninhibitor, "NS" for Non-substrate, and "S" for substrate. And M for moderate. Additionally, "H" denotes High, "L" represents Low, "A" indicates Active, and "I" stands for Inactive.

SN	Compound CID	Absorption	Distribution	Metabolism						Excretion	Toxicity					
				CYP450 inhibitor			CYP450 substrate			Renal clearance (ml/min/kg)	Hepatotoxicity	Carcinogenicity	Mutagenicity	Immunogenicity	Cytotoxicity	Rat LD_{50} value (mg/kg)
		HIA	BBB penetration	CYP4502C9	CYP4502D6	CYP4503A4	CYP4502C9	CYP4502D6	CYP4503A4							
1	5363254	L	No	NI	NI	NI	NS	NS	NS	M	I	I	I	I	I	15000
2	8973	L	No	NI	NI	NI	NS	NS	NS	Low	I	I	I	I	I	20000
3	91701131	H	No	NI	NI	NI	NS	NS	S	M	I	A	I	I	I	386
4	102861	H	Yes	NI	NI	NI	NS	NS	NS	M	I	I	I	I	I	5000
5	7150	H	Yes	NI	NI	NI	NS	NS	NS	M	I	I	I	I	I	1177
6	557905	L	Yes	NI	NI	NI	NS	NS	NS	M	I	I	I	I	I	15380
7	136654	H	Yes	NI	NI	NI	NS	NS	NS	M	I	I	I	I	I	2450
8	536476	H	Yes	NI	NI	NI	NS	NS	NS	M	A	I	I	I	I	2100

9	8 5365371	L	No	NI	NI	NI	S	NS	NS	Low	I	I	I	I	I	750
10	94042	L	No	NI	NI	NI	S	NS	S	Low	I	I	I	I	I	850
11	138824	H	Yes	NI	NI	NI	NS	NS	NS	M	I	I	I	I	I	1000
12	16491	H	Yes	NI	NI	NI	NS	NS	NS	M	I	A	I	I	I	2280

Table S7. This table provides the drug-ability profile of the 12 most interactive phytochemicals. “MW” stands for molecular weight, “HBA” for hydrogen bond acceptor, “HBD” for hydrogen bond donor, “TPSA” for topological surface area, and RB for rotatable bonds.

SN	**Compound CID**	**Drug-ability profile**									
		Physicochemical properties						**Lipophilicity (cLOGPo/w)**	**Water solubility [LogS (ESOL)]**	**Lipinski's Rule of Five (RO5) violation**	**Synthetic accessibility score**
		MW (g/mol)	**No. of HBA**	**No. of HBD**	**Heavy atoms**	**TPSA (Å²)**	**No. of RB**				
1	5363254	322.57	1	0	23	17.07	17	5.58	-6.12	1	4.23 (Easy)
2	8973	194.18	6	4	13	107.220	6	-2.56	1.17	1	3.52 (Easy)
3	91701131	406.60	4	0	29	52.6	19	5	-6.61	1	5.46 (Moderately easy)
4	102861	226.31	3	0	16	43.37	7	2.04	-2.46	0	2.91 (Easy)
5	7150	136.15	2	0	10	26.3	2	1.93	-2.33	0	1 (Very easy)
6	557905	168.32	0	0	12	0.0	2	5	-4.12	1	3.09 (Easy)
7	136654	164.24	1	0	12	17.07	0	2.49	-2.4	0	3.23 (Easy)
8	5364768	294.47	2	2	21	40.46	14	3.39	-4.41	0	4.49 (Easy)
9	5365371	337.58	1	1	24	43.09	19	5.06	-6.45	1	3.44 (Easy)
10	94042	338.57	2	0	24	26.3	15	5.47	-6.25	1	4.09 (Easy)
11	138824	228.41	1	1	16	20.23	10	4.2	-4.39	1	2.89 (Easy)
12	16491	258.44	2	1	18	29.46	15	3.53	-4.35	0	3.01 (Easy)

Table 8. This table presents the molecular docking interactions and the interacting residues of the LasR quorum sensing protein with the best phytochemical compounds and native ligands from specific docked complexes.

Compounds	Docking Score (Kcal/mol)	H-Bond with LasR	Other interaction LasR
Methyl dihydrojasmonate (CID 102861)	-5.923	TYR56, ASP73	LEU36, GLY38, LEU39, LEU40, TYR47, ALA50, ILE52, ARG61, TYR64, ASP65, ALA70, THR75, VAL76, CYS79, THR80, THR115, LEU125, GLY126, ALA127, SER229
Methyl benzoate (CID 7150)	-5.811	TYR56, SER129	LEU36, TRP60, TYR64, ASP73, THR75, VAL76, TRP88, TYR93, PHE101, ALA105, LEU110, THR115, ALA127
4a-Methyl-4,4a,5,6,7,8-hexahydro-2(3H)-naphthalenone (CID 136654)	-5.472	-	LEU36, GLY38, LEU39, LEU40, TYR47, ALA50, ILE52, ARG61, TYR64, ASP65, ALA70, CYS79, VAL76, LEU125, GLY126, ALA127
N-3-Oxo-Dodecanoyl-L-Homoserine Lactone (CID 3246941) LasR native compound	-5.375	TRP60	LEU36, GLY38, LEU39, LEU40, TRY47, ALA50, ILE52, TYR56, ARG61, TYR64, ASP65, ALA70, ASP73, THR75, VAL76, CYS79, THR80, TRP88, TYR93, PHE101, PHE102, ALA105, LEU110, THR115, LEU125, GLY126, ALA127, SER129, SER 131

Table 9. This table showcases the additional molecular docking interactions of the LpxC lipid A biosynthesis protein with the best phytochemical compounds and the native ligand, enabling a comprehensive analysis of the phytochemicals' multi-targeting capabilities.

SN	PubChem identifier	Compounds	Docking score	XP GScore
1	CID 9823454 (LpxC native ligand)	(2R)-N-hydroxy-3-naphthalen-2-yl-2-(naphthalen-2-ylsulfonylamino)propanamide	-4.604	-4.619
2	CID 102861	Methyl dihydrojasmonate	-4.772	-4.772
3	CID 136654	Methyl benzoate	-4.688	-4.688
4	CID 7150	4a-Methyl-4,4a,5,6,7,8-hexahydro-2(3H)-naphthalene	-3.505	-3.505