Table S1: Some properties of inhibitors natural essential oil against **Aerial** part of *C. sulphurea*

Molécule	Name	IUPAC name	Pub Chem CID	Molar mass (g/mol)	Formula
L1	α-Pinene	2,6,6-trimethylbicyclo[3.1.1]hept-2-ene	6654	136.23	C10H16
L2	Sabinene	4-methylidene-1-propan-2-ylbicyclo[3.1.0]hexane	18818	136.23	C10H16
L3	β-pinene	6,6-dimethyl-2-methylidenebicyclo[3.1.1]heptane	14896	136.23	C10H16
L4	Myrcene	7-methyl-3-methylideneocta-1,6-diene	31253	136.23	C10H16
L5	p-Cymene	1-methyl-4-propan-2-ylbenzene	7463	134.22	C10H14
L6	Limonene	1-methyl-4-prop-1-en-2-ylcyclohexene	22311	136.23	C10H16
L7	(Z)-β-ocimene	(3Z)-3,7-dimethylocta-1,3,6-triene	5320250	136.23	C10H16
L8	(E)-β-ocimene	(3E)-3,7-dimethylocta-1,3,6-triene	5281553	136.23	C10H16
L9	Nonanal	nonanal	31289	142.24	C9H18O
L10	Linalool	3,7-dimethylocta-1,6-dien-3-ol	6549	154.25	C10H18O
L11	Terpinen-4-ol	4-methyl-1-propan-2-ylcyclohex-3-en-1-ol	11230	154.25	C10H18O
L12	methyl-Salicylate	methyl 2-hydroxybenzoate	4133	152.15	C8H8O3
L13	Decanol	decan-1-ol	8174	158.28	C10H22O
L14	α-Copaene	1,3-dimethyl-8-propan-2-yltricyclo[4.4.0.02,7]dec-3-ene	19725	204.35	C15H24
L15	(E)-β-Caryophyllene	(1R,4E,9S)-4,11,11-trimethyl-8-methylidenebicyclo[7.2.0]undec-4-ene	5281515	204.35	C15H24
L16	α-Humulene	(1E,4E,8E)-2,6,6,9-tetramethylcycloundeca-1,4,8-triene	5281520	204.35	C15H24
L17	Germacrene-D	(1Z,6Z,8S)-1-methyl-5-methylidene-8-propan-2-ylcyclodeca-1,6-diene	91723653	204.35	C15H24
L18	β-Selinene	(3R,4aS,8aR)-8a-methyl-5-methylidene-3-prop-1-en-2-yl-1,2,3,4,4a,6,7,8-octahydronaphthalene	442393	204.35	C15H24
L19	4-epi-Cubebol	(1S,4S,5S,6S,7R,10S)-4,10-dimethyl-7-propan-2-yltricyclo[4.4.0.01,5]decan-4-ol	12304217	222.37	C15H26O

L20	Bicyclogermacrene	(1S,2E,6E,10R)-3,7,11,11-tetramethylbicyclo[8.1.0]undeca-2,6-diene	13894537	204.35	C15H24
L21	α-Muurolene	(1S,4aS,8aR)-4,7-dimethyl-1-propan-2-yl-1,2,4a,5,6,8a-hexahydronaphthalene	12306047	204.35	C15H24
L25	Germacrene-D-4-ol	(2E,7E)-1,7-dimethyl-4-propan-2-ylcyclodeca-2,7-dien-1-ol	5352847	222.37	C15H26O
L26	Caryophyllene oxyde	4,12,12-trimethyl-9-methylidene-5-oxatricyclo[8.2.0.04,6]dodecane	14350	220.35	C15H24O
L27	Salvial-4(14)-en-1-one	(1S,3aR,8aS)-3a-methyl-7-methylidene-1-propan-2-yl-2,3,5,6,8,8a-hexahydro-1H-azulen-4-one	42608172	220.35	C15H24O
L28	Viridiflorol	(1aR,4S,4aS,7R,7aS,7bS)-1,1,4,7-tetramethyl-2,3,4a,5,6,7,7a,7b-octahydro-1aH-cyclopropa[e]azulen-4-ol	11996452	222.37	C15H26O
L29	Humuleneepoxyde II	(3Z,7E)-1,5,5,8-tetramethyl-12-oxabicyclo[9.1.0]dodeca-3,7-diene	5463721	220.35	C15H24O
L31	epi-Cubenol	(1S,4R,4aS,8aR)-4,7-dimethyl-1-propan-2-yl-2,3,4,5,6,8a-hexahydro-1H-naphthalen-4a-ol	12046149	222.37	C15H26O
L32	τ-Muurolol	(1S,4S,4aR,8aS)-1,6-dimethyl-4-propan-2-yl-3,4,4a,7,8,8a-hexahydro-2H-naphthalen-1-ol	3084331	222.37	C15H26O
L34	α-Cadinol	(1R,4S,4aR,8aR)-1,6-dimethyl-4-propan-2-yl-3,4,4a,7,8,8a-hexahydro-2H-naphthalen-1-ol	10398656	222.37	C15H26O
L35	α-Eudesmol	2-[(2R,4aR,8aR)-4a,8-dimethyl-2,3,4,5,6,8a-hexahydro-1H-naphthalen-2-yl]propan-2-ol	92762	222.37	C15H26O
L37	Eudesma-4(15),7-dien-1β -ol	(1R,8aR)-8a-methyl-4-methylidene-6-propan-2-yl-1,2,3,4a,5,8-hexahydronaphthalen-1-ol	6429131	220.35	C15H24O
L38	Tetradecanol	tetradecan-1-ol	8209	214.39	C14H30O

Table S2: Some properties of inhibitors natural essential oil against **Root** part of *C. sulphurea*

Molecule	Name	IUPAC name	Pub Chem CID	Weight (g/mol)	Formula
L43	Hex-3-en-1-ol (E)	(E)-hex-3-en-1-ol	5284503	100.16	C6H12O
L44	Hex-3-en-1-ol (Z)	(Z)-hex-3-en-1-ol	5281167	100.16	C6H12O
L45	α-Thujene	2-methyl-5-propan-2-ylbicyclo[3.1.0]hex-2-ene	17868	136.23	C10H16
L46	β-pinene	6,6-dimethyl-2-methylidenebicyclo[3.1.1]heptane	14896	136.23	C10H16
L47	methyl-Salicylate	methyl 2-hydroxybenzoate	4133	152.15	C8H8O3
L48	Decanol	decan-1-ol	8174	158.28	C10H22O
L49	Dec-3-en-2-one	(E)-dec-3-en-2-one	5363233	154.25	C10H18O
L51	α-Copaene	1,3-dimethyl-8-propan-2-yltricyclo[4.4.0.02,7]dec-3-ene	19725	204.35	C15H24
L52	Dodecanal	dodecanal	8194	184.32	C12H24O
L53	(E)-β-Caryophyllene	(1R,4E,9S)-4,11,11-trimethyl-8-methylidenebicyclo[7.2.0]undec-4-ene	5281515	204.35	C15H24
L54	α-Humulene	(1E,4E,8E)-2,6,6,9-tetramethylcycloundeca-1,4,8-triene	5281520	204.35	C15H24
L55	Germacrene-D	(1Z,6Z,8S)-1-methyl-5-methylidene-8-propan-2-ylcyclodeca-1,6-diene	91723653	204.35	C15H24
L56	Caryophyllene oxyde	4,12,12-trimethyl-9-methylidene-5-oxatricyclo[8.2.0.04,6]dodecane	14350	220.35	C15H24O
L57	Humuleneepoxyde II	(3Z,7E)-1,5,5,8-tetramethyl-12-oxabicyclo[9.1.0]dodeca-3,7-diene	5463721	220.35	C15H24O

Table S3. Energy (binding affinity) of **other** complexes formed by natural compounds (Kcal/mol) with the pocket of the ***catalase*** target.

Mol	Score	RMSD-refine	E-Conf	E-PLACE	E-REFINE	rmsd
Lref (Native)	**-7.97096014**	**4.68782759**	**-722.341064**	**-56.5938377**	**-29.9442215**	**1.287**
L1	-3.98895788	2.59013176	38.2863731	-22.9999352	-10.3836775	1.101
L2	-3.88704371	1.21237528	30.6284142	-34.1589203	-8.03204155	0.231
L3	-3.94628	1.11452448	19.6354332	-36.5459633	-10.104681	0.151
L4	-4.55995321	1.26810312	3.4000299	-41.6391563	-12.9062834	0.405
L5	-4.31294489	1.6795876	23.7007504	-36.9787025	-12.7957802	0.240
L6	-4.24678135	2.32827258	24.4138355	-38.4764977	-10.3571377	0.105
L7	-4.63459826	0.80311048	22.1834126	-37.6015015	-11.5327673	0.071
L8	-4.40625525	3.86050892	19.7765789	-37.639225	-12.3703632	0.186
L9	-4.66843081	1.29199898	-2.58940005	-42.1385002	-12.2455978	0.118
L10	-4.67725086	1.95574021	14.1400661	-41.0474396	-13.0402174	0.097
L11	-4.19324493	1.56141019	26.1478539	-41.6175385	-13.2336178	0.234
L12	-4.2321372	1.94384146	22.0518665	-63.2284546	-11.6995354	0.141
L13	-4.87165976	0.716219127	-3.67760944	-59.6669884	-12.0080776	0.261
L14	-4.6683259	2.09637737	49.688221	-41.6238899	-14.2940207	0.272
L15	-4.36114502	3.20033979	60.4819107	-47.2253075	-12.8066206	0.151
L16	-4.55383825	1.90766406	63.6945992	-42.1987381	-12.5069418	1.071
L17	-4.57506704	3.35696459	40.505024	-35.3185463	-13.3276224	0.532
L18	-4.0977416	2.71517467	47.431881	-47.5162964	-12.8394489	0.356
L19	-4.99567032	2.46123052	41.7866516	-48.5986137	-13.7355928	0.427
L20	-4.69868898	1.20911908	62.9069977	-41.3514328	-11.1247225	0.316
L21	-4.75638676	0.661210179	40.244648	-55.6263962	-7.03142071	0.236
L25	-4.62917185	2.53696036	34.9913177	-41.2908936	-11.6854525	0.258
L26	-4.49333096	2.48852944	53.9551048	-33.3199577	-16.0133057	0.238
L27	-4.52912569	3.28587341	48.2331848	-48.6194572	-15.9582672	0.319
L28	-4.52298212	3.256078	63.402832	-48.4812775	-12.752758	0.212
L29	-4.81293726	2.08405995	69.3171005	-39.6858788	-15.3131933	0.246
L31	-4.73594141	0.731017649	47.0833549	-36.8992348	-15.1315441	0.192
L32	-4.63027239	3.51910138	40.4549713	-54.8345413	-16.2687168	0.207
L34	-4.82514524	1.82431555	37.2686043	-55.1147346	-12.8953199	0.306
L35	-4.64924383	2.06205535	45.2310524	-52.5151253	-12.6898384	0.262
L37	-4.93070602	1.24613357	14.4794188	-67.3982162	-14.2452564	0.222
L38	-4.256355	1.325658	15.236535	-563256354	-123.525653	0.2356
L43	-3.59877467	1.30459833	2.60804319	-35.2643356	-6.84670687	0.128
L44	-3.81998968	1.21585739	11.0346546	-35.2956848	-8.45313549	0.070
L45	-4.48522472	1.10241115	29.9271927	-30.5219498	-9.03198051	0.083
L46	-3.82427931	0.824638844	25.8639469	-23.777956	0.603183985	0.088
L47	-4.5938282	0.934319556	33.1085548	-54.815239	-11.1250544	0.117
L48	-4.82161379	1.38320065	-3.77851653	-43.7966957	-11.3690357	0.160
L49	-4.7997489	1.44501567	-5.9522171	-46.6148033	-14.142457	0.174
L51	-4.21852636	2.02631927	50.182251	-57.0978699	-11.8984489	0.189
L52	-4.74782705	0.737626314	-5.68534279	-46.3250999	-15.2927198	0.189
L53	-4.836936	1.95184958	60.3355751	-26.3364162	-15.0616941	0.143
L54	-4.40791798	1.40854919	64.750618	-30.32617	-8.24160576	0.238
L55	-4.38038158	2.29839063	40.2982025	-43.6075706	-12.984643	0.347
L56	-4.96466064	1.42215419	53.9763756	-49.9227905	-16.1066895	0.425
L57	-3.82165098	2.89302421	66.7069244	-39.9659081	-8.7645216	0.234

Table S4 . Results of energy (binding affinity) of the **best** complex formed by antioxidants drug molecules with the pocket of the ***catalase*** target.

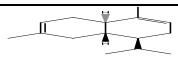
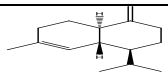
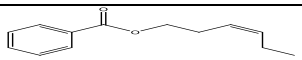
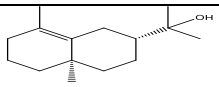
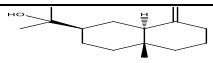
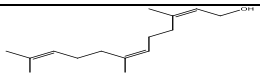
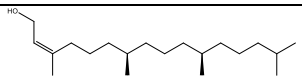
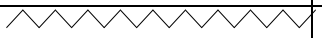
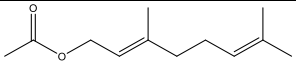
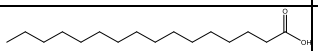
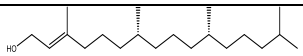
	Chemical Structure	**Binding Energy (Kcal/mole)**	**Rmsd -refine**	**Energy-Conf**	**Energy-Place**	**Energy-Refine**	**RMSD**
β-Cadinene		-5.528	2.355	43.482193	-52.9849396	-15.390	1.327
δ-Cadinene		-5.351	1.159	16.569	-47.146	-15.205	0.086
3-(Z)-Hexenyl-benzoate		-5.478	1.930	27.476	-48.967	-16.140337	0.237
ϒ-Eudesmol		-5.286	1.428	40.253	-54.067	-16.033	0.282
β-Eudesmol		-5.070	2.654	8.3214	-51.109	-14.573	0.204
(Z,Z)-Farnesol		-5.717	2.840	30.338	-50.508	-18.749	0.246
(Z)-Phytol		-7.184	2.225	24.944	-67.679	-22.707	0.306
Heneicosane		-6.809	2.181	16.027	-58.416	-20.155	0.237
Eicosane		-7.158	1.879	14.769	-40.716	-19.400	0.150
Geranyl acetate		-5.268	1.295	-18.100	-51.625	-15.292	0.231
Aplotaxene		-6.130	1.630	37.518	-53.907	-19.592	0.281
Hexadecanoic acid		-6.266	1.053	-79.371	-61.458	-20.364	0.310
(E)-Phytol		-6.908	1.747	24.898	-63.211	-19.590	0.321

Table S5 : S-score (Energy) and interactions between compounds and the active site residues of catalase target.

Nº	Compounds	S-score (kcal/mol	Bonds between atoms of compounds and residues of the active site					
			Atom of compound	Involved Receptor atoms	Involved Receptor residues	Type of interaction bond	Distances (Å)	Energies (kcal/mol
	Catalase (Cal)							
L24	3-(Z)-Hexenyl-benzoate	-5.478	6-ring	NZ	LYS 237	pi-cation	3.83	-1.3
L33	β-Eudesmol	-5.070	O1 1	6-ring	PHE 198	H-pi	4.49	-0.7
L5	p-Cymene	-4.312	6-ring	6-ring	PHE 198	pi-pi	3.89	-0.0
L10	Linalool	-4.677	O1 1 O1 1	O NH	HOH1444 ARG203	H-donor H-acceptor	2.39 2.63	8.0 -1.5
L12	methyl-Salicylate	-4.232	O3 3 6-ring	O CD	HOH 1533 ARG 203	H-acceptor pi-H	2.44 4.33	2.9 -0.7
L13	Decanol	-4.871	O1 1 O1 1	O O	HOH 1414 HOH 1484	H-donor H-acceptor	2.64 2.34	-0.4 13.3
L14	α-Copaene	-4.668	C11 11	6-ring	PHE 198	H-pi	3.77	-0.6
L22	β-Cadinene	-5.528	C3 3	6-ring	PHE 198	H-pi	4.00	-0.6
L27	Salvial-4(14)-en-1-one	-4.529	C6 6	5-ring	HIS 305	H-pi	3.80	-1.0
L29	Humuleneepoxyde II	-4.812	C8 8	5-ring	HIS 305	H-pi	3.75	-1.0
L32	τ-Muurolol	-4.630	O1 1	O	HOH 1444	H-acceptor	2.60	-1.1
L33	β-Eudesmol	-5.002	O1 1	O	HOH1533	H-donor	2.72	-1.2
L36	(Z,Z)-Farnesol	-5.130	O1 1	O	HOH 1465	H-donor	2.59	-0.6
L45	α-Thujene	-4.485	C4 4	6-ring	PHE198	H-pi	4.21	-0.6
L47	methyl-Salicylate	-4.593	O2 2	O	ASN 149	H-donor	2.47	-0.4
L48	Decanol	-4.821	O1 1	O	HOH 1465	H-donor	2.54	0.8
L49	Dec-3-en-2-one	-4.799	O1 1 O1 1	O O	HOH 1465 HOH 1533	H-acceptor H-acceptor	2.63 2.52	-1.7 0.5
L50	Geranylacetate	-5.432	O2 2	N	HIS 305	H-acceptor	2.74	-3.6
L52	Dodecanal	-4.747	O1 1	O	HOH 1608	H-acceptor	2.55	-0.7
L56	Caryophyllene oxyde	-4.964	O1 1 C15 15	N 5-ring	HIS 305 HIS 305	H-acceptor H-pi	2.61 4.60	-2.7 -0.6

H = Conventional hydrogen bond, C = Carbon hydrogen bond, Aa = Alkyl-alkyl, Ap = Alkyl-Pi, Aps = Amide-Pi stacked, Ppt = Pi-pi T-shaped, X = Halogen

Table S6. The docking energies of **other** DNA inhibitors.

Ligand	Compound	DE*(kcal/mol) *ctDNA*	DE*(kcal/mol) ***Catalase***	ETOR (kT)	VDW (kT)	EIE (kT)
BHT		-4.743	-5.052	330.721	413.487	-1942.09
EDTA		-4.965	-5.591	330.722	413.486	-1942.09
Lref		-5.900	-8.043	330.722	413.486	-1942.09
L22	β-Cadinene	-4.741	-5.528	330.704	413.378	-1942.04
L23	δ-Cadinene	-5.507	-5.351	330.722	413.682	-1942.18
L24	3-(Z)-Hexenyl-benzoate	-5.757	-5.478	330.723	413.680	-1942.19
L30	ϒ-Eudesmol	-4.824	-5.286	330.723	413.681	-1942.19
L33	β-Eudesmol	-4.793	-5.070	330.724	413.680	-1942.19
L36	(Z,Z)-Farnesol	-5.482	-5.717	330.723	413.317	-1942.01
L50	Geranyl acetate	-5.029	-5.268	330.724	413.316	-1942.01
L58	Aplotaxene	-6.406	-6.130	330.725	413.315	-1942.01
	DE: Energy ETOR: Energy Tortion VDW: Van Der Walls EIE: Electostatic					

Table S7: Interaction profiles of **other** compounds for three *Endogenous Enzymatic* inhibitors

Nº	Compound	Targets	Energy (kcal/mol	Energy Tortion (kT)	Van Der Walls (kcal/mol	Electrostatic (kcal/mol)
L22	β-Cadinene	CAT	-5.528	2516.749	8577.675	-22121.4
		SOD	-3.422	621.834	3664.946	-10248.4
		GPX	-4.462	1072.848	4669.599	-12257.0
L23	δ-Cadinene	CAT	-5.351	2514.223	8580.197	-22145.5
		SOD	-3.532	625.892	3646.372	-10224.6
		GPX	-4.053	1072.109	4693.851	-12282.4
L24	3-(Z)-Hexenyl-benzoate	CAT	-5.470	2526.529	8570.499	-22161.7
		SOD	-3.693	624.144	3701.304	-10248.5
		GPX	-4.380	1080.134	4729.110	-12320.9
L30	ϒ-Eudesmol	CAT	-5.286	2550.548	9178.920	-22166.9
		SOD	-3.182	628.255	3698.876	-10299.3
		GPX	-4.227	1085.522	4744.378	-12365.9
L33	β-Eudesmol	CAT	-5.070	2545.981	8611.407	-22208.9
		SOD	-3.494	634.114	3849.729	-10525.8
		GPX	-4.000	1089.727	4790.189	-12429.4
L36	(Z,Z)-Farnesol	CAT	-5.717	2538.600	8615.747	-22258.9
		SOD	-3.782	622.721	3627.715	-10134.0
		GPX	-4.356	1071.766	4784.062	-12419.4
L50	Geranyl acetate	CAT	-5.268	2532.317	9171.650	-22260.7
		SOD	-4.173	600.814	3709.599	-10307.0
		GPX	-4.337	1081.093	4770.511	-12436.6
L58	Aplotaxene	CAT	-6.130	2523.155	9149.877	-22190.6
		SOD	-3.714	592.475	3706.447	-10286.5
		GPX	-4.664	1073.626	4769.966	-12422.9
DE: docking energy; ETOR: Torsion energy; VDW: Van der Waals; EIE: Electrostatic Interaction Energy						

Table S8 . Predicted of toxicity risks **other** test compounds

Ligands	Mutagenic	Tumorigenic	Irritant	Reproductive effective
Lref				
BHT				
EDTA				
L22				
L23				
L24				
L30				
L33				
L36				
L50				
L58				
green = good, yellow = tolerable, red = bad.				

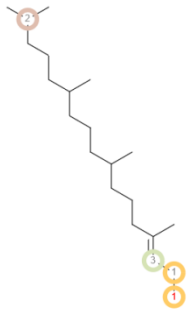
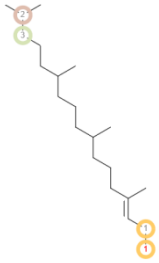
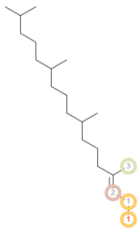
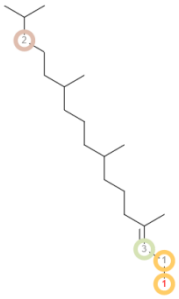
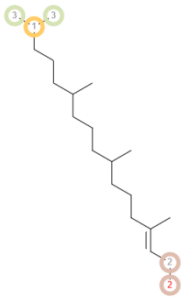
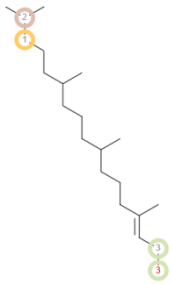
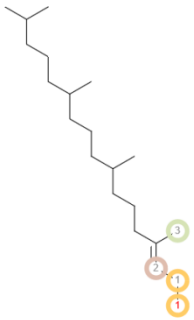
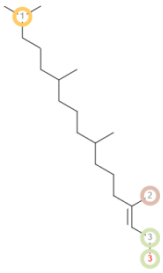
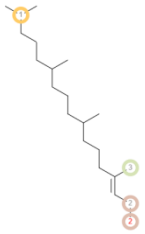
Table S9. Drug-likeness prediction through OSIRIS Property Explorer of the best inhibitors

S. number	**Ligand**	***c* log *P***	**Solubility log *S***	**Molecular weight**	**TPSA Å²**	**Druglikness**	**Drug score**
BHT31404		4.82	-3.98	220.35	20.23	-9.12	0.05
EDTA6049		-6.14	1.67	292.24	155.68	-7.63	0.17
Lref		-11.59	0.95	745.2	393.58	-36.39	0.26
01	L22	4.25	-3.48	204.36	00.00	-2.48	0.44
02	L23	4.33	-3.64	204.36	00.00	-6.30	0.41
03	L24	3.54	-2.91	204.27	26.30	-5.32	0.27
04	L30	3.73	-3.27	222.37	20.23	-4.04	0.45
05	L33	3.64	-3.48	222.37	20.23	-7.00	0.44
06	L36	5.66	-2.87	222.37	20.23	-3.38	0.20
10	L50	3.97	-2.30	196.29	26.30	-2.88	0.08
11	L58	6.85	-4.29	232.41	00.00	-23.02	0.17
MW: molecular weight, MLogP: logarithm of partition coefficient of the compound between water and n-octanol: n-OHNH donors: number of hydrogen bonds donors. n-ON acceptors: number of hydrogen bond acceptors. n-ROTB: number of rotatable bonds							

Table S10 . Details of in-silico ADME profile of eight selected best ligands using the Swiss ADME online server

			L22	L23	L30	L33	L39	L40	L42	L60
ADMET PROFILE	**Physiochemicalparameters**	**Formula**	$C_{15}H_{24}$	$C_{15}H_{24}$	$C_{15}H_{26}O$	$C_{15}H_{26}O$	$C_{20}H_{40}O$	$C_{21}H_{44}$	$C_{20}H_{42}$	$C_{20}H_{40}O$
		Molecularweight	204.35 g/mol	204.35 g/mol	222.37 g/mol	222.37 g/mol	296.53 g/mol	296.57 g/mol	282.55 g/mol	296.53 g/mol
		Mol. refractivity	69.04	69.04	70.46	70.46	98.94	103.06	98.25	98.94
	Lipophilicity	**ILOGP**	3.36	3.39	3.16	3.07	4.78	5.85	5.64	4.77
		SILICOS-IT	3.73	4.01	3.75	3.64	6.57	8.43	7.98	6.57
	Water Solubility	**Log S (ESOL), Class**	-3.56	-3.76	-3.29	-3.51	-5.98	-7.41	-7.05	-5.98
		Log S (Ali), Class	-3.70	-4.02	-3.49	-3.86	-8.47	-10.96	-10.40	-8.47
		SILICOS-IT, Class	-3.07	-3.32	-3.41	-3.21	-5.51	-8.34	-7.94	-5.51
	Pharmacokinetics	**GI absorption**	Low	Low	High	High	Low	Low	Low	Low
		BBB permeant	No	No	Yes	Yes	No	No	No	No
		Log K_p(skin perm.)	-4.71 cm/s	-4.49 cm/s	-5.25cm/s	-5.00cm/s	-2.29 cm/s	-0.31 cm/s	-0.60 cm/s	-2.29 cm/s
		CYP1A2	No	No	No	No	No	Yes	Yes	No
		CYP2C19	Yes	Yes	No	No	No	No	No	No
		CYP2C9	Yes	Yes	No	Yes	Yes	No	No	Yes
		CYP2D6	No	No	No	No	No	No	No	No
		CYP3A4	No	No	No	No	No	No	No	No

Table S11. Results of the P450 sites of metabolism prediction study of best ligand molecules

Names of P450 isoenzymes	**(Z)-Phytol** **L39**	**Names of P450 isoenzymes**	**(Z)-Phytol** **L39**	**Names of P450 isoenzymes**	**(Z)-Phytol** **L39**
1A2		2C8		2D6	
2A6		2C9		2E1	
2B6		2C19		3A4	

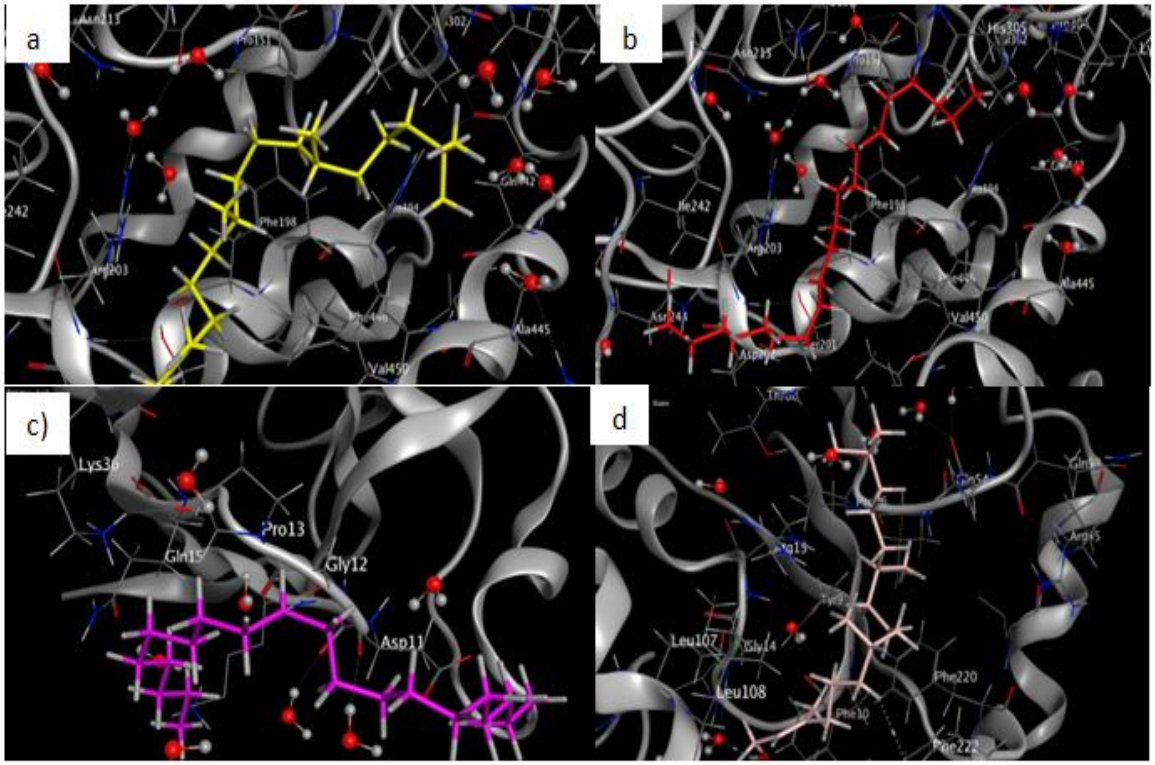


Figure S1. 3D representations of the best pose interactions between the ligands and their receptor. The proteins are represented in solid ribbon model and the ligands are represented in stick model. A. interaction between Z-phytol and Cat, B. interaction between Eicosane and Cat, C. interaction between Eicosane and Cat.D. interaction between E-phytol and GPX.

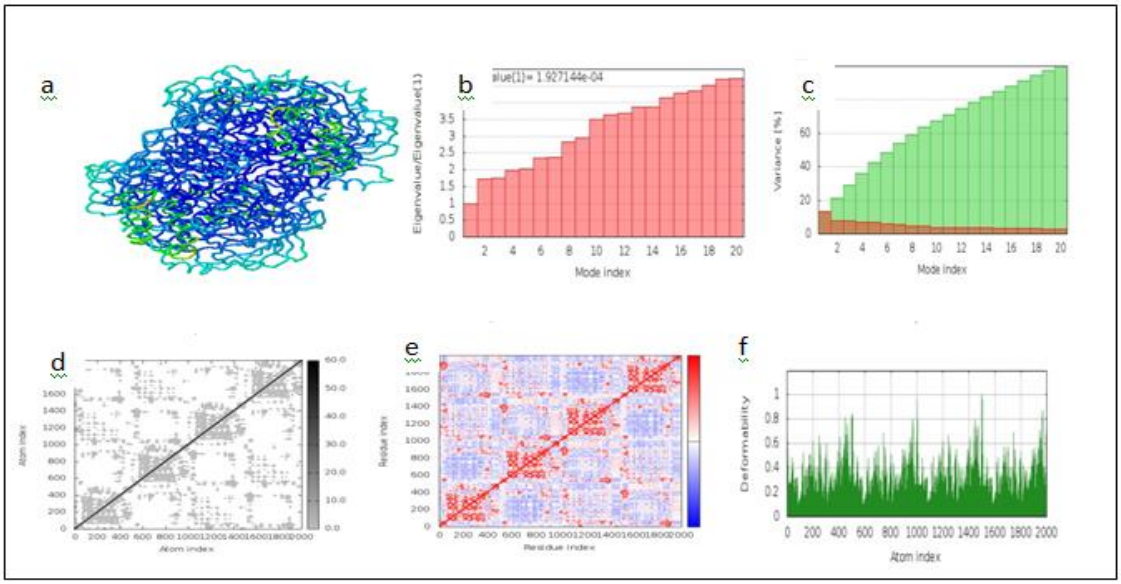


Figure S2. Results of molecular dynamics simulation of (Z)-Phytol – Catalase (*Cat*) docked complex. (a) NMA mobility, (b) eigenvalue, (c) variance (red color indicates individual variances and green color indicates cumulative variances), (d) elastic network (darker grey regions indicate stiffer regions) of the complex, e) co-variance map (correlated (red), uncorrelated (white) or anti-correlated (blue) motions)

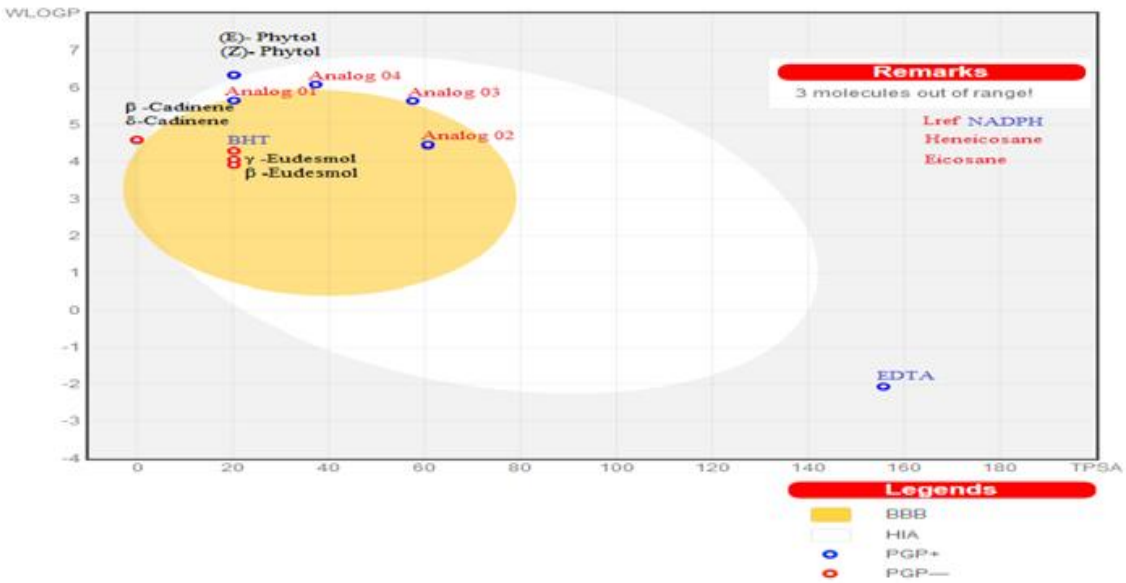


Figure S 3. BOILED-Egg plot. Points located in the BOILED-Egg's yolk (yellow) represent the molecules predicted to passively permeate through the blood-brain barrier (BBB). whereas the ones in the egg white are relative to the molecules predicted to be passively absorbed by the gastrointestinal tract; the blue dots indicate the molecules for which it was expected to be effluated from the central nervous system (CNS)