Comparative Molecular Docking Analysis of *Ocimum sanctum* Compounds and Anti-Allergic Drugs Against Allergic Rhinitis Targets

Supplementary Table 1

ST1: List of PubChem IDs of the phytocompounds and chemical names

	Compound name	Chemical name	PubChem id
1.	Borneol	Bicyclo[2.2.1]heptan-2-ol, 1,7,7-trimethyl-, (1s-endo)-	439569
2.	Eugenol	Eugenol	3314
3.	Cyclohexane	Cyclohexane, 1-ethenyl-1-methyl-2,4-bis(1-methylethenyl)-, [1S-1.alpha., 2.beta., 4.beta.)]-	6431151
4.	Isoaromadendrene epoxide	Isoaromadendrene epoxide	534398
5.	Isocaryophyllene	bicyclo[7.2.0]undec-4-ene, 4,11,11-trimethyl-8-methylene-, [1r-(1r*,4e,9s)	5322111
6.	Germacrene D	1,6-Cyclodecadiene, 1-methyl-5-methylene-8-(1-methylethyl)-, [s-(e,e)]	5373727
7.	β-Selinene	Naphthalene, decahydro-4a-methyl-1-methylene-7-(1-methylethenyl)-,	442393
8.	α-selinene	alpha.-selinene	10123
9.	Choline	Choline	305
10.	β-Caryophyllene epoxide	(-)-5 Oxatricyclo[8.2.0.0(4,6)]dodecane,,12-trimethyl-9-methylene-, [1r]	14350
11.	Humulene epoxide II	(1R,3E,7E,11R)-1,5,5,8-Tetramethyl-12-oxabicyclo[9.1.0]dodeca-3,7-diene	5318104
12.	β-Costol	2-((2R,4aR,8aS)-4a-Methyl-8-methylenedecahydronaphthalen-2-yl)prop-2-en-1-ol	12304104
13.	Epiglobulol	1,1,4,7-Tetramethyldecahydro-1H-cyclopropa[e]azulene-4,7-dio	178322
14.	Pseudoephedrine	Pseudoephedrine	7028
15.	Levocetirizine	Levocetirizine	1549000

Supplementary Table 2: Toxicity prediction of the best binding molecules and control drugs

Pubchem IDs	**5373727**	**10123**	**534398**	**305**	**7028**
Predicted LD50	5300mg/kg	5000mg/kg	5000mg/kg	1391mg/kg	404mg/kg
Predicted toxicity clsaa	5	5	5	4	4
Hepatotoxicity (Probability of prediction)	0.80 (Inactive)	0.82 (Inactive)	0.79 (Inactive)	0.94 (Inactive)	0.96 (Inactive)
Carcinogenicity (Probability of prediction)	0.73 (Inactive)	0.70 (Inactive)	0.56 (Inactive)	0.78 (Inactive)	0.64 (Inactive)
Mutagenicity (Probability of prediction)	0.87 (Inactive)	0.85 (Inactive)	0.78 (Inactive)	0.91 (Inactive)	0.86 (Inactive)
Immunotoxicity (Probability of prediction)	0.80 (Active)	0.99 (Inactive)	0.93 (Inactive)	0.99 (Inactive)	0.99 (Inactive)
Cytotoxicity (Probability of prediction)	0.83 (Inactive)	0.73 (Inactive)	0.79 (Inactive)	0.82 (Inactive)	0.78 (Inactive)

Supplementary Table 3: ADMET properties of the compounds along with control drugs

ADMET Properties	PubChem ID				
	5373727	**10123**	**534398**	**7028**	**305**
Molecular weight (g/mol)	204.35	204.35	220.35	165.28	104.17
Topological polar surface area (TPSA) (A°)	0	0	12.53	32.26	20.23
Num. H-bond acceptors	0	0	1	2	1
Num. H-bond donors	0	0	0	2	1
Molar refractivity	70.68	68.78	66.63	49.79	29.69
XLOGP	4.74	5.2	3.76	0.93	-0.04
iLOGP	3.32	3.31	3.23	2.25	-2.14
MLOGP	4.53	4.63	3.81	1.56	-3.46
WLOGP	4.89	4.73	3.48	1.00	-0.32
Lipinski	1	1	0	1	0
Ghose	0	0	0	1	2
Veber	0	0	0	1	1
Egan	0	0	0	1	0
Muegge	1	2	1	1	1
Bioavailability score	0.55	0.55	0.55	0.55	0.55
Gastrointestinal (GI) absorption	Low	Low	High	High	Low
Blood brain barrier (BBB) permeability	No	No	Yes	Yes	No
P-gp substrate	No	No	No	No	No
CYP1A2 inhibitor	No	No	Yes	No	No
CYP2C19 inhibitor	No	Yes	Yes	No	No
CYP2C9 inhibitor	Yes	Yes	No	No	No
CYP2D6 inhibitor	No	No	No	No	No
CYP3A4 inhibitor	No	No	No	No	No
Log Kp (skin permeation) cm/s	-4.18	-3.85	-4.97	-6.65	-7.22
Pan assay interference compounds (PAINS)	0	0	0	0	0
Brenk	1	1	1	0	1
Leadlikeness	2	2	2	1	1
Synthetic accessibility	4.55	4.22	3.96	1.76	1