**Supplementary Materials** 

Chemical composition and toxicity studies on Lantana camara L. flower essential oil and its in-silico binding and pharmacokinetics to superoxide dismutase 1 for amyotrophic lateral sclerosis (ALS) therapy

Abdullah Haikal, Ahmed R. Ali

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## **Molecular Docking Simulation Methodology**

Molecular docking simulation was calculated using AutoDock 4.2 included in LigandScout Software. In addition to intramolecular terms and a "full" desolvation model, the AutoDock semi-empirical force field takes directionality in hydrogen bonds into account. The total of the torsional degrees of freedom is used to compute the conformational entropy. The water contribution (dispersion/repulsion, hydrogen bonding, electrostatics, and desolvation) is estimated using pair-wise atomic terms; weights are provided for calibration (based on experimental data), but water molecules are not explicitly represented. In summary, the evaluation phase involves determining the energy of the protein and ligand in their unbound states first. Next, determine the protein-ligand complex's energy. The difference between 1 and 2 is then calculated.

$$\begin{split} \Delta G = (V_{\text{bound}}^{\text{L}-\text{L}} - V_{\text{unbound}}^{\text{L}-\text{L}}) + (V_{\text{bound}}^{\text{P}-\text{P}} - V_{\text{unbound}}^{\text{P}-\text{P}}) \\ + (V_{\text{bound}}^{\text{P}-\text{L}} - V_{\text{unbound}}^{\text{P}-\text{L}} + \Delta S_{\text{conf}}) \end{split}$$

where P stands for protein, L for ligand, V for the pairwise assessments previously indicated, and  $\Delta S$ ~conf~ for conformational entropy lost during binding.

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The following are the parameters used in the docking run. Genetic algorithm runs (the specified number of docking runs using the simulated annealing search engine) was set to 20. RMSD cluster tolerance (the RMSD threshold (in Å) for joining together multiple docking results and show them as one entry in the list of docked poses) was set to 2.0 Å. Number of individuals in population (the size of the initial population for the genetic algorithm search) was set to 150. Max. number of energy evaluations (maximum number of energy evaluations performed during each genetic algorithm search run) was set to 2,500,000. Max. number of generations (maximum number of generations simulated during each genetic algorithm search run) was set to 27,000.

# **Results from OSIRIS Software (Table 4):**

### • 2-Thujene



### • *α*-pinene

enter composite non-composite and non-	KS
Interview	(S ? ? ? ? ? ? ? ? ? ? ? ? ? ? ? ? ? ? ?

### • Camphene



### • Sabinene



### • β-Myrcene



### • 3-Carene

Enter c	ompound name, SMILES or CAS-no:	<ctrl-v clipboard="" from="" paste="" to=""></ctrl-v>	Toxicity Risks
ներին			🖯 mutagenic ?
*≠			😑 tumorigenic 🛛 ?
FR			😑 irritant 🛛 🝸
			effective
			cLogP ?
1			Solubility ?
			-2.52
00			Molweight
00			<b>O</b> 136.0
+ -		known chirality	TPSA ?
C Si	. un	Known chirality	• 0.0
NP			Druglikeness [?]
0 \$			Drug Score 2
F CI			
Br I			
H ?			

## • o-Cymene

Enter compound name, SMILES or CAS-no:	<ctrl-v clipboard="" from="" paste="" to=""></ctrl-v>	Toxicity Risks
ներերություն		🖯 mutagenic ?
×.		🖯 tumorigenic ?
FR ~		🖯 irritant 💽
¥ 🖍		reproductive ? effective
Text		cLogP ?
		3.19
		Solubility ?
		-2.83
	$\triangleleft$	Molweight
		134.0
+ -	$\checkmark$	TPSA ?
C Si		0.0
N P		Druglikeness [?
0 5		Drug-Score 2
F CI		0.47
Br I		
H ?		

## • Eucalyptol

Enter compound name, SMILES or CAS-no:	<ctrl-v clipboard="" from="" paste="" to=""></ctrl-v>	Toxicity Risks
		mutagenic ?     tumorigenic ?     irritant ?
in text		effective
		Solubility ?
		Molweight 154.0
C Si N P		Druglikeness ?
0 S F C1 Br 1		
H ?		

### • β-cis-Ocimene

![](_page_6_Figure_1.jpeg)

## • y-Terpinene

Enter compound name, SMILES or CAS-no:	<ctrl-v clipboard="" from="" paste="" to=""></ctrl-v>	Toxicity Risks
Gen Uth		😑 mutagenic 🛛 ?
× =		😑 tumorigenic 🛛 🕐
CR and		😑 irritant 🛛 💽
Text		effective
	1	<b>cLogP</b> ?
	$\wedge$	Solubility ?
		Molweight
+ - C Si		<b>TPSA</b> ?
N P		Druglikeness ?
F CI Br L		Drug-Score ?
H ?		

### • Terpinen-4-ol

![](_page_7_Figure_1.jpeg)

### • α-Copaene

Enter compound name, SMILES or CAS-no:	<ctrl-v clipboard="" from="" paste="" to=""></ctrl-v>	Toxicity Risks
Gen Uth		😑 mutagenic 🛛 ?
× -		😑 tumorigenic 🛛 🕐
R.		😑 irritant 🛛 ?
Tr als		effective
🖉 Text		
$\smallsetminus$		CLOGP [?]
N 34		Solubility ?
		Molweight
	$\sim$	<b>6</b> 204.0
+-		TPSA ?
C Si	A A	0.0 O
NP		Druglikeness [?]
0 \$	Ť	Drug-Score 2
F CI	I	
Br I u	nknown chirality	
H  ?		

### • Caryophyllene

![](_page_8_Figure_1.jpeg)

### • Humulene

Enter compour	nd name, SMILES or CAS-no:	<ctrl-v clipboard="" from="" paste="" to=""></ctrl-v>	Toxicity Risks
<mark>Կ</mark> ես կին			🖯 mutagenic 🔋
**			🖯 tumorigenic ?
R			😑 irritant 🛛 ?
₩ 🖍			oreproductive Productive effective
🖌 Text			cLogP ?
			6.24
			Solubility ?
음분			-3.4
			Molweight
			204.0
		<sup>∎</sup> L J	
		X	Druglikeness ?
N P			-4.72
			Drug-Score ?
Pr L			0.28
BT 1			
H f			

### Germacrene D

![](_page_9_Figure_1.jpeg)

#### • Bicyclogermacrene

![](_page_9_Figure_3.jpeg)

### • Aromandendrene

![](_page_10_Figure_1.jpeg)

### • trans-Nerolidol

![](_page_10_Figure_3.jpeg)

### • Caryophyllene oxide

![](_page_11_Figure_1.jpeg)

### • Longifolenaldehyde

![](_page_11_Figure_3.jpeg)

### • Isospathulenol

![](_page_12_Figure_1.jpeg)

### • Aromadendrene oxide l

![](_page_12_Figure_3.jpeg)

# **Results from SwissADME (Table 5):**

• 2-Thujene

Molecule 1			(
<b># Θ Ο 🖉</b> Σ			Water Solubility
	LIPO	Log S (ESOL) 📀	-2.77
C	H <sub>3</sub>	Solubility	2.33e-01 mg/ml ; 1.71e-03 mol/l
	FLEX	Class 🔞	Soluble
		Log S (Ali) 🥹	-3.09
	>	Solubility	1.11e-01 mg/ml ; 8.13e-04 mol/l
		Class 🛞	Soluble
н₄с—	INSATU	Log S (SILICOS-IT) 📀	-1.78
з \ <sub>СН</sub>		Solubility	2.27e+00 mg/ml ; 1.67e-02 mol/l
G '3		Class 🔞	Soluble
	INSOLU		Pharmacokinetics
SMILES C[C@H]1C=CC2(	C1C2)C(C)C	GI absorption 📀	Low
P	hysicochemical Properties	BBB permeant 📀	Yes
Formula	C10H16	P-gp substrate 📀	No
Molecular weight	136.23 g/mol	CYP1A2 inhibitor 📀	No
Num. heavy atoms	10	CYP2C19 inhibitor 📀	No
Num. arom. heavy atoms	0	CYP2C9 inhibitor 📀	No
Fraction Csp3	0.80	CYP2D6 inhibitor 🤨	No
Num. rotatable bonds	1	CYP3A4 inhibitor 📀	No
Num. H-bond acceptors	0	Log K <sub>n</sub> (skin permeation) 📀	-4.71 cm/s
Num. H-bond donors	0	e protection of	Druglikeness
Molar Refractivity	45.22	Lipinski 📀	Yes: 1 violation: MLOGP>4.15
TPSA 🥹	0.00 A <sup>2</sup>	Ghose 🔞	No; 1 violation: MW<160
	Lipophilicity	Veber 😣	Yes
Log P <sub>o/w</sub> (ILOGP)	2.65	Egan 📀	Yes
Log P <sub>o/w</sub> (XLOGP3) 📀	3.41	Muegge 📀	No: 2 violations: MW<200. Heteroatoms<2
Log P <sub>o/w</sub> (WLOGP) 📀	2.85	Bioavailability Score 🥹	0.55
Log P <sub>o/w</sub> (MLOGP) 📀	4.29	,	Medicinal Chemistry
Log P <sub>o/w</sub> (SILICOS-IT) 📀	2.55	PAINS ()	0 alert
Consensus Log P <sub>o/w</sub> 📀	3.15	Brenk 🛞	1 alert: isolated_alkene 📀
		Leadlikeness 🛞	No; 1 violation: MW<250
		Synthetic accessibility 📀	4.19

## • α-pinene

Molecule 1			
<b># Θ Ο 🖉</b> Σ			Water Solubility
	LIPO	Log S (ESOL) 📀	-3.51
		Solubility	4.24e-02 mg/ml ; 3.11e-04 mol/l
	CH <sub>3</sub> FLEX SIZE	Class 📀	Soluble
/		Log S (Ali) 📀	-4.20
H <sub>2</sub> C,		Solubility	8.59e-03 mg/ml ; 6.31e-05 mol/l
		Class 🛞	Moderately soluble
H <sub>3</sub> C /	INSATU	Log S (SILICOS-IT) 🔞	-2.23
		Solubility	8.06e-01 mg/ml ; 5.92e-03 mol/l
		Class 🛞	Soluble
	INSOLU		Pharmacokinetics
SMILES CC1=CCC2CC10	C2(C)C	GI absorption <sup>(2)</sup>	Low
F	Physicochemical Properties	BBB permeant 📀	Yes
Formula	C10H16	P-gp substrate 📀	No
Molecular weight	136.23 g/mol	CYP1A2 inhibitor 📀	No
Num. heavy atoms	10	CYP2C19 inhibitor 📀	No
Num. arom. heavy atoms	0	CYP2C9 inhibitor 📀	Yes
Fraction Csp3	0.80	CYP2D6 inhibitor 📀	No
Num. rotatable bonds	0	CYP3A4 inhibitor 📀	No
Num. H-bond acceptors	0	Log $K_{\rm p}$ (skin permeation) $^{(0)}$	-3.95 cm/s
Num. H-bond donors	0		Druglikeness
	45.22	Lipinski 🔞	Yes; 1 violation: MLOGP>4.15
IP5A 💿	U.UU A-	Ghose 📀	No; 1 violation: MW<160
	2.63	Veber 🛞	Yes
	2.00	Egan 📀	Yes
LOG P <sub>0/W</sub> (XLOGP3)	4.48	Muegge 📀	No; 2 violations: MW<200, Heteroatoms<2
Log P <sub>o/w</sub> (WLOGP) 🧐	3.00	Bioavailability Score 📀	0.55
Log P <sub>o/w</sub> (MLOGP) 🧐	4.29		Medicinal Chemistry
Log P <sub>o/w</sub> (SILICOS-IT) 📀	2.79	PAINS 🛞	0 alert
Consensus Log P <sub>o/w</sub> 📀	3.44	Brenk 🛞	1 alert: isolated_alkene 🥹
		Leadlikeness 📀	No; 2 violations: MW<250, XLOGP3>3.5
		Synthetic accessibility 📀	4.44

## • Camphene

Molecule 1			٤
<b># Θ Ο </b> <i>ω</i> Σ			Water Solubility
	LIPO	Log <i>S</i> (ESOL) 📀	-3.34
HC		Solubility	6.18e-02 mg/ml ; 4.54e-04 mol/l
	FLEX SIZE	Class 📀	Soluble
Υ /		Log S (Ali) 😗	-3.93
		Solubility	1.60e-02 ma/ml : 1.17e-04 mol/l
130		Class 🔞	Soluble
	INSATU	Log <i>S</i> (SILICOS-IT) 📀	-2.48
H <sub>3</sub> C		Solubility	4.55e-01 mg/ml ; 3.34e-03 mol/l
		Class 📀	Soluble
	INSOLU		Pharmacokinetics
SMILES C=C1C2CCC(C1)	(C)C)C2	GI absorption 📀	Low
P	hysicochemical Properties	BBB permeant 🧐	Yes
Formula	C10H16	P-gp substrate 📀	No
Molecular weight	136.23 g/mol	CYP1A2 inhibitor 📀	No
Num. heavy atoms	10	CYP2C19 inhibitor 📀	No
Num. arom. heavy atoms	0	CYP2C9 inhibitor 📀	Yes
Fraction Csp3	0.80	CYP2D6 inhibitor 📀	No
Num. rotatable bonds	0	CYP3A4 inhibitor 📀	No
Num. H-bond acceptors	0	Log <i>K</i> p (skin permeation) 📀	-4.13 cm/s
Num. H-bond donors	0		Druglikeness
Molar Refractivity	45.22	Lipinski 📀	Yes; 1 violation: MLOGP>4.15
IPSA 🥑	0.00 A <sup>2</sup>	Ghose 📀	No; 1 violation: MW<160
		Veber 🐵	Yes
Log P <sub>o/w</sub> (ILOGP)	2.58	Egan 🐵	Yes
Log P <sub>o/w</sub> (XLOGP3) 🧐	4.22	Muegge 📀	No; 2 violations: MW<200, Heteroatoms<2
Log P <sub>o/w</sub> (WLOGP) 📀	3.00	Bioavailability Score 📀	0.55
Log P <sub>o/w</sub> (MLOGP) 🥹	4.29	,	Medicinal Chemistry
Log P <sub>o/w</sub> (SILICOS-IT) 📀	3.08	PAINS 😢	0 alert
Consensus Log P <sub>o/w</sub> 📀	3.43	Brenk 😢	1 alert: isolated_alkene 📀
		Leadlikeness 📀	No; 2 violations: MW<250, XLOGP3>3.5
		Synthetic accessibility 🥹	3.50

## • Sabinene

Molecule 1			۵
<b>†† ⊕ Ο </b> <i>ω</i> Σ			Water Solubility
	LIPO	Log S (ESOL) 📀	-2.57
CH <sub>3</sub>		Solubility	3.71e-01 mg/ml ; 2.72e-03 mol/l
H₃C—	FLEX	Class 📀	Soluble
		Log S (Ali) 🥹	-2.76
	$\mathbf{N}$	Solubility	2.38e-01 mg/ml : 1.75e-03 mol/l
		Class 🔞	Soluble
M	INSATU	Log <i>S</i> (SILICOS-IT) 📀	-2.48
		Solubility	4.55e-01 mg/ml ; 3.34e-03 mol/l
) í		Class 🔞	Soluble
	INSOLU		Pharmacokinetics
SMILES C=C1CCC2(C1C	C2)C(C)C	GI absorption 📀	Low
	Physicochemical Properties	BBB permeant 🛞	Yes
Formula	C10H16	P-gp substrate 📀	No
Molecular weight	136.23 g/mol	CYP1A2 inhibitor 📀	No
Num. heavy atoms	10	CYP2C19 inhibitor 📀	No
Num. arom. heavy atoms	0	CYP2C9 inhibitor 📀	No
Fraction Csp3	0.80	CYP2D6 inhibitor 📀	No
Num. rotatable bonds	1	CYP3A4 inhibitor 📀	No
Num. H-bond acceptors	0	Log K <sub>n</sub> (skin permeation) 📀	-4.94 cm/s
Num. H-bond donors	0	ор( ; )	Druglikeness
Molar Refractivity	45.22	Lipinski 😗	Yes: 1 violation: MLOGP>4.15
TPSA 🥹	0.00 A <sup>2</sup>	Ghose 😗	No: 1 violation: MW<160
	Lipophilicity	Veber 📀	Yes
Log P <sub>o/w</sub> (iLOGP) 🧐	2.65	Egan 📀	Yes
Log P <sub>o/w</sub> (XLOGP3) 📀	3.09	Muegge 📀	No: 2 violations: MW<200, Heteroatoms<2
Log P <sub>o/w</sub> (WLOGP) 📀	3.00	Bioavailability Score 🛞	0.55
Log P <sub>o/w</sub> (MLOGP) 📀	4.29		Medicinal Chemistry
Log P <sub>o/w</sub> (SILICOS-IT) 📀	3.23	PAINS <sup>(9)</sup>	0 alert
Consensus Log Poly	3.25	Brenk 📀	1 alert: isolated alkene 3
0.00		Leadlikeness 📀	No; 1 violation: MW<250
		Synthetic accessibility 🥹	2.87

S17

# • β-Myrcene

Molecule 1			
<b>₩ ⊕ Ο ₽</b> Σ			Water Solubility
	LIPO	Log S (ESOL) 📀	-3.05
		Solubility	1.22e-01 mg/ml ; 8.96e-04 mol/l
	FLEX	Class 📀	Soluble
сн, сн,		Log <i>S</i> (Ali) 📀	-3.88
		Solubility	1.80e-02 mg/ml ; 1.32e-04 mol/l
н,с		Class 📀	Soluble
	INSATU	Log <i>S</i> (SILICOS-IT) 📀	-2.42
		Solubility	5.24e-01 mg/ml ; 3.85e-03 mol/l
	NICOLU	Class 🤨	Soluble
	INSOLU		Pharmacokinetics
SMILES C=CC(=C)CCC=	C(C)C	GI absorption 📀	Low
F	Physicochemical Properties	BBB permeant 📀	Yes
Formula	C10H16	P-gp substrate 📀	No
Molecular weight	136.23 g/mol	CYP1A2 inhibitor 🛞	No
Num. heavy atoms	10	CYP2C19 inhibitor 🛞	No
Num. arom. heavy atoms	0	CYP2C9 inhibitor 📀	No
Fraction Csp3	0.40	CYP2D6 inhibitor 🧐	No
Num. rotatable bonds	4	CYP3A4 inhibitor 📀	No
Num. H-bond acceptors	0	Log $K_{\rm p}$ (skin permeation) $^{(0)}$	-4.17 cm/s
Num. H-bond donors	0		Druglikeness
Molar Refractivity	48.76	Lipinski 🧐	Yes; 0 violation
TPSA 👽	0.00 A <sup>2</sup>	Ghose 📀	No; 1 violation: MW<160
	2.90	Veber 📀	Yes
	2.09	Egan 🔞	Yes
Log P <sub>o/w</sub> (XLOGP3)	4.17	Muegge 📀	No; 2 violations: MW<200, Heteroatoms<2
Log P <sub>o/w</sub> (WLOGP) 🧐	3.48	Bioavailability Score 📀	0.55
Log P <sub>o/w</sub> (MLOGP) 📀	3.56		Medicinal Chemistry
Log P <sub>o/w</sub> (SILICOS-IT) 📀	3.05	PAINS 🛞	0 alert
Consensus Log P <sub>o/w</sub> 📀	3.43	Brenk 📀	2 alerts: isolated_alkene, polyene 🥺
		Leadlikeness 📀	No; 2 violations: MW<250, XLOGP3>3.5
		Synthetic accessibility 📀	2.85

## • 3-Carene

Molecule 1			۵
<b>Η Θ Ο </b> <i>ω</i> Σ			Water Solubility
	LIPO	Log S (ESOL) 📀	-3.44
		Solubility	4.90e-02 mg/ml ; 3.60e-04 mol/l
	FLEX	Class 🔞	Soluble
	CH3	Log S (Ali) 🥹	-4 10
H <sub>3</sub> C		Solubility	1.09e-02 ma/ml : 8.01e-05 mol/l
H <sub>3</sub> C		Class ()	Moderately soluble
~	INSATU	Log S (SILICOS-IT) 📀	-2.23
		Solubility	8.06e-01 mg/ml ; 5.92e-03 mol/l
		Class 🔞	Soluble
	INSOLU		Pharmacokinetics
SMILES CC1=CCC2C(C1)	C2(C)C	GI absorption 📀	Low
PI	hysicochemical Properties	BBB permeant 📀	Yes
Formula	C10H16	P-gp substrate 📀	No
Molecular weight	136.23 g/mol	CYP1A2 inhibitor 🗐	No
Num. heavy atoms	10	CYP2C19 inhibitor 📀	No
Num. arom. heavy atoms	0	CYP2C9 inhibitor 📀	Yes
Fraction Csp3	0.80	CYP2D6 inhibitor 📀	No
Num. rotatable bonds	0	CYP3A4 inhibitor 📀	No
Num. H-bond acceptors	0	Log $K_{\rm p}$ (skin permeation) 📀	-4.02 cm/s
Num. H-bond donors	0		Druglikeness
Molar Refractivity	45.22	Lipinski 📀	Yes; 1 violation: MLOGP>4.15
TPSA 🥑	0.00 A <sup>2</sup>	Ghose 📀	No; 1 violation: MW<160
	Lipophilicity	Veber 🔞	Yes
Log P <sub>o/w</sub> (ILOGP)	2.63	Egan 🛞	Yes
Log P <sub>o/w</sub> (XLOGP3) 🧐	4.38	Muegge 📀	No; 2 violations: MW<200, Heteroatoms<2
Log P <sub>o/w</sub> (WLOGP) 🛞	3.00	Bioavailability Score 📀	0.55
Log P <sub>o/w</sub> (MLOGP) 📀	4.29		Medicinal Chemistry
Log P <sub>o/w</sub> (SILICOS-IT) 😣	2.79	PAINS (?)	0 alert
Consensus Log P <sub>o/w</sub> 📀	3.42	Brenk 🛞	1 alert: isolated_alkene 📀
		Leadlikeness 🛞	No; 2 violations: MW<250, XLOGP3>3.5
		Synthetic accessibility 📀	3.84

## • o-Cymene

Molecule 1			
<b>₩ ⊕ Ο </b>			Water Solubility
	LIPO	Log S (ESOL) 📀	-3.81
		Solubility	2.08e-02 mg/ml ; 1.55e-04 mol/l
CH <sub>3</sub>	CH <sub>3</sub> FLEX SIZE	Class 📀	Soluble
			-4.10
		Solubility	1 08e-02 mg/ml · 8 01e-05 mol/l
$H_{3}C^{2}$ I		Class ()	Mederately celuble
	INSATU POLAR	Log S (SILICOS-IT)	-3.57
	▼	Solubility	3.58e-02 mg/ml ; 2.67e-04 mol/l
	INSOLU	Class 🤨	Soluble
		Ol shaamtian 0	Pharmacokinetics
SIVILES CO(CTCCCCCTC)	Physicochemical Properties		Low
Formula	C10H14	BBB permeant	res
Molecular weight	134 22 g/mol	P-gp substrate 👽	No
Num, heavy atoms	10	CYP2C10 inhibitor	No
Num. arom. heavy atoms	6	CYP2C19 Inhibitor	No
Fraction Csp3	0.40	CYP2C9 Inhibitor	Vec
Num. rotatable bonds	1	CYP244 inhibitor	No
Num. H-bond acceptors	0	Log K (skin permeation)	4.01 cm/c
Num. H-bond donors	0	Log Ap (Skill permeation)	-4.01 cm/s
Molar Refractivity	45.99	Lininald 🙆	Druglikeness
TPSA 📀	0.00 Ų		res, I violation: MLOGP>4.15
	Lipophilicity	Gnose 👽	
Log P <sub>o/w</sub> (iLOGP) 📀	2.43	Veber	res
Log P <sub>o/w</sub> (XLOGP3) 📀	4.38	Egan 👽	Tes
Log P <sub>o/w</sub> (WLOGP) 📀	3.12	Nuegge	
Log P <sub>o/w</sub> (MLOGP) 📀	4.47		Medicinal Chemistry
Log Poly (SILICOS-IT)	3.29	PAINS ()	
	3.54	Brenk	
Concorroug Log / 0/W	0.01		No: 2 violations: MW<250 XLOGP3>3.5
		Synthetic accessibility @	1.00

## • Eucalyptol

Molecule 1			
<b># Θ Ο 🖉</b> Σ			Water Solubility
	LIPO	Log <i>S</i> (ESOL) 📀	-2.52
H₃C		Solubility	4.63e-01 mg/ml ; 3.00e-03 mol/l
	FLEX	Class 📀	Soluble
H <sub>3</sub> C		Log S (Ali) 😗	-2.59
		Solubility	3.98e-01 mg/ml ; 2.58e-03 mol/l
0		Class 📀	Soluble
Ť			-2.45
	INSATU	Solubility	$5.45e_{-0.1}$ mg/ml $: 3.53e_{-0.3}$ mg/l
CH <sub>3</sub>	3	Class ()	Soluble
	INSOLU		Pharmacokinetics
SMILES CC12CCC(CC1)C	C(O2)(C)C	GI absorption 📀	High
P	Physicochemical Properties	BBB permeant (9)	Yes
Formula	C10H18O	P-gp substrate 📀	No
Molecular weight	154.25 g/mol	CYP1A2 inhibitor 🛞	No
Num. heavy atoms	11	CYP2C19 inhibitor 📀	No
Num. arom. heavy atoms	0	CYP2C9 inhibitor 📀	No
Fraction Csp3	1.00	CYP2D6 inhibitor 📀	No
Num. rotatable bonds	0	CYP3A4 inhibitor 📀	No
Num. H-bond acceptors	1	Log $K_{\rm p}$ (skin permeation) 📀	-5.30 cm/s
Num. H-bond donors	0	, ,	Druglikeness
	47.12	Lipinski 🤨	Yes; 0 violation
IPSA 🐨	9.23 A*	Ghose 📀	No; 1 violation: MW<160
Log P. (il OGP) 😗	2.58	Veber 🐵	Yes
$\log P$ , (YLOGP2)	0.74	Egan 🛞	Yes
	2.14	Muegge 📀	No; 2 violations: MW<200, Heteroatoms<2
Log P <sub>o/w</sub> (WLOGP) 🥹	2.74	Bioavailability Score 📀	0.55
Log P <sub>o/w</sub> (MLOGP) 🧐	2.45		Medicinal Chemistry
Log P <sub>o/w</sub> (SILICOS-IT) 😣	2.86	PAINS 📀	0 alert
Consensus Log P <sub>o/w</sub> 📀	2.67	Brenk 📀	0 alert
		Leadlikeness 📀	No; 1 violation: MW<250
		Synthetic accessibility 📀	3.65

## • β-cis-Ocimene

Molecule 1			٤
<b>₩ ⊕ Ο ₽</b> Σ			Water Solubility
	LIPO	Log <i>S</i> (ESOL) 📀	-3.17
		Solubility	9.20e-02 mg/ml ; 6.75e-04 mol/l
н.с.	FLEX	Class 📀	Soluble
<u> </u>		Log S (Ali) 😗	-3.97
	-CH3	Solubility	1.45e-02 ma/ml : 1.07e-04 mol/l
H <sub>3</sub> C		Class (2)	Soluble
CH2	INSATU	Log S (SILICOS-IT) 😣	-2.04
		Solubility	1.24e+00 mg/ml ; 9.10e-03 mol/l
		Class 📀	Soluble
	INSOLU		Pharmacokinetics
SMILES C=C/C(=C\CC=C(	(C)C)/C	GI absorption 📀	Low
P	hysicochemical Properties	BBB permeant 📀	Yes
Formula	C10H16	P-gp substrate 📀	No
Molecular weight	136.23 g/mol	CYP1A2 inhibitor 📀	No
Num. heavy atoms	10	CYP2C19 inhibitor 📀	No
Num. arom. heavy atoms	0	CYP2C9 inhibitor 📀	No
Fraction Csp3	0.40	CYP2D6 inhibitor 📀	No
Num. rotatable bonds	3	CYP3A4 inhibitor 📀	No
Num. H-bond acceptors	0	Log $K_{\rm p}$ (skin permeation) 📀	-4.11 cm/s
Num. H-bond donors	0	- p · · · ·	Druglikeness
Molar Refractivity	48.76	Lipinski 📀	Yes; 0 violation
TPSA 🥑	0.00 A <sup>2</sup>	Ghose 📀	No; 1 violation: MW<160
	Lipophilicity	Veber 🐵	Yes
Log P <sub>o/w</sub> (ILOGP)	2.91	Egan 📀	Yes
Log P <sub>o/w</sub> (XLOGP3) 😢	4.26	Muegge 📀	No; 2 violations: MW<200, Heteroatoms<2
Log P <sub>o/w</sub> (WLOGP) 📀	3.48	Bioavailability Score (9)	0.55
Log P <sub>o/w</sub> (MLOGP) 🤨	3.56		Medicinal Chemistry
Log P <sub>o/w</sub> (SILICOS-IT) 😣	2.88	PAINS 😢	0 alert
Consensus Log P <sub>o/w</sub> 📀	3.42	Brenk 🐵	2 alerts: isolated_alkene, polyene 📀
		Leadlikeness 📀	No; 2 violations: MW<250, XLOGP3>3.5
		Synthetic accessibility 📀	3.63

## • y-Terpinene

Molecule 1			
<b>Η 🛛 🖓 Σ</b>			Water Solubility
	LIPO	Log S (ESOL) 📀	-3.45
		Solubility	4.79e-02 mg/ml ; 3.52e-04 mol/l
	FLEX	Class 🛞	Soluble
		Log S (Ali) 🔞	-4.22
		Solubility	8.19e-03 mg/ml ; 6.01e-05 mol/l
		Class 🔞	Moderately soluble
	INSATU	Log S (SILICOS-IT)	-2.23
		Solubility	8.06e-01 mg/ml ; 5.92e-03 mol/l
H <sub>3</sub> C <sup>°</sup> CH <sub>3</sub>		Class 📀	Soluble
	INSOLU		Pharmacokinetics
SMILES CC1=CCC(=CC1	)C(C)C	GI absorption 📀	Low
F	Physicochemical Properties	BBB permeant 📀	Yes
Formula	C10H16	P-gp substrate 📀	No
Molecular weight	136.23 g/mol	CYP1A2 inhibitor 📀	No
Num. heavy atoms	10	CYP2C19 inhibitor 📀	No
Num. arom. heavy atoms	0	CYP2C9 inhibitor 📀	No
Fraction Csp3	0.60	CYP2D6 inhibitor 📀	No
Num. rotatable bonds	1	CYP3A4 inhibitor 📀	No
Num. H-bond acceptors	0	Log K <sub>p</sub> (skin permeation) 📀	-3.94 cm/s
Num. H-bond donors	0	• p ,	Drualikeness
Molar Refractivity	47.12	Lipinski 😗	Yes: 0 violation
TPSA 🧐	0.00 A <sup>2</sup>	Ghose 😗	No; 1 violation: MW<160
	Lipophilicity	Veber 📀	Yes
Log P <sub>o/w</sub> (ILOGP)	2.73	Egan 🐵	Yes
Log P <sub>o/w</sub> (XLOGP3) 🥹	4.50	Mueage 📀	No: 2 violations: MW<200. Heteroatoms<2
Log P <sub>o/w</sub> (WLOGP) 📀	3.31	Bioavailability Score ()	0.55
Log P <sub>o/w</sub> (MLOGP) 📀	3.27	,	Medicinal Chemistry
Log P <sub>o/w</sub> (SILICOS-IT) 📀	2.95	PAINS 😣	0 alert
Consensus Log P <sub>o/w</sub> 📀	3.35	Brenk 🛞	1 alert: isolated_alkene 🥹
		Leadlikeness 🛞	No; 2 violations: MW<250, XLOGP3>3.5
		Synthetic accessibility 📀	3.11

## • Terpinen-4-ol

Molecule 1			<b>(</b>
<b># @ Ο </b>			Water Solubility
	LIPO	Log <i>S</i> (ESOL) 📀	-2.78
CH <sub>3</sub>		Solubility	2.54e-01 mg/ml ; 1.64e-03 mol/l
Н₃С— ( ОН	FLEX	Class 🛞	Soluble
X		Log S (Ali) 😢	-3.36
		Solubility	6.75e-02 mg/ml ; 4.38e-04 mol/l
		Class 😢	Soluble
	INSATU	Log S (SILICOS-IT) 📀	-1.91
		Solubility	1.92e+00 mg/ml ; 1.24e-02 mol/l
CU3	INCOLU	Class 🛞	Soluble
	INSOLU		Pharmacokinetics
SMILES CC1=CCC(CC1)(C	D)C(C)C	GI absorption 📀	High
PI	nysicochemical Properties	BBB permeant 📀	Yes
Formula	C10H18O	P-gp substrate 📀	No
Molecular weight	154.25 g/mol	CYP1A2 inhibitor 📀	No
Num. heavy atoms	11	CYP2C19 inhibitor 📀	No
Num. arom. heavy atoms	0	CYP2C9 inhibitor 📀	No
Fraction Csp3	0.80	CYP2D6 inhibitor 📀	No
Num. rotatable bonds	1	CYP3A4 inhibitor 📀	No
Num. H-bond acceptors	1	Log $K_{\rm p}$ (skin permeation) 📀	-4.93 cm/s
Num. H-bond donors	1	- p · · · ·	Druglikeness
Molar Refractivity	48.80	Lipinski 😑	Yes; 0 violation
TPSA 🧐	20.23 A <sup>2</sup>	Ghose 📀	No; 1 violation: MW<160
	Lipophilicity	Veber 🐵	Yes
Log P <sub>o/w</sub> (ILOGP)	2.51	Egan 🐵	Yes
Log P <sub>o/w</sub> (XLOGP3) 🧐	3.26	Muegge 📀	No; 2 violations: MW<200, Heteroatoms<2
Log P <sub>o/w</sub> (WLOGP) 📀	2.50	Bioavailability Score 📀	0.55
Log P <sub>o/w</sub> (MLOGP) 📀	2.30		Medicinal Chemistry
Log P <sub>o/w</sub> (SILICOS-IT) 📀	2.44	PAINS (9)	0 alert
Consensus Log P <sub>o/w</sub> 📀	2.60	Brenk 📀	1 alert: isolated_alkene 🧐
		Leadlikeness 📀	No; 1 violation: MW<250
		Synthetic accessibility 📀	3.28

## • α-Copaene

Molecule 1			
<b>Η Θ Ο </b> <i>ω</i> Σ			Water Solubility
	LIPO	Log S (ESOL) 😢	-3.86
H₃C		Solubility	2.84e-02 mg/ml ; 1.39e-04 mol/l
NX1	FLEX	Class 📀	Soluble
$\langle 1 \rangle$			-4.19
		Solubility	-4.13
		Class (9)	Mederately coluble
H <sub>3</sub> C )	-CH3		
	INSATU	Log S (SILICOS-IT)	-3.07
H <sub>3</sub> C		Solubility	1./4e-01 mg/ml ; 8.51e-04 mol/l
	INSOLU	Class 🧐	Soluble
SMILES 00/010000/02/		Ol shaamtian 🙆	Pharmacokinetics
	Physicschemical Properties		Low
Formula	C15H24	BBB permeant	tes
Molecular weight	204 35 g/mol	P-gp substrate	NO
Num, heavy atoms	15		Vee
Num. arom. heavy atoms	0		Ves
Fraction Csp3	0.87		No
Num. rotatable bonds	1		No
Num. H-bond acceptors	0	Log K (skin permeation)	4.97 om/o
Num. H-bond donors	0	Log Ap (skill permeation)	-4.37 cm/s
Molar Refractivity	67.14	Lininalii 🙆	Drugiikeness
TPSA 📀	0.00 Ų		Voc
	Lipophilicity	Vobor 🙆	Vae
Log P <sub>o/w</sub> (iLOGP) 🛞	3.40		Ves
Log P <sub>o/w</sub> (XLOGP3) 📀	4.47	Eyan 🐨	No: 1 violation: Hateroatome-2
Log P <sub>o/w</sub> (WLOGP) 📀	4.27	Bioavailability Score 🤷	
Log P <sub>o/w</sub> (MLOGP) 📀	5.65		Medicinal Chemistry
Log Poly (SILICOS-IT)	3.73	PAINS ()	0 alert
Consensus Log Patro	4.30	Brenk 🔞	1 alert: isolated, alkene ??
Conservation Log / O/W	-100	Leadlikeness 🛞	No: 2 violations: MW<250, XLOGP3>3.5
		Synthetic accessibility @	4.62

## Caryophyllene

Molecule 1			
$\mathbf{H} \odot \bigcirc \mathscr{O} \simeq \Sigma$			Water Solubility
	LIPO	Log S (ESOL) 📀	-3.87
		Solubility	2.78e-02 mg/ml; 1.36e-04 mol/l
н"с	CH3 FLEX SIZE	Class 📀	Soluble
н_с		Log S (Ali) 😣	-4.10
	<b>}</b>	Solubility	1.64e-02 mg/ml ; 8.01e-05 mol/l
, and the second se	8	Class 🛞	Moderately soluble
			-3 77
H <sub>2</sub> C	INGATO	Solubility	3.49e-02 ma/ml : 1.71e-04 mal/l
		Class 🕑	Soluble
	INSOLU		Pharmacokinetics
SMILES CC1=CCCC(=C)C	C2C(CC1)C(C2)(C)C	GI absorption 📀	Low
P	Physicochemical Properties	BBB permeant 📀	No
Formula	C15H24	P-gp substrate 📀	No
Molecular weight	204.35 g/mol	CYP1A2 inhibitor 😣	No
Num. heavy atoms	15	CYP2C19 inhibitor 🛞	Yes
Num. arom. heavy atoms	0	CYP2C9 inhibitor 🤨	Yes
Fraction Csp3	0.73	CYP2D6 inhibitor 🤨	No
Num. rotatable bonds	0	CYP3A4 inhibitor 📀	No
Num. H-bond acceptors	0	Log K <sub>p</sub> (skin permeation) 📀	-4.44 cm/s
Num. H-bond donors	0	F	Druglikeness
Molar Refractivity	68.78	Lipinski 🔞	Yes; 1 violation: MLOGP>4.15
TPSA 🔮	0.00 A <sup>2</sup>	Ghose 🛞	Yes
		Veber 🛞	Yes
$Log P_{o/W}$ (ILOGP)	3.29	Egan 📀	Yes
Log P <sub>o/w</sub> (XLOGP3)	4.38	Muegge 📀	No; 1 violation: Heteroatoms<2
Log P <sub>o/w</sub> (WLOGP) 📀	4.73	Bioavailability Score 📀	0.55
Log P <sub>o/w</sub> (MLOGP) 🛞	4.63		Medicinal Chemistry
Log P <sub>o/w</sub> (SILICOS-IT) 📀	4.19	PAINS <sup>(9)</sup>	0 alert
Consensus Log P <sub>o/w</sub> 📀	4.24	Brenk 😣	1 alert: isolated_alkene 🧐
		Leadlikeness 📀	No; 2 violations: MW<250, XLOGP3>3.5
		Synthetic accessibility 📀	4.51

## • Humulene

Molecule 1			۵
<b># ⊕ Ο </b>			Water Solubility
	LIPO	Log <i>S</i> (ESOL) 🧐	-3.97
H <sub>3</sub> C CH <sub>3</sub>		Solubility	2.17e-02 mg/ml ; 1.06e-04 mol/l
m V.m	FLEX	Class 📀	Soluble
C' Am,		Loa S (Ali) 🥹	-4.27
\\ н с		Solubility	1.09e-02 mg/ml ; 5.34e-05 mol/l
H <sub>3</sub> C		Class 😗	Moderately soluble
	INSATU	Log S (SILICOS-IT) 📀	-3.52
		Solubility	6.19e-02 mg/ml ; 3.03e-04 mol/l
MA		Class 📀	Soluble
	INSOLU		Pharmacokinetics
SMILES CC1=CCC(C)(C)C	=CCC(=CCC1)C	GI absorption 📀	Low
Pł	nysicochemical Properties	BBB permeant 📀	No
Formula	C15H24	P-gp substrate 📀	No
Molecular weight	204.35 g/mol	CYP1A2 inhibitor 📀	No
Num. heavy atoms	15	CYP2C19 inhibitor 📀	No
Num. arom. heavy atoms	0	CYP2C9 inhibitor 📀	Yes
Fraction Csp3	0.60	CYP2D6 inhibitor 📀	No
Num. rotatable bonds	0	CYP3A4 inhibitor 📀	No
Num. H-bond acceptors	0	Log <i>K</i> <sub>p</sub> (skin permeation) 📀	-4.32 cm/s
Num. H-bond donors	0	с р. т. ,	Druglikeness
Molar Refractivity	70.42	Lipinski 🤨	Yes; 1 violation: MLOGP>4.15
TPSA 🥹	0.00 A <sup>2</sup>	Ghose 📀	Yes
	Lipophilicity	Veber 📀	Yes
Log P <sub>o/w</sub> (iLOGP) 🧐	3.27	Egan 🛞	Yes
Log P <sub>o/w</sub> (XLOGP3) 📀	4.55	Muegae 📀	No: 1 violation: Heteroatoms<2
Log P <sub>o/w</sub> (WLOGP) 📀	5.04	Bioavailability Score 📀	0.55
Log P <sub>o/w</sub> (MLOGP) 😣	4.53		Medicinal Chemistry
Log P <sub>o/w</sub> (SILICOS-IT) 😣	3.91	PAINS 😢	0 alert
Consensus Log Po/w 📀	4.26	Brenk 📀	1 alert: isolated_alkene 📀
		Leadlikeness 📀	No; 2 violations: MW<250, XLOGP3>3.5
		Synthetic accessibility 🧐	3.66

### Germacrene D

Molecule 1			
<b># Θ Ο </b>			Water Solubility
	LIPO	Log S (ESOL) 😣	-4.03
H-C		Solubility	1.92e-02 mg/ml ; 9.39e-05 mol/l
	FLEX	Class 📀	Moderately soluble
<i>[</i> -	- 34	Log S (Ali)	-4 47
		Solubility	6.93e-03 ma/ml : 3.39e-05 mol/l
H <sub>3</sub> C H <sub>2</sub> C		Class <sup>(2)</sup>	Moderately soluble
	INSATU	Log S (SILICOS-IT) 😣	-3.32
H₃C		Solubility	9.83e-02 mg/ml ; 4.81e-04 mol/l
		Class 📀	Soluble
	INSOLU		Pharmacokinetics
SMILES CC1=CCCC(=C)	C=CC(CC1)C(C)C	GI absorption 📀	Low
F	Physicochemical Properties	BBB permeant 📀	No
Formula	C15H24	P-gp substrate 📀	No
Molecular weight	204.35 g/mol	CYP1A2 inhibitor 📀	No
Num. heavy atoms	15	CYP2C19 inhibitor <sup>(2)</sup>	No
Num. arom. heavy atoms	0	CYP2C9 inhibitor 📀	Yes
Fraction Csp3	0.60	CYP2D6 inhibitor 📀	No
Num. rotatable bonds	1	CYP3A4 inhibitor 🤨	No
Num. H-bond acceptors	0	Log $K_{\rm p}$ (skin permeation) 📀	-4.18 cm/s
Num. H-bond donors	0		Druglikeness
Molar Refractivity	70.68	Lipinski 🔞	Yes; 1 violation: MLOGP>4.15
IPSA 🧐	U.UU A <sup>2</sup>	Ghose 🔞	Yes
		Veber 🔞	Yes
Log P <sub>o/w</sub> (ILOGP) 🐨	3.32	Egan 🗐	Yes
Log P <sub>o/w</sub> (XLOGP3) 🧐	4.74	Muegge <sup>(3)</sup>	No; 1 violation: Heteroatoms<2
Log P <sub>o/w</sub> (WLOGP) 📀	4.89	Bioavailability Score 📀	0.55
Log P <sub>o/w</sub> (MLOGP) 📀	4.53		Medicinal Chemistry
Log P <sub>o/w</sub> (SILICOS-IT) 📀	4.01	PAINS 🛞	0 alert
Consensus Log P <sub>o/w</sub> 📀	4.30	Brenk 🛞	1 alert: isolated_alkene 📀
		Leadlikeness 📀	No; 2 violations: MW<250, XLOGP3>3.5
		Synthetic accessibility 📀	4.55

## • Bicyclogermacrene

Molecule 1			٤
<b># Θ Ο </b> <i>ω</i> Σ			Water Solubility
	LIPO	Log <i>S</i> (ESOL) 🤨	-3.72
		Solubility	3.94e-02 mg/ml ; 1.93e-04 mol/l
	CH- FLEX SIZE	Class 📀	Soluble
		Log S (Ali) 📀	-3.85
нъс.		Solubility	2.90e-02 mg/ml ; 1.42e-04 mol/l
	1 <sub>3</sub>	Class 📀	Soluble
H <sub>3</sub> C Mu	INSATU POLAR	Log S (SILICOS-IT) 📀	-3.52
		Solubility	6.19e-02 mg/ml ; 3.03e-04 mol/l
	INCOLL	Class 📀	Soluble
	INSOLU		Pharmacokinetics
SMILES CC1=CCCC(=CC2	2C(CC1)C2(C)C)C	GI absorption 🛞	Low
P	hysicochemical Properties	BBB permeant 📀	No
Formula	C15H24	P-gp substrate 📀	No
Molecular weight	204.35 g/mol	CYP1A2 inhibitor 📀	No
Num. heavy atoms	15	CYP2C19 inhibitor 📀	Yes
Num. arom. heavy atoms	0	CYP2C9 inhibitor 📀	Yes
Fraction Csp3	0.73	CYP2D6 inhibitor 📀	No
Num. rotatable bonds	0	CYP3A4 inhibitor 📀	No
Num. H-bond acceptors	0	Log K <sub>p</sub> (skin permeation) 📀	-4.61 cm/s
Num. H-bond donors	0		Druglikeness
Molar Refractivity	68.78	Lipinski 🤨	Yes; 1 violation: MLOGP>4.15
TPSA 🧐	0.00 A <sup>2</sup>	Ghose 🧐	Yes
	Lipophilicity	Veber 📀	Yes
Log P <sub>o/w</sub> (ILOGP)	3.34	Egan 📀	Yes
Log P <sub>o/w</sub> (XLOGP3) 🧐	4.14	Mueage 📀	No; 1 violation: Heteroatoms<2
Log P <sub>o/w</sub> (WLOGP) 📀	4.73	Bioavailability Score 📀	0.55
Log P <sub>o/w</sub> (MLOGP) 📀	4.63	,	Medicinal Chemistry
Log P <sub>o/w</sub> (SILICOS-IT) 📀	3.91	PAINS ()	0 alert
Consensus Log P <sub>o/w</sub> 📀	4.15	Brenk 📀	1 alert: isolated_alkene 📀
		Leadlikeness 📀	No; 2 violations: MW<250, XLOGP3>3.5
		Synthetic accessibility 🧐	4.34

## • Aromandendrene

Molecule 1			
<b>₩ ⊕ Ο </b>			Water Solubility
	LIPO	Log <i>S</i> (ESOL) 📀	-3.72
		Solubility	3.94e-02 mg/ml ; 1.93e-04 mol/l
	CH. FLEX SIZE	Class 📀	Soluble
		Log S (Ali) 😗	-3.85
н.с.		Solubility	2.90e-02 mg/ml ; 1.42e-04 mol/l
	H <sub>3</sub> `}	Class 📀	Soluble
H3C M			-3.52
-	POLAR	Solubility	6 19e-02 mg/ml : 3 03e-04 mol/l
		Class ()	Soluble
	INSOLU		Pharmacokinetics
SMILES CC1=CCCC(=CC	2C(CC1)C2(C)C)C	GI absorption (9)	Low
P	Physicochemical Properties	BBB permeant ()	No
Formula	C15H24	P-gp substrate 📀	No
Molecular weight	204.35 g/mol	CYP1A2 inhibitor 😢	No
Num. heavy atoms	15	CYP2C19 inhibitor 📀	Yes
Num. arom. heavy atoms	0	CYP2C9 inhibitor 📀	Yes
Fraction Csp3	0.73	CYP2D6 inhibitor 📀	No
Num. rotatable bonds	0	CYP3A4 inhibitor 📀	No
Num. H-bond acceptors	0	Log $K_{\rm p}$ (skin permeation) $^{(0)}$	-4.61 cm/s
Num. H-bond donors	0		Druglikeness
Molar Refractivity	68.78	Lipinski 📀	Yes; 1 violation: MLOGP>4.15
IPSA 🐨	0.00 A <sup>2</sup>	Ghose 📀	Yes
	2.24	Veber 🔞	Yes
$\log F_{0/W} (\text{ICOGP}) \bigcirc$	3.34	Egan 🛞	Yes
$\log P_{o/W}$ (XLOGP3)	4.14	Muegge 📀	No; 1 violation: Heteroatoms<2
Log P <sub>o/w</sub> (WLOGP) 🥹	4.73	Bioavailability Score 📀	0.55
Log P <sub>o/w</sub> (MLOGP) 📀	4.63		Medicinal Chemistry
Log P <sub>o/w</sub> (SILICOS-IT) 🛞	3.91	PAINS 📀	0 alert
Consensus Log P <sub>o/w</sub> 📀	4.15	Brenk 😗	1 alert: isolated_alkene 📀
		Leadlikeness 📀	No; 2 violations: MW<250, XLOGP3>3.5
		Synthetic accessibility 📀	4.34

# • trans-Nerolidol

Molecule 1			
<b>₩ ⊕ Ο </b>			Water Solubility
	CH_	Log S (ESOL)	-3.80
_		Solubility	3.53e-02 mg/ml ; 1.59e-04 mol/l
/_	CH, FLEX SIZE	Class 🔞	Soluble
=		Log S (Ali) 🔞	-4.99
<sup>д<sup>2</sup> сн,</sup>		Solubility	2.29e-03 mg/ml ; 1.03e-05 mol/l
н.с. >		Class 😗	Moderately soluble
он	INSATU	Log S (SILICOS-IT) 📀	-3.15
		Solubility	1.56e-01 mg/ml ; 7.00e-04 mol/l
`сн <sub>а</sub>		Class 🛞	Soluble
	INSOLU		Pharmacokinetics
SMILES C=CC(CCC=C(C	CC=C(C)C)C)(O)C	GI absorption 📀	High
F	Physicochemical Properties	BBB permeant 📀	Yes
Formula	C15H26O	P-gp substrate 📀	No
Molecular weight	222.37 g/mol	CYP1A2 inhibitor 📀	Yes
Num. heavy atoms	16	CYP2C19 inhibitor 📀	No
Num. arom. heavy atoms	0	CYP2C9 inhibitor 📀	Yes
Fraction Csp3	0.60	CYP2D6 inhibitor 📀	No
Num. rotatable bonds	7	CYP3A4 inhibitor 📀	No
Num. H-bond acceptors	1	Log K <sub>p</sub> (skin permeation) 📀	-4.23 cm/s
Num. H-bond donors	1	- p	Drualikeness
Molar Refractivity	74.00	Lipinski 😗	Yes: 0 violation
TPSA 🧐	20.23 A <sup>2</sup>	Ghose 📀	Yes
	Lipophilicity	Veber 📀	Yes
Log P <sub>o/w</sub> (iLOGP) 🧐	3.64	Egan 📀	Yes
Log P <sub>o/w</sub> (XLOGP3) 📀	4.83	Muegge 📀	No: 1 violation: Heteroatoms<2
Log P <sub>o/w</sub> (WLOGP) 📀	4.40	Bioavailability Score @	0.55
Log P <sub>o/w</sub> (MLOGP) 📀	3.86	Dioartanability Oobro -	Medicinal Chemistry
Log P <sub>o/w</sub> (SILICOS-IT) 📀	4.21	PAINS 😣	0 alert
Consensus Log P <sub>o/w</sub> 📀	4.19	Brenk 🛞	1 alert: isolated_alkene 🤨
		Leadlikeness 🛞	No; 2 violations: MW<250, XLOGP3>3.5
		Synthetic accessibility 📀	3.53

## • Caryophyllene oxide

Molecule 1			Sector 2013
<b>₩ ⊕ () &amp;</b> Σ			Water Solubility
	LIPO	Log S (ESOL) 📀	-3.45
		Solubility	7.84e-02 mg/ml ; 3.56e-04 mol/l
CH <sub>2</sub>	FLEX	Class 🔞	Soluble
		Log S (Ali) 🔞	-3.51
		Solubility	6.83e-02 mg/ml ; 3.10e-04 mol/l
	-сн.	Class 🛞	Soluble
н,с /	INSATU POLAR	Log S (SILICOS-IT) 📀	-3.51
		Solubility	6.81e-02 mg/ml ; 3.09e-04 mol/l
	NICOLU	Class 📀	Soluble
	INSOLU		Pharmacokinetics
SMILES C=C1CCC2OC2(C	CCC2C1CC2(C)C)C	GI absorption 📀	High
P	hysicochemical Properties	BBB permeant 📀	Yes
Formula	C15H24O	P-gp substrate 📀	No
Molecular weight	220.35 g/mol	CYP1A2 inhibitor 📀	No
Num. heavy atoms	16	CYP2C19 inhibitor 📀	Yes
Num. arom. heavy atoms	0	CYP2C9 inhibitor 📀	Yes
Fraction Csp3	0.87	CYP2D6 inhibitor 📀	No
Num. rotatable bonds	0	CYP3A4 inhibitor 📀	No
Num. H-bond acceptors	1	Log K <sub>n</sub> (skin permeation) 📀	-5.12 cm/s
Num. H-bond donors	0	ор(; ; )	Drualikeness
Molar Refractivity	68.27	Lipinski 😗	Yes: 0 violation
TPSA 🥹	12.53 A²	Ghose 😗	Yes
	Lipophilicity	Veber 🛞	Yes
Log P <sub>o/w</sub> (iLOGP) 🧐	3.15	Egan 🛞	Yes
Log P <sub>o/w</sub> (XLOGP3) 🧐	3.56	Muegge 📀	No: 1 violation: Heteroatoms<2
Log P <sub>o/w</sub> (WLOGP) 📀	3.94	Bioavailability Score 0	0.55
Log P <sub>o/w</sub> (MLOGP) 📀	3.67		Medicinal Chemistry
Log P <sub>o/w</sub> (SILICOS-IT) 🥹	4.07	PAINS 😢	0 alert
Consensus Log P <sub>o/w</sub> 📀	3.68	Brenk 📀	2 alerts: Three-membered_heterocycle, isolated_alkene 0
		Leadlikeness 📀	No; 2 violations: MW<250, XLOGP3>3.5
		Synthetic accessibility 📀	4.35

# Longifolenaldehyde

Molecule 1			
<b>†† ⊕ Ο </b> <i>ω</i> Σ			Water Solubility
H.C.	LIPO	Log <i>S</i> (ESOL) 📀	-3.87
п <sub>3</sub> с		Solubility	2.94e-02 mg/ml ; 1.34e-04 mol/l
	, O FLEX SIZE	Class 📀	Soluble
		Log S (Ali) 📀	-4.41
		Solubility	8.51e-03 mg/ml ; 3.86e-05 mol/l
		Class 🛞	Moderately soluble
X	INSATU	Log <i>S</i> (SILICOS-IT) 📀	-3.10
H <sub>3</sub> C∕ \		Solubility	1.75e-01 mg/ml ; 7.93e-04 mol/l
CH3	NOOLI	Class 📀	Soluble
	INSOLU		Pharmacokinetics
SMILES O=CC1C2CCC3C	C1(C)CCCC(C23)(C)C	GI absorption 📀	High
P	Physicochemical Properties	BBB permeant 🧐	Yes
Formula	C15H24O	P-gp substrate 📀	No
Molecular weight	220.35 g/mol	CYP1A2 inhibitor 📀	No
Num. heavy atoms	16	CYP2C19 inhibitor 📀	Yes
Num. arom. heavy atoms	0	CYP2C9 inhibitor 📀	Yes
Fraction Csp3	0.93	CYP2D6 inhibitor 📀	No
Num. rotatable bonds	1	CYP3A4 inhibitor 📀	No
Num. H-bond acceptors	1	Log $K_{\rm p}$ (skin permeation) $^{(0)}$	-4.56 cm/s
Num. H-bond donors	0	σρτ	Drualikeness
Molar Refractivity	67.56	Lininski	Yes: 0 violation
TPSA 🕗	17.07 Ų	Ghose (9)	Yes
	Lipophilicity	Veher 🖗	Yes
Log P <sub>o/w</sub> (iLOGP) 🧐	2.66	Fgan	Yes
Log P <sub>o/w</sub> (XLOGP3) 😢	4.34	Muegge	No: 1 violation: Heteroatoms<2
Log P <sub>o/w</sub> (WLOGP) 📀	3.67	Bioavailability Score	0.55
Log P <sub>o/w</sub> (MLOGP) 🤨	3.67		Medicinal Chemistry
Log P <sub>o/w</sub> (SILICOS-IT) 🛞	3.59	PAINS 🤨	0 alert
Consensus Log P <sub>o/w</sub> 📀	3.59	Brenk 📀	1 alert: aldehyde 🤨
		Leadlikeness 📀	No; 2 violations: MW<250, XLOGP3>3.5
		Synthetic accessibility 📀	3.45

## • Isospathulenol

Molecule 1			۵
<b>₩ ⊕ Ο </b>			Water Solubility
	LIPO	Log S (ESOL) 📀	-2.86
	,сн <sub>3</sub>	Solubility	3.06e-01 mg/ml ; 1.39e-03 mol/l
	FLEX SIZE	Class 🔞	Soluble
		Log S (Ali) 🤗	-2.69
		Solubility	4.45e-01 mg/ml : 2.02e-03 mol/l
		Class 📀	Soluble
	INSATU	Log S (SILICOS-IT) 😗	-3.17
H <sub>3</sub> C HO	CH-	Solubility	1.51e-01 mg/ml ; 6.84e-04 mol/l
		Class 📀	Soluble
	INSOLU		Pharmacokinetics
SMILES CC1=C2CCC(C2C	C2C(CC1)C2(C)C)(C)O	GI absorption 📀	High
PI	hysicochemical Properties	BBB permeant 📀	Yes
Formula	C15H24O	P-gp substrate 📀	No
Molecular weight	220.35 g/mol	CYP1A2 inhibitor 📀	No
Num. heavy atoms	16	CYP2C19 inhibitor 📀	No
Num. arom. heavy atoms	0	CYP2C9 inhibitor 📀	No
Fraction Csp3	0.87	CYP2D6 inhibitor 📀	No
Num. rotatable bonds	0	CYP3A4 inhibitor 📀	No
Num. H-bond acceptors	1	Log K <sub>p</sub> (skin permeation) 📀	-5.78 cm/s
Num. H-bond donors	1		Druglikeness
	00.04 20.02 Å2	Lipinski 🔞	Yes; 0 violation
IF SA V	Lipophilicity	Ghose 📀	Yes
Log P. (il OGP) 🤫	2.89	Veber 🐵	Yes
	2.00	Egan 🛞	Yes
$\log P_{0/W}$ (ALOGPS)	2.02	Muegge 📀	No; 1 violation: Heteroatoms<2
Log P <sub>o/w</sub> (WLOGP)	3.53	Bioavailability Score 📀	0.55
Log P <sub>o/w</sub> (MLOGP) 🧐	3.67		Medicinal Chemistry
Log P <sub>o/w</sub> (SILICOS-IT) 😣	3.38	PAINS 😕	0 alert
Consensus Log P <sub>o/w</sub> 📀	3.22	Brenk 🛞	1 alert: isolated_alkene 🥹
		Leadlikeness 🛞	No; 1 violation: MW<250
		Synthetic accessibility 📀	4.35

### • Aromadendrene oxide I

Molecule 1			٤
<b># Θ Ο </b> <i>ω</i> Σ			Water Solubility
	LIPO	Log <i>S</i> (ESOL) 🧐	-3.52
		Solubility	6.58e-02 mg/ml ; 2.99e-04 mol/l
CH3	FLEX	Class <sup>(2)</sup>	Soluble
		Log S (Ali) 📀	-3.63
		Solubility	5.13e-02 mg/ml ; 2.33e-04 mol/l
	CH3	Class 📀	Soluble
	CH3 INSATU POLAR	Log S (SILICOS-IT) 😣	-2.93
		Solubility	2.57e-01 mg/ml ; 1.16e-03 mol/l
		Class 📀	Soluble
	INSOLU		Pharmacokinetics
SMILES CC1CCC2C1C1C	(C1(C)C)CCC12OC1	GI absorption 🔞	High
P	hysicochemical Properties	BBB permeant 📀	Yes
Formula	C15H24O	P-gp substrate 📀	No
Molecular weight	220.35 g/mol	CYP1A2 inhibitor 📀	Yes
Num. heavy atoms	16	CYP2C19 inhibitor 📀	Yes
Num. arom. heavy atoms	0	CYP2C9 inhibitor 📀	Yes
Fraction Csp3	1.00	CYP2D6 inhibitor 📀	No
Num. rotatable bonds	0	CYP3A4 inhibitor 📀	No
Num. H-bond acceptors	1	Log <i>K</i> <sub>p</sub> (skin permeation) 📀	-5.03 cm/s
Num. H-bond donors	0	- p	Druglikeness
Molar Refractivity	66.63	Lipinski 📀	Yes: 0 violation
TPSA 🧐	12.53 A <sup>2</sup>	Ghose 📀	Yes
	Lipophilicity	Veber 📀	Yes
Log P <sub>o/w</sub> (iLOGP) 🧐	3.17	Egan 📀	Yes
Log P <sub>o/w</sub> (XLOGP3) 😢	3.68	Muegae 📀	No: 1 violation: Heteroatoms<2
Log P <sub>o/w</sub> (WLOGP) 📀	3.48	Bioavailability Score 📀	0.55
Log P <sub>o/w</sub> (MLOGP) 🥹	3.81		Medicinal Chemistry
Log P <sub>o/w</sub> (SILICOS-IT) 😣	3.57	PAINS ()	0 alert
Consensus Log P <sub>o/w</sub> 📀	3.54	Brenk 📀	1 alert: Three-membered_heterocycle 🥹
		Leadlikeness 📀	No; 2 violations: MW<250, XLOGP3>3.5
		Synthetic accessibility 📀	4.03