Supplementary Information (SI) for RSC Advances.

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

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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.

$$\Delta G = (V^{\mathrm{L-L}}_{\mathrm{bound}} - V^{\mathrm{L-L}}_{\mathrm{unbound}}) + (V^{\mathrm{P-P}}_{\mathrm{bound}} - V^{\mathrm{P-P}}_{\mathrm{unbound}}) + (V^{\mathrm{P-L}}_{\mathrm{bound}} - V^{\mathrm{P-L}}_{\mathrm{unbound}} + \Delta S_{\mathrm{conf}})$$

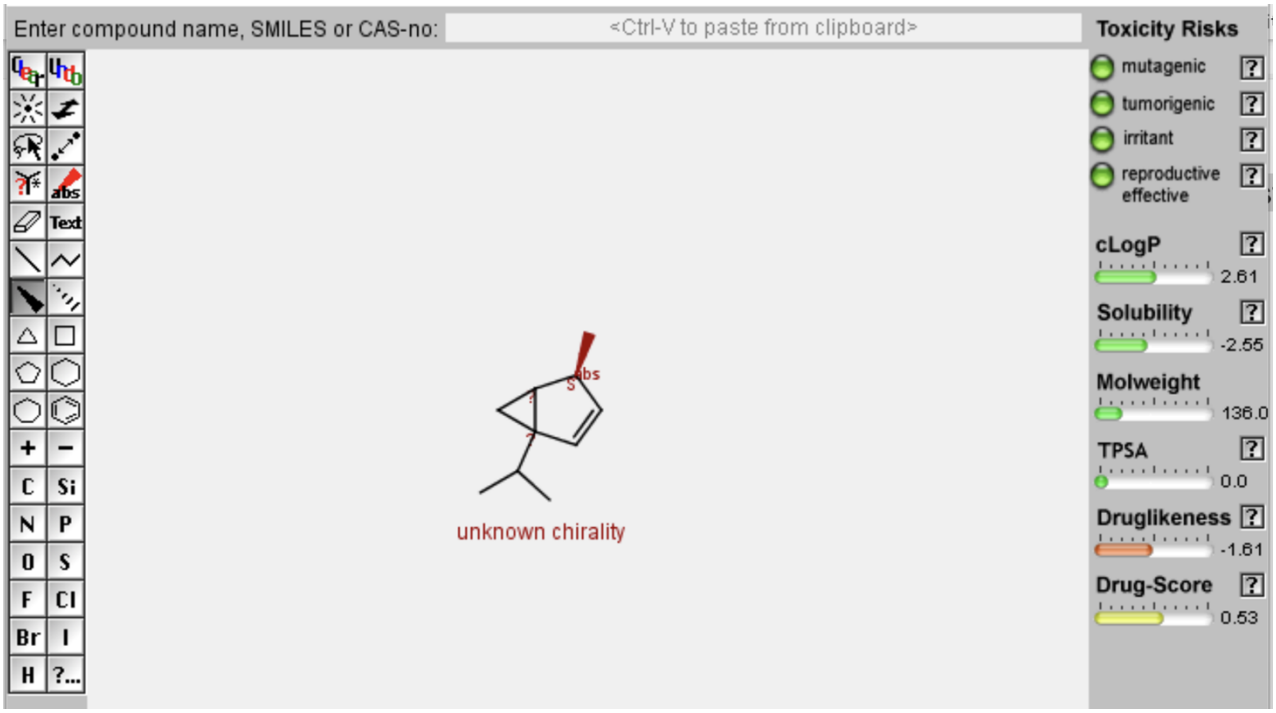
where P stands for protein, L for ligand, V for the pairwise assessments previously indicated, and ΔS~conf~ for conformational entropy lost during binding.

doi:10.1002/jcc.20634.

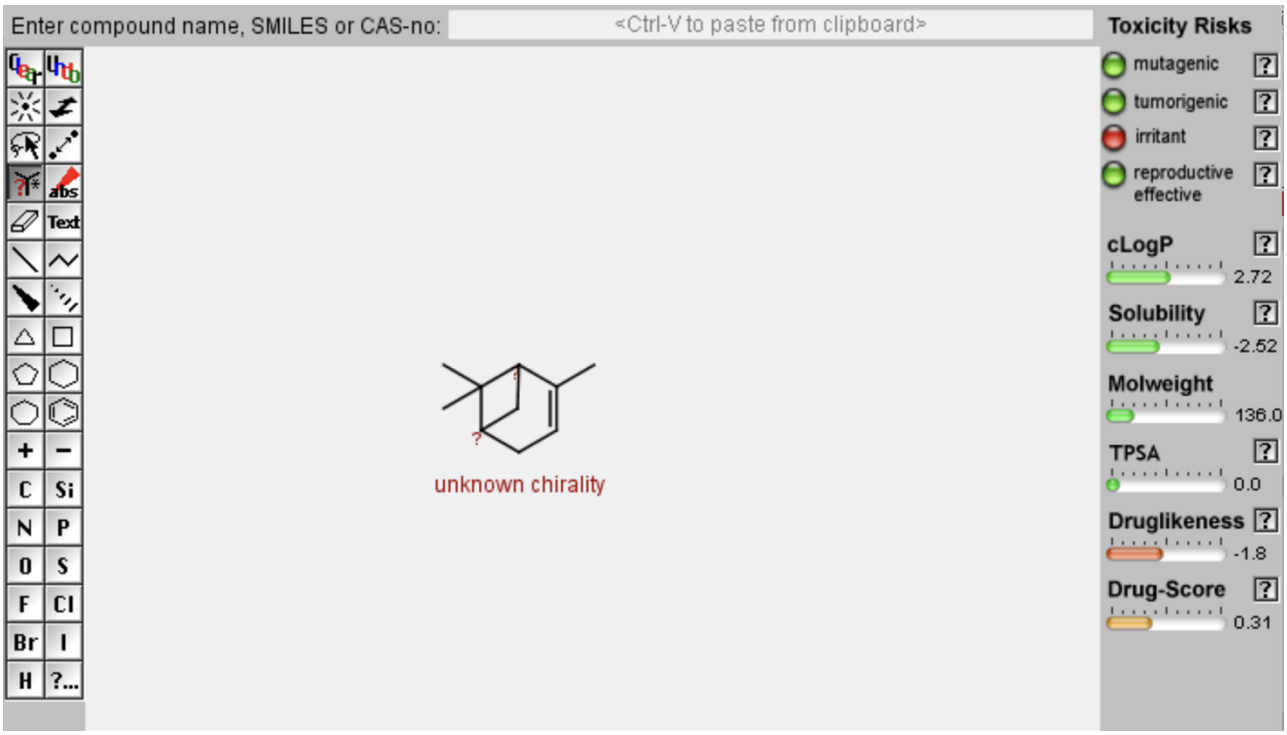
The following are the parameters used in the docking run. Genetic algorithm runs (the specified number of docking runs using the simulated annealing search engine) was set to 20. RMSD cluster tolerance (the RMSD threshold (in Å) for joining together multiple docking results and show them as one entry 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):

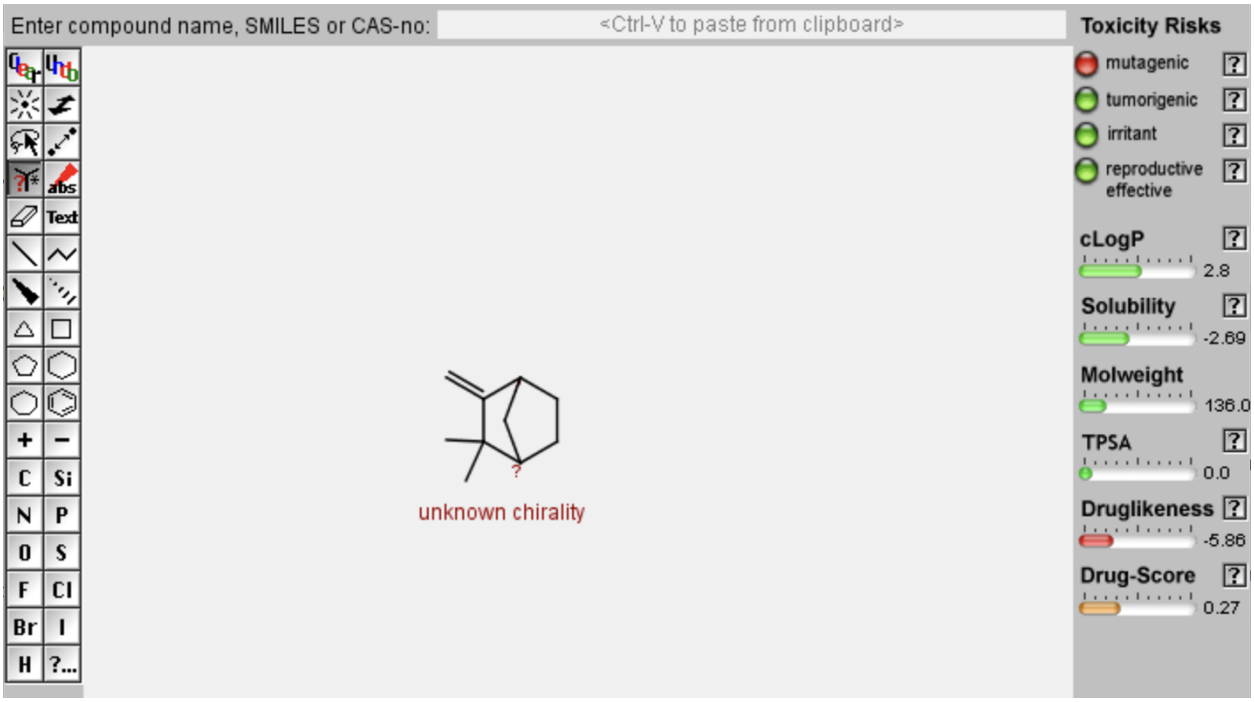
- **2-Thujene**



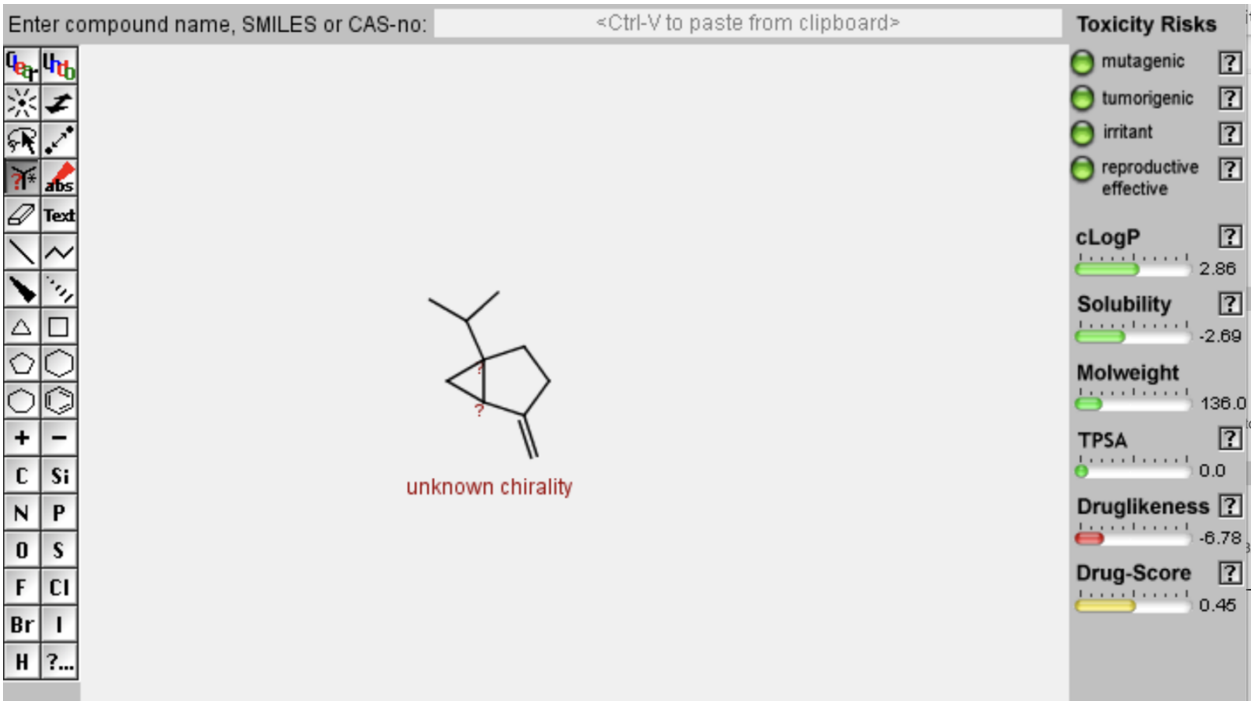
- ***α*-pinene**



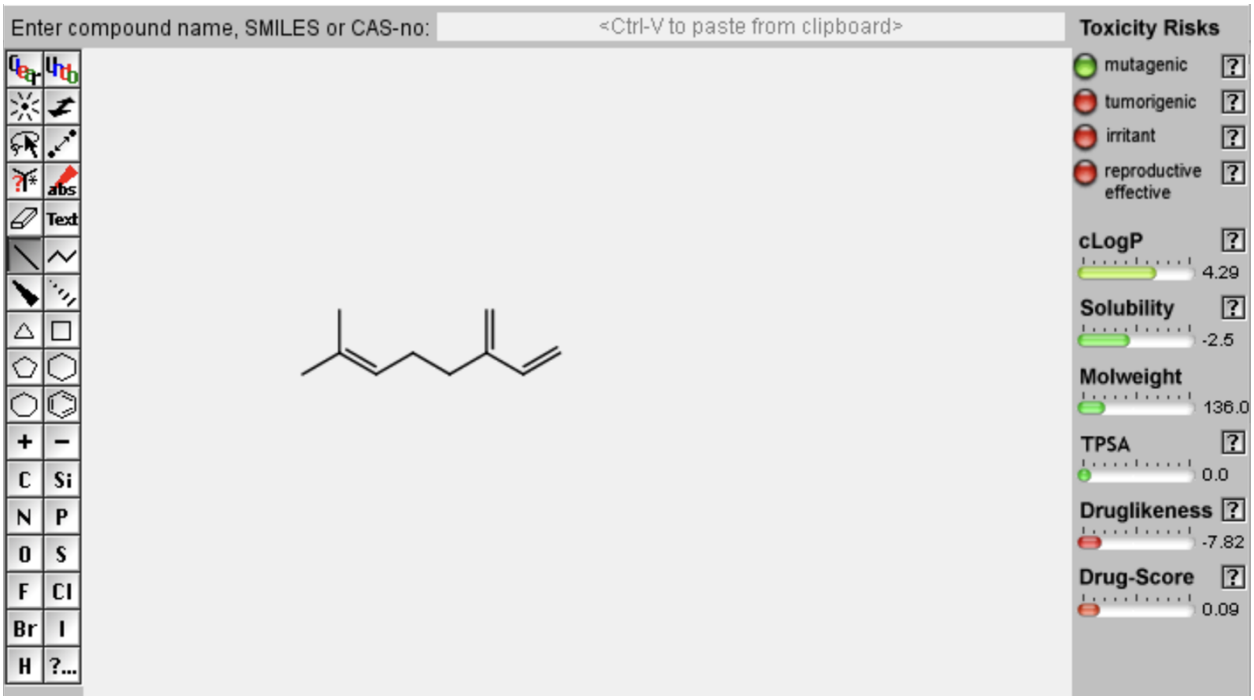
- **Camphene**



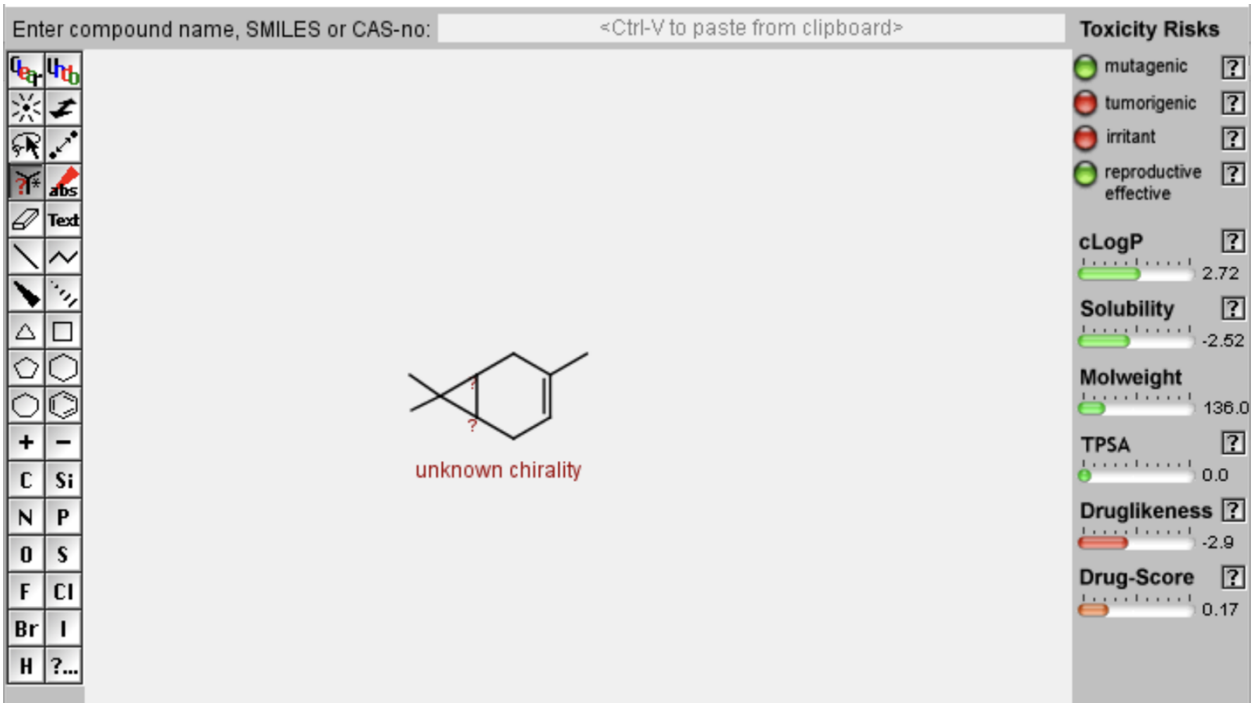
- **Sabinene**



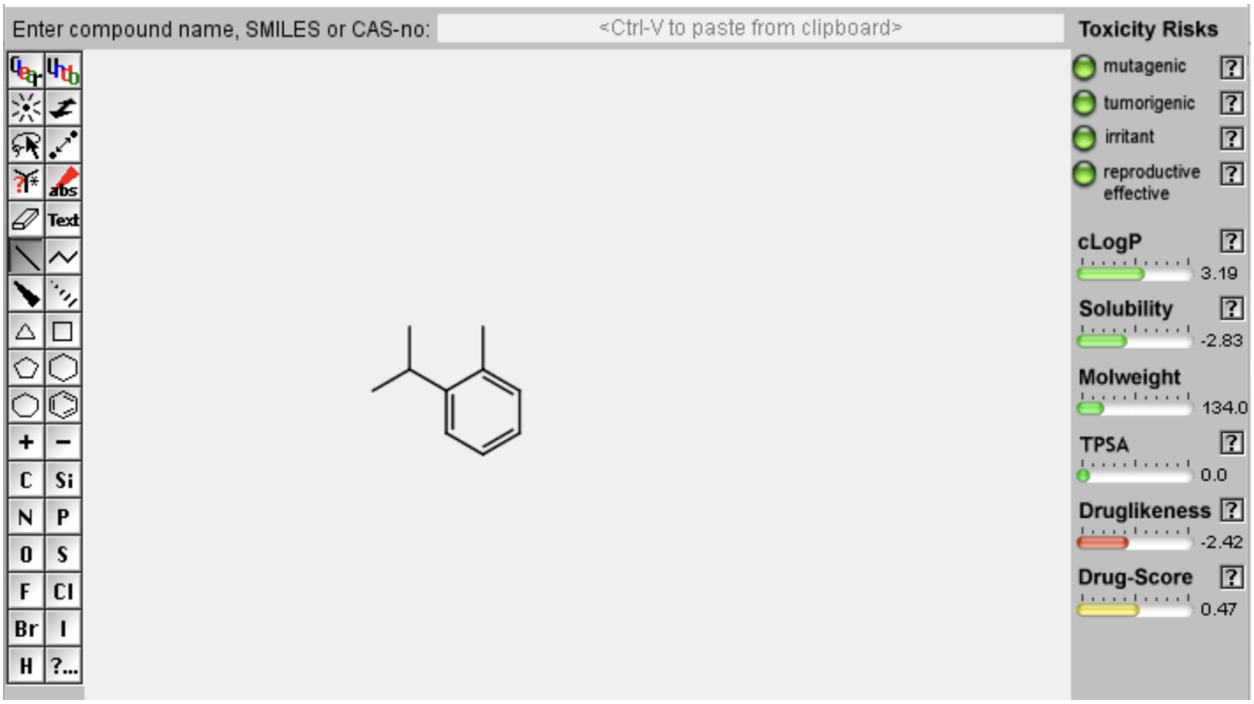
- ***β*-Myrcene**



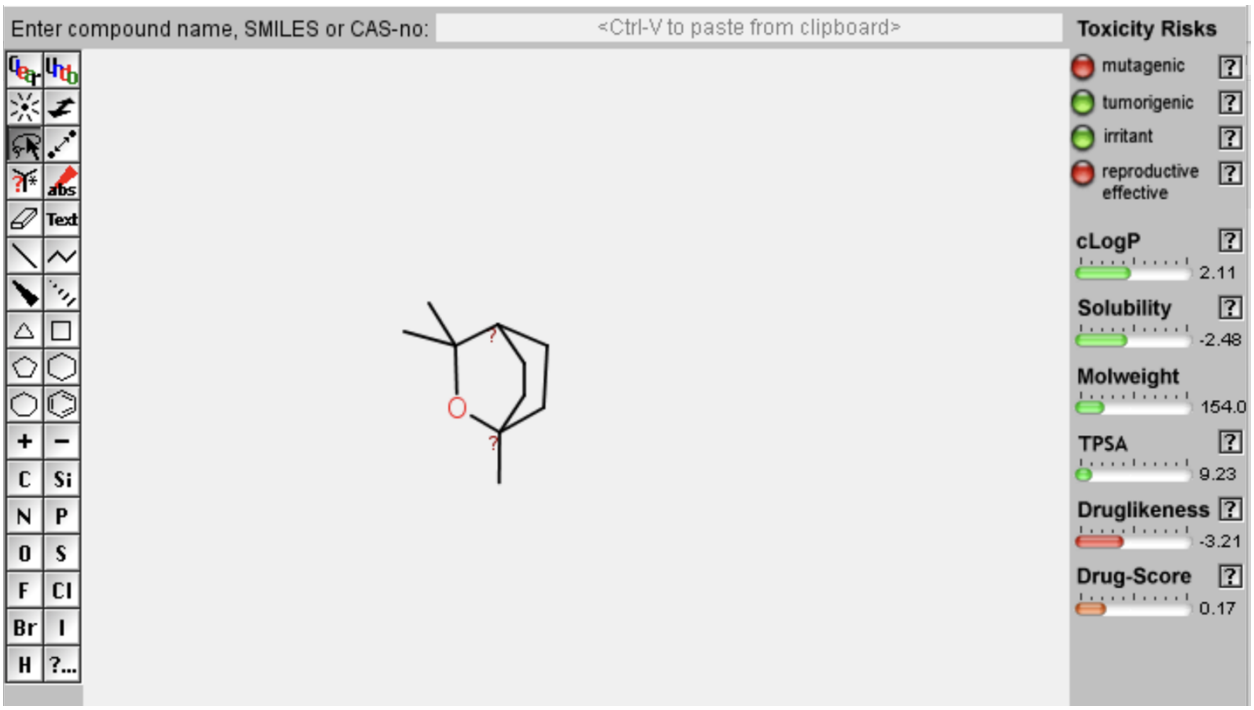
- **3-Carene**



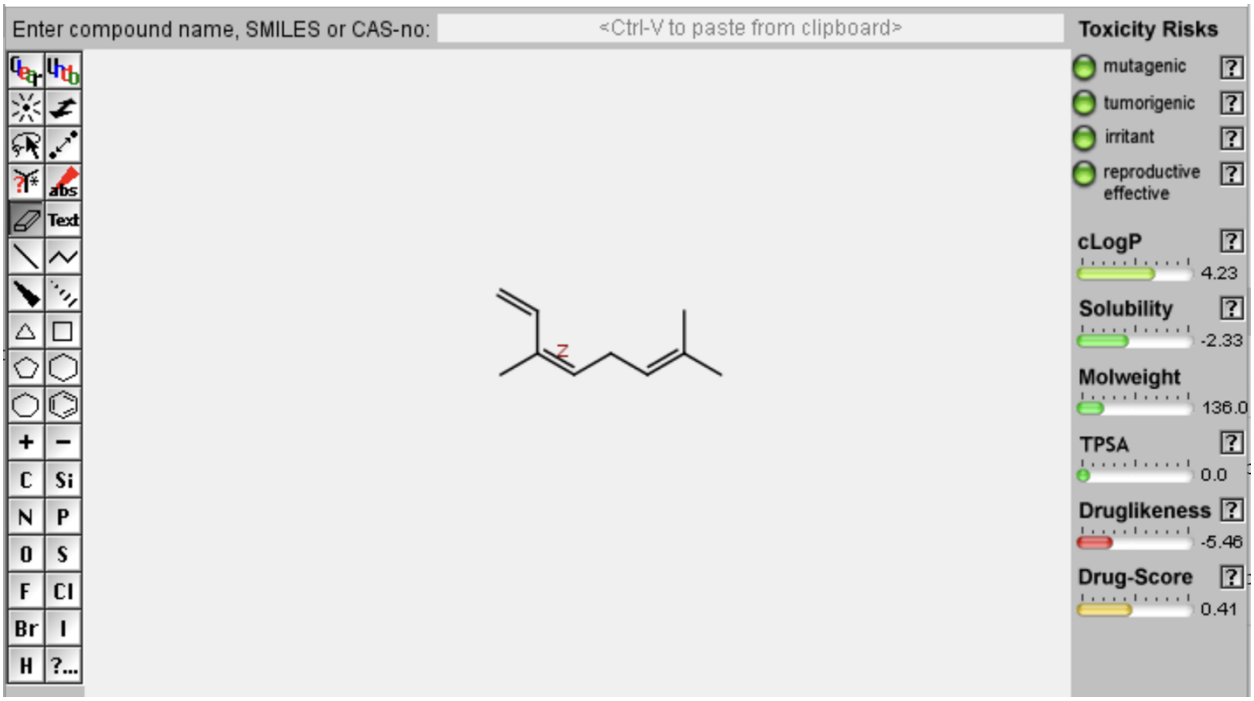
- ***o*-Cymene**



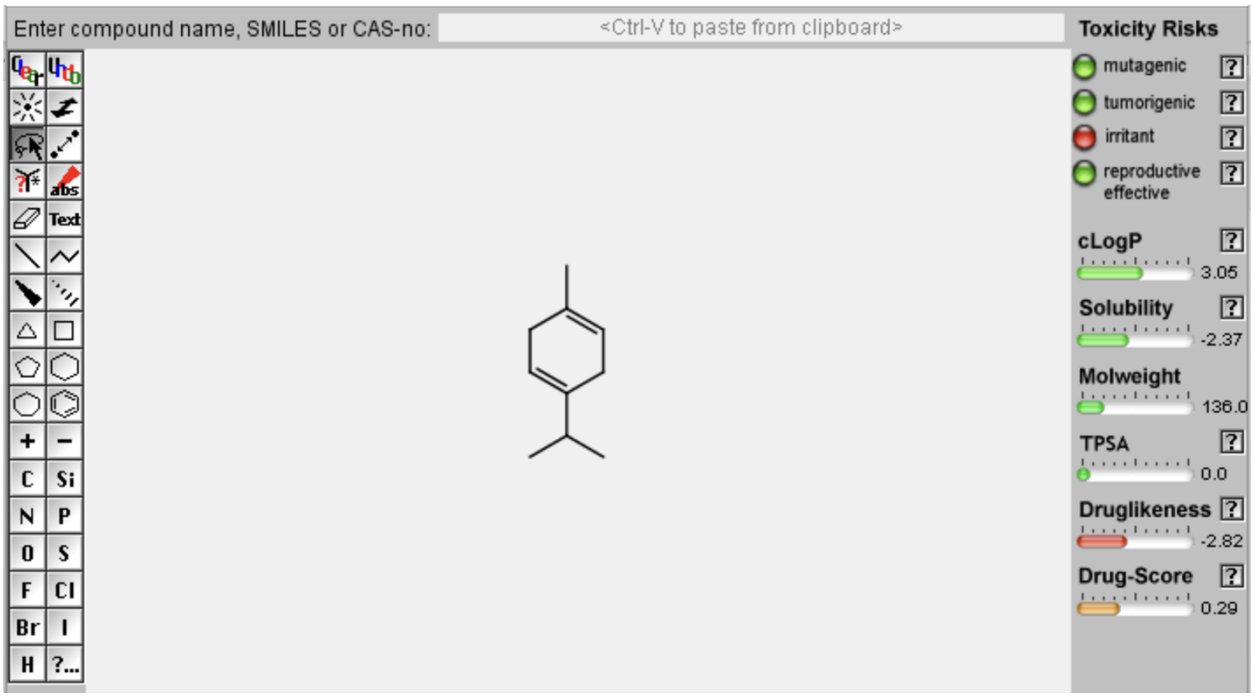
- **Eucalyptol**



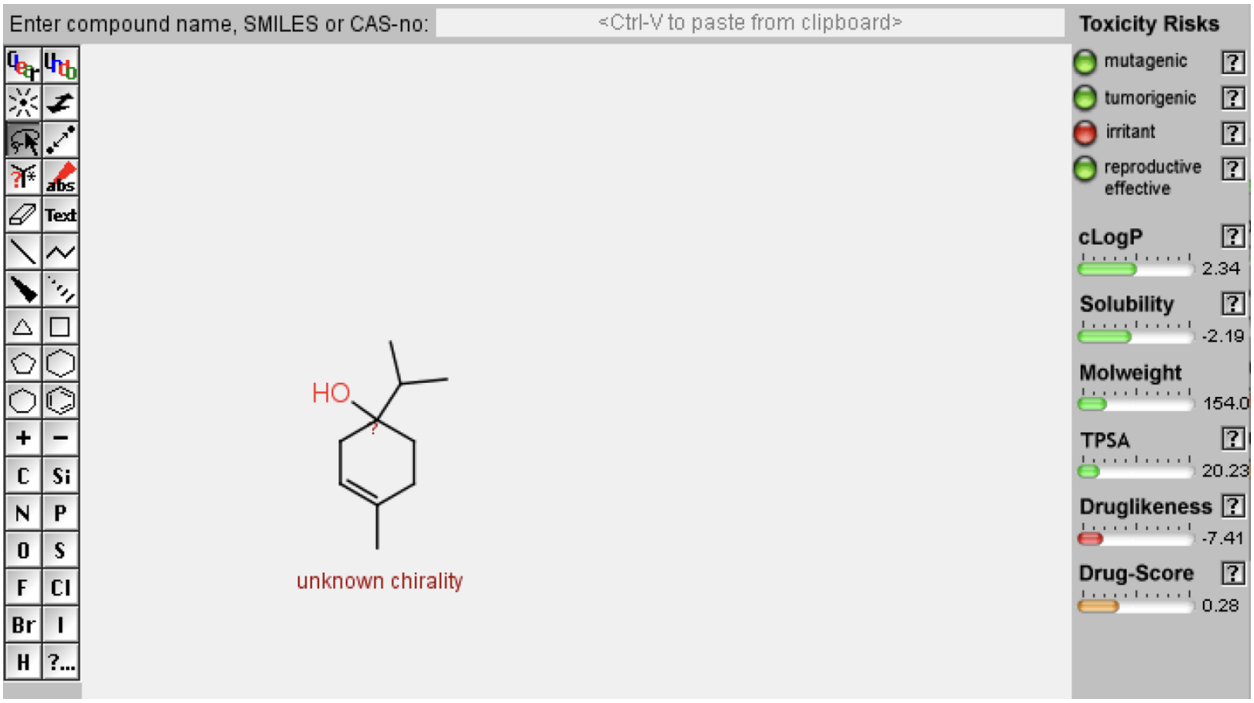
- ***β*-cis-Ocimene**



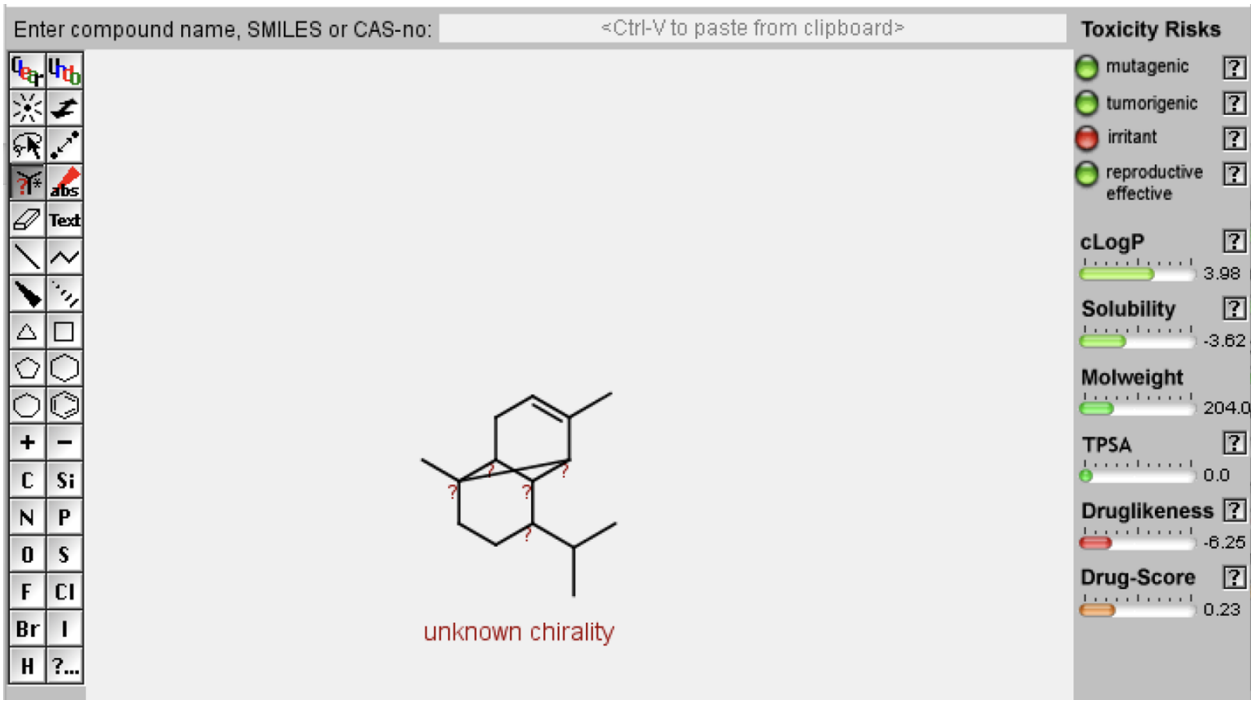
- ***γ*-Terpinene**



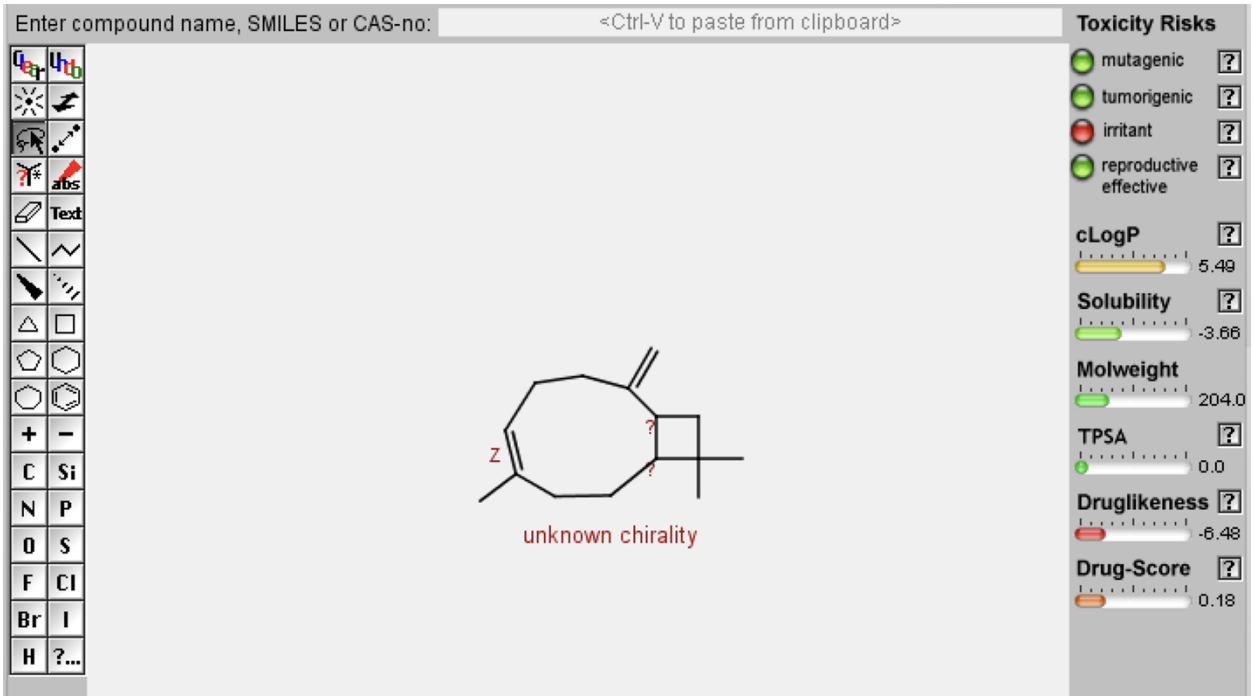
- **Terpinen-4-ol**



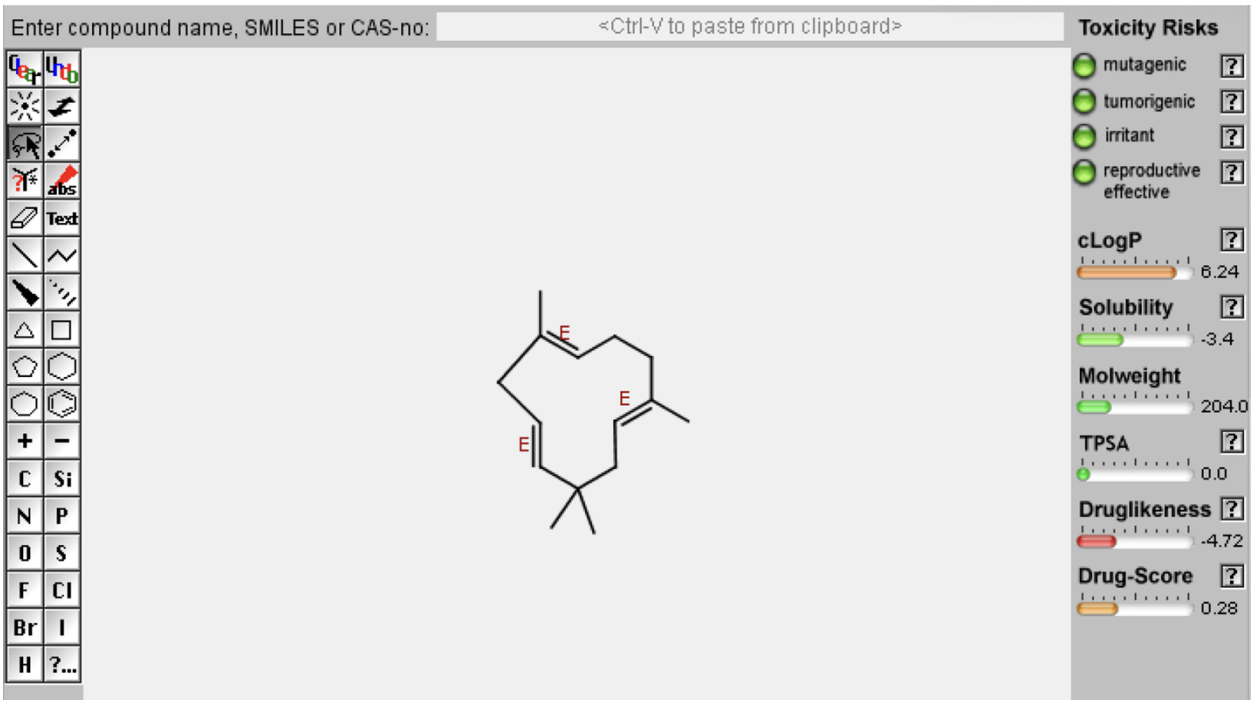
- ***α*-Copaene**



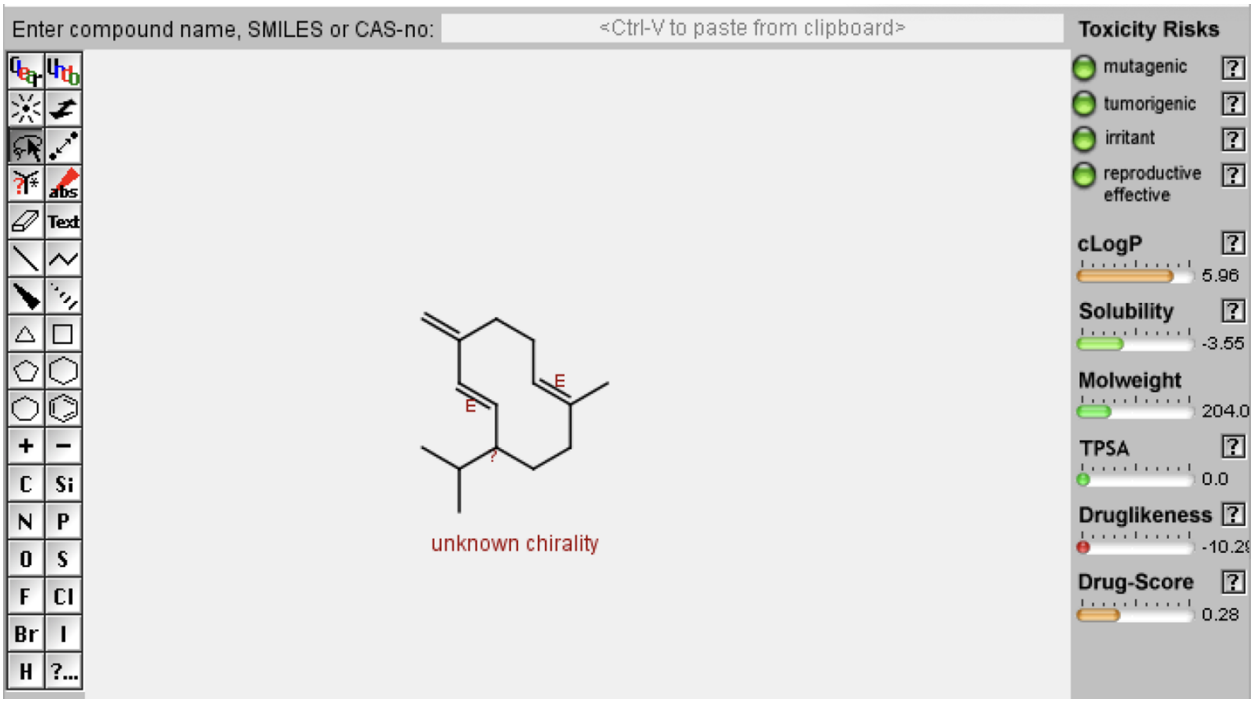
- **Caryophyllene**



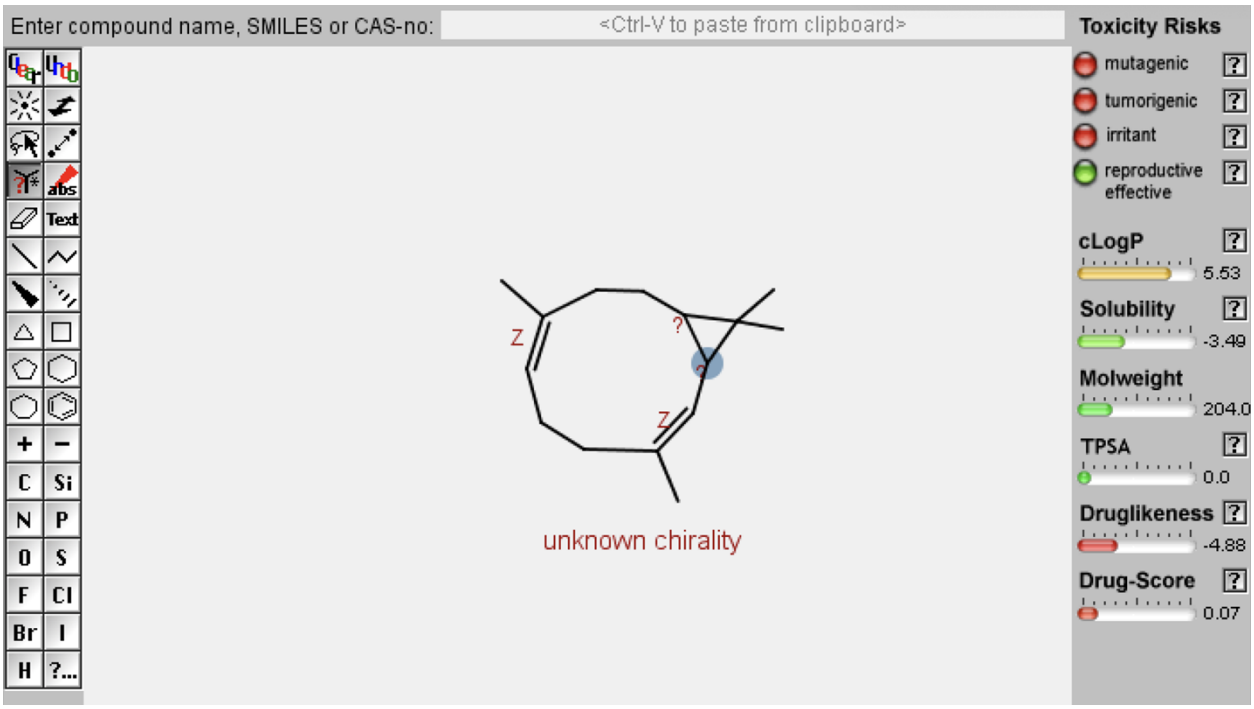
- **Humulene**



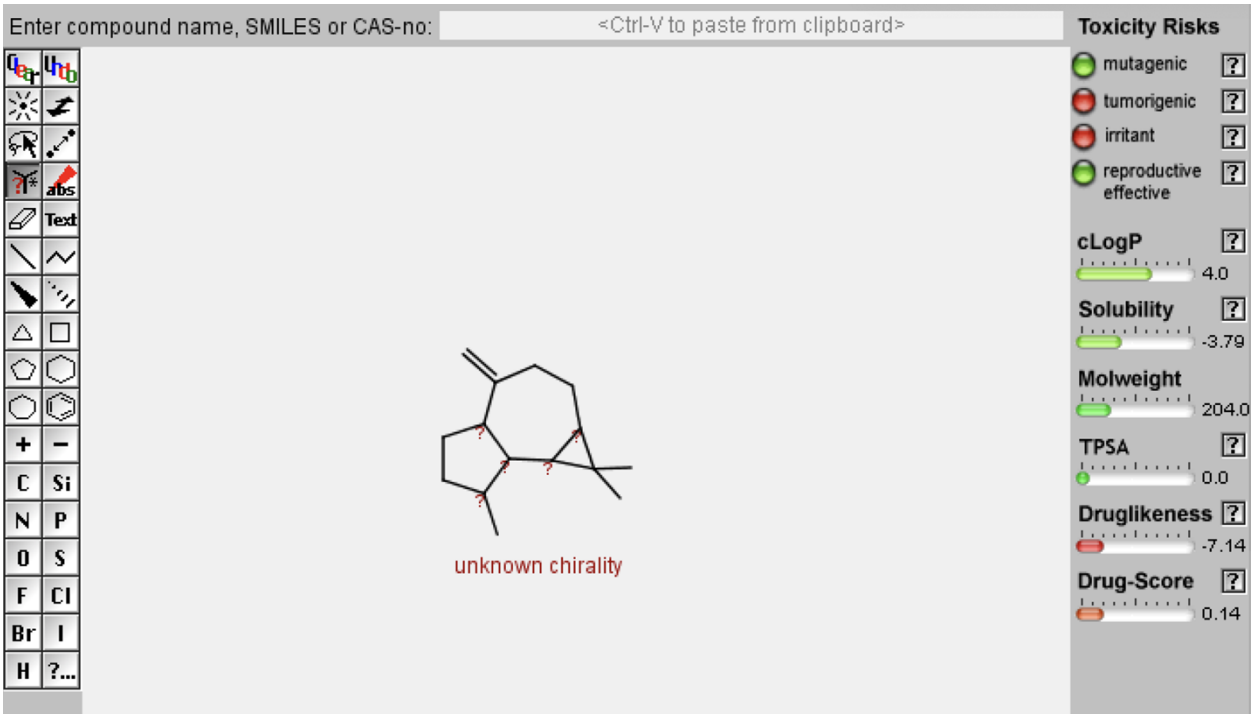
- **Germacrene D**



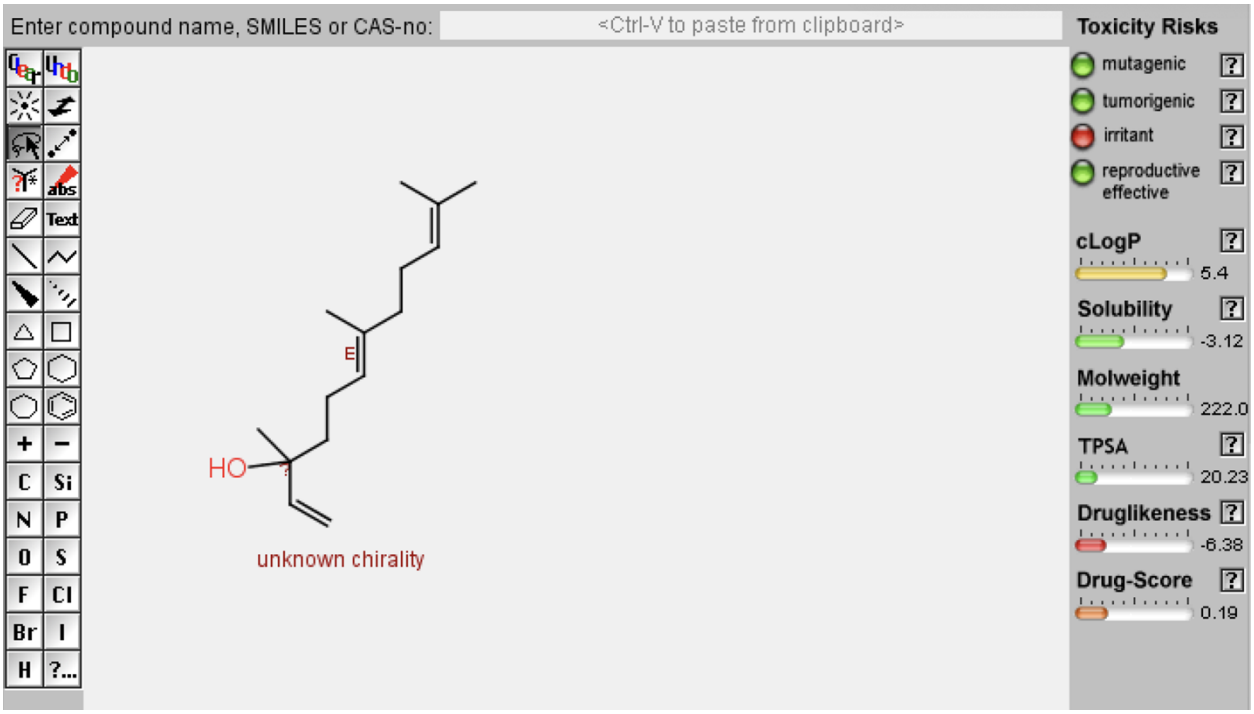
- **Bicyclogermacrene**



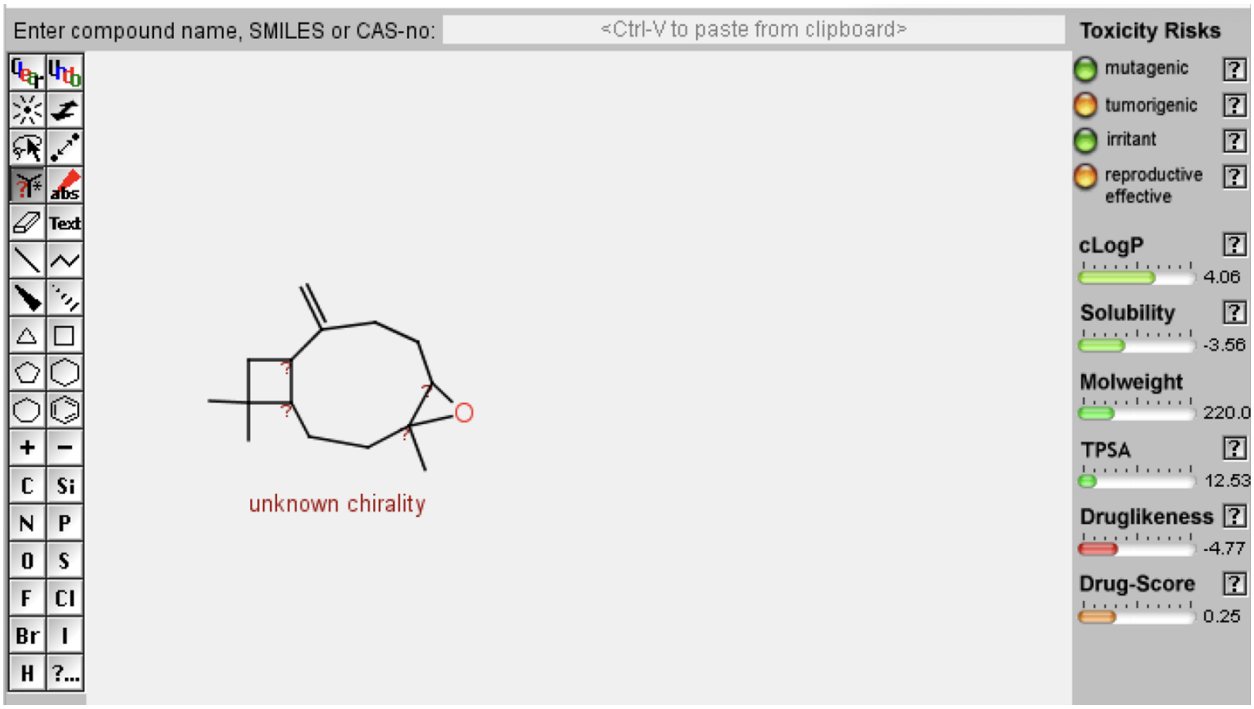
- **Aromandendrene**



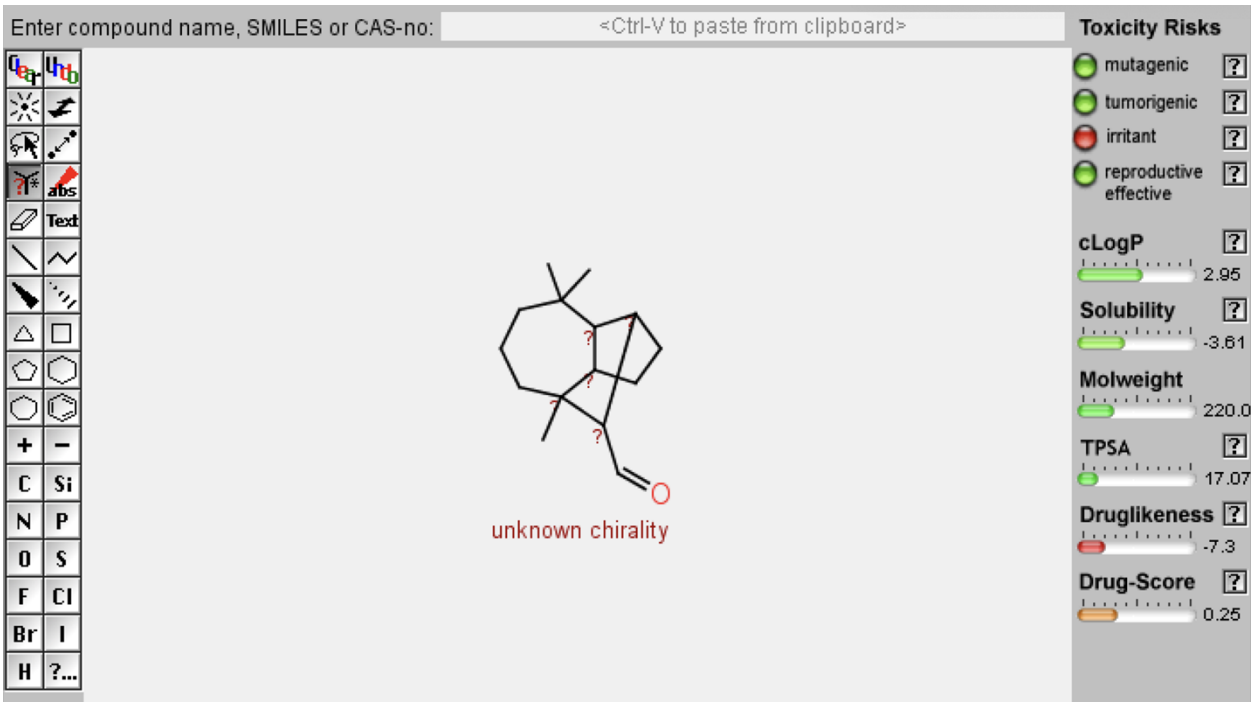
- **trans-Nerolidol**



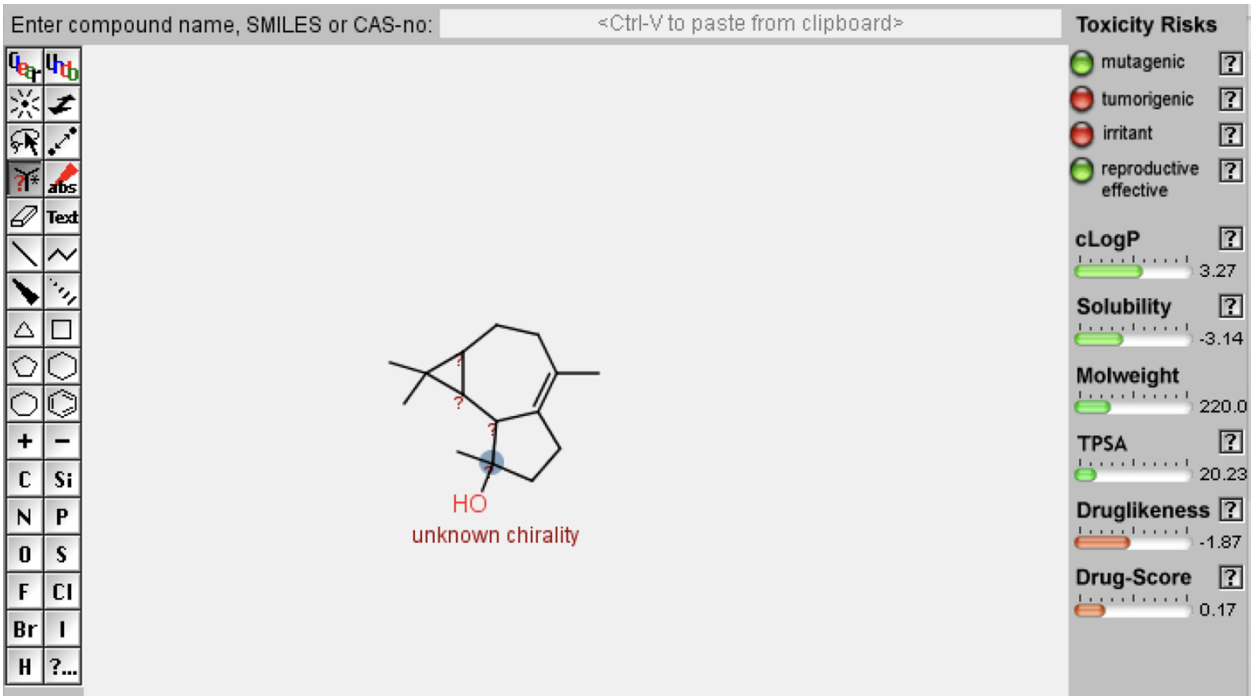
- **Caryophyllene oxide**



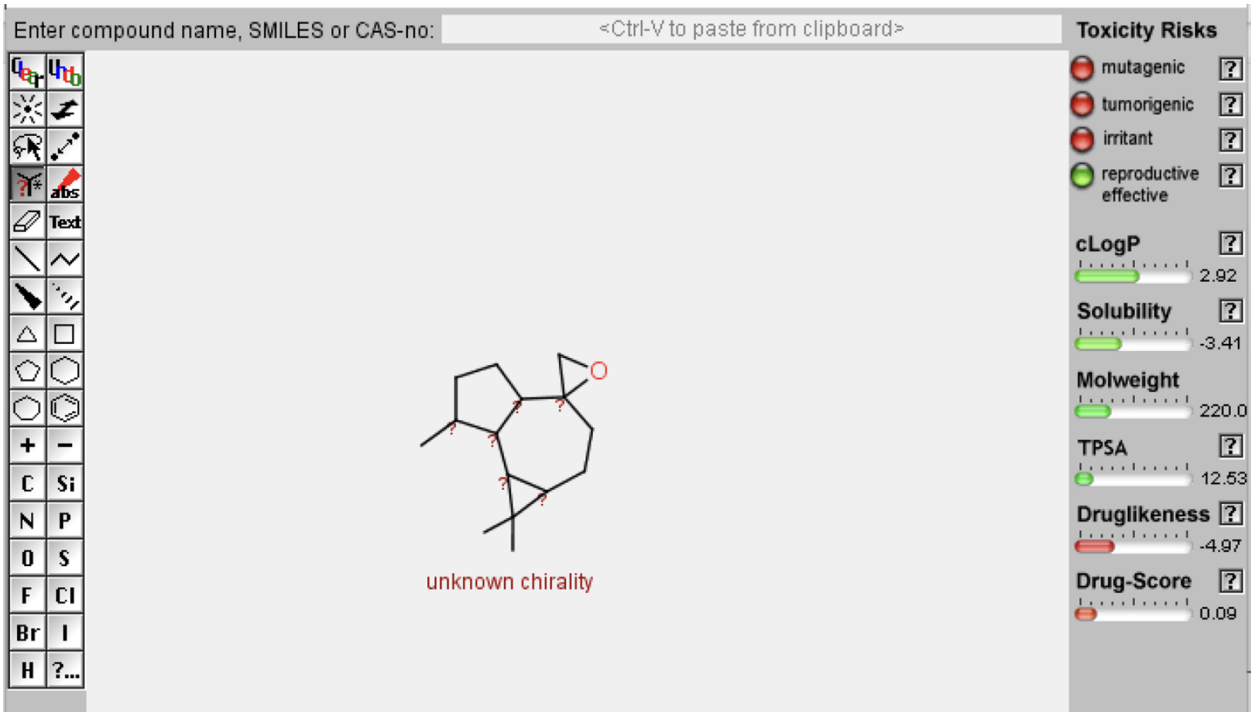
- **Longifolenaldehyde**



- **Isospathulenol**



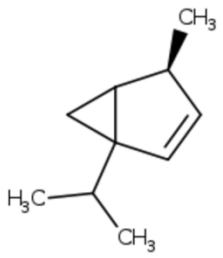
- **Aromadendrene oxide I**

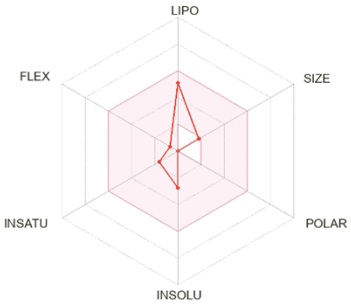


Results from SwissADME (Table 5):

- **2-Thujene**

Molecule 1





SMILES C[C@H]1C=CC2(C1C2)C(C)C

Physicochemical Properties	
Formula	C10H16
Molecular weight	136.23 g/mol
Num. heavy atoms	10
Num. arom. heavy atoms	0
Fraction Csp3	0.80
Num. rotatable bonds	1
Num. H-bond acceptors	0
Num. H-bond donors	0
Molar Refractivity	45.22
TPSA	0.00 Å²

Lipophilicity	
Log $P_{o/w}$ (iLOGP)	2.65
Log $P_{o/w}$ (XLOGP3)	3.41
Log $P_{o/w}$ (WLOGP)	2.85
Log $P_{o/w}$ (MLOGP)	4.29
Log $P_{o/w}$ (SILICOS-IT)	2.55
Consensus Log $P_{o/w}$	3.15

Water Solubility	
Log *S* (ESOL)	-2.77
Solubility	2.33e-01 mg/ml ; 1.71e-03 mol/l
Class	Soluble
Log *S* (Ali)	-3.09
Solubility	1.11e-01 mg/ml ; 8.13e-04 mol/l
Class	Soluble
Log *S* (SILICOS-IT)	-1.78
Solubility	2.27e+00 mg/ml ; 1.67e-02 mol/l
Class	Soluble

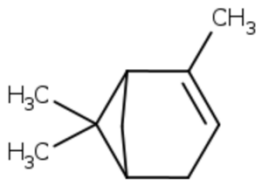
Pharmacokinetics	
GI absorption	Low
BBB permeant	Yes
P-gp substrate	No
CYP1A2 inhibitor	No
CYP2C19 inhibitor	No
CYP2C9 inhibitor	No
CYP2D6 inhibitor	No
CYP3A4 inhibitor	No
Log K_p (skin permeation)	-4.71 cm/s

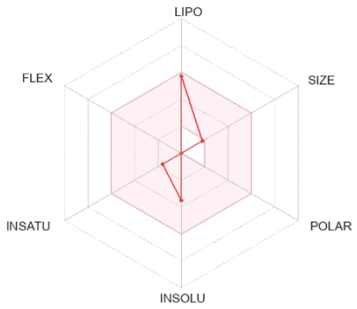
Druglikeness	
Lipinski	Yes; 1 violation: MLOGP>4.15
Ghose	No; 1 violation: MW<160
Veber	Yes
Egan	Yes
Muegge	No; 2 violations: MW<200, Heteroatoms<2
Bioavailability Score	0.55

Medicinal Chemistry	
PAINS	0 alert
Brenk	1 alert: isolated_alkene
Leadlikeness	No; 1 violation: MW<250
Synthetic accessibility	4.19

- ***α*-pinene**

Molecule 1





SMILES CC1=CCC2CC1C2(C)C

Physicochemical Properties	
Formula	C10H16
Molecular weight	136.23 g/mol
Num. heavy atoms	10
Num. arom. heavy atoms	0
Fraction Csp3	0.80
Num. rotatable bonds	0
Num. H-bond acceptors	0
Num. H-bond donors	0
Molar Refractivity	45.22
TPSA	0.00 Å²

Lipophilicity	
Log $P_{o/w}$ (iLOGP)	2.63
Log $P_{o/w}$ (XLOGP3)	4.48
Log $P_{o/w}$ (WLOGP)	3.00
Log $P_{o/w}$ (MLOGP)	4.29
Log $P_{o/w}$ (SILICOS-IT)	2.79
Consensus Log $P_{o/w}$	3.44

Water Solubility	
Log *S* (ESOL)	-3.51
Solubility	4.24e-02 mg/ml ; 3.11e-04 mol/l
Class	Soluble
Log *S* (Ali)	-4.20
Solubility	8.59e-03 mg/ml ; 6.31e-05 mol/l
Class	Moderately soluble
Log *S* (SILICOS-IT)	-2.23
Solubility	8.06e-01 mg/ml ; 5.92e-03 mol/l
Class	Soluble

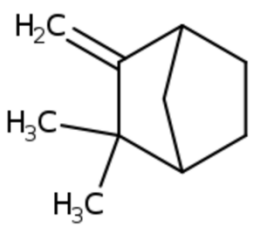
Pharmacokinetics	
GI absorption	Low
BBB permeant	Yes
P-gp substrate	No
CYP1A2 inhibitor	No
CYP2C19 inhibitor	No
CYP2C9 inhibitor	Yes
CYP2D6 inhibitor	No
CYP3A4 inhibitor	No
Log K_p (skin permeation)	-3.95 cm/s

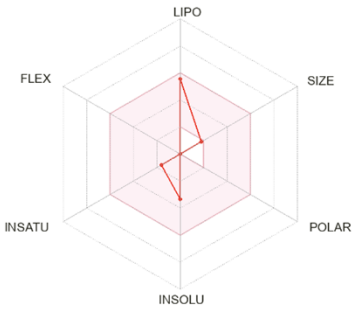
Druglikeness	
Lipinski	Yes; 1 violation: MLOGP>4.15
Ghose	No; 1 violation: MW<160
Veber	Yes
Egan	Yes
Muegge	No; 2 violations: MW<200, Heteroatoms<2
Bioavailability Score	0.55

Medicinal Chemistry	
PAINS	0 alert
Brenk	1 alert: isolated_alkene
Leadlikeness	No; 2 violations: MW<250, XLOGP3>3.5
Synthetic accessibility	4.44

- **Camphene**

Molecule 1





SMILES C=C1C2CCC(C1(C)C)C2

Physicochemical Properties	
Formula	C10H16
Molecular weight	136.23 g/mol
Num. heavy atoms	10
Num. arom. heavy atoms	0
Fraction Csp3	0.80
Num. rotatable bonds	0
Num. H-bond acceptors	0
Num. H-bond donors	0
Molar Refractivity	45.22
TPSA	0.00 Å²

Lipophilicity	
Log $P_{o/w}$ (iLOGP)	2.58
Log $P_{o/w}$ (XLOGP3)	4.22
Log $P_{o/w}$ (WLOGP)	3.00
Log $P_{o/w}$ (MLOGP)	4.29
Log $P_{o/w}$ (SILICOS-IT)	3.08
Consensus Log $P_{o/w}$	3.43

Water Solubility	
Log *S* (ESOL)	-3.34
Solubility	6.18e-02 mg/ml ; 4.54e-04 mol/l
Class	Soluble
Log *S* (Ali)	-3.93
Solubility	1.60e-02 mg/ml ; 1.17e-04 mol/l
Class	Soluble
Log *S* (SILICOS-IT)	-2.48
Solubility	4.55e-01 mg/ml ; 3.34e-03 mol/l
Class	Soluble

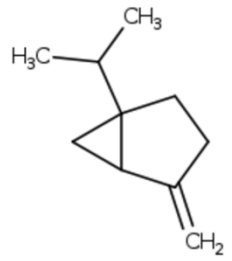
Pharmacokinetics	
GI absorption	Low
BBB permeant	Yes
P-gp substrate	No
CYP1A2 inhibitor	No
CYP2C19 inhibitor	No
CYP2C9 inhibitor	Yes
CYP2D6 inhibitor	No
CYP3A4 inhibitor	No
Log K_p (skin permeation)	-4.13 cm/s

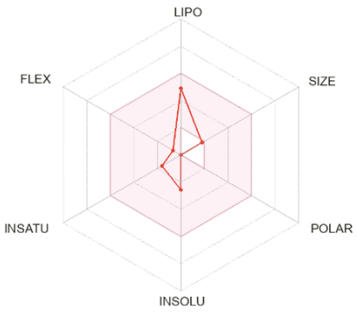
Druglikeness	
Lipinski	Yes; 1 violation: MLOGP>4.15
Ghose	No; 1 violation: MW<160
Veber	Yes
Egan	Yes
Muegge	No; 2 violations: MW<200, Heteroatoms<2
Bioavailability Score	0.55

Medicinal Chemistry	
PAINS	0 alert
Brenk	1 alert: isolated_alkene
Leadlikeness	No; 2 violations: MW<250, XLOGP3>3.5
Synthetic accessibility	3.50

- **Sabinene**

Molecule 1





SMILES C=C1CCC2(C1C2)C(C)C

Physicochemical Properties	
Formula	C10H16
Molecular weight	136.23 g/mol
Num. heavy atoms	10
Num. arom. heavy atoms	0
Fraction Csp3	0.80
Num. rotatable bonds	1
Num. H-bond acceptors	0
Num. H-bond donors	0
Molar Refractivity	45.22
TPSA	0.00 Å²

Lipophilicity	
Log $P_{o/w}$ (iLOGP)	2.65
Log $P_{o/w}$ (XLOGP3)	3.09
Log $P_{o/w}$ (WLOGP)	3.00
Log $P_{o/w}$ (MLOGP)	4.29
Log $P_{o/w}$ (SILICOS-IT)	3.23
Consensus Log $P_{o/w}$	3.25

Water Solubility	
Log *S* (ESOL)	-2.57
Solubility	3.71e-01 mg/ml ; 2.72e-03 mol/l
Class	Soluble
Log *S* (Ali)	-2.76
Solubility	2.38e-01 mg/ml ; 1.75e-03 mol/l
Class	Soluble
Log *S* (SILICOS-IT)	-2.48
Solubility	4.55e-01 mg/ml ; 3.34e-03 mol/l
Class	Soluble

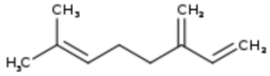
Pharmacokinetics	
GI absorption	Low
BBB permeant	Yes
P-gp substrate	No
CYP1A2 inhibitor	No
CYP2C19 inhibitor	No
CYP2C9 inhibitor	No
CYP2D6 inhibitor	No
CYP3A4 inhibitor	No
Log K_p (skin permeation)	-4.94 cm/s

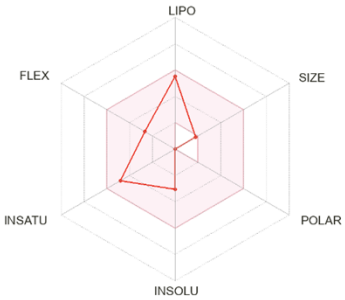
Druglikeness	
Lipinski	Yes; 1 violation: MLOGP>4.15
Ghose	No; 1 violation: MW<160
Veber	Yes
Egan	Yes
Muegge	No; 2 violations: MW<200, Heteroatoms<2
Bioavailability Score	0.55

Medicinal Chemistry	
PAINS	0 alert
Brenk	1 alert: isolated_alkene
Leadlikeness	No; 1 violation: MW<250
Synthetic accessibility	2.87

- ***β*-Myrcene**

Molecule 1





SMILES C=CC(=C)CCC=C(C)C

Physicochemical Properties	
Formula	C10H16
Molecular weight	136.23 g/mol
Num. heavy atoms	10
Num. arom. heavy atoms	0
Fraction Csp3	0.40
Num. rotatable bonds	4
Num. H-bond acceptors	0
Num. H-bond donors	0
Molar Refractivity	48.76
TPSA	0.00 Å²

Lipophilicity	
Log $P_{o/w}$ (iLOGP)	2.89
Log $P_{o/w}$ (XLOGP3)	4.17
Log $P_{o/w}$ (WLOGP)	3.48
Log $P_{o/w}$ (MLOGP)	3.56
Log $P_{o/w}$ (SILICOS-IT)	3.05
Consensus Log $P_{o/w}$	3.43

Water Solubility	
Log *S* (ESOL)	-3.05
Solubility	1.22e-01 mg/ml ; 8.96e-04 mol/l
Class	Soluble
Log *S* (Ali)	-3.88
Solubility	1.80e-02 mg/ml ; 1.32e-04 mol/l
Class	Soluble
Log *S* (SILICOS-IT)	-2.42
Solubility	5.24e-01 mg/ml ; 3.85e-03 mol/l
Class	Soluble

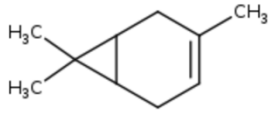
Pharmacokinetics	
GI absorption	Low
BBB permeant	Yes
P-gp substrate	No
CYP1A2 inhibitor	No
CYP2C19 inhibitor	No
CYP2C9 inhibitor	No
CYP2D6 inhibitor	No
CYP3A4 inhibitor	No
Log K_p (skin permeation)	-4.17 cm/s

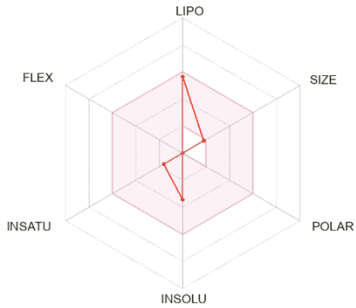
Druglikeness	
Lipinski	Yes; 0 violation
Ghose	No; 1 violation: MW<160
Veber	Yes
Egan	Yes
Muegge	No; 2 violations: MW<200, Heteroatoms<2
Bioavailability Score	0.55

Medicinal Chemistry	
PAINS	0 alert
Brenk	2 alerts: isolated_alkene, polyene
Leadlikeness	No; 2 violations: MW<250, XLOGP3>3.5
Synthetic accessibility	2.85

- **3-Carene**

Molecule 1





SMILES CC1=CCC2C(C1)C2(C)C

Physicochemical Properties	
Formula	C10H16
Molecular weight	136.23 g/mol
Num. heavy atoms	10
Num. arom. heavy atoms	0
Fraction Csp3	0.80
Num. rotatable bonds	0
Num. H-bond acceptors	0
Num. H-bond donors	0
Molar Refractivity	45.22
TPSA	0.00 Å²

Lipophilicity	
Log $P_{o/w}$ (iLOGP)	2.63
Log $P_{o/w}$ (XLOGP3)	4.38
Log $P_{o/w}$ (WLOGP)	3.00
Log $P_{o/w}$ (MLOGP)	4.29
Log $P_{o/w}$ (SILICOS-IT)	2.79
Consensus Log $P_{o/w}$	3.42

Water Solubility	
Log *S* (ESOL)	-3.44
Solubility	4.90e-02 mg/ml ; 3.60e-04 mol/l
Class	Soluble
Log *S* (Ali)	-4.10
Solubility	1.09e-02 mg/ml ; 8.01e-05 mol/l
Class	Moderately soluble
Log *S* (SILICOS-IT)	-2.23
Solubility	8.06e-01 mg/ml ; 5.92e-03 mol/l
Class	Soluble

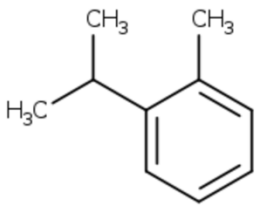
Pharmacokinetics	
GI absorption	Low
BBB permeant	Yes
P-gp substrate	No
CYP1A2 inhibitor	No
CYP2C19 inhibitor	No
CYP2C9 inhibitor	Yes
CYP2D6 inhibitor	No
CYP3A4 inhibitor	No
Log K_p (skin permeation)	-4.02 cm/s

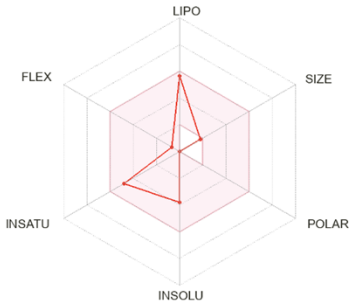
Druglikeness	
Lipinski	Yes; 1 violation: MLOGP>4.15
Ghose	No; 1 violation: MW<160
Veber	Yes
Egan	Yes
Muegge	No; 2 violations: MW<200, Heteroatoms<2
Bioavailability Score	0.55

Medicinal Chemistry	
PAINS	0 alert
Brenk	1 alert: isolated_alkene
Leadlikeness	No; 2 violations: MW<250, XLOGP3>3.5
Synthetic accessibility	3.84

- ***o*-Cymene**

Molecule 1





SMILES CC(c1ccccc1C)C

Physicochemical Properties	
Formula	C10H14
Molecular weight	134.22 g/mol
Num. heavy atoms	10
Num. arom. heavy atoms	6
Fraction Csp3	0.40
Num. rotatable bonds	1
Num. H-bond acceptors	0
Num. H-bond donors	0
Molar Refractivity	45.99
TPSA	0.00 Å²

Lipophilicity	
Log $P_{o/w}$ (iLOGP)	2.43
Log $P_{o/w}$ (XLOGP3)	4.38
Log $P_{o/w}$ (WLOGP)	3.12
Log $P_{o/w}$ (MLOGP)	4.47
Log $P_{o/w}$ (SILICOS-IT)	3.29
Consensus Log $P_{o/w}$	3.54

Water Solubility	
Log *S* (ESOL)	-3.81
Solubility	2.08e-02 mg/ml ; 1.55e-04 mol/l
Class	Soluble
Log *S* (Ali)	-4.10
Solubility	1.08e-02 mg/ml ; 8.01e-05 mol/l
Class	Moderately soluble
Log *S* (SILICOS-IT)	-3.57
Solubility	3.58e-02 mg/ml ; 2.67e-04 mol/l
Class	Soluble

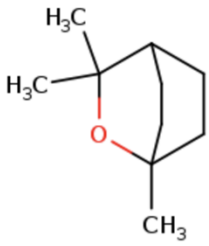
Pharmacokinetics	
GI absorption	Low
BBB permeant	Yes
P-gp substrate	No
CYP1A2 inhibitor	No
CYP2C19 inhibitor	No
CYP2C9 inhibitor	No
CYP2D6 inhibitor	Yes
CYP3A4 inhibitor	No
Log K_p (skin permeation)	-4.01 cm/s

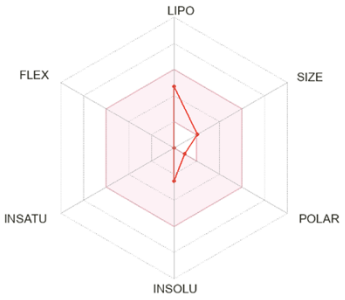
Druglikeness	
Lipinski	Yes; 1 violation: MLOGP>4.15
Ghose	No; 1 violation: MW<160
Veber	Yes
Egan	Yes
Muegge	No; 2 violations: MW<200, Heteroatoms<2
Bioavailability Score	0.55

Medicinal Chemistry	
PAINS	0 alert
Brenk	0 alert
Leadlikeness	No; 2 violations: MW<250, XLOGP3>3.5
Synthetic accessibility	1.00

- **Eucalyptol**

Molecule 1





SMILES CC12CCC(CC1)C(O2)(C)C

Physicochemical Properties	
Formula	C10H18O
Molecular weight	154.25 g/mol
Num. heavy atoms	11
Num. arom. heavy atoms	0
Fraction Csp3	1.00
Num. rotatable bonds	0
Num. H-bond acceptors	1
Num. H-bond donors	0
Molar Refractivity	47.12
TPSA	9.23 Å²

Lipophilicity	
Log $P_{o/w}$ (iLOGP)	2.58
Log $P_{o/w}$ (XLOGP3)	2.74
Log $P_{o/w}$ (WLOGP)	2.74
Log $P_{o/w}$ (MLOGP)	2.45
Log $P_{o/w}$ (SILICOS-IT)	2.86
Consensus Log $P_{o/w}$	2.67

Water Solubility	
Log *S* (ESOL)	-2.52
Solubility	4.63e-01 mg/ml ; 3.00e-03 mol/l
Class	Soluble
Log *S* (Ali)	-2.59
Solubility	3.98e-01 mg/ml ; 2.58e-03 mol/l
Class	Soluble
Log *S* (SILICOS-IT)	-2.45
Solubility	5.45e-01 mg/ml ; 3.53e-03 mol/l
Class	Soluble

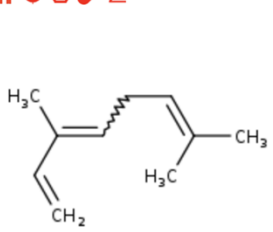
Pharmacokinetics	
GI absorption	High
BBB permeant	Yes
P-gp substrate	No
CYP1A2 inhibitor	No
CYP2C19 inhibitor	No
CYP2C9 inhibitor	No
CYP2D6 inhibitor	No
CYP3A4 inhibitor	No
Log K_p (skin permeation)	-5.30 cm/s

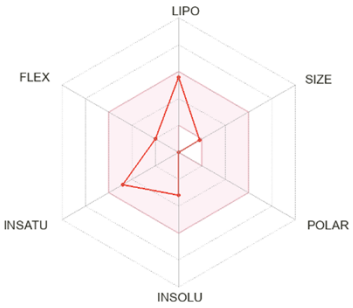
Druglikeness	
Lipinski	Yes; 0 violation
Ghose	No; 1 violation: MW<160
Veber	Yes
Egan	Yes
Muegge	No; 2 violations: MW<200, Heteroatoms<2
Bioavailability Score	0.55

Medicinal Chemistry	
PAINS	0 alert
Brenk	0 alert
Leadlikeness	No; 1 violation: MW<250
Synthetic accessibility	3.65

- ***β*-cis-Ocimene**

Molecule 1





SMILES C=C/C(=C\CC=C(C)C)/C

Physicochemical Properties	
Formula	C10H16
Molecular weight	136.23 g/mol
Num. heavy atoms	10
Num. arom. heavy atoms	0
Fraction Csp3	0.40
Num. rotatable bonds	3
Num. H-bond acceptors	0
Num. H-bond donors	0
Molar Refractivity	48.76
TPSA	0.00 Å²

Lipophilicity	
Log $P_{o/w}$ (iLOGP)	2.91
Log $P_{o/w}$ (XLOGP3)	4.26
Log $P_{o/w}$ (WLOGP)	3.48
Log $P_{o/w}$ (MLOGP)	3.56
Log $P_{o/w}$ (SILICOS-IT)	2.88
Consensus Log $P_{o/w}$	3.42

Water Solubility	
Log *S* (ESOL)	-3.17
Solubility	9.20e-02 mg/ml ; 6.75e-04 mol/l
Class	Soluble
Log *S* (Ali)	-3.97
Solubility	1.45e-02 mg/ml ; 1.07e-04 mol/l
Class	Soluble
Log *S* (SILICOS-IT)	-2.04
Solubility	1.24e+00 mg/ml ; 9.10e-03 mol/l
Class	Soluble

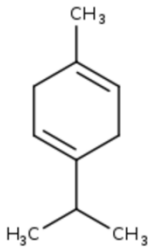
Pharmacokinetics	
GI absorption	Low
BBB permeant	Yes
P-gp substrate	No
CYP1A2 inhibitor	No
CYP2C19 inhibitor	No
CYP2C9 inhibitor	No
CYP2D6 inhibitor	No
CYP3A4 inhibitor	No
Log K_p (skin permeation)	-4.11 cm/s

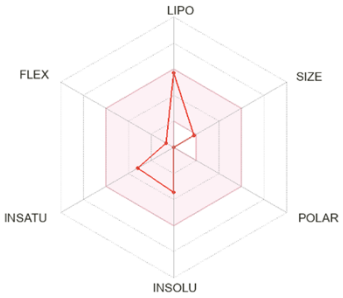
Druglikeness	
Lipinski	Yes; 0 violation
Ghose	No; 1 violation: MW<160
Veber	Yes
Egan	Yes
Muegge	No; 2 violations: MW<200, Heteroatoms<2
Bioavailability Score	0.55

Medicinal Chemistry	
PAINS	0 alert
Brenk	2 alerts: isolated_alkene, polyene
Leadlikeness	No; 2 violations: MW<250, XLOGP3>3.5
Synthetic accessibility	3.63

- ***γ*-Terpinene**

Molecule 1





SMILES CC1=CCC(=CC1)C(C)C

Physicochemical Properties	
Formula	C10H16
Molecular weight	136.23 g/mol
Num. heavy atoms	10
Num. arom. heavy atoms	0
Fraction Csp3	0.60
Num. rotatable bonds	1
Num. H-bond acceptors	0
Num. H-bond donors	0
Molar Refractivity	47.12
TPSA	0.00 Å²

Lipophilicity	
Log $P_{o/w}$ (iLOGP)	2.73
Log $P_{o/w}$ (XLOGP3)	4.50
Log $P_{o/w}$ (WLOGP)	3.31
Log $P_{o/w}$ (MLOGP)	3.27
Log $P_{o/w}$ (SILICOS-IT)	2.95
Consensus Log $P_{o/w}$	3.35

Water Solubility	
Log *S* (ESOL)	-3.45
Solubility	4.79e-02 mg/ml ; 3.52e-04 mol/l
Class	Soluble
Log *S* (Ali)	-4.22
Solubility	8.19e-03 mg/ml ; 6.01e-05 mol/l
Class	Moderately soluble
Log *S* (SILICOS-IT)	-2.23
Solubility	8.06e-01 mg/ml ; 5.92e-03 mol/l
Class	Soluble

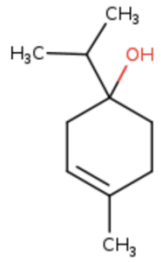
Pharmacokinetics	
GI absorption	Low
BBB permeant	Yes
P-gp substrate	No
CYP1A2 inhibitor	No
CYP2C19 inhibitor	No
CYP2C9 inhibitor	No
CYP2D6 inhibitor	No
CYP3A4 inhibitor	No
Log K_p (skin permeation)	-3.94 cm/s

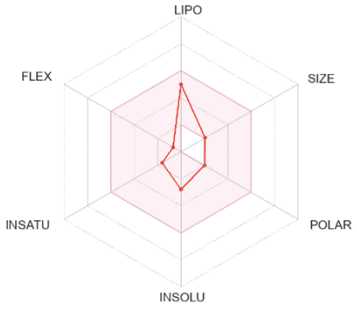
Druglikeness	
Lipinski	Yes; 0 violation
Ghose	No; 1 violation: MW<160
Veber	Yes
Egan	Yes
Muegge	No; 2 violations: MW<200, Heteroatoms<2
Bioavailability Score	0.55

Medicinal Chemistry	
PAINS	0 alert
Brenk	1 alert: isolated_alkene
Leadlikeness	No; 2 violations: MW<250, XLOGP3>3.5
Synthetic accessibility	3.11

- **Terpinen-4-ol**

Molecule 1





SMILES CC1=CCC(CC1)(O)C(C)C

Physicochemical Properties	
Formula	C10H18O
Molecular weight	154.25 g/mol
Num. heavy atoms	11
Num. arom. heavy atoms	0
Fraction Csp3	0.80
Num. rotatable bonds	1
Num. H-bond acceptors	1
Num. H-bond donors	1
Molar Refractivity	48.80
TPSA	20.23 Å²

Lipophilicity	
Log $P_{o/w}$ (iLOGP)	2.51
Log $P_{o/w}$ (XLOGP3)	3.26
Log $P_{o/w}$ (WLOGP)	2.50
Log $P_{o/w}$ (MLOGP)	2.30
Log $P_{o/w}$ (SILICOS-IT)	2.44
Consensus Log $P_{o/w}$	2.60

Water Solubility	
Log *S* (ESOL)	-2.78
Solubility	2.54e-01 mg/ml ; 1.64e-03 mol/l
Class	Soluble
Log *S* (Ali)	-3.36
Solubility	6.75e-02 mg/ml ; 4.38e-04 mol/l
Class	Soluble
Log *S* (SILICOS-IT)	-1.91
Solubility	1.92e+00 mg/ml ; 1.24e-02 mol/l
Class	Soluble

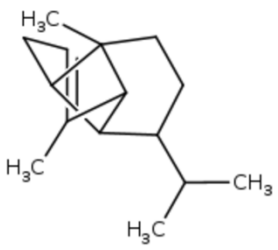
Pharmacokinetics	
GI absorption	High
BBB permeant	Yes
P-gp substrate	No
CYP1A2 inhibitor	No
CYP2C19 inhibitor	No
CYP2C9 inhibitor	No
CYP2D6 inhibitor	No
CYP3A4 inhibitor	No
Log K_p (skin permeation)	-4.93 cm/s

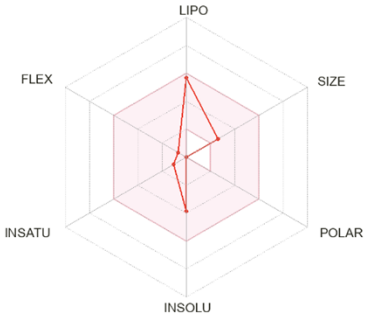
Druglikeness	
Lipinski	Yes; 0 violation
Ghose	No; 1 violation: MW<160
Veber	Yes
Egan	Yes
Muegge	No; 2 violations: MW<200, Heteroatoms<2
Bioavailability Score	0.55

Medicinal Chemistry	
PAINS	0 alert
Brenk	1 alert: isolated_alkene
Leadlikeness	No; 1 violation: MW<250
Synthetic accessibility	3.28

- ***α*-Copaene**

Molecule 1





SMILES CC(C1CCC2(C3C1C2C(=CC3)C)C)C

Physicochemical Properties	
Formula	C15H24
Molecular weight	204.35 g/mol
Num. heavy atoms	15
Num. arom. heavy atoms	0
Fraction Csp3	0.87
Num. rotatable bonds	1
Num. H-bond acceptors	0
Num. H-bond donors	0
Molar Refractivity	67.14
TPSA	0.00 Å²

Lipophilicity	
Log $P_{o/w}$ (iLOGP)	3.40
Log $P_{o/w}$ (XLOGP3)	4.47
Log $P_{o/w}$ (WLOGP)	4.27
Log $P_{o/w}$ (MLOGP)	5.65
Log $P_{o/w}$ (SILICOS-IT)	3.73
Consensus Log $P_{o/w}$	4.30

Water Solubility	
Log *S* (ESOL)	-3.86
Solubility	2.84e-02 mg/ml ; 1.39e-04 mol/l
Class	Soluble
Log *S* (Ali)	-4.19
Solubility	1.32e-02 mg/ml ; 6.46e-05 mol/l
Class	Moderately soluble
Log *S* (SILICOS-IT)	-3.07
Solubility	1.74e-01 mg/ml ; 8.51e-04 mol/l
Class	Soluble

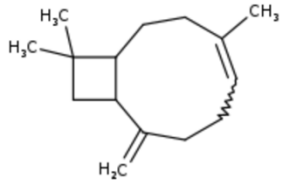
Pharmacokinetics	
GI absorption	Low
BBB permeant	Yes
P-gp substrate	No
CYP1A2 inhibitor	Yes
CYP2C19 inhibitor	Yes
CYP2C9 inhibitor	Yes
CYP2D6 inhibitor	No
CYP3A4 inhibitor	No
Log K_p (skin permeation)	-4.37 cm/s

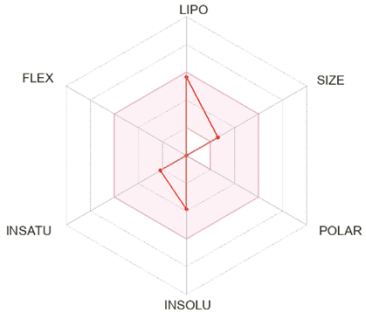
Druglikeness	
Lipinski	Yes; 1 violation: MLOGP>4.15
Ghose	Yes
Veber	Yes
Egan	Yes
Muegge	No; 1 violation: Heteroatoms<2
Bioavailability Score	0.55

Medicinal Chemistry	
PAINS	0 alert
Brenk	1 alert: isolated_alkene
Leadlikeness	No; 2 violations: MW<250, XLOGP3>3.5
Synthetic accessibility	4.62

- **Caryophyllene**

Molecule 1





SMILES CC1=CCCC(=C)C2C(CC1)C(C2)(C)C

Physicochemical Properties	
Formula	C15H24
Molecular weight	204.35 g/mol
Num. heavy atoms	15
Num. arom. heavy atoms	0
Fraction Csp3	0.73
Num. rotatable bonds	0
Num. H-bond acceptors	0
Num. H-bond donors	0
Molar Refractivity	68.78
TPSA	0.00 Å²

Lipophilicity	
Log $P_{o/w}$ (iLOGP)	3.29
Log $P_{o/w}$ (XLOGP3)	4.38
Log $P_{o/w}$ (WLOGP)	4.73
Log $P_{o/w}$ (MLOGP)	4.63
Log $P_{o/w}$ (SILICOS-IT)	4.19
Consensus Log $P_{o/w}$	4.24

Water Solubility	
Log *S* (ESOL)	-3.87
Solubility	2.78e-02 mg/ml ; 1.36e-04 mol/l
Class	Soluble
Log *S* (Ali)	-4.10
Solubility	1.64e-02 mg/ml ; 8.01e-05 mol/l
Class	Moderately soluble
Log *S* (SILICOS-IT)	-3.77
Solubility	3.49e-02 mg/ml ; 1.71e-04 mol/l
Class	Soluble

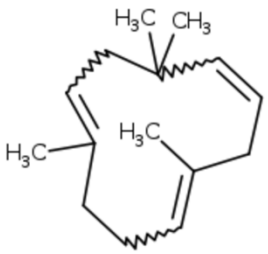
Pharmacokinetics	
GI absorption	Low
BBB permeant	No
P-gp substrate	No
CYP1A2 inhibitor	No
CYP2C19 inhibitor	Yes
CYP2C9 inhibitor	Yes
CYP2D6 inhibitor	No
CYP3A4 inhibitor	No
Log K_p (skin permeation)	-4.44 cm/s

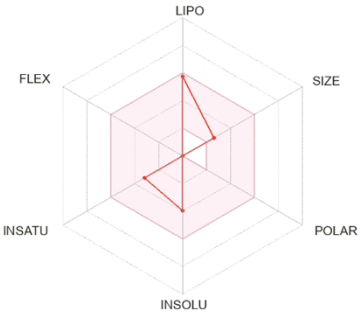
Druglikeness	
Lipinski	Yes; 1 violation: MLOGP>4.15
Ghose	Yes
Veber	Yes
Egan	Yes
Muegge	No; 1 violation: Heteroatoms<2
Bioavailability Score	0.55

Medicinal Chemistry	
PAINS	0 alert
Brenk	1 alert: isolated_alkene
Leadlikeness	No; 2 violations: MW<250, XLOGP3>3.5
Synthetic accessibility	4.51

- **Humulene**

Molecule 1





SMILES CC1=CCC(C)(C)C=CCC(=CCC1)C

Physicochemical Properties	
Formula	C15H24
Molecular weight	204.35 g/mol
Num. heavy atoms	15
Num. arom. heavy atoms	0
Fraction Csp3	0.60
Num. rotatable bonds	0
Num. H-bond acceptors	0
Num. H-bond donors	0
Molar Refractivity	70.42
TPSA	0.00 Å²

Lipophilicity	
Log $P_{o/w}$ (iLOGP)	3.27
Log $P_{o/w}$ (XLOGP3)	4.55
Log $P_{o/w}$ (WLOGP)	5.04
Log $P_{o/w}$ (MLOGP)	4.53
Log $P_{o/w}$ (SILICOS-IT)	3.91
Consensus Log $P_{o/w}$	4.26

Water Solubility	
Log *S* (ESOL)	-3.97
Solubility	2.17e-02 mg/ml ; 1.06e-04 mol/l
Class	Soluble
Log *S* (Ali)	-4.27
Solubility	1.09e-02 mg/ml ; 5.34e-05 mol/l
Class	Moderately soluble
Log *S* (SILICOS-IT)	-3.52
Solubility	6.19e-02 mg/ml ; 3.03e-04 mol/l
Class	Soluble

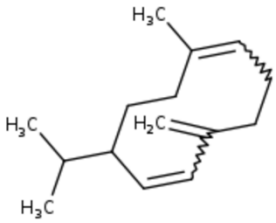
Pharmacokinetics	
GI absorption	Low
BBB permeant	No
P-gp substrate	No
CYP1A2 inhibitor	No
CYP2C19 inhibitor	No
CYP2C9 inhibitor	Yes
CYP2D6 inhibitor	No
CYP3A4 inhibitor	No
Log K_p (skin permeation)	-4.32 cm/s

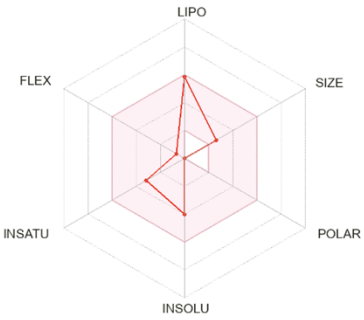
Druglikeness	
Lipinski	Yes; 1 violation: MLOGP>4.15
Ghose	Yes
Veber	Yes
Egan	Yes
Muegge	No; 1 violation: Heteroatoms<2
Bioavailability Score	0.55

Medicinal Chemistry	
PAINS	0 alert
Brenk	1 alert: isolated_alkene
Leadlikeness	No; 2 violations: MW<250, XLOGP3>3.5
Synthetic accessibility	3.66

- **Germacrene D**

Molecule 1





SMILES CC1=CCCC(=C)C=CC(CC1)C(C)C

Physicochemical Properties	
Formula	C15H24
Molecular weight	204.35 g/mol
Num. heavy atoms	15
Num. arom. heavy atoms	0
Fraction Csp3	0.60
Num. rotatable bonds	1
Num. H-bond acceptors	0
Num. H-bond donors	0
Molar Refractivity	70.68
TPSA	0.00 Å²

Lipophilicity	
Log $P_{o/w}$ (iLOGP)	3.32
Log $P_{o/w}$ (XLOGP3)	4.74
Log $P_{o/w}$ (WLOGP)	4.89
Log $P_{o/w}$ (MLOGP)	4.53
Log $P_{o/w}$ (SILICOS-IT)	4.01
Consensus Log $P_{o/w}$	4.30

Water Solubility	
Log *S* (ESOL)	-4.03
Solubility	1.92e-02 mg/ml ; 9.39e-05 mol/l
Class	Moderately soluble
Log *S* (Ali)	-4.47
Solubility	6.93e-03 mg/ml ; 3.39e-05 mol/l
Class	Moderately soluble
Log *S* (SILICOS-IT)	-3.32
Solubility	9.83e-02 mg/ml ; 4.81e-04 mol/l
Class	Soluble

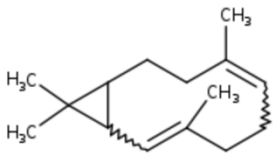
Pharmacokinetics	
GI absorption	Low
BBB permeant	No
P-gp substrate	No
CYP1A2 inhibitor	No
CYP2C19 inhibitor	No
CYP2C9 inhibitor	Yes
CYP2D6 inhibitor	No
CYP3A4 inhibitor	No
Log K_p (skin permeation)	-4.18 cm/s

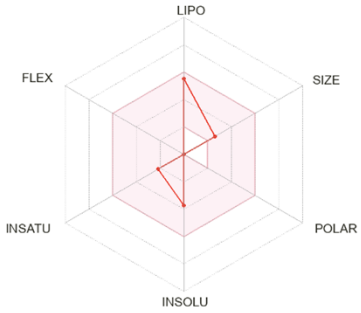
Druglikeness	
Lipinski	Yes; 1 violation: MLOGP>4.15
Ghose	Yes
Veber	Yes
Egan	Yes
Muegge	No; 1 violation: Heteroatoms<2
Bioavailability Score	0.55

Medicinal Chemistry	
PAINS	0 alert
Brenk	1 alert: isolated_alkene
Leadlikeness	No; 2 violations: MW<250, XLOGP3>3.5
Synthetic accessibility	4.55

- **Bicyclogermacrene**

Molecule 1





SMILES CC1=CCCC(=CC2C(CC1)C2(C)C)C

Physicochemical Properties	
Formula	C15H24
Molecular weight	204.35 g/mol
Num. heavy atoms	15
Num. arom. heavy atoms	0
Fraction Csp3	0.73
Num. rotatable bonds	0
Num. H-bond acceptors	0
Num. H-bond donors	0
Molar Refractivity	68.78
TPSA	0.00 Å²

Lipophilicity	
Log $P_{o/w}$ (iLOGP)	3.34
Log $P_{o/w}$ (XLOGP3)	4.14
Log $P_{o/w}$ (WLOGP)	4.73
Log $P_{o/w}$ (MLOGP)	4.63
Log $P_{o/w}$ (SILICOS-IT)	3.91
Consensus Log $P_{o/w}$	4.15

Water Solubility	
Log *S* (ESOL)	-3.72
Solubility	3.94e-02 mg/ml ; 1.93e-04 mol/l
Class	Soluble
Log *S* (Ali)	-3.85
Solubility	2.90e-02 mg/ml ; 1.42e-04 mol/l
Class	Soluble
Log *S* (SILICOS-IT)	-3.52
Solubility	6.19e-02 mg/ml ; 3.03e-04 mol/l
Class	Soluble

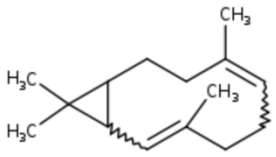
Pharmacokinetics	
GI absorption	Low
BBB permeant	No
P-gp substrate	No
CYP1A2 inhibitor	No
CYP2C19 inhibitor	Yes
CYP2C9 inhibitor	Yes
CYP2D6 inhibitor	No
CYP3A4 inhibitor	No
Log K_p (skin permeation)	-4.61 cm/s

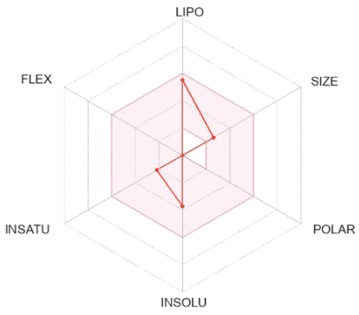
Druglikeness	
Lipinski	Yes; 1 violation: MLOGP>4.15
Ghose	Yes
Veber	Yes
Egan	Yes
Muegge	No; 1 violation: Heteroatoms<2
Bioavailability Score	0.55

Medicinal Chemistry	
PAINS	0 alert
Brenk	1 alert: isolated_alkene
Leadlikeness	No; 2 violations: MW<250, XLOGP3>3.5
Synthetic accessibility	4.34

- **Aromandendrene**

Molecule 1





SMILES CC1=CCCC(=CC2C(CC1)C2(C)C)C

Physicochemical Properties	
Formula	C15H24
Molecular weight	204.35 g/mol
Num. heavy atoms	15
Num. arom. heavy atoms	0
Fraction Csp3	0.73
Num. rotatable bonds	0
Num. H-bond acceptors	0
Num. H-bond donors	0
Molar Refractivity	68.78
TPSA	0.00 Å²

Lipophilicity	
Log $P_{o/w}$ (iLOGP)	3.34
Log $P_{o/w}$ (XLOGP3)	4.14
Log $P_{o/w}$ (WLOGP)	4.73
Log $P_{o/w}$ (MLOGP)	4.63
Log $P_{o/w}$ (SILICOS-IT)	3.91
Consensus Log $P_{o/w}$	4.15

Water Solubility	
Log *S* (ESOL)	-3.72
Solubility	3.94e-02 mg/ml ; 1.93e-04 mol/l
Class	Soluble
Log *S* (Ali)	-3.85
Solubility	2.90e-02 mg/ml ; 1.42e-04 mol/l
Class	Soluble
Log *S* (SILICOS-IT)	-3.52
Solubility	6.19e-02 mg/ml ; 3.03e-04 mol/l
Class	Soluble

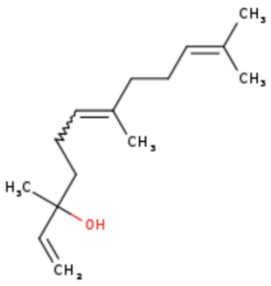
Pharmacokinetics	
GI absorption	Low
BBB permeant	No
P-gp substrate	No
CYP1A2 inhibitor	No
CYP2C19 inhibitor	Yes
CYP2C9 inhibitor	Yes
CYP2D6 inhibitor	No
CYP3A4 inhibitor	No
Log K_p (skin permeation)	-4.61 cm/s

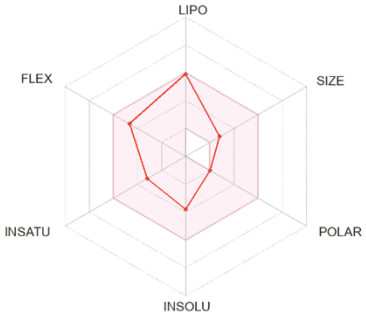
Druglikeness	
Lipinski	Yes; 1 violation: MLOGP>4.15
Ghose	Yes
Veber	Yes
Egan	Yes
Muegge	No; 1 violation: Heteroatoms<2
Bioavailability Score	0.55

Medicinal Chemistry	
PAINS	0 alert
Brenk	1 alert: isolated_alkene
Leadlikeness	No; 2 violations: MW<250, XLOGP3>3.5
Synthetic accessibility	4.34

- **trans-Nerolidol**

Molecule 1





SMILES C=CC(CCC=C(CCC=C(C)C)C)(O)C

Physicochemical Properties	
Formula	C15H26O
Molecular weight	222.37 g/mol
Num. heavy atoms	16
Num. arom. heavy atoms	0
Fraction Csp3	0.60
Num. rotatable bonds	7
Num. H-bond acceptors	1
Num. H-bond donors	1
Molar Refractivity	74.00
TPSA	20.23 Å²

Lipophilicity	
Log $P_{o/w}$ (iLOGP)	3.64
Log $P_{o/w}$ (XLOGP3)	4.83
Log $P_{o/w}$ (WLOGP)	4.40
Log $P_{o/w}$ (MLOGP)	3.86
Log $P_{o/w}$ (SILICOS-IT)	4.21
Consensus Log $P_{o/w}$	4.19

Water Solubility	
Log *S* (ESOL)	-3.80
Solubility	3.53e-02 mg/ml ; 1.59e-04 mol/l
Class	Soluble
Log *S* (Ali)	-4.99
Solubility	2.29e-03 mg/ml ; 1.03e-05 mol/l
Class	Moderately soluble
Log *S* (SILICOS-IT)	-3.15
Solubility	1.56e-01 mg/ml ; 7.00e-04 mol/l
Class	Soluble

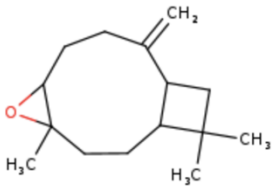
Pharmacokinetics	
GI absorption	High
BBB permeant	Yes
P-gp substrate	No
CYP1A2 inhibitor	Yes
CYP2C19 inhibitor	No
CYP2C9 inhibitor	Yes
CYP2D6 inhibitor	No
CYP3A4 inhibitor	No
Log K_p (skin permeation)	-4.23 cm/s

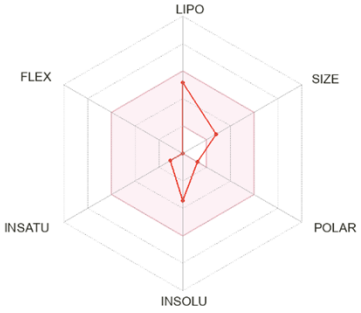
Druglikeness	
Lipinski	Yes; 0 violation
Ghose	Yes
Veber	Yes
Egan	Yes
Muegge	No; 1 violation: Heteroatoms<2
Bioavailability Score	0.55

Medicinal Chemistry	
PAINS	0 alert
Brenk	1 alert: isolated_alkene
Leadlikeness	No; 2 violations: MW<250, XLOGP3>3.5
Synthetic accessibility	3.53

- **Caryophyllene oxide**

Molecule 1





SMILES C=C1CCC2OC2(CCC2C1CC2(C)C)C

Physicochemical Properties	
Formula	C15H24O
Molecular weight	220.35 g/mol
Num. heavy atoms	16
Num. arom. heavy atoms	0
Fraction Csp3	0.87
Num. rotatable bonds	0
Num. H-bond acceptors	1
Num. H-bond donors	0
Molar Refractivity	68.27
TPSA	12.53 Å²

Lipophilicity	
Log $P_{o/w}$ (iLOGP)	3.15
Log $P_{o/w}$ (XLOGP3)	3.56
Log $P_{o/w}$ (WLOGP)	3.94
Log $P_{o/w}$ (MLOGP)	3.67
Log $P_{o/w}$ (SILICOS-IT)	4.07
Consensus Log $P_{o/w}$	3.68

Water Solubility	
Log *S* (ESOL)	-3.45
Solubility	7.84e-02 mg/ml ; 3.56e-04 mol/l
Class	Soluble
Log *S* (Ali)	-3.51
Solubility	6.83e-02 mg/ml ; 3.10e-04 mol/l
Class	Soluble
Log *S* (SILICOS-IT)	-3.51
Solubility	6.81e-02 mg/ml ; 3.09e-04 mol/l
Class	Soluble

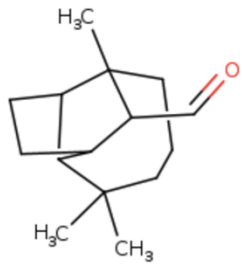
Pharmacokinetics	
GI absorption	High
BBB permeant	Yes
P-gp substrate	No
CYP1A2 inhibitor	No
CYP2C19 inhibitor	Yes
CYP2C9 inhibitor	Yes
CYP2D6 inhibitor	No
CYP3A4 inhibitor	No
Log K_p (skin permeation)	-5.12 cm/s

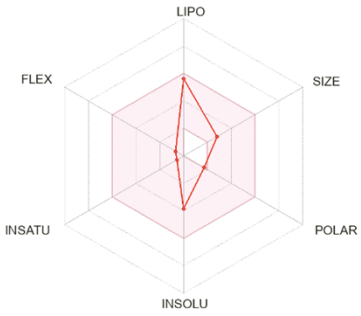
Druglikeness	
Lipinski	Yes; 0 violation
Ghose	Yes
Veber	Yes
Egan	Yes
Muegge	No; 1 violation: Heteroatoms<2
Bioavailability Score	0.55

Medicinal Chemistry	
PAINS	0 alert
Brenk	2 alerts: Three-membered_heterocycle, isolated_alkene
Leadlikeness	No; 2 violations: MW<250, XLOGP3>3.5
Synthetic accessibility	4.35

- **Longifolenaldehyde**

Molecule 1





SMILES O=CC1C2CCC3C1(C)CCCC(C23)(C)C

Physicochemical Properties	
Formula	C15H24O
Molecular weight	220.35 g/mol
Num. heavy atoms	16
Num. arom. heavy atoms	0
Fraction Csp3	0.93
Num. rotatable bonds	1
Num. H-bond acceptors	1
Num. H-bond donors	0
Molar Refractivity	67.56
TPSA	17.07 Å²

Lipophilicity	
Log $P_{o/w}$ (iLOGP)	2.66
Log $P_{o/w}$ (XLOGP3)	4.34
Log $P_{o/w}$ (WLOGP)	3.67
Log $P_{o/w}$ (MLOGP)	3.67
Log $P_{o/w}$ (SILICOS-IT)	3.59
Consensus Log $P_{o/w}$	3.59

Water Solubility	
Log *S* (ESOL)	-3.87
Solubility	2.94e-02 mg/ml ; 1.34e-04 mol/l
Class	Soluble
Log *S* (Ali)	-4.41
Solubility	8.51e-03 mg/ml ; 3.86e-05 mol/l
Class	Moderately soluble
Log *S* (SILICOS-IT)	-3.10
Solubility	1.75e-01 mg/ml ; 7.93e-04 mol/l
Class	Soluble

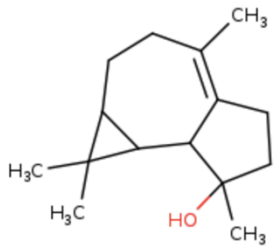
Pharmacokinetics	
GI absorption	High
BBB permeant	Yes
P-gp substrate	No
CYP1A2 inhibitor	No
CYP2C19 inhibitor	Yes
CYP2C9 inhibitor	Yes
CYP2D6 inhibitor	No
CYP3A4 inhibitor	No
Log K_p (skin permeation)	-4.56 cm/s

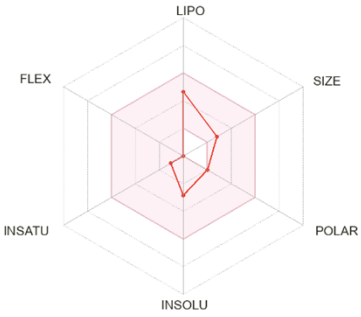
Druglikeness	
Lipinski	Yes; 0 violation
Ghose	Yes
Veber	Yes
Egan	Yes
Muegge	No; 1 violation: Heteroatoms<2
Bioavailability Score	0.55

Medicinal Chemistry	
PAINS	0 alert
Brenk	1 alert: aldehyde
Leadlikeness	No; 2 violations: MW<250, XLOGP3>3.5
Synthetic accessibility	3.45

- **Isospathulenol**

Molecule 1





SMILES CC1=C2CCC(C2C2C(CC1)C2(C)C)(C)O

Physicochemical Properties	
Formula	C15H24O
Molecular weight	220.35 g/mol
Num. heavy atoms	16
Num. arom. heavy atoms	0
Fraction Csp3	0.87
Num. rotatable bonds	0
Num. H-bond acceptors	1
Num. H-bond donors	1
Molar Refractivity	68.34
TPSA	20.23 Å²

Lipophilicity	
Log $P_{o/w}$ (iLOGP)	2.89
Log $P_{o/w}$ (XLOGP3)	2.62
Log $P_{o/w}$ (WLOGP)	3.53
Log $P_{o/w}$ (MLOGP)	3.67
Log $P_{o/w}$ (SILICOS-IT)	3.38
Consensus Log $P_{o/w}$	3.22

Water Solubility	
Log *S* (ESOL)	-2.86
Solubility	3.06e-01 mg/ml ; 1.39e-03 mol/l
Class	Soluble
Log *S* (Ali)	-2.69
Solubility	4.45e-01 mg/ml ; 2.02e-03 mol/l
Class	Soluble
Log *S* (SILICOS-IT)	-3.17
Solubility	1.51e-01 mg/ml ; 6.84e-04 mol/l
Class	Soluble

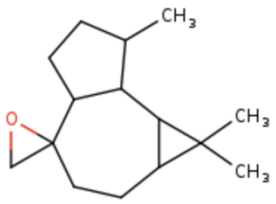
Pharmacokinetics	
GI absorption	High
BBB permeant	Yes
P-gp substrate	No
CYP1A2 inhibitor	No
CYP2C19 inhibitor	No
CYP2C9 inhibitor	No
CYP2D6 inhibitor	No
CYP3A4 inhibitor	No
Log K_p (skin permeation)	-5.78 cm/s

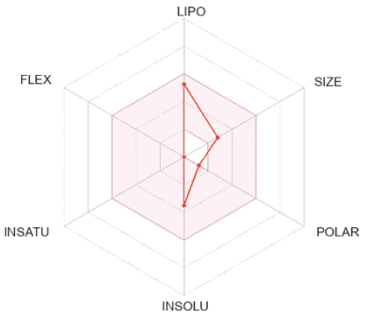
Druglikeness	
Lipinski	Yes; 0 violation
Ghose	Yes
Veber	Yes
Egan	Yes
Muegge	No; 1 violation: Heteroatoms<2
Bioavailability Score	0.55

Medicinal Chemistry	
PAINS	0 alert
Brenk	1 alert: isolated_alkene
Leadlikeness	No; 1 violation: MW<250
Synthetic accessibility	4.35

- **Aromadendrene oxide I**

Molecule 1





SMILES CC1CCC2C1C1C(C1(C)C)CCC12OC1

Physicochemical Properties	
Formula	C15H24O
Molecular weight	220.35 g/mol
Num. heavy atoms	16
Num. arom. heavy atoms	0
Fraction Csp3	1.00
Num. rotatable bonds	0
Num. H-bond acceptors	1
Num. H-bond donors	0
Molar Refractivity	66.63
TPSA	12.53 Å²

Lipophilicity	
Log $P_{o/w}$ (iLOGP)	3.17
Log $P_{o/w}$ (XLOGP3)	3.68
Log $P_{o/w}$ (WLOGP)	3.48
Log $P_{o/w}$ (MLOGP)	3.81
Log $P_{o/w}$ (SILICOS-IT)	3.57
Consensus Log $P_{o/w}$	3.54

Water Solubility	
Log *S* (ESOL)	-3.52
Solubility	6.58e-02 mg/ml ; 2.99e-04 mol/l
Class	Soluble
Log *S* (Ali)	-3.63
Solubility	5.13e-02 mg/ml ; 2.33e-04 mol/l
Class	Soluble
Log *S* (SILICOS-IT)	-2.93
Solubility	2.57e-01 mg/ml ; 1.16e-03 mol/l
Class	Soluble

Pharmacokinetics	
GI absorption	High
BBB permeant	Yes
P-gp substrate	No
CYP1A2 inhibitor	Yes
CYP2C19 inhibitor	Yes
CYP2C9 inhibitor	Yes
CYP2D6 inhibitor	No
CYP3A4 inhibitor	No
Log K_p (skin permeation)	-5.03 cm/s

Druglikeness	
Lipinski	Yes; 0 violation
Ghose	Yes
Veber	Yes
Egan	Yes
Muegge	No; 1 violation: Heteroatoms<2
Bioavailability Score	0.55

Medicinal Chemistry	
PAINS	0 alert
Brenk	1 alert: Three-membered_heterocycle
Leadlikeness	No; 2 violations: MW<250, XLOGP3>3.5
Synthetic accessibility	4.03