

S1 - Targethunter analysis of the major compounds of *Virola surinamensis essential* oil.

<b><math>\alpha</math>-Pinene</b>							
ID	ChEMBL Similar Compound	Name Similar Compound	SMILES Similar Compound	DOI Articles	Bioactivity value (IC50, Ki, etc)*	Antibacterial test	Bacterial species
1	CHEMBL1236329	(+)-alpha - Pinene	<chem>CC1=CC[C@@H]2C[C@H]1C2(C)C</chem>	10.1021/jf034936d	20,80%	Gi	<i>S. aureus</i>
2	CHEMBL1689085	(1R,2E,4R,7E,11S,12R)-2,7,18-Dolabellatriene	<chem>C[C@@H]1CCC=C(CC[C@H]2[C@@H](C[C@@]2/C=C1)C=C(C)C</chem>	10.1021/np1006586	128 µg/ml	MIC	<i>S. aureus</i>

<b><math>\beta</math>-Maaliene</b>							
ID	ChEMBL Similar Compound	Name Similar Compound	SMILES Similar Compound	DOI Articles	Bioactivity value (IC50, Ki, etc)*	Antibacterial test	Bacterial species
1	CHEMBL1171157	(4S,4aS,6aR,6bS,8aR,11R,12S,12aR,14aR,14bS)-4,6a,6b,8a,11,12,14b-heptamethyl-1,2,3,4,4a,5,6,7,8,9,10,11,12,12a,14,14a-hexadecahydricene	<chem>C[C@H]1CCC[C@]2([C@H]1CC[C@@]3([C@@H]2CC=C4[C@]3(CC[C@@]5([C@H]4[C@H]([C@@H](CC5)C)C)C)C)C</chem>	10.1016/j.bmcl.2010.	100 µg/ml	MIC	<i>M. tuberculosis</i>

<b><math>\beta</math>-Pinene</b>							
ID	ChEMBL Similar Compound	Name Similar Compound	SMILES Similar Compound	Articles	Bioactivity value (IC50, Ki, etc)*	Antibacterial test	Bacterial species
1	CHEMBL2269085	(+)-beta - Pinene	<chem>CC1([C@@H]2CCC(=C)[C@H]1C2)C</chem>	10.1021/jf034936d	17,60%	Gi	<i>S. aureus</i>
2	CHEMBL2269083	(+)-Aromadendrene	<chem>C[C@@H]1CC[C@@H]2[C@@H]1[C@H]3[C@H](C3(C)C)CCC2=C</chem>	10.1021/jf034936d	24,20%	Gi	<i>E. coli</i>

<b>δ-Selinene</b>							
ID	ChEMBL Similar Compound	Name Similar Compound	SMILES Similar Compound	DOI Articles	Bioactivity value (IC50, Ki, etc)*	Antibacterial test	Bacterial species
1	CHEMBL1171156	Stigmasta-3,5-diene	<chem>CCC(CC[C@@H](C)[C@H]1CC[C@@H]2[C@@]1(CC[C@H]3[C@H]2CC=C4[C@@]3(CCC=C4)C)C(C)C</chem>	10.1016/j.bmcl.2010.	100 µg/ml	MIC	<i>M. tuberculosis</i>
<b>Limonene</b>							
ID	ChEMBL Similar Compound	Name Similar Compound	SMILES Similar Compound	DOI Articles	Bioactivity value (IC50, Ki, etc)*	Antibacterial test	Bacterial species
1	CHEMBL1689074	(1S,3aR,5E,12aS)-3a,6,10-trimethyl-1-prop-1-en-2-yl-2,3,4,7,8,11,12,12a-octahydro-1H-cyclopenta[11]annulene	<chem>CC1=CCC/C(=C/C[C@]2(CC[C@@H]([C@@H]2CC1)C(=C)C)C)/C</chem>	10.1021/np1006586	64 µg/ml	MIC	<i>S. aureus</i>
2	CHEMBL1689085	(1R,2E,4R,7E,11S,12R)-2,7,18-Dolabellatriene	<chem>C[C@@H]1CCC=C(CC[C@H]2[C@@H](CC[C@@]2/C=C1)C)C(=C)C</chem>	10.1021/np1006586	>128 µg/ml	MIC	<i>S. aureus</i>
<b>Myrcene</b>							
ID	ChEMBL Similar Compound	Name Similar Compound	SMILES Similar Compound	DOI Articles	Bioactivity value (IC50, Ki, etc)*	Antibacterial test	Bacterial species
1	CHEMBL458402	Squalene	<chem>CC(=CCC/C(=C/CC/C(=C/CC/C=C(/CC/C=C(/CCC=C(C)C)\C)\C)/C)/C</chem>	10.1021/np800082e	100 µg/ml	MIC	<i>M. tuberculosis</i>

\*All bioactivity values refer to the inhibition tests against the bacterial species

