

Molecular docking analysis of *Mentha X Piperita* derived ligands for targeting migraine receptors: Identification and evaluation of high-affinity compounds

Bhavani Muthulakshmi Muthumurgan¹, Sindumathi Subramani¹, Subha Prabakaran¹, Premnath Dhanaraj² & Indiraleka Muthiah^{1*}

¹Mepco Schlenk Engineering College (Autonomous), Sivakasi, Virudhunagar-626 005, Tamil Nadu, India

²School of Agriculture and Biosciences, Karunya Institute of Technology and Sciences (Deemed to be University), Coimbatore-641 114, Tamil Nadu, India

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Supplementary Data

Suppl. Table S1 — Molecular interaction of *Mentha X Piperita* leaf ligands with 5HT_{1A}

Ligand	Lipinski's rule	Docking score (Kcal/mol)	Molecular weight (Da)
(+)-beta-phellandrene	Passed	-5.5	136.24
(+)-delta-cadinene	Passed	-6.5	204.36
(+)-gamma-cadinene	Passed	-7.2	204.36
(+)-isomenthal	Passed	-5.1	156.27
(-)-beta bourbone	Passed	-6.9	204.36
(+)-germacerene A	Passed	-6.5	204.36
(-)-isopulegol	Passed	-5.4	154.25
(1R)-2-methyl-5-propan-2-ylbicyclo[3.1.0]hex-2-ene	Passed	-5.3	136.24
(1S,2R,5S)-2-isopropyl-5-methylcyclohexyl acetate	Passed	-5.6	198.31
(1S,2S,3Z,6S)-3-enthylyl-3,7,7-trimethyl-2-prop-1-en-2-ylbicyclo[4.1.0]heptane	Passed	-6.4	204.36
(S,1Z,6Z)-8-Isopropyl-1-methyl-5-methylenecyclodeca-1,6-diene	Passed	-7	204.36
(Z)-beta-Ocimene	Passed	-4.9	136.24
3-Octanol	Passed	-3.9	130.23
4-Carvomenthenol	Passed	-5.7	154.25
alpha-Pinene	Passed	-6.2	136.24
alpha-Terpinene	Passed	-5.7	136.24
alpha-Terpineol	Passed	-5.5	154.25
Azulene	Passed	-5.9	128.17
beta-Caryophyllene	Passed	-6.9	204.36
beta-Cubebene	Passed	-6.5	204.36
beta-Elementene	Passed	-6.9	204.36
beta-Farnesene	Passed	-5.3	204.36
beta-Pinene	Passed	-5.4	136.24
Bicyclogermacrene	Passed	-6.3	204.36
Carvone	Passed	-5.3	150.22
Caryophyllene oxide	Passed	-6.9	220.36
Chrysanthenone	Passed	-5.6	150.22
cis-beta-Farnesene	Passed	-5.2	204.36
cis-Dihydrocarvone	Passed	-5.7	152.24
cis-Sabinene hydrate	Passed	-5.1	138.25
Durohydroquinone	Passed	-5.8	166.22
Eriodictyol	Passed	-8.4	288.26
Eucalyptol	Passed	-6.4	154.25

gamma-Terpinene	Passed	-5.2	136.24
Humulene	Passed	-6.9	204.36
Isomenthone	Passed	-5.4	154.25
Isomenthyl acetate	Passed	-5.5	198.31
Isopulegone	Passed	-5.3	152.24
Jasmone	Passed	-6	164.25
Limonene	Passed	-5.4	136.24
Linalool	Passed	-4.8	154.25
Luteolin	Passed	-8.6	286.24
Menthofuran	Passed	-5.9	150.22
Menthol	Passed	-5.4	156.27
Menthone	Passed	-5.4	154.25
Myrcene	Passed	-4.8	136.24
o-Menth-8-ene	Passed	-6.2	138.25
p-Cymene	Passed	-5.8	134.22
p-Menthan-3-one	Passed	-5.2	154.25
Piperitenone oxide	Passed	-6.3	166.22
Piperitone	Passed	-5.6	152.24
Pulegone	Passed	-5.9	152.24
Rosmarinic acid	Passed	-7.8	360.32
Sabinene	Passed	-5.2	136.24
Spathulenol	Passed	-6.6	220.36
Terpinolene	Passed	-5.7	136.24
trans-Sabinene hydrate	Passed	-6	154.25
Viridiflorol	Passed	-6.7	222.37
Zizanene	Passed	-6.6	204.36

Suppl. Table S2 — Molecular interaction of *Mentha X Piperita* leaf ligands with 5HT_{1F}

Ligand	Lipinski's rule	Docking score (Kcal/mol)	Molecular weight (Da)
(+)-beta-phellandrene	Passed	-5.1	136.24
(+)-delta-cadinene	Passed	-6.6	204.36
(+)-gamma-cadinene	Passed	-6.7	204.36
(-)-beta bourbone	Passed	-6.4	204.36
(-)-isopulegol	Passed	-5	154.25
(1R)-2-methyl-5-propan-2-ylbicyclo[3.1.0]hex-2-ene	Passed	-5.5	136.24
(1S,2R,5S)-2-isopropyl-5-methylcyclohexyl acetate	Passed	-5.1	198.31
(1S,2S,3,6S)-3-enthnyl-3,7,7-trimethyl-2-prop-1-en-2-ylbicyclo[4.1.0]heptane	Passed	-6.2	204.36
(S,1Z,6Z)-8-Isopropyl-1-methyl-5-methylenecyclodeca-1,6-diene	Passed	-6.3	204.36
(Z)-beta-Ocimene	Passed	-4.7	136.24
3-Octanol	Passed	-4.1	130.23
4-Carvomenthenol	Passed	-5	154.25
alpha-Pinene	Passed	-6.2	136.24
alpha-Terpinene	Passed	-5.5	136.24
alpha-Terpineol	Passed	-5	154.25
Azulene	Passed	-5.7	128.17
beta-Caryophyllene	Passed	-6.1	204.36
beta-Cubebene	Passed	-6.7	204.36
beta-Elementene	Passed	-6.5	204.36
beta-Farnesene	Passed	-5.2	204.36
beta-Pinene	Passed	-6.1	136.24
Bicyclogermacrene	Passed	-5.9	204.36
Carvone	Passed	-5.5	150.22
Caryophyllene oxide	Passed	-6.2	220.36
Chrysanthenone	Passed	-5.7	150.22
cis-beta-Farnesene	Passed	-4.7	204.36
cis-Dihydrocarvone	Passed	-5.5	152.24
cis-Sabinene hydrate	Passed	-4.9	138.25
Durohydroquinone	Passed	-5.3	166.22

Eriodictyol	Passed	-8.4	288.26
Eucalyptol	Passed	-5.1	154.25
gamma-Terpinene	Passed	-5.3	136.24
Humulene	Passed	-6.3	204.36
Isomenthone	Passed	-5.3	154.25
Isomenthyl acetate	Passed	-4.9	198.31
Isopulegone	Passed	-5.1	152.24
Jasmone	Passed	-4.7	164.25
Limonene	Passed	-6	136.24
Linalool	Passed	-4.6	154.25
Luteolin	Passed	-8.9	286.24
Menthofuran	Passed	-5.1	150.22
Menthol	Passed	-4.8	156.27
Menthone	Passed	-5	154.25
Myrcene	Passed	-4.9	136.24
o-Menth-8-ene	Passed	-5.1	138.25
p-Cymene	Passed	-5.3	134.22
p-Menthan-3-one	Passed	-5.2	154.25
Piperitenone oxide	Passed	-4.7	166.22
Piperitone	Passed	-5.8	152.24
Pulegone	Passed	-5.2	152.24
Rosmarinic acid	Passed	-7.5	360.32
Sabinene	Passed	-5.1	136.24
Spathulenol	Passed	-6.6	220.36
Terpinolene	Passed	-5.4	136.24
trans-Sabinene hydrate	Passed	-4.8	154.25
Viridiflorol	Passed	-6.5	222.37
Zizanene	Passed	-7.4	204.36
(+)-isomenthal	Passed	-5.1	156.27
(+)-germacerene A	Passed	-6.5	204.36

Suppl. Table S3 — Molecular interaction of *Mentha X Piperita* leaf ligand with RAMP

Ligand	Lipinski's rule	Dockingscore (Kcal/mol)	Molecular weight (Da)
(+)-beta-phellandrene	Passed	-5.6	136.24
(+)-delta-cadinene	Passed	-5.2	204.36
(+)-gamma-cadinene	Passed	-6.4	204.36
(+)-isomenthal	Passed	-4.6	156.27
(-)-beta bourbone	Passed	-6.2	204.36
(+)-germacerene A	Passed	-6.2	204.36
(-)-isopulegol	Passed	-5.3	154.25
(1R)-2-methyl-5-propan-2-ylbicyclo[3.1.0]hex-2-ene	Passed	-5.1	136.24
(1S,2R,5S)-2-isopropyl-5-methylcyclohexyl acetate	Passed	-4.9	198.31
(1S,2S,3,6S)-3-enthnyl-3,7,7-trimethyl-2-prop-1-en-2-ylbicyclo[4.1.0]heptane	Passed	-5.5	204.36
(S,1Z,6Z)-8-Isopropyl-1-methyl-5-methylenecyclodeca-1,6-diene	Passed	-5.9	204.36
(Z)-beta-Ocimene	Passed	-4.6	136.24
3-Octanol	Passed	-3.6	130.23
4-Carvomenthenol	Passed	-5.4	154.25
alpha-Pinene	Passed	-5	136.24
alpha-Terpinene	Passed	-5.5	136.24
alpha-Terpineol	Passed	-4.9	154.25
Azulene	Passed	-6	128.17
beta-Caryophyllene	Passed	-6.3	204.36
beta-Cubebene	Passed	-6.5	204.36
beta-Elementene	Passed	-5.5	204.36
beta-Farnesene	Passed	-5.3	204.36
beta-Pinene	Passed	-5	136.24
Bicyclogermacrene	Passed	-5.9	204.36

Carvone	Passed	-5.6	150.22
Caryophyllene oxide	Passed	-5.8	220.36
Chrysanthenone	Passed	-4.9	150.22
cis-beta-Farnesene	Passed	-4.9	204.36
cis-Dihydrocarvone	Passed	-5.1	152.24
cis-Sabinene hydrate	Passed	-4.7	138.25
Durohydroquinone	Passed	-5.4	166.22
Eriodictyol	Passed	-7	288.26
Eucalyptol	Passed	-4.7	154.25
gamma-Terpinene	Passed	-5.2	136.24
Humulene	Passed	-6	204.36
Isomenthone	Passed	-5.1	154.25
Isomenthyl acetate	Passed	-5.1	198.31
Isopulegone	Passed	-4.9	152.24
Jasmone	Passed	-4.9	164.25
limonene	Passed	-5.5	136.24
Linalool	Passed	-4.2	154.25
Luteolin	Passed	-6.7	286.24
Menthofuran	Passed	-5.2	150.22
Menthol	Passed	-5.2	156.27
Menthone	Passed	-4.8	154.25
Myrcene	Passed	-4.2	136.24
o-Menth-8-ene	Passed	-5.1	138.25
p-Cymene	Passed	-5.7	134.22
p-Menthan-3-one	Passed	-4.7	154.25
Piperitenone oxide	Passed	-5.4	166.22
Piperitone	Passed	-4.9	152.24
Pulegone	Passed	-5.4	152.24
Rosmarinic acid	Passed	-5.5	360.32
Sabinene	Passed	-5.6	136.24
Spathulenol	Passed	-6.2	220.36
Terpinolene	Passed	-5.4	136.24
Trans-Sabinene hydrate	Passed	-4.8	154.25
Viridiflorol	Passed	-6	222.37
Zizanene	Passed	-6.2	204.36