Target Name	MAO-A
Target TTD ID	TTDS00289

Target Species	Human
Chemical Type	Propargyl (clorgyline analogues)
Mode of Action	Inhibitor
QSAR Model 1	$\text{i-MAO-A} = -1.32\chi_1(C_{sat}) - 2.56\chi_2(\text{Het}) + 0.46\alpha_0(\text{Het}) + 1.69\alpha_1(\text{Het}) + 1.16MR_1 + 1.21 + 7.12MR_2(C_{unsat}) - 1.71MR_0(\text{Het}) - 2.95 \cdot \log P_0 - 5.6 \cdot \log P_2(C_{unsat})$ $\lambda = 0.36 \quad F = 273.93 \quad p < 0.01$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** ${}^k\chi(G)$: molecular or group electro-negativities; ${}^kMR(G)$: refractivities; ${}^k\alpha(G)$: polarizabilities; $\log {}^kP$: logarithms of water/*n*-octanol partition coefficients; *G*: atoms included in a specific group; i-MAO-A: MAO-A inhibitory activity score; *W*: Wilk's λ statistic; *F*: the Fisher ratio; *p*: the *p*-level.
Reference	A QSAR Model for in Silico Screening of MAO-A Inhibitors. Prediction, Synthesis, and Biological Assay of Novel Coumarins. *J. Med. Chem.* 2006, 49, 1149-1156

Target Species	Human
Chemical Type	Benzamide (moclobemide analogues)
Mode of Action	Inhibitor

QSAR Model 1	$\text{i-MAO-A} = -1.32\chi_1(C_{sat}) - 2.56\chi_2(\text{Het}) + 0.46\alpha_0(\text{Het}) + 1.69\alpha_1(\text{Het}) + 1.16MR_1 + 1.21$ $+ 7.12MR_2(C_{unsat}) - 1.71MR_0(\text{Het}) - 2.95 \cdot \log P_0 - 5.6 \cdot \log P_2(C_{unsat})$ $\lambda = 0.36 \quad F = 273.93 \quad p < 0.01$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** $^k\chi(G)$: molecular or group electro-negativities; $^kMR(G)$: refractivities; $^k\alpha(G)$: polarizabilities; $\log^kP$: logarithms of water/*n*-octanol partition coefficients; *G*: atoms included in a specific group; i-MAO-A: MAO-A inhibitory activity score; *W*: Wilk's λ statistic; *F*: the Fisher ratio; *p*: the *p*-level.
Reference	A QSAR Model for in Silico Screening of MAO-A Inhibitors. Prediction, Synthesis, and Biological Assay of Novel Coumarins. *J. Med. Chem.* 2006, 49, 1149-1156

Target Species	Human
Chemical Type	Phenylethylamines
Mode of Action	Inhibitor
QSAR Model 1	$\text{i-MAO-A} = -1.32\chi_1(C_{sat}) - 2.56\chi_2(\text{Het}) + 0.46\alpha_0(\text{Het}) + 1.69\alpha_1(\text{Het}) + 1.16MR_1 + 1.21$ $+ 7.12MR_2(C_{unsat}) - 1.71MR_0(\text{Het}) - 2.95 \cdot \log P_0 - 5.6 \cdot \log P_2(C_{unsat})$ $\lambda = 0.36 \quad F = 273.93 \quad p < 0.01$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** $^k\chi(G)$: molecular or group electro-negativities; $^kMR(G)$: refractivities; $^k\alpha(G)$: polarizabilities; $\log^kP$: logarithms of water/*n*-octanol partition coefficients; *G*: atoms included in a specific group; i-MAO-A: MAO-A inhibitory activity score; *W*: Wilk's λ statistic; *F*: the Fisher ratio; *p*: the *p*-level.
Reference	A QSAR Model for in Silico Screening of MAO-A Inhibitors. Prediction, Synthesis, and Biological Assay of Novel Coumarins. *J. Med. Chem.* 2006, 49, 1149-1156

Target	Human

Species	
Chemical Type	Indoles
Mode of Action	Inhibitor
QSAR Model 1	$\text{i-MAO-A} = -1.32\chi_1(\text{C}_{\text{sat}}) - 2.56\chi_2(\text{Het}) + 0.46\alpha_0(\text{Het}) + 1.69\alpha_1(\text{Het}) + 1.16\text{MR}_1 + 1.21 + 7.12\text{MR}_2(\text{C}_{\text{unsat}}) - 1.71\text{MR}_0(\text{Het}) - 2.95 \cdot \log P_0 - 5.6 \cdot \log P_2(\text{C}_{\text{unsat}})$ $\lambda = 0.36 \quad F = 273.93 \quad p < 0.01$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** ${}^k\chi(G)$: molecular or group electro-negativities; ${}^kMR(G)$: refractivities; ${}^k\alpha(G)$: polarizabilities; $\log {}^kP$: logarithms of water/*n*-octanol partition coefficients; *G*: atoms included in a specific group; i-MAO-A: MAO-A inhibitory activity score; *W*: Wilk's λ statistic; *F*: the Fisher ratio; *p*: the *p*-level.
Reference	A QSAR Model for in Silico Screening of MAO-A Inhibitors. Prediction, Synthesis, and Biological Assay of Novel Coumarins. *J. Med. Chem.* 2006, 49, 1149-1156

Target Species	Human
Chemical Type	Coumarins
Mode of Action	Inhibitor
QSAR Model 1	$\text{i-MAO-A} = -1.32\chi_1(\text{C}_{\text{sat}}) - 2.56\chi_2(\text{Het}) + 0.46\alpha_0(\text{Het}) + 1.69\alpha_1(\text{Het}) + 1.16\text{MR}_1 + 1.21 + 7.12\text{MR}_2(\text{C}_{\text{unsat}}) - 1.71\text{MR}_0(\text{Het}) - 2.95 \cdot \log P_0 - 5.6 \cdot \log P_2(\text{C}_{\text{unsat}})$ $\lambda = 0.36 \quad F = 273.93 \quad p < 0.01$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** ${}^k\chi(G)$: molecular or group electro-negativities; ${}^kMR(G)$: refractivities; ${}^k\alpha(G)$: polarizabilities; $\log {}^kP$: logarithms of water/*n*-octanol partition coefficients; *G*: atoms included in a specific group; i-MAO-A:

	MAO-A inhibitory activity score; *W*: Wilk's λ statistic; *F*: the Fisher ratio; *p*: the *p*-level.
Reference	A QSAR Model for in Silico Screening of MAO-A Inhibitors. Prediction, Synthesis, and Biological Assay of Novel Coumarins. *J. Med. Chem.* 2006, 49, 1149-1156

Target Species	Human
Chemical Type	Thioxanthenes
Mode of Action	Inhibitor
QSAR Model 1	$\text{i-MAO-A} = -1.32\chi_1(C_{sat}) - 2.56\chi_2(\text{Het}) + 0.46\alpha_0(\text{Het}) + 1.69\alpha_1(\text{Het}) + 1.16MR_1 + 1.21$ $+ 7.12MR_2(C_{unsat}) - 1.71MR_0(\text{Het}) - 2.95 \cdot \log P_0 - 5.6 \cdot \log P_2(C_{unsat})$ $\lambda = 0.36 \quad F = 273.93 \quad p < 0.01$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** ${}^k\chi(G)$: molecular or group electro-negativities; ${}^kMR(G)$: refractivities; ${}^k\alpha(G)$: polarizabilities; $\log {}^kP$: logarithms of water/*n*-octanol partition coefficients; *G*: atoms included in a specific group; i-MAO-A: MAO-A inhibitory activity score; *W*: Wilk's λ statistic; *F*: the Fisher ratio; *p*: the *p*-level.
Reference	A QSAR Model for in Silico Screening of MAO-A Inhibitors. Prediction, Synthesis, and Biological Assay of Novel Coumarins. *J. Med. Chem.* 2006, 49, 1149-1156

Target Species	Human
Chemical Type	Oxadiazolidone (toloxatone analogues)
Mode of Action	Inhibitor

QSAR Model 1	$\text{i-MAO-A} = -1.32\chi_1(C_{sat}) - 2.56\chi_2(\text{Het}) + 0.46\alpha_0(\text{Het}) + 1.69\alpha_1(\text{Het}) + 1.16MR_1 + 1.21$ $+ 7.12MR_2(C_{unsat}) - 1.71MR_0(\text{Het}) - 2.95 \cdot \log P_0 - 5.6 \cdot \log P_2(C_{unsat})$ $\lambda = 0.36 \quad F = 273.93 \quad p < 0.01$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** $^k\chi(G)$: molecular or group electro-negativities; $^kMR(G)$: refractivities; $^k\alpha(G)$: polarizabilities; $\log^kP$: logarithms of water/*n*-octanol partition coefficients; *G*: atoms included in a specific group; i-MAO-A: MAO-A inhibitory activity score; *W*: Wilk's λ statistic; *F*: the Fisher ratio; *p*: the *p*-level.
Reference	A QSAR Model for in Silico Screening of MAO-A Inhibitors. Prediction, Synthesis, and Biological Assay of Novel Coumarins. *J. Med. Chem.* 2006, 49, 1149-1156

Target Species	Human
Chemical Type	Diazoheterocyclic derivatives
Mode of Action	Inhibitor
QSAR Model 1	$\text{i-MAO-A} = -1.32\chi_1(C_{sat}) - 2.56\chi_2(\text{Het}) + 0.46\alpha_0(\text{Het}) + 1.69\alpha_1(\text{Het}) + 1.16MR_1 + 1.21$ $+ 7.12MR_2(C_{unsat}) - 1.71MR_0(\text{Het}) - 2.95 \cdot \log P_0 - 5.6 \cdot \log P_2(C_{unsat})$ $\lambda = 0.36 \quad F = 273.93 \quad p < 0.01$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** $^k\chi(G)$: molecular or group electro-negativities; $^kMR(G)$: refractivities; $^k\alpha(G)$: polarizabilities; $\log^kP$: logarithms of water/*n*-octanol partition coefficients; *G*: atoms included in a specific group; i-MAO-A: MAO-A inhibitory activity score; *W*: Wilk's λ statistic; *F*: the Fisher ratio; *p*: the *p*-level.
Reference	A QSAR Model for in Silico Screening of MAO-A Inhibitors. Prediction, Synthesis, and Biological Assay of Novel Coumarins. *J. Med. Chem.* 2006, 49, 1149-1156