

Reprogramming MAO-A-Driven Oxidative Stress: Computational Discovery of Neuroprotective Leads for Diabetic Neuropathy

Table S1: Scoring parameters of generated pharmacophore hypotheses and selection of the optimal AAHRR model.

Row	ID	Survival	-Survival	Post-hoc	Site	Vector	Volume	# Matches	Energy	Activity	Inactive	Cluster Number	Cluster Size
1	AAHHR.59	4.271	1.538	3.807	1.00	1.000	0.809	5	0.000	5.874	2.733	2	1
2	AAHHR.37	4.270	1.538	3.806	1.00	1.000	0.809	5	0.000	5.874	2.732	1	2
3	AAHHR.47	4.270	1.538	3.806	1.00	1.000	0.809	5	0.000	5.874	2.732	1	2
4	AAHHR.41	4.169	2.061	3.838	1.00	0.999	0.840	4	0.080	5.783	2.107	29	1
5	AAHHR.17	4.168	2.444	3.837	1.00	0.999	0.840	4	0.080	5.783	1.724	3	2
6	AAHHR.24	4.168	2.444	3.837	1.00	0.999	0.840	4	0.080	5.783	1.724	3	2
7	AAHHR.63	4.168	2.008	3.837	1.00	0.999	0.840	4	0.080	5.783	2.159	30	1
8	AAHHR.39	4.167	2.027	3.836	1.00	0.999	0.840	4	0.080	5.783	2.140	31	1
9	AAHHR.70	4.167	2.023	3.836	1.00	1.000	0.840	4	0.080	5.783	2.144	4	2
10	AAHHR.69	4.167	2.023	3.836	1.00	0.999	0.840	4	0.080	5.783	2.144	4	2
11	AAHHR.1	4.166	1.855	3.836	1.00	0.999	0.839	4	0.080	5.783	2.311	32	1
12	AAHHR.7	4.165	1.855	3.834	1.00	0.999	0.839	4	0.080	5.783	2.309	33	1

Supplementary Table 2. Best 1000 ligands screened for MAOA protein interaction using pharmacophore hypothesis

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ZINC05613217	ZINC12550279	ZINC37639989	ZINC07695851	ZINC04026787
ZINC09601596	ZINC09421529	ZINC37640081	ZINC38590883	ZINC13643595
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Table S3: Docking scores of 591 compounds interacting with the protein, G-score < -4 kcal/mol

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ZINC02123682	-7.54	ZINC08893796	-4.91	ZINC11758257	-4.37
ZINC11758317	-7.51	ZINC10364454	-4.9	ZINC38590851-2	-4.36
ZINC02123667	-7.5	ZINC14668899	-4.89	ZINC37640000	-4.36
ZINC48876098-3	-7.41	ZINC08901574-2	-4.89	ZINC72260171	-4.35
ZINC17271461-2	-7.12	ZINC22239971	-4.89	ZINC02687531	-4.35
ZINC80449468	-6.99	ZINC72380208-4	-4.89	ZINC45530043-3	-4.35
ZINC80449468-2	-6.77	ZINC06760443-2	-4.89	ZINC10003280-2	-4.34
ZINC10364442	-6.72	ZINC24780460	-4.89	ZINC78031815-2	-4.33
ZINC02123590	-6.64	ZINC11758277	-4.88	ZINC02956972	-4.33
ZINC04084916	-6.58	ZINC10332407	-4.86	ZINC11758319	-4.33
ZINC09087286-2	-6.52	ZINC10248454	-4.86	ZINC32833050	-4.33
ZINC07319822-2	-6.45	ZINC08879606-2	-4.86	ZINC11758264	-4.33
ZINC02957032	-6.42	ZINC48876094-2	-4.85	ZINC10248452-2	-4.32
ZINC34602317	-6.39	ZINC08232978	-4.85	ZINC72260180	-4.32
ZINC00664889	-6.39	ZINC01110235	-4.85	ZINC78031818-3	-4.32
ZINC11458823	-6.27	ZINC06589269-2	-4.85	ZINC10332455-2	-4.32
ZINC48876098	-6.26	ZINC37640081	-4.84	ZINC01258128-3	-4.32
ZINC02956922	-6.2	ZINC06607592	-4.84	ZINC34729393	-4.32
ZINC17271466	-6.18	ZINC72260235	-4.83	ZINC06291892-2	-4.32
ZINC15463133	-6.16	ZINC04348995	-4.83	ZINC02334884	-4.31
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