

The discovery of monoamine oxidase inhibitors: Virtual screening and *in vitro* inhibition potencies

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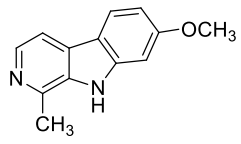
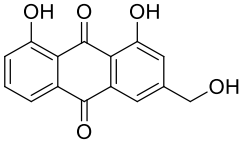
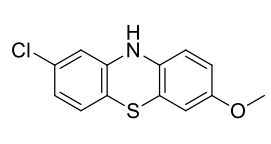
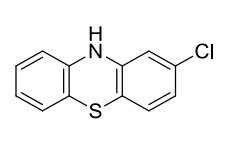
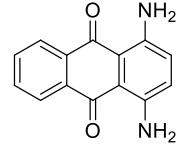
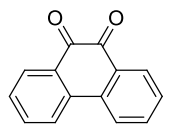
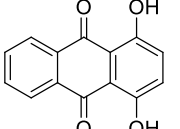
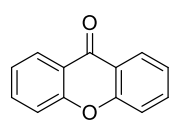
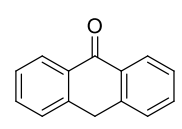
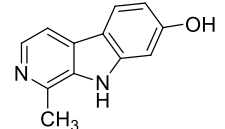
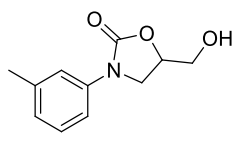
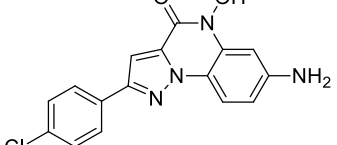
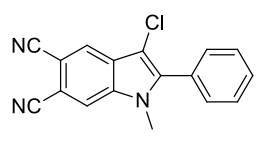
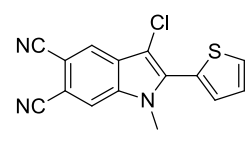
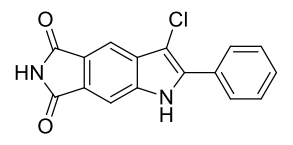
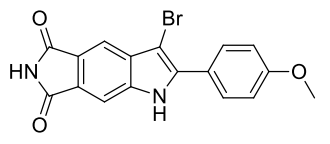
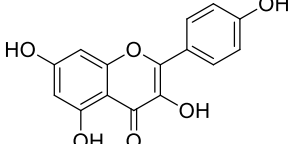
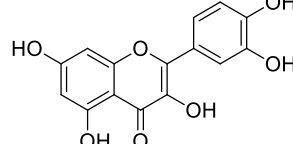
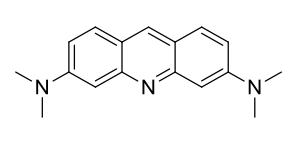
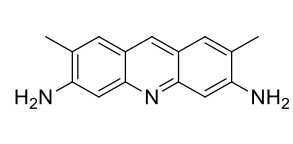
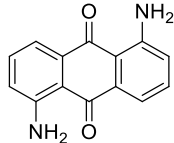
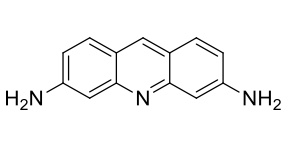
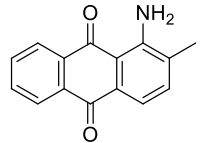
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Table S1 The 23 known inhibitors of MAO-A and 24 known MAO-B inhibitors that were selected from the literature to determine EF^{10%} and ROC-AUC values

MAO-A Inhibitors				
 MAO-A: IC₅₀ = 0.0041 μM MAO-B: IC₅₀ = NI (Myburg <i>et al.</i>, 2022)	 MAO-A: IC₅₀ = 1.77 μM MAO-B: IC₅₀ = 21.9 μM (Lefin <i>et al.</i>, 2022)	 MAO-A: IC₅₀ = 0.576 μM MAO-B: IC₅₀ = 1.34 μM (Lefin <i>et al.</i>, 2022)	 MAO-A: IC₅₀ = 1.22 μM MAO-B: IC₅₀ = NI (Lefin <i>et al.</i>, 2022)	 MAO-A: IC₅₀ = 1.06 μM MAO-B: IC₅₀ = NI (Lefin <i>et al.</i>, 2022)
 MAO-A: IC₅₀ = 1.92 μM MAO-B: IC₅₀ = NI (Lefin <i>et al.</i>, 2022)	 MAO-A: IC₅₀ = 0.065 μM MAO-B: IC₅₀ = 110 μM (Lefin <i>et al.</i>, 2022)	 MAO-A: IC₅₀ = 0.623 μM MAO-B: IC₅₀ = NI (Lefin <i>et al.</i>, 2022)	 MAO-A: IC₅₀ = 1.89 μM MAO-B: IC₅₀ = NI (Lefin <i>et al.</i>, 2022)	 MAO-A: IC₅₀ = 0.211 μM MAO-B: IC₅₀ = NI (Myburg <i>et al.</i>, 2022)
 MAO-A: IC₅₀ = 1.67 μM MAO-B: IC₅₀ = NI (Stear <i>et al.</i>, 2024)	 MAO-A: IC₅₀ = 0.345 μM MAO-B: IC₅₀ = NI (Panova <i>et al.</i>, 2021)	 MAO-A: IC₅₀ = 0.142 μM MAO-B: IC₅₀ = NI (Chirkova <i>et al.</i>, 2015)	 MAO-A: IC₅₀ = 0.035 μM MAO-B: IC₅₀ = NI (Chirkova <i>et al.</i>, 2015)	 MAO-A: IC₅₀ = 0.250 μM MAO-B: IC₅₀ = NI (Chirkova <i>et al.</i>, 2016)
 MAO-A: IC₅₀ = 0.011 μM MAO-B: IC₅₀ = 6.64 μM (Chirkova <i>et al.</i>, 2019)	 MAO-A: IC₅₀ = 0.525 μM MAO-B: IC₅₀ = NI (Gidaro <i>et al.</i>, 2016)	 MAO-A: IC₅₀ = 3.98 μM MAO-B: IC₅₀ = NI (Gidaro <i>et al.</i>, 2016)	 MAO-A: IC₅₀ = 0.017 μM MAO-B: IC₅₀ = 12.4 μM (De Beer <i>et al.</i>, 2020)	 MAO-A: IC₅₀ = 0.350 μM MAO-B: IC₅₀ = 11.9 μM (De Beer <i>et al.</i>, 2020)
 MAO-A: IC₅₀ = 0.585 μM MAO-B: IC₅₀ = NI (De Beer <i>et al.</i>, 2020)	 MAO-A: IC₅₀ = 0.507 μM MAO-B: IC₅₀ = 32.5 μM (De Beer <i>et al.</i>, 2020)	 MAO-A: IC₅₀ = 0.450 μM MAO-B: IC₅₀ = NI (De Beer <i>et al.</i>, 2020)		

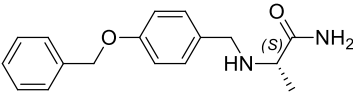
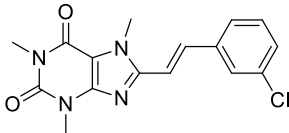
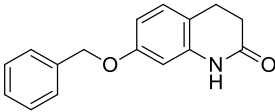
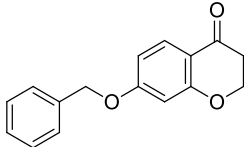
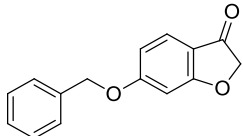
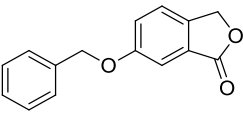
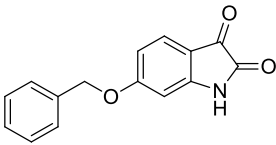
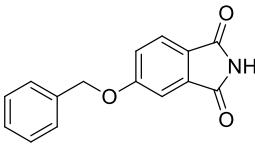
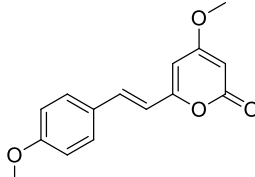
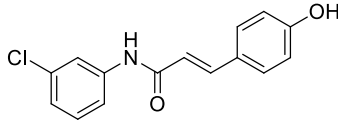
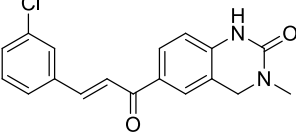
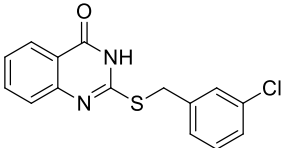
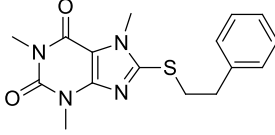
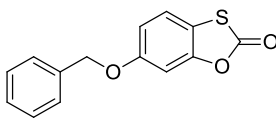
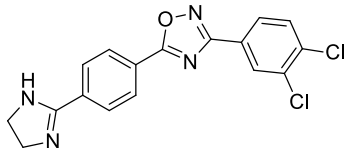
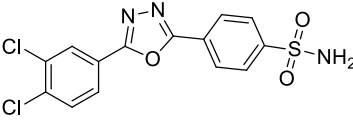
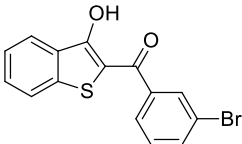
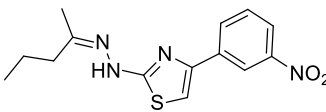
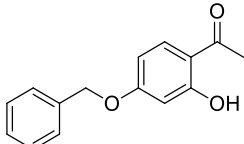
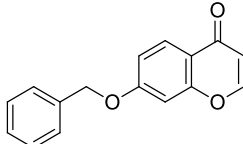
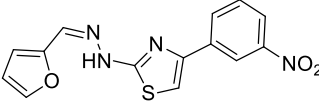
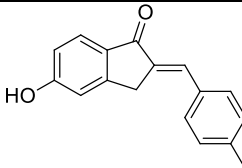
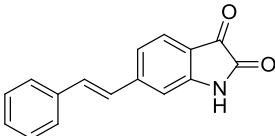
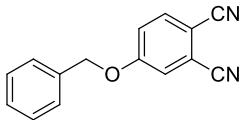
MAO-B Inhibitors				
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 MAO-A: IC₅₀ = 1.19 μM MAO-B: IC₅₀ = 0.024 μM (Strydom et al., 2013)	 MAO-A: IC₅₀ = 72.4 μM MAO-B: IC₅₀ = 0.138 μM (Manley-King et al., 2011a)	 MAO-A: IC₅₀ = 4.17 μM MAO-B: IC₅₀ = 0.043 μM (Manley-King et al., 2011b)	 MAO-A: IC₅₀ = 1.29 μM MAO-B: IC₅₀ = 0.085 μM (Prinsloo et al., 2019)	 MAO-A: IC₅₀ = 47.3 μM MAO-B: IC₅₀ = 0.032 μM (Legoabe et al., 2011)
 MAO-A: IC₅₀ = 44.2 μM MAO-B: IC₅₀ = 0.350 μM (Marais et al., 2020)	 MAO-A: IC₅₀ = NI MAO-B: IC₅₀ = 0.230 μM (Qhobosheane et al., 2018)	 MAO-A: IC₅₀ = 18.7 μM MAO-B: IC₅₀ = 0.271 μM (Mostert et al., 2012)	 MAO-A: IC₅₀ = 5.41 μM MAO-B: IC₅₀ = 0.051 μM (Mostert et al., 2016)	 MAO-A: IC₅₀ = 1.11 μM MAO-B: IC₅₀ = 0.012 μM (Shetnev et al., 2019a)
 MAO-A: IC₅₀ = 46.2 μM MAO-B: IC₅₀ = 0.0027 μM (Shetnev et al., 2019b)	 MAO-A: IC₅₀ = 63.2 μM MAO-B: IC₅₀ = 0.35 μM (Guglielmi et al., 2019)	 MAO-A: IC₅₀ = 38.0 μM MAO-B: IC₅₀ = 0.055 μM (Carradori et al., 2018)	 MAO-A: IC₅₀ = 8.36 μM MAO-B: IC₅₀ = 0.007 μM (Legoabe et al., 2015)	 MAO-A: IC₅₀ = 5.33 μM MAO-B: IC₅₀ = 0.085 μM (Legoabe et al., 2012)
 MAO-A: IC₅₀ = 8.98 μM MAO-B: IC₅₀ = 0.095 μM (Secchi et al., 2019)	 MAO-A: IC₅₀ = 3.22 μM MAO-B: IC₅₀ = 0.0052 μM (Nel et al., 2016)	 MAO-A: IC₅₀ = 22 μM MAO-B: IC₅₀ = 0.56 μM (Van der Walt et al., 2009)	 MAO-A: IC₅₀ = 1.79 μM MAO-B: IC₅₀ = 0.0079 μM (Manley-King et al., 2012)	

Table S2 RMSD as validation metric for redocking of co-crystallised ligands into the active site of MAO-B with *CDOcker* and scoring the resulting poses with selected scoring functions

PDB Code	Best pose (rank)	Scoring functions										
		Native - 1st ^c	LigScore 1 - 1st (rank)	LigScore 2 - 1st (rank)	PLP 1 - 1st (rank)	PLP 2 - 1st (rank)	Jain - 1st (rank)	PMF - 1st (rank)	PMF 4 - 1st (rank)	Ludi 1 - 1st (rank)	Ludi 2 - 1st (rank)	Ludi 3 - 1st (rank)
2V5Z	0.4 (1)	0.4	0.4 (1)	0.4 (1)	0.4 (1)	0.4 (1)	0.4 (1)	1.6 (7)	1.6 (6)	0.4 (1)	0.4 (1)	0.4 (1)
1OJ9	0.7 (8)	1.0	0.8 (2)	0.8 (7)	1.0 (1)	1.0 (1)	0.8 (7)	0.8 (6)	1.0 (5)	0.8 (2)	0.8 (6)	0.8 (6)
1OJA	1.7 (8)	1.9	2.0 (10)	2.0 (10)	1.8 (5)	1.8 (5)	1.8 (6)	2.4 (9)	2.4 (9)	1.9 (1)	2.0 (10)	1.9 (1)
1OJD	2.2 (8)	8.7	2.6 (3)	2.6 (3)	2.6 (3)	9.2 (6)	2.2 (9)	2.6 (2)	2.6 (3)	2.6 (2)	2.3 (7)	2.2 (9)
2BK3	1.6 (8)	2.0	8.2 (10)	2.3 (3)	2.4 (7)	2.4 (7)	1.6 (8)	2.3 (3)	1.6 (8)	2.3 (3)	2.3 (3)	2.3 (3)
2V60	0.8 (7)	0.8	0.8 (9)	0.8 (9)	0.8 (2)	0.8 (10)	0.8 (1)	0.8 (9)	0.8 (10)	0.8 (10)	0.8 (2)	0.8 (1)
2V61	3.0 (4)	3.0	3.0 (3)	8.3 (9)	8.3 (9)	3.0 (3)	3.2 (8)	3.0 (7)	3.0 (3)	3.0 (6)	3.0 (5)	8.7 (10)
3PO7	1.5 (2)	2.7	2.7 (1)	5.2 (9)	1.5 (2)	1.5 (2)	8.0 (3)	5.6 (6)	1.5 (2)	2.7 (1)	2.7 (1)	2.7 (1)
4A79	3.0 (4)	3.0	3.5 (6)	3.4 (5)	3.0 (3)	3.0 (1)	3.5 (7)	3.0 (3)	3.0 (2)	3.5 (9)	3.4 (5)	3.3 (10)
4A7A	1.2 (6)	1.2	1.2 (1)	1.2 (6)	1.4 (4)	1.4 (4)	1.2 (2)	1.3 (8)	1.3 (5)	1.2 (7)	1.2 (3)	1.2 (2)
4CRT	3.2 (5)	8.0	8.0 (4)	8.2 (8)	3.2 (6)	3.2 (6)	3.4 (7)	3.2 (6)	3.2 (6)	3.2 (6)	8.0 (3)	8.0 (3)
5MRL	3.0 (3)	3.2	3.2 (1)	8.6 (7)	3.2 (1)	3.2 (1)	8.5 (5)	3.1 (6)	3.1 (6)	8.6 (7)	3.1 (6)	3.1 (6)
6FVZ	0.7 (7)	0.8	0.8 (6)	0.8 (6)	0.8 (6)	1.7 (10)	0.7 (7)	0.9 (4)	0.8 (6)	0.8 (3)	0.8 (6)	1.7 (10)
6FW0	2.1 (2)	2.2	2.2 (1)	2.2 (1)	7.9 (7)	7.9 (6)	2.2 (1)	2.1 (2)	7.9 (10)	2.1 (2)	7.9 (9)	7.9 (5)
6FWC	0.7 (6)	0.8	0.8 (9)	0.7 (4)	0.7 (6)	0.7 (5)	0.8 (7)	0.8 (1)	0.8 (2)	0.7 (4)	0.8 (7)	0.7 (4)
6RKB	2.2 (6)	2.4	2.4 (1)	2.4 (1)	2.4 (10)	2.4 (10)	2.4 (3)	2.2 (6)	2.2 (6)	2.6 (8)	2.2 (6)	2.4 (3)
6RKP	1.8 (10)	1.9	2.0 (9)	2.0 (9)	2.0 (9)	2.0 (7)	1.9 (3)	1.8 (5)	2.0 (9)	1.8 (10)	2.0 (7)	2.0 (7)
6RLE	1.7 (4)	2.4	2.1 (8)	1.7 (4)	2.4 (2)	2.2 (5)	2.2 (3)	2.1 (8)	2.1 (8)	2.1 (6)	2.2 (7)	2.1 (6)
6YT2	4.9 (9)	4.9	4.9 (2)	4.9 (10)	4.9 (1)	4.9 (1)	4.9 (2)	4.9 (10)	4.9 (9)	4.9 (1)	4.9 (2)	4.9 (2)
7B0V	0.5 (8)	8.5	8.5 (2)	8.5 (1)	8.4 (6)	8.5 (1)	8.5 (3)	0.6 (10)	8.4 (6)	8.4 (4)	8.4 (4)	0.5 (7)
7B0Z	0.7 (4)	0.7	0.7 (4)	0.7 (4)	0.8 (10)	0.7 (4)	0.8 (8)	0.8 (10)	0.7 (4)	0.7 (2)	0.8 (10)	0.7 (2)
Total ^a	13	9	9	10	10	9	10	9	10	9	8	9
Ave. RMSD	1.8	2.9	2.9	3.2	2.9	3.0	2.9	2.2	2.6	2.6	2.9	2.8
Success rate ^b	62	43	43	48	48	43	48	43	48	43	38	43

^a Number of ligands with an RMSD value < 2 Å^b Percentage of ligands with and RMSD value < 2 Å^c Native scoring function for CDOCKER – CDOCKER Energy

Table S3 RMSD as validation metric for redocking of co-crystallised ligands into the active site of MAO-B with *LibDock* and scoring the resulting poses with selected scoring functions

PDB Code	Best pose (rank)	Scoring functions										
		Native - 1st ^c	LigScore 1 - 1st (rank)	LigScore 2 - 1st (rank)	PLP 1 - 1st (rank)	PLP 2 - 1st (rank)	Jain - 1st (rank)	PMF - 1st (rank)	PMF 4 - 1st (rank)	Ludi 1 - 1st (rank)	Ludi 2 - 1st (rank)	Ludi 3 - 1st (rank)
2V5Z	1.0 (60)	2.0	1.2 (12)	1.2 (49)	1.4 (6)	9.5 (20)	9.2 (82)	2.3 (33)	2.3 (33)	1.7 (19)	1.2 (12)	9.2 (40)
1OJ9	1.2 (64)	3.1	2.6 (21)	2.6 (21)	2.6 (11)	2.3 (10)	2.0 (87)	1.2 (64)	1.5 (85)	1.7 (60)	2.1 (84)	3.0 (2)
1OJA	1.2 (6)	2.0	2.0 (1)	2.0 (1)	2.0 (1)	2.5 (4)	10.0 (22)	3.9 (2)	3.9 (2)	3.2 (3)	3.2 (3)	3.2 (3)
1OJD	1.9 (10)	1.9	2.6 (36)	9.6 (12)	1.9 (1)	9.4 (6)	3.0 (37)	9.6 (20)	2.7 (78)	2.3 (30)	3.0 (37)	2.1 (3)
2BK3	1.5 (17)	3.0	2.2 (6)	8.5 (21)	2.2 (6)	8.9 (4)	2.5 (7)	2.2 (6)	1.5 (17)	2.4 (43)	2.4 (43)	2.4 (43)
2V60	1.0 (11)	1.9	1.0 (11)	1.0 (11)	2.2 (8)	2.2 (5)	2.0 (53)	1.0 (11)	2.2 (5)	1.4 (45)	3.1 (25)	3.0 (73)
2V61	1.0 (16)	2.2	3.2 (14)	8.2 (25)	8.2 (25)	8.2 (25)	3.4 (47)	1.0 (16)	3.5 (9)	3.5 (20)	3.2 (50)	3.9 (3)
3PO7	1.5 (26)	1.8	2.1 (21)	2.1 (21)	4.2 (3)	4.3 (7)	7.1 (69)	4.3 (34)	1.7 (17)	4.2 (3)	4.2 (3)	4.3 (34)
4A79	1.7 (3)	4.0	4.0 (1)	4.0 (1)	4.0 (2)	3.2 (6)	9.7 (10)	4.0 (2)	4.0 (1)	3.2 (6)	3.2 (6)	4.0 (1)
4A7A	1.4 (45)	7.8	2.0 (25)	2.0 (25)	7.8 (1)	1.8 (26)	2.0 (44)	8.5 (63)	1.6 (19)	2.0 (25)	2.0 (25)	3.1 (88)
4CRT	2.6 (19)	2.8	8.0 (22)	8.0 (22)	7.9 (4)	7.9 (4)	8.3 (20)	3.7 (57)	8.0 (8)	2.8 (2)	8.4 (41)	4.2 (31)
5MRL	2.0 (41)	2.4	3.0 (26)	2.7 (34)	2.4 (1)	2.4 (3)	3.0 (26)	3.0 (21)	3.0 (21)	5.0 (80)	2.8 (77)	5.2 (81)
6FVZ	1.0 (1)	1.0	2.8 (17)	1.7 (4)	8.1 (2)	8.1 (2)	2.6 (21)	1.9 (10)	2.0 (22)	1.7 (6)	2.4 (8)	2.4 (8)
6FW0	0.9 (54)	1.0	1.4 (9)	1.0 (1)	1.0 (1)	2.5 (15)	7.7 (16)	1.4 (9)	1.0 (1)	7.7 (27)	7.7 (43)	2.1 (5)
6FWC	0.8 (1)	0.8	2.0 (33)	0.8 (1)	0.8 (1)	7.4 (3)	3.4 (58)	1.9 (14)	0.8 (1)	3.4 (58)	3.4 (58)	2.4 (18)
6RKB	2.5 (31)	3.1	3.2 (12)	3.2 (12)	8.8 (8)	8.8 (9)	2.6 (41)	2.6 (26)	2.6 (32)	8.6 (49)	8.6 (83)	8.5 (67)
6RKP	1.7 (84)	2.2	9.5 (10)	9.5 (10)	9.5 (10)	9.5 (10)	9.4 (7)	2.5 (13)	9.6 (2)	2.0 (74)	2.0 (92)	9.6 (23)
6RLE	1.7 (98)	2.6	2.3 (3)	2.3 (3)	9.0 (6)	9.0 (6)	3.0 (76)	2.6 (9)	2.6 (9)	2.8 (27)	9.5 (14)	2.6 (1)
6YT2	1.6 (2)	5.0	4.8 (5)	4.7 (3)	1.6 (2)	1.6 (2)	7.4 (59)	2.3 (6)	5.2 (34)	5.0 (1)	7.4 (59)	2.3 (6)
7B0V	0.6 (23)	8.5	8.5 (7)	1.1 (34)	8.5 (2)	7.8 (20)	7.8 (20)	0.9 (57)	8.5 (7)	7.8 (20)	7.8 (20)	7.8 (20)
7B0Z	0.8 (23)	1.1	1.0 (15)	1.0 (24)	8.3 (38)	1.1 (11)	1.0 (18)	8.3 (34)	1.0 (18)	8.3 (41)	8.3 (31)	8.5 (49)
Total ^a	19	8	6	8	5	3	1	7	8	6	2	0
Ave. RMSD	1.4	2.9	3.3	3.7	4.9	5.6	5.1	3.3	3.3	3.8	4.6	4.5
Success rate ^b	90	38	29	38	24	14	5	33	38	29	10	0

^a Number of ligands with an RMSD value < 2 Å^b Percentage of ligands with and RMSD value < 2 Å^c Native scoring function for LibDock – LibDock Score

Table S4 RMSD as validation metric for redocking of co-crystallised ligands into the active site of MAO-B with *LigandFit* and scoring the resulting poses with selected scoring functions

PDB Code	Best pose (rank)	Scoring functions										
		Native - 1st ^c	LigScore 1 - 1st (rank)	LigScore 2 - 1st (rank)	PLP 1 - 1st (rank)	PLP 2 - 1st (rank)	Jain - 1st (rank)	PMF - 1st (rank)	PMF 4 - 1st (rank)	Ludi 1 - 1st (rank)	Ludi 2 - 1st (rank)	Ludi 3 - 1st (rank)
2V5Z	1.3 (1)	1.3	1.3 (5)	1.3 (4)	9.2 (8)	9.2 (8)	1.3 (5)	1.3 (1)	1.3 (1)	1.3 (5)	1.3 (5)	9.2 (8)
1OJ9	0.6 (9)	0.7	0.9 (5)	0.9 (5)	0.9 (5)	0.9 (5)	0.9 (7)	0.7 (2)	0.8 (6)	0.7 (1)	0.9 (7)	0.7 (2)
1OJA ^d	—	—	—	—	—	—	—	—	—	—	—	—
1OJD	2.0 (1)	2.0	2.0 (1)	2.6 (10)	2.3 (7)	2.0 (2)	2.6 (8)	2.4 (5)	2.0 (1)	2.0 (2)	2.6 (8)	2.6 (8)
2BK3	8.3 (9)	8.7	8.7 (1)	8.7 (1)	8.7 (1)	8.7 (1)	8.5 (3)	8.6 (2)	8.6 (2)	8.4 (7)	8.4 (7)	8.4 (8)
2V60	0.9 (9)	2.2	2.2 (1)	2.2 (1)	2.2 (1)	2.2 (1)	2.1 (10)	1.0 (3)	0.9 (9)	1.9 (4)	2.2 (1)	2.2 (1)
2V61	3.1 (10)	8.1	3.2 (3)	8.1 (1)	3.1 (10)	3.3 (5)	8.4 (6)	3.1 (10)	3.1 (10)	3.3 (5)	3.1 (10)	8.1 (8)
3PO7 ^d	—	—	—	—	—	—	—	—	—	—	—	—
4A79	3.3 (6)	3.6	3.6 (1)	3.6 (1)	3.4 (4)	3.4 (4)	3.6 (1)	3.6 (1)	3.6 (1)	3.5 (5)	3.4 (7)	3.6 (1)
4A7A	0.9 (9)	2.1	2.1 (2)	2.0 (3)	0.9 (9)	2.0 (4)	2.0 (4)	0.9 (6)	2.1 (1)	2.1 (1)	2.1 (2)	2.2 (7)
4CRT	7.9 (8)	8.0	8.0 (2)	8.0 (1)	8.0 (1)	8.0 (2)	8.0 (10)	8.0 (9)	7.9 (8)	8.0 (1)	8.1 (3)	8.1 (3)
5MRL ^d	—	—	—	—	—	—	—	—	—	—	—	—
6FVZ	0.7 (2)	0.7	0.7 (8)	0.7 (6)	0.7 (4)	0.7 (8)	2.0 (9)	0.7 (4)	0.7 (6)	2.0 (9)	2.0 (9)	0.7 (8)
6FW0	0.9 (10)	2.1	0.9 (9)	0.9 (9)	0.9 (9)	0.9 (9)	2.1 (4)	0.9 (9)	2.1 (2)	2.1 (1)	2.1 (1)	0.9 (9)
6FWC	7.5 (1)	7.5	7.5 (2)	7.5 (1)	7.5 (5)	7.5 (8)	7.5 (5)	7.5 (4)	7.5 (4)	7.5 (7)	7.5 (1)	7.5 (4)
6RKB	2.3 (1)	2.3	2.6 (10)	2.6 (10)	2.5 (6)	2.5 (6)	2.5 (4)	2.5 (2)	2.5 (2)	2.5 (2)	2.5 (8)	2.4 (3)
6RKP	1.8 (8)	2.1	9.4 (10)	9.4 (10)	2.3 (4)	2.3 (3)	9.4 (9)	1.8 (8)	9.4 (10)	2.1 (7)	2.1 (6)	2.3 (3)
6RLE	2.1 (3)	2.1	2.1 (1)	2.1 (1)	2.1 (1)	2.1 (2)	2.5 (6)	2.2 (4)	2.2 (4)	2.1 (1)	2.4 (10)	2.4 (10)
6YT2 ^d	—	—	—	—	—	—	—	—	—	—	—	—
7B0V	0.7 (5)	0.8	0.9 (7)	0.9 (7)	0.7 (3)	0.7 (3)	1.0 (9)	0.8 (2)	0.8 (2)	0.8 (2)	0.9 (8)	0.8 (4)
7B0Z	8.0 (6)	8.1	8.1 (2)	8.1 (2)	8.0 (6)	8.0 (6)	8.1 (2)	8.1 (2)	8.1 (5)	8.1 (1)	8.1 (9)	8.1 (9)
Total ^a	9	5	6	5	5	4	4	8	6	5	4	4
Ave. RMSD	2.5	3.0	3.8	4.1	3.7	3.8	4.3	3.2	3.8	3.4	3.5	4.1
Success rate ^b	43	24	29	24	24	19	19	38	29	24	19	19

^a Number of ligands with an RMSD value < 2 Å^b Percentage of ligands with and RMSD value < 2 Å^c Native scoring function for LigandFit – Dock Score^d No poses generated

Table S5 EF^{10%} and ROC-AUC values as validation metrics for identifying 24 known MAO-B inhibitors within the DUD-E and Schrödinger decoy datasets. Docking was carried out with *LigandFit* and the resulting poses were scored with selected scoring functions

	LigandFit		LigandFit	
	DUD-E^b		Schrödinger^c	
	EF^{10%}	ROC-AUC	EF^{10%}	ROC-AUC
Native^a	8.72	0.89	8.72	0.839
LigScore 1	6.64	0.804	4.15	0.646
LigScore 2	8.72	0.897	8.72	0.887
PLP 1	8.30	0.892	1.66	0.684
PLP 2	6.64	0.843	1.66	0.57
Jain	0.83	0.346	0.00	0.239
PMF	8.30	0.847	0.42	0.511
PMF 4	5.40	0.777	2.08	0.563
Ludi 1	2.49	0.61	0.83	0.369
Ludi 2	2.49	0.536	0.42	0.382
Ludi 3	7.89	0.879	2.08	0.59

^a Native scoring function for LigandFit – Dock Score

^b Maximum EF^{10%} = 10.0 (2590 total compounds /24 active compounds)

^c Maximum EF^{10%} = 10.0 (1046 total compounds /24 active compounds)

Table S6 EF^{10%} and ROC-AUC values as validation metrics for identifying 23 known MAO-A inhibitors within the DUD-E and Schrödinger decoy datasets. Docking was carried out with *LigandFit* and the resulting poses were scored with selected scoring functions

	LigandFit		LigandFit	
	DUD-E^b		Schrödinger^c	
	EF^{10%}	ROC-AUC	EF^{10%}	ROC-AUC
Native^a	3.03	0.647	3.47	0.549
LigScore 1	3.46	0.708	3.47	0.57
LigScore 2	3.90	0.682	3.90	0.64
PLP 1	1.73	0.462	1.30	0.296
PLP 2	0.00	0.462	1.73	0.292
Jain	0.43	0.457	1.30	0.359
PMF	1.73	0.579	1.73	0.408
PMF 4	0.00	0.446	1.73	0.382
Ludi 1	1.73	0.559	2.17	0.459
Ludi 2	0.43	0.388	0.87	0.397
Ludi 3	3.03	0.804	2.60	0.567

^a Native scoring function for LigandFit – Dock Score

^b Maximum EF^{10%} = 10.0 (2590 total compounds /23 active compounds)

^c Maximum EF^{10%} = 10.0 (1046 total compounds /23 active compounds)

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