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**Supplementary information**

Lists of compounds used to validate the maximum size of MAO-B active site.

**4-phenyl-R-substituted MPTP derivatives.**

All of them have the same length as MPTP (1) (10.07 Å) and are issued from references 12 and 14

R	kcat/Km
2-Me	1275
2-Et	295
2-n-Pr	86
2-OMe	233
2-Cl	1353
2-i-Pr	53
2-CF <sub>3</sub>	520

R	kcat/Km
2,6-diMe	209
3-Me	650
3-F	900
3-Cl	1132
3-Br	2036
3-OMe	944
3-CF <sub>3</sub>	514

**4-(R-substituted-phenoxy)-N-methyl-1,2,3,6-tetrahydropyridine and 4-(aryloxy)-N-methyl-1,2,3,6-tetrahydropyridine derivatives.**

All of them have the same length as 4-phenoxy derivative 33 (6.60 Å) and are issued from reference 28 and 6

R	kcat/Km
2'-Me	1782
2'-NO <sub>2</sub>	786
2'-OMe	746
2'-Cl	822
2'-Ph	132
3'-Me	1747
3'-NO <sub>2</sub>	1410
3'-OMe	721
3'-Cl	729
3'-Ph	637

R	kcat/Km
4'-Me	2019
4'-NO <sub>2</sub>	191
4'-OMe	746
4'-Cl	1401
4'-Ph	363
4'-n-Bu	1090
4'-t-Bu	395
4-a-Naph	565
4-b-Naph	1214

**4-(R-substituted-benzyl)-N-methyl-1,2,3,6-tetrahydropyridine and 4-(arylmethyl)-N-methyl-1,2,3,6-tetrahydropyridine derivatives.**

All of them have the same length as 4-benzyl derivative **25** (6.72 Å) and are issued from reference <sup>32</sup>

R	kcat/Km
2-F	1440
2-OMe	145
3-Me	603
3-F	2330
4-Me	615

R	kcat/Km
4-F	1140
4-I	1190
-a-Naph	105
-b-Naph	310
-9-Phen	inactive

**4-(R-substituted-phenylethenyl)-N-methyl-1,2,3,6-tetrahydropyridine and 4-(arylethenyl)-N-methyl-1,2,3,6-tetrahydropyridine derivatives.**

All of *cis* isomers have the same length as 4-phenylethenyl derivative **31** (7.96 Å), all of the *trans* isomers have the same length as 4-phenylethenyl derivative **30** (12.16 Å) and are issued from reference <sup>31</sup> and <sup>21</sup>

R ( <i>cis</i> )	kcat/Km
2'-Br	107
2'-OMe	93
3'-Br	1056
4'-Br	890
-a-Naph	49

R ( <i>trans</i> )	kcat/Km
2'-OMe	16
2'-Br	617
2'-Me	< 10%
3'-Br	6
4'-Br	98
4'-F	138
4'-Me	59
4'-N(Me) <sub>2</sub>	67
4'-OMe	53
-a-Naph	21

**N-R<sub>1</sub>-4-R<sub>2</sub>-1,2,3,6-tetrahydropyridine derivatives.**

Data are issued from reference 32, 5, 15, 3, 10, 12

R <sub>1</sub>	R <sub>2</sub>	kcat/Km	Length
Me	methyl-thien-2-yl	3270	8.0
Me	a-naphthylethyl	62	7.8
Me	b-naphthylethyl	76	7.8
Me	ethyl-thien-2-yl	1059	8.4
Me	thien-3-yl	160	8.5
Me	methyl-thien-3-yl	785	8.1
Me	ethyl-thien-3-yl	890	7.8
Me	ethyl	41 %	/ 7.8
n-butyl	phenyl	MPTP	13.5
cPr methyl	phenyl	inactive	12.2
2-ethanol	phenyl	inactive	12.0
		inactive	