Supporting Information

(Supplemental materials may be accessed free of charge online at http://pubs.acs.org)

Characterization of 4-Nitrophenylpropyl-*N*-alkylamine Interactions with Sigma Receptors

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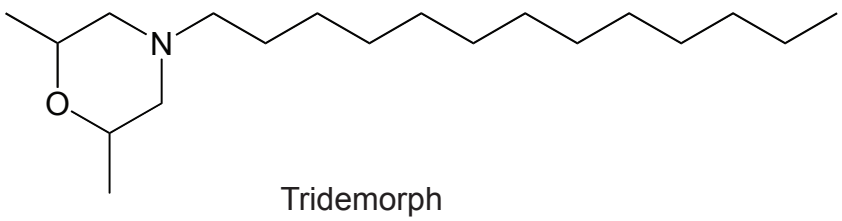
Figure Legend

Figure S-1: Structure of tridemorph

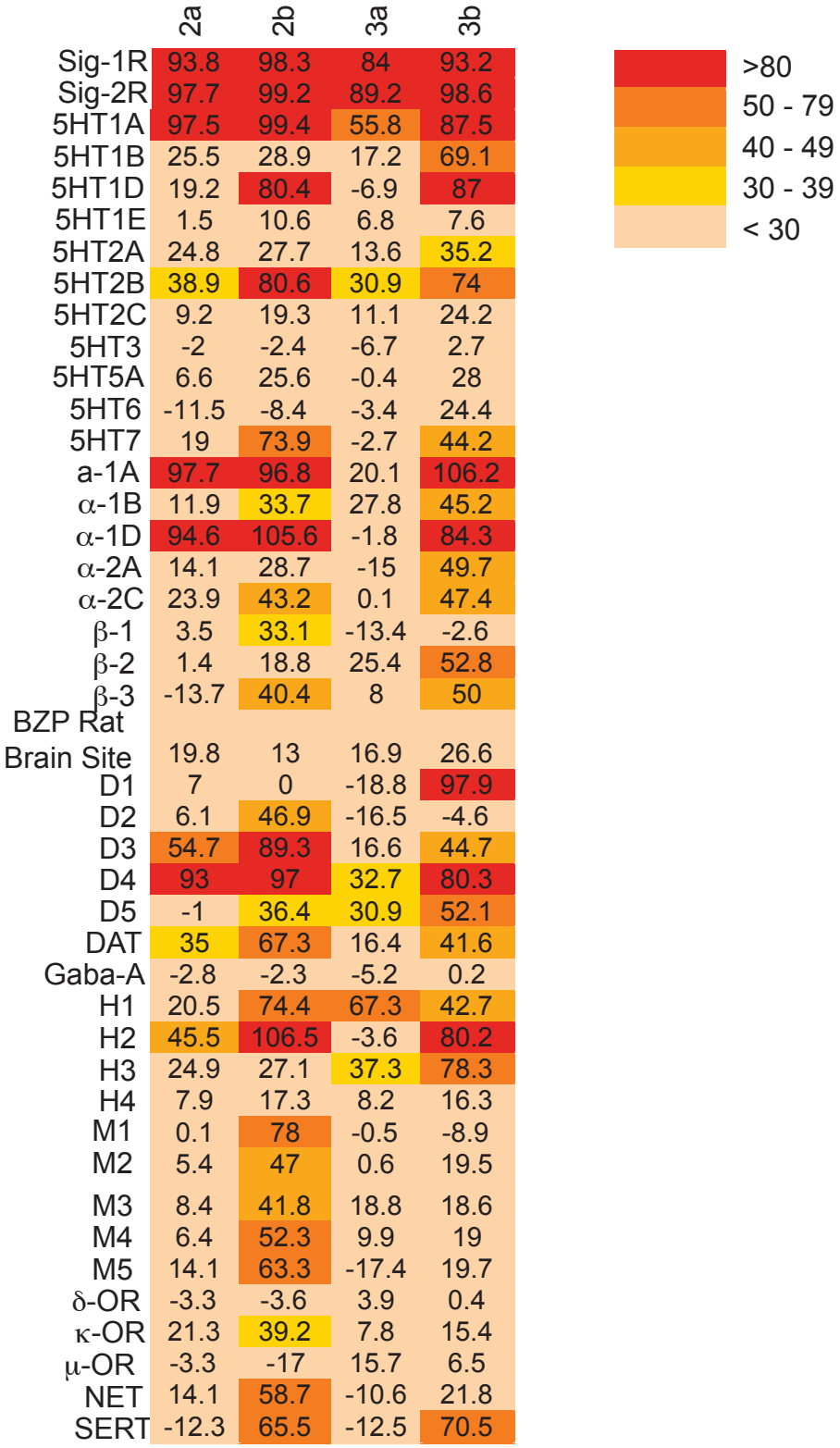
Figure S-2. A heat map of the percent inhibition of PPC7, 4-NPPC7, PPC12, and 4-NPPC12 for a panel of membrane receptors and transporters. Data represent mean % inhibition (n = 4 determinations) at a default concentration of 10 μM for each of the *N*-alkylamine derivatives tested. Significant inhibition is considered at ≥50%. *N*-alkylamine derivatives showing ≥50% inhibition at any of these targets was subsequently tested in competitive displacement secondary assays to determine the actual K_I values utilizing the Cheng-Prusoff equation (see Table 3).

Figure S-1



Tridemorph

Figure S-2


2a
2b
3a
3b
Sig-1R 93.8 98.3 84 93.2
Sig-2R 97.7 99.2 89.2 98.6
5HT1A 97.5 99.4 55.8 87.5
5HT1B 25.5 28.9 17.2 69.1
5HT1D 19.2 80.4 -6.9 87
5HT1E 1.5 10.6 6.8 7.6
5HT2A 24.8 27.7 13.6 35.2
5HT2B 38.9 80.6 30.9 74
5HT2C 9.2 19.3 11.1 24.2
5HT3 -2 -2.4 -6.7 2.7
5HT5A 6.6 25.6 -0.4 28
5HT6 -11.5 -8.4 -3.4 24.4
5HT7 19 73.9 -2.7 44.2
a-1A 97.7 96.8 20.1 106.2
α-1B 11.9 33.7 27.8 45.2
α-1D 94.6 105.6 -1.8 84.3
α-2A 14.1 28.7 -15 49.7
α-2C 23.9 43.2 0.1 47.4
β-1 3.5 33.1 -13.4 -2.6
β-2 1.4 18.8 25.4 52.8
β-3 -13.7 40.4 8 50
BZP Rat Brain Site 19.8 13 16.9 26.6
D1 7 0 -18.8 97.9
D2 6.1 46.9 -16.5 -4.6
D3 54.7 89.3 16.6 44.7
D4 93 97 32.7 80.3
D5 -1 36.4 30.9 52.1
DAT 35 67.3 16.4 41.6
Gaba-A -2.8 -2.3 -5.2 0.2
H1 20.5 74.4 67.3 42.7
H2 45.5 106.5 -3.6 80.2
H3 24.9 27.1 37.3 78.3
H4 7.9 17.3 8.2 16.3
M1 0.1 78 -0.5 -8.9
M2 5.4 47 0.6 19.5
M3 8.4 41.8 18.8 18.6
M4 6.4 52.3 9.9 19
M5 14.1 63.3 -17.4 19.7
δ-OR -3.3 -3.6 3.9 0.4
κ-OR 21.3 39.2 7.8 15.4
μ-OR -3.3 -17 15.7 6.5
NET 14.1 58.7 -10.6 21.8
SERT -12.3 65.5 -12.5 70.5
>80
50 - 79
40 - 49
30 - 39
< 30