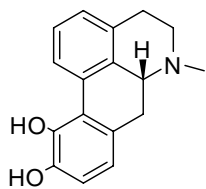
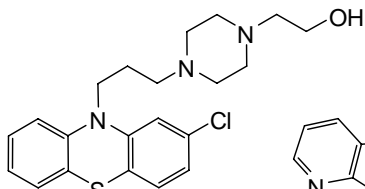


Supplementary Figure 1

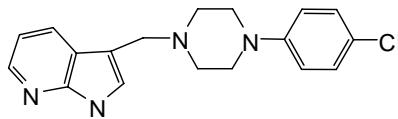
a



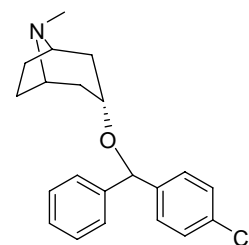
6
Apomorphine
Cluster 84
p-value = 8.86E-30
Target(s): DRD1a,
DRD2, DRD4



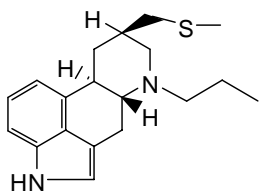
26
Perphenazine
Cluster 130
p-value = 9.30E-29
Target(s): DRD1a,
DRD2, ADRA1a



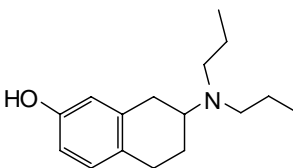
43
L-745,870
Cluster 44
p-value = 8.86E-30
Target(s): DRD4



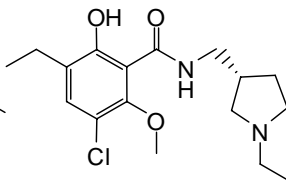
44
4--Chloro-3-alpha-
(diphenylmethoxy) tropane
Cluster 29
p-value = 1.98E-22
Target(s): Reuptake Blocker



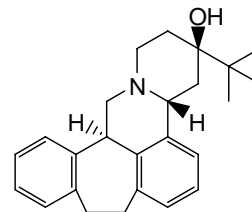
45
Pergolide
Cluster 51
p-value = 3.95E-03
Target(s): DRD1,
DRD2, 5-HT2B



46
(±)-7-Hydroxy-DPAT
Cluster 8
p-value = 6.12E-29
Target(s): DRD2,
DRD3

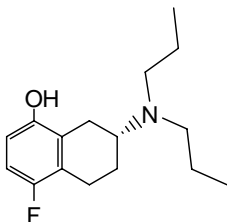


47
S-(-)-Eticlopride
Cluster 126
p-value = 1.25E-07
Target(s): DRD2,
DRD3

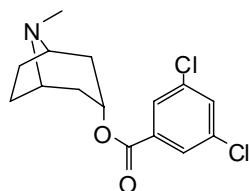


4
(+)-Butaclamol
Cluster 68
p-value = 8.86E-30
Target(s): DRD1/
DRD2, NaCh, 5-HT1F

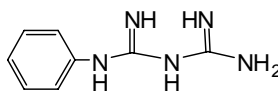
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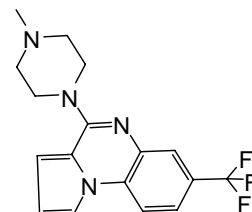
48
R(+)-UH-301
Cluster 127
p-value = 5.92E-03
Target(s): 5-HT1A



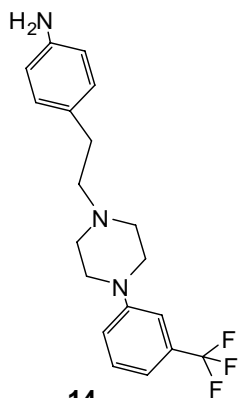
49
3-Tropanyl-3,5-
dichlorobenzoate
Cluster 29
p-value = 9.09E-10
Target(s): 5-HT3



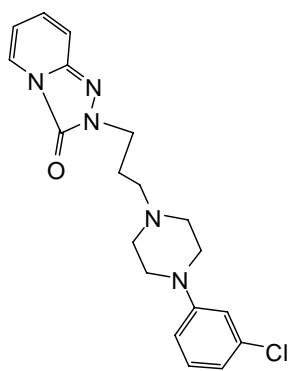
50
1-Phenylbiguanide
Cluster 136
p-value = 3.58E-03
Target(s): 5-HT3



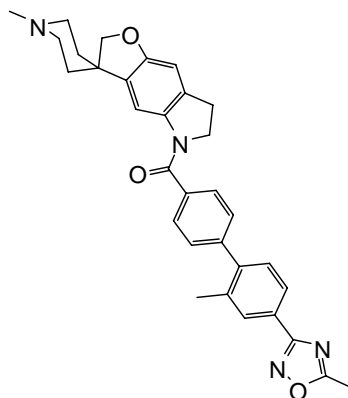
40
CGS-12066A
Cluster 71 (singleton)
p-value = 5.01E-03
Target(s): 5-HT1B



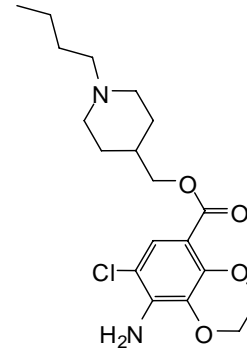
14
PAPP
Cluster 94 (singleton)
p-value = 3.78E-27
Target(s): 5-HT1A,
5-HT1D, DRD2



51
Trazodone
Cluster 122
p-value = 4.10E-03
Target(s): 5-HT2A,
SLC6A4, SLC6A2,
ADRA2A, HRH1



52
SB 224289
Cluster 11
p-value = 8.52E-07
Target(s): 5-HT1B



53
SB 204070
Cluster 116 (singleton)
p-value = 1.98E-09
Target(s): 5-HT4

Supplementary Figure 1 | Bioactive neuromodulators display a rich intra-class chemical diversity. (a) 8 of the 22 bioactive agents identified as dopamine signaling regulators. All 8 molecules are found in unique clusters when grouped based on 2D chemical fingerprint. A total of 10 different clusters were identified within the 22 agents known to act on the dopamine pathways. (b) 8 of the 12 bioactive agents identified as serotonin signaling regulators. All 8 molecules are found in unique clusters when grouped based on 2D chemical fingerprint. A total of 10 different clusters were identified within the 12 agents known to act on the serotonin pathway. P-value represents the original significance testing performed from the screening data. Reported drug targets displayed in this figure represents curated data published in Drugbank¹ and inhouse.

Reference

1. Wishart,D.S. *et al.* DrugBank: a comprehensive resource for in silico drug discovery and exploration. *Nucleic Acids Res.* 34, D668-D672 (2006).