

Supporting Information

High affinity dopamine D₃ receptor (D₃R)-selective antagonists attenuate heroin self-administration in wildtype but not D₃R knockout mice

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Table S1: Microanalysis Data:

Compound	C	H	N	C	H	N
	Calculated			Found		
14; BAK-04-51	60.38	6.33	11.74	60.27	6.43	11.63
15; BAK-04-52	58.11	6.18	6.78	58.13	5.99	6.85
16; BAK-04-54	68.05	6.87	11.76	68.00	6.81	11.52
17; BAK-04-55	64.67	6.98	10.77	64.68	6.70	10.85
18; BAK-04-56	66.15	6.13	7.98	66.06	6.08	7.97
19; BAK-04-57	63.66	5.99	7.68	63.39	6.02	7.67
20; CJB-038	55.27	5.24	11.21	54.97	5.17	10.93
21; OMO6-016	52.73	4.78	9.84	52.51	4.84	9.56
22; OMO4-013	63.77	6.34	11.02	63.49	6.32	10.92
23; OMO3-053	61.82	6.15	10.68	61.56	6.03	10.53
24; OMO4-015	61.59	5.93	10.64	61.32	5.97	10.47
25; OMO3-056	65.70	6.51	12.26	65.52	6.44	12.13
26; OMO2-088	69.10	6.96	12.89	68.91	6.98	12.68
27; OMO3-012	69.10	6.96	12.89	68.91	6.98	12.68
28; OMO2-086	66.35	6.46	12.38	66.08	6.37	12.21
29; OMO2-084	66.29	7.38	11.89	66.29	7.25	11.72
30; OMO2-063	56.40	6.04	9.07	56.38	6.05	9.15
31; OMO2-092	50.98	6.50	9.51	50.74	6.34	9.57
32; CAB02-015	67.59	6.15	10.51	67.34	6.07	10.43
33; CAB02-017*						
34; CAB02-029	58.27	5.89	10.07	58.17	5.67	10.22
35; CAB02-027	61.66	6.42	11.50	61.90	6.17	11.21
36; OMO6-018	55.23	4.81	9.91	54.97	4.85	9.65
37; OMO6-010	52.10	4.88	9.35	51.75	4.53	9.38

* The Free base compound purity was determined by using the HRMS to identify m/z 455.2443 (M+H)⁺, See Figure S2.

Table S2: Selected Reaction Monitoring (SRM) transitions of D3R-selective ligands.

Compound Name	Parent Mass	Product Mass
6	461.148	143.989, 213.106
16	427.100	267.257, 144.026
20	462.810	161.979, 233.111
21	479.008	161.994, 231.089
26	435.261	156.041
32	439.219	155.980
33	456.250	128.021, 156.025
34	453.010	128.019, 156.027
36	475.007	174.004, 245.110
37	491.046	145.993, 174.012

Figure S2: Mass spectrum Analysis of 33 in THA using HRMS

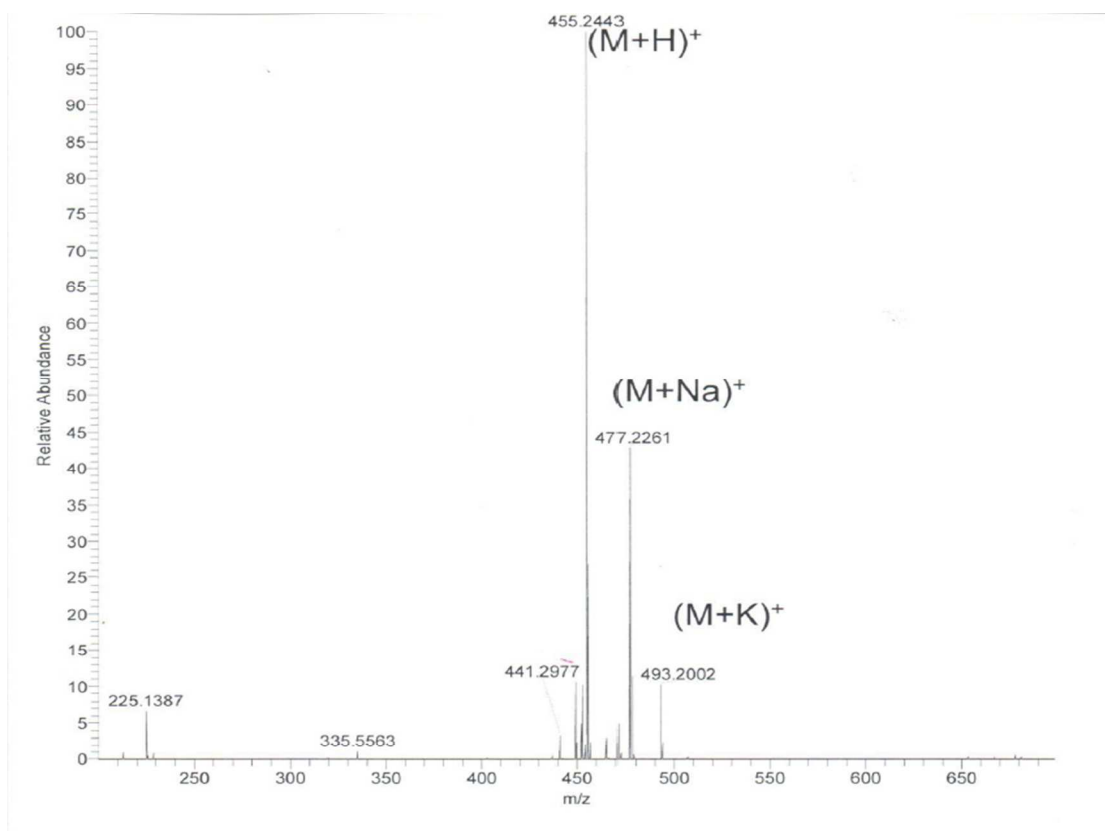


Table S3. K and t1/2 values for analogues tested

Unsubstituted

Compound	k	t1/2 (min.)
32	-0.017	41.8
16	-0.010	67.5
34	-0.077	9.0
20	-0.032	21.9

Substituted

Compound	k	t1/2 (min.)
26	-0.032	21.9
33	-0.029	24.3
21	-0.033	21.2
37	-0.058	11.9
36	-0.050	13.9
6	-0.037	18.8