

QSAR-based Computational Approaches to Accelerate the Discovery of Sigma-2 Receptor (S2R) Ligands as Therapeutic Drugs

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Figure S1. Virtual screening cascade is depicted in Figure 1, basically involving QSAR modeling, pharmacophore screening, and shape-based screening.

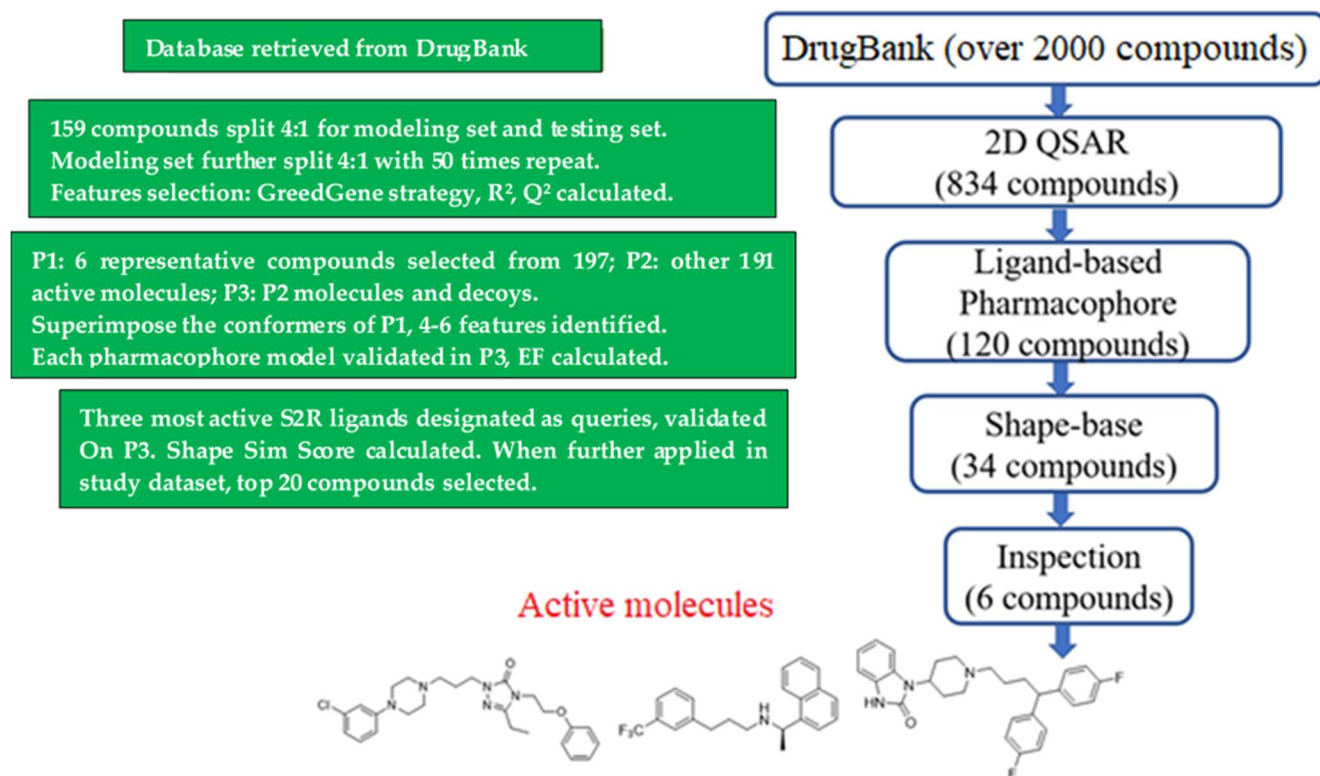


Table S1: Structures and activity data of all S2R ligands pooled from different sources for the present 2D-QSAR studies ¹⁻¹⁵

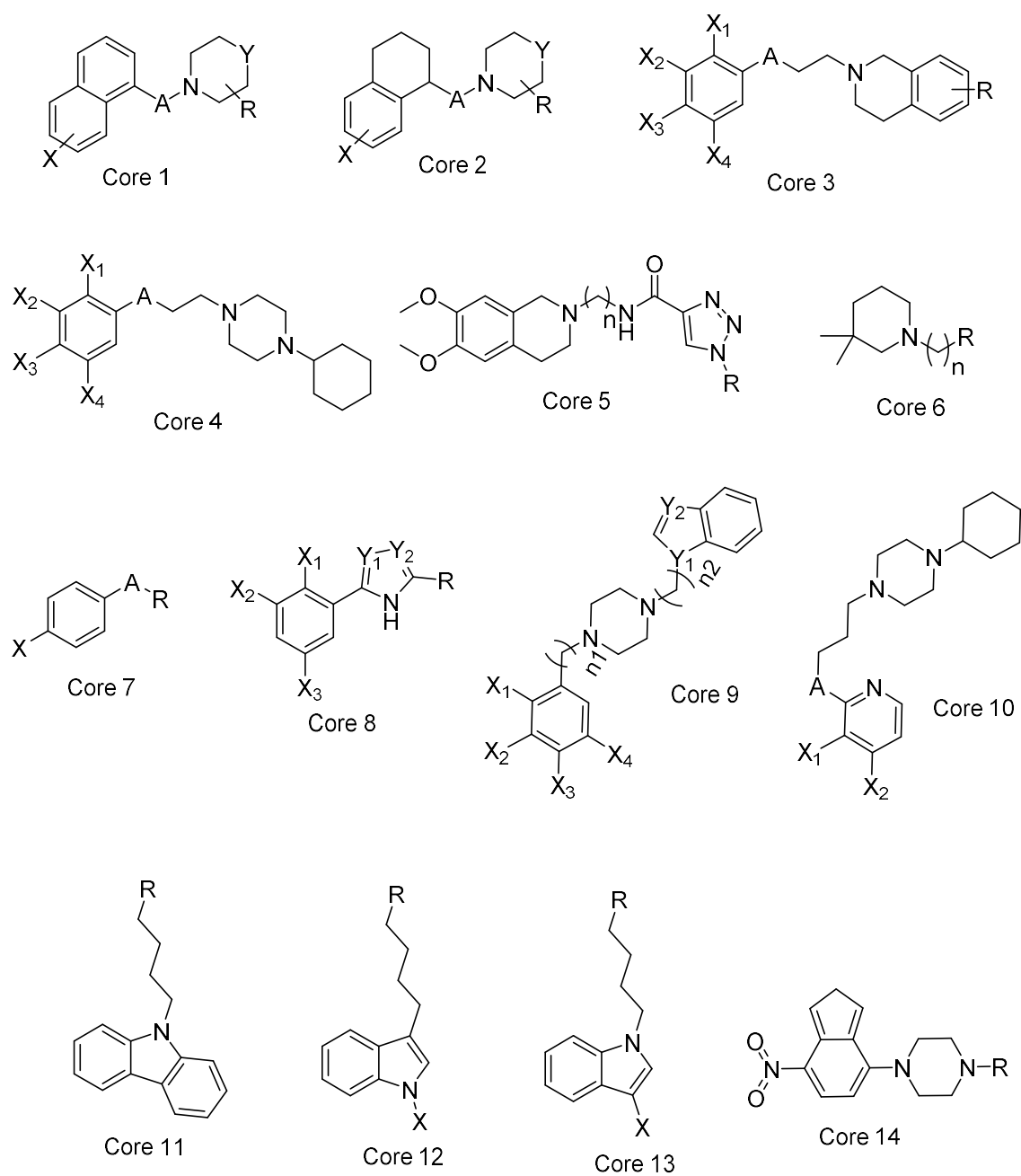
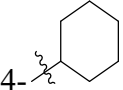
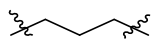
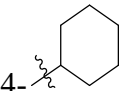
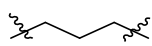
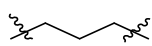
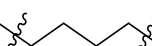
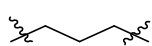
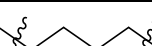
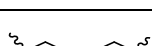
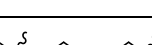
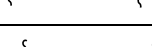
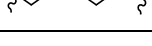
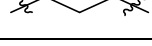
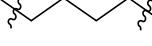
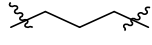
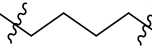
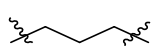
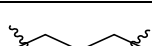
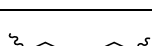
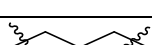
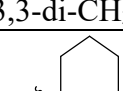


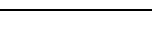
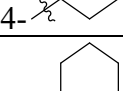
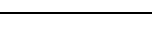
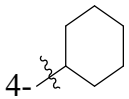
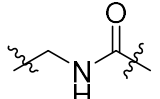
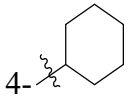
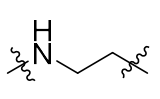
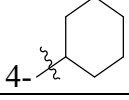
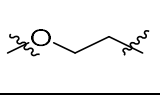
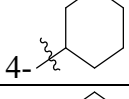
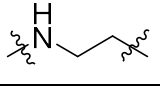
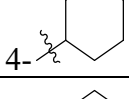
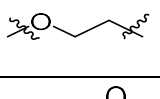
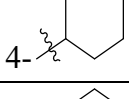
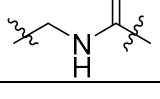
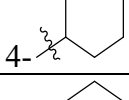
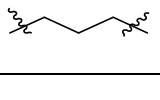
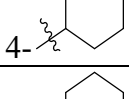
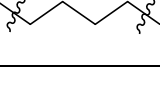
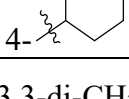
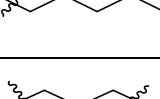
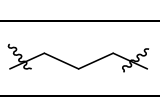
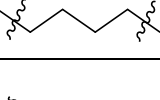
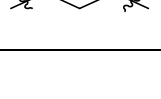
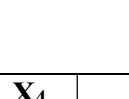
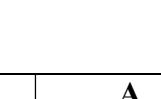
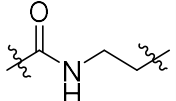
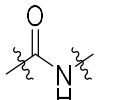
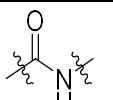
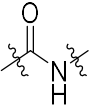
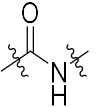
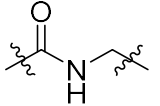
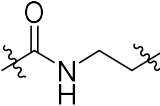
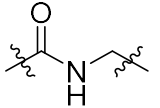
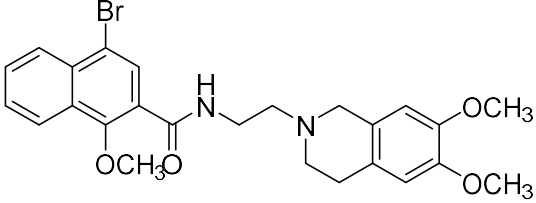
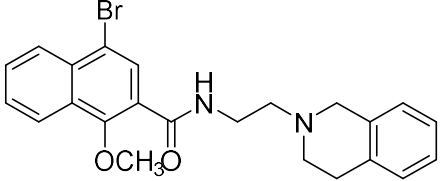
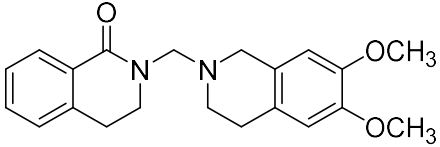
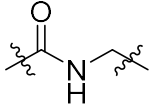
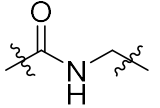
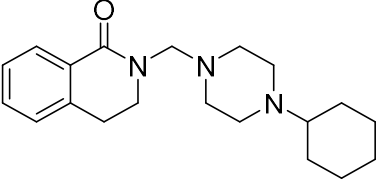
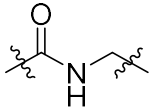
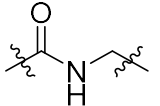


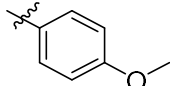
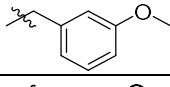
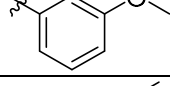
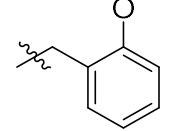
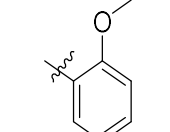
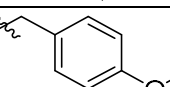
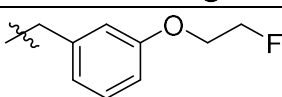
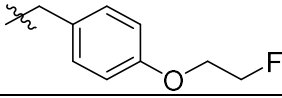
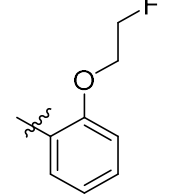
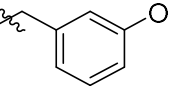
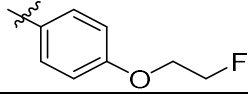
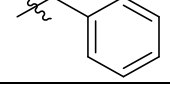
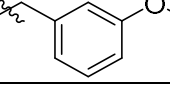
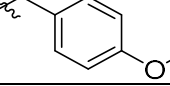
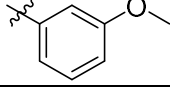
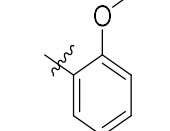
Table S2. Summary of the specific scaffold (core), nature of the substituents X, Y, A, etc., values of the experimental and QSAR model-predicted pK_i, the Residual (Res.) = Exp. pK_i – Pred. pK_i, and the identification of the dataset.

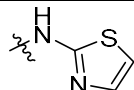
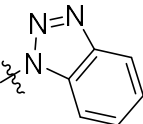
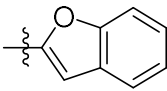
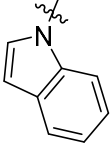
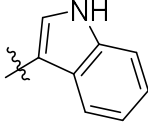
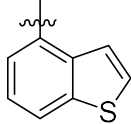
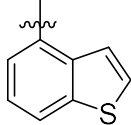
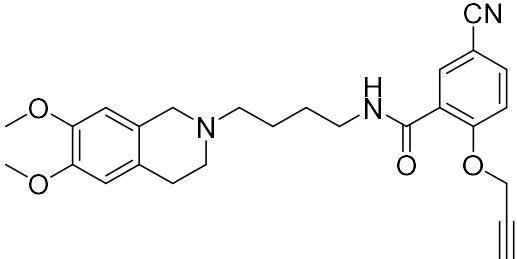
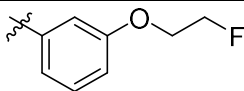
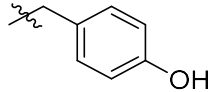
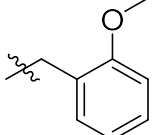
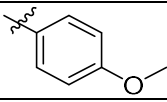
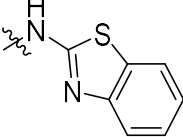

No	Core	X	Y	R	A	Exp. pK _i	Pred. pK _i	Res. #	Set
1	1	6-OCH ₃	NH			8.03	7.99	-0.04	M
2	1	H	NH			9.16	8.04	-1.12	M
3	1	5-OCH ₃	CH ₂	H		6.76	7.11	0.35	M
4	1	5-OCH ₃	CH ₂	H		6.82	7.55	0.73	M
5	1	5-OCH ₃	CH ₂	2,2-di-CH ₃		7.04	6.95	-0.09	M
6	1	5-OCH ₃	CH ₂	3,3-di-CH ₃		7.17	7.53	0.36	M
7	1	5-OCH ₃	CH ₂	4,4-di-CH ₃		7.58	7.19	-0.39	M
8	1	5-OCH ₃	CH ₂	4-CH ₃		7.75	7.62	-0.13	M
9	1	5-OCH ₃	CH ₂	4,4-di-CH ₃		7.75	7.63	-0.12	M
10	1	5-OCH ₃	CH ₂	2-CH ₃		7.06	7.05	-0.01	M
11	1	5-OCH ₃	CH ₂	2-CH ₃		7.19	7.56	0.37	M
12	1	5-OCH ₃	CH ₂	3-CH ₃		7.22	7.12	-0.1	M
13	1	5-OCH ₃	CH ₂	2-CH ₃		7.31	7.51	0.2	M
14	1	5-OCH ₃	CH ₂	H		7.58	7.34	-0.24	M
15	1	4-OCH ₃	CH ₂	3,3-di-CH ₃		6.17	7.00	0.83	M
16	1	6-OCH ₃	CH ₂	3,3-di-CH ₃		6.19	6.96	0.77	M
17	1	5-OH	CH ₂	3,3-di-CH ₃		6.22	6.81	0.59	M
18	1	4-OH	CH ₂	3,3-di-CH ₃		6.39	6.77	0.38	M
19	1	5-OH	NH			7.58	7.79	0.21	M
20	1	4-OH	NH			7.93	7.76	-0.17	M
21	1	5-OCH ₃	NH			8.04	8.06	0.02	M

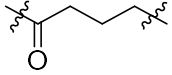
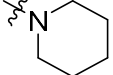
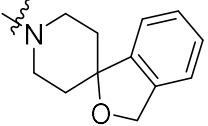
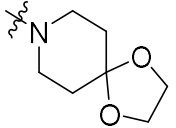
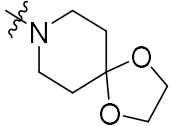
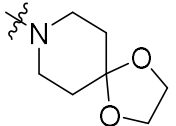
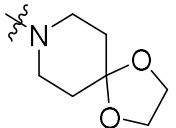
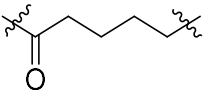
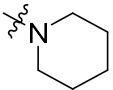
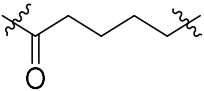
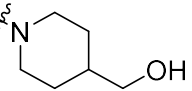
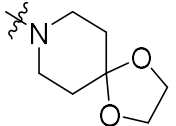
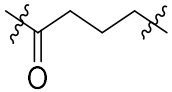
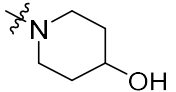
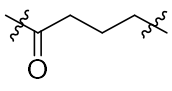
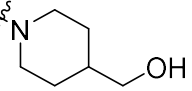
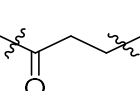
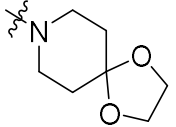
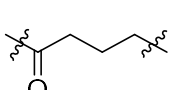
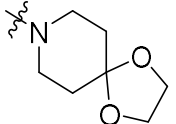
22	1	6-OCH ₃	NH			7.63	6.91	-0.72	M
23	1	6-OCH ₃	NH			7.73	7.51	-0.22	M
24	1	6-OCH ₃	NH			8.62	7.79	-0.83	M
25	2	6-O-CH ₃	NH			7.84	7.99	0.15	M
26	2	6-O-CH ₃	NH			7.95	8.26	0.31	M
27	2	6-O-CH ₃	NH			8.23	7.39	-0.84	M
28	2	6-O-CH ₃	NH			9.31	8.22	-1.09	M
29	1	H	NH			7.52	8.43	0.91	EE
30	1	H	NH			9.24	8.80	-0.44	EE
31	1	5-OCH ₃	CH ₂	3,3-di-CH ₃		6.62	7.08	0.46	EE
32	1	5-OCH ₃	CH ₂	4-CH ₃		7.41	7.18	-0.23	EE
33	1	5-OCH ₃	CH ₂	2,2-di-CH ₃		7.54	7.42	-0.12	EE
34	1	4-OCH ₃	NH			8.08	8.00	-0.08	EE

No	Core	X ₁	X ₂	X ₃	X ₄	R	A	pK _i exp	pK _i pred	Res. [#]	Set
35	3	-OCH ₃	-OCH ₃	H	Br	5,6-di-OCH ₃		8.09	7.98	-0.11	M
36	3	-OCH ₃	-OCH ₃	H	Br	H		6.14	7.14	1	M
37	3	-OCH ₃	-OCH ₃	H	Br	5,6-di-OCH ₃		7.79	7.15	-0.64	M

38	3	⁻ OCH ₃	H	H	⁻ CH ₃	5,6-di- OCH ₃		7.88	7.23	-0.65	M
39	3	⁻ OCH ₃	H	H	Br	5,6-di- OCH ₃		7.91	7.23	-0.68	M
40	3	Br	H	⁻ OC H ₃	⁻ OC H ₃	5,6-di- OCH ₃		7.29	7.67	0.38	M
41	3	⁻ OCH ₃	H	H	⁻ CH ₃	5,6-di- OCH ₃		8.06	8.05	-0.01	M
42	3	⁻ OCH ₃	H	H	⁻ CH ₃	5,6-di- OCH ₃		8.58	7.65	-0.93	M
43	3							7.67	7.88	0.21	M
44	3							7.32	7.79	0.47	M
45	3							8.32	7.91	-0.41	M
46	4	⁻ OCH ₃	H	H	⁻ CH ₃	-		7.58	7.81	0.23	M
47	4	⁻ OCH ₃	⁻ OCH ₃	H	Br	-		7.67	7.70	0.03	M
48	4							7.58	8.01	0.43	M
49	3	⁻ OCH ₃	H	H	⁻ CH ₃	5,6-di- OCH ₃		7.99	8.05	0.06	EE
50	3	⁻ OCH ₃	⁻ OCH ₃	H	Br	5,6-di- OCH ₃		7.89	7.58	-0.31	EE

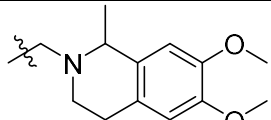
No	Core	n	R	pK _i exp	pK _i pred	Res. #	Set
51	5	2		6.39	7.16	0.77	M
52	5	2		6.67	7.21	0.54	M
53	5	2		6.74	7.11	0.37	M
54	5	2		6.81	7.16	0.35	M
55	5	2		6.82	7.06	0.24	M
56	5	2		7.03	7.25	0.22	M
57	5	4		7.21	7.58	0.37	M
58	5	4		7.32	7.65	0.33	M
59	5	4		7.62	7.43	-0.19	M
60	5	4		7.65	7.64	-0.01	M
61	5	4		7.66	7.58	-0.08	M
62	5	4		7.91	7.88	-0.03	M
63	5	4		7.97	7.91	-0.06	M
64	5	4		8.30	7.95	-0.35	M
65	5	4		8.52	7.84	-0.68	M
66	5	4		8.82	7.79	-1.03	M

67	6	3		5.48	5.98	0.5	M
68	6	3		5.70	6.56	0.86	M
69	6	1		5.74	6.42	0.68	M
70	6	3		6.71	6.64	-0.07	M
71	6	3		6.96	6.68	-0.28	M
72	6	3		7.20	7.12	-0.08	M
73	6	3		7.37	7.05	-0.32	M
74				7.91	8.21	0.3	M
75	5	4	H	5.99	6.92	0.93	EE
76	5	4		7.6	7.51	-0.09	EE
77	5	4		7.94	7.66	-0.28	EE
78	5	4		8.01	7.87	-0.14	EE
79	5	4		8.26	7.88	-0.38	EE
80	6	3		6.13	6.91	0.78	EE
81	6	4		7.71	7.08	-0.63	EE

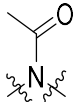
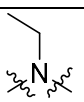
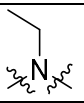
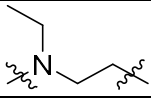
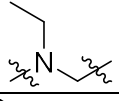
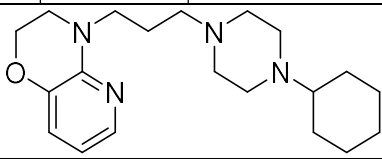
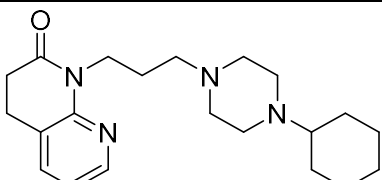
No	Core	X	A	R	pK _i exp	pK _i pred	Res. #	Set
82	7	F			6.49	6.52	0.03	M
83	7	- OCH ₂ CH ₂ F	-CH ₂ -		6.56	7.13	0.57	M
84	7	Br	-CH ₂ -		6.63	6.66	0.03	M
85	7	I	-CH ₂ -		6.63	6.66	0.03	M
86	7	F	-CH ₂ -		6.79	6.65	-0.14	M
87	7	- OCH ₂ CH ₂ F	-CH ₂ -		6.79	6.66	-0.13	M
88	7	F			6.97	6.96	-0.01	M
89	7	F			7.05	6.76	-0.29	M
90	7	- OCH ₃	-CH ₂ -		6.28	6.79	0.51	EE
91	7	F			6.30	6.30	0	EE
92	7	F			6.46	6.34	-0.12	EE
93	7	F			6.51	7.19	0.68	EE
94	7	F			6.75	7.63	0.88	EE

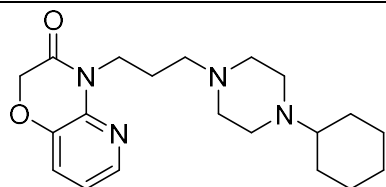
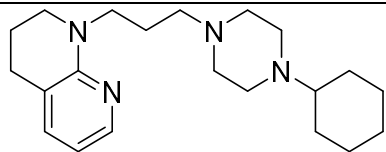
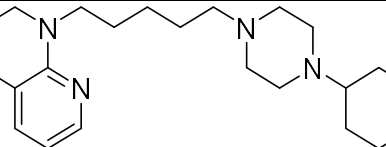
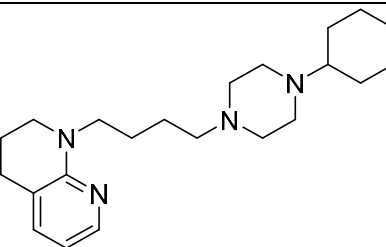

95	7	F			6.86	6.53	-0.33	EE
96	7	F			6.93	6.74	-0.19	EE
97	7	F			7.64	6.97	-0.67	EE

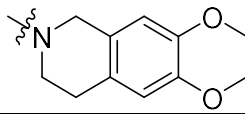
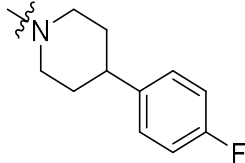
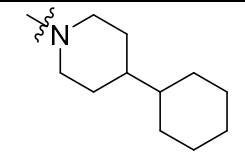
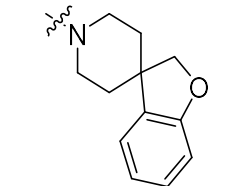
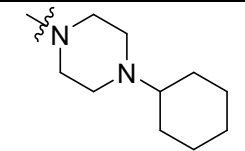
No	Core	X ₁	X ₂	X ₃	Y ₁	Y ₂	R	pK _i exp	pK _i pred	Res. #	Set
98	8	⁻ OCH ₃	⁻ OCH ₃	Br	N	CH		6.39	6.57	0.18	M
99	8	⁻ OCH ₃	⁻ OCH ₃	H	N	O		6.60	6.65	0.05	M
100	8	⁻ OCH ₃	⁻ OCH ₃	Br	N	CH		6.85	6.85	0	M
101	8	⁻ OCH ₃	⁻ OCH ₃	Br	N	CH		6.95	6.69	-0.26	M
102	8	⁻ OCH ₃	⁻ OCH ₃	Br	CH	CH		6.29	5.77	-0.52	M
104	8	⁻ OCH ₃	⁻ OCH ₃	Br	CH	CH		6.34	6.83	0.49	M
105	8	⁻ OCH ₃	⁻ OCH ₃	Br	CH	CH		6.45	7.10	0.65	M
106	8	⁻ OCH ₃	⁻ OCH ₃	Br	CH	CH		6.51	6.69	0.18	M
107	8	⁻ OCH ₃	⁻ OCH ₃	Br	CH	CH		6.66	6.98	0.32	M
108	8	⁻ OCH ₃	⁻ OCH ₃	Br	CH	CH		7.06	7.15	0.09	M
109	8	⁻ OCH ₃	⁻ OCH ₃	Br	CH	CH		7.28	6.69	-0.59	M
110	8	⁻ OCH ₃	⁻ OCH ₃	Br	CH	CH		7.59	7.35	-0.24	M

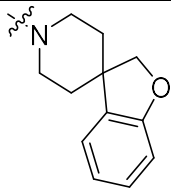
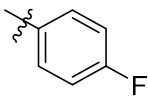
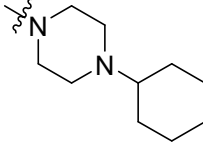
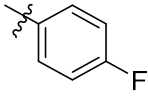
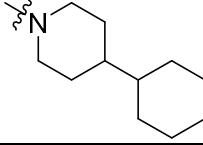
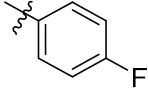
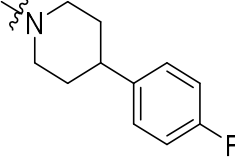
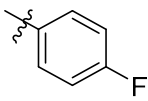
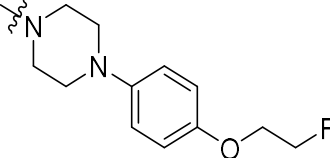
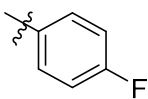
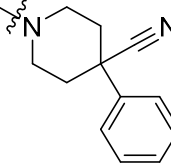
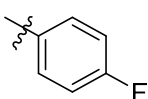
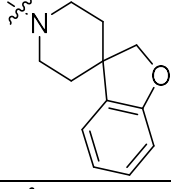
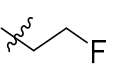
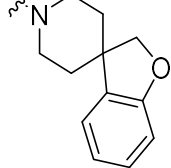
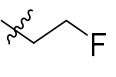
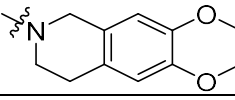
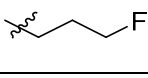
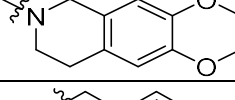
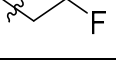
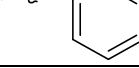
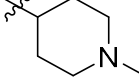
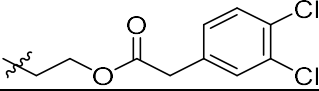
103	8	- OCH ₃	- OCH ₃	Br	CH	CH		6.30	6.67	0.37	EE
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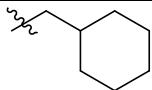
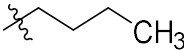
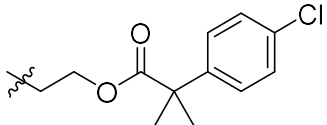
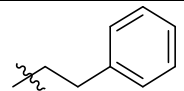
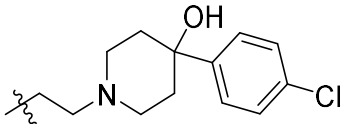
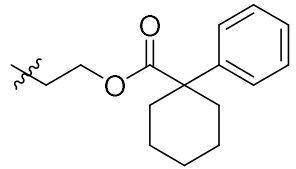
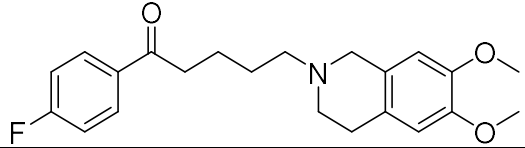
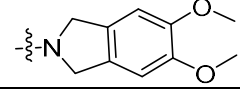
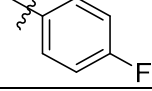
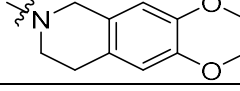
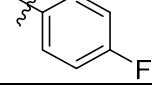
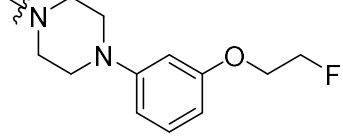
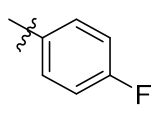

No	Core	X ₁	X ₂	X ₃	X ₄	Y ₁	Y ₂	n ₁	n ₂	pK _i exp	pK _i pred	Res. #	Set
111	9	H	H	F	H	C	N	0	1	6.18	6.86	0.68	M
112	9	H	H	H	H	N	C-CH ₃	2	1	7.25	7.15	-0.1	M
113	9	F	H	H	H	N	CH	0	3	8.00	7.58	-0.42	M
114	9	F	H	H	F	C	N	1	1	6.38	6.85	0.47	EE
115	9	H	F	F	H	C	N	1	1	6.89	6.93	0.04	EE
116	9	H	H	F	H	N	CH	0	3	7.70	7.65	-0.05	EE

No	Core	X ₁	X ₂	A	pK _i exp	pK _i pred	Res. #	Set
117	10	H	-OCH ₃		6.61	6.97	0.36	M
118	10	H	H	-NH-	7.15	7.06	-0.09	M
119	10	H	-OCH ₃	-NH-	7.22	7.09	-0.13	M
120	10	H	-OCH ₃		7.52	7.72	0.2	M
121	10	H	H		7.83	7.15	-0.68	M
122	10	H	H		8.17	8.52	0.35	M
123	10	H	H		8.45	8.15	-0.3	M
124	10				7.73	7.70	-0.03	M
125	10				7.79	7.60	-0.19	M

126	10				7.80	7.63	-0.17	M
127	10				8.01	7.67	-0.34	M
128	10				8.19	8.43	0.24	M
129	10				8.79	8.06	-0.73	M
130	10	H	H		6.51	6.92	0.41	EE

No	Core	R	X	pK _i exp	pK _i pred	Res. #	Set
131	11		-	10.40	8.62	-1.78	M
132	11		-	7.93	8.75	0.82	M
133	11		-	8.12	8.71	0.59	M
134	11		-	8.49	9.02	0.53	M
135	12		H	8.19	7.99	-0.2	M

136	12			7.90	8.60	0.7	M
137	12			7.54	8.18	0.64	M
138	12			8.14	8.26	0.12	M
139	12			9.57	8.30	-1.27	M
140	12			7.17	8.11	0.94	M
141	12			8.52	8.41	-0.11	M
142	12			7.36	7.92	0.56	M
143	13			7.53	7.92	0.39	M
144	13			7.55	7.39	-0.16	M
145	13			7.56	7.38	-0.18	M
146	14		-	5.33	5.86	0.53	M
147	14		-	6.24	5.65	-0.59	M
148	14		-	6.41	6.57	0.16	M

149	14		-	6.42	6.09	-0.33	M
150	14		-	6.45	5.55	-0.9	M
151	14		-	6.56	6.40	-0.16	M
152	14		-	6.65	6.26	-0.39	M
153	14		-	6.68	6.77	0.09	M
154	14		-	7.25	6.80	-0.45	M
155				7.91	7.76	-0.15	M
156	12			7.27	8.17	0.9	EE
157	12			7.31	8.19	0.88	EE
158	12			7.32	8.04	0.72	EE
159	14		-	6.50	5.66	-0.84	EE

#: Res. (Residual) = pK_i pred - pK_i exp; *: M: Modeling dataset; EE: External evaluation dataset

Table S3: SMILES structure for all S2R ligands used in the present study.

No	SMILES structure
1	<chem>C(CCC1c2c([nH]c1)cccc2)C[N+]1CCN(C2CCCCC2)CC1</chem>
2	<chem>C(C[N+]1CCN(C2CCCCC2)CC1)Cn1c2c(c3c1cccc3)cccc2</chem>
3	<chem>C(CCN1c2c(c3c1cccc3)cccc2)C[N+]1CCC(C2CCCCC2)CC1</chem>
4	<chem>Fc1ccc(C2CC[N+](CCCCn3c4c(c5c3cccc5)cccc4)CC2)cc1</chem>
5	<chem>C(CCN1c2c(c3c1cccc3)cccc2)C[N+]1CCC2(OCc3c2cccc3)CC1</chem>
6	<chem>O(C)c1c(OC)cc2c(c1)C[N+](CCCCn1c3c(c4c1cccc4)cccc3)CC2</chem>
7	<chem>Fc1ccc(-n2c3c(c(CCCC[N+]4CCC(C5CCCCC5)CC4)c2)cccc3)cc1</chem>
8	<chem>Fc1ccc(-n2c3c(c(CCCC[N+]4CCN(C5CCCCC5)CC4)c2)cccc3)cc1</chem>
9	<chem>Fc1ccc(-n2c3c(c(CCCC[N+]4CCC(c5ccc(F)cc5)CC4)c2)cccc3)cc1</chem>
10	<chem>Fc1ccc(-n2c3c(c(CCCC[N+]4CCC5(OCc6c5cccc6)CC4)c2)cccc3)cc1</chem>
11	<chem>Fc1ccc(-n2c3c(c(CCCC[N+]4Cc5c(cc(OC)c(OC)c5)CC4)c2)cccc3)cc1</chem>
12	<chem>Fc1ccc(-n2c3c(c(CCCC[N+]Cc4ccc(OC)cc4)c2)cccc3)cc1</chem>
13	<chem>Fc1ccc(-n2c3c(c(CCCC[N+]Cc4cc(OC)ccc4)c2)cccc3)cc1</chem>
14	<chem>Fc1ccc(-n2c3c(c(CCCC[N+]CCc4cc(OC)ccc4)c2)cccc3)cc1</chem>
15	<chem>Fc1ccc(-n2c3c(c(CCCC[N+](CCc4ccc(OC)cc4)C)c2)cccc3)cc1</chem>
16	<chem>Fc1ccc(-n2c3c(c(CCCC[N+](CCc4cc(OC)ccc4)C)c2)cccc3)cc1</chem>
17	<chem>Fc1ccc(-n2c3c(c(CCCC[N+](CC)Cc4cc(OC)ccc4)c2)cccc3)cc1</chem>
18	<chem>Fc1ccc(-n2c3c(c(CCCC[N+](CC)Cc4ccc(OC)cc4)c2)cccc3)cc1</chem>
19	<chem>Fc1ccc(-n2c3c(c(CCCC[N+]Cc4cc(OC)c(OC)cc4)c2)cccc3)cc1</chem>
20	<chem>Fc1ccc(-n2c3c(c(CCCC[N+]4Cc5c(cc(OC)c(OC)c5)CC4)c2)cccc3)cc1</chem>
21	<chem>Fc1ccc(-n2c3c(c(CCCC[N+](CCc4cc(OC)c(OC)cc4)C)c2)cccc3)cc1</chem>
22	<chem>Fc1ccc(-n2c3c(c(CCCC[N+](CC)Cc4cc(OC)c(OC)cc4)c2)cccc3)cc1</chem>
23	<chem>O(C)c1cc2c(c(CCC[N+]3CCCCC3)ccc2)cc1</chem>
24	<chem>O(C)c1cc2c(c(CCCC[N+]3CCCCC3)ccc2)cc1</chem>
25	<chem>O(C)c1cc2c(c(CCC[N+]3[C@H](C)CCCC3)ccc2)cc1</chem>
26	<chem>O(C)c1cc2c(c(CCC[N+]3[C@H](C)CCC3)ccc2)cc1</chem>
27	<chem>O(C)c1cc2c(c(CCC[N+]3CCC(C)CC3)ccc2)cc1</chem>
28	<chem>O(C)c1cc2c(c(CCC[N+]3C(C)(C)CCCC3)ccc2)cc1</chem>
29	<chem>O(C)c1cc2c(c(CCCC[N+]3[C@H](C)CCC3)ccc2)cc1</chem>
30	<chem>O(C)c1cc2c(c(CCCC[N+]3[C@H](C)CCCC3)ccc2)cc1</chem>
31	<chem>O(C)c1cc2c(c(CCC[N+]3CCC(C)(C)CC3)ccc2)cc1</chem>
32	<chem>O(C)c1cc2c(c(CCCC[N+]3CCC(C)CC3)ccc2)cc1</chem>
33	<chem>O(C)c1cc2c(c(CCCC[N+]3CC(C)(C)CCC3)ccc2)cc1</chem>
34	<chem>O(C)c1cc2c(c(CCCC[N+]3C(C)(C)CCCC3)ccc2)cc1</chem>
35	<chem>O(C)c1cc2c(c(CCCC[N+]3CCC(C)(C)CC3)ccc2)cc1</chem>
36	<chem>OC1cc2c(c(CCC[N+]3CC(C)(C)CCC3)ccc2)cc1</chem>
37	<chem>OC1cc2c(CCC[N+]3CC(C)(C)CCC3)cccc2cc1</chem>
38	<chem>O(C)c1cc2c(CCC[N+]3CC(C)(C)CCC3)cccc2cc1</chem>
39	<chem>O(C)c1c2c(c(CCC[N+]3CC(C)(C)CCC3)ccc2)ccc1</chem>
40	<chem>O(C)c1cc2c(c(CCC[N+]3CC(C)(C)CCC3)ccc2)cc1</chem>
41	<chem>OC1cc2c(c(CCC[N+]3CCN(C4CCCCC4)CC3)ccc2)cc1</chem>
42	<chem>OC1cc2c(CCC[N+]3CCN(C4CCCCC4)CC3)cccc2cc1</chem>
43	<chem>O(C)c1c2c(c(CCC[N+]3CCN(C4CCCCC4)CC3)ccc2)ccc1</chem>
44	<chem>O(C)c1cc2c(c(CCC[N+]3CCN(C4CCCCC4)CC3)ccc2)cc1</chem>
45	<chem>O(C)c1cc2c(CCC[N+]3CCN(C4CCCCC4)CC3)cccc2cc1</chem>
46	<chem>O(C)c1c2c(c(NCC[N+]3CCN(C4CCCCC4)CC3)ccc2)ccc1</chem>
47	<chem>O(CC[N+]1CCN(C2CCCCC2)CC1)c1c2c(c(OC)ccc2)ccc1</chem>
48	<chem>O(C)c1c2c([C@H](CCC[N+]3CCN(C4CCCCC4)CC3)CCC2)ccc1</chem>
49	<chem>O(C)c1c2c([C@H](NCCN3CC[N+](C4CCCCC4)CC3)CCC2)ccc1</chem>
50	<chem>O(CC[N+]1CCN(C2CCCCC2)CC1)[C@H]1c2c(c(OC)ccc2)CCC1</chem>

51	<chem>O=C(Nc1c2c(c(OC)ccc2)ccc1)CN1CC[N+](C2CCCCC2)CC1</chem>
52	<chem>O=C(N[C@H]1c2c(c(OC)ccc2)CCC1)CN1CC[N+](C2CCCCC2)CC1</chem>
53	<chem>O=[N+](O-)[c1cc2c(cc1)CC[N+](CCCCN1C(=O)c3c(C1=O)cccc3)C2</chem>
54	<chem>O=[N+](O-)[c1cc2c(cc1)CC[N+](CCCCNC(=O)c1c(OC)c(OC)c(OC)cc1)C2</chem>
55	<chem>C(CCC1CCCCC1)C[N+](C)CCC1</chem>
56	<chem>C(C[N+](C)CCC1)Cn1c2c(cc1)cccc2</chem>
57	<chem>C(C[N+](C)CCC1)Cc1c2c([nH]c1)cccc2</chem>
58	<chem>C(C[N+](C)CCC1)Cc1c2c(occ2)ccc1</chem>
59	<chem>C(C[N+](C)CCC1)Cc1c2c(scc2)ccc1</chem>
60	<chem>N(CCC[N+](C)CCC1)c1sc2c(n1)cccc2</chem>
61	<chem>O=C(OC1CC2[N+](CCCC[N+])C(C1)CCC2)Nc1c(OC)ccc(C)c1</chem>
62	<chem>O=C(OC1CC2[N+](CCCCC[N+])C(C1)CCC2)Nc1c(OC)ccc(C)c1</chem>
63	<chem>O=C(OC1CC2[N+](CCCCCCCCC[N+])C(C1)CCC2)Nc1c(OC)ccc(C)c1</chem>
64	<chem>Brc1cc(C[N+](CCCC[N+])2C3CC(OC(=O)Nc4c(OC)ccc(C)c4)CC2CCC3)ccc1</chem>
65	<chem>Fc1cc(C[N+](CCCC[N+])2C3CC(OC(=O)Nc4c(OC)ccc(C)c4)CC2CCC3)ccc1</chem>
66	<chem>lc1cc(C[N+](CCCC[N+])2C3CC(OC(=O)Nc4c(OC)ccc(C)c4)CC2CCC3)ccc1</chem>
67	<chem>Brc1ccc(C[N+](CCCC[N+])2C3CC(OC(=O)Nc4c(OC)ccc(C)c4)CC2CCC3)cc1</chem>
68	<chem>Fc1ccc(C[N+](CCCC[N+])2C3CC(OC(=O)Nc4c(OC)ccc(C)c4)CC2CCC3)cc1</chem>
69	<chem>lc1ccc(C[N+](CCCC[N+])2C3CC(OC(=O)Nc4c(OC)ccc(C)c4)CC2CCC3)cc1</chem>
70	<chem>Brc1cc(C[N+](CCCCC[N+])2C3CC(OC(=O)Nc4c(OC)ccc(C)c4)CC2CCC3)ccc1</chem>
71	<chem>Fc1cc(C[N+](CCCCC[N+])2C3CC(OC(=O)Nc4c(OC)ccc(C)c4)CC2CCC3)ccc1</chem>
72	<chem>lc1cc(C[N+](CCCCC[N+])2C3CC(OC(=O)Nc4c(OC)ccc(C)c4)CC2CCC3)ccc1</chem>
73	<chem>Brc1ccc(C[N+](CCCCC[N+])2C3CC(OC(=O)Nc4c(OC)ccc(C)c4)CC2CCC3)cc1</chem>
74	<chem>Fc1ccc(C[N+](CCCCC[N+])2C3CC(OC(=O)Nc4c(OC)ccc(C)c4)CC2CCC3)cc1</chem>
75	<chem>lc1ccc(C[N+](CCCCC[N+])2C3CC(OC(=O)Nc4c(OC)ccc(C)c4)CC2CCC3)cc1</chem>
76	<chem>Clc1ccc(C(=O)NCCCCC[N+])2C3CC(OC(=O)Nc4c(OC)ccc(C)c4)CC2CCC3)cc1</chem>
77	<chem>Brc1ccc(C(=O)NCCCCC[N+])2C3CC(OC(=O)Nc4c(OC)ccc(C)c4)CC2CCC3)cc1</chem>
78	<chem>Fc1ccc(C(=O)NCCCCC[N+])2C3CC(OC(=O)Nc4c(OC)ccc(C)c4)CC2CCC3)cc1</chem>
79	<chem>lc1ccc(C(=O)NCCCCC[N+])2C3CC(OC(=O)Nc4c(OC)ccc(C)c4)CC2CCC3)cc1</chem>
80	<chem>O=C(NCC[N+](C)Cc2c(cc(OC)c(OC)c2)CC1)c1c(OC)ccc(C)c1</chem>
81	<chem>O=C(NCCCC[N+](C)Cc2c(cc(OC)c(OC)c2)CC1)c1c(OC)ccc(C)c1</chem>
82	<chem>Brc1cc(OC)c(OC)c(C(=O)NCC[N+])2Cc3c(cccc3)CC2)c1</chem>
83	<chem>Brc1c2c(c(OC)c(C(=O)NCC[N+])3Cc4c(cccc4)CC3)c1)cccc2</chem>
84	<chem>Brc1cc(C(=O)NCC[N+])2Cc3c(cc(OC)c(OC)c3)CC2)c(OC)cc1</chem>
85	<chem>Brc1cc(OC)c(OC)c(C(=O)NCC[N+])2Cc3c(cc(OC)c(OC)c3)CC2)c1</chem>
86	<chem>Brc1c2c(c(OC)c(C(=O)NCC[N+])3Cc4c(cc(OC)c(OC)c4)CC3)c1)cccc2</chem>
87	<chem>Brc1cc(OC)c(OC)c(C(=O)NCCCC[N+])2Cc3c(cc(OC)c(OC)c3)CC2)c1</chem>
88	<chem>N(CCC[N+](C)CCN(C2CCCCC2)CC1)c1ncccc1</chem>
89	<chem>N(CCC[N+](C)CCN(C2CCCCC2)CC1)(CC)c1ncccc1</chem>
90	<chem>O(C)c1cc(NCCC[N+])2CCN(C3CCCCC3)CC2)ncc1</chem>
91	<chem>C(C[N+](C)CCN(C2CCCCC2)CC1)CN1c2ncccc2CCC1</chem>
92	<chem>O=C(N(CCC[N+](C)CCN(C2CCCCC2)CC1)c1ncccc1)C</chem>
93	<chem>C(C[N+](C)CCN(C2CCCCC2)CC1)CN1c2ncccc2OCC1</chem>
94	<chem>N(CCCC[N+](C)CCN(C2CCCCC2)CC1)(CC)c1ncccc1</chem>
95	<chem>O=C1N(CCC[N+])2CCN(C3CCCCC3)CC2)c2ncccc2CC1</chem>
96	<chem>C(CCN1c2ncccc2CCC1)C[N+](C)CCN(C2CCCCC2)CC1</chem>
97	<chem>O=C1N(CCC[N+])2CCN(C3CCCCC3)CC2)c2ncccc2OC1</chem>
98	<chem>N(CCCCC[N+](C)CCN(C2CCCCC2)CC1)(CC)c1ncccc1</chem>
99	<chem>O(C)c1cc(N(CCC[N+])2CCN(C3CCCCC3)CC2)CC)ncc1</chem>
100	<chem>C(CC[N+](C)CCN(C2CCCCC2)CC1)CCN1c2ncccc2CCC1</chem>
101	<chem>O=C(N(CCC[N+](C)CCN(C2CCCCC2)CC1)c1nccc(OC)c1)C</chem>
102	<chem>O=C1N(CCC[N+])2CCN(C3CCCCC3)CC2)CCc2c1cccc2</chem>
103	<chem>O(C)c1c(OC)cc2c(c1)C[N+](CCCCN1C(=O)c3c(cccc3)CC1)CC2</chem>
104	<chem>Brc1cc(OC)c(OC)c(C(=O)NCCC[N+])2CCN(C3CCCCC3)CC2)c1</chem>
105	<chem>Brc1c(C(=O)NCCC[N+])2Cc3c(cc(OC)c(OC)c3)CC2)cc(OC)c(OC)c1</chem>
106	<chem>Brc1cc(OC)c(OC)c(C(=O)NCCC[N+])2Cc3c(cc(OC)c(OC)c3)CC2)c1</chem>
107	<chem>O[C@@H]1C([N+])2C3CC(c4cccc4)CC2CC3)CCCC1</chem>

108	<chem>O[C@@H]1C([N+]2C3CC(c4cccc4)CC2CC3)Cc2c(cccc2)C1</chem>
109	<chem>Fc1ccc(CN2CC([N+]3C4CC(c5cccc5)CC3CC4)[C@@H](O)CC2)cc1</chem>
110	<chem>lc1cc(CN2CC([N+]3C4CC(c5cccc5)CC3CC4)[C@@H](O)CC2)ccc1</chem>
111	<chem>Brc1ccc(C[C@H](O)C[N+]2C3CC(c4cccc4)CC2CC3)cc1</chem>
112	<chem>O[C@H](C[N+]1C2CC(c3cccc3)CC1CC2)c1cccc1</chem>
113	<chem>Brc1c([C@H](O)C[N+]2C3CC(c4cccc4)CC2CC3)cccc1</chem>
114	<chem>Brc1cc([C@H](O)C[N+]2C3CC(c4cccc4)CC2CC3)ccc1</chem>
115	<chem>Brc1ccc([C@H](O)C[N+]2C3CC(c4cccc4)CC2CC3)cc1</chem>
116	<chem>Clc1c([C@H](O)C[N+]2C3CC(c4cccc4)CC2CC3)c(Cl)ccc1</chem>
117	<chem>Clc1c(Cl)ccc([C@H](O)C[N+]2C3CC(c4cccc4)CC2CC3)c1</chem>
118	<chem>Fc1ccc(C(=O)C[N+]2C3CC(c4cccc4)CC2CC3)cc1</chem>
119	<chem>Fc1ccc(C(=O)CC[N+]2C3CC(c4cccc4)CC2CC3)cc1</chem>
120	<chem>Brc1c2c(c(OC)c(C(=O)N[C@@H]3C[N+](C4C5CCCC4CCC5)CC3)c1)cccc2</chem>
121	<chem>Brc1c2c(c(OC)c(C(=O)N[C@@H]3C[N+](C4C5CC6CC4CC(C5)C6)CC3)c1)cccc2</chem>
122	<chem>Brc1c2c(c(OC)c(C(=O)N[C@H]3[N+](C4C5CCCC4CCC5)CC3)c1)cccc2</chem>
123	<chem>Brc1c2c(c(OC)c(C(=O)N[C@H]3[N+](C4C5CC6CC4CC(C5)C6)CC3)c1)cccc2</chem>
124	<chem>Brc1c2c(c(OC)c(C(=O)NC3CC4[N+](C5CCCCC5)C(C3)CCC4)c1)cccc2</chem>
125	<chem>Brc1c2c(c(OC)c(C(=O)NC3CC4[N+](C5CCCCC5)C(C3)CCC4)c1)cccc2</chem>
126	<chem>Brc1c2c(c(OC)c(C(=O)NC3CC[N+](C4C5CCCC4CCC5)CC3)c1)cccc2</chem>
127	<chem>Brc1c2c(c(OC)c(C(=O)NC3CC[N+](C4C5CC6CC4CC(C5)C6)CC3)c1)cccc2</chem>
128	<chem>O=C(NCC[N+]1Cc2c(cc(OC)c(OC)c2)CC1)c1nnn(-c2ccc(OC)cc2)c1</chem>
129	<chem>O=C(NCC[N+]1Cc2c(cc(OC)c(OC)c2)CC1)c1nnn(-c2cc(OC)ccc2)c1</chem>
130	<chem>O=C(NCC[N+]1Cc2c(cc(OC)c(OC)c2)CC1)c1nnn(-c2c(OC)cccc2)c1</chem>
131	<chem>O=C(NCCCC[N+]1Cc2c(cc(OC)c(OC)c2)CC1)c1c(OCC#C)ccc(C#N)c1</chem>
132	<chem>O=C(NCCCC[N+]1Cc2c(cc(OC)c(OC)c2)CC1)c1nnn(Cc2cccc2)c1</chem>
133	<chem>O=C(NCC[N+]1Cc2c(cc(OC)c(OC)c2)CC1)c1nnn(Cc2cc(OC)ccc2)c1</chem>
134	<chem>O=C(NCC[N+]1Cc2c(cc(OC)c(OC)c2)CC1)c1nnn(Cc2c(OC)cccc2)c1</chem>
135	<chem>O=C(NCC[N+]1Cc2c(cc(OC)c(OC)c2)CC1)c1nnn(Cc2ccc(OC)cc2)c1</chem>
136	<chem>O=C(NCCCC[N+]1Cc2c(cc(OC)c(OC)c2)CC1)c1nnn(Cc2cc(O)ccc2)c1</chem>
137	<chem>O=C(NCCCC[N+]1Cc2c(cc(OC)c(OC)c2)CC1)c1nnn(Cc2ccc(O)cc2)c1</chem>
138	<chem>O=C(NCCCC[N+]1Cc2c(cc(OC)c(OC)c2)CC1)c1nnn(-c2ccc(OC)cc2)c1</chem>
139	<chem>O=C(NCCCC[N+]1Cc2c(cc(OC)c(OC)c2)CC1)c1nnn(-c2cc(OC)ccc2)c1</chem>
140	<chem>O=C(NCCCC[N+]1Cc2c(cc(OC)c(OC)c2)CC1)c1nnn(-c2c(OC)cccc2)c1</chem>
141	<chem>O=C(NCCCC[N+]1Cc2c(cc(OC)c(OC)c2)CC1)c1nnn(Cc2cc(OC)ccc2)c1</chem>
142	<chem>O=C(NCCCC[N+]1Cc2c(cc(OC)c(OC)c2)CC1)c1nnn(Cc2c(OC)cccc2)c1</chem>
143	<chem>O=C(NCCCC[N+]1Cc2c(cc(OC)c(OC)c2)CC1)c1nnn(Cc2ccc(OC)cc2)c1</chem>
144	<chem>FCCn1nnc(-c2ccc(C(=O)NCCCC[N+]3Cc4c(cc(OC)c(OC)c4)CC3)cc2)c1</chem>
145	<chem>FCCOc1cc(-n2nnc(C(=O)NCCCC[N+]3Cc4c(cc(OC)c(OC)c4)CC3)c2)ccc1</chem>
146	<chem>FCCOc1c(-n2nnc(C(=O)NCCCC[N+]3Cc4c(cc(OC)c(OC)c4)CC3)c2)cccc1</chem>
147	<chem>FCCOc1ccc(-n2nnc(C(=O)NCCCC[N+]3Cc4c(cc(OC)c(OC)c4)CC3)c2)cc1</chem>
148	<chem>Clc1c(Cl)ccc(CC(=O)OCCN2CCN(c3c4c(c([N+](=O)[O-])cc3)C=CC4)CC2)c1</chem>
149	<chem>Clc1ccc(C(C(=O)OCCN2CCN(c3c4c(c([N+](=O)[O-])cc3)C=CC4)CC2)(C)C)cc1</chem>
150	<chem>O=[N+](O)c1c2c(c(N3CCN(CCOC(=O)C4(c5cccc5)CCCC4)CC3)cc1)CC=C2</chem>
151	<chem>O=[N+](O)c1c2c(c(N3CCN(CC4CCCC4)CC3)cc1)CC=C2</chem>
152	<chem>O=[N+](O)c1c2c(c(N3CCN(CCCC)CC3)cc1)CC=C2</chem>
153	<chem>Clc1cc(C2(O)CCN(CCN3CCN(c4c5c(c([N+](=O)[O-])cc4)C=CC5)CC3)CC2)ccc1</chem>
154	<chem>O=[N+](O)c1c2c(c(N3CCN(CC4CCCC4)CC3)cc1)CC=C2</chem>
155	<chem>O=[N+](O)c1c2c(c(N3CCN(C4CCCC4)CC3)cc1)CC=C2</chem>
156	<chem>Fc1cc2n(-c3ccc(F)cc3)cc(CCCCN3Cc4c(cc(OC)c(OC)c4)CC3)c2cc1</chem>
157	<chem>Fc1ccc(-n2c3c(c(CCCCN4Cc5c(cc(OC)c(OC)c5)C4)c2)cccc3)cc1</chem>
158	<chem>Fc1ccc(-n2c3c(c(CCCCN4Cc5c(cc(OC)c(OC)c5)CC4)c2)cccc3)cc1</chem>
159	<chem>FCCOc1cc(N2CCN(CCCc3c4c(n(-c5ccc(F)cc5)c3)cccc4)CC2)ccc1</chem>

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