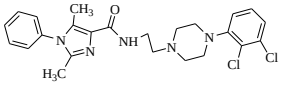
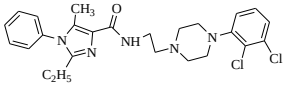
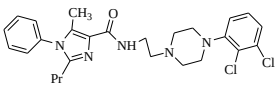
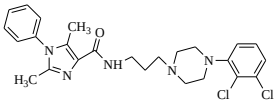
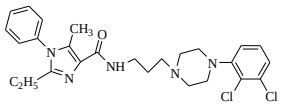
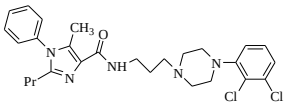
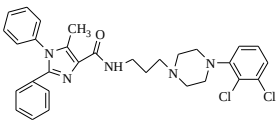
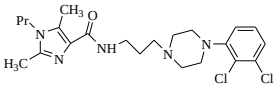
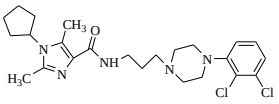
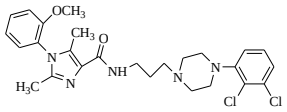
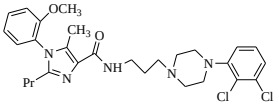
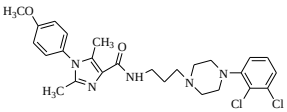
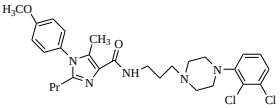
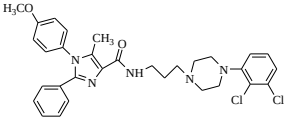
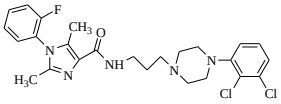
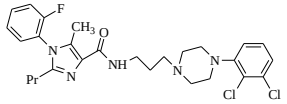
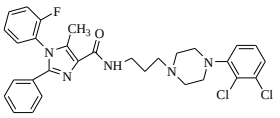
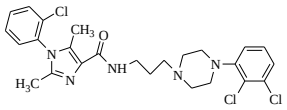
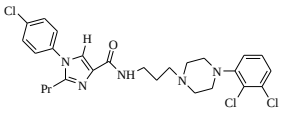
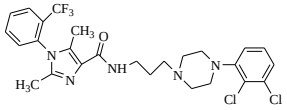
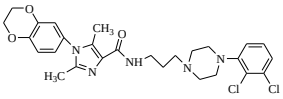
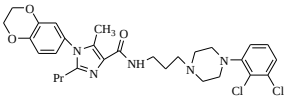
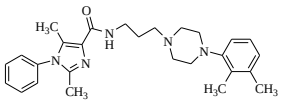
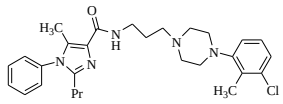
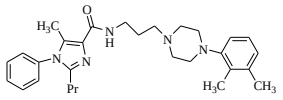
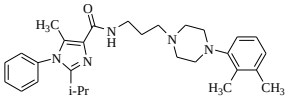
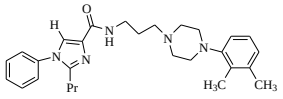
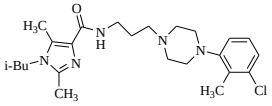
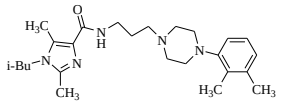
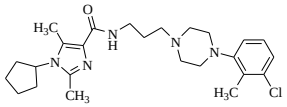
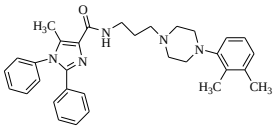
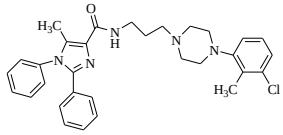
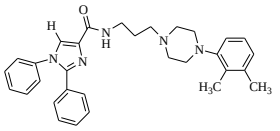
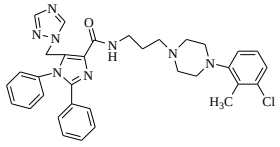
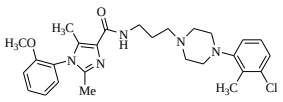
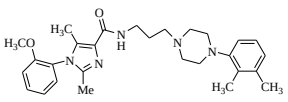
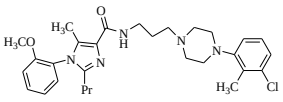
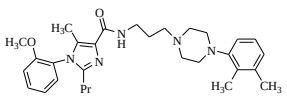
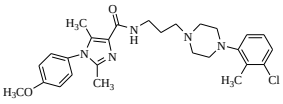
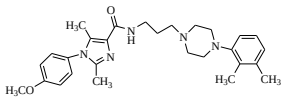
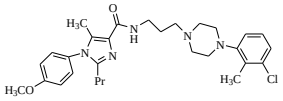
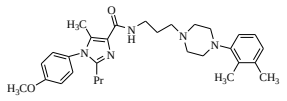
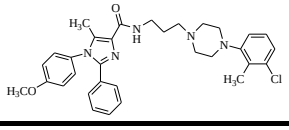
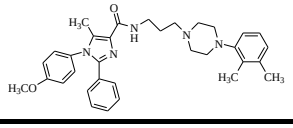
Mechanism Exploration of Arylpiperazine Derivatives Targeting the 5-HT$_{2A}$ Receptor by In Silico Methods

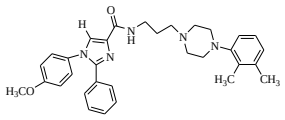
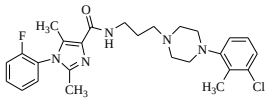
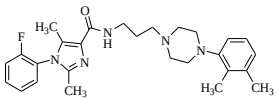
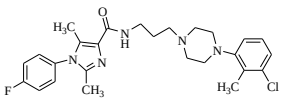
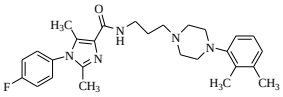
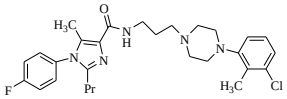
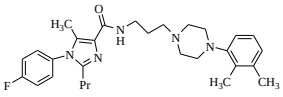
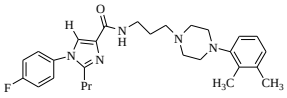
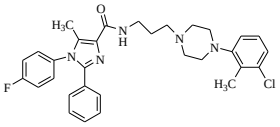
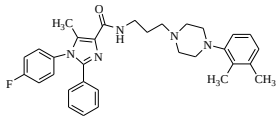
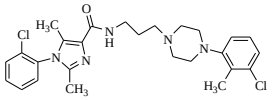
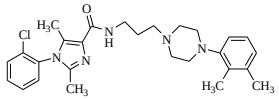
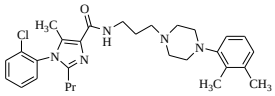
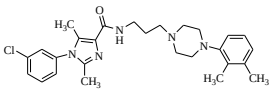
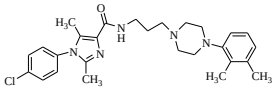
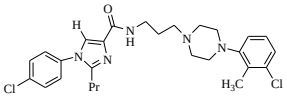
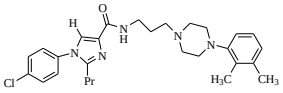
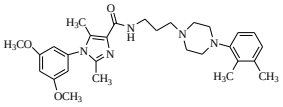
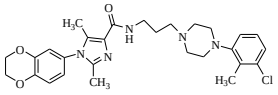
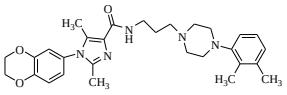
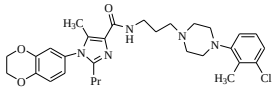
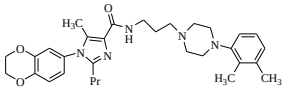
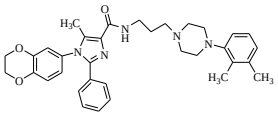
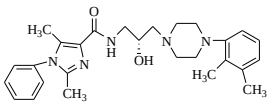
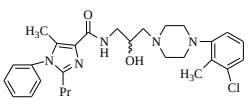
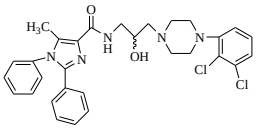
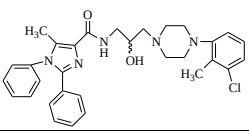
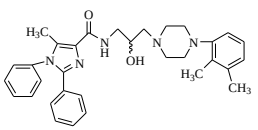
Feng Lin [1,2], Feng Li [3], Chao Wang [2], Jinghui Wang [2], Yinfeng Yang [2], Ling Yang [4] and Yan Li [1,2,*]

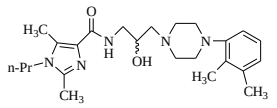
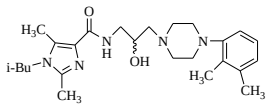
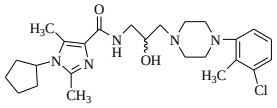
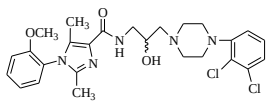
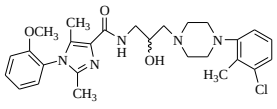
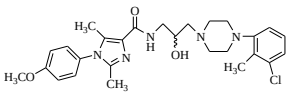
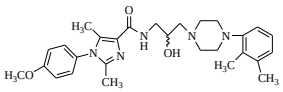
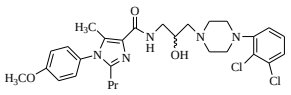
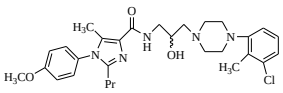
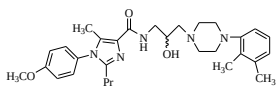
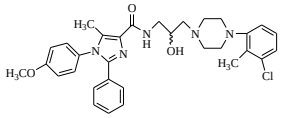
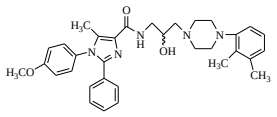
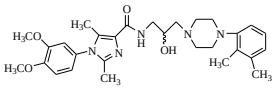
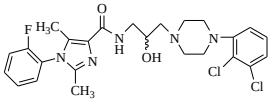
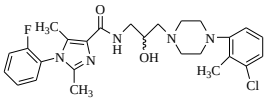
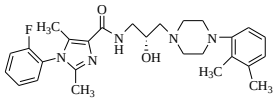
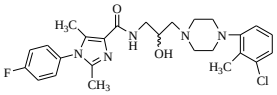
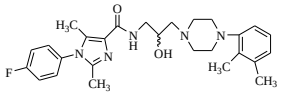
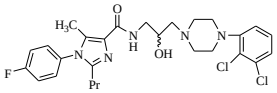
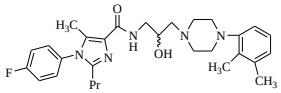
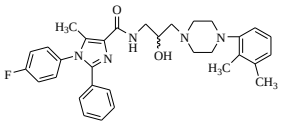
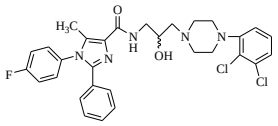
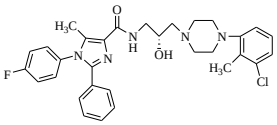
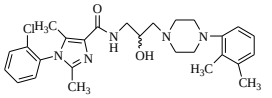
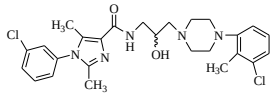
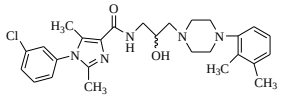
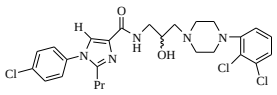
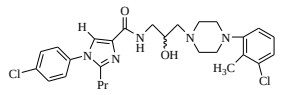
[1] Key Laboratory of Xinjiang Endemic Phytomedicine Resources, Pharmacy School, Shihezi University, Shihezi 832002, Xinjiang, China; fenglin_dut@yeah.net
[2] Key Laboratory of Industrial Ecology and Environmental Engineering (MOE), Faculty of Chemical, Environmental and Biological Science and Technology, Dalian University of Technology, Dalian 116024, Liaoning, China; chaowang_dlou@163.com (C.W.); jhwang_dlut@163.com (J.W.); yinfengyang@yeah.net (Y.Y.)
[3] Department of Civil Engineering, Henan Institute of Engineering, Zhengzhou 451191, Henan, China; fengli@haue.edu.cn
[4] Institute of Interdisciplinary Integrative Medicine Research, Shanghai University of Traditional Chinese Medicine, Shanghai 201203, China; yling@dicp.ac.cn
* Correspondence: yanli@dlut.edu.cn; Tel.: +86-0411-8498-6062

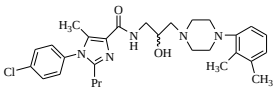
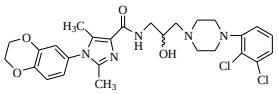
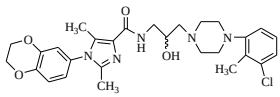
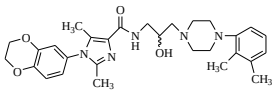
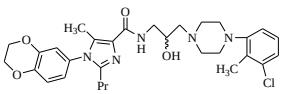
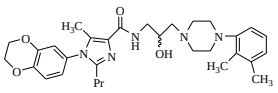
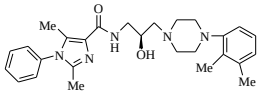
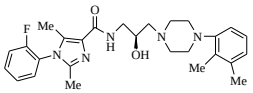
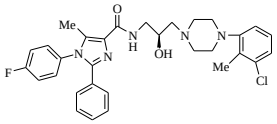
Table S1. Molecular structures and pIC$_{50}$ values of arylpiperazine derivatives.

No.	Structure	pIC$_{50}$ (M)	No.	Structure	pIC$_{50}$ (M)
1		7.509	2		7.569
3		7.409	4		7.730
5[t]		7.319	6		7.678
7		7.848	8[t]		7.585
9		7.260	10		7.987
11		6.857	12		7.699
13		8.287	14		7.886
15		7.775	16[t]		7.678

17[t]		7.710	18		7.523
19		7.149	20		7.237
21		8.064	22		6.975
23		7.041	24[t]		6.812
25		7.125	26		6.979
27[t]		6.876	28		7.342
29		6.664	30		7.094
31		7.532	32		7.857
33		7.879	34		7.910
35[t]		7.893	36		6.842
37[t]		6.767	38		6.597
39		7.636	40[t]		7.203
41[t]		7.818	42[t]		7.150
43		7.678	44		7.620

45		7.721	46[t]		7.398
47		7.188	48		7.420
49		6.928	50[t]		7.268
51		7.509	52		6.851
53[t]		7.914	54		7.556
55		7.538	56[t]		7.097
57		7.046	58		7.014
59		7.174	60[t]		7.699
61		7.489	62		7.495
63[t]		7.553	64		7.391
65		7.328	66		6.618
67		7.721	68[t]		7.140
69		6.697	70		7.620
71		7.244	72		7.232

73[t]		6.076	74		5.995
75		7.011	76		7.283
77		6.432	78[t]		7.252
79		6.757	80		7.200
81		6.235	82		6.900
83[t]		6.770	84		6.733
85		6.689	86[t]		6.983
87		6.706	88[t]		6.569
89		6.595	90		7.106
91		6.708	92[t]		6.485
93		7.149	94		7.027
95		7.022	96		6.498
97		6.740	98		6.561
99		6.753	100[t]		6.971

101		6.833	102		8.006
103		6.896	104[t]		6.635
105		6.625	106[t]		6.532
107		6.190	108		6.613
109		7.697			

[t] Compounds belonging to the test set.