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Electronic Supplementary Information (ESI)

Structure–activity relationship analysis of a series of nonsteroidal analogues as androgen receptor antagonists

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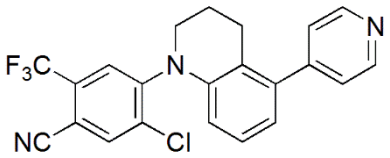
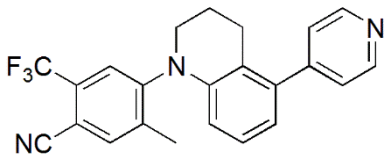
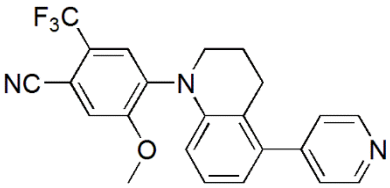
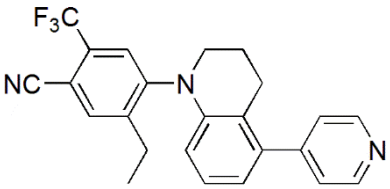
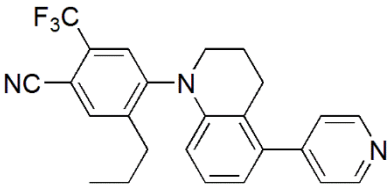
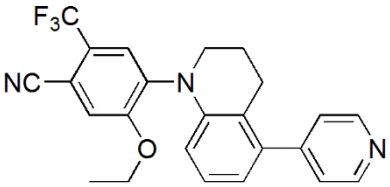
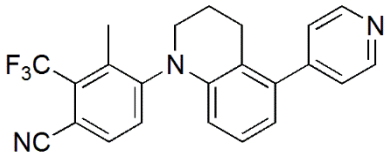
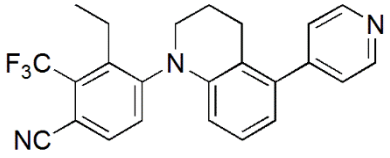
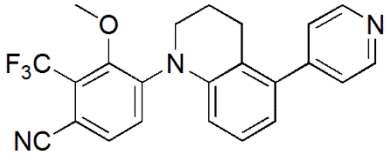
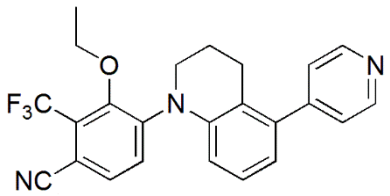
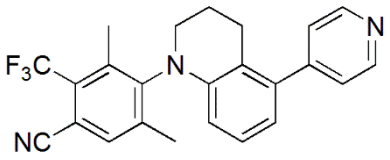
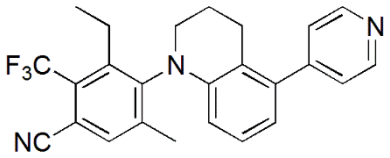
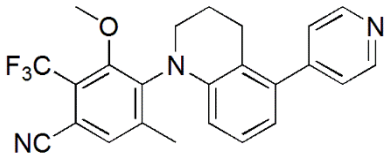
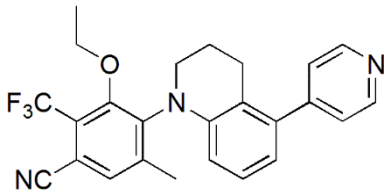
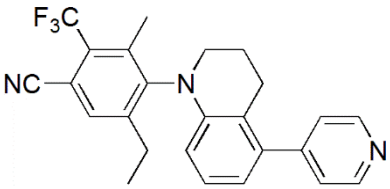
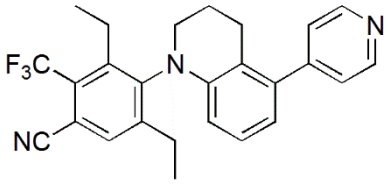
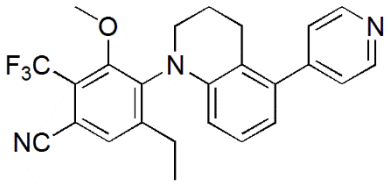
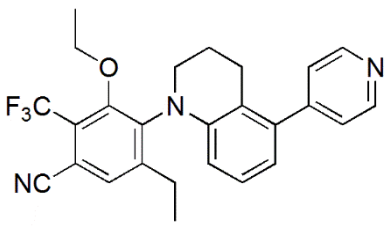
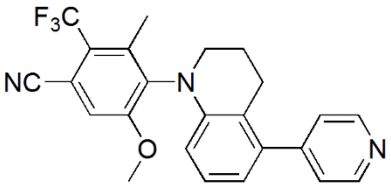
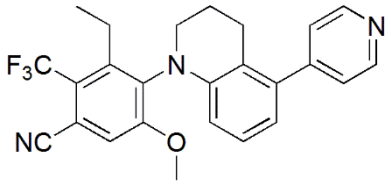
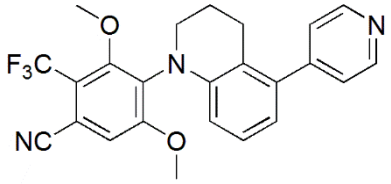
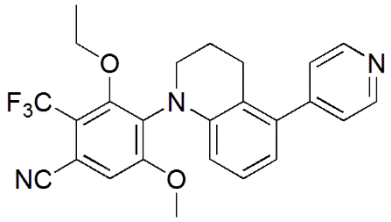
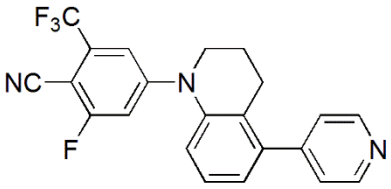
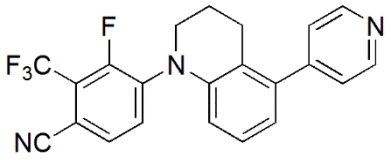
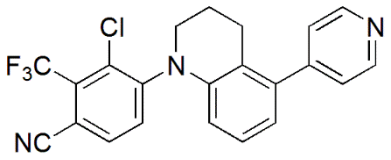
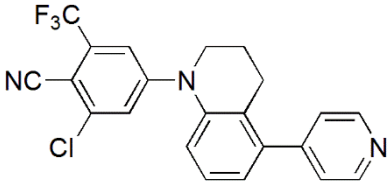
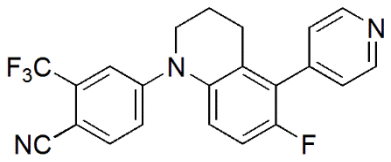
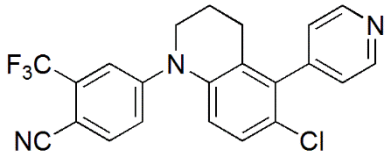
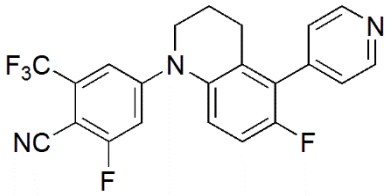
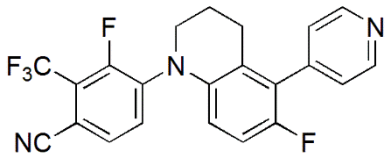
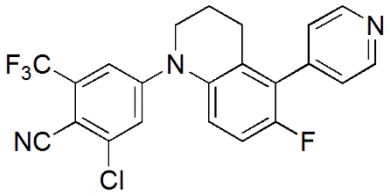
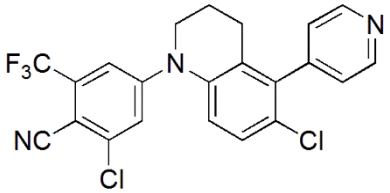
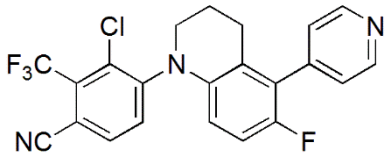
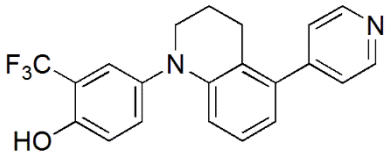
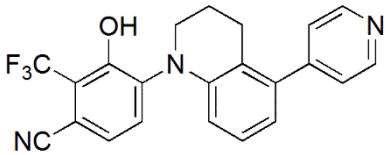
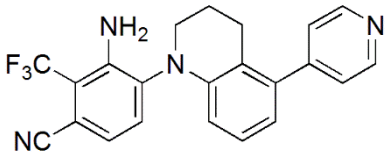
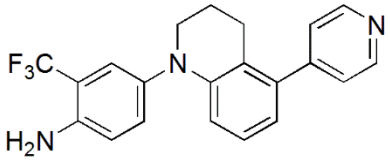
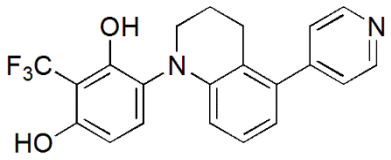
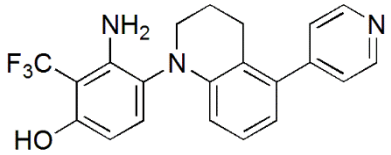
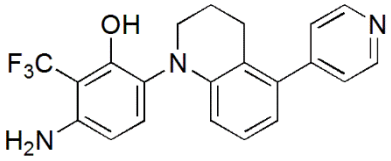
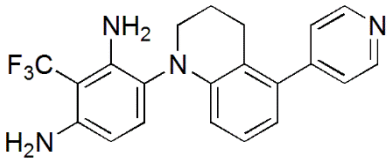
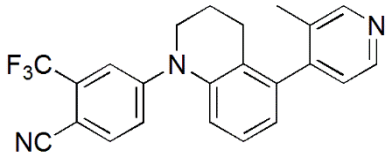
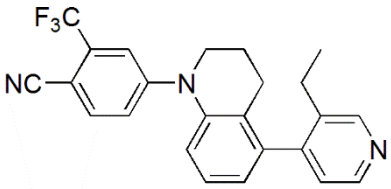
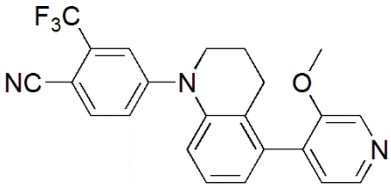
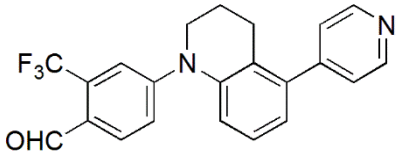
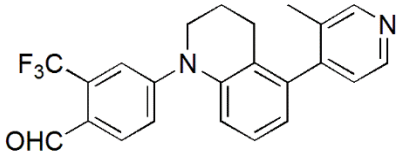
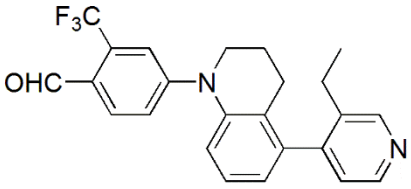
Table S1. The designed new molecules based on the constructed 3D-QSAR models.

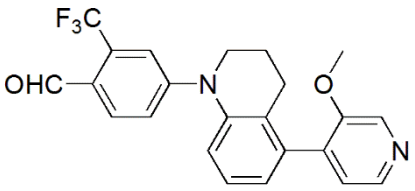
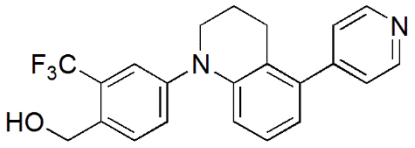
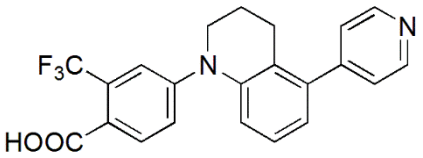
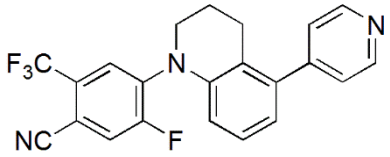
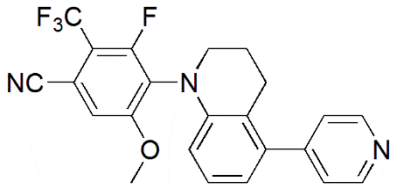
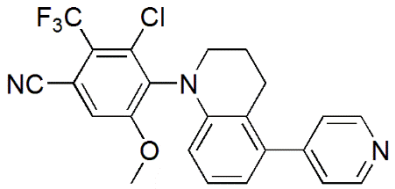
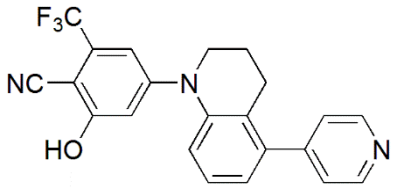
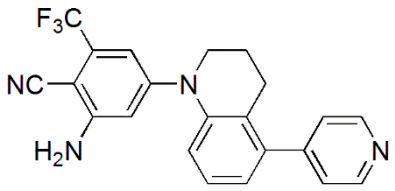
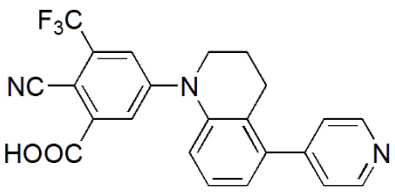
ID	Structure	Predicted pIC_{50}	
		CoMFA	CoMSIA
01* (D1)		7.198	7.211
02* (D2)		7.237	7.214
03* (D3)		7.250	7.240
04		6.878	7.021
05		6.958	7.061
06		7.146	7.259
07		7.025	7.135
08		6.753	7.005
09		6.937	7.075

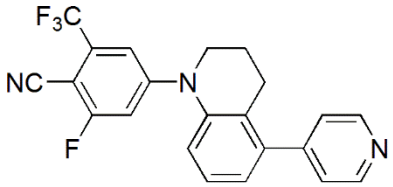
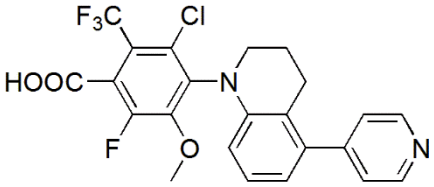
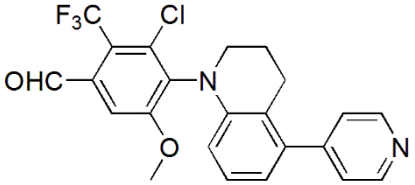
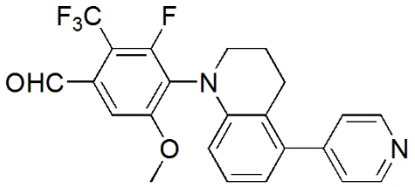
10		6.928	7.069
11		7.094	7.155
12		6.624	6.748
13		6.961	7.003
14		6.951	6.995
15		6.870	7.003
16		6.950	6.865
17		7.108	7.024
18		7.051	7.023

19		7.152	7.210
20		6.856	7.076
21		7.028	7.111
22		7.021	7.109
23		7.173	7.158
24* (D4)		7.222	7.197
25* (D5)		7.168	7.228
26		7.152	7.244
27		7.017	7.189

28		7.007	7.178
29		7.048	7.175
30		7.096	7.212
31		7.027	7.261
32		7.017	7.250
33		7.050	7.246
34		7.137	7.227
35		7.144	7.134
36		7.098	6.950
37		7.073	7.092

38		6.874	7.139
39		6.848	7.001
40		6.809	7.022
41		6.808	6.890
42		7.021	7.170
43		6.806	7.136
44		6.977	6.992
45* (D8)		7.191	7.334
46		7.066	7.332
47		6.858	7.300

48		7.026	7.155
49		6.923	7.223
50		6.881	6.792
51		7.143	7.207
52* (D6)		7.268	7.273
53* (D7)		7.285	7.309
54		7.067	7.037
55		7.107	6.955
56		7.148	7.263

57		7.174	7.157
58		7.199	7.164
59* (D9)		7.264	7.405
60* (D10)		7.324	7.422

*Selected novel compounds.