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Supplementary material to:

PROBING THE ORIGINS OF AROMATASE INHIBITORY ACTIVITY OF DISUBSTITUTED COUMARINS VIA QSAR AND MOLECULAR DOCKING

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Name	SMILES	MW	nHDon	nHAcc	ALOGP	IC50 (uM)
1	O=C1OC2=CC(OCC3=CC=CC=C3)=CC=C2C(CN4C=CN=C4)=C1	332,38	0	4	3,104	0,150
2	O=C1OC2=CC(OCC3=CC=CC(C)=C3)=CC=C2C(CN4C=CN=C4)=C1	346,41	0	4	3,59	0,114
3	O=C1OC2=CC(OCC3=CC=CC(F)=C3)=CC=C2C(CN4C=CN=C4)=C1	350,37	0	5	3,309	0,113
4	O=C1OC2=CC(OCC3=CC=CC(Cl)=C3)=CC=C2C(CN4C=CN=C4)=C1	366,82	0	4	3,768	0,130
5	O=C1OC2=CC(OCC3=CC=CC(C(F)(F)F)=C3)=CC=C2C(CN4C=CN=C4)=C1	400,38	0	7	4,046	0,235
6	O=C1OC2=CC(OCC3=CC=CC(OC(F)(F)F)=C3)=CC=C2C(CN4C=CN=C4)=C1	416,38	0	8	5,224	0,207
7	O=C1OC2=CC(OCC3=CC=CC([N+]([O-])=O)=C3)=CC=C2C(CN4C=CN=C4)=C1	377,38	0	6	2,998	0,141
8	O=C1OC2=CC(OCC3=CC=C(F)C=C3)=CC=C2C(CN4C=CN=C4)=C1	350,37	0	5	3,309	0,267
9	O=C1OC2=CC(OCC3=CC=C(Cl)C=C3)=CC=C2C(CN4C=CN=C4)=C1	366,82	0	4	3,768	0,178
10	O=C1OC2=CC(OCC3=CC=C(OC)C=C3)=CC=C2C(CN4C=CN=C4)=C1	362,41	0	5	3,087	0,127
11	O=C1OC2=CC(OCC3=CC=C(C=C3)OC(F)(F)F)=CC=C2C(CN4C=CN=C4)=C1	416,38	0	8	5,224	0,481
12	O=C1OC2=CC(OC3=CC=CC=C3)=CC=C2C(CN4C=CN=C4)=C1	318,35	0	4	3,097	0,169
13	O=C1OC2=CC(OCC3=CC=C(F)C(F)=C3)=CC=C2C(CN4C=CN=C4)=C1	368,36	0	6	3,515	0,165
14	O=C1OC2=CC(OC3=CC=CC=C3)=CC=C2C(CN4C=CN=C4)=C1	318,35	0	4	3,097	0,051
15	O=C1OC2=CC(OC3=CC=CC(F)=C3)=CC=C2C(CN4C=CN=C4)=C1	336,34	0	5	3,302	0,072
16	O=C1OC2=CC(OC3=CC=CC(Cl)=C3)=CC=C2C(CN4C=CN=C4)=C1	352,79	0	4	3,761	0,072
17	O=C1OC2=CC(OC3=CC=CC(OC)=C3)=CC=C2C(CN4C=CN=C4)=C1	348,38	0	5	3,08	0,292
18	O=C1OC2=CC(OC3=CC=C(C)C=C3)=CC=C2C(CN4C=CN=C4)=C1	332,38	0	4	3,583	0,690
19	O=C1OC2=CC(OC3=CC=C(Cl)C=C3)=CC=C2C(CN4C=CN=C4)=C1	352,79	0	4	3,761	0,112
20	O=C1OC2=CC(OC3=CC=C(C#N)C=C3)=CC=C2C(CN4C=CN=C4)=C1	343,36	0	5	2,976	0,164

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21	O=C1OC2=CC(OC3=CC=C(C(C)=O)C=C3)=CC=C2C(CN4C=CN=C4)=C1	360,39	0	5	2,837	0,296
22	O=C1OC2=CC(OC3=CC=C(N(C)C)C=C3)=CC=C2C(CN4C=CN=C4)=C1	361,43	0	5	3,259	0,081
23	O=C1OC2=CC(OC3=CC(F)=CC(F)=C3)=CC=C2C(CN4C=CN=C4)=C1	354,33	0	6	3,508	0,070
24	O=C1OC2=CC(OC3=CC=C(F)C(F)=C3)=CC=C2C(CN4C=CN=C4)=C1	354,33	0	6	3,508	0,047
25	O=C1OC2=CC(NC3=CC=CC=C3)=CC=C2C(CN4C=CN=C4)=C1	317,37	1	4	3,087	0,105
27	O=C1OC2=CC(OC)=CC=C2C(CN3C=CN=C3)=C1	256,28	0	4	1,52	0,280
28	O=C1OC2=CC(OC)=CC=C2C([C@@H](N3C=CN=C3)C4=CC=CC=C4)=C1	332,38	0	4	3,132	0,455
29	O=C1OC2=CC(OC3=CC=CC=C3)=CC=C2C([C@@H](N4C=CN=C4)C5=CC=CC=C5)=C1	394,45	0	4	4,709	0,067
30	O=C1OC2=CC(OC3=CC=C(F)C(F)=C3)=CC=C2C([C@@H](N4C=CN=C4)C5=CC=CC=C5)=C1	430,43	0	6	5,12	0,317
31	O=C1OC2=CC(OC3=CC=CC=C3)=CC=C2C([C@@H](N4C=CN=C4)C5=CC=C(Cl)C=C5)=C1	428,89	0	4	5,373	0,532
32	O=C1OC2=CC(OC3=CC=CC=C3)=CC=C2C([C@@H](N4C=CN=C4)C5=CC=C(C#N)C=C5)=C1	419,46	0	5	4,588	4,010
33	O=C1OC2=CC(OC)=CC=C2C=C1CN3C=NC=C3	256,28	0	4	1,52	2,820
34	O=C1OC2=CC(OC3=CC=CC=C3)=CC=C2C=C1[C@@H](C4=CC=CC=C4)N5C=NC=C5	394,45	0	4	4,709	0,313