

Table S1 SMILES notation for the ligands obtained within the presented study

Ligand	SMILES notation
2	<chem>ClC1=CC=CC=C1CNC(N2C)=NC3=C2C(N(CC)C(N3C)=O)=O</chem>
5	<chem>O=C1C2=C(N=C(NCC3=C(F)C=CC=C3Cl)N2C)N(C)C(N1CCC)=O</chem>
6	<chem>ClC1=CC=CC=C1CNC(N2C)=NC3=C2C(N(CCCC)C(N3C)=O)=O</chem>
7	<chem>ClC1=CC=CC=C1CNC(N2C)=NC3=C2C(N(CCCCC)C(N3C)=O)=O</chem>
8	<chem>ClC1=CC=CC=C1CNC(N2C)=NC3=C2C(N(CCCCCC)C(N3C)=O)=O</chem>
9	<chem>ClC1=CC=CC=C1CNC(N2C)=NC3=C2C(N(CC4=CC=CC=C4)C(N3C)=O)=O</chem>
10	<chem>ClC1=CC=CC=C1CNC(N2C)=NC3=C2C(N(CC4=CC=C(Cl)C=C4)C(N3C)=O)=O</chem>
11	<chem>ClC1=CC=CC=C1CNC(N2C)=NC3=C2C(N(CC4=CC(Cl)=C(Cl)C=C4)C(N3C)=O)=O</chem>
12	<chem>O=C1C2=C(N=C(NCC3=CC=CC=C3Br)N2C)N(C)C(N1CCC)=O</chem>
13	<chem>O=C1C2=C(N=C(NCC3=CC=CC=C3F)N2C)N(C)C(N1CCC)=O</chem>
14	<chem>O=C1C2=C(N=C(NCC3=C(F)C=CC=C3Cl)N2C)N(C)C(N1CCC)=O</chem>
15	<chem>O=C1C2=C(N=C(NCC3=CC=CC(Cl)=C3)N2C)N(C)C(N1CCC)=O</chem>
16	<chem>O=C1C2=C(N=C(NCC3=CC=CC(Br)=C3)N2C)N(C)C(N1CCC)=O</chem>
17	<chem>O=C1C2=C(N=C(NCC3=CC=CC(OC)=C3)N2C)N(C)C(N1CCC)=O</chem>
18	<chem>O=C1C2=C(N=C(NCC3=CC=C(OC)C(OC)=C3)N2C)N(C)C(N1CCC)=O</chem>
19	<chem>O=C1C2=C(N=C(NCC3=CC=CC=C3Cl)N2C)N(C)C(N1CC#C)=O</chem>
20	<chem>O=C1C2=C(N=C(NCC3=CC=CC=C3Br)N2C)N(C)C(N1CC#C)=O</chem>
21	<chem>O=C1C2=C(N=C(NCC3=CC=CC=C3F)N2C)N(C)C(N1CC#C)=O</chem>
22	<chem>O=C1C2=C(N=C(NCC3=C(F)C=CC=C3Cl)N2C)N(C)C(N1CC#C)=O</chem>
23	<chem>O=C1C2=C(N=C(NCC3=CC=CC(Cl)=C3)N2C)N(C)C(N1CC#C)=O</chem>
24	<chem>O=C1C2=C(N=C(NCC3=CC=CC(Br)=C3)N2C)N(C)C(N1CC#C)=O</chem>
25	<chem>O=C1C2=C(N=C(NCC3=CC=CC(OC)=C3)N2C)N(C)C(N1CC#C)=O</chem>
26	<chem>O=C1C2=C(N=C(NCC3=CC=C(OC)C(OC)=C3)N2C)N(C)C(N1CC#C)=O</chem>
27	<chem>O=C1C2=C(N=C(NCC3=CC=CC=C3Cl)N2C)N(C4CC4)C(N1CC#C)=O</chem>
28	<chem>O=C1C2=C(N=C(NCC3=CC=CC=C3F)N2C)N(C4CC4)C(N1CC#C)=O</chem>
29	<chem>O=C1C2=C(N=C(NCC3=C(F)C=CC=C3Cl)N2C)N(C4CC4)C(N1CC#C)=O</chem>