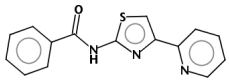
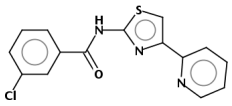
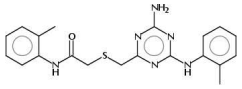
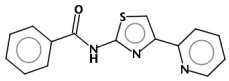
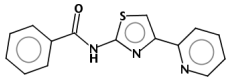
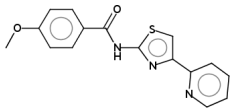
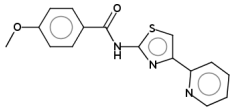
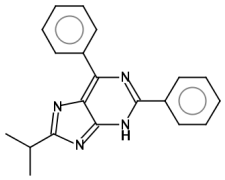
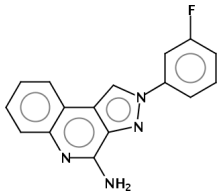
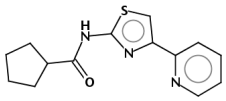
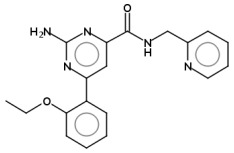
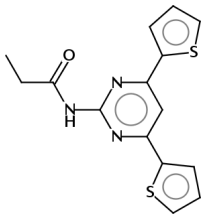
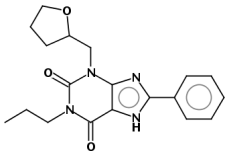
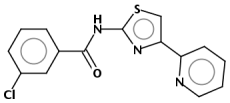
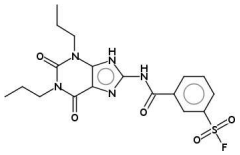
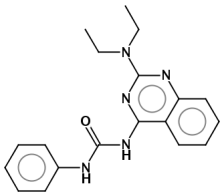
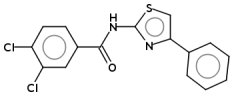
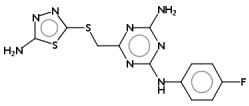
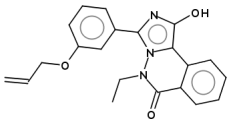
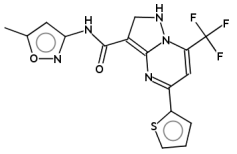
Table S2: Compounds in ChEMBL most similar to the ligands identified in this study.

ID	Closest ChEMBL	sim_T	2D-Structure
7	CHEMBL164087	0.53	
8	CHEMBL163040	0.64	
9	CHEMBL605584	0.47	
10	CHEMBL164087	0.57	
11	CHEMBL164087	0.56	
12	CHEMBL165784	0.72	
13	CHEMBL165784	0.60	
14	CHEMBL204780	0.25	
15	CHEMBL321441	0.30	
16	CHEMBL162808	0.46	
17	CHEMBL611964	0.49	
18	CHEMBL1650339	0.41	

continued on next page

Table S2 continued

19	CHEMBL597167	0.41	
20	CHEMBL163040	0.71	
21	CHEMBL93600	0.39	
22	CHEMBL305516	0.32	
23	CHEMBL293437	0.50	
24	CHEMBL600404	0.42	
25	CHEMBL1097489	0.30	
26	CHEMBL1098786	0.27