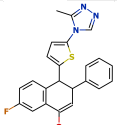
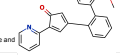
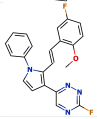
RAW RNN SMILES	SCORE	Notes	2D	EC50Chembl(uM)	Ion Regulation Activity	Most Acidic pKa	Most Basic pKa	Ptal EC50 (Inh)	Ptal (3D7) IC50 (Broad)	Ptal (Dd2) IC50 (Broad)	Ptal (K1) IC50 (Avery)	Ptal (K1) IC50 (Guy)	Ptal IC50 (Avery)	Ptal IC50 (Dundee)	Ptal IC50 (GSK)	Ptal IC50 (Guy)	Ptal IC50 (Ralph)	Ptal IC50 (Syngene)	Single Shot Inhibition %	logS	logS @ pH7.4	logD	2C9 pKi	hERG pIC50	BBB log[[brain]:[blood]]
CC1=C(C=C2CCC(c3ccccc3OC)C(=C2S1)c4ccccc4F)n5cnnc5	0.0427	The aromatic ring with a sulphur would be considered unusual and one would wonder how prone to oxidation that might be		5.944	0.2544	6.984	4.684	5.776	6.23	6.15	6.062	5.974	7.558	5.374	7.232	6.274	7.542	5.648	61.35	-0.784	0.0864	4.989	5.93	5.854	-0.0945
Cc1nncn1-c2ccc(s2)C3c4ccc(cc4C(=CC3c5ccccc5)OC)F	0.04102	This compound is OK but the fact that you have a saturated bond between the phenyl bearing carbon and the thiophene bearing carbon would make one think that this would oxidise and make the aromatic naphthalene ring. Also you haven't indicated stereochemistry here, does that matter to your model (I would guess not but there are 4 possible compounds which match this structure and all would be quite different conformationally)		5.822	0.4428	7.02	4.918	5.889	5.93	5.849	6.09	6.005	7.587	5.403	7.126	6.285	7.3	5.673	74.95	-0.2528	-0.0164	5.053	6.09	5.879	-0.2361
COc1ccc(cc1-c2ccccc2/C/3=C/C(=O)/C(=C3)/c4ccccn4)F	0.04021	Cyclopentadienone is unstable and will polymerise in solution.		6.325	0.0545	7.22	3.719	5.975	6.334	6.344	5.731	5.812	7.578	5.457	7.109	6.2	7.407	5.92	57.24	-0.7848	-0.3093	4.213	5.922	5.326	-0.0945
MODIFIED RNN SMILES	SCORE		2D	EC50Chembl(uM)_1	Ion Regulation Activity_1	Most Acidic pKa_1	Most Basic pKa_1	Ptal EC50 (Inh)_1	Ptal (3D7) IC50 (Broad)_1	Ptal (Dd2) IC50 (Broad)_1	Ptal (K1) IC50 (Avery)_1	Ptal (K1) IC50 (Guy)_1	Ptal IC50 (Avery)_1	Ptal IC50 (Dundee)_1	Ptal IC50 (GSK)_1	Ptal IC50 (Guy)_1	Ptal IC50 (Ralph)_1	Ptal IC50 (Syngene)_	Single Shot Inhibition %_1	logS_1	logS @ pH7.4_1	logD_1	2C9 pKi_1	hERG pIC50_1	BBB log[[brain]:[blood]]_1
CS/C1=C(/C=C\N(c2ccccc2)/C(=C1)c3ccc(cc3)OC(F)F)n4ccnc4	0.02257			5.835	0.1805	7.001	4.819	5.675	6.053	5.853	5.821	5.702	7.245	5.344	7.265	6.029	7.388	5.937	58.25	-0.3236	0.3102	4.476	5.914	5.725	0.1686
CC1=C(C=C2C(=O(c3ccccc3F)/C(=C\O2)/c4ccccc4OC)S1)n5cnnc5	0.01277			5.99	0.0856	6.995	5.128	5.716	5.858	5.651	6.3	5.523	6.883	5.176	7.219	5.813	7.109	5.344	49.33	-0.3099	0.4872	3.715	5.854	5.517	-0.2398
COc1ccc(cc1C=Cc2o(con2-c3ccccc3)-c4ccc(nn4)F)F	0.01206			5.947	0.2702	7.003	4.602	5.898	6.32	6.322	5.903	5.571	6.188	5.454	6.22	5.82	6.483	6.083	31.8	-0.7378	-0.6311	4.656	6.023	6.012	-0.1973