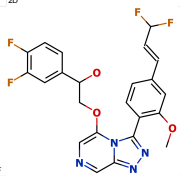
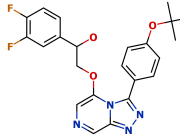


Notes	SMILES	2D	EC50	Chembi	(uM Ion Regulation A)	Most Acidic pKa	Most Basic pKa	Pfal	EC50 (Inh)	Pfal	(3D7)	IC50	(Pfal	(Dd2)	IC50	(Pfal	(K1)	IC50	(A Pfal	(K1)	IC50	(G Pfal	IC50	(Avery)	Pfal	IC50	(Dunde	Pfal	IC50	(GSK)	Pfal	IC50	(Gay)	Pfal	IC50	(Ralph)	Pfal	IC50	(Syngae	Single Shot	Inhib	logS	logS	@	pH7.4	logD	2C9	pKi_1	HERG	pIC50_1	BBB	log[brain]
Best molecule predicted	<chem>COc1c(ccc1c2nc3ncoc(n3)OCC)(c4cc(c(c4)F)F)O)C=CC(F)F</chem>		5.743	0.92	10.15	4.646	6.809	5.973	5.819	6.3	6.005	6.316	6.605	6.316	6.605	6.536	6.159	6.653	6.362	69.62	-0.0123	0.0393	3.575	6.083	6.072	-0.4706																										
Best molecule predicted which does not contain CHF2	<chem>CC(C)C(O)C1cc(c(c1)c2nc3ncoc(n3)OCC)(c4cc(c(c4)F)F)O</chem>		5.856	0.91	11.36	4.653	7.174	6.259	6.004	6.143	5.995	5.311	6.418	6.474	6.165	6.371	6.389	84.49	0.1353	0.0909	3.699	6.062	6.16	-0.4527																												