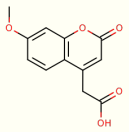
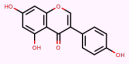
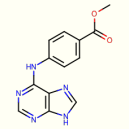
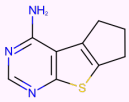
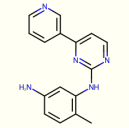
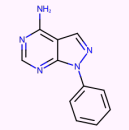
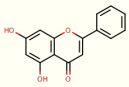
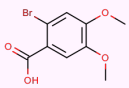
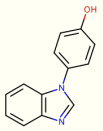
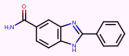
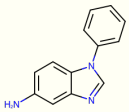
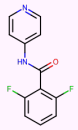
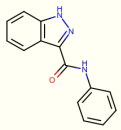
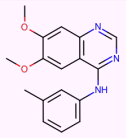
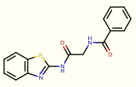
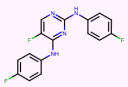
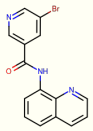
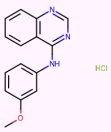
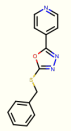
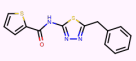
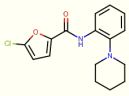
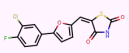
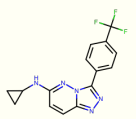
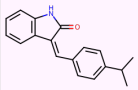
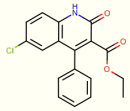
df_frag_final_oe.csv								
Molecule	pKas in [3,11]	XlogP	MolWt	Availability (mg)	Price ($/100 mg)	N_Rot	eMolecules ID	eMolecules SMILES
	[3.621]	0.67	234.21	3439.8	223.0	3	490595	COc1ccc2c(c1)oc(=O)cc2CC(=O)O
	[8.584, 9.84, 10.869]	0.89	270.24	1015.0	168.0	1	532754	Oc1ccc(cc1)c1coc2c(c1=O)c(O)cc(c2)O
	[3.923, 9.999]	0.85	269.26	108.0	275.0	4	4934119	COC(=O)c1ccc(cc1)Nc1ncnc2c1nc[nH]2
	[4.048]	1.04	191.25	1026.0	168.0	0	2867544	Nc1ncnc2c1c1CCCc1s2
	[3.887, 4.98]	1.30	277.32	101.1	400.0	3	2727697	Nc1ccc(c(c1)Nc1nccc(n1)c1cccnc1)C
	[3.869]	1.50	211.22	3430.0	414.0	1	719540	Nc1ncnc2c1cnn2c1ccccc1
	[8.416, 10.823]	1.71	254.24	1056.0	168.0	1	493608	Oc1cc(O)c2c(c1)oc(cc2=O)c1ccccc1
	[3.005]	1.70	261.07	10134.0	168.0	3	508324	COc1cc(C(=O)O)c(cc1OC)Br
	[5.82, 8.709]	2.22	210.23	21650.2	148.0	1	37095168	Oc1ccc(cc1)n1cnc2c1cccc2
	[6.342]	2.19	237.26	2000.0	168.0	2	37053191	NC(=O)c1ccc2c(c1)nc([nH]2)c1ccccc1
	[6.348]	2.33	209.25	50213.0	148.0	1	31653344	Nc1ccc2c(c1)ncn2c1ccccc1
	[4.714, 10.538]	2.30	234.20	100.0	168.0	3	2042282	O=C(c1c(F)cccc1F)Nc1ccncc1

	[8.398]	2.64	237.26	762.8	223.0	3	13419113	O=C(c1n[nH]c2c1cccc2)Nc1ccccc1
	[4.267]	2.60	295.34	1864.0	414.0	4	5828805	COc1cc2c(ncnc2cc1OC)Nc1cccc(c1)C
	[8.672]	2.72	311.36	149.1	148.0	6	23354217	O=C(Nc1nc2c(s1)cccc2)CNC(=O)c1ccccc1
	[3.892]	2.81	316.28	105.0	168.0	4	1698122	Fc1ccc(cc1)Nc1ncc(c(n1)Nc1ccc(cc1)F)F
	[4.001, 10.328]	2.92	328.16	406.0	148.0	3	18893169	Brc1cncc(c1)C(=O)Nc1cccc2c1nccc2
	[4.05]	3.14	287.74	119.7	148.0	3	1865544	COc1cccc(c1)Nc1ncnc2c1cccc2.Cl
	[4.902]	3.31	269.32	170.0	168.0	4	1444229	c1ccc(cc1)CSc1nnc(o1)c1ccncc1
	[7.12]	3.61	301.39	379.0	148.0	5	1228629	O=C(c1cccs1)Nc1nnc(s1)Cc1ccccc1
	[5.346]	3.79	304.77	424.3	148.0	4	18908671	Clc1ccc(o1)C(=O)Nc1ccccc1N1CCCCC1
	[8.052]	3.91	323.73	125.0	168.0	2	25775231	O=C1S/C(=C/c2ccc(o2)c2ccc(c(c2)Cl)F)/C(=O)N1
	[4.394]	4.13	319.28	3175.0	414.0	4	5784088	FC(c1ccc(cc1)c1nnc2n1nc(cc2)NC1CC1)(F)F

	[3.158]	4.23	263.33	283.7	400.0	2	45809595	O=C1Nc2c(/C/1=C/c1ccc(cc1)C(C)C)cccc2
	[8.549]	4.52	327.76	1059.0	168.0	4	703997	CCOC(=O)c1c(=O)[nH]c2c(c1c1ccccc1)cc(cc2)Cl