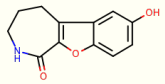
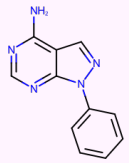
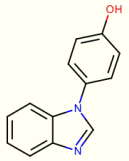
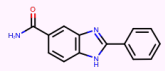
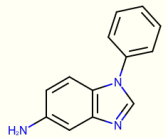
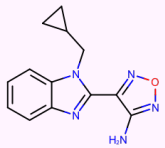
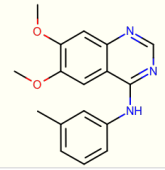
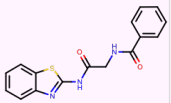
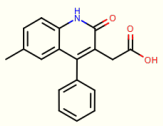
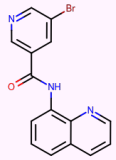
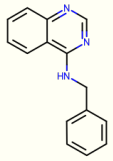
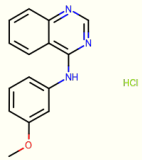
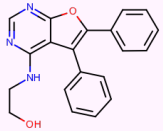
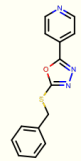
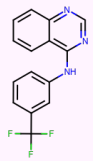
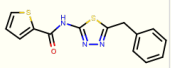
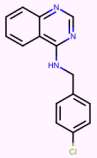
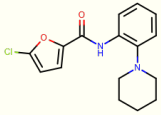
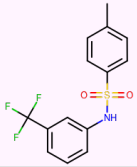
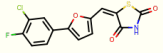
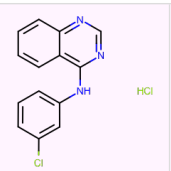
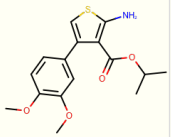
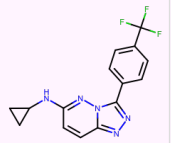
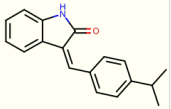
df_frag_final_oe.csv														
Molecule	pKas in [3,11]	XlogP	MolWt	Availability (mg)	Price	group	N_Rot	N_UV_chrom	Selection	Bin index	Priority	Final list	eMolecules SMILES	canonical isomeric SMILES
	[9.119]	0.72	217.221	184.0	533.0	fragment-like	0	27	picked	4	1	True	Oc1cc2c3CCCNC(=O)c3oc2cc1	c1cc2c(cc1O)c3c(o2)C(=O)NCCC3
	[3.869]	1.50	211.223	3430.0	414.0	fragment-like	1	31	picked	8	1	True	Nc1ncnc2c1cnn2c1ccccc1	c1ccc(cc1)n2c3c(cn2)c(ncn3)N
	[5.82, 8.709]	2.22	210.231	21650.2	148.0	fragment-like	1	40	picked	11	1	True	Oc1ccc(cc1)n1cnc2c1cccc2	c1ccc2c(c1)ncn2c3ccc(cc3)O
	[6.342]	2.19	237.257	2000.0	168.0	fragment-like	2	42	picked	11	2	True	NC(=O)c1ccc2c(c1)nc([nH]2)c1ccccc1	c1ccc(cc1)c2[nH]c3ccc(cc3n2)C(=O)N
	[6.348]	2.33	209.247	50213.0	148.0	fragment-like	1	40	picked	12	1	True	Nc1ccc2c(c1)ncn2c1ccccc1	c1ccc(cc1)n2cnc3c2ccc(c3)N
	[4.082]	2.44	255.275	300.0	168.0	fragment-like	3	28	picked	12	2	True	Nc1nonc1c1nc2c(n1CC1CC1)cccc2	c1ccc2c(c1)nc(n2CC3CC3)c4c(non4)N
	[4.267]	2.60	295.336	1864.0	414.0	fragment-like	4	36	picked	13	2	True	COc1cc2c(ncnc2cc1OC)Nc1cccc(c1)C	Cc1cccc(c1)Nc2c3cc(c(cc3ncn2)OC)OC

	[8.672]	2.72	311.358	149.1	148.0	fragment-like	6	28	picked	14	1	True	O=C(Nc1nc2c(s1)cccc2)CNC(=O)c1ccccc1	c1ccc(cc1)C(=O)NCC(=O)Nc2nc3ccccc3s2
	[4.109]	2.80	293.317	232.1	223.0	fragment-like	3	59	picked	14	2	True	OC(=O)Cc1c(=O)[nH]c2c(c1c1ccccc1)cc(cc2)C	Cc1ccc2c(c1)c(c(c(=O)[nH]2)CC(=O)O)c3ccccc3
	[4.001, 10.328]	2.92	328.163	406.0	148.0	fragment-like	3	37	picked	15	1	True	Brc1cncc(c1)C(=O)Nc1cccc2c1nccc2	c1cc2cccnc2c(c1)NC(=O)c3cc(cnc3)Br
	[5.564]	2.91	235.284	208.7	223.0	fragment-like	3	36	picked	15	2	True	c1ccc(cc1)CNc1ncnc2c1cccc2	c1ccc(cc1)CNc2c3ccccc3ncn2
	[4.714, 9.847]	2.93	267.111	385.0	275.0	fragment-like	3	20	picked	15	3	True	O=C(c1c(Cl)cccc1Cl)Nc1ccncc1	c1cc(c(c(c1)Cl)C(=O)Nc2ccncc2)Cl
	[4.05]	3.14	287.744	119.7	148.0	fragment-like	3	36	picked	16	1	True	COc1cccc(c1)Nc1ncnc2c1cccc2.Cl	COc1cccc(c1)Nc2c3ccccc3ncn2.Cl
	[4.294]	3.08	331.368	159.0	168.0	fragment-like	5	71	picked	16	2	True	OCCNc1ncnc2c1c(c1ccccc1)c(o2)c1ccccc1	c1ccc(cc1)c2c3c(ncnc3oc2c4ccccc4)NCCO

	[4.902]	3.31	269.322	170.0	168.0	fragment-like	4	30	picked	17	1	True	c1ccc(cc1)CSc1nnc(o1)c1ccncc1	c1ccc(cc1)CSc2nnc(o2)c3ccncc3
	[4.05]	3.27	289.255	101.0	355.0	fragment-like	3	36	picked	17	2	True	FC(c1cccc(c1)Nc1ncnc2c1cccc2)(F)F	c1ccc2c(c1)c(ncn2)Nc3cccc(c3)C(F)(F)F
	[7.12]	3.61	301.387	379.0	148.0	fragment-like	5	14	picked	18	1	True	O=C(c1cccs1)Nc1nnc(s1)Cc1ccccc1	c1ccc(cc1)Cc2nnc(s2)NC(=O)c3cccs3
	[5.564]	3.52	269.729	415.5	148.0	fragment-like	3	36	picked	18	2	True	Clc1ccc(cc1)CNc1ncnc2c1cccc2	c1ccc2c(c1)c(ncn2)NCc3ccc(cc3)Cl
	[5.346]	3.79	304.771	424.3	148.0	fragment-like	4	18	picked	19	1	True	Clc1ccc(o1)C(=O)Nc1ccccc1N1CCCCC1	c1ccc(c(c1)NC(=O)c2ccc(o2)Cl)N3CCCCC3
	[7.903]	3.75	315.311	527.0	168.0	fragment-like	4	24	picked	19	2	True	Cc1ccc(cc1)S(=O)(=O)Nc1cccc(c1)C(F)(F)F	Cc1ccc(cc1)S(=O)(=O)Nc2cccc(c2)C(F)(F)F
	[8.052]	3.91	323.727	125.0	168.0	fragment-like	2	31	picked	20	1	True	O=C1S/C(=C/c2ccc(o2)c2ccc(c(c2)Cl)F)/C(=O)N1	c1cc(c(cc1c2ccc(o2)/C=C/3\C(=O)NC(=O)S3)Cl)F

	[4.05]	3.90	292.163	7366.0	414.0	fragment-like	2	36	picked	20	2	True	Clc1cccc(c1)Nc1ncnc2c1cccc2.Cl	c1ccc2c(c1)c(ncn2)Nc3cccc(c3)Cl.Cl
	[10.184]	4.08	321.391	10117.0	168.0	fragment-like	6	28	picked	21	1	True	COc1cc(ccc1OC)c1csc(c1C(=O)OC(C)C)N	CC(C)OC(=O)c1c(csc1N)c2ccc(c(c2)OC)OC
	[4.394]	4.13	319.284	3175.0	414.0	fragment-like	4	32	picked	21	2	True	FC(c1ccc(cc1)c1nnc2n1nc(cc2)NC1CC1)(F)F	c1cc(ccc1c2nnc3n2nc(cc3)NC4CC4)C(F)(F)F
	[3.158]	4.23	263.334	283.7	400.0	fragment-like	2	24	picked	22	1	True	O=C1Nc2c(/C/1=C/c1ccc(cc1)C(C)C)cccc2	CC(C)c1ccc(cc1)/C=C\2/c3ccccc3NC2=O