df_frag_final_oe.csv									
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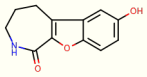
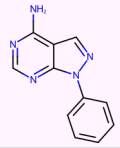
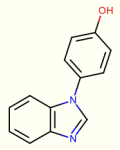
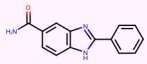
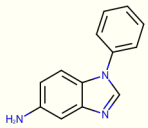
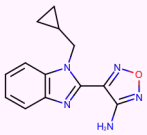
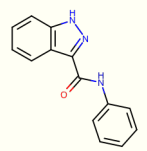
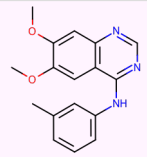
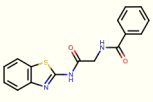
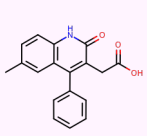
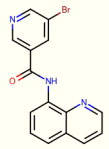
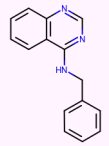
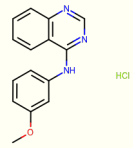
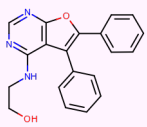
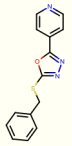
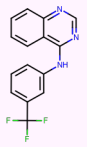
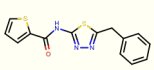
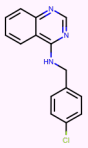
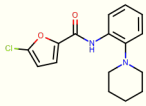
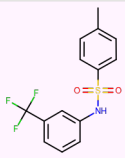
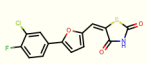
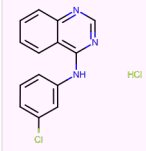
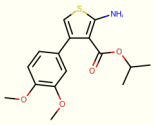
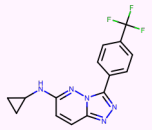
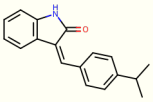
	Oc1cc2c3CCCNC(=O)c3oc2cc1	[9.119]	0.7199999690055847	217.221	184.0	533.0	0	c1cc2c(cc1O)c3c(o2)C(=O)NCCC3	6679830
	Nc1ncnc2c1cnn2c1ccccc1	[3.869]	1.4990001916885376	211.223	3430.0	414.0	1	c1ccc(cc1)n2c3c(cn2)c(ncn3)N	719540
	Oc1ccc(cc1)n1cnc2c1cccc2	[5.82, 8.709]	2.2190003395080566	210.231	21650.2	148.0	1	c1ccc2c(c1)ncn2c3ccc(cc3)O	37095168
	NC(=O)c1ccc2c(c1)nc([nH]2)c1ccccc1	[6.342]	2.1920003890991206	237.257	2000.0	168.0	2	c1ccc(cc1)c2[nH]c3ccc(cc3n2)C(=O)N	37053191
	Nc1ccc2c(c1)ncn2c1ccccc1	[6.348]	2.3329999446868896	209.247	50213.0	148.0	1	c1ccc(cc1)n2cnc3c2ccc(c3)N	31653344
	Nc1nonc1c1nc2c(n1CC1CC1)cccc2	[4.082]	2.43999981880188	255.275	300.0	168.0	3	c1ccc2c(c1)nc(n2CC3CC3)c4c(non4)N	8332960
	O=C(c1n[nH]c2c1cccc2)Nc1ccccc1	[8.398]	2.6429998874664307	237.257	762.8	223.0	3	c1ccc(cc1)NC(=O)c2c3ccccc3[nH]n2	13419113
	COc1cc2c(ncnc2cc1OC)Nc1cccc(c1)C	[4.267]	2.5950002670288086	295.336	1864.0	414.0	4	Cc1cccc(c1)Nc2c3cc(c(cc3ncn2)OC)OC	5828805
	O=C(Nc1nc2c(s1)cccc2)CNC(=O)c1ccccc1	[8.672]	2.7179999351501465	311.358	149.1	148.0	6	c1ccc(cc1)C(=O)NCC(=O)Nc2nc3ccccc3s2	23354217
	OC(=O)Cc1c(=O)[nH]c2c(c1c1ccccc1)cc(cc2)C	[4.109]	2.8030002117156982	293.317	232.1	223.0	3	Cc1ccc2c(c1)c(c(c(=O)[nH]2)CC(=O)O)c3ccccc3	1367649

	Brc1cncc(c1)C(=O)Nc1cccc2c1nccc2	[4.001, 10.328]	2.922999620437622	328.163	406.0	148.0	3	c1cc2cccnc2c(c1)NC(=O)c3cc(cnc3)Br	18893169
	c1ccc(cc1)CNc1ncnc2c1cccc2	[5.564]	2.9070003032684326	235.284	208.7	223.0	3	c1ccc(cc1)CNc2c3ccccc3ncn2	1327878
	COc1cccc(c1)Nc1ncnc2c1cccc2.Cl	[4.05]	3.138999938964844	287.744	119.7	148.0	3	COc1cccc(c1)Nc2c3ccccc3ncn2.Cl	1865544
	OCCNc1ncnc2c1c(c1ccccc1)c(o2)c1ccccc1	[4.294]	3.0820000171661377	331.36800000000005	159.0	168.0	5	c1ccc(cc1)c2c3c(ncnc3oc2c4ccccc4)NCCO	1415762
	c1ccc(cc1)CSc1nnc(o1)c1ccncc1	[4.902]	3.3059999942779537	269.322	170.0	168.0	4	c1ccc(cc1)CSc2nnc(o2)c3ccncc3	1444229
	FC(c1cccc(c1)Nc1ncnc2c1cccc2)(F)F	[4.05]	3.2689995765686035	289.255	101.0	355.0	3	c1ccc2c(c1)c(ncn2)Nc3cccc(c3)C(F)(F)F	1327907
	O=C(c1cccs1)Nc1nnc(s1)Cc1ccccc1	[7.12]	3.6050002574920654	301.387	379.0	148.0	5	c1ccc(cc1)Cc2nnc(s2)NC(=O)c3cccs3	1228629
	Clc1ccc(cc1)CNc1ncnc2c1cccc2	[5.564]	3.523000240325928	269.72900000000004	415.5	148.0	3	c1ccc2c(c1)c(ncn2)NCc3ccc(cc3)Cl	30719859
	Clc1ccc(o1)C(=O)Nc1ccccc1N1CCCCC1	[5.346]	3.794999837875366	304.771	424.3	148.0	4	c1ccc(c(c1)NC(=O)c2ccc(o2)Cl)N3CCCCC3	18908671
	Cc1ccc(cc1)S(=O)(=O)Nc1cccc(c1)C(F)(F)F	[7.903]	3.747999668121338	315.311	527.0	168.0	4	Cc1ccc(cc1)S(=O)(=O)Nc2cccc(c2)C(F)(F)F	1377874
	O=C1S/C(=C/c2ccc(o2)c2ccc(c(c2)Cl)F)/C(=O)N1	[8.052]	3.9079997539520255	323.72700000000001	125.0	168.0	2	c1cc(c(cc1c2ccc(o2)/C=C/3\C(=O)NC(=O)S3)Cl)F	25775231

	Clc1cccc(c1)Nc1ncnc2c1cccc2.Cl	[4.05]	3.89900016784668	292.163	7366.0	414.0	2	c1ccc2c(c1)c(ncn2)Nc3cccc(c3)Cl.Cl	1859493
	COc1cc(ccc1OC)c1csc(c1C(=O)OC(C)C)N	[10.184]	4.079999923706056	321.391	10117.0	168.0	6	CC(C)OC(=O)c1c(csc1N)c2ccc(c(c2)OC)OC	837243
	FC(c1ccc(cc1)c1nnc2n1nc(cc2)NC1CC1)(F)F	[4.394]	4.128999710083009	319.284	3175.0	414.0	4	c1cc(ccc1c2nnc3n2nc(cc3)NC4CC4)C(F)(F)F	5784088
	O=C1Nc2c(/C/1=C/c1ccc(cc1)C(C)C)cccc2	[3.158]	4.2330002784728995	263.334	283.7	400.0	2	CC(C)c1ccc(cc1)/C=C\2/c3ccccc3NC2=O	45809595