df_drug_final_supplier_oe.csv

Molecule	eMolecules SMILES	pKas in [3,11]	XlogP	MolWt	Availability (mg)	Price	group	N_Rot	N_UV_chrom	Selection	Bin index	Priority	Final list	Supplier Name	Catalog Number	canonical isomeric SMILES	eMolecules ID
	O=C(Nc1ncc(s1)Cc1ccc(c(c1)F)F)CCc1nc2ccccc2c(=O)[nH]1	[9.381, 10.773]	3.34	426.439	247.7	223.0	drug-like	7	37	picked	0.0	2	True	Enamine Screening Compounds	Z278071350	c1ccc2c(c1)c(=O)[nH]c(n2)CCC(=O)Nc3ncc(s3)Cc4ccc(c(c4)F)F	18897105
	CCOc1ccc2c(c1)sc(n2)NC(=O)Cc1ccc(c(c1)Cl)Cl	[9.167]	5.17	381.276	489.9	148.0	drug-like	6	28	picked	3.0	1	True	Enamine Screening Compounds	Z30206127	CCOc1ccc2c(c1)sc(n2)NC(=O)Cc3ccc(c(c3)Cl)Cl	3365457
	O=C(Nc1cccc(c1Cl)Cl)Nc1cc(nn1c1ccccc1)C(C)(C)C	[4.113]	5.78	403.305	324.5	148.0	drug-like	6	35	picked	4.0	1	True	Enamine Screening Compounds	Z2216889245	CC(C)(C)c1cc(n(n1)c2ccccc2)NC(=O)Nc3cccc(c3Cl)Cl	10794751
	Brc1ccc(cc1)CSc1nnc(s1)NC(=O)c1ccccc1Cl	[6.525]	5.90	440.765	239.5	400.0	drug-like	6	24	picked	4.0	2	True	Life Chemicals	F0417-1895	c1ccc(c(c1)C(=O)Nc2nnc(s2)SCc3ccc(cc3)Br)Cl	5428718
	O=C(c1ccccc1)Nc1ccc(cc1)Oc1ncnc2c1c1CCCCc1s2	[3.199]	4.72	401.481	636.9	249.0	drug-like	5	34	picked	3.0	3	True	UORSY	PB31167343	c1ccc(cc1)C(=O)Nc2ccc(cc2)Oc3c4c5c(sc4ncn3)CCCC5	3064762
	Ic1cc(I)c2c(c1O)nccc2	[3.511, 6.794]	3.37	396.951	239.0	168.0	drug-like	0	29	picked	0.0	1	True	Vitas M Labs	STK070581	c1cc2c(cc(c(c2nc1)O)I)I	536848
	CCOC(=O)c1ccc(cc1)Nc1cc(C)nc(n1)Nc1ccc(cc1)C(=O)OCC	[6.336]	2.94	420.461	319.0	168.0	drug-like	10	28	picked	0.0	3	True	Vitas M Labs	STK097966	CCOC(=O)c1ccc(cc1)Nc2cc(nc(n2)Nc3ccc(cc3)C(=O)OCC)C	4375254
	Brc1cccc(c1)Nc1ncc(c(n1)Nc1cccc(c1)Br)F	[3.892]	4.14	438.092	222.0	168.0	drug-like	4	28	picked	2.0	1	True	Vitas M Labs	STL368658	c1cc(cc(c1)Br)Nc2c(cnc(n2)Nc3cccc(c3)Br)F	1574612
	O=C1NC(=O)/C(=C\c2cccc(c2)OCc2ccc(cc2Cl)Cl)/S1	[8.05]	5.24	380.245	154.0	219.0	drug-like	4	24	picked	3.0	2	True	Vitas M Labs	STL282831	c1cc(cc(c1)OCc2ccc(cc2Cl)Cl)/C=C/3\C(=O)NC(=O)S3	46568819
	OCCNc1ncnc2c1c(c1ccc(cc1)OC)c(o2)c1ccc(cc1)OC	[4.829]	2.79	391.42	398.0	168.0	drug-like	7	71	picked		1	True	Vitas M Labs	STK090644	COc1ccc(cc1)c2c3c(ncnc3oc2c4ccc(cc4)OC)NCCO	1415746