SUPPLEMENTARY MATERIAL

An Invitation to Open Innovation in Malaria Drug Discovery: 47 Quality Starting Points From the (TCAMS)

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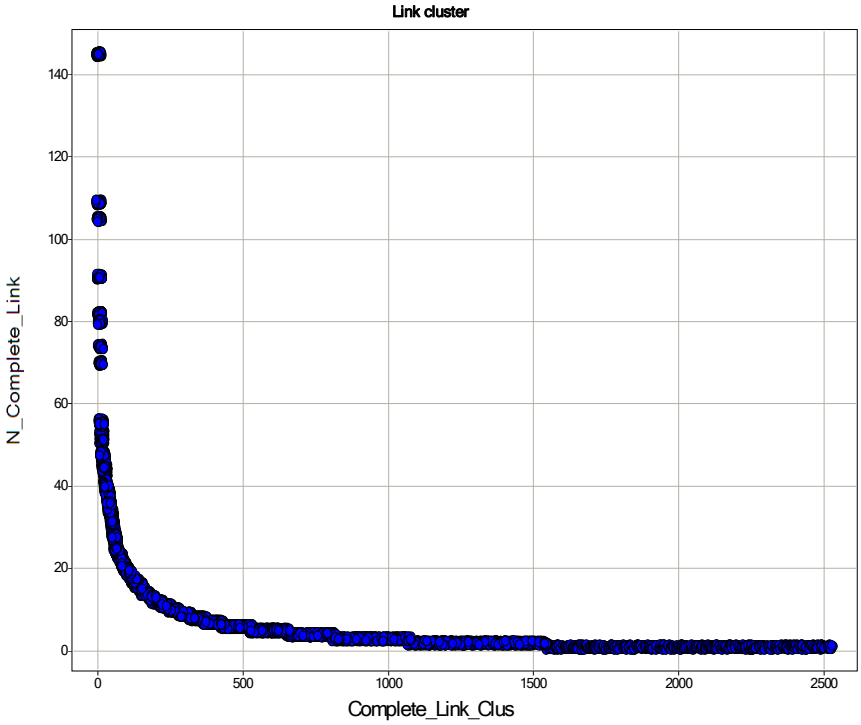
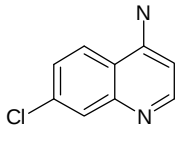
1. Overview of the cluster analysis



A graph showing the number of clusters (Complete Link Clus) *vs.* the number of compounds in each cluster (N_Complete_Link) showing that after carrying out the clustering process on TCAMS, most clusters contain less than 20 compounds with many clusters only containing one compound.

2.- known antimalarials Scaffolds examinated



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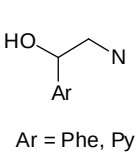

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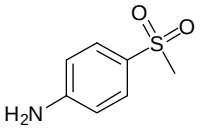

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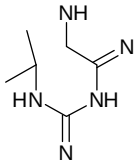

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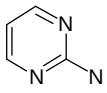

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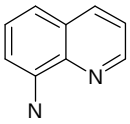

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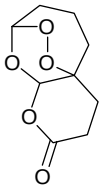

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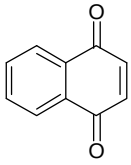

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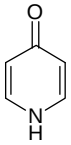

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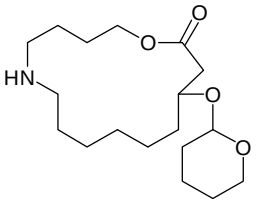

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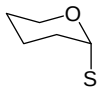

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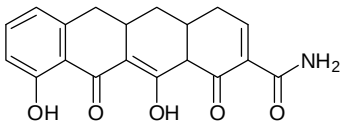


10c

Chloro-aminoquinolines **1** (chloroquine, amodiaquine, piperaquine), aminoalcohols **2** (quinine, quinidine, mefloquine, halomefantrine, lumefantrine), sulfonamides and sulfones **3** (sulfadoxine, sulfalene, dapsone), biguanides **4** (proguanil, chlorproguanil), diaminopyrimidine **5** (pyrimethamine), 8-aminoquinoline **6** (primaquine), sesquiterpene lactones **7** (artemisin, arteether, artemether, artesunate, dihydroartemisinin), naphthoquinone **8** (atovaquone), quinolone **9** and antibiotics **10a-c** (azythromycin, clindamycin, doxycycline, tetracycline)

3.- Experimental Details

Pf XC_{50}'s, *Pf* IC_{50}'s and cytoxicities in a HepG2 cell line (Cytox) were determined according to reference 12; cLogP was calculated using Daylight software.

Plasmodium falciparum Hypoxanthine Assay

Equipment and Materials Instrument Cell Harvester TOMTEC (Perkin Elmer), Instrument Microbeta counter Wallac (Perkin Elmer), 96 well cell culture plates, flat bottom with lid, tissue culture treated, polystyrene, sterile (Costar, Catalog # 3599), 96 well cell culture plates, V-bottom with lid, tissue culture treated, polystyrene, sterile (Costar, Catalog # 3894), printed Filtermat A, glass fibre filter (Wallac, Catalog # 1450-421), MeltiLex A melt-on scintillator sheets (PerkinElmer, Catalog # 1450-441).

Biological and Molecular Reagents Red blood cells ABStorage 4ºC (source Spanish Red Cross Blood Bank), Plasmodium falciparum 3D7A strain (source MR4)

Chemical Reagents Hypoxanthine (Fluka, Catalog Number 56700, molecular weight 136.11), 3H-hypoxanthine (Amersham Biosciences, Catalog Number TRK74) - safety relevant information (known hazards, MSDS) radiolabelled. RPMI-1640 medium (Sigma Catalog Number R5886), 25mM HEPES and NaHCO3 without L-glutamine, Albumax II (Gibco, Catalog Number 11021-037), L-glutamine, (Merck, Catalog Number 1.00229).

Solutions Albumax II 100g/L, D-sucrose 40g/L, L-glutamine 6g/L, hypoxanthine 15 mM (100x), hypoxanthine 2 g/L (guideline add NaOH to dissolve).

Experimental protocol Sensitivity of P. falciparum infected erythrocytes to the drugs was determined using a modification of the in vitro 3H-hypoxanthine incorporation method (see Desjardins, R.E., Canfield, C. J., Haynes, J.D. and Chulay J.D. Quantitative assessment of antimalarial activity in vitro by a semiautomated microdilution technique Antimicrob. Agents Chemother. 1979, 16, 710-718). This assay relies on the parasite incorporation of labeled hypoxanthine that is proportional to P. falciparum growth. A culture of parasitized red blood cells (RBC) of strain 3D7A with a 0.5% parasitemia and 2% haematocrit in RPMI-1640, albumax and 5uM hypoxanthine was exposed to 2-fold serial dilutions of the compound. Plates were incubated 24h at 37ºC, 5% CO2, 5%O2, 95% N2. After 24h of incubation, 3H-hypoxanthine was added and plates were incubated for additiona 24h. After that period, plates were harvested on glass fiber filters using a TOMTEC Cell harvester 96. Filters were dried and melt-on scintillator sheets used to determine the incorporation of 3H-hypoxanthine. Radioactivity was measured using a microbeta counter. Data are normalized using the incorporation of the

positive control, (parasitized red blood cells without drug). IC50s (50% inhibitory concentrations) values were determined using Excel and Grafit 5 software. The assays were performed in three independent experiments, and standard desviation has been calculated.

Data Management, Plate Setup / Control Values, Concentration Response Curve - Control Curves (up to 4 CRCs)

Test agent chloroquine diphosphate salt (# Sigma C-6628), starting conc. (M) 50 ng/mL, dilution factor applied dilution factor:2, no. points in each CRC 9, locations on test 5 plate variable, expected activity value IC50= 15 ng/mL. Test agent "atovaquone", starting Conc. (M) 60 ng/mL, dilution factor applied dilution factor: 3, no. points in each CRC 9 dilutions, locations on test plate variable, expected activity value IC50=0.2 ng/mL.

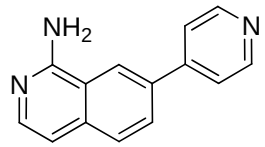
Microsome Assay

930 uL of microsomes 0.645mg/mL(0.5mg/mL), 6uL of compound at 100uM (0.5uM), 150uL of NADPH (2mM) and 108uL MgCl (55mg/mL) were incubated at 37ºC. Remove 100 uL aliquots at 0, 5, 10, 15, 20, 25, and 30 minutes and place into a 96-deepwell plate containing 200 uL (2 volumes) of Stop Solution with Internal Standard. Precipitate protein by centrifugation (37000 rpm, 15minutes) and analyse by HPLC.

hERG Dofetilide Binding Assay

The FP assay uses membranes from CHO cells stably expressing hERG and measures the binding of a fluorescent ligand (Cy3b dofetilide). This is a high-throughput 384 well plate-based assay. Test compounds that bind to hERG compete with the fluorescent compound and to decrease the FP signal.

4. Ligand efficiency structures



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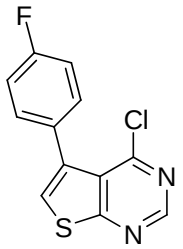

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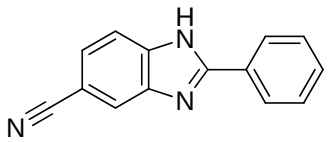

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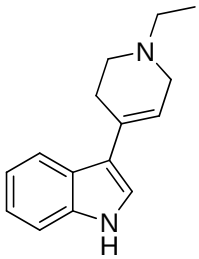

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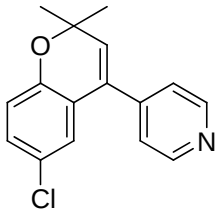

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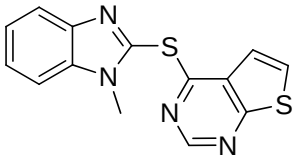

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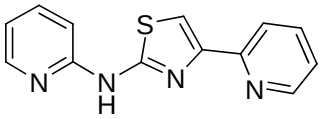

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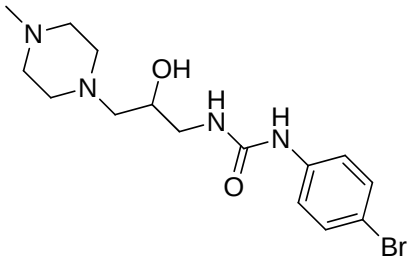

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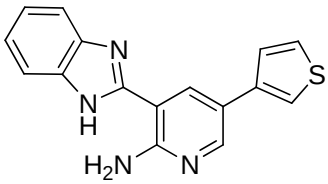

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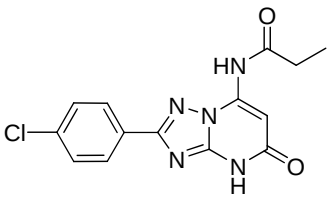

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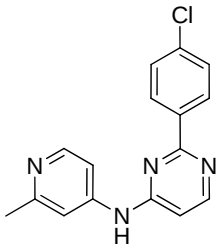

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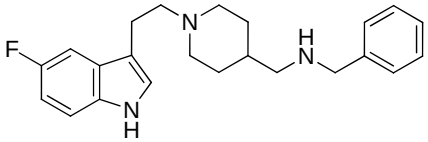

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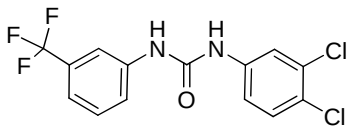

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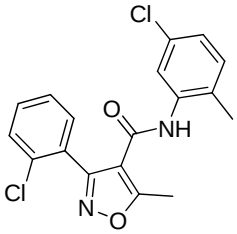

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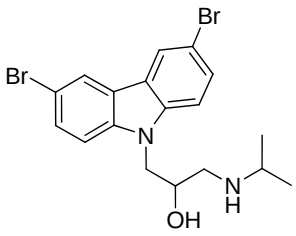

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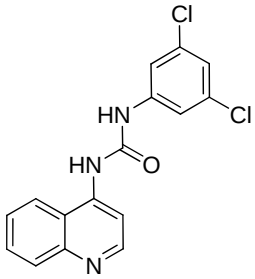

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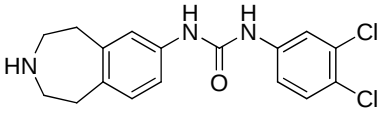

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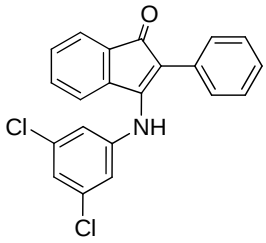

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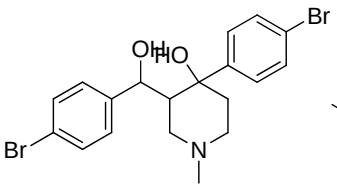

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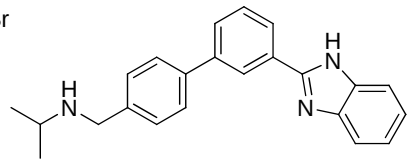

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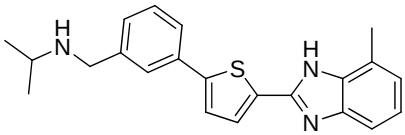

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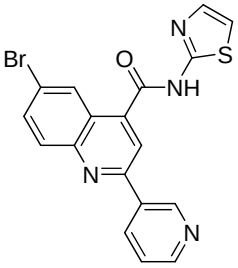

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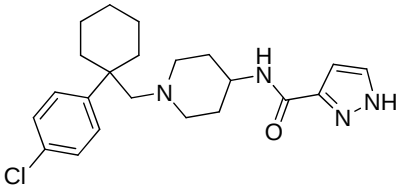

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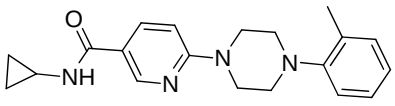

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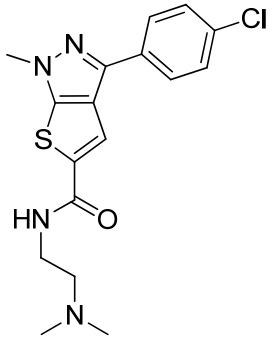

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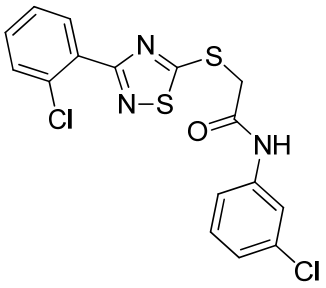

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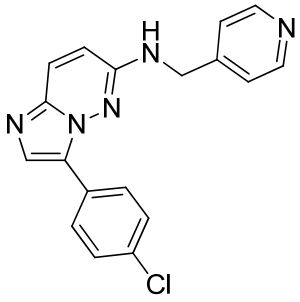

TCMDC-136682

5. Embedded XL spreadsheets

FAST-TRACK SET

TCAMS- ID	3D7 XC50	PXC50	FAST-TRACK SERIES	number of comp. in cluster	clogP	N_Acceptors	N_Donors	N_Heavy_Atoms	Molecular_ Weight	Total_Polar_Surface_Area	Total Score Fast track	SMILES
TCMDC-137332	0.007	8.15	1	3	4.619	2	1	21	303.81	38.33	22	CC(C)(C)C(=O)Nc1ccccc1Oc1ccc(Cl)cc1
TCMDC-125481	0.042	7.38	1	3	2.815	1	1	12	204.06	29.1	20	CC(=O)Nc1ccc(Cl)c(Cl)c1
TCMDC-124303	0.159	6.8	1	3	5.613	2	2	23	392.07	58.2	11	Clc1cc(Cl)cc(NC(=O)CC(=O)Nc2cc(Cl)cc(Cl)c2)c1
TCMDC-133193	0.09	7.05	2	33	6.554	3	3	33	429.51	93.6	19	O=C(Nc1cccc(c1)C#N)Nc1cccc(c1)-c1cccc(c1)-c1nc2ccccc2[nH]1
TCMDC-133152	0.139	6.86	2	33	6.918	2	3	32	418.53	69.81	13	Cc1cccc2nc([nH]c12)-c1cccc(c1)-c1cccc(NC(=O)Nc2ccccc2)c1
TCMDC-133155	0.715	6.15	2	33	6.918	2	3	32	418.53	69.81	13	Cc1cccc2nc([nH]c12)-c1ccc(cc1)-c1cccc(NC(=O)Nc2ccccc2)c1
TCMDC-133171	0.756	6.12	2	33	5.538	2	3	28	370.49	69.81	16	CCNC(=O)Nc1ccc(cc1)-c1cccc(c1)-c1nc2cccc(C)c2[nH]1
TCMDC-133172	1.038	5.98	2	33	5.538	2	3	28	370.49	69.81	13	CCNC(=O)Nc1cccc(c1)-c1cccc(c1)-c1nc2cccc(C)c2[nH]1
TCMDC-133173	0.678	6.17	2	33	6.058	2	3	31	424.46	69.81	13	CCNC(=O)Nc1cccc(c1)-c1cccc(c1)-c1nc2cc(ccc2[nH]1)C(F)(F)F
TCMDC-133179	0.236	6.63	2	33	7.933	2	3	33	452.97	69.81	13	Cc1cccc2nc([nH]c12)-c1cccc(c1)-c1cccc(NC(=O)Nc2ccc(Cl)cc2)c1
TCMDC-133192	0.187	6.73	2	33	7.053	3	3	34	443.54	93.6	13	Cc1cccc2nc([nH]c12)-c1cccc(c1)-c1ccc(NC(=O)Nc2cccc(c2)C#N)cc1
TCMDC-133194	0.104	6.98	2	33	7.053	3	3	34	443.54	93.6	13	Cc1cccc2nc([nH]c12)-c1cccc(c1)-c1cccc(NC(=O)Nc2cccc(c2)C#N)c1
TCMDC-133196	0.114	6.94	2	33	7.053	3	3	34	443.54	93.6	13	Cc1cccc2nc([nH]c12)-c1ccc(cc1)-c1ccc(NC(=O)Nc2cccc(c2)C#N)cc1
TCMDC-133197	0.225	6.65	2	33	6.775	3	3	34	447.5	93.6	13	Fc1ccc2[nH]c(nc2c1)-c1cccc(c1)-c1cccc(NC(=O)Nc2cccc(c2)C#N)c1
TCMDC-133198	0.544	6.26	2	33	7.053	3	3	34	443.54	93.6	13	Cc1cccc2nc([nH]c12)-c1cccc(c1)-c1cccc(NC(=O)Nc2cccc(c2)C#N)c1
TCMDC-133199	0.275	6.56	2	33	6.775	3	3	34	447.5	93.6	13	Fc1ccc2[nH]c(nc2c1)-c1cccc(c1)-c1ccc(NC(=O)Nc2cccc(c2)C#N)cc1
TCMDC-133204	0.096	7.02	2	33	7.021	2	3	34	448.56	79.04	19	COc1ccccc1NC(=O)Nc1cccc(c1)-c1cccc(c1)-c1nc2cccc(C)c2[nH]1
TCMDC-133238	0.189	6.72	2	33	6.376	2	3	30	398.55	69.81	14	CCC(C)NC(=O)Nc1ccc(cc1)-c1cccc(c1)-c1nc2cccc(C)c2[nH]1
TCMDC-133239	0.809	6.09	2	33	6.376	2	3	30	398.55	69.81	14	CCC(C)NC(=O)Nc1cccc(c1)-c1cccc(c1)-c1nc2cccc(C)c2[nH]1
TCMDC-133240	0.624	6.2	2	33	6.896	2	3	33	452.52	69.81	13	CCC(C)NC(=O)Nc1ccc(cc1)-c1cccc(c1)-c1nc2cc(ccc2[nH]1)C(F)(F)F
TCMDC-133241	0.821	6.09	2	33	5.877	2	3	29	384.52	69.81	16	CCC(C)NC(=O)Nc1ccc(cc1)-c1cccc(c1)-c1nc2ccccc2[nH]1
TCMDC-133245	0.142	6.85	2	33	7.021	2	3	34	448.56	79.04	13	COc1ccc(NC(=O)Nc2ccc(cc2)-c2cccc(c2)-c2nc3cccc(C)c3[nH]2)cc1
TCMDC-133247	0.4	6.4	2	33	7.021	2	3	34	448.56	79.04	13	COc1ccc(NC(=O)Nc2cccc(c2)-c2cccc(c2)-c2nc3cccc(C)c3[nH]2)cc1
TCMDC-133251	0.754	6.12	2	33	5.847	2	3	29	384.52	69.81	16	CC(C)NC(=O)Nc1ccc(cc1)-c1cccc(c1)-c1nc2ccccc2[nH]1
TCMDC-133260	0.273	6.56	2	33	8.487	3	3	40	544.57	96.11	13	CCOC(=O)c1ccc(NC(=O)Nc2ccc(cc2)-c2ccc(cc2)-c2nc3cc(ccc3[nH]2)C(F)(F)F)cc1
TCMDC-133261	0.212	6.67	2	33	8.487	3	3	40	544.57	96.11	13	CCOC(=O)c1ccc(NC(=O)Nc2cccc(c2)-c2ccc(cc2)-c2nc3cc(ccc3[nH]2)C(F)(F)F)cc1
TCMDC-133262	0.145	6.84	2	33	7.967	3	3	37	490.6	96.11	13	CCOC(=O)c1ccc(NC(=O)Nc2ccc(cc2)-c2cccc(c2)-c2nc3cccc(C)c3[nH]2)cc1
TCMDC-133263	0.069	7.16	2	33	7.468	3	3	36	476.57	96.11	19	CCOC(=O)c1ccc(NC(=O)Nc2cccc(c2)-c2cccc(c2)-c2nc3ccccc3[nH]2)cc1
TCMDC-133264	0.106	6.97	2	33	7.967	3	3	37	490.6	96.11	13	CCOC(=O)c1ccc(NC(=O)Nc2cccc(c2)-c2cccc(c2)-c2nc3cccc(C)c3[nH]2)cc1
TCMDC-133265	0.022	7.66	2	33	7.468	3	3	36	476.57	96.11	19	CCOC(=O)c1ccc(NC(=O)Nc2ccc(cc2)-c2ccc(cc2)-c2nc3ccccc3[nH]2)cc1
TCMDC-133266	0.212	6.67	2	33	7.468	3	3	36	476.57	96.11	13	CCOC(=O)c1ccc(NC(=O)Nc2cccc(c2)-c2ccc(cc2)-c2nc3ccccc3[nH]2)cc1
TCMDC-133267	0.094	7.03	2	33	7.688	3	3	37	494.56	96.11	19	CCOC(=O)c1ccc(NC(=O)Nc2cccc(c2)-c2ccc(cc2)-c2nc3cc(F)ccc3[nH]2)cc1
TCMDC-133268	0.095	7.02	2	33	7.688	3	3	37	494.56	96.11	19	CCOC(=O)c1ccc(NC(=O)Nc2cccc(c2)-c2cccc(c2)-c2nc3cc(F)ccc3[nH]2)cc1
TCMDC-133269	0.122	6.91	2	33	7.688	3	3	37	494.56	96.11	13	CCOC(=O)c1ccc(NC(=O)Nc2ccc(cc2)-c2cccc(c2)-c2nc3cc(F)ccc3[nH]2)cc1
TCMDC-133270	0.145	6.84	2	33	7.468	3	3	36	476.57	96.11	13	CCOC(=O)c1ccc(NC(=O)Nc2ccc(cc2)-c2cccc(c2)-c2nc3ccccc3[nH]2)cc1
TCMDC-133277	0.375	6.43	2	33	8.632	2	3	34	487.41	69.81	13	Cc1cccc2nc([nH]c12)-c1cccc(c1)-c1cccc(NC(=O)Nc2ccc(Cl)c(Cl)c2)c1
TCMDC-135371	0.034	7.47	3	74	3.458	4	4	39	554.82	110.77	24	Cl.CCNc1cc(cc(c1)C(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC12CCC(CC1)C2)N1CCCCS1(=O)=O
TCMDC-132413	0.518	6.29	3	74	3.948	4	4	42	594.84	120	18	OC=O.CCNc1cc(cc(c1)C(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNCc1cccc(OC)c1C)N1CCCCS1(=O)=O
TCMDC-134521	0.721	6.14	3	74	3.891	4	3	41	581.79	117.2	18	Cl.CCOc1cc(cc(c1)C(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNCc1cccc(OC)c1)N1CCCCS1(=O)=O
TCMDC-134522	0.73	6.14	3	74	4.2	4	3	42	595.82	117.2	15	Cl.COc1cccc(CNC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)c2cc(OC(C)C)cc(c2)N2CCCCS2(=O)=O)c1
TCMDC-134523	0.599	6.22	3	74	5.323	4	3	43	605.86	107.97	14	Cl.COc1cccc(CNC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)c2cc(cc(c2)N2CCCCS2(=O)=O)C2CCCC2)c1
TCMDC-134524	0.519	6.28	3	74	3.98	4	3	43	611.82	126.43	17	Cl.CCOc1cc(cc(c1)C(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNCc1cc(OC)cc(OC)c1)N1CCCCS1(=O)=O
TCMDC-134525	0.59	6.23	3	74	4.289	4	3	44	625.85	126.43	14	Cl.COc1cc(CNC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)c2cc(OC(C)C)cc(c2)N2CCCCS2(=O)=O)cc(OC)c1
TCMDC-134561	0.704	6.15	3	74	5.412	4	3	45	635.89	117.2	14	Cl.COc1cc(CNC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)c2cc(cc(c2)N2CCCCS2(=O)=O)C2CCCC2)cc(OC)c1
TCMDC-134660	0.412	6.39	3	74	4.068	4	4	41	578.84	110.77	15	CCNc1cc(cc(c1)C(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC(C)C)N1CC(CCS1(=O)=O)c1ccccc1
TCMDC-134673	0.689	6.16	3	74	3.397	4	4	43	610.84	129.23	17	CCNc1cc(N2CCCCS2(=O)=O)c(OC)c(c1)C(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNCc1cccc(OC)c1
TCMDC-134674	0.03	7.52	3	74	4.911	5	3	49	693	128.28	20	CCCN(CCC)C(=O)c1cc(cc(c1)C(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC(C)(C)c1cccc(OC)c1)N1CCCCS1(=O)=O
TCMDC-134675	0.036	7.44	3	74	5.875	5	3	51	730.97	119.05	20	CCCN(CCC)C(=O)c1cc(cc(c1)C(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC(C)(C)c1cccc(c1)C(F)(F)F)N1CCCCS1(=O)=O
TCMDC-134676	0.17	6.77	3	74	3.703	4	4	38	542.81	110.77	18	CCNc1cc(cc(c1)C(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC1CCCC1)N1CCCCS1(=O)=O
TCMDC-134678	0.613	6.21	3	74	4.749	4	4	45	654.76	110.77	14	Cl.CCNc1cc(cc(c1)C(=O)N[C@@H](Cc1cc(F)cc(F)c1)[C@H](O)CNCc1cccc(c1)C(F)(F)F)N1CCCCS1(=O)=O
TCMDC-134703	0.156	6.81	3	74	4.222	4	4	39	556.84	110.77	15	Cl.CCNc1cc(cc(c1)C(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC1(C)CCCCC1)N1CCCCS1(=O)=O
TCMDC-134706	0.555	6.26	3	74	3.994	4	4	41	576.82	110.77	18	CCNc1cc(cc(c1)C(=O)N[C@@H](Cc1ccccc1)[C@H](O)CN[C@@H]1CCc2ccccc12)N1CCCCS1(=O)=O
TCMDC-134842	1.14	5.94	3	74	3.777	4	4	44	624.87	129.23	14	Cl.CCNc1cc(cc(c1)C(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNCCc1cc(OC)cc(OC)c1)N1CCCCS1(=O)=O
TCMDC-134938	0.202	6.69	3	74	3.128	5	3	40	569.83	107.97	18	OC=O.O[C@H](CNC1CCOCC1)[C@H](Cc1ccccc1)NC(=O)c1cc(cc(c1)N1CCCCS1(=O)=O)C1CCCC1
TCMDC-135059	0.749	6.13	3	74	3.715	4	4	43	616.79	120	17	Cl.CCNc1cc(cc(c1)C(=O)N[C@@H](Cc1ccc(F)c(F)c1)[C@H](O)CNCc1cccc(OC)c1)N1CCCCS1(=O)=O
TCMDC-135060	0.117	6.93	3	74	3.919	4	4	40	578.79	110.77	18	Cl.CCNc1cc(cc(c1)C(=O)N[C@@H](Cc1ccc(F)c(F)c1)[C@H](O)CNC1CCCCC1)N1CCCCS1(=O)=O
TCMDC-135107	0.237	6.63	3	74	3.978	4	4	39	554.82	110.77	18	Cl.CCNc1cc(cc(c1)C(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC1CC2CCC1C2)N1CCCCS1(=O)=O
TCMDC-135108	0.647	6.19	3	74	4.741	4	4	40	570.87	110.77	15	Cl.CCNc1cc(cc(c1)C(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC1CCC(C)(C)CC1)N1CCCCS1(=O)=O
TCMDC-135165	0.797	6.1	3	74	3.551	4	4	39	562.82	110.77	18	OC=O.CCNc1cc(N2CCCCS2(=O)=O)c(F)c(c1)C(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNCCC(C)(C)C
TCMDC-135166	1.008	6	3	74	4.259	4	4	41	590.88	110.77	12	CCNc1cc(N2CCCCS2(=O)=O)c(F)c(c1)C(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC(C)(C)CC(C)(C)C
TCMDC-135167	1.115	5.95	3	74	3.461	4	4	39	562.82	110.77	15	OC=O.CCNc1cc(N2CCCCS2(=O)=O)c(F)c(c1)C(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC(C)CC(C)C
TCMDC-135171	0.936	6.03	3	74	3.769	4	4	40	564.81	110.77	18	Cl.CCNc1cc(cc(c1)C(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNCCc1ccccc1)N1CCCCS1(=O)=O

TCMDC-135176	1.606	5.79	3	74	3.074	4	4	37	528.78	110.77	15	Cl.CCNc1cc(cc(c1)C(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC1(CC)CC1)N1CCCCS1(=O)=O
TCMDC-135177	0.398	6.4	3	74	3.259	4	4	36	516.77	110.77	18	Cl.CCCCNC[C@@H](O)[C@H](Cc1ccccc1)NC(=O)c1cc(NCC)cc(c1)N1CCCCS1(=O)=O
TCMDC-135189	1.355	5.87	3	74	3.504	4	4	43	608.82	129.23	14	OC=O.CCNc1cc(cc(c1)C(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNCc1ccc2OCCOc2c1)N1CCCCS1(=O)=O
TCMDC-135192	1.082	5.97	3	74	3.603	4	4	38	542.81	110.77	15	Cl.CCCC1(CC1)NC[C@@H](O)[C@H](Cc1ccccc1)NC(=O)c1cc(NCC)cc(c1)N1CCCCS1(=O)=O
TCMDC-135194	0.82	6.09	3	74	3.837	4	4	38	544.83	110.77	18	Cl.CCNc1cc(cc(c1)C(=O)N[C@@H](Cc1ccccc1)[C@H](O)CN[C@H](C)C(C)(C)C)N1CCCCS1(=O)=O
TCMDC-135201	0.15	6.82	3	74	4.416	4	4	39	577.25	110.77	15	Cl.CCNc1cc(cc(c1)C(=O)N[C@@H](Cc1ccc(Cl)cc1)[C@H](O)CNC1CCCCC1)N1CCCCS1(=O)=O
TCMDC-135203	0.103	6.99	3	74	4.012	4	4	39	556.84	110.77	15	OC=O.CC(C)Nc1cc(cc(c1)C(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC1CCCCC1)N1CCCCS1(=O)=O
TCMDC-135204	0.079	7.1	3	74	5.48	4	4	46	660.87	110.77	20	OC=O.CC(C)Nc1cc(cc(c1)C(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC(C)(C)c1cccc(c1)C(F)(F)F)N1CCCCS1(=O)=O
TCMDC-135205	0.784	6.11	3	74	3.808	4	4	42	594.84	120	18	OC=O.COc1cccc(CNC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)c2cc(NC(C)C)cc(c2)N2CCCCS2(=O)=O)c1
TCMDC-135206	0.206	6.69	3	74	5.733	4	4	42	600.95	110.77	14	OC=O.CC(C)CCCC(C)(C)NC[C@@H](O)[C@H](Cc1ccccc1)NC(=O)c1cc(NC(C)C)cc(c1)N1CCCCS1(=O)=O
TCMDC-135209	0.265	6.58	3	74	4.751	4	4	40	570.87	110.77	15	Cl.CCNc1cc(cc(c1)C(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC1(CC)CCCCC1)N1CCCCS1(=O)=O
TCMDC-135211	0.446	6.35	3	74	5.424	4	4	41	586.92	110.77	15	OC=O.CCNc1cc(cc(c1)C(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC(C)(C)CCCC(C)C)N1CCCCS1(=O)=O
TCMDC-135216	0.147	6.83	3	74	5.392	4	3	39	555.85	98.74	15	Cl.CCCC(C)NC[C@@H](O)[C@H](Cc1ccccc1)NC(=O)c1cc(cc(c1)N1CCCCS1(=O)=O)C1CCCC1
TCMDC-135218	0.995	6	3	74	4.317	4	4	38	544.83	110.77	15	Cl.CCCCCCNC[C@@H](O)[C@H](Cc1ccccc1)NC(=O)c1cc(NCC)cc(c1)N1CCCCS1(=O)=O
TCMDC-135221	0.052	7.28	3	74	5.131	4	4	42	613.28	110.77	20	Cl.CCNc1cc(cc(c1)C(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC(CC)c1cccc(Cl)c1)N1CCCCS1(=O)=O
TCMDC-135223	0.803	6.1	3	74	4.416	4	4	39	577.25	110.77	15	Cl.CCNc1cc(cc(c1)C(=O)N[C@@H](Cc1ccccc1Cl)[C@H](O)CNC1CCCCC1)N1CCCCS1(=O)=O
TCMDC-135224	0.928	6.03	3	74	5.738	4	4	41	607.33	110.77	14	Cl.CCNc1cc(cc(c1)C(=O)N[C@@H](Cc1ccccc1Cl)[C@H](O)CNC(C)CCCC(C)C)N1CCCCS1(=O)=O
TCMDC-135225	0.285	6.55	3	74	5.738	4	4	41	607.33	110.77	14	Cl.CCNc1cc(cc(c1)C(=O)N[C@@H](Cc1cccc(Cl)c1)[C@H](O)CNC(C)CCCC(C)C)N1CCCCS1(=O)=O
TCMDC-135226	0.163	6.79	3	74	3.568	4	4	37	530.8	110.77	18	Cl.CCCC(C)NC[C@@H](O)[C@H](Cc1ccccc1)NC(=O)c1cc(NCC)cc(c1)N1CCCCS1(=O)=O
TCMDC-135245	1.077	5.97	3	74	4.531	4	4	40	570.87	110.77	12	Cl.CCNc1cc(cc(c1)C(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC1(CCC(C)C)CC1)N1CCCCS1(=O)=O
TCMDC-135258	1.018	5.99	3	74	4.002	4	4	39	556.84	110.77	12	Cl.CCNc1cc(cc(c1)C(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC1(CC(C)C)CC1)N1CCCCS1(=O)=O
TCMDC-135261	0.505	6.3	3	74	4.721	4	4	40	570.87	110.77	15	Cl.CCCC1(CCCC1)NC[C@@H](O)[C@H](Cc1ccccc1)NC(=O)c1cc(NCC)cc(c1)N1CCCCS1(=O)=O
TCMDC-135262	0.247	6.61	3	74	5.28	4	4	41	584.9	110.77	15	Cl.CCCC1(CCCCC1)NC[C@@H](O)[C@H](Cc1ccccc1)NC(=O)c1cc(NCC)cc(c1)N1CCCCS1(=O)=O
TCMDC-135269	0.224	6.65	3	74	2.73	4	4	35	502.74	110.77	18	Cl.CCCNC[C@@H](O)[C@H](Cc1ccccc1)NC(=O)c1cc(NCC)cc(c1)N1CCCCS1(=O)=O
TCMDC-135293	0.398	6.4	3	74	4.626	4	4	39	558.86	110.77	15	Cl.CCCCCC(C)NC[C@@H](O)[C@H](Cc1ccccc1)NC(=O)c1cc(NCC)cc(c1)N1CCCCS1(=O)=O
TCMDC-135302	0.138	6.86	3	74	4.182	4	4	39	556.84	110.77	15	Cl.CCNc1cc(cc(c1)C(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC1CCC(C)(C)C1)N1CCCCS1(=O)=O
TCMDC-135304	1.01	6	3	74	2.879	4	4	37	532.77	123.91	15	Cl.CCNc1cc(cc(c1)C(=O)N[C@@H](Cc1ccco1)[C@H](O)CNC1CCCC1)N1CCCCS1(=O)=O
TCMDC-135307	0.596	6.22	3	74	5.168	4	4	41	590.88	110.77	15	Cl.CCNc1cc(cc(c1)C(=O)N[C@@H](Cc1cccc(F)c1)[C@H](O)CNC(C)CCCC(C)C)N1CCCCS1(=O)=O
TCMDC-135309	0.887	6.05	3	74	5.19	4	4	43	627.31	110.77	14	Cl.CCNc1cc(cc(c1)C(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC(C)(C)Cc1cccc(Cl)c1)N1CCCCS1(=O)=O
TCMDC-135352	0.219	6.66	3	74	4.331	4	4	42	594.89	110.77	15	Cl.CCNc1cc(cc(c1)C(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC12CC3CC(CC(C3)C1)C2)N1CCCCS1(=O)=O
TCMDC-135374	0.72	6.14	3	74	4.162	4	4	39	556.84	110.77	15	Cl.CCCC1(CCC1)NC[C@@H](O)[C@H](Cc1ccccc1)NC(=O)c1cc(NCC)cc(c1)N1CCCCS1(=O)=O
TCMDC-135375	0.685	6.16	3	74	4.032	4	4	39	556.84	110.77	15	Cl.CCNc1cc(cc(c1)C(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC1(CCC1)C(C)C)N1CCCCS1(=O)=O
TCMDC-135383	1.177	5.93	3	74	5.385	4	4	44	639.32	110.77	11	Cl.CCNc1cc(cc(c1)C(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC1(Cc2cccc(Cl)c2)CCC1)N1CCCCS1(=O)=O
TCMDC-135390	0.063	7.2	3	74	4.017	4	4	40	568.85	110.77	21	Cl.CCNc1cc(cc(c1)C(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC12CCC(CC1)CC2)N1CCCCS1(=O)=O
TCMDC-135411	0.619	6.21	3	74	4.201	4	4	39	562.85	123.91	15	Cl.CCNc1cc(cc(c1)C(=O)N[C@@H](Cc1ccco1)[C@H](O)CNC(C)CCCC(C)C)N1CCCCS1(=O)=O
TCMDC-135412	0.496	6.3	3	74	4.791	4	4	42	613.28	110.77	14	Cl.CCNc1cc(cc(c1)C(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC(C)Cc1cccc(Cl)c1)N1CCCCS1(=O)=O
TCMDC-135424	0.668	6.18	3	74	5.371	4	4	42	594.89	110.77	15	Cl.CCNc1cc(cc(c1)C(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC1C2CC3CC(C2)CC1C3)N1CCCCS1(=O)=O
TCMDC-135445	0.166	6.78	3	74	2.166	5	3	39	561.78	107.97	18	CCCc1cc(N2CCCCS2(=O)=O)c(F)c(c1)C(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC1CCOCC1
TCMDC-135448	0.212	6.67	3	74	2.583	4	4	41	596.78	110.77	18	OC=O.CCNc1cc(N2CCCCS2(=O)=O)c(F)c(c1)C(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC1CCC(F)(F)CC1
TCMDC-135451	0.109	6.96	3	74	5.942	4	3	47	672.88	101.98	14	CCN1CCc2c1cc(cc2N1CCCCS1(=O)=O)C(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC(C)(C)c1cccc(c1)C(F)(F)F
TCMDC-135510	0.029	7.54	3	74	5.574	4	3	46	651.91	107.97	20	OC=O.COc1cccc(c1)C(C)(C)NC[C@@H](O)[C@H](Cc1ccccc1)NC(=O)c1cc(cc(N2CCCCS2(=O)=O)c1F)C1CCCC1
TCMDC-135538	0.794	6.1	3	74	4.267	4	4	45	650.8	110.77	14	OC=O.CC(C)Nc1cc(N2CCCCS2(=O)=O)c(F)c(c1)C(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNCc1cccc(c1)C(F)(F)F
TCMDC-135540	0.219	6.66	3	74	5.227	4	4	43	618.94	110.77	14	OC=O.CC(C)CCCC(C)(C)NC[C@@H](O)[C@H](Cc1ccccc1)NC(=O)c1cc(NC(C)C)cc(N2CCCCS2(=O)=O)c1F
TCMDC-135541	0.183	6.74	3	74	1.107	5	4	40	576.8	120	18	OC=O.CC(C)Nc1cc(N2CCCCS2(=O)=O)c(F)c(c1)C(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC1CCOCC1
TCMDC-135686	0.15	6.82	3	74	2.012	5	4	40	572.84	120	18	CC(C)(C)Nc1cc(cc(c1)C(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC1CCOCC1)N1CCCCS1(=O)=O
TCMDC-138883	0.876	6.06	3	74	5.167	5	3	49	702.91	119.05	14	CCCN(CCC)C(=O)c1cc(cc(c1)C(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNCc1cccc(c1)C(F)(F)F)N1CCCCS1(=O)=O
TCMDC-138892	0.156	6.81	3	74	2.959	5	3	41	584.85	119.05	18	CCCN(CCC)C(=O)c1cc(cc(c1)C(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC1CC1)N1CCCCS1(=O)=O
TCMDC-138893	0.549	6.26	3	74	4.203	5	3	47	664.94	128.28	14	CCCN(CCC)C(=O)c1cc(cc(c1)C(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNCc1cccc(OC)c1)N1CCCCS1(=O)=O
TCMDC-138418	0.032	7.49	4	30	8.393	1	1	32	446	28.16	19	Fc1ccc(Nc2ccnc3cc(ccc23)-c2cccc(CN3CCCCC3)c2)c(Cl)c1
TCMDC-138412	0.809	6.09	4	30	7.113	1	2	32	449.01	40.19	13	CN(C)CCNCc1cccc(c1)-c1ccc2c(Nc3ccc(F)cc3Cl)ccnc2c1
TCMDC-138413	0.549	6.26	4	30	6.237	2	3	33	465.01	60.42	13	CN(C)CCNCc1cccc(c1)-c1ccc2c(Nc3cc(O)c(Cl)cc3F)ccnc2c1
TCMDC-138414	0.142	6.85	4	30	7.102	2	2	35	491.05	49.42	13	Fc1ccc(Nc2ccnc3cc(ccc23)-c2cccc(CNCCN3CCOCC3)c2)c(Cl)c1
TCMDC-138415	0.68	6.17	4	30	6.904	2	2	31	435.96	46.18	13	COCCNCc1cccc(c1)-c1ccc2c(Nc3ccc(F)cc3Cl)ccnc2c1
TCMDC-138416	0.11	6.96	4	30	7.655	1	1	33	463.04	31.4	13	CN(C)CCN(C)Cc1cccc(c1)-c1ccc2c(Nc3ccc(F)cc3Cl)ccnc2c1
TCMDC-138417	0.156	6.81	4	30	7.674	1	1	33	461.02	31.4	13	CN1CCN(Cc2cccc(c2)-c2ccc3c(Nc4ccc(F)cc4Cl)ccnc3c2)CC1
TCMDC-138429	0.114	6.94	4	30	6.028	3	3	32	451.96	66.41	13	COCCNCc1cccc(c1)-c1ccc2c(Nc3cc(O)c(Cl)cc3F)ccnc2c1
TCMDC-138430	0.77	6.11	4	30	6.797	2	2	34	477.02	51.63	13	CN1CCN(Cc2cccc(c2)-c2ccc3c(Nc4cc(O)c(Cl)cc4F)ccnc3c2)CC1
TCMDC-138432	0.237	6.63	4	30	6.778	2	2	34	479.04	51.63	13	CN(C)CCN(C)Cc1cccc(c1)-c1ccc2c(Nc3cc(O)c(Cl)cc3F)ccnc2c1
TCMDC-138433	0.102	6.99	4	30	7.516	2	2	33	462	48.39	13	Oc1cc(Nc2ccnc3cc(ccc23)-c2cccc(CN3CCCC3)c2)c(F)cc1Cl
TCMDC-138434	0.207	6.68	4	30	6.236	3	2	33	463.97	57.62	13	Oc1cc(Nc2ccnc3cc(ccc23)-c2cccc(CN3CCOCC3)c2)c(F)cc1Cl
TCMDC-138435	0.254	6.6	4	30	4.918	4	3	34	500.02	91.32	15	CS(=O)(=O)CCNCc1cccc(c1)-c1ccc2c(Nc3cc(O)c(Cl)cc3F)ccnc2c1
TCMDC-138460	0.728	6.14	4	30	9.334	2	1	39	535.13	40.63	13	CN1CCN(Cc2cccc(c2)-c2cc3nccc(Nc4ccc(Oc5ccccc5)cc4)c3cc2Cl)CC1
TCMDC-138461	1.384	5.86	4	30	8.565	3	2	37	510.07	55.41	10	COCCNCc1cccc(c1)-c1cc2nccc(Nc3ccc(Oc4ccccc4)cc3)c2cc1Cl
TCMDC-138462	0.625	6.2	4	30	7.455	4	2	39	558.13	80.32	13	CS(=O)(=O)CCNCc1cccc(c1)-c1cc2nccc(Nc3ccc(Oc4ccccc4)cc3)c2cc1Cl
TCMDC-138472	0.836	6.08	4	30	4.628	4	3	33	461.62	91.32	15	Cc1ccc(O)cc1Nc1ccnc2cc(ccc12)-c1cccc(CNCCS(C)(=O)=O)c1
TCMDC-138473	0.441	6.36	4	30	8.213	2	2	37	488.68	49.42	13	CN(C)CCNCc1cccc(c1)-c1ccc2c(Nc3ccc(Oc4ccccc4)cc3)ccnc2c1
TCMDC-138474	0.391	6.41	4	30	8.201	3	2	40	530.72	58.65	13	C(CN1CCOCC1)NCc1cccc(c1)-c1ccc2c(Nc3ccc(Oc4ccccc4)cc3)ccnc2c1

TCMDC-138475	0.336	6.47	4	30	8.212	3	1	37	487.64	46.62	13	C(N1CCOCC1)c1cccc(c1)-c1ccc2c(Nc3ccc(Oc4ccccc4)cc3)ccnc2c1
TCMDC-138476	0.226	6.65	4	30	8.773	2	1	38	500.69	40.63	13	CN1CCN(Cc2cccc(c2)-c2ccc3c(Nc4ccc(Oc5ccccc5)cc4)ccnc3c2)CC1
TCMDC-138477	0.691	6.16	4	30	6.894	4	2	38	523.69	80.32	13	CS(=O)(=O)CCNCc1cccc(c1)-c1ccc2c(Nc3ccc(Oc4ccccc4)cc3)ccnc2c1
TCMDC-138478	0.517	6.29	4	30	8.004	3	2	36	475.63	55.41	13	COCCNCc1cccc(c1)-c1ccc2c(Nc3ccc(Oc4ccccc4)cc3)ccnc2c1
TCMDC-138487	0.178	6.75	4	30	6.507	4	2	36	476.62	68.3	13	COCCNCc1cccc(c1)-c1ccc2c(Nc3ccc(Oc4cccnc4)cc3)ccnc2c1
TCMDC-138488	0.142	6.85	4	30	5.397	5	2	38	524.68	93.21	15	CS(=O)(=O)CCNCc1cccc(c1)-c1ccc2c(Nc3ccc(Oc4cccnc4)cc3)ccnc2c1
TCMDC-138489	0.192	6.72	4	30	7.276	3	1	38	501.68	53.52	13	CN1CCN(Cc2cccc(c2)-c2ccc3c(Nc4ccc(Oc5ccccc5)cc4)ccnc3c2)CC1
TCMDC-138490	0.305	6.52	4	30	6.715	4	1	37	488.63	59.51	13	C(N1CCOCC1)c1cccc(c1)-c1ccc2c(Nc3ccc(Oc4cccnc4)cc3)ccnc2c1
TCMDC-138491	0.124	6.91	4	30	7.995	3	1	37	486.66	50.28	13	C(N1CCCCC1)c1cccc(c1)-c1ccc2c(Nc3ccc(Oc4cccnc4)cc3)ccnc2c1
TCMDC-138492	0.112	6.95	4	30	6.704	4	2	40	531.71	71.54	13	C(CN1CCOCC1)NCc1cccc(c1)-c1ccc2c(Nc3ccc(Oc4cccnc4)cc3)ccnc2c1
TCMDC-138493	0.233	6.63	4	30	6.716	3	2	37	489.67	62.31	13	CN(C)CCNCc1cccc(c1)-c1ccc2c(Nc3ccc(Oc4ccccn4)cc3)ccnc2c1
TCMDC-123738	0.032	7.49	5	2	3.291	2	1	23	323.44	44.7	20	CN(C)c1ccc(C=C2SC(=O)NC2=Nc2ccccc2)cc1
TCMDC-123697	0.47	6.33	5	2	3.134	2	1	24	340.42	59.92	14	COc1ccc(C=C2SC(=O)NC2=Nc2ccccc2)c(OC)c1
TCMDC-131984	0.033	7.48	6	5	4.585	0	2	27	365.54	31.06	17	Cl.Fc1ccc2[nH]cc(CCN3CCC(CNCc4ccccc4)CC3)c2c1
TCMDC-131457	1.274	5.89	6	5	4.77	1	1	27	369.61	37.27	8	Cl.CC1CC(C)CN(CCCC(=O)NCCc2c(C)n(C)c3ccccc23)C1
TCMDC-131970	0.597	6.22	6	5	4.262	0	1	27	365.54	22.27	11	OC(=O)C(F)(F)F.CN(Cc1ccccc1)C1CCN(CCc2c[nH]c3ccc(F)cc23)CC1
TCMDC-131975	0.71	6.15	6	5	3.194	1	3	28	381.54	51.29	14	OC(=O)C(F)(F)F.OC1(CNCc2ccccc2)CCN(CCc2c[nH]c3ccc(F)cc23)CC1
TCMDC-131991	0.878	6.06	6	5	5.164	1	2	34	455.62	48.13	10	Fc1ccc2[nH]cc(CCN3CCC(CC3)(NC(=O)Cc3ccccc3)c3ccccc3)c2c1
TCMDC-135696	0.046	7.34	7	11	4.317	7	2	45	625.7	131.24	17	CC(c1cccc(Nc2nccc(n2)-c2c(nn3nccxx23)-c2cccc(NC(=O)c3c(F)cccc3F)c2)c1)S(C)(=O)=O
TCMDC-134631	0.726	6.14	7	11	5.88	5	2	39	519.55	97.1	12	Fc1cccc(F)c1C(=O)Nc1cccc(c1)-c1nn2nccccc2c1-c1ccnc(Nc2ccccc2)n1
TCMDC-135544	0.158	6.8	7	11	5.336	6	2	45	604.67	109.57	11	Fc1cccc(F)c1C(=O)Nc1cccc(c1)-c1nn2nccccc2c1-c1ccnc(Nc2ccc(cc2)N2CCOCC2)n1
TCMDC-135548	0.184	6.74	7	11	4.899	6	3	43	576.61	126.2	12	CC(=O)Nc1cccc(Nc2nccc(n2)-c2c(nn3nccxx23)-c2cccc(NC(=O)c3c(F)cccc3F)c2)c1
TCMDC-135549	0.648	6.19	7	11	6.82	5	2	43	587.55	97.1	10	Fc1cccc(F)c1C(=O)Nc1cccc(c1)-c1nn2nccccc2c1-c1ccnc(Nc2cccc(c2)C(F)(F)F)n1
TCMDC-135550	0.166	6.78	7	11	5.673	6	2	44	586.6	123.13	12	Fc1cccc(F)c1C(=O)Nc1cccc(c1)-c1nn2nccccc2c1-c1ccnc(Nc2cccc(c2)-c2cnco2)n1
TCMDC-135635	0.528	6.28	7	11	4.494	6	2	39	520.54	109.99	12	Cl.Fc1cccc(F)c1C(=O)Nc1cccc(c1)-c1nn2nccccc2c1-c1ccnc(Nc2cccnc2)n1
TCMDC-135681	0.162	6.79	7	11	4.008	7	2	44	611.67	131.24	11	CS(=O)(=O)Cc1ccc(Nc2nccc(n2)-c2c(nn3nccxx23)-c2cccc(NC(=O)c3c(F)cccc3F)c2)cc1
TCMDC-135682	1.032	5.99	7	11	4.905	7	2	46	641.7	140.47	8	CCS(=O)(=O)c1ccc(OC)c(Nc2nccc(n2)-c2c(nn3nccxx23)-c2cccc(NC(=O)c3c(F)cccc3F)c2)c1
TCMDC-135684	0.033	7.48	7	11	5.032	5	2	45	609.64	124.79	17	COc1cc(Nc2nccc(n2)-c2c(nn3nccxx23)-c2cccc(NC(=O)c3c(F)cccc3F)c2)cc(OC)c1OC
TCMDC-135812	0.201	6.7	7	11	4.818	7	2	42	581.75	131.24	12	CS(=O)(=O)Cc1ccc(Nc2nccc(n2)-c2c(nn3nccxx23)-c2cccc(NC(=O)C3CCCCC3)c2)cc1
TCMDC-123794	0.054	7.27	8	2	2.843	3	1	35	476.55	87.26	19	Cc1cc(C(=O)OCC(=O)Nc2c(C)n(C)n(-c3ccccc3)c2=O)c(C)n1-c1ccc(F)cc1
TCMDC-123812	0.331	6.48	8	2	3.004	2	1	21	290.32	74.32	14	Cc1cc(C(=O)OCC(N)=O)c(C)n1-c1ccc(F)cc1
TCMDC-134379	0.057	7.24	9	1	2.882	5	0	22	326.46	85.16	20	Cl.CC(C)N(C)C(=O)n1cnc(n1)S(=O)(=O)C1CC2CCC1C2
TCMDC-123553	0.058	7.24	10	2	3.776	4	2	29	441.94	87.74	19	Cc1ccc(NCC(=O)Nc2ccc(F)c(Cl)c2)cc1S(=O)(=O)N1CCOCC1
TCMDC-125117	0.92	6.04	10	2	4.395	4	1	32	478.05	78.95	10	CCN(CC)S(=O)(=O)c1ccc(C=CC(=O)Nc2cc(Cl)ccc2N2CCOCC2)cc1
TCMDC-125454	0.06	7.22	11	3	3.495	3	1	27	372.38	59.81	20	FC(F)(F)c1ccc(c(NC(=O)C2(CC2)c2ccccc2)c1)-n1cncn1
TCMDC-125455	0.455	6.34	11	3	3.201	3	1	24	338.82	59.81	14	Clc1ccc(c(NC(=O)C2(CC2)c2ccccc2)c1)-n1cncn1
TCMDC-124870	0.321	6.49	11	3	4.313	3	1	29	401.43	63.05	10	CC1Cc2ccccc2N1CC(=O)Nc1cc(ccc1-n1cncn1)C(F)(F)F
TCMDC-124492	0.062	7.21	12	4	3.361	4	1	29	404.44	75.42	19	Cc1ccnc2nc(nn12)C(=O)Nc1cc(ccc1N1CCCCC1)C(F)(F)F
TCMDC-125466	0.251	6.6	12	4	3.392	4	1	28	393.41	81.41	14	CCCOc1ccc(cc1NC(=O)c1nc2nc(C)cc(C)n2n1)C(F)(F)F
TCMDC-123614	0.119	6.92	12	4	2.481	5	1	30	420.44	84.65	13	Cc1cc(C)n2nc(nc2n1)C(=O)Nc1cc(ccc1N1CCOCC1)C(F)(F)F
TCMDC-124435	1.236	5.91	12	4	1.745	5	1	26	372.85	84.65	11	Cc1ccnc2nc(nn12)C(=O)Nc1cc(Cl)ccc1N1CCOCC1
TCMDC-135093	0.071	7.15	13	3	5.839	3	1	35	486.96	69.04	16	CC(=O)Nc1cccc(c1)-c1cn(-c2ccc(OCc3cccc(F)c3)c(Cl)c2)c2ncncc12
TCMDC-135092	1.032	5.99	13	3	4.387	4	1	34	477.97	82.68	7	Fc1cccc(COc2ccc(cc2Cl)-n2ccc3c(NCCCn4ccnc4)ncnc23)n1
TCMDC-135377	0.171	6.77	13	3	4.879	4	1	34	473.92	81.93	10	Fc1cccc(COc2ccc(cc2Cl)-n2cc(NC(=O)c3ccncc3)c3cncnc23)c1
TCMDC-133427	0.033	7.48	14	10	2.436	1	2	24	320.43	71.25	20	OC(=O)C(F)(F)F.CN(C)CC(=O)Nc1ccc(cc1)-c1ccc2ccnc(N)c2c1
TCMDC-133409	0.92	6.04	14	10	3.268	1	3	23	304.38	80.04	14	Nc1ccc(cn1)-c1ccc(NC(=O)Nc2ccccc2)cc1
TCMDC-125114	0.035	7.46	15	3	4.772	3	2	27	441.37	74.43	16	CC(Sc1nnc([nH]1)-c1ccccc1Br)C(=O)c1c(C)[nH]c2ccccc12
TCMDC-125010	1.804	5.74	15	3	3.623	3	2	24	354.47	74.43	11	CC(Sc1nnc([nH]1)-c1cccs1)C(=O)c1c[nH]c2ccccc12
TCMDC-123710	0.982	6.01	15	3	3.964	3	2	25	413.31	74.43	13	Brc1ccccc1-c1nnc(SCC(=O)c2c[nH]c3ccccc23)[nH]1
TCMDC-142012	0.038	7.42	16	25	3.047	2	1	16	229.68	41.57	20	Clc1ccc2nc([nH]c2c1)-c1cccnc1
TCMDC-123507	1.115	5.95	16	25	4.389	3	2	24	311.37	70.25	8	c1ccc2[nH]c(nc2c1)-c1cccc(n1)-c1nc2ccccc2[nH]1
TCMDC-137279	0.04	7.4	17	1	3.186	3	0	20	307.82	38.25	20	Clc1ccc(Sc2cncnc2N2CCOCC2)cc1
TCMDC-139046	0.041	7.39	18	13	6.176	2	1	35	497.43	63.69	16	COc1cc2CCN(C(=O)Nc3cc(OC(F)(F)F)cc(c3)-c3cccnc3)c2cc1C(F)(F)F
TCMDC-139014	0.71	6.15	18	13	6.352	1	1	34	469.55	44.81	10	COc1cc2CCN(C(=O)Nc3ccccc(c3)-c3ccc(CN(C)C)cc3)c2cc1C(F)(F)F
TCMDC-139015			18	13	4.63	2	1	25	416.22	54.46	8	COc1cc2CCN(C(=O)Nc3ccc(Br)cn3)c2cc1C(F)(F)F
TCMDC-139024	0.864	6.06	18	13	5.962	2	1	31	492.32	54.46	12	COc1cc2CCN(C(=O)Nc3cc(Br)cc(c3)-c3cccnc3)c2cc1C(F)(F)F
TCMDC-139030	0.702	6.15	18	13	5.771	2	1	32	439.47	54.46	12	COc1cc2CCN(C(=O)Nc3cc(C=C)cc(c3)-c3cccnc3)c2cc1C(F)(F)F
TCMDC-139039	0.5	6.3	18	13	4.286	3	1	31	432.41	67.35	12	COc1cc2CCN(C(=O)Nc3cc(F)cc(c3)-c3cncnc3)c2cc1C(F)(F)F
TCMDC-139040	0.619	6.21	18	13	5.447	3	1	36	490.52	67.35	12	COc1cc2CCN(C(=O)Nc3cc(cc(c3)-c3cccnc3)-c3cccnc3)c2cc1C(F)(F)F
TCMDC-139045	0.275	6.56	18	13	4.236	3	1	31	432.41	67.35	12	COc1cc2CCN(C(=O)Nc3cc(F)cc(c3)-c3cccnn3)c2cc1C(F)(F)F
TCMDC-139061	0.626	6.2	18	13	5.333	2	1	32	449.41	54.46	12	COc1cc2CCN(C(=O)Nc3cc(F)c(F)c(c3)-c3cccnc3)c2cc1C(F)(F)F
TCMDC-139848	0.966	6.02	18	13	6.071	2	1	33	476.47	57.7	10	CN(C)CCOc1ncc(NC(=O)N2CCc3cc(C)c(cc23)C(F)(F)F)cc1C(F)(F)F
TCMDC-139850	0.905	6.04	18	13	6.254	1	1	33	475.48	44.81	10	Cl.CN(C)CCOc1ccc(NC(=O)N2CCc3cc(C)c(cc23)C(F)(F)F)cc1C(F)(F)F
TCMDC-139873	0.708	6.15	18	13	6.254	1	1	33	475.48	44.81	10	Cl.CN(C)CCOc1cc(NC(=O)N2CCc3cc(C)c(cc23)C(F)(F)F)cc(c1)C(F)(F)F
TCMDC-140341	0.259	6.59	18	13	7.93	1	1	37	531.6	44.81	10	Cl.CC(C)N(CCOc1cc(NC(=O)N2CCc3cc(C)c(cc23)C(F)(F)F)cc(c1)C(F)(F)F)C(C)C
TCMDC-123870	0.045	7.35	19	3	3.852	2	0	22	292.36	46.34	20	CN(C)c1ccc(C=Cc2nc(=O)c3ccccc3o2)cc1
TCMDC-123878	1.052	5.98	19	3	4.55	2	0	20	328.17	43.1	8	Brc1ccc(C=Cc2nc(=O)c3ccccc3o2)cc1

TCMDC-124577	0.064	7.19	19	3	3.345	2	0	23	309.34	61.56	20	COc1cccc(C=Cc2nc(=O)c3ccccc3o2)c1OC
TCMDC-136672	0.074	7.13	20	4	4.764	2	2	22	310.8	45.15	17	OCc1ccc(cc1)-c1cncc(Nc2cccc(Cl)c2)c1
TCMDC-136669	0.773	6.11	20	4	3.424	4	1	26	369.42	104.88	14	CS(=O)(=O)c1ccc(cc1)-c1cncc(Nc2cccc(c2)N(=O)=O)c1
TCMDC-136670			20	4	3.915	3	2	24	321.36	90.97	10	OCc1ccc(cc1)-c1cncc(Nc2cccc(c2)N(=O)=O)c1
TCMDC-136671	0.089	7.05	20	4	4.944	2	2	23	328.79	45.15	17	OCc1ccc(cc1)-c1cncc(Nc2ccc(F)c(Cl)c2)c1
TCMDC-135629	0.082	7.09	21	2	5.353	2	1	28	391.93	45.23	17	Cl.Clc1ccc(\C=C\C(=O)Nc2ccc3nc(CN4CCCC4)ccc3c2)cc1
TCMDC-135628	0.255	6.59	21	2	5.353	2	1	28	391.93	45.23	11	Cl.Clc1cccc(\C=C\C(=O)Nc2ccc3nc(CN4CCCC4)ccc3c2)c1
TCMDC-125243	0.084	7.08	22	10	3.605	4	1	30	424.56	86.37	21	Cc1ccc(cc1)S(=O)(=O)N1CCCN(CC1)C(=O)c1cc([nH]n1)-c1ccccc1
TCMDC-124703	0.357	6.45	22	10	4.027	4	1	28	481.41	86.37	12	Brc1ccc(cc1)S(=O)(=O)N1CCN(CC1)C(=O)c1cc(n[nH]1)-c1cccs1
TCMDC-124702	0.292	6.53	22	10	3.877	4	1	28	436.96	86.37	15	Clc1ccc(cc1)S(=O)(=O)N1CCN(CC1)C(=O)c1cc(n[nH]1)-c1cccs1
TCMDC-124701	0.868	6.06	22	10	3.612	4	1	27	442.98	86.37	15	Clc1ccc(s1)S(=O)(=O)N1CCN(CC1)C(=O)c1cc(n[nH]1)-c1cccs1
TCMDC-124700	0.866	6.06	22	10	4.162	4	1	29	430.58	86.37	12	Cc1ccc(c(C)c1)S(=O)(=O)N1CCN(CC1)C(=O)c1cc(n[nH]1)-c1cccs1
TCMDC-124699	0.497	6.3	22	10	3.532	4	1	28	465.35	99.51	15	Brc1ccc(cc1)S(=O)(=O)N1CCN(CC1)C(=O)c1cc(n[nH]1)-c1ccco1
TCMDC-124698	0.356	6.45	22	10	3.383	4	1	28	420.9	99.51	15	Clc1ccc(cc1)S(=O)(=O)N1CCN(CC1)C(=O)c1cc(n[nH]1)-c1ccco1
TCMDC-124697	0.925	6.03	22	10	3.732	4	1	28	436.96	86.37	15	Clc1ccc(s1)S(=O)(=O)N1CCN(CC1)C(=O)c1cc(n[nH]1)-c1ccccc1
TCMDC-124401	0.603	6.22	22	10	3.782	4	1	29	410.53	86.37	15	Cc1ccc(cc1)S(=O)(=O)N1CCN(CC1)C(=O)c1cc(n[nH]1)-c1ccccc1
TCMDC-124398	1.159	5.94	22	10	3.183	4	1	31	440.56	95.6	12	COc1ccccc1-c1cc([nH]n1)C(=O)N1CCN(CC1)S(=O)(=O)c1ccc(C)cc1
TCMDC-125225	0.088	7.06	23	2	3.728	2	0	20	309.83	29.54	20	CC1CN(CC(C)O1)C(=O)c1sc2ccccc2c1Cl
TCMDC-125624	0.176	6.75	23	2	4.227	2	0	21	323.86	29.54	11	CC1CN(CC(C)O1)C(=O)c1sc2cc(C)ccc2c1Cl
TCMDC-123859	0.239	6.62	24	6	3.386	1	2	19	252.35	57.94	16	CN(C)c1ccc(cc1)-c1nc2cc(N)ccc2[nH]1
TCMDC-124395	0.941	6.03	24	6	3.79	1	2	20	259.33	54.7	16	Cl.Nc1ccc(cc1)-c1nc2c(ccc3ccccc23)[nH]1
TCMDC-124391	0.892	6.05	24	6	2.563	1	3	18	238.32	80.72	16	Cc1cc(N)cc2nc([nH]c12)-c1ccc(N)cc1
TCMDC-137223	0.698	6.16	24	6	3.276	2	1	17	219.26	52.47	16	N#Cc1ccc2[nH]c(nc2c1)-c1ccccc1
TCMDC-124242	1.207	5.92	24	6	2.513	1	3	18	238.32	80.72	13	Cc1c(N)ccc2[nH]c(nc12)-c1ccc(N)cc1
TCMDC-123486	0.512	6.29	24	6	5.157	2	4	33	430.55	109.4	12	Nc1ccc(cc1)-c1nc2cc(Cc3ccc4[nH]c(nc4c3)-c3ccc(N)cc3)ccc2[nH]1
TCMDC-136679	0.255	6.59	25	8	2.885	4	1	26	340.42	78.9	16	N#Cc1ccc(cc1)-c1cnc2ccc(NCCc3cccnc3)nn12
TCMDC-134177	0.772	6.11	25	8	2.966	2	0	24	324.42	51.89	16	OC=O.COc1ccc(cc1OC)-c1cnc2ccc(nn12)N1CCCC1
TCMDC-136680	0.857	6.07	25	8	4.163	3	1	25	349.85	55.11	13	Clc1ccc(cc1)-c1cnc2ccc(NCCc3cccnc3)nn12
TCMDC-136683	0.672	6.17	25	8	2.181	3	2	24	328.41	80.91	16	COc1ccc(cc1OC)-c1cnc2ccc(NCCCO)nn12
TCMDC-136691	0.978	6.01	25	8	3.967	3	2	27	358.48	62.45	16	OC1CCC(CC1)Nc1ccc2ncc(-c3ccc4ccccc4c3)n2n1
TCMDC-136692	0.995	6	25	8	2.601	5	2	26	352.43	99.75	16	OC1CCC(CC1)Nc1ccc2ncc(-c3ccc(cc3)C(O)=O)n2n1
TCMDC-136693	0.824	6.08	25	8	3.508	3	2	24	342.86	62.45	16	OC1CCC(CC1)Nc1ccc2ncc(-c3ccc(Cl)cc3)n2n1
TCMDC-136694	0.715	6.15	25	8	2.177	4	2	25	339.44	84.57	16	COc1ccc(cn1)-c1cnc2ccc(NC3CCC(O)CC3)nn12
TCMDC-125317	0.331	6.48	26	13	3.649	2	0	17	264.71	25.78	16	Fc1ccc(cc1)-c1csc2ncnc(Cl)c12
TCMDC-123811	0.46	6.34	26	13	4.219	2	0	17	281.16	25.78	13	Clc1ccc(cc1)-c1csc2ncnc(Cl)c12
TCMDC-125437			26	13	4.004	2	0	17	260.75	25.78	9	Cc1nc(Cl)c2c(csc2n1)-c1ccccc1
TCMDC-125318	0.886	6.05	26	13	4.369	2	0	17	325.61	25.78	13	Clc1ncnc2scc(-c3ccc(Br)cc3)c12
TCMDC-125316	0.769	6.11	26	13	3.177	2	0	20	306.78	44.24	16	COc1ccc(cc1OC)-c1csc2ncnc(Cl)c12
TCMDC-123805	0.781	6.11	26	13	3.444	2	0	18	276.75	35.01	16	COc1ccc(cc1)-c1csc2ncnc(Cl)c12
TCMDC-125523	0.357	6.45	26	13	3.676	2	0	21	320.81	44.24	16	COc1ccc(cc1OC)-c1csc2nc(C)nc(Cl)c12
TCMDC-125643	0.934	6.03	27	7	3.686	2	1	25	362.78	55.13	16	Cc1onc(c1C(=O)Nc1cc(C)ccc1F)-c1c(F)cccc1Cl
TCMDC-125477	0.916	6.04	27	7	3.774	2	1	28	441.71	73.59	15	COc1cc(NC(=O)c2c(C)onc2-c2c(Cl)cccc2Cl)c(OC)cc1Cl
TCMDC-125644	0.952	6.02	27	7	3.707	2	1	24	456.66	55.13	15	Cc1onc(c1C(=O)Nc1ccccc1I)-c1c(F)cccc1Cl
TCMDC-123664	0.701	6.15	27	7	2.936	2	1	27	390.82	73.59	16	COc1ccc(OC)c(NC(=O)c2c(C)onc2-c2c(F)cccc2Cl)c1
TCMDC-123635	0.861	6.06	27	7	3.454	2	1	28	425.26	73.59	15	COc1cc(NC(=O)c2c(C)onc2-c2c(F)cccc2Cl)c(OC)cc1Cl
TCMDC-123514	1.182	5.93	27	7	4.683	2	1	25	416.09	55.13	9	Cc1onc(c1C(=O)Nc1cc(Cl)c(Cl)cc1Cl)-c1ccccc1Cl
TCMDC-124175	0.192	6.72	27	7	4.062	2	1	24	361.24	55.13	13	Cc1onc(c1C(=O)Nc1cc(Cl)ccc1C)-c1ccccc1Cl
TCMDC-133315	0.605	6.22	28	51	3.187	4	3	36	511.03	117.59	18	OC(=O)C(F)(F)F.COC(=O)c1ccc(NC(=O)Nc2ccc(Cn3ncc(N4CCCNCC4)c(Cl)c3=O)cc2)cc1
TCMDC-133312	1.139	5.94	28	51	5.282	3	3	37	523.14	91.29	12	OC(=O)C(F)(F)F.CCCCCc1ccc(NC(=O)Nc2ccc(Cn3ncc(N4CCCNCC4)c(Cl)c3=O)cc2)cc1
TCMDC-133313	1.027	5.99	28	51	4.623	3	3	36	509.11	91.29	12	OC(=O)C(F)(F)F.CCC(C)c1ccc(NC(=O)Nc2ccc(Cn3ncc(N4CCCNCC4)c(Cl)c3=O)cc2)cc1
TCMDC-133314	0.752	6.12	28	51	4.493	3	3	36	509.11	91.29	15	OC(=O)C(F)(F)F.CC(C)(C)c1ccc(NC(=O)Nc2ccc(Cn3ncc(N4CCCNCC4)c(Cl)c3=O)cc2)cc1
TCMDC-133316	0.987	6.01	28	51	4.765	4	3	39	545.09	100.52	15	OC(=O)C(F)(F)F.Clc1c(cnn(Cc2ccc(NC(=O)Nc3cccc(Oc4ccccc4)c3)cc2)c1=O)N1CCCNCC1
TCMDC-133317	0.767	6.12	28	51	4.328	3	3	37	538.98	91.29	15	OC(=O)C(F)(F)F.Fc1cc(NC(=O)Nc2ccc(Cn3ncc(N4CCCNCC4)c(Cl)c3=O)cc2)cc(c1)C(F)(F)F
TCMDC-133318	0.923	6.03	28	51	5.944	3	3	40	567.2	100.52	15	OC(=O)C(F)(F)F.CCCCCCCOc1ccc(NC(=O)Nc2ccc(Cn3ncc(N4CCCNCC4)c(Cl)c3=O)cc2)cc1
TCMDC-133319	0.822	6.09	28	51	4.538	3	3	40	559.12	100.52	15	OC(=O)C(F)(F)F.Clc1c(cnn(Cc2ccc(NC(=O)Nc3ccc(OCc4ccccc4)cc3)cc2)c1=O)N1CCCNCC1
TCMDC-133320	0.529	6.28	28	51	4.335	3	3	37	553.05	91.29	15	OC(=O)C(F)(F)F.FC(F)(F)Sc1ccc(NC(=O)Nc2ccc(Cn3ncc(N4CCCNCC4)c(Cl)c3=O)cc2)cc1
TCMDC-133321	0.675	6.17	28	51	4.335	3	3	37	553.05	91.29	15	OC(=O)C(F)(F)F.FC(F)(F)Sc1cccc(NC(=O)Nc2ccc(Cn3ncc(N4CCCNCC4)c(Cl)c3=O)cc2)c1
TCMDC-133322	1.118	5.95	28	51	4.093	3	3	33	578.89	91.29	12	OC(=O)C(F)(F)F.Clc1c(cnn(Cc2ccc(NC(=O)Nc3ccc(I)cc3)cc2)c1=O)N1CCCNCC1
TCMDC-133323	0.739	6.13	28	51	4.774	4	3	39	553.12	117.59	15	OC(=O)C(F)(F)F.CCCCOC(=O)c1ccc(NC(=O)Nc2ccc(Cn3ncc(N4CCCNCC4)c(Cl)c3=O)cc2)cc1
TCMDC-133324	0.708	6.15	28	51	3.349	5	3	40	569.07	143.89	18	OC(=O)C(F)(F)F.COC(=O)c1ccc(NC(=O)Nc2ccc(Cn3ncc(N4CCCNCC4)c(Cl)c3=O)cc2)cc(c1)C(=O)OC
TCMDC-133325	1.049	5.98	28	51	4.094	3	3	35	495.08	91.29	12	OC(=O)C(F)(F)F.CC(C)c1ccc(NC(=O)Nc2ccc(Cn3ncc(N4CCCNCC4)c(Cl)c3=O)cc2)cc1
TCMDC-133326	0.866	6.06	28	51	4.502	3	3	34	521.87	91.29	15	OC(=O)C(F)(F)F.Clc1cc(Cl)cc(NC(=O)Nc2ccc(Cn3ncc(N4CCCNCC4)c(Cl)c3=O)cc2)c1
TCMDC-133327	0.588	6.23	28	51	5.148	3	3	40	588.99	91.29	15	OC(=O)C(F)(F)F.FC(F)(F)c1ccc(NC(=O)Nc2ccc(Cn3ncc(N4CCCNCC4)c(Cl)c3=O)cc2)cc(c1)C(F)(F)F
TCMDC-133328	0.731	6.14	28	51	4.08	3	3	36	520.99	91.29	15	OC(=O)C(F)(F)F.FC(F)(F)c1ccc(NC(=O)Nc2ccc(Cn3ncc(N4CCCNCC4)c(Cl)c3=O)cc2)cc1
TCMDC-133329	1.137	5.94	28	51	3.833	3	3	33	531.88	91.29	15	OC(=O)C(F)(F)F.Clc1c(cnn(Cc2ccc(NC(=O)Nc3ccc(Br)cc3)cc2)c1=O)N1CCCNCC1
TCMDC-133330	0.443	6.35	28	51	3.716	4	3	37	525.06	117.59	18	OC(=O)C(F)(F)F.CCOC(=O)c1ccc(NC(=O)Nc2ccc(Cn3ncc(N4CCCNCC4)c(Cl)c3=O)cc2)cc1
TCMDC-133331	0.783	6.11	28	51	3.683	3	3	33	487.43	91.29	18	OC(=O)C(F)(F)F.Clc1ccc(NC(=O)Nc2ccc(Cn3ncc(N4CCCNCC4)c(Cl)c3=O)cc2)cc1

TCMDC-133332	0.918	6.04	28	51	3.166	3	3	33	467.02	91.29	18	OC(=O)C(F)(F)F.Cc1ccc(NC(=O)Nc2ccc(Cn3ncc(N4CCCNCC4)c(Cl)c3=O)cc2)cc1
TCMDC-141693	0.713	6.15	28	51	4.195	3	2	37	514.07	79.26	15	OC(=O)C(F)(F)F.Clc1nn(Cc2ccc(NC(=O)c3ccc(cc3)-c3ccccc3)cc2)c(=O)cc1N1CCCNCC1
TCMDC-141694	0.369	6.43	28	51	4.508	3	3	37	515.06	91.29	15	OC(=O)C(F)(F)F.Clc1nn(Cc2cccc(NC(=O)Nc3ccc(cc3)-c3ccccc3)c2)c(=O)cc1N1CCNCC1
TCMDC-141695	0.676	6.17	28	51	4.555	3	3	38	529.09	91.29	15	OC(=O)C(F)(F)F.Clc1nn(Cc2cccc(NC(=O)Nc3ccc(cc3)-c3ccccc3)c2)c(=O)cc1N1CCCNCC1
TCMDC-141696	0.843	6.07	28	51	4.555	3	3	38	529.09	91.29	15	OC(=O)C(F)(F)F.Clc1nn(Cc2ccc(NC(=O)Nc3ccc(cc3)-c3ccccc3)cc2)c(=O)cc1N1CCCNCC1
TCMDC-141697	0.667	6.18	28	51	4.494	3	3	39	543.12	91.29	15	OC(=O)C(F)(F)F.Cc1ccc(Cn2nc(Cl)c(cc2=O)N2CCCNCC2)cc1NC(=O)Nc1ccc(cc1)-c1ccccc1
TCMDC-141698	0.675	6.17	28	51	4.447	3	3	38	529.09	91.29	15	OC(=O)C(F)(F)F.Cc1ccc(Cn2nc(Cl)c(cc2=O)N2CCNCC2)cc1NC(=O)Nc1ccc(cc1)-c1ccccc1
TCMDC-141699	1.382	5.86	28	51	4.397	3	3	38	529.09	91.29	12	OC(=O)C(F)(F)F.Cc1c(Cn2nc(Cl)c(cc2=O)N2CCNCC2)cccc1NC(=O)Nc1ccc(cc1)-c1ccccc1
TCMDC-141700	0.753	6.12	28	51	4.508	3	3	37	515.06	91.29	15	OC(=O)C(F)(F)F.Clc1nn(Cc2ccc(NC(=O)Nc3ccc(cc3)-c3ccccc3)cc2)c(=O)cc1N1CCNCC1
TCMDC-141724	0.364	6.44	28	51	4.658	3	3	40	559.12	100.52	15	OC(=O)C(F)(F)F.COc1ccc(NC(=O)Nc2ccc(cc2)-c2ccccc2)cc1Cn1nc(Cl)c(cc1=O)N1CCCNCC1
TCMDC-141920	0.456	6.34	28	51	4.508	3	3	37	515.06	91.29	15	OC(=O)C(F)(F)F.Clc1c(cnn(Cc2cccc(NC(=O)Nc3ccc(cc3)-c3ccccc3)c2)c1=O)N1CCNCC1
TCMDC-141921	1.117	5.95	28	51	4.447	3	3	38	529.09	91.29	12	OC(=O)C(F)(F)F.Cc1ccc(Cn2ncc(N3CCNCC3)c(Cl)c2=O)cc1NC(=O)Nc1ccc(cc1)-c1ccccc1
TCMDC-141922	0.591	6.23	28	51	4.508	3	3	37	515.06	91.29	15	OC(=O)C(F)(F)F.Clc1c(cnn(Cc2ccc(NC(=O)Nc3ccc(cc3)-c3ccccc3)cc2)c1=O)N1CCNCC1
TCMDC-141923	0.225	6.65	28	51	4.555	3	3	38	529.09	91.29	15	Clc1c(cnn(Cc2cccc(NC(=O)Nc3ccc(cc3)-c3ccccc3)c2)c1=O)N1CCCNCC1
TCMDC-141924	0.625	6.2	28	51	4.494	3	3	39	543.12	91.29	15	Cc1ccc(Cn2ncc(N3CCCNCC3)c(Cl)c2=O)cc1NC(=O)Nc1ccc(cc1)-c1ccccc1
TCMDC-141925	0.64	6.19	28	51	4.08	3	3	36	520.99	91.29	15	OC(=O)C(F)(F)F.FC(F)(F)c1cccc(NC(=O)Nc2ccc(Cn3ncc(N4CCCNCC4)c(Cl)c3=O)cc2)c1
TCMDC-141926	1.099	5.96	28	51	3.307	4	3	36	515.98	137.11	15	Fc1ccc(NC(=O)Nc2ccc(Cn3ncc(N4CCCNCC4)c(Cl)c3=O)cc2)c(c1)N(=O)=O
TCMDC-141927	0.815	6.09	28	51	4.555	3	3	38	529.09	91.29	15	Clc1c(cnn(Cc2ccc(NC(=O)Nc3ccc(cc3)-c3ccccc3)cc2)c1=O)N1CCCNCC1
TCMDC-141928	0.797	6.1	28	51	4.555	3	3	38	529.09	91.29	15	OC(=O)C(F)(F)F.Clc1c(cnn(Cc2ccc(NC(=O)Nc3ccc(cc3)-c3ccccc3)cc2)c1=O)N1CCCNCC1
TCMDC-141929	0.657	6.18	28	51	4.58	3	4	39	543.12	100.08	15	OC(=O)C(F)(F)F.Cc1ccc(Cn2ncc(NC3CCNCC3)c(Cl)c2=O)cc1NC(=O)Nc1ccc(cc1)-c1ccccc1
TCMDC-141930	1.14	5.94	28	51	3.917	3	3	38	529.09	105.28	15	OC(=O)C(F)(F)F.NC1CCN(CC1)c1cnn(Cc2cccc(NC(=O)Nc3ccc(cc3)-c3ccccc3)c2)c(=O)c1Cl
TCMDC-141931	0.697	6.16	28	51	3.806	3	3	39	543.12	105.28	18	OC(=O)C(F)(F)F.Cc1c(Cn2ncc(N3CCC(N)CC3)c(Cl)c2=O)cccc1NC(=O)Nc1ccc(cc1)-c1ccccc1
TCMDC-141932	0.917	6.04	28	51	3.856	3	3	39	543.12	105.28	18	OC(=O)C(F)(F)F.Cc1ccc(Cn2ncc(N3CCC(N)CC3)c(Cl)c2=O)cc1NC(=O)Nc1ccc(cc1)-c1ccccc1
TCMDC-141933	0.818	6.09	28	51	5.07	3	3	37	535.02	91.29	15	OC(=O)C(F)(F)F.CC1CN(CC(C)N1)c1cnn(Cc2cccc(NC(=O)Nc3cccc(c3)C(F)(F)F)c2)c(=O)c1Cl
TCMDC-141934	0.866	6.06	28	51	4.298	4	3	37	530.01	137.11	15	OC(=O)C(F)(F)F.CC1CN(CC(C)N1)c1cnn(Cc2cccc(NC(=O)Nc3ccc(F)cc3N(=O)=O)c2)c(=O)c1Cl
TCMDC-141935	0.34	6.47	28	51	5.546	3	3	39	543.12	91.29	15	OC(=O)C(F)(F)F.CC1CN(CC(C)N1)c1cnn(Cc2cccc(NC(=O)Nc3ccc(cc3)-c3ccccc3)c2)c(=O)c1Cl
TCMDC-141936	0.596	6.22	28	51	5.435	3	3	40	557.15	91.29	15	OC(=O)C(F)(F)F.CC1CN(CC(C)N1)c1cnn(Cc2cccc(NC(=O)Nc3ccc(cc3)-c3ccccc3)c2C)c(=O)c1Cl
TCMDC-141937	0.739	6.13	28	51	5.485	3	3	40	557.15	91.29	15	OC(=O)C(F)(F)F.CC1CN(CC(C)N1)c1cnn(Cc2cccc(C)c(NC(=O)Nc3ccc(cc3)-c3ccccc3)c2)c(=O)c1Cl
TCMDC-141938	0.94	6.03	28	51	5.07	3	3	37	535.02	91.29	15	OC(=O)C(F)(F)F.CC1CN(CC(C)N1)c1cnn(Cc2ccc(NC(=O)Nc3cccc(c3)C(F)(F)F)cc2)c(=O)c1Cl
TCMDC-141939	0.808	6.09	28	51	4.298	4	3	37	530.01	137.11	15	OC(=O)C(F)(F)F.CC1CN(CC(C)N1)c1cnn(Cc2ccc(NC(=O)Nc3ccc(F)cc3N(=O)=O)cc2)c(=O)c1Cl
TCMDC-141940	0.367	6.44	28	51	5.546	3	3	39	543.12	91.29	15	OC(=O)C(F)(F)F.CC1CN(CC(C)N1)c1cnn(Cc2ccc(NC(=O)Nc3ccc(cc3)-c3ccccc3)cc2)c(=O)c1Cl
TCMDC-136814	0.189	6.72	29	24	5.418	1	1	27	363.55	58.69	16	OC=O.CCCCC(CC)CN1C(N)=NC(C1=O)(c1ccccc1)c1ccccc1
TCMDC-132351	1.228	5.91	29	24	3.654	2	2	29	385.5	78.92	16	NC1=NC(C(=O)N1CCCc1ccccc1)(c1ccccc1)c1cccc(O)c1
TCMDC-132352	0.836	6.08	29	24	3.654	2	2	29	385.5	78.92	19	NC1=NC(C(=O)N1CCCc1ccccc1)(c1ccccc1)c1cccc(O)c1
TCMDC-136488	0.76	6.12	29	24	4.85	1	1	29	383.53	58.69	16	OC=O.NC1=NC(C(=O)N1CCCCc1ccccc1)(c1ccccc1)c1ccccc1
TCMDC-136491	0.97	6.01	29	24	4.36	1	1	25	335.49	58.69	16	OC=O.CCC(CC)CN1C(N)=NC(C1=O)(c1ccccc1)c1ccccc1
TCMDC-136492	0.26	6.59	29	24	4.159	1	1	32	429.56	77.15	15	OC=O.COc1cccc(c1)C1(N=C(N)N(CCCc2ccccc2)C1=O)c1cccc(OC)c1
TCMDC-136493	0.844	6.07	29	24	3.954	1	1	28	371.47	67.92	19	NC1=NC(C(=O)N1CCOc1ccccc1)(c1ccccc1)c1ccccc1
TCMDC-136503	1.054	5.98	29	24	4.24	1	1	30	399.53	67.92	13	OC(=O)C(F)(F)F.COc1ccc(CCCN2C(N)=NC(C2=O)(c2ccccc2)c2ccccc2)cc1
TCMDC-136504	0.265	6.58	29	24	4.24	1	1	30	399.53	67.92	16	OC(=O)C(F)(F)F.COc1ccccc1CCCN1C(N)=NC(C1=O)(c1ccccc1)c1ccccc1
TCMDC-136505	0.598	6.22	29	24	4.217	1	1	28	367.48	58.69	16	OC(=O)C(F)(F)F.NC1=NC(C(=O)N1CC=Cc1ccccc1)(c1ccccc1)c1ccccc1
TCMDC-136516	0.805	6.09	29	24	3.741	1	1	24	321.46	58.69	19	OC=O.CCC(CC)N1C(N)=NC(C1=O)(c1ccccc1)c1ccccc1
TCMDC-136522	0.858	6.07	29	24	4.769	1	1	31	413.56	67.92	15	OC(=O)C(F)(F)F.COc1ccc(CCCCN2C(N)=NC(C2=O)(c2ccccc2)c2ccccc2)cc1
TCMDC-136547	0.891	6.05	29	24	3.811	1	1	24	321.46	58.69	19	CCC1(N=C(N)N(CCCc2ccccc2)C1=O)c1ccccc1
TCMDC-136715	0.971	6.01	29	24	4.486	1	1	31	412.58	61.93	15	OC(=O)C(F)(F)F.CN(C)c1ccc(cc1)C1(N=C(N)N(CCCc2ccccc2)C1=O)c1ccccc1
TCMDC-136760	0.515	6.29	29	24	3.701	1	1	24	321.46	58.69	19	OC=O.CC(C)(C)CN1C(N)=NC(C1=O)(c1ccccc1)c1ccccc1
TCMDC-136761	0.661	6.18	29	24	3.786	1	1	25	333.47	58.69	19	OC=O.NC1=NC(C(=O)N1C1CCCCC1)(c1ccccc1)c1ccccc1
TCMDC-136775	0.753	6.12	29	24	3.377	1	1	24	319.44	58.69	19	OC=O.NC1=NC(C(=O)N1CC1CCC1)(c1ccccc1)c1ccccc1
TCMDC-136799	0.712	6.15	29	24	3.831	1	1	24	321.46	58.69	19	OC=O.CCC(C)CN1C(N)=NC(C1=O)(c1ccccc1)c1ccccc1
TCMDC-136807	0.659	6.18	29	24	3.831	1	1	26	345.48	58.69	19	OC=O.NC1=NC(C(=O)N1C(CC=C)CC=C)(c1ccccc1)c1ccccc1
TCMDC-136877	0.793	6.1	29	24	3.961	1	1	24	321.46	58.69	19	CCCCCN1C(N)=NC(C1=O)(c1ccccc1)c1ccccc1
TCMDC-136878	0.182	6.74	29	24	6.476	1	1	29	391.61	58.69	14	OC=O.CCCCC(CCCC)CN1C(N)=NC(C1=O)(c1ccccc1)c1ccccc1
TCMDC-136879	0.136	6.87	29	24	4.87	1	1	29	383.53	58.69	16	OC=O.CCC(CN1C(N)=NC(C1=O)(c1ccccc1)c1ccccc1)c1ccccc1
TCMDC-137006	0.815	6.09	29	24	2.705	2	2	27	364.49	87.79	19	CC(C)CNC(=O)CN1C(N)=NC(C1=O)(c1ccccc1)c1ccccc1
TCMDC-137051	1.062	5.97	29	24	3.321	1	1	20	273.42	58.69	16	OC(=O)C(F)(F)F.CCC(CC)CN1C(N)=NC(C)(C1=O)c1ccccc1
TCMDC-140688	0.757	6.12	30	34	5.649	3	3	33	501.87	73.83	15	Cl.CC(C)(CNCc1ccc(Cl)c(Cl)c1)c1nc(c([nH]1)-c1ccncc1)-c1ccc(Cl)c(O)c1
TCMDC-140762	0.736	6.13	30	34	2.315	3	3	25	356.89	73.83	19	Cl.CNCC(C)(C)c1nc(c([nH]1)-c1ccncc1)-c1ccc(Cl)c(O)c1
TCMDC-140369	0.756	6.12	30	34	2.169	3	3	24	342.86	87.82	19	Cl.CC(C)(CN)c1nc(c([nH]1)-c1ccncc1)-c1ccc(Cl)c(O)c1
TCMDC-140389	0.537	6.27	30	34	4.343	3	3	31	432.99	73.83	15	Cl.CC(C)(CNCc1ccccc1)c1nc(c([nH]1)-c1ccncc1)-c1ccc(Cl)c(O)c1
TCMDC-140538	0.357	6.45	30	34	4.262	3	3	33	463.02	83.06	15	Cl.COc1ccc(CNCC(C)(C)c2nc(c([nH]2)-c2ccncc2)-c2ccc(Cl)c(O)c2)cc1
TCMDC-140548	0.476	6.32	30	34	5.056	3	3	32	467.43	73.83	15	Cl.CC(C)(CNCc1ccc(Cl)cc1)c1nc(c([nH]1)-c1ccncc1)-c1ccc(Cl)c(O)c1
TCMDC-140549	0.601	6.22	30	34	4.171	3	3	29	413.01	73.83	15	Cl.CC(C)(C)CNCC(C)(C)c1nc(c([nH]1)-c1ccncc1)-c1ccc(Cl)c(O)c1
TCMDC-140650	0.708	6.15	30	34	4.711	3	3	38	534.16	86.3	15	Cl.CN(C)CCCOc1ccc(CNCC(C)(C)c2nc(c([nH]2)-c2ccncc2)-c2ccc(Cl)c(O)c2)cc1
TCMDC-140672	0.66	6.18	30	34	4.559	3	3	33	468.97	73.83	15	Cl.CC(C)(CNCc1ccc(F)c(F)c1)c1nc(c([nH]1)-c1ccncc1)-c1ccc(Cl)c(O)c1
TCMDC-140674	0.769	6.11	30	34	2.815	2	2	25	401.34	76.82	18	Cl.COc1cc(ccc1Br)-c1nc([nH]c1-c1ccncc1)C(C)(C)CN
TCMDC-140680	0.965	6.02	30	34	2.369	3	3	24	387.31	87.82	19	Cl.CC(C)(CN)c1nc(c([nH]1)-c1ccncc1)-c1ccc(Br)c(O)c1
TCMDC-140687	0.693	6.16	30	34	4.262	3	3	33	463.02	83.06	15	Cl.COc1cccc(CNCC(C)(C)c2nc(c([nH]2)-c2ccncc2)-c2ccc(Cl)c(O)c2)c1

TCMDC-140689	0.734	6.13	30	34	5.226	3	3	35	500.99	73.83	15	Cl.CC(C)(CNCc1ccc(cc1)C(F)(F)F)c1nc(c([nH]1)-c1ccncc1)-c1ccc(Cl)c(O)c1
TCMDC-140700	1	6	30	34	2.805	4	3	33	466.03	94.14	18	Cl.CN1CCC=C(C1)C(=O)NCC(C)(C)c1nc(c([nH]1)-c1ccncc1)-c1ccc(Cl)c(O)c1
TCMDC-140708	0.545	6.26	30	34	5.371	3	3	36	516.99	83.06	15	Cl.CC(C)(CNCc1ccc(OC(F)(F)F)cc1)c1nc(c([nH]1)-c1ccncc1)-c1ccc(Cl)c(O)c1
TCMDC-140736	0.643	6.19	30	34	5.348	4	3	44	620.26	112.6	14	Cl.COc1ccc(cc1OCCN(C(C)C)C(C)C)C(=O)NCC(C)(C)c1nc(c([nH]1)-c1ccncc1)-c1ccc(Cl)c(O)c1
TCMDC-140792	0.911	6.04	30	34	2.196	5	3	36	556.56	103.37	18	Cl.COCCN1CCC(CC1)C(=O)NCC(C)(C)c1nc(c([nH]1)-c1ccncc1)-c1ccc(Br)c(O)c1
TCMDC-140898	0.753	6.12	30	34	3.175	4	3	35	498.13	86.3	18	Cl.COCCN1CCC(CNCC(C)(C)c2nc(c([nH]2)-c2ccncc2)-c2ccc(Cl)c(O)c2)CC1
TCMDC-140899	1.031	5.99	30	34	3.711	4	2	36	512.16	77.51	15	Cl.COCCN1CCC(CN(C)CC(C)(C)c2nc(c([nH]2)-c2ccncc2)-c2ccc(Cl)c(O)c2)CC1
TCMDC-140926	0.717	6.14	30	34	2.556	4	3	34	484.1	86.3	18	Cl.COCCN1CCC(CC1)NCC(C)(C)c1nc(c([nH]1)-c1ccncc1)-c1ccc(Cl)c(O)c1
TCMDC-140954	0.866	6.06	30	34	2.777	4	3	38	534.11	107.28	18	Cl.CC(C)(CNC(=O)C1CCN(Cc2ccoc2)CC1)c1nc(c([nH]1)-c1ccncc1)-c1ccc(Cl)c(O)c1
TCMDC-141060	1.274	5.89	30	34	2.242	4	4	31	439.99	102.93	15	Cl.CC(C)(CNC(=O)[C@H]1CCCN1)c1nc(c([nH]1)-c1ccncc1)-c1ccc(Cl)c(O)c1
TCMDC-141070	0.727	6.14	30	34	2.801	4	4	32	454.02	102.93	18	Cl.CC(C)(CNC(=O)[C@H]1CCCCN1)c1nc(c([nH]1)-c1ccncc1)-c1ccc(Cl)c(O)c1
	0.841	6.08	30	34	2.801	4	4	32	454.02	102.93	18	Cl.CC(C)(CNC(=O)[C@@H]1CCCCN1)c1nc(c([nH]1)-c1ccncc1)-c1ccc(Cl)c(O)c1
TCMDC-141122	0.62	6.21	30	34	3.616	5	3	42	588.21	103.37	18	Cl.CC(C)(CNC(=O)C1CCN(CCOCc2ccccc2)CC1)c1nc(c([nH]1)-c1ccncc1)-c1ccc(Cl)c(O)c1
TCMDC-141124	0.709	6.15	30	34	4.549	4	3	42	608.62	103.37	14	Cl.CC(C)(CNC(=O)C1CCN(CCOc2ccc(Cl)cc2)CC1)c1nc(c([nH]1)-c1ccncc1)-c1ccc(Cl)c(O)c1
TCMDC-141125	0.881	6.06	30	34	5.717	4	3	42	608.62	103.37	14	Cl.CC(C)(CNC(=O)[C@@H]1CCCN(CCOc2ccc(Cl)cc2)CC1)c1nc(c([nH]1)-c1ccncc1)-c1ccc(Cl)c(O)c1
TCMDC-141136	0.316	6.5	30	34	4.101	4	3	43	610.16	103.37	14	Cl.CC(C)(CNC(=O)C1CCN(CCOc2ccc(F)c(F)c2)CC1)c1nc(c([nH]1)-c1ccncc1)-c1ccc(Cl)c(O)c1
TCMDC-141137	0.722	6.14	30	34	5.269	4	3	43	610.16	103.37	14	Cl.CC(C)(CNC(=O)[C@@H]1CCCN(CCOc2ccc(F)c(F)c2)CC1)c1nc(c([nH]1)-c1ccncc1)-c1ccc(Cl)c(O)c1
TCMDC-141138	0.623	6.21	30	34	4.314	4	3	40	578.59	94.14	15	Cl.CC(C)(CNC(=O)C1CCN(Cc2ccc(Cl)cc2)CC1)c1nc(c([nH]1)-c1ccncc1)-c1ccc(Cl)c(O)c1
TCMDC-141139	0.941	6.03	30	34	5.393	4	3	40	578.59	94.14	15	Cl.CC(C)(CNC(=O)[C@@H]1CCCN(Cc2ccc(Cl)cc2)CC1)c1nc(c([nH]1)-c1ccncc1)-c1ccc(Cl)c(O)c1
TCMDC-141147	0.888	6.05	30	34	4.293	4	3	39	550.21	94.14	15	Cl.CC(C)(CNC(=O)C1CCN(CC2CCCC2)CC1)c1nc(c([nH]1)-c1ccncc1)-c1ccc(Cl)c(O)c1
TCMDC-141154	0.744	6.13	30	34	3.482	3	3	27	382.93	87.82	19	Cl.NCC1(CCCCC1)c1nc(c([nH]1)-c1ccncc1)-c1ccc(Cl)c(O)c1
TCMDC-141155	0.125	6.9	30	34	6.369	3	3	35	507.5	73.83	13	Cl.Oc1cc(ccc1Cl)-c1nc([nH]c1-c1ccncc1)C1(CNCc2ccc(Cl)cc2)CCCCC1
TCMDC-123580	0.665	6.18	31	10	3.577	2	1	24	362.91	50.16	16	CN(C)CCNC(=O)c1cc2c(nn(C)c2s1)-c1ccc(Cl)cc1
TCMDC-124731	1.098	5.96	31	10	3.924	2	1	31	460.09	53.4	12	CCCN1CCN(CCCNC(=O)c2cc3c(nn(C)c3s2)-c2ccc(Cl)cc2)CC1
TCMDC-124566	1.089	5.96	31	10	5.56	2	1	34	476.66	50.16	9	Cc1cccc(CN2CCC(CNC(=O)c3cc4c(nn(C)c4s3)-c3ccccc3F)CC2)c1
TCMDC-123585	0.955	6.02	31	10	5.074	2	1	35	493.65	62.63	12	COc1cccc(c1)-c1nn(C)c2sc(cc12)C(=O)NCCN1CCN(CC1)c1ccccc1F
TCMDC-123584	0.948	6.02	31	10	3.326	3	1	26	364.45	69.04	16	COc1cccc(c1)-c1nn(C)c2sc(cc12)C(=O)Nc1ccccn1
TCMDC-123583	0.814	6.09	31	10	4.64	2	1	31	434.6	59.39	12	COc1cccc(c1)-c1nn(C)c2sc(cc12)C(=O)NCCN(C)Cc1ccccc1
TCMDC-123582	0.789	6.1	31	10	4.442	2	1	32	448.6	50.16	12	Cn1nc(-c2ccccc2F)c2cc(sc12)C(=O)NC1CCN(Cc2ccccc2)CC1
TCMDC-123581	0.81	6.09	31	10	3.55	3	1	25	352.41	59.81	16	Cn1nc(-c2ccccc2F)c2cc(sc12)C(=O)Nc1ccccn1
TCMDC-123579	0.788	6.1	31	10	4.736	2	1	27	402.98	50.16	12	CCN1CCCC1CNC(=O)c1cc2c(nn(C)c2s1)-c1ccc(Cl)cc1
TCMDC-124416	0.721	6.14	31	10	3.562	3	1	27	404.95	59.39	15	Cn1nc(-c2ccc(Cl)cc2)c2cc(sc12)C(=O)NCCN1CCOCC1
TCMDC-141261	0.721	6.14	32	27	3.444	1	3	31	481.48	60.16	18	CNC(=O)C1Cc2c([nH]c3cc(Br)ccc23)C2(CCN(CCc3ccccc3)CC2)N1
TCMDC-141085	1.139	5.94	32	27	5.058	1	3	35	472.74	60.16	12	CCCCCCNC(=O)C1Cc2c([nH]c3ccccc23)C2(CCN(CCc3ccccc3)CC2)N1
TCMDC-141090	0.932	6.03	32	27	4.759	1	3	34	458.71	60.16	15	CC(C)CCNC(=O)C1Cc2c([nH]c3ccc(C)cc23)C2(CCN(Cc3ccccc3)CC2)N1
TCMDC-141091	0.982	6.01	32	27	5.418	1	3	35	472.74	60.16	15	CCCCCCNC(=O)C1Cc2c([nH]c3ccc(C)cc23)C2(CCN(Cc3ccccc3)CC2)N1
TCMDC-141092	1.271	5.9	32	27	5.557	1	3	36	486.77	60.16	12	CCCCCCNC(=O)C1Cc2c([nH]c3ccc(C)cc23)C2(CCN(CCc3ccccc3)CC2)N1
TCMDC-141178	0.817	6.09	32	27	5.291	1	3	34	523.57	60.16	15	CC(C)CCNC(=O)C1Cc2c([nH]c3ccc(Br)cc23)C2(CCN(Cc3ccccc3)CC2)N1
TCMDC-141179	0.688	6.16	32	27	5.43	1	3	35	537.6	60.16	15	CC(C)CCNC(=O)C1Cc2c([nH]c3ccc(Br)cc23)C2(CCN(CCc3ccccc3)CC2)N1
TCMDC-141180	0.908	6.04	32	27	4.417	1	3	34	521.55	60.16	15	Brc1ccc2[nH]c3c(CC(NC33CCN(CCc4ccccc4)CC3)C(=O)NCC3CC3)c2c1
TCMDC-141181	0.722	6.14	32	27	5.95	1	3	35	537.6	60.16	15	CCCCCCNC(=O)C1Cc2c([nH]c3ccc(Br)cc23)C2(CCN(Cc3ccccc3)CC2)N1
TCMDC-141182	0.788	6.1	32	27	6.089	1	3	36	551.63	60.16	13	CCCCCCNC(=O)C1Cc2c([nH]c3ccc(Br)cc23)C2(CCN(CCc3ccccc3)CC2)N1
TCMDC-141183	0.873	6.06	32	27	5.185	1	3	36	543.55	60.16	15	Brc1ccc2[nH]c3c(CC(NC33CCN(Cc4ccccc4)CC3)C(=O)NCc3ccccc3)c2c1
TCMDC-141184	0.678	6.17	32	27	4.502	1	3	33	509.54	60.16	15	CCCNC(=O)C1Cc2c([nH]c3ccc(Br)cc23)C2(CCN(CCc3ccccc3)CC2)N1
TCMDC-141185	0.919	6.04	32	27	3.444	1	3	31	481.48	60.16	18	CNC(=O)C1Cc2c([nH]c3ccc(Br)cc23)C2(CCN(CCc3ccccc3)CC2)N1
TCMDC-141244	1.366	5.86	32	27	4.653	1	3	36	478.69	60.16	12	Cc1cccc2c3CC(NC4(CCN(Cc5ccccc5)CC4)c3[nH]c12)C(=O)NCc1ccccc1
TCMDC-141245	1.002	6	32	27	4.792	1	3	37	492.72	60.16	12	Cc1cccc2c3CC(NC4(CCN(CCc5ccccc5)CC4)c3[nH]c12)C(=O)NCc1ccccc1
TCMDC-141258	0.792	6.1	32	27	5.291	1	3	34	523.57	60.16	15	CC(C)CCNC(=O)C1Cc2c([nH]c3cc(Br)ccc23)C2(CCN(Cc3ccccc3)CC2)N1
TCMDC-141259	0.91	6.04	32	27	5.43	1	3	35	537.6	60.16	15	CC(C)CCNC(=O)C1Cc2c([nH]c3cc(Br)ccc23)C2(CCN(CCc3ccccc3)CC2)N1
TCMDC-141260	0.972	6.01	32	27	4.502	1	3	33	509.54	60.16	15	CCCNC(=O)C1Cc2c([nH]c3cc(Br)ccc23)C2(CCN(CCc3ccccc3)CC2)N1
TCMDC-141285	0.893	6.05	32	27	3.294	1	3	31	437.03	60.16	18	CNC(=O)C1Cc2c([nH]c3ccc(Cl)cc23)C2(CCN(CCc3ccccc3)CC2)N1
TCMDC-141294	0.69	6.16	32	27	5.28	1	3	35	493.15	60.16	15	CC(C)CCNC(=O)C1Cc2c([nH]c3cc(Cl)ccc23)C2(CCN(CCc3ccccc3)CC2)N1
TCMDC-141295	1.38	5.86	32	27	4.411	1	3	30	431.08	60.16	12	CCCN1CCC2(CC1)NC(Cc1c2[nH]c2cc(Cl)ccc12)C(=O)NCCC(C)C
TCMDC-141296	0.903	6.04	32	27	5.8	1	3	35	493.15	60.16	15	CCCCCCNC(=O)C1Cc2c([nH]c3cc(Cl)ccc23)C2(CCN(Cc3ccccc3)CC2)N1
TCMDC-141297	0.88	6.06	32	27	4.9	1	3	31	445.11	60.16	15	CCCCCCNC(=O)C1Cc2c([nH]c3cc(Cl)ccc23)C2(CCN(CCC)CC2)N1
TCMDC-141298	0.815	6.09	32	27	5.589	1	3	36	507.18	60.16	15	CC(C)CC(C)NC(=O)C1Cc2c([nH]c3cc(Cl)ccc23)C2(CCN(CCc3ccccc3)CC2)N1
TCMDC-141299	0.934	6.03	32	27	3.294	1	3	31	437.03	60.16	18	CNC(=O)C1Cc2c([nH]c3cc(Cl)ccc23)C2(CCN(CCc3ccccc3)CC2)N1
TCMDC-141303	0.871	6.06	32	27	5.23	1	3	35	476.7	60.16	15	CCCCCCNC(=O)C1Cc2c([nH]c3ccc(F)cc23)C2(CCN(Cc3ccccc3)CC2)N1
TCMDC-141304	0.97	6.01	32	27	4.88	1	3	35	476.7	60.16	15	CC(C)CC(C)NC(=O)C1Cc2c([nH]c3ccc(F)cc23)C2(CCN(Cc3ccccc3)CC2)N1
TCMDC-132459	0.734	6.13	33	7	3.133	3	0	29	388.48	61.92	16	Fc1cccc(Cn2cncc2CN(CC2CC2)C(=O)c2ccccc2C#N)c1
TCMDC-132457	0.614	6.21	33	7	4.886	3	0	33	454.54	61.92	12	CC(C)CCN(Cc1cncn1Cc1cccc(c1)C(F)(F)F)C(=O)c1ccccc1C#N
TCMDC-132458	0.774	6.11	33	7	6.064	3	0	37	506.62	51.02	10	CC(C)CCN(Cc1cncn1Cc1cccc(c1)C(F)(F)F)C(=O)c1cncc(c1)-c1ccccc1
TCMDC-132464	0.804	6.09	33	7	4.311	3	0	33	440.56	51.02	12	Fc1ccccc1Cn1cncc1CN(CC1CC1)C(=O)c1cncc(c1)-c1ccccc1
TCMDC-132465	0.762	6.12	33	7	5.894	3	0	34	473.06	51.02	12	CC(C)CCN(Cc1cncn1Cc1cccc(Cl)c1)C(=O)c1cncc(c1)-c1ccccc1
TCMDC-132470	0.791	6.1	33	7	5.324	3	0	34	456.61	51.02	12	CC(C)CCN(Cc1cncn1Cc1ccccc1F)C(=O)c1cncc(c1)-c1ccccc1
TCMDC-132536	1.041	5.98	33	7	4.688	3	0	31	461.43	60.25	9	OC(=O)C(F)(F)F.COc1ccc(Cn2cncc2CN(CCC(C)C)C(=O)c2ccc(Cl)nc2Cl)cc1
TCMDC-136483	0.85	6.07	34	13	3.686	2	2	27	364.54	62.71	16	CC(C)(C)c1nn(-c2ccccc2)c2[nH]c(=O)c(CNC3CCCC3)cc12

TCMDC-125381	0.866	6.06	34	13	4.311	2	2	30	400.57	62.71	12	CC(C)(C)c1nn(-c2ccccc2)c2[nH]c(=O)c(CNCCc3ccccc3)cc12
TCMDC-125352	0.804	6.09	34	13	4.892	2	2	31	416.54	62.71	12	Fc1ccc(cc1)-c1nn(-c2ccccc2)c2[nH]c(=O)c(CNC3CCCCC3)cc12
TCMDC-125867	0.945	6.02	34	13	4.892	2	2	31	416.54	62.71	12	Fc1cccc(c1)-c1nn(-c2ccccc2)c2[nH]c(=O)c(CNC3CCCCC3)cc12
TCMDC-125351	0.148	6.83	34	13	4.692	2	2	35	495.07	81.17	12	COc1ccc(CCNCc2cc3c(nn(-c4ccc(Cl)cc4)c3[nH]c2=O)C(C)(C)C)cc1OC
TCMDC-124897	1.007	6	34	13	4.329	2	1	30	416.58	53.92	9	Cc1cccc(c1)-c1nn(-c2ccccc2)c2[nH]c(=O)c(CN3CCSCC3)cc12
TCMDC-123911	1.046	5.98	34	13	3.372	2	2	29	386.54	62.71	13	CC(C)(C)c1nn(-c2ccccc2)c2[nH]c(=O)c(CNCc3ccccc3)cc12
TCMDC-123910	1.047	5.98	34	13	3.337	2	2	32	430.55	81.17	12	CC(C)(C)c1nn(-c2ccccc2)c2[nH]c(=O)c(CNCc3ccc4OCOc4c3)cc12
TCMDC-123551	1.249	5.9	34	13	4.245	2	2	28	378.57	62.71	10	CC(C)(C)c1nn(-c2ccccc2)c2[nH]c(=O)c(CNC3CCCCC3)cc12
TCMDC-123909	0.234	6.63	34	13	4.409	2	2	28	398.98	62.71	13	CC(C)(C)c1nn(-c2ccc(Cl)cc2)c2[nH]c(=O)c(CNC3CCCC3)cc12
TCMDC-123908	0.759	6.12	34	13	3.971	2	2	29	427	62.71	15	CC(C)(C)c1nn(-c2ccc(Cl)cc2)c2[nH]c(=O)c(CNCc3cccs3)cc12
TCMDC-136662	0.81	6.09	34	13	4.06	2	2	33	464.99	81.17	12	CC(C)(C)c1nn(-c2ccc(Cl)cc2)c2[nH]c(=O)c(CNCc3ccc4OCOc4c3)cc12
TCMDC-136663	0.759	6.12	34	13	4.687	2	2	30	398.55	62.71	13	Cc1cccc(c1)-c1nn(-c2ccccc2)c2[nH]c(=O)c(CNC3CCCC3)cc12
TCMDC-125605	0.977	6.01	35	7	3.748	3	1	25	346.43	59.81	16	O=C(Nc1ccncc1)c1cn(nc1-c1cccs1)-c1ccccc1
TCMDC-123623	0.97	6.01	35	7	4.351	3	1	25	386.89	59.81	13	Clc1ccc(s1)-c1nn(cc1C(=O)Nc1nccs1)-c1ccccc1
TCMDC-124531	0.911	6.04	35	7	4.096	3	1	25	366.48	59.81	13	Cc1csc(NC(=O)c2cn(nc2-c2cccs2)-c2ccccc2)n1
TCMDC-124433	0.945	6.02	35	7	4.096	3	1	25	366.48	59.81	13	Cc1cnc(NC(=O)c2cn(nc2-c2cccs2)-c2ccccc2)s1
TCMDC-124055	0.869	6.06	35	7	3.748	3	1	25	346.43	59.81	16	O=C(Nc1ccncc1)c1cn(nc1-c1cccs1)-c1ccccc1
TCMDC-124032	0.258	6.59	35	7	4.9	3	2	35	487.67	79.26	12	CCN(CC)CCNC(=O)c1ccc(NC(=O)c2cn(nc2-c2cccs2)-c2ccccc2)cc1
TCMDC-124022	0.379	6.42	35	7	5.999	3	1	35	488.65	76.46	12	Cl.CCN(CC)CCOC(=O)c1ccc(NC(=O)c2cn(nc2-c2cccs2)-c2ccccc2)cc1
TCMDC-136321	0.886	6.05	36	5	2.739	2	1	29	389.49	65.79	16	OC(=O)C(F)(F)F.O=C(Nc1cccc(CN2CCN(CC2)C(=O)c2ccccc2)c1)c1ccco1
TCMDC-125463	0.703	6.15	36	5	4.617	2	2	30	427.97	74.58	12	CCN(CC)CCNC(=O)c1ccc(NC(=O)c2oc3c(Cl)cccc3c2C)cc1
TCMDC-134620	0.909	6.04	36	5	6.163	1	1	31	419.62	48.72	10	OC(=O)C(F)(F)F.CCCCCCN1CCN(Cc2cccc(NC(=O)c3cc4ccccc4o3)c2)CC1
TCMDC-134622	1.18	5.93	36	5	4.573	2	2	33	441.57	68.95	9	OC(=O)C(F)(F)F.Oc1ccc(CN2CCN(Cc3cccc(NC(=O)c4cc5ccccc5o4)c3)CC2)cc1
TCMDC-136322	0.438	6.36	36	5	3.528	2	1	30	423.93	65.79	15	OC(=O)C(F)(F)F.Clc1cccc(c1)C(=O)N1CCN(Cc2cccc(NC(=O)c3ccco3)c2)CC1
TCMDC-133384	0.157	6.8	37	3	4.293	1	0	34	473.51	45.67	10	COc1ccc(F)cc1-c1ccc(cc1)C(=O)N1CCCN(CC1)c1ccc(cn1)C(F)(F)F
TCMDC-133385	0.112	6.95	37	3	2.892	2	0	32	430.52	69.46	13	COc1ccc(F)cc1-c1ccc(cc1)C(=O)N1CCCN(CC1)c1ccc(cn1)C#N
TCMDC-140216	1.194	5.92	37	3	6.06	0	1	42	574.7	49.86	5	OC(=O)C(F)(F)F.FC(F)(F)c1ccc(nc1)N1CCCN(Cc2cccc(c2)-c2ccccc2CNCc2ccc3OCOc3c2)CC1
TCMDC-134142	0.251	6.6	37	5	4.615	2	0	34	471.58	54.26	10	CC(C)(C)c1cc(C(=O)N2CCN(CC2)c2ncccc2C(F)(F)F)n(Cc2ccccc2)n1
TCMDC-133771	0.907	6.04	37	5	4.468	4	0	33	460.65	67.15	10	CC(C)(C)c1cc(C(=O)N2CCN(CC2)c2ncnc3ccsc23)n(Cc2ccccc2)n1
TCMDC-133778	1.136	5.94	37	5	2.819	4	0	30	404.57	67.15	10	CC(C)(C)c1cc(C(=O)N2CCN(CC2)c2cnccn2)n(Cc2ccccc2)n1
TCMDC-134141	0.759	6.12	37	5	2.527	5	0	32	429.58	90.94	13	CC(C)(C)c1cc(C(=O)N2CCN(CC2)c2nccnc2C#N)n(Cc2ccccc2)n1
TCMDC-123791	0.978	6.01	37	5	4.758	2	0	35	489.57	54.26	10	CC(C)(C)c1cc(C(=O)N2CCN(CC2)c2ccc(cn2)C(F)(F)F)n(Cc2ccc(F)cc2)n1
TCMDC-125347	0.947	6.02	37	6	2.759	3	1	29	392.44	84.5	16	COc1ccc(cc1OC)C1CC(=NN1C(=O)c1ccco1)c1ccccc1O
TCMDC-125623	0.513	6.29	37	6	5.14	2	0	25	480.18	45.81	12	Brc1ccc(o1)C(=O)N1N=C(CC1c1ccc(Br)cc1)c1cccs1
TCMDC-125610	0.887	6.05	37	6	4.776	2	0	25	415.32	45.81	12	Cc1ccc(cc1)C1CC(=NN1C(=O)c1ccc(Br)o1)c1cccs1
TCMDC-123796	0.172	6.76	37	6	3.072	2	0	27	382.46	64.27	16	COc1ccc(cc1OC)C1CC(=NN1C(=O)c1ccco1)c1cccs1
TCMDC-124921	0.397	6.4	37	6	3.687	2	0	26	346.41	55.04	16	COc1ccccc1C1CC(=NN1C(=O)c1ccco1)c1ccccc1
TCMDC-123705	0.323	6.49	37	6	4.55	2	0	27	425.3	55.04	12	COc1ccc(cc1)C1CC(=NN1C(=O)c1ccc(Br)o1)c1ccccc1
TCMDC-124828	0.084	7.08	38	8	4.807	2	2	28	401	61.02	18	Cl.Clc1ccc(cc1)C1(CN2CCC(CC2)NC(=O)c2cc[nH]n2)CCCCC1
TCMDC-124833	0.09	7.04	38	8	3.61	2	1	27	387.9	58.37	20	Cc1cc(on1)C(=O)NC1CCN(CC2(CCC2)c2ccc(Cl)cc2)CC1
TCMDC-124840	0.892	6.05	38	8	4.86	2	2	32	438.68	70.25	12	CCc1n[nH]c(C(=O)NC2CCN(CC3(CCCCC3)c3ccc(OC)cc3)CC2)c1C
TCMDC-124839	0.225	6.65	38	8	4.593	2	2	28	380.59	61.02	13	Cc1ccc(cc1)C1(CN2CCC(CC2)NC(=O)c2cc[nH]n2)CCCCC1
TCMDC-124838	0.321	6.49	38	8	4.576	2	2	29	415.03	61.02	12	Cc1ccc(cc1)C1(CN2CCC(CC2)NC(=O)c2n[nH]cc2Cl)CCCCC1
TCMDC-124837	0.997	6	38	8	3.678	2	2	27	370.52	61.02	16	Fc1ccccc1C1(CN2CCC(CC2)NC(=O)c2cc[nH]n2)CCCC1
TCMDC-124836	1.043	5.98	38	8	3.348	2	2	27	386.97	61.02	13	Clc1c[nH]nc1C(=O)NC1CCN(CC2(CCCC2)c2ccccc2)CC1
TCMDC-124830	0.421	6.38	38	8	3.689	2	2	26	372.94	61.02	16	Clc1ccc(cc1)C1(CN2CCC(CC2)NC(=O)c2cc[nH]n2)CCC1
TCMDC-134633	0.23	6.64	39	7	0.739	3	2	22	326.8257	67.84	16	OC(=O)C(F)(F)F.CN1CCN(CC(O)CNC(=O)Nc2ccc(Cl)cc2)CC1
TCMDC-134634	0.149	6.83	39	7	1.268	3	2	23	340.8525	67.84	16	OC(=O)C(F)(F)F.CCN1CCN(CC(O)CNC(=O)Nc2ccc(Cl)cc2)CC1
TCMDC-134635	0.149	6.83	39	7	0.889	3	2	22	371.2767	67.84	16	OC(=O)C(F)(F)F.CN1CCN(CC(O)CNC(=O)Nc2ccc(Br)cc2)CC1
TCMDC-134636	1.052	5.98	39	7	3.9	3	2	23	384.3154	64.6	13	OC(=O)C(F)(F)F.CC1CC(C)CN(CC(O)CNC(=O)Nc2ccc(Br)cc2)C1
TCMDC-134638	0.063	7.2	39	7	1.947	3	2	24	399.3303	67.84	22	OC(=O)C(F)(F)F.CCCN1CCN(CC(O)CNC(=O)Nc2ccc(Br)cc2)CC1
TCMDC-134645	0.097	7.01	39	7	1.797	3	2	24	354.8793	67.84	22	OC(=O)C(F)(F)F.CCCCN1CCN(CC(O)CNC(=O)Nc2ccc(Cl)cc2)CC1
TCMDC-134646	0.069	7.16	39	7	2.326	3	2	25	368.9061	67.84	22	OC(=O)C(F)(F)F.CCCCN1CCN(CC(O)CNC(=O)Nc2ccc(Cl)cc2)CC1
TCMDC-125475	0.351	6.45	40	6	1.686	2	4	23	311.3433	92.15	16	CC(C)CC(=O)Nc1cc(=O)[nH]c2nc(nn12)-c1ccccc1
TCMDC-125474	0.416	6.38	40	6	2.26	2	4	25	337.3811	92.15	16	O=C(Nc1cc(=O)[nH]c2nc(nn12)-c1ccccc1)C1CCCCC1
TCMDC-125473	0.57	6.24	40	6	1.473	2	4	22	317.7348	92.15	16	CCC(=O)Nc1cc(=O)[nH]c2nc(nn12)-c1ccc(Cl)cc1
TCMDC-125323	0.844	6.07	40	6	1.991	2	4	27	363.3753	105.29	16	CCC(C(=O)Nc1cc(=O)[nH]c2nc(nn12)-c1ccco1)c1ccccc1
TCMDC-125002	0.708	6.15	40	6	2.531	2	4	24	345.7884	92.15	16	CCCCC(=O)Nc1cc(=O)[nH]c2nc(nn12)-c1ccc(Cl)cc1
TCMDC-125001	0.421	6.38	40	6	1.566	2	4	23	311.3433	92.15	16	CC(C)C(=O)Nc1cc(=O)[nH]c2nc(nn12)-c1cccc(C)c1
TCMDC-134577	0.901	6.05	41	21	3.443	1	1	25	338.4524	48.47	19	OC(=O)C(F)(F)F.CC(C)NC(=O)c1ccc(nc1)N1CCN(CC1)c1ccccc1C
TCMDC-134578	0.459	6.34	41	21	3.189	1	1	25	336.4366	48.47	19	OC(=O)C(F)(F)F.Cc1ccccc1N1CCN(CC1)c1ccc(cn1)C(=O)NC1CC1
TCMDC-134579	1.339	5.87	41	21	3.694	1	1	26	370.8817	48.47	16	OC(=O)C(F)(F)F.Clc1ccc(CN2CCN(CC2)c2ccc(cn2)C(=O)NC2CC2)cc1
TCMDC-134582	0.587	6.23	41	21	4.394	1	1	28	372.4696	48.47	16	OC(=O)C(F)(F)F.Cc1ccccc1N1CCN(CC1)c1ccc(cn1)C(=O)Nc1ccccc1
TCMDC-134585	1.417	5.85	41	21	3.398	1	1	30	405.4746	61.36	15	OC(=O)C(F)(F)F.Fc1ccc(CCNC(=O)c2ccc(nc2)N2CCN(CC2)c2ccncc2)cc1
TCMDC-134587	1.061	5.97	41	21	4.561	1	1	31	456.3747	61.36	12	OC(=O)C(F)(F)F.Clc1ccccc(CCNC(=O)c2ccc(nc2)N2CCN(CC2)c2ccncc2)c1Cl
TCMDC-134588	1.39	5.86	41	21	3.704	1	1	30	401.5113	61.36	15	OC(=O)C(F)(F)F.Cc1ccccc1CCNC(=O)c1ccc(nc1)N1CCN(CC1)c1ccncc1
TCMDC-134595	1.148	5.94	41	21	3.967	1	1	32	451.9554	70.59	15	OC(=O)C(F)(F)F.COc1ccccc1CCNC(=O)c1cnc(N2CCN(CC2)c2ccncc2)c(Cl)c1

TCMDC-134597	0.702	6.15	41	21	5.354	1	1	32	490.8198	61.36	15	OC(=O)C(F)(F)F.Clc1cccc(CCNC(=O)c2cnc(N3CCN(CC3)c3ccncc3)c(Cl)c2)c1Cl
TCMDC-134598	1.065	5.97	41	21	4.497	1	1	31	435.9564	61.36	12	OC(=O)C(F)(F)F.Cc1ccccc1CCNC(=O)c1cnc(N2CCN(CC2)c2ccncc2)c(Cl)c1
TCMDC-134599	0.735	6.13	41	21	3.927	1	1	29	411.8661	61.36	18	OC(=O)C(F)(F)F.Fc1ccc(NC(=O)c2cnc(N3CCN(CC3)c3ccncc3)c(Cl)c2)cc1
TCMDC-134600	0.963	6.02	41	21	4.497	1	1	29	428.3211	61.36	15	OC(=O)C(F)(F)F.Clc1cccc(NC(=O)c2cnc(N3CCN(CC3)c3ccncc3)c(Cl)c2)c1
TCMDC-134601	0.847	6.07	41	21	4.487	1	1	27	405.3268	48.47	15	OC(=O)C(F)(F)F.Clc1ccc(CN2CCN(CC2)c2ncc(cc2Cl)C(=O)NC2CC2)cc1
TCMDC-134602	0.628	6.2	41	21	3.982	1	1	26	370.8817	48.47	19	OC(=O)C(F)(F)F.Cc1ccccc1N1CCN(CC1)c1ncc(cc1Cl)C(=O)NC1CC1
TCMDC-134603	0.965	6.02	41	21	4.239	1	1	29	407.9028	61.36	15	OC(=O)C(F)(F)F.Cc1ccc(NC(=O)c2cnc(N3CCN(CC3)c3ccncc3)c(Cl)c2)cc1
TCMDC-134604	1.309	5.88	41	21	4.273	1	1	27	384.9085	48.47	13	GSK1971678A
TCMDC-134607	0.905	6.04	41	21	4.63	1	1	28	423.3169	48.47	15	OC(=O)C(F)(F)F.Fc1cccc(Cl)c1CN1CCN(CC1)c1ncc(cc1Cl)C(=O)NC1CC1
TCMDC-134625	0.678	6.17	41	21	4.239	1	1	29	407.9028	61.36	15	OC(=O)C(F)(F)F.Cc1cccc(NC(=O)c2cnc(N3CCN(CC3)c3ccncc3)c(Cl)c2)c1
TCMDC-134626	1.289	5.89	41	21	4.418	1	1	30	421.9296	61.36	12	GSK1977998A
TCMDC-134627	1.39	5.86	41	21	4.062	1	1	30	425.8929	61.36	12	OC(=O)C(F)(F)F.Fc1ccc(CNC(=O)c2cnc(N3CCN(CC3)c3ccncc3)c(Cl)c2)cc1
TCMDC-134628	1.149	5.94	41	21	3.838	1	1	31	437.9286	70.59	15	OC(=O)C(F)(F)F.COc1cccc(CNC(=O)c2cnc(N3CCN(CC3)c3ccncc3)c(Cl)c2)c1
TCMDC-125224	0.777	6.11	42	6	4.097	1	4	27	374.8295	67.77	13	Cc1c(Cl)ccc2c(cc(nc12)-c1ccncc1)C(=O)Nc1ccncc1
TCMDC-125217	0.744	6.13	42	6	3.083	1	4	25	395.2149	80.91	16	Brc1ccc2nc(cc(C(=O)Nc3ccon3)c2c1)-c1ccccc1
TCMDC-125215	0.403	6.39	42	6	3.596	1	4	25	411.2819	67.77	15	Brc1ccc2nc(cc(C(=O)Nc3nccs3)c2c1)-c1ccccc1
TCMDC-125212	0.64	6.19	42	6	3.748	1	4	26	405.2537	67.77	15	Brc1ccc2nc(cc(C(=O)Nc3ccccn3)c2c1)-c1ccccc1
TCMDC-124361	1.062	5.97	42	6	3.598	1	4	26	360.8027	67.77	13	Clc1ccc2nc(cc(C(=O)Nc3ccccn3)c2c1)-c1ccccc1
TCMDC-124360	0.786	6.1	42	6	2.933	1	4	25	350.7639	80.91	16	Clc1ccc2nc(cc(C(=O)Nc3ccon3)c2c1)-c1ccccc1
TCMDC-132030	0.14	6.85	43	8	4.974	1	0	21	270.3336	38.91	13	Nc1c2ccccc2nc2ccc(cc12)-c1ccccc1
TCMDC-133424	0.052	7.28	43	8	3.267	1	1	21	271.3217	51.8	22	OC(=O)C(F)(F)F.Nc1nccc2ccc(cc12)-c1cccc2ncccc12
TCMDC-133426	0.112	6.95	43	8	3.267	1	1	21	271.3217	51.8	16	OC(=O)C(F)(F)F.Nc1nccc2ccc(cc12)-c1ccc2ncccc2c1
TCMDC-136762	0.796	6.1	43	8	2.153	2	0	18	235.2887	64.93	16	Nc1cccc(c1)-c1ccc2ccnc(N)c2c1
TCMDC-136763	0.682	6.17	43	8	2.153	2	0	18	235.2887	64.93	16	Nc1ccc(cc1)-c1ccc2ccnc(N)c2c1
TCMDC-136788	0.614	6.21	43	8	2.189	1	2	22	313.3795	85.08	16	OC(=O)C(F)(F)F.CS(=O)(=O)Nc1ccc(cc1)-c1ccc2ccnc(N)c2c1
TCMDC-136895	1.536	5.81	43	8	3.146	2	0	19	269.7338	64.93	13	Nc1cc(ccc1Cl)-c1ccc2c(N)nccc2c1
TCMDC-138929	0.249	6.6	43	8	1.883	1	1	17	221.2619	51.8	16	Nc1nccc2ccc(cc12)-c1ccncc1
TCMDC-125258	0.879	6.06	44	6	3.657	0	4	23	342.4456	52.83	16	COCCn1c(Sc2ncnc3sccc23)nc2ccccc12
TCMDC-124602	0.663	6.18	44	6	3.554	0	3	19	284.3662	43.08	16	S(c1ncc2ccccn12)c1ncnc2sccc12
TCMDC-124553	0.823	6.08	44	6	4.742	1	3	21	312.4198	54.46	13	CCc1cc2c(Sc3nc4ccccc4[nH]3)ncnc2s1
TCMDC-124514	0.191	6.72	44	6	3.729	0	3	20	298.393	43.6	16	Cn1c(Sc2ncnc3sccc23)nc2ccccc12
TCMDC-125539	0.734	6.13	44	6	4.229	0	3	19	301.4173	38.67	13	S(c1nc2ccccc2s1)c1ncnc2sccc12
TCMDC-123835	0.255	6.59	44	6	4.662	1	3	21	312.4198	54.46	13	Cc1sc2ncnc(Sc3nc4ccccc4[nH]3)c2c1C
TCMDC-133074	1.56	5.81	45	17	4.835	2	1	25	395.2585	76.82	10	OC(=O)C(F)(F)F.COc1ccc(cc1)-c1cnc(N)c(c1)-c1nc2cc(Br)ccc2[nH]1
TCMDC-133132	0.175	6.76	45	17	4.253	2	1	24	322.3168	67.59	13	OC(=O)C(F)(F)F.Nc1ncc(cc1-c1nc2cc(F)ccc2[nH]1)-c1cccc(F)c1
TCMDC-133133	0.193	6.71	45	17	3.646	2	2	25	329.3368	91.38	16	OC(=O)C(F)(F)F.Nc1ncc(cc1-c1nc2cc(ccc2[nH]1)C#N)-c1cccc(F)c1
TCMDC-133557	0.851	6.07	45	17	3.631	2	1	21	292.3648	67.59	16	Nc1ncc(cc1-c1nc2ccccc2[nH]1)-c1ccsc1
TCMDC-133558	0.672	6.17	45	17	3.831	2	3	29	407.4959	113.76	15	Cc1cc2nc([nH]c2cc1C)-c1cc(cnc1N)-c1cccc(NS(C)(=O)=O)c1
TCMDC-135292	0.124	6.91	45	17	5.169	2	1	24	334.8085	67.59	13	OC(=O)C(F)(F)F.Cc1cccc2[nH]c(nc12)-c1cc(cnc1N)-c1cccc(Cl)c1
TCMDC-135320	0.211	6.68	45	17	5.879	2	2	32	420.47	93.89	12	COC(=O)c1ccc2nc([nH]c2c1)-c1cc(cnc1N)-c1cccc(c1)-c1ccccc1
TCMDC-135560	0.281	6.55	45	17	4.961	2	2	28	372.426	93.89	13	CCOC(=O)c1ccc(cc1)-c1cnc(N)c(c1)-c1nc2cccc(C)c2[nH]1
TCMDC-135807	0.861	6.06	45	17	3.409	3	2	25	330.3892	87.82	16	OC(=O)C(F)(F)F.Cc1ccc2[nH]c(nc2c1)-c1cc(cnc1N)-c1ccc(CO)cc1
TCMDC-135808	0.117	6.93	45	17	3.9	2	2	25	325.3735	91.38	16	OC(=O)C(F)(F)F.Cc1ccc2[nH]c(nc2c1)-c1cc(cnc1N)-c1cccc(c1)C#N
TCMDC-135839	1.676	5.78	45	17	6.23	2	1	31	406.4868	76.82	7	OC(=O)C(F)(F)F.Cc1ccc2[nH]c(nc2c1)-c1cc(cnc1N)-c1ccc(OCc2ccccc2)cc1
TCMDC-138783	0.263	6.58	45	17	4.818	2	1	24	338.7718	67.59	13	Cl.Nc1ncc(cc1-c1nc2cc(Cl)c(F)cc2[nH]1)-c1ccccc1
TCMDC-138790	0.652	6.19	45	17	4.914	2	1	28	384.3595	76.82	13	Cl.COc1cccc(c1)-c1cnc(N)c(c1)-c1nc2ccc(cc2[nH]1)C(F)(F)F
TCMDC-138791	0.85	6.07	45	17	4.115	2	1	25	334.3525	76.82	13	Cl.COc1cccc(c1)-c1cnc(N)c(c1)-c1nc2ccc(F)cc2[nH]1
TCMDC-138792	0.536	6.27	45	17	4.832	2	1	26	368.7976	76.82	13	COc1cccc(c1)-c1cnc(N)c(c1)-c1nc2cc(Cl)c(F)cc2[nH]1
TCMDC-138793	0.191	6.72	45	17	3.361	2	1	28	376.414	95.28	16	Cl.COc1cc(cc(OC)c1OC)-c1cnc(N)c(c1)-c1nc2ccccc2[nH]1
TCMDC-138810	0.753	6.12	45	17	4.823	2	1	24	338.7718	67.59	13	Nc1ncc(cc1-c1nc2ccc(Cl)cc2[nH]1)-c1ccc(F)cc1
TCMDC-132502	0.639	6.19	46	23	5.055	2	3	31	413.5183	69.22	15	CCN(CC(C)O)C(=O)c1ccc(cc1)-c1cccc(c1)-c1nc2cccc(C)c2[nH]1
TCMDC-132503	0.84	6.08	46	23	5.055	2	3	31	413.5183	69.22	15	CCN(CC(C)O)C(=O)c1ccc(cc1)-c1ccc(cc1)-c1nc2cccc(C)c2[nH]1
TCMDC-132538	1.664	5.78	46	23	5.503	2	1	26	339.4399	40.71	13	OC(=O)C(F)(F)F.C(NC1CC1)c1ccc(cc1)-c1cccc(c1)-c1nc2ccccc2[nH]1
TCMDC-132539	0.717	6.14	46	23	5.299	2	1	28	370.4974	43.95	16	OC(=O)C(F)(F)F.CN(C)CCNCc1ccc(cc1)-c1cccc(c1)-c1nc2ccccc2[nH]1
TCMDC-132541	0.113	6.95	46	23	5.158	2	2	31	407.5185	58.53	15	OC(=O)C(F)(F)F.C(CNCc1ccc(cc1)-c1cccc(c1)-c1nc2ccccc2[nH]1)Cn1ccnc1
TCMDC-132547	0.626	6.2	46	23	6.376	2	1	27	355.4825	40.71	14	OC(=O)C(F)(F)F.CC(C)CNCc1ccc(cc1)-c1cccc(c1)-c1nc2ccccc2[nH]1
TCMDC-132550	0.231	6.64	46	23	5.757	2	1	26	341.4557	40.71	16	OC(=O)C(F)(F)F.CC(C)NCc1ccc(cc1)-c1cccc(c1)-c1nc2ccccc2[nH]1
TCMDC-132558	0.194	6.71	46	23	5.375	2	3	35	481.6173	74.85	15	OC(=O)C(F)(F)F.CS(=O)(=O)c1ccc(CCNCc2ccc(cc2)-c2cccc(c2)-c2nc3ccccc3[nH]2)cc1
TCMDC-132561	0.945	6.02	46	23	4.832	2	3	31	434.5614	78.09	15	OC(=O)C(F)(F)F.CN(CCNCc1ccc(cc1)-c1cccc(c1)-c1nc2ccccc2[nH]1)S(C)(=O)=O
TCMDC-132567	0.751	6.12	46	23	5.84	1	1	29	384.5242	35.16	16	OC(=O)C(F)(F)F.CN(C)CCN(C)Cc1ccc(cc1)-c1cccc(c1)-c1nc2ccccc2[nH]1
TCMDC-132568	0.55	6.26	46	23	5.448	2	1	25	327.4289	40.71	16	OC(=O)C(F)(F)F.CCNCc1ccc(cc1)-c1cccc(c1)-c1nc2ccccc2[nH]1
TCMDC-132680	0.766	6.12	46	23	5.299	2	1	28	370.4974	43.95	16	OC(=O)C(F)(F)F.CN(C)CCNCc1cccc(c1)-c1cccc(c1)-c1nc2ccccc2[nH]1
TCMDC-132682	0.682	6.17	46	23	5.798	2	1	29	384.5242	43.95	16	OC(=O)C(F)(F)F.CN(C)CCNCc1cccc(c1)-c1ccc(cc1)-c1nc2cccc(C)c2[nH]1
TCMDC-132738	0.336	6.47	46	23	6.256	2	1	27	355.4825	40.71	14	OC(=O)C(F)(F)F.CC(C)NCc1cccc(c1)-c1cccc(c1)-c1nc2cccc(C)c2[nH]1
TCMDC-132744	0.676	6.17	46	23	6.256	2	1	27	355.4825	40.71	14	OC(=O)C(F)(F)F.CC(C)NCc1ccc(cc1)-c1ccc(cc1)-c1nc2cccc(C)c2[nH]1
TCMDC-132746	0.761	6.12	46	23	5.757	2	1	26	341.4557	40.71	16	OC(=O)C(F)(F)F.CC(C)NCc1cccc(c1)-c1ccc(cc1)-c1nc2ccccc2[nH]1
TCMDC-132748	0.799	6.1	46	23	5.757	2	1	26	341.4557	40.71	16	OC(=O)C(F)(F)F.CC(C)NCc1cccc(c1)-c1cccc(c1)-c1nc2ccccc2[nH]1

TCMDC-132803	0.405	6.39	46	23	6.875	2	1	28	369.5093	40.71	14	OC(=O)C(F)(F)F.CC(C)CNCc1ccc(cc1)-c1ccc(cc1)-c1nc2cccc(C)c2[nH]1
TCMDC-132804	0.818	6.09	46	23	6.018	2	1	27	351.4509	40.71	14	OC(=O)C(F)(F)F.Cc1cccc2nc([nH]c12)-c1cccc(c1)-c1ccc(CNCC#C)cc1
TCMDC-132825	0.766	6.12	46	23	5.204	3	1	28	370.4974	52.74	16	OC(=O)C(F)(F)F.CNCCNCc1cccc(c1)-c1cccc(c1)-c1nc2cccc(C)c2[nH]1
TCMDC-132831	0.798	6.1	46	23	5.204	3	1	28	370.4974	52.74	16	OC(=O)C(F)(F)F.CNCCNCc1cccc(c1)-c1ccc(cc1)-c1nc2cccc(C)c2[nH]1
TCMDC-132837	0.67	6.17	46	23	5.204	3	1	28	370.4974	52.74	16	OC(=O)C(F)(F)F.CNCCNCc1ccc(cc1)-c1ccc(cc1)-c1nc2cccc(C)c2[nH]1
TCMDC-132839	0.743	6.13	46	23	4.705	3	1	27	356.4706	52.74	16	OC(=O)C(F)(F)F.CNCCNCc1cccc(c1)-c1ccc(cc1)-c1nc2ccccc2[nH]1
TCMDC-136673	0.7	6.15	47	16	5.284	1	2	27	377.877	45.46	13	CN(C)c1cccc(c1)-c1cnc2ccc(NCc3cccc(Cl)c3)nn12
TCMDC-136674	0.928	6.03	47	16	3.005	1	3	24	319.3416	55.11	16	Fc1ccc(CNc2ccc3ncc(-c4cccnc4)n3n2)cc1
TCMDC-136675	0.834	6.08	47	16	4.167	1	2	28	378.4051	60.68	13	COc1ccc(cc1OC)-c1cnc2ccc(NCc3ccc(F)cc3)nn12
TCMDC-136676	1.084	5.96	47	16	3.963	2	3	25	334.3525	62.45	13	Oc1cccc(c1)-c1cnc2ccc(NCc3ccc(F)cc3)nn12
TCMDC-136677	0.698	6.16	47	16	4.863	2	3	33	483.4006	74.56	12	CN(C)CCNC(=O)c1cccc(c1)-c1cnc2ccc(NCc3ccc(Cl)c(Cl)c3)nn12
TCMDC-136678	0.913	6.04	47	16	4.863	2	3	33	483.4006	74.56	12	CN(C)CCNC(=O)c1ccc(cc1)-c1cnc2ccc(NCc3ccc(Cl)c(Cl)c3)nn12
TCMDC-136681	0.866	6.06	47	16	3.918	1	3	28	385.3476	64.34	16	FC(F)(F)Oc1ccc(cc1)-c1cnc2ccc(NCc3ccncc3)nn12
TCMDC-136682	0.891	6.05	47	16	3.514	1	3	24	335.7966	55.11	16	Clc1ccc(cc1)-c1cnc2ccc(NCc3ccncc3)nn12
TCMDC-136684	0.588	6.23	47	16	4.505	2	3	33	442.564	74.56	12	CN(C)CCNC(=O)c1cccc(c1)-c1cnc2ccc(NCc3ccc(C)cc3C)nn12
TCMDC-136685	0.578	6.24	47	16	3.579	2	4	32	463.4384	111.61	15	NS(=O)(=O)c1ccc(CNc2ccc3ncc(-c4ccc(OC(F)(F)F)cc4)n3n2)cc1
TCMDC-124515	0.785	6.11	47	16	1.898	2	5	29	404.4524	126.17	15	NS(=O)(=O)c1ccc(CNc2ccc3ncc(-c4ccc(cc4)C#N)n3n2)cc1
TCMDC-136686	0.284	6.55	47	16	3.175	2	4	28	413.8874	102.38	15	NS(=O)(=O)c1ccc(CNc2ccc3ncc(-c4ccc(Cl)cc4)n3n2)cc1
TCMDC-136687	0.796	6.1	47	16	2.469	2	4	29	409.4681	111.61	15	COc1ccc(cc1)-c1cnc2ccc(NCc3ccc(cc3)S(N)(=O)=O)nn12
TCMDC-136688	0.867	6.06	47	16	1.844	2	5	29	410.4562	124.5	15	COc1ccc(cn1)-c1cnc2ccc(NCc3ccc(cc3)S(N)(=O)=O)nn12
TCMDC-136689	0.834	6.08	47	16	5.433	1	2	35	482.5075	57.93	12	CN1CCN(CC1)c1ccc(CNc2ccc3ncc(-c4ccc(OC(F)(F)F)cc4)n3n2)cc1

LIGAND EFFICIENCY SET

TCAMS-ID	Fast-track series	le	lle	3D7 XC50	PXC50	number of comp. in cluster	clogP	MW	PSA	Total Score Fast track
TCMDC-138929	series 43	0.53	4.72	0.249	6.6	8	1.883	221.28	51.8	16
TCMDC-125317	series 26	0.52	2.83	0.331	6.48	7	3.649	264.71	25.78	16
TCMDC-137223	series 24	0.5	2.88	0.698	6.16	6	3.276	219.26	52.47	16
TCMDC-124447	similar scaffold as series 6	0.48	2.79	1.028	5.99	17	3.204	226.35	19.03	13
TCMDC-131771	new	0.46	1.92	0.43	6.37	5	4.453	271.76	22.12	11
TCMDC-124514	series 44	0.46	2.99	0.191	6.72	6	3.729	298.4	43.6	16

TCMDC-124275	new	0.45	3.23	1.15	5.94	9	2.712	254.33	50.7	13
TCMDC-134635	series 39	0.43	5.94	0.149	6.83	7	0.889	371.32	67.84	16
TCMDC-133557	series 45	0.4	2.44	0.851	6.07	17	3.631	292.38	67.59	16
TCMDC-125473	series 40	0.39	4.77	0.57	6.24	6	1.473	317.76	92.15	16
TCMDC-141398	new	0.39	1.57	1.04	5.98	6	4.415	296.78	50.7	10
TCMDC-131984	series 6	0.38	2.9	0.033	7.48	5	4.585	365.54	31.06	17
TCMDC-124202	similar scaffold as series 2	0.38	0.26	0.735	6.13	15	5.871	349.15	41.13	13

TCMDC-124175	same scaffold as series 27	0.38	2.66	0.192	6.72	8	4.062	361.24	55.13	13
TCMDC-124100	new	0.38	1.02	0.451	6.35	5	5.326	440.2	37.19	10
TCMDC-139375	same scaffold as series 4	0.38	0.69	0.745	6.13	10	5.438	332.2	54.02	13
TCMDC-133731	similar scaffold as series 2	0.37	1.68	0.532	6.27	10	4.586	350.27	53.16	13
TCMDC-125500	new	0.35	0.27	0.372	6.43	9	6.162	366.25	29.1	11
TCMDC-132076	new	0.35	2.01	0.731	6.14	8	4.125	455.21	43.7	12

TCMDC-132550	series 46	0.35	0.88	0.231	6.64	23	5.757	341.49	40.71	16
TCMDC-132743	same scaffold as series 24	0.35	0.27	0.231	6.64	39	6.372	361.54	40.71	14
TCMDC-125215	series 42	0.35	2.79	0.403	6.39	6	3.596	411.29	67.77	15
TCMDC-124828	series 38	0.35	2.27	0.084	7.08	7	4.807	401	61.02	18
TCMDC-134578	series 41	0.35	3.15	0.459	6.34	21	3.189	336.48	48.47	19
TCMDC-123580	series 48	0.35	2.6	0.665	6.18	10	3.577	362.91	50.16	16

TCMDC-124548	new	0.35	1.14	0.787	6.1	8	4.964	396.32	54.88	13
TCMDC-136682	series 47	0.35	2.54	0.891	6.05	16	3.514	335.82	55.11	16