SUPPLEMENTARY TABLES

Supplementary Table 1. List of all commercial and non-commercial compounds tested using the RED assay in this study. Each compound is listed with their respective chemical structure in SMILES format (Simplified molecular-input line-entry system) and physicochemical properties [(1)].

Name or ID #	Source / Description	SMILES	*fu* (%)	MW	Arom_ Rings	Mol_ Sol	Sp2	IW1_ VS	Plasma PB
Ethambutol	Anti-TB drug	CC[C@@H](CO)NCCN[C@@H](CC)CO	38.8	204.3	0	-1.418	0	0.080	0.916
Isoniazid	Anti-TB drug	c1cnccc1C(=O)NN	67.2	137.1	1	-0.951	6	0.131	0.916
Pyrazinamide	Anti-TB drug	c1cnc(cn1)C(=N)O	62.0						
p-aminosalicylic acid	Anti-TB drug	c1cc(C(O)=O)c(O)cc1N	51.1	153.1	1	-0.9	7	0.134	0.916
Rifampicin	Anti-TB drug	C[C@H]1/C=C/C=C(\C(=O)NC2=C(C(=C3C(=C2O)C(=C(C4=C3C(=O)[C@](O4)(O/C=C/[C@@H]([C@H]([C@H]([C@@H]([C@@H]([C@@H]([C@@H]1O)C)O)C)OC(=O)C)C)OC)C)C)O)O)/C=N/N5CCN(CC5)C)/C	7.3	822.9	2	-6.389	20	0.014	0.500
Rifapentine	Anti-TB drug	C[C@H]1/C=C/C=C(\C(=O)NC2=C(C(=C3C(=C2O)C(=C(C4=C3C(=O)[C@](O4)(O/C=C/[C@@H]([C@H]([C@H]([C@@H]([C@@H]([C@@H]([C@@H]1O)C)O)C)OC(=O)C)C)OC)C)C)O)O)/C=N/N5CCN(CC5)C6CCCC6)/C	1.1	877.0	2	-7.541	20	0.023	0.500
Moxifloxacin	Anti-TB drug	COc1c2c(cc(c1N3C[C@@H]4CCCN[C@@H]4C3)F)c(=O)c(cn2C5CC5)C(=O)O	16.8	401.4	2	-3.066	10	0.110	0.916
Levofloxacin	Anti-TB drug	C[C@H]1COc2c3n1cc(c(=O)c3cc(c2N4CCN(CC4)C)F)C(=O)O	16.3	361.4	2	-1.607	10	0.104	0.916
Gatifloxacin	Anti-TB drug	CC1CN(CCN1)c2c(cc3c(c2OC)n(cc(c3=O)C(=O)O)C4CC4)F	18.8	375.4	2	-2.658	10	0.093	0.916
Linezolid	Anti-TB drug	CC(=O)NC[C@H]1CN(C(=O)O1)c2ccc(c(c2)F)N3CCOCC3	27.9	337.3	1	-1.927	8	0.038	0.916
Posizolid	Anti-TB drug	c1conc1OC[C@H]2CN(C(=O)O2)c3cc(c(c(c3)F)C4=CCN(CC4)C(=O)[C@H](CO)O)F	17.6	465.4	2	-3.267	13	0.069	0.200
Sutezolid	Anti-TB drug	CC(=O)NC[C@H]1CN(C(=O)O1)c2ccc(c(c2)F)N3CCSCC3	21.7	353.4	1	-2.875	8	0.059	0.916

Radezolid	Anti-TB drug	CC(=O)NC[C@H]1CN(C(=O)O1)C2=CC(=C(C=C2)C3=CC=C(C=C3)CNCC4=CN=NN4)F	7.6	438.5	3	-5.041	16	0.048	0.771
Tedizolid	Anti-TB drug	CN1N=C(N=N1)C2=NC=C(C=C2)C3=C(C=C(C=C3)N4C[C@@H](OC4=O)CO)F	13.7	450.3	3	-2.934	13	0.061	0.771
Clofazimine	Anti-TB drug	CC(C)/N=c/1\cc-2n(c3ccccc3nc2cc1Nc4ccc(cc4)Cl)c5ccc (cc5)Cl	<0.01	473.4	4	-8.969	24	0.033	0.099
Bedaquiline	Anti-TB drug	CN(C)CC[C@@](c1cccc2c1cccc2)([C@H](c3ccccc3)c4cc5cc(ccc5nc4OC)Br)O	<0.01	555.5	5	-10.636	25	0.026	0.179
PA-824	Anti-TB drug	c1cc(ccc1CO[C@H]2Cn3cc(nc3OC2)[N+](=O)[O-])OC(F)(F)F	3.6	359.3	2	-4.814	9	0.067	0.154
OPC67683	Anti-TB drug	C[C@@]1(Cn2cc(nc2O1)[N+](=O)[O-])COc3ccc(cc3)N4CCC(CC4)Oc5ccc(cc5)OC(F)(F)F	0.02	534.5	3	-7.203	15	0.069	0.164
LLY001	Eli Lilly, UBA	Cc1ncc(n1CCO)N(=O)=O	63.2	171.2	1	-1.293	3	0.062	0.916
LLY002	Eli Lilly, UBA	CN(c1ccc(C(=O)N[C@H](C(=O)O)CCC(=O)O)cc1)Cc1[n]c2c([n]c1)[n]c([n]c2N)N	15.3	454.4	3	-3.639	15	0.072	0.771
LLY003	Eli Lilly, UBA	CC(C)(C)NC[C@H](c1ccc(c(c1)CO)O)O	34.0	239.3	1	-2.341	6	0.126	0.916
LLY004	Eli Lilly, UBA	CN1C(=C(c2ccccc2S1(=O)=O)O)C(=O)Nc3ccccn3	22.8	331.3	2	-3.302	14	0.079	0.771
LLY005	Eli Lilly, UBA	CC(C)(C)NC[C@H](c1cc(cc(c1)OC(=O)N(C)C)OC(=O)N(C)C)O	28.1	367.4	1	-3.383	8	0.032	0.916
LLY006	Eli Lilly, UBA	OC(=O)[C@H]1N(CSC1)C(=O)[C@H]1NC(=O)CC1	79.05	244.3	0	-0.69	3	0.117	0.916
LLY007	Eli Lilly, UBA	Cc1cnc(cn1)C(=O)NCCc2ccc(cc2)S(=O)(=O)NC(=O)NC3CCCCC3	10	445.5	2	-5.77	12	0.053	0.143
LLY008	Eli Lilly, UBA	C1CCN(CC1)c2c3c(c(nc(n3)N(CCO)CCO)N4CCCCC4)nc(n2)N(CCO)CCO	1.78	504.6	2	-0.856	6	0.026	0.500
LLY009	Eli Lilly, UBA	COc1cc(c(cc1C(=O)N[C@H]2CCN(C[C@H]2OC)CCCOc3ccc(cc3)F)Cl)N	2.37	465.9	2	-5.48	13	0.015	0.164
LLY010	Eli Lilly, UBA	c1ccc2c(c1)N(c3cc(ccc3S2)Cl)CCCN4CCN(CC4)CCO	0.11	404.0	2	-4.403	12	0.089	0.056
LLY011	Eli Lilly, UBA	CN(C)CCCN1c2ccccc2Sc3c1cc(cc3)Cl	0.08	318.9	2	-4.848	12	0.026	0.179
LLY012	Eli Lilly, UBA	CCCc1nc2c(cc(cc2n1Cc3ccc(cc3)c4ccccc4C(=O)O)c5nc6ccccc6n5C)C	0.75	514.6	6	-11.079	27	0.033	0.164
LLY013	Eli Lilly, UBA	CC(C)COCC(CN(Cc1ccccc1)c2ccccc2)N3CCCC3.Cl	0.4	366.5	2	-5.524	12	0.018	0.164

LLY014	Eli Lilly, UBA	CN(C)CCCN1c2ccccc2CCc3c1cc(cc3)Cl.Cl	0.21	314.9	2	-5.325	12	0.025	0.179
LLY015	Eli Lilly, UBA	[H][C@]12CN(C[C@]1([C@@H]2N)[H])c3c(cc4c(=O)c(cn(c4n3)c5ccc(cc5F)F)C(=O)O)F	12.1	416.4	3	-4.037	15	0.029	0.771
LLY016	Eli Lilly, UBA	Cn1c(nc(=O)c(n1)O)SCC2=C(N3[C@@H]([C@@H](C3=O)NC(=O)/C(=N/OC)/c4csc(n4)N)SC2)C(=O)[O-].[Na+]	24.4	554.6	2	-3.982	12	0.100	0.333
DDD00031548	DDU, PZA analog	Cc1cnc(C(Nc2ccc(OC(F)(F)F)cc2)=O)cn1	0.87	297.2	2	-4.714	11	0.084	0.099
DDD00085385	DDU, PZA analog	Oc1ccc(c2cnc3c(n2)nc(O)nc3O)cc1	24.29	256.2	3	-2.29	12	0.139	0.771
DDD00309053	DDU, PZA analog	Nc1nccnc1C(O)=O	86.78	139.1	1	-0.548	5	0.120	0.916
DDD00401795	DDU, PZA analog	CC1CN(S(N2CCN(C(c3nccnc3N)=O)CC2)(=O)=O)CC(O1)C	45.93	384.5	1	-0.525	5	0.046	0.500
DDD00404833	DDU, PZA analog	Cc1cnc(C(Nc2cc(C(C)(C)C)nn2c3ccc(F)cc3)=O)cn1	1.19	353.4	3	-5.865	14	0.043	0.099
DDD00486000	DDU, PZA analog	Cc1cc(C)c(NC(c2cnccn2)=O)c(C)c1	25.58	241.3	2	-4.031	11	0.130	0.099
DDD00497644	DDU, PZA analog	COc1ccc(NC(c2nccnc2N)=O)cn1	23.2	245.2	2	-2.105	10	0.078	0.771
DDD00529297	DDU, PZA analog	COc1ccc(NC(c2cnc3c(n2)cccc3)=O)cn1	7.18	280.3	3	-3.761	14	0.084	0.771
DDD00771048	DDU, PZA analog	CNC(c1nccnc1N)=O	>99.9	152.2	1	-0.736	5	0.119	0.916
DDD01012369	DDU, PZA analog	COC(c1nc(Cl)c(N)nc1N)=O	51.84	202.6	1	-1.385	5	0.106	0.916
DDD01012370	DDU, PZA analog	NC(c1cnc(N)cn1)=O	>99.9	138.1	1	-0.562	5	0.085	0.916
DDD01012371	DDU, PZA analog	Cc1cnc(C(Nc2nnc(C(F)(F)F)[nH]2)=O)cn1	>99.9	272.2	2	-3.394	7	0.117	0.916
DDD01012372	DDU, PZA analog	Cc1cnc(C(Nc2ccccc2C(N3CCCC3)=O)=O)cn1	39.92	310.4	2	-3.505	12	0.068	0.099
DDD01012374	DDU, PZA analog	FC(COc1ccc(S(N2CCCC2)(=O)=O)cc1NC(c3cnccn3)=O)(F)F	2.42	430.4	2	-4.281	11	0.036	0.099
DDD01012375	DDU, PZA analog	Nc1nccnc1C(Nc2cccc(CNC(Nc3ccccc3Cl)=O)c2)=O	0.58	396.8	3	-5.435	18	0.028	0.099
DDD01012376	DDU, PZA analog	Cc1c(c2ccccc2)sc(NC(c3cnccn3)=O)c1C(N4CCOCC4)=O	1.71	408.5	3	-5.058	16	0.064	0.099

DDD01012377	DDU, PZA analog	CC(Oc1ccc(CNC(c2cnc(C)cn2)=O)cn1)C	16.36	286.3	2	-3.691	10	0.088	0.771
DDD01012378	DDU, PZA analog	Cc1cnc(C(NCc2ccccc2S(N3CCCCC3)(=O)=O)=O)cn1	7.61	374.5	2	-4.007	11	0.063	0.099
DDD01012379	DDU, PZA analog	CCc1cccc(C)c1NC(c2cnc3c(n2)cccc3)=O	1.22	291.3	3	-5.434	15	0.079	0.099
DDD01012380	DDU, PZA analog	CCN(CCNC(c1nccnc1NC(c2ccccc2)=O)=O)CC	31.31	341.4	2	-3.708	12	0.058	0.889
DDD01012381	DDU, PZA analog	O=C(c1cnccn1)Nc2cn[nH]c2	>99.9	189.2	2	-1.2	8	0.072	0.916
DDD01012382	DDU, PZA analog	Cc1c(NC(c2cnccn2)=O)cccc1C(N)=O	>99.9	256.3	2	-3.125	12	0.049	0.771
DDD01012383	DDU, PZA analog	CS(NCCNC(c1nccnc1N)=O)(=O)=O	>99.9	259.3	1	-1.334	5	0.059	0.916
DDD01012384	DDU, PZA analog	COc1cc(CNC(c2nccnc2N)=O)ccc1O	80.48	274.3	2	-2.359	11	0.052	0.771
DDD01012385	DDU, PZA analog	NC(c1cnc2c(n1)cccc2)=O	>99.9	173.2	2	-2.16	9	0.173	0.916
DDD01012386	DDU, PZA analog	Nc1nccnc1C(NCc2cc3c([nH]2)cccc3)=O	4.02	267.3	3	-3.32	13	0.130	0.771
DDD01012387	DDU, PZA analog	CC(c1cnc2c(n1)cccc2)=O	33.22	172.2	2	-2.537	9	0.115	0.916
DDD01012388	DDU, PZA analog	Nc1nc2c(nc1C(O)=O)cccc2	51.64	189.2	2	-1.894	9	0.176	0.916
DDD01012461	DDU, PZA analog	CS(N1CCC(CNC(c2cnccn2)=O)CC1)(=O)=O	31.77	298.4	1	-1.952	5	0.061	0.916
DDD01012463	DDU, PZA analog	Cc1cnc(C(N2CCN(c3ncccn3)CC2)=O)cn1	35.97	284.3	2	-1.464	9	0.055	0.500
DDD01012464	DDU, PZA analog	OC(c1nccnc1C(Nc2ccc(S(N3CCOCC3)(=O)=O)cc2)=O)=O	18.36	392.4	2	-2.672	12	0.063	0.771
DDD01012612	DDU, PZA analog	O=C(c1cnccn1)NCC2CC2	>99.9	177.2	1	-1.659	5	0.157	0.916
DDD01010956	NIH / DDU, TB-active	Nc1cccc(F)c1C(O)=O	36.8	155.1	1	-1.613	7	0.205	0.916
DDD00301814	NIH / DDU, TB-active	Nc1ccc(F)cc1C(O)=O	47.25	155.1	1	-1.618	7	0.151	0.916
DDD01270522	NIH / DDU, TB-active	Nc1cc(F)ccc1C(O)=O	31.8	155.1	1	-1.612	7	0.056	0.916
DDD01010955	NIH / DDU, TB-active	Nc1c(F)cccc1C(O)=O	43.8	155.1	1	-1.604	7	0.118	0.916

DDD00630425	NIH / DDU, TB-active	COc1ccc(c2[nH]c3c(c2CCC(Nc4ccc5c(NC(C(O5)C)=O)c4)=O)cccc3)cc1	0.0799	455.5	4	-7.222	22	0.073	0.099
DDD00613993	NIH / DDU, TB-active	CC(n1ncc2c1nc(c3ccccc3)cc2C(NCC(c4ccco4)N5CCCC5)=O)C	0.0129	443.5	4	-6.735	17	0.052	0.164
DDD00806527	NIH / DDU, TB-active	CN(c1cc(C(Nc2ccccc2)=O)ncn1)Cc3ccc(Cl)c(Cl)c3	0.1	387.3	3	-6.237	17	0.021	0.164
DDD00685697	NIH / DDU, TB-active	Fc1ccc(OCc2nc(CSc3nnc(c4ccncc4)o3)cs2)cc1	0.43	400.5	4	-6.497	16	0.029	0.099
DDD00281126	NIH / DDU, TB-active	Clc1ccc(c2cc3c(s2)c(n4cnnc4C#N)ncn3)cc1	0.013	338.8	4	-6.053	14	0.149	0.099
DDD01009187	NIH / DDU, TB-active	COc1ccc(c2n(C)c3c([n+]2CC(OC4CC(CCC4C(C)C)C)=O)cccc3)cc1	0.016	435.6	3	-7.817	14	0.033	0.164
DDD00935077	NIH / DDU, TB-active	Cc1onc(c2ccccc2Cl)c1C(Oc3cccc4c3nccc4)=O	0.19	364.8	4	-6.767	19	0.043	0.099
DDD01010816	NIH / DDU, TB-active	CCCc1cc(c2nc(c3ccc(OC(F)F)cc3)cs2)ccn1	0.003	346.4	3	-7.602	14	0.056	0.099
DDD00302363	NIH / DDU, TB-active	CCCc1cc(c2nc(c3cccc(OC)c3)cs2)ccn1	0.0018	310.4	3	-6.559	14	0.011	0.099
DDD01009188	NIH / DDU, TB-active	CC1CCC(C(OC(C[n+]2c(c3ccccc3)n(C)c4c2cccc4)=O)C1)C(C)C	0.136	405.6	3	-7.72	14	0.034	0.164
DDD00054958	NIH / DDU, TB-active	Fc1ccc(c2nonc2NC(c3sc4c(c3Cl)cccc4)=O)cc1	0.0168	373.8	4	-6.867	17	0.093	0.099
DDD00853474	NIH / DDU, TB-active	CC1=CC(NC(n2nc(C)cc2NC(COc3ccc(Cl)cc3)=O)=N1)=O	1.22	373.8	3	-4.562	14	0.033	0.154
DDD00309396	NIH / DDU, TB-active	Cc1nc2n(c(NCc3ccccn3)c1C)ncc2c4ccccc4	0.029	329.4	4	-5.365	17	0.018	0.164
DDD00664718	NIH / DDU, TB-active	NS(c1ccc2c(CCN2Cc3nc4c(n3CCO)cc(Cl)cc4)c1)(=O)=O	8.02	406.9	3	-4.479	13	0.074	0.154
DDD00709278	NIH / DDU, TB-active	CCc1nc2n(n1)c(O)c(Cc3ccc(Cl)cc3)c(C)n2	4.75	302.8	3	-4.178	11	0.069	0.099
DDD01008487	NIH / DDU, TB-active	Cc1nn2c(c1c3ccccc3)nc(c4ccc(F)cc4)cc2O	0.37	319.3	4	-5.186	18	0.072	0.099
DDD00696423	NIH / DDU, TB-active	Cc1cccc(N2CCN(CC2)CCNC(CCN3C=Nc4c(C3=O)c(CCCC5)c5s4)=O)c1	0.29	479.6	3	-5.795	13	0.044	0.056
DDD01008622	NIH / DDU, TB-active	FC(Oc1ccc2c(c1)oc(NC(c3cccc(C(F)(F)F)c3)=O)n2)(F)F	0.016	390.2	3	-6.891	14	0.039	0.099
DDD00054872	NIH / DDU, TB-active	Clc1c(C(Nc2nonc2c3cccs3)=O)sc4c1cccc4	0.16	361.8	4	-6.617	15	0.109	0.099
DDD00546354	NIH / DDU, TB-active	CC(C(Nc1ccc(C(F)(F)F)cc1)=O)Nc2ccc3c(OCCO3)c2	0.33	366.3	2	-5.26	13	0.070	0.099

DDD00003013	NIH / DDU, TB-active	COc1ccc(c2csc3c2C(OC(c4ccccc4OC)=N3)=O)cc1	0.038	365.4	4	-6.106	18	0.052	0.099
DDD00507713	NIH / DDU, TB-active	CCc1cccc2c1[nH]cc2C(Cn3nnc(c4cccs4)n3)=O	0.11	337.4	4	-5.473	14	0.071	0.099
DDD00175986	NIH / DDU, TB-active	Cc1nc(C)c(c2cc(O)n3c(n2)c(c4ccccc4)c(C)n3)s1	1.04	336.4	4	-5.391	15	0.062	0.099
DDD00275330	NIH / DDU, TB-active	CCCc1ccc(NC(C(Nc2ccc3c(NC(N3)=O)c2)=O)C)cc1	0.74	338.4	3	-5.091	14	0.142	0.099
DDD00304844	NIH / DDU, TB-active	COc1ccc(CNc2nc3n(C(C4=C(N3)CCC4)=O)n2)cc1	26.7	311.3	3	-3.04	11	0.010	0.099
DDD01008485	NIH / DDU, TB-active	CCCc1cc(O)n2c(n1)c(c3ccc(Cl)cc3)cn2	0.62	287.7	3	-4.404	12	0.102	0.099
DDD01008654	NIH / DDU, TB-active	Fc1cc(C(Nc2nc3c(o2)cc(OC(F)(F)F)cc3)=O)ccc1C#N	0.44	365.2	3	-6.06	14	0.034	0.099
DDD01010817	NIH / DDU, TB-active	CCCc1cc(c2nc(c3ccc(S(C)(=O)=O)cc3)cs2)ccn1	0.3	358.5	3	-6.716	14	0.040	0.099
DDD01009141	NIH / DDU, TB-active	CC1(c2ccc(OC(F)F)cc2)NC(N(C1=O)CC(c3ccc(Cl)s3)=O)=O	0.34	414.8	2	-6.14	13	0.053	0.099
DDD00401639	NIH / DDU, TB-active	CCN(c1nc2c(s1)cc(C(Nc3ccc4c(OCO4)c3)=O)s2)CC	0.13	375.5	3	-4.678	12	0.075	0.099
DDD00055473	NIH / DDU, TB-active	CCCc1ccc(Oc2cc(n3ncc(C(C)=O)c3C)ncn2)cc1	0.02	336.4	3	-5.616	14	0.116	0.099
DDD01012298	NIH / DDU, TB-active	Fc1ccc(C(Nc2nc3c(o2)cc(Cl)cn3)=O)cc1OC(F)(F)F	0.67	375.7	3	-6.055	13	0.087	0.099
DDD00285816	NIH / DDU, TB-active	CCn1c(CSc2nccc(C)n2)nc3c1ccc(NS(C)(=O)=O)c3	22.3	377.5	3	-5.145	11	0.072	0.164
DDD00067798	NIH / DDU, TB-active	Cc1ccc(c2cc(C(Oc3ccc(C)cc3C)=O)no2)cc1	0.014	307.3	3	-6.097	16	0.017	0.099
DDD00082485	NIH / DDU, TB-active	CC1=CC(NC(n2nc(C)cc2NC(c3cc4c(o3)cccc4)=O)=N1)=O	0.19	349.3	4	-4.789	16	0.038	0.164
DDD00247711	NIH / DDU, TB-active	CC1(c2ccc(OC(F)F)cc2)NC(N(C1=O)CC(c3ccc(F)cc3)=O)=O	1.02	392.3	2	-5.865	15	0.003	0.099
DDD01009327	NIH / DDU, TB-active	CCOc1ccc(C2CC(NC3=C2C(NC(SCC=C)=N3)=O)=O)cc1	2.1	357.4	2	-4.379	13	0.064	0.714
DDD00036467	NIH / DDU, TB-active	CC(c1ccc2c(OCCO2)c1)NC(c3ccc(Cl)cc3)=O	1.84	317.8	2	-4.764	13	0.037	0.099
DDD00013032	NIH / DDU, TB-active	CSc1ccc(CCNC(c2ccc3c(c2)nns3)=O)cc1	0.94	329.4	3	-5.864	13	0.107	0.099
DDD01009316	NIH / DDU, TB-active	CCc1ccc(C2CC(NC3=C2C(NC(SCC=C)=N3)=O)=O)cc1	1.07	341.4	2	-4.876	13	0.067	0.164

DDD01009694	NIH / DDU, TB-active	Fc1cc(C(Nc2nc3c(o2)cc(Cl)cn3)=O)ccc1OC(F)(F)F	0.148	375.7	3	-6.076	13	0.098	0.099
DDD00336009	NIH / DDU, TB-active	O=C(N1CCc2c1cccc2)CNS(c3ccc4c(OCCCO4)c3)(=O)=O	3.76	388.4	2	-3.471	13	0.044	0.200
DDD01009143	NIH / DDU, TB-active	CC1(c2ccc(OC(F)F)cc2)NC(N(C1=O)CC(c3ccccc3)=O)=O	1.08	374.3	2	-5.52	15	0.055	0.099
DDD00303559	NIH / DDU, TB-active	CCC(C(Nc1nc2c([nH]1)cccc2)=O)N3N=Nc4c(C3=O)cccc4	0.76	348.4	4	-4.502	15	0.024	0.099
DDD00507097	NIH / DDU, TB-active	Cc1ccc(C(CN2C(NC(c3ccc(OC(F)F)cc3)(C2=O)C)=O)=O)s1	0.86	394.4	2	-5.883	13	0.057	0.099
DDD00757679	NIH / DDU, TB-active	O=C(c1ccc(n2cccn2)cc1)Nc3nc(c4ccccn4)cs3	0.0067	347.4	4	-5.568	18	0.030	0.099
DDD00309343	NIH / DDU, TB-active	Oc1cc(c2ccccc2)nc3n1ncc3c4ccccc4	0.59	287.3	4	-4.528	18	0.100	0.099
DDD00649697	NIH / DDU, TB-active	O=C(c1cnc2c(n1)cccc2)NCc3ccc(N4CCOCC4)nc3	8.34	349.4	3	-3.798	14	0.029	0.771
DDD00052492	NIH / DDU, TB-active	COc1ccc2c(C(C=C(N2CC(Nc3ccccc3OC)=O)C)=O)c1	0.82	352.4	3	-3.935	16	0.071	0.099
DDD00174774	NIH / DDU, TB-active	Cc1nc2n(c1C(NCc3ccc(Cl)cc3)=O)ccs2	5.86	305.8	3	-4.431	12	0.076	0.099
DDD01009325	NIH / DDU, TB-active	COc1ccc(C2CC(NC3=C2C(NC(SCC#C)=N3)=O)=O)cc1	6.69	341.4	2	-3.148	11	0.046	0.154
DDD00306436	NIH / DDU, TB-active	COc1ccc(C2CC(NC3=C2C(NC(SCC=C)=N3)=O)=O)cc1	11.1	343.4	2	-4.044	13	0.053	0.714
DDD00553694	NIH / DDU, TB-active	FC(n1ccnc1COC(CCc2c[nH]c3c2cccc3)=O)F	0.0576	319.3	3	-5.205	12	0.078	0.164
DDD00078890	NIH / DDU, TB-active	COc1ccc2c(c1)nc(C)c(C(Nc3cc(C)ccn3)=O)c2	2.05	307.3	3	-5.158	15	0.049	0.099
DDD00512622	NIH / DDU, TB-active	FC(c1csc(NC(Cc2ccc(N3CCCC3=O)cc2)=O)n1)(F)F	2.87	369.4	2	-4.812	11	0.049	0.099
DDD00282186	NIH / DDU, TB-active	Cc1nc(SCCN2CCOC2=O)c3c(n1)scc3c4cccs4	0.64	377.5	3	-5.783	11	0.026	0.099
DDD00080579	NIH / DDU, TB-active	CNc1nc(c2ccsc2)nc3c1cccc3	1.17	241.3	3	-4.515	12	0.031	0.164
DDD01009324	NIH / DDU, TB-active	CCSC1=NC2=C(C(N1)=O)C(c3ccc(OC)cc3)CC(N2)=O	7.13	331.4	2	-3.671	11	0.083	0.154
DDD00756232	NIH / DDU, TB-active	CC1(c2ccc(C#N)cc2)NC(N(C1=O)CC(c3ccc(F)cc3F)=O)=O	2.956	369.3	2	-5.216	15	0.029	0.099
DDD00293239	NIH / DDU, TB-active	Cc1nn(c2nc3c(s2)cccc3)c(O)c1CCC#N	22.4	284.3	3	-4.37	10	0.078	0.099

DDD00097738	NIH / DDU, TB-active	CC1CCN(Cc2c(O)ccc3c2C(C=C(c4ccco4)O3)=O)CC1	2.16	339.4	3	-3.887	13	0.028	0.164
DDD00302941	NIH / DDU, TB-active	C[C@@]([H])(C(Nc1nc2c(s1)cccc2)=O)N3N=Nc4c(C3=O)cccc4	0.54	351.4	4	-5.3	15	0.057	0.099
DDD00055877	NIH / DDU, TB-active	COc1cnc(c2ccccc2)nc1N3CCCC3	0.12	255.3	2	-3.198	10	0.033	0.164
DDD00175988	NIH / DDU, TB-active	Cc1nn2c(c1c3ccccc3)nc(c4cnccn4)cc2O	4.5	303.3	4	-3.938	16	0.103	0.099
DDD01009328	NIH / DDU, TB-active	C=CCSC1=NC2=C(C(N1)=O)C(c3ccc4c(OCO4)c3)CC(N2)=O	3.68	357.4	2	-3.291	13	0.062	0.771
DDD00806486	NIH / DDU, TB-active	O=C(C1CC1)Nc2ccc(C3=Nc4c(C(O3)=O)cccc4)cc2	0.169	306.3	3	-4.482	15	0.032	0.099
DDD00242108	NIH / DDU, TB-active	CCc1cccc2c1[nH]cc2C(CN3C(Nc4c(C3=O)cccc4)=O)=O	0.3	347.4	4	-4.766	17	0.081	0.099
DDD00000113	NIH / DDU, TB-active	Cc1cccc(Cn2ccc(NC(c3ccco3)=O)n2)c1	5.06	281.3	3	-4.693	14	0.053	0.099
DDD00651173	NIH / DDU, TB-active	CC1NC(N(c2ccc(c3cn4c(n3)scc4)cc2)C1=O)=S	5.45	328.4	3	-4.773	13	0.035	0.099
DDD01009128	NIH / DDU, TB-active	CC1(c2ccc(C#N)cc2)NC(N(C1=O)CC(c3ccc(F)c(F)c3)=O)=O	2.24	369.3	2	-5.199	15	0.024	0.099
DDD00304195	NIH / DDU, TB-active	COc1ccc(Cn2c(C)c(C)n3c2nc(N(C(NC4=O)=O)C)c34)cc1	3.41	353.4	4	-3.427	13	0.098	0.771
DDD00853663	NIH / DDU, TB-active	FC1(CCC(NC(CSC2=Nc3c(C(N2)=O)cccc3)=O)CC1)F	13	353.4	2	-3.998	9	0.046	0.875
DDD00081512	NIH / DDU, TB-active	CS(c1cccc(C(Nc2nc3c(o2)ccc(Cl)c3)=O)c1)(=O)=O	4.29	350.8	3	-5.068	14	0.073	0.099
DDD00409494	NIH / DDU, TB-active	[O-][n+]1ccccc1SCCS(Oc2ccccc2)(=O)=O	46.6	311.4	2	-3.583	11	0.070	0.771
DDD00957045	NIH / DDU, TB-active	CN1C(C(C(N(C1=O)C)=O)C(Nc2ccc(SC(F)(F)F)cc2)=O)=O	0.59	375.3	1	-4.883	10	0.047	0.916
DDD01009094	NIH / DDU, TB-active	CC(C(Nc1nc2c([nH]1)cccc2)=O)N3C=Nc4c(C3=O)cccc4	4.07	333.3	4	-4.245	16	0.030	0.099
DDD00293274	NIH / DDU, TB-active	C[C@@]([H])(C(Nc1nc2c([nH]1)cccc2)=O)N3C=Nc4c(C3=O)cccc4	2.92	333.3	4	-4.245	16	0.040	0.099
DDD00946831	NIH / DDU, TB-active	O=C(NCC1CCCCC1)CSC2=Nc3c(C(N2)=O)cccc3	4.19	331.4	2	-4.752	9	0.057	0.241
DDD00957083	NIH / DDU, TB-active	FC(c1cccc(C(Cc2nc3c(o2)cccc3)=O)c1)(F)F	0.0039	305.3	3	-5.651	14	0.072	0.099
DDD00361107	NIH / DDU, TB-active	FC(c1nnc(NC(CCc2ncc(c3ccccc3)o2)=O)[nH]1)(F)F	5.2	351.3	3	-5.33	12	0.146	0.099

DDD00713267	NIH / DDU, TB-active	CCC(C(Nc1nc2c([nH]1)cccc2)=O)N3C(Nc4c(C3=O)cccc4)=O	0.7	363.4	4	-4.105	16	0.035	0.099
DDD00935026	NIH / DDU, TB-active	CC1=CC(NC(n2nc(C)cc2NC(c3ccccc3)=O)=N1)=O	4.8	309.3	3	-3.849	14	0.026	0.771
DDD00057463	NIH / DDU, TB-active	COCCNc1nc(SC)nc2c1cccc2	10.86	249.3	2	-3.507	8	0.067	0.154
DDD00057794	NIH / DDU, TB-active	COc1ccc(S(CC(Nc2nnc(C(F)(F)F)s2)=O)(=O)=O)cc1	9.25	381.4	2	-4.199	9	0.114	0.916
DDD01012425	NIH / DDU, TB-active	Fc1cc(C(Nc2nc3c(o2)cc(Cl)cn3)=O)ccc1C#N	2.69	316.7	3	-4.848	13	0.087	0.099
DDD01007953	NIH / DDU, TB-active	FC(C(Cc1nc2c(o1)ccc(Cl)c2)=O)(F)F	3.03	263.6	2	-4.872	8	0.151	0.099
DDD01009186	NIH / DDU, TB-active	CC(C1CCC(CC1NC(c2cccc(C(F)(F)F)c2)=O)C)C	0.015	327.4	1	-6.12	7	0.080	0.099
DDD00284199	NIH / DDU, TB-active	Nc1ccc(N2CCCCC2)c3c1cncc3	2.49	227.3	2	-3.414	9	0.122	0.099
DDD00079282	NIH / DDU, TB-active	Cc1n[nH]c(C)c1S(Nc2ccc3c(c2)[nH]nc3)(=O)=O	13.125	291.3	3	-2.859	10	0.062	0.771
DDD00711226	NIH / DDU, TB-active	C[C@@]([H])(C(Nc1nc2c([nH]1)cccc2)=O)N3C(Nc4c(C3=O)cccc4)=O	1.47	349.3	4	-3.953	16	0.039	0.771
DDD00806477	NIH / DDU, TB-active	Cc1ccsc1\C=C(\S2)/C(=O)N=C2N3CCCCC3	3.12	292.4	1	-4.253	8	0.064	0.164
DDD00304160	NIH / DDU, TB-active	CN1C(NC(c2c1nc3n2cc(C)n3Cc4ccc(C)cc4)=O)=O	9.9	323.3	4	-3.431	13	0.145	0.771
DDD00935323	NIH / DDU, TB-active	CN(C(c1[nH]c(C)c(S(Nc2ccc3c(c2)cn[nH]3)(=O)=O)c1C)=O)C	32.65	361.4	3	-3.486	12	0.080	0.200
DDD00080629	NIH / DDU, TB-active	Cc1noc(C)c1S(Nc2ccc3c(c2)[nH]nc3)(=O)=O	10.665	292.3	3	-3.259	10	0.059	0.771
DDD00957043	NIH / DDU, TB-active	CN1C(C(C(N(C1=O)C)=O)C(Nc2cccc(C(F)(F)F)c2)=O)=O	1.87	343.3	1	-4.79	10	0.056	0.916
DDD00203282	NIH / DDU, TB-active	Cc1n[nH]c(C)c1S(Nc2ccc3c(c2)cn[nH]3)(=O)=O	29	291.3	3	-2.866	10	0.034	0.771
DDD00203278	NIH / DDU, TB-active	Cc1noc(C)c1S(Nc2ccc3c(c2)cn[nH]3)(=O)=O	7.92	292.3	3	-3.266	10	0.032	0.771
DDD00005964	NIH / DDU, TB-active	O=C(C1COc2c(O1)cccc2)NC3CCCCC3	3.05	261.3	1	-3.212	7	0.083	0.875
DDD01007956	NIH / DDU, TB-active	Fc1ccc2c(c1)oc(CC(C(F)(F)F)=O)n2	12.2	247.1	2	-4.328	8	0.071	0.099
DDD00017596	NIH / DDU, TB-active	O=C(C1COc2c(O1)cccc2)NC3CCCC3	9.06	247.3	1	-2.733	7	0.090	0.875

DDD00957048	NIH / DDU, TB-active	CC(c1ccc(NC(C2C(N(C(N(C2=O)C)=O)C)=O)=O)cc1)C	0.95	317.3	1	-4.06	10	0.113	0.916
DDD00520827	NIH / DDU, TB-active	CN1C(NC(c2c1ncc(C(c3cc(F)ccc3O)=O)c2)=O)=O	3.8	315.3	3	-2.993	14	0.056	0.771
DDD00023831	NIH / DDU, TB-active	CCOC(c1cc2c(nc1N)cccc2)=O	1.46	216.2	2	-2.93	10	0.128	0.771
DDD00022015	NIH / DDU, TB-active	CC1(CC(C=C(Nc2ccc(C(O)=O)c(O)c2)C1)=O)C	48.58	275.3	1	-3.472	10	0.089	0.099
DDD01007954	NIH / DDU, TB-active	FC(C(Cc1nc2c(o1)cccc2)=O)F	23.1	211.2	2	-3.866	8	0.148	0.099
DDD00956999	NIH / DDU, TB-active	CN1C(C(C(N(C1=O)C)=O)C(Nc2ccccc2)=O)=O	17.1	275.3	1	-2.882	10	0.102	0.916
DDD00935325	NIH / DDU, TB-active	Cc1[nH]c(C(Nc2ccc(F)cc2)=O)c(C)c1S(Nc3ccc4c(c3)cn[nH]4)(=O)=O	0.811	427.5	4	-5.452	18	0.037	0.099
DDD00935330	NIH / DDU, TB-active	Cc1[nH]c(C(Nc2cccnc2)=O)c(C)c1S(Nc3ccc4c(c3)cn[nH]4)(=O)=O	5.13	410.5	4	-4.719	17	0.057	0.771
DDD00935328	NIH / DDU, TB-active	Cc1[nH]c(C(Nc2ccccc2)=O)c(C)c1S(Nc3ccc4c(c3)cn[nH]4)(=O)=O	1.07	409.5	4	-5.168	18	0.076	0.099
DDD00809430	DDU, TB-active	CN1C(Nc2c(C(F)(F)F)ccc(C(F)(F)F)c2)=NC(C(F)(F)F)=CC1=O	0.41	405.2	2	-8.187	10	0.031	0.099
DDD00898006	DDU, TB-active	Cc1nc(n2c(C)c1)nc(S(Nc3c(Cl)cccc3Cl)(=O)=O)n2	26.63	372.2	3	-4.556	11	0.034	0.099
DDD00911186	DDU, TB-active	CC(c1ccc(Br)cc1)NC(C(=O)c(c2C3=O)cccn2)=C3Cl	0.78	391.6	2	-6.258	15	0.070	0.164
DDD00810551	DDU, TB-active	COc1nc(c2cc1)c(n3nc4c(CC(NC\C=C\c5ccccc5)CC4)c3)ccn2	0.09	411.5	4	-7.639	19	0.055	0.164
DDD00816928	DDU, TB-active	Cc1cc(Nc2sc(c3ncccc3)cn2)ncc1	0.18	268.3	3	-4.618	13	0.023	0.099
DDD00812162	DDU, TB-active	CS(NC(CCc1c(c2ccc(Cl)cc2)nn(c3ccc(Br)cc3)c1)=O)(=O)=O	0.14	482.8	3	-7.735	16	0.073	0.099
DDD00898780	DDU, TB-active	Fc1cc(C(C(=O)N(CCc2ccccc2)c(c34)nc(N5CCNCC5)nc3)=N4)cc(F)c1	0.09	448.5	4	-5.451	18	0.061	0.164
DDD00923606	DDU, TB-active	Cc1nc(n2c(C)c1)nc(C(NS(c3c(Cl)cccc3)(=O)=O)=O)n2	18.06	365.8	3	-4.111	12	0.111	0.771
DDD00911207	DDU, TB-active	Cc1cc(NC(C(=O)c(c2C3=O)cccn2)=C3Cl)c(C)cc1	0.32	312.8	2	-5.301	15	0.077	0.099
DDD01053390	DDU, TB-active	CN1C(Nc2c(C(F)(F)F)cc(C(F)(F)F)cc2)=NC(C(F)(F)F)=CC1=O	0.26	405.2	2	-8.112	10	0.003	0.099
DDD00931564	DDU, TB-active	CCCS(c1c(S(NC(c2c(n3nn2)nc(C)cc3C)=O)(=O)=O)cccc1)(=O)=O	26.21	437.5	3	-3.982	12	0.039	0.771

DDD00810203	DDU, TB-active	CCOc1n(c2nc(CF)c1)nc(S(Nc3c(Cl)c(C)ccc3Cl)(=O)=O)n2	6.52	434.3	3	-4.985	11	0.071	0.099
DDD01053330	DDU, TB-active	COc1n(c2nc(CF)c1)nc(S(Nc3c(Cl)c(C)ccc3Cl)(=O)=O)n2	10.71	420.2	3	-4.765	11	0.083	0.099
DDD00898025	DDU, TB-active	Cc1nc(n2cc1)nc(S(Nc3c(F)cccc3F)(=O)=O)n2	42.79	325.3	3	-3.244	11	0.061	0.771
DDD00909564	DDU, TB-active	CC(C(Nc1ccc(Br)cc1)=O)N2C(=O)c(c3C(C)=N2)noc3C	3.39	391.2	3	-5.152	12	0.048	0.099
DDD00817112	DDU, TB-active	Cc1nc(n2c(Oc3c(c4c(Cl)cc3)nccc4)c1)ncn2	>99.9	311.7	4	-4.217	14	0.107	0.099
DDD00923584	DDU, TB-active	Cc1nc(n2c(C)c1)c(C(NS(c3c(Br)cccc3Br)(=O)=O)=O)nn2	2.97	489.1	3	-5.377	12	0.036	0.099
DDD00902271	DDU, TB-active	CCn1c(c2c(S(NC(c3c(n4nn3)nc(C)cc4C)=O)(=O)=O)cccc2)nnn1	27.23	427.4	4	-4.034	13	0.052	0.333
DDD01269631	DDU, TB-active	COc1c(N2C(=O)OC(OC(C)C)=N2)ccc(c3ccccc3)c1	0.1	326.3	3	-4.625	14	0.070	0.099
DDD01053249	DDU, TB-active	CN(C(C(=O)c(c1C2=O)cncc1)=C2Cl)Cc3ccccc3	0.68	312.8	2	-4.492	15	0.098	0.714
DDD00899979	DDU, TB-active	CN(C1C(C)(C)S(=O)(=O)C1c2c(Cl)cccc2)C	10.22	287.8	1	-3.583	6	0.077	0.889
DDD01053427	DDU, TB-active	CC(c1c(c2ccccc2)nn(c3ccc(C(F)(F)F)cc3)c1O)=O	1.3	346.3	3	-5.817	16	0.097	0.099
DDD00816149	DDU, TB-active	CS(C(S(C)(=O)=O)CC(N)=O)(=O)=O	52.16	229.3	0	-1.278	1	0.016	0.916
DDD01306067	DDU, TB-active	CN(C1C(C)(C)C2C1S(=O)(=O)C2)C	49.81	203.3	0	-0.999	0	0.135	0.916
DDD00813226	DDU, TB-active	N[C@@H](C(O)=O)[C@H]1ON=C(Cl)C1	48.23	178.6	0	-1.198	2	0.208	0.916
DDD00913915	DDU, TB-active	CCc1c(c2c(O)cc1)cccn2	0.7	173.2	2	-2.991	9	0.156	0.099
DDD00908944	DDU, TB-active	CC1SC(Nc2ccc(C(C)C)cc2)=NC(=O)C1	1.07	262.4	1	-4.176	8	0.075	0.164
DDD01008683	Eli Lilly / IDRI, TB-active	Cc1n(c2ccccc2)nc(CN3CCC4(c(c5CCO4)cccc5)CC3)c1	0.725	373.5	3	-6.403	15	0.055	0.164
DDD01009593	Eli Lilly / IDRI, TB-active	Cc1n(c2c(F)cccc2)nc(CN3CCC4(OCCCC4)CC3)c1	15.16	343.4	2	-5.263	9	0.039	0.164
DDD01270367	TAMU, TB-active	CNC(c1c(c2oc1c3ccc(O)cc3)c(CN4CCCCC4)c(O)cc2)=O	5.37	380.4	3	-4.857	15	0.045	0.164
DDD01305150	Eli Lilly / IDRI, TB-active	Cc1n(c2ccc(C(O)=O)cc2)nc(CN3CCC4(c(c5CCO4)cccc5)CC3)c1	14.97	417.5	3	-6.314	16	0.084	0.164
DDD01307205	TAMU, TB-active	CNC(c1c(c2oc1c3ccc(O)cc3)c(CN4CC5(COC5)C4)c(O)cc2)=O	9.81	394.4	3	-4.057	15	0.027	0.771

DDD01510098	TAMU, TB-active	CNC(c1c(c2oc1c3ccc(O)cc3)c(CN4CC5(COCC5)C4)c(O)cc2)=O	8.01	408.4	3	-4.453	15	0.025	0.771
DDD01510167	TAMU, TB-active	CNC(c1c(c2oc1c3ccc(O)cc3)c(CN4C[C@H](O)CCC4)c(O)cc2)=O	8.51	396.4	3	-4.004	15	0.037	0.154
DDD01510238	TAMU, TB-active	Oc1ccc(c2c(C#N)c(c3o2)c(CN4CCCCC4)c(O)cc3)cc1	0.3	348.4	3	-5.047	14	0.044	0.164
DDD01510278	Eli Lilly / IDRI, TB-active	Cc1n(c2cc(C(O)=O)ccc2)nc(CN3CCC4(c(c5CCO4)cccc5)CC3)c1	15.7	417.5	3	-6.248	16	0.074	0.164
DDD01510283	TAMU, TB-active	CNC(c1c(c2oc1c3ccc(O)cc3)c(CN4CC(F)CCC4)c(O)cc2)=O	3.86	398.4	3	-4.761	15	0.033	0.164
DDD01510824	Eli Lilly / IDRI, TB-active	Cc1n(c2ccc(C(O)=O)cc2)nc(CN3CCC4(c(c5CCO4)ccc(F)c5)CC3)c1	12.23	435.5	3	-6.337	16	0.052	0.164
DDD01510825	Eli Lilly / IDRI, TB-active	Cc1n(c2ccc(C(O)=O)cc2)nc(CN3CCC4(c(c5CCO4)cc(F)cc5)CC3)c1	12.81	435.5	3	-6.32	16	0.070	0.164
H3DTB-0000994	UCT, TB-active	CN(c1ncnc(C(Nc2ccccc2)=O)c1)Cc3ccc(C(F)(F)F)cc3	0.1	386.4	3	-6.137	17	0.043	0.164
H3DTB-0002745	UCT, TB-active	CN(c1ncnc(C(Nc2ccc(N3CCN(C)CC3)cc2)=O)c1)Cc4ccc(C(F)(F)F)cc4	0.06	484.5	3	-5.736	17	0.039	0.056
H3DTB-0002574	UCT, TB-active	CN(c1ncnc(C(Nc2scnn2)=O)c1)Cc3cnc(C(F)(F)F)cc3	3.59	395.4	3	-4.879	12	0.065	0.154
H3DTB-0001208	UCT, TB-active	CN(c1ncnc(C(Nc2scnn2)=O)c1)Cc3ccc(F)cc3	0.52	344.4	3	-4.01	13	0.099	0.154
H3DTB-0001620	UCT, TB-active	CN(c1ncnc(C(Nc2scnn2)=O)c1)Cc3ccc(C(F)(F)F)cc3	0.07	394.4	3	-5.223	13	0.084	0.164
H3DTB-0005893	UCT, TB-active	O=C(c1cc(N(Cc2ccc(F)cc2)C)ncn1)Nc3scc(CN(C)C)n3	0.6	400.5	3	-4.649	14	0.030	0.179
H3DTB-0002846	UCT, TB-active	Cc1scc(c2ccc(Oc3nnc(C(=O)OC)cc3)c(F)c2)n1	3.02	345.3	3	-5.194	14	0.060	0.099
H3DTB-0002841	UCT, TB-active	O=C(Nc1c(C(=O)O)cccc1)CCc2ccc(C(F)(F)F)cc2	4.12	337.3	2	-5.555	14	0.044	0.099
H3DTB-0002899	UCT, TB-active	O=C(O)c1ccccc1NC(=O)CCc2ccc(c3ccc(Cl)cc3)cc2	0.09	379.8	3	-7.283	20	0.094	0.099
H3DTB-0002895	UCT, TB-active	O=C(O)c1ccccc1NC(=O)CNc2ccc(Br)cc2	3.27	349.2	2	-4.686	14	0.093	0.099
H3DTB-0001187	UCT, TB-active	Nc1cnc(C(=O)O)cc1	>99.9	138.1	1	-0.924	6	0.170	0.916
H3DTB-0002563	UCT, TB-active	Cc1sc(C(c2sc(c3n2)cccc3)=NO)nn1	5.33	276.3	3	-4.439	10	0.076	0.099
H3DTB-0002900	UCT, TB-active	ON=C(c1sc(c2n1)cccc2)c3sc(C(F)(F)F)nn3	0.27	330.3	3	-5.157	10	0.119	0.099

H3DTB-0002461	UCT, TB-active	Cc1nc(c2c(N)c(c3c(C)n2)C(=O)N(Cc4cc(Cl)ccc4)C3=O)on1	0.11	383.8	3	-4.787	15	0.059	0.099
X-001	Sanofi, TB-active	CN(c1c(c2nc(c13)C(C)=CN(c4sccn4)C3=O)cccc2C(F)(F)F)CC(O)(C)C	<0.01	462.5	4	-5.848	15	0.024	0.099
X-002	Sanofi, TB-active	CN(C1CN(c2c(c3nc(c24)C(C)=CN(c5sccn5)C4=O)cccc3C(F)(F)F)CC1)C	0.04	473.5	4	-5.237	15	0.051	0.179
X-003	Sanofi, TB-active	Nc1c(c2[nH]c1c3nnc(c4ccccc4)o3)ncc(c25)cccc5	<0.01	327.3	5	-5.692	19	0.095	0.099
X-004	Sanofi, TB-active	CN(c1ccccc1)C(CN2CCN(c3ncnc(n4ccc4)c3)CC2)=O	11.77	377.4	3	-2.66	14	0.085	0.200
X-005	Sanofi, TB-active	CCn1ncc(c2c(c3c(c4n2)[nH]nc4N)cccc3)c1	3.99	278.3	4	-4.211	13	0.106	0.099
X-006	Sanofi, TB-active	Nc1c(c2[nH]c1c3nc(c4ccccc4)no3)ncc(c25)cccc5	<0.01	327.3	5	-5.696	19	0.008	0.099
X-007	Sanofi, TB-active	Nc1c(c2[nH]n1)nc(c3sc(c4c3)cccc4)c(c25)cccc5	<0.01	316.4	5	-6.687	18	0.093	0.099
X-008	Sanofi, TB-active	CCC(OC(c1c(N)c(c2[nH]1)c(C)nc(c23)c(C)cc(N(CC)CC)c3)=O)C	<0.01	382.5	3	-5.75	12	0.059	0.099
X-009	Sanofi, TB-active	CN1c(c2C(=O)N1c3cc(C(F)(F)F)ccc3)nc(c4c2O)c(C(F)(F)F)ccc4	<0.01	427.3	4	-5.922	16	0.013	0.099
X-010	Sanofi, TB-active	CCc1c(N2C(=O)N=C(NC)N=C2)c(CC)cc(Br)c1	13.62	337.2	2	-5.101	9	0.083	0.099
X-011	Sanofi, TB-active	CC(c1c(c(N2CCOCC2)c(c3n1)cccc3C(F)(F)F)C(=O)N4c5sccn5)=C4	<0.01	446.4	4	-5.036	15	0.016	0.099
X-012	Sanofi, TB-active	Oc1c(c2nc(C(F)F)c1C(Nc3sccn3)=O)cccc2C(F)(F)F	0.33	389.3	3	-5.584	13	0.070	0.099
X-013	Sanofi, TB-active	CC1c(c2C(=O)N1c3sccn3)nc(c4c2O)c(C(F)(F)F)ccc4C(F)(F)F	0.09	433.3	3	-5.403	13	0.064	0.099
X-014	Sanofi, TB-active	Oc1c(c2nc(C(Cl)Cl)c1C(Nc3sc(c4n3)cccc4)=O)cccc2C(F)(F)F	0.03	472.3	4	-7.79	17	0.049	0.099
X-015	Sanofi, TB-active	CCCNC(N=CN(c1c(CC)cccc1CC)C2=O)=N2	18.39	286.4	2	-4.63	9	0.031	0.099
X-016	Sanofi, TB-active	CON1c(c2C(=O)C(C(NN)=O)=C1C)ccc(Cl)c2	50.57	281.7	2	-2.718	10	0.166	0.916
X-017	Sanofi, TB-active	CN1CCN(c2c(c3nc(c24)C(C)=CN(c5sccn5)C4=O)cccc3C(F)(F)F)CC1	<0.01	459.5	4	-4.854	15	0.051	0.056
X-018	Sanofi, TB-active	CC(c(c1C(=O)N2c3sccn3)nc(c4c1O)c(C(F)(F)F)ccc4)=C2	<0.01	377.3	4	-4.801	15	0.033	0.099
IDR-0469041	IDRI, TB-active	CC(c1ccc(n2c(c3c(C4CCN(Cc5ccccc5)CC4)c2)cccc3)cc1)(C)C	<0.01	422.6	4	-9.981	20	0.013	0.164

IDR-0514734	IDRI, TB-active	COCc1ccc(n2c(c3c(C4CCN(Cc5ccccc5)CC4)n2)cccc3)cc1	0.02	411.5	4	-7.869	19	0.028	0.164
IDR-0527745	IDRI, TB-active	COc1snc(c2ccc(n3c(c4c(C5CCN(Cc6ccccc6)CC5)c3)cccc4)cc2)n1	<0.01	480.6	5	-9.243	22	0.067	0.164
IDR-0528696	IDRI, TB-active	COc1scc(c2ccc(n3c(c4c(C5CCN(Cc6ccccc6)CC5)c3)cccc4)cc2)n1	<0.01	479.6	5	-9.899	23	0.050	0.164
IDR-0532279	IDRI, TB-active	COCc1cnc(n2c(c3c(C4CCN(Cc5ccccc5)CC4)n2)cccc3)cc1	0.02	412.5	4	-7.265	18	0.027	0.164
IDR-0497562	IDRI, TB-active	CNc1c2c(CCCO2)nc(SC)n1	20.83	211.3	1	-2.109	4	0.042	0.916
IDR-0528776	IDRI, TB-active	CNc1c2c(CCCO2)nc(OC)n1	64.37	195.2	1	-1.394	4	0.059	0.916
IDR-0528780	IDRI, TB-active	COc1nc(NCCOc2ccccc2)c3c(CCCO3)n1	1.95	301.3	2	-3.422	10	0.066	0.099
IDR-0532039	IDRI, TB-active	CNc1c2c(CCCO2)nc(C(C)C)n1	26.45	207.3	1	-2.425	4	0.028	0.916
IDR-0532131	IDRI, TB-active	CNc1nc(SC)nc(c12)cccc2	8.01	205.3	2	-3.092	8	0.045	0.154
IDR-0532133	IDRI, TB-active	CCOc1nc(NC)c2c(CCCO2)n1	53.97	209.2	1	-1.712	4	0.038	0.916
IDR-0504706	IDRI, TB-active	COc1ncc(n2c(C)cc(CN3CCC4(c(c5CCO4)cccc5)CC3)n2)cc1	1.31	404.5	3	-6.003	14	0.050	0.154
IDR-0021254	IDRI, TB-active	Cc1oc(c2ccccc2)cc1CN3CCC4(c5c(ccs5)CCO4)CC3	0.03	379.5	3	-7.377	14	0.025	0.164
IDR-0514759	IDRI, TB-active	Cc1n(c2ccc(OC(F)(F)F)cc2)nc(CN3CCC4(c(c5CCO4)ccc(F)c5)CC3)c1	0.3	475.5	3	-7.808	15	0.050	0.164
IDR-0484833	IDRI, TB-active	NC(c1sc(n2cncc2)cc1OCCc3cc(F)ccc3)=O	6.32	331.4	3	-4.937	14	0.079	0.099
IDR-0338595	IDRI, TB-active	COc1ccc(CCOc2cc(N3CCOCC3)sc2C(=O)N)cc1	5.71	362.4	2	-3.983	11	0.081	0.099
IDR-0492028	IDRI, TB-active	CNC(c1c(OCCc2ccc(OC)cc2)ccc(N3CCOCC3)c1)=O	6.5	370.4	2	-4.323	13	0.021	0.099
IDR-0275902	IDRI, TB-active	NC(c1sc(N2CCOCC2)cc1OCCc3ccccc3)=O	6.18	332.4	2	-3.864	11	0.107	0.099
IDR-0341930	IDRI, TB-active	CCc1n(CCCCOc2ccccc2)c(c3n1)cc(C)cc3	0.15	308.4	3	-6.618	13	0.022	0.164
IDR-0390228	IDRI, TB-active	CCc1n(CCCSc2oc(c3ccc(Cl)cc3)nn2)c(c4n1)cc(C)cc4	0.09	412.9	4	-8.359	15	0.024	0.164
IDR-0461471	IDRI, TB-active	CC(CC(N1CCC(c2ccccc2)CC1)(C)C)(C)C	3.76	273.5	1	-5.828	6	0.012	0.164
IDR-0376022	IDRI, TB-active	CCC1(N2CCC(c3ccccc3)CC2)CCCCC1	3.16	271.4	1	-5.855	6	0.016	0.164
IDR-0303213	IDRI, TB-active	C(c1cccc(c12)cccn2)N3CCC(c4[nH]c(c5n4)cccc5)CC3	8.02	342.4	4	-6.009	16	0.023	0.164
IDR-0351615	IDRI, TB-active	Fc1ccc(Cn2c(c3cn2)ccnc3c4occc4)cc1	0.33	293.3	4	-5.558	16	0.056	0.099

IDR-0469026	IDRI, TB-active	COc1ccc(c2nccc(c23)n(Cc4ccc(F)cc4)nc3)cc1	0.09	333.4	4	-6.42	18	0.035	0.099
IDR-0392810	IDRI, TB-active	C(c1ccc(Oc2ccccc2)cc1)n3c(c4cn3)ccnc4N5CCCCC5	<0.01	384.5	4	-6.653	18	0.020	0.241
GSK001	GSK, TB-active	CCc1nn(CC)c(C(N[C@H]2CN(C(c3c(c4oc3)cccc4)=O)[C@H](C(=O)N)C2)=O)c1	7.43	423.5	3	-4.998	14	0.058	0.200
GSK002	GSK, TB-active	Cc1nc([C@@](c2sc(Nc3nn(Cc4nc(C)sc4)cc3)nn2)(O)C)sc1	8.42	419.5	4	-5.831	11	0.023	0.099
GSK003	GSK, TB-active	CCc1nccc(C(=S)N)c1	36.62	166.2	1	-3.531	6	0.056	0.916

(1) Acronyms: UBA, undefined bactericidal activity; PZA, pyrazinamide; NIH, National Institute of Health; DDU, Drug Discovery Unit University of Dundee; TAMU, Texas A&M University; UCT, University of Cape Town; IDRI, Infectious Disease Research Institute; GSK, GlaxoSmithKline. Molecular Descriptors: Arom_Rings, Number of aromatic rings; Mol_Sol, solubility; sp2, sp2 carbon count; IW1_VS, hydrophobicity / lipophilicity unbalance; plasma PB, predicted plasma protein binding

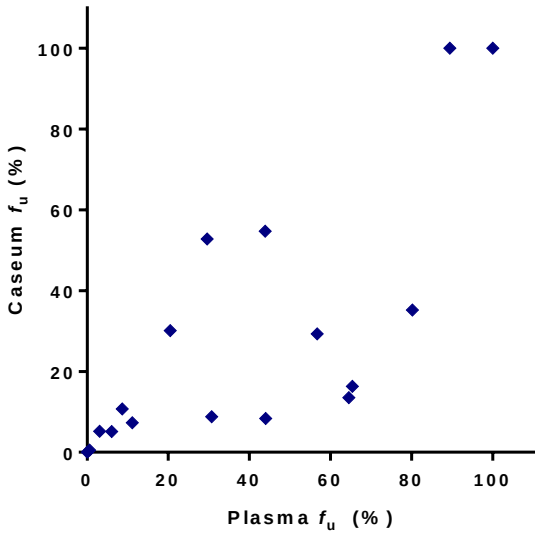
Supplementary Table 2. List of all 69 calculated molecular descriptors evaluated. Descriptors that were included in Principal Component Analysis (PCA) and / or building the consensus model are indicated with a 'Y'. Descriptors that were not included in PCA are indicated with an 'N'.

Descriptor	Source	PCA	Model
HAC	Stardrop	Y	Y
AromaticRings	Stardrop	Y	Y
C_count	Stardrop	Y	Y
Sp3_count	Stardrop	Y	Y
TPSA	Stardrop	Y	Y
logD	Stardrop	Y	Y
HBD	Stardrop	Y	Y
HBA	Stardrop	Y	Y
Flexibility	Stardrop	Y	Y
RotBonds	Stardrop	Y	Y
FU4	Volsurf+	Y	Y
FU8	Volsurf+	Y	Y
A	Volsurf+	Y	Y
ACACAC	Volsurf+	Y	Y
ACACDO	Volsurf+	Y	Y
ACDODO	Volsurf+	Y	Y
AUS7_4	Volsurf+	Y	Y
CD1	Volsurf+	Y	Y
CP	Volsurf+	Y	Y
CW2	Volsurf+	Y	Y
D1	Volsurf+	Y	Y
DD8	Volsurf+	Y	Y
DIFF	Volsurf+	Y	Y
DODODO	Volsurf+	Y	Y
DRACAC	Volsurf+	Y	Y
DRACDO	Volsurf+	Y	Y
DRDOD	Volsurf+	Y	Y
DRDRAC	Volsurf+	Y	Y
DRDRDO	Volsurf+	Y	Y
DRDRDR	Volsurf+	Y	Y
FLEX	Volsurf+	Y	Y
FLEX_RB	Volsurf+	Y	Y
G	Volsurf+	Y	Y
HL1	Volsurf+	Y	Y
HAS	Volsurf+	Y	Y

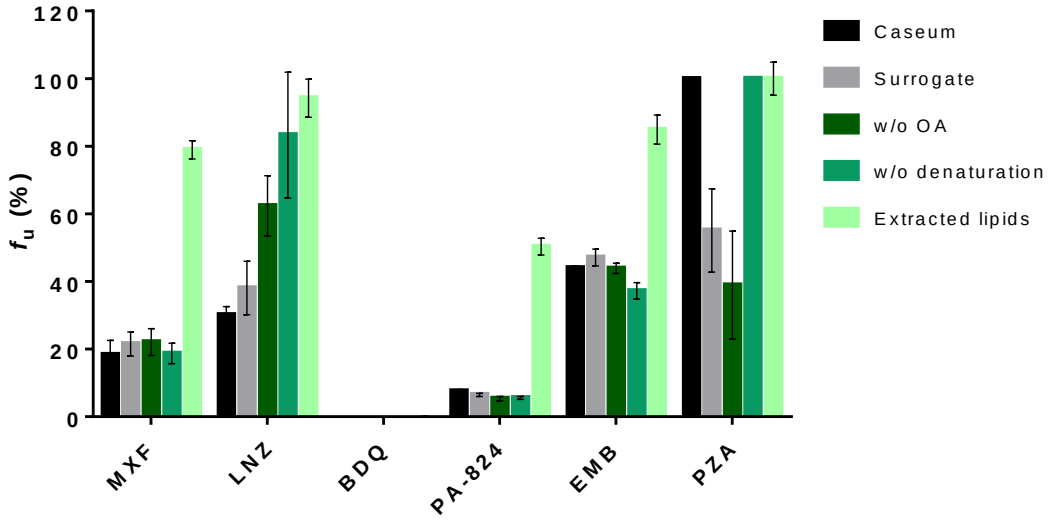
ID1	Volsurf+	Y	Y
IW1	Volsurf+	Y	Y
L4LgS	Volsurf+	Y	Y
LOGP_cHex	Volsurf+	Y	Y
LOGP_nOct	Volsurf+	Y	Y
LgD8	Volsurf+	Y	Y
MW	Volsurf+	Y	Y
PB	Volsurf+	Y	Y
PHSAR	Volsurf+	Y	Y
POL	Volsurf+	Y	Y
PSA	Volsurf+	Y	Y
PSAR	Volsurf+	Y	Y
R	Volsurf+	Y	Y
S	Volsurf+	Y	Y
V	Volsurf+	Y	Y
VD	Volsurf+	Y	Y
W2	Volsurf+	Y	Y
W6	Volsurf+	Y	Y
WN6	Volsurf+	Y	Y
WO5	Volsurf+	Y	Y
FmF	PipelinePilot	Y	Y
Ring_count	PipelinePilot	Y	Y
Mol_sol	PipelinePilot	Y	Y
sp2	PipelinePilot	Y	Y
fSP3	PipelinePilot	Y	Y
Alogp_MR	PipelinePilot	Y	Y
Wiener	PipelinePilot	Y	Y
Zagreb	PipelinePilot	Y	Y
N_O_Count	PipelinePilot	Y	Y
Num_SpiroAtoms	PipelinePilot	N	Y
E-state_Keys	PipelinePilot	N	Y
E-state_Counts	PipelinePilot	N	Y
SCFP_4	PipelinePilot	N	Y
FCFP12	PipelinePilot	N	Y

SUPPLEMENTARY FIGURES

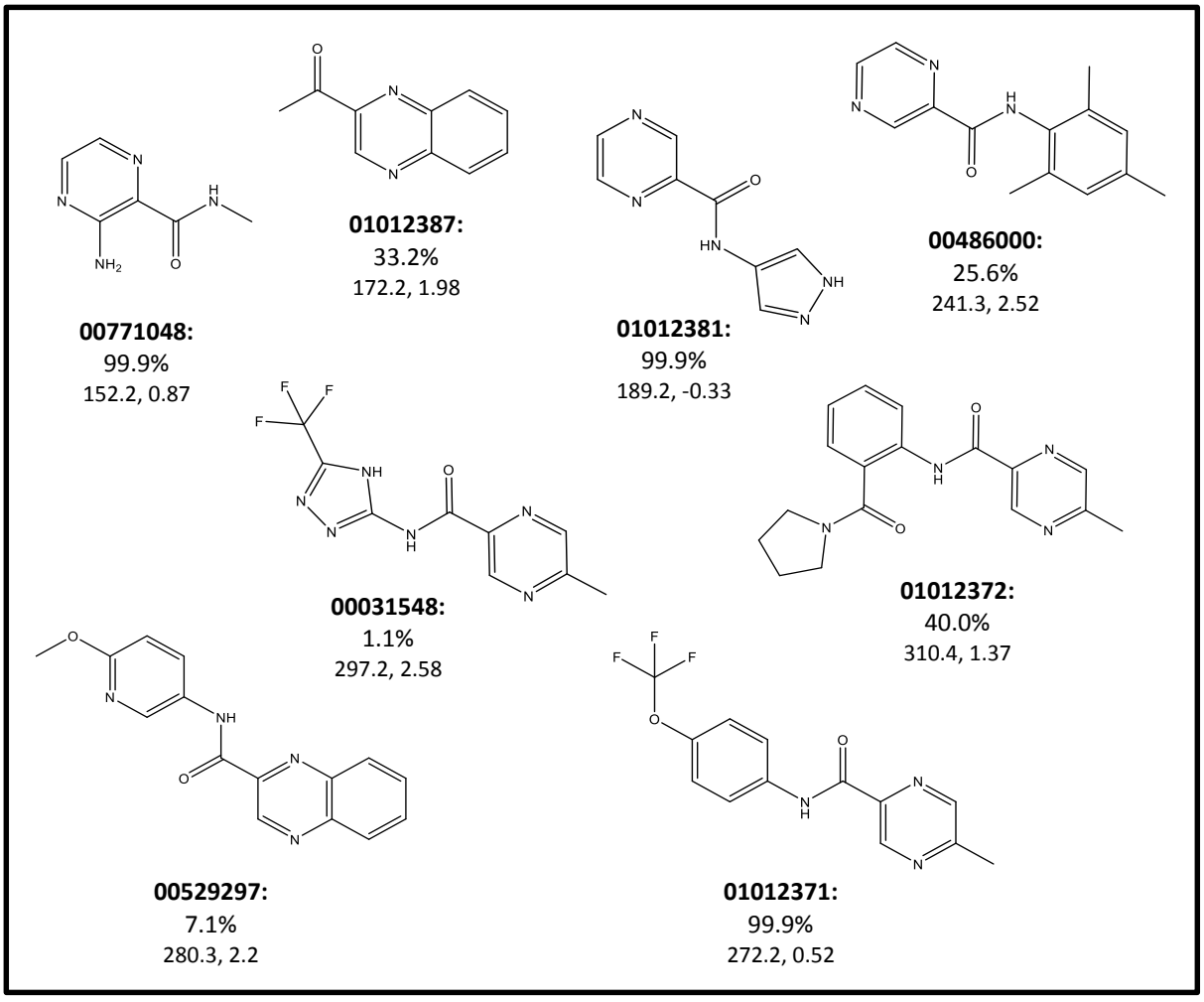
Supplementary Figure 1. Plasma protein binding versus caseum binding for anti-tuberculosis drugs. Protein binding was measured in rabbit plasma and rabbit caseum for 20 drugs using the rapid equilibrium dialysis assay.



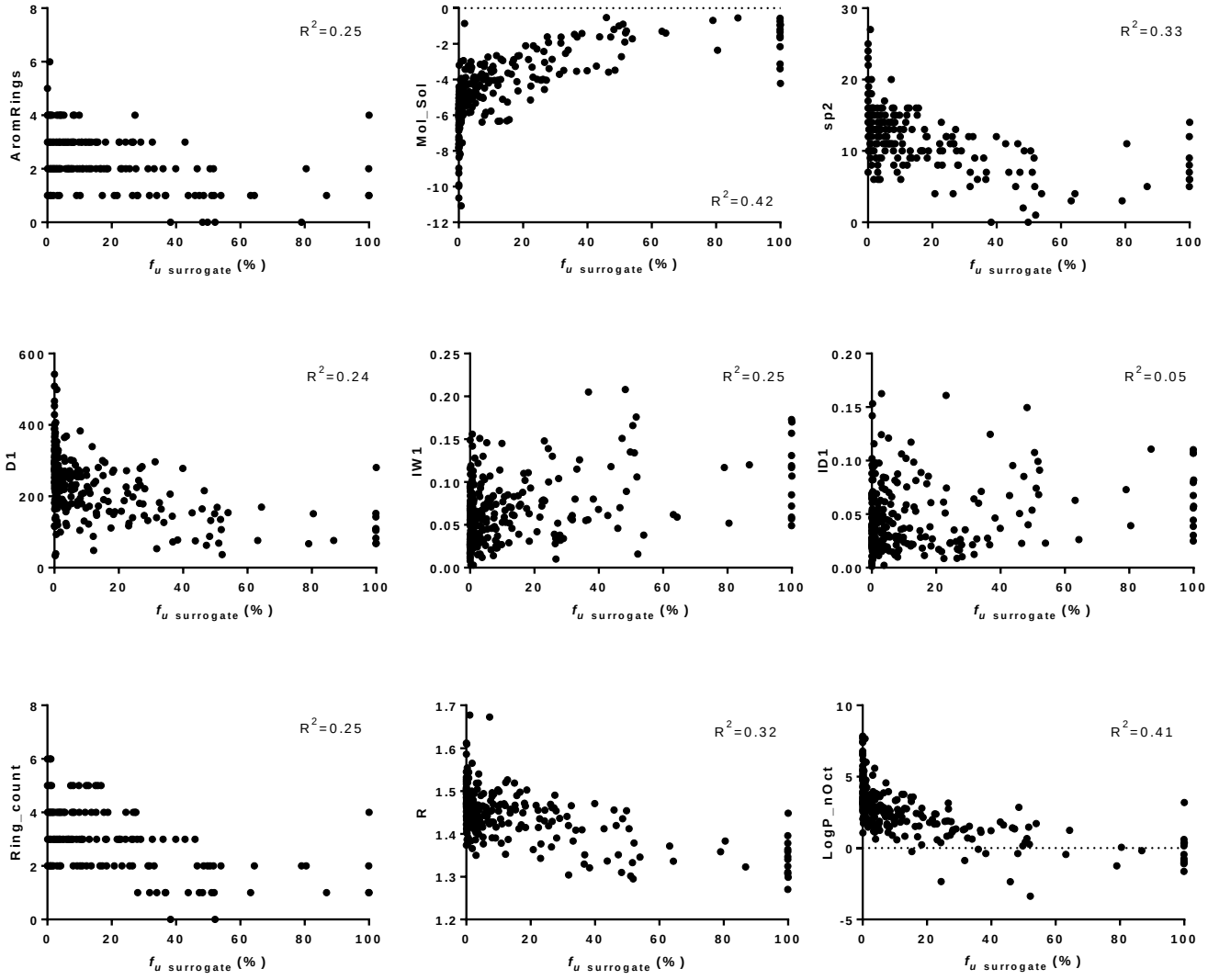
Supplementary Figure 2. Effect of modulation of the lipid and protein contents in the surrogate matrix on drug binding. Several versions of the surrogate were generated in which we (i) omitted induction of lipid droplet formation with OA, (ii) omitted the protein denaturing step or (iii) extracted the lipids only. These assays were performed in the cassette format with moxifloxacin (MXF), linezolid (LNZ), bedaquiline (BDQ), PA-824, ethambutol (EMB) and pyrazinamide (PZA). Each bar is the average of three representative experiments with standard deviations (error bars). Manipulating the composition of the surrogate matrix affected binding of each drug to different degrees. Only bedaquiline binding remained high and constant (f_u < 0.01) under all conditions.



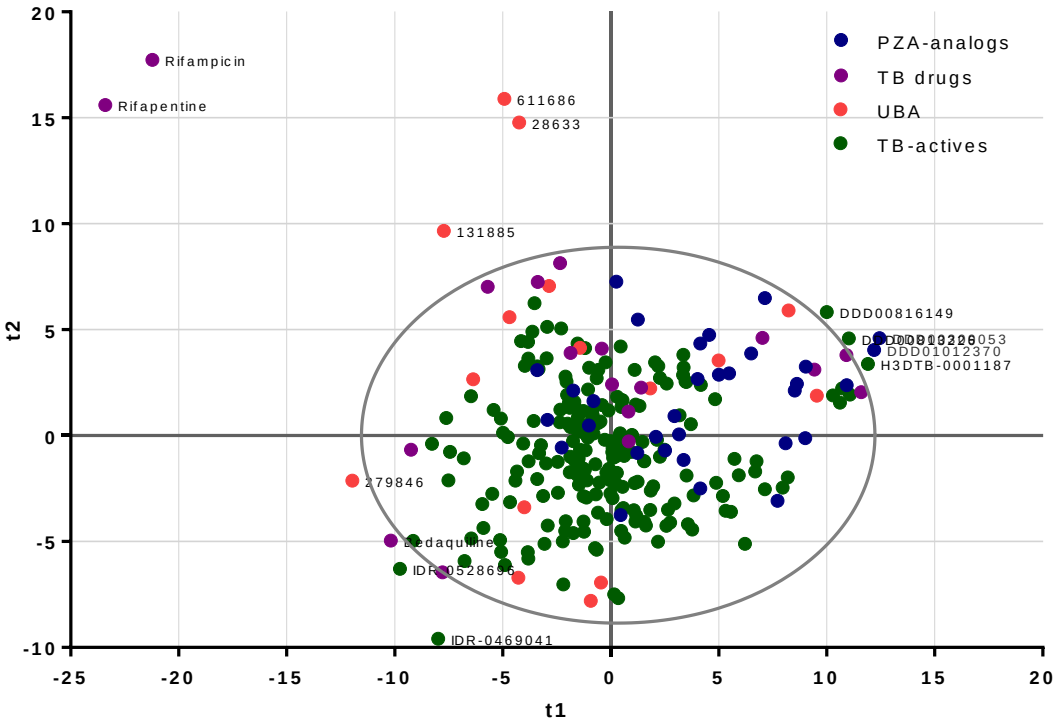
Supplementary Figure 3. Fraction unbound in caseum surrogate (%), molecular weight and cLogP of selected compounds containing the pyrazinamide scaffold.



Supplementary Figure 4a Parameters that show the strongest correlation with the unbound fractions of 279 compounds in caseum surrogate (based on the p1 and p2 PCA loadings).



Supplementary Figure 4b The PCA scores t1 and t2 are new variables summarizing how the different compounds (described by the set of 64 molecular descriptors) are situated with respect to each other. The plot shows the presence of outliers, similarities, groups and other patterns in the data set.



Supplementary Figure 4c. Correlation between ciPFI (cLogP + #Ar) of 279 compounds and their unbound fractions in caseum surrogate.