Training dataset curated from R-SIM database for the “Riboswitch” model in RSAPred

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
221	C1=NC2=NC=NC(=C2N1)N	GGACAUAUAAUCGCGUGGAUAUGGCACGCAAGUUUCUACCGGGCACCGUAAAUGUCCGAUUAUGUCC	Adenine	Target_lig_165	ADENINE RIBOSWITCH	Target_69	6.3979400086 7204
222	C1=C2C(=NC(=N1)N)N=CN2	GGACAUAUAAUCGCGUGGAUAUGGCACGCAAGUUUCUACCGGGCACCGUAAAUGUCCGAUUAUGUCC	2-aminopurine	Target_lig_166	ADENINE RIBOSWITCH	Target_69	5.7891466346 8511
223	C1=C(N=C(N=C1N)N)N	GGACAUAUAAUCGCGUGGAUAUGGCACGCAAGUUUCUACCGGGCACCGUAAAUGUCCGAUUAUGUCC	2,4,6-triaminopyrimidine	Target_lig_167	ADENINE RIBOSWITCH	Target_69	4.6989700043 3602
224	C1=NC2=NC(=NC(=C2N1)N)N	GGACAUAUAAUCGCGUGGAUAUGGCACGCAAGUUUCUACCGGGCACCGUAAAUGUCCGAUUAUGUCC	2,6- diaminopurine	Target_lig_168	ADENINE RIBOSWITCH	Target_69	7.6989700043 3602
225	C1=NC(=NC2(C1=NC=N2)N)N	GGACAUAUAAUCGCGUGGAUAUGGCACGCAAGUUUCUACCGGGCACCGUAAAUGUCCGAUUAUGUCC	2,4-diaminopurine	Target_lig_169	ADENINE RIBOSWITCH	Target_69	8.3979400086 7204
231	CC1=CC2=C(C=C1C)N(C=N2)C3C(C(C(O3)CO)OP(=O)([O-])OC(C)CNC(=O)CCC4(C(C5C6(C(C(C(=N6)C(=C7C(C(C(=N7)C=C8C(C(C(=N8)C(=C4[N-]5)C)CCC(=O)N)(C)C)CCC(=O)N)(C)CC(=O)N)C)CCC(=O)N)(C)CC(=O)N)C)CC(=O)N)C)O.[CH2-]C1C(C(C(O1)N2C=NC3=C(N=CN=C32)N)O)O.[Co+3]	GCCGGUCCUGUGAGUUAAUAGGGAAUCCAGUGCGAAUCUGGAGCUGACGCGCAGCGGUAAGGAAAGGUGCGAUGAUUGCGUUAUGCGGACACUGCCAUUCGGUGGGAAGUCAUCAUCUCUUAGUAUCUUAGAUACCCCUCCAAGCCCGAAGACCUGCCGGCCAACGUCGCAUCUGGUUCUCAUCAUCGCGUAAUAUUGAUGA	deoxy_adenosylcobalamin	Target_lig_173	Riboswitch	Target_70	6.5228787452 8034
315	C1=NC2=NC=NC(=C2N1)N	GGACAUAUAAUCGCGUGGAUAUGGCACGCAAGUUUCUACCGGGCACCGUAAAUGUCCGACUAUGUCC	Adenine	Target_lig_165	Guanine riboswitch	Target_74	6.3288271572 8492
316	C1=NC2=C(N1)C(=O)N=CN2	GGACAUAUAAUCGCGUGGAUAUGGCACGCAAGUUUCUACCGGGCACCGUAAAUGUCCGACUAUGUCC	Hypoxanthine	Target_lig_162	Guanine riboswitch	Target_74	7.3010299956 6398
317	C1=NC2=C(N1)C(=O)NC(=N2)N	GGACAUAUAAUCGCGUGGAUAUGGCACGCAAGUUUCUACCGGGCACCGUAAAUGUCCGACUAUGUCC	GUANINE	Target_lig_248	Guanine riboswitch	Target_74	8.3010299956 6398
318	C1=NC(=NC2(C1=NC=N2)N)N	GGACAUAUAAUCGCGUGGAUAUGGCACGCAAGUUUCUACCGGGCACCGUAAAUGUCCGACUAUGUCC	2,4-diaminopurine	Target_lig_169	Guanine riboswitch	Target_74	7.7695510786 2173
319	C1=NC2=C(N1)C(=NC(=N2)N)NO	GGACAUAUAAUCGCGUGGAUAUGGCACGCAAGUUUCUACCGGGCACCGUAAAUGUCCGACUAUGUCC	2-AMINO-N6-HYDROXYADENINE	Target_lig_249	Guanine riboswitch	Target_74	7.6989700043 3602

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
320	C1(=C(N=C(NC1=O)N)N)N	GGACAUAUAAUCGCGUGGAUAUGGCACGCAAGUUUCUACCGGGCACCGUAAAUGUCCGACUAUGUCC	2,5,6-TRIAMINO-PYRIMIDINE-4-ONE	Target_lig_250	Guanine riboswitch	Target_74	7
392	C[S+](CCC(C(=O)[O-])N)CC1C(C(C(O1)N2C=NC3=C(N=CN=C32)N)O)O	GGCUUAUCAAGAGAGGUGGAGGGACUGGCCCGAUGAAACCCGGCAACCAGAAAUGGUGCCAAUUCCUGCAGCGGAAACGUUGAAAGAUGAGCCA	S-adenosyl methionine	Target_lig_314	S_Adenosyl_methionine_riboswitch	Target_71	8
398	CC1=C(SC=[N+]1CC2=CN=C(N=C2N)C)CCOP(=O)(O)OP(=O)(O)[O-]	GGACUCGGGGUGCCCUUCUGCGUGAAGGCUGAGAAAUACCCGUAUCACCUGAUCUGGAUAAUGCCAGCGUAGGGAAGUUC	Thiamine_Pyrophosphate(TPP)	Target_lig_318	thiamine_BOX_Riboswitch	Target_72	6.2218487496 1636
410	C1=NC2=NC=NC(=C2N1)N	GGAAUAAUUGUAUAACCUCAAUAAUAUGGUUUGAGGGUGUCUACCAGGAACCGUAAAAUCCUGAUUACAA	Adenine	Target_lig_165	B_subtilis_pbuE_Adenine riboswitch	Target_73	6.2358238676 0967
412	CC1=CC2=C(C=C1C)N(C3=NC(=O)NC(=O)C3=N2)CC(C(C(COP(=O)(O)O)O)O)O	GGCGUGUAGGAUAUGCUUCGGCAGAAGGACACGCC	FMN	Target_lig_68	FMN RIBOSWITCH APTAMER	Target_36	8.9208187539 5238
413	C1=C(C2=C(N1)N=C(NC2=O)N)CN	AGUAGAUGUGCUAGCAAAACAUCUUUAAAAAACUAGACUUGGGGUGCAAGUCCCCUUUUUUAUUGCUUAAAUUU	preQ1 (7-Aminomethyl-7-deazaguanine)	Target_lig_331	PreQ1_riboswitch_Fusobacterium	Target_75	6.5482135644 7571
414	CC1=C(SC=[N+]1CC2=CN=C(N=C2N)C)CCOP(=O)(O)OP(=O)(O)[O-]	GGUAACCACUAGGGGUGUCCUUCAUAAGGGCUGAGAUAAAAGUGUGACUUUUAGACCCUCAUAACUUGAACAGGUUCAGACCUGCGUAGGGAAGUGGAGC	Thiamine_Pyrophosphate(TPP)	Target_lig_318	TPP RIBOSWITCH APTAMER	Target_37	6.3053948010 6643
415	C[S+](CCC(C(=O)[O-])N)CC1C(C(C(O1)N2C=NC3=C(N=CN=C32)N)O)O	GGCUUAUCAAGAGAGGUGGAGGGACUGGCCCGAUGAAACCCGGCAACCAGAAAUGGUGCCAAUUCCUGCAGCGGAAACGUUGAAAGAUGAGCCA	SAM	Target_lig_1248	S_Adenosyl_methionine	Target_71	5.8696662315 0499
416	C(CCN)C[C@@H](C(=O)O)N	GAAGAUAGAGGUGCGAACUUCAAGAGUAUGCCUUUGGAGAAAGAUGGAUUCUGUGAAAAAGGCUGAAAGGGGAGCGUCGCCGAAGCAAAUAAAACCCCAUCGGUAUUAUUUGCUGGCCGUGCAUUGAAUAAAUGUAAGGCUGUCAAGAAAUCAUUUUCUUGGAGGGCUAUCUCGUUGUUCAUAAUCAUUUAUGAUGAUUAAUUGAUAAGCAAUGAGAGUAUUCCUCUCAUUGCUUUUUU	lysine	Target_lig_31	LYSINE RIBOSWITCH APTAMER	Target_38	5.7447274948 9669
739	CC1=C(SC=[N+]1CC2=CN=C(N=C2N)C)CCOP(=O)(O)OP(=O)(O)	GGUAACCACUAGGGGUGUCCUUCAUAAGGGCUGAGAUAAAAG	Thiamine_Pyrophosphate(TPP)	Target_lig_318	B.subtilis tenA TPP riboswitch	Target_76	7.3010299956 6398

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	[O-]	UGUGACUUUUAGACCCUCAUAACUUGAACAGGUUCAGACCUGCGUAGGGAAGUGGAGC					
740	CC1=C(SC=[N+]1CC2=CN=C(N=C2N)C)CCO	GGUAACCACUAGGGGUGUCCUUCAUAAGGGCUGAGAUAAAAGUGUGACUUUUAGACCCUCAUAACUUGAACAGGUUCAGACCUGCGUAGGGAAGUGGAGC	Thiamine_mol	Target_lig_502	B.subtilis tenA TPP riboswitch	Target_76	4.3010299956 6398
741	CC1=C(C=CC=[N+]1CC2=CN=C(N=C2N)C)CCO.Br.[Br-]	GGUAACCACUAGGGGUGUCCUUCAUAAGGGCUGAGAUAAAAGUGUGACUUUUAGACCCUCAUAACUUGAACAGGUUCAGACCUGCGUAGGGAAGUGGAGC	Pyrithiamine_mol	Target_lig_503	B.subtilis tenA TPP riboswitch	Target_76	5.2218487496 1636
742	n1c(ncc(c1N)CN1=CC=CC(=C1)CCO[P@@](=O)(O)P(=O)(O)O)C	GGUAACCACUAGGGGUGUCCUUCAUAAGGGCUGAGAUAAAAGUGUGACUUUUAGACCCUCAUAACUUGAACAGGUUCAGACCUGCGUAGGGAAGUGGAGC	Pyrithiamine_Pyrophosphate_der	Target_lig_504	B.subtilis tenA TPP riboswitch	Target_76	6.7958800173 4408
743	CC1=CC2=C(C=C1C)N(C3=NC(=O)NC(=O)C3=N2)CC(C(C(COP(=O)(O)O)O)O)O	GGAAGGACAAAUGAAUAAAGAUUGUAUCCUUCGGGGCAGGGUGGAAAUCCCGACCGGCGGUAGUAAAGCACAUUUGCUUUAGAGCCCGUGACCCGUGUGCAAUAGCACGCGGUGGAUUCAGUUUAAGCUGAAGCCGACAGUGAAAGUCUGGAUGGGAGAAGGAUG	FMN	Target_lig_68	B.subtilis tenA FMN riboswitch	Target_77	8.3010299956 6398
744	CC1=CC2=C(C=C1C)N(C3=NC(=O)NC(=O)C3=N2)CC(C(C(CO)O)O)O	GGAAGGACAAAUGAAUAAAGAUUGUAUCCUUCGGGGCAGGGUGGAAAUCCCGACCGGCGGUAGUAAAGCACAUUUGCUUUAGAGCCCGUGACCCGUGUGCAAUAGCACGCGGUGGAUUCAGUUUAAGCUGAAGCCGACAGUGAAAGUCUGGAUGGGAGAAGGAUG	riboflavin	Target_lig_70	B.subtilis tenA FMN riboswitch	Target_77	5.5228787452 8034
745	CC1=CC2=C(C=C1N(C)C)N(C3=NC(=O)NC(=O)C3=N2)CC(C(C(CO)O)O)O	GGAAGGACAAAUGAAUAAAGAUUGUAUCCUUCGGGGCAGGGUGGAAAUCCCGACCGGCGGUAGUAAAGCACAUUUGCUUUAGAGCCCGUGACCCGUGUGCAAUAGCACGCGGUGGAUUCAGUUUAAGCUGAAGCCGACAGUGAAAGUCUGGAUGGGAGAAGGAUG	Roseoflavin	Target_lig_505	B.subtilis tenA FMN riboswitch	Target_77	7
746	C(CCN=C(N)N)C[C@@H](C(=O)O)N	GAAGAUAGAGGUGCGAACUUCAAGAGUAUGCCUUUGGAGAAAGAUGGAUUCUGUGAAAAAGGCUGAAAGGGGAGCGUCGCCGAA	L-homoarginine	Target_lig_57	B.subtilis lysine riboswitch	Target_78	5.1549019599 8574

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		GCAAAUAAAACCCC AUCGGUAUUAUUUG CUGGCCGUGCAUUG AAUAAAUGUAAGGC UGUCAAGAAAUCAU UUUCUUGGAGGGCU AUCUCGUUGUUCAU AAUCAUUUAUGAUG AUUAAUUGAUAAGC AAUGAGAGUAUUCC UCUCAUUGCUUUUU U					
747	C(CCN)C[C@@H](C(=O)O)N	GAAGAUAGAGGUGC GAACUUCAAGAGUA UGCCUUUGGAGAAA GAUGGAUUCUGUGA AAAAGGCUGAAAGG GGAGCGUCGCCGAA GCAAAUAAAACCCC AUCGGUAUUAUUUG CUGGCCGUGCAUUG AAUAAAUGUAAGGC UGUCAAGAAAUCAU UUUCUUGGAGGGCU AUCUCGUUGUUCAU AAUCAUUUAUGAUG AUUAAUUGAUAAGC AAUGAGAGUAUUCC UCUCAUUGCUUUUU U	lysine	Target_lig_31	B.subtilis lysine riboswitch	Target_78	6.4436974992 3271
748	C(COC[C@@H](C(=O)O)N)N	GAAGAUAGAGGUGC GAACUUCAAGAGUA UGCCUUUGGAGAAA GAUGGAUUCUGUGA AAAAGGCUGAAAGG GGAGCGUCGCCGAA GCAAAUAAAACCCC AUCGGUAUUAUUUG CUGGCCGUGCAUUG AAUAAAUGUAAGGC UGUCAAGAAAUCAU UUUCUUGGAGGGCU AUCUCGUUGUUCAU AAUCAUUUAUGAUG AUUAAUUGAUAAGC AAUGAGAGUAUUCC UCUCAUUGCUUUUU U	L-4 L_4_Oxalysine	Target_lig_506	B.subtilis lysine riboswitch	Target_78	4.8860566476 9316
749	CCC1CC1(C(=O)O)N	GAAGAUAGAGGUGC GAACUUCAAGAGUA UGCCUUUGGAGAAA GAUGGAUUCUGUGA AAAAGGCUGAAAGG GGAGCGUCGCCGAA GCAAAUAAAACCCC AUCGGUAUUAUUUG CUGGCCGUGCAUUG AAUAAAUGUAAGGC UGUCAAGAAAUCAU UUUCUUGGAGGGCU AUCUCGUUGUUCAU AAUCAUUUAUGAUG AUUAAUUGAUAAGC AAUGAGAGUAUUCC UCUCAUUGCUUUUU U	AEC	Target_lig_507	B.subtilis lysine riboswitch	Target_78	4.5228787452 8034
750	C(CS(=O)(=O)C[C@@H](C(=O)[O-])[NH3+])[NH3+]	GAAGAUAGAGGUGC GAACUUCAAGAGUA UGCCUUUGGAGAAA GAUGGAUUCUGUGA AAAAGGCUGAAAGG GGAGCGUCGCCGAA GCAAAUAAAACCCC	L-3-[(2-AMINOETHYL)-SULFONYL]-ALANINE	Target_lig_508	B.subtilis lysine riboswitch	Target_78	5.6020599913 2796

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		AUCGGUAUUAUUUG CUGGCCGUGCAUUG AAUAAAUGUAAGGC UGUCAAGAAAUCAU UUUCUUGGAGGGCU AUCUCGUUGUUCAU AAUCAUUUAUGAUG AUUAAUUGAUAAGC AAUGAGAGUAUUCC UCUCAUUGCUUUUU U					
751	C(/C=C/ C[NH3+])C(C(=O) [O-])[NH3+]	GAAGAUAGAGGUGC GAACUUCAAGAGUA UGCCUUUGGAGAAA GAUGGAUUCUGUGA AAAAGGCUGAAAGG GGAGCGUCGCCGAA GCAAAUAAAACCCC AUCGGUAUUAUUUG CUGGCCGUGCAUUG AAUAAAUGUAAGGC UGUCAAGAAAUCAU UUUCUUGGAGGGCU AUCUCGUUGUUCAU AAUCAUUUAUGAUG AUUAAUUGAUAAGC AAUGAGAGUAUUCC UCUCAUUGCUUUUU U	DL-TRANS-2,6-DIAMINO-4-HEXENOIC ACID	Target_lig_509	B.subtilis lysine riboswitch	Target_78	6.0132282657 3376
1157	CC(CCN1C2=CC(C)= C(C)C=C2N=C2C(=O) [N-]C(=O)N=C12)C1= CC=C(F)C=C1	GGAAGGACAAAUGA AUAAAGAUUGUAUC CUUCGGGGCAGGGU GGAAAUCCCGACCG GCGGUAGUAAAGCA CAUUUGCUUUAGAG CCCGUGACCCGUGU GCAAUAGCACGCGG UGGAUUCAGUUUAA GCUGAAGCCGACAG UGAAAGUCUGGAUG GGAGAAGGAUG	5FDQD	Target_lig_662	165 ribD FMN Riboswitch Aptamer, B. subtilis	Target_189	8.1249387366 083
1159	CNC1=NC=C(C=N1)C N2CCC[C@@H] (C2)C3=NC(=CC(=O) N3)C4=CC=CS4	GGAUCUUCGGGGCA GGGUGAAAUUCCCG ACCGGUGGUAUAGU CCACGAAAGUAUUU GCUUUGAUUUGGUG AAAUUCCAAAACCG ACAGUAGAGUCUGG AUGAGAGAAGAUUC	Ribocil-B	Target_lig_663	FMN Riboswitch Aptamer, E. Coli	Target_190	8.1804560644 5813
1160	C1C[C@@H] (CN(C1)CC2=CN(C= N2)C3=NC=CC=N3)C 4=NC(=CC(=O)N4)C5 =CC=CS5	GGAUCUUCGGGGCA GGGUGAAAUUCCCG ACCGGUGGUAUAGU CCACGAAAGUAUUU GCUUUGAUUUGGUG AAAUUCCAAAACCG ACAGUAGAGUCUGG AUGAGAGAAGAUUC	Ribocil-C	Target_lig_664	FMN Riboswitch Aptamer, E. Coli	Target_190	9
1161	C1C[C@@H] (CN(C1)CC2=CN(C= N2)C3=NC=CC=N3)C 4=NC(=CC(=O)N4)C5 =CC=CS5	UAAUUCUUUCGGGG CAGGGUGAAAUUCC CAACCGGCAGUAAA UAAAGCCUGCGACC UGCUAAUAUGUUUC AUAUUAGUGGCUGA UCUAGUGAGAUUCU AGAGCCGACAGUUA AAGUCUGGAUGGGA GAAAGAAUGUUAAU UAUCGACAAAGAUA AUGUAGCGUAUUUG UAAAAAUGUGUACA AAUAGGCUUAUUUA ACGAUAAAUUUUUC	Ribocil-C	Target_lig_664	FMN Riboswitch Aptamer SA1, S. Aureus	Target_191	7.2365720064 3706

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		UCCUUGCAUCUUAAUUCAUGAUGUGAGGAUU					
1162	C1C[C@@H](CN(C1)CC2=CN(C=N2)C3=NC=CC=N3)C4=NC(=CC(=O)N4)C5=CC=CS5	AUUCAUCUUCGGGGUCGGGUGUAAUUCCCAACCGGCAGUAAAUAAAGCCUGCGACCUGCUAGUAUGUAUCAUAUUAGUGGCUGAUCUAGUGAGAUUCUAGAGCCGACAGUAUAGUCUGGAUGGGAGAAGAUGGAGGUUUUUUGUUGUGCAAUAAUCCUCCUAUUCUUACGAGAUGAAUGGAAGGAGAAAAUU	Ribocil-C	Target_lig_664	FMN Riboswitch Aptamer SA2, S. Aureus	Target_192	7.4814860601 2211
1163	CC1=CC2=C(C=C1N(C)C)N(C3=NC(=O)NC(=O)C3=N2)CC(C(C(CO)O)O)O	GGUACCAGAAGCAGCGCACUCCGGGGUCGGUGAAAGUCCGAACCGGCGGUUACAGUCCGCGACCCGACCGCUUCCAGCGGCCGGUUGACCAGGUGAAAUUCCUGGACCGACGGUUAAAGUCCGGAUGGGAGGCAGUGCGCGCGGCGGGCGG	Roseoflavin	Target_lig_505	FMN Riboswitch, S. Davawensis	Target_193	8
1164	NC1=NC(N)=C2NC=NC2=N1	GGAAUAAUUGUAUAACCUCAAUAAUAUGGUUUGAGGGUGUCUACCAGGAACCGUAAAAUCCUGAUUACAA	2,6-Diaminopurine	Target_lig_1254	PbuE Riboswitch	Target_73	7.6020599913 2796
1165	CC1=C(C=CC=[N+]1CC2=CN=C(N=C2N)C)CCO.Br.[Br-]	GGUAACCACUAGGGGUGUCCUUCAUAAGGGCUGAGAUAAAAGUGUGACUUUUAGACCCUCAUAACUUGAACAGGUUCAGACCUGCGUAGGGAAGUGGAGC	Pyrithiamine	Target_lig_503	TPP Riboswitch, B. Subtilis	Target_194	5.2218487496 1636
1166	C1=NC2=C(N1)C(=NC(=N2)N)NO	GGACAUAUAAUCGCGUGGAUAUGGCACGCAAGUUUCUACCGGGCACCGUAAAUGUCCGACUAUGUCC	2-Amino-N6-Hydroxyadenine	Target_lig_665	xpt-pbuX Guanine Riboswitch, B. Subtilis	Target_74	7.6989700043 3602
1167	NC1=NC(=O)C(N)=C(N)N1	GGACAUAUAAUCGCGUGGAUAUGGCACGCAAGUUUCUACCGGGCACCGUAAAUGUCCGACUAUGUCC	PC1	Target_lig_1255	Guanine Riboswitch	Target_74	7
1168	C[N+]1=C2C(=C3C=CC(=C(C3=C1)OC)OC)C=CC4=CC5=C(C=C42)OCO5	GUAUAUGGUAAACUAUGAAAAAACACGAUUCGGUUGGUAGUCCGGAUGCAUGAUUGAGAAUGUCAGUAACCUUCCCCUCCUCGGGAUGUCCAUCAUUCUUUAAUAUCU	Chelerythrine	Target_lig_666	108 nt yjdF Riboswitch Construct, B. subtilis, Mutant 1	Target_195	8.6197887582 8839
1169	CC1=[N+](C2=CC=CC=C2C(=C1)N)CCCCCCCCCC[N+]3=C(C=C(C4=CC=CC=C43)N)C	GUAUAUGGUAAACUAUGAAAAAACACGAUUCGGUUGGUAGUCCGGAUGCAUGAUUGAGAAUGUCAGUAACCUUCCCCUCCUCGGGAUGUCCAUCAUUCUUUAAUAUCU	Dequalinium	Target_lig_667	108 nt yjdF Riboswitch Construct, B. subtilis, Mutant 1	Target_195	8
1170	CC1=NC=CC2=C1NC3=CC=CC=C23	GUAUAUGGUAAACUAUGAAAAAACACGA	Harmane	Target_lig_668	108 nt yjdF Riboswitch	Target_195	7

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		UUCGGUUGGUAGUC CGGAUGCAUGAUUG AGAAUGUCAGUAAC CUUCCCCUCCUCGG GAUGUCCAUCAUUC UUUAAUAUCU			Construct, B. subtilis, Mutant 1		
1171	C1=CC(=CC2=NC3=C(C=CC(=C3)N)C=C21)N	GUAUAUGGUAAACU AUGAAAAAACACGA UUCGGUUGGUAGUC CGGAUGCAUGAUUG AGAAUGUCAGUAAC CUUCCCCUCCUCGG GAUGUCCAUCAUUC UUUAAUAUCU	Proflavin	Target_lig_336	108 nt yjdF Riboswitch Construct, B. subtilis, Mutant 1	Target_195	8.2146701649 8923
1172	C[C@@]12[C@@H]([C@@H](C[C@@H](O1)N3C4=CC=CC=C4C5=C6C(=C7C8=CC=CC=C8N2C7=C53)CNC6=O)NC)OC	GUAUAUGGUAAACU AUGAAAAAACACGA UUCGGUUGGUAGUC CGGAUGCAUGAUUG AGAAUGUCAGUAAC CUUCCCCUCCUCGG GAUGUCCAUCAUUC UUUAAUAUCU	Staurosporine	Target_lig_669	108 nt yjdF Riboswitch Construct, B. subtilis, Mutant 1	Target_195	7
1279	C1CCC(CC1)NC2=NC3=C(C(=O)N2)NC=N3	GGAUCAUAUAAUCG CGUGGAUAUGGCAC GCAAGUUUCUACCG GGCACCGUAAAUGU CCGACUAUGGUC	Guanine Analog 25f	Target_lig_714	C. difficile guaA riboswitch	Target_228	5.1870866433 5714
1280	[NH3+]CCS(=O)(=O)C[C@H]([NH3+])C([O-])=O	GAAGAUAGAGGUGC GAACUUCAAGAGUA UGCCUUUGGAGAAA GAUGGAUUCUGUGA AAAAGGCUGAAAGG GGAGCGUCGCCGAA GCAAAUAAAACCCC AUCGGUAUUAUUUG CUGGCCGUGCAUUG AAUAAAUAUAAGGC UGUCAAGAAAUCAU UUUCUUGGAGGGCU AUCUCGUUGUUCAU AAUCAUUUAUGAUG AUUAAUUGAUAAGC AAUGAGAGUAUUCC UCUCAUUGCUUUUU U	Lysine Analog 8	Target_lig_1260	lysC riboswitch	Target_229	5.6020599913 2796
1282	[NH3+]CCS(=O)(=O)C[C@H]([NH3+])C([O-])=O	GAAGAUAGAGGUGC GAACUUCAAGAGUA UGCCUUUGGAGAAA GAUGGAUUCUGUGA AAAAGGCUGAAGGG GAGCGUCGCCGAAG CAAAUAAAACCCCA UCGGUAUUAUUUGC UGGCCGUGCAUUGA AUAAAUGUAAGGCU GUCAAGAAAUCAUU UUCUUGGAGGGCUA UCUCGUUGUUCAUA AUCAUUUAUGAUGA UUAAUUGAUAAGCA AUGAGAGUAUUCCU CUCAUUGCUUUUUU	Lysine Analog 8	Target_lig_1260	lysC riboswitch mutant 1 (M2)	Target_230	4.6197887582 8839
1283	[NH3+]CCOC[C@H]([NH3+])C([O-])=O	GAAGAUAGAGGUGC GAACUUCAAGAGUA UGCCUUUGGAGAAA GAUGGAUUCUGUGA AAAAGGCUGAAAGG GGAGCGUCGCCGAA GCAAAUAAAACCCC AUCGGUAUUAUUUG CUGGCCGUGCAUUG	Lysine Analog 9	Target_lig_1261	lysC riboswitch	Target_229	4.8860566476 9316

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		AAUAAAUAUAAGGC UGUCAAGAAAUCAU UUUCUUGGAGGGCU AUCUCGUUGUUCAU AAUCAUUUAUGAUG AUUAAUUGAUAAGC AAUGAGAGUAUUCC UCUCAUUGCUUUUU U					
1285	[NH3+]CCOC[C@H]([NH3+])C([O-])=O	GAAGAUAGAGGUGC GAACUUCAAGAGUA UGCCUUUGGAGAAA GAUGGAUUCUGUGA AAAAGGCUGAAGGG GAGCGUCGCCGAAG CAAAUAAAACCCCA UCGGUAUUAUUUGC UGGCCGUGCAUUGA AUAAAUGUAAGGCU GUCAAGAAAUCAUU UUCUUGGAGGGCUA UCUCGUUGUUCAUA AUCAUUUAUGAUGA UUAAUUGAUAAGCA AUGAGAGUAUUCCU CUCAUUGCUUUUUU	Lysine Analog 9	Target_lig_1261	lysC riboswitch mutant 1 (M2)	Target_230	4.1249387366083
1889	C1=NC(=C(N1C2C(C(C(O2)COP(=O)(O)O)O)O)N)C(=O)N	UAUCAGUUAUAUGA CUGACGGAACGUGG AAUUAACCACAUGA AGUAUAACGAUGAC AAUGCCGACCGUCU GGGCG	AIZA analog 1	Target_lig_1044	Fusibacterium ulcerans ZTP riboswitch	Target_352	6.4948500216 8009
1890	Ccn1c2ccc(cc2c2c1ccc2)N1CCNCC1	UAUCAGUUAUAUGA CUGACGGAACGUGG AAUUAACCACAUGA AGUAUAACGAUGAC AAUGCCGACCGUCU GGGCG	AIZA analog 2	Target_lig_1045	Fusibacterium ulcerans ZTP riboswitch	Target_352	4.3872161432 8026
1891	C1=NC(=C(N1C2C(C(C(O2)CO)O)O)N)C(=O)N	UAUCAGUUAUAUGA CUGACGGAACGUGG AAUUAACCACAUGA AGUAUAACGAUGAC AAUGCCGACCGUCU GGGCG	AIZA analog 5	Target_lig_1046	Fusibacterium ulcerans ZTP riboswitch	Target_352	5.6382721639 8241
1892	C1=CN=CC=C1N2C=NC(=C2N)C(=O)N	UAUCAGUUAUAUGA CUGACGGAACGUGG AAUUAACCACAUGA AGUAUAACGAUGAC AAUGCCGACCGUCU GGGCG	AIZA analog 7	Target_lig_1047	Fusibacterium ulcerans ZTP riboswitch	Target_352	5.8538719643 2176
1893	C1CNCCC1N2C=NC(=C2N)C(=O)N	UAUCAGUUAUAUGA CUGACGGAACGUGG AAUUAACCACAUGA AGUAUAACGAUGAC AAUGCCGACCGUCU GGGCG	AIZA analog 8	Target_lig_1048	Fusibacterium ulcerans ZTP riboswitch	Target_352	5.0604807473 8138
1894	C1=NC(=C(N1CCO)N)C(=O)N	UAUCAGUUAUAUGA CUGACGGAACGUGG AAUUAACCACAUGA AGUAUAACGAUGAC AAUGCCGACCGUCU GGGCG	AIZA analog 10	Target_lig_1049	Fusibacterium ulcerans ZTP riboswitch	Target_352	3.8239087409 4432
1895	NC(=O)c1ncn(c1N)c1ccccn1	UAUCAGUUAUAUGA CUGACGGAACGUGG AAUUAACCACAUGA AGUAUAACGAUGAC AAUGCCGACCGUCU GGGCG	AIZA analog 12	Target_lig_1050	Fusibacterium ulcerans ZTP riboswitch	Target_352	5.25181197299 38
1896	C1=CC(=CN=C1)N2C	UAUCAGUUAUAUGA	AIZA analog 13	Target_lig_105	Fusibacterium	Target_352	6.2218

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	=NC(=C2N)C(=O)N	CUGACGGAACGUGGAAUUAACCACAUGAAGUAUAACGAUGACAAUGCCGACCGUCUGGGCG		1	ulcerans ZTP riboswitch		4874961636
2044	C1(=C(N=C(N=C1N)N)N)N	GGACAUAUAAUCGCGUGGAUAUGGCACGCAAGUUUCUACCGGGCACCGUAAAUGUCCGAUUAUGUCC	2,4,5,6-tetraaminopyrimidine	Target_lig_1121	ADENINE RIBOSWITCH	Target_69	4.69897000433602
2045	C1=CN=C(N=C1N)N	GGACAUAUAAUCGCGUGGAUAUGGCACGCAAGUUUCUACCGGGCACCGUAAAUGUCCGAUUAUGUCC	2,4-diaminopyrimidine	Target_lig_1122	ADENINE RIBOSWITCH	Target_69	3
2046	Nc1nc(N)nc(n1)N	GGACAUAUAAUCGCGUGGAUAUGGCACGCAAGUUUCUACCGGGCACCGUAAAUGUCCGAUUAUGUCC	2,4,6-triamino-1,3,5-triazine	Target_lig_1123	ADENINE RIBOSWITCH	Target_69	4.69897000433602
2136	C[S+](CCC(C(=O)[O-])N)CC1C(C(C(O1)N2C=NC3=C(N=CN=C32)N)O)O	GGUACAAUCUAAAAACUUAUCAAGAGCGGCUGAGGGACUGGACCUAUGAAGCCCGGCAACCUGCAUAGUUUGUAAGGUGCUACUUCCAGCAAAAUGAAUUCCAUUUUGAAAGAUAAGGGCUGCAUGCUGUUCCUGUCUUUCUUUCCGCCGAUUGAAAGUUUUUU	S-adenosyl methionine	Target_lig_314	B.subtilis cysH	Target_405	6
2137	C1=NC(=C2C(=N1)N(C=N2)C3C(C(C(O3)CSCCC(C(=O)O)N)O)O)N	GGUACAAUCUAAAAACUUAUCAAGAGCGGCUGAGGGACUGGACCUAUGAAGCCCGGCAACCUGCAUAGUUUGUAAGGUGCUACUUCCAGCAAAAUGAAUUCCAUUUUGAAAGAUAAGGGCUGCAUGCUGUUCCUGUCUUUCUUUCCGCCGAUUGAAAGUUUUUU	SAH	Target_lig_1153	B.subtilis cysH	Target_405	3.096910013000806
2138	C1=NC(=C2C(=N1)N(C=N2)C3C(C(C(O3)CSCC(C(=O)O)N)O)O)N	GGUACAAUCUAAAAACUUAUCAAGAGCGGCUGAGGGACUGGACCUAUGAAGCCCGGCAACCUGCAUAGUUUGUAAGGUGCUACUUCCAGCAAAAUGAAUUCCAUUUUGAAAGAUAAGGGCUGCAUGCUGUUCCUGUCUUUCUUUCCGCCGAUUGAAAGUUUUUU	SAC	Target_lig_1154	B.subtilis cysH	Target_405	3
2139	C[S+](CCC(C(=O)[O-])N)CC1C(C(C(O1)N2C=NC3=C(N=CN=C32)N)O)O	GGAGCUUAUCAAGAGAAGCGGAGGGAACUGGCCCGGCGAAGCUCGGCAACCUGCUUAUAGAAAGCAAGGUGCUAAAUCCAGCAAAAUGGAUUCCAUUUUGAAAGAUAAGGUAAAAUAUAUUACCGAACAGUCUUUUCGAAAUGGGAAAGAUUUUUUUUAU	S-adenosyl methionine	Target_lig_314	B.anthracis cysH	Target_406	8
2140	C1=NC(=C2C(=N1)N(C=N2)C3C(C(C(O3)C	GGAGCUUAUCAAGAGAAGCGGAGGGAAC	SAH	Target_lig_1153	B.anthracis cysH	Target_406	5.5228787452

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	SCCC(C(=O)O)N)O)O)N	UGGCCCGGCGAAGCUCGGCAACCUGCUUAUAGAAAGCAAGGUGCUAAAUCCAGCAAAAUGGAUUCCAUUUUGAAAGAUAAGGUAAAAUAUAUUACCGAACAGUCUUUUCGAAAUGGGAAAGAUUUUUUUUUAU					8034
2141	C1=NC(=C2C(=N1)N(C=N2)C3C(C(C(O3)CSCC(C(=O)O)N)O)O)N	GGAGCUUAUCAAGAGAAGCGGAGGGAACUGGCCCGGCGAAGCUCGGCAACCUGCUUAUAGAAAGCAAGGUGCUAAAUCCAGCAAAAUGGAUUCCAUUUUGAAAGAUAAGGUAAAAUAUAUUACCGAACAGUCUUUUCGAAAUGGGAAAGAUUUUUUUUUAU	SAC	Target_lig_1154	B.anthracis cysH	Target_406	3
2259	CC1(C2CC3C(C(=O)C(=C(C3(C(=O)C2=C(C4=C1C=CC=C4O)O)O)O)C(=O)N)N(C)C)O	GGGCCUAGAACAUACCAGAUCGCCACCCGCGCUUUAAUCUGGAGAGGUGAAGAAUACGACCACCUAGGCUC	tetracyclin	Target_lig_74	Tetracycline riboswitch A08G mutant	Target_412	8.9788107009 3006
2260	CC1(C2CC3C(C(=O)C(=C(C3(C(=O)C2=C(C4=C1C=CC=C4O)O)O)O)C(=O)N)N(C)C)O	GGGCCUAAGACAUACCAGAUCGCCACCCGCGCUUUAAUCUGGAGAGGUGAAGAAUACGACCACCUAGGCUC	tetracyclin	Target_lig_74	Tetracycline riboswitch A09G mutant	Target_413	6.7904849854 5737
2261	CC1(C2CC3C(C(=O)C(=C(C3(C(=O)C2=C(C4=C1C=CC=C4O)O)O)O)C(=O)N)N(C)C)O	GGGCCUAAAACAUUCCAGAUCGCCACCCGCGCUUUAAUCUGGAGAGGUGAAGAAUACGACCACCUAGGCUC	tetracyclin	Target_lig_74	Tetracycline riboswitch A13U mutant	Target_414	6.6536470255 4936
2262	CC1(C2CC3C(C(=O)C(=C(C3(C(=O)C2=C(C4=C1C=CC=C4O)O)O)O)C(=O)N)N(C)C)O	GGGCCUAAAACAUACCAGAUCGCCACCCGCGCUUUAAUCUGGAGAGGUGAUGAAUACGACCACCUAGGCUC	tetracyclin	Target_lig_74	Tetracycline riboswitch A50U mutant	Target_415	6.7077439286 4352
2263	CC1(C2CC3C(C(=O)C(=C(C3(C(=O)C2=C(C4=C1C=CC=C4O)O)O)O)C(=O)N)N(C)C)O	GGGCCUAAAACAUACCAGAUCGCCACCCGCGCUUUAAUCUGGAGAGGUGAAUAAUACGACCACCUAGGCUC	tetracyclin	Target_lig_74	Tetracycline riboswitch G51U mutant	Target_416	8.5331323796 4589
2264	CC1(C2CC3C(C(=O)C(=C(C3(C(=O)C2=C(C4=C1C=CC=C4O)O)O)O)C(=O)N)N(C)C)O	GGGCCUAAAACAUACCAGAUCGCCACCCGCGCUUUAAUCUGGAGAGGUGAAGAAGACGACCACCUAGGCUC	tetracyclin	Target_lig_74	Tetracycline riboswitch U54G mutant	Target_417	8.5800442515 1024
2265	CC1(C2CC3C(C(=O)C(=C(C3(C(=O)C2=C(C4=C1C=CC=C4O)O)O)O)C(=O)N)N(C)C)O	GGGCCUAAAACAUACCAGAUCGCCACCCGCGCUUUAAUCUGGAGAGGUGAAGAAUGCGACCACCUAGGCUC	tetracyclin	Target_lig_74	Tetracycline riboswitch A55G mutant	Target_418	8.77211329538 633
2266	CN(C1C(=O)C(=C(C2(C1CC1C(=C(O)c3c(C1(C)O)c(Cl)ccc3O)C2=O)O)O)C(=O)N)C	GGGCCUAAAACAUACCAGAUCGCCACCCGCGCUUUAAUCUGGAGAGGUGAAGAAUACGACCACCUAGGCU	cltc	Target_lig_1164	Tetracycline riboswitch	Target_411	9.2418453780 3261

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		C					
2267	NC(=O)C1=C(O)C2(C(CC1=O)CC1C(=C(O)c3c(C1(C)O)cccc3O)C2=O)O	GGGCCUAAAACAUACCAGAUCGCCACCCGCGCUUUAAUCUGGAGAGGUGAAGAAUACGACCACCUAGGCUC	cmt1	Target_lig_1165	Tetracycline riboswitch	Target_411	8.70553377383841
2268	NC(=O)C1=C(O)C2(C(C(C1=O)O)CC1C(=C(O)c3c(C1(C)O)cccc3O)C2=O)O	GGGCCUAAAACAUACCAGAUCGCCACCCGCGCUUUAAUCUGGAGAGGUGAAGAAUACGACCACCUAGGCUC	cmt6	Target_lig_1166	Tetracycline riboswitch	Target_411	8.55752023093555
2269	NNC1=C2C(=O)C3(O)C(CC2C(c2c1c(O)ccc2)(C)O)CC(=O)C(=C3O)C(=O)N	GGGCCUAAAACAUACCAGAUCGCCACCCGCGCUUUAAUCUGGAGAGGUGAAGAAUACGACCACCUAGGCUC	cmt5	Target_lig_1167	Tetracycline riboswitch	Target_411	9.00436480540245
2270	N#CC1=C(O)C2(C(C(C1=O)N(C)C)CC1C(=C(O)c3c(C1(C)O)cccc3O)C2=O)O	GGGCCUAAAACAUACCAGAUCGCCACCCGCGCUUUAAUCUGGAGAGGUGAAGAAUACGACCACCUAGGCUC	cmt2	Target_lig_1168	Tetracycline riboswitch	Target_411	8.00877392430751
2271	CN(C1C(=O)C(=C(C2(C1C(O)C1C(=C(O)c3c(C1(C)O)cccc3O)C2=O)O)O)C(=O)N)C	GGGCCUAAAACAUACCAGAUCGCCACCCGCGCUUUAAUCUGGAGAGGUGAAGAAUACGACCACCUAGGCUC	otc	Target_lig_1169	Tetracycline riboswitch	Target_411	8.74957999769111
2272	C[C@H]1[C@H]([C@H](C[C@@H](O1)O[C@H]2C[C@@](CC3=C2C(=C4C(=C3O)C(=O)C5=C(C4=O)C(=CC=C5)OC)O)(C(=O)CO)O)N)O	GGGCCUAAAACAUACCAGAUCGCCACCCGCGCUUUAAUCUGGAGAGGUGAAGAAUACGACCACCUAGGCUC	dox	Target_lig_496	Tetracycline riboswitch	Target_411	6.92811799269388
2273	NC(=O)C1=C(O)C2(C(CC1=O)C(O)C1C(=C(O)c3c(C1C)cccc3O)C2=O)O	GGGCCUAAAACAUACCAGAUCGCCACCCGCGCUUUAAUCUGGAGAGGUGAAGAAUACGACCACCUAGGCUC	cmt8	Target_lig_1171	Tetracycline riboswitch	Target_411	6.26201267366657
2274	C[N+]1=C2C(=C3C=CC4=C(C3=C1)OCO4)C=CC5=CC6=C(C=C52)OCO6	GGGCCUAAAACAUACCAGAUCGCCACCCGCGCUUUAAUCUGGAGAGGUGAAGAAUACGACCACCUAGGCUC	san	Target_lig_18	Tetracycline riboswitch	Target_411	7.65364702554936
2275	CN(C1C(=O)C(=C(C2(C1CC1C(C)c3cccc(c3C(=C1C2=O)O)O)O)O)O)C(=O)N)C	GGGCCUAAAACAUACCAGAUCGCCACCCGCGCUUUAAUCUGGAGAGGUGAAGAAUACGACCACCUAGGCUC	atc	Target_lig_1173	Tetracycline riboswitch	Target_411	8.45593195564972
2276	CN(C1C(=O)C(=C(C2(C1C(O)C1C(=C(O)c3c(C1(C)O)cccc3O)C2=O)O)O)C(=O)N)C	GGGCCUAAGACAUACCAGAUCGCCACCCGCGCUUUAAUCUGGAGAGGUGAAGAAUACGACCACCUAGGCUC	otc	Target_lig_1169	Tetracycline riboswitch A09G mutant	Target_413	6.35163998901907
2277	N#CC1=C(O)C2(C(C(C1=O)N(C)C)CC1C(=C(O)c3c(C1(C)O)cccc3O)C2=O)O	GGGCCUAAGACAUACCAGAUCGCCACCCGCGCUUUAAUCUGGAGAGGUGAAGAAUACGACCACCUAGGCU	cmt2	Target_lig_1168	Tetracycline riboswitch A09G mutant	Target_413	5.57839607313017

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		C					
2278	C[C@H]1[C@H]([C@H](C[C@@H](O1)O[C@H]2C[C@@](CC3=C2C(=C4C(=C3O)C(=O)C5=C(C4=O)C(=CC=C5)OC)O)(C(=O)CO)O)N)O	GGGCCUAAGACAUACCAGAUCGCCACCCGCGCUUUAAUCUGGAGAGGUGAAGAAUACGACCACCUAGGCUC	dox	Target_lig_496	Tetracycline riboswitch A09G mutant	Target_413	4.7520267336 3819
2279	CN(C1C(=O)C(=C(C2(C1C(O)C1C(=C(O)c3c(C1(C)O)cccc3O)C2=O)O)O)C(=O)N)C	GGGCCUAAAACAUUCCAGAUCGCCACCCGCGCUUUAAUCUGGAGAGGUGAAGAAUACGACCACCUAGGCUC	otc	Target_lig_1169	Tetracycline riboswitch A13U mutant	Target_414	6.2740883677 0495
2280	N#CC1=C(O)C2(C(C(C1=O)N(C)C)CC1C(=C(O)c3c(C1(C)O)cccc3O)C2=O)O	GGGCCUAAAACAUUCCAGAUCGCCACCCGCGCUUUAAUCUGGAGAGGUGAAGAAUACGACCACCUAGGCUC	cmt2	Target_lig_1168	Tetracycline riboswitch A13U mutant	Target_414	5.7695510786 2173
2281	C[C@H]1[C@H]([C@H](C[C@@H](O1)O[C@H]2C[C@@](CC3=C2C(=C4C(=C3O)C(=O)C5=C(C4=O)C(=CC=C5)OC)O)(C(=O)CO)O)N)O	GGGCCUAAAACAUUCCAGAUCGCCACCCGCGCUUUAAUCUGGAGAGGUGAAGAAUACGACCACCUAGGCUC	dox	Target_lig_496	Tetracycline riboswitch A13U mutant	Target_414	5.6161846340 1957
2282	CN(C1C(=O)C(=C(C2(C1C(O)C1C(=C(O)c3c(C1(C)O)cccc3O)C2=O)O)O)C(=O)N)C	GGGCCUAAAACAUACCAGAUCGCCACCCGCGCUUUAAUCUGGAGAGGUGAUGAAUACGACCACCUAGGCUC	otc	Target_lig_1169	Tetracycline riboswitch A50U mutant	Target_415	6.2218487496 1636
2283	N#CC1=C(O)C2(C(C(C1=O)N(C)C)CC1C(=C(O)c3c(C1(C)O)cccc3O)C2=O)O	GGGCCUAAAACAUACCAGAUCGCCACCCGCGCUUUAAUCUGGAGAGGUGAUGAAUACGACCACCUAGGCUC	cmt2	Target_lig_1168	Tetracycline riboswitch A50U mutant	Target_415	5.5900668766 6871
2284	C[C@H]1[C@H]([C@H](C[C@@H](O1)O[C@H]2C[C@@](CC3=C2C(=C4C(=C3O)C(=O)C5=C(C4=O)C(=CC=C5)OC)O)(C(=O)CO)O)N)O	GGGCCUAAAACAUACCAGAUCGCCACCCGCGCUUUAAUCUGGAGAGGUGAUGAAUACGACCACCUAGGCUC	dox	Target_lig_496	Tetracycline riboswitch A50U mutant	Target_415	4.9788107009 3006
2320	CNC1=NC=C(C=N1)CN2CCC[C@@H](C2)C3=NC(=CC(=O)N3)C4=CC=CS4	GGCGUGUAGGAUAUGCUUCGGCAGAAGGACACGCC	Ribocil	Target_lig_663	FMN RIBOSWITCH APTAMER	Target_36	7.7958800173 4408
2321	CNc1ncc(cn1)CN1CCC[C@H](C1)c1nc(O)cc(n1)c1ccccs1	GGCGUGUAGGAUAUGCUUCGGCAGAAGGACACGCC	Ribocil-A	Target_lig_1187	FMN RIBOSWITCH APTAMER	Target_36	5
2322	CNC1=NC=C(C=N1)CN2CCC[C@@H](C2)C3=NC(=CC(=O)N3)C4=CC=CS4	GGCGUGUAGGAUAUGCUUCGGCAGAAGGACACGCC	Ribocil-B	Target_lig_663	FMN RIBOSWITCH APTAMER	Target_36	8.1804560644 5813
2323	C1C[C@@H](CN(C1)CC2=CN(C=N2)C3=NC=CC=N3)C4=NC(=CC(=O)N4)C5=CC=CS5	GGCGUGUAGGAUAUGCUUCGGCAGAAGGACACGCC	Ribocil-C	Target_lig_664	FMN RIBOSWITCH APTAMER	Target_36	9