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

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
100	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	GAGCGUCACACCUUCGGGUGAAGUCGCUC	tetracyclin	Target_lig_74	A-site 16S rRNA_E_coli (1)	Target_3	5.45593195564972
101	CC1CC(=O)C2(C(O1)OC3C(C(C(C3O2)NC)O)NC)O)O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Spectinomycin	Target_lig_75	A-site 16S rRNA_E_coli (1)	Target_3	6.58502665202918
103	CC1(COC(C(C1NC)O)OC2C(CC(C(C2O)OC3C(CCC(O3)CN)N)N)N)O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	gentamicin_mol_c1a	Target_lig_76	A-site 16S rRNA_E_coli (1)	Target_3	5.76955107862173
104	C1C(C(C(C(C1N)OC2C(C(C(C(O2)CN)O)O)O)O)OC3C(C(C(C(O3)CO)O)N)O)N	GAGCGUCACACCUUCGGGUGAAGUCGCUC	kanamycin	Target_lig_7	A-site 16S rRNA_E_coli (1)	Target_3	6.90308998699194
107	CC1C(CC(C(O1)OC2C(C(C(C(C2O)O)O)O)O)N)N=C(C(=O)O)N	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Kasugamycin	Target_lig_78	A-site 16S rRNA_E_coli (1)	Target_3	4.82390874094432
108	CNC1C(C2C(CC(C(O2)OC3C(CC(C(C3O)O)N)N)N)OC1OC4C(C(C(C(O4)CO)N)O)O)O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	apramycin	Target_lig_79	A-site 16S rRNA_E_coli (1)	Target_3	7.09691001300806
109	C1C(C(C(C(C1N)OC2C(C(C(C(O2)CN)O)O)N)O)O)N	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Neamine	Target_lig_80	A-site 16S rRNA_E_coli (1)	Target_3	6.30102999566398
110	C1=CC=C2C(=C1)NC(=N2)N	GAGCGUCACACCUUCGGGUGAAGUCGCUC	1H-1,3-benzodiazol-2-amine	Target_lig_81	A-site 16S rRNA_E_coli (1)	Target_3	3.63827216398241
111	CC1=CC2=C(C=C1C)N=CN2	GAGCGUCACACCUUCGGGUGAAGUCGCUC	5,6-dimethyl-1H-1,3-benzodiazole	Target_lig_82	A-site 16S rRNA_E_coli (1)	Target_3	3.09151498112135
112	CC1=CC(=C2C(=C1)NC(=N2)N)C	GAGCGUCACACCUUCGGGUGAAGUCGCUC	4,6-dimethyl-1H-1,3-benzodiazol-2-amine	Target_lig_83	A-site 16S rRNA_E_coli (1)	Target_3	3.58502665202918
113	CC1=CC(=NC2=CC=CC=C12)N	GAGCGUCACACCUUCGGGUGAAGUCGCUC	4-methylquinolin-2-amine	Target_lig_84	A-site 16S rRNA_E_coli (1)	Target_3	4.04575749056068
114	CC1=CC2=C(C=C1C)N=C(N2)N	GAGCGUCACACCUUCGGGUGAAGUCGCUC	5,6-dimethyl-1H-1,3-benzodiazol-2-amine	Target_lig_85	A-site 16S rRNA_E_coli (1)	Target_3	3.65757731917779
115	CC1=C(C2=C(C=C1)NC(=N2)N)C	GAGCGUCACACCUUCGGGUGAAGUCGCUC	6,7-dimethyl-1H-1,3-benzodiazol-2-amine	Target_lig_86	A-site 16S rRNA_E_coli (1)	Target_3	3.79588001734407
116	CC1=CC(=NC2=C1C=CC(=C2)NC(=O)CC3=CC=NC=C3)N(C)C	GAGCGUCACACCUUCGGGUGAAGUCGCUC	dimethylamino_methylquinolinyl_pyridinyl_acetamide	Target_lig_87	A-site 16S rRNA_E_coli (1)	Target_3	4.74472749489669
117	CN(C)C1=NC2=CC=CC=C2C(=C1)NC(=O)CC3=CC=C(C=C3)O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	dimethylamino_quinolinyl_pyridinyl_acetamide	Target_lig_88	A-site 16S rRNA_E_coli (1)	Target_3	5.04575749056068
118	CC1=CC2=C(C=C1)C(=CC(=N2)N)C	GAGCGUCACACCUUCGGGUGAAGUCGCUC	N,4-dimethylquinolin-2-amine	Target_lig_89	A-site 16S rRNA_E_coli (1)	Target_3	4.22184874961636
119	CC1=C(C2=C(C=C1)C(=CC(=N2)N)C)C	GAGCGUCACACCUUCGGGUGAAGUCGCUC	N,N,4-trimethylquinolin-2-amine	Target_lig_90	A-site 16S rRNA_E_coli (1)	Target_3	3.76955107862173
120	CN(C)C1=NC2=CC=CC=C2C=C1	GAGCGUCACACCUUCGGGUGAAGUCGCUC	N,N-dimethylquinolin-2-amine	Target_lig_91	A-site 16S rRNA_E_coli (1)	Target_3	3.00436480540245
121	CC1=C(N=CC=C1)NCCN	GAGCGUCACACCUUCGGGUGAAGUCGCU	methylpyridine_der_1	Target_lig_92	A-site 16S rRNA_E_coli	Target_3	3.22184874961636

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		C			(1)		
122	CC1=CC(=NC=C1)NCCN	GAGCGUCACACCUUCGGGUGAAGUCGCUC	methylpyridine_der_2	Target_lig_93	A-site 16S rRNA_E_coli (1)	Target_3	5.52287874528034
123	CC1=CC(=NC=C1)NCCCN	GAGCGUCACACCUUCGGGUGAAGUCGCUC	methylpyridine_der_3	Target_lig_94	A-site 16S rRNA_E_coli (1)	Target_3	4.69897000433602
124	CC1=CN=C(C=C1)NCCN	GAGCGUCACACCUUCGGGUGAAGUCGCUC	methylpyridine_der_4	Target_lig_95	A-site 16S rRNA_E_coli (1)	Target_3	4.65757731917779
125	C1=CC(=NC=C1[N+](=O)[O-])NCCN	GAGCGUCACACCUUCGGGUGAAGUCGCUC	methylpyridine_der_5	Target_lig_96	A-site 16S rRNA_E_coli (1)	Target_3	2
126	CC1=NC(=CC=C1)NCCN	GAGCGUCACACCUUCGGGUGAAGUCGCUC	methylpyridine_der_6	Target_lig_97	A-site 16S rRNA_E_coli (1)	Target_3	3.97881070093006
127	C1=CC=NC(=C1)NCCN	GAGCGUCACACCUUCGGGUGAAGUCGCUC	methylpyridine_der_7	Target_lig_98	A-site 16S rRNA_E_coli (1)	Target_3	4.16749108729376
128	CC1=CC(=NC2=C1C=CC(=C2)N)N(C)C	GAGCGUCACACCUUCGGGUGAAGUCGCUC	2-N,2-N,4-trimethylquinoline-2,7-diamine	Target_lig_99	A-site 16S rRNA_E_coli (1)	Target_3	4.45593195564972
129	CN(C)C1=NC2=CC=CC=C2C(=C1)N	GAGCGUCACACCUUCGGGUGAAGUCGCUC	2-N,2-N-dimethylquinoline-2,4-diamine	Target_lig_100	A-site 16S rRNA_E_coli (1)	Target_3	4.22184874961636
130	CNC1=NC2=CC=CC=C2C=C1	GAGCGUCACACCUUCGGGUGAAGUCGCUC	N-methylquinolin-2-amine	Target_lig_101	A-site 16S rRNA_E_coli (1)	Target_3	3.30980391997149
132	C1CCN(CC1)CN2CCN(C2=S)CN3CCCCC3	GAGCGUCACACCUUCGGGUGAAGUCGCUC	1,3-bis(piperidin-1-ylmethyl)imidazolidine-2-thione	Target_lig_103	A-site 16S rRNA_E_coli (1)	Target_3	3.96257350205938
133	C1CN(CCN1CC2=CNC3=CC=CC=C32)CC4=CNC5=CC=CC=C54	GAGCGUCACACCUUCGGGUGAAGUCGCUC	1,4-bis((1H-indol-3-yl)methyl)piperazine	Target_lig_104	A-site 16S rRNA_E_coli (1)	Target_3	3.66554624884907
134	CC1(CC(CC(N1)(C)C)NCC2=CC=CC=C2O)C	GAGCGUCACACCUUCGGGUGAAGUCGCUC	2-((2,2,6,6-tetramethylpiperidin-4-ylamino)methyl)phenol	Target_lig_105	A-site 16S rRNA_E_coli (1)	Target_3	3.68613277963085
135	OCC1=C=C=C(c2nc(C3=C=NC4=C(C=C=C=C4)C3)c(C3=C=C=C=C=C3)[nH]2)C=C1O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	2-(hydroxymethyl)-5-(5-phenyl-4-(quinolin-3-yl)-1H-imidazol-2-yl)phenol	Target_lig_106	A-site 16S rRNA_E_coli (1)	Target_3	3.95467702121334
136	CC1=CC=CC=C1OCCNC2=C(C=CC(=C2)N3CCNCC3)[N+](=O)[O-]	GAGCGUCACACCUUCGGGUGAAGUCGCUC	2-nitro-5-(piperazin-1-yl)-N-(2-(o-tolyloxy)ethyl)aniline	Target_lig_107	A-site 16S rRNA_E_coli (1)	Target_3	3.6903698325741
137	CCC1=CC2=C(C(=C1O)CN3CCOCC3)OC=C(C2=O)C4=NC5=CC=CC=C5N4	GAGCGUCACACCUUCGGGUGAAGUCGCUC	3-(1H-benzo[d]imidazol-2-yl)-6-ethyl-7-hydroxy-8-(morpholinomethyl)-4H-chromen-4-one	Target_lig_108	A-site 16S rRNA_E_coli (1)	Target_3	3.60032627851896
138	CN1CCN(CC1)CCCN2C=NC3=C(C2=O)NC4=CC=CC=C43	GAGCGUCACACCUUCGGGUGAAGUCGCUC	3-(3-(4-methylpiperazin-1-yl)propyl)-3H-pyrimido[5,4-b]indol-4(5H)-one	Target_lig_109	A-site 16S rRNA_E_coli (1)	Target_3	3.37059040089728

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
139	CC1=C(C(=O)C2=CC=CC=C2N1)CN3CCCCCC3	GAGCGUCACACCUUCGGGUGAAGUCGCUC	3-(azepan-1-ylmethyl)-2-methylquinolin-4-ol	Target_lig_110	A-site 16S rRNA_E_coli (1)	Target_3	3.39685562737982
140	CN1C2=C(C(=O)NC1=O)N(C=N2)CCN3CCCCC3	GAGCGUCACACCUUCGGGUGAAGUCGCUC	3-methyl-7-(2-(piperidin-1-yl)ethyl)-1H-purine-2,6(3H,7H)-dione	Target_lig_111	A-site 16S rRNA_E_coli (1)	Target_3	3.67366413907125
141	C1CCCN(CC1)CC2=C(N(N=N2)C3=NON=C3N)CN4CCCCCC4	GAGCGUCACACCUUCGGGUGAAGUCGCUC	4-(4,5-bis(azepan-1-ylmethyl)-1H-1,2,3-triazol-1-yl)-1,2,5-oxadiazol-3-amine	Target_lig_112	A-site 16S rRNA_E_coli (1)	Target_3	3.53610701101409
142	C1CCN(C1)CCNC2=NN=C(C3=CC=CC=C32)C4=CC=C(C=C4)Cl	GAGCGUCACACCUUCGGGUGAAGUCGCUC	4-(4-chlorophenyl)-N-(2-(pyrrolidin-1-yl)ethyl)phthalazin-1-amine	Target_lig_113	A-site 16S rRNA_E_coli (1)	Target_3	3.83564714421556
143	CC1=CC=C(C=C1)C2=C(C(=CC(=N2)CN3CCCCC3)CN4CCCCC4)O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	4,6-bis(piperidin-1-ylmethyl)-2-p-tolylpyridin-3-ol	Target_lig_114	A-site 16S rRNA_E_coli (1)	Target_3	3.84466396253494
144	C1CCN(CC1)CCCNC(=O)C2=C(C3=CC=CC=C3NC2=O)O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	4-hydroxy-2-oxo-N-(3-(piperidin-1-yl)propyl)-1,2-dihydroquinoline-3-carboxamide	Target_lig_115	A-site 16S rRNA_E_coli (1)	Target_3	3.61618463401957
145	CC1=CC2=C(C=C1)OC=C(C2=O)CN3CCCN(CC3)C	GAGCGUCACACCUUCGGGUGAAGUCGCUC	6-methyl-3-((4-methyl-1,4-diazepan-1-yl)methyl)-4H-chromen-4-one	Target_lig_116	A-site 16S rRNA_E_coli (1)	Target_3	3.73518217699046
146	N1(CCCCCCC1)CCN1C=NC=2N(C(NC(C12)=O)=O)C	GAGCGUCACACCUUCGGGUGAAGUCGCUC	7-(2-(azocan-1-yl)ethyl)-3-methyl-1H-purine-2,6(3H,7H)-dione	Target_lig_117	A-site 16S rRNA_E_coli (1)	Target_3	3.54821356447571
147	C(C1=CC=CC=C1)N1C(=NC=2N(C(NC(C12)=O)=O)C)N1CCNCC1	GAGCGUCACACCUUCGGGUGAAGUCGCUC	7-benzyl-3-methyl-8-(piperazin-1-yl)-1H-purine-2,6(3H,7H)-dione	Target_lig_1111	A-site 16S rRNA_E_coli (1)	Target_3	3.60906489289662
148	C1CN(CCN1)CCN2C=NC3=C(C2=O)NC4=C3C=C(C=C4)Br	GAGCGUCACACCUUCGGGUGAAGUCGCUC	8-bromo-3-(2-(piperazin-1-yl)ethyl)-3H-pyrimido[5,4-b]indol-4(5H)-one	Target_lig_118	A-site 16S rRNA_E_coli (1)	Target_3	3.57839607313017
149	CC1=CC2=C(C=C1)NC3=C2N=CN(C3=O)CCN4CCCC4	GAGCGUCACACCUUCGGGUGAAGUCGCUC	8-methyl-3-(2-(pyrrolidin-1-yl)ethyl)-3H-pyrimido[5,4-b]indol-4(5H)-one	Target_lig_119	A-site 16S rRNA_E_coli (1)	Target_3	3.4672456210075
150	N=C(N)CCCOC1=C=C=C=C=C1C1=C=C=C=C=C1	GAGCGUCACACCUUCGGGUGAAGUCGCUC	biphenyl_derivative	Target_lig_120	A-site 16S rRNA_E_coli (1)	Target_3	4.27572413039921
151	C1CN(CCC1C(=O)NCCN2CCOCC2)CC3=CC=CC4=CC=CC=C43	GAGCGUCACACCUUCGGGUGAAGUCGCUC	N-(2-morpholinoethyl)-1-(naphthalen-1-ylmethyl)piperidi	Target_lig_121	A-site 16S rRNA_E_coli (1)	Target_3	3.63264407897398

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
			ne-4-carboxamide				
152	CCN1CCN(CC1)CCC(=O)NC2=CC(=C(C=C2)Br)C	GAGCGUCACACCUUCGGGUGAAGUCGCUC	N-(4-bromo-3-methylphenyl)-3-(4-ethylpiperazin-1-yl)propanamide	Target_lig_122	A-site 16S rRNA_E_coli (1)	Target_3	3.3777859770337
153	COC=1C=C(C2=CC(=CC=C2C1)OC)NCCCC(C)N	GAGCGUCACACCUUCGGGUGAAGUCGCUC	N1-(3,7-dimethoxynaphthalen-1-yl)pentane-1,4-diamine	Target_lig_123	A-site 16S rRNA_E_coli (1)	Target_3	3.68613277963085
154	N=C(N)SCc1nc2C=C=C=Cc2n1CCC1=C=C=C=C=C1	GAGCGUCACACCUUCGGGUGAAGUCGCUC	benzodiazolyl_methyl_sulfanylmethanimidamide	Target_lig_124	A-site 16S rRNA_E_coli (1)	Target_3	3.75696195131371
155	COC1=CC=CC=C1C2=COC3=C(C2=O)C=CC(=C3CN4CCCCC4)O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	7-hydroxy-3-(2-methoxyphenyl)-8-(piperidin-1-ylmethyl)-4H-chromen-4-one	Target_lig_125	A-site 16S rRNA_E_coli (1)	Target_3	3.40340290437354
156	CC(=O)C1=CCC2C1(CC=C3C2CCC4=CC(=O)C=CC43C)C	GAGCGUCACACCUUCGGGUGAAGUCGCUC	tetraene_mol	Target_lig_126	A-site 16S rRNA_E_coli (1)	Target_3	4.45593195564972
157	O=C1NC(=O)N(C2=C=C=C(Br)C=C2)C(=O)/C/1=C/NCCN1CCNCC1	GAGCGUCACACCUUCGGGUGAAGUCGCUC	5E1bromophenyl52piperazin1	Target_lig_127	A-site 16S rRNA_E_coli (1)	Target_3	3.86327943284359
158	CN1CCCN(CC1)CC2=COC3=C(C2=O)C=C(C=C3)Cl	GAGCGUCACACCUUCGGGUGAAGUCGCUC	6-chloro-3-((4-methyl-1,4-diazepan-1-yl)methyl)-4H-chromen-4-one	Target_lig_128	A-site 16S rRNA_E_coli (1)	Target_3	3.80687540164554
159	O=C(NCCN1CCCCC1)c1c(O)c2C=C=C=Cc2[nH]c1=O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	dihydroquinoline-3-carboxamide_derivative	Target_lig_129	A-site 16S rRNA_E_coli (1)	Target_3	3.65364702554936
160	C1CCN(CC1)CCCNCC2C3=CC=CC=C3CCO2	GAGCGUCACACCUUCGGGUGAAGUCGCUC	N-(isochroman-1-ylmethyl)-3-(piperidin-1-yl)propan-1-amine	Target_lig_130	A-site 16S rRNA_E_coli (1)	Target_3	4.74472749489669
161	CC1=CC=C(C=C1)C(=O)N2CCN(CC2)CCNC(=O)C(=O)NC(C)C	GAGCGUCACACCUUCGGGUGAAGUCGCUC	N1-isopropyl-N2-(2-(4-(4-methylbenzoyl)piperazin-1-yl)ethyl)oxalamide	Target_lig_131	A-site 16S rRNA_E_coli (1)	Target_3	3.51144928349956
162	C1CN(CCC1C(=O)NCCN2CCOCC2)CC3=CC=C(C=C3)Cl	GAGCGUCACACCUUCGGGUGAAGUCGCUC	1-(4-chlorobenzyl)-N-(2-morpholinoethyl)piperidine-4-carboxamide	Target_lig_132	A-site 16S rRNA_E_coli (1)	Target_3	3.60205999132796
163	CN1CCCN(CC1)CC2=C(C=C(C=C2)OC)OC	GAGCGUCACACCUUCGGGUGAAGUCGCUC	1-(2,4-dimethoxybenzyl)-4-methyl-1,4-diazepane	Target_lig_133	A-site 16S rRNA_E_coli (1)	Target_3	4.50863830616573
164	Cn1c2nc(N/N=C\3/C4=C(C=C=C=C4)NC3=O)n(CC3=C=C=C(Cl)C=C3)c2c(=O)[nH]c1=O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	DIONE_DERIVATIVE	Target_lig_134	A-site 16S rRNA_E_coli (1)	Target_3	4.30102999566398
165	OC1C(C(NC=2CCCCC12)=O)C(=O)NCCCN1CCCCC1	GAGCGUCACACCUUCGGGUGAAGUCGCUC	4-hydroxy-2-oxo-N-(3-(piperidin-1-yl)propyl)-	Target_lig_135	A-site 16S rRNA_E_coli (1)	Target_3	4.76955107862173

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
			1,2,3,4,5,6,7,8-octahydroquinoline-3-carboxamide				
166	NC[C@H]1O[C@H](O[C@H]2[C@H](CO)O[C@H](O[C@H]3[C@H]([C@H](N)C[C@H]([C@H]3O[C@H]3O[C@H](CO)[C@@H](O)[C@H](O)[C@@H]3N)N)O)[C@H]2O)[C@@H](N)[C@H](O)[C@@H]1O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	pyran-3,4-diol_derivative	Target_lig_136	A-site 16S rRNA_E_coli (1)	Target_3	4.9100948885606
167	C1C(C(C(C(C1N)OC2C(C(C(C(O2)CN)O)O)N)OC3C(C(C(O3)CO)OC4C(C(C(C(O4)CN)O)O)N)O)O)N	GCACCGGCUAACUCCGUGCCAGCAGCGCGGUAAUACGGAGGGUGC	Neomycin	Target_lig_4	16S rRNA_neomycin	Target_96	7.22184874961636
196	C1C(C(C(C(C1N)OC2C(C(C(C(O2)CO)O)O)N)OC3C(C(C(O3)CO)OC4C(C(C(C(O4)CN)O)O)N)O)O)N	AAAUUGAAGAGUUUGAUCAUGGCUCAGAUUGAACGCUGGCGGCAGGCCUAACACAUGCAAGUCGAACGGUAACAGGAAGAAGCUUGCUUCUUUGCUGACGAGUGGCGGACGGGUGAGUAAUGUCUGGGAAACUGCCUGAUGGAGGGGGAUAACUACUGGAAACGGUAGCUAAUACCGCAUAACGUCGCAAGACCAAAGAGGGGGACCUUCGGGCCUCUUGCCAUCGGAUGUGCCCAGAUGGGAUUAGCUAGUAGGUGGGGUAACGGCUCACCUAGGCGACGAUCCCUAGCUGGUCUGAGAGGAUGACCAGCCACACUGGAACUGAGACACGGUCCAGACUCCUACGGGAGGCAGCAGUGGGGAAUAUUGCACAAUGGGCGCAAGCCUGAUGCAGCCAUGCCGCGUGUAUGAAGAAGGCCUUCGGGUUGUAAAGUACUUUCAGCGGGGAGGAAGGGAGUAAAGUUAAUACCUUUGCUCAUUGACGUUACCCGCAGAAGAAGCACCGGCUAACUCCGUGCCAGCAGCCGCGGUAAUACGGAGGGUGCAAGCGUUAAUCGGAAUUACUGGGCGUAAAGCGCACGCAGGCGGUUUGUUAAGUCAGAUGUGAAAUCCCCGGGCUCAACCUGGGAACUGCAUCUGAUACUGGCAAGCUUGAGUCUCGUAGAGGGGGGUAGAAUUCCAGGUGUAGCGGUGAAAUGCGUAGAGAUCUGG	Paromomycin_mol_mol	Target_lig_1116	decoding region 16SrRNA	Target_97	5.73282827159699

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		AGGAAUACCGGUG GCGAAGGCGGCCCC CUGGACGAAGACUG ACGCUCAGGUGCGA AAGCGUGGGGAGC AAACAGGAUUAGA UACCCUGGUAGUCC ACGCCGUAAACGAU GUCGACUUGGAGG UUGUGCCCUUGAGG CGUGGCUUCCGGAG CUAACGCGUUAAGU CGACCGCCUGGGGA GUACGGCCGCAAGG UUAAAACUCAAAU GAAUUGACGGGGG CCCGCACAAGCGGU GGAGCAUGUGGUU UAAUUCGAUGCAAC GCGAAGAACCUUAC CUGGUCUUGACAUC CACGGAAGUUUUCA GAGAUGAGAAUGU GCCUUCGGGAACCG UGAGACAGGUGCU GCAUGGCUGUCGUC AGCUCGUGUUGUG AAAUGUUGGGUUA AGUCCCGCAACGAG CGCAACCCUUAUCC UUUGUUGCCAGCGG UCCGGCCGGGAACU CAAAGGAGACUGCC AGUGAUAAACUGG AGGAAGGUGGGGA UGACGUCAAGUCAU CAUGGCCCUUACGA CCAGGGCUACACAC GUGCUACAAUGGCG CAUACAAAGAGAA GCGACCUCGCGAGA GCAAGCGGACCUCA UAAAGUGCGUCGU AGUCCGGAUUGGA GUCUGCAACUCGAC UCCAUGAAGUCGGA AUCGCUAGUAAUCG UGGAUCAGAAUGCC ACGGUGAAUACGU UCCCGGGCCUUGUA CACACCGCCCGUCA CACCAUGGGAGUGG GUUGCAAAAGAAG UAGGUAGCUUAACC UUCGGGAGGGCGCU UACCACUUUGUGAU UCAUGACUGGGGU GAAGUCGUAACAA GGUAACCGUAGGG GAACCUGCGGUUGG AUCACCUCCUUA					
197	[C@H]1([C@H](C[C@H]([C@H]([C@H]1O)O[C@@H]1[C@@H](C[C@@H]([C@@H](O1)CN)O)N)N)O[C@@H]1[C@H]([C@@H]([C@H]([C@@H](O1)CNc1c2ccccc2nc2c1cccc2)O)N)O	AAAUUGAAGAGUU UGAUCAUGGCUCAG AUUGAACGCUGGCG GCAGGCCUAACACA UGCAAGUCGAACGG UAACAGGAAGAAG CUUGCUUCUUUGCU GACGAGUGGCGGAC GGGUGAGUAAUGU CUGGGAAACUGCCU GAUGGAGGGGGAU AACUACUGGAAACG GUAGCUAAUACCGC AUAACGUCGCAAGA	Tobramycin	Target_lig_540	decoding region 16SrRNA	Target_97	5.772113295386333

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		CCAAAGAGGGGGAC CUUCGGGCCUCUUG CCAUCGGAUGUGCC CAGAUGGGAUUAG CUAGUAGGUGGGG UAACGGCUCACCUA GGCGACGAUCCCUA GCUGGUCUGAGAG GAUGACCAGCCACA CUGGAACUGAGACA CGGUCCAGACUCCU ACGGGAGGCAGCAG UGGGGAAUAUUGC ACAAUGGGCGCAAG CCUGAUGCAGCCAU GCCGCGUGUAUGAA GAAGGCCUUCGGGU UGUAAAGUACUUU CAGCGGGGAGGAA GGGAGUAAAGUUA AUACCUUUGCUCAU UGACGUUACCCGCA GAAGAAGCACCGGC UAACUCCGUGCCAG CAGCCGCGGUAAUA CGGAGGGUGCAAGC GUUAAUCGGAAUU ACUGGGCGUAAAGC GCACGCAGGCGGUU UGUUAAGUCAGAU GUGAAAUCCCCGGG CUCAACCUGGGAAC UGCAUCUGAUACUG GCAAGCUUGAGUCU CGUAGAGGGGGGU AGAAUUCCAGGUG UAGCGGUGAAAUG CGUAGAGAUCUGG AGGAAUACCGGUG GCGAAGGCGGCCCC CUGGACGAAGACUG ACGCUCAGGUGCGA AAGCGUGGGGAGC AAACAGGAUUAGA UACCCUGGUAGUCC ACGCCGUAAACGAU GUCGACUUGGAGG UUGUGCCCUUGAGG CGUGGCUUCCGGAG CUAACGCGUUAAGU CGACCGCCUGGGGA GUACGGCCGCAAGG UUAAAACUCAAAU GAAUUGACGGGGG CCCGCACAAGCGGU GGAGCAUGUGGUU UAAUUCGAUGCAAC GCGAAGAACCUUAC CUGGUCUUGACAUC CACGGAAGUUUUCA GAGAUGAGAAUGU GCCUUCGGGAACCG UGAGACAGGUGCU GCAUGGCUGUCGUC AGCUCGUGUUGUG AAAUGUUGGGUUA AGUCCCGCAACGAG CGCAACCCUUAUCC UUUGUUGCCAGCGG UCCGGCCGGGAACU CAAAGGAGACUGCC AGUGAUAAACUGG AGGAAGGUGGGGA UGACGUCAAGUCAU CAUGGCCCUUACGA					

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		CCAGGGCUACACAC GUGCUACAAUGGCG CAUACAAAGAGAA GCGACCUCGCGAGA GCAAGCGGACCUCA UAAAGUGCGUCGU AGUCCGGAUUGGA GUCUGCAACUCGAC UCCAUGAAGUCGGA AUCGCUAGUAAUCG UGGAUCAGAAUGCC ACGGUGAAUACGU UCCCGGGCCUUGUA CACACCGCCCGUCA CACCAUGGGAGUGG GUUGCAAAAGAAG UAGGUAGCUUAACC UUCGGGAGGGCGCU UACCACUUUGUGAU UCAUGACUGGGGU GAAGUCGUAACAA GGUAACCGUAGGG GAACCUGCGGUUGG AUCACCUCCUUA					
198	C1C(C(C(C(C1N)OC2C(C(C(C(O2)CO)O)N)O)O)OC3C(C(C(C(O3)CN)O)O)O)N)N	AAAUUGAAGAGUU UGAUCAUGGCUCAG AUUGAACGCUGGCG GCAGGCCUAACACA UGCAAGUCGAACGG UAACAGGAAGAAG CUUGCUUCUUUGCU GACGAGUGGCGGAC GGGUGAGUAAUGU CUGGGAAACUGCCU GAUGGAGGGGGAU AACUACUGGAAACG GUAGCUAAUACCGC AUAACGUCGCAAGA CCAAAGAGGGGGAC CUUCGGGCCUCUUG CCAUCGGAUGUGCC CAGAUGGGAUUAG CUAGUAGGUGGGG UAACGGCUCACCUA GGCGACGAUCCCUA GCUGGUCUGAGAG GAUGACCAGCCACA CUGGAACUGAGACA CGGUCCAGACUCCU ACGGGAGGCAGCAG UGGGGAAUAUUGC ACAAUGGGCGCAAG CCUGAUGCAGCCAU GCCGCGUGUAUGAA GAAGGCCUUCGGGU UGUAAAGUACUUU CAGCGGGGAGGAA GGGAGUAAAGUUA AUACCUUUGCUCAU UGACGUUACCCGCA GAAGAAGCACCGGC UAACUCCGUGCCAG CAGCCGCGGUAAUA CGGAGGGUGCAAGC GUUAAUCGGAAUU ACUGGGCGUAAAGC GCACGCAGGCGGUU UGUUAAGUCAGAU GUGAAAUCCCCGGG CUCAACCUGGGAAC UGCAUCUGAUACUG GCAAGCUUGAGUCU CGUAGAGGGGGGU AGAAUUCCAGGUG UAGCGGUGAAAUG	KANAMYCIN B	Target_lig_8	decoding region 16SrRNA	Target_97	5.66958622665081

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		CGUAGAGAUCUGG AGGAAUACCGGUG GCGAAGGCGGCCCC CUGGACGAAGACUG ACGCUCAGGUGCGA AAGCGUGGGGAGC AAACAGGAUUAGA UACCCUGGUAGUCC ACGCCGUAAACGAU GUCGACUUGGAGG UUGUGCCCUUGAGG CGUGGCUUCCGGAG CUAACGCGUUAAGU CGACCGCCUGGGGA GUACGGCCGCAAGG UUAAAACUCAAAU GAAUUGACGGGGG CCCGCACAAGCGGU GGAGCAUGUGGUU UAAUUCGAUGCAAC GCGAAGAACCUUAC CUGGUCUUGACAUC CACGGAAGUUUUCA GAGAUGAGAAUGU GCCUUCGGGAACCG UGAGACAGGUGCU GCAUGGCUGUCGUC AGCUCGUGUUGUG AAAUGUUGGGUUA AGUCCCGCAACGAG CGCAACCCUUAUCC UUUGUUGCCAGCGG UCCGGCCGGGAACU CAAAGGAGACUGCC AGUGAUAAACUGG AGGAAGGUGGGGA UGACGUCAAGUCAU CAUGGCCCUUACGA CCAGGGCUACACAC GUGCUACAAUGGCG CAUACAAAGAGAA GCGACCUCGCGAGA GCAAGCGGACCUCA UAAAGUGCGUCGU AGUCCGGAUUGGA GUCUGCAACUCGAC UCCAUGAAGUCGGA AUCGCUAGUAAUCG UGGAUCAGAAUGCC ACGGUGAAUACGU UCCCGGGCCUUGUA CACACCGCCCGUCA CACCAUGGGAGUGG GUUGCAAAAGAAG UAGGUAGCUUAACC UUCGGGAGGGCGCU UACCACUUUGUGAU UCAUGACUGGGGU GAAGUCGUAACAA GGUAACCGUAGGG GAACCUGCGGUUGG AUCACCUCCUUA					
199	C1C(C(C(C(C1N)OC2C(C(C(C(O2)CN)O)O)N)OC3C(C(C(O3)CO)OC4C(C(C(C(O4)CN)O)O)N)O)O)N	AAAUUGAAGAGUU UGAUCAUGGCUCAG AUUGAACGCUGGCG GCAGGCCUAACACA UGCAAGUCGAACGG UAACAGGAAGAAG CUUGCUUCUUUGCU GACGAGUGGCGGAC GGGUGAGUAAUGU CUGGGAAACUGCCU GAUGGAGGGGGAU AACUACUGGAAACG GUAGCUAAUACCGC	Neomycin_B	Target_lig_1246	decoding region 16SrRNA	Target_97	6.87942606879415

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		AUAACGUCGCAAGA CCAAAGAGGGGGAC CUUCGGGCCUCUUG CCAUCGGAUGUGCC CAGAUGGGAUUAG CUAGUAGGUGGGG UAACGGCUCACCUA GGCGACGAUCCCUA GCUGGUCUGAGAG GAUGACCAGCCACA CUGGAACUGAGACA CGGUCCAGACUCCU ACGGGAGGCAGCAG UGGGGAAUAUUGC ACAAUGGGCGCAAG CCUGAUGCAGCCAU GCCGCGUGUAUGAA GAAGGCCUUCGGGU UGUAAAGUACUUU CAGCGGGGAGGAA GGGAGUAAAGUUA AUACCUUUGCUCAU UGACGUUACCCGCA GAAGAAGCACCGGC UAACUCCGUGCCAG CAGCCGCGGUAAUA CGGAGGGUGCAAGC GUUAAUCGGAAUU ACUGGGCGUAAAGC GCACGCAGGCGGUU UGUUAAGUCAGAU GUGAAAUCCCCGGG CUCAACCUGGGAAC UGCAUCUGAUACUG GCAAGCUUGAGUCU CGUAGAGGGGGGU AGAAUUCCAGGUG UAGCGGUGAAAUG CGUAGAGAUCUGG AGGAAUACCGGUG GCGAAGGCGGCCCC CUGGACGAAGACUG ACGCUCAGGUGCGA AAGCGUGGGGAGC AAACAGGAUUAGA UACCCUGGUAGUCC ACGCCGUAAACGAU GUCGACUUGGAGG UUGUGCCCUUGAGG CGUGGCUUCCGGAG CUAACGCGUUAAGU CGACCGCCUGGGGA GUACGGCCGCAAGG UUAAAACUCAAAU GAAUUGACGGGGG CCCGCACAAGCGGU GGAGCAUGUGGUU UAAUUCGAUGCAAC GCGAAGAACCUUAC CUGGUCUUGACAUC CACGGAAGUUUUCA GAGAUGAGAAUGU GCCUUCGGGAACCG UGAGACAGGUGCU GCAUGGCUGUCGUC AGCUCGUGUUGUG AAAUGUUGGGUUA AGUCCCGCAACGAG CGCAACCCUUAUCC UUUGUUGCCAGCGG UCCGGCCGGGAACU CAAAGGAGACUGCC AGUGAUAAACUGG AGGAAGGUGGGGA UGACGUCAAGUCAU					

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		CAUGGCCCUUACGA CCAGGGCUACACAC GUGCUACAAUGGCG CAUACAAAGAGAA GCGACCUCGCGAGA GCAAGCGGACCUCA UAAAGUGCGUCGU AGUCCGGAUUGGA GUCUGCAACUCGAC UCCAUGAAGUCGGA AUCGCUAGUAAUCG UGGAUCAGAAUGCC ACGGUGAAUACGU UCCCGGGCCUUGUA CACACCGCCCGUCA CACCAUGGGAGUGG GUUGCAAAAGAAG UAGGUAGCUUAACC UUCGGGAGGGCGCU UACCACUUUGUGAU UCAUGACUGGGGU GAAGUCGUAACAA GGUAACCGUAGGG GAACCUGCGGUUGG AUCACCUCCUUA					
200	CC1(COC(C(C1NC)O) OC2C(CC(C(C2O)OC3 C(CCC(O3)CN)N)N)N)O	AAAUUGAAGAGUU UGAUCAUGGCUCAG AUUGAACGCUGGCG GCAGGCCUAACACA UGCAAGUCGAACGG UAACAGGAAGAAG CUUGCUUCUUUGCU GACGAGUGGCGGAC GGGUGAGUAAUGU CUGGGAAACUGCCU GAUGGAGGGGGAU AACUACUGGAAACG GUAGCUAAUACCGC AUAACGUCGCAAGA CCAAAGAGGGGGAC CUUCGGGCCUCUUG CCAUCGGAUGUGCC CAGAUGGGAUUAG CUAGUAGGUGGGG UAACGGCUCACCUA GGCGACGAUCCCUA GCUGGUCUGAGAG GAUGACCAGCCACA CUGGAACUGAGACA CGGUCCAGACUCCU ACGGGAGGCAGCAG UGGGGAAUAUUGC ACAAUGGGCGCAAG CCUGAUGCAGCCAU GCCGCGUGUAUGAA GAAGGCCUUCGGGU UGUAAAGUACUUU CAGCGGGGAGGAA GGGAGUAAAGUUA AUACCUUUGCUCAU UGACGUUACCCGCA GAAGAAGCACCGGC UAACUCCGUGCCAG CAGCCGCGGUAAUA CGGAGGGUGCAAGC GUUAAUCGGAAUU ACUGGGCGUAAAGC GCACGCAGGCGGUU UGUUAAGUCAGAU GUGAAAUCCCCGGG CUCAACCUGGGAAC UGCAUCUGAUACUG GCAAGCUUGAGUCU CGUAGAGGGGGGU AGAAUUCCAGGUG	gentamicin_mol_c	Target_lig_76	decoding region 16SrRNA	Target_97	5.73518217699046

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		UAGCGGUGAAAUG CGUAGAGAUCUGG AGGAAUACCGGUG GCGAAGGCGGCCCC CUGGACGAAGACUG ACGCUCAGGUGCGA AAGCGUGGGGAGC AAACAGGAUUAGA UACCCUGGUAGUCC ACGCCGUAAACGAU GUCGACUUGGAGG UUGUGCCCUUGAGG CGUGGCUUCCGGAG CUAACGCGUUAAGU CGACCGCCUGGGGA GUACGGCCGCAAGG UUAAAACUCAAAU GAAUUGACGGGGG CCCGCACAAGCGGU GGAGCAUGUGGUU UAAUUCGAUGCAAC GCGAAGAACCUUAC CUGGUCUUGACAUC CACGGAAGUUUUCA GAGAUGAGAAUGU GCCUUCGGGAACCG UGAGACAGGUGCU GCAUGGCUGUCGUC AGCUCGUGUUGUG AAAUGUUGGGUUA AGUCCCGCAACGAG CGCAACCCUUAUCC UUUGUUGCCAGCGG UCCGGCCGGGAACU CAAAGGAGACUGCC AGUGAUAAACUGG AGGAAGGUGGGGA UGACGUCAAGUCAU CAUGGCCCUUACGA CCAGGGCUACACAC GUGCUACAAUGGCG CAUACAAAGAGAA GCGACCUCGCGAGA GCAAGCGGACCUCA UAAAGUGCGUCGU AGUCCGGAUUGGA GUCUGCAACUCGAC UCCAUGAAGUCGGA AUCGCUAGUAAUCG UGGAUCAGAAUGCC ACGGUGAAUACGU UCCCGGGCCUUGUA CACACCGCCCGUCA CACCAUGGGAGUGG GUUGCAAAAGAAG UAGGUAGCUUAACC UUCGGGAGGGCGCU UACCACUUUGUGAU UCAUGACUGGGGU GAAGUCGUAACAA GGUAACCGUAGGG GAACCUGCGGUUGG AUCACCUCCUUA					
201	CC(C)CC(C(=O)NC(CC1=CNC2=CC=CC=C21)C(=O)N3CCCC3C(=O)O)NC(=O)C(CCC(=O)N)NC(=O)C4CCCN4C(=O)C(CCCCN)N	AAAUUGAAGAGUU UGAUCAUGGCUCAG AUUGAACGCUGGCG GCAGGCCUAACACA UGCAAGUCGAACGG UAACAGGAAGAAG CUUGCUUCUUUGCU GACGAGUGGCGGAC GGGUGAGUAAUGU CUGGGAAACUGCCU GAUGGAGGGGGAU AACUACUGGAAACG	CRP	Target_lig_147	decoding region 16SrRNA	Target_97	6.78251605578609

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		GUAGCUAAUACCGC AUAACGUCGCAAGA CCAAAGAGGGGGAC CUUCGGGCCUCUUG CCAUCGGAUGUGCC CAGAUGGGAUUAG CUAGUAGGUGGGG UAACGGCUCACCUA GGCGACGAUCCCUA GCUGGUCUGAGAG GAUGACCAGCCACA CUGGAACUGAGACA CGGUCCAGACUCCU ACGGGAGGCAGCAG UGGGGAAUAUUGC ACAAUGGGCGCAAG CCUGAUGCAGCCAU GCCGCGUGUAUGAA GAAGGCCUUCGGGU UGUAAAGUACUUU CAGCGGGGAGGAA GGGAGUAAAGUUA AUACCUUUGCUCAU UGACGUUACCCGCA GAAGAAGCACCGGC UAACUCCGUGCCAG CAGCCGCGGUAAUA CGGAGGGUGCAAGC GUUAAUCGGAAUU ACUGGGCGUAAAGC GCACGCAGGCGGUU UGUUAAGUCAGAU GUGAAAUCCCCGGG CUCAACCUGGGAAC UGCAUCUGAUACUG GCAAGCUUGAGUCU CGUAGAGGGGGGU AGAAUUCCAGGUG UAGCGGUGAAAUG CGUAGAGAUCUGG AGGAAUACCGGUG GCGAAGGCGGCCCC CUGGACGAAGACUG ACGCUCAGGUGCGA AAGCGUGGGGAGC AAACAGGAUUAGA UACCCUGGUAGUCC ACGCCGUAAACGAU GUCGACUUGGAGG UUGUGCCCUUGAGG CGUGGCUUCCGGAG CUAACGCGUUAAGU CGACCGCCUGGGGA GUACGGCCGCAAGG UUAAAACUCAAAU GAAUUGACGGGGG CCCGCACAAGCGGU GGAGCAUGUGGUU UAAUUCGAUGCAAC GCGAAGAACCUUAC CUGGUCUUGACAUC CACGGAAGUUUUCA GAGAUGAGAAUGU GCCUUCGGGAACCG UGAGACAGGUGCU GCAUGGCUGUCGUC AGCUCGUGUUGUG AAAUGUUGGGUUA AGUCCCGCAACGAG CGCAACCCUUAUCC UUUGUUGCCAGCGG UCCGGCCGGGAACU CAAAGGAGACUGCC AGUGAUAAACUGG AGGAAGGUGGGGA					

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		UGACGUCAAGUCAU CAUGGCCCUUACGA CCAGGGCUACACAC GUGCUACAAUGGCG CAUACAAAGAGAA GCGACCUCGCGAGA GCAAGCGGACCUCA UAAAGUGCGUCGU AGUCCGGAUUGGA GUCUGCAACUCGAC UCCAUGAAGUCGGA AUCGCUAGUAAUCG UGGAUCAGAAUGCC ACGGUGAAUACGU UCCCGGGCCUUGUA CACACCGCCCGUCA CACCAUGGGAGUGG GUUGCAAAAGAAG UAGGUAGCUUAACC UUCGGGAGGGCGCU UACCACUUUGUGAU UCAUGACUGGGGU GAAGUCGUAACAA GGUAACCGUAGGG GAACCUGCGGUUGG AUCACCUCCUUA					
226	C1C(C(C(C(C1N)OC2C(C(C(C(O2)CN)O)O)N)OC3C(C(C(O3)CO)OC4C(C(C(C(O4)CN)O)O)N)O)O)N	GAGCGUCACACCUU CGGGUGAAGUCGCU C	Neomycin	Target_lig_4	A-site	Target_3	7.22184874961636
228	CC1=CC(=NC2=C1C=CC(=C2)N)N(C)C	GAGCGUCACACCUU CGGGUGAAGUCGCU C	quinolinediamine_trimethyl_der	Target_lig_170	A-site	Target_3	4.45593195564972
229	C1=CC=C2C(=C1)C=C(C=N2)C(=O)N	GAGCGUCACACCUU CGGGUGAAGUCGCU C	3-quinolinecarboxamide	Target_lig_171	A-site	Target_3	4.76955107862173
230	CC1=CC(=NC2=C1C=CC(=C2)NC(=O)CC3=CC=NC=C3)N(C)C	GAGCGUCACACCUU CGGGUGAAGUCGCU C	4-pyridineacetamide, N- [2-(dimethylamino)-4-methyl-7-quinolinyl]	Target_lig_172	A-site	Target_3	4.74472749489669
232	CCC1C2(C(C(C(=O)C(CC(C(C(C(=O)C(C(=O)O1)C)C)OC3C(C(CC(O3)C)N(C)C)O)(C)OCC=CC4=CC5=CC=CC=C5N=C4)C)C)NC(=O)O2)C	UUGGCUACUAUGCC AGCUGGUGGAUUG CUCGGCUCAGGCGC UGAUGAAGGACGU GCCAAGCUGCGAUA AGCCAUGGGGAGCC GCACGGAGGCGAAG AACCAUGGAUUUCC GAAUGAGAAUCUC UCUAACAAUUGCUU CGCGCAAUGAGGAA CCCCGAGAACUGAA ACAUCUCAGUAUCG GGAGGAACAGAAA ACGCAAUGUGAUG UCGUUAGUAACCGC GAGUGAACGCGAU ACAGCCCAAACCGA AGCCCUCACGGGCA AUGUGGUGUCAGG GCUACCUCUCAUCA GCCGACCGUCUCGA CGAAGUCUCUUGGA ACAGAGCGUGAUAC AGGGUGACAACCCC GUACUCGAGACCAG UACGACGUGCGGUA GUGCCAGAGUAGCG GGGGUUGGAUAUC	Cethromycin	Target_lig_174	U2609_Ecoli_ribosome	Target_99	8.88605664769316

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		CCUCGCGAAUAACG CAGGCAUCGACUGC GAAGGCUAAACACA ACCUGAGACCGAUA GUGAACAAGUAGU GUGAACGAACGCUG CAAAGUACCCUCAG AAGGGAGGCGAAA UAGAGCAUGAAAU CAGUUGGCGAUCGA GCGACAGGGCAUAC AAGGUCCCUCGACG AAUGACCGACGCGC GAGCGUCCAGUAAG ACUCACGGGAAGCC GAUGUUCUGUCGU ACGUUUUGAAAAA CGAGCCAGGGAGUG UGUCUGCAUGGCAA GUCUAACCGGAGUA UCCGGGGAGGCACA GGGAAACCGACAUG GCCGCAGGGCUUUG CCCGAGGGCCGCCG UCUUCAAGGGCGGG GAGCCAUGUGGACA CGACCCGAAUCCGG ACGAUCUACGCAUG GACAAGAUGAAGC GUGCCGAAAGGCAC GUGGAAGUCUGUU AGAGUUGGUGUCC UACAAUACCCUCUC GUGAUCUAUGUGU AGGGGUGAAAGGC CCAUCGAGUCCGGC AACAGCUGGUUCCA AUCGAAACAUGUCG AAGCAUGACCUCCG CCGAGGUAGUCUGU GAGGUAGAGCGACC GAUUGGUGUGUCC GCCUCCGAGAGGAG UCGGCACACCUGUC AAACUCCAAACUUA CAGACGCCGUUUGA CGCGGGGAUUCCGG UGCGCGGGGUAAGC CUGUGUACCAGGAG GGGAACAACCCAGA GAUAGGUUAAGGU CCCCAAGUGUGGAU UAAGUGUAAUCCUC UGAAGGUGGUCUC GAGCCCUAGACAGC CGGGAGGUGAGCU UAGAAGCAGCUACC CUCUAAGAAAAGCG UAACAGCUUACCGG CCGAGGUUUGAGGC GCCCAAAAUGAUCG GGACUCAAAUCCAC CACCGAGACCUGUC CGUACCACUCAUAC UGGUAAUCGAGUA GAUUGGCGCUCUAA UUGGAUGGAAGUA GGGGUGAAAACUCC UAUGGACCGAUUA GUGACGAAAAUCCU GGCCAUAGUAGCAG CGAUAGUCGGGUG AGAACCCCGACGGC CUAAUGGAUAAGG GUUCCUCAGCACUG					

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		CUGAUCAGCUGAGG GUUAGCCGGUCCUA AGUCAUACCGCAAC UCGACUAUGACGAA AUGGGAAACGGGU UAAUAUUCCCGUGC CACUAUGCAGUGAA AGUUGACGCCCUGG GGUCGAUCACGCUG GGCAUUCGCCCAGU CGAACCGUCCAACU CCGUGGAAGCCGUA AUGGCAGGAAGCG GACGAACGGCGGCA UAGGGAAACGUGA UUCAACCUGGGGCC CAUGAAAAGACGA GCAUAGUGUCCGUA CCGAGAACCGACAC AGGUGUCCAUGGCG GCGAAAGCCAAGGC CUGUCGGGAGCAAC CAACGUUAGGGAA UUCGGCAAGUUAG UCCCGUACCUUCGG AAGAAGGGAUGCC UGCUCCGGAACGGA GCAGGUCGCAGUGA CUCGGAAGCUCGGA CUGUCUAGUAACAA CAUAGGUGACCGCA AAUCCGCAAGGACU CGUACGGUCACUGA AUCCUGCCCAGUGC AGGUAUCUGAACAC CUCGUACAAGAGGA CGAAGGACCUGUCA ACGGCGGGGGUAAC UAUGACCCUCUUAA GGUAGCGUAGUACC UUGCCGCAUCAGUA GCGGCUUGCAUGAA UGGAUUAACCAGA GCUUCACUGUCCCA ACGUUGGGCCCGGU GAACUGUACAUUCC AGUGCGGAGUCUG GAGACACCCAGGGG GAAGCGAAGACCCU AUGGAGCUUUACU GCAGGCUGUCGCUG AGACGUGGUCGCCG AUGUGCAGCAUAG GUAGGAGACACUAC ACAGGUACCCGCGC UAGCGGGCCACCGA GUCAACAGUGAAA UACUACCCGUCGGU GACUGCGACUCUCA CUCCGGGAGGAGGA CACCGAUAGCCGGG CAGUUUGACUGGG GCGGUACGCGCUCG AAAAGAUAUCGAG CGCGCCCUAUGGCU AUCUCAGCCGGGAC AGAGACCCGGCGAA GAGUGCAAGAGCA AAAGAUAGCUUGA CAGUGUUCUUCCCA ACGAGGAACGCUGA CGCGAAAGCGUGGU CUAGCGAACCAAUU AGCCUGCUUGAUGC GGGCAAUUGAUGA					

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		CAGAAAAGCUACCC UAGGGAUAACAGA GUCGUCACUCGCAA GAGCACAUAUCGAC CGAGUGGCUUGCUA CCUCGAUGUCGGUU CCCUCCAUCCUGCC CGUGCAGAAGCGGG CAAGGGUGAGGUU GUUCGCCUAUUAAA GGAGGUCGUGAGC UGGGUUUAGACCG UCGUGAGACAGGUC GGCUGCUAUCUACU GGGUGUGUAAUGG UGUCUGACAAGAAC GACCGUAUAGUACG AGAGGAACUACGG UUGGUGGCCACUGG UGUACCGGUUGUUC GAGAGAGCACGUGC CGGGUAGCCACGCC ACACGGGGUAAGA GCUGAACGCAUCUA AGCUCGAAACCCAC UUGGAAAAGAGAC ACCGCCGAGGUCCC GCGUACAAGACGCG GUCGAUAGACUCGG GGUGUGCGCGUCGA GGUAACGAGACGU UAAGCCCACGAGCA CUAACAGACCAAAG CCAUCAU					
282	C1C(C(C(C(C1NC(=O)C(CCN)O)OC2C(C(C(C(O2)CO)O)O)N)O)O)OC3C(C(C(C(O3)CN)O)O)O)N	GAGCGUCACACCUU CGGGUGAAGUCGCU C	Amikacin	Target_lig_175	A-site for Amikacin	Target_3	7.259637310505 76
283	CC(=O)OC1C(CNC1CC2=CC=C(C=C2)OC)O	UUGGCUACUAUGCC AGCUGGUGGAUUG CUCGGCUCAGGCGC UGAUGAAGGACGU GCCAAGCUGCGAUA AGCCAUGGGGAGCC GCACGGAGGCGAAG AACCAUGGAUUUCC GAAUGAGAAUCUC UCUAACAAUUGCUU CGCGCAAUGAGGAA CCCCGAGAACUGAA ACAUCUCAGUAUCG GGAGGAACAGAAA ACGCAAUGUGAUG UCGUUAGUAACCGC GAGUGAACGCGAU ACAGCCCAAACCGA AGCCCUCACGGGCA AUGUGGUGUCAGG GCUACCUCUCAUCA GCCGACCGUCUCGA CGAAGUCUCUUGGA ACAGAGCGUGAUAC AGGGUGACAACCCC GUACUCGAGACCAG UACGACGUGCGGUA GUGCCAGAGUAGCG GGGGUUGGAUAUC CCUCGCGAAUAACG CAGGCAUCGACUGC GAAGGCUAAACACA ACCUGAGACCGAUA GUGAACAAGUAGU GUGAACGAACGCUG	Anisomycin	Target_lig_222	Ribosome (PTC)	Target_99	7

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		CAAAGUACCCUCAG AAGGGAGGCGAAA UAGAGCAUGAAAU CAGUUGGCGAUCGA GCGACAGGGCAUAC AAGGUCCCUCGACG AAUGACCGACGCGC GAGCGUCCAGUAAG ACUCACGGGAAGCC GAUGUUCUGUCGU ACGUUUUGAAAAA CGAGCCAGGGAGUG UGUCUGCAUGGCAA GUCUAACCGGAGUA UCCGGGGAGGCACA GGGAAACCGACAUG GCCGCAGGGCUUUG CCCGAGGGCCGCCG UCUUCAAGGGCGGG GAGCCAUGUGGACA CGACCCGAAUCCGG ACGAUCUACGCAUG GACAAGAUGAAGC GUGCCGAAAGGCAC GUGGAAGUCUGUU AGAGUUGGUGUCC UACAAUACCCUCUC GUGAUCUAUGUGU AGGGGUGAAAGGC CCAUCGAGUCCGGC AACAGCUGGUUCCA AUCGAAACAUGUCG AAGCAUGACCUCCG CCGAGGUAGUCUGU GAGGUAGAGCGACC GAUUGGUGUGUCC GCCUCCGAGAGGAG UCGGCACACCUGUC AAACUCCAAACUUA CAGACGCCGUUUGA CGCGGGGAUUCCGG UGCGCGGGGUAAGC CUGUGUACCAGGAG GGGAACAACCCAGA GAUAGGUUAAGGU CCCCAAGUGUGGAU UAAGUGUAAUCCUC UGAAGGUGGUCUC GAGCCCUAGACAGC CGGGAGGUGAGCU UAGAAGCAGCUACC CUCUAAGAAAAGCG UAACAGCUUACCGG CCGAGGUUUGAGGC GCCCAAAAUGAUCG GGACUCAAAUCCAC CACCGAGACCUGUC CGUACCACUCAUAC UGGUAAUCGAGUA GAUUGGCGCUCUAA UUGGAUGGAAGUA GGGGUGAAAACUCC UAUGGACCGAUUA GUGACGAAAAUCCU GGCCAUAGUAGCAG CGAUAGUCGGGUG AGAACCCCGACGGC CUAAUGGAUAAGG GUUCCUCAGCACUG CUGAUCAGCUGAGG GUUAGCCGGUCCUA AGUCAUACCGCAAC UCGACUAUGACGAA AUGGGAAACGGGU UAAUAUUCCCGUGC					

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		CACUAUGCAGUGAA AGUUGACGCCCUGG GGUCGAUCACGCUG GGCAUUCGCCCAGU CGAACCGUCCAACU CCGUGGAAGCCGUA AUGGCAGGAAGCG GACGAACGGCGGCA UAGGGAAACGUGA UUCAACCUGGGGCC CAUGAAAAGACGA GCAUAGUGUCCGUA CCGAGAACCGACAC AGGUGUCCAUGGCG GCGAAAGCCAAGGC CUGUCGGGAGCAAC CAACGUUAGGGAA UUCGGCAAGUUAG UCCCGUACCUUCGG AAGAAGGGAUGCC UGCUCCGGAACGGA GCAGGUCGCAGUGA CUCGGAAGCUCGGA CUGUCUAGUAACAA CAUAGGUGACCGCA AAUCCGCAAGGACU CGUACGGUCACUGA AUCCUGCCCAGUGC AGGUAUCUGAACAC CUCGUACAAGAGGA CGAAGGACCUGUCA ACGGCGGGGGUAAC UAUGACCCUCUUAA GGUAGCGUAGUACC UUGCCGCAUCAGUA GCGGCUUGCAUGAA UGGAUUAACCAGA GCUUCACUGUCCCA ACGUUGGGCCCGGU GAACUGUACAUUCC AGUGCGGAGUCUG GAGACACCCAGGGG GAAGCGAAGACCCU AUGGAGCUUUACU GCAGGCUGUCGCUG AGACGUGGUCGCCG AUGUGCAGCAUAG GUAGGAGACACUAC ACAGGUACCCGCGC UAGCGGGCCACCGA GUCAACAGUGAAA UACUACCCGUCGGU GACUGCGACUCUCA CUCCGGGAGGAGGA CACCGAUAGCCGGG CAGUUUGACUGGG GCGGUACGCGCUCG AAAAGAUAUCGAG CGCGCCCUAUGGCU AUCUCAGCCGGGAC AGAGACCCGGCGAA GAGUGCAAGAGCA AAAGAUAGCUUGA CAGUGUUCUUCCCA ACGAGGAACGCUGA CGCGAAAGCGUGGU CUAGCGAACCAAUU AGCCUGCUUGAUGC GGGCAAUUGAUGA CAGAAAAGCUACCC UAGGGAUAACAGA GUCGUCACUCGCAA GAGCACAUAUCGAC CGAGUGGCUUGCUA CCUCGAUGUCGGUU					

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		CCCUCCAUCCUGCC CGUGCAGAAGCGGG CAAGGGUGAGGUU GUUCGCCUAUUAAA GGAGGUCGUGAGC UGGGUUUAGACCG UCGUGAGACAGGUC GGCUGCUAUCUACU GGGUGUGUAAUGG UGUCUGACAAGAAC GACCGUAUAGUACG AGAGGAACUACGG UUGGUGGCCACUGG UGUACCGGUUGUUC GAGAGAGCACGUGC CGGGUAGCCACGCC ACACGGGGUAAGA GCUGAACGCAUCUA AGCUCGAAACCCAC UUGGAAAAGAGAC ACCGCCGAGGUCCC GCGUACAAGACGCG GUCGAUAGACUCGG GGUGUGCGCGUCGA GGUAACGAGACGU UAAGCCCACGAGCA CUAACAGACCAAAG CCAUCAU					
284	CCC1C(C(C(N(CC(CC(C(C(C(C(=O)O1)C)OC2CC(C(C(O2)C)O)(C)OC)C)OC3C(C(CC(O3)C)N(C)C)O)(C)O)C)C)O)(C)O	UUGGCUACUAUGCC AGCUGGUGGAUUG CUCGGCUCAGGCGC UGAUGAAGGACGU GCCAAGCUGCGAUA AGCCAUGGGGAGCC GCACGGAGGCGAAG AACCAUGGAUUUCC GAAUGAGAAUCUC UCUAACAAUUGCUU CGCGCAAUGAGGAA CCCCGAGAACUGAA ACAUCUCAGUAUCG GGAGGAACAGAAA ACGCAAUGUGAUG UCGUUAGUAACCGC GAGUGAACGCGAU ACAGCCCAAACCGA AGCCCUCACGGGCA AUGUGGUGUCAGG GCUACCUCUCAUCA GCCGACCGUCUCGA CGAAGUCUCUUGGA ACAGAGCGUGAUAC AGGGUGACAACCCC GUACUCGAGACCAG UACGACGUGCGGUA GUGCCAGAGUAGCG GGGGUUGGAUAUC CCUCGCGAAUAACG CAGGCAUCGACUGC GAAGGCUAAACACA ACCUGAGACCGAUA GUGAACAAGUAGU GUGAACGAACGCUG CAAAGUACCCUCAG AAGGGAGGCGAAA UAGAGCAUGAAAU CAGUUGGCGAUCGA GCGACAGGGCAUAC AAGGUCCCUCGACG AAUGACCGACGCGC GAGCGUCCAGUAAG ACUCACGGGAAGCC GAUGUUCUGUCGU ACGUUUUGAAAAA CGAGCCAGGGAGUG	Azithromycin	Target_lig_223	Ribosome (PTC)	Target_99	8.42021640338319

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		UGUCUGCAUGGCAA GUCUAACCGGAGUA UCCGGGGAGGCACA GGGAAACCGACAUG GCCGCAGGGCUUUG CCCGAGGGCCGCCG UCUUCAAGGGCGGG GAGCCAUGUGGACA CGACCCGAAUCCGG ACGAUCUACGCAUG GACAAGAUGAAGC GUGCCGAAAGGCAC GUGGAAGUCUGUU AGAGUUGGUGUCC UACAAUACCCUCUC GUGAUCUAUGUGU AGGGGUGAAAGGC CCAUCGAGUCCGGC AACAGCUGGUUCCA AUCGAAACAUGUCG AAGCAUGACCUCCG CCGAGGUAGUCUGU GAGGUAGAGCGACC GAUUGGUGUGUCC GCCUCCGAGAGGAG UCGGCACACCUGUC AAACUCCAAACUUA CAGACGCCGUUUGA CGCGGGGAUUCCGG UGCGCGGGGUAAGC CUGUGUACCAGGAG GGGAACAACCCAGA GAUAGGUUAAGGU CCCCAAGUGUGGAU UAAGUGUAAUCCUC UGAAGGUGGUCUC GAGCCCUAGACAGC CGGGAGGUGAGCU UAGAAGCAGCUACC CUCUAAGAAAAGCG UAACAGCUUACCGG CCGAGGUUUGAGGC GCCCAAAAUGAUCG GGACUCAAAUCCAC CACCGAGACCUGUC CGUACCACUCAUAC UGGUAAUCGAGUA GAUUGGCGCUCUAA UUGGAUGGAAGUA GGGGUGAAAACUCC UAUGGACCGAUUA GUGACGAAAAUCCU GGCCAUAGUAGCAG CGAUAGUCGGGUG AGAACCCCGACGGC CUAAUGGAUAAGG GUUCCUCAGCACUG CUGAUCAGCUGAGG GUUAGCCGGUCCUA AGUCAUACCGCAAC UCGACUAUGACGAA AUGGGAAACGGGU UAAUAUUCCCGUGC CACUAUGCAGUGAA AGUUGACGCCCUGG GGUCGAUCACGCUG GGCAUUCGCCCAGU CGAACCGUCCAACU CCGUGGAAGCCGUA AUGGCAGGAAGCG GACGAACGGCGGCA UAGGGAAACGUGA UUCAACCUGGGGCC CAUGAAAAGACGA GCAUAGUGUCCGUA					

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		CCGAGAACCGACAC AGGUGUCCAUGGCG GCGAAAGCCAAGGC CUGUCGGGAGCAAC CAACGUUAGGGAA UUCGGCAAGUUAG UCCCGUACCUUCGG AAGAAGGGAUGCC UGCUCCGGAACGGA GCAGGUCGCAGUGA CUCGGAAGCUCGGA CUGUCUAGUAACAA CAUAGGUGACCGCA AAUCCGCAAGGACU CGUACGGUCACUGA AUCCUGCCCAGUGC AGGUAUCUGAACAC CUCGUACAAGAGGA CGAAGGACCUGUCA ACGGCGGGGGUAAC UAUGACCCUCUUAA GGUAGCGUAGUACC UUGCCGCAUCAGUA GCGGCUUGCAUGAA UGGAUUAACCAGA GCUUCACUGUCCCA ACGUUGGGCCCGGU GAACUGUACAUUCC AGUGCGGAGUCUG GAGACACCCAGGGG GAAGCGAAGACCCU AUGGAGCUUUACU GCAGGCUGUCGCUG AGACGUGGUCGCCG AUGUGCAGCAUAG GUAGGAGACACUAC ACAGGUACCCGCGC UAGCGGGCCACCGA GUCAACAGUGAAA UACUACCCGUCGGU GACUGCGACUCUCA CUCCGGGAGGAGGA CACCGAUAGCCGGG CAGUUUGACUGGG GCGGUACGCGCUCG AAAAGAUAUCGAG CGCGCCCUAUGGCU AUCUCAGCCGGGAC AGAGACCCGGCGAA GAGUGCAAGAGCA AAAGAUAGCUUGA CAGUGUUCUUCCCA ACGAGGAACGCUGA CGCGAAAGCGUGGU CUAGCGAACCAAUU AGCCUGCUUGAUGC GGGCAAUUGAUGA CAGAAAAGCUACCC UAGGGAUAACAGA GUCGUCACUCGCAA GAGCACAUAUCGAC CGAGUGGCUUGCUA CCUCGAUGUCGGUU CCCUCCAUCCUGCC CGUGCAGAAGCGGG CAAGGGUGAGGUU GUUCGCCUAUUAAA GGAGGUCGUGAGC UGGGUUUAGACCG UCGUGAGACAGGUC GGCUGCUAUCUACU GGGUGUGUAAUGG UGUCUGACAAGAAC GACCGUAUAGUACG AGAGGAACUACGG					

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		UUGGUGGCCACUGG UGUACCGGUUGUUC GAGAGAGCACGUGC CGGGUAGCCACGCC ACACGGGGUAAGA GCUGAACGCAUCUA AGCUCGAAACCCAC UUGGAAAAGAGAC ACCGCCGAGGUCCC GCGUACAAGACGCG GUCGAUAGACUCGG GGUGUGCGCGUCGA GGUAACGAGACGU UAAGCCCACGAGCA CUAACAGACCAAAG CCAUCAU					
289	C1=CC(=CC=C1C(C(CO)NC(=O)C(Cl)Cl)O)[N+](=O)[O-]	GGUUAAGCGACUA AGCGUACACGGUGG AUGCCCUGGCAGUC AGAGGCGAUGAAG GACGUGCUAAUCUG CGAUAAGCGUCGGU AAGGUGAUAUGAA CCGUUAUAACCGGC GAUUUCCGAAUGG GGAAACCCAGUGUG UUUCGACACACUAU CAUUAACUGAAUCC AUAGGUUAAUGAG GCGAACCGGGGGAA CUGAAACAUCUAAG UACCCCGAGGAAAA GAAAUCAACCGAGA UUCCCCCAGUAGCG GCGAGCGAACGGGG AGCAGCCCAGAGCC UGAAUCAGUGUGU GUGUUAGUGGAAG CGUCUGGAAAGGCG CGCGAUACAGGGUG ACAGCCCCGUACAC AAAAAUGCACAUGC UGUGAGCUCGAUG AGUAGGGCGGGAC ACGUGGUAUCCUGU CUGAAUAUGGGGG GACCAUCCUCCAAG GCUAAAUACUCCUG ACUGACCGAUAGUG AACCAGUACCGUGA GGGAAAGGCGAAA AGAACCCCGGCGAG GGGAGUGAAAAAG AACCUGAAACCGUG UACGUACAAGCAGU GGGAGCACGCUUAG GCGUGUGACUGCGU ACCUUUUGUAUAA UGGGUCAGCGACUU AUAUUCUGUAGCA AGGUUAACCGAAU AGGGGAGCCGAAG GGAAACCGAGUCUU AACUGGGCGUUAA GUUGCAGGGUAUA GACCCGAAACCCGG UGAUCUAGCCAUGG GCAGGUUGAAGGU UGGGUAACACUAAC UGGAGGACCGAACC GACUAAUGUUGAA AAAUUAGCGGAUG ACUUGUGGCUGGG GGUGAAAGGCCAA UCAAACCGGGAGAU	Chloramphenicol	Target_lig_228	50S subunit	Target_100	5.69897000433602

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		AGCUGGUUCUCCCC GAAAGCUAUUUAG GUAGCGCCUCGUGA AUUCAUCUCCGGGG GUAGAGCACUGUU UCGGCAAGGGGGUC ACUUACCAACCCGA UGCAAACUGCGAAU ACCGGAGAAUGUU AUCACGGGAGACAC ACGGCGGGUGCUAA CGUCCGUCGUGAAG AGGGAAACAACCCA GACCGCCAGCUAAG GUCCCAAAGUCAUG GUUAAGUGGGAAA CGAUGUGGGAAGG CCCAGACAGCCAGG AUGUUGGCUUAGA AGCAGCCAUCAUUU AAAGAAAGCGUAA UAGCUCACUGGUCG AGUCGGCCUGCGCG GAAGAUGUAACGG GGCUAAACCAUGCA CCGAAGCUGCGGCA GCGACGCUUAUGCG UUGUUGGGUAGGG GAGCGUUCUGUAA GCCUGCGAAGGUGU GCUGUGAGGCAUGC UGGAGGUAUCAGA AGUGCGAAUGCUG ACAUAAGUAACGA UAAAGCGGGUGAA AAGCCCGCUCGCCG GAAGACCAAGGGU UCCUGUCCAACGUU AAUCGGGGCAGGG UGAGUCGACCCCUA AGGCGAGGCCGAAA GGCGUAGUCGAUG GGAAACAGGUUAA UAUUCCUGUACUUG GUGUUACUGCGAA GGGGGGACGGAGA AGGCUAUGUUGGCC GGGCGACGGUUGUC CCGGUUUAAGCGUG UAGGCUGGUUUUCC AGGCAAAUCCGGAA AAUCAAGGCUGAG GCGUGAUGACGAG GCACUACGGUGCUG AAGCAACAAAUGCC CUGCUUCCAGGAAA AGCCUCUAAGCAUC AGGUAACAUCAAA UCGUACCCCAAACC GACACAGGUGGUCA GGUAGAGAAUACC AAGGCGCUUGAGA GAACUCGGGUGAA GGAACUAGGCAAA AUGGUGCCGUAACU UCGGGAGAAGGCAC GCUGAUAUGUAGG UGAGGUCCCUCGCG GAUGGAGCUGAAA UCAGUCGAAGAUAC CAGCUGGCUGCAAC UGUUUAUUAAAAA CACAGCACUGUGCA AACACGAAAGUGG ACGUAUACGGUGU					

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		GACGCCUGCCCGGU GCCGGAAGGUUAA UUGAUGGGGUUAG CGCAAGCGAAGCUC UUGAUCGAAGCCCC GGUAAACGGCGGCC GUAACXAUAACGG UCCUAAGGUAGCGA AAUUCCUUGUCGGG UAAGUUCCGACCUG CACGAAUGGCGUAA UGAUGGCCAGGCUG UCUCCACCCGAGAC UCAGUGAAAUUGA ACUCGCUGUGAAGA UGCAGUGUACCCGC GGCAAGACGGAAA GACCCCGUGAACCU UUACUAUAGCUUG ACACUGAACAUUGA GCCUUGAUGUGUA GGAUAGGUGGGAG GCUUUGAAGUGUG GACGCCAGUCUGCA UGGAGCCGACCUUG AAAUACCACCCUUU AAUGUUUGAUGUU CUAACGUUGACCCG UAAUCCGGGUUGCG GACAGUGUCUGGU GGGUAGUUUGACU GGGGCGGUCUCCUC CUAAAGAGUAACG GAGGAGCACGAAG GUUGGCUAAUCCUG GUCGGACAUCAGGA GGUUAGUGCAAUG GCAUAAGCCAGCUU GACUGCGAGCGUGA CGGCGCGAGCAGGU GCGAAAGCAGGUCA UAGUGAUCCGGUG GUUCUGAAUGGAA GGGCCAUCGCUCAA CGGAUAAAAGGUA CUCCGGGGAUAACA GGCUGAUACCGCCC AAGAGUUCAUAUC GACGGCGGUGUUU GGCACCUCGAUGUC GGCUCAUCACAUCC UGGGGCUGAAGUA GGUCCCAAGGGUAU GGCUGUUCGCCAUU UAAAGUGGUACGC GAGCUGGGUUUAG AACGUCGUGAGACA GUUCGGUCCCUAUC UGCCGUGGGCGCUG GAGAACUGAGGGG GGCUGCUCCUAGUA CGAGAGGACCGGAG UGGACGCAUCACUG GUGUUCGGGUUGU CAUGCCAAUGGCAC UGCCCGGUAGCUAA AUGCGGAAGAGAU AAGUGCUGAAAGC AUCUAAGCACGAAA CUUGCCCCGAGAUG AGUUCUCCCUGACC CUUUAAGGGUCCUG AAGGAACGUUGAA GACGACGACGUUGA UAGGCCGGGUGUG					

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		UAAGCGCAGCGAUG CGUUGAGCUAACCG GUACUAAUGAACCG UGAGGCUUAACCU					
290	CC[C@@H]1C(=O)N2 CCC[C@H]2C(=O)N([C@H] (C(=O)N3CCC(=O)C[C@H]3C(=O)N[C@H] (C(=O)O[C@@H] ([C@@H] (C(=O)N1)NC(=O)C4= C(C=CC=N4)O)C)C5= CC=CC=C5)CC6=CC= C(C=C6)N(C)C)C	GGUUAAGCGACUA AGCGUACACGGUGG AUGCCCUGGCAGUC AGAGGCGAUGAAG GACGUGCUAAUCUG CGAUAAGCGUCGGU AAGGUGAUAUGAA CCGUUAUAACCGGC GAUUUCCGAAUGG GGAAACCCAGUGUG UUUCGACACACUAU CAUUAACUGAAUCC AUAGGUUAAUGAG GCGAACCGGGGGAA CUGAAACAUCUAAG UACCCCGAGGAAAA GAAAUCAACCGAGA UUCCCCCAGUAGCG GCGAGCGAACGGGG AGCAGCCCAGAGCC UGAAUCAGUGUGU GUGUUAGUGGAAG CGUCUGGAAAGGCG CGCGAUACAGGGUG ACAGCCCCGUACAC AAAAAUGCACAUGC UGUGAGCUCGAUG AGUAGGGCGGGAC ACGUGGUAUCCUGU CUGAAUAUGGGGG GACCAUCCUCCAAG GCUAAAUACUCCUG ACUGACCGAUAGUG AACCAGUACCGUGA GGGAAAGGCGAAA AGAACCCCGGCGAG GGGAGUGAAAAAG AACCUGAAACCGUG UACGUACAAGCAGU GGGAGCACGCUUAG GCGUGUGACUGCGU ACCUUUUGUAUAA UGGGUCAGCGACUU AUAUUCUGUAGCA AGGUUAACCGAAU AGGGGAGCCGAAG GGAAACCGAGUCUU AACUGGGCGUUAA GUUGCAGGGUAUA GACCCGAAACCCGG UGAUCUAGCCAUGG GCAGGUUGAAGGU UGGGUAACACUAAC UGGAGGACCGAACC GACUAAUGUUGAA AAAUUAGCGGAUG ACUUGUGGCUGGG GGUGAAAGGCCAA UCAAACCGGGAGAU AGCUGGUUCUCCCC GAAAGCUAUUUAG GUAGCGCCUCGUGA AUUCAUCUCCGGGG GUAGAGCACUGUU UCGGCAAGGGGGUC ACUUACCAACCCGA UGCAAACUGCGAAU ACCGGAGAAUGUU AUCACGGGAGACAC ACGGCGGGUGCUAA CGUCCGUCGUGAAG	Streptogramin_B	Target_lig_229	50S subunit	Target_100	7.22914798835786

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		AGGGAAACAACCCA GACCGCCAGCUAAG GUCCCAAAGUCAUG GUUAAGUGGGAAA CGAUGUGGGAAGG CCCAGACAGCCAGG AUGUUGGCUUAGA AGCAGCCAUCAUUU AAAGAAAGCGUAA UAGCUCACUGGUCG AGUCGGCCUGCGCG GAAGAUGUAACGG GGCUAAACCAUGCA CCGAAGCUGCGGCA GCGACGCUUAUGCG UUGUUGGGUAGGG GAGCGUUCUGUAA GCCUGCGAAGGUGU GCUGUGAGGCAUGC UGGAGGUAUCAGA AGUGCGAAUGCUG ACAUAAGUAACGA UAAAGCGGGUGAA AAGCCCGCUCGCCG GAAGACCAAGGGU UCCUGUCCAACGUU AAUCGGGGCAGGG UGAGUCGACCCCUA AGGCGAGGCCGAAA GGCGUAGUCGAUG GGAAACAGGUUAA UAUUCCUGUACUUG GUGUUACUGCGAA GGGGGGACGGAGA AGGCUAUGUUGGCC GGGCGACGGUUGUC CCGGUUUAAGCGUG UAGGCUGGUUUUCC AGGCAAAUCCGGAA AAUCAAGGCUGAG GCGUGAUGACGAG GCACUACGGUGCUG AAGCAACAAAUGCC CUGCUUCCAGGAAA AGCCUCUAAGCAUC AGGUAACAUCAAA UCGUACCCCAAACC GACACAGGUGGUCA GGUAGAGAAUACC AAGGCGCUUGAGA GAACUCGGGUGAA GGAACUAGGCAAA AUGGUGCCGUAACU UCGGGAGAAGGCAC GCUGAUAUGUAGG UGAGGUCCCUCGCG GAUGGAGCUGAAA UCAGUCGAAGAUAC CAGCUGGCUGCAAC UGUUUAUUAAAAA CACAGCACUGUGCA AACACGAAAGUGG ACGUAUACGGUGU GACGCCUGCCCGGU GCCGGAAGGUUAA UUGAUGGGGUUAG CGCAAGCGAAGCUC UUGAUCGAAGCCCC GGUAAACGGCGGCC GUAACXAUAACGG UCCUAAGGUAGCGA AAUUCCUUGUCGGG UAAGUUCCGACCUG CACGAAUGGCGUAA UGAUGGCCAGGCUG					

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		UCUCCACCCGAGAC UCAGUGAAAUUGA ACUCGCUGUGAAGA UGCAGUGUACCCGC GGCAAGACGGAAA GACCCCGUGAACCU UUACUAUAGCUUG ACACUGAACAUUGA GCCUUGAUGUGUA GGAUAGGUGGGAG GCUUUGAAGUGUG GACGCCAGUCUGCA UGGAGCCGACCUUG AAAUACCACCCUUU AAUGUUUGAUGUU CUAACGUUGACCCG UAAUCCGGGUUGCG GACAGUGUCUGGU GGGUAGUUUGACU GGGGCGGUCUCCUC CUAAAGAGUAACG GAGGAGCACGAAG GUUGGCUAAUCCUG GUCGGACAUCAGGA GGUUAGUGCAAUG GCAUAAGCCAGCUU GACUGCGAGCGUGA CGGCGCGAGCAGGU GCGAAAGCAGGUCA UAGUGAUCCGGUG GUUCUGAAUGGAA GGGCCAUCGCUCAA CGGAUAAAAGGUA CUCCGGGGAUAACA GGCUGAUACCGCCC AAGAGUUCAUAUC GACGGCGGUGUUU GGCACCUCGAUGUC GGCUCAUCACAUCC UGGGGCUGAAGUA GGUCCCAAGGGUAU GGCUGUUCGCCAUU UAAAGUGGUACGC GAGCUGGGUUUAG AACGUCGUGAGACA GUUCGGUCCCUAUC UGCCGUGGGCGCUG GAGAACUGAGGGG GGCUGCUCCUAGUA CGAGAGGACCGGAG UGGACGCAUCACUG GUGUUCGGGUUGU CAUGCCAAUGGCAC UGCCCGGUAGCUAA AUGCGGAAGAGAU AAGUGCUGAAAGC AUCUAAGCACGAAA CUUGCCCCGAGAUG AGUUCUCCCUGACC CUUUAAGGGUCCUG AAGGAACGUUGAA GACGACGACGUUGA UAGGCCGGGUGUG UAAGCGCAGCGAUG CGUUGAGCUAACCG GUACUAAUGAACCG UGAGGCUUAACCU					
291	CC1CC(=O)C2(C(O1)OC3C(C(C(C(C3O2)NC)O)NC)O)O	AAAUUGAAGAGUU UGAUCAUGGCUCAG AUUGAACGCUGGCG GCAGGCCUAACACA UGCAAGUCGAACGG UAACAGGAAGAAG CUUGCUUCUUUGCU GACGAGUGGCGGAC	Spectinomycin	Target_lig_75	Small subunit	Target_101	6.58502665202918

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		GGGUGAGUAAUGU CUGGGAAACUGCCU GAUGGAGGGGGAU AACUACUGGAAACG GUAGCUAAUACCGC AUAACGUCGCAAGA CCAAAGAGGGGGAC CUUCGGGCCUCUUG CCAUCGGAUGUGCC CAGAUGGGAUUAG CUAGUAGGUGGGG UAACGGCUCACCUA GGCGACGAUCCCUA GCUGGUCUGAGAG GAUGACCAGCCACA CUGGAACUGAGACA CGGUCCAGACUCCU ACGGGAGGCAGCAG UGGGGAAUAUUGC ACAAUGGGCGCAAG CCUGAUGCAGCCAU GCCGCGUGUAUGAA GAAGGCCUUCGGGU UGUAAAGUACUUU CAGCGGGGAGGAA GGGAGUAAAGUUA AUACCUUUGCUCAU UGACGUUACCCGCA GAAGAAGCACCGGC UAACUCCGUGCCAG CAGCCGCGGUAAUA CGGAGGGUGCAAGC GUUAAUCGGAAUU ACUGGGCGUAAAGC GCACGCAGGCGGUU UGUUAAGUCAGAU GUGAAAUCCCCGGG CUCAACCUGGGAAC UGCAUCUGAUACUG GCAAGCUUGAGUCU CGUAGAGGGGGGU AGAAUUCCAGGUG UAGCGGUGAAAUG CGUAGAGAUCUGG AGGAAUACCGGUG GCGAAGGCGGCCCC CUGGACGAAGACUG ACGCUCAGGUGCGA AAGCGUGGGGAGC AAACAGGAUUAGA UACCCUGGUAGUCC ACGCCGUAAACGAU GUCGACUUGGAGG UUGUGCCCUUGAGG CGUGGCUUCCGGAG CUAACGCGUUAAGU CGACCGCCUGGGGA GUACGGCCGCAAGG UUAAAACUCAAAU GAAUUGACGGGGG CCCGCACAAGCGGU GGAGCAUGUGGUU UAAUUCGAUGCAAC GCGAAGAACCUUAC CUGGUCUUGACAUC CACGGAAGUUUUCA GAGAUGAGAAUGU GCCUUCGGGAACCG UGAGACAGGUGCU GCAUGGCUGUCGUC AGCUCGUGUUGUG AAAUGUUGGGUUA AGUCCCGCAACGAG CGCAACCCUUAUCC UUUGUUGCCAGCGG					

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		UCCGGCCGGGAACU CAAAGGAGACUGCC AGUGAUAAACUGG AGGAAGGUGGGGA UGACGUCAAGUCAU CAUGGCCCUUACGA CCAGGGCUACACAC GUGCUACAAUGGCG CAUACAAAGAGAA GCGACCUCGCGAGA GCAAGCGGACCUCA UAAAGUGCGUCGU AGUCCGGAUUGGA GUCUGCAACUCGAC UCCAUGAAGUCGGA AUCGCUAGUAAUCG UGGAUCAGAAUGCC ACGGUGAAUACGU UCCCGGGCCUUGUA CACACCGCCCGUCA CACCAUGGGAGUGG GUUGCAAAAGAAG UAGGUAGCUUAACC UUCGGGAGGGCGCU UACCACUUUGUGAU UCAUGACUGGGGU GAAGUCGUAACAA GGUAACCGUAGGG GAACCUGCGGUUGG AUCACCUCCUUA					
292	CN(C)C1C2CC3CC4=C(C=CC(=C4C(=C3C(=O)C2(C(=C(C1=O)C(=O)N)O)O)O)O)N(C)C	AAAUUGAAGAGUU UGAUCAUGGCUCAG AUUGAACGCUGGCG GCAGGCCUAACACA UGCAAGUCGAACGG UAACAGGAAGAAG CUUGCUUCUUUGCU GACGAGUGGCGGAC GGGUGAGUAAUGU CUGGGAAACUGCCU GAUGGAGGGGGAU AACUACUGGAAACG GUAGCUAAUACCGC AUAACGUCGCAAGA CCAAAGAGGGGGAC CUUCGGGCCUCUUG CCAUCGGAUGUGCC CAGAUGGGAUUAG CUAGUAGGUGGGG UAACGGCUCACCUA GGCGACGAUCCCUA GCUGGUCUGAGAG GAUGACCAGCCACA CUGGAACUGAGACA CGGUCCAGACUCCU ACGGGAGGCAGCAG UGGGGAAUAUUGC ACAAUGGGCGCAAG CCUGAUGCAGCCAU GCCGCGUGUAUGAA GAAGGCCUUCGGGU UGUAAAGUACUUU CAGCGGGGAGGAA GGGAGUAAAGUUA AUACCUUUGCUCAU UGACGUUACCCGCA GAAGAAGCACCGGC UAACUCCGUGCCAG CAGCCGCGGUAAUA CGGAGGGUGCAAGC GUUAAUCGGAAUU ACUGGGCGUAAAGC GCACGCAGGCGGUU UGUUAAGUCAGAU GUGAAAUCCCCGGG	Minocycline	Target_lig_230	Small subunit	Target_101	7

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		CUCAACCUGGGAAC UGCAUCUGAUACUG GCAAGCUUGAGUCU CGUAGAGGGGGGU AGAAUUCCAGGUG UAGCGGUGAAAUG CGUAGAGAUCUGG AGGAAUACCGGUG GCGAAGGCGGCCCC CUGGACGAAGACUG ACGCUCAGGUGCGA AAGCGUGGGGAGC AAACAGGAUUAGA UACCCUGGUAGUCC ACGCCGUAAACGAU GUCGACUUGGAGG UUGUGCCCUUGAGG CGUGGCUUCCGGAG CUAACGCGUUAAGU CGACCGCCUGGGGA GUACGGCCGCAAGG UUAAAACUCAAAU GAAUUGACGGGGG CCCGCACAAGCGGU GGAGCAUGUGGUU UAAUUCGAUGCAAC GCGAAGAACCUUAC CUGGUCUUGACAUC CACGGAAGUUUUCA GAGAUGAGAAUGU GCCUUCGGGAACCG UGAGACAGGUGCU GCAUGGCUGUCGUC AGCUCGUGUUGUG AAAUGUUGGGUUA AGUCCCGCAACGAG CGCAACCCUUAUCC UUUGUUGCCAGCGG UCCGGCCGGGAACU CAAAGGAGACUGCC AGUGAUAAACUGG AGGAAGGUGGGGA UGACGUCAAGUCAU CAUGGCCCUUACGA CCAGGGCUACACAC GUGCUACAAUGGCG CAUACAAAGAGAA GCGACCUCGCGAGA GCAAGCGGACCUCA UAAAGUGCGUCGU AGUCCGGAUUGGA GUCUGCAACUCGAC UCCAUGAAGUCGGA AUCGCUAGUAAUCG UGGAUCAGAAUGCC ACGGUGAAUACGU UCCCGGGCCUUGUA CACACCGCCCGUCA CACCAUGGGAGUGG GUUGCAAAAGAAG UAGGUAGCUUAACC UUCGGGAGGGCGCU UACCACUUUGUGAU UCAUGACUGGGGU GAAGUCGUAACAA GGUAACCGUAGGG GAACCUGCGGUUGG AUCACCUCCUUA					
293	CC(C) (C)NCC(=O)NC1=CC(=C2CC3CC4C(C(=O)C (=C(C4(C(=O)C3=C(C 2=C1O)O)O)O)C(=O) N)N(C)C)N(C)C	AAAUUGAAGAGUU UGAUCAUGGCUCAG AUUGAACGCUGGCG GCAGGCCUAACACA UGCAAGUCGAACGG UAACAGGAAGAAG CUUGCUUCUUUGCU	Tigecycline_mol	Target_lig_231	Small subunit	Target_101	8

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		GACGAGUGGCGGAC GGGUGAGUAAUGU CUGGGAAACUGCCU GAUGGAGGGGGAU AACUACUGGAAACG GUAGCUAAUACCGC AUAACGUCGCAAGA CCAAAGAGGGGGAC CUUCGGGCCUCUUG CCAUCGGAUGUGCC CAGAUGGGAUUAG CUAGUAGGUGGGG UAACGGCUCACCUA GGCGACGAUCCCUA GCUGGUCUGAGAG GAUGACCAGCCACA CUGGAACUGAGACA CGGUCCAGACUCCU ACGGGAGGCAGCAG UGGGGAAUAUUGC ACAAUGGGCGCAAG CCUGAUGCAGCCAU GCCGCGUGUAUGAA GAAGGCCUUCGGGU UGUAAAGUACUUU CAGCGGGGAGGAA GGGAGUAAAGUUA AUACCUUUGCUCAU UGACGUUACCCGCA GAAGAAGCACCGGC UAACUCCGUGCCAG CAGCCGCGGUAAUA CGGAGGGUGCAAGC GUUAAUCGGAAUU ACUGGGCGUAAAGC GCACGCAGGCGGUU UGUUAAGUCAGAU GUGAAAUCCCCGGG CUCAACCUGGGAAC UGCAUCUGAUACUG GCAAGCUUGAGUCU CGUAGAGGGGGGU AGAAUUCCAGGUG UAGCGGUGAAAUG CGUAGAGAUCUGG AGGAAUACCGGUG GCGAAGGCGGCCCC CUGGACGAAGACUG ACGCUCAGGUGCGA AAGCGUGGGGAGC AAACAGGAUUAGA UACCCUGGUAGUCC ACGCCGUAAACGAU GUCGACUUGGAGG UUGUGCCCUUGAGG CGUGGCUUCCGGAG CUAACGCGUUAAGU CGACCGCCUGGGGA GUACGGCCGCAAGG UUAAAACUCAAAU GAAUUGACGGGGG CCCGCACAAGCGGU GGAGCAUGUGGUU UAAUUCGAUGCAAC GCGAAGAACCUUAC CUGGUCUUGACAUC CACGGAAGUUUUCA GAGAUGAGAAUGU GCCUUCGGGAACCG UGAGACAGGUGCU GCAUGGCUGUCGUC AGCUCGUGUUGUG AAAUGUUGGGUUA AGUCCCGCAACGAG CGCAACCCUUAUCC					

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		UUUGUUGCCAGCGG UCCGGCCGGGAACU CAAAGGAGACUGCC AGUGAUAAACUGG AGGAAGGUGGGGA UGACGUCAAGUCAU CAUGGCCCUUACGA CCAGGGCUACACAC GUGCUACAAUGGCG CAUACAAAGAGAA GCGACCUCGCGAGA GCAAGCGGACCUCA UAAAGUGCGUCGU AGUCCGGAUUGGA GUCUGCAACUCGAC UCCAUGAAGUCGGA AUCGCUAGUAAUCG UGGAUCAGAAUGCC ACGGUGAAUACGU UCCCGGGCCUUGUA CACACCGCCCGUCA CACCAUGGGAGUGG GUUGCAAAAGAAG UAGGUAGCUUAACC UUCGGGAGGGCGCU UACCACUUUGUGAU UCAUGACUGGGGU GAAGUCGUAACAA GGUAACCGUAGGG GAACCUGCGGUUGG AUCACCUCCUUA					
294	CCC1C(C(C(C(=O)C(CC(C(C(C(C(=O)O1)C)OC2CC(C(C(O2)C)O) (C)OC)C)OC3C(C(CC(O3)C)N(C)C)O) (C)OC)C)C)O)(C)O	UUGGCUACUAUGCC AGCUGGUGGAUUG CUCGGCUCAGGCGC UGAUGAAGGACGU GCCAAGCUGCGAUA AGCCAUGGGGAGCC GCACGGAGGCGAAG AACCAUGGAUUUCC GAAUGAGAAUCUC UCUAACAAUUGCUU CGCGCAAUGAGGAA CCCCGAGAACUGAA ACAUCUCAGUAUCG GGAGGAACAGAAA ACGCAAUGUGAUG UCGUUAGUAACCGC GAGUGAACGCGAU ACAGCCCAAACCGA AGCCCUCACGGGCA AUGUGGUGUCAGG GCUACCUCUCAUCA GCCGACCGUCUCGA CGAAGUCUCUUGGA ACAGAGCGUGAUAC AGGGUGACAACCCC GUACUCGAGACCAG UACGACGUGCGGUA GUGCCAGAGUAGCG GGGGUUGGAUAUC CCUCGCGAAUAACG CAGGCAUCGACUGC GAAGGCUAAACACA ACCUGAGACCGAUA GUGAACAAGUAGU GUGAACGAACGCUG CAAAGUACCCUCAG AAGGGAGGCGAAA UAGAGCAUGAAAU CAGUUGGCGAUCGA GCGACAGGGCAUAC AAGGUCCCUCGACG AAUGACCGACGCGC GAGCGUCCAGUAAG ACUCACGGGAAGCC	Clarithromycin	Target_lig_232	PTC	Target_99	8.20760831050175

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		GAUGUUCUGUCGU ACGUUUUGAAAAA CGAGCCAGGGAGUG UGUCUGCAUGGCAA GUCUAACCGGAGUA UCCGGGGAGGCACA GGGAAACCGACAUG GCCGCAGGGCUUUG CCCGAGGGCCGCCG UCUUCAAGGGCGGG GAGCCAUGUGGACA CGACCCGAAUCCGG ACGAUCUACGCAUG GACAAGAUGAAGC GUGCCGAAAGGCAC GUGGAAGUCUGUU AGAGUUGGUGUCC UACAAUACCCUCUC GUGAUCUAUGUGU AGGGGUGAAAGGC CCAUCGAGUCCGGC AACAGCUGGUUCCA AUCGAAACAUGUCG AAGCAUGACCUCCG CCGAGGUAGUCUGU GAGGUAGAGCGACC GAUUGGUGUGUCC GCCUCCGAGAGGAG UCGGCACACCUGUC AAACUCCAAACUUA CAGACGCCGUUUGA CGCGGGGAUUCCGG UGCGCGGGGUAAGC CUGUGUACCAGGAG GGGAACAACCCAGA GAUAGGUUAAGGU CCCCAAGUGUGGAU UAAGUGUAAUCCUC UGAAGGUGGUCUC GAGCCCUAGACAGC CGGGAGGUGAGCU UAGAAGCAGCUACC CUCUAAGAAAAGCG UAACAGCUUACCGG CCGAGGUUUGAGGC GCCCAAAAUGAUCG GGACUCAAAUCCAC CACCGAGACCUGUC CGUACCACUCAUAC UGGUAAUCGAGUA GAUUGGCGCUCUAA UUGGAUGGAAGUA GGGGUGAAAACUCC UAUGGACCGAUUA GUGACGAAAAUCCU GGCCAUAGUAGCAG CGAUAGUCGGGUG AGAACCCCGACGGC CUAAUGGAUAAGG GUUCCUCAGCACUG CUGAUCAGCUGAGG GUUAGCCGGUCCUA AGUCAUACCGCAAC UCGACUAUGACGAA AUGGGAAACGGGU UAAUAUUCCCGUGC CACUAUGCAGUGAA AGUUGACGCCCUGG GGUCGAUCACGCUG GGCAUUCGCCCAGU CGAACCGUCCAACU CCGUGGAAGCCGUA AUGGCAGGAAGCG GACGAACGGCGGCA UAGGGAAACGUGA					

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		UUCAACCUGGGGCC CAUGAAAAGACGA GCAUAGUGUCCGUA CCGAGAACCGACAC AGGUGUCCAUGGCG GCGAAAGCCAAGGC CUGUCGGGAGCAAC CAACGUUAGGGAA UUCGGCAAGUUAG UCCCGUACCUUCGG AAGAAGGGAUGCC UGCUCCGGAACGGA GCAGGUCGCAGUGA CUCGGAAGCUCGGA CUGUCUAGUAACAA CAUAGGUGACCGCA AAUCCGCAAGGACU CGUACGGUCACUGA AUCCUGCCCAGUGC AGGUAUCUGAACAC CUCGUACAAGAGGA CGAAGGACCUGUCA ACGGCGGGGGUAAC UAUGACCCUCUUAA GGUAGCGUAGUACC UUGCCGCAUCAGUA GCGGCUUGCAUGAA UGGAUUAACCAGA GCUUCACUGUCCCA ACGUUGGGCCCGGU GAACUGUACAUUCC AGUGCGGAGUCUG GAGACACCCAGGGG GAAGCGAAGACCCU AUGGAGCUUUACU GCAGGCUGUCGCUG AGACGUGGUCGCCG AUGUGCAGCAUAG GUAGGAGACACUAC ACAGGUACCCGCGC UAGCGGGCCACCGA GUCAACAGUGAAA UACUACCCGUCGGU GACUGCGACUCUCA CUCCGGGAGGAGGA CACCGAUAGCCGGG CAGUUUGACUGGG GCGGUACGCGCUCG AAAAGAUAUCGAG CGCGCCCUAUGGCU AUCUCAGCCGGGAC AGAGACCCGGCGAA GAGUGCAAGAGCA AAAGAUAGCUUGA CAGUGUUCUUCCCA ACGAGGAACGCUGA CGCGAAAGCGUGGU CUAGCGAACCAAUU AGCCUGCUUGAUGC GGGCAAUUGAUGA CAGAAAAGCUACCC UAGGGAUAACAGA GUCGUCACUCGCAA GAGCACAUAUCGAC CGAGUGGCUUGCUA CCUCGAUGUCGGUU CCCUCCAUCCUGCC CGUGCAGAAGCGGG CAAGGGUGAGGUU GUUCGCCUAUUAAA GGAGGUCGUGAGC UGGGUUUAGACCG UCGUGAGACAGGUC GGCUGCUAUCUACU GGGUGUGUAAUGG					

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		UGUCUGACAAGAAC GACCGUAUAGUACG AGAGGAACUACGG UUGGUGGCCACUGG UGUACCGGUUGUUC GAGAGAGCACGUGC CGGGUAGCCACGCC ACACGGGGUAAGA GCUGAACGCAUCUA AGCUCGAAACCCAC UUGGAAAAGAGAC ACCGCCGAGGUCCC GCGUACAAGACGCG GUCGAUAGACUCGG GGUGUGCGCGUCGA GGUAACGAGACGU UAAGCCCACGAGCA CUAACAGACCAAAG CCAUCAU					
295	CCC1C(C(C(C(=O)C(CC(C(C(C(C(=O)O1)C)OC2CC(C(C(O2)C)O)(C)OC)C)OC3C(C(CC(O3)C)N(C)C)O)(C)O)C)C)O)(C)O	UUGGCUACUAUGCC AGCUGGUGGAUUG CUCGGCUCAGGCGC UGAUGAAGGACGU GCCAAGCUGCGAUA AGCCAUGGGGAGCC GCACGGAGGCGAAG AACCAUGGAUUUCC GAAUGAGAAUCUC UCUAACAAUUGCUU CGCGCAAUGAGGAA CCCCGAGAACUGAA ACAUCUCAGUAUCG GGAGGAACAGAAA ACGCAAUGUGAUG UCGUUAGUAACCGC GAGUGAACGCGAU ACAGCCCAAACCGA AGCCCUCACGGGCA AUGUGGUGUCAGG GCUACCUCUCAUCA GCCGACCGUCUCGA CGAAGUCUCUUGGA ACAGAGCGUGAUAC AGGGUGACAACCCC GUACUCGAGACCAG UACGACGUGCGGUA GUGCCAGAGUAGCG GGGGUUGGAUAUC CCUCGCGAAUAACG CAGGCAUCGACUGC GAAGGCUAAACACA ACCUGAGACCGAUA GUGAACAAGUAGU GUGAACGAACGCUG CAAAGUACCCUCAG AAGGGAGGCGAAA UAGAGCAUGAAAU CAGUUGGCGAUCGA GCGACAGGGCAUAC AAGGUCCCUCGACG AAUGACCGACGCGC GAGCGUCCAGUAAG ACUCACGGGAAGCC GAUGUUCUGUCGU ACGUUUUGAAAAA CGAGCCAGGGAGUG UGUCUGCAUGGCAA GUCUAACCGGAGUA UCCGGGGAGGCACA GGGAAACCGACAUG GCCGCAGGGCUUUG CCCGAGGGCCGCCG UCUUCAAGGGCGGG GAGCCAUGUGGACA CGACCCGAAUCCGG	Eryrthromycin	Target_lig_233	PTC	Target_99	6.00436480540245

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		ACGAUCUACGCAUG GACAAGAUGAAGC GUGCCGAAAGGCAC GUGGAAGUCUGUU AGAGUUGGUGUCC UACAAUACCCUCUC GUGAUCUAUGUGU AGGGGUGAAAGGC CCAUCGAGUCCGGC AACAGCUGGUUCCA AUCGAAACAUGUCG AAGCAUGACCUCCG CCGAGGUAGUCUGU GAGGUAGAGCGACC GAUUGGUGUGUCC GCCUCCGAGAGGAG UCGGCACACCUGUC AAACUCCAAACUUA CAGACGCCGUUUGA CGCGGGGAUUCCGG UGCGCGGGGUAAGC CUGUGUACCAGGAG GGGAACAACCCAGA GAUAGGUUAAGGU CCCCAAGUGUGGAU UAAGUGUAAUCCUC UGAAGGUGGUCUC GAGCCCUAGACAGC CGGGAGGUGAGCU UAGAAGCAGCUACC CUCUAAGAAAAGCG UAACAGCUUACCGG CCGAGGUUUGAGGC GCCCAAAAUGAUCG GGACUCAAAUCCAC CACCGAGACCUGUC CGUACCACUCAUAC UGGUAAUCGAGUA GAUUGGCGCUCUAA UUGGAUGGAAGUA GGGGUGAAAACUCC UAUGGACCGAUUA GUGACGAAAAUCCU GGCCAUAGUAGCAG CGAUAGUCGGGUG AGAACCCCGACGGC CUAAUGGAUAAGG GUUCCUCAGCACUG CUGAUCAGCUGAGG GUUAGCCGGUCCUA AGUCAUACCGCAAC UCGACUAUGACGAA AUGGGAAACGGGU UAAUAUUCCCGUGC CACUAUGCAGUGAA AGUUGACGCCCUGG GGUCGAUCACGCUG GGCAUUCGCCCAGU CGAACCGUCCAACU CCGUGGAAGCCGUA AUGGCAGGAAGCG GACGAACGGCGGCA UAGGGAAACGUGA UUCAACCUGGGGCC CAUGAAAAGACGA GCAUAGUGUCCGUA CCGAGAACCGACAC AGGUGUCCAUGGCG GCGAAAGCCAAGGC CUGUCGGGAGCAAC CAACGUUAGGGAA UUCGGCAAGUUAG UCCCGUACCUUCGG AAGAAGGGAUGCC UGCUCCGGAACGGA					

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		GCAGGUCGCAGUGA CUCGGAAGCUCGGA CUGUCUAGUAACAA CAUAGGUGACCGCA AAUCCGCAAGGACU CGUACGGUCACUGA AUCCUGCCCAGUGC AGGUAUCUGAACAC CUCGUACAAGAGGA CGAAGGACCUGUCA ACGGCGGGGGUAAC UAUGACCCUCUUAA GGUAGCGUAGUACC UUGCCGCAUCAGUA GCGGCUUGCAUGAA UGGAUUAACCAGA GCUUCACUGUCCCA ACGUUGGGCCCGGU GAACUGUACAUUCC AGUGCGGAGUCUG GAGACACCCAGGGG GAAGCGAAGACCCU AUGGAGCUUUACU GCAGGCUGUCGCUG AGACGUGGUCGCCG AUGUGCAGCAUAG GUAGGAGACACUAC ACAGGUACCCGCGC UAGCGGGCCACCGA GUCAACAGUGAAA UACUACCCGUCGGU GACUGCGACUCUCA CUCCGGGAGGAGGA CACCGAUAGCCGGG CAGUUUGACUGGG GCGGUACGCGCUCG AAAAGAUAUCGAG CGCGCCCUAUGGCU AUCUCAGCCGGGAC AGAGACCCGGCGAA GAGUGCAAGAGCA AAAGAUAGCUUGA CAGUGUUCUUCCCA ACGAGGAACGCUGA CGCGAAAGCGUGGU CUAGCGAACCAAUU AGCCUGCUUGAUGC GGGCAAUUGAUGA CAGAAAAGCUACCC UAGGGAUAACAGA GUCGUCACUCGCAA GAGCACAUAUCGAC CGAGUGGCUUGCUA CCUCGAUGUCGGUU CCCUCCAUCCUGCC CGUGCAGAAGCGGG CAAGGGUGAGGUU GUUCGCCUAUUAAA GGAGGUCGUGAGC UGGGUUUAGACCG UCGUGAGACAGGUC GGCUGCUAUCUACU GGGUGUGUAAUGG UGUCUGACAAGAAC GACCGUAUAGUACG AGAGGAACUACGG UUGGUGGCCACUGG UGUACCGGUUGUUC GAGAGAGCACGUGC CGGGUAGCCACGCC ACACGGGGUAAGA GCUGAACGCAUCUA AGCUCGAAACCCAC UUGGAAAAGAGAC ACCGCCGAGGUCCC					

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		GCGUACAAGACGCG GUCGAUAGACUCGG GGUGUGCGCGUCGA GGUAACGAGACGU UAAGCCCACGAGCA CUAACAGACCAAAG CCAUCAU					
296	CC1C=CC(=O)NCC=C C(=CC(CC(=O)CC2=N C(=CO2)C(=O)N3CCC =C3C(=O)OC1C(C)C) O)C	UUGGCUACUAUGCC AGCUGGUGGAUUG CUCGGCUCAGGCGC UGAUGAAGGACGU GCCAAGCUGCGAUA AGCCAUGGGGAGCC GCACGGAGGCGAAG AACCAUGGAUUUCC GAAUGAGAAUCUC UCUAACAAUUGCUU CGCGCAAUGAGGAA CCCCGAGAACUGAA ACAUCUCAGUAUCG GGAGGAACAGAAA ACGCAAUGUGAUG UCGUUAGUAACCGC GAGUGAACGCGAU ACAGCCCAAACCGA AGCCCUCACGGGCA AUGUGGUGUCAGG GCUACCUCUCAUCA GCCGACCGUCUCGA CGAAGUCUCUUGGA ACAGAGCGUGAUAC AGGGUGACAACCCC GUACUCGAGACCAG UACGACGUGCGGUA GUGCCAGAGUAGCG GGGGUUGGAUAUC CCUCGCGAAUAACG CAGGCAUCGACUGC GAAGGCUAAACACA ACCUGAGACCGAUA GUGAACAAGUAGU GUGAACGAACGCUG CAAAGUACCCUCAG AAGGGAGGCGAAA UAGAGCAUGAAAU CAGUUGGCGAUCGA GCGACAGGGCAUAC AAGGUCCCUCGACG AAUGACCGACGCGC GAGCGUCCAGUAAG ACUCACGGGAAGCC GAUGUUCUGUCGU ACGUUUUGAAAAA CGAGCCAGGGAGUG UGUCUGCAUGGCAA GUCUAACCGGAGUA UCCGGGGAGGCACA GGGAAACCGACAUG GCCGCAGGGCUUUG CCCGAGGGCCGCCG UCUUCAAGGGCGGG GAGCCAUGUGGACA CGACCCGAAUCCGG ACGAUCUACGCAUG GACAAGAUGAAGC GUGCCGAAAGGCAC GUGGAAGUCUGUU AGAGUUGGUGUCC UACAAUACCCUCUC GUGAUCUAUGUGU AGGGGUGAAAGGC CCAUCGAGUCCGGC AACAGCUGGUUCCA AUCGAAACAUGUCG AAGCAUGACCUCCG	Pristinamycin IIA	Target_lig_234	PTC	Target_99	6.85387196432176

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		CCGAGGUAGUCUGU GAGGUAGAGCGACC GAUUGGUGUGUCC GCCUCCGAGAGGAG UCGGCACACCUGUC AAACUCCAAACUUA CAGACGCCGUUUGA CGCGGGGAUUCCGG UGCGCGGGGUAAGC CUGUGUACCAGGAG GGGAACAACCCAGA GAUAGGUUAAGGU CCCCAAGUGUGGAU UAAGUGUAAUCCUC UGAAGGUGGUCUC GAGCCCUAGACAGC CGGGAGGUGAGCU UAGAAGCAGCUACC CUCUAAGAAAAGCG UAACAGCUUACCGG CCGAGGUUUGAGGC GCCCAAAAUGAUCG GGACUCAAAUCCAC CACCGAGACCUGUC CGUACCACUCAUAC UGGUAAUCGAGUA GAUUGGCGCUCUAA UUGGAUGGAAGUA GGGGUGAAAACUCC UAUGGACCGAUUA GUGACGAAAAUCCU GGCCAUAGUAGCAG CGAUAGUCGGGUG AGAACCCCGACGGC CUAAUGGAUAAGG GUUCCUCAGCACUG CUGAUCAGCUGAGG GUUAGCCGGUCCUA AGUCAUACCGCAAC UCGACUAUGACGAA AUGGGAAACGGGU UAAUAUUCCCGUGC CACUAUGCAGUGAA AGUUGACGCCCUGG GGUCGAUCACGCUG GGCAUUCGCCCAGU CGAACCGUCCAACU CCGUGGAAGCCGUA AUGGCAGGAAGCG GACGAACGGCGGCA UAGGGAAACGUGA UUCAACCUGGGGCC CAUGAAAAGACGA GCAUAGUGUCCGUA CCGAGAACCGACAC AGGUGUCCAUGGCG GCGAAAGCCAAGGC CUGUCGGGAGCAAC CAACGUUAGGGAA UUCGGCAAGUUAG UCCCGUACCUUCGG AAGAAGGGAUGCC UGCUCCGGAACGGA GCAGGUCGCAGUGA CUCGGAAGCUCGGA CUGUCUAGUAACAA CAUAGGUGACCGCA AAUCCGCAAGGACU CGUACGGUCACUGA AUCCUGCCCAGUGC AGGUAUCUGAACAC CUCGUACAAGAGGA CGAAGGACCUGUCA ACGGCGGGGGUAAC UAUGACCCUCUUAA					

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		GGUAGCGUAGUACC UUGCCGCAUCAGUA GCGGCUUGCAUGAA UGGAUUAACCAGA GCUUCACUGUCCCA ACGUUGGGCCCGGU GAACUGUACAUUCC AGUGCGGAGUCUG GAGACACCCAGGGG GAAGCGAAGACCCU AUGGAGCUUUACU GCAGGCUGUCGCUG AGACGUGGUCGCCG AUGUGCAGCAUAG GUAGGAGACACUAC ACAGGUACCCGCGC UAGCGGGCCACCGA GUCAACAGUGAAA UACUACCCGUCGGU GACUGCGACUCUCA CUCCGGGAGGAGGA CACCGAUAGCCGGG CAGUUUGACUGGG GCGGUACGCGCUCG AAAAGAUAUCGAG CGCGCCCUAUGGCU AUCUCAGCCGGGAC AGAGACCCGGCGAA GAGUGCAAGAGCA AAAGAUAGCUUGA CAGUGUUCUUCCCA ACGAGGAACGCUGA CGCGAAAGCGUGGU CUAGCGAACCAAUU AGCCUGCUUGAUGC GGGCAAUUGAUGA CAGAAAAGCUACCC UAGGGAUAACAGA GUCGUCACUCGCAA GAGCACAUAUCGAC CGAGUGGCUUGCUA CCUCGAUGUCGGUU CCCUCCAUCCUGCC CGUGCAGAAGCGGG CAAGGGUGAGGUU GUUCGCCUAUUAAA GGAGGUCGUGAGC UGGGUUUAGACCG UCGUGAGACAGGUC GGCUGCUAUCUACU GGGUGUGUAAUGG UGUCUGACAAGAAC GACCGUAUAGUACG AGAGGAACUACGG UUGGUGGCCACUGG UGUACCGGUUGUUC GAGAGAGCACGUGC CGGGUAGCCACGCC ACACGGGGUAAGA GCUGAACGCAUCUA AGCUCGAAACCCAC UUGGAAAAGAGAC ACCGCCGAGGUCCC GCGUACAAGACGCG GUCGAUAGACUCGG GGUGUGCGCGUCGA GGUAACGAGACGU UAAGCCCACGAGCA CUAACAGACCAAAG CCAUCAU					
297	CCC1C(=O)N2CCCC2C(=O)N(C(C(=O)N3CC(C(=O)CC3C(=O)NC(C(=O)OC(C(C(=O)N1)NC(=O)C4=C(C=CC=	UUGGCUACUAUGCC AGCUGGUGGAUUG CUCGGCUCAGGCGC UGAUGAAGGACGU GCCAAGCUGCGAUA	Quinupristin	Target_lig_235	PTC	Target_99	6.49485002168009

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	N4)O)C)C5=CC=CC=C5)CSC6CN7CCC6CC7)CC8=CC=C(C=C8)N(C)C)C	AGCCAUGGGGAGCC GCACGGAGGCGAAG AACCAUGGAUUUCC GAAUGAGAAUCUC UCUAACAAUUGCUU CGCGCAAUGAGGAA CCCCGAGAACUGAA ACAUCUCAGUAUCG GGAGGAACAGAAA ACGCAAUGUGAUG UCGUUAGUAACCGC GAGUGAACGCGAU ACAGCCCAAACCGA AGCCCUCACGGGCA AUGUGGUGUCAGG GCUACCUCUCAUCA GCCGACCGUCUCGA CGAAGUCUCUUGGA ACAGAGCGUGAUAC AGGGUGACAACCCC GUACUCGAGACCAG UACGACGUGCGGUA GUGCCAGAGUAGCG GGGGUUGGAUAUC CCUCGCGAAUAACG CAGGCAUCGACUGC GAAGGCUAAACACA ACCUGAGACCGAUA GUGAACAAGUAGU GUGAACGAACGCUG CAAAGUACCCUCAG AAGGGAGGCGAAA UAGAGCAUGAAAU CAGUUGGCGAUCGA GCGACAGGGCAUAC AAGGUCCCUCGACG AAUGACCGACGCGC GAGCGUCCAGUAAG ACUCACGGGAAGCC GAUGUUCUGUCGU ACGUUUUGAAAAA CGAGCCAGGGAGUG UGUCUGCAUGGCAA GUCUAACCGGAGUA UCCGGGGAGGCACA GGGAAACCGACAUG GCCGCAGGGCUUUG CCCGAGGGCCGCCG UCUUCAAGGGCGGG GAGCCAUGUGGACA CGACCCGAAUCCGG ACGAUCUACGCAUG GACAAGAUGAAGC GUGCCGAAAGGCAC GUGGAAGUCUGUU AGAGUUGGUGUCC UACAAUACCCUCUC GUGAUCUAUGUGU AGGGGUGAAAGGC CCAUCGAGUCCGGC AACAGCUGGUUCCA AUCGAAACAUGUCG AAGCAUGACCUCCG CCGAGGUAGUCUGU GAGGUAGAGCGACC GAUUGGUGUGUCC GCCUCCGAGAGGAG UCGGCACACCUGUC AAACUCCAAACUUA CAGACGCCGUUUGA CGCGGGGAUUCCGG UGCGCGGGGUAAGC CUGUGUACCAGGAG GGGAACAACCCAGA GAUAGGUUAAGGU					

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		CCCCAAGUGUGGAU UAAGUGUAAUCCUC UGAAGGUGGUCUC GAGCCCUAGACAGC CGGGAGGUGAGCU UAGAAGCAGCUACC CUCUAAGAAAAGCG UAACAGCUUACCGG CCGAGGUUUGAGGC GCCCAAAAUGAUCG GGACUCAAAUCCAC CACCGAGACCUGUC CGUACCACUCAUAC UGGUAAUCGAGUA GAUUGGCGCUCUAA UUGGAUGGAAGUA GGGGUGAAAACUCC UAUGGACCGAUUA GUGACGAAAAUCCU GGCCAUAGUAGCAG CGAUAGUCGGGUG AGAACCCCGACGGC CUAAUGGAUAAGG GUUCCUCAGCACUG CUGAUCAGCUGAGG GUUAGCCGGUCCUA AGUCAUACCGCAAC UCGACUAUGACGAA AUGGGAAACGGGU UAAUAUUCCCGUGC CACUAUGCAGUGAA AGUUGACGCCCUGG GGUCGAUCACGCUG GGCAUUCGCCCAGU CGAACCGUCCAACU CCGUGGAAGCCGUA AUGGCAGGAAGCG GACGAACGGCGGCA UAGGGAAACGUGA UUCAACCUGGGGCC CAUGAAAAGACGA GCAUAGUGUCCGUA CCGAGAACCGACAC AGGUGUCCAUGGCG GCGAAAGCCAAGGC CUGUCGGGAGCAAC CAACGUUAGGGAA UUCGGCAAGUUAG UCCCGUACCUUCGG AAGAAGGGAUGCC UGCUCCGGAACGGA GCAGGUCGCAGUGA CUCGGAAGCUCGGA CUGUCUAGUAACAA CAUAGGUGACCGCA AAUCCGCAAGGACU CGUACGGUCACUGA AUCCUGCCCAGUGC AGGUAUCUGAACAC CUCGUACAAGAGGA CGAAGGACCUGUCA ACGGCGGGGGUAAC UAUGACCCUCUUAA GGUAGCGUAGUACC UUGCCGCAUCAGUA GCGGCUUGCAUGAA UGGAUUAACCAGA GCUUCACUGUCCCA ACGUUGGGCCCGGU GAACUGUACAUUCC AGUGCGGAGUCUG GAGACACCCAGGGG GAAGCGAAGACCCU AUGGAGCUUUACU GCAGGCUGUCGCUG					

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		AGACGUGGUCGCCG AUGUGCAGCAUAG GUAGGAGACACUAC ACAGGUACCCGCGC UAGCGGGCCACCGA GUCAACAGUGAAA UACUACCCGUCGGU GACUGCGACUCUCA CUCCGGGAGGAGGA CACCGAUAGCCGGG CAGUUUGACUGGG GCGGUACGCGCUCG AAAAGAUAUCGAG CGCGCCCUAUGGCU AUCUCAGCCGGGAC AGAGACCCGGCGAA GAGUGCAAGAGCA AAAGAUAGCUUGA CAGUGUUCUUCCCA ACGAGGAACGCUGA CGCGAAAGCGUGGU CUAGCGAACCAAUU AGCCUGCUUGAUGC GGGCAAUUGAUGA CAGAAAAGCUACCC UAGGGAUAACAGA GUCGUCACUCGCAA GAGCACAUAUCGAC CGAGUGGCUUGCUA CCUCGAUGUCGGUU CCCUCCAUCCUGCC CGUGCAGAAGCGGG CAAGGGUGAGGUU GUUCGCCUAUUAAA GGAGGUCGUGAGC UGGGUUUAGACCG UCGUGAGACAGGUC GGCUGCUAUCUACU GGGUGUGUAAUGG UGUCUGACAAGAAC GACCGUAUAGUACG AGAGGAACUACGG UUGGUGGCCACUGG UGUACCGGUUGUUC GAGAGAGCACGUGC CGGGUAGCCACGCC ACACGGGGUAAGA GCUGAACGCAUCUA AGCUCGAAACCCAC UUGGAAAAGAGAC ACCGCCGAGGUCCC GCGUACAAGACGCG GUCGAUAGACUCGG GGUGUGCGCGUCGA GGUAACGAGACGU UAAGCCCACGAGCA CUAACAGACCAAAG CCAUCAU					
298	CCN(CC)CCSCC(=O)OC1CC(C(C(C23CCC(C1(C2C(=O)CC3)C)C)C)O)(C)C=C	UUGGCUACUAUGCC AGCUGGUGGAUUG CUCGGCUCAGGCGC UGAUGAAGGACGU GCCAAGCUGCGAUA AGCCAUGGGGAGCC GCACGGAGGCGAAG AACCAUGGAUUUCC GAAUGAGAAUCUC UCUAACAAUUGCUU CGCGCAAUGAGGAA CCCCGAGAACUGAA ACAUCUCAGUAUCG GGAGGAACAGAAA ACGCAAUGUGAUG UCGUUAGUAACCGC GAGUGAACGCGAU	Tiamulin	Target_lig_236	PTC	Target_99	6.82681373158773

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		ACAGCCCAAACCGA AGCCCUCACGGGCA AUGUGGUGUCAGG GCUACCUCUCAUCA GCCGACCGUCUCGA CGAAGUCUCUUGGA ACAGAGCGUGAUAC AGGGUGACAACCCC GUACUCGAGACCAG UACGACGUGCGGUA GUGCCAGAGUAGCG GGGGUUGGAUAUC CCUCGCGAAUAACG CAGGCAUCGACUGC GAAGGCUAAACACA ACCUGAGACCGAUA GUGAACAAGUAGU GUGAACGAACGCUG CAAAGUACCCUCAG AAGGGAGGCGAAA UAGAGCAUGAAAU CAGUUGGCGAUCGA GCGACAGGGCAUAC AAGGUCCCUCGACG AAUGACCGACGCGC GAGCGUCCAGUAAG ACUCACGGGAAGCC GAUGUUCUGUCGU ACGUUUUGAAAAA CGAGCCAGGGAGUG UGUCUGCAUGGCAA GUCUAACCGGAGUA UCCGGGGAGGCACA GGGAAACCGACAUG GCCGCAGGGCUUUG CCCGAGGGCCGCCG UCUUCAAGGGCGGG GAGCCAUGUGGACA CGACCCGAAUCCGG ACGAUCUACGCAUG GACAAGAUGAAGC GUGCCGAAAGGCAC GUGGAAGUCUGUU AGAGUUGGUGUCC UACAAUACCCUCUC GUGAUCUAUGUGU AGGGGUGAAAGGC CCAUCGAGUCCGGC AACAGCUGGUUCCA AUCGAAACAUGUCG AAGCAUGACCUCCG CCGAGGUAGUCUGU GAGGUAGAGCGACC GAUUGGUGUGUCC GCCUCCGAGAGGAG UCGGCACACCUGUC AAACUCCAAACUUA CAGACGCCGUUUGA CGCGGGGAUUCCGG UGCGCGGGGUAAGC CUGUGUACCAGGAG GGGAACAACCCAGA GAUAGGUUAAGGU CCCCAAGUGUGGAU UAAGUGUAAUCCUC UGAAGGUGGUCUC GAGCCCUAGACAGC CGGGAGGUGAGCU UAGAAGCAGCUACC CUCUAAGAAAAGCG UAACAGCUUACCGG CCGAGGUUUGAGGC GCCCAAAAUGAUCG GGACUCAAAUCCAC CACCGAGACCUGUC					

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		CGUACCACUCAUAC UGGUAAUCGAGUA GAUUGGCGCUCUAA UUGGAUGGAAGUA GGGGUGAAAACUCC UAUGGACCGAUUA GUGACGAAAAUCCU GGCCAUAGUAGCAG CGAUAGUCGGGUG AGAACCCCGACGGC CUAAUGGAUAAGG GUUCCUCAGCACUG CUGAUCAGCUGAGG GUUAGCCGGUCCUA AGUCAUACCGCAAC UCGACUAUGACGAA AUGGGAAACGGGU UAAUAUUCCCGUGC CACUAUGCAGUGAA AGUUGACGCCCUGG GGUCGAUCACGCUG GGCAUUCGCCCAGU CGAACCGUCCAACU CCGUGGAAGCCGUA AUGGCAGGAAGCG GACGAACGGCGGCA UAGGGAAACGUGA UUCAACCUGGGGCC CAUGAAAAGACGA GCAUAGUGUCCGUA CCGAGAACCGACAC AGGUGUCCAUGGCG GCGAAAGCCAAGGC CUGUCGGGAGCAAC CAACGUUAGGGAA UUCGGCAAGUUAG UCCCGUACCUUCGG AAGAAGGGAUGCC UGCUCCGGAACGGA GCAGGUCGCAGUGA CUCGGAAGCUCGGA CUGUCUAGUAACAA CAUAGGUGACCGCA AAUCCGCAAGGACU CGUACGGUCACUGA AUCCUGCCCAGUGC AGGUAUCUGAACAC CUCGUACAAGAGGA CGAAGGACCUGUCA ACGGCGGGGGUAAC UAUGACCCUCUUAA GGUAGCGUAGUACC UUGCCGCAUCAGUA GCGGCUUGCAUGAA UGGAUUAACCAGA GCUUCACUGUCCCA ACGUUGGGCCCGGU GAACUGUACAUUCC AGUGCGGAGUCUG GAGACACCCAGGGG GAAGCGAAGACCCU AUGGAGCUUUACU GCAGGCUGUCGCUG AGACGUGGUCGCCG AUGUGCAGCAUAG GUAGGAGACACUAC ACAGGUACCCGCGC UAGCGGGCCACCGA GUCAACAGUGAAA UACUACCCGUCGGU GACUGCGACUCUCA CUCCGGGAGGAGGA CACCGAUAGCCGGG CAGUUUGACUGGG GCGGUACGCGCUCG					

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		AAAAGAUAUCGAG CGCGCCCUAUGGCU AUCUCAGCCGGGAC AGAGACCCGGCGAA GAGUGCAAGAGCA AAAGAUAGCUUGA CAGUGUUCUUCCCA ACGAGGAACGCUGA CGCGAAAGCGUGGU CUAGCGAACCAAUU AGCCUGCUUGAUGC GGGCAAUUGAUGA CAGAAAAGCUACCC UAGGGAUAACAGA GUCGUCACUCGCAA GAGCACAUAUCGAC CGAGUGGCUUGCUA CCUCGAUGUCGGUU CCCUCCAUCCUGCC CGUGCAGAAGCGGG CAAGGGUGAGGUU GUUCGCCUAUUAAA GGAGGUCGUGAGC UGGGUUUAGACCG UCGUGAGACAGGUC GGCUGCUAUCUACU GGGUGUGUAAUGG UGUCUGACAAGAAC GACCGUAUAGUACG AGAGGAACUACGG UUGGUGGCCACUGG UGUACCGGUUGUUC GAGAGAGCACGUGC CGGGUAGCCACGCC ACACGGGGUAAGA GCUGAACGCAUCUA AGCUCGAAACCCAC UUGGAAAAGAGAC ACCGCCGAGGUCCC GCGUACAAGACGCG GUCGAUAGACUCGG GGUGUGCGCGUCGA GGUAACGAGACGU UAAGCCCACGAGCA CUAACAGACCAAAG CCAUCAU					
299	CC1CCC23CCC(=O)C2C1(C(CC(C(C3C)O)(C)C=C)OC(=O)CSC(C)(C)CNC(=O)C(C(C)C)N)C	UUGGCUACUAUGCC AGCUGGUGGAUUG CUCGGCUCAGGCGC UGAUGAAGGACGU GCCAAGCUGCGAUA AGCCAUGGGGAGCC GCACGGAGGCGAAG AACCAUGGAUUUCC GAAUGAGAAUCUC UCUAACAAUUGCUU CGCGCAAUGAGGAA CCCCGAGAACUGAA ACAUCUCAGUAUCG GGAGGAACAGAAA ACGCAAUGUGAUG UCGUUAGUAACCGC GAGUGAACGCGAU ACAGCCCAAACCGA AGCCCUCACGGGCA AUGUGGUGUCAGG GCUACCUCUCAUCA GCCGACCGUCUCGA CGAAGUCUCUUGGA ACAGAGCGUGAUAC AGGGUGACAACCCC GUACUCGAGACCAG UACGACGUGCGGUA GUGCCAGAGUAGCG GGGGUUGGAUAUC	Valnemulin	Target_lig_237	PTC	Target_99	11.301029995664

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		CCUCGCGAAUAACG CAGGCAUCGACUGC GAAGGCUAAACACA ACCUGAGACCGAUA GUGAACAAGUAGU GUGAACGAACGCUG CAAAGUACCCUCAG AAGGGAGGCGAAA UAGAGCAUGAAAU CAGUUGGCGAUCGA GCGACAGGGCAUAC AAGGUCCCUCGACG AAUGACCGACGCGC GAGCGUCCAGUAAG ACUCACGGGAAGCC GAUGUUCUGUCGU ACGUUUUGAAAAA CGAGCCAGGGAGUG UGUCUGCAUGGCAA GUCUAACCGGAGUA UCCGGGGAGGCACA GGGAAACCGACAUG GCCGCAGGGCUUUG CCCGAGGGCCGCCG UCUUCAAGGGCGGG GAGCCAUGUGGACA CGACCCGAAUCCGG ACGAUCUACGCAUG GACAAGAUGAAGC GUGCCGAAAGGCAC GUGGAAGUCUGUU AGAGUUGGUGUCC UACAAUACCCUCUC GUGAUCUAUGUGU AGGGGUGAAAGGC CCAUCGAGUCCGGC AACAGCUGGUUCCA AUCGAAACAUGUCG AAGCAUGACCUCCG CCGAGGUAGUCUGU GAGGUAGAGCGACC GAUUGGUGUGUCC GCCUCCGAGAGGAG UCGGCACACCUGUC AAACUCCAAACUUA CAGACGCCGUUUGA CGCGGGGAUUCCGG UGCGCGGGGUAAGC CUGUGUACCAGGAG GGGAACAACCCAGA GAUAGGUUAAGGU CCCCAAGUGUGGAU UAAGUGUAAUCCUC UGAAGGUGGUCUC GAGCCCUAGACAGC CGGGAGGUGAGCU UAGAAGCAGCUACC CUCUAAGAAAAGCG UAACAGCUUACCGG CCGAGGUUUGAGGC GCCCAAAAUGAUCG GGACUCAAAUCCAC CACCGAGACCUGUC CGUACCACUCAUAC UGGUAAUCGAGUA GAUUGGCGCUCUAA UUGGAUGGAAGUA GGGGUGAAAACUCC UAUGGACCGAUUA GUGACGAAAAUCCU GGCCAUAGUAGCAG CGAUAGUCGGGUG AGAACCCCGACGGC CUAAUGGAUAAGG GUUCCUCAGCACUG					

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		CUGAUCAGCUGAGG GUUAGCCGGUCCUA AGUCAUACCGCAAC UCGACUAUGACGAA AUGGGAAACGGGU UAAUAUUCCCGUGC CACUAUGCAGUGAA AGUUGACGCCCUGG GGUCGAUCACGCUG GGCAUUCGCCCAGU CGAACCGUCCAACU CCGUGGAAGCCGUA AUGGCAGGAAGCG GACGAACGGCGGCA UAGGGAAACGUGA UUCAACCUGGGGCC CAUGAAAAGACGA GCAUAGUGUCCGUA CCGAGAACCGACAC AGGUGUCCAUGGCG GCGAAAGCCAAGGC CUGUCGGGAGCAAC CAACGUUAGGGAA UUCGGCAAGUUAG UCCCGUACCUUCGG AAGAAGGGAUGCC UGCUCCGGAACGGA GCAGGUCGCAGUGA CUCGGAAGCUCGGA CUGUCUAGUAACAA CAUAGGUGACCGCA AAUCCGCAAGGACU CGUACGGUCACUGA AUCCUGCCCAGUGC AGGUAUCUGAACAC CUCGUACAAGAGGA CGAAGGACCUGUCA ACGGCGGGGGUAAC UAUGACCCUCUUAA GGUAGCGUAGUACC UUGCCGCAUCAGUA GCGGCUUGCAUGAA UGGAUUAACCAGA GCUUCACUGUCCCA ACGUUGGGCCCGGU GAACUGUACAUUCC AGUGCGGAGUCUG GAGACACCCAGGGG GAAGCGAAGACCCU AUGGAGCUUUACU GCAGGCUGUCGCUG AGACGUGGUCGCCG AUGUGCAGCAUAG GUAGGAGACACUAC ACAGGUACCCGCGC UAGCGGGCCACCGA GUCAACAGUGAAA UACUACCCGUCGGU GACUGCGACUCUCA CUCCGGGAGGAGGA CACCGAUAGCCGGG CAGUUUGACUGGG GCGGUACGCGCUCG AAAAGAUAUCGAG CGCGCCCUAUGGCU AUCUCAGCCGGGAC AGAGACCCGGCGAA GAGUGCAAGAGCA AAAGAUAGCUUGA CAGUGUUCUUCCCA ACGAGGAACGCUGA CGCGAAAGCGUGGU CUAGCGAACCAAUU AGCCUGCUUGAUGC GGGCAAUUGAUGA					

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		CAGAAAAGCUACCC UAGGGAUAACAGA GUCGUCACUCGCAA GAGCACAUAUCGAC CGAGUGGCUUGCUA CCUCGAUGUCGGUU CCCUCCAUCCUGCC CGUGCAGAAGCGGG CAAGGGUGAGGUU GUUCGCCUAUUAAA GGAGGUCGUGAGC UGGGUUUAGACCG UCGUGAGACAGGUC GGCUGCUAUCUACU GGGUGUGUAAUGG UGUCUGACAAGAAC GACCGUAUAGUACG AGAGGAACUACGG UUGGUGGCCACUGG UGUACCGGUUGUUC GAGAGAGCACGUGC CGGGUAGCCACGCC ACACGGGGUAAGA GCUGAACGCAUCUA AGCUCGAAACCCAC UUGGAAAAGAGAC ACCGCCGAGGUCCC GCGUACAAGACGCG GUCGAUAGACUCGG GGUGUGCGCGUCGA GGUAACGAGACGU UAAGCCCACGAGCA CUAACAGACCAAAG CCAUCAU					
310	CC1C(C(CC(O1)OC2C (OC3(CC2O)OC4C(OC (C(C4(O3)C)O)OC5C(C(OC(C5OC)C)OC6C(OC(C(C6O)OC)OC7C(C8C(CO7)OC9(O8)C1 C(C(CO9)OC(=O)C2= C(C=C(C=C2C)O)O)O CO1)O)COC)O)C)C)O C1CC(C(C(O1)C)OC) (C)[N+](=O) [O-])OC(=O)C1=C(C(= C(C(=C1OC)Cl)O)Cl)C	GGUUAAGCGACUA AGCGUACACGGUGG AUGCCCUGGCAGUC AGAGGCGAUGAAG GACGUGCUAAUCUG CGAUAAGCGUCGGU AAGGUGAUAUGAA CCGUUAUAACCGGC GAUUUCCGAAUGG GGAAACCCAGUGUG UUUCGACACACUAU CAUUAACUGAAUCC AUAGGUUAAUGAG GCGAACCGGGGGAA CUGAAACAUCUAAG UACCCCGAGGAAAA GAAAUCAACCGAGA UUCCCCCAGUAGCG GCGAGCGAACGGGG AGCAGCCCAGAGCC UGAAUCAGUGUGU GUGUUAGUGGAAG CGUCUGGAAAGGCG CGCGAUACAGGGUG ACAGCCCCGUACAC AAAAAUGCACAUGC UGUGAGCUCGAUG AGUAGGGCGGGAC ACGUGGUAUCCUGU CUGAAUAUGGGGG GACCAUCCUCCAAG GCUAAAUACUCCUG ACUGACCGAUAGUG AACCAGUACCGUGA GGGAAAGGCGAAA AGAACCCCGGCGAG GGGAGUGAAAAAG AACCUGAAACCGUG UACGUACAAGCAGU GGGAGCACGCUUAG GCGUGUGACUGCGU	Evernimicin	Target_lig_247	Bacterial 23S rRNA hairpins 82 and 91	Target_102	4.52287874528034

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		ACCUUUUGUAUAA UGGGUCAGCGACUU AUAUUCUGUAGCA AGGUUAACCGAAU AGGGGAGCCGAAG GGAAACCGAGUCUU AACUGGGCGUUAA GUUGCAGGGUAUA GACCCGAAACCCGG UGAUCUAGCCAUGG GCAGGUUGAAGGU UGGGUAACACUAAC UGGAGGACCGAACC GACUAAUGUUGAA AAAUUAGCGGAUG ACUUGUGGCUGGG GGUGAAAGGCCAA UCAAACCGGGAGAU AGCUGGUUCUCCCC GAAAGCUAUUUAG GUAGCGCCUCGUGA AUUCAUCUCCGGGG GUAGAGCACUGUU UCGGCAAGGGGGUC AUCCCGACUUACCA ACCCGAUGCAAACU GCGAAUACCGGAGA AUGUUAUCACGGG AGACACACGGCGGG UGCUAACGUCCGUC GUGAAGAGGGAAA CAACCCAGACCGCC AGCUAAGGUCCCAA AGUCAUGGUUAAG UGGGAAACGAUGU GGGAAGGCCCAGAC AGCCAGGAUGUUG GCUUAGAAGCAGCC AUCAUUUAAAGAA AGCGUAAUAGCUCA CUGGUCGAGUCGGC CUGCGCGGAAGAUG UAACGGGGCUAAAC CAUGCACCGAAGCU GCGGCAGCGACGCU UAUGCGUUGUUGG GUAGGGGAGCGUU CUGUAAGCCUGCGA AGGUGUGCUGUGA GGCAUGCUGGAGG UAUCAGAAGUGCG AAUGCUGACAUAA GUAACGAUAAAGC GGGUGAAAAGCCCG CUCGCCGGAAGACC AAGGGUUCCUGUCC AACGUUAAUCGGG GCAGGGUGAGUCG ACCCCUAAGGCGAG GCCGAAAGGCGUAG UCGAUGGGAAACA GGUUAAUAUUCCU GUACUUGGUGUUA CUGCGAAGGGGGG ACGGAGAAGGCUA UGUUGGCCGGGCGA CGGUUGUCCCGGUU UAAGCGUGUAGGC UGGUUUUCCAGGCA AAUCCGGAAAAUCA AGGCUGAGGCGUG AUGACGAGGCACUA CGGUGCUGAAGCAA CAAAUGCCCUGCUU CCAGGAAAAGCCUC					

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		UAAGCAUCAGGUA ACAUCAAAUCGUAC CCCAAACCGACACU GGUGGUCAGGUAG AGAAUACCAAGGCG CUUGAGAGAACUCG GGUGAAGGAACUA GGCAAAAUGGUGCC GUAACUUCGGGAG AAGGCACGCUGAUA UGUAGGUGAGGUC CCUCGCGGAUGGAG CUGAAAUCAGUCGA AGAUACCAGCUGGC UGCAACUGUUUAU UAAAAACACAGCAC UGUGCAAACACGAA AGUGGACGUAUAC GGUGUGACGCCUGC CCGGUGCCGGAAGG UUAAUUGAUGGGG UUAGCGCAAGCGAA GCUCUUGAUCGAAG CCCCGGUAAACGGC GGCCGUAACUAUAA CGGUCCUAAGGUAG CGAAAUUCCUUGUC GGGUAAGUUCCGAC CUGCACGAAUGGCG UAAUGAUGGCCAG GCUGUCUCCACCCG AGACUCAGUGAAA UUGAACUCGCUGUG CAGAUGCAGUGUAC CCGCGGCAAGACGG AAAGACCCCGUGAA CCUUUACUAUAGCU UGACACUGAACAUU GAGCCUUGAUGUG UAGGAUAGGUGGG AGGCUUUGAAGUG UGGACGCCAGUCUG CAUGGAGCCGACCU UGAAAUACCACCCU UUAAUGUUUGAUG UUCUAACGUUGACC CGUAAUCCGGGUUG CGGACAGUGUCUGG UGGGUAGUUUGAC UGGGGCGGUCUCCU CCUAAAGAGUAACG GAGGAGCACGAAG GUUGGCUAAUCCUG GUCGGACAUCAGGA GGUUAGUGCAAUG GCAUAAGCCAGCUU GACUGCGAGCGUGA CGGCGCGAGCAGGU GCGAAAGCAGGUCA UAGUGAUCCGGUG GUUCUGAAUGGAA GGGCCAUCGCUCAA CGGAUAAAAGGUA CUCCGGGGAUAACA GGCUGAUACCGCCC AAGAGUUCAUAUC GACGGCGGUGUUU GGCACCUCGAUGUC GGCUCAUCACAUCC UGGGGCUGAAGUA GGUCCCAAGGGUAU GGCUGUUCGCCAUU UAAAGUGGUACGC GAGCUGGGUUUAG AACGUCGUGAGACA					

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		GUUCGGUCCCUAUC UGCCGUGGGCGCUG GAGAACUGAGGGG GGCUGCUCCUAGUA CGAGAGGACCGGAG UGGACGCAUCACUG GUGUUCGGGUUGU CAUGCCAAUGGCAC UGCCCGGUAGCUAA AUGCGGAAGAGAU AAGUGCUGAAAGC AUCUAAGCACGAAA CUUGCCCCGAGAUG AGUUCUCCCUGACC CUUUAAGGGUCCUG AAGGAACGUUGAA GACGACGACGUUGA UAGGCCGGGUGUG UAAGCGCAGCGAUG CGUUGAGCUAACCG GUACUAAUGAACCG UGAGGCUUAACCUU					
321	[C@H]1([C@H](C[C@H]([C@H]([C@H]1O)O[C@@H]1[C@@H](C[C@@H]([C@@H](O1)CN)O)N)N)O[C@@H]1[C@H]([C@@H]([C@H]([C@@H](O1)CNc1c2ccccc2nc2c1cccc2)O)N)O	GAGCGUCACACCUU CGGGUGAAGUCGCU C	Tobramycin	Target_lig_540	Bacterial ribosomal A-site	Target_3	7
323	C1C(C(C(C(C1N)OC2C(C(C(C(O2)CN)O)O)N)OC3C(C(C(O3)CO)O)O)O)N	GAGCGUCACACCUU CGGGUGAAGUCGCU C	ribostamycin	Target_lig_9	Bacterial ribosomal A-site	Target_3	5.76955107862173
324	C1C(C(C(C(C1N)OC2C(CC(C(O2)CO)O)N)OC3C(C(C(O3)CO)OC4C(C(C(C(O4)CN)OC5C(C(C(C(O5)CO)O)O)O)O)N)O)O)N	GAGCGUCACACCUU CGGGUGAAGUCGCU C	Lividomycin A	Target_lig_1247	Bacterial ribosomal A-site	Target_3	7.55284196865778
325	[C@@H]1([C@H]([C@@H]([C@H](O[C@@H]1CO)O[C@@H]1[C@H]([C@@H]([C@H](C[C@H]1N)N)O)O[C@H]1O[C@H]([C@H]([C@@H]1OCCc1ccccc1)O[C@@H]1[C@H]([C@@H]([C@@H]([C@@H](O1)N)O)O)N)CO)N)O)O	GAGCGUCACACCUU CGGGUGAAGUCGCU C	Phenyl ether paromomycin derivative 1	Target_lig_251	Bacterial ribosomal A-site	Target_3	5.42021640338319
326	[C@H]1([C@H]([C@@H]([C@H](O[C@@H]1CO)O[C@H]1[C@@H]([C@@H]([C@@H](C[C@@H]1N)N)O)O[C@@H]1OC[C@@H]([C@H]1OCCNc1cnccc1)O[C@@H]1[C@H]([C@@H](C[C@@H](O1)CN)O)N)N)O)O	GAGCGUCACACCUU CGGGUGAAGUCGCU C	Aminoglycoside derivative 1	Target_lig_252	Bacterial ribosomal A-site	Target_3	6.22184874961636
327	[C@@H]1([C@@H]([C@@H]([C@@H](O[C@H]1CO)O[C@@H]1[C@H]([C@@H]	GAGCGUCACACCUU CGGGUGAAGUCGCU C	Aminoglycoside derivative 2	Target_lig_253	Bacterial ribosomal A-site	Target_3	6.04575749056068

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	([C@H](C[C@H]1N)N)O)O[C@H]1OC[C@@H]([C@@H]1OCCNCc1ncccc1)O[C@@H]1[C@H]([C@@H](C[C@@H](O1)CN)O)N)N)O)O						
328	[C@H]1([C@@H]([C@H]([C@@H](O[C@H]1CO)O[C@H]1[C@@H]([C@@H]([C@H](C[C@@H]1N)N)O)O[C@@H]1OC[C@H]([C@@H]1OCCNCCCN)O[C@H]1[C@@H]([C@H](C[C@H](O1)CN)O)N)N)O)O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Aminoglycoside derivative 3	Target_lig_254	Bacterial ribosomal A-site	Target_3	6.39794000867204
329	[C@@H]1([C@@H]([C@H]([C@H](O[C@@H]1CO)O[C@H]1[C@@H]([C@H]([C@H](C[C@H]1N)N)O)O[C@@H]1OC[C@@H]([C@H]1OCCNCCN)O[C@@H]1[C@H]([C@@H](C[C@@H](O1)CN)O)N)N)O)O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Aminoglycoside derivative 4	Target_lig_255	Bacterial ribosomal A-site	Target_3	6.15490195998574
330	[C@@H]1([C@@H]([C@H]([C@@H](O[C@@H]1CO)O[C@@H]1[C@H]([C@@H]([C@H](C[C@@H]1N)N)O)O[C@H]1OC[C@H]([C@@H]1OCCN)O[C@H]1[C@@H]([C@H](C[C@H](O1)CN)O)N)N)O)O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Aminoglycoside derivative 6	Target_lig_256	Bacterial ribosomal A-site	Target_3	6.52287874528034
331	[C@H]1([C@H]([C@@H]([C@@H](O[C@H]1CO)O[C@@H]1[C@@H]([C@@H]([C@H](C[C@H]1N)N)O)O[C@@H]1OC[C@@H]([C@H]1OCCNCCNCCN)O[C@@H]1[C@@H]([C@H](C[C@H](O1)CN)O)N)N)O)O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Aminoglycoside derivative 7	Target_lig_257	Bacterial ribosomal A-site	Target_3	5.03621217265444
332	[C@@H]1([C@@H]([C@H]([C@@H](O[C@@H]1CO)O[C@@H]1[C@H]([C@@H]([C@H](C[C@H]1N)N)O)O[C@@H]1OC[C@H]([C@@H]1OCCNCCN1CCNCC1)O[C@H]1[C@H]([C@@H](C[C@@H](O1)CN)O)N)N)O)O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Aminoglycoside derivative 8	Target_lig_258	Bacterial ribosomal A-site	Target_3	5.88605664769316
333	[C@H]1([C@H]([C@@H]([C@H](O[C@H]1CO)O[C@H]1[C@@H]([C@H]([C@@H](C[C@@H]1N)N)O)O[C@@H]1OC[C@H]	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Aminoglycoside derivative 9	Target_lig_259	Bacterial ribosomal A-site	Target_3	7

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	([C@H]1OCCNC1CCNCC1)O[C@H]1[C@@H]([C@H](C[C@H](O1)CN)O)N)N)O)O						
334	[C@@H]1([C@H]([C@@H]([C@H](O[C@@H]1CO)O[C@H]1[C@@H]([C@@H]([C@H](C[C@@H]1N)N)O)O[C@H]1OC[C@H]([C@@H]1OCCNC[C@H]1CNCCC1)O[C@@H]1[C@@H]([C@H](C[C@@H](O1)CN)O)N)N)O)O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Aminoglycoside derivative 10	Target_lig_260	Bacterial ribosomal A-site	Target_3	6.52287874528034
335	[C@H]1([C@H]([C@H]([C@@H](O[C@@H]1CO)O[C@@H]1[C@@H]([C@H]([C@@H](C[C@@H]1N)N)O)O[C@@H]1OC[C@@H]([C@H]1OCCNc1ccnc2c1cccc2)O[C@@H]1[C@H]([C@@H](C[C@@H](O1)CN)O)N)N)O)O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Aminoglycoside derivative 12	Target_lig_261	Bacterial ribosomal A-site	Target_3	7
336	[C@H]1([C@H]([C@@H]([C@H](O[C@H]1CO)O[C@@H]1[C@H]([C@@H]([C@H](C[C@H]1N)N)O)O[C@H]1OC[C@H]([C@@H]1OCCNC1CCCCC1)O[C@H]1[C@@H]([C@H](C[C@H](O1)CN)O)N)N)O)O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Aminoglycoside derivative 13	Target_lig_262	Bacterial ribosomal A-site	Target_3	7
337	[C@@H]1([C@@H]([C@H]([C@H](O[C@@H]1CO)O[C@@H]1[C@H]([C@@H]([C@@H](C[C@@H]1N)N)O)O[C@H]1OC[C@@H]([C@H]1OCCNCCc1cnccc1)O[C@@H]1[C@H]([C@@H](C[C@@H](O1)CN)O)N)N)O)O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Aminoglycoside derivative 14	Target_lig_263	Bacterial ribosomal A-site	Target_3	6.69897000433602
338	[C@H]1([C@H]([C@@H]([C@H](O[C@H]1CO)O[C@H]1[C@@H]([C@@H]([C@@H](C[C@H]1N)N)O)O[C@H]1OC[C@@H]([C@H]1OCCNCCc1ccccc1)O[C@@H]1[C@H]([C@@H](C[C@@H](O1)CN)O)N)N)O)O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Aminoglycoside derivative 15	Target_lig_264	Bacterial ribosomal A-site	Target_3	7
339	[C@H]1([C@@H]([C@H]([C@@H](O[C@H]1CO)O[C@H]1[C@@H]([C@H]([C@@H](C[C@@H]1N)N)O)O[C@@H]1OC[C@@H]([C@H]1OCCNCc1ccc	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Aminoglycoside derivative 16	Target_lig_265	Bacterial ribosomal A-site	Target_3	7

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	cc1)O[C@@H]1[C@H]([C@@H](C[C@@H](O1)CN)O)N)N)O)O						
340	[C@H]1([C@H]([C@H]([C@@H](O[C@H]1CO)O[C@H]1[C@@H]([C@@H]([C@H](C[C@H]1N)N)O)O[C@@H]1OC[C@H]([C@H]1OCCNc1cccc(c1)O)O[C@@H]1[C@@H]([C@H](C[C@@H](O1)CN)O)N)N)O)O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Aminoglycoside derivative 17	Target_lig_266	Bacterial ribosomal A-site	Target_3	6.22184874961636
341	[C@H]1([C@H]([C@@H]([C@@H](O[C@@H]1CO)O[C@@H]1[C@@H]([C@H]([C@H](C[C@@H]1N)N)O)O[C@@H]1OC[C@H]([C@H]1OCCNCc1cnc(cc1)N)O[C@@H]1[C@@H]([C@H](C[C@@H](O1)CN)O)N)N)O)O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Aminoglycoside derivative 18	Target_lig_267	Bacterial ribosomal A-site	Target_3	7
342	[C@H]1([C@H]([C@@H]([C@H](O[C@@H]1CO)O[C@@H]1[C@H]([C@H]([C@@H](C[C@H]1N)N)O)O[C@H]1OC[C@@H]([C@H]1OCCNCc1ccnc(c1)N)O[C@H]1[C@H]([C@@H](C[C@H](O1)CN)O)N)N)O)O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Aminoglycoside derivative 19	Target_lig_268	Bacterial ribosomal A-site	Target_3	7.69897000433602
343	[C@H]1([C@H]([C@@H]([C@@H](O[C@H]1CO)O[C@@H]1[C@H]([C@@H]([C@H](C[C@@H]1N)N)O)O[C@H]1OC[C@@H]([C@@H]1OCCNc1nccc1)O[C@@H]1[C@H]([C@@H](C[C@@H](O1)CN)O)N)N)O)O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Aminoglycoside derivative 20	Target_lig_269	Bacterial ribosomal A-site	Target_3	5.30102999566398
344	[C@@H]1([C@@H]([C@H]([C@H](O[C@H]1CO)O[C@H]1[C@@H]([C@H]([C@@H](C[C@H]1N)N)O)O[C@@H]1OC[C@@H]([C@H]1OCCNCCC(C)(C)C)O[C@H]1[C@H]([C@@H](C[C@@H](O1)CN)O)N)N)O)O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Aminoglycoside derivative 21	Target_lig_270	Bacterial ribosomal A-site	Target_3	5.60205999132796
345	[C@H]1([C@H]([C@@H]([C@H](O[C@H]1CO)O[C@@H]1[C@H]([C@H]([C@@H](C[C@H]1N)N)O)O[C@H]1OC[C@H]([C@@H]1OCCNCCCc1ccccc1)O[C@@H]1[	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Aminoglycoside derivative 22	Target_lig_271	Bacterial ribosomal A-site	Target_3	6

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	C@@H]([C@H](C[C@@H](O1)CN)O)N)N)O)O						
346	[C@H]1([C@H]([C@H]([C@@H](O[C@H]1CO)O[C@@H]1[C@H]([C@@H]([C@@H](C[C@H]1N)N)O)O[C@H]1OC[C@@H]([C@H]1OCCNCCCCc1ccccc1)O[C@H]1[C@@H]([C@H](C[C@H](O1)CN)O)N)N)O)O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Aminoglycoside derivative 24	Target_lig_272	Bacterial ribosomal A-site	Target_3	6.154901959985 74
347	[C@H]1([C@H]([C@@H]([C@H](O[C@H]1CO)O[C@@H]1[C@H]([C@H]([C@@H](C[C@H]1N)N)O)O[C@@H]1OC[C@@H]([C@@H]1OCCNCCc1ccc(cc1)c1ccccc1)O[C@H]1[C@H]([C@@H](C[C@@H](O1)CN)O)N)N)O)O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Aminoglycoside derivative 25	Target_lig_273	Bacterial ribosomal A-site	Target_3	6.045757490 56068
348	[C@H]1([C@H]([C@@H]([C@H](O[C@H]1CO)O[C@H]1[C@@H]([C@@H]([C@H](C[C@H]1N)N)O)O[C@@H]1OC[C@@H]([C@H]1OCCN)O[C@@H]1[C@H]([C@@H](C[C@@H](O1)CN)O)NCCc1cc2c(cc1)cccc2)N)O)O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Aminoglycoside derivative 33	Target_lig_274	Bacterial ribosomal A-site	Target_3	6.154901959985 74
349	[C@@H]1([C@H]([C@H]([C@@H](O[C@H]1CN(C)C)O[C@H]1[C@@H]([C@H]([C@H](C[C@H]1N)N)O)O[C@@H]1O[C@@H]([C@@H]([C@@H]1O)O[C@H]1CO[C@@H]([C@@H]([C@H]1O)O)CN)CO)N)O)O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Perazidoparomomycin derivative 1	Target_lig_275	Bacterial ribosomal A-site	Target_3	6.221848749 61636
350	[C@@H]1([C@H]([C@H]([C@H](O[C@@H]1CNCCCN)O[C@H]1[C@@H]([C@H]([C@H](C[C@H]1N)N)O)O[C@@H]1O[C@@H]([C@H]([C@@H]1O)O[C@@H]1CO[C@@H]([C@@H]([C@H]1O)O)CN)CO)N)O)O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Perazidoparomomycin derivative 2	Target_lig_276	Bacterial ribosomal A-site	Target_3	5.795880017 34408
351	[C@@H]1([C@@H]([C@H]([C@H](O[C@H]1CCN1CCOCC1)O[C@H]1[C@@H]([C@H]([C@H](C[C@H]1N)N)O)O[C@@H]1O[C@@H]	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Perazidoparomomycin derivative 3	Target_lig_277	Bacterial ribosomal A-site	Target_3	5.443697499 23271

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	([C@H]([C@@H]1O)O[C@@H]1CO[C@@H]([C@@H]([C@H]1O)O)CN)CO)N)O)O						
352	[C@@H]1([C@H]([C@H]([C@H](O[C@H]1CNNC(=O)OC(C)(C)C)O[C@H]1[C@@H]([C@H]([C@H](C[C@H]1N)N)O)O[C@H]1O[C@@H]([C@H]([C@@H]1O)O[C@@H]1CO[C@H]([C@@H]([C@H]1O)O)CN)CO)N)O)O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Perazidoparomomycin derivative 4	Target_lig_278	Bacterial ribosomal A-site	Target_3	8
353	[C@H]1([C@H]([C@H]([C@H](O[C@H]1CNC)O[C@H]1[C@@H]([C@H]([C@H](C[C@H]1N)N)O)O[C@@H]1O[C@@H]([C@H]([C@@H]1O)O[C@@H]1CO[C@@H]([C@@H]([C@H]1O)O)CN)CO)N)O)O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Perazidoparomomycin derivative 5	Target_lig_279	Bacterial ribosomal A-site	Target_3	6.39794000867204
354	[C@@H]1([C@H]([C@H]([C@H](O[C@@H]1CNCCCCN)O[C@H]1[C@@H]([C@H]([C@H](C[C@H]1N)N)O)O[C@H]1O[C@@H]([C@H]([C@@H]1O)O[C@@H]1CO[C@H]([C@@H]([C@H]1O)O)CN)CO)N)O)O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Perazidoparomomycin derivative 6	Target_lig_280	Bacterial ribosomal A-site	Target_3	5.20065945054642
355	[C@H]1([C@@H]([C@H]([C@H](O[C@@H]1CNCC(C)C)O[C@H]1[C@@H]([C@H]([C@H](C[C@H]1N)N)O)O[C@H]1O[C@@H]([C@H]([C@@H]1O)O[C@@H]1CO[C@H]([C@@H]([C@H]1O)O)CN)CO)N)O)O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Perazidoparomomycin derivative 8	Target_lig_281	Bacterial ribosomal A-site	Target_3	5.92081875395238
356	[C@@H]1([C@@H]([C@H]([C@H](O[C@H]1CNN)O[C@H]1[C@@H]([C@H]([C@H](C[C@H]1N)N)O)O[C@@H]1O[C@@H]([C@H]([C@@H]1O)O[C@@H]1CO[C@@H]([C@@H]([C@H]1O)O)CN)CO)N)O)O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Perazidoparomomycin derivative 9	Target_lig_282	Bacterial ribosomal A-site	Target_3	6.22184874961636

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
357	[C@H]1([C@H]([C@H]([C@H](O[C@@H]1CNCCc1ccccc1)O[C@H]1[C@@H]([C@H]([C@H](C[C@H]1N)N)O)O[C@H]1O[C@@H]([C@@H]([C@@H]1O)O[C@H]1CO[C@@H]([C@@H]([C@H]1O)O)CN)CO)N)O)O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Perazidoparomomycin derivative 10	Target_lig_283	Bacterial ribosomal A-site	Target_3	6.30102999566398
358	[C@@H]1([C@@H]([C@H]([C@H](O[C@H]1CN(CCc1ccccc1)C)O[C@H]1[C@@H]([C@H]([C@H](C[C@H]1N)N)O)O[C@@H]1O[C@@H]([C@@H]([C@H]1O)O[C@H]1CO[C@@H]([C@@H]([C@H]1O)O)CN)CO)N)O)O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Perazidoparomomycin derivative 11	Target_lig_284	Bacterial ribosomal A-site	Target_3	5.65757731917779
359	[C@@H]1([C@H]([C@@H]([C@H](O[C@@H]1CNCCCc1ccccc1)O[C@H]1[C@@H]([C@H]([C@H](C[C@H]1N)N)O)O[C@H]1O[C@@H]([C@H]([C@@H]([C@@H]1O)O[C@@H]1CO[C@@H]([C@@H]([C@H]1O)O)CN)CO)N)O)O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Perazidoparomomycin derivative 12	Target_lig_285	Bacterial ribosomal A-site	Target_3	5.85387196432176
360	[C@H]1([C@H]([C@H]([C@H](O[C@@H]1CNCCc1ccc(cc1)C1CCCCC1)O[C@H]1[C@@H]([C@H]([C@H](C[C@H]1N)N)O)O[C@H]1O[C@@H]([C@@H]([C@@H]1O)O[C@H]1CO[C@@H]([C@@H]([C@H]1O)O)CN)CO)N)O)O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Perazidoparomomycin derivative 13	Target_lig_286	Bacterial ribosomal A-site	Target_3	5.31875876262441
361	[C@@H]1([C@@H]([C@H]([C@H](O[C@H]1CNCCc1c(cccc1)OC)O[C@H]1[C@@H]([C@H]([C@H](C[C@H]1N)N)O)O[C@H]1O[C@@H]([C@H]([C@@H]([C@@H]1O)O[C@@H]1CO[C@@H]([C@@H]([C@H]1O)O)CN)CO)N)O)O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Perazidoparomomycin derivative 14	Target_lig_287	Bacterial ribosomal A-site	Target_3	5.09691001300806
362	[C@H]1([C@H]([C@H]([C@H](O[C@H]1CNCCc1ccc(cc1)F)O[C@H]1[C@@H]([C@H]([C@H](C[C@H]1N)N)O)O[C@@H]1O[C@@H]	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Perazidoparomomycin derivative 15	Target_lig_288	Bacterial ribosomal A-site	Target_3	2.85387196432176

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	([C@@H]([C@@H]1O)O[C@H]1CO[C@@H]([C@@H]([C@H]1O)O)CN)CO)N)O)O						
363	[C@H]1([C@H]([C@H]([C@H](O[C@@H]1CN[C@@H](Cc1ccccc1)C)O[C@H]1[C@@H]([C@H]([C@H](C[C@H]1N)N)O)O[C@H]1O[C@@H]([C@H]([C@@H]1O)O[C@@H]1CO[C@@H]([C@@H]([C@H]1O)O)CN)CO)N)O)O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Perazidoparomomycin derivative 16	Target_lig_289	Bacterial ribosomal A-site	Target_3	2.63827216398241
364	[C@H]1([C@H]([C@H]([C@H](O[C@@H]1CNCCc1ccc(cc1)C(F)(F)F)O[C@H]1[C@@H]([C@H]([C@H](C[C@H]1N)N)O)O[C@@H]1O[C@@H]([C@@H]([C@@H]1O)O[C@H]1CO[C@@H]([C@@H]([C@H]1O)O)CN)CO)N)O)O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Perazidoparomomycin derivative 17	Target_lig_290	Bacterial ribosomal A-site	Target_3	2.53760200210104
365	[C@@H]1([C@H]([C@H]([C@H](O[C@@H]1CNCCc1ccc(cc1)OC)O[C@H]1[C@@H]([C@H]([C@H](C[C@H]1N)N)O)O[C@@H]1O[C@@H]([C@H]([C@@H]1O)O[C@@H]1CO[C@@H]([C@@H]([C@H]1O)O)CN)CO)N)O)O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Perazidoparomomycin derivative 18	Target_lig_291	Bacterial ribosomal A-site	Target_3	2.20760831050175
366	[C@H]1([C@H]([C@H]([C@H](O[C@@H]1CN1C[C@H]2[C@H](C1)CCCC2)O[C@H]1[C@@H]([C@H]([C@H](C[C@H]1N)N)O)O[C@H]1O[C@@H]([C@@H]([C@@H]1O)O[C@H]1CO[C@@H]([C@@H]([C@H]1O)O)CN)CO)N)O)O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Perazidoparomomycin derivative 19	Target_lig_292	Bacterial ribosomal A-site	Target_3	1.88941028970075
367	[C@@H]1([C@@H]([C@H]([C@H](O[C@H]1CN[C@@H]([C@@H](c1ccccc1)O)C)O[C@H]1[C@@H]([C@H]([C@H](C[C@H]1N)N)O)O[C	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Perazidoparomomycin derivative 20	Target_lig_293	Bacterial ribosomal A-site	Target_3	1.78781239559604

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	@H]1O[C@@H]([C@H]([C@@H]1O)O[C@@H]1CO[C@@H]([C@@H]([C@H]1O)O)CN)CO)N)O)O						
368	[C@H]1([C@H]([C@H]([C@H](O[C@H]1CNCCc1ccc(ccc1)C(F)(F)F)O[C@H]1[C@@H]([C@H]([C@H](C[C@H]1N)N)O)O[C@@H]1O[C@@H]([C@@H]([C@@H]1O)O[C@H]1CO[C@@H]([C@H]([C@H]1O)O)CN)CO)N)O)O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Perazidoparomomycin derivative 21	Target_lig_294	Bacterial ribosomal A-site	Target_3	1.69464863055338
369	[C@H]1([C@H]([C@H]([C@H](O[C@@H]1CNCCc1cc(ccc1)OC)O[C@H]1[C@@H]([C@H]([C@H](C[C@H]1N)N)O)O[C@H]1O[C@@H]([C@@H]([C@@H]1O)O[C@H]1CO[C@@H]([C@H]([C@H]1O)O)CN)CO)N)O)O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Perazidoparomomycin derivative 22	Target_lig_295	Bacterial ribosomal A-site	Target_3	7
370	[C@H]1([C@H]([C@@H]([C@H](O[C@@H]1CCN1C[C@@H]2[C@H](C1)CCCC2)O[C@H]1[C@@H]([C@H]([C@H](C[C@H]1N)N)O)O[C@H]1O[C@@H]([C@H]([C@@H]1O)O[C@@H]1CO[C@@H]([C@@H]([C@H]1O)O)CN)CO)N)O)O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Perazidoparomomycin derivative 23	Target_lig_296	Bacterial ribosomal A-site	Target_3	3
371	[C@@H]1([C@H]([C@H]([C@H](O[C@@H]1CNCC[C@H]1CCCNC1)O[C@H]1[C@@H]([C@H]([C@H](C[C@H]1N)N)O)O[C@H]1O[C@@H]([C@@H]([C@@H]1O)O[C@H]1CO[C@@H]([C@@H]([C@H]1O)O)CN)CO)N)O)O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Perazidoparomomycin derivative 26	Target_lig_297	Bacterial ribosomal A-site	Target_3	5.2839966563652
372	[C@@H]1([C@H]([C@H]([C@H](O[C@@H]1CNCC[C@H]1NCCCC1)O[C@H]1[C@@H]([C@H]([C@H](C[C@H]1N)N)O)O[C@@H]1O[C@@H]([C@H]	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Perazidoparomomycin derivative 27	Target_lig_298	Bacterial ribosomal A-site	Target_3	5.44369749923271

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	([C@@H]1O)O[C@@H]1CO[C@@H]([C@@H]([C@H]1O)O)CN)CO)N)O)O						
373	[C@H]1([C@H]([C@@H]([C@H](C[C@@H]1CO)O[C@@H]1[C@@H]([C@H]([C@@H](C[C@@H]1N)N)O)O[C@@H]1O[C@@H]([C@H]([C@H]1OCCN(CCc1ccccc1)C(=O)c1ccccc1)O[C@@H]1[C@H]([C@H]([C@@H]([C@H](O1)N)O)O)N)CO)N)O)O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Benzoyl paromomycin derivative	Target_lig_299	Bacterial ribosomal A-site	Target_3	5.4089353929735
374	[C@@H]1([C@@H]([C@H]([C@@H](C[C@@H]1CO)O[C@@H]1[C@H]([C@H]([C@@H](C[C@@H]1N)N)O)O[C@H]1O[C@H]([C@H]([C@@H]1OCCN(CCc1ccccc1)C(=O)C)O[C@@H]1[C@H]([C@@H]([C@H]([C@H](O1)N)O)O)N)CO)N)O)O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Acetyl parmomycin derivative	Target_lig_300	Bacterial ribosomal A-site	Target_3	5.82390874094432
375	[C@@H]1([C@@H]([C@H]([C@@H](C[C@@H]1CO)O[C@@H]1[C@H]([C@H]([C@@H](C[C@@H]1N)N)O)O[C@H]1O[C@H]([C@H]([C@@H]1OCCN(CCc1ccccc1)C(=O)C)O[C@@H]1[C@H]([C@@H]([C@H]([C@H](O1)N)O)O)N)CO)N)O)O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Ether paromomycin derivative 1	Target_lig_1112	Bacterial ribosomal A-site	Target_3	6.04575749056068
376	[C@@H]1([C@H]([C@H]([C@@H](C[C@H]1CO)O[C@H]1[C@H]([C@H]([C@@H](C[C@@H]1N)N)O)O[C@@H]1O[C@@H]([C@H]([C@@H]1OC[C@@H](O)c1ccccc1)O[C@H]1[C@H]([C@@H]([C@H]([C@H](O1)N)O)O)N)CO)N)O)O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Ether paromomycin derivative 3	Target_lig_301	Bacterial ribosomal A-site	Target_3	5.56863623584101
377	[C@H]1([C@@H]([C@H]([C@@H](C[C@H]1CO)O[C@@H]1[C@@H]([C@H]([C@@H](C[C@@H]1N)N)O)O[C@H]1O[C@@H]([C@H]([C@@H]1O)O)N)CO)N)O)O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Ether paromomycin derivative 4	Target_lig_302	Bacterial ribosomal A-site	Target_3	4.72124639904717

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	([C@@H]([C@@H]1OCCN)O)CO)N)O)O						
378	[C@H]1([C@H]([C@H]([C@@H](C[C@@H]1CO)O[C@H]1[C@@H]([C@@H]([C@H](C[C@H]1N)N)O)O[C@@H]1O[C@@H]([C@H]([C@H]1OCCNCN)O)CO)N)O)O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Ether paromomycin derivative 5	Target_lig_303	Bacterial ribosomal A-site	Target_3	5.036212172654 44
379	[C@H]1([C@@H]([C@H]([C@H](C[C@@H]1CO)O[C@H]1[C@@H]([C@@H]([C@H](C[C@H]1N)N)O)O[C@@H]1O[C@@H]([C@H]([C@H]1O)O[C@H]1[C@@H]([C@H]([C@@H]([C@@H](O1)CN)O)O)N)COCN(C)C)N)O)O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Ethyl paromomycin derivative 2	Target_lig_304	Bacterial ribosomal A-site	Target_3	5.387216143280 26
380	[C@H]1([C@H]([C@@H]([C@@H](C[C@H]1CO)O[C@@H]1[C@H]([C@H]([C@@H](C[C@@H]1N)N)O)O[C@@H]1O[C@@H]([C@H]([C@H]1O)O[C@@H]1[C@@H]([C@H]([C@H]([C@H](O1)CN)O)O)N)COF)N)O)O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Deoxy fluoro paromomycin	Target_lig_305	Bacterial ribosomal A-site	Target_3	5.958607314841 77
381	C1C(C(C(C(C1N)OC2C(C(C(O2)CO)O)N)O)O)OC3C(C(C(C(O3)CN)O)O)O)N)N	GAGCGUCACACCUUCGGGUGAAGUCGCUC	KANAMYCIN B	Target_lig_8	A-site for Kanamycin B	Target_3	7.096910013008 06
382	CC1C(CC(C(O1)OC2C(C(C(C2O)O)O)O)O)N)N=C(C(=O)O)N	UUGGCUACUAUGCCAGCUGGUGGAUUGCUCGGCUCAGGCGCUGAUGAAGGACGUGCCAAGCUGCGAUAAGCCAUGGGGAGCCGCACGGAGGCGAAGAACCAUGGAUUUCCGAAUGAGAAUCUCUCUAACAAUUGCUUCGCGCAAUGAGGAACCCCGAGAACUGAAACAUCUCAGUAUCGGGAGGAACAGAAAACGCAAUGUGAUGUCGUUAGUAACCGCGAGUGAACGCGAUACAGCCCAAACCGAAGCCCUCACGGGCAAUGUGGUGUCAGGGCUACCUCUCAUCAGCCGACCGUCUCGACGAAGUCUCUUGGAACAGAGCGUGAUACAGGGUGACAACCCCGUACUCGAGACCAGUACGACGUGCGGUAGUGCCAGAGUAGCGGGGGUUGGAUAUC	Kasugamycin	Target_lig_78	Bacterial 70S ribosome	Target_99	4.823908740944 32

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		CCUCGCGAAUAACG CAGGCAUCGACUGC GAAGGCUAAACACA ACCUGAGACCGAUA GUGAACAAGUAGU GUGAACGAACGCUG CAAAGUACCCUCAG AAGGGAGGCGAAA UAGAGCAUGAAAU CAGUUGGCGAUCGA GCGACAGGGCAUAC AAGGUCCCUCGACG AAUGACCGACGCGC GAGCGUCCAGUAAG ACUCACGGGAAGCC GAUGUUCUGUCGU ACGUUUUGAAAAA CGAGCCAGGGAGUG UGUCUGCAUGGCAA GUCUAACCGGAGUA UCCGGGGAGGCACA GGGAAACCGACAUG GCCGCAGGGCUUUG CCCGAGGGCCGCCG UCUUCAAGGGCGGG GAGCCAUGUGGACA CGACCCGAAUCCGG ACGAUCUACGCAUG GACAAGAUGAAGC GUGCCGAAAGGCAC GUGGAAGUCUGUU AGAGUUGGUGUCC UACAAUACCCUCUC GUGAUCUAUGUGU AGGGGUGAAAGGC CCAUCGAGUCCGGC AACAGCUGGUUCCA AUCGAAACAUGUCG AAGCAUGACCUCCG CCGAGGUAGUCUGU GAGGUAGAGCGACC GAUUGGUGUGUCC GCCUCCGAGAGGAG UCGGCACACCUGUC AAACUCCAAACUUA CAGACGCCGUUUGA CGCGGGGAUUCCGG UGCGCGGGGUAAGC CUGUGUACCAGGAG GGGAACAACCCAGA GAUAGGUUAAGGU CCCCAAGUGUGGAU UAAGUGUAAUCCUC UGAAGGUGGUCUC GAGCCCUAGACAGC CGGGAGGUGAGCU UAGAAGCAGCUACC CUCUAAGAAAAGCG UAACAGCUUACCGG CCGAGGUUUGAGGC GCCCAAAAUGAUCG GGACUCAAAUCCAC CACCGAGACCUGUC CGUACCACUCAUAC UGGUAAUCGAGUA GAUUGGCGCUCUAA UUGGAUGGAAGUA GGGGUGAAAACUCC UAUGGACCGAUUA GUGACGAAAAUCCU GGCCAUAGUAGCAG CGAUAGUCGGGUG AGAACCCCGACGGC CUAAUGGAUAAGG GUUCCUCAGCACUG					

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		CUGAUCAGCUGAGG GUUAGCCGGUCCUA AGUCAUACCGCAAC UCGACUAUGACGAA AUGGGAAACGGGU UAAUAUUCCCGUGC CACUAUGCAGUGAA AGUUGACGCCCUGG GGUCGAUCACGCUG GGCAUUCGCCCAGU CGAACCGUCCAACU CCGUGGAAGCCGUA AUGGCAGGAAGCG GACGAACGGCGGCA UAGGGAAACGUGA UUCAACCUGGGGCC CAUGAAAAGACGA GCAUAGUGUCCGUA CCGAGAACCGACAC AGGUGUCCAUGGCG GCGAAAGCCAAGGC CUGUCGGGAGCAAC CAACGUUAGGGAA UUCGGCAAGUUAG UCCCGUACCUUCGG AAGAAGGGAUGCC UGCUCCGGAACGGA GCAGGUCGCAGUGA CUCGGAAGCUCGGA CUGUCUAGUAACAA CAUAGGUGACCGCA AAUCCGCAAGGACU CGUACGGUCACUGA AUCCUGCCCAGUGC AGGUAUCUGAACAC CUCGUACAAGAGGA CGAAGGACCUGUCA ACGGCGGGGGUAAC UAUGACCCUCUUAA GGUAGCGUAGUACC UUGCCGCAUCAGUA GCGGCUUGCAUGAA UGGAUUAACCAGA GCUUCACUGUCCCA ACGUUGGGCCCGGU GAACUGUACAUUCC AGUGCGGAGUCUG GAGACACCCAGGGG GAAGCGAAGACCCU AUGGAGCUUUACU GCAGGCUGUCGCUG AGACGUGGUCGCCG AUGUGCAGCAUAG GUAGGAGACACUAC ACAGGUACCCGCGC UAGCGGGCCACCGA GUCAACAGUGAAA UACUACCCGUCGGU GACUGCGACUCUCA CUCCGGGAGGAGGA CACCGAUAGCCGGG CAGUUUGACUGGG GCGGUACGCGCUCG AAAAGAUAUCGAG CGCGCCCUAUGGCU AUCUCAGCCGGGAC AGAGACCCGGCGAA GAGUGCAAGAGCA AAAGAUAGCUUGA CAGUGUUCUUCCCA ACGAGGAACGCUGA CGCGAAAGCGUGGU CUAGCGAACCAAUU AGCCUGCUUGAUGC GGGCAAUUGAUGA					

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		CAGAAAAGCUACCC UAGGGAUAACAGA GUCGUCACUCGCAA GAGCACAUAUCGAC CGAGUGGCUUGCUA CCUCGAUGUCGGUU CCCUCCAUCCUGCC CGUGCAGAAGCGGG CAAGGGUGAGGUU GUUCGCCUAUUAAA GGAGGUCGUGAGC UGGGUUUAGACCG UCGUGAGACAGGUC GGCUGCUAUCUACU GGGUGUGUAAUGG UGUCUGACAAGAAC GACCGUAUAGUACG AGAGGAACUACGG UUGGUGGCCACUGG UGUACCGGUUGUUC GAGAGAGCACGUGC CGGGUAGCCACGCC ACACGGGGUAAGA GCUGAACGCAUCUA AGCUCGAAACCCAC UUGGAAAAGAGAC ACCGCCGAGGUCCC GCGUACAAGACGCG GUCGAUAGACUCGG GGUGUGCGCGUCGA GGUAACGAGACGU UAAGCCCACGAGCA CUAACAGACCAAAG CCAUCAU					
383	CC1=C(C(=O)NC(=O)N1)C=CC(=O)NC(CO)CS(=O)CSC	UUGGCUACUAUGCC AGCUGGUGGAUUG CUCGGCUCAGGCGC UGAUGAAGGACGU GCCAAGCUGCGAUA AGCCAUGGGGAGCC GCACGGAGGCGAAG AACCAUGGAUUUCC GAAUGAGAAUCUC UCUAACAAUUGCUU CGCGCAAUGAGGAA CCCCGAGAACUGAA ACAUCUCAGUAUCG GGAGGAACAGAAA ACGCAAUGUGAUG UCGUUAGUAACCGC GAGUGAACGCGAU ACAGCCCAAACCGA AGCCCUCACGGGCA AUGUGGUGUCAGG GCUACCUCUCAUCA GCCGACCGUCUCGA CGAAGUCUCUUGGA ACAGAGCGUGAUAC AGGGUGACAACCCC GUACUCGAGACCAG UACGACGUGCGGUA GUGCCAGAGUAGCG GGGGUUGGAUAUC CCUCGCGAAUAACG CAGGCAUCGACUGC GAAGGCUAAACACA ACCUGAGACCGAUA GUGAACAAGUAGU GUGAACGAACGCUG CAAAGUACCCUCAG AAGGGAGGCGAAA UAGAGCAUGAAAU CAGUUGGCGAUCGA GCGACAGGGCAUAC AAGGUCCCUCGACG	Sparsomycin	Target_lig_306	Bacterial 70S ribosome	Target_99	5.39794000867204

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		AAUGACCGACGCGC GAGCGUCCAGUAAG ACUCACGGGAAGCC GAUGUUCUGUCGU ACGUUUUGAAAAA CGAGCCAGGGAGUG UGUCUGCAUGGCAA GUCUAACCGGAGUA UCCGGGGAGGCACA GGGAAACCGACAUG GCCGCAGGGCUUUG CCCGAGGGCCGCCG UCUUCAAGGGCGGG GAGCCAUGUGGACA CGACCCGAAUCCGG ACGAUCUACGCAUG GACAAGAUGAAGC GUGCCGAAAGGCAC GUGGAAGUCUGUU AGAGUUGGUGUCC UACAAUACCCUCUC GUGAUCUAUGUGU AGGGGUGAAAGGC CCAUCGAGUCCGGC AACAGCUGGUUCCA AUCGAAACAUGUCG AAGCAUGACCUCCG CCGAGGUAGUCUGU GAGGUAGAGCGACC GAUUGGUGUGUCC GCCUCCGAGAGGAG UCGGCACACCUGUC AAACUCCAAACUUA CAGACGCCGUUUGA CGCGGGGAUUCCGG UGCGCGGGGUAAGC CUGUGUACCAGGAG GGGAACAACCCAGA GAUAGGUUAAGGU CCCCAAGUGUGGAU UAAGUGUAAUCCUC UGAAGGUGGUCUC GAGCCCUAGACAGC CGGGAGGUGAGCU UAGAAGCAGCUACC CUCUAAGAAAAGCG UAACAGCUUACCGG CCGAGGUUUGAGGC GCCCAAAAUGAUCG GGACUCAAAUCCAC CACCGAGACCUGUC CGUACCACUCAUAC UGGUAAUCGAGUA GAUUGGCGCUCUAA UUGGAUGGAAGUA GGGGUGAAAACUCC UAUGGACCGAUUA GUGACGAAAAUCCU GGCCAUAGUAGCAG CGAUAGUCGGGUG AGAACCCCGACGGC CUAAUGGAUAAGG GUUCCUCAGCACUG CUGAUCAGCUGAGG GUUAGCCGGUCCUA AGUCAUACCGCAAC UCGACUAUGACGAA AUGGGAAACGGGU UAAUAUUCCCGUGC CACUAUGCAGUGAA AGUUGACGCCCUGG GGUCGAUCACGCUG GGCAUUCGCCCAGU CGAACCGUCCAACU CCGUGGAAGCCGUA					

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		AUGGCAGGAAGCG GACGAACGGCGGCA UAGGGAAACGUGA UUCAACCUGGGGCC CAUGAAAAGACGA GCAUAGUGUCCGUA CCGAGAACCGACAC AGGUGUCCAUGGCG GCGAAAGCCAAGGC CUGUCGGGAGCAAC CAACGUUAGGGAA UUCGGCAAGUUAG UCCCGUACCUUCGG AAGAAGGGAUGCC UGCUCCGGAACGGA GCAGGUCGCAGUGA CUCGGAAGCUCGGA CUGUCUAGUAACAA CAUAGGUGACCGCA AAUCCGCAAGGACU CGUACGGUCACUGA AUCCUGCCCAGUGC AGGUAUCUGAACAC CUCGUACAAGAGGA CGAAGGACCUGUCA ACGGCGGGGGUAAC UAUGACCCUCUUAA GGUAGCGUAGUACC UUGCCGCAUCAGUA GCGGCUUGCAUGAA UGGAUUAACCAGA GCUUCACUGUCCCA ACGUUGGGCCCGGU GAACUGUACAUUCC AGUGCGGAGUCUG GAGACACCCAGGGG GAAGCGAAGACCCU AUGGAGCUUUACU GCAGGCUGUCGCUG AGACGUGGUCGCCG AUGUGCAGCAUAG GUAGGAGACACUAC ACAGGUACCCGCGC UAGCGGGCCACCGA GUCAACAGUGAAA UACUACCCGUCGGU GACUGCGACUCUCA CUCCGGGAGGAGGA CACCGAUAGCCGGG CAGUUUGACUGGG GCGGUACGCGCUCG AAAAGAUAUCGAG CGCGCCCUAUGGCU AUCUCAGCCGGGAC AGAGACCCGGCGAA GAGUGCAAGAGCA AAAGAUAGCUUGA CAGUGUUCUUCCCA ACGAGGAACGCUGA CGCGAAAGCGUGGU CUAGCGAACCAAUU AGCCUGCUUGAUGC GGGCAAUUGAUGA CAGAAAAGCUACCC UAGGGAUAACAGA GUCGUCACUCGCAA GAGCACAUAUCGAC CGAGUGGCUUGCUA CCUCGAUGUCGGUU CCCUCCAUCCUGCC CGUGCAGAAGCGGG CAAGGGUGAGGUU GUUCGCCUAUUAAA GGAGGUCGUGAGC UGGGUUUAGACCG					

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		UCGUGAGACAGGUC GGCUGCUAUCUACU GGGUGUGUAAUGG UGUCUGACAAGAAC GACCGUAUAGUACG AGAGGAACUACGG UUGGUGGCCACUGG UGUACCGGUUGUUC GAGAGAGCACGUGC CGGGUAGCCACGCC ACACGGGGUAAGA GCUGAACGCAUCUA AGCUCGAAACCCAC UUGGAAAAGAGAC ACCGCCGAGGUCCC GCGUACAAGACGCG GUCGAUAGACUCGG GGUGUGCGCGUCGA GGUAACGAGACGU UAAGCCCACGAGCA CUAACAGACCAAAG CCAUCAU					
384	CC(=O)NCC1CN(C(=O)O1)C2=CC(=C(C=C2)N3CCOCC3)F	UUGGCUACUAUGCC AGCUGGUGGAUUG CUCGGCUCAGGCGC UGAUGAAGGACGU GCCAAGCUGCGAUA AGCCAUGGGGAGCC GCACGGAGGCGAAG AACCAUGGAUUUCC GAAUGAGAAUCUC UCUAACAAUUGCUU CGCGCAAUGAGGAA CCCCGAGAACUGAA ACAUCUCAGUAUCG GGAGGAACAGAAA ACGCAAUGUGAUG UCGUUAGUAACCGC GAGUGAACGCGAU ACAGCCCAAACCGA AGCCCUCACGGGCA AUGUGGUGUCAGG GCUACCUCUCAUCA GCCGACCGUCUCGA CGAAGUCUCUUGGA ACAGAGCGUGAUAC AGGGUGACAACCCC GUACUCGAGACCAG UACGACGUGCGGUA GUGCCAGAGUAGCG GGGGUUGGAUAUC CCUCGCGAAUAACG CAGGCAUCGACUGC GAAGGCUAAACACA ACCUGAGACCGAUA GUGAACAAGUAGU GUGAACGAACGCUG CAAAGUACCCUCAG AAGGGAGGCGAAA UAGAGCAUGAAAU CAGUUGGCGAUCGA GCGACAGGGCAUAC AAGGUCCCUCGACG AAUGACCGACGCGC GAGCGUCCAGUAAG ACUCACGGGAAGCC GAUGUUCUGUCGU ACGUUUUGAAAAA CGAGCCAGGGAGUG UGUCUGCAUGGCAA GUCUAACCGGAGUA UCCGGGGAGGCACA GGGAAACCGACAUG GCCGCAGGGCUUUG CCCGAGGGCCGCCG	Linezolid	Target_lig_307	Bacterial ribosome	Target_99	4.39794000867204

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		UCUUCAAGGGCGGG GAGCCAUGUGGACA CGACCCGAAUCCGG ACGAUCUACGCAUG GACAAGAUGAAGC GUGCCGAAAGGCAC GUGGAAGUCUGUU AGAGUUGGUGUCC UACAAUACCCUCUC GUGAUCUAUGUGU AGGGGUGAAAGGC CCAUCGAGUCCGGC AACAGCUGGUUCCA AUCGAAACAUGUCG AAGCAUGACCUCCG CCGAGGUAGUCUGU GAGGUAGAGCGACC GAUUGGUGUGUCC GCCUCCGAGAGGAG UCGGCACACCUGUC AAACUCCAAACUUA CAGACGCCGUUUGA CGCGGGGAUUCCGG UGCGCGGGGUAAGC CUGUGUACCAGGAG GGGAACAACCCAGA GAUAGGUUAAGGU CCCCAAGUGUGGAU UAAGUGUAAUCCUC UGAAGGUGGUCUC GAGCCCUAGACAGC CGGGAGGUGAGCU UAGAAGCAGCUACC CUCUAAGAAAAGCG UAACAGCUUACCGG CCGAGGUUUGAGGC GCCCAAAAUGAUCG GGACUCAAAUCCAC CACCGAGACCUGUC CGUACCACUCAUAC UGGUAAUCGAGUA GAUUGGCGCUCUAA UUGGAUGGAAGUA GGGGUGAAAACUCC UAUGGACCGAUUA GUGACGAAAAUCCU GGCCAUAGUAGCAG CGAUAGUCGGGUG AGAACCCCGACGGC CUAAUGGAUAAGG GUUCCUCAGCACUG CUGAUCAGCUGAGG GUUAGCCGGUCCUA AGUCAUACCGCAAC UCGACUAUGACGAA AUGGGAAACGGGU UAAUAUUCCCGUGC CACUAUGCAGUGAA AGUUGACGCCCUGG GGUCGAUCACGCUG GGCAUUCGCCCAGU CGAACCGUCCAACU CCGUGGAAGCCGUA AUGGCAGGAAGCG GACGAACGGCGGCA UAGGGAAACGUGA UUCAACCUGGGGCC CAUGAAAAGACGA GCAUAGUGUCCGUA CCGAGAACCGACAC AGGUGUCCAUGGCG GCGAAAGCCAAGGC CUGUCGGGAGCAAC CAACGUUAGGGAA UUCGGCAAGUUAG					

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		UCCCGUACCUUCGG AAGAAGGGAUGCC UGCUCCGGAACGGA GCAGGUCGCAGUGA CUCGGAAGCUCGGA CUGUCUAGUAACAA CAUAGGUGACCGCA AAUCCGCAAGGACU CGUACGGUCACUGA AUCCUGCCCAGUGC AGGUAUCUGAACAC CUCGUACAAGAGGA CGAAGGACCUGUCA ACGGCGGGGGUAAC UAUGACCCUCUUAA GGUAGCGUAGUACC UUGCCGCAUCAGUA GCGGCUUGCAUGAA UGGAUUAACCAGA GCUUCACUGUCCCA ACGUUGGGCCCGGU GAACUGUACAUUCC AGUGCGGAGUCUG GAGACACCCAGGGG GAAGCGAAGACCCU AUGGAGCUUUACU GCAGGCUGUCGCUG AGACGUGGUCGCCG AUGUGCAGCAUAG GUAGGAGACACUAC ACAGGUACCCGCGC UAGCGGGCCACCGA GUCAACAGUGAAA UACUACCCGUCGGU GACUGCGACUCUCA CUCCGGGAGGAGGA CACCGAUAGCCGGG CAGUUUGACUGGG GCGGUACGCGCUCG AAAAGAUAUCGAG CGCGCCCUAUGGCU AUCUCAGCCGGGAC AGAGACCCGGCGAA GAGUGCAAGAGCA AAAGAUAGCUUGA CAGUGUUCUUCCCA ACGAGGAACGCUGA CGCGAAAGCGUGGU CUAGCGAACCAAUU AGCCUGCUUGAUGC GGGCAAUUGAUGA CAGAAAAGCUACCC UAGGGAUAACAGA GUCGUCACUCGCAA GAGCACAUAUCGAC CGAGUGGCUUGCUA CCUCGAUGUCGGUU CCCUCCAUCCUGCC CGUGCAGAAGCGGG CAAGGGUGAGGUU GUUCGCCUAUUAAA GGAGGUCGUGAGC UGGGUUUAGACCG UCGUGAGACAGGUC GGCUGCUAUCUACU GGGUGUGUAAUGG UGUCUGACAAGAAC GACCGUAUAGUACG AGAGGAACUACGG UUGGUGGCCACUGG UGUACCGGUUGUUC GAGAGAGCACGUGC CGGGUAGCCACGCC ACACGGGGUAAGA GCUGAACGCAUCUA					

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		AGCUCGAAACCCAC UUGGAAAAGAGAC ACCGCCGAGGUCCC GCGUACAAGACGCG GUCGAUAGACUCGG GGUGUGCGCGUCGA GGUAACGAGACGU UAAGCCCACGAGCA CUAACAGACCAAAG CCAUCAU					
386	CC=C1C2=NC(=CS2)C(=O)NC(C3=NC(=CS3)C(=O)NC(C4=NC(=CS4)C5=C(C=CC(=N5)C6=NC(=CS6)C7=NC(=CS7)C(=O)NC(=CC)C(=O)NCC(C)O)C8=NC(=CS8)C(=O)NC(C(=O)N1)C(C)O)C(C)O)C(C)C	GCUGGGAUGUUGG CUUAGAAGCAGCCA UCAUUUAAAGAGU GCGUAACAGCUCAC CAGC	Micrococcin	Target_lig_309	L11 binding BD RNA	Target_122	7.09691001300806
387	CC=C1C2=NC(=CS2)C(=O)NC3CC(C(=O)OCC4=C5C(=C(C(=O)SCC(C6=NC(=CS6)C7=NC(=C(C=C7C8=NC(=CS8)C(=O)NC(C(=O)N1)C(C)O)O)C9=NC(=CS9)C(=O)NC(=C)C(=O)N)NC(=O)C1=CSC3=N1)NC5=CC=C4)C)O	GCUGGGAUGUUGG CUUAGAAGCAGCCA UCAUUUAAAGAGU GCGUAACAGCUCAC CAGC	Nosiheptide	Target_lig_310	L11 binding BD RNA	Target_122	5.30102999566398
389	C1C(C(C(C(C1N)OC2C(C(C(C(O2)CO)O)O)N)O)O)N	UACCUGGUUGAUCC UGCCAGUAGCAUAU GCUUGUCUCAAAGA UUAAGCCAUGCAUG UCUAAGUACGCACG GCCGGUACAGUGAA ACUGCGAAUGGCUC AUUAAAUCAGUUA UGGUUCCUUUGGUC GCUCGCUCCUCUCC CACUUGGAUAACUG UGGUAAUUCUAGA GCUAAUACAUGCCG ACGGGCGCUGACCC CCUUCGCGGGGGGG AUGCGUGCAUUUA UCAGAUCAAAACCA ACCCGGUCAGCCCC UCUCCGGCCCCGGC CGGGGGGCGGGCGC CGGCGGCUUUGGUG ACUCUAGAUAACCU CGGGCCGAUCGCAC GCCCCCCGUGGCGG CGACGACCCAUUCG AACGUCUGCCCUAU CAACUUUCGAUGGU AGUCGCCGUGCCUA CCAUGGUGACCACG GGUGACGGGGAAU CAGGGUUCGAUUCC GGAGAGGGAGCCU GAGAAACGGCUACC ACAUCCAAGGAAGG CAGCAGGCGCGCAA AUUACCCACUCCCG ACCCGGGGAGGUAG UGACGAAAAAUAA CAAUACAGGACUCU UUCGAGGCCCUGUA AUUGGAAUGAGUC CACUUUAAAUCCUU CCGCGAGGAUCCAU	Paromamine	Target_lig_311	Human A-site	Target_103	4

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		UGGAGGGCAAGUC UGGUGCCAGCAGCC GCGGUAAUUCCAGC UCCAAUAGCGUAUA UUAAAGUUGCUGC AGUUAAAAAGCUC GUAGUUGGAUCUU GGGAGCGGGCGGGC GGUCCGCCGCGAGG CGAGCCACCGCCCG UCCCCGCCCCUUGC CUCUCGGCGCCCCC UCGAUGCUCUUAGC UGAGUGUCCCGCGG GGCCCGAAGCAUUU ACUUUGAAAAAAU UAGAGUGUUCAAA GCAGGCCCGAGCCG CCUGGAUACCGCAG CUAGGAAUAAUGG AAUAGGACCGCGGU UCUAUUUUGUUGG UUUUCGGAACUGA GGCCAUGAUUAAG AGGGACGGCCGGGG GCAUUCGUAUUGCG CCGCUAGAGGUGAA AUUCUUGGACCGGC GCAAGACGGACCAG AGCGAAAGCAUUU GCCAAGAAUGUUU UCAUUAAUCAAGA ACGAAAGUCGGAG GUUCGAAGACGAUC AGAUACCGUCGUAG UUCCGACCAUAAAC GAUGCCGACUGGCG AUGCGGCGGCGUUA UUCCCAUGACCCGC CGGGCAGCUUCCGG GAAACCAAAGUCUU UGGGUUCCGGGGG GAGUAUGGUUGCA AAGCUGAAACUUA AAGGAAUUGACGG AAGGGCACCACCAG GAGUGGAGCCUGCG GCUUAAUUUGACUC AACACGGGAAACCU CACCCGGCCCGGAC ACGGACAGGAUUG ACAGAUUGAUAGC UCUUUCUCGAUUCC GUGGGUGGUGGUG CAUGGCCGUUCUUA GUUGGUGGAGCGA UUUGUCUGGUUAA UUCCGAUAACGAAC GAGACUCUGGCAUG CUAACUAGUUACGC GACCCCCGAGCGGU CGGCGUCCCCCAAC UUCUUAGAGGGAC AAGUGGCGUUCAGC CACCCGAGAUUGAG CAAUAACAGGUCUG UGAUGCCCUUAGAU GUCCGGGGCUGCAC GCGCGCUACACUGA CUGGCUCAGCGUGU GCCUACCCUACGCC GGCAGGCGCGGGUA ACCCGUUGAACCCC AUUCGUGAUGGGG AUCGGGGAUUGCA					

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		AUUAUUCCCCAUGA ACGAGGAAUUCCCA GUAAGUGCGGGUC AUAAGCUUGCGUU GAUUAAGUCCCUGC CCUUUGUACACACC GCCCGUCGCUACUA CCGAUUGGAUGGU UUAGUGAGGCCCUC GGAUCGGCCCCGCC GGGGUCGGCCCACG GCCCUGGCGGAGCG CUGAGAAGACGGUC GAACUUGACUAUCU AGAGGAAGUAAAA GUCGUAACAAGGU UUCCGUAGGUGAAC CUGCGGAAGGAUCA UUA					
390	CN(C)C1=NC=NC2=C1N=CN2C3C(C(C(O3)CO)NC(=O)C(CC4=CC=C(C=C4)OC)N)O	GGUUAAGCGACUA AGCGUACACGGUGG AUGCCCUGGCAGUC AGAGGCGAUGAAG GACGUGCUAAUCUG CGAUAAGCGUCGGU AAGGUGAUAUGAA CCGUUAUAACCGGC GAUUUCCGAAUGG GGAAACCCAGUGUG UUUCGACACACUAU CAUUAACUGAAUCC AUAGGUUAAUGAG GCGAACCGGGGGAA CUGAAACAUCUAAG UACCCCGAGGAAAA GAAAUCAACCGAGA UUCCCCCAGUAGCG GCGAGCGAACGGGG AGCAGCCCAGAGCC UGAAUCAGUGUGU GUGUUAGUGGAAG CGUCUGGAAAGGCG CGCGAUACAGGGUG ACAGCCCCGUACAC AAAAAUGCACAUGC UGUGAGCUCGAUG AGUAGGGCGGGAC ACGUGGUAUCCUGU CUGAAUAUGGGGG GACCAUCCUCCAAG GCUAAAUACUCCUG ACUGACCGAUAGUG AACCAGUACCGUGA GGGAAAGGCGAAA AGAACCCCGGCGAG GGGAGUGAAAAAG AACCUGAAACCGUG UACGUACAAGCAGU GGGAGCACGCUUAG GCGUGUGACUGCGU ACCUUUUGUAUAA UGGGUCAGCGACUU AUAUUCUGUAGCA AGGUUAACCGAAU AGGGGAGCCGAAG GGAAACCGAGUCUU AACUGGGCGUUAA GUUGCAGGGUAUA GACCCGAAACCCGG UGAUCUAGCCAUGG GCAGGUUGAAGGU UGGGUAACACUAAC UGGAGGACCGAACC GACUAAUGUUGAA AAAUUAGCGGAUG	Puromycin	Target_lig_312	50S A-site for puromycin	Target_100	3.31875876262441

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		ACUUGUGGCUGGG GGUGAAAGGCCAA UCAAACCGGGAGAU AGCUGGUUCUCCCC GAAAGCUAUUUAG GUAGCGCCUCGUGA AUUCAUCUCCGGGG GUAGAGCACUGUU UCGGCAAGGGGGUC ACUUACCAACCCGA UGCAAACUGCGAAU ACCGGAGAAUGUU AUCACGGGAGACAC ACGGCGGGUGCUAA CGUCCGUCGUGAAG AGGGAAACAACCCA GACCGCCAGCUAAG GUCCCAAAGUCAUG GUUAAGUGGGAAA CGAUGUGGGAAGG CCCAGACAGCCAGG AUGUUGGCUUAGA AGCAGCCAUCAUUU AAAGAAAGCGUAA UAGCUCACUGGUCG AGUCGGCCUGCGCG GAAGAUGUAACGG GGCUAAACCAUGCA CCGAAGCUGCGGCA GCGACGCUUAUGCG UUGUUGGGUAGGG GAGCGUUCUGUAA GCCUGCGAAGGUGU GCUGUGAGGCAUGC UGGAGGUAUCAGA AGUGCGAAUGCUG ACAUAAGUAACGA UAAAGCGGGUGAA AAGCCCGCUCGCCG GAAGACCAAGGGU UCCUGUCCAACGUU AAUCGGGGCAGGG UGAGUCGACCCCUA AGGCGAGGCCGAAA GGCGUAGUCGAUG GGAAACAGGUUAA UAUUCCUGUACUUG GUGUUACUGCGAA GGGGGGACGGAGA AGGCUAUGUUGGCC GGGCGACGGUUGUC CCGGUUUAAGCGUG UAGGCUGGUUUUCC AGGCAAAUCCGGAA AAUCAAGGCUGAG GCGUGAUGACGAG GCACUACGGUGCUG AAGCAACAAAUGCC CUGCUUCCAGGAAA AGCCUCUAAGCAUC AGGUAACAUCAAA UCGUACCCCAAACC GACACAGGUGGUCA GGUAGAGAAUACC AAGGCGCUUGAGA GAACUCGGGUGAA GGAACUAGGCAAA AUGGUGCCGUAACU UCGGGAGAAGGCAC GCUGAUAUGUAGG UGAGGUCCCUCGCG GAUGGAGCUGAAA UCAGUCGAAGAUAC CAGCUGGCUGCAAC UGUUUAUUAAAAA					

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		CACAGCACUGUGCA AACACGAAAGUGG ACGUAUACGGUGU GACGCCUGCCCGGU GCCGGAAGGUUAA UUGAUGGGGUUAG CGCAAGCGAAGCUC UUGAUCGAAGCCCC GGUAAACGGCGGCC GUAACXAUAACGG UCCUAAGGUAGCGA AAUUCCUUGUCGGG UAAGUUCCGACCUG CACGAAUGGCGUAA UGAUGGCCAGGCUG UCUCCACCCGAGAC UCAGUGAAAUUGA ACUCGCUGUGAAGA UGCAGUGUACCCGC GGCAAGACGGAAA GACCCCGUGAACCU UUACUAUAGCUUG ACACUGAACAUUGA GCCUUGAUGUGUA GGAUAGGUGGGAG GCUUUGAAGUGUG GACGCCAGUCUGCA UGGAGCCGACCUUG AAAUACCACCCUUU AAUGUUUGAUGUU CUAACGUUGACCCG UAAUCCGGGUUGCG GACAGUGUCUGGU GGGUAGUUUGACU GGGGCGGUCUCCUC CUAAAGAGUAACG GAGGAGCACGAAG GUUGGCUAAUCCUG GUCGGACAUCAGGA GGUUAGUGCAAUG GCAUAAGCCAGCUU GACUGCGAGCGUGA CGGCGCGAGCAGGU GCGAAAGCAGGUCA UAGUGAUCCGGUG GUUCUGAAUGGAA GGGCCAUCGCUCAA CGGAUAAAAGGUA CUCCGGGGAUAACA GGCUGAUACCGCCC AAGAGUUCAUAUC GACGGCGGUGUUU GGCACCUCGAUGUC GGCUCAUCACAUCC UGGGGCUGAAGUA GGUCCCAAGGGUAU GGCUGUUCGCCAUU UAAAGUGGUACGC GAGCUGGGUUUAG AACGUCGUGAGACA GUUCGGUCCCUAUC UGCCGUGGGCGCUG GAGAACUGAGGGG GGCUGCUCCUAGUA CGAGAGGACCGGAG UGGACGCAUCACUG GUGUUCGGGUUGU CAUGCCAAUGGCAC UGCCCGGUAGCUAA AUGCGGAAGAGAU AAGUGCUGAAAGC AUCUAAGCACGAAA CUUGCCCCGAGAUG AGUUCUCCCUGACC CUUUAAGGGUCCUG					

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		AAGGAACGUUGAA GACGACGACGUUGA UAGGCCGGGUGUG UAAGCGCAGCGAUG CGUUGAGCUAACCG GUACUAAUGAACCG UGAGGCUUAACCU					
391	CC1CCC23CCC(=O)C 2C1(C(CC(C(C3C)O) (C)C=C)OC(=O)CSC4 CC5CCC(C4)N5C)C	GGUUAAGCGACUA AGCGUACACGGUGG AUGCCCUGGCAGUC AGAGGCGAUGAAG GACGUGCUAAUCUG CGAUAAGCGUCGGU AAGGUGAUAUGAA CCGUUAUAACCGGC GAUUUCCGAAUGG GGAAACCCAGUGUG UUUCGACACACUAU CAUUAACUGAAUCC AUAGGUUAAUGAG GCGAACCGGGGGAA CUGAAACAUCUAAG UACCCCGAGGAAAA GAAAUCAACCGAGA UUCCCCCAGUAGCG GCGAGCGAACGGGG AGCAGCCCAGAGCC UGAAUCAGUGUGU GUGUUAGUGGAAG CGUCUGGAAAGGCG CGCGAUACAGGGUG ACAGCCCCGUACAC AAAAAUGCACAUGC UGUGAGCUCGAUG AGUAGGGCGGGAC ACGUGGUAUCCUGU CUGAAUAUGGGGG GACCAUCCUCCAAG GCUAAAUACUCCUG ACUGACCGAUAGUG AACCAGUACCGUGA GGGAAAGGCGAAA AGAACCCCGGCGAG GGGAGUGAAAAAG AACCUGAAACCGUG UACGUACAAGCAGU GGGAGCACGCUUAG GCGUGUGACUGCGU ACCUUUUGUAUAA UGGGUCAGCGACUU AUAUUCUGUAGCA AGGUUAACCGAAU AGGGGAGCCGAAG GGAAACCGAGUCUU AACUGGGCGUUAA GUUGCAGGGUAUA GACCCGAAACCCGG UGAUCUAGCCAUGG GCAGGUUGAAGGU UGGGUAACACUAAC UGGAGGACCGAACC GACUAAUGUUGAA AAAUUAGCGGAUG ACUUGUGGCUGGG GGUGAAAGGCCAA UCAAACCGGGAGAU AGCUGGUUCUCCCC GAAAGCUAUUUAG GUAGCGCCUCGUGA AUUCAUCUCCGGGG GUAGAGCACUGUU UCGGCAAGGGGGUC ACUUACCAACCCGA UGCAAACUGCGAAU ACCGGAGAAUGUU	Retapamulin	Target_lig_313	large ribosomal subunit from Deinococcus radiodurans	Target_100	8.69897000433602

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		AUCACGGGAGACAC ACGGCGGGUGCUAA CGUCCGUCGUGAAG AGGGAAACAACCCA GACCGCCAGCUAAG GUCCCAAAGUCAUG GUUAAGUGGGAAA CGAUGUGGGAAGG CCCAGACAGCCAGG AUGUUGGCUUAGA AGCAGCCAUCAUUU AAAGAAAGCGUAA UAGCUCACUGGUCG AGUCGGCCUGCGCG GAAGAUGUAACGG GGCUAAACCAUGCA CCGAAGCUGCGGCA GCGACGCUUAUGCG UUGUUGGGUAGGG GAGCGUUCUGUAA GCCUGCGAAGGUGU GCUGUGAGGCAUGC UGGAGGUAUCAGA AGUGCGAAUGCUG ACAUAAGUAACGA UAAAGCGGGUGAA AAGCCCGCUCGCCG GAAGACCAAGGGU UCCUGUCCAACGUU AAUCGGGGCAGGG UGAGUCGACCCCUA AGGCGAGGCCGAAA GGCGUAGUCGAUG GGAAACAGGUUAA UAUUCCUGUACUUG GUGUUACUGCGAA GGGGGGACGGAGA AGGCUAUGUUGGCC GGGCGACGGUUGUC CCGGUUUAAGCGUG UAGGCUGGUUUUCC AGGCAAAUCCGGAA AAUCAAGGCUGAG GCGUGAUGACGAG GCACUACGGUGCUG AAGCAACAAAUGCC CUGCUUCCAGGAAA AGCCUCUAAGCAUC AGGUAACAUCAAA UCGUACCCCAAACC GACACAGGUGGUCA GGUAGAGAAUACC AAGGCGCUUGAGA GAACUCGGGUGAA GGAACUAGGCAAA AUGGUGCCGUAACU UCGGGAGAAGGCAC GCUGAUAUGUAGG UGAGGUCCCUCGCG GAUGGAGCUGAAA UCAGUCGAAGAUAC CAGCUGGCUGCAAC UGUUUAUUAAAAA CACAGCACUGUGCA AACACGAAAGUGG ACGUAUACGGUGU GACGCCUGCCCGGU GCCGGAAGGUUAA UUGAUGGGGUUAG CGCAAGCGAAGCUC UUGAUCGAAGCCCC GGUAAACGGCGGCC GUAACXAUAACGG UCCUAAGGUAGCGA AAUUCCUUGUCGGG					

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		UAAGUUCCGACCUG CACGAAUGGCGUAA UGAUGGCCAGGCUG UCUCCACCCGAGAC UCAGUGAAAUUGA ACUCGCUGUGAAGA UGCAGUGUACCCGC GGCAAGACGGAAA GACCCCGUGAACCU UUACUAUAGCUUG ACACUGAACAUUGA GCCUUGAUGUGUA GGAUAGGUGGGAG GCUUUGAAGUGUG GACGCCAGUCUGCA UGGAGCCGACCUUG AAAUACCACCCUUU AAUGUUUGAUGUU CUAACGUUGACCCG UAAUCCGGGUUGCG GACAGUGUCUGGU GGGUAGUUUGACU GGGGCGGUCUCCUC CUAAAGAGUAACG GAGGAGCACGAAG GUUGGCUAAUCCUG GUCGGACAUCAGGA GGUUAGUGCAAUG GCAUAAGCCAGCUU GACUGCGAGCGUGA CGGCGCGAGCAGGU GCGAAAGCAGGUCA UAGUGAUCCGGUG GUUCUGAAUGGAA GGGCCAUCGCUCAA CGGAUAAAAGGUA CUCCGGGGAUAACA GGCUGAUACCGCCC AAGAGUUCAUAUC GACGGCGGUGUUU GGCACCUCGAUGUC GGCUCAUCACAUCC UGGGGCUGAAGUA GGUCCCAAGGGUAU GGCUGUUCGCCAUU UAAAGUGGUACGC GAGCUGGGUUUAG AACGUCGUGAGACA GUUCGGUCCCUAUC UGCCGUGGGCGCUG GAGAACUGAGGGG GGCUGCUCCUAGUA CGAGAGGACCGGAG UGGACGCAUCACUG GUGUUCGGGUUGU CAUGCCAAUGGCAC UGCCCGGUAGCUAA AUGCGGAAGAGAU AAGUGCUGAAAGC AUCUAAGCACGAAA CUUGCCCCGAGAUG AGUUCUCCCUGACC CUUUAAGGGUCCUG AAGGAACGUUGAA GACGACGACGUUGA UAGGCCGGGUGUG UAAGCGCAGCGAUG CGUUGAGCUAACCG GUACUAAUGAACCG UGAGGCUUAACCU					
394	CC1CC=CC=CC(C(CC(C(C(C(CC(=O)O1)O)OC)OC2C(C(C(C(O2)C)OC3CC(C(C(O3)C)O)	GGUUAAGCGACUA AGCGUACACGGUGG AUGCCCUGGCAGUC AGAGGCGAUGAAG GACGUGCUAAUCUG	Spiramycin A	Target_lig_315	50S exit tunnel for SPIRAMYCIN A	Target_100	5.74472749489669

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	(C)O)N(C)C)O)CC=O)C)OC4CCC(C(O4)C)N(C)C	CGAUAAGCGUCGGU AAGGUGAUAUGAA CCGUUAUAACCGGC GAUUUCCGAAUGG GGAAACCCAGUGUG UUUCGACACACUAU CAUUAACUGAAUCC AUAGGUUAAUGAG GCGAACCGGGGGAA CUGAAACAUCUAAG UACCCCGAGGAAAA GAAAUCAACCGAGA UUCCCCCAGUAGCG GCGAGCGAACGGGG AGCAGCCCAGAGCC UGAAUCAGUGUGU GUGUUAGUGGAAG CGUCUGGAAAGGCG CGCGAUACAGGGUG ACAGCCCCGUACAC AAAAAUGCACAUGC UGUGAGCUCGAUG AGUAGGGCGGGAC ACGUGGUAUCCUGU CUGAAUAUGGGGG GACCAUCCUCCAAG GCUAAAUACUCCUG ACUGACCGAUAGUG AACCAGUACCGUGA GGGAAAGGCGAAA AGAACCCCGGCGAG GGGAGUGAAAAAG AACCUGAAACCGUG UACGUACAAGCAGU GGGAGCACGCUUAG GCGUGUGACUGCGU ACCUUUUGUAUAA UGGGUCAGCGACUU AUAUUCUGUAGCA AGGUUAACCGAAU AGGGGAGCCGAAG GGAAACCGAGUCUU AACUGGGCGUUAA GUUGCAGGGUAUA GACCCGAAACCCGG UGAUCUAGCCAUGG GCAGGUUGAAGGU UGGGUAACACUAAC UGGAGGACCGAACC GACUAAUGUUGAA AAAUUAGCGGAUG ACUUGUGGCUGGG GGUGAAAGGCCAA UCAAACCGGGAGAU AGCUGGUUCUCCCC GAAAGCUAUUUAG GUAGCGCCUCGUGA AUUCAUCUCCGGGG GUAGAGCACUGUU UCGGCAAGGGGGUC ACUUACCAACCCGA UGCAAACUGCGAAU ACCGGAGAAUGUU AUCACGGGAGACAC ACGGCGGGUGCUAA CGUCCGUCGUGAAG AGGGAAACAACCCA GACCGCCAGCUAAG GUCCCAAAGUCAUG GUUAAGUGGGAAA CGAUGUGGGAAGG CCCAGACAGCCAGG AUGUUGGCUUAGA AGCAGCCAUCAUUU AAAGAAAGCGUAA					

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		UAGCUCACUGGUCG AGUCGGCCUGCGCG GAAGAUGUAACGG GGCUAAACCAUGCA CCGAAGCUGCGGCA GCGACGCUUAUGCG UUGUUGGGUAGGG GAGCGUUCUGUAA GCCUGCGAAGGUGU GCUGUGAGGCAUGC UGGAGGUAUCAGA AGUGCGAAUGCUG ACAUAAGUAACGA UAAAGCGGGUGAA AAGCCCGCUCGCCG GAAGACCAAGGGU UCCUGUCCAACGUU AAUCGGGGCAGGG UGAGUCGACCCCUA AGGCGAGGCCGAAA GGCGUAGUCGAUG GGAAACAGGUUAA UAUUCCUGUACUUG GUGUUACUGCGAA GGGGGGACGGAGA AGGCUAUGUUGGCC GGGCGACGGUUGUC CCGGUUUAAGCGUG UAGGCUGGUUUUCC AGGCAAAUCCGGAA AAUCAAGGCUGAG GCGUGAUGACGAG GCACUACGGUGCUG AAGCAACAAAUGCC CUGCUUCCAGGAAA AGCCUCUAAGCAUC AGGUAACAUCAAA UCGUACCCCAAACC GACACAGGUGGUCA GGUAGAGAAUACC AAGGCGCUUGAGA GAACUCGGGUGAA GGAACUAGGCAAA AUGGUGCCGUAACU UCGGGAGAAGGCAC GCUGAUAUGUAGG UGAGGUCCCUCGCG GAUGGAGCUGAAA UCAGUCGAAGAUAC CAGCUGGCUGCAAC UGUUUAUUAAAAA CACAGCACUGUGCA AACACGAAAGUGG ACGUAUACGGUGU GACGCCUGCCCGGU GCCGGAAGGUUAA UUGAUGGGGUUAG CGCAAGCGAAGCUC UUGAUCGAAGCCCC GGUAAACGGCGGCC GUAACXAUAACGG UCCUAAGGUAGCGA AAUUCCUUGUCGGG UAAGUUCCGACCUG CACGAAUGGCGUAA UGAUGGCCAGGCUG UCUCCACCCGAGAC UCAGUGAAAUUGA ACUCGCUGUGAAGA UGCAGUGUACCCGC GGCAAGACGGAAA GACCCCGUGAACCU UUACUAUAGCUUG ACACUGAACAUUGA GCCUUGAUGUGUA					

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		GGAUAGGUGGGAG GCUUUGAAGUGUG GACGCCAGUCUGCA UGGAGCCGACCUUG AAAUACCACCCUUU AAUGUUUGAUGUU CUAACGUUGACCCG UAAUCCGGGUUGCG GACAGUGUCUGGU GGGUAGUUUGACU GGGGCGGUCUCCUC CUAAAGAGUAACG GAGGAGCACGAAG GUUGGCUAAUCCUG GUCGGACAUCAGGA GGUUAGUGCAAUG GCAUAAGCCAGCUU GACUGCGAGCGUGA CGGCGCGAGCAGGU GCGAAAGCAGGUCA UAGUGAUCCGGUG GUUCUGAAUGGAA GGGCCAUCGCUCAA CGGAUAAAAGGUA CUCCGGGGAUAACA GGCUGAUACCGCCC AAGAGUUCAUAUC GACGGCGGUGUUU GGCACCUCGAUGUC GGCUCAUCACAUCC UGGGGCUGAAGUA GGUCCCAAGGGUAU GGCUGUUCGCCAUU UAAAGUGGUACGC GAGCUGGGUUUAG AACGUCGUGAGACA GUUCGGUCCCUAUC UGCCGUGGGCGCUG GAGAACUGAGGGG GGCUGCUCCUAGUA CGAGAGGACCGGAG UGGACGCAUCACUG GUGUUCGGGUUGU CAUGCCAAUGGCAC UGCCCGGUAGCUAA AUGCGGAAGAGAU AAGUGCUGAAAGC AUCUAAGCACGAAA CUUGCCCCGAGAUG AGUUCUCCCUGACC CUUUAAGGGUCCUG AAGGAACGUUGAA GACGACGACGUUGA UAGGCCGGGUGUG UAAGCGCAGCGAUG CGUUGAGCUAACCG GUACUAAUGAACCG UGAGGCUUAACCU					
396	CCC1C2(C(C(C(=O)C(CC(C(C(C(=O)C(C(=O)O1)C)C)OC3C(C(CC(O3)C)N(C)C)O)(C)OC)C)C)N(C(=O)O2)CCCCN4C=C(N=C4)C5=CN=CC=C5)C	GGUUAAGCGACUA AGCGUACACGGUGG AUGCCCUGGCAGUC AGAGGCGAUGAAG GACGUGCUAAUCUG CGAUAAGCGUCGGU AAGGUGAUAUGAA CCGUUAUAACCGGC GAUUUCCGAAUGG GGAAACCCAGUGUG UUUCGACACACUAU CAUUAACUGAAUCC AUAGGUUAAUGAG GCGAACCGGGGGAA CUGAAACAUCUAAG UACCCCGAGGAAAA GAAAUCAACCGAGA	Telithromycin	Target_lig_317	Large subunit (TELITHROMYCIN)	Target_100	8.886056647693 16

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		UUCCCCCAGUAGCG GCGAGCGAACGGGG AGCAGCCCAGAGCC UGAAUCAGUGUGU GUGUUAGUGGAAG CGUCUGGAAAGGCG CGCGAUACAGGGUG ACAGCCCCGUACAC AAAAAUGCACAUGC UGUGAGCUCGAUG AGUAGGGCGGGAC ACGUGGUAUCCUGU CUGAAUAUGGGGG GACCAUCCUCCAAG GCUAAAUACUCCUG ACUGACCGAUAGUG AACCAGUACCGUGA GGGAAAGGCGAAA AGAACCCCGGCGAG GGGAGUGAAAAAG AACCUGAAACCGUG UACGUACAAGCAGU GGGAGCACGCUUAG GCGUGUGACUGCGU ACCUUUUGUAUAA UGGGUCAGCGACUU AUAUUCUGUAGCA AGGUUAACCGAAU AGGGGAGCCGAAG GGAAACCGAGUCUU AACUGGGCGUUAA GUUGCAGGGUAUA GACCCGAAACCCGG UGAUCUAGCCAUGG GCAGGUUGAAGGU UGGGUAACACUAAC UGGAGGACCGAACC GACUAAUGUUGAA AAAUUAGCGGAUG ACUUGUGGCUGGG GGUGAAAGGCCAA UCAAACCGGGAGAU AGCUGGUUCUCCCC GAAAGCUAUUUAG GUAGCGCCUCGUGA AUUCAUCUCCGGGG GUAGAGCACUGUU UCGGCAAGGGGGUC ACUUACCAACCCGA UGCAAACUGCGAAU ACCGGAGAAUGUU AUCACGGGAGACAC ACGGCGGGUGCUAA CGUCCGUCGUGAAG AGGGAAACAACCCA GACCGCCAGCUAAG GUCCCAAAGUCAUG GUUAAGUGGGAAA CGAUGUGGGAAGG CCCAGACAGCCAGG AUGUUGGCUUAGA AGCAGCCAUCAUUU AAAGAAAGCGUAA UAGCUCACUGGUCG AGUCGGCCUGCGCG GAAGAUGUAACGG GGCUAAACCAUGCA CCGAAGCUGCGGCA GCGACGCUUAUGCG UUGUUGGGUAGGG GAGCGUUCUGUAA GCCUGCGAAGGUGU GCUGUGAGGCAUGC UGGAGGUAUCAGA AGUGCGAAUGCUG					

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		ACAUAAGUAACGA UAAAGCGGGUGAA AAGCCCGCUCGCCG GAAGACCAAGGGU UCCUGUCCAACGUU AAUCGGGGCAGGG UGAGUCGACCCCUA AGGCGAGGCCGAAA GGCGUAGUCGAUG GGAAACAGGUUAA UAUUCCUGUACUUG GUGUUACUGCGAA GGGGGGACGGAGA AGGCUAUGUUGGCC GGGCGACGGUUGUC CCGGUUUAAGCGUG UAGGCUGGUUUUCC AGGCAAAUCCGGAA AAUCAAGGCUGAG GCGUGAUGACGAG GCACUACGGUGCUG AAGCAACAAAUGCC CUGCUUCCAGGAAA AGCCUCUAAGCAUC AGGUAACAUCAAA UCGUACCCCAAACC GACACAGGUGGUCA GGUAGAGAAUACC AAGGCGCUUGAGA GAACUCGGGUGAA GGAACUAGGCAAA AUGGUGCCGUAACU UCGGGAGAAGGCAC GCUGAUAUGUAGG UGAGGUCCCUCGCG GAUGGAGCUGAAA UCAGUCGAAGAUAC CAGCUGGCUGCAAC UGUUUAUUAAAAA CACAGCACUGUGCA AACACGAAAGUGG ACGUAUACGGUGU GACGCCUGCCCGGU GCCGGAAGGUUAA UUGAUGGGGUUAG CGCAAGCGAAGCUC UUGAUCGAAGCCCC GGUAAACGGCGGCC GUAACXAUAACGG UCCUAAGGUAGCGA AAUUCCUUGUCGGG UAAGUUCCGACCUG CACGAAUGGCGUAA UGAUGGCCAGGCUG UCUCCACCCGAGAC UCAGUGAAAUUGA ACUCGCUGUGAAGA UGCAGUGUACCCGC GGCAAGACGGAAA GACCCCGUGAACCU UUACUAUAGCUUG ACACUGAACAUUGA GCCUUGAUGUGUA GGAUAGGUGGGAG GCUUUGAAGUGUG GACGCCAGUCUGCA UGGAGCCGACCUUG AAAUACCACCCUUU AAUGUUUGAUGUU CUAACGUUGACCCG UAAUCCGGGUUGCG GACAGUGUCUGGU GGGUAGUUUGACU GGGGCGGUCUCCUC CUAAAGAGUAACG					

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		GAGGAGCACGAAG GUUGGCUAAUCCUG GUCGGACAUCAGGA GGUUAGUGCAAUG GCAUAAGCCAGCUU GACUGCGAGCGUGA CGGCGCGAGCAGGU GCGAAAGCAGGUCA UAGUGAUCCGGUG GUUCUGAAUGGAA GGGCCAUCGCUCAA CGGAUAAAAGGUA CUCCGGGGAUAACA GGCUGAUACCGCCC AAGAGUUCAUAUC GACGGCGGUGUUU GGCACCUCGAUGUC GGCUCAUCACAUCC UGGGGCUGAAGUA GGUCCCAAGGGUAU GGCUGUUCGCCAUU UAAAGUGGUACGC GAGCUGGGUUUAG AACGUCGUGAGACA GUUCGGUCCCUAUC UGCCGUGGGCGCUG GAGAACUGAGGGG GGCUGCUCCUAGUA CGAGAGGACCGGAG UGGACGCAUCACUG GUGUUCGGGUUGU CAUGCCAAUGGCAC UGCCCGGUAGCUAA AUGCGGAAGAGAU AAGUGCUGAAAGC AUCUAAGCACGAAA CUUGCCCCGAGAUG AGUUCUCCCUGACC CUUUAAGGGUCCUG AAGGAACGUUGAA GACGACGACGUUGA UAGGCCGGGUGUG UAAGCGCAGCGAUG CGUUGAGCUAACCG GUACUAAUGAACCG UGAGGCUUAACCU					
397	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	AAAUUGAAGAGUU UGAUCAUGGCUCAG AUUGAACGCUGGCG GCAGGCCUAACACA UGCAAGUCGAACGG UAACAGGAAGAAG CUUGCUUCUUUGCU GACGAGUGGCGGAC GGGUGAGUAAUGU CUGGGAAACUGCCU GAUGGAGGGGGAU AACUACUGGAAACG GUAGCUAAUACCGC AUAACGUCGCAAGA CCAAAGAGGGGGAC CUUCGGGCCUCUUG CCAUCGGAUGUGCC CAGAUGGGAUUAG CUAGUAGGUGGGG UAACGGCUCACCUA GGCGACGAUCCCUA GCUGGUCUGAGAG GAUGACCAGCCACA CUGGAACUGAGACA CGGUCCAGACUCCU ACGGGAGGCAGCAG UGGGGAAUAUUGC ACAAUGGGCGCAAG CCUGAUGCAGCCAU	tetracyclin	Target_lig_74	Small subunit tetracycline	Target_101	5.45593195564972

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		GCCGCGUGUAUGAA GAAGGCCUUCGGGU UGUAAAGUACUUU CAGCGGGGAGGAA GGGAGUAAAGUUA AUACCUUUGCUCAU UGACGUUACCCGCA GAAGAAGCACCGGC UAACUCCGUGCCAG CAGCCGCGGUAAUA CGGAGGGUGCAAGC GUUAAUCGGAAUU ACUGGGCGUAAAGC GCACGCAGGCGGUU UGUUAAGUCAGAU GUGAAAUCCCCGGG CUCAACCUGGGAAC UGCAUCUGAUACUG GCAAGCUUGAGUCU CGUAGAGGGGGGU AGAAUUCCAGGUG UAGCGGUGAAAUG CGUAGAGAUCUGG AGGAAUACCGGUG GCGAAGGCGGCCCC CUGGACGAAGACUG ACGCUCAGGUGCGA AAGCGUGGGGAGC AAACAGGAUUAGA UACCCUGGUAGUCC ACGCCGUAAACGAU GUCGACUUGGAGG UUGUGCCCUUGAGG CGUGGCUUCCGGAG CUAACGCGUUAAGU CGACCGCCUGGGGA GUACGGCCGCAAGG UUAAAACUCAAAU GAAUUGACGGGGG CCCGCACAAGCGGU GGAGCAUGUGGUU UAAUUCGAUGCAAC GCGAAGAACCUUAC CUGGUCUUGACAUC CACGGAAGUUUUCA GAGAUGAGAAUGU GCCUUCGGGAACCG UGAGACAGGUGCU GCAUGGCUGUCGUC AGCUCGUGUUGUG AAAUGUUGGGUUA AGUCCCGCAACGAG CGCAACCCUUAUCC UUUGUUGCCAGCGG UCCGGCCGGGAACU CAAAGGAGACUGCC AGUGAUAAACUGG AGGAAGGUGGGGA UGACGUCAAGUCAU CAUGGCCCUUACGA CCAGGGCUACACAC GUGCUACAAUGGCG CAUACAAAGAGAA GCGACCUCGCGAGA GCAAGCGGACCUCA UAAAGUGCGUCGU AGUCCGGAUUGGA GUCUGCAACUCGAC UCCAUGAAGUCGGA AUCGCUAGUAAUCG UGGAUCAGAAUGCC ACGGUGAAUACGU UCCCGGGCCUUGUA CACACCGCCCGUCA CACCAUGGGAGUGG					

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		GUUGCAAAAGAAG UAGGUAGCUUAACC UUCGGGAGGGCGCU UACCACUUUGUGAU UCAUGACUGGGGU GAAGUCGUAACAA GGUAACCGUAGGG GAACCUGCGGUUGG AUCACCUCCUUA					
399	CCC(C)C1C(=O)NC(C(=O)NC(=C)C(=O)NC(C(=O)NC23CCC(=NC2C4=CSC(=N4)C(C(OC(=O)C5=NC6=C(C=CC(C6O)N1)C(=C5)C(C)O)C)NC(=O)C7=CSC(=N7)C(NC(=O)C8CSC(=N8)C(=CC)NC(=O)C(NC(=O)C9=CSC3=N9)C(C)O)C(C)(C(C)O)O)C1=NC(=CS1)C(=O)NC(=C)C(=O)NC(=C)C(=O)N)C)C	GCUGGGAUGUUGG CUUAGAAGCAGCCA UCAUUUAAAGAGU GCGUAACAGCUCAC CAGC	Thiostrepton	Target_lig_319	L11 BD RNA	Target_122	5.88605664769316
400	CCC1C(C=C(C=CC(=O)C(CC(C(C(C(CC(=O)O1)O)C)OC2C(C(C(C(O2)C)OC3CC(C(C(O3)C)O)(C)O)N(C)C)O)CC=O)C)C)COC4C(C(C(C(O4)C)O)OC)OC	GGUUAAGCGACUA AGCGUACACGGUGG AUGCCCUGGCAGUC AGAGGCGAUGAAG GACGUGCUAAUCUG CGAUAAGCGUCGGU AAGGUGAUAUGAA CCGUUAUAACCGGC GAUUUCCGAAUGG GGAAACCCAGUGUG UUUCGACACACUAU CAUUAACUGAAUCC AUAGGUUAAUGAG GCGAACCGGGGGAA CUGAAACAUCUAAG UACCCCGAGGAAAA GAAAUCAACCGAGA UUCCCCCAGUAGCG GCGAGCGAACGGGG AGCAGCCCAGAGCC UGAAUCAGUGUGU GUGUUAGUGGAAG CGUCUGGAAAGGCG CGCGAUACAGGGUG ACAGCCCCGUACAC AAAAAUGCACAUGC UGUGAGCUCGAUG AGUAGGGCGGGAC ACGUGGUAUCCUGU CUGAAUAUGGGGG GACCAUCCUCCAAG GCUAAAUACUCCUG ACUGACCGAUAGUG AACCAGUACCGUGA GGGAAAGGCGAAA AGAACCCCGGCGAG GGGAGUGAAAAAG AACCUGAAACCGUG UACGUACAAGCAGU GGGAGCACGCUUAG GCGUGUGACUGCGU ACCUUUUGUAUAA UGGGUCAGCGACUU AUAUUCUGUAGCA AGGUUAACCGAAU AGGGGAGCCGAAG GGAAACCGAGUCUU AACUGGGCGUUAA GUUGCAGGGUAUA GACCCGAAACCCGG UGAUCUAGCCAUGG	Tylosin	Target_lig_320	Exit tunnel for TYLOSIN	Target_100	8.56066730616974

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		GCAGGUUGAAGGU UGGGUAACACUAAC UGGAGGACCGAACC GACUAAUGUUGAA AAAUUAGCGGAUG ACUUGUGGCUGGG GGUGAAAGGCCAA UCAAACCGGGAGAU AGCUGGUUCUCCCC GAAAGCUAUUUAG GUAGCGCCUCGUGA AUUCAUCUCCGGGG GUAGAGCACUGUU UCGGCAAGGGGGUC ACUUACCAACCCGA UGCAAACUGCGAAU ACCGGAGAAUGUU AUCACGGGAGACAC ACGGCGGGUGCUAA CGUCCGUCGUGAAG AGGGAAACAACCCA GACCGCCAGCUAAG GUCCCAAAGUCAUG GUUAAGUGGGAAA CGAUGUGGGAAGG CCCAGACAGCCAGG AUGUUGGCUUAGA AGCAGCCAUCAUUU AAAGAAAGCGUAA UAGCUCACUGGUCG AGUCGGCCUGCGCG GAAGAUGUAACGG GGCUAAACCAUGCA CCGAAGCUGCGGCA GCGACGCUUAUGCG UUGUUGGGUAGGG GAGCGUUCUGUAA GCCUGCGAAGGUGU GCUGUGAGGCAUGC UGGAGGUAUCAGA AGUGCGAAUGCUG ACAUAAGUAACGA UAAAGCGGGUGAA AAGCCCGCUCGCCG GAAGACCAAGGGU UCCUGUCCAACGUU AAUCGGGGCAGGG UGAGUCGACCCCUA AGGCGAGGCCGAAA GGCGUAGUCGAUG GGAAACAGGUUAA UAUUCCUGUACUUG GUGUUACUGCGAA GGGGGGACGGAGA AGGCUAUGUUGGCC GGGCGACGGUUGUC CCGGUUUAAGCGUG UAGGCUGGUUUUCC AGGCAAAUCCGGAA AAUCAAGGCUGAG GCGUGAUGACGAG GCACUACGGUGCUG AAGCAACAAAUGCC CUGCUUCCAGGAAA AGCCUCUAAGCAUC AGGUAACAUCAAA UCGUACCCCAAACC GACACAGGUGGUCA GGUAGAGAAUACC AAGGCGCUUGAGA GAACUCGGGUGAA GGAACUAGGCAAA AUGGUGCCGUAACU UCGGGAGAAGGCAC GCUGAUAUGUAGG					

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		UGAGGUCCCUCGCG GAUGGAGCUGAAA UCAGUCGAAGAUAC CAGCUGGCUGCAAC UGUUUAUUAAAAA CACAGCACUGUGCA AACACGAAAGUGG ACGUAUACGGUGU GACGCCUGCCCGGU GCCGGAAGGUUAA UUGAUGGGGUUAG CGCAAGCGAAGCUC UUGAUCGAAGCCCC GGUAAACGGCGGCC GUAACXAUAACGG UCCUAAGGUAGCGA AAUUCCUUGUCGGG UAAGUUCCGACCUG CACGAAUGGCGUAA UGAUGGCCAGGCUG UCUCCACCCGAGAC UCAGUGAAAUUGA ACUCGCUGUGAAGA UGCAGUGUACCCGC GGCAAGACGGAAA GACCCCGUGAACCU UUACUAUAGCUUG ACACUGAACAUUGA GCCUUGAUGUGUA GGAUAGGUGGGAG GCUUUGAAGUGUG GACGCCAGUCUGCA UGGAGCCGACCUUG AAAUACCACCCUUU AAUGUUUGAUGUU CUAACGUUGACCCG UAAUCCGGGUUGCG GACAGUGUCUGGU GGGUAGUUUGACU GGGGCGGUCUCCUC CUAAAGAGUAACG GAGGAGCACGAAG GUUGGCUAAUCCUG GUCGGACAUCAGGA GGUUAGUGCAAUG GCAUAAGCCAGCUU GACUGCGAGCGUGA CGGCGCGAGCAGGU GCGAAAGCAGGUCA UAGUGAUCCGGUG GUUCUGAAUGGAA GGGCCAUCGCUCAA CGGAUAAAAGGUA CUCCGGGGAUAACA GGCUGAUACCGCCC AAGAGUUCAUAUC GACGGCGGUGUUU GGCACCUCGAUGUC GGCUCAUCACAUCC UGGGGCUGAAGUA GGUCCCAAGGGUAU GGCUGUUCGCCAUU UAAAGUGGUACGC GAGCUGGGUUUAG AACGUCGUGAGACA GUUCGGUCCCUAUC UGCCGUGGGCGCUG GAGAACUGAGGGG GGCUGCUCCUAGUA CGAGAGGACCGGAG UGGACGCAUCACUG GUGUUCGGGUUGU CAUGCCAAUGGCAC UGCCCGGUAGCUAA AUGCGGAAGAGAU					

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		AAGUGCUGAAAGC AUCUAAGCACGAAA CUUGCCCCGAGAUG AGUUCUCCCUGACC CUUUAAGGGUCCUG AAGGAACGUUGAA GACGACGACGUUGA UAGGCCGGGUGUG UAAGCGCAGCGAUG CGUUGAGCUAACCG GUACUAAUGAACCG UGAGGCUUAACCU					
401	CCCC1CC(N(C1)C)C(=O)NC(C2C(C(C(C(O2)SC)O)O)O)C(C)Cl	GGUUAAGCGACUA AGCGUACACGGUGG AUGCCCUGGCAGUC AGAGGCGAUGAAG GACGUGCUAAUCUG CGAUAAGCGUCGGU AAGGUGAUAUGAA CCGUUAUAACCGGC GAUUUCCGAAUGG GGAAACCCAGUGUG UUUCGACACACUAU CAUUAACUGAAUCC AUAGGUUAAUGAG GCGAACCGGGGGAA CUGAAACAUCUAAG UACCCCGAGGAAAA GAAAUCAACCGAGA UUCCCCCAGUAGCG GCGAGCGAACGGGG AGCAGCCCAGAGCC UGAAUCAGUGUGU GUGUUAGUGGAAG CGUCUGGAAAGGCG CGCGAUACAGGGUG ACAGCCCCGUACAC AAAAAUGCACAUGC UGUGAGCUCGAUG AGUAGGGCGGGAC ACGUGGUAUCCUGU CUGAAUAUGGGGG GACCAUCCUCCAAG GCUAAAUACUCCUG ACUGACCGAUAGUG AACCAGUACCGUGA GGGAAAGGCGAAA AGAACCCCGGCGAG GGGAGUGAAAAAG AACCUGAAACCGUG UACGUACAAGCAGU GGGAGCACGCUUAG GCGUGUGACUGCGU ACCUUUUGUAUAA UGGGUCAGCGACUU AUAUUCUGUAGCA AGGUUAACCGAAU AGGGGAGCCGAAG GGAAACCGAGUCUU AACUGGGCGUUAA GUUGCAGGGUAUA GACCCGAAACCCGG UGAUCUAGCCAUGG GCAGGUUGAAGGU UGGGUAACACUAAC UGGAGGACCGAACC GACUAAUGUUGAA AAAUUAGCGGAUG ACUUGUGGCUGGG GGUGAAAGGCCAA UCAAACCGGGAGAU AGCUGGUUCUCCCC GAAAGCUAUUUAG GUAGCGCCUCGUGA AUUCAUCUCCGGGG	Clindamycin	Target_lig_324	50S ribosome (CLINDAMYCIN)	Target_100	5.096910013008 06

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		GUAGAGCACUGUU UCGGCAAGGGGGUC ACUUACCAACCCGA UGCAAACUGCGAAU ACCGGAGAAUGUU AUCACGGGAGACAC ACGGCGGGUGCUAA CGUCCGUCGUGAAG AGGGAAACAACCCA GACCGCCAGCUAAG GUCCCAAAGUCAUG GUUAAGUGGGAAA CGAUGUGGGAAGG CCCAGACAGCCAGG AUGUUGGCUUAGA AGCAGCCAUCAUUU AAAGAAAGCGUAA UAGCUCACUGGUCG AGUCGGCCUGCGCG GAAGAUGUAACGG GGCUAAACCAUGCA CCGAAGCUGCGGCA GCGACGCUUAUGCG UUGUUGGGUAGGG GAGCGUUCUGUAA GCCUGCGAAGGUGU GCUGUGAGGCAUGC UGGAGGUAUCAGA AGUGCGAAUGCUG ACAUAAGUAACGA UAAAGCGGGUGAA AAGCCCGCUCGCCG GAAGACCAAGGGU UCCUGUCCAACGUU AAUCGGGGCAGGG UGAGUCGACCCCUA AGGCGAGGCCGAAA GGCGUAGUCGAUG GGAAACAGGUUAA UAUUCCUGUACUUG GUGUUACUGCGAA GGGGGGACGGAGA AGGCUAUGUUGGCC GGGCGACGGUUGUC CCGGUUUAAGCGUG UAGGCUGGUUUUCC AGGCAAAUCCGGAA AAUCAAGGCUGAG GCGUGAUGACGAG GCACUACGGUGCUG AAGCAACAAAUGCC CUGCUUCCAGGAAA AGCCUCUAAGCAUC AGGUAACAUCAAA UCGUACCCCAAACC GACACAGGUGGUCA GGUAGAGAAUACC AAGGCGCUUGAGA GAACUCGGGUGAA GGAACUAGGCAAA AUGGUGCCGUAACU UCGGGAGAAGGCAC GCUGAUAUGUAGG UGAGGUCCCUCGCG GAUGGAGCUGAAA UCAGUCGAAGAUAC CAGCUGGCUGCAAC UGUUUAUUAAAAA CACAGCACUGUGCA AACACGAAAGUGG ACGUAUACGGUGU GACGCCUGCCCGGU GCCGGAAGGUUAA UUGAUGGGGUUAG CGCAAGCGAAGCUC					

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		UUGAUCGAAGCCCC GGUAAACGGCGGCC GUAACXAUAACGG UCCUAAGGUAGCGA AAUUCCUUGUCGGG UAAGUUCCGACCUG CACGAAUGGCGUAA UGAUGGCCAGGCUG UCUCCACCCGAGAC UCAGUGAAAUUGA ACUCGCUGUGAAGA UGCAGUGUACCCGC GGCAAGACGGAAA GACCCCGUGAACCU UUACUAUAGCUUG ACACUGAACAUUGA GCCUUGAUGUGUA GGAUAGGUGGGAG GCUUUGAAGUGUG GACGCCAGUCUGCA UGGAGCCGACCUUG AAAUACCACCCUUU AAUGUUUGAUGUU CUAACGUUGACCCG UAAUCCGGGUUGCG GACAGUGUCUGGU GGGUAGUUUGACU GGGGCGGUCUCCUC CUAAAGAGUAACG GAGGAGCACGAAG GUUGGCUAAUCCUG GUCGGACAUCAGGA GGUUAGUGCAAUG GCAUAAGCCAGCUU GACUGCGAGCGUGA CGGCGCGAGCAGGU GCGAAAGCAGGUCA UAGUGAUCCGGUG GUUCUGAAUGGAA GGGCCAUCGCUCAA CGGAUAAAAGGUA CUCCGGGGAUAACA GGCUGAUACCGCCC AAGAGUUCAUAUC GACGGCGGUGUUU GGCACCUCGAUGUC GGCUCAUCACAUCC UGGGGCUGAAGUA GGUCCCAAGGGUAU GGCUGUUCGCCAUU UAAAGUGGUACGC GAGCUGGGUUUAG AACGUCGUGAGACA GUUCGGUCCCUAUC UGCCGUGGGCGCUG GAGAACUGAGGGG GGCUGCUCCUAGUA CGAGAGGACCGGAG UGGACGCAUCACUG GUGUUCGGGUUGU CAUGCCAAUGGCAC UGCCCGGUAGCUAA AUGCGGAAGAGAU AAGUGCUGAAAGC AUCUAAGCACGAAA CUUGCCCCGAGAUG AGUUCUCCCUGACC CUUUAAGGGUCCUG AAGGAACGUUGAA GACGACGACGUUGA UAGGCCGGGUGUG UAAGCGCAGCGAUG CGUUGAGCUAACCG GUACUAAUGAACCG UGAGGCUUAACCU					

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
403	CC1C=CC(=O)NCC=CC(=CC(CC(=O)CC2=NC(=CO2)C(=O)N3CCC=C3C(=O)OC1C(C)C)O)C	GGUUAAGCGACUA AGCGUACACGGUGG AUGCCCUGGCAGUC AGAGGCGAUGAAG GACGUGCUAAUCUG CGAUAAGCGUCGGU AAGGUGAUAUGAA CCGUUAUAACCGGC GAUUUCCGAAUGG GGAAACCCAGUGUG UUUCGACACACUAU CAUUAACUGAAUCC AUAGGUUAAUGAG GCGAACCGGGGGAA CUGAAACAUCUAAG UACCCCGAGGAAAA GAAAUCAACCGAGA UUCCCCCAGUAGCG GCGAGCGAACGGGG AGCAGCCCAGAGCC UGAAUCAGUGUGU GUGUUAGUGGAAG CGUCUGGAAAGGCG CGCGAUACAGGGUG ACAGCCCCGUACAC AAAAAUGCACAUGC UGUGAGCUCGAUG AGUAGGGCGGGAC ACGUGGUAUCCUGU CUGAAUAUGGGGG GACCAUCCUCCAAG GCUAAAUACUCCUG ACUGACCGAUAGUG AACCAGUACCGUGA GGGAAAGGCGAAA AGAACCCCGGCGAG GGGAGUGAAAAAG AACCUGAAACCGUG UACGUACAAGCAGU GGGAGCACGCUUAG GCGUGUGACUGCGU ACCUUUUGUAUAA UGGGUCAGCGACUU AUAUUCUGUAGCA AGGUUAACCGAAU AGGGGAGCCGAAG GGAAACCGAGUCUU AACUGGGCGUUAA GUUGCAGGGUAUA GACCCGAAACCCGG UGAUCUAGCCAUGG GCAGGUUGAAGGU UGGGUAACACUAAC UGGAGGACCGAACC GACUAAUGUUGAA AAAUUAGCGGAUG ACUUGUGGCUGGG GGUGAAAGGCCAA UCAAACCGGGAGAU AGCUGGUUCUCCCC GAAAGCUAUUUAG GUAGCGCCUCGUGA AUUCAUCUCCGGGG GUAGAGCACUGUU UCGGCAAGGGGGUC ACUUACCAACCCGA UGCAAACUGCGAAU ACCGGAGAAUGUU AUCACGGGAGACAC ACGGCGGGUGCUAA CGUCCGUCGUGAAG AGGGAAACAACCCA GACCGCCAGCUAAG GUCCCAAAGUCAUG GUUAAGUGGGAAA	Virginiamycin M	Target_lig_1113	50S ribosome (Virginiamycin M)	Target_100	5.09691001300806

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		CGAUGUGGGAAGG CCCAGACAGCCAGG AUGUUGGCUUAGA AGCAGCCAUCAUUU AAAGAAAGCGUAA UAGCUCACUGGUCG AGUCGGCCUGCGCG GAAGAUGUAACGG GGCUAAACCAUGCA CCGAAGCUGCGGCA GCGACGCUUAUGCG UUGUUGGGUAGGG GAGCGUUCUGUAA GCCUGCGAAGGUGU GCUGUGAGGCAUGC UGGAGGUAUCAGA AGUGCGAAUGCUG ACAUAAGUAACGA UAAAGCGGGUGAA AAGCCCGCUCGCCG GAAGACCAAGGGU UCCUGUCCAACGUU AAUCGGGGCAGGG UGAGUCGACCCCUA AGGCGAGGCCGAAA GGCGUAGUCGAUG GGAAACAGGUUAA UAUUCCUGUACUUG GUGUUACUGCGAA GGGGGGACGGAGA AGGCUAUGUUGGCC GGGCGACGGUUGUC CCGGUUUAAGCGUG UAGGCUGGUUUUCC AGGCAAAUCCGGAA AAUCAAGGCUGAG GCGUGAUGACGAG GCACUACGGUGCUG AAGCAACAAAUGCC CUGCUUCCAGGAAA AGCCUCUAAGCAUC AGGUAACAUCAAA UCGUACCCCAAACC GACACAGGUGGUCA GGUAGAGAAUACC AAGGCGCUUGAGA GAACUCGGGUGAA GGAACUAGGCAAA AUGGUGCCGUAACU UCGGGAGAAGGCAC GCUGAUAUGUAGG UGAGGUCCCUCGCG GAUGGAGCUGAAA UCAGUCGAAGAUAC CAGCUGGCUGCAAC UGUUUAUUAAAAA CACAGCACUGUGCA AACACGAAAGUGG ACGUAUACGGUGU GACGCCUGCCCGGU GCCGGAAGGUUAA UUGAUGGGGUUAG CGCAAGCGAAGCUC UUGAUCGAAGCCCC GGUAAACGGCGGCC GUAACXAUAACGG UCCUAAGGUAGCGA AAUUCCUUGUCGGG UAAGUUCCGACCUG CACGAAUGGCGUAA UGAUGGCCAGGCUG UCUCCACCCGAGAC UCAGUGAAAUUGA ACUCGCUGUGAAGA UGCAGUGUACCCGC					

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		GGCAAGACGGAAA GACCCCGUGAACCU UUACUAUAGCUUG ACACUGAACAUUGA GCCUUGAUGUGUA GGAUAGGUGGGAG GCUUUGAAGUGUG GACGCCAGUCUGCA UGGAGCCGACCUUG AAAUACCACCCUUU AAUGUUUGAUGUU CUAACGUUGACCCG UAAUCCGGGUUGCG GACAGUGUCUGGU GGGUAGUUUGACU GGGGCGGUCUCCUC CUAAAGAGUAACG GAGGAGCACGAAG GUUGGCUAAUCCUG GUCGGACAUCAGGA GGUUAGUGCAAUG GCAUAAGCCAGCUU GACUGCGAGCGUGA CGGCGCGAGCAGGU GCGAAAGCAGGUCA UAGUGAUCCGGUG GUUCUGAAUGGAA GGGCCAUCGCUCAA CGGAUAAAAGGUA CUCCGGGGAUAACA GGCUGAUACCGCCC AAGAGUUCAUAUC GACGGCGGUGUUU GGCACCUCGAUGUC GGCUCAUCACAUCC UGGGGCUGAAGUA GGUCCCAAGGGUAU GGCUGUUCGCCAUU UAAAGUGGUACGC GAGCUGGGUUUAG AACGUCGUGAGACA GUUCGGUCCCUAUC UGCCGUGGGCGCUG GAGAACUGAGGGG GGCUGCUCCUAGUA CGAGAGGACCGGAG UGGACGCAUCACUG GUGUUCGGGUUGU CAUGCCAAUGGCAC UGCCCGGUAGCUAA AUGCGGAAGAGAU AAGUGCUGAAAGC AUCUAAGCACGAAA CUUGCCCCGAGAUG AGUUCUCCCUGACC CUUUAAGGGUCCUG AAGGAACGUUGAA GACGACGACGUUGA UAGGCCGGGUGUG UAAGCGCAGCGAUG CGUUGAGCUAACCG GUACUAAUGAACCG UGAGGCUUAACCU					
404	CC(=O)NCC1CN(C(=O)O1)C2=CC(=C(C=C2)N3CCOCC3)F	GGUUAAGCGACUA AGCGUACACGGUGG AUGCCCUGGCAGUC AGAGGCGAUGAAG GACGUGCUAAUCUG CGAUAAGCGUCGGU AAGGUGAUAUGAA CCGUUAUAACCGGC GAUUUCCGAAUGG GGAAACCCAGUGUG UUUCGACACACUAU CAUUAACUGAAUCC	Linezolid	Target_lig_307	23SrRNA	Target_104	6

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		AUAGGUUAAUGAG GCGAACCGGGGGAA CUGAAACAUCUAAG UACCCCGAGGAAAA GAAAUCAACCGAGA UUCCCCCAGUAGCG GCGAGCGAACGGGG AGCAGCCCAGAGCC UGAAUCAGUGUGU GUGUUAGUGGAAG CGUCUGGAAAGGCG CGCGAUACAGGGUG ACAGCCCCGUACAC AAAAAUGCACAUGC UGUGAGCUCGAUG AGUAGGGCGGGAC ACGUGGUAUCCUGU CUGAAUAUGGGGG GACCAUCCUCCAAG GCUAAAUACUCCUG ACUGACCGAUAGUG AACCAGUACCGUGA GGGAAAGGCGAAA AGAACCCCGGCGAG GGGAGUGAAAAAG AACCUGAAACCGUG UACGUACAAGCAGU GGGAGCACGCUUAG GCGUGUGACUGCGU ACCUUUUGUAUAA UGGGUCAGCGACUU AUAUUCUGUAGCA AGGUUAACCGAAU AGGGGAGCCGAAG GGAAACCGAGUCUU AACUGGGCGUUAA GUUGCAGGGUAUA GACCCGAAACCCGG UGAUCUAGCCAUGG GCAGGUUGAAGGU UGGGUAACACUAAC UGGAGGACCGAACC GACUAAUGUUGAA AAAUUAGCGGAUG ACUUGUGGCUGGG GGUGAAAGGCCAA UCAAACCGGGAGAU AGCUGGUUCUCCCC GAAAGCUAUUUAG GUAGCGCCUCGUGA AUUCAUCUCCGGGG GUAGAGCACUGUU UCGGCAAGGGGGUC AUCCCGACUUACCA ACCCGAUGCAAACU GCGAAUACCGGAGA AUGUUAUCACGGG AGACACACGGCGGG UGCUAACGUCCGUC GUGAAGAGGGAAA CAACCCAGACCGCC AGCUAAGGUCCCAA AGUCAUGGUUAAG UGGGAAACGAUGU GGGAAGGCCCAGAC AGCCAGGAUGUUG GCUUAGAAGCAGCC AUCAUUUAAAGAA AGCGUAAUAGCUCA CUGGUCGAGUCGGC CUGCGCGGAAGAUG UAACGGGGCUAAAC CAUGCACCGAAGCU GCGGCAGCGACGCU UAUGCGUUGUUGG					

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		GUAGGGGAGCGUU CUGUAAGCCUGCGA AGGUGUGCUGUGA GGCAUGCUGGAGG UAUCAGAAGUGCG AAUGCUGACAUAA GUAACGAUAAAGC GGGUGAAAAGCCCG CUCGCCGGAAGACC AAGGGUUCCUGUCC AACGUUAAUCGGG GCAGGGUGAGUCG ACCCCUAAGGCGAG GCCGAAAGGCGUAG UCGAUGGGAAACA GGUUAAUAUUCCU GUACUUGGUGUUA CUGCGAAGGGGGG ACGGAGAAGGCUA UGUUGGCCGGGCGA CGGUUGUCCCGGUU UAAGCGUGUAGGC UGGUUUUCCAGGCA AAUCCGGAAAAUCA AGGCUGAGGCGUG AUGACGAGGCACUA CGGUGCUGAAGCAA CAAAUGCCCUGCUU CCAGGAAAAGCCUC UAAGCAUCAGGUA ACAUCAAAUCGUAC CCCAAACCGACACU GGUGGUCAGGUAG AGAAUACCAAGGCG CUUGAGAGAACUCG GGUGAAGGAACUA GGCAAAAUGGUGCC GUAACUUCGGGAG AAGGCACGCUGAUA UGUAGGUGAGGUC CCUCGCGGAUGGAG CUGAAAUCAGUCGA AGAUACCAGCUGGC UGCAACUGUUUAU UAAAAACACAGCAC UGUGCAAACACGAA AGUGGACGUAUAC GGUGUGACGCCUGC CCGGUGCCGGAAGG UUAAUUGAUGGGG UUAGCGCAAGCGAA GCUCUUGAUCGAAG CCCCGGUAAACGGC GGCCGUAACUAUAA CGGUCCUAAGGUAG CGAAAUUCCUUGUC GGGUAAGUUCCGAC CUGCACGAAUGGCG UAAUGAUGGCCAG GCUGUCUCCACCCG AGACUCAGUGAAA UUGAACUCGCUGUG CAGAUGCAGUGUAC CCGCGGCAAGACGG AAAGACCCCGUGAA CCUUUACUAUAGCU UGACACUGAACAUU GAGCCUUGAUGUG UAGGAUAGGUGGG AGGCUUUGAAGUG UGGACGCCAGUCUG CAUGGAGCCGACCU UGAAAUACCACCCU UUAAUGUUUGAUG UUCUAACGUUGACC					

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		CGUAAUCCGGGUUG CGGACAGUGUCUGG UGGGUAGUUUGAC UGGGGCGGUCUCCU CCUAAAGAGUAACG GAGGAGCACGAAG GUUGGCUAAUCCUG GUCGGACAUCAGGA GGUUAGUGCAAUG GCAUAAGCCAGCUU GACUGCGAGCGUGA CGGCGCGAGCAGGU GCGAAAGCAGGUCA UAGUGAUCCGGUG GUUCUGAAUGGAA GGGCCAUCGCUCAA CGGAUAAAAGGUA CUCCGGGGAUAACA GGCUGAUACCGCCC AAGAGUUCAUAUC GACGGCGGUGUUU GGCACCUCGAUGUC GGCUCAUCACAUCC UGGGGCUGAAGUA GGUCCCAAGGGUAU GGCUGUUCGCCAUU UAAAGUGGUACGC GAGCUGGGUUUAG AACGUCGUGAGACA GUUCGGUCCCUAUC UGCCGUGGGCGCUG GAGAACUGAGGGG GGCUGCUCCUAGUA CGAGAGGACCGGAG UGGACGCAUCACUG GUGUUCGGGUUGU CAUGCCAAUGGCAC UGCCCGGUAGCUAA AUGCGGAAGAGAU AAGUGCUGAAAGC AUCUAAGCACGAAA CUUGCCCCGAGAUG AGUUCUCCCUGACC CUUUAAGGGUCCUG AAGGAACGUUGAA GACGACGACGUUGA UAGGCCGGGUGUG UAAGCGCAGCGAUG CGUUGAGCUAACCG GUACUAAUGAACCG UGAGGCUUAACCUU					
405	CC(=O)NC[C@H]1CN(C(=O)O1)C2=CC(=C(C=C2)N3CCN(CC3)C(=O)CO)F	GGUUAAGCGACUA AGCGUACACGGUGG AUGCCCUGGCAGUC AGAGGCGAUGAAG GACGUGCUAAUCUG CGAUAAGCGUCGGU AAGGUGAUAUGAA CCGUUAUAACCGGC GAUUUCCGAAUGG GGAAACCCAGUGUG UUUCGACACACUAU CAUUAACUGAAUCC AUAGGUUAAUGAG GCGAACCGGGGGAA CUGAAACAUCUAAG UACCCCGAGGAAAA GAAAUCAACCGAGA UUCCCCCAGUAGCG GCGAGCGAACGGGG AGCAGCCCAGAGCC UGAAUCAGUGUGU GUGUUAGUGGAAG CGUCUGGAAAGGCG CGCGAUACAGGGUG	LINEZOLID_DERIVATIVE_1	Target_lig_326	23SrRNA	Target_104	3.709965383863748

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		ACAGCCCCGUACAC AAAAAUGCACAUGC UGUGAGCUCGAUG AGUAGGGCGGGAC ACGUGGUAUCCUGU CUGAAUAUGGGGG GACCAUCCUCCAAG GCUAAAUACUCCUG ACUGACCGAUAGUG AACCAGUACCGUGA GGGAAAGGCGAAA AGAACCCCGGCGAG GGGAGUGAAAAAG AACCUGAAACCGUG UACGUACAAGCAGU GGGAGCACGCUUAG GCGUGUGACUGCGU ACCUUUUGUAUAA UGGGUCAGCGACUU AUAUUCUGUAGCA AGGUUAACCGAAU AGGGGAGCCGAAG GGAAACCGAGUCUU AACUGGGCGUUAA GUUGCAGGGUAUA GACCCGAAACCCGG UGAUCUAGCCAUGG GCAGGUUGAAGGU UGGGUAACACUAAC UGGAGGACCGAACC GACUAAUGUUGAA AAAUUAGCGGAUG ACUUGUGGCUGGG GGUGAAAGGCCAA UCAAACCGGGAGAU AGCUGGUUCUCCCC GAAAGCUAUUUAG GUAGCGCCUCGUGA AUUCAUCUCCGGGG GUAGAGCACUGUU UCGGCAAGGGGGUC AUCCCGACUUACCA ACCCGAUGCAAACU GCGAAUACCGGAGA AUGUUAUCACGGG AGACACACGGCGGG UGCUAACGUCCGUC GUGAAGAGGGAAA CAACCCAGACCGCC AGCUAAGGUCCCAA AGUCAUGGUUAAG UGGGAAACGAUGU GGGAAGGCCCAGAC AGCCAGGAUGUUG GCUUAGAAGCAGCC AUCAUUUAAAGAA AGCGUAAUAGCUCA CUGGUCGAGUCGGC CUGCGCGGAAGAUG UAACGGGGCUAAAC CAUGCACCGAAGCU GCGGCAGCGACGCU UAUGCGUUGUUGG GUAGGGGAGCGUU CUGUAAGCCUGCGA AGGUGUGCUGUGA GGCAUGCUGGAGG UAUCAGAAGUGCG AAUGCUGACAUAA GUAACGAUAAAGC GGGUGAAAAGCCCG CUCGCCGGAAGACC AAGGGUUCCUGUCC AACGUUAAUCGGG GCAGGGUGAGUCG					

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		ACCCCUAAGGCGAG GCCGAAAGGCGUAG UCGAUGGGAAACA GGUUAAUAUUCCU GUACUUGGUGUUA CUGCGAAGGGGGG ACGGAGAAGGCUA UGUUGGCCGGGCGA CGGUUGUCCCGGUU UAAGCGUGUAGGC UGGUUUUCCAGGCA AAUCCGGAAAAUCA AGGCUGAGGCGUG AUGACGAGGCACUA CGGUGCUGAAGCAA CAAAUGCCCUGCUU CCAGGAAAAGCCUC UAAGCAUCAGGUA ACAUCAAAUCGUAC CCCAAACCGACACU GGUGGUCAGGUAG AGAAUACCAAGGCG CUUGAGAGAACUCG GGUGAAGGAACUA GGCAAAAUGGUGCC GUAACUUCGGGAG AAGGCACGCUGAUA UGUAGGUGAGGUC CCUCGCGGAUGGAG CUGAAAUCAGUCGA AGAUACCAGCUGGC UGCAACUGUUUAU UAAAAACACAGCAC UGUGCAAACACGAA AGUGGACGUAUAC GGUGUGACGCCUGC CCGGUGCCGGAAGG UUAAUUGAUGGGG UUAGCGCAAGCGAA GCUCUUGAUCGAAG CCCCGGUAAACGGC GGCCGUAACUAUAA CGGUCCUAAGGUAG CGAAAUUCCUUGUC GGGUAAGUUCCGAC CUGCACGAAUGGCG UAAUGAUGGCCAG GCUGUCUCCACCCG AGACUCAGUGAAA UUGAACUCGCUGUG CAGAUGCAGUGUAC CCGCGGCAAGACGG AAAGACCCCGUGAA CCUUUACUAUAGCU UGACACUGAACAUU GAGCCUUGAUGUG UAGGAUAGGUGGG AGGCUUUGAAGUG UGGACGCCAGUCUG CAUGGAGCCGACCU UGAAAUACCACCCU UUAAUGUUUGAUG UUCUAACGUUGACC CGUAAUCCGGGUUG CGGACAGUGUCUGG UGGGUAGUUUGAC UGGGGCGGUCUCCU CCUAAAGAGUAACG GAGGAGCACGAAG GUUGGCUAAUCCUG GUCGGACAUCAGGA GGUUAGUGCAAUG GCAUAAGCCAGCUU GACUGCGAGCGUGA CGGCGCGAGCAGGU					

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		GCGAAAGCAGGUCA UAGUGAUCCGGUG GUUCUGAAUGGAA GGGCCAUCGCUCAA CGGAUAAAAGGUA CUCCGGGGAUAACA GGCUGAUACCGCCC AAGAGUUCAUAUC GACGGCGGUGUUU GGCACCUCGAUGUC GGCUCAUCACAUCC UGGGGCUGAAGUA GGUCCCAAGGGUAU GGCUGUUCGCCAUU UAAAGUGGUACGC GAGCUGGGUUUAG AACGUCGUGAGACA GUUCGGUCCCUAUC UGCCGUGGGCGCUG GAGAACUGAGGGG GGCUGCUCCUAGUA CGAGAGGACCGGAG UGGACGCAUCACUG GUGUUCGGGUUGU CAUGCCAAUGGCAC UGCCCGGUAGCUAA AUGCGGAAGAGAU AAGUGCUGAAAGC AUCUAAGCACGAAA CUUGCCCCGAGAUG AGUUCUCCCUGACC CUUUAAGGGUCCUG AAGGAACGUUGAA GACGACGACGUUGA UAGGCCGGGUGUG UAAGCGCAGCGAUG CGUUGAGCUAACCG GUACUAAUGAACCG UGAGGCUUAACCUU					
406	CC(=O)NC[C@@H]1CN(C(=O)O1)C2=CC(=C(C=C2)N3CCN(CC3)C(=O)CO)F	GGUUAAGCGACUA AGCGUACACGGUGG AUGCCCUGGCAGUC AGAGGCGAUGAAG GACGUGCUAAUCUG CGAUAAGCGUCGGU AAGGUGAUAUGAA CCGUUAUAACCGGC GAUUUCCGAAUGG GGAAACCCAGUGUG UUUCGACACACUAU CAUUAACUGAAUCC AUAGGUUAAUGAG GCGAACCGGGGGAA CUGAAACAUCUAAG UACCCCGAGGAAAA GAAAUCAACCGAGA UUCCCCCAGUAGCG GCGAGCGAACGGGG AGCAGCCCAGAGCC UGAAUCAGUGUGU GUGUUAGUGGAAG CGUCUGGAAAGGCG CGCGAUACAGGGUG ACAGCCCCGUACAC AAAAAUGCACAUGC UGUGAGCUCGAUG AGUAGGGCGGGAC ACGUGGUAUCCUGU CUGAAUAUGGGGG GACCAUCCUCCAAG GCUAAAUACUCCUG ACUGACCGAUAGUG AACCAGUACCGUGA GGGAAAGGCGAAA AGAACCCCGGCGAG	LINEZOLID_DERIVATIVE_2	Target_lig_327	23SrRNA	Target_104	3.11861534322943

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		GGGAGUGAAAAAG AACCUGAAACCGUG UACGUACAAGCAGU GGGAGCACGCUUAG GCGUGUGACUGCGU ACCUUUUGUAUAA UGGGUCAGCGACUU AUAUUCUGUAGCA AGGUUAACCGAAU AGGGGAGCCGAAG GGAAACCGAGUCUU AACUGGGCGUUAA GUUGCAGGGUAUA GACCCGAAACCCGG UGAUCUAGCCAUGG GCAGGUUGAAGGU UGGGUAACACUAAC UGGAGGACCGAACC GACUAAUGUUGAA AAAUUAGCGGAUG ACUUGUGGCUGGG GGUGAAAGGCCAA UCAAACCGGGAGAU AGCUGGUUCUCCCC GAAAGCUAUUUAG GUAGCGCCUCGUGA AUUCAUCUCCGGGG GUAGAGCACUGUU UCGGCAAGGGGGUC AUCCCGACUUACCA ACCCGAUGCAAACU GCGAAUACCGGAGA AUGUUAUCACGGG AGACACACGGCGGG UGCUAACGUCCGUC GUGAAGAGGGAAA CAACCCAGACCGCC AGCUAAGGUCCCAA AGUCAUGGUUAAG UGGGAAACGAUGU GGGAAGGCCCAGAC AGCCAGGAUGUUG GCUUAGAAGCAGCC AUCAUUUAAAGAA AGCGUAAUAGCUCA CUGGUCGAGUCGGC CUGCGCGGAAGAUG UAACGGGGCUAAAC CAUGCACCGAAGCU GCGGCAGCGACGCU UAUGCGUUGUUGG GUAGGGGAGCGUU CUGUAAGCCUGCGA AGGUGUGCUGUGA GGCAUGCUGGAGG UAUCAGAAGUGCG AAUGCUGACAUAA GUAACGAUAAAGC GGGUGAAAAGCCCG CUCGCCGGAAGACC AAGGGUUCCUGUCC AACGUUAAUCGGG GCAGGGUGAGUCG ACCCCUAAGGCGAG GCCGAAAGGCGUAG UCGAUGGGAAACA GGUUAAUAUUCCU GUACUUGGUGUUA CUGCGAAGGGGGG ACGGAGAAGGCUA UGUUGGCCGGGCGA CGGUUGUCCCGGUU UAAGCGUGUAGGC UGGUUUUCCAGGCA AAUCCGGAAAAUCA					

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		AGGCUGAGGCGUG AUGACGAGGCACUA CGGUGCUGAAGCAA CAAAUGCCCUGCUU CCAGGAAAAGCCUC UAAGCAUCAGGUA ACAUCAAAUCGUAC CCCAAACCGACACU GGUGGUCAGGUAG AGAAUACCAAGGCG CUUGAGAGAACUCG GGUGAAGGAACUA GGCAAAAUGGUGCC GUAACUUCGGGAG AAGGCACGCUGAUA UGUAGGUGAGGUC CCUCGCGGAUGGAG CUGAAAUCAGUCGA AGAUACCAGCUGGC UGCAACUGUUUAU UAAAAACACAGCAC UGUGCAAACACGAA AGUGGACGUAUAC GGUGUGACGCCUGC CCGGUGCCGGAAGG UUAAUUGAUGGGG UUAGCGCAAGCGAA GCUCUUGAUCGAAG CCCCGGUAAACGGC GGCCGUAACUAUAA CGGUCCUAAGGUAG CGAAAUUCCUUGUC GGGUAAGUUCCGAC CUGCACGAAUGGCG UAAUGAUGGCCAG GCUGUCUCCACCCG AGACUCAGUGAAA UUGAACUCGCUGUG CAGAUGCAGUGUAC CCGCGGCAAGACGG AAAGACCCCGUGAA CCUUUACUAUAGCU UGACACUGAACAUU GAGCCUUGAUGUG UAGGAUAGGUGGG AGGCUUUGAAGUG UGGACGCCAGUCUG CAUGGAGCCGACCU UGAAAUACCACCCU UUAAUGUUUGAUG UUCUAACGUUGACC CGUAAUCCGGGUUG CGGACAGUGUCUGG UGGGUAGUUUGAC UGGGGCGGUCUCCU CCUAAAGAGUAACG GAGGAGCACGAAG GUUGGCUAAUCCUG GUCGGACAUCAGGA GGUUAGUGCAAUG GCAUAAGCCAGCUU GACUGCGAGCGUGA CGGCGCGAGCAGGU GCGAAAGCAGGUCA UAGUGAUCCGGUG GUUCUGAAUGGAA GGGCCAUCGCUCAA CGGAUAAAAGGUA CUCCGGGGAUAACA GGCUGAUACCGCCC AAGAGUUCAUAUC GACGGCGGUGUUU GGCACCUCGAUGUC GGCUCAUCACAUCC UGGGGCUGAAGUA					

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		GGUCCCAAGGGUAU GGCUGUUCGCCAUU UAAAGUGGUACGC GAGCUGGGUUUAG AACGUCGUGAGACA GUUCGGUCCCUAUC UGCCGUGGGCGCUG GAGAACUGAGGGG GGCUGCUCCUAGUA CGAGAGGACCGGAG UGGACGCAUCACUG GUGUUCGGGUUGU CAUGCCAAUGGCAC UGCCCGGUAGCUAA AUGCGGAAGAGAU AAGUGCUGAAAGC AUCUAAGCACGAAA CUUGCCCCGAGAUG AGUUCUCCCUGACC CUUUAAGGGUCCUG AAGGAACGUUGAA GACGACGACGUUGA UAGGCCGGGUGUG UAAGCGCAGCGAUG CGUUGAGCUAACCG GUACUAAUGAACCG UGAGGCUUAACCUU					
407	CC(=S)NC[C@@H]1CN(C(=O)O1)C2=CC(=C(C=C2)N3CCS(=O)CC3)F	GGUUAAGCGACUA AGCGUACACGGUGG AUGCCCUGGCAGUC AGAGGCGAUGAAG GACGUGCUAAUCUG CGAUAAGCGUCGGU AAGGUGAUAUGAA CCGUUAUAACCGGC GAUUUCCGAAUGG GGAAACCCAGUGUG UUUCGACACACUAU CAUUAACUGAAUCC AUAGGUUAAUGAG GCGAACCGGGGGAA CUGAAACAUCUAAG UACCCCGAGGAAAA GAAAUCAACCGAGA UUCCCCCAGUAGCG GCGAGCGAACGGGG AGCAGCCCAGAGCC UGAAUCAGUGUGU GUGUUAGUGGAAG CGUCUGGAAAGGCG CGCGAUACAGGGUG ACAGCCCCGUACAC AAAAAUGCACAUGC UGUGAGCUCGAUG AGUAGGGCGGGAC ACGUGGUAUCCUGU CUGAAUAUGGGGG GACCAUCCUCCAAG GCUAAAUACUCCUG ACUGACCGAUAGUG AACCAGUACCGUGA GGGAAAGGCGAAA AGAACCCCGGCGAG GGGAGUGAAAAAG AACCUGAAACCGUG UACGUACAAGCAGU GGGAGCACGCUUAG GCGUGUGACUGCGU ACCUUUUGUAUAA UGGGUCAGCGACUU AUAUUCUGUAGCA AGGUUAACCGAAU AGGGGAGCCGAAG GGAAACCGAGUCUU AACUGGGCGUUAA	LINEZOLID_DERIVATIVE_3	Target_lig_328	23SrRNA	Target_104	4.0268721464003

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		GUUGCAGGGUAUA GACCCGAAACCCGG UGAUCUAGCCAUGG GCAGGUUGAAGGU UGGGUAACACUAAC UGGAGGACCGAACC GACUAAUGUUGAA AAAUUAGCGGAUG ACUUGUGGCUGGG GGUGAAAGGCCAA UCAAACCGGGAGAU AGCUGGUUCUCCCC GAAAGCUAUUUAG GUAGCGCCUCGUGA AUUCAUCUCCGGGG GUAGAGCACUGUU UCGGCAAGGGGGUC AUCCCGACUUACCA ACCCGAUGCAAACU GCGAAUACCGGAGA AUGUUAUCACGGG AGACACACGGCGGG UGCUAACGUCCGUC GUGAAGAGGGAAA CAACCCAGACCGCC AGCUAAGGUCCCAA AGUCAUGGUUAAG UGGGAAACGAUGU GGGAAGGCCCAGAC AGCCAGGAUGUUG GCUUAGAAGCAGCC AUCAUUUAAAGAA AGCGUAAUAGCUCA CUGGUCGAGUCGGC CUGCGCGGAAGAUG UAACGGGGCUAAAC CAUGCACCGAAGCU GCGGCAGCGACGCU UAUGCGUUGUUGG GUAGGGGAGCGUU CUGUAAGCCUGCGA AGGUGUGCUGUGA GGCAUGCUGGAGG UAUCAGAAGUGCG AAUGCUGACAUAA GUAACGAUAAAGC GGGUGAAAAGCCCG CUCGCCGGAAGACC AAGGGUUCCUGUCC AACGUUAAUCGGG GCAGGGUGAGUCG ACCCCUAAGGCGAG GCCGAAAGGCGUAG UCGAUGGGAAACA GGUUAAUAUUCCU GUACUUGGUGUUA CUGCGAAGGGGGG ACGGAGAAGGCUA UGUUGGCCGGGCGA CGGUUGUCCCGGUU UAAGCGUGUAGGC UGGUUUUCCAGGCA AAUCCGGAAAAUCA AGGCUGAGGCGUG AUGACGAGGCACUA CGGUGCUGAAGCAA CAAAUGCCCUGCUU CCAGGAAAAGCCUC UAAGCAUCAGGUA ACAUCAAAUCGUAC CCCAAACCGACACU GGUGGUCAGGUAG AGAAUACCAAGGCG CUUGAGAGAACUCG GGUGAAGGAACUA					

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		GGCAAAAUGGUGCC GUAACUUCGGGAG AAGGCACGCUGAUA UGUAGGUGAGGUC CCUCGCGGAUGGAG CUGAAAUCAGUCGA AGAUACCAGCUGGC UGCAACUGUUUAU UAAAAACACAGCAC UGUGCAAACACGAA AGUGGACGUAUAC GGUGUGACGCCUGC CCGGUGCCGGAAGG UUAAUUGAUGGGG UUAGCGCAAGCGAA GCUCUUGAUCGAAG CCCCGGUAAACGGC GGCCGUAACUAUAA CGGUCCUAAGGUAG CGAAAUUCCUUGUC GGGUAAGUUCCGAC CUGCACGAAUGGCG UAAUGAUGGCCAG GCUGUCUCCACCCG AGACUCAGUGAAA UUGAACUCGCUGUG CAGAUGCAGUGUAC CCGCGGCAAGACGG AAAGACCCCGUGAA CCUUUACUAUAGCU UGACACUGAACAUU GAGCCUUGAUGUG UAGGAUAGGUGGG AGGCUUUGAAGUG UGGACGCCAGUCUG CAUGGAGCCGACCU UGAAAUACCACCCU UUAAUGUUUGAUG UUCUAACGUUGACC CGUAAUCCGGGUUG CGGACAGUGUCUGG UGGGUAGUUUGAC UGGGGCGGUCUCCU CCUAAAGAGUAACG GAGGAGCACGAAG GUUGGCUAAUCCUG GUCGGACAUCAGGA GGUUAGUGCAAUG GCAUAAGCCAGCUU GACUGCGAGCGUGA CGGCGCGAGCAGGU GCGAAAGCAGGUCA UAGUGAUCCGGUG GUUCUGAAUGGAA GGGCCAUCGCUCAA CGGAUAAAAGGUA CUCCGGGGAUAACA GGCUGAUACCGCCC AAGAGUUCAUAUC GACGGCGGUGUUU GGCACCUCGAUGUC GGCUCAUCACAUCC UGGGGCUGAAGUA GGUCCCAAGGGUAU GGCUGUUCGCCAUU UAAAGUGGUACGC GAGCUGGGUUUAG AACGUCGUGAGACA GUUCGGUCCCUAUC UGCCGUGGGCGCUG GAGAACUGAGGGG GGCUGCUCCUAGUA CGAGAGGACCGGAG UGGACGCAUCACUG GUGUUCGGGUUGU					

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		CAUGCCAAUGGCAC UGCCCGGUAGCUAA AUGCGGAAGAGAU AAGUGCUGAAAGC AUCUAAGCACGAAA CUUGCCCCGAGAUG AGUUCUCCCUGACC CUUUAAGGGUCCUG AAGGAACGUUGAA GACGACGACGUUGA UAGGCCGGGUGUG UAAGCGCAGCGAUG CGUUGAGCUAACCG GUACUAAUGAACCG UGAGGCUUAACCUU					
408	CC(=S)NC[C@@H]1CN(C(=O)O1)C2=CC(=C(C=C2)N3CCS(=O)CC3)F	GGUUAAGCGACUA AGCGUACACGGUGG AUGCCCUGGCAGUC AGAGGCGAUGAAG GACGUGCUAAUCUG CGAUAAGCGUCGGU AAGGUGAUAUGAA CCGUUAUAACCGGC GAUUUCCGAAUGG GGAAACCCAGUGUG UUUCGACACACUAU CAUUAACUGAAUCC AUAGGUUAAUGAG GCGAACCGGGGGAA CUGAAACAUCUAAG UACCCCGAGGAAAA GAAAUCAACCGAGA UUCCCCCAGUAGCG GCGAGCGAACGGGG AGCAGCCCAGAGCC UGAAUCAGUGUGU GUGUUAGUGGAAG CGUCUGGAAAGGCG CGCGAUACAGGGUG ACAGCCCCGUACAC AAAAAUGCACAUGC UGUGAGCUCGAUG AGUAGGGCGGGAC ACGUGGUAUCCUGU CUGAAUAUGGGGG GACCAUCCUCCAAG GCUAAAUACUCCUG ACUGACCGAUAGUG AACCAGUACCGUGA GGGAAAGGCGAAA AGAACCCCGGCGAG GGGAGUGAAAAAG AACCUGAAACCGUG UACGUACAAGCAGU GGGAGCACGCUUAG GCGUGUGACUGCGU ACCUUUUGUAUAA UGGGUCAGCGACUU AUAUUCUGUAGCA AGGUUAACCGAAU AGGGGAGCCGAAG GGAAACCGAGUCUU AACUGGGCGUUAA GUUGCAGGGUAUA GACCCGAAACCCGG UGAUCUAGCCAUGG GCAGGUUGAAGGU UGGGUAACACUAAC UGGAGGACCGAACC GACUAAUGUUGAA AAAUUAGCGGAUG ACUUGUGGCUGGG GGUGAAAGGCCAA UCAAACCGGGAGAU AGCUGGUUCUCCCC	LINEZOLID_DERIVATIVE_4	Target_lig_329	23SrRNA	Target_104	3.32422165832591

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		GAAAGCUAUUUAG GUAGCGCCUCGUGA AUUCAUCUCCGGGG GUAGAGCACUGUU UCGGCAAGGGGGUC AUCCCGACUUACCA ACCCGAUGCAAACU GCGAAUACCGGAGA AUGUUAUCACGGG AGACACACGGCGGG UGCUAACGUCCGUC GUGAAGAGGGAAA CAACCCAGACCGCC AGCUAAGGUCCCAA AGUCAUGGUUAAG UGGGAAACGAUGU GGGAAGGCCCAGAC AGCCAGGAUGUUG GCUUAGAAGCAGCC AUCAUUUAAAGAA AGCGUAAUAGCUCA CUGGUCGAGUCGGC CUGCGCGGAAGAUG UAACGGGGCUAAAC CAUGCACCGAAGCU GCGGCAGCGACGCU UAUGCGUUGUUGG GUAGGGGAGCGUU CUGUAAGCCUGCGA AGGUGUGCUGUGA GGCAUGCUGGAGG UAUCAGAAGUGCG AAUGCUGACAUAA GUAACGAUAAAGC GGGUGAAAAGCCCG CUCGCCGGAAGACC AAGGGUUCCUGUCC AACGUUAAUCGGG GCAGGGUGAGUCG ACCCCUAAGGCGAG GCCGAAAGGCGUAG UCGAUGGGAAACA GGUUAAUAUUCCU GUACUUGGUGUUA CUGCGAAGGGGGG ACGGAGAAGGCUA UGUUGGCCGGGCGA CGGUUGUCCCGGUU UAAGCGUGUAGGC UGGUUUUCCAGGCA AAUCCGGAAAAUCA AGGCUGAGGCGUG AUGACGAGGCACUA CGGUGCUGAAGCAA CAAAUGCCCUGCUU CCAGGAAAAGCCUC UAAGCAUCAGGUA ACAUCAAAUCGUAC CCCAAACCGACACU GGUGGUCAGGUAG AGAAUACCAAGGCG CUUGAGAGAACUCG GGUGAAGGAACUA GGCAAAAUGGUGCC GUAACUUCGGGAG AAGGCACGCUGAUA UGUAGGUGAGGUC CCUCGCGGAUGGAG CUGAAAUCAGUCGA AGAUACCAGCUGGC UGCAACUGUUUAU UAAAAACACAGCAC UGUGCAAACACGAA AGUGGACGUAUAC GGUGUGACGCCUGC					

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		CCGGUGCCGGAAGG UUAAUUGAUGGGG UUAGCGCAAGCGAA GCUCUUGAUCGAAG CCCCGGUAAACGGC GGCCGUAACUAUAA CGGUCCUAAGGUAG CGAAAUUCCUUGUC GGGUAAGUUCCGAC CUGCACGAAUGGCG UAAUGAUGGCCAG GCUGUCUCCACCCG AGACUCAGUGAAA UUGAACUCGCUGUG CAGAUGCAGUGUAC CCGCGGCAAGACGG AAAGACCCCGUGAA CCUUUACUAUAGCU UGACACUGAACAUU GAGCCUUGAUGUG UAGGAUAGGUGGG AGGCUUUGAAGUG UGGACGCCAGUCUG CAUGGAGCCGACCU UGAAAUACCACCCU UUAAUGUUUGAUG UUCUAACGUUGACC CGUAAUCCGGGUUG CGGACAGUGUCUGG UGGGUAGUUUGAC UGGGGCGGUCUCCU CCUAAAGAGUAACG GAGGAGCACGAAG GUUGGCUAAUCCUG GUCGGACAUCAGGA GGUUAGUGCAAUG GCAUAAGCCAGCUU GACUGCGAGCGUGA CGGCGCGAGCAGGU GCGAAAGCAGGUCA UAGUGAUCCGGUG GUUCUGAAUGGAA GGGCCAUCGCUCAA CGGAUAAAAGGUA CUCCGGGGAUAACA GGCUGAUACCGCCC AAGAGUUCAUAUC GACGGCGGUGUUU GGCACCUCGAUGUC GGCUCAUCACAUCC UGGGGCUGAAGUA GGUCCCAAGGGUAU GGCUGUUCGCCAUU UAAAGUGGUACGC GAGCUGGGUUUAG AACGUCGUGAGACA GUUCGGUCCCUAUC UGCCGUGGGCGCUG GAGAACUGAGGGG GGCUGCUCCUAGUA CGAGAGGACCGGAG UGGACGCAUCACUG GUGUUCGGGUUGU CAUGCCAAUGGCAC UGCCCGGUAGCUAA AUGCGGAAGAGAU AAGUGCUGAAAGC AUCUAAGCACGAAA CUUGCCCCGAGAUG AGUUCUCCCUGACC CUUUAAGGGUCCUG AAGGAACGUUGAA GACGACGACGUUGA UAGGCCGGGUGUG UAAGCGCAGCGAUG					

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		CGUUGAGCUAACCG GUACUAAUGAACCG UGAGGCUUAACCUU					
419	CC1CCC23CCC(=O)C2C1(C(CC(C(C3C)O)(C)C=C)OC(=O)CSC4CCNCC4)C	GGUUAAGCGACUA AGCGUACACGGUGG AUGCCCUGGCAGUC AGAGGCGAUGAAG GACGUGCUAAUCUG CGAUAAGCGUCGGU AAGGUGAUAUGAA CCGUUAUAACCGGC GAUUUCCGAAUGG GGAAACCCAGUGUG UUUCGACACACUAU CAUUAACUGAAUCC AUAGGUUAAUGAG GCGAACCGGGGGAA CUGAAACAUCUAAG UACCCCGAGGAAAA GAAAUCAACCGAGA UUCCCCCAGUAGCG GCGAGCGAACGGGG AGCAGCCCAGAGCC UGAAUCAGUGUGU GUGUUAGUGGAAG CGUCUGGAAAGGCG CGCGAUACAGGGUG ACAGCCCCGUACAC AAAAAUGCACAUGC UGUGAGCUCGAUG AGUAGGGCGGGAC ACGUGGUAUCCUGU CUGAAUAUGGGGG GACCAUCCUCCAAG GCUAAAUACUCCUG ACUGACCGAUAGUG AACCAGUACCGUGA GGGAAAGGCGAAA AGAACCCCGGCGAG GGGAGUGAAAAAG AACCUGAAACCGUG UACGUACAAGCAGU GGGAGCACGCUUAG GCGUGUGACUGCGU ACCUUUUGUAUAA UGGGUCAGCGACUU AUAUUCUGUAGCA AGGUUAACCGAAU AGGGGAGCCGAAG GGAAACCGAGUCUU AACUGGGCGUUAA GUUGCAGGGUAUA GACCCGAAACCCGG UGAUCUAGCCAUGG GCAGGUUGAAGGU UGGGUAACACUAAC UGGAGGACCGAACC GACUAAUGUUGAA AAAUUAGCGGAUG ACUUGUGGCUGGG GGUGAAAGGCCAA UCAAACCGGGAGAU AGCUGGUUCUCCCC GAAAGCUAUUUAG GUAGCGCCUCGUGA AUUCAUCUCCGGGG GUAGAGCACUGUU UCGGCAAGGGGGUC ACUUACCAACCCGA UGCAAACUGCGAAU ACCGGAGAAUGUU AUCACGGGAGACAC ACGGCGGGUGCUAA CGUCCGUCGUGAAG AGGGAAACAACCCA	SB-280080	Target_lig_334	50S SB 280080	Target_100	8.1249387366083

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		GACCGCCAGCUAAG GUCCCAAAGUCAUG GUUAAGUGGGAAA CGAUGUGGGAAGG CCCAGACAGCCAGG AUGUUGGCUUAGA AGCAGCCAUCAUUU AAAGAAAGCGUAA UAGCUCACUGGUCG AGUCGGCCUGCGCG GAAGAUGUAACGG GGCUAAACCAUGCA CCGAAGCUGCGGCA GCGACGCUUAUGCG UUGUUGGGUAGGG GAGCGUUCUGUAA GCCUGCGAAGGUGU GCUGUGAGGCAUGC UGGAGGUAUCAGA AGUGCGAAUGCUG ACAUAAGUAACGA UAAAGCGGGUGAA AAGCCCGCUCGCCG GAAGACCAAGGGU UCCUGUCCAACGUU AAUCGGGGCAGGG UGAGUCGACCCCUA AGGCGAGGCCGAAA GGCGUAGUCGAUG GGAAACAGGUUAA UAUUCCUGUACUUG GUGUUACUGCGAA GGGGGGACGGAGA AGGCUAUGUUGGCC GGGCGACGGUUGUC CCGGUUUAAGCGUG UAGGCUGGUUUUCC AGGCAAAUCCGGAA AAUCAAGGCUGAG GCGUGAUGACGAG GCACUACGGUGCUG AAGCAACAAAUGCC CUGCUUCCAGGAAA AGCCUCUAAGCAUC AGGUAACAUCAAA UCGUACCCCAAACC GACACAGGUGGUCA GGUAGAGAAUACC AAGGCGCUUGAGA GAACUCGGGUGAA GGAACUAGGCAAA AUGGUGCCGUAACU UCGGGAGAAGGCAC GCUGAUAUGUAGG UGAGGUCCCUCGCG GAUGGAGCUGAAA UCAGUCGAAGAUAC CAGCUGGCUGCAAC UGUUUAUUAAAAA CACAGCACUGUGCA AACACGAAAGUGG ACGUAUACGGUGU GACGCCUGCCCGGU GCCGGAAGGUUAA UUGAUGGGGUUAG CGCAAGCGAAGCUC UUGAUCGAAGCCCC GGUAAACGGCGGCC GUAACXAUAACGG UCCUAAGGUAGCGA AAUUCCUUGUCGGG UAAGUUCCGACCUG CACGAAUGGCGUAA UGAUGGCCAGGCUG UCUCCACCCGAGAC				

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		UCAGUGAAAUUGA ACUCGCUGUGAAGA UGCAGUGUACCCGC GGCAAGACGGAAA GACCCCGUGAACCU UUACUAUAGCUUG ACACUGAACAUUGA GCCUUGAUGUGUA GGAUAGGUGGGAG GCUUUGAAGUGUG GACGCCAGUCUGCA UGGAGCCGACCUUG AAAUACCACCCUUU AAUGUUUGAUGUU CUAACGUUGACCCG UAAUCCGGGUUGCG GACAGUGUCUGGU GGGUAGUUUGACU GGGGCGGUCUCCUC CUAAAGAGUAACG GAGGAGCACGAAG GUUGGCUAAUCCUG GUCGGACAUCAGGA GGUUAGUGCAAUG GCAUAAGCCAGCUU GACUGCGAGCGUGA CGGCGCGAGCAGGU GCGAAAGCAGGUCA UAGUGAUCCGGUG GUUCUGAAUGGAA GGGCCAUCGCUCAA CGGAUAAAAGGUA CUCCGGGGAUAACA GGCUGAUACCGCCC AAGAGUUCAUAUC GACGGCGGUGUUU GGCACCUCGAUGUC GGCUCAUCACAUCC UGGGGCUGAAGUA GGUCCCAAGGGUAU GGCUGUUCGCCAUU UAAAGUGGUACGC GAGCUGGGUUUAG AACGUCGUGAGACA GUUCGGUCCCUAUC UGCCGUGGGCGCUG GAGAACUGAGGGG GGCUGCUCCUAGUA CGAGAGGACCGGAG UGGACGCAUCACUG GUGUUCGGGUUGU CAUGCCAAUGGCAC UGCCCGGUAGCUAA AUGCGGAAGAGAU AAGUGCUGAAAGC AUCUAAGCACGAAA CUUGCCCCGAGAUG AGUUCUCCCUGACC CUUUAAGGGUCCUG AAGGAACGUUGAA GACGACGACGUUGA UAGGCCGGGUGUG UAAGCGCAGCGAUG CGUUGAGCUAACCG GUACUAAUGAACCG UGAGGCUUAACCU					
420	[C@@H]1(C[C@] ([C@@H]([C@@H] ([C@]23[C@@H] ([C@]1([C@@H] (CC3)C)C)C(=O) [C@H](C2)O)C)O) (C)C=C)OC(=O)NC(= O)c1ccc(nn1)N	GGUUAAGCGACUA AGCGUACACGGUGG AUGCCCUGGCAGUC AGAGGCGAUGAAG GACGUGCUAAUCUG CGAUAAGCGUCGGU AAGGUGAUAUGAA CCGUUAUAACCGGC GAUUUCCGAAUGG	SB-571519	Target_lig_335	50S SB571519	Target_100	7.95467702121334

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		GGAAACCCAGUGUG UUUCGACACACUAU CAUUAACUGAAUCC AUAGGUUAAUGAG GCGAACCGGGGGAA CUGAAACAUCUAAG UACCCCGAGGAAAA GAAAUCAACCGAGA UUCCCCCAGUAGCG GCGAGCGAACGGGG AGCAGCCCAGAGCC UGAAUCAGUGUGU GUGUUAGUGGAAG CGUCUGGAAAGGCG CGCGAUACAGGGUG ACAGCCCCGUACAC AAAAAUGCACAUGC UGUGAGCUCGAUG AGUAGGGCGGGAC ACGUGGUAUCCUGU CUGAAUAUGGGGG GACCAUCCUCCAAG GCUAAAUACUCCUG ACUGACCGAUAGUG AACCAGUACCGUGA GGGAAAGGCGAAA AGAACCCCGGCGAG GGGAGUGAAAAAG AACCUGAAACCGUG UACGUACAAGCAGU GGGAGCACGCUUAG GCGUGUGACUGCGU ACCUUUUGUAUAA UGGGUCAGCGACUU AUAUUCUGUAGCA AGGUUAACCGAAU AGGGGAGCCGAAG GGAAACCGAGUCUU AACUGGGCGUUAA GUUGCAGGGUAUA GACCCGAAACCCGG UGAUCUAGCCAUGG GCAGGUUGAAGGU UGGGUAACACUAAC UGGAGGACCGAACC GACUAAUGUUGAA AAAUUAGCGGAUG ACUUGUGGCUGGG GGUGAAAGGCCAA UCAAACCGGGAGAU AGCUGGUUCUCCCC GAAAGCUAUUUAG GUAGCGCCUCGUGA AUUCAUCUCCGGGG GUAGAGCACUGUU UCGGCAAGGGGGUC ACUUACCAACCCGA UGCAAACUGCGAAU ACCGGAGAAUGUU AUCACGGGAGACAC ACGGCGGGUGCUAA CGUCCGUCGUGAAG AGGGAAACAACCCA GACCGCCAGCUAAG GUCCCAAAGUCAUG GUUAAGUGGGAAA CGAUGUGGGAAGG CCCAGACAGCCAGG AUGUUGGCUUAGA AGCAGCCAUCAUUU AAAGAAAGCGUAA UAGCUCACUGGUCG AGUCGGCCUGCGCG GAAGAUGUAACGG GGCUAAACCAUGCA				

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		CCGAAGCUGCGGCA GCGACGCUUAUGCG UUGUUGGGUAGGG GAGCGUUCUGUAA GCCUGCGAAGGUGU GCUGUGAGGCAUGC UGGAGGUAUCAGA AGUGCGAAUGCUG ACAUAAGUAACGA UAAAGCGGGUGAA AAGCCCGCUCGCCG GAAGACCAAGGGU UCCUGUCCAACGUU AAUCGGGGCAGGG UGAGUCGACCCCUA AGGCGAGGCCGAAA GGCGUAGUCGAUG GGAAACAGGUUAA UAUUCCUGUACUUG GUGUUACUGCGAA GGGGGGACGGAGA AGGCUAUGUUGGCC GGGCGACGGUUGUC CCGGUUUAAGCGUG UAGGCUGGUUUUCC AGGCAAAUCCGGAA AAUCAAGGCUGAG GCGUGAUGACGAG GCACUACGGUGCUG AAGCAACAAAUGCC CUGCUUCCAGGAAA AGCCUCUAAGCAUC AGGUAACAUCAAA UCGUACCCCAAACC GACACAGGUGGUCA GGUAGAGAAUACC AAGGCGCUUGAGA GAACUCGGGUGAA GGAACUAGGCAAA AUGGUGCCGUAACU UCGGGAGAAGGCAC GCUGAUAUGUAGG UGAGGUCCCUCGCG GAUGGAGCUGAAA UCAGUCGAAGAUAC CAGCUGGCUGCAAC UGUUUAUUAAAAA CACAGCACUGUGCA AACACGAAAGUGG ACGUAUACGGUGU GACGCCUGCCCGGU GCCGGAAGGUUAA UUGAUGGGGUUAG CGCAAGCGAAGCUC UUGAUCGAAGCCCC GGUAAACGGCGGCC GUAACXAUAACGG UCCUAAGGUAGCGA AAUUCCUUGUCGGG UAAGUUCCGACCUG CACGAAUGGCGUAA UGAUGGCCAGGCUG UCUCCACCCGAGAC UCAGUGAAAUUGA ACUCGCUGUGAAGA UGCAGUGUACCCGC GGCAAGACGGAAA GACCCCGUGAACCU UUACUAUAGCUUG ACACUGAACAUUGA GCCUUGAUGUGUA GGAUAGGUGGGAG GCUUUGAAGUGUG GACGCCAGUCUGCA UGGAGCCGACCUUG					

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		AAAUACCACCCUUU AAUGUUUGAUGUU CUAACGUUGACCCG UAAUCCGGGUUGCG GACAGUGUCUGGU GGGUAGUUUGACU GGGGCGGUCUCCUC CUAAAGAGUAACG GAGGAGCACGAAG GUUGGCUAAUCCUG GUCGGACAUCAGGA GGUUAGUGCAAUG GCAUAAGCCAGCUU GACUGCGAGCGUGA CGGCGCGAGCAGGU GCGAAAGCAGGUCA UAGUGAUCCGGUG GUUCUGAAUGGAA GGGCCAUCGCUCAA CGGAUAAAAGGUA CUCCGGGGAUAACA GGCUGAUACCGCCC AAGAGUUCAUAUC GACGGCGGUGUUU GGCACCUCGAUGUC GGCUCAUCACAUCC UGGGGCUGAAGUA GGUCCCAAGGGUAU GGCUGUUCGCCAUU UAAAGUGGUACGC GAGCUGGGUUUAG AACGUCGUGAGACA GUUCGGUCCCUAUC UGCCGUGGGCGCUG GAGAACUGAGGGG GGCUGCUCCUAGUA CGAGAGGACCGGAG UGGACGCAUCACUG GUGUUCGGGUUGU CAUGCCAAUGGCAC UGCCCGGUAGCUAA AUGCGGAAGAGAU AAGUGCUGAAAGC AUCUAAGCACGAAA CUUGCCCCGAGAUG AGUUCUCCCUGACC CUUUAAGGGUCCUG AAGGAACGUUGAA GACGACGACGUUGA UAGGCCGGGUGUG UAAGCGCAGCGAUG CGUUGAGCUAACCG GUACUAAUGAACCG UGAGGCUUAACCU					
596	C1C(C(C(C(C1N)OC2C(C(C(C(O2)CO)O)O)N)OC3C(C(C(O3)CO)OC4C(C(C(C(O4)CN)O)O)N)O)O)N	GAGCGUCACACCUU CGGGUGAAGUCGCU C	Paromomycin_mol_mol	Target_lig_1116	16s_rRNA A SITE	Target_3	6.886056647693 16
600	C1C(C(C(C(C1N)OC2C(C(C(C(O2)CN)O)O)N)OC3C(C(C(O3)CO)OC4C(C(C(C(O4)CN)O)O)N)O)O)N	GAGCGUCACACCUU CGGGUGAAGUCGCU C	Neomycin B	Target_lig_1251	16s_rRNA A SITE	Target_3	5.823908740944 32
607	[C@H]1([C@@H]([C@@H]([C@@H](O[C@@H]1CN)O[C@@H]1[C@@H]([C@@H]([C@@H](C[C@@H]1N)N)O)OCC(=O)NCCCCCNC(=O)CO[C@@H]1[C@@H]([C@H](C[C@@H]	GAGCGUCACACCUU CGGGUGAAGUCGCU C	Bifunctional_aminoglycoside_derivative_1	Target_lig_353	16s_rRNA A SITE	Target_3	6.096910013008 06

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	([C@H]1O)N)N)O[C@H]1[C@H]([C@H]([C@H]([C@@H](O1)CN)O)O)N)N)O)O						
608	[C@H]1([C@@H]([C@@H]([C@@H](O[C@H]1CN)O[C@H]1[C@H]([C@H]([C@H](C[C@@H]1N)N)O)OC[C@@H](CN(CCCCN(C[C@@H](CO[C@H]1[C@@H]([C@H](C[C@H]([C@@H]1O)N)N)O[C@H]1[C@H]([C@@H]([C@@H]([C@@H](O1)CN)O)O)N)O)C)C)O)N)O)O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Bifunctional_aminoglycoside_derivative_2	Target_lig_354	16s_rRNA A SITE	Target_3	7.397940000867204
609	[C@@H]1([C@H]([C@H]([C@@H](O[C@@H]1CN)OC[C@@H](CN(CCCCCCN(C)C[C@H](CO[C@@H]1O[C@H]([C@@H]([C@@H]([C@H]1N)O)O)CN)O)C)O)N)O)O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Bifunctional_aminoglycoside_derivative_3	Target_lig_355	16s_rRNA A SITE	Target_3	4.958607314841 77
610	[C@@H]1([C@H]([C@H]([C@@H]([C@@H](C1)N)OC[C@@H](CN(CCCCCCN(C)C[C@@H](CO[C@@H]1[C@@H](C[C@H]([C@@H]([C@H]1O)O)N)N)O)C)O)O)O)N	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Bifunctional_aminoglycoside_derivative_4	Target_lig_356	16s_rRNA A SITE	Target_3	4.677780705266 08
611	[C@H]1([C@H]([C@@H]([C@H](O[C@H]1CO)OC[C@@H](CN(CCCCCCN(C)C[C@H](CO[C@@H]1O[C@H]([C@@H]([C@@H]([C@H]1N)O)O)CO)O)C)O)N)O)O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Bifunctional_aminoglycoside_derivative_5	Target_lig_357	16s_rRNA A SITE	Target_3	4.283996656365 2
612	[C@H]1([C@H]([C@@H]([C@H](C1)N)OC[C@@H](CN(CCCCCCN(C)C[C@H](CO[C@@H]1O[C@@H]([C@H]([C@H]([C@H]1N)O)O)CO)O)C)O)O)O)N	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Bifunctional_aminoglycoside_derivative_6	Target_lig_358	16s_rRNA A SITE	Target_3	4.408935392973 5
613	[C@H]1([C@H]([C@@H]([C@H](C1)N)OC[C@@H](CN(CCCCCCN(C)C[C@H](CO[C@@H]1O[C@H]([C@@H]([C@@H]([C@H]1N)O)O)CN)O)C)O)O)O)N	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Bifunctional_aminoglycoside_derivative_7	Target_lig_359	16s_rRNA A SITE	Target_3	4.494850021680 09
614	[C@H]1([C@H]	GAGCGUCACACCUU	Neamine	Target_lig_36	16s_rRNA A	Target_3	2.92081875

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	([C@@H]([C@@H](O[C@@H]1CN)O[C@@H]1[C@@H]([C@H]([C@@H](C[C@@H]1N)NC(=O)[C@@H](CCN)O)OCCNCCN)O)N)O)O	CGGGUGAAGUCGCUC	derivative_1	0	SITE		395238
615	C1[C@@H]([C@H]([C@@H]([C@H]([C@@H]1NC(=O)[C@H](CCN)O)OCCNCCCN)O)O[C@@H]2[C@@H]([C@H]([C@@H]([C@H](O2)CN)O)O)N)N	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Neamine derivative_2	Target_lig_361	16s_rRNA A SITE	Target_3	5.22914798835786
616	[C@H]1([C@H]([C@@H]([C@@H](O[C@@H]1CN)O[C@H]1[C@H]([C@@H]([C@H](C[C@H]1N)NC(=O)[C@@H](CCN)O)OCCNCCCCN)O)N)O)O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Neamine derivative_3	Target_lig_362	16s_rRNA A SITE	Target_3	5.4089353929735
617	[C@@H]1([C@@H]([C@H]([C@H](O[C@H]1CN)O[C@@H]1[C@@H]([C@H]([C@@H](C[C@H]1N)N)OCCNCCCN)O)N)O)O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Neamine derivative_4	Target_lig_363	16s_rRNA A SITE	Target_3	5.79588001734408
618	[C@H]1([C@@H]([C@H]([C@H](O[C@@H]1CN)O[C@@H]1[C@@H]([C@H](C[C@H]1N)NC(=O)[C@H](CCN)O)OCCN(CCCN)C(=O)[C@H](CCN)O)O)N)O)O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Neamine derivative_5	Target_lig_364	16s_rRNA A SITE	Target_3	4.95860731484177
619	[C@H]1([C@H]([C@@H]([C@@H](O[C@H]1CN)O[C@@H]1[C@@H]([C@H]([C@@H](C[C@H]1N)NC(=O)Cc1ccc(cc1)N)OCCNCCCCN)O)N)O)O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Neamine derivative_6	Target_lig_365	16s_rRNA A SITE	Target_3	4.61978875828839
620	[C@H]1([C@H]([C@@H]([C@@H](O[C@@H]1CN)O[C@H]1[C@H]([C@H]([C@@H](C[C@H]1N)NC(=O)Cc1cccc(c1)N)OCCNCCCCN)O)N)O)O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Neamine derivative_7	Target_lig_366	16s_rRNA A SITE	Target_3	4.61978875828839
621	[C@H]1([C@H]([C@@H]([C@H](O[C@H]1CO)O[C@H]1[C@@H]([C@H](O[C@H]([C@@H]1N)OC)CN)O)N)O)O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Neamine mimic_1	Target_lig_367	16s_rRNA A SITE	Target_3	4.30980391997149
622	[C@@H]1([C@@H]([C@H]([C@H](O[C@@H]1CN)O[C@@H]1[C@H]	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Neamine mimic_2	Target_lig_368	16s_rRNA A SITE	Target_3	4.43179827593301

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	([C@@H](O[C@@H]([C@H]1N)OC)CN)O)N)O)O						
623	[C@@H]1([C@H]([C@H]([C@H](O[C@@H]1CN)O[C@H]1[C@H]([C@@H]([C@H](O[C@H]1CO)OC)N)O)N)O)O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Neamine mimic_3	Target_lig_369	16s_rRNA A SITE	Target_3	4.39794000867204
624	[C@@H]1([C@@H]([C@H]([C@H](O[C@@H]1CO)O[C@H]1[C@H]([C@@H]([C@H](O[C@@H]1CN)OC)N)O)N)O)O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Neamine mimic_4	Target_lig_370	16s_rRNA A SITE	Target_3	4.58502665202918
625	[C@@H]1([C@H]([C@H]([C@@H](O[C@@H]1CN)O[C@@H]1[C@@H]([C@H]([C@@H](O[C@H]1CN)OC)N)O)N)O)O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Neamine mimic_5	Target_lig_371	16s_rRNA A SITE	Target_3	4.95860731484177
626	[C@H]1([C@H]([C@@H]([C@H](O[C@H]1CN)O[C@@H]1[C@H]([C@@H]([C@H](O[C@H]1CN)OC)N)O)N)O)O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Neamine mimic_6	Target_lig_372	16s_rRNA A SITE	Target_3	4.4089353929735
627	[C@H]1([C@H]([C@@H]([C@@H](O[C@@H]1CN)O[C@@H]1[C@@H]([C@H](O[C@H]([C@@H]1N)OC)CN)O[C@H]1[C@@H]([C@H]([C@H]([C@H](O1)C)N)O)O)N)O)O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Neamine mimic_7	Target_lig_373	16s_rRNA A SITE	Target_3	3.55129368009492
628	[C@H]1([C@@H]([C@@H]([C@H](O[C@H]1CN)O[C@@H]1[C@@H]([C@@H]([C@H](O[C@@H]1CN)OC)N)O[C@H]1[C@H]([C@H]([C@@H](O1)CO)O)O)N)O)O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Neamine mimic_8	Target_lig_374	16s_rRNA A SITE	Target_3	4.36653154442041
629	[C@H]1([C@H]([C@@H]([C@@H](O[C@@H]1CN)O[C@@H]1[C@H]([C@@H]([C@H](O[C@H]1CN)OC)N)O[C@@H]1[C@H]([C@H]([C@H]([C@H](O1)C)N)O)O)N)O)O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Neamine mimic_9	Target_lig_375	16s_rRNA A SITE	Target_3	5.69897000433602
630	C1[C@@H]([C@@H]([C@H]([C@@H]([C@@H]1N)O[C@H]1O[C@H]([C@@H]([C@H]([C@@H]1N)O)O)CO)O[C@@H]1[C@H]([C@H]([C@H](O1)CO)O[C@H]1O[C@@H]([C@@H]	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Paromomycin_mol derivative 1 16S A-site RNA	Target_lig_376	16s_rRNA A SITE	Target_3	6.63827216398241

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	([C@H]([C@@H]1N)O)O)CN)OCCN)O)N						
631	C1[C@@H]([C@@H]([C@H]([C@H]([C@@H]1N)O[C@@H]1O[C@H]([C@@H]([C@@H]([C@@H]1N)O)O)CO)O[C@@H]1[C@H]([C@H]([C@H](O1)CO)O[C@H]1O[C@H]([C@@H]([C@H]([C@@H]1N)O)O)CN)OCCCN)O)N	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Paromomycin_mol derivative 2 16S A-site RNA	Target_lig_377	16s_rRNA A SITE	Target_3	7
632	C1[C@@H]([C@@H]([C@@H]([C@H]([C@@H]1N)O[C@@H]1O[C@H]([C@@H]([C@@H]([C@@H]1N)O)O)CO)O[C@@H]1[C@H]([C@@H]([C@H](O1)CO)O[C@H]1O[C@H]([C@@H]([C@H]([C@@H]1N)O)O)CN)OCc1cccnc1)O)N	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Paromomycin_mol derivative 3 16S A-site RNA	Target_lig_378	16s_rRNA A SITE	Target_3	6.88605664769316
633	C1[C@@H]([C@H]([C@@H]([C@H]([C@@H]1N)OCN2C=NC3=C2N=CNC3=O)O)O)N	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Heterocyclic paromomycin derivative 1	Target_lig_379	16s_rRNA A SITE	Target_3	4
634	C1[C@@H]([C@H]([C@@H]([C@H]([C@@H]1N)OCN2C=CN=C2)O)O)N	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Heterocyclic paromomycin derivative 2	Target_lig_380	16s_rRNA A SITE	Target_3	3.56066730616974
635	C1[C@@H]([C@H]([C@@H]([C@H]([C@@H]1N)OCN2C=CN=N2)O)O)N	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Heterocyclic paromomycin derivative 3	Target_lig_381	16s_rRNA A SITE	Target_3	3.44977164694491
636	C1[C@@H]([C@H]([C@@H]([C@H]([C@@H]1N)OCN2C=NC=N2)O)O)N	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Heterocyclic paromomycin derivative 4	Target_lig_382	16s_rRNA A SITE	Target_3	3.42250820016277
637	C1[C@@H](N)[C@@H](O)[C@H]([C@@H]([C@H]1N)OCSc1ccnc2c1ccc(c2)C(F)(F)F)O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Quinolinyl_DOS_der	Target_lig_383	16s_rRNA A SITE	Target_3	4.16749108729376
638	C1[C@@H](N)[C@H](O)[C@H]([C@@H]([C@H]1N)OCSc1ccnc2c1ccc(c2)C(F)(F)F)O[C@@H]1O[C@@H]([C@H]([C@H]1O)O[C@H]1[C@@H]([C@H]([C@@H]([C@@H](O1)CN)O)O)N)CO	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Quinolinyl_DOS_paromomycin_der_1	Target_lig_384	16s_rRNA A SITE	Target_3	6
639	C1[C@H](N)[C@@H](OCCNCCCN)[C@H]([C@H]([C@@H]1N)OCSc1ccnc2c1ccc(c2)C(F)(F)F)O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Quinolinyl_DOS_paromomycin_der_2	Target_lig_385	16s_rRNA A SITE	Target_3	5.82390874094432
640	C1[C@H]([C@@H]([C@H]([C@@H]([C@H]1N)OCSC2=C3C=CC(=CC3=NC=C2)	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Quinolinyl_DOS_paromomycin_der_3	Target_lig_386	16s_rRNA A SITE	Target_3	5.69897000433602

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	C(F)(F)F)OCCNCCCN)O)N						
641	c1cccc(c1)c1ccc(cc1)CO[C@H](CO[C@@H]1O[C@@H]([C@H](O)[C@@H](O)[C@H]1N)CN)CN	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Acyclic DOS mimic 1_biphenyl substituent	Target_lig_387	16s_rRNA A SITE	Target_3	5.63827216398241
642	C(O[C@@H](CO[C@@H]1O[C@H]([C@@H](O)[C@H](O)[C@H]1N)CN)CN)c1cc2ccccc2cc1	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Acyclic DOS mimic 2_naphthyl substituent	Target_lig_388	16s_rRNA A SITE	Target_3	5.55284196865778
643	C(O[C@@H](CO[C@@H]1O[C@H]([C@H](O)[C@@H](O)[C@H]1N)CN)CN)c1ccccc1	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Acyclic DOS mimic 3_benzyl substituent	Target_lig_389	16s_rRNA A SITE	Target_3	3
649	O1[C@H](O[C@@H]2C[C@@H](NCC[C@H]2N)CO)[C@H]([C@@H]([C@H]([C@@H]1CN)O)O)N	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Azepane aminoglycoside mimic 1	Target_lig_395	16s_rRNA A SITE	Target_3	4.95860731484177
650	O1[C@H](O[C@@H]2C[C@@H](NCC[C@H]2N)CO)[C@H]([C@@H]([C@H]([C@@H]1CN)O)O)N	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Azepane aminoglycoside mimic 2	Target_lig_1114	16s_rRNA A SITE	Target_3	4.92081875395238
651	O1[C@H](O[C@@H]2C[C@H](NCC[C@H]2N)CO)[C@H]([C@@H]([C@H]([C@@H]1CN)O)O)N	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Azepane aminoglycoside mimic 3	Target_lig_396	16s_rRNA A SITE	Target_3	4.09691001300806
653	C1[C@H](CN(C[C@H]1N)c1nc(nc(N2C[C@H](C[C@@H](C2)N)N)n1)Nc1ccc(cc1)NC(=O)c1c(cc2c(c1)cccc2)O)N	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Diamino_piperidinyl_triazine_2	Target_lig_398	16s_rRNA A SITE	Target_3	8.69897000433602
655	C1CNCCC1C2=NC3=C(N2)C=C(C=C3)N	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Benzimidazole 16S A-site RNA	Target_lig_417	16s_rRNA A SITE	Target_3	3.30102999566398
656	C1CNCCC1C2=NC3=C(N2)C=C(C=C3)[N+](=O)[O-]	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Nitro substituted benzimidazole 16S A-site RNA	Target_lig_418	16s_rRNA A SITE	Target_3	3.51144928349956
657	C1CNCCC1C2=NC3=CC(=C(C=C3N2)Cl)Cl	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Halogen substituted benzimidazole	Target_lig_419	16s_rRNA A SITE	Target_3	3.7594507517174
658	C1C[C@@H](C[C@@H]1C2=NC3=C(N2)C=C(C=C3)[N+](=O)[O-])N	GAGCGUCACACCUUCGGGUGAAGUCGCUC	benzimidazole_analog_rRNA_1	Target_lig_420	16s_rRNA A SITE	Target_3	3.30102999566398
660	COC(=O)C1=CC=C(C=C1)CN2C3=CC(=C(C=C3N=C2C4CCNCC4)Cl)Cl	GAGCGUCACACCUUCGGGUGAAGUCGCUC	benzimidazole_analog_rRNA_3	Target_lig_446	16s_rRNA A SITE	Target_3	3
661	C1CCC(CC1)C2=NC3=C(N2)C=C(C=C3)[N+](=O)[O-]	GAGCGUCACACCUUCGGGUGAAGUCGCUC	benzimidazole_analog_rRNA_4	Target_lig_421	16s_rRNA A SITE	Target_3	3
662	C1=CC2=C(C=C1[N+](=O)	GAGCGUCACACCUUCGGGUGAAGUCGCU	benzimidazole_analog_rRNA_5	Target_lig_422	16s_rRNA A SITE	Target_3	3

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	[O-])NC(=N2)C3=CC=NC=C3	C					
663	C1=CC(=CN=C1)C2=NC3=C(N2)C=C(C=C3)[N+](=O)[O-]	GAGCGUCACACCUUCGGGUGAAGUCGCUC	benzimidazole_analog_rRNA_6	Target_lig_423	16s_rRNA A SITE	Target_3	3
664	C1=CC(=CC=C1C2=NC3=C(N2)C=C(C=C3)[N+](=O)[O-])N	GAGCGUCACACCUUCGGGUGAAGUCGCUC	benzimidazole_analog_rRNA_7	Target_lig_424	16s_rRNA A SITE	Target_3	3
665	C1=CC(=CC(=C1)N)C2=NC3=C(N2)C=C(C=C3)[N+](=O)[O-]	GAGCGUCACACCUUCGGGUGAAGUCGCUC	benzimidazole_analog_rRNA_8	Target_lig_425	16s_rRNA A SITE	Target_3	3.9100948885606
666	C1CC(CCC1C2=NC3=C(N2)C=C(C=C3)[N+](=O)[O-])N	GAGCGUCACACCUUCGGGUGAAGUCGCUC	benzimidazole_analog_rRNA_9	Target_lig_426	16s_rRNA A SITE	Target_3	3.97881070093006
667	c1c(cc2c(c1)[nH]c(n2)[C@H]1C[C@H](CCC1)N)N(=O)O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	benzimidazole_analog_rRNA_10	Target_lig_427	16s_rRNA A SITE	Target_3	3.65560772631489
668	CC(=O)N1CCC(CC1)C2=NC3=C(N2)C=C(C=C3)[N+](=O)[O-]	GAGCGUCACACCUUCGGGUGAAGUCGCUC	benzimidazole_analog_rRNA_11	Target_lig_428	16s_rRNA A SITE	Target_3	3
669	CN1CCC(CC1)C2=NC3=C(N2)C=C(C=C3)[N+](=O)[O-]	GAGCGUCACACCUUCGGGUGAAGUCGCUC	benzimidazole_analog_rRNA_12	Target_lig_429	16s_rRNA A SITE	Target_3	3
670	COC1=CC2=C(C=C1)N=C(N2)C3CCNCC3	GAGCGUCACACCUUCGGGUGAAGUCGCUC	benzimidazole_analog_rRNA_13	Target_lig_430	16s_rRNA A SITE	Target_3	3.23062267392386
671	CC1=CC2=C(C=C1)N=C(N2)C3CCNCC3	GAGCGUCACACCUUCGGGUGAAGUCGCUC	benzimidazole_analog_rRNA_14	Target_lig_431	16s_rRNA A SITE	Target_3	3.35753547975788
672	C1CNCCC1C2=NC3=C(N2)C=C(C=C3)Br	GAGCGUCACACCUUCGGGUGAAGUCGCUC	benzimidazole_analog_rRNA_15	Target_lig_432	16s_rRNA A SITE	Target_3	3.44249279809434
673	C1CNCCC1C2=NC3=C(N2)C=C(C=C3)Cl	GAGCGUCACACCUUCGGGUGAAGUCGCUC	benzimidazole_analog_rRNA_16	Target_lig_433	16s_rRNA A SITE	Target_3	3.29413628771608
674	C1CNCCC1C2=NC3=C(N2)C=C(C=C3)C(F)(F)F	GAGCGUCACACCUUCGGGUGAAGUCGCUC	benzimidazole_analog_rRNA_17	Target_lig_434	16s_rRNA A SITE	Target_3	3.55129368009492
675	CC1=CC2=C(C=C1Cl)N=C(N2)C3CCNCC3	GAGCGUCACACCUUCGGGUGAAGUCGCUC	benzimidazole_analog_rRNA_18	Target_lig_435	16s_rRNA A SITE	Target_3	3.42021640338319
676	c1(c(cc2c(c1)[nH]c(n2)C1CCNCC1)Cl)Cl	GAGCGUCACACCUUCGGGUGAAGUCGCUC	benzimidazole_analog_rRNA_19	Target_lig_1115	16s_rRNA A SITE	Target_3	3.7594507517174
677	C1CNCCC1C2=NC3=CC=CC=C3N2	GAGCGUCACACCUUCGGGUGAAGUCGCUC	benzimidazole_analog_rRNA_20	Target_lig_436	16s_rRNA A SITE	Target_3	3.74472749489669
678	C1CNCCC1C2=NC3=C(N2)C=NC=C3	GAGCGUCACACCUUCGGGUGAAGUCGCUC	benzimidazole_analog_rRNA_21	Target_lig_437	16s_rRNA A SITE	Target_3	3.95860731484177
679	C1CNCCC1C2=NC3=C(N2)C=CC=N3	GAGCGUCACACCUUCGGGUGAAGUCGCUC	benzimidazole_analog_rRNA_22	Target_lig_438	16s_rRNA A SITE	Target_3	3.27164621797877
680	C1CNCCC1C2=NC3=NC=NC=C3N2	GAGCGUCACACCUUCGGGUGAAGUCGCUC	benzimidazole_analog_rRNA_23	Target_lig_439	16s_rRNA A SITE	Target_3	3.03905380426617
681	C1CNCCC1C2=NC3=CC=CC=C3S2	GAGCGUCACACCUUCGGGUGAAGUCGCUC	benzimidazole_analog_rRNA_24	Target_lig_440	16s_rRNA A SITE	Target_3	3
682	C1CNCCC1C2=NC3=CC(=C(C=C3N2CC4=CC=C(C=C4)C(F)	GAGCGUCACACCUUCGGGUGAAGUCGCUC	benzimidazole_analog_rRNA_25	Target_lig_441	16s_rRNA A SITE	Target_3	3.66958622665081

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	(F)F)Cl)Cl						
683	C1CNCCC1C2=NC3=CC(=C(C=C3N2CC4=C(C=C(C=C4)C(F)(F)F)C(F)(F)F)Cl)Cl	GAGCGUCACACCUUCGGGUGAAGUCGCUC	benzimidazole_analog_rRNA_26	Target_lig_442	16s_rRNA A SITE	Target_3	3.79860287567955
684	C1CNCCC1C2=NC3=CC(=C(C=C3N2CC4=C(C(=C(C(=C4F)F)F)F)F)Cl)Cl	GAGCGUCACACCUUCGGGUGAAGUCGCUC	benzimidazole_analog_rRNA_27	Target_lig_443	16s_rRNA A SITE	Target_3	3.6252516539899
685	C1CNCCC1C2=NC3=CC(=C(C=C3N2CC4=C(C(=C(C(=C4F)F)C(F)(F)F)F)F)Cl)Cl	GAGCGUCACACCUUCGGGUGAAGUCGCUC	benzimidazole_analog_rRNA_28	Target_lig_444	16s_rRNA A SITE	Target_3	3.93181413825384
686	C1CNCCC1C2=NC3=CC(=C(C=C3N2CC4=CC=C(C=C4)[N+](=O)[O-])Cl)Cl	GAGCGUCACACCUUCGGGUGAAGUCGCUC	benzimidazole_analog_rRNA_29	Target_lig_445	16s_rRNA A SITE	Target_3	3.61798295742513
687	COC(=O)C1=CC=C(C=C1)CN2C3=CC(=C(C=C3N=C2C4CCNCC4)Cl)Cl	GAGCGUCACACCUUCGGGUGAAGUCGCUC	benzimidazole_analog_rRNA_30	Target_lig_446	16s_rRNA A SITE	Target_3	3.64975198166584
688	C1CNCCC1C2=NC3=CC(=C(C=C3N2CC4=CC=C(C=C4)I)Cl)Cl	GAGCGUCACACCUUCGGGUGAAGUCGCUC	benzimidazole_analog_rRNA_31	Target_lig_447	16s_rRNA A SITE	Target_3	3.70333480973847
689	C1CNCCC1C2=NC3=CC(=C(C=C3N2CC4=CC(=CC=C4)I)Cl)Cl	GAGCGUCACACCUUCGGGUGAAGUCGCUC	benzimidazole_analog_rRNA_32	Target_lig_448	16s_rRNA A SITE	Target_3	3.39254497678533
690	C1CNCCC1C2=NC3=CC(=C(C=C3N2CC4=CC=C(C=C4)Br)Cl)Cl	GAGCGUCACACCUUCGGGUGAAGUCGCUC	benzimidazole_analog_rRNA_33	Target_lig_449	16s_rRNA A SITE	Target_3	3.36251027048749
691	CC(C)(C)C1=CC=C(C=C1)CN2C3=CC(=C(C=C3N=C2C4CCNCC4)Cl)Cl	GAGCGUCACACCUUCGGGUGAAGUCGCUC	benzimidazole_analog_rRNA_34	Target_lig_450	16s_rRNA A SITE	Target_3	3.24033215531037
692	C1CNCCC1C2=NC3=CC(=C(C=C3N2CC4=CC=NC=C4)Cl)Cl	GAGCGUCACACCUUCGGGUGAAGUCGCUC	benzimidazole_analog_rRNA_35	Target_lig_451	16s_rRNA A SITE	Target_3	4.22184874961636
693	C1CNCCC1C2=NC3=CC(=C(C=C3N2CC4=CN=CC=C4)Cl)Cl	GAGCGUCACACCUUCGGGUGAAGUCGCUC	benzimidazole_analog_rRNA_36	Target_lig_452	16s_rRNA A SITE	Target_3	4.17392519729917
694	CCCCN1C2=CC(=C(C=C2N=C1C3CCNCC3)Cl)Cl	GAGCGUCACACCUUCGGGUGAAGUCGCUC	benzimidazole_analog_rRNA_37	Target_lig_453	16s_rRNA A SITE	Target_3	3.55595520408192
695	CN1C2=CC(=C(C=C2N=C1C3CCNCC3)Cl)Cl	GAGCGUCACACCUUCGGGUGAAGUCGCUC	benzimidazole_analog_rRNA_38	Target_lig_454	16s_rRNA A SITE	Target_3	3.62160209905186
696	COC(=O)CN1C2=CC(=C(C=C2N=C1C3CCNCC3)Cl)Cl	GAGCGUCACACCUUCGGGUGAAGUCGCUC	benzimidazole_analog_rRNA_39	Target_lig_455	16s_rRNA A SITE	Target_3	3.52143350440616
697	C1CNCCC1C2=NC3=CC(=C(C=C3N2CC4=CC=CC=C4Br)Cl)Cl	GAGCGUCACACCUUCGGGUGAAGUCGCUC	benzimidazole_analog_rRNA_40	Target_lig_456	16s_rRNA A SITE	Target_3	3.22694530663574
698	C1CNCCC1C2=NC3=CC(=C(C=C3N2CC4=CSC5=C4C=C(C=C5)Cl)Cl)Cl	GAGCGUCACACCUUCGGGUGAAGUCGCUC	benzimidazole_analog_rRNA_41	Target_lig_457	16s_rRNA A SITE	Target_3	3
699	c1(c(cc2c(c1)nc(n2Cc1ccc(cc1N(=O)O)C(F)(F)F)C1CCNCC1)Cl)Cl	GAGCGUCACACCUUCGGGUGAAGUCGCUC	benzimidazole_analog_rRNA_42	Target_lig_458	16s_rRNA A SITE	Target_3	3.91364016932525
700	c1(c(cc2c(c1)nc(n2Cc1ccc(cc1N(=O)O)N(=O)O)C1CCNCC1)Cl)Cl	GAGCGUCACACCUUCGGGUGAAGUCGCUC	benzimidazole_analog_rRNA_43	Target_lig_459	16s_rRNA A SITE	Target_3	3.61439372640169
701	c1(c(cc2c(c1)nc(n2Cc1	GAGCGUCACACCUU	benzimidazole_a	Target_lig_46	16s_rRNA A	Target_3	3.17263072

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	ncccn1)C1CCNCC1)Cl)Cl	CGGGUGAAGUCGCUC	nalog_rRNA_44	0	SITE		694617
702	c1(c(cc2c(c1)nc(n2CS(=O)(=O)c1ccc(cc1)C)C1CCNCC1)Cl)Cl	GAGCGUCACACCUUCGGGUGAAGUCGCUC	benzimidazole_analog_rRNA_45	Target_lig_461	16s_rRNA A SITE	Target_3	3
703	c1(c(cc2c(c1)nc(n2CC(=O)Oc1ccc(cc1)C)C1CCNCC1)Cl)Cl	GAGCGUCACACCUUCGGGUGAAGUCGCUC	benzimidazole_analog_rRNA_46	Target_lig_462	16s_rRNA A SITE	Target_3	3
875	c12c(c(c3c(n1)cccc3)Nc1ccc(cc1)CN)cccc2C(=O)N[C@@H](C(=O)N[C@H](C(=O)N[C@H](C(=O)O)CCCCN)CCCCN)CN	AAAUUGAAGAGUUUGAUCAUGGCUCAGAUUGAACGCUGGCGGCAGGCCUAACACAUGCAAGUCGAACGGUAACAGGAAGAAGCUUGCUUCUUUGCUGACGAGUGGCGGACGGGUGAGUAAUGUCUGGGAAACUGCCUGAUGGAGGGGGAUAACUACUGGAAACGGUAGCUAAUACCGCAUAACGUCGCAAGACCAAAGAGGGGGACCUUCGGGCCUCUUGCCAUCGGAUGUGCCCAGAUGGGAUUAGCUAGUAGGUGGGGUAACGGCUCACCUAGGCGACGAUCCCUAGCUGGUCUGAGAGGAUGACCAGCCACACUGGAACUGAGACACGGUCCAGACUCCUACGGGAGGCAGCAGUGGGGAAUAUUGCACAAUGGGCGCAAGCCUGAUGCAGCCAUGCCGCGUGUAUGAAGAAGGCCUUCGGGUUGUAAAGUACUUUCAGCGGGGAGGAAGGGAGUAAAGUUAAUACCUUUGCUCAUUGACGUUACCCGCAGAAGAAGCACCGGCUAACUCCGUGCCAGCAGCCGCGGUAAUACGGAGGGUGCAAGCGUUAAUCGGAAUUACUGGGCGUAAAGCGCACGCAGGCGGUUUGUUAAGUCAGAUGUGAAAUCCCCGGGCUCAACCUGGGAACUGCAUCUGAUACUGGCAAGCUUGAGUCUCGUAGAGGGGGGUAGAAUUCCAGGUGUAGCGGUGAAAUGCGUAGAGAUCUGGAGGAAUACCGGUGGCGAAGGCGGCCCCCUGGACGAAGACUGACGCUCAGGUGCGAAAGCGUGGGGAGCAAACAGGAUUAGAUACCCUGGUAGUCCACGCCGUAAACGAUGUCGACUUGGAGGUUGUGCCCUUGAGGCGUGGCUUCCGGAGCUAACGCGUUAAGU	HTP 21	Target_lig_528	Helix 22 of E.coli 16s RNA	Target_98	4.795880017344 08

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		CGACCGCCUGGGGA GUACGGCCGCAAGG UUAAAACUCAAAU GAAUUGACGGGGG CCCGCACAAGCGGU GGAGCAUGUGGUU UAAUUCGAUGCAAC GCGAAGAACCUUAC CUGGUCUUGACAUC CACGGAAGUUUUCA GAGAUGAGAAUGU GCCUUCGGGAACCG UGAGACAGGUGCU GCAUGGCUGUCGUC AGCUCGUGUUGUG AAAUGUUGGGUUA AGUCCCGCAACGAG CGCAACCCUUAUCC UUUGUUGCCAGCGG UCCGGCCGGGAACU CAAAGGAGACUGCC AGUGAUAAACUGG AGGAAGGUGGGGA UGACGUCAAGUCAU CAUGGCCCUUACGA CCAGGGCUACACAC GUGCUACAAUGGCG CAUACAAAGAGAA GCGACCUCGCGAGA GCAAGCGGACCUCA UAAAGUGCGUCGU AGUCCGGAUUGGA GUCUGCAACUCGAC UCCAUGAAGUCGGA AUCGCUAGUAAUCG UGGAUCAGAAUGCC ACGGUGAAUACGU UCCCGGGCCUUGUA CACACCGCCCGUCA CACCAUGGGAGUGG GUUGCAAAAGAAG UAGGUAGCUUAACC UUCGGGAGGGCGCU UACCACUUUGUGAU UCAUGACUGGGGU GAAGUCGUAACAA GGUAACCGUAGGG GAACCUGCGGUUGG AUCACCUCCUUA					
898	CC(=O)C1=CC2=C(C=C1)SC3=CC=CC=C3N2CCCN(C)C	GAGCGUCACACCUU CGGGUGAAGUCGCU C	Acetylpromazine	Target_lig_176	A-site bindings	Target_3	3.44369749923271
946	c12cc(ccc1c(c1c(n2)ccc(c1)OC)NCCCCc1c(nc(nc1N)N)N)Cl	GAGCGUCACACCUU CGGGUGAAGUCGCU C	MBNL CCUG ligand 3	Target_lig_563	RNA A	Target_3	3.52287874528034
1802	CC1=C(C2=C(N=C1C)N=C(C=C2)NCCN)C	GAGCGUCACACCUU CGGGUGAAGUCGCU C	ATMND-C2-NH2	Target_lig_1012	Bacterial rRNA A-site	Target_3	6.35654732351381
1804	CC1=C(C2=C(N=C1C)N=C(C=C2)NCCCN)C	GAGCGUCACACCUU CGGGUGAAGUCGCU C	ATMND-C3-NH2	Target_lig_1014	Bacterial rRNA A-site	Target_3	6
1805	NCCCCNc1ccc2c(n1)nc(c(c2C)C)C	GAGCGUCACACCUU CGGGUGAAGUCGCU C	ATMND-C4-NH2	Target_lig_1015	Bacterial rRNA A-site	Target_3	5.79588001734408
1806	NCCNc1ccc2c(n1)nccc2	GAGCGUCACACCUU CGGGUGAAGUCGCU C	AMND-C2-NH2	Target_lig_1016	Bacterial rRNA A-site	Target_3	4.58502665202918
1807	NCCNc1ccc2c(n1)nc(cc2C)C	GAGCGUCACACCUU CGGGUGAAGUCGCU C	ADMND-C2-NH2	Target_lig_1017	Bacterial rRNA A-site	Target_3	5.63827216398241

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
1808	Cc1cc(NCCN)ncc1	GAGCGUCACACCUU CGGGUGAAGUCGCU C	MPED	Target_lig_1277	Bacterial rRNA A-site	Target_3	4.92081875395238
2101	CCC1C(C(C(N(CC(CC(C(C(C(C(=O)O1)C)OC2CC(C(C(O2)C)O)(C)OC)C)OC3C(C(CC(O3)C)N(C)C)O)(C)O)C)C)O)(C)O	GGUUAAGCGACUA AGCGUACACGGUGG AUGCCCUGGCAGUC AGAGGCGAUGAAG GACGUGCUAAUCUG CGAUAAGCGUCGGU AAGGUGAUAUGAA CCGUUAUAACCGGC GAUUUCCGAAUGG GGAAACCCAGUGUG UUUCGACACACUAU CAUUAACUGAAUCC AUAGGUUAAUGAG GCGAACCGGGGGAA CUGAAACAUCUAAG UACCCCGAGGAAAA GAAAUCAACCGAGA UUCCCCCAGUAGCG GCGAGCGAACGGGG AGCAGCCCAGAGCC UGAAUCAGUGUGU GUGUUAGUGGAAG CGUCUGGAAAGGCG CGCGAUACAGGGUG ACAGCCCCGUACAC AAAAAUGCACAUGC UGUGAGCUCGAUG AGUAGGGCGGGAC ACGUGGUAUCCUGU CUGAAUAUGGGGG GACCAUCCUCCAAG GCUAAAUACUCCUG ACUGACCGAUAGUG AACCAGUACCGUGA GGGAAAGGCGAAA AGAACCCCGGCGAG GGGAGUGAAAAAG AACCUGAAACCGUG UACGUACAAGCAGU GGGAGCACGCUUAG GCGUGUGACUGCGU ACCUUUUGUAUAA UGGGUCAGCGACUU AUAUUCUGUAGCA AGGUUAACCGAAU AGGGGAGCCGAAG GGAAACCGAGUCUU AACUGGGCGUUAA GUUGCAGGGUAUA GACCCGAAACCCGG UGAUCUAGCCAUGG GCAGGUUGAAGGU UGGGUAACACUAAC UGGAGGACCGAACC GACUAAUGUUGAA AAAUUAGCGGAUG ACUUGUGGCUGGG GGUGAAAGGCCAA UCAAACCGGGAGAU AGCUGGUUCUCCCC GAAAGCUAUUUAG GUAGCGCCUCGUGA AUUCAUCUCCGGGG GUAGAGCACUGUU UCGGCAAGGGGGUC ACUUACCAACCCGA UGCAAACUGCGAAU ACCGGAGAAUGUU AUCACGGGAGACAC ACGGCGGGUGCUAA CGUCCGUCGUGAAG AGGGAAACAACCCA	Azithromycin	Target_lig_223	50S subunit	Target_100	8.42021640338319

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		GACCGCCAGCUAAG GUCCCAAAGUCAUG GUUAAGUGGGAAA CGAUGUGGGAAGG CCCAGACAGCCAGG AUGUUGGCUUAGA AGCAGCCAUCAUUU AAAGAAAGCGUAA UAGCUCACUGGUCG AGUCGGCCUGCGCG GAAGAUGUAACGG GGCUAAACCAUGCA CCGAAGCUGCGGCA GCGACGCUUAUGCG UUGUUGGGUAGGG GAGCGUUCUGUAA GCCUGCGAAGGUGU GCUGUGAGGCAUGC UGGAGGUAUCAGA AGUGCGAAUGCUG ACAUAAGUAACGA UAAAGCGGGUGAA AAGCCCGCUCGCCG GAAGACCAAGGGU UCCUGUCCAACGUU AAUCGGGGCAGGG UGAGUCGACCCCUA AGGCGAGGCCGAAA GGCGUAGUCGAUG GGAAACAGGUUAA UAUUCCUGUACUUG GUGUUACUGCGAA GGGGGGACGGAGA AGGCUAUGUUGGCC GGGCGACGGUUGUC CCGGUUUAAGCGUG UAGGCUGGUUUUCC AGGCAAAUCCGGAA AAUCAAGGCUGAG GCGUGAUGACGAG GCACUACGGUGCUG AAGCAACAAAUGCC CUGCUUCCAGGAAA AGCCUCUAAGCAUC AGGUAACAUCAAA UCGUACCCCAAACC GACACAGGUGGUCA GGUAGAGAAUACC AAGGCGCUUGAGA GAACUCGGGUGAA GGAACUAGGCAAA AUGGUGCCGUAACU UCGGGAGAAGGCAC GCUGAUAUGUAGG UGAGGUCCCUCGCG GAUGGAGCUGAAA UCAGUCGAAGAUAC CAGCUGGCUGCAAC UGUUUAUUAAAAA CACAGCACUGUGCA AACACGAAAGUGG ACGUAUACGGUGU GACGCCUGCCCGGU GCCGGAAGGUUAA UUGAUGGGGUUAG CGCAAGCGAAGCUC UUGAUCGAAGCCCC GGUAAACGGCGGCC GUAACXAUAACGG UCCUAAGGUAGCGA AAUUCCUUGUCGGG UAAGUUCCGACCUG CACGAAUGGCGUAA UGAUGGCCAGGCUG UCUCCACCCGAGAC				

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		UCAGUGAAAUUGA ACUCGCUGUGAAGA UGCAGUGUACCCGC GGCAAGACGGAAA GACCCCGUGAACCU UUACUAUAGCUUG ACACUGAACAUUGA GCCUUGAUGUGUA GGAUAGGUGGGAG GCUUUGAAGUGUG GACGCCAGUCUGCA UGGAGCCGACCUUG AAAUACCACCCUUU AAUGUUUGAUGUU CUAACGUUGACCCG UAAUCCGGGUUGCG GACAGUGUCUGGU GGGUAGUUUGACU GGGGCGGUCUCCUC CUAAAGAGUAACG GAGGAGCACGAAG GUUGGCUAAUCCUG GUCGGACAUCAGGA GGUUAGUGCAAUG GCAUAAGCCAGCUU GACUGCGAGCGUGA CGGCGCGAGCAGGU GCGAAAGCAGGUCA UAGUGAUCCGGUG GUUCUGAAUGGAA GGGCCAUCGCUCAA CGGAUAAAAGGUA CUCCGGGGAUAACA GGCUGAUACCGCCC AAGAGUUCAUAUC GACGGCGGUGUUU GGCACCUCGAUGUC GGCUCAUCACAUCC UGGGGCUGAAGUA GGUCCCAAGGGUAU GGCUGUUCGCCAUU UAAAGUGGUACGC GAGCUGGGUUUAG AACGUCGUGAGACA GUUCGGUCCCUAUC UGCCGUGGGCGCUG GAGAACUGAGGGG GGCUGCUCCUAGUA CGAGAGGACCGGAG UGGACGCAUCACUG GUGUUCGGGUUGU CAUGCCAAUGGCAC UGCCCGGUAGCUAA AUGCGGAAGAGAU AAGUGCUGAAAGC AUCUAAGCACGAAA CUUGCCCCGAGAUG AGUUCUCCCUGACC CUUUAAGGGUCCUG AAGGAACGUUGAA GACGACGACGUUGA UAGGCCGGGUGUG UAAGCGCAGCGAUG CGUUGAGCUAACCG GUACUAAUGAACCG UGAGGCUUAACCU					
2104	CC1CC=CC=CC(C(CC(C(C(C(CC(=O)O1)O)OC)OC2C(C(C(C(O2)C)OC3CC(C(C(O3)C)O)(C)C)N(C)C)O)CC=O)C)O	GGUUAAGCGACUA AGCGUACACGGUGG AUGCCCUGGCAGUC AGAGGCGAUGAAG GACGUGCUAAUCUG CGAUAAGCGUCGGU AAGGUGAUAUGAA CCGUUAUAACCGGC GAUUUCCGAAUGG	Kitasamycin	Target_lig_1144	50S subunit	Target_100	8.17069622716898

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		GGAAACCCAGUGUG UUUCGACACACUAU CAUUAACUGAAUCC AUAGGUUAAUGAG GCGAACCGGGGGAA CUGAAACAUCUAAG UACCCCGAGGAAAA GAAAUCAACCGAGA UUCCCCCAGUAGCG GCGAGCGAACGGGG AGCAGCCCAGAGCC UGAAUCAGUGUGU GUGUUAGUGGAAG CGUCUGGAAAGGCG CGCGAUACAGGGUG ACAGCCCCGUACAC AAAAAUGCACAUGC UGUGAGCUCGAUG AGUAGGGCGGGAC ACGUGGUAUCCUGU CUGAAUAUGGGGG GACCAUCCUCCAAG GCUAAAUACUCCUG ACUGACCGAUAGUG AACCAGUACCGUGA GGGAAAGGCGAAA AGAACCCCGGCGAG GGGAGUGAAAAAG AACCUGAAACCGUG UACGUACAAGCAGU GGGAGCACGCUUAG GCGUGUGACUGCGU ACCUUUUGUAUAA UGGGUCAGCGACUU AUAUUCUGUAGCA AGGUUAACCGAAU AGGGGAGCCGAAG GGAAACCGAGUCUU AACUGGGCGUUAA GUUGCAGGGUAUA GACCCGAAACCCGG UGAUCUAGCCAUGG GCAGGUUGAAGGU UGGGUAACACUAAC UGGAGGACCGAACC GACUAAUGUUGAA AAAUUAGCGGAUG ACUUGUGGCUGGG GGUGAAAGGCCAA UCAAACCGGGAGAU AGCUGGUUCUCCCC GAAAGCUAUUUAG GUAGCGCCUCGUGA AUUCAUCUCCGGGG GUAGAGCACUGUU UCGGCAAGGGGGUC ACUUACCAACCCGA UGCAAACUGCGAAU ACCGGAGAAUGUU AUCACGGGAGACAC ACGGCGGGUGCUAA CGUCCGUCGUGAAG AGGGAAACAACCCA GACCGCCAGCUAAG GUCCCAAAGUCAUG GUUAAGUGGGAAA CGAUGUGGGAAGG CCCAGACAGCCAGG AUGUUGGCUUAGA AGCAGCCAUCAUUU AAAGAAAGCGUAA UAGCUCACUGGUCG AGUCGGCCUGCGCG GAAGAUGUAACGG GGCUAAACCAUGCA				

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		CCGAAGCUGCGGCA GCGACGCUUAUGCG UUGUUGGGUAGGG GAGCGUUCUGUAA GCCUGCGAAGGUGU GCUGUGAGGCAUGC UGGAGGUAUCAGA AGUGCGAAUGCUG ACAUAAGUAACGA UAAAGCGGGUGAA AAGCCCGCUCGCCG GAAGACCAAGGGU UCCUGUCCAACGUU AAUCGGGGCAGGG UGAGUCGACCCCUA AGGCGAGGCCGAAA GGCGUAGUCGAUG GGAAACAGGUUAA UAUUCCUGUACUUG GUGUUACUGCGAA GGGGGGACGGAGA AGGCUAUGUUGGCC GGGCGACGGUUGUC CCGGUUUAAGCGUG UAGGCUGGUUUUCC AGGCAAAUCCGGAA AAUCAAGGCUGAG GCGUGAUGACGAG GCACUACGGUGCUG AAGCAACAAAUGCC CUGCUUCCAGGAAA AGCCUCUAAGCAUC AGGUAACAUCAAA UCGUACCCCAAACC GACACAGGUGGUCA GGUAGAGAAUACC AAGGCGCUUGAGA GAACUCGGGUGAA GGAACUAGGCAAA AUGGUGCCGUAACU UCGGGAGAAGGCAC GCUGAUAUGUAGG UGAGGUCCCUCGCG GAUGGAGCUGAAA UCAGUCGAAGAUAC CAGCUGGCUGCAAC UGUUUAUUAAAAA CACAGCACUGUGCA AACACGAAAGUGG ACGUAUACGGUGU GACGCCUGCCCGGU GCCGGAAGGUUAA UUGAUGGGGUUAG CGCAAGCGAAGCUC UUGAUCGAAGCCCC GGUAAACGGCGGCC GUAACXAUAACGG UCCUAAGGUAGCGA AAUUCCUUGUCGGG UAAGUUCCGACCUG CACGAAUGGCGUAA UGAUGGCCAGGCUG UCUCCACCCGAGAC UCAGUGAAAUUGA ACUCGCUGUGAAGA UGCAGUGUACCCGC GGCAAGACGGAAA GACCCCGUGAACCU UUACUAUAGCUUG ACACUGAACAUUGA GCCUUGAUGUGUA GGAUAGGUGGGAG GCUUUGAAGUGUG GACGCCAGUCUGCA UGGAGCCGACCUUG					

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		AAAUACCACCCUUU AAUGUUUGAUGUU CUAACGUUGACCCG UAAUCCGGGUUGCG GACAGUGUCUGGU GGGUAGUUUGACU GGGGCGGUCUCCUC CUAAAGAGUAACG GAGGAGCACGAAG GUUGGCUAAUCCUG GUCGGACAUCAGGA GGUUAGUGCAAUG GCAUAAGCCAGCUU GACUGCGAGCGUGA CGGCGCGAGCAGGU GCGAAAGCAGGUCA UAGUGAUCCGGUG GUUCUGAAUGGAA GGGCCAUCGCUCAA CGGAUAAAAGGUA CUCCGGGGAUAACA GGCUGAUACCGCCC AAGAGUUCAUAUC GACGGCGGUGUUU GGCACCUCGAUGUC GGCUCAUCACAUCC UGGGGCUGAAGUA GGUCCCAAGGGUAU GGCUGUUCGCCAUU UAAAGUGGUACGC GAGCUGGGUUUAG AACGUCGUGAGACA GUUCGGUCCCUAUC UGCCGUGGGCGCUG GAGAACUGAGGGG GGCUGCUCCUAGUA CGAGAGGACCGGAG UGGACGCAUCACUG GUGUUCGGGUUGU CAUGCCAAUGGCAC UGCCCGGUAGCUAA AUGCGGAAGAGAU AAGUGCUGAAAGC AUCUAAGCACGAAA CUUGCCCCGAGAUG AGUUCUCCCUGACC CUUUAAGGGUCCUG AAGGAACGUUGAA GACGACGACGUUGA UAGGCCGGGUGUG UAAGCGCAGCGAUG CGUUGAGCUAACCG GUACUAAUGAACCG UGAGGCUUAACCU					
2105	CC1CC=CC=CC(C(CC(C(C(C(CC(=O)O1)OC(=O)C)OC)OC2C(C(C(C(O2)C)OC3CC(C(C(O3)C)OC(=O)CC(C)C)(C)O)N(C)C)O)CC=O)C)O	GGUUAAGCGACUA AGCGUACACGGUGG AUGCCCUGGCAGUC AGAGGCGAUGAAG GACGUGCUAAUCUG CGAUAAGCGUCGGU AAGGUGAUAUGAA CCGUUAUAACCGGC GAUUUCCGAAUGG GGAAACCCAGUGUG UUUCGACACACUAU CAUUAACUGAAUCC AUAGGUUAAUGAG GCGAACCGGGGGAA CUGAAACAUCUAAG UACCCCGAGGAAAA GAAAUCAACCGAGA UUCCCCCAGUAGCG GCGAGCGAACGGGG AGCAGCCCAGAGCC UGAAUCAGUGUGU	Josamycin	Target_lig_1145	50S subunit	Target_100	8.08884239126002

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		GUGUUAGUGGAAG CGUCUGGAAAGGCG CGCGAUACAGGGUG ACAGCCCCGUACAC AAAAAUGCACAUGC UGUGAGCUCGAUG AGUAGGGCGGGAC ACGUGGUAUCCUGU CUGAAUAUGGGGG GACCAUCCUCCAAG GCUAAAUACUCCUG ACUGACCGAUAGUG AACCAGUACCGUGA GGGAAAGGCGAAA AGAACCCCGGCGAG GGGAGUGAAAAAG AACCUGAAACCGUG UACGUACAAGCAGU GGGAGCACGCUUAG GCGUGUGACUGCGU ACCUUUUGUAUAA UGGGUCAGCGACUU AUAUUCUGUAGCA AGGUUAACCGAAU AGGGGAGCCGAAG GGAAACCGAGUCUU AACUGGGCGUUAA GUUGCAGGGUAUA GACCCGAAACCCGG UGAUCUAGCCAUGG GCAGGUUGAAGGU UGGGUAACACUAAC UGGAGGACCGAACC GACUAAUGUUGAA AAAUUAGCGGAUG ACUUGUGGCUGGG GGUGAAAGGCCAA UCAAACCGGGAGAU AGCUGGUUCUCCCC GAAAGCUAUUUAG GUAGCGCCUCGUGA AUUCAUCUCCGGGG GUAGAGCACUGUU UCGGCAAGGGGGUC ACUUACCAACCCGA UGCAAACUGCGAAU ACCGGAGAAUGUU AUCACGGGAGACAC ACGGCGGGUGCUAA CGUCCGUCGUGAAG AGGGAAACAACCCA GACCGCCAGCUAAG GUCCCAAAGUCAUG GUUAAGUGGGAAA CGAUGUGGGAAGG CCCAGACAGCCAGG AUGUUGGCUUAGA AGCAGCCAUCAUUU AAAGAAAGCGUAA UAGCUCACUGGUCG AGUCGGCCUGCGCG GAAGAUGUAACGG GGCUAAACCAUGCA CCGAAGCUGCGGCA GCGACGCUUAUGCG UUGUUGGGUAGGG GAGCGUUCUGUAA GCCUGCGAAGGUGU GCUGUGAGGCAUGC UGGAGGUAUCAGA AGUGCGAAUGCUG ACAUAAGUAACGA UAAAGCGGGUGAA AAGCCCGCUCGCCG GAAGACCAAGGGU					

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		UCCUGUCCAACGUU AAUCGGGGCAGGG UGAGUCGACCCCUA AGGCGAGGCCGAAA GGCGUAGUCGAUG GGAAACAGGUUAA UAUUCCUGUACUUG GUGUUACUGCGAA GGGGGGACGGAGA AGGCUAUGUUGGCC GGGCGACGGUUGUC CCGGUUUAAGCGUG UAGGCUGGUUUUCC AGGCAAAUCCGGAA AAUCAAGGCUGAG GCGUGAUGACGAG GCACUACGGUGCUG AAGCAACAAAUGCC CUGCUUCCAGGAAA AGCCUCUAAGCAUC AGGUAACAUCAAA UCGUACCCCAAACC GACACAGGUGGUCA GGUAGAGAAUACC AAGGCGCUUGAGA GAACUCGGGUGAA GGAACUAGGCAAA AUGGUGCCGUAACU UCGGGAGAAGGCAC GCUGAUAUGUAGG UGAGGUCCCUCGCG GAUGGAGCUGAAA UCAGUCGAAGAUAC CAGCUGGCUGCAAC UGUUUAUUAAAAA CACAGCACUGUGCA AACACGAAAGUGG ACGUAUACGGUGU GACGCCUGCCCGGU GCCGGAAGGUUAA UUGAUGGGGUUAG CGCAAGCGAAGCUC UUGAUCGAAGCCCC GGUAAACGGCGGCC GUAACXAUAACGG UCCUAAGGUAGCGA AAUUCCUUGUCGGG UAAGUUCCGACCUG CACGAAUGGCGUAA UGAUGGCCAGGCUG UCUCCACCCGAGAC UCAGUGAAAUUGA ACUCGCUGUGAAGA UGCAGUGUACCCGC GGCAAGACGGAAA GACCCCGUGAACCU UUACUAUAGCUUG ACACUGAACAUUGA GCCUUGAUGUGUA GGAUAGGUGGGAG GCUUUGAAGUGUG GACGCCAGUCUGCA UGGAGCCGACCUUG AAAUACCACCCUUU AAUGUUUGAUGUU CUAACGUUGACCCG UAAUCCGGGUUGCG GACAGUGUCUGGU GGGUAGUUUGACU GGGGCGGUCUCCUC CUAAAGAGUAACG GAGGAGCACGAAG GUUGGCUAAUCCUG GUCGGACAUCAGGA GGUUAGUGCAAUG					

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		GCAUAAGCCAGCUU GACUGCGAGCGUGA CGGCGCGAGCAGGU GCGAAAGCAGGUCA UAGUGAUCCGGUG GUUCUGAAUGGAA GGGCCAUCGCUCAA CGGAUAAAAGGUA CUCCGGGGAUAACA GGCUGAUACCGCCC AAGAGUUCAUAUC GACGGCGGUGUUU GGCACCUCGAUGUC GGCUCAUCACAUCC UGGGGCUGAAGUA GGUCCCAAGGGUAU GGCUGUUCGCCAUU UAAAGUGGUACGC GAGCUGGGUUUAG AACGUCGUGAGACA GUUCGGUCCCUAUC UGCCGUGGGCGCUG GAGAACUGAGGGG GGCUGCUCCUAGUA CGAGAGGACCGGAG UGGACGCAUCACUG GUGUUCGGGUUGU CAUGCCAAUGGCAC UGCCCGGUAGCUAA AUGCGGAAGAGAU AAGUGCUGAAAGC AUCUAAGCACGAAA CUUGCCCCGAGAUG AGUUCUCCCUGACC CUUUAAGGGUCCUG AAGGAACGUUGAA GACGACGACGUUGA UAGGCCGGGUGUG UAAGCGCAGCGAUG CGUUGAGCUAACCG GUACUAAUGAACCG UGAGGCUUAACCU					
2106	CCCC(=O)OC1C(OC(CC1(C)OC(=O)CC)OC2C(OC(C(C2N(C)C)O)OC3C(CC(C(C=CC=CCC(OC(=O)CC(C3OC)O)C)O)C)CC=O)C)C	GGUUAAGCGACUA AGCGUACACGGUGG AUGCCCUGGCAGUC AGAGGCGAUGAAG GACGUGCUAAUCUG CGAUAAGCGUCGGU AAGGUGAUAUGAA CCGUUAUAACCGGC GAUUUCCGAAUGG GGAAACCCAGUGUG UUUCGACACACUAU CAUUAACUGAAUCC AUAGGUUAAUGAG GCGAACCGGGGGAA CUGAAACAUCUAAG UACCCCGAGGAAAA GAAAUCAACCGAGA UUCCCCCAGUAGCG GCGAGCGAACGGGG AGCAGCCCAGAGCC UGAAUCAGUGUGU GUGUUAGUGGAAG CGUCUGGAAAGGCG CGCGAUACAGGGUG ACAGCCCCGUACAC AAAAAUGCACAUGC UGUGAGCUCGAUG AGUAGGGCGGGAC ACGUGGUAUCCUGU CUGAAUAUGGGGG GACCAUCCUCCAAG GCUAAAUACUCCUG ACUGACCGAUAGUG	Rokitamycin	Target_lig_1146	50S subunit	Target_100	7.71331903064507

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		AACCAGUACCGUGA GGGAAAGGCGAAA AGAACCCCGGCGAG GGGAGUGAAAAAG AACCUGAAACCGUG UACGUACAAGCAGU GGGAGCACGCUUAG GCGUGUGACUGCGU ACCUUUUGUAUAA UGGGUCAGCGACUU AUAUUCUGUAGCA AGGUUAACCGAAU AGGGGAGCCGAAG GGAAACCGAGUCUU AACUGGGCGUUAA GUUGCAGGGUAUA GACCCGAAACCCGG UGAUCUAGCCAUGG GCAGGUUGAAGGU UGGGUAACACUAAC UGGAGGACCGAACC GACUAAUGUUGAA AAAUUAGCGGAUG ACUUGUGGCUGGG GGUGAAAGGCCAA UCAAACCGGGAGAU AGCUGGUUCUCCCC GAAAGCUAUUUAG GUAGCGCCUCGUGA AUUCAUCUCCGGGG GUAGAGCACUGUU UCGGCAAGGGGGUC ACUUACCAACCCGA UGCAAACUGCGAAU ACCGGAGAAUGUU AUCACGGGAGACAC ACGGCGGGUGCUAA CGUCCGUCGUGAAG AGGGAAACAACCCA GACCGCCAGCUAAG GUCCCAAAGUCAUG GUUAAGUGGGAAA CGAUGUGGGAAGG CCCAGACAGCCAGG AUGUUGGCUUAGA AGCAGCCAUCAUUU AAAGAAAGCGUAA UAGCUCACUGGUCG AGUCGGCCUGCGCG GAAGAUGUAACGG GGCUAAACCAUGCA CCGAAGCUGCGGCA GCGACGCUUAUGCG UUGUUGGGUAGGG GAGCGUUCUGUAA GCCUGCGAAGGUGU GCUGUGAGGCAUGC UGGAGGUAUCAGA AGUGCGAAUGCUG ACAUAAGUAACGA UAAAGCGGGUGAA AAGCCCGCUCGCCG GAAGACCAAGGGU UCCUGUCCAACGUU AAUCGGGGCAGGG UGAGUCGACCCCUA AGGCGAGGCCGAAA GGCGUAGUCGAUG GGAAACAGGUUAA UAUUCCUGUACUUG GUGUUACUGCGAA GGGGGGACGGAGA AGGCUAUGUUGGCC GGGCGACGGUUGUC CCGGUUUAAGCGUG					

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		UAGGCUGGUUUUCC AGGCAAAUCCGGAA AAUCAAGGCUGAG GCGUGAUGACGAG GCACUACGGUGCUG AAGCAACAAAUGCC CUGCUUCCAGGAAA AGCCUCUAAGCAUC AGGUAACAUCAAA UCGUACCCCAAACC GACACAGGUGGUCA GGUAGAGAAUACC AAGGCGCUUGAGA GAACUCGGGUGAA GGAACUAGGCAAA AUGGUGCCGUAACU UCGGGAGAAGGCAC GCUGAUAUGUAGG UGAGGUCCCUCGCG GAUGGAGCUGAAA UCAGUCGAAGAUAC CAGCUGGCUGCAAC UGUUUAUUAAAAA CACAGCACUGUGCA AACACGAAAGUGG ACGUAUACGGUGU GACGCCUGCCCGGU GCCGGAAGGUUAA UUGAUGGGGUUAG CGCAAGCGAAGCUC UUGAUCGAAGCCCC GGUAAACGGCGGCC GUAACXAUAACGG UCCUAAGGUAGCGA AAUUCCUUGUCGGG UAAGUUCCGACCUG CACGAAUGGCGUAA UGAUGGCCAGGCUG UCUCCACCCGAGAC UCAGUGAAAUUGA ACUCGCUGUGAAGA UGCAGUGUACCCGC GGCAAGACGGAAA GACCCCGUGAACCU UUACUAUAGCUUG ACACUGAACAUUGA GCCUUGAUGUGUA GGAUAGGUGGGAG GCUUUGAAGUGUG GACGCCAGUCUGCA UGGAGCCGACCUUG AAAUACCACCCUUU AAUGUUUGAUGUU CUAACGUUGACCCG UAAUCCGGGUUGCG GACAGUGUCUGGU GGGUAGUUUGACU GGGGCGGUCUCCUC CUAAAGAGUAACG GAGGAGCACGAAG GUUGGCUAAUCCUG GUCGGACAUCAGGA GGUUAGUGCAAUG GCAUAAGCCAGCUU GACUGCGAGCGUGA CGGCGCGAGCAGGU GCGAAAGCAGGUCA UAGUGAUCCGGUG GUUCUGAAUGGAA GGGCCAUCGCUCAA CGGAUAAAAGGUA CUCCGGGGAUAACA GGCUGAUACCGCCC AAGAGUUCAUAUC GACGGCGGUGUUU					

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		GGCACCUCGAUGUC GGCUCAUCACAUCC UGGGGCUGAAGUA GGUCCCAAGGGUAU GGCUGUUCGCCAUU UAAAGUGGUACGC GAGCUGGGUUUAG AACGUCGUGAGACA GUUCGGUCCCUAUC UGCCGUGGGCGCUG GAGAACUGAGGGG GGCUGCUCCUAGUA CGAGAGGACCGGAG UGGACGCAUCACUG GUGUUCGGGUUGU CAUGCCAAUGGCAC UGCCCGGUAGCUAA AUGCGGAAGAGAU AAGUGCUGAAAGC AUCUAAGCACGAAA CUUGCCCCGAGAUG AGUUCUCCCUGACC CUUUAAGGGUCCUG AAGGAACGUUGAA GACGACGACGUUGA UAGGCCGGGUGUG UAAGCGCAGCGAUG CGUUGAGCUAACCG GUACUAAUGAACCG UGAGGCUUAACCU					
2107	CCC1C(C(C(C(=O)C(CC(C(C(C(C(C(=O)O1)C)OC2CC(C(C(O2)C)O)(C)OC)C)OC3C(C(CC(O3)C)N(C)C)O)(C)O)C)C)O)(C)O	GGUUAAGCGACUA AGCGUACACGGUGG AUGCCCUGGCAGUC AGAGGCGAUGAAG GACGUGCUAAUCUG CGAUAAGCGUCGGU AAGGUGAUAUGAA CCGUUAUAACCGGC GAUUUCCGAAUGG GGAAACCCAGUGUG UUUCGACACACUAU CAUUAACUGAAUCC AUAGGUUAAUGAG GCGAACCGGGGGAA CUGAAACAUCUAAG UACCCCGAGGAAAA GAAAUCAACCGAGA UUCCCCCAGUAGCG GCGAGCGAACGGGG AGCAGCCCAGAGCC UGAAUCAGUGUGU GUGUUAGUGGAAG CGUCUGGAAAGGCG CGCGAUACAGGGUG ACAGCCCCGUACAC AAAAAUGCACAUGC UGUGAGCUCGAUG AGUAGGGCGGGAC ACGUGGUAUCCUGU CUGAAUAUGGGGG GACCAUCCUCCAAG GCUAAAUACUCCUG ACUGACCGAUAGUG AACCAGUACCGUGA GGGAAAGGCGAAA AGAACCCCGGCGAG GGGAGUGAAAAAG AACCUGAAACCGUG UACGUACAAGCAGU GGGAGCACGCUUAG GCGUGUGACUGCGU ACCUUUUGUAUAA UGGGUCAGCGACUU AUAUUCUGUAGCA AGGUUAACCGAAU	Eryrthromycin	Target_lig_233	50S subunit	Target_100	8.11350927482752

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		AGGGGAGCCGAAG GGAAACCGAGUCUU AACUGGGCGUUAA GUUGCAGGGUAUA GACCCGAAACCCGG UGAUCUAGCCAUGG GCAGGUUGAAGGU UGGGUAACACUAAC UGGAGGACCGAACC GACUAAUGUUGAA AAAUUAGCGGAUG ACUUGUGGCUGGG GGUGAAAGGCCAA UCAAACCGGGAGAU AGCUGGUUCUCCCC GAAAGCUAUUUAG GUAGCGCCUCGUGA AUUCAUCUCCGGGG GUAGAGCACUGUU UCGGCAAGGGGGUC ACUUACCAACCCGA UGCAAACUGCGAAU ACCGGAGAAUGUU AUCACGGGAGACAC ACGGCGGGUGCUAA CGUCCGUCGUGAAG AGGGAAACAACCCA GACCGCCAGCUAAG GUCCCAAAGUCAUG GUUAAGUGGGAAA CGAUGUGGGAAGG CCCAGACAGCCAGG AUGUUGGCUUAGA AGCAGCCAUCAUUU AAAGAAAGCGUAA UAGCUCACUGGUCG AGUCGGCCUGCGCG GAAGAUGUAACGG GGCUAAACCAUGCA CCGAAGCUGCGGCA GCGACGCUUAUGCG UUGUUGGGUAGGG GAGCGUUCUGUAA GCCUGCGAAGGUGU GCUGUGAGGCAUGC UGGAGGUAUCAGA AGUGCGAAUGCUG ACAUAAGUAACGA UAAAGCGGGUGAA AAGCCCGCUCGCCG GAAGACCAAGGGU UCCUGUCCAACGUU AAUCGGGGCAGGG UGAGUCGACCCCUA AGGCGAGGCCGAAA GGCGUAGUCGAUG GGAAACAGGUUAA UAUUCCUGUACUUG GUGUUACUGCGAA GGGGGGACGGAGA AGGCUAUGUUGGCC GGGCGACGGUUGUC CCGGUUUAAGCGUG UAGGCUGGUUUUCC AGGCAAAUCCGGAA AAUCAAGGCUGAG GCGUGAUGACGAG GCACUACGGUGCUG AAGCAACAAAUGCC CUGCUUCCAGGAAA AGCCUCUAAGCAUC AGGUAACAUCAAA UCGUACCCCAAACC GACACAGGUGGUCA GGUAGAGAAUACC					

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		AAGGCGCUUGAGA GAACUCGGGUGAA GGAACUAGGCAAA AUGGUGCCGUAACU UCGGGAGAAGGCAC GCUGAUAUGUAGG UGAGGUCCCUCGCG GAUGGAGCUGAAA UCAGUCGAAGAUAC CAGCUGGCUGCAAC UGUUUAUUAAAAA CACAGCACUGUGCA AACACGAAAGUGG ACGUAUACGGUGU GACGCCUGCCCGGU GCCGGAAGGUUAA UUGAUGGGGUUAG CGCAAGCGAAGCUC UUGAUCGAAGCCCC GGUAAACGGCGGCC GUAACXAUAACGG UCCUAAGGUAGCGA AAUUCCUUGUCGGG UAAGUUCCGACCUG CACGAAUGGCGUAA UGAUGGCCAGGCUG UCUCCACCCGAGAC UCAGUGAAAUUGA ACUCGCUGUGAAGA UGCAGUGUACCCGC GGCAAGACGGAAA GACCCCGUGAACCU UUACUAUAGCUUG ACACUGAACAUUGA GCCUUGAUGUGUA GGAUAGGUGGGAG GCUUUGAAGUGUG GACGCCAGUCUGCA UGGAGCCGACCUUG AAAUACCACCCUUU AAUGUUUGAUGUU CUAACGUUGACCCG UAAUCCGGGUUGCG GACAGUGUCUGGU GGGUAGUUUGACU GGGGCGGUCUCCUC CUAAAGAGUAACG GAGGAGCACGAAG GUUGGCUAAUCCUG GUCGGACAUCAGGA GGUUAGUGCAAUG GCAUAAGCCAGCUU GACUGCGAGCGUGA CGGCGCGAGCAGGU GCGAAAGCAGGUCA UAGUGAUCCGGUG GUUCUGAAUGGAA GGGCCAUCGCUCAA CGGAUAAAAGGUA CUCCGGGGAUAACA GGCUGAUACCGCCC AAGAGUUCAUAUC GACGGCGGUGUUU GGCACCUCGAUGUC GGCUCAUCACAUCC UGGGGCUGAAGUA GGUCCCAAGGGUAU GGCUGUUCGCCAUU UAAAGUGGUACGC GAGCUGGGUUUAG AACGUCGUGAGACA GUUCGGUCCCUAUC UGCCGUGGGCGCUG GAGAACUGAGGGG GGCUGCUCCUAGUA					

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		CGAGAGGACCGGAG UGGACGCAUCACUG GUGUUCGGGUUGU CAUGCCAAUGGCAC UGCCCGGUAGCUAA AUGCGGAAGAGAU AAGUGCUGAAAGC AUCUAAGCACGAAA CUUGCCCCGAGAUG AGUUCUCCCUGACC CUUUAAGGGUCCUG AAGGAACGUUGAA GACGACGACGUUGA UAGGCCGGGUGUG UAAGCGCAGCGAUG CGUUGAGCUAACCG GUACUAAUGAACCG UGAGGCUUAACCU					
2286	CCC1C(C=C(C=CC(=O)C(CC(C(C(C(CC(=O)O1)O)C)OC2C(C(C(O2)C)OC3CC(C(C(O3)C)O)(C)O)N(C)C)O)CC=O)C)C)COC4C(C(C(C(O4)C)O)OC)OC	UUGGCUACUAUGCC AGCUGGUGGAUUG CUCGGCUCAGGCGC UGAUGAAGGACGU GCCAAGCUGCGAUA AGCCAUGGGGAGCC GCACGGAGGCGAAG AACCAUGGAUUUCC GAAUGAGAAUCUC UCUAACAAUUGCUU CGCGCAAUGAGGAA CCCCGAGAACUGAA ACAUCUCAGUAUCG GGAGGAACAGAAA ACGCAAUGUGAUG UCGUUAGUAACCGC GAGUGAACGCGAU ACAGCCCAAACCGA AGCCCUCACGGGCA AUGUGGUGUCAGG GCUACCUCUCAUCA GCCGACCGUCUCGA CGAAGUCUCUUGGA ACAGAGCGUGAUAC AGGGUGACAACCCC GUACUCGAGACCAG UACGACGUGCGGUA GUGCCAGAGUAGCG GGGGUUGGAUAUC CCUCGCGAAUAACG CAGGCAUCGACUGC GAAGGCUAAACACA ACCUGAGACCGAUA GUGAACAAGUAGU GUGAACGAACGCUG CAAAGUACCCUCAG AAGGGAGGCGAAA UAGAGCAUGAAAU CAGUUGGCGAUCGA GCGACAGGGCAUAC AAGGUCCCUCGACG AAUGACCGACGCGC GAGCGUCCAGUAAG ACUCACGGGAAGCC GAUGUUCUGUCGU ACGUUUUGAAAAA CGAGCCAGGGAGUG UGUCUGCAUGGCAA GUCUAACCGGAGUA UCCGGGGAGGCACA GGGAAACCGACAUG GCCGCAGGGCUUUG CCCGAGGGCCGCCG UCUUCAAGGGCGGG GAGCCAUGUGGACA CGACCCGAAUCCGG ACGAUCUACGCAUG	Tylosin	Target_lig_320	U2609_Ecoli_ribosome	Target_99	7.12027350336042

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		GACAAGAUGAAGC GUGCCGAAAGGCAC GUGGAAGUCUGUU AGAGUUGGUGUCC UACAAUACCCUCUC GUGAUCUAUGUGU AGGGGUGAAAGGC CCAUCGAGUCCGGC AACAGCUGGUUCCA AUCGAAACAUGUCG AAGCAUGACCUCCG CCGAGGUAGUCUGU GAGGUAGAGCGACC GAUUGGUGUGUCC GCCUCCGAGAGGAG UCGGCACACCUGUC AAACUCCAAACUUA CAGACGCCGUUUGA CGCGGGGAUUCCGG UGCGCGGGGUAAGC CUGUGUACCAGGAG GGGAACAACCCAGA GAUAGGUUAAGGU CCCCAAGUGUGGAU UAAGUGUAAUCCUC UGAAGGUGGUCUC GAGCCCUAGACAGC CGGGAGGUGAGCU UAGAAGCAGCUACC CUCUAAGAAAAGCG UAACAGCUUACCGG CCGAGGUUUGAGGC GCCCAAAAUGAUCG GGACUCAAAUCCAC CACCGAGACCUGUC CGUACCACUCAUAC UGGUAAUCGAGUA GAUUGGCGCUCUAA UUGGAUGGAAGUA GGGGUGAAAACUCC UAUGGACCGAUUA GUGACGAAAAUCCU GGCCAUAGUAGCAG CGAUAGUCGGGUG AGAACCCCGACGGC CUAAUGGAUAAGG GUUCCUCAGCACUG CUGAUCAGCUGAGG GUUAGCCGGUCCUA AGUCAUACCGCAAC UCGACUAUGACGAA AUGGGAAACGGGU UAAUAUUCCCGUGC CACUAUGCAGUGAA AGUUGACGCCCUGG GGUCGAUCACGCUG GGCAUUCGCCCAGU CGAACCGUCCAACU CCGUGGAAGCCGUA AUGGCAGGAAGCG GACGAACGGCGGCA UAGGGAAACGUGA UUCAACCUGGGGCC CAUGAAAAGACGA GCAUAGUGUCCGUA CCGAGAACCGACAC AGGUGUCCAUGGCG GCGAAAGCCAAGGC CUGUCGGGAGCAAC CAACGUUAGGGAA UUCGGCAAGUUAG UCCCGUACCUUCGG AAGAAGGGAUGCC UGCUCCGGAACGGA GCAGGUCGCAGUGA					

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		CUCGGAAGCUCGGA CUGUCUAGUAACAA CAUAGGUGACCGCA AAUCCGCAAGGACU CGUACGGUCACUGA AUCCUGCCCAGUGC AGGUAUCUGAACAC CUCGUACAAGAGGA CGAAGGACCUGUCA ACGGCGGGGGUAAC UAUGACCCUCUUAA GGUAGCGUAGUACC UUGCCGCAUCAGUA GCGGCUUGCAUGAA UGGAUUAACCAGA GCUUCACUGUCCCA ACGUUGGGCCCGGU GAACUGUACAUUCC AGUGCGGAGUCUG GAGACACCCAGGGG GAAGCGAAGACCCU AUGGAGCUUUACU GCAGGCUGUCGCUG AGACGUGGUCGCCG AUGUGCAGCAUAG GUAGGAGACACUAC ACAGGUACCCGCGC UAGCGGGCCACCGA GUCAACAGUGAAA UACUACCCGUCGGU GACUGCGACUCUCA CUCCGGGAGGAGGA CACCGAUAGCCGGG CAGUUUGACUGGG GCGGUACGCGCUCG AAAAGAUAUCGAG CGCGCCCUAUGGCU AUCUCAGCCGGGAC AGAGACCCGGCGAA GAGUGCAAGAGCA AAAGAUAGCUUGA CAGUGUUCUUCCCA ACGAGGAACGCUGA CGCGAAAGCGUGGU CUAGCGAACCAAUU AGCCUGCUUGAUGC GGGCAAUUGAUGA CAGAAAAGCUACCC UAGGGAUAACAGA GUCGUCACUCGCAA GAGCACAUAUCGAC CGAGUGGCUUGCUA CCUCGAUGUCGGUU CCCUCCAUCCUGCC CGUGCAGAAGCGGG CAAGGGUGAGGUU GUUCGCCUAUUAAA GGAGGUCGUGAGC UGGGUUUAGACCG UCGUGAGACAGGUC GGCUGCUAUCUACU GGGUGUGUAAUGG UGUCUGACAAGAAC GACCGUAUAGUACG AGAGGAACUACGG UUGGUGGCCACUGG UGUACCGGUUGUUC GAGAGAGCACGUGC CGGGUAGCCACGCC ACACGGGGUAAGA GCUGAACGCAUCUA AGCUCGAAACCCAC UUGGAAAAGAGAC ACCGCCGAGGUCCC GCGUACAAGACGCG					

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		GUCGAUAGACUCGG GGUGUGCGCGUCGA GGUAACGAGACGU UAAGCCCACGAGCA CUAACAGACCAAAG CCAUCAU					
2288	CCCC1CC(N(C1)C)C(=O)NC(C2C(C(C(C(O2)SC)O)O)O)O)C(C)O	GGUUAAGCGACUA AGCGUACACGGUGG AUGCCCUGGCAGUC AGAGGCGAUGAAG GACGUGCUAAUCUG CGAUAAGCGUCGGU AAGGUGAUAUGAA CCGUUAUAACCGGC GAUUUCCGAAUGG GGAAACCCAGUGUG UUUCGACACACUAU CAUUAACUGAAUCC AUAGGUUAAUGAG GCGAACCGGGGGAA CUGAAACAUCUAAG UACCCCGAGGAAAA GAAAUCAACCGAGA UUCCCCCAGUAGCG GCGAGCGAACGGGG AGCAGCCCAGAGCC UGAAUCAGUGUGU GUGUUAGUGGAAG CGUCUGGAAAGGCG CGCGAUACAGGGUG ACAGCCCCGUACAC AAAAAUGCACAUGC UGUGAGCUCGAUG AGUAGGGCGGGAC ACGUGGUAUCCUGU CUGAAUAUGGGGG GACCAUCCUCCAAG GCUAAAUACUCCUG ACUGACCGAUAGUG AACCAGUACCGUGA GGGAAAGGCGAAA AGAACCCCGGCGAG GGGAGUGAAAAAG AACCUGAAACCGUG UACGUACAAGCAGU GGGAGCACGCUUAG GCGUGUGACUGCGU ACCUUUUGUAUAA UGGGUCAGCGACUU AUAUUCUGUAGCA AGGUUAACCGAAU AGGGGAGCCGAAG GGAAACCGAGUCUU AACUGGGCGUUAA GUUGCAGGGUAUA GACCCGAAACCCGG UGAUCUAGCCAUGG GCAGGUUGAAGGU UGGGUAACACUAAC UGGAGGACCGAACC GACUAAUGUUGAA AAAUUAGCGGAUG ACUUGUGGCUGGG GGUGAAAGGCCAA UCAAACCGGGAGAU AGCUGGUUCUCCCC GAAAGCUAUUUAG GUAGCGCCUCGUGA AUUCAUCUCCGGGG GUAGAGCACUGUU UCGGCAAGGGGGUC ACUUACCAACCCGA UGCAAACUGCGAAU ACCGGAGAAUGUU AUCACGGGAGACAC	Lincomycin	Target_lig_1175	50S ribosome (CLINDAMYCIN)	Target_100	5.30102999566398

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		ACGGCGGGUGCUAA CGUCCGUCGUGAAG AGGGAAACAACCCA GACCGCCAGCUAAG GUCCCAAAGUCAUG GUUAAGUGGGAAA CGAUGUGGGAAGG CCCAGACAGCCAGG AUGUUGGCUUAGA AGCAGCCAUCAUUU AAAGAAAGCGUAA UAGCUCACUGGUCG AGUCGGCCUGCGCG GAAGAUGUAACGG GGCUAAACCAUGCA CCGAAGCUGCGGCA GCGACGCUUAUGCG UUGUUGGGUAGGG GAGCGUUCUGUAA GCCUGCGAAGGUGU GCUGUGAGGCAUGC UGGAGGUAUCAGA AGUGCGAAUGCUG ACAUAAGUAACGA UAAAGCGGGUGAA AAGCCCGCUCGCCG GAAGACCAAGGGU UCCUGUCCAACGUU AAUCGGGGCAGGG UGAGUCGACCCCUA AGGCGAGGCCGAAA GGCGUAGUCGAUG GGAAACAGGUUAA UAUUCCUGUACUUG GUGUUACUGCGAA GGGGGGACGGAGA AGGCUAUGUUGGCC GGGCGACGGUUGUC CCGGUUUAAGCGUG UAGGCUGGUUUUCC AGGCAAAUCCGGAA AAUCAAGGCUGAG GCGUGAUGACGAG GCACUACGGUGCUG AAGCAACAAAUGCC CUGCUUCCAGGAAA AGCCUCUAAGCAUC AGGUAACAUCAAA UCGUACCCCAAACC GACACAGGUGGUCA GGUAGAGAAUACC AAGGCGCUUGAGA GAACUCGGGUGAA GGAACUAGGCAAA AUGGUGCCGUAACU UCGGGAGAAGGCAC GCUGAUAUGUAGG UGAGGUCCCUCGCG GAUGGAGCUGAAA UCAGUCGAAGAUAC CAGCUGGCUGCAAC UGUUUAUUAAAAA CACAGCACUGUGCA AACACGAAAGUGG ACGUAUACGGUGU GACGCCUGCCCGGU GCCGGAAGGUUAA UUGAUGGGGUUAG CGCAAGCGAAGCUC UUGAUCGAAGCCCC GGUAAACGGCGGCC GUAACXAUAACGG UCCUAAGGUAGCGA AAUUCCUUGUCGGG UAAGUUCCGACCUG					

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		CACGAAUGGCGUAA UGAUGGCCAGGCUG UCUCCACCCGAGAC UCAGUGAAAUUGA ACUCGCUGUGAAGA UGCAGUGUACCCGC GGCAAGACGGAAA GACCCCGUGAACCU UUACUAUAGCUUG ACACUGAACAUUGA GCCUUGAUGUGUA GGAUAGGUGGGAG GCUUUGAAGUGUG GACGCCAGUCUGCA UGGAGCCGACCUUG AAAUACCACCCUUU AAUGUUUGAUGUU CUAACGUUGACCCG UAAUCCGGGUUGCG GACAGUGUCUGGU GGGUAGUUUGACU GGGGCGGUCUCCUC CUAAAGAGUAACG GAGGAGCACGAAG GUUGGCUAAUCCUG GUCGGACAUCAGGA GGUUAGUGCAAUG GCAUAAGCCAGCUU GACUGCGAGCGUGA CGGCGCGAGCAGGU GCGAAAGCAGGUCA UAGUGAUCCGGUG GUUCUGAAUGGAA GGGCCAUCGCUCAA CGGAUAAAAGGUA CUCCGGGGAUAACA GGCUGAUACCGCCC AAGAGUUCAUAUC GACGGCGGUGUUU GGCACCUCGAUGUC GGCUCAUCACAUCC UGGGGCUGAAGUA GGUCCCAAGGGUAU GGCUGUUCGCCAUU UAAAGUGGUACGC GAGCUGGGUUUAG AACGUCGUGAGACA GUUCGGUCCCUAUC UGCCGUGGGCGCUG GAGAACUGAGGGG GGCUGCUCCUAGUA CGAGAGGACCGGAG UGGACGCAUCACUG GUGUUCGGGUUGU CAUGCCAAUGGCAC UGCCCGGUAGCUAA AUGCGGAAGAGAU AAGUGCUGAAAGC AUCUAAGCACGAAA CUUGCCCCGAGAUG AGUUCUCCCUGACC CUUUAAGGGUCCUG AAGGAACGUUGAA GACGACGACGUUGA UAGGCCGGGUGUG UAAGCGCAGCGAUG CGUUGAGCUAACCG GUACUAAUGAACCG UGAGGCUUAACCU					
2292	CCC1C(=O)N2CCCC2C(=O)N(C(C(=O)N3CCC(=O)CC3C(=O)NC(C(=O)OC(C(C(=O)N1)NC(=O)C4=C(C=CC=N4)O)C)C5=CC=CC=	GGUUAAGCGACUA AGCGUACACGGUGG AUGCCCUGGCAGUC AGAGGCGAUGAAG GACGUGCUAAUCUG CGAUAAGCGUCGGU	Virginiamycin S	Target_lig_1176	50S ribosome (Virginiamycin M)	Target_100	6.39794000867204

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	C5)CC6=CC=CC=C6)C	AAGGUGAUAUGAA CCGUUAUAACCGGC GAUUUCCGAAUGG GGAAACCCAGUGUG UUUCGACACACUAU CAUUAACUGAAUCC AUAGGUUAAUGAG GCGAACCGGGGGAA CUGAAACAUCUAAG UACCCCGAGGAAAA GAAAUCAACCGAGA UUCCCCCAGUAGCG GCGAGCGAACGGGG AGCAGCCCAGAGCC UGAAUCAGUGUGU GUGUUAGUGGAAG CGUCUGGAAAGGCG CGCGAUACAGGGUG ACAGCCCCGUACAC AAAAAUGCACAUGC UGUGAGCUCGAUG AGUAGGGCGGGAC ACGUGGUAUCCUGU CUGAAUAUGGGGG GACCAUCCUCCAAG GCUAAAUACUCCUG ACUGACCGAUAGUG AACCAGUACCGUGA GGGAAAGGCGAAA AGAACCCCGGCGAG GGGAGUGAAAAAG AACCUGAAACCGUG UACGUACAAGCAGU GGGAGCACGCUUAG GCGUGUGACUGCGU ACCUUUUGUAUAA UGGGUCAGCGACUU AUAUUCUGUAGCA AGGUUAACCGAAU AGGGGAGCCGAAG GGAAACCGAGUCUU AACUGGGCGUUAA GUUGCAGGGUAUA GACCCGAAACCCGG UGAUCUAGCCAUGG GCAGGUUGAAGGU UGGGUAACACUAAC UGGAGGACCGAACC GACUAAUGUUGAA AAAUUAGCGGAUG ACUUGUGGCUGGG GGUGAAAGGCCAA UCAAACCGGGAGAU AGCUGGUUCUCCCC GAAAGCUAUUUAG GUAGCGCCUCGUGA AUUCAUCUCCGGGG GUAGAGCACUGUU UCGGCAAGGGGGUC ACUUACCAACCCGA UGCAAACUGCGAAU ACCGGAGAAUGUU AUCACGGGAGACAC ACGGCGGGUGCUAA CGUCCGUCGUGAAG AGGGAAACAACCCA GACCGCCAGCUAAG GUCCCAAAGUCAUG GUUAAGUGGGAAA CGAUGUGGGAAGG CCCAGACAGCCAGG AUGUUGGCUUAGA AGCAGCCAUCAUUU AAAGAAAGCGUAA UAGCUCACUGGUCG					

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		AGUCGGCCUGCGCG GAAGAUGUAACGG GGCUAAACCAUGCA CCGAAGCUGCGGCA GCGACGCUUAUGCG UUGUUGGGUAGGG GAGCGUUCUGUAA GCCUGCGAAGGUGU GCUGUGAGGCAUGC UGGAGGUAUCAGA AGUGCGAAUGCUG ACAUAAGUAACGA UAAAGCGGGUGAA AAGCCCGCUCGCCG GAAGACCAAGGGU UCCUGUCCAACGUU AAUCGGGGCAGGG UGAGUCGACCCCUA AGGCGAGGCCGAAA GGCGUAGUCGAUG GGAAACAGGUUAA UAUUCCUGUACUUG GUGUUACUGCGAA GGGGGGACGGAGA AGGCUAUGUUGGCC GGGCGACGGUUGUC CCGGUUUAAGCGUG UAGGCUGGUUUUCC AGGCAAAUCCGGAA AAUCAAGGCUGAG GCGUGAUGACGAG GCACUACGGUGCUG AAGCAACAAAUGCC CUGCUUCCAGGAAA AGCCUCUAAGCAUC AGGUAACAUCAAA UCGUACCCCAAACC GACACAGGUGGUCA GGUAGAGAAUACC AAGGCGCUUGAGA GAACUCGGGUGAA GGAACUAGGCAAA AUGGUGCCGUAACU UCGGGAGAAGGCAC GCUGAUAUGUAGG UGAGGUCCCUCGCG GAUGGAGCUGAAA UCAGUCGAAGAUAC CAGCUGGCUGCAAC UGUUUAUUAAAAA CACAGCACUGUGCA AACACGAAAGUGG ACGUAUACGGUGU GACGCCUGCCCGGU GCCGGAAGGUUAA UUGAUGGGGUUAG CGCAAGCGAAGCUC UUGAUCGAAGCCCC GGUAAACGGCGGCC GUAACXAUAACGG UCCUAAGGUAGCGA AAUUCCUUGUCGGG UAAGUUCCGACCUG CACGAAUGGCGUAA UGAUGGCCAGGCUG UCUCCACCCGAGAC UCAGUGAAAUUGA ACUCGCUGUGAAGA UGCAGUGUACCCGC GGCAAGACGGAAA GACCCCGUGAACCU UUACUAUAGCUUG ACACUGAACAUUGA GCCUUGAUGUGUA GGAUAGGUGGGAG					

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		GCUUUGAAGUGUG GACGCCAGUCUGCA UGGAGCCGACCUUG AAAUACCACCCUUU AAUGUUUGAUGUU CUAACGUUGACCCG UAAUCCGGGUUGCG GACAGUGUCUGGU GGGUAGUUUGACU GGGGCGGUCUCCUC CUAAAGAGUAACG GAGGAGCACGAAG GUUGGCUAAUCCUG GUCGGACAUCAGGA GGUUAGUGCAAUG GCAUAAGCCAGCUU GACUGCGAGCGUGA CGGCGCGAGCAGGU GCGAAAGCAGGUCA UAGUGAUCCGGUG GUUCUGAAUGGAA GGGCCAUCGCUCAA CGGAUAAAAGGUA CUCCGGGGAUAACA GGCUGAUACCGCCC AAGAGUUCAUAUC GACGGCGGUGUUU GGCACCUCGAUGUC GGCUCAUCACAUCC UGGGGCUGAAGUA GGUCCCAAGGGUAU GGCUGUUCGCCAUU UAAAGUGGUACGC GAGCUGGGUUUAG AACGUCGUGAGACA GUUCGGUCCCUAUC UGCCGUGGGCGCUG GAGAACUGAGGGG GGCUGCUCCUAGUA CGAGAGGACCGGAG UGGACGCAUCACUG GUGUUCGGGUUGU CAUGCCAAUGGCAC UGCCCGGUAGCUAA AUGCGGAAGAGAU AAGUGCUGAAAGC AUCUAAGCACGAAA CUUGCCCCGAGAUG AGUUCUCCCUGACC CUUUAAGGGUCCUG AAGGAACGUUGAA GACGACGACGUUGA UAGGCCGGGUGUG UAAGCGCAGCGAUG CGUUGAGCUAACCG GUACUAAUGAACCG UGAGGCUUAACCU					
2348	[C@H]1([C@H]([C@@H]([C@H](O[C@H]1CO)O[C@H]1[C@@H]([C@H](O[C@H]([C@@H]1N)OC)CN)O)N)O)O	GAGCGUCACACCUU CGGGUGAAGUCGCU C	Neamine mimic_10	Target_lig_1285	16s_rRNA A SITE	Target_3	4.16115090926274
2349	N[C@@H]1C[C@H](N)[C@H]([C@@H]([C@H]1OCn1cnc2c1ccc2)O)O	GAGCGUCACACCUU CGGGUGAAGUCGCU C	Neamine_derivative_14	Target_lig_1201	16s_rRNA A SITE	Target_3	3.17587416608345
2350	N[C@@H]1C[C@H](N)[C@H]([C@@H]([C@H]1OCn1c2ccccc2nc1C(F)(F)F)O)O	GAGCGUCACACCUU CGGGUGAAGUCGCU C	Neamine_derivative_15	Target_lig_1202	16s_rRNA A SITE	Target_3	3.35753547975788
2351	N[C@@H]1C[C@H]	GAGCGUCACACCUU	Neamine_derivat	Target_lig_12	16s_rRNA A	Target_3	3.16621562

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	(N)[C@H]([C@@H]([C@H]1OCn1ccc(n1)I)O)O	CGGGUGAAGUCGCUC	ive_18	03	SITE		534352
2352	N[C@@H]1C[C@H](N)[C@H]([C@@H]([C@H]1OSc1cncnc1)O)O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Neamine_derivative_19	Target_lig_1204	16s_rRNA A SITE	Target_3	3.31158017799729
2353	N[C@@H]1C[C@H](N)[C@H]([C@@H]([C@H]1OSc1cnc(nc1)C(F)(F)F)O)O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Neamine_derivative_20	Target_lig_1205	16s_rRNA A SITE	Target_3	2.96697855531709
2354	N[C@@H]1C[C@H](N)[C@H]([C@@H]([C@H]1OC[N+]1N=Nc2c1nccc2)O)O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Neamine_derivative_26	Target_lig_1206	16s_rRNA A SITE	Target_3	3.25649023527157
2355	N[C@@H]1C[C@H](N)[C@H]([C@@H]([C@H]1OC[N+]1N=Nc2c1cccn2)O)O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Neamine_derivative_27	Target_lig_1207	16s_rRNA A SITE	Target_3	3.25649023527157
2356	N[C@@H]1C[C@H](N)[C@H]([C@@H]([C@H]1OCn1nc2c(n1)cccn2)O)O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Neamine_derivative_28	Target_lig_1208	16s_rRNA A SITE	Target_3	3.25649023527157
2357	N[C@@H]1C[C@H](N)[C@H]([C@@H]([C@H]1OCn1ccc(n1)C(F)(F)F)O)O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Neamine_derivative_29	Target_lig_1209	16s_rRNA A SITE	Target_3	3.35556141053216
2358	N[C@@H]1C[C@H](N)[C@H]([C@@H]([C@H]1OCn1nccc1C(F)(F)F)O)O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Neamine_derivative_30	Target_lig_1210	16s_rRNA A SITE	Target_3	3.35556141053216
2359	N[C@@H]1C[C@H](N)[C@H]([C@@H]([C@H]1OCn1cnc2c1nc[nH]c2=O)O)O	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Neamine_derivative_33	Target_lig_1211	16s_rRNA A SITE	Target_3	4
2361	CNC1C(OC2OC(Cn3nnc(c3)CCC(=O)Nc3ccccc(c3)c3csc(n3)NC(=O)C)C(C(C2O)O)N)OC2C(C1O)OC(C(C2)N)OC1C(N)CC(C(C1O)O)N	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Apramycin	Target_lig_772	16s_rRNA A SITE	Target_3	5.69897000433602
2362	C1C(C(C(C(C1N)OC2C(C(C(C(O2)CO)O)N)O)O)OC3C(C(C(C(O3)CN)O)O)O)N)N	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Bekanamycin	Target_lig_1286	16s_rRNA A SITE	Target_3	5.69897000433602
2364	C1C(C(C(C(C1N)OC2C(C(C(C(O2)CO)O)O)N)OC3C(C(C(O3)CO)OC4C(C(C(C(O4)CN)O)O)N)O)O)N	GAGCGUCACACCUUCGGGUGAAGUCGCUC	Paromomycin	Target_lig_5	16s_rRNA A SITE	Target_3	6.95860731484177