Training dataset curated from R-SIM database for the "Aptamers" model in RSAPred

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
39	C1=CC=C2C(=C1)C(=O)C3=C(C2=O)C(=C(C=C3NC4=CC(=C(C=C4)NC5=NC(=NC(=N5)NC6=CC=CC=C6S(=O)(=O)O)Cl)S(=O)(=O)O)S(=O)(=O)O)N	GGGAGAATTCCCGCGGCAGAAGCCCACCTGGCTTTGAACTCTATGTTATTGGGTGGGGGAAACTTAAGAAAACTACCACCCTTCAACATTACCGCCCTTCAGCCTGCCAGCGCCCTGCAGCCCGGGAAGCTT	Cibacron blue	Target_lig_27	RNA_APTAMER_CB_42	Target_4	4
40	C1=CC=C2C(=C1)C(=O)C3=C(C2=O)C(=C(C=C3NC4=CC(=C(C=C4)S(=O)(=O)O)NC5=NC(=NC(=N5)Cl)Cl)S(=O)(=O)O)N	GGGAGAAUUCCCGCGGCGUUGGCCCAGGAUAAUAGGACGAAAUCCGAAAAAUCCGUACCCAACAUGAACCCCCCAGCGCUCACACGGACGCCCCAUUACGGCUAACCGAACGCCUGCAGCCCGGGAAGCUU	Reactive Blue 4	Target_lig_28	RNA_APTAMER_B4_25	Target_5	3.2218487496 1636
91	C1=NC(=C2C(=N1)N(C=N2)C3C(C(C(O3)COP(=O)(O)OP(=O)(O)OP(=O)(O)O)O)O)N	GGGAAGGGAAGAAACUGCGGCUUCGGCCGGCUUCCC	ATP	Target_lig_65	RNA_Aptamer	Target_6	5.3979400086 7204
92	C1=NC(=C2C(=N1)N(C=N2)C3C(C(C(O3)COP(=O)(O)O)O)O)N	GGGAAGGGAAGAAACUGCGGCUUCGGCCGGCUUCCC	AMP	Target_lig_66	RNA_Aptamer	Target_6	8.3010256527 4088
93	CC1=CC2=C(C=C1C)N(C3=NC(=O)NC(=O)C3=N2)CC(C(C(COP(=O)(O)OP(=O)(O)OCC4C(C(C(O4)N5C=NC6=C(N=CN=C65)N)O)O)O)O)O	GGCGUGUAGGAUAUGCUUCGGCAGAAGGACACGCC	FAD	Target_lig_67	35 nucleotide RNA	Target_26	4.6382721639 8241
94	CC1=CC2=C(C=C1C)N(C3=NC(=O)NC(=O)C3=N2)CC(C(C(COP(=O)(O)O)O)O)O	GGCGUGUAGGAUAUGCUUCGGCAGAAGGACACGCC	FMN	Target_lig_68	35 nucleotide RNA	Target_26	6.3010299956 6398
95	C1=NC(=C2C(=N1)N(C=N2)C3C(C(C(O3)CO)O)O)N	GGCGUGUAGGAUAUGCUUCGGCAGAAGGACACGCC	ADENOSINE	Target_lig_69	35 nucleotide RNA	Target_26	2.3979400086 7204
96	CC1=CC2=C(C=C1C)N(C3=NC(=O)NC(=O)C3=N2)CC(C(C(CO)O)O)O	GGAACGAGGGAUGGAGGAGGAGUCGUUCC	riboflavin	Target_lig_70	Riboflavin binding RNA aptamer	Target_29	-0.4771212547 19662
97	C1=CC(=C[N+](=C1)C2C(C(C(O2)COP(=O)(O)[O-])O)O)C(=O)N	GGAACCCAACUAGGCGUUUGAGGGGAUUCGGCCACGGUAACAACCCCUC	NMN	Target_lig_71	NMN binding RNA aptamer	Target_30	5.6020599913 2796
98	CC1=CC2=C(C=C1C)N(C=N2)C3C(C(C(O3)CO)OP(=O)	CGGGUGCGCAUAACCACCUCAGUGCGAGCAA	cyanocobalamine	Target_lig_72	cyanocobalamin 35 nt RNA aptamer	Target_31	7.0604807473 8138

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	([O-])OC(C)CNC(=O)CCC4(C(C5C6(C(C(C(=N6)C(=C7C(C(C(=N7)C=C8C(C(C(=N8)C(=C4[N-]5)C)CCC(=O)N)(C)C)CCC(=O)N)(C)CC(=O)N)C)CCC(=O)N)(C)CC(=O)N)C)CC(=O)N)C)O.[C-]#N.[Co+3]						
99	C/C/1=C/2\[C@@]([C@@H](C(=N2)/C=C\3/C([C@@H](C(=N3)/C(=C\4/[C@]([C@H](C([N-]4)[C@]5([C@@]([C@@H](C1=N5)CCC(=O)N)(C)CC(=O)N)C)CC(=O)N)(C)CCC(=O)NCC(C)O)/C)CCC(=O)N)(C)C)CCC(=O)N)(C)CC(=O)N.[C-]#N.[C-]#N.[Co]	CGGGUGCGCAUAACCACCUCAGUGCGAGCAA	cobinamide dicyanide	Target_lig_73	cyanocobalamin 35 nt RNA aptamer	Target_31	4.705533773833841
210	CN1C2=C(C(=O)N(C1=O)C)NC=N2	AAGUGAUACCAGCAUCGUCUUGAUGCCCUUGGCAGCACUUCA	Theophylline	Target_lig_154	TCT8-4 RNA Aptamer	Target_32	6.494850021680009
211	CN1C=NC2=C1C(=O)N(C(=O)N2C)C	AAGUGAUACCAGCAUCGUCUUGAUGCCCUUGGCAGCACUUCA	caffeine	Target_lig_155	TCT8-4 RNA Aptamer	Target_32	2.455931955649972
213	CN1C2=C(C(=O)N(C1=O)C)NC(=O)N2	AAGUGAUACCAGCAUCGUCUUGAUGCCCUUGGCAGCACUUCA	1,3-dimethyluric acid	Target_lig_157	TCT8-4 RNA Aptamer	Target_32	3
214	CN1C=NC2=C1C(=O)NC(=O)N2C	AAGUGAUACCAGCAUCGUCUUGAUGCCCUUGGCAGCACUUCA	3,7-dimethylxanthine	Target_lig_158	TCT8-4 RNA Aptamer	Target_32	3.30102999566398
215	CN1C2=C(C(=O)NC1=O)NC=N2	AAGUGAUACCAGCAUCGUCUUGAUGCCCUUGGCAGCACUUCA	3-methylxanthine	Target_lig_159	TCT8-4 RNA Aptamer	Target_32	5.698970004336602
216	CN1C=NC2=C1C(=O)NC(=O)N2	AAGUGAUACCAGCAUCGUCUUGAUGCCCUUGGCAGCACUUCA	7-methylxanthine	Target_lig_160	TCT8-4 RNA Aptamer	Target_32	3.30102999566398
217	CN1C2=C(C(=O)N(C1=O)CCC(=O)O)NC=N2	AAGUGAUACCAGCAUCGUCUUGAUGCCCUUGGCAGCACUUCA	CP-theophylline	Target_lig_161	TCT8-4 RNA Aptamer	Target_32	6.031517051446607
218	C1=NC2=C(N1)C(=O)N=CN2	AAGUGAUACCAGCAUCGUCUUGAUGCCCUUGGCAGCACUUCA	Hypoxanthine	Target_lig_162	TCT8-4 RNA Aptamer	Target_32	4.309803919997149
219	CN1C(=O)C2=C(NC1=O)N=CN2	AAGUGAUACCAGCAUCGUCUUGAUGCCCUUGGCAGCACUUCA	xanthine	Target_lig_156	TCT8-4 RNA Aptamer	Target_32	5.070581074285571
285	[C@@H]1([C@H]([C@H](O)[C@H]([C@@H]	CGCGCGUGUGCGCG	B-12	Target_lig_224	RNA hairpin loop	Target_120	4.602059991327796

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	(C1)N)O)OCCCc1cn(nn1)Cc1cccc(Cn2cc(nn2)CCCO[C@H]2[C@@H](C[C@@H]([C@@H](O)[C@H]2O)N)N)c1)N						
288	C1C2C(C(S1)CCCCC(=O)O)NC(=O)N2	GGAACACUAUCCGAUGGCACCGACCAUAGGCUCGGGUUGCCAGAGGUUCCACACUUUCAUCGAAAAGCCUAUGCUAGGCAAUGACAUGGACUCCUUGGUCAUUAGGAUCG	biotin_molecule	Target_lig_227	Biotin aptamer	Target_33	5.2438966284149
309	C1C(C(C(C(C1N)OC2C(C(C(C(O2)CO)O)N)O)O)OC3C(CC(C(O3)CN)O)N)N	GGGUCUCGAGUUUUCGAAGACCC	Ethidium bromide	Target_lig_6	Bulge_A_RNA	Target_121	5.48148606012211
311	CC1=CC2=C(C=C1C)N(C3=NC(=O)NC(=O)C3=N2)CC(C(C(COP(=O)(O)O)O)O)O	GGCGUGUAGGAUAUGCUUCGGCAGAAGGACACGCC	FMN	Target_lig_68	FMN aptamer	Target_34	8.30102999566398
385	CN(C)C1=CC=C(C=C1)C(=C2C=CC(=[N+](C)C)C=C2)C3=CC=CC=C3.[Cl-]	GGGAAGGGAAGAAACUGCGGCUUCGGCCGGCUUCCC	Malachite green	Target_lig_308	Aptamer	Target_6	7.30102999566398
417	CC1(C2CC3C(C(=O)C(=C(C3(C(=O)C2=C(C4=C1C=CC=C4O)O)O)O)O)C(=O)N)N(C)C)O	GGGCCUAAAACAUACCAGAUCGCCACCCGCGCUUUAAUCUGGAGAGGUGAAGAAUACGACACCUAGGCUC	tetracyclin	Target_lig_74	Tetracycline in vitro aptamer	Target_39	9.09691001300806
457	CC1=C2C=CN=CC2=C(C3=C1NC4=CC=CC=C43)C	AAA	Ellipticine	Target_lig_342	ss_PolyA	Target_40	5.33724216831843
752	C1CN(CCN1C[C@@H]2[C@H](OC(=O)N2)COC(=O)CC3=CC=CC=C3)C4=CC=CC=C4	GAGGGUGGAACCGCGCUUCGGCGUCCCUC	phenylacetate derivative	Target_lig_510	T-box riboswitch	Target_79	5.18045606445813
753	CC(=O)C1=CC=C(C=C1)NC(=O)OC[C@@H]2[C@H](NC(=O)O2)CN3CCN(CC3)C4=CC=CC=C4	GAGGGUGGAACCGCGCUUCGGCGUCCCUC	methyl N-(4-acetylphenyl)carbamate derivative	Target_lig_511	T-box riboswitch	Target_79	6.04575749056068

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
778	CC1C(C(C(C(O1)OC2C3CC#CC4C(O4)(C#CC3=CC2OC(=O)C5=C(C=CC6=C5C=C(C=C6C)OC)O)C7COC(=O)O7)NC)O)O	GUCCGAUGCGUGUUUCACGCAGUUCGGAC	neocarzinostatin	Target_lig_148	RNA XIII	Target_123	5.958607314844177
779	c12c(cccc1)[C@]1(C(=O)C=C2)[C@@H](O[C@@H]2[C@@H]1c1c(C2=O)cc2c(c1)cccc2)O[C@@H]1[C@H]([C@@H]([C@H]([C@H](O1)CO)O)O)N	GUCCGAUGCGUGUUUCACGCAGUUCGGAC	Neocarzinostatin_chromophore_derivative_2	Target_lig_150	RNA XIII	Target_123	4.677780705266608
780	c12c(cccc1)[C@]1([C@@H](C=C2)O[C@H]2[C@@H]([C@H]([C@@H]([C@@H](O2)CO)O)O)N)C(=O)O[C@H]2[C@@H]1c1c(C2=O)cc2c(c1)cccc2	GUCCGAUGCGUGUUUCACGCAGUUCGGAC	Neocarzinostatin_chromophore_derivative_3	Target_lig_151	RNA XIII	Target_123	4.657577319177779
781	c12c(cc(cc1)OC)[C@@]1(C(=O)C=C2)C=C[C@@H]2[C@@H]1c1c([C@H]2O[C@@H]2[C@H]([C@@H]([C@@H]([C@@H](O2)C)O)O)NC)cc2c(c1)cccc2	GUCCGAUGCGUGUUUCACGCAGUUCGGAC	Neocarzinostatin_chromophore_derivative_5	Target_lig_152	RNA XIII	Target_123	5.886056647693316
782	c12c(cccc1)[C@]1(C(=O)C=C2)[C@@H](O[C@@H]2[C@@H]1c1c(C2=O)cc2c(c1)cccc2)O[C@@H]1[C@H]([C@@H]([C@H]([C@H](O1)CO)O)O)N	GUCCGAUGCGUGUUUCACGCAGUCGGAC	Neocarzinostatin_chromophore_derivative_2	Target_lig_150	RNA XIV	Target_124	4.721246399047717
783	c12c(cccc1)[C@]1([C@@H](C=C2)O[C@H]2[C@@H]([C@H]([C@@H]([C@@H](O2)CO)O)O)N)C(=O)O[C@H]2[C@@H]1c1c(C2=O)cc2c(c1)cccc2	GUCCGAUGCGUGUUUCACGCAGUCGGAC	Neocarzinostatin_chromophore_derivative_3	Target_lig_151	RNA XIV	Target_124	4.167491087293376
784	c12c(cccc1)[C@]1(C(=O)C	GUCCGAUGCGUGUUUCACGCAUCGGAC	Neocarzinostatin_chromophore_d	Target_lig_150	RNA XV	Target_125	4.698970004333602

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	=C2)[C@@H](O[C@@H]2[C@@H]1c1c(C2=O)cc2c(c1)cccc2)O[C@@H]1[C@H]([C@@H]([C@H]([C@H](O1)CO)O)O)N		erivative_2				
785	c12c(cc(cc1)OC)[C@@]1(C(=O)C=C2)C=C[C@@H]2[C@@H]1c1c([C@H]2O[C@@H]2[C@H]([C@@H]([C@H]([C@H](O2)CO)O)O)N)cc2c(c1)cccc2	GUCCGAUGCGUGUUUCACGCAUCGGAC	Neocarzinostatin_chromophore_derivative_4	Target_lig_526	RNA XV	Target_125	5.30102999566398
786	c12c(cc(cc1)OC)[C@@]1(C(=O)C=C2)C=C[C@@H]2[C@@H]1c1c([C@H]2O[C@@H]2[C@H]([C@@H]([C@@H]([C@@H](O2)C)O)O)NC)cc2c(c1)cccc2	GUCCGAUGCGUGUUUCACGCAUCGGAC	Neocarzinostatin_chromophore_derivative_5	Target_lig_152	RNA XV	Target_125	5.309803919971149
787	c12c(cc(cc1)OC)[C@@]1(C(=O)C=C2)C=C[C@H]2[C@H]1c1c([C@@H]2O[C@@H]2[C@H]([C@@H]([C@@H]([C@@H](O2)C)O)O)NC)cc2c(c1)cccc2	GUCCGAUGCGUGUUUCACGCAUCGGAC	Neocarzinostatin_chromophore_derivative_6	Target_lig_153	RNA XV	Target_125	4.920818753955238
788	c12c(cc(cc1)OC)[C@@]1(C(=O)C=C2)C=C[C@@H]2[C@@H]1c1c([C@H]2O[C@@H]2[C@H]([C@@H]([C@@H]([C@@H](O2)C)O)O)NC)cc2c(c1)cccc2	GUCCGAUGCGUGUUUUCACGCAGUUCGGAC	Neocarzinostatin_chromophore_derivative_5	Target_lig_152	RNA XVII	Target_126	5.795880017344408
789	c12c(cc(cc1)OC)[C@@]1(C(=O)C=C2)C=C[C@H]2[C@H]1c1c([C@@H]2O[C@@H]2[C@H]([C@@H]([C@@H]([C@@H](O2)C)O)O)NC)cc2c(c1)cccc2	GUCCGAUGCGUGUUUUCACGCAGUUCGGAC	Neocarzinostatin_chromophore_derivative_6	Target_lig_153	RNA XVII	Target_126	5.552841968665778
790	CC1C(C(C(O1)OC2C(C(C(C(C2O)O)N=C(N)N	GAGGGUGGAACCGCGCUUCGGCGUCCCUC	Streptomycin	Target_lig_63	T box antiterminator RNA	Target_112	3.102372908709956

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	)O)N=C(N)N)OC3C(C(C(C(O3)CO)O)O)NC)(C=O)O						
791	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	GAGGGUGGAACCGCGCUUCGGCGUCCCUC	Paromomycin_mol_mol	Target_lig_1116	T box antiterminator RNA	Target_112	4.30102999566398
792	[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)N)O[C@@H]1[C@H]([C@@H]([C@H]([C@@H](O1)CNc1c2ccccc2nc2c1cccc2)O)N)O	GAGGGUGGAACCGCGCUUCGGCGUCCCUC	Tobramycin	Target_lig_540	T box antiterminator RNA	Target_112	4.420216403383319
793	C1C(C(C(C(C1N)OC2C(C(C(O2)CN)O)O)O)O)OC3C(C(C(C(O3)CO)O)N)O)N	GAGGGUGGAACCGCGCUUCGGCGUCCCUC	Kanamycin A	Target_lig_7	T box antiterminator RNA	Target_112	3.677780705266608
794	C1C(C(C(C(C1N)OC2C(C(C(O2)CO)O)N)O)O)OC3C(C(C(C(O3)CN)O)O)N)N	GAGGGUGGAACCGCGCUUCGGCGUCCCUC	KANAMYCIN B	Target_lig_8	T box antiterminator RNA	Target_112	3.823908740944432
795	C1C(C(C(C(C1N)OC2C(C(C(O2)CN)O)O)N)OC3C(C(C(O3)CO)OC4C(C(C(C(O4)CN)O)O)N)O)O)N	GAGGGUGGAACCGCGCUUCGGCGUCCCUC	Neomycin_B	Target_lig_1246	T box antiterminator RNA	Target_112	5.070581074285571
796	CC1(COC(C(C1NC)O)OC2C(CC(C(C2O)OC3C(CCC(O3)CN)N)N)N)O	GAGGGUGGAACCGCGCUUCGGCGUCCCUC	gentamicin_mol_c	Target_lig_76	T box antiterminator RNA	Target_112	3.920818753955237
797	C1C(C(C(C(C1NC(=O)C(CCN)O)OC2C(C(C(O2)CO)O)N)O)O)OC3C(C(C(C(O3)CN)O)O)O)N	GAGGGUGGAACCGCGCUUCGGCGUCCCUC	Amikacin	Target_lig_175	T box antiterminator RNA	Target_112	3.119186407719 21
801	CC1CC(=O)C2(C(O1)OC3C(CC(C(C3O2)NC)O)NC)O)O	AUUUUUCCUCGAACUUGGCGGAACGCAGAAAAAU	Spectinomycin	Target_lig_75	SLI of Rep A	Target_127	5.397940008667204
802	CNC1CC(C(C(C1O)OC2C3C(C(C(O2)CO)O)OC4(O3)C(C(C(C(O4)C(CO)N)O)O)O)O)N	AUUUUUCCUCGAACUUGGCGGAACGCAGAAAAAU	Hygromycin_B	Target_lig_3	SLI of Rep A	Target_127	5.397940008667204
803	C1C(C(C(C(C1	AUUUUUCCUCGAAC	Neomycin	Target_lig_4	SLI of Rep A	Target_127	7.0969100130

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	N)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	UUGGCGGAACGCAGAAAAAU					0806
804	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	AUUUUUCCUCGAACUUGGCGGAACGCAGAAAAAU	Paromomycin_mol_mol	Target_lig_1116	SLI of Rep A	Target_127	7.397940008667204
805	[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)CNc1c2cccc2nc2c1cccc2)O)N)O	AUUUUUCCUCGAACUUGGCGGAACGCAGAAAAAU	Tobramycin	Target_lig_540	SLI of Rep A	Target_127	7.397940008667204
806	C1C(C(C(C(C1N)OC2C(C(C(O2)CN)O)O)O)O)OC3C(C(C(C(O3)CO)O)N)O)N	AUUUUUCCUCGAACUUGGCGGAACGCAGAAAAAU	Kanamycin A	Target_lig_7	SLI of Rep A	Target_127	6.769551078622173
807	C1C(C(C(C(C1N)OC2C(C(C(O2)CO)O)N)O)O)OC3C(C(C(C(O3)CN)O)O)N)N	AUUUUUCCUCGAACUUGGCGGAACGCAGAAAAAU	KANAMYCIN B	Target_lig_8	SLI of Rep A	Target_127	6.958607314841177
808	CC1(COC(C(C1NC)O)OC2C(CC(C(C2O)OC3C(CC=C(O3)CN)N)N)N)O	AUUUUUCCUCGAACUUGGCGGAACGCAGAAAAAU	sisomicin	Target_lig_10	SLI of Rep A	Target_127	7.522878745280034
809	C1C(C(C(C(C1NC(=O)C(CCN)O)OC2C(C(C(C(O2)CO)O)N)O)O)OC3C(C(C(C(O3)CN)O)O)O)N	AUUUUUCCUCGAACUUGGCGGAACGCAGAAAAAU	Amikacin	Target_lig_175	SLI of Rep A	Target_127	7.096910013000806
810	CC1(COC(C(C1NC)O)OC2C(CC(C(C2O)OC3C(CCC(O3)CN)N)N)N)O	AUUUUUCCUCGAACUUGGCGGAACGCAGAAAAAU	gentamicin_mol	Target_lig_76	SLI of Rep A	Target_127	7.096910013000806
811	C1C(C(C(C(C1NC(=O)C(CCN)O)O)OC2C(C(C(O2)CO)O)O)OC3C(C(C(C(O3)CN)O)O)N)N	AUUUUUCCUCGAACUUGGCGGAACGCAGAAAAAU	Butirosin	Target_lig_220	SLI of Rep A	Target_127	6.698970004336602
812	C1C(C(C(C(C1N)OC2C(C(C(O2)CN)O)O)N)OC3C(C(C(O3)CO)OC4C(C(C(	CCCCCCCGCCGCGCCAUGCCUGUGGCCGGUCGG	Neomycin	Target_lig_4	Thymidylate synthase m-RNA	Target_63	6.056505484093 9

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	C(O4)CN)O)O)N)O)O)N						
813	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	CCCCCCCGCCGCGCCAUGCCUGUGGCCGGUCGG	Paromomycin_mol_mol	Target_lig_1116	Thymidylate synthase m-RNA	Target_63	5.634324859544408
814	[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)N)O[C@@H]1[C@H]([C@@H]([C@H]([C@@H](O1)CNc1c2ccccc2nc2c1cccc2)O)N)O	CCCCCCCGCCGCGCCAUGCCUGUGGCCGGUCGG	Tobramycin	Target_lig_540	Thymidylate synthase m-RNA	Target_63	5.6929320493387
815	C1C(C(C(C(C1N)OC2C(C(C(O2)CO)O)N)O)O)OC3C(C(C(C(O3)CN)O)O)N)N	CCCCCCCGCCGCGCCAUGCCUGUGGCCGGUCGG	KANAMYCIN B	Target_lig_8	Thymidylate synthase m-RNA	Target_63	5.660548558669356
816	CC1(COC(C(C1NC)O)OC2C(CC(C(C2O)OC3C(CCC(O3)CN)N)N)N)O	CCCCCCCGCCGCGCCAUGCCUGUGGCCGGUCGG	gentamicin_mol	Target_lig_76	Thymidylate synthase m-RNA	Target_63	5.565750547603 53
817	CC1C(C(C(O1)OC2C(C(C(C(2O)O)N=C(N)N)O)N=C(N)N)OC3C(C(C(C(O3)CO)O)O)NC)(C=O)O	GGCUGACCAUCAAUAAGGAAGAAGCCCUUCAGCGGCCAGUA	Streptomycin	Target_lig_63	Bcr-Abl m-RNA	Target_64	4.698970004336 02
818	CC1CC(=O)C2(C(O1)OC3C(CC(C(C3O2)NC)O)NC)O)O	GGCUGACCAUCAAUAAGGAAGAAGCCCUUCAGCGGCCAGUA	Spectinomycin	Target_lig_75	Bcr-Abl m-RNA	Target_64	4
819	CNC1CC(C(C(C1O)OC2C3C(C(C(O2)CO)O)OC4(O3)C(C(C(C(O4)C(CO)N)O)O)O)O)N	GGCUGACCAUCAAUAAGGAAGAAGCCCUUCAGCGGCCAGUA	Hygromycin_B	Target_lig_3	Bcr-Abl m-RNA	Target_64	4
820	C1C(C(C(C(C1N)OC2C(C(C(O2)CN)O)O)N)OC3C(C(C(O3)CO)OC4C(C(C(C(O4)CN)O)O)N)O)O)N	GGCUGACCAUCAAUAAGGAAGAAGCCCUUCAGCGGCCAGUA	Neomycin	Target_lig_4	Bcr-Abl m-RNA	Target_64	5.823908740944432
821	C1C(C(C(C(C1N)OC2C(C(C(O2)CO)O)O)N)OC3C(C(C(O3)CO)OC4C(C(C(C(O4)CN)O)O)N)O)O)N	GGCUGACCAUCAAUAAGGAAGAAGCCCUUCAGCGGCCAGUA	Paromomycin_mol_mol	Target_lig_1116	Bcr-Abl m-RNA	Target_64	5.769551078621 73
822	CNC1C(C2C(CC(C(O2)OC3C(	GGCUGACCAUCAAUAAGGAAGAAGCCCU	apramycin	Target_lig_79	Bcr-Abl m-RNA	Target_64	4.698970004336 02

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	CC(C(C3O)O)N)N)OC1OC4C(C(C(C(O4)CO)N)O)O)O	UCAGCGGCCAGUA					
823	C1C(C(C(C(C1N)OC2C(C(C(O2)CN)O)O)N)O)O)N	GGCUGACCAUCAAUAAGGAAGAAGCCCUUCAGCGGCCAGUA	Neamine	Target_lig_80	Bcr-Abl m-RNA	Target_64	4.769551078622173
824	CC(C1C(C(C(C(O1)OC2C(CC(C(C2O)OC3C(C(CO3)(C)O)NC)O)N)N)N)O)O)O	GGCUGACCAUCAAUAAGGAAGAAGCCCUUCAGCGGCCAGUA	Geneticin	Target_lig_140	Bcr-Abl m-RNA	Target_64	4.698970004336602
825	[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	GGCUGACCAUCAAUAAGGAAGAAGCCCUUCAGCGGCCAGUA	Tobramycin	Target_lig_540	Bcr-Abl m-RNA	Target_64	5.443697499233271
826	C1C(C(C(C(C1N)OC2C(C(C(O2)CN)O)O)O)O)OC3C(C(C(C(O3)CO)O)N)O)N	GGCUGACCAUCAAUAAGGAAGAAGCCCUUCAGCGGCCAGUA	Kanamycin A	Target_lig_7	Bcr-Abl m-RNA	Target_64	5
827	C1C(C(C(C(C1N)OC2C(C(C(O2)CO)O)N)O)O)OC3C(C(C(C(O3)CN)O)O)N)N	GGCUGACCAUCAAUAAGGAAGAAGCCCUUCAGCGGCCAGUA	KANAMYCIN B	Target_lig_8	Bcr-Abl m-RNA	Target_64	5.602059991327796
828	C1C(C(C(C(C1N)OC2C(C(C(O2)CN)O)O)N)OC3C(C(C(O3)CO)O)O)O)N	GGCUGACCAUCAAUAAGGAAGAAGCCCUUCAGCGGCCAGUA	ribostamycin	Target_lig_9	Bcr-Abl m-RNA	Target_64	4.096910013006806
829	C1C(C(C(C(C1NC(=O)C(CCN)O)OC2C(C(C(O2)CO)O)N)O)O)OC3C(C(C(C(O3)CN)O)O)O)N	GGCUGACCAUCAAUAAGGAAGAAGCCCUUCAGCGGCCAGUA	Amikacin	Target_lig_175	Bcr-Abl m-RNA	Target_64	5
830	CC1(COC(C(C1NC)O)OC2C(CC(C(C2O)OC3C(CCC(O3)CN)N)N)N)O	GGCUGACCAUCAAUAAGGAAGAAGCCCUUCAGCGGCCAGUA	gentamicin_mol	Target_lig_76	Bcr-Abl m-RNA	Target_64	5.522878745228034
831	C1C(C(C(C(C1NC(=O)C(CCN)O)O)OC2C(C(C(O2)CO)O)O)O)OC3C(C(C(C(O3)CN)O)O)N)N	GGCUGACCAUCAAUAAGGAAGAAGCCCUUCAGCGGCCAGUA	Butirosin	Target_lig_220	Bcr-Abl m-RNA	Target_64	4.823908740944432
832	CC1C(C(C(O1)OC2C(C(C(C2O)O)N=C(N)N)O)N=C(N)N)O	GGAUUUAAGCAGAGUUCAAAAGCCCUUCAGCGGCCAGUAG	Streptomycin	Target_lig_63	PAX3-FKHR m-RNA	Target_65	4.602059991327796

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	C3C(C(C(C(O3)CO)O)O)NC)(C=O)O						
833	CC1CC(=O)C2(C(O1)OC3C(C(C(C(C3O2)NC)O)NC)O)O	GGAUUUAAGCAGAGUUCAAAAGCCCUUCAGCGGCCAGUAG	Spectinomycin	Target_lig_75	PAX3-FKHR m-RNA	Target_65	4
834	CNC1CC(C(C(C1O)OC2C3C(C(C(O2)CO)O)OC4(O3)C(C(C(C(O4)C(CO)N)O)O)O)O)N	GGAUUUAAGCAGAGUUCAAAAGCCCUUCAGCGGCCAGUAG	Hygromycin_B	Target_lig_3	PAX3-FKHR m-RNA	Target_65	4
835	C1C(C(C(C(C1N)OC2C(C(C(O2)CN)O)O)N)OC3C(C(C(O3)CO)OC4C(C(C(C(O4)CN)O)O)N)O)O)N	GGAUUUAAGCAGAGUUCAAAAGCCCUUCAGCGGCCAGUAG	Neomycin	Target_lig_4	PAX3-FKHR m-RNA	Target_65	5.823908740944432
836	C1C(C(C(C(C1N)OC2C(C(C(O2)CO)O)O)N)OC3C(C(C(O3)CO)OC4C(C(C(C(O4)CN)O)O)N)O)O)N	GGAUUUAAGCAGAGUUCAAAAGCCCUUCAGCGGCCAGUAG	Paromomycin_mol_mol	Target_lig_1116	PAX3-FKHR m-RNA	Target_65	5.744727494889669
837	CNC1C(C2C(CC(C(O2)OC3C(CC(C(C3O)O)N)N)N)OC1OC4C(C(C(C(O4)CO)N)O)O)O	GGAUUUAAGCAGAGUUCAAAAGCCCUUCAGCGGCCAGUAG	apramycin	Target_lig_79	PAX3-FKHR m-RNA	Target_65	4.698970004336020
838	C1C(C(C(C(C1N)OC2C(C(C(O2)CN)O)O)N)O)O)N	GGAUUUAAGCAGAGUUCAAAAGCCCUUCAGCGGCCAGUAG	Neamine	Target_lig_80	PAX3-FKHR m-RNA	Target_65	4.698970004336020
839	CC(C1C(C(C(C(O1)OC2C(CC(C(C2O)OC3C(C(C(CO3)(C)O)NC)O)N)N)N)O)O)O	GGAUUUAAGCAGAGUUCAAAAGCCCUUCAGCGGCCAGUAG	Geneticin	Target_lig_140	PAX3-FKHR m-RNA	Target_65	4.522878745280340
840	[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)N)O[C@@H]1[C@H]([C@@H]([C@H]([C@@H](O1)CNc1c2ccccc2nc2c1cccc2)O)N)O	GGAUUUAAGCAGAGUUCAAAAGCCCUUCAGCGGCCAGUAG	Tobramycin	Target_lig_540	PAX3-FKHR m-RNA	Target_65	5.744727494889669
841	C1C(C(C(C(C1N)OC2C(C(C(O2)CN)O)O)O)O)OC3C(C(C(C(O3)CO)O)N)O)N	GGAUUUAAGCAGAGUUCAAAAGCCCUUCAGCGGCCAGUAG	Kanamycin A	Target_lig_7	PAX3-FKHR m-RNA	Target_65	4.698970004336020
842	C1C(C(C(C(C1N)OC2C(C(C(O2)CO)O)N)O)O)OC3C(C(C(C	GGAUUUAAGCAGAGUUCAAAAGCCCUUCAGCGGCCAGUAG	KANAMYCIN B	Target_lig_8	PAX3-FKHR m-RNA	Target_65	5.301029995636398

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	(O3)CN)O)O)N)N						
843	C1C(C(C(C(C1N)OC2C(C(C(O2)CN)O)O)N)OC3C(C(C(O3)CO)O)O)O)N	GGAUUUAAGCAGAGUUCAAAAGCCCUUCAGCGGCCAGUAG	ribostamycin	Target_lig_9	PAX3-FKHR m-RNA	Target_65	4.045757490560 68
844	C1C(C(C(C(C1NC(=O)C(CCN)O)OC2C(C(C(O2)CO)O)N)O)O)OC3C(C(C(C(O3)CN)O)O)O)N	GGAUUUAAGCAGAGUUCAAAAGCCCUUCAGCGGCCAGUAG	Amikacin	Target_lig_175	PAX3-FKHR m-RNA	Target_65	4.823908740944 32
845	CC1(COC(C(C1NC)O)OC2C(CC(C(C2O)OC3C(CCC(O3)CN)N)N)N)O	GGAUUUAAGCAGAGUUCAAAAGCCCUUCAGCGGCCAGUAG	gentamicin_mol	Target_lig_76	PAX3-FKHR m-RNA	Target_65	5.221848749616 36
846	C1C(C(C(C(C1NC(=O)C(CCN)O)O)OC2C(C(C(O2)CO)O)O)OC3C(C(C(C(O3)CN)O)O)N)N	GGAUUUAAGCAGAGUUCAAAAGCCCUUCAGCGGCCAGUAG	Butirosin	Target_lig_220	PAX3-FKHR m-RNA	Target_65	4.602059991327 96
871	c12c(c(c3c(n1)ccc3)Nc1ccc(cc1)CNC(=O)[C@H](C(C)C)NC(=O)[C@H](NC(=O)CCCN)CO)cccc2C(=O)N[C@@H](C(=O)N)CCCNC(=N)N	GGGCGGUUUUUCGAAGCUUGAGUCUCGUAGAGGGCUUCGGCCUGGCGAAUUAGACUGACGCUC	HTP 20	Target_lig_527	RNA aptamer_1	Target_56	7.677780705266 608
872	c12c(c(c3c(n1)ccc3)Nc1ccc(cc1)CNC(=O)[C@H](C(C)C)NC(=O)[C@H](NC(=O)CCCN)CO)cccc2C(=O)N[C@@H](C(=O)N)CCCNC(=N)N	GGGCGGUUUUUCGAAGCUUGAGUCUUACGUAGAGGGCUUCGGCCUGGCGAUAGACUGACGCUC	HTP 20	Target_lig_527	RNA aptamer_2	Target_57	6.838631997765 03
873	c12c(c(c3c(n1)ccc3)Nc1ccc(cc1)CNC(=O)[C@H](C(C)C)NC(=O)[C@H](NC(=O)CCCN)CO)cccc2C(=O)N[C@@H](C(=O)N)CCCNC(=N)N	GGGCGGUUUUUCGAAGCUUGAGUCUCUCGUAGAGGGCUUCGGCCUGGGCGCAAGACUGACGCUC	HTP 20	Target_lig_527	RNA aptamer_3	Target_58	6.113509274827 52
874	c12c(c(c3c(n1)ccc3)Nc1ccc(cc1)CNC(=O)[C@H](C(C)C)NC(=O)[C@H](NC(=O)CCCN)CO)cccc2C(=O)N[C@@H](C(=O)N)CCCNC(=N)N	GGGCGGUUUUUCGAAGCUUGAGUCUCGUAGAGGGCUUCGGCCUGGCGUAGACUGACGCUC	HTP 20	Target_lig_527	RNA aptamer_4	Target_59	7.045757490560 68

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
901	COC1=CC=C(C=C1)N2[C@@H]([C@H](OC2=O)COC(=O)CC3=CC=CC=C3)CC4=CC=CC=C4	GAGGGUGGAACCGCGCUUCGGCGUCCCUC	Oxazolidinone 2	Target_lig_543	T-box RNA	Target_113	5.468521082958774
902	C1=CC=C(C=C1)C[C@@H]2[C@H](OC(=O)N2)COC(=O)CC3=CC=CC=C3	GAGGGUGGAACCGCGCUUCGGCGUCCCUC	Oxazolidinone 6	Target_lig_544	T-box RNA	Target_113	5.045757490560 68
903	COC1=CC=C(C=C1)N2[C@@H]([C@H](OC2=O)COC(=O)CC3=CC=CC=C3)CC4=CC=CC=C4	GAGGGUGGAAUCGCGCUUCGGCGUCCCUC	Oxazolidinone 2	Target_lig_543	T-box C11U	Target_114	4.602059991327796
904	C1=CC=C(C=C1)C[C@@H]2[C@H](OC(=O)N2)COC(=O)CC3=CC=CC=C3	GAGGGUGGAAUCGCGCUUCGGCGUCCCUC	Oxazolidinone 6	Target_lig_544	T-box C11U	Target_114	3.903089986991 94
905	COC(=O)C1C(CCC2C1CC3C4=C(CCN3C2)C5=CC=CC=C5N4)O	UUCCUGCUUCAACAGUGCUUGGACGGAA	Yohimbine	Target_lig_193	fIIRE	Target_132	5.408935392 9735
906	COC(=O)C1C(CCC2C1CC3C4=C(CCN3C2)C5=CC=CC=C5N4)O	ACAUUACCGGGAGCAGUGUCUUCUGUAAUGU	Yohimbine	Target_lig_193	TfR_IRE	Target_133	5.136677139879954
907	COC(=O)C1C(CCC2C1CC3C4=C(CCN3C2)C5=CC=CC=C5N4)O	ACAUUACCGGGAGCAGUGUCUUCUGUAAUGU	Yohimbine	Target_lig_193	TfR_IRE_C24U	Target_134	5.229147988358786
909	COC(=O)C1C(CCC2C1CC3C4=C(CCN3C2)C5=CC=CC=C5N4)O	GGGCGAAUUGGGUACCGGGCCCCCCC	Yohimbine	Target_lig_193	Yohimbine_XII_RNA	Target_135	5.036212172654444
910	C1[C@@H](N)[C@@H](O)[C@H]([C@@H]([C@H]1N)OCSc1ccnc2c1ccc(c2)C(F)(F)F)O	CGCGCGUGUGCGCG	DOS	Target_lig_383	RNA_XIX	Target_136	3
911	[C@H]1([C@H](OCCCCCCCCCCCCO[C@H]2[C@@H](C[C@H](N)[C@@H](O)[C@H]2O)N)[C@H](O)[C@H]([C@@H](C1)N)O)N	CGCGCGUGUGCGCG	DOS_der_1	Target_lig_546	RNA_XIX	Target_136	4.468521082958774
912	[C@H]1([C@H](OCc2ccc(cc2)CCc2ccc(cc2)CO[C@H]2[C@@H](C[C@H](N)	CGCGCGUGUGCGCG	DOS_der_2	Target_lig_547	RNA_XIX	Target_136	4.795880017344408

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	[C@@H](O)[C@@H]2O)N)[C@@H](O)[C@@H]([C@H](C1)N)O)N						
913	[C@H]1([C@@H]([C@H](O)[C@H]([C@H](C1)N#N)O)OCc1ccc(cc1)c1ccc(cc1)CO[C@H]1[C@H](C[C@@H]([C@@H](O)[C@@H]1O)N#N)N#N)N#N	CGCGCGUGUGCGCG	DOS_der_3	Target_lig_548	RNA_XIX	Target_136	3.602059991327796
914	OCc1ccc(cc1)CCc1ccc(cc1)CO[C@H]1[C@@H](C[C@H](N)[C@@H](O)[C@@H]1O)N	CGCGCGUGUGCGCG	DOS_der_4	Target_lig_549	RNA_XIX	Target_136	3
915	C1[C@@H](N)[C@@H](O)[C@H]([C@@H]([C@H]1N)OCSc1ccnc2c1ccc(c2)C(F)(F)F)O	CGCGCAGUGUAGCGCG	DOS	Target_lig_383	RNA_XX	Target_137	3
916	[C@H]1([C@H](OCCCCCCCCCCCCCO[C@H]2[C@@H](C[C@H](N)[C@@H](O)[C@H]2O)N)[C@H](O)[C@H]([C@@H](C1)N)O)N	CGCGCAGUGUAGCGCG	DOS_der_1	Target_lig_546	RNA_XX	Target_137	4.958607314884177
917	[C@H]1([C@H](OCc2ccc(cc2)CCc2ccc(cc2)CO[C@H]2[C@@H](C[C@H](N)[C@@H](O)[C@@H]2O)N)[C@@H](O)[C@@H]([C@H](C1)N)O)N	CGCGCAGUGUAGCGCG	DOS_der_2	Target_lig_547	RNA_XX	Target_137	5.221848749616636
918	[C@H]1([C@@H]([C@H](O)[C@H]([C@H](C1)N#N)O)OCc1ccc(cc1)c1ccc(cc1)CO[C@H]1[C@H](C[C@@H]([C@@H](O)[C@@H]1O)N#N)N#N)N#N	CGCGCAGUGUAGCGCG	DOS_der_3	Target_lig_548	RNA_XX	Target_137	3.602059991327796
919	OCc1ccc(cc1)CCc1ccc(cc1)CO[C@H]1[C@@H](C[C@H](N)[C@@H](O)[C@@H]1O)N	CGCGCAGUGUAGCGCG	DOS_der_4	Target_lig_549	RNA_XX	Target_137	3
920	C1[C@@H](N)	CGCGCAGUAGUAGC	DOS	Target_lig_38	RNA_XXI	Target_138	3

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	[C@@H](O)[C@H]([C@@H]([C@H]1N)OCSc1ccnc2c1ccc(c2)C(F)(F)F)O	GCG		3			
921	[C@H]1([C@H](OCCCCCCCCCCCCCO[C@H]2[C@@H](C[C@H](N)[C@@H](O)[C@H]2O)N)[C@H](O)[C@H]([C@@H](C1)N)O)N	CGCGCAGUAGUAGCGCG	DOS_der_1	Target_lig_546	RNA_XXI	Target_138	4.958607314884177
922	[C@H]1([C@H](OCc2ccc(cc2)CCc2ccc(cc2)CO[C@H]2[C@@H](C[C@H](N)[C@@H](O)[C@@H]2O)N)[C@@H](O)[C@@H]([C@H](C1)N)O)N	CGCGCAGUAGUAGCGCG	DOS_der_2	Target_lig_547	RNA_XXI	Target_138	5.221848749616636
923	[C@H]1([C@@H]([C@H](O)[C@H]([C@H](C1)N#N)O)OCc1ccc(cc1)c1ccc(cc1)CO[C@H]1[C@H](C[C@@H]([C@@H](O)[C@@H]1O)N#N)N#N)N#N	CGCGCAGUAGUAGCGCG	DOS_der_3	Target_lig_548	RNA_XXI	Target_138	3.602059991327796
924	OCc1ccc(cc1)CCc1ccc(cc1)CO[C@H]1[C@@H](C[C@H](N)[C@@H](O)[C@@H]1O)N	CGCGCAGUAGUAGCGCG	DOS_der_4	Target_lig_549	RNA_XXI	Target_138	3
925	C1[C@@H](N)[C@@H](O)[C@H]([C@@H]([C@H]1N)OCSc1ccnc2c1ccc(c2)C(F)(F)F)O	CGCGCAGUCAGUAGCGCG	DOS	Target_lig_383	RNA_XXII	Target_139	3
926	[C@H]1([C@H](OCCCCCCCCCCCCCO[C@H]2[C@@H](C[C@H](N)[C@@H](O)[C@H]2O)N)[C@H](O)[C@H]([C@@H](C1)N)O)N	CGCGCAGUCAGUAGCGCG	DOS_der_1	Target_lig_546	RNA_XXII	Target_139	5.096910013008806
927	[C@H]1([C@H](OCc2ccc(cc2)CCc2ccc(cc2)CO[C@H]2[C@@H](C[C@H](N)[C@@H](O)[C@@H]2O)N)[C@@H](O)	CGCGCAGUCAGUAGCGCG	DOS_der_2	Target_lig_547	RNA_XXII	Target_139	5.221848749616636

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	[C@@H]([C@H](C1)N)O)N						
928	[C@H]1([C@@H]([C@H](O)[C@H]([C@H](C1)N#N)O)OCc1ccc(cc1)c1ccc(cc1)CO[C@H]1[C@H](C[C@@H]([C@@H](O)[C@@H]1O)N#N)N#N)N#N	CGCGCAGUCAGUAGCGCG	DOS_der_3	Target_lig_548	RNA_XXII	Target_139	3.602059991327796
929	OCc1ccc(cc1)CCc1ccc(cc1)CO[C@H]1[C@@H](C[C@H](N)[C@@H](O)[C@@H]1O)N	CGCGCAGUCAGUAGCGCG	DOS_der_4	Target_lig_549	RNA_XXII	Target_139	3
930	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	GGGGCGAAAGCCUUAU	Neomycin_B	Target_lig_1246	GNRA tetraloop construct XVIII	Target_141	4.522878745280034
931	C1=NC2=NC=NC(=C2N1)N	CUCGGUACCGCAAAAGCGUUUUUCGCAUACCUAUUCGUUAUAGGUCGAUUGUACCGAG	Adenine	Target_lig_165	Spiegelmer L-A42d RNA (58 mer)	Target_142	1.787812395596604
932	C1=NC(=C2C(=N1)N(C=N2)[C@H]3[C@@H]([C@@H]([C@H](O3)CO)O)O)N	CUCGGUACCGCAAAAGCGUUUUUCGCAUACCUAUUCGUUAUAGGUCGAUUGUACCGAG	D_Adenosine	Target_lig_551	Spiegelmer L-A42d RNA (58 mer)	Target_142	5.657577319177779
933	CO[C@@H]1[C@H](O[C@H]([C@@H]1O)N2C=NC3=C(N=CN=C32)N)CO	CUCGGUACCGCAAAAGCGUUUUUCGCAUACCUAUUCGUUAUAGGUCGAUUGUACCGAG	3-O-methyl-D-Adenosine	Target_lig_552	Spiegelmer L-A42d RNA (58 mer)	Target_142	5.853871964321762
934	C1=NC2=C(N1[C@H]3[C@@H]([C@@H]([C@H](O3)CO)O)O)N=C(NC2=O)N	CUCGGUACCGCAAAAGCGUUUUUCGCAUACCUAUUCGUUAUAGGUCGAUUGUACCGAG	D-guanosine	Target_lig_553	Spiegelmer L-A42d RNA (58 mer)	Target_142	5.318758762624412
935	C1[C@H](O[C@H]([C@@H]1O)N2C=NC3=C(N=CN=C32)N)CO	CUCGGUACCGCAAAAGCGUUUUUCGCAUACCUAUUCGUUAUAGGUCGAUUGUACCGAG	3-deoxy-D-Adenosine	Target_lig_554	Spiegelmer L-A42d RNA (58 mer)	Target_142	5.096910013008806
936	C1[C@@H]([C@H](O[C@H]1N2C=NC3=C(N=CN=C32)N)CO)O	CUCGGUACCGCAAAAGCGUUUUUCGCAUACCUAUUCGUUAUAGGUCGAUUGUACCGAG	2-deoxy-D-Adenosine	Target_lig_555	Spiegelmer L-A42d RNA (58 mer)	Target_142	2.853871964321762
937	C1=CN(C(=O)NC1=O)[C@H]2[C@@H]([C@@H]([C@H](O2)CO)O)O	CUCGGUACCGCAAAAGCGUUUUUCGCAUACCUAUUCGUUAUAGGUCGAUUGUACCGAG	D-uridine	Target_lig_556	Spiegelmer L-A42d RNA (58 mer)	Target_142	2.638272163981241
938	C1=NC(=C2C(=N1)N(C=N2)[C@H]3[C@@	CUCGGUACCGCAAAAGCGUUUUUCGCAUACCUAUUCGUUAUA	D-adenosine triphosphate	Target_lig_557	Spiegelmer L-A42d RNA (58 mer)	Target_142	2.537602002101104

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	H]([C@@H]([C@H](O3)COP(=O)(O)OP(=O)(O)OP(=O)(O)O)O)N	GGUCGAUUGUACCGAG					
939	C1=CN(C(=O)N=C1N)[C@H]2[C@@H]([C@@H]([C@H](O2)CO)O)O	CUCGGUACCGCAAAAGCGUUUUUCGCAUACCUAUUCGUUAUAGGUCGAUUGUACCGAG	D-Cytidine	Target_lig_558	Spiegelmer L-A42d RNA (58 mer)	Target_142	2.20760831050175
940	CO[C@@H]1[C@@H]([C@H](O[C@H]1N2C=NC3=C(N=CN=C32)N)CO)O	CUCGGUACCGCAAAAGCGUUUUUCGCAUACCUAUUCGUUAUAGGUCGAUUGUACCGAG	2-O-methyl-D-Adenosine	Target_lig_559	Spiegelmer L-A42d RNA (58 mer)	Target_142	1.88941028970075
941	C1=NC(=C2C(=N1)N(C=N2)[C@@H]3[C@H]([C@H]([C@@H](O3)CO)O)O)N	CUCGGUACCGCAAAAGCGUUUUUCGCAUACCUAUUCGUUAUAGGUCGAUUGUACCGAG	L_Adenosine	Target_lig_560	Spiegelmer L-A42d RNA (58 mer)	Target_142	1.69464863055338
942	CN1C2=C(C(=O)N(C1=O)C)NC=N2	GGUGAUACCAGCCGAAAGGCCCUUGGCAGCACC	Theophylline	Target_lig_154	T alpha aptamer	Target_60	6.823908740944432
943	N=C1N[C@@H]2CS[C@@H]([C@H]2N1)CCCCC(=O)NCCOCCOCCNC(=O)CCCC[C@H]1[C@@H]2NC(=N)N[C@H]2CS1	GGACCGUCAGAGGACACGGUUAAAAAGUCCUCU	biotin dimer	Target_lig_561	B alpha aptamer	Target_61	5.677780705266608
944	N=C1N[C@H]2CS[C@H]([C@@H]2N1)CCCCC(=O)NCCOCCOCCN	GGACCGUCAGAGGACACGGUUAAAAAGUCCUCU	biotin PEO Amine	Target_lig_562	B alpha aptamer	Target_61	4.853871964321776
947	c12cc(ccc1c(c1c(n2)ccc(c1)OC)NCCCCc1c(nc(nc1N)N)N)Cl	CUGGCCUGGCGCGCCUGCCCAG	MBNL CCUG ligand 3	Target_lig_563	RNA B	Target_144	4.585026652029218
948	c12cc(ccc1c(c1c(n2)ccc(c1)OC)NCCCCc1c(nc(nc1N)N)N)Cl	CUGGCUGCGCGCGCCGCCAG	MBNL CCUG ligand 3	Target_lig_563	RNA C	Target_145	3.782516055778609
970	C1(=O)O[C@H]([C@H](N1)CN1CCN(CC1)c1ccccc1)COC(=O)Cc1ccccc1	GAGGGUGGAACCGCGCUUCGGCGUCCCUC	racemic_oxazolidinones	Target_lig_585	Antiterminator model RNA AM1A	Target_147	4.886056647693316
971	C1(=O)O[C@H]([C@H](N1)CN1CCN(CC1)c1ccccc1)COC(=O)Nc1ccc(cc1)C(=O)C	GAGGGUGGAACCGCGCUUCGGCGUCCCUC	racemic_oxazolidinones_2	Target_lig_586	Antiterminator model RNA AM1A	Target_147	5.397940008677204
1006	COC1=C(C=C(C=C1)NCC2=CC=C(S2)[N+](=O)[O-])OC	AUCACCUCCUUAUAAGGAGGUGAU	SL3 RNA_ligand4	Target_lig_607	Double stranded RNA seq	Target_149	5.494850021680009
1007	C1=CC=C2C=C(C=CC2=C1)/C=C/3\C(=O)NC(=S)N	AUCACCUCCUUAUAAGGAGGUGAU	SL3 RNA_ligand5	Target_lig_608	Double stranded RNA seq	Target_149	5.086186147661628

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	3						
1008	C1=CC=C(C=C1)C[N+]2=CC=C(C=C2)C(=O)N/N=C\C3=CC=C(C=C3)Br	AUCACCUCCUUAUAAGGAGGUGAU	SL3 RNA_ligand6	Target_lig_609	Double stranded RNA seq	Target_149	5.080921907623 93
1009	CC1CCN(CC1)C2=CC=C(C=C2)N	AUCACCUCCUUAUAAGGAGGUGAU	SL3 RNA_ligand7	Target_lig_610	Double stranded RNA seq	Target_149	3.723538195826 76
1010	C1=CC2=C(C=CC(=C2N=C1)SCCO)[N+](=O)[O-]	AUCACCUCCUUAUAAGGAGGUGAU	SL3 RNA_ligand9	Target_lig_612	Double stranded RNA seq	Target_149	5.659555885159 88
1011	C1=CC=C(C(=C1)/C=C\2/C(=O)N(C(=O)N2)/C=C/3\C(=O)C4=CC=CC=C4OC3=O)O	AUCACCUCCUUAUAAGGAGGUGAU	SL3 RNA_ligand10	Target_lig_613	Double stranded RNA seq	Target_149	5.292429823902 06
1012	C1=CC=C2C(=C1)C(=O)C3=C(C2=O)C(=C(C=C3NC4=CC=C(C=C4)S(=O)(=O)N)S(=O)(=O)O)N	AUCACCUCCUUAUAAGGAGGUGAU	SL3 RNA_ligand11	Target_lig_614	Double stranded RNA seq	Target_149	4.950781977329 82
1013	c12ccccc1C(=O)[C@H]1[C@H](C2=O)C(=CC=C1NCCO)NCCO	AUCACCUCCUUAUAAGGAGGUGAU	SL3 RNA_ligand12	Target_lig_615	Double stranded RNA seq	Target_149	5.075720713938 12
1014	CC1=CC=CN2C1=NC3=C(C2=O)C=C(C(=N)N3CCCO)C(=O)NC	AUCACCUCCUUAUAAGGAGGUGAU	SL3 RNA_ligand13	Target_lig_616	Double stranded RNA seq	Target_149	4.920818753955 238
1015	CN1CCN(CC1)CCCN2C3=CC=CC=C3SC4=C2C=C(C=C4)C(F)(F)F	AUCACCUCCUUAUAAGGAGGUGAU	SL3 RNA_ligand17	Target_lig_620	Double stranded RNA seq	Target_149	2.955068453855 084
1016	COC1=C(C=C(C=C1)NCC2=CC=C(S2)[N+](=O)[O-])OC	AUCACCUCCUUA	SL3 RNA_ligand4	Target_lig_607	single stranded RNA seq	Target_150	5.657577319177 779
1017	C1=CC=C2C=C(C=CC2=C1)/C=C/3\C(=O)NC(=S)N3	AUCACCUCCUUA	SL3 RNA_ligand5	Target_lig_608	single stranded RNA seq	Target_150	5.022276394711 115
1018	C1=CC=C(C=C1)C[N+]2=CC=C(C=C2)C(=O)N/N=C\C3=CC=C(C=C3)Br	AUCACCUCCUUA	SL3 RNA_ligand6	Target_lig_609	single stranded RNA seq	Target_150	4.928117992693 88
1019	CC1CCN(CC1)C2=CC=C(C=C2)N	AUCACCUCCUUA	SL3 RNA_ligand7	Target_lig_610	single stranded RNA seq	Target_150	3.552841968657 78
1020	C1=CC2=C(C=CC(=C2N=C1)SCCO)[N+](=O)[O-]	AUCACCUCCUUA	SL3 RNA_ligand9	Target_lig_612	single stranded RNA seq	Target_150	5.698970004336 02
1021	C1=CC=C(C(=	AUCACCUCCUUA	SL3	Target_lig_61	single stranded	Target_150	5.3872161432

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	C1)/C=C\2/C(=O)N(C(=O)N2)/C=C/3\C(=O)C4=CC=CC=C4OC3=O)O		RNA_ligand10	3	RNA seq		8026
1022	C1=CC=C2C(=C1)C(=O)C3=C(C2=O)C(=C(C=C3NC4=CC=C(C=C4)S(=O)(=O)N)S(=O)(=O)O)N	AUCACCUCCUUA	SL3 RNA_ligand11	Target_lig_614	single stranded RNA seq	Target_150	5.05060999335509
1023	c12ccccc1C(=O)[C@H]1[C@H](C2=O)C(=CC=C1NCCO)NCCO	AUCACCUCCUUA	SL3 RNA_ligand12	Target_lig_615	single stranded RNA seq	Target_150	4.853871964321 76
1024	CC1=CC=CN2C1=NC3=C(C2=O)C=C(C(=N)N3CCCO)C(=O)NC	AUCACCUCCUUA	SL3 RNA_ligand13	Target_lig_616	single stranded RNA seq	Target_150	5.12493873660 83
1025	CN1CCN(CC1)CCCN2C3=CC=CC=C3SC4=C2C=C(C=C4)C(F)(F)F	AUCACCUCCUUA	SL3 RNA_ligand17	Target_lig_620	single stranded RNA seq	Target_150	3.218963061377887
1030	O1COc2c1cc(C(=O)N1[C@H](C(=O)N[C@H](C(=O)N[C@@H](C(=O)NCCCN)CCCCN)CSSC[C@H](NC(=O)[C@@H]3CCCN3C(=O)c3cc4OCOc4cc3)C(=O)N[C@H](C(=O)NCCCN)CCCCN)CCC1)cc2	CCGCUGCUGCUGCUGCGG	ligand 3-3	Target_lig_621	RNA seq A	Target_151	5.267606240177703
1031	n1c2c(cc(C(=O)N3[C@H](C(=O)N[C@H](C(=O)N[C@@H](C(=O)NCCCN)CCCCN)CSSC[C@H](NC(=O)[C@@H]4CCCN4C(=O)c4cc5c(nc4CC)cccc5)C(=O)N[C@@H](C(=O)NCCCN)CCCCN)CCC3)c1CC)cccc2	CCGCUGCUGCUGCUGCGG	ligand 4-4	Target_lig_622	RNA seq A	Target_151	5.173925197299917
1032	n1c2c(cc(C(=O)N[C@H](C(=O)N[C@@H](C(=O)N[C@H](C(=O)NCCCN)CCCCN)CSSC[C@H](NC(=O)[C@@H]3CCCN3C(=O)c3cc4c(nc3CC)cccc4)C(=O)N[C@@H](C(=O)NCCCN)	CCGCUGCUGCUGCUGCGG	ligand 2-4	Target_lig_623	RNA seq A	Target_151	5.346787486224 66

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	CCCCN)CC(=O)N)c1CC)cccc2						
1033	O1COc2c1cc(C(=O)N1[C@H](C(=O)N[C@@H](C(=O)N[C@H](C(=O)NCCCN)CCCCN)CSSC[C@H](NC(=O)[C@@H]3CCCN3C(=O)c3cc4c(nc3CC)cccc4)C(=O)N[C@@H](C(=O)NCCCN)CCCCN)CCC1)cc2	CCGCUGCUGCUGCUGCGG	ligand 3-4	Target_lig_624	RNA seq A	Target_151	5.387216143280026
1034	O1COc2c1cc(C(=O)N1[C@H](C(=O)N[C@H](C(=O)N[C@@H](C(=O)NCCCN)CCCCN)CSSC[C@H](NC(=O)[C@@H]3CCCN3C(=O)c3cc4OCOc4cc3)C(=O)N[C@H](C(=O)NCCCN)CCCCN)CCC1)cc2	CCGCUGCUGCUGCUGCGG	ligand 3-3	Target_lig_621	RNA seq A (20 x t-RNA)	Target_152	4.853871964321776
1035	n1c2c(cc(C(=O)N3[C@H](C(=O)N[C@H](C(=O)N[C@@H](C(=O)NCCCN)CCCCN)CSSC[C@H](NC(=O)[C@@H]4CCCN4C(=O)c4cc5c(nc4CC)cccc5)C(=O)N[C@@H](C(=O)NCCCN)CCCCN)CCC3)c1CC)cccc2	CCGCUGCUGCUGCUGCGG	ligand 4-4	Target_lig_622	RNA seq A (20 x t-RNA)	Target_152	4.744727494889669
1036	n1c2c(cc(C(=O)N[C@H](C(=O)N[C@@H](C(=O)N[C@H](C(=O)NCCCN)CCCCN)CSSC[C@H](NC(=O)[C@@H]3CCCN3C(=O)c3cc4c(nc3CC)cccc4)C(=O)N[C@@H](C(=O)NCCCN)CCCCN)CC(=O)N)c1CC)cccc2	CCGCUGCUGCUGCUGCGG	ligand 2-4	Target_lig_623	RNA seq A (20 x t-RNA)	Target_152	5
1037	O1COc2c1cc(C(=O)N1[C@H](C(=O)N[C@@H](C(=O)N[C@H](C(=O)NCCCN)CCCCN)CSSC[C@H](NC(=O)[C@@H]3CCCN3C(=O)c3cc4c	CCGCUGCUGCUGCUGCGG	ligand 3-4	Target_lig_624	RNA seq A (20 x t-RNA)	Target_152	5.017728766960643

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	(nc3CC)cccc4)C(=O)N[C@@H](C(=O)NCCCN)CCCCN)CCC1)cc2						
1038	O1COc2c1cc(C(=O)N1[C@H](C(=O)N[C@H](C(=O)N[C@@H](C(=O)NCCCN)CCCCN)CSSC[C@H](NC(=O)[C@@H]3CCCN3C(=O)c3cc4OCOc4cc3)C(=O)N[C@H](C(=O)NCCCN)CCCCN)CCC1)cc2	GGGCUGCUGCUGCUGCUGGGG	ligand 3-3	Target_lig_621	RNA seq B	Target_153	5.602059991327796
1039	n1c2c(cc(C(=O)N3[C@H](C(=O)N[C@H](C(=O)N[C@@H](C(=O)NCCCN)CCCCN)CSSC[C@H](NC(=O)[C@@H]4CCCN4C(=O)c4cc5c(nc4CC)cccc5)C(=O)N[C@@H](C(=O)NCCCN)CCCCN)CCC3)c1CC)cccc2	GGGCUGCUGCUGCUGCUGGGG	ligand 4-4	Target_lig_622	RNA seq B	Target_153	5.677780705266608
1040	n1c2c(cc(C(=O)N[C@H](C(=O)N[C@@H](C(=O)N[C@H](C(=O)NCCCN)CCCCN)CSSC[C@H](NC(=O)[C@@H]3CCCN3C(=O)c3cc4c(nc3CC)cccc4)C(=O)N[C@@H](C(=O)NCCCN)CCCCN)CC(=O)N)c1CC)cccc2	GGGCUGCUGCUGCUGCUGGGG	ligand 2-4	Target_lig_623	RNA seq B	Target_153	5.677780705266608
1041	O1COc2c1cc(C(=O)N1[C@H](C(=O)N[C@@H](C(=O)N[C@H](C(=O)NCCCN)CCCCN)CSSC[C@H](NC(=O)[C@@H]3CCCN3C(=O)c3cc4c(nc3CC)cccc4)C(=O)N[C@@H](C(=O)NCCCN)CCCCN)CCC1)cc2	GGGCUGCUGCUGCUGCUGGGG	ligand 3-4	Target_lig_624	RNA seq B	Target_153	5.721246399047717
1042	O1COc2c1cc(C(=O)N1[C@H](C(=O)N[C@H](C(=O)N[C@@H](C(=O)NCCCN)CCCCN)CSSC[	CCGCUGGGCAACCUGCGG	ligand 3-3	Target_lig_621	RNA seq C	Target_154	5.031517051446077

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	C@H](NC(=O)[C@@H]3CCCN3C(=O)c3cc4OCOc4cc3)C(=O)N[C@H](C(=O)NCCCN)CCCCN)CCC1)cc2						
1043	n1c2c(cc(C(=O)N3[C@H](C(=O)N[C@H](C(=O)N[C@@H](C(=O)NCCCN)CCCCN)CSSC[C@H](NC(=O)[C@@H]4CCCN4C(=O)c4cc5c(nc4CC)cccc5)C(=O)N[C@@H](C(=O)NCCCN)CCCCN)CCC3)c1CC)cccc2	CCGCUGGGCAACCUGCGG	ligand 4-4	Target_lig_622	RNA seq C	Target_154	5.14874165128092
1044	n1c2c(cc(C(=O)N[C@H](C(=O)N[C@@H](C(=O)N[C@H](C(=O)NCCCN)CCCCN)CSSC[C@H](NC(=O)[C@@H]3CCCN3C(=O)c3cc4c(nc3CC)cccc4)C(=O)N[C@@H](C(=O)NCCCN)CCCCN)CC(=O)N)c1CC)cccc2	CCGCUGGGCAACCUGCGG	ligand 2-4	Target_lig_623	RNA seq C	Target_154	5.193820026001611
1045	O1COc2c1cc(C(=O)N1[C@H](C(=O)N[C@@H](C(=O)N[C@H](C(=O)NCCCN)CCCCN)CSSC[C@H](NC(=O)[C@@H]3CCCN3C(=O)c3cc4c(nc3CC)cccc4)C(=O)N[C@@H](C(=O)NCCCN)CCCCN)CCC1)cc2	CCGCUGGGCAACCUGCGG	ligand 3-4	Target_lig_624	RNA seq C	Target_154	5.327902142006428
1046	O1COc2c1cc(C(=O)N1[C@H](C(=O)N[C@H](C(=O)N[C@@H](C(=O)NCCCN)CCCCN)CSSC[C@H](NC(=O)[C@@H]3CCCN3C(=O)c3cc4OCOc4cc3)C(=O)N[C@H](C(=O)NCCCN)CCCCN)CCC1)cc2	CGCGCUGCUGCGCG	ligand 3-3	Target_lig_621	RNA seq D	Target_155	5.124938736608 3
1047	n1c2c(cc(C(=O)N3[C@H](C(=O)N[C@H](C(=O)N[C@@	CGCGCUGCUGCGCG	ligand 4-4	Target_lig_622	RNA seq D	Target_155	5.070581074285571

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	H](C(=O)NCCCN)CCCCN)CSSC[C@H](NC(=O)[C@@H]4CCCN4C(=O)c4cc5c(nc4CC)cccc5)C(=O)N[C@@H](C(=O)NCCCN)CCCCN)CCC3)c1CC)cccc2						
1048	n1c2c(cc(C(=O)N[C@H](C(=O)N[C@@H](C(=O)N[C@H](C(=O)NCCCN)CCCCN)CSSC[C@H](NC(=O)[C@@H]3CCCN3C(=O)c3cc4c(nc3CC)cccc4)C(=O)N[C@@H](C(=O)NCCCN)CCCCN)CC(=O)N)c1CC)cccc2	CGCGCUGCUGCGCG	ligand 2-4	Target_lig_623	RNA seq D	Target_155	5.337242168318 43
1049	O1COc2c1cc(C(=O)N1[C@H](C(=O)N[C@@H](C(=O)N[C@H](C(=O)NCCCN)CCCCN)CSSC[C@H](NC(=O)[C@@H]3CCCN3C(=O)c3cc4c(nc3CC)cccc4)C(=O)N[C@@H](C(=O)NCCCN)CCCCN)CCC1)cc2	CGCGCUGCUGCGCG	ligand 3-4	Target_lig_624	RNA seq D	Target_155	5.221848749616 36
1050	O1COc2c1cc(C(=O)N1[C@H](C(=O)N[C@H](C(=O)N[C@@H](C(=O)NCCCN)CCCCN)CSSC[C@H](NC(=O)[C@@H]3CCCN3C(=O)c3cc4OCOc4cc3)C(=O)N[C@H](C(=O)NCCCN)CCCCN)CCC1)cc2	CCAGCUGGCAACAGCUGG	ligand 3-3	Target_lig_621	RNA seq E	Target_156	4.677780705266 08
1051	n1c2c(cc(C(=O)N3[C@H](C(=O)N[C@H](C(=O)N[C@@H](C(=O)NCCCN)CCCCN)CSSC[C@H](NC(=O)[C@@H]4CCCN4C(=O)c4cc5c(nc4CC)cccc5)C(=O)N[C@@H](C(=O)NCCCN)CCCCN)CCC3)c1CC)cccc2	CCAGCUGGCAACAGCUGG	ligand 4-4	Target_lig_622	RNA seq E	Target_156	4.397940008672 04
1052	n1c2c(cc(C(=O)	CCAGCUGGCAACAG	ligand 2-4	Target_lig_62	RNA seq E	Target_156	4.7099653886

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	N[C@H](C(=O)N[C@@H](C(=O)N[C@H](C(=O)NCCCN)CCCCN)CSSC[C@H](NC(=O)[C@@H]3CCCN3C(=O)c3cc4c(nc3CC)cccc4)C(=O)N[C@@H](C(=O)NCCCN)CCCCN)CC(=O)N)c1CC)cccc2	CUGG		3			3748
1053	O1COc2c1cc(C(=O)N1[C@H](C(=O)N[C@@H](C(=O)N[C@H](C(=O)NCCCN)CCCCN)CSSC[C@H](NC(=O)[C@@H]3CCCN3C(=O)c3cc4c(nc3CC)cccc4)C(=O)N[C@@H](C(=O)NCCCN)CCCCN)CCC1)cc2	CCAGCUGGCAACAGCUGG	ligand 3-4	Target_lig_624	RNA seq E	Target_156	4.67778070526608
1054	O1COc2c1cc(C(=O)N1[C@H](C(=O)N[C@H](C(=O)N[C@@H](C(=O)NCCCN)CCCCN)CSSC[C@H](NC(=O)[C@@H]3CCCN3C(=O)c3cc4OCOc4cc3)C(=O)N[C@H](C(=O)NCCCN)CCCCN)CCC1)cc2	GGCCUUCCCACAAGGGAAGGCC	ligand 3-3	Target_lig_621	RNA seq F	Target_157	4.387216143280 26
1055	n1c2c(cc(C(=O)N3[C@H](C(=O)N[C@H](C(=O)N[C@@H](C(=O)NCCCN)CCCCN)CSSC[C@H](NC(=O)[C@@H]4CCCN4C(=O)c4cc5c(nc4CC)cccc5)C(=O)N[C@@H](C(=O)NCCCN)CCCCN)CCC3)c1CC)cccc2	GGCCUUCCCACAAGGGAAGGCC	ligand 4-4	Target_lig_622	RNA seq F	Target_157	4.619788758288839
1056	n1c2c(cc(C(=O)N[C@H](C(=O)N[C@@H](C(=O)N[C@H](C(=O)NCCCN)CCCCN)CSSC[C@H](NC(=O)[C@@H]3CCCN3C(=O)c3cc4c(nc3CC)cccc4)C(=O)N[C@@H](C(=O)NCCCN)CCCCN)CC(=O	GGCCUUCCCACAAGGGAAGGCC	ligand 2-4	Target_lig_623	RNA seq F	Target_157	4.657577319177779

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	)N)c1CC)cccc2						
1057	O1COc2c1cc(C(=O)N1[C@H](C(=O)N[C@@H](C(=O)N[C@H](C(=O)NCCCN)CCCCN)CSSC[C@H](NC(=O)[C@@H]3CCCN3C(=O)c3cc4c(nc3CC)cccc4)C(=O)N[C@@H](C(=O)NCCCN)CCCCN)CCC1)cc2	GGCCUUCCCACAAGGGAAGGCC	ligand 3-4	Target_lig_624	RNA seq F	Target_157	4.795880017344408
1058	[NH3+]CCCC[C@H]([NH3+])C(=O)NC1=CC2=C(C=C1)C1C3=CC=C(NC(=O)[C@@H]([NH3+])CCCC[NH3+])C=C3C2C2=C1C=CC(NC(=O)[C@@H]([NH3+])CCCC[NH3+])=C2	AUCGAUUGAGAGGAUUUGAAUGACUGACAAAAUGCAAAGUUUAGCUUUAGCCCCAGUUGGCAACGCAGCUAACGCGUGGCCGAUGUUGUCGGCUGACGAGGAGCGGGCGCUGGCUGAAAAGCUGCAUUACCAUGGCGCACCUGCGGUUUGUUGUUCAUAUUGCUCGUAAUUAUGCGGGCUAUGGC	Triptycene 1	Target_lig_625	RpoH σ32mRNA factor	Target_158	5.602059991132796
1059	NC(=[NH2+])NCCC[C@H]([NH3+])C(=O)NC1=CC2=C(C=C1)C1C3=CC=C(NC(=O)[C@@H]([NH3+])CCCNC(N)=[NH2+])C=C3C2C2=C1C=CC(NC(=O)[C@@H]([NH3+])CCCNC(N)=[NH2+])=C2	AUCGAUUGAGAGGAUUUGAAUGACUGACAAAAUGCAAAGUUUAGCUUUAGCCCCAGUUGGCAACGCAGCUAACGCGUGGCCGAUGUUGUCGGCUGACGAGGAGCGGGCGCUGGCUGAAAAGCUGCAUUACCAUGGCGCACCUGCGGUUUGUUGUUCAUAUUGCUCGUAAUUAUGCGGGCUAUGGC	Triptycene 2	Target_lig_626	RpoH σ32mRNA factor	Target_158	5.823908740944432
1118	CCC1=C(C=C2C=C3C=CC=CC3=CC2=N1)C(=O)N1CCC[C@H]1C(=O)N[C@@H](C\C=C/C[C@H](NC(=O)[C@@H]1CCCN1C(=O)C1=C(CC)N=C2C=C3C=CC=CC3=CC2=C1)C(=O)N[C@@H](CCCC[NH3+])C(=O)NCCC[NH3+])C(=O)N[C@@H](CCCC[NH3+])C(=O)NCCC[NH3+]	AAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAUUUUUUUUUUUUUUUUUUUUUUUUUUUUUU	DCC 4 (2012)	Target_lig_652	RNA duplex	Target_2	7.173925197299917
1173	C[N+]1=C(C=CC2=CC=CC=C21)/C=C/C3=CC4=CC=CC=C4N3	UGGGGGACGGGUAGGGGCGGGAGGUAGGGG	Methylquinolinium 15	Target_lig_670	A10-RNA-WT QGRS in ADAM10 mRNA	Target_196	5.468521082955774

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
1174	CCN1C2=C(C=C(C=C2)/C=C/C3=[N+](C4=CC=CC=C4C=C3)C)C5=CC=CC=C51	UGGGGGACGGGUAGGGGCGGGAGGUAGGGG	Methylquinolinium 16	Target_lig_671	A10-RNA-WT QGRS in ADAM10 mRNA	Target_196	4.71669877129645
1175	C[NH+]1CCN(CC1)C1=C2C=CC=CC2=[N+](C)C(C=CC2=CC=C(C=C2)N2CCOCC2)=C1	UGGGGGACGGGUAGGGGCGGGAGGUAGGGG	Methylquinolinium 22	Target_lig_672	A10-RNA-WT QGRS in ADAM10 mRNA	Target_196	5.585026652029 18
1176	C[NH+]1CCN(CC1)C1=C2C=CC=CC2=[N+](C)C(C=CC2=CC3=CC=CC=C3N2)=C1	UGGGGGACGGGUAGGGGCGGGAGGUAGGGG	Methylquinolinium 23	Target_lig_673	A10-RNA-WT QGRS in ADAM10 mRNA	Target_196	5.744727494894669
1178	CCN1C2=C(C=CC=C2)C2=C1C=CC(C=CC1=CC(N3CC[NH+](C)CC3)=C3C=CC=CC3=[N+]1C)=C2	UGGGGGACGGGUAGGGGCGGGAGGUAGGGG	Methylquinolinium 24	Target_lig_674	A10-RNA-WT QGRS in ADAM10 mRNA Mutant	Target_197	0.154901959985743
1179	CCN1C2=C(C=CC=C2)C2=C1C=CC(C=CC1=CC(N3CC[NH+](C)CC3)=C3C=CC=CC3=[N+]1C)=C2	UGGGGGACGGGUAGGGGCGGGAGGUAGGGG	Methylquinolinium 24	Target_lig_674	A10-RNA-WT QGRS in ADAM10 mRNA	Target_196	5.309803919997149
1180	NC1=CC=C(C=C1)C1=CC2=CC=C(C=C2N1)C1=[NH+]CCN1	GGCAGUGUGAGUACCUUCAUACGUC	Compound 1	Target_lig_675	DDPAC MAPT A Bulge	Target_198	5
1181	NC(=[NH2+])C1=CC=C(NC2=CC=C(C=C2)C2=CC3=CC=C(C=C3N2)C(N)=[NH2+])C=C1	GGCAGUGUGAGUACCUUCAUACGUC	Compound 2	Target_lig_676	DDPAC MAPT A Bulge	Target_198	4.853871964321 76
1182	NC(=[NH2+])C1=CC=C(NC2=CC=C(C=C2)C2=CC3=CC=C(C=C3N2)C(N)=[NH2+])C=C1	GGCAGUGUGAGUACCUUCAUACGUC	Compound 2	Target_lig_676	DDPAC + I17T Mutant	Target_199	4
1183	NC(=[NH2+])C1=CC=C(NC2=CC=C(C=C2)C2=CC3=CC=C(C=C3N2)C(N)=[NH2+])C=C1	GGCAGUGUGAGUACCUUCAUACGUC	Compound 2	Target_lig_676	MAPT A WT	Target_200	4.853871964321 76
1208	C1=CC(=CC(=C1)N)C2=NC3=C(N2)C=C(C=C3)C4=CC5=C(C=C4)N=C(N5)C6=CC(=CC=C6)N	GGGAGAGGGUUUAAUUAAAAGUCGACGAAAGUCGUCGCUAAUUGGAUCCGCAAGG	H1	Target_lig_684	Fully Paired RNA	Target_207	6.721246399047717
1217	C1CCN(C1)C2=NC(=C3C(=C2)C(=C(N=C3N)N4CCCC4)C#N)N	CGCUGCGGAAACGCUGCG	Naphthyridine 2	Target_lig_686	1 X 1 UU Hairpin	Target_208	6.275724130399921

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
1218	C1CCN(C1)C2=NC(=C3C(=C2)C(=C(N=C3N)N4CCCC4)C#N)N	CGCAGCGGAAACGCUGCG	Naphthyridine 2	Target_lig_686	AU stem	Target_209	4.602059991327796
1220	C1=CC(=CC=C1C(=O)NC2=NC=C(C=C2)NC(=O)C3=CC=NC=C3)F	GCGCGCGCGAAAGCGCGCGC	p7	Target_lig_687	GC Stem Loop	Target_211	4.522878745280034
1221	C1=CC(=CC=C1C(=O)NC2=NC=C(C=C2)NC(=O)C3=CC=NC=C3)F	CGCGAATTCGCGTTTTCGCGAATTCGCG	p7	Target_lig_687	AT Hairpin DNA	Target_212	4.301029995566398
1263	CCN(CC)CCOC1=CC=C(C=C1)NC2=NC(=NC3=CC=CC=C32)C4=CC=CC=C4NC(=O)CCN5CCN(CC5)C	CGCGAATTCGCGTTTTCGCGAATTCGCG	Compound 1 (2017)	Target_lig_707	Hairpin DNA	Target_212	4.673664139071125
1267	C[NH+]1CCN(CC1)C1=CC=C(C=C1)C1=CC=C2NC(=NC2=C1)C1=CC(=C(OCCCC(=O)NCCCN=[N+]=[N-])C(=C1)C(C)(C)C)C(C)(C)C	GGGAGAGGGUUUAUGACGAAAGUCUAUGGAUCCGCAAGG	Targaprimir-18a	Target_lig_708	G_U/CUA Bulge in miR-18a	Target_223	4.522878745280034
1268	C[NH+]1CCN(CC1)C1=CC=C(C=C1)C1=CC=C2NC(=NC2=C1)C1=CC(=C(OCCCC(=O)NCCCN=[N+]=[N-])C(=C1)C(C)(C)C)C(C)(C)C	GGGAGAGGGUUUAUAGACGAAAGUCUAUGGAUCCGCAAGG	Targaprimir-18a	Target_lig_708	GAU/CUA Stem Mutant	Target_224	4
1269	C[NH+]1CCN(CC1)C1=CC=C(C=C1)C1=CC=C2NC(=NC2=C1)C1=CC(=C(OCCCC(=O)NCCCN=[N+]=[N-])C(=C1)C(C)(C)C)C(C)(C)C	GGGAGAGGGUUUAGAUACGAAAGUACUGGAUCCGCAAGG	Targaprimir-18a	Target_lig_708	GAU/A_C Bulge in miR-18a	Target_225	4.494850021680009
1270	C[NH+]1CCN(CC1)C1=CC=C(C=C1)C1=CC=C2NC(=NC2=C1)C1=CC(=C(OCCCC(=O)NCCCN=[N+]=[N-])C(=C1)C(C)(C)C)C(C)(C)C	GGGAGAGGGUUUAGGUACGAAAGUACUGGAUCCGCAAGG	Targaprimir-18a	Target_lig_708	GGU/A_C Bulge Mutant	Target_226	4.397940008672047
1287	NC(=[NH2+])C1=CC=C(N=C1)C1=CC=C(O1)C1=CC=C(O1)C1=NC=C(C=C1)C(N)=[NH2+]	GGGGCCGGGGCCGGGGCCGGGGGCC	DB1246	Target_lig_716	G4C2 repeat G-quadruplex RNA	Target_232	6.387216143280026

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		GGGGCCGGGGCCGGGGCCGGGGCCGGGGCCGGGGCCGGGGCC					
1288	NC(=[NH2+])C1=CC=C(N=C1)C1=CC=C(S1)C1=CC=C(S1)C1=NC=C(C=C1)C(N)=[NH2+]	GGGGCC	DB1247	Target_lig_717	G4C2 repeat G-quadruplex RNA	Target_232	6.588380294003677
1291	C1=C(C=C(C(=C1O)O)O)C2=C(C(=O)C3=C(C=C(C=C3O2)O)O)O	GGAGAGGGUUUAAUCAGUACGAAAGUAGACAUUGGAUCCGCAAGG	Myricetin	Target_lig_718	5′CAG/3′GAC x 2 repeat RNA	Target_235	7.195860567666465
1292	C1=C(C=C(C(=C1O)O)O)C2=C(C(=O)C3=C(C=C(C=C3O2)O)O)O	GGAGAGGGUUUAAUCAGUACGAAAGUAGACAUUGGAUCCGCAAGG	Myricetin	Target_lig_718	5′CAG/3′GAC x 3 repeat RNA	Target_236	8.236572006437706
1293	C1=C(C=C(C(=C1O)O)O)C2=C(C(=O)C3=C(C=C(C=C3O2)O)O)O	GGAGAGGGUUUAAUCAGUACGAAAGUAGACAUUGGAUCCGCAAGG	Myricetin	Target_lig_718	5′CAG/3′GAC x 4 repeat RNA	Target_237	7.386158178123937
1294	C1=C(C=C(C(=C1O)O)O)C2=C(C(=O)C3=C(C=C(C=C3O2)O)O)O	GGAGAGGGUUUAAUCAGUACGAAAGUAGACAUUGGAUCCGCAAGG	Myricetin	Target_lig_718	5′CAG/3′GAC x 5 repeat RNA	Target_238	7.244125144327751
1295	C1=C(C=C(C(=C1O)O)O)C2=C(C(=O)C3=C(C=C(C=C3O2)O)O)O	GGAGAGGGUUUAAUCAGUACGAAAGUAGUCAUUGGAUCCGCAAGG	Myricetin	Target_lig_718	5'CAG/3'GUC x 6 repeat RNA	Target_234	7.136677139879954
1296	C1=C(C=C(C(=C1O)O)O)C2=C(C(=O)C3=C(C=C(C=C3O2)O)O)O	GGAGAGGGUUUAAUCAGUACGAAAGUAGACAUUGGAUCCGCAAGG	Myricetin	Target_lig_718	5′CAG/3′GAC x 33 repeat RNA	Target_239	8.769551078621773
1297	C1=C(C=C(C(=C1O)O)O)C2=C(C(=O)C3=C(C=C(C=C3O2)O)O)O	GGAGAGGGUUUAAUCAGUACGAAAGUAGACAUUGGAUCCGCAAGG	Myricetin	Target_lig_718	5′CAG/3′GAC internal loop	Target_240	6.602059991327796
1298	C1=C(C=C(C(=C1O)O)O)C2=C(C(=O)C3=C(C=C(C=C3O2)O)O)O	GGAGAGGGUUUAAUCAGUACGAAAGUAGUCAUUGGAUCCGCAAGG	Myricetin	Target_lig_718	5'CAG/3'GUC internal loop	Target_241	3.694648630553338
1299	[NH3+]CCNC1=C2OC=CC2=C(NCC[NH3+])C2=C1C(=O)C1=CC=CC=C1C2=O	GCGGCGGCGGAGGCA	Anthrafurandione 2a	Target_lig_719	KRAS RNA G-quadruplex utr-1	Target_242	7.124938736608 3
1300	[NH3+]CCNC1=C2OC=CC2=C	GGCGGCGGCAGUGGCGGCGG	Anthrafurandione 2a	Target_lig_719	KRAS RNA G-quadruplex utr-	Target_243	6.600326278518896

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	(NCC[NH3+])C2=C1C(=O)C1=CC=CC=C1C2=O				z		
1301	[NH3+]CCNC1=C2OC=CC2=C(NCC[NH3+])C2=C1C(=O)C1=CC=CC=C1C2=O	CAGCAGCGGCGGCGGCAGUGG	Anthrafurandione 2a	Target_lig_719	KRAS RNA G-quadruplex utr-4	Target_244	7.0177287669 6043
1302	[NH3+]CCNC1=C2OC=CC2=C(NCC[NH3+])C2=C1C(=O)C1=CC=CC=C1C2=O	CCGCCGCAGUGGCGGCGG	Anthrafurandione 2a	Target_lig_719	RNA Hairpin	Target_245	6.2890368810 0472
1304	[NH3+]CCNC1=C2SC=CC2=C(NCC[NH3+])C2=C1C(=O)C1=CC=CC=C1C2=O	GCGGCGGCGGAGGCA	Anthrathiophenedione 2b	Target_lig_720	KRAS RNA G-quadruplex utr-1	Target_242	7.0409586076 7891
1305	[NH3+]CCNC1=C2SC=CC2=C(NCC[NH3+])C2=C1C(=O)C1=CC=CC=C1C2=O	GGCGGCGGCAGUGGCGGCGG	Anthrathiophenedione 2b	Target_lig_720	KRAS RNA G-quadruplex utr-z	Target_243	6.5316526695 8784
1306	[NH3+]CCNC1=C2SC=CC2=C(NCC[NH3+])C2=C1C(=O)C1=CC=CC=C1C2=O	CAGCAGCGGCGGCGGCAGUGG	Anthrathiophenedione 2b	Target_lig_720	KRAS RNA G-quadruplex utr-4	Target_244	7.0809219076 2393
1307	[NH3+]CCNC1=C2SC=CC2=C(NCC[NH3+])C2=C1C(=O)C1=CC=CC=C1C2=O	CCGCCGCAGUGGCGGCGG	Anthrathiophenedione 2b	Target_lig_720	RNA Hairpin	Target_245	6.3169529617 6115
1310	CC[NH+]1CCN(C[C@@H]1C)C1=CC=C2C=C(C3=CN4C=C(C)N=C(C)C4=N3)C(=O)OC2=C1	AGAAGGAAGGUGCUC	SMN-C2	Target_lig_722	Oligo-4, an AGGAAG-containing RNA 15-mer	Target_248	4.7958800173 4408
1311	CC[NH+]1CCN(C[C@@H]1C)C1=CC=C2C=C(C3=CN4C=C(C)N=C(C)C4=N3)C(=O)OC2=C1	AAUUAAGGAGUAAGU	SMN-C2	Target_lig_722	Oligo-7, an AAGGAG-containing RNA 15-mer	Target_249	4.3372421683 1843
1312	CC[NH+]1CCN(C[C@@H]1C)C1=CC=C2C=C(C3=CN4C=C(C)N=C(C)C4=N3)C(=O)OC2=C1	CUUCCUUUAUUUUCC	SMN-C2	Target_lig_722	Oligo-1, a pyrimidine-rich RNA 15-mer	Target_250	3.7958800173 4407
1313	CC[NH+]1CCN(C[C@@H]1C)C1=CC=C2C=C(C3=CN4C=C(C)N=C(C)C4=N3)C(=O)OC2=C1	GGUUUUAGACAAAAU	SMN-C2	Target_lig_722	Oligo-2, an RNA 15-mer	Target_251	3.7958800173 4407

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
1314	CC[NH+]1CCN(C[C@@H]1C)C1=CC=C2C=C(C3=CN4C=C(C)N=C(C)C4=N3)C(=O)OC2=C1	AAAAUCAAAAAGAAG	SMN-C2	Target_lig_722	Oligo-3, a purine-rich RNA 15-mer	Target_252	3.795880017344407
1315	CC[NH+]1CCN(C[C@@H]1C)C1=CC=C2C=C(C3=CN4C=C(C)N=C(C)C4=N3)C(=O)OC2=C1	UGCUCACAUUCCUUA	SMN-C2	Target_lig_722	Oligo-5, an RNA 15-mer	Target_253	3.795880017344407
1316	CC[NH+]1CCN(C[C@@H]1C)C1=CC=C2C=C(C3=CN4C=C(C)N=C(C)C4=N3)C(=O)OC2=C1	CCUUAAAUUAAGGAG	SMN-C2	Target_lig_722	Oligo-6, an RNA 15-mer	Target_254	3.795880017344407
1318	C(CN1C=C(CNC2=C3C=CC=CC3=[NH+]C3=C2OC2=C3C=CC=C2)N=N1)C[NH+]1CCCCC1	GGGUUAGGGU	Quindoline CK1-14	Target_lig_723	Telomeric DNA G-quadruplex (HTG22)	Target_256	4.779891911959995
1319	C(CN1C=C(CNC2=C3C=CC=CC3=[NH+]C3=C2OC2=C3C=CC=C2)N=N1)C[NH+]1CCCCC1	CGCGAATTCGCGTTTTCGCGAATTCGCG	Quindoline CK1-14	Target_lig_723	Hairpin DNA	Target_212	0.467245621007502
1320	C(CN1C=C(CNC2=C3C=CC=CC3=[NH+]C3=C2OC2=C3C=CC=C2)N=N1)C[NH+]1CCCCC1	AGGGUUAGGGUUAGGGUUAGGG	Quindoline CK1-14	Target_lig_723	TERRA G-quadruplex (TERRA22)	Target_255	6.657577319177779
1323	C(CN1C=C(CNC2=C3C=CC=CC3=[NH+]C3=C2OC2=C3C=CC=C2)N=N1)C[NH+]1CCCCC1	AGGGGGCCGUGGGGUGGGAGCUGGGG	Quindoline CK1-14	Target_lig_723	BCL2 RNA G-quadruplex	Target_258	5.530177984002184
1324	C(CN1C=C(CNC2=C3C=CC=CC3=[NH+]C3=C2OC2=C3C=CC=C2)N=N1)C[NH+]1CCCCC1	UGUGGGAGGGGCGGGUCUGGG	Quindoline CK1-14	Target_lig_723	NRAS RNA G-quadruplex	Target_259	6.356547323513381
1325	C(CN1C=C(CNC2=C3C=CC=CC3=[NH+]C3=C2OC2=C3C=CC=C2)N=N1)C[NH+]1CCCCC1	TGAGGGTGGGTAGGGTGGGTAA	Quindoline CK1-14	Target_lig_723	Pu22 DNA G-quadruplex	Target_260	5.148741651280092
1326	C(CN1C=C(CNC2=C3C=CC=CC3=[NH+]C3=C2OC2=C3C=CC=C2)N=N1)C[NH+]1CCCCC1	GGGUUAGGGU	Quindoline CK1-14	Target_lig_723	TRF2:Telomeric duplex DNA (hTELO-dup)	Target_261	7.231731983548445
1327	C(CN1C=C(CNC2=C3C=CC=CC3=[NH+]C3=C2OC2=C3C=CC=C2)N=N1)C[NH+]1CCCCC1	GGGUUAGGGU	Quindoline CK1-14	Target_lig_723	TRF2:TERRA G-quadruplex (TERRA22):Telomeric duplex DNA (hTELO-dup)	Target_262	6.272784179091511

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
1505	O=c1n2Cc3nc4scc(c4c(=O)n3Cc2nc2c1c(cs2)c1ccoc1)c1ccco1	AGGGUUAGGGUUAGGGUUAGGG	RGB-1	Target_lig_815	TERRA G-quadruplex	Target_255	5.229147988335786
1517	C1=CC(=CC=C1/C=N/N=C(N)N)C2=CC3=C(S2)C=C(C=C3)/C=N/N=C(N)N	GGCAGUGUGAGUACCUUCAUACGUC	Compound 3	Target_lig_823	DDPAC hairpin A-bulge	Target_198	5.1249387366083
1518	CCC1=C(C=C2C=C3C=CC=CC3=CC2=N1)C(=O)N(C)[C@@H](C\C=C\C[C@H](N(C)C(=O)C1=C(CC)N=C2C=C3C=CC=CC3=CC2=C1)C(=O)N1CCC[C@H]1C(=O)N(C)[C@@H](CC1=CC=CC=C1)C(=O)NCCC[NH3+])C(=O)N1CCC[C@H]1C(=O)N(C)[C@@H](CC1=CC=CC=C1)C(=O)NCCC[NH3+]	GGCAGUGUGAGUACCUUCAUACGUC	Compound 4	Target_lig_654	DDPAC hairpin A-bulge	Target_198	5.443697499233271
1519	Cn1c(NCc2cccc(c2)C(=O)C)ncc1c1ccc(cc1)C(=O)C	GGCAGUGUGAGUACCUUCAUACGUC	Compound 5	Target_lig_813	DDPAC hairpin A-bulge	Target_198	4.7851561519523
1520	OC1CN(C1)Cc1ccc(cc1)C1CCN(CC1)C(=O)c1cn(c2c1cccc2)C	GGCAGUGUGAGUACCUUCAUACGUC	Compound 6	Target_lig_826	DDPAC hairpin A-bulge	Target_198	4.818156412055523
1521	OC1CN(C1)Cc1ccc(cc1)C1CCN(CC1)C(=O)c1c(C)nc2n1ccs2	GGCAGUGUGAGUACCUUCAUACGUC	Compound 7	Target_lig_827	DDPAC hairpin A-bulge	Target_198	4.772113295338633
1522	Oc1ccc2c(c1)c1c(C)c3c[n+](CCN4CCCCC4)ccc3c(c1[nH]2)C	GGCAGUGUGAGUACCUUCAUACGUC	Compound 8	Target_lig_1265	DDPAC hairpin A-bulge	Target_198	5.318758762622441
1600	CC[NH+]1CCN(C[C@@H]1C)C1=CC=C2C=C(C3=CN4C=C(C)N=C(C)C4=N3)C(=O)OC2=C1	AAAAGAAGGAAGUGCUCACAUUCCUUAAAUUAAGGAGUAAGUCUGC	SMN-C2	Target_lig_722	SMN2 pre-mRNA GA-rich sequence	Target_284	5.267606240117703
1601	CC1=CN2C=C(C=C(C2=N1)F)C3=CC(=O)N4C=C(C=CC4=N3)N5CCN(CC5)C	AAAAGAAGGAAGUGCUCACAUUCCUUAAAUUAAGGAGUAAGUCUGC	SMN-C5	Target_lig_858	SMN2 pre-mRNA GA-rich sequence	Target_284	5.096910013000806
1602	C[C@H]1CN(CCN1)C2=CC3=C(C=C2)C=C(C(=O)O3)C4=CN5C=C(N=C(C5=N4)C)C	AAAAGAAGGAAGUGCUCACAUUCCUUAAAUUAAGGAGUAAGUCUGC	SMN2_compound_1	Target_lig_859	SMN2 pre-mRNA GA-rich sequence	Target_284	4.732828271599699
1603	O=C(OC(C)	AAAAGAAGGAAGUG	SMN2_compoun	Target_lig_86	SMN2 pre-	Target_284	4.2924298239

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	(C)C)NCCN1CCN(C[C@@H]1C)c1ccc2c(c1)oc(=O)c(c2)c1cn2c(n1)c(C)nc(c2)C	CUCACAUUCCUUAAAUUAAGGAGUAAGUCUGC	d_2	0	mRNA GA-rich sequence		0206
1604	CN1CCN(CC1)c1ccc2c(c1)oc(=O)c(c2)c1ccccc1Cl	AAAAGAAGGAAGUGCUCACAUUCCUUAAAUUAAGGAGUAAGUCUGC	SMN2_compound_3	Target_lig_861	SMN2 pre-mRNA GA-rich sequence	Target_284	4
1605	CN1CCN(CC1)c1ccc2c(c1)oc(=O)c(c2)c1cccc(c1)Cl	AAAAGAAGGAAGUGCUCACAUUCCUUAAAUUAAGGAGUAAGUCUGC	SMN2_compound_4	Target_lig_862	SMN2 pre-mRNA GA-rich sequence	Target_284	4.444905551421682168
1606	CN1CCN(CC1)c1ccc2c(c1)oc(=O)c(c2)c1ccc(cc1)Cl	AAAAGAAGGAAGUGCUCACAUUCCUUAAAUUAAGGAGUAAGUCUGC	SMN2_compound_5	Target_lig_863	SMN2 pre-mRNA GA-rich sequence	Target_284	4.514278573518421842
1607	CN1CCN(CC1)c1cc(F)c2c(c1)oc(=O)c(c2)c1cccc(c1)Cl	AAAAGAAGGAAGUGCUCACAUUCCUUAAAUUAAGGAGUAAGUCUGC	SMN2_compound_6	Target_lig_864	SMN2 pre-mRNA GA-rich sequence	Target_284	4.484126156288832
1608	CN1CCN(CC1)c1cc(F)c2c(c1)oc(=O)c(c2)c1ccc(cc1)Cl	AAAAGAAGGAAGUGCUCACAUUCCUUAAAUUAAGGAGUAAGUCUGC	SMN2_compound_7	Target_lig_865	SMN2 pre-mRNA GA-rich sequence	Target_284	4.510041520575517
1609	CN1CCN(CC1)c1ccc2c(c1)oc(=O)c(c2C)c1cccc(c1)Cl	AAAAGAAGGAAGUGCUCACAUUCCUUAAAUUAAGGAGUAAGUCUGC	SMN2_compound_8	Target_lig_866	SMN2 pre-mRNA GA-rich sequence	Target_284	4
1610	CN1CCN(CC1)c1ccc2c(c1)oc(=O)c(c2C)c1ccc(cc1)Cl	AAAAGAAGGAAGUGCUCACAUUCCUUAAAUUAAGGAGUAAGUCUGC	SMN2_compound_9	Target_lig_867	SMN2 pre-mRNA GA-rich sequence	Target_284	4
1611	C1CN(CCN1)C2=CC3=C(C=C2)C=C(C(=O)O3)C4=CN5C=CC=CC5=N4	AAAAGAAGGAAGUGCUCACAUUCCUUAAAUUAAGGAGUAAGUCUGC	SMN2_compound_10	Target_lig_868	SMN2 pre-mRNA GA-rich sequence	Target_284	4.838631997765503
1612	COc1ncc2n(c1)cc(n2)c1cc2ccc(cc2oc1=O)N1CCNCC1	AAAAGAAGGAAGUGCUCACAUUCCUUAAAUUAAGGAGUAAGUCUGC	SMN2_compound_11	Target_lig_869	SMN2 pre-mRNA GA-rich sequence	Target_284	4.943095148663353
1613	CC[NH+]1CCN(C[C@@H]1C)C1=CC=C2C=C(C3=CN4C=C(C)N=C(C)C4=N3)C(=O)OC2=C1	UGAAGGAAGGUUUCGACCUUCCUUCA	SMN-C2	Target_lig_722	Seq20	Target_285	4
1614	CC[NH+]1CCN(C[C@@H]1C)C1=CC=C2C=C(C3=CN4C=C(C)N=C(C)C4=N3)C(=O)OC2=C1	GCGCCGACUGAAGGAAGGAGUCGGCGC	SMN-C2	Target_lig_722	Seq21	Target_286	5.337242168318431843
1615	CC[NH+]1CCN(C[C@@H]1C)C1=CC=C2C=C(C3=CN4C=C(C)N=C(C)C4=N3)C(=O)OC2=C1	GTGCCAGTTCGCTGGCACTGAAGGAAGGT	SMN-C2	Target_lig_722	Seq22	Target_287	4.958607314841774177
1616	CC[NH+]1CCN(C[C@@H]1C)C1=CC=C2C=C	GCCAGGCGCACUUUCGAGUGCGCGAAGGAAGGCUGGC	SMN-C2	Target_lig_722	Seq23	Target_288	5.251811972993938

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	(C3=CN4C=C(C)N=C(C)C4=N3)C(=O)OC2=C1						
1765	[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)N)O[C@@H]1[C@H]([C@@H]([C@H]([C@@H](O1)CNc1c2cccc2nc2c1cccc2)O)N)O	GGCUUAGUAUAGCGAGGUUUAGCUACACUCGUGCUGAGCC	Tobramycin	Target_lig_540	J6f1 RNA	Target_307	8.28819277095881
1766	OCC1OC(OC2C(N)CC(C(C2O)OC2OC(CNC(=O)c3ccc(c(c3)C(=O)O)c3c4ccc(=[N+](C)C)cc4oc4c3cc(c4)N(C)C)C(CC2N)O)N)C(C(C1O)N)O	GGCUUAGUAUAGCGAGGUUUAGCUACACUCGUGCUGAGCC	Tobramycin-CRT	Target_lig_993	J6f1 RNA	Target_307	6.715343717211148
1767	[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)N)O[C@@H]1[C@H]([C@@H]([C@H]([C@@H](O1)CNc1c2cccc2nc2c1cccc2)O)N)O	GGCUUAGUAUAGCUAGGUUUAGCUACACUCGUGCUGAGCC	Tobramycin	Target_lig_540	J6fd6 RNA	Target_308	6.829738284605040
1768	OCC1OC(OC2C(N)CC(C(C2O)OC2OC(CNC(=O)c3ccc(c(c3)C(=O)O)c3c4ccc(=[N+](C)C)cc4oc4c3cc(c4)N(C)C)C(CC2N)O)N)C(C(C1O)N)O	GGCUUAGUAUAGCUAGGUUUAGCUACACUCGUGCUGAGCC	Tobramycin-CRT	Target_lig_993	J6fd6 RNA	Target_308	7.468521082957774
1769	[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)N)O[C@@H]1[C@H]([C@@H]([C@H]([C@@H](O1)CNc1c2cccc2nc2c1cccc2)O)N)O	GGCUUAGUAUAGCGAGGUUUGGCUACACUCGUGCUGAGCC	Tobramycin	Target_lig_540	J6f15 RNA	Target_309	7.744727494889669

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
1770	OCC1OC(OC2C(N)CC(C(C2O)OC2OC(CNC(=O)c3ccc(c(c3)C(=O)O)c3c4ccc(=[N+](C)C)cc4oc4c3ccc(c4)N(C)C)C(CC2N)O)N)C(C(C1O)N)O	GGCUUAGUAUAGCGAGGUUUGGCUACACUCGUGCUGAGCC	Tobramycin-CRT	Target_lig_993	J6f15 RNA	Target_309	6.3707943428977
1771	[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)N)O[C@@H]1[C@H]([C@@H]([C@H]([C@@H](O1)CNc1c2ccccc2nc2c1cccc2)O)N)O	GGCUUAGUAUAGCGAGGUUUAACUACACUCGUGCUGAGCC	Tobramycin	Target_lig_540	J6f16 RNA	Target_310	8.59345981956604
1772	OCC1OC(OC2C(N)CC(C(C2O)OC2OC(CNC(=O)c3ccc(c(c3)C(=O)O)c3c4ccc(=[N+](C)C)cc4oc4c3ccc(c4)N(C)C)C(CC2N)O)N)C(C(C1O)N)O	GGCUUAGUAUAGCGAGGUUUAACUACACUCGUGCUGAGCC	Tobramycin-CRT	Target_lig_993	J6f16 RNA	Target_310	7.22184874961636
1773	[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)N)O[C@@H]1[C@H]([C@@H]([C@H]([C@@H](O1)CNc1c2ccccc2nc2c1cccc2)O)N)O	GGCUUAGUAUAGCGAGGUUUAGUUACACUCGUGCUGAGCC	Tobramycin	Target_lig_540	J6f17 RNA	Target_311	7.74472749489669
1774	OCC1OC(OC2C(N)CC(C(C2O)OC2OC(CNC(=O)c3ccc(c(c3)C(=O)O)c3c4ccc(=[N+](C)C)cc4oc4c3ccc(c4)N(C)C)C(CC2N)O)N)C(C(C1O)N)O	GGCUUAGUAUAGCGAGGUUUAGUUACACUCGUGCUGAGCC	Tobramycin-CRT	Target_lig_993	J6f17 RNA	Target_311	6.3763372926438
1835	C1CN=C(N1)NN=CC2=C3C=CC=CC3=C(C4=CC=CC=C42)C=NNC5=NCCN5	GGGAGAGGGUUUAAUUCAGUACGAAAGUACGGAUUGGAUCCGCAAGG	Bisantrene	Target_lig_1031	(5'CAG/3'GGC) x 1	Target_334	5.39794000867204
1836	C1CN=C(N1)NN=CC2=C3C=CC=CC3=C(C4=	GGGAGAGGGUUUAAUUCCGUACGAAAGUACAGAUUGGAUCCG	Bisantrene	Target_lig_1031	(5'CCG/3'GAC) x 1	Target_335	5.92081875395238

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	CC=CC=C42)C=NNC5=NCCN5	CAAGG					
1837	C1CN=C(N1)NN=CC2=C3C=CC=CC3=C(C4=CC=CC=C42)C=NNC5=NCCN5	GGGAGAGGGUUUAAUUCGGUACGAAAGUACAGAUUGGAUCCGCAAGG	Bisantrene	Target_lig_1031	(5'CGG/3'GAC) x 1	Target_336	5.22184874961636
1838	C1CN=C(N1)NN=CC2=C3C=CC=CC3=C(C4=CC=CC=C42)C=NNC5=NCCN5	GGGAGAGGGUUUAAUUCCGUACGAAAGUACUGAUUGGAUCCGCAAGG	Bisantrene	Target_lig_1031	(5'CCG/3'GUC) x 1	Target_337	5.337242168318431
1839	C1CN=C(N1)NN=CC2=C3C=CC=CC3=C(C4=CC=CC=C42)C=NNC5=NCCN5	GGGAGAGGGUUUAAUUCAGUACGAAAGUACCGAUUGGAUCCGCAAGG	Bisantrene	Target_lig_1031	(5'CAG/3'GCC) x 1	Target_338	5.958607314841177
1840	C1CN=C(N1)NN=CC2=C3C=CC=CC3=C(C4=CC=CC=C42)C=NNC5=NCCN5	GGGAGAGGGUUUAAUUCUGUACGAAAGUACCGAUUGGAUCCGCAAGG	Bisantrene	Target_lig_1031	(5'CUG/3'GCC) x 1	Target_339	5.920818753955238
1841	C1CN=C(N1)NN=CC2=C3C=CC=CC3=C(C4=CC=CC=C42)C=NNC5=NCCN5	GGGAGAGGGUUUAAUUCGGUACGAAAGUACGGAUUGGAUCCGCAAGG	Bisantrene	Target_lig_1031	(5'CGG/3'GCC) x 1	Target_340	6.468521082958774
1842	C1CN=C(N1)NN=CC2=C3C=CC=CC3=C(C4=CC=CC=C42)C=NNC5=NCCN5	GGGAGAGGGUUUAAUUCAGUACGAAAGUACAGAUUGGAUCCGCAAGG	Bisantrene	Target_lig_1031	(5'CAG/3'GAC) x 1	Target_341	5.795880017344408
1843	C1CN=C(N1)NN=CC2=C3C=CC=CC3=C(C4=CC=CC=C42)C=NNC5=NCCN5	GGGAGAGGGUUUAAUUCCGUACGAAAGUACGGAUUGGAUCCGCAAGG	Bisantrene	Target_lig_1031	(5'CCG/3'GGC) x 1	Target_342	5.537602002101040
1844	C1CN=C(N1)NN=CC2=C3C=CC=CC3=C(C4=CC=CC=C42)C=NNC5=NCCN5	GGGAGAGGGUUUAAUUCUGUACGAAAGUACUGAUUGGAUCCGCAAGG	Bisantrene	Target_lig_1031	(5'CUG/3'GUC) x 1	Target_343	5.431798275933301
1845	C1CN=C(N1)NN=CC2=C3C=CC=CC3=C(C4=CC=CC=C42)C=NNC5=NCCN5	GGGAGAGGGUUUAAUUCAGUACGAAAGUACUGAUUGGAUCCGCAAGG	Bisantrene	Target_lig_1031	(5'CAG/3'CUG) x 1	Target_344	5.552841968665778
1846	NC(=[NH2+])C1=CC=C(N=C1)C1=CC=C(O1)C1=CC=C(O1)C1=NC=C(C=C1)C(N)=[NH2+]	GGGAGAGGGUUUAAUUCGGUACGAAAGUACGGAUUGGAUCCGCAAGG	B1	Target_lig_716	(5'CGG/3'GGC) x1	Target_345	6.619788758288839
1847	C[NH+](C)CCC[NH+]=C(C1=CC=C(C=C1)C(=[NH+]CCC[NH+]	GGGAGAGGGUUUAAUUCGGUACGAAAGUACGGAUUGGAUCCGCAAGG	B2	Target_lig_693	(5'CGG/3'GGC) x1	Target_345	5.958607314841177

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	(C)C)N)N						
1848	CN(C)CCCN=C(C1=CC=C(C=C1)C2=CC=C(O2)C3=NC4=C(N3)C=C(C=C4)C(=NCCCN(C)C)N)N	GGGAGAGGGUUUAAUUCGGUACGAAAGUACGGAUUGGAUCCGCAAGG	B3	Target_lig_246	(5'CGG/3'GGC) x1	Target_345	5.45593195564972
1849	CC(C)C1=CC2=C(C=C1)N=C3C=CC(=CN3C2=O)C(=O)NCCN(C)C	GGGAGAGGGUUUAAUUCGGUACGAAAGUACGGAUUGGAUCCGCAAGG	B4	Target_lig_1035	(5'CGG/3'GGC) x1	Target_345	6.48148606012211
1850	COC1=CC(=CC(=C1O)OC)C2=NC3=C(N2)C=C4C(=C3)NC(=O)N4	GGGAGAGGGUUUAAUUCGGUACGAAAGUACGGAUUGGAUCCGCAAGG	B5	Target_lig_957	(5'CGG/3'GGC) x1	Target_345	5.853871964321 76
1851	C1C[NH+]=C(N1)C2=CC=C(C=C2)C3=CC=C(O3)C4=CC=C(C=C4)C5=[NH+]CCN5	GGGAGAGGGUUUAAUUCGGUACGAAAGUACGGAUUGGAUCCGCAAGG	B6	Target_lig_696	(5'CGG/3'GGC) x1	Target_345	6.40893539297 35
1852	C1=CC(=CC=C1C2=CC=C(O2)C3=CC=C(C=C3)C(=[NH2+])N)C(=[NH2+])N	GGGAGAGGGUUUAAUUCGGUACGAAAGUACGGAUUGGAUCCGCAAGG	B7	Target_lig_697	(5'CGG/3'GGC) x1	Target_345	6.56863623584101
1853	C1N(C2=CC=CC=C2N(C1)C(=O)/C=C/C3=CC=CC=C3)C(=O)/C=C/C4=CC=CC=C4	GGGAGAGGGUUUAAUUCGGUACGAAAGUACGGAUUGGAUCCGCAAGG	B8	Target_lig_1039	(5'CGG/3'GGC) x1	Target_345	5.853871964321 76
1854	CCN(CC)CC(=O)NC1=CC=CC2=C1C(=O)C3=C(C4=CC=CC=C4C(=C3C2=O)O)O	GGGAGAGGGUUUAAUUCGGUACGAAAGUACGGAUUGGAUCCGCAAGG	B9	Target_lig_1040	(5'CGG/3'GGC) x1	Target_345	5.63827216398241
1855	C1CC2=C(CC1C(=O)O)C(=NC(=N2)NCC3=CC=CC=C3)NCC4=CC=CC=C4	GGGAGAGGGUUUAAUUCGGUACGAAAGUACGGAUUGGAUCCGCAAGG	B10	Target_lig_1041	(5'CGG/3'GGC) x1	Target_345	5.27572413039921
1856	C1COCCN1CCNC2=C3C(=C(C=C2)NCCN4CCOCC4)C(=O)C5=CC=CC=C5C3=O	GGGAGAGGGUUUAAUUCGGUACGAAAGUACGGAUUGGAUCCGCAAGG	B11	Target_lig_1042	(5'CGG/3'GGC) x1	Target_345	6.44369749923271
1858	NC(=[NH2+])C1=CC=C(N=C1)C1=CC=C(O1)C1=CC=C(O1)C1=NC=C(C=C1)C(N)=[NH2+]	GGGAGAGGGUUUAAUUCAGUACGAAAGUACUGAUUGGAUCCGCAAGG	B1	Target_lig_716	(5'CAG/3'GUC) x1	Target_346	5.44369749923271
1859	C[NH+](C)CCC[NH+]=C(C1=CC=C(C=C1)C(=[NH+]CCC[NH+](C)C)N)N	GGGAGAGGGUUUAAUUCAGUACGAAAGUACUGAUUGGAUCCGCAAGG	B2	Target_lig_693	(5'CAG/3'GUC) x1	Target_346	6.43179827593301
1860	CN(C)CCCN=C(C1=CC=C(C=C1)C2=CC=C(O2)C3=NC4=C(	GGGAGAGGGUUUAAUUCAGUACGAAAGUACUGAUUGGAUCCGCAAGG	B3	Target_lig_246	(5'CAG/3'GUC) x1	Target_346	5.85387196432176

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	N3)C=C(C=C4)C(=NCCCN(C)C)N)N						
1861	CC(C)C1=CC2=C(C=C1)N=C3C=CC(=CN3C2=O)C(=O)NCCN(C)C	GGGAGAGGGUUUAAUUCAGUACGAAAGUACUGAUUGGAUCCGCAAGG	B4	Target_lig_1035	(5'CAG/3'GUC) x1	Target_346	5.309803919997149
1862	COC1=CC(=CC(=C1O)OC)C2=NC3=C(N2)C=C4C(=C3)NC(=O)N4	GGGAGAGGGUUUAAUUCAGUACGAAAGUACUGAUUGGAUCCGCAAGG	B5	Target_lig_957	(5'CAG/3'GUC) x1	Target_346	5.823908740944432
1863	C1C[NH+]=C(N1)C2=CC=C(C=C2)C3=CC=C(O3)C4=CC=C(C=C4)C5=[NH+]CCN5	GGGAGAGGGUUUAAUUCAGUACGAAAGUACUGAUUGGAUCCGCAAGG	B6	Target_lig_696	(5'CAG/3'GUC) x1	Target_346	5.886056647693316
1864	C1=CC(=CC=C1C2=CC=C(O2)C3=CC=C(C=C3)C(=[NH2+])N)C(=[NH2+])N	GGGAGAGGGUUUAAUUCAGUACGAAAGUACUGAUUGGAUCCGCAAGG	B7	Target_lig_697	(5'CAG/3'GUC) x1	Target_346	5.721246399047717
1865	C1N(C2=CC=CC=C2N(C1)C(=O)/C=C/C3=CC=CC=C3)C(=O)/C=C/C4=CC=CC=C4	GGGAGAGGGUUUAAUUCAGUACGAAAGUACUGAUUGGAUCCGCAAGG	B8	Target_lig_1039	(5'CAG/3'GUC) x1	Target_346	6.154901959985574
1866	CCN(CC)CC(=O)NC1=CC=CC2=C1C(=O)C3=C(C4=CC=CC=C4C(=C3C2=O)O)O	GGGAGAGGGUUUAAUUCAGUACGAAAGUACUGAUUGGAUCCGCAAGG	B9	Target_lig_1040	(5'CAG/3'GUC) x1	Target_346	5.318758762624441
1867	C1CC2=C(CC1C(=O)O)C(=NC(=N2)NCC3=CC=CC=C3)NCC4=CC=CC=C4	GGGAGAGGGUUUAAUUCAGUACGAAAGUACUGAUUGGAUCCGCAAGG	B10	Target_lig_1041	(5'CAG/3'GUC) x1	Target_346	5.387216143280026
1868	C1COCCN1CCNC2=C3C(=C(C=C2)NCCN4CCOCC4)C(=O)C5=CC=CC=C5C3=O	GGGAGAGGGUUUAAUUCAGUACGAAAGUACUGAUUGGAUCCGCAAGG	B11	Target_lig_1042	(5'CAG/3'GUC) x1	Target_346	5.267606240177703
1903	C1CCN(CC1)C2CCN(CC2)CCCNC3=NC(=NC4=CC=CC=C43)C5=NN=C(O5)C6=CC=CC=C6	UGUGGGAGGGGCGGGUCUGGG	NRAS SAR 1	Target_lig_1053	NRAS G4 motif	Target_259	5.920818753955238
1904	Fc1ccc(cc1)c1nnc(o1)c1nc(NCCc2ccco2)c2c(n1)cccc2	UGUGGGAGGGGCGGGUCUGGG	NRAS SAR 2	Target_lig_1054	NRAS G4 motif	Target_259	6.585026652029218
1905	C1CCC(CC1)NC2=NC(=NC3=CC=CC=C32)C4=NN=C(O4)C5=CC=C(C=C5)F	UGUGGGAGGGGCGGGUCUGGG	NRAS SAR 3	Target_lig_1055	NRAS G4 motif	Target_259	6.366531544422041
1906	CCCSCCCNC1=NC(=NC2=CC=CC=C21)C3=NN=C(O3)C4=CC=CC=C4	UGUGGGAGGGGCGGGUCUGGG	NRAS SAR 6	Target_lig_1056	NRAS G4 motif	Target_259	6.130768280269026

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
1907	C1=CC=C(C=C1)C2=NN=C(O2)C3=NC4=CC=CC=C4C(=N3)NCCC5=CC=CS5	UGUGGGAGGGGCGGGUCUGGG	NRAS SAR 7	Target_lig_1057	NRAS G4 motif	Target_259	6.44369749923271
1908	Clc1ccc(cc1)c1nnc(o1)c1nc2ccccc2c(n1)c1ccc(cc1)N(C)C	UGUGGGAGGGGCGGGUCUGGG	NRAS SAR 8	Target_lig_1058	NRAS G4 motif	Target_259	5.522878745280034
1909	CC1=CC(=CC=C1)C2=NN=C(O2)C3=NC4=CC=CC=C4C(=N3)NCCC5=CN=CN5	UGUGGGAGGGGCGGGUCUGGG	NRAS SAR 10	Target_lig_1059	NRAS G4 motif	Target_259	6.318758762624441
1910	CC1=CC(=CC=C1)C2=NN=C(O2)C3=NC4=CC=CC=C4C(=N3)NCCN5CCOCC5	UGUGGGAGGGGCGGGUCUGGG	NRAS SAR 12	Target_lig_1060	NRAS G4 motif	Target_259	6.522878745280034
1911	CC1=CC(=CC=C1)C2=NN=C(O2)C3=NC4=CC=CC=C4C(=N3)NCCC5=C(ON=C5C)C	UGUGGGAGGGGCGGGUCUGGG	NRAS SAR 14	Target_lig_1061	NRAS G4 motif	Target_259	6.552841968665778
1912	CC1=CC=C(C=C1)C2=NN=C(O2)C3=NC4=CC=CC=C4C(=N3)N5CCCCC5	UGUGGGAGGGGCGGGUCUGGG	NRAS SAR 16	Target_lig_1062	NRAS G4 motif	Target_259	6.455931955564972
1913	Cc1ccc(cc1)c1nnc(o1)c1nc(NCc2cccc3c2OCO3)c2c(n1)cccc2	UGUGGGAGGGGCGGGUCUGGG	NRAS SAR 17	Target_lig_1063	NRAS G4 motif	Target_259	6.251811972993 8
1914	CC1=CC=C(C=C1)C2=NN=C(O2)C3=NC4=CC=CC=C4C(=N3)NCCC5=CC=C(C=C5)S(=O)(=O)N	UGUGGGAGGGGCGGGUCUGGG	NRAS SAR 18	Target_lig_1064	NRAS G4 motif	Target_259	6.602059991327796
1915	CC1=CC=C(C=C1)C2=NN=C(O2)C3=NC4=CC=CC=C4C(=N3)NCCN5CCCC5	UGUGGGAGGGGCGGGUCUGGG	NRAS SAR 24	Target_lig_1065	NRAS G4 motif	Target_259	6.301029995663398
1916	CC1=CC=C(C=C1)C2=NN=C(O2)C3=NC4=CC=CC=C4C(=N3)NCCCN5CCC6=CC=CC=C6C5	UGUGGGAGGGGCGGGUCUGGG	NRAS SAR 25	Target_lig_1066	NRAS G4 motif	Target_259	6.022276394711115
1917	C1CCN(CC1)C1CCN(CC1)CCCCNc1nc(nc2ccccc2)c1nnc(o1)c1ccccc1	UGUGGGAGGGGCGGGUCUGGG	NRAS compound 1	Target_lig_1052	NRAS G4 motif	Target_259	6.346787486224466
1918	C1COCC1C2=NOC(=N2)C3=CC(=CC(=C3)CN)NC(=O)C4=CC=CC=N4	UGUGGGAGGGGCGGGUCUGGG	Hit S1	Target_lig_1067	NRAS G4 motif	Target_259	4.962573502059938
1919	CC1=CN=C(C=	UGUGGGAGGGGCGG	Hit S2	Target_lig_10	NRAS G4	Target_259	4.5951662833

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	C1)NCCCNC(=O)C2=CN(N=N2)CCN	GUCUGGG		68	motif		8006
1920	C1CN2CCC1C(C2)NCC3=C(N=CC=C3)OC4=CC(=C(C=C4)F)F	UGUGGGAGGGGCGGGUCUGGG	Hit S3	Target_lig_1069	NRAS G4 motif	Target_259	4.841637507904475
1921	CN1C2=C(C(=CC=C2)Cl)C(=N1)CN3CCCCC(C3)N	UGUGGGAGGGGCGGGUCUGGG	Hit S4	Target_lig_1070	NRAS G4 motif	Target_259	4.554395796726 4
1922	C1CN(CCC1N2CCC(CC2)O)C3=NC=NC(=C3)CCN	UGUGGGAGGGGCGGGUCUGGG	Hit S5	Target_lig_1071	NRAS G4 motif	Target_259	4.408935392973 5
1923	CC1=CC(=NC(=N1)N)N2CCN(CC2)C(=O)CCC3=NN4CCNCC4=C3	UGUGGGAGGGGCGGGUCUGGG	Hit S6	Target_lig_1072	NRAS G4 motif	Target_259	4.031517051446 07
1924	CC(CCC1=CC=CO1)NC2CCC3(CC2)CCNCC3	UGUGGGAGGGGCGGGUCUGGG	Hit S7	Target_lig_1073	NRAS G4 motif	Target_259	4.017728766960 43
1925	COC1=C(C=C(C=C1)CN2CCC(CC2)N3CCN(CC3)CCO)OCC4=CC=CC=C4	UGUGGGAGGGGCGGGUCUGGG	Hit S8	Target_lig_1074	NRAS G4 motif	Target_259	4
1926	C1=CN=CC=C1C2=NC(=NC=C2)NCCCC3=NN=C(S3)N	UGUGGGAGGGGCGGGUCUGGG	Hit S9	Target_lig_1075	NRAS G4 motif	Target_259	4.317854923626 17
1927	CC(C)OC(=O)C1=CC=C(C=C1)NC2=NC3=CC=CC=C3C4=NN=CN42	UGUGGGAGGGGCGGGUCUGGG	Hit S11	Target_lig_1076	NRAS G4 motif	Target_259	4
1928	C1CCCN(CC1)CC2=NC(=NC(=N2)NC3=CC=C(C=C3)F)N	UGUGGGAGGGGCGGGUCUGGG	Hit S12	Target_lig_1077	NRAS G4 motif	Target_259	4
1943	COC1=C(C=CC(=C1)C=CC(=O)CC(=O)C=CC2=CC(=C(C=C2)O)OC)O	GGGAGAGGGUUUAAUUCAGUACGAAAGUACGGAUUGGAUCCGCAAGG	Curcumin	Target_lig_1092	(5'CAG/3'GGC) x 1	Target_334	6.124938736 6083
1944	COC1=C(C=CC(=C1)C=CC(=O)CC(=O)C=CC2=CC(=C(C=C2)O)OC)O	GGGAGAGGGUUUAAUUCCGUACGAAAGUACAGAUUGGAUCCGCAAGG	Curcumin	Target_lig_1092	(5'CCG/3'GAC) x 1	Target_335	5.978810700930 06
1945	COC1=C(C=CC(=C1)C=CC(=O)CC(=O)C=CC2=CC(=C(C=C2)O)OC)O	GGGAGAGGGUUUAAUUCGGUACGAAAGUACAGAUUGGAUCCGCAAGG	Curcumin	Target_lig_1092	(5'CGG/3'GAC) x 1	Target_336	6.244125144 32751
1946	COC1=C(C=CC(=C1)C=CC(=O)CC(=O)C=CC2=CC(=C(C=C2)O)OC)O	GGGAGAGGGUUUAAUUCCGUACGAAAGUACUGAUUGGAUCCGCAAGG	Curcumin	Target_lig_1092	(5'CCG/3'GUC) x 1	Target_337	6.107905397 30952
1947	COC1=C(C=CC(=C1)C=CC(=O)CC(=O)C=CC2=CC(=C(C=C2)	GGGAGAGGGUUUAAUUCAGUACGAAAGUACCGAUUGGAUCCGCAAGG	Curcumin	Target_lig_1092	(5'CAG/3'GCC) x 1	Target_338	6.356547323 51381

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	O)OC)O						
1948	COC1=C(C=CC(=C1)C=CC(=O)CC(=O)C=CC2=CC(=C(C=C2)O)OC)O	GGGAGAGGGUUUAAUUCUGUACGAAAGUACCGAUUGGAUCCGCAAGG	Curcumin	Target_lig_1092	(5'CUG/3'GCC) x 1	Target_339	6.18045606445813
1949	COC1=C(C=CC(=C1)C=CC(=O)CC(=O)C=CC2=CC(=C(C=C2)O)OC)O	GGGAGAGGGUUUAAUUCGGUACGAAAGUACGGAUUGGAUCCGCAAGG	Curcumin	Target_lig_1092	(5'CGG/3'GCC) x 1	Target_340	6.92081875395238
1950	COC1=C(C=CC(=C1)C=CC(=O)CC(=O)C=CC2=CC(=C(C=C2)O)OC)O	GGGAGAGGGUUUAAUUCAGUACGAAAGUACAGAUUGGAUCCGCAAGG	Curcumin	Target_lig_1092	(5'CAG/3'GAC) x 1	Target_341	6.2518119729938
1951	COC1=C(C=CC(=C1)C=CC(=O)CC(=O)C=CC2=CC(=C(C=C2)O)OC)O	GGGAGAGGGUUUAAUUCCGUACGAAAGUACGGAUUGGAUCCGCAAGG	Curcumin	Target_lig_1092	(5'CCG/3'GGC) x 1	Target_342	6.06550154875643
1952	COC1=C(C=CC(=C1)C=CC(=O)CC(=O)C=CC2=CC(=C(C=C2)O)OC)O	GGGAGAGGGUUUAAUUCUGUACGAAAGUACUGAUUGGAUCCGCAAGG	Curcumin	Target_lig_1092	(5'CUG/3'GUC) x 1	Target_343	6.130768280269 02
1953	COC1=C(C=CC(=C1)C=CC(=O)CC(=O)C=CC2=CC(=C(C=C2)O)OC)O	GGGAGAGGGUUUAAUUCAGUACGAAAGUACUGAUUGGAUCCGCAAGG	Curcumin	Target_lig_1092	(5'CAG/3'CUG) x 1	Target_344	5.67778070526608
2042	CC1=CC2=C(C=C1C)N(C=N2)C3C(C(C(O3)CO)OP(=O)([O-])OC(C)CNC(=O)CCC4(CC5C6(C(C(C(=N6)C(=C7C(C(C(=N7)C=C8C(C(C(=N8)C(=C4[N-]5)C)CCC(=O)N)(C)C)CCC(=O)N)(C)CC(=O)N)C)CCC(=O)N)(C)CC(=O)N)C)CC(=O)N)C)O.[C-]#N.[Co+3]	CCGGTGCGCATAACCACCTCAGTGCGAGCAACGATGGCC	cyanocobalamine	Target_lig_72	B12.9	Target_372	6.49485002168009
2043	C/C/1=C/2\[C@@](C[C@@H](C(=N2)/C=C\3/C([C@@H](C(=N3)/C(=C\4/[C@](C[C@H](C([N-]4)[C@]5([C@@](C[C@@H](C1=N5)CCC(=O)N)(C)CC(=O)N)CC(=O)N)(C)CCC(=O)NCC(C)O)/C)CCC(=O)N)(C)C)CCC(=O)N)(C)CC(=O)N.[C-]#N.[C-]#N.	CCGGTGCGCATAACCACCTCAGTGCGAGCAACGATGGCC	cobinamide dicyanide	Target_lig_73	B12.9	Target_372	5.05551732784983

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	[Co]						
2062	N[C@@H]1C[C@H](N)[C@H]([C@H]([C@H]1OCCCc1nnn(c1)Cc1ccc(cc1)Cn1nnc(c1)CCCO[C@@H]1[C@H](N)C[C@H]([C@@H]([C@H]1O)O)N)O)O	CGCGCGAAAGCGCG	B-11	Target_lig_1137	RNA hairpin loop I	Target_375	5.24184537803261
2063	N[C@@H]1C[C@H](N)[C@H]([C@H]([C@H]1OCCCc1nnn(c1)Cc1c(C)cc(c(c1C)Cn1nnc(c1)CCCO[C@@H]1[C@H](N)C[C@H]([C@@H]([C@H]1O)O)N)C)O)O	CGCGCGAAAGCGCG	B-13	Target_lig_1138	RNA hairpin loop I	Target_375	6.20065945054642
2064	N[C@@H]1C[C@H](N)[C@H]([C@H]([C@H]1OCCCc1nnn(c1)Cc1ccc(n1)Cn1nnc(c1)CCCO[C@@H]1[C@H](N)C[C@H]([C@@H]([C@H]1O)O)N)O)O	CGCGCGAAAGCGCG	B-14	Target_lig_1139	RNA hairpin loop I	Target_375	5.29584948311602
2066	[C@@H]1([C@H]([C@H](O)[C@H]([C@@H](C1)N)O)OCCCc1cn(nn1)Cc1ccc(Cn2cc(nn2)CCCO[C@H]2[C@@H](C[C@@H]([C@@H](O)[C@H]2O)N)N)c1)N	CGCGCGAAAGCGCG	B-12	Target_lig_224	RNA hairpin loop Ia	Target_375	5.866461091629978
2069	N[C@@H]1C[C@H](N)[C@H]([C@H]([C@H]1OCCCc1nnn(c1)Cc1ccc(cc1)Cn1nnc(c1)CCCO[C@@H]1[C@H](N)C[C@H]([C@@H]([C@H]1O)O)N)O)O	CGCGCUUCGGCGCG	B-11	Target_lig_1137	RNA hairpin loop Ib	Target_376	5.199282921717762
2070	[C@@H]1([C@H]([C@H](O)[C@H]([C@@H](C1)N)O)OCCCc1cn(nn1)Cc1ccc(Cn2cc(nn2)CCCO[C@H]2[C@@H]	CGCGCUUCGGCGCG	B-12	Target_lig_224	RNA hairpin loop Ib	Target_376	5.812479279163546

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	(C[C@@H]([C@@H](O)[C@H]2O)N)N)c1)N						
2071	N[C@@H]1C[C@H](N)[C@H]([C@H]([C@H]1OCCCc1nnn(c1)Cc1c(C)cc(c(c1C)Cn1nnc(c1)CCCO[C@@H]1[C@H](N)C[C@H]([C@@H]([C@H]1O)O)N)C)O)O	CGCGCUUCGGCGCG	B-13	Target_lig_1138	RNA hairpin loop Ib	Target_376	6.075720713938 12
2072	N[C@@H]1C[C@H](N)[C@H]([C@H]([C@H]1OCCCc1nnn(c1)Cc1ccccc(n1)Cn1nnc(c1)CCCO[C@@H]1[C@H](N)C[C@H]([C@@H]([C@H]1O)O)N)O)O	CGCGCUUCGGCGCG	B-14	Target_lig_1139	RNA hairpin loop Ib	Target_376	5.103473782510 45
2073	N[C@@H]1C[C@H](N)[C@H]([C@H]([C@H]1OCCCc1nnn(c1)Cc1ccc(cc1)Cn1nnc(c1)CCCO[C@@H]1[C@H](N)C[C@H]([C@@H]([C@H]1O)O)N)O)O	CGCGCAGUGUAGCGCG	B-11	Target_lig_1137	RNA hairpin loop II	Target_377	5.684029654543 08
2074	[C@@H]1([C@H]([C@H](O)[C@H]([C@@H](C1)N)O)OCCCc1cn(nn1)Cc1ccccc(Cn2cc(nn2)CCCO[C@H]2[C@@H](C[C@@H]([C@@H](O)[C@H]2O)N)N)c1)N	CGCGCAGUGUAGCGCG	B-12	Target_lig_224	RNA hairpin loop II	Target_377	4.998699066979 958
2075	N[C@@H]1C[C@H](N)[C@H]([C@H]([C@H]1OCCCc1nnn(c1)Cc1c(C)cc(c(c1C)Cn1nnc(c1)CCCO[C@@H]1[C@H](N)C[C@H]([C@@H]([C@H]1O)O)N)C)O)O	CGCGCAGUGUAGCGCG	B-13	Target_lig_1138	RNA hairpin loop II	Target_377	6.221848749616 36
2076	N[C@@H]1C[C@H](N)[C@H]([C@H]([C@H]1OCCCc1nnn(c1)Cc1ccccc(n1)Cn1nnc(c	CGCGCAGUGUAGCGCG	B-14	Target_lig_1139	RNA hairpin loop II	Target_377	5.340083799930 15

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	1)CCCO[C@@H]1[C@H](N)C[C@H]([C@@H]([C@H]1O)O)N)O)O						
2077	N[C@@H]1C[C@H](N)[C@H]([C@H]([C@H]1OCCCc1nnn(c1)Cc1ccc(cc1)Cn1nnc(c1)CCCO[C@@H]1[C@H](N)C[C@H]([C@@H]([C@H]1O)O)N)O)O	CGCGCAGUAGUAGCGCG	B-11	Target_lig_1137	RNA hairpin loop III	Target_378	5.844663962534494
2078	[C@@H]1([C@H]([C@H](O)[C@H]([C@@H](C1)N)O)OCCCc1cn(nn1)Cc1ccc(Cn2cc(nn2)CCCO[C@H]2[C@@H](C[C@@H]([C@@H](O)[C@H]2O)N)N)c1)N	CGCGCAGUAGUAGCGCG	B-12	Target_lig_224	RNA hairpin loop III	Target_378	5.005682847330336
2079	N[C@@H]1C[C@H](N)[C@H]([C@H]([C@H]1OCCCc1nnn(c1)Cc1c(C)cc(c(c1C)Cn1nnc(c1)CCCO[C@@H]1[C@H](N)C[C@H]([C@@H]([C@H]1O)O)N)C)O)O	CGCGCAGUAGUAGCGCG	B-13	Target_lig_1138	RNA hairpin loop III	Target_378	5.593459819566604
2080	N[C@@H]1C[C@H](N)[C@H]([C@H]([C@H]1OCCCc1nnn(c1)Cc1ccc(n1)Cn1nnc(c1)CCCO[C@@H]1[C@H](N)C[C@H]([C@@H]([C@H]1O)O)N)O)O	CGCGCAGUAGUAGCGCG	B-14	Target_lig_1139	RNA hairpin loop III	Target_378	5.896196279044404
2081	N[C@@H]1C[C@H](N)[C@H]([C@H]([C@H]1OCCCc1nnn(c1)Cc1ccc(cc1)Cn1nnc(c1)CCCO[C@@H]1[C@H](N)C[C@H]([C@@H]([C@H]1O)O)N)O)O	CGCGCACAAGUAGCGCG	B-11	Target_lig_1137	RNA hairpin loop IIIa	Target_379	5.563837352955924
2082	[C@@H]1([C@H]([C@H](O)[C@H]([C@@H]	CGCGCACAAGUAGCGCG	B-12	Target_lig_224	RNA hairpin loop IIIa	Target_379	5.651695136951184

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	(C1)N)O)OCCCc1cn(nn1)Cc1ccccc(Cn2cc(nn2)CCCO[C@H]2[C@@H](C[C@@H]([C@@H](O)[C@H]2O)N)N)c1)N						
2083	N[C@@H]1C[C@H](N)[C@H]([C@H]([C@H]1OCCCc1nnn(c1)Cc1c(C)cc(c(c1C)Cn1nnc(c1)CCCO[C@@H]1[C@H](N)C[C@H]([C@@H]([C@H]1O)O)N)C)O)O	CGCGCACAAGUAGCGCG	B-13	Target_lig_1138	RNA hairpin loop IIIa	Target_379	6.35654732351381
2084	N[C@@H]1C[C@H](N)[C@H]([C@H]([C@H]1OCCCc1nnn(c1)Cc1ccccc(n1)Cn1nnc(c1)CCCO[C@@H]1[C@H](N)C[C@H]([C@@H]([C@H]1O)O)N)O)O	CGCGCACAAGUAGCGCG	B-14	Target_lig_1139	RNA hairpin loop IIIa	Target_379	5.45593195564972
2085	N[C@@H]1C[C@H](N)[C@H]([C@H]([C@H]1OCCCc1nnn(c1)Cc1ccc(cc1)Cn1nnc(c1)CCCO[C@@H]1[C@H](N)C[C@H]([C@@H]([C@H]1O)O)N)O)O	CGCGCACAACAAGCGCG	B-11	Target_lig_1137	RNA hairpin loop IIIb	Target_380	5.692503962086679
2086	[C@@H]1([C@H]([C@H](O)[C@H]([C@@H](C1)N)O)OCCCc1cn(nn1)Cc1ccccc(Cn2cc(nn2)CCCO[C@H]2[C@@H](C[C@@H]([C@@H](O)[C@H]2O)N)N)c1)N	CGCGCACAACAAGCGCG	B-12	Target_lig_224	RNA hairpin loop IIIb	Target_380	5.621602099055186
2087	N[C@@H]1C[C@H](N)[C@H]([C@H]([C@H]1OCCCc1nnn(c1)Cc1c(C)cc(c(c1C)Cn1nnc(c1)CCCO[C@@H]1[C@H](N)C[C@H]([C@@H]([C@H]1O)O)N)C)O)O	CGCGCACAACAAGCGCG	B-13	Target_lig_1138	RNA hairpin loop IIIb	Target_380	6.327902142066428
2088	N[C@@H]1C[C	CGCGCACAACAAGC	B-14	Target_lig_11	RNA hairpin	Target_380	5.4659738939

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	@H](N)[C@H]([C@H]([C@H]1OCCCc1nnn(c1)Cc1ccccc(n1)Cn1nnc(c1)CCCO[C@@H]1[C@H](N)C[C@H]([C@@H]([C@H]1O)O)N)O)O	GCG		39	loop IIIb		4387
2089	N[C@@H]1C[C@H](N)[C@H]([C@H]([C@H]1OCCCc1nnn(c1)Cc1ccc(cc1)Cn1nnc(c1)CCCO[C@@H]1[C@H](N)C[C@H]([C@@H]([C@H]1O)O)N)O)O	CGCGCAGUCAGUAGCGCG	B-11	Target_lig_1137	RNA hairpin loop IV	Target_381	5.511449283499956
2090	[C@@H]1([C@H]([C@H](O)[C@H]([C@@H](C1)N)O)OCCCc1cn(nn1)Cc1ccccc(Cn2cc(nn2)CCCO[C@H]2[C@@H](C[C@@H]([C@@H](O)[C@H]2O)N)N)c1)N	CGCGCAGUCAGUAGCGCG	B-12	Target_lig_224	RNA hairpin loop IV	Target_381	6.494850021680009
2091	N[C@@H]1C[C@H](N)[C@H]([C@H]([C@H]1OCCCc1nnn(c1)Cc1c(C)cc(c(c1C)Cn1nnc(c1)CCCO[C@@H]1[C@H](N)C[C@H]([C@@H]([C@H]1O)O)N)C)O)O	CGCGCAGUCAGUAGCGCG	B-13	Target_lig_1138	RNA hairpin loop IV	Target_381	6.387216143280026
2092	N[C@@H]1C[C@H](N)[C@H]([C@H]([C@H]1OCCCc1nnn(c1)Cc1ccccc(n1)Cn1nnc(c1)CCCO[C@@H]1[C@H](N)C[C@H]([C@@H]([C@H]1O)O)N)O)O	CGCGCAGUCAGUAGCGCG	B-14	Target_lig_1139	RNA hairpin loop IV	Target_381	5.522878745280034
2093	N[C@@H]1C[C@H](N)[C@H]([C@H]([C@H]1OCCCc1nnn(c1)Cc1ccc(cc1)Cn1nnc(c1)CCCO[C@@H]1[C@H](N)C[C@H]([C@@H]([C@H]1O)O)N)O)O	CGCGCUUGCGAGUGCGCG	B-11	Target_lig_1137	RNA hairpin loop Iva	Target_382	5.692503962086679

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
2094	[C@@H]1([C@H]([C@H](O)[C@H]([C@@H](C1)N)O)OCCCc1cn(nn1)Cc1ccccc(Cn2cc(nn2)CCCO[C@H]2[C@@H](C[C@@H]([C@@H](O)[C@H]2O)N)N)c1)N	CGCGCUUGCGAGUGCGCG	B-12	Target_lig_224	RNA hairpin loop Iva	Target_382	6.823908740944432
2095	N[C@@H]1C[C@H](N)[C@H]([C@H]([C@H]1OCCCc1nnn(c1)Cc1c(C)cc(c(c1C)Cn1nnc(c1)CCCO[C@@H]1[C@H](N)C[C@H]([C@@H]([C@H]1O)O)N)C)O)O	CGCGCUUGCGAGUGCGCG	B-13	Target_lig_1138	RNA hairpin loop Iva	Target_382	6.318758762624441
2096	N[C@@H]1C[C@H](N)[C@H]([C@H]([C@H]1OCCCc1nnn(c1)Cc1ccccc(n1)Cn1nnc(c1)CCCO[C@@H]1[C@H](N)C[C@H]([C@@H]([C@H]1O)O)N)O)O	CGCGCUUGCGAGUGCGCG	B-14	Target_lig_1139	RNA hairpin loop Iva	Target_382	5.649751981666584
2112	CN(C)C1=CC2=C(C=C1)C(=C3C=CC(=[N+](C)C)C=C3O2)C4=CC=CC=C4	GGGAAGGGAAGAAACUGCGGCUUCGGCCGGCUUCCC	Tetramethylrosamine (TMR)	Target_lig_1151	Aptamer	Target_6	7.301029995666398
2113	CN(C)C1=CC2=C(C=C1)C=C3C=CC(=[N+](C)C)C=C3O2.[Cl-]	GGGAAGGGAAGAAACUGCGGCUUCGGCCGGCUUCCC	Pyronin Y	Target_lig_1152	Aptamer	Target_6	6.647817481888864
2114	CN(C)C1=CC2=C(C=C1)C(=C3C=CC(=[N+](C)C)C=C3O2)C4=CC=CC=C4	GGUACCCGACUGGCGAGAGCCAGGCAACGAAUGGUACC	Tetramethylrosamine (TMR)	Target_lig_1151	Aptamer mutant C25	Target_383	6.434152181326 48
2115	CN(C)C1=CC2=C(C=C1)C(=C3C=CC(=[N+](C)C)C=C3O2)C4=CC=CC=C4	GGUACCCGACUGGCGAGAGCCAGGGAACGAAUGGUACC	Tetramethylrosamine (TMR)	Target_lig_1151	Aptamer mutant G25	Target_384	5.721246399047717
2116	CN(C)C1=CC2=C(C=C1)C(=C3C=CC(=[N+](C)C)C=C3O2)C4=CC=CC=C4	GGUACCCGACUGGCGAGAGCCAGGAAACGAAUGGUACC	Tetramethylrosamine (TMR)	Target_lig_1151	Aptamer mutant A25	Target_385	5.259637310505076
2117	CN(C)C1=CC2=C(C=C1)C(=C3C=CC(=[N+](C)C)C=C3O2)C4=CC=CC=C4	GGUACCCGCCUGGCGAGAGCCAGGUAACGAAUGGUACC	Tetramethylrosamine (TMR)	Target_lig_1151	Aptamer mutant C9	Target_386	5.537602002101 04
2118	CN(C)C1=CC2=C(C=C1)C(=C	GGUACCCGGCUGGCGAGAGCCAGGUAAC	Tetramethylrosamine (TMR)	Target_lig_1151	Aptamer mutant G9	Target_387	7.193820026016 11

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	3C=CC(=[N+](C)C)C=C3O2)C4=CC=CC=C4	GAAUGGUACC					
2119	CN(C)C1=CC2=C(C=C1)C(=C3C=CC(=[N+](C)C)C=C3O2)C4=CC=CC=C4	GGUACCCGUCUGGCGAGAGCCAGGUAACGAAUGGUACC	Tetramethylrosamine (TMR)	Target_lig_1151	Aptamer mutant U9	Target_388	6.85387196432176
2120	CN(C)C1=CC2=C(C=C1)C(=C3C=CC(=[N+](C)C)C=C3O2)C4=CC=CC=C4	GGUACCCGACUGGCGAGAGCCAGGUAACGGAUGGUACC	Tetramethylrosamine (TMR)	Target_lig_1151	Aptamer mutant G30	Target_389	5.79588001734408
2121	CN(C)C1=CC2=C(C=C1)C(=C3C=CC(=[N+](C)C)C=C3O2)C4=CC=CC=C4	GGUACCCGACUGGCGAGAGCCAGGUAACGCAUGGUACC	Tetramethylrosamine (TMR)	Target_lig_1151	Aptamer mutant C30	Target_390	6.30102999566398
2122	CN(C)C1=CC2=C(C=C1)C(=C3C=CC(=[N+](C)C)C=C3O2)C4=CC=CC=C4	GGUACCCGACUGGCGAGAGCCAGGUAACGUAUGGUACC	Tetramethylrosamine (TMR)	Target_lig_1151	Aptamer mutant U30	Target_391	5.337242168318 43
2123	CN(C)C1=CC2=C(C=C1)C(=C3C=CC(=[N+](C)C)C=C3O2)C4=CC=CC=C4	GGUACCCGACUGGCGAGAGCCAGGUACCGAAUGGUACC	Tetramethylrosamine (TMR)	Target_lig_1151	Aptamer mutant C27	Target_392	5.396855627379982
2124	CN(C)C1=CC2=C(C=C1)C(=C3C=CC(=[N+](C)C)C=C3O2)C4=CC=CC=C4	GGUACCCGACUGGCGAGAGCCAGGUAGCGAAUGGUACC	Tetramethylrosamine (TMR)	Target_lig_1151	Aptamer mutant G27	Target_393	5.455559862682 31
2125	CN(C)C1=CC2=C(C=C1)C(=C3C=CC(=[N+](C)C)C=C3O2)C4=CC=CC=C4	GGUACCCGACUGGCGAGAGCCAGGUAUCGAAUGGUACC	Tetramethylrosamine (TMR)	Target_lig_1151	Aptamer mutant U27	Target_394	5.124938736 6083
2126	CN(C)C1=CC2=C(C=C1)C(=C3C=CC(=[N+](C)C)C=C3O2)C4=CC=CC=C4	GGUACCCGAGUGGCGAGAGCCACGUAACGAAUGGUACC	Tetramethylrosamine (TMR)	Target_lig_1151	Aptamer mutant G10C23	Target_395	6.471083299722235
2127	CN(C)C1=CC2=C(C=C1)C(=C3C=CC(=[N+](C)C)C=C3O2)C4=CC=CC=C4	GGUACCCGACUGGCGAGAGCCAGGUGACGAAUGGUACC	Tetramethylrosamine (TMR)	Target_lig_1151	Aptamer mutant G26	Target_396	5.070581074285 71
2128	CN(C)C1=CC2=C(C=C1)C(=C3C=CC(=[N+](C)C)C=C3O2)C4=CC=CC=C4	GGUACCCGACUGGCGAGAGCCAGGUUACGAAUGGUACC	Tetramethylrosamine (TMR)	Target_lig_1151	Aptamer mutant U26	Target_397	5.346787486224 66
2129	CN(C)C1=CC2=C(C=C1)C(=C3C=CC(=[N+](C)C)C=C3O2)C4=CC=CC=C4	GGUACCCGACUGGCGAGAGCCAGGUCACGAAUGGUACC	Tetramethylrosamine (TMR)	Target_lig_1151	Aptamer mutant C26	Target_398	5.221848749616 36
2130	CN(C)C1=CC2=C(C=C1)C(=C3C=CC(=[N+](C)C)C=C3O2)C4=CC=CC=C4	GGUACCCGACAGGCGAGAGCCUGGUAACGAAUGGUACC	Tetramethylrosamine (TMR)	Target_lig_1151	Aptamer mutant A11U22	Target_399	7.318758762624 41
2131	CN(C)C1=CC2=C(C=C1)C(=C3C=CC(=[N+](C)C)C=C3O2)	GGUACCCGACUGGCGAGAGCCAGCUAACGAAUGGUACC	Tetramethylrosamine (TMR)	Target_lig_1151	Aptamer mutant C24	Target_400	6.290730039024 17

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	C4=CC=CC=C4						
2132	CN(C)C1=CC2=C(C=C1)C(=C3C=CC(=[N+](C)C)C=C3O2)C4=CC=CC=C4	GGUACCCGACUGGCGAGAGCCAGGUAACGAGUGGUACC	Tetramethylrosamine (TMR)	Target_lig_1151	Aptamer mutant G31	Target_401	5.14266750356873
2133	CN(C)C1=CC2=C(C=C1)C(=C3C=CC(=[N+](C)C)C=C3O2)C4=CC=CC=C4	GGUACCCGACUGGCGAGAGCCAGGUAACGACUGGUACC	Tetramethylrosamine (TMR)	Target_lig_1151	Aptamer mutant C31	Target_402	5.92081875395238
2134	CN(C)C1=CC2=C(C=C1)C(=C3C=CC(=[N+](C)C)C=C3O2)C4=CC=CC=C4	GGUACCCGACUGGCGAGAGCCAGGUAACGAUUGGUACC	Tetramethylrosamine (TMR)	Target_lig_1151	Aptamer mutant U31	Target_403	5.70996538863748
2135	CN(C)C1=CC2=C(C=C1)C(=C3C=CC(=[N+](C)C)C=C3O2)C4=CC=CC=C4	GGUACCCCACUGGCGAGAGCCAGGUAAGGAAUGGUACC	Tetramethylrosamine (TMR)	Target_lig_1151	Aptamer mutant C8G28	Target_404	5.25963731050576
2170	CC1(COC(C(C1NC)O)OC2C(CC(C(C2O)OC3C(CC=C(O3)CN)N)N)N)O	GAAGACAGCCGCUUCUACGAGCAU	sisomicin	Target_lig_10	E. coli transglycosidase mRNA	Target_407	4.92081875395238
2171	[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)N)O[C@@H]1[C@H]([C@@H]([C@H]([C@@H](O1)CNc1c2cccc2nc2c1cccc2)O)N)O	GAAGACAGCCGCUUCUACGAGCAU	Tobramycin	Target_lig_540	E. coli transglycosidase mRNA	Target_407	4.721246399047717
2172	C1C(C(C(C(C1N)OC2C(C(C(O2)CN)O)O)N)OC3C(C(C(O3)CO)OC4C(C(C(C(O4)CN)O)O)N)O)O)N	GAAGACAGCCGCUUCUACGAGCAU	Neomycin B	Target_lig_1251	E. coli transglycosidase mRNA	Target_407	5.552841968665778
2173	NCC1OC(OC2C(N)CC(C(C2O)OC2OC(CN)C(C(C2O)O)N)N)C(CC1O)N	GAAGACAGCCGCUUCUACGAGCAU	Compd 32	Target_lig_1155	E. coli transglycosidase mRNA	Target_407	4.958607314844177
2174	NCC1OC(OC2C(N)CC(C(C2O)OC2OC(CN)C(CC2N)O)N)C(C(C1OC1OC(CO)C(C(C1O)O)N)N)O	GAAGACAGCCGCUUCUACGAGCAU	Compd 33	Target_lig_1156	E. coli transglycosidase mRNA	Target_407	5.744727494889669
2175	NCC1OC(OC2C(N)CC(C(C2O)OC2OC(CN)C(CC2N)O)N)C(C(C1OC1OC(CO)C(C(C1O)N)O)O)N	GAAGACAGCCGCUUCUACGAGCAU	Compd 34	Target_lig_1157	E. coli transglycosidase mRNA	Target_407	6.207608310500175

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
2176	NCC1OC(OC2C(N)CC(C(C2O)OC2OC(CN)C(C(C2O)N)O)N)C(CC1O)N	GAAGACAGCCGCUUCUACGAGCAU	Compd 35	Target_lig_1158	E. coli transglycosidase mRNA	Target_407	5.309803919997149
2177	NCC1OC(OC2C(N)CC(C(C2O)OC2OC(COC3OC(CO)C(C(C3N)O)O)C(C(C2N)O)O)N)C(CC1O)N	GAAGACAGCCGCUUCUACGAGCAU	Compd 36	Target_lig_1163	E. coli transglycosidase mRNA	Target_407	5.275724130399921
2178	NCC1OC(OC2C(N)CC(C(C2O)OC2OC(CN)C(CC2N)O)N)C(C(C1O)OC1OC(CO)C(C(C1O)O)N)O	GAAGACAGCCGCUUCUACGAGCAU	Compd 37	Target_lig_1159	E. coli transglycosidase mRNA	Target_407	4.853871964321762176
2179	NCC1OC(OC2C(N)CC(C(C2O)OC2OC(CN)C(CC2N)O)N)C(C(C1OC1OC(CO)C(C(C1N)O)O)N)O	GAAGACAGCCGCUUCUACGAGCAU	Compd 38	Target_lig_1160	E. coli transglycosidase mRNA	Target_407	6
2180	NCC1OC(OC2C(N)CC(C(C2O)OC2OC(COC3OC(CN)C(C(C3O)O)O)C(C(C2N)O)N)N)C(CC1O)N	GAAGACAGCCGCUUCUACGAGCAU	Compd 39	Target_lig_1161	E. coli transglycosidase mRNA	Target_407	6.376750709602 1
2181	NCC1OC(OC2C(N)CC(C(C2O)OC2OC(COC3OC(CN)C(C(C3O)O)O)C(C(C2N)O)N)N)C(CC1O)N	GAAGACAGCCGCUUCUACGAGCAU	Compd 40	Target_lig_1281	E. coli transglycosidase mRNA	Target_407	5.096910013 00806
2182	NCC1OC(OC2C(N)CC(C(C2O)OC2OC(CN)C(CC2N)O)N)C(C(C1O)OC1OC(CO)C(C(C1N)O)O)N	GAAGACAGCCGCUUCUACGAGCAU	Compd 41	Target_lig_1162	E. coli transglycosidase mRNA	Target_407	6.173925197 29917
2183	NCC1OC(OC2C(N)CC(C(C2O)OC2OC(CN)C(CC2N)O)N)C(C(C1O)OC1OC(CO)C(C(C1N)O)O)N	GAAGACAGCCGCUUCUACGAGCAU	Compd 42	Target_lig_1282	E. coli transglycosidase mRNA	Target_407	5.602059991 32796
2184	NCC1OC(OC2C(N)CC(C(C2O)OC2OC(CN)C(CC2N)O)N)C(C(C1OC1OC(CO)C(C(C1N)O)O)N)O	GAAGACAGCCGCUUCUACGAGCAU	Compd 43	Target_lig_1283	E. coli transglycosidase mRNA	Target_407	5.769551078 62173
2245	CC1(COC(C(C1NC)O)OC2C(CC(C(C2O)OC3C(CC=C(O3)CN)N)N)N)O	GCCAACCCACCUAACUACGGAAAACCUGAUCCC	sisomicin	Target_lig_10	human tyrosine sulfotransferase mRNA	Target_410	4.431798275 93301
2246	[C@H]1([C@H](C[C@H]([C@H]	GCCAACCCACCUAACUACGGAAAACCUGAUCCC	Tobramycin	Target_lig_540	human tyrosine sulfotransferase mRNA	Target_410	4.187086643 35714

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	([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						
2247	C1C(C(C(C(C1N)OC2C(C(C(C(O2)CN)O)O)N)OC3C(C(C(O3)CO)O)C4C(C(C(C(O4)CN)O)O)N)O)O)N	GCCAACCCACCUAACUACGGAAAACCUGAUCCC	Neomycin B	Target_lig_1251	human tyrosine sulfotransferase mRNA	Target_410	6.522878745280034
2248	NCC1OC(OC2C(N)CC(C(C2O)OC2OC(CN)C(C(C2O)O)N)N)C(CC1O)N	GCCAACCCACCUAACUACGGAAAACCUGAUCCC	Compd 32	Target_lig_1155	human tyrosine sulfotransferase mRNA	Target_410	4.602059991327796
2249	NCC1OC(OC2C(N)CC(C(C2O)OC2OC(CN)C(CC2N)O)N)C(C(C1OC1OC(CO)C(C(C1O)O)N)N)O	GCCAACCCACCUAACUACGGAAAACCUGAUCCC	Compd 33	Target_lig_1156	human tyrosine sulfotransferase mRNA	Target_410	5.795880017344408
2250	NCC1OC(OC2C(N)CC(C(C2O)OC2OC(CN)C(CC2N)O)N)C(C(C1OC1OC(CO)C(C(C1O)N)O)O)N	GCCAACCCACCUAACUACGGAAAACCUGAUCCC	Compd 34	Target_lig_1157	human tyrosine sulfotransferase mRNA	Target_410	5.026872146400 3
2251	NCC1OC(OC2C(N)CC(C(C2O)OC2OC(CN)C(C(C2O)N)O)N)C(CC1O)N	GCCAACCCACCUAACUACGGAAAACCUGAUCCC	Compd 35	Target_lig_1158	human tyrosine sulfotransferase mRNA	Target_410	5.091514981121 35
2252	NCC1OC(OC2C(N)CC(C(C2O)OC2OC(CN)C(CC2N)O)N)C(C(C1O)OC1OC(CO)C(C(C1O)O)N)O	GCCAACCCACCUAACUACGGAAAACCUGAUCCC	Compd 37	Target_lig_1159	human tyrosine sulfotransferase mRNA	Target_410	4.283996656 3652
2253	NCC1OC(OC2C(N)CC(C(C2O)OC2OC(CN)C(CC2N)O)N)C(C(C1OC1OC(CO)C(C(C1N)O)O)N)O	GCCAACCCACCUAACUACGGAAAACCUGAUCCC	Compd 38	Target_lig_1160	human tyrosine sulfotransferase mRNA	Target_410	4.853871964 32176
2254	NCC1OC(OC2C(N)CC(C(C2O)OC2OC(COC3OC(CN)C(C(C3O)O)O)C(C(C2N)O)N)N)C(CC1O)N	GCCAACCCACCUAACUACGGAAAACCUGAUCCC	Compd 39	Target_lig_1161	human tyrosine sulfotransferase mRNA	Target_410	5.017728766 96043
2255	NCC1OC(OC2C(N)CC(C(C2O)OC2OC(COC3OC(CN)C(C(C3	GCCAACCCACCUAACUACGGAAAACCUGAUCCC	Compd 40	Target_lig_1281	human tyrosine sulfotransferase mRNA	Target_410	4.886056647693316

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	O)O)O)C(C(C2N)O)N)N)C(CC1O)N						
2256	NCC1OC(OC2C(N)CC(C(C2O)OC2OC(CN)C(CC2N)O)N)C(C(C1O)OC1OC(CO)C(C(C1N)O)O)N	GCCAACCCACCUAACUACGGAAAACCUGAUCCC	Compd 41	Target_lig_1162	human tyrosine sulfotransferase mRNA	Target_410	5.026872146403
2257	NCC1OC(OC2C(N)CC(C(C2O)OC2OC(CN)C(CC2N)O)N)C(C(C1O)OC1OC(CO)C(C(C1N)O)O)N	GCCAACCCACCUAACUACGGAAAACCUGAUCCC	Compd 42	Target_lig_1282	human tyrosine sulfotransferase mRNA	Target_410	5.408935392973 5
2258	NCC1OC(OC2C(N)CC(C(C2O)OC2OC(CN)C(CC2N)O)N)C(C(C1OC1OC(CO)C(C(C1N)O)O)N)O	GCCAACCCACCUAACUACGGAAAACCUGAUCCC	Compd 43	Target_lig_1283	human tyrosine sulfotransferase mRNA	Target_410	5.292429823 90206
2398	Coc1ccc2c(c1)c(Nc1ccc(c(c1)CN1CCN(CC1)C)O)c1c(n2)cc(cc1)Cl	AUCACCUCCUUA	Acridine_derivative_2 (AD2)	Target_lig_1231	Duplex RNA	Target_436	6.060480747 38138
2399	CCOC(=O)C1=C2C=CC=CN2C3=C1C(=O)C4=CC=CC=C4C3=O	AUCACCUCCUUA	NSC119236	Target_lig_1232	Duplex RNA	Target_436	5.522878745 28034
2400	C[N+](CCN[N+]1(C)CCCc2c1cccc2)(C)C	AUCACCUCCUUA	SL3_compound_6	Target_lig_1233	Duplex RNA	Target_436	5.214670164 98923
2401	CC1=NC2=NC(=NN2C(=C1)N3CCN(CC3)C)C4=CC=C(C=C4)Cl	AUCACCUCCUUA	methylpiperazine derivative	Target_lig_498	Duplex RNA	Target_436	4.161150909 26274
2402	CC1=C(C(=O)C2=C(C1=O)N3C[C@H]4[C@@H](C3=C2COC(=O)N)N4C)OC	AUCACCUCCUUA	methyl_carbamate derivative	Target_lig_499	Duplex RNA	Target_436	3.462180904 92673
2403	Coc1ccc2c(c1)c(Nc1ccc(c(c1)CN1CCN(CC1)C)O)c1c(n2)cc(cc1)Cl	AUCACCUCCUUA	Acridine_derivative_2 (AD2)	Target_lig_1231	Single_stranded_RNA	Target_437	5.522878745 28034
2404	CCOC(=O)C1=C2C=CC=CN2C3=C1C(=O)C4=CC=CC=C4C3=O	AUCACCUCCUUA	NSC119236	Target_lig_1232	Single_stranded_RNA	Target_437	5.638272163 98241
2405	C[N+](CCN[N+]1(C)CCCc2c1cccc2)(C)C	AUCACCUCCUUA	SL3_compound_6	Target_lig_1233	Single_stranded_RNA	Target_437	5.107905397 30952
2406	CC1=NC2=NC(=NN2C(=C1)N3CCN(CC3)C)C4=CC=C(C=C4)Cl	AUCACCUCCUUA	methylpiperazine derivative	Target_lig_498	Single_stranded_RNA	Target_437	3.559090917 93478

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
2407	CC1=C(C(=O)C2=C(C1=O)N3C[C@H]4[C@@H](C3=C2COC(=O)N)N4C)OC	AUCACCUCCUUA	methyl_carbamate derivative	Target_lig_499	Single_stranded_RNA	Target_437	2.309803919977149
2408	C[N+](CCN[N+]1(C)CCCc2c1cccc2)(C)C	GGACUAGCGCUAGUCC	SL3_compound_6	Target_lig_1233	SL3_duplex_RNA	Target_438	4.853871964321776
2409	CC1=NC2=NC(=NN2C(=C1)N3CCN(CC3)C)C4=CC=C(C=C4)Cl	GGACUAGCGCUAGUCC	methylpiperazine derivative	Target_lig_498	SL3_duplex_RNA	Target_438	4.236572006437706
2410	CC1=C(C(=O)C2=C(C1=O)N3C[C@H]4[C@@H](C3=C2COC(=O)N)N4C)OC	GGUGCGAGAGCGUC	methyl_carbamate derivative	Target_lig_499	SL4 RNA	Target_439	4.102372908709560
2411	CC1=NC2=NC(=NN2C(=C1)N3CCN(CC3)C)C4=CC=C(C=C4)Cl	GGCGACUGGUGAGUACGCC	methylpiperazine derivative	Target_lig_498	SL2 RNA	Target_440	4.337242168318431
2412	CC1=NC2=NC(=NN2C(=C1)N3CCN(CC3)C)C4=CC=C(C=C4)Cl	GGUGCGAGAGCGUC	methylpiperazine derivative	Target_lig_498	SL4 RNA	Target_439	4.154901959985574
2413	CC(=[NH+]CCCC[C@@H](C(=O)[O-])[NH3+])N	GAGGGUGGAACCGCGCUUCGGCGUCCCUC	N6-1-Iminoethyl-L-lysine	Target_lig_1235	T-box riboswitch	Target_79	4.958607314841777
2414	C1C(C(C(C(C1NC(=O)C(CCN)O)O)OC2C(C(C(O2)CO)O)O)OC3C(C(C(C(O3)CN)O)O)N)N	AUUUUUCCUCGAACCCGGCGGAACGCAGAAAAAU	Butirosin	Target_lig_220	U15C,U16C SLI_mutant	Target_441	6.698970004336021
2415	C1C(C(C(C(C1NC(=O)C(CCN)O)OC2C(C(C(O2)CO)O)N)O)O)OC3C(C(C(C(O3)CN)O)O)O)N	AUUUUUCCUCGAACCCGGCGGAACGCAGAAAAAU	Amikacin	Target_lig_175	U15C,U16C SLI_mutant	Target_441	7.154901959985574
2416	C1C(C(C(C(C1N)OC2C(C(C(O2)CN)O)O)N)OC3C(C(C(O3)CO)OC4C(C(C(C(O4)CN)O)O)N)O)O)N	AUUUUUCCUCGAACCCGGCGGAACGCAGAAAAAU	Neomycin	Target_lig_4	U15C,U16C SLI_mutant	Target_441	7.154901959985574
2417	C1C(C(C(C(C1N)OC2C(C(C(O2)CO)O)N)O)O)OC3C(C(C(C(O3)CN)O)O)N)N	AUUUUUCCUCGAACCCGGCGGAACGCAGAAAAAU	KANAMYCIN B	Target_lig_8	U15C,U16C SLI_mutant	Target_441	6.958607314841777
2418	C1C(C(C(C(C1N)OC2C(C(C(O2)CN)O)O)O)O)OC3C(C(C(C(O3)CO)O)N)O)N	AUUUUUCCUCGAACCCGGCGGAACGCAGAAAAAU	Kanamycin A	Target_lig_7	U15C,U16C SLI_mutant	Target_441	6.537602002101104
2419	CC1(COC(C(C1	AUUUUUCCUCGAAC	gentamicin_mol	Target_lig_76	U15C,U16C	Target_441	7.2218487496

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	NC)O)OC2C(CC(C(C2O)OC3C(CCC(O3)CN)N)N)N)O	CCGGCGGAACGCAGAAAAAU			SLI_mutant		1636
2420	[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)N)O[C@@H]1[C@H]([C@@H]([C@H]([C@@H](O1)CNc1c2ccccc2nc2c1cccc2)O)N)O	AUUUUUCCUCGAACCCGGCGGAACGCAGAAAAAU	Tobramycin	Target_lig_540	U15C,U16C SLI_mutant	Target_441	7.045757490560 68
2421	CC1(COC(C(C1NC)O)OC2C(CC(C(C2O)OC3C(CC=C(O3)CN)N)N)N)O	AUUUUUCCUCGAACCCGGCGGAACGCAGAAAAAU	sisomicin	Target_lig_10	U15C,U16C SLI_mutant	Target_441	7.397940008672 04
2422	C1C(C(C(C(C1N)OC2C(C(C(O2)CO)O)O)N)OC3C(C(C(O3)CO)OC4C(C(C(C(O4)CN)O)O)N)O)O)N	AUUUUUCCUCGAACCCGGCGGAACGCAGAAAAAU	Paromomycin_mol_mol	Target_lig_1116	U15C,U16C SLI_mutant	Target_441	7.397940008672 04
2423	C1C(C(C(C(C1NC(=O)C(CCN)O)O)OC2C(C(C(O2)CO)O)O)OC3C(C(C(C(O3)CN)O)O)N)N	AUUUUUCCUCGAACUUAACGGAACGCAGAAAAAU	Butirosin	Target_lig_220	G17A,G18A SLI_mutant	Target_442	6.698970004336 02
2424	C1C(C(C(C(C1NC(=O)C(CCN)O)OC2C(C(C(O2)CO)O)N)O)O)OC3C(C(C(C(O3)CN)O)O)O)N	AUUUUUCCUCGAACUUAACGGAACGCAGAAAAAU	Amikacin	Target_lig_175	G17A,G18A SLI_mutant	Target_442	6.886056647693 16
2425	C1C(C(C(C(C1N)OC2C(C(C(O2)CN)O)O)N)OC3C(C(C(O3)CO)OC4C(C(C(C(O4)CN)O)O)N)O)O)N	AUUUUUCCUCGAACUUAACGGAACGCAGAAAAAU	Neomycin	Target_lig_4	G17A,G18A SLI_mutant	Target_442	7.301029995663 98
2426	C1C(C(C(C(C1N)OC2C(C(C(O2)CO)O)N)O)O)OC3C(C(C(C(O3)CN)O)O)N)N	AUUUUUCCUCGAACUUAACGGAACGCAGAAAAAU	KANAMYCIN B	Target_lig_8	G17A,G18A SLI_mutant	Target_442	7
2427	C1C(C(C(C(C1N)OC2C(C(C(O2)CN)O)O)O)O)OC3C(C(C(C(O3)CO)O)N)O)N	AUUUUUCCUCGAACUUAACGGAACGCAGAAAAAU	Kanamycin A	Target_lig_7	G17A,G18A SLI_mutant	Target_442	6.920818753952 38
2428	CC1(COC(C(C1NC)O)OC2C(CC(C(C2O)OC3C(CCC(O3)CN)N)N)N)O	AUUUUUCCUCGAACUUAACGGAACGCAGAAAAAU	gentamicin_mol	Target_lig_76	G17A,G18A SLI_mutant	Target_442	7

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
2429	[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)N)O[C@@H]1[C@H]([C@@H]([C@H]([C@@H](O1)CNc1c2cccc2nc2c1cccc2)O)N)O	AUUUUUCCUCGAACUUAACGGAACGCAGAAAAAU	Tobramycin	Target_lig_540	G17A,G18A SLI_mutant	Target_442	7.522878745280034
2430	CC1(COC(C(C1NC)O)OC2C(CC(C(C2O)OC3C(CC=C(O3)CN)N)N)N)O	AUUUUUCCUCGAACUUAACGGAACGCAGAAAAAU	sisomicin	Target_lig_10	G17A,G18A SLI_mutant	Target_442	7.397940008677204
2431	C1C(C(C(C(C1N)OC2C(C(C(O2)CO)O)O)N)OC3C(C(C(O3)CO)OC4C(C(C(C(O4)CN)O)O)N)O)O)N	AUUUUUCCUCGAACUUAACGGAACGCAGAAAAAU	Paromomycin_mol_mol	Target_lig_1116	G17A,G18A SLI_mutant	Target_442	7.301029995566398
2432	C1C(C(C(C(C1NC(=O)C(CCN)O)O)OC2C(C(C(O2)CO)O)O)OC3C(C(C(C(O3)CN)O)O)N)N	AUUUUUCCUCGAACUUGGUAGAACGCAGAAAAAU	Butirosin	Target_lig_220	C19U,G20A SLI_mutant	Target_443	6.823908740944432
2433	C1C(C(C(C(C1NC(=O)C(CCN)O)OC2C(C(C(O2)CO)O)N)O)O)OC3C(C(C(C(O3)CN)O)O)O)N	AUUUUUCCUCGAACUUGGUAGAACGCAGAAAAAU	Amikacin	Target_lig_175	C19U,G20A SLI_mutant	Target_443	7.154901959985574
2434	C1C(C(C(C(C1N)OC2C(C(C(O2)CN)O)O)N)OC3C(C(C(O3)CO)OC4C(C(C(C(O4)CN)O)O)N)O)O)N	AUUUUUCCUCGAACUUGGUAGAACGCAGAAAAAU	Neomycin	Target_lig_4	C19U,G20A SLI_mutant	Target_443	7.301029995566398
2435	C1C(C(C(C(C1N)OC2C(C(C(O2)CO)O)N)O)O)OC3C(C(C(C(O3)CN)O)O)N)N	AUUUUUCCUCGAACUUGGUAGAACGCAGAAAAAU	KANAMYCIN B	Target_lig_8	C19U,G20A SLI_mutant	Target_443	7
2436	C1C(C(C(C(C1N)OC2C(C(C(O2)CN)O)O)O)O)OC3C(C(C(C(O3)CO)O)N)O)N	AUUUUUCCUCGAACUUGGUAGAACGCAGAAAAAU	Kanamycin A	Target_lig_7	C19U,G20A SLI_mutant	Target_443	6.522878745280034
2437	CC1(COC(C(C1NC)O)OC2C(CC(C(C2O)OC3C(CCC(O3)CN)N)N)N)O	AUUUUUCCUCGAACUUGGUAGAACGCAGAAAAAU	gentamicin_mol	Target_lig_76	C19U,G20A SLI_mutant	Target_443	7.154901959985574
2438	[C@H]1([C@H](C[C@H]([C@H]([C@H]1O)O[C	AUUUUUCCUCGAACUUGGUAGAACGCAGAAAAAU	Tobramycin	Target_lig_540	C19U,G20A SLI_mutant	Target_443	7.221848749661636

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	@@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)CNc1c2cccc2nc2c1cccc2)O)N)O						
2439	CC1(COC(C(C1NC)O)OC2C(CC(C(C2O)OC3C(CC=C(O3)CN)N)N)N)O	AUUUUUCCUCGAACUUGGUAGAACGCAGAAAAAU	sisomicin	Target_lig_10	C19U,G20ASLI_mutant	Target_443	7.522878745280034
2440	C1C(C(C(C(C1N)OC2C(C(C(O2)CO)O)O)N)OC3C(C(C(O3)CO)OC4C(C(C(C(O4)CN)O)O)N)O)O)N	AUUUUUCCUCGAACUUGGUAGAACGCAGAAAAAU	Paromomycin_mol_mol	Target_lig_1116	C19U,G20ASLI_mutant	Target_443	7.301029995566398
2441	C1C(C(C(C(C1NC(=O)C(CCN)O)O)OC2C(C(C(O2)CO)O)O)OC3C(C(C(C(O3)CN)O)O)N)N	AUUUUUCCUCGAACUUGGCGAGACGCAGAAAAAU	Butirosin	Target_lig_220	G21A,A22GSLI_mutant	Target_444	6.585026652029 18
2442	C1C(C(C(C(C1NC(=O)C(CCN)O)OC2C(C(C(O2)CO)O)N)O)O)OC3C(C(C(C(O3)CN)O)O)O)N	AUUUUUCCUCGAACUUGGCGAGACGCAGAAAAAU	Amikacin	Target_lig_175	G21A,A22GSLI_mutant	Target_444	6.920818753955238
2443	C1C(C(C(C(C1N)OC2C(C(C(O2)CN)O)O)N)OC3C(C(C(O3)CO)OC4C(C(C(C(O4)CN)O)O)N)O)O)N	AUUUUUCCUCGAACUUGGCGAGACGCAGAAAAAU	Neomycin	Target_lig_4	G21A,A22GSLI_mutant	Target_444	7.522878745280034
2444	C1C(C(C(C(C1N)OC2C(C(C(O2)CO)O)N)O)O)OC3C(C(C(C(O3)CN)O)O)N)N	AUUUUUCCUCGAACUUGGCGAGACGCAGAAAAAU	KANAMYCIN B	Target_lig_8	G21A,A22GSLI_mutant	Target_444	6.886056647693 16
2445	C1C(C(C(C(C1N)OC2C(C(C(O2)CN)O)O)O)O)OC3C(C(C(C(O3)CO)O)N)O)N	AUUUUUCCUCGAACUUGGCGAGACGCAGAAAAAU	Kanamycin A	Target_lig_7	G21A,A22GSLI_mutant	Target_444	6.619788758288839
2446	CC1(COC(C(C1NC)O)OC2C(CC(C(C2O)OC3C(CCC(O3)CN)N)N)N)O	AUUUUUCCUCGAACUUGGCGAGACGCAGAAAAAU	gentamicin_mol	Target_lig_76	G21A,A22GSLI_mutant	Target_444	7.045757490560 68
2447	[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)	AUUUUUCCUCGAACUUGGCGAGACGCAGAAAAAU	Tobramycin	Target_lig_540	G21A,A22GSLI_mutant	Target_444	7.154901959985574

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	N)O[C@@H]1[C@H]([C@@H]([C@H]([C@@H](O1)CNc1c2ccccc2nc2c1cccc2)O)N)O						
2448	CC1(COC(C(C1NC)O)OC2C(CC(C(C2O)OC3C(CC=C(O3)CN)N)N)N)O	AUUUUUCCUCGAACUUGGCGAGACGCAGAAAAAU	sisomicin	Target_lig_10	G21A,A22G SLI_mutant	Target_444	7.221848749616361636
2449	C1C(C(C(C(C1N)OC2C(C(C(O2)CO)O)O)N)OC3C(C(C(O3)CO)OC4C(C(C(C(O4)CN)O)O)N)O)O)N	AUUUUUCCUCGAACUUGGCGAGACGCAGAAAAAU	Paromomycin_mol_mol	Target_lig_1116	G21A,A22G SLI_mutant	Target_444	7.301029995566398
2450	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	CCCCCCCGCCGCGCCAUGCCUGUGGCCGGUCGG	CRP	Target_lig_147	Thymidylate synthase m-RNA	Target_63	6.134896025358887
2451	CNC1C(O)C(OCC1(C)O)OC1C(N)CC(C(C1O)OC1OC(CCC1N)C(CCNC(=O)c1ccc(c(c1)C(=O)O)c1c2ccc(=[N+](C)C)cc2oc2c1ccc(c2)N(C)C)C)N	CCCCCCCGCCGCGCCAUGCCUGUGGCCGGUCGG	CRG	Target_lig_1236	Thymidylate synthase m-RNA	Target_63	6.071092309775605
2452	OCC1OC(OC2C(N)CC(C(C2O)OC2OC(CNC(=O)c3ccc(c(c3)C(=O)O)c3c4ccc(=[N+](C)C)cc4oc4c3ccc(c4)N(C)C)C(CC2N)O)N)C(C(C1O)N)O	CCCCCCCGCCGCGCCAUGCCUGUGGCCGGUCGG	CRT	Target_lig_993	Thymidylate synthase m-RNA	Target_63	6.088842391260002
2453	OCC1OC(OC2C(N)CC(C(C2O)OC2OC(CNC(=O)c3ccc(c(c3)C(=O)O)c3c4ccc(=[N+](C)C)cc4oc4c3ccc(c4)N(C)C)C(C(C2N)O)O)N)C(C(C1O)N)O	CCCCCCCGCCGCGCCAUGCCUGUGGCCGGUCGG	CRK	Target_lig_1238	Thymidylate synthase m-RNA	Target_63	6.023650020996673
2454	C1C(C(C(C(C1N)OC2C(C(C(O2)CN)O)O)N)OC3C(C(C(O3)CO)OC4C(C(C(C(O4)CN)O)O)N)O)O)N	CCCCCCCGCCGCGCCAUGCCUGUGGCCGGGGGG	Neomycin	Target_lig_4	TS mRNA Construct_4	Target_445	6.010105436281238123
2455	C1C(C(C(C(C1N)OC2C(C(C(O2)CO)O)O)N)	CCCCCCCGCCGCGCCAUGCCUGUGGCCGGGGGG	Paromomycin_mol_mol	Target_lig_1116	TS mRNA Construct_4	Target_445	5.729787145110376

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	OC3C(C(C(O3)CO)OC4C(C(C(O4)CN)O)O)N)O)O)N						
2456	CC1(COC(C(C1NC)O)OC2C(CC(C(C2O)OC3C(CCC(O3)CN)N)N)N)O	CCCCCCCGCCGCGCCAUGCCUGUGGCCGGGGGG	gentamicin_mol	Target_lig_76	TS mRNA Construct_4	Target_445	5.594482893023362
2457	[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)N)O[C@@H]1[C@H]([C@@H]([C@H]([C@@H](O1)CNc1c2ccccc2nc2c1cccc2)O)N)O	CCCCCCCGCCGCGCCAUGCCUGUGGCCGGGGGG	Tobramycin	Target_lig_540	TS mRNA Construct_4	Target_445	5.639785386704650
2458	C1C(C(C(C(C1N)OC2C(C(C(O2)CO)O)N)O)O)OC3C(C(C(C(O3)CN)O)O)N)N	CCCCCCCGCCGCGCCAUGCCUGUGGCCGGGGGG	KANAMYCIN B	Target_lig_8	TS mRNA Construct_4	Target_445	5.614751317596678
2459	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	CCCCCCCGCCGCGCCAUGCCUGUGGCCGGGGGG	CRP	Target_lig_147	TS mRNA Construct_4	Target_445	6.146301788223830
2460	CNC1C(O)C(OCC1(C)O)OC1C(N)CC(C(C1O)OC1OC(CCC1N)C(CCNC(=O)c1ccc(c(c1)C(=O)O)c1c2ccc(=[N+](C)C)cc2oc2c1ccc(c2)N(C)C)C)N	CCCCCCCGCCGCGCCAUGCCUGUGGCCGGGGGG	CRG	Target_lig_1236	TS mRNA Construct_4	Target_445	6.036684488613890
2461	OCC1OC(OC2C(N)CC(C(C2O)OC2OC(CNC(=O)c3ccc(c(c3)C(=O)O)c3c4ccc(=[N+](C)C)cc4oc4c3ccc(c4)N(C)C)C(CC2N)O)N)C(C(C1O)N)O	CCCCCCCGCCGCGCCAUGCCUGUGGCCGGGGGG	CRT	Target_lig_993	TS mRNA Construct_4	Target_445	6.057000406633396
2462	OCC1OC(OC2C(N)CC(C(C2O)OC2OC(CNC(=O)c3ccc(c(c3)C(=O)O)c3c4ccc(=[N+](C)C)cc4oc4c3ccc(c4)N(C)C)C(C(C2N)O)O)N)C(C(C1O)N)O	CCCCCCCGCCGCGCCAUGCCUGUGGCCGGGGGG	CRK	Target_lig_1238	TS mRNA Construct_4	Target_445	5.955852379121280

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
2463	C1C(C(C(C(C1N)OC2C(C(C(O2)CN)O)O)N)OC3C(C(C(O3)CO)OC4C(C(C(O4)CN)O)O)N)O)O)N	CCCCCGCCACCUUCGGGUGGCCGGGG	Neomycin	Target_lig_4	TS mRNA Construct_5	Target_446	5.839231438138887
2464	C1C(C(C(C(C1N)OC2C(C(C(O2)CO)O)O)N)OC3C(C(C(O3)CO)OC4C(C(C(O4)CN)O)O)N)O)O)N	CCCCCGCCACCUUCGGGUGGCCGGGG	Paromomycin_mol_mol	Target_lig_1116	TS mRNA Construct_5	Target_446	5.649558143466494
2465	CC1(COC(C(C1NC)O)OC2C(CC(C(C2O)OC3C(CCC(O3)CN)N)N)O)O	CCCCCGCCACCUUCGGGUGGCCGGGG	gentamicin_mol	Target_lig_76	TS mRNA Construct_5	Target_446	5.547753425479956
2466	[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)N)O[C@@H]1[C@H]([C@@H]([C@H]([C@@H](O1)CNc1c2ccccc2nc2c1cccc2)O)N)O	CCCCCGCCACCUUCGGGUGGCCGGGG	Tobramycin	Target_lig_540	TS mRNA Construct_5	Target_446	5.477816682381318
2467	C1C(C(C(C(C1N)OC2C(C(C(O2)CO)O)N)O)O)OC3C(C(C(O3)CN)O)O)N)N	CCCCCGCCACCUUCGGGUGGCCGGGG	KANAMYCIN B	Target_lig_8	TS mRNA Construct_5	Target_446	5.456925764966647
2468	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	CCCCCGCCACCUUCGGGUGGCCGGGG	CRP	Target_lig_147	TS mRNA Construct_5	Target_446	5.951946826884439
2469	CNC1C(O)C(OCC1(C)O)OC1C(N)CC(C(C1O)OC1OC(CCC1N)C(CCNC(=O)c1ccc(c(c1)C(=O)O)c1c2ccc(=[N+](C)C)cc2oc2c1ccc(c2)N(C)C)C)N	CCCCCGCCACCUUCGGGUGGCCGGGG	CRG	Target_lig_1236	TS mRNA Construct_5	Target_446	5.904830648568825
2470	OCC1OC(OC2C(N)CC(C(C2O)OC2OC(CNC(=O)c3ccc(c(c3)C(=O)O)c3c4ccc(=[N+](C)C)cc4oc4c3ccc(c4)N(C)C)C(CC2N)O)N)C(C(C1O)N)O	CCCCCGCCACCUUCGGGUGGCCGGGG	CRT	Target_lig_993	TS mRNA Construct_5	Target_446	5.883060353449924

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
2471	OCC1OC(OC2C(N)CC(C(C2O)OC2OC(CNC(=O)c3ccc(c(c3)C(=O)O)c3c4ccc(=[N+](C)C)cc4oc4c3ccc(c4)N(C)C)C(C(C2N)O)O)N)C(C(C1O)N)O	CCCCCGCCACCUUCGGGUGGCCGGGG	CRK	Target_lig_1238	TS mRNA Construct_5	Target_446	5.829151796356669
2497	O=C(Cc1ccccc1)OC[C@H]1OC(=O)NC1CN1CCN(CC1)c1ccccc1	GAGGGUGGAACCGCGCUUCGGCGUCCCUC	Compound (4R,5S)-1	Target_lig_1239	Antiterminator model RNA AM1A	Target_147	4.920818753952238
2498	O=C(Cc1ccccc1)OCC1OC(=O)N[C@H]1CN1CCN(CC1)c1ccccc1	GAGGGUGGAACCGCGCUUCGGCGUCCCUC	Compound (4S,5R)-1	Target_lig_1240	Antiterminator model RNA AM1A	Target_147	4.795880017344408
2499	O=C(Nc1ccc(cc1)C(=O)C)OC[C@H]1OC(=O)NC1CN1CCN(CC1)c1ccccc1	GAGGGUGGAACCGCGCUUCGGCGUCCCUC	Compound (4R,5S)-2	Target_lig_1241	Antiterminator model RNA AM1A	Target_147	5.522878745280034
2500	O=C(Nc1ccc(cc1)C(=O)C)OCC1OC(=O)N[C@H]1CN1CCN(CC1)c1ccccc1	GAGGGUGGAACCGCGCUUCGGCGUCCCUC	Compound (4S,5R)-2	Target_lig_1242	Antiterminator model RNA AM1A	Target_147	5.795880017344408
2501	O=C(Nc1ccc(cc1)C(=O)C)OC[C@H]1OC(=O)N[C@H]1CN1CCN(CC1)c1ccccc1	GAGGGUGGAACCGCGCUUCGGCGUCCCUC	Compound cis-2	Target_lig_1243	Antiterminator model RNA AM1A	Target_147	5.744727494896669