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

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
1060	CCCN(CC(=O)N(CCC)CC(=O)N(CC(N)=O)CC1=CN(CCCNC(=O)CCCOC2=C(C=C(C=C2C(C)(C)C)C2=NC3=CC(=CC=C3N2)N2CC[NH+](C)CC2)C(C)(C)C)N=N1)C(=O)CCCOC1=CC=CC(=C1)C1=NC2=CC(=CC=C2N1)C1=NC2=CC(=CC=C2N1)N1CC[NH+](C)CC1	GGGAGAGGGUUUAAUUACGAAAGUAAUUGGAUCCGCAAGG	Targaprimir-96	Target_lig_627	Pri-miR-96 RNAC (UU loop mutant to AU basepair)	Target_159	5.397940008667204
1061	CCCN(CC(=O)N(CCC)CC(=O)N(CC(N)=O)CC1=CN(CCCNC(=O)CCCOC2=C(C=C(C=C2C(C)(C)C)C2=NC3=CC(=CC=C3N2)N2CC[NH+](C)CC2)C(C)(C)C)N=N1)C(=O)CCCOC1=CC=CC(=C1)C1=NC2=CC(=CC=C2N1)C1=NC2=CC(=CC=C2N1)N1CC[NH+](C)CC1	GGGAGAGGGUUUAUUUACGAAAGUAUAUGGAUCCGCAAGG	Targaprimir-96	Target_lig_627	Pri-miR-96 RNA1 (Drosha processing site only)	Target_160	5.920818753955238
1062	CCCN(CC(=O)N(CCC)CC(=O)N(CC(N)=O)CC1=CN(CCCNC(=O)CCCOC2=C(C=C(C=C2C(C)(C)C)C2=NC3=CC(=CC=C3N2)N2CC[NH+](C)CC2)C(C)(C)C)N=N1)C(=O)CCCOC1=CC=CC(=C1)C1=NC2=CC(=CC=C2N1)C1=NC2=CC(=CC=C2N1)N1CC[NH+](C)CC1	GGGAGAGGGUUUACGAACGAAAGUUGGUGGAUCCGCAAGG	Targaprimir-96	Target_lig_627	Pri-miR-96 RNA2 (desired GG loop only)	Target_161	6.045757490560068
1063	CCCN(CC(=O)N(CCC)CC(=O)N(CC(N)=O)CC1=CN(CCCNC(=O)CCCOC2=C(C=C(C=C2C(C)(C)C)C2=NC3=CC(=CC=C3N2)N2CC[NH+](C)CC2)C(C)(C)C)N=N1)C(=O)CCCOC1=CC=CC(=C1)C1=NC2=CC(=CC=C2N1)C1=NC2=CC(=CC=C2N1)N1CC[NH+](C)CC1	GGGAGAGGGUUUACGAUUUACGAAAGUAUAUGGUGGAUCCGCAAGG	Targaprimir-96	Target_lig_627	Pri-miR-96 RNA3 (both the Drosha target site and adjacent target site)	Target_162	4.698970004336020
1064	CCCN(CC(=O)N(CCC)CC(=O)N(CC(N)=O)CC1=CN(CCCNC(=O)CCCOC2=C(C=C(C=C2C(C)(C)C)C2=NC3=CC(=CC=C3N2)N2CC[NH+](C)CC2)C(C)(C)C)N=N1)C(=O)CCCOC1=CC=CC(=C1)C1=NC2=CC(=CC=C2N1)C1=NC2=CC(=CC=C2N1)N1CC[NH+](C)CC1	GGGAGAGGGUUUACGAUUUACGAAAGUAUAUCGUGGAUCCGCAAGG	Targaprimir-96	Target_lig_627	Pri-miR-96 RNA4 (GG to GC loop mutation)	Target_163	5.920818753955238

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
1065	CCCN(CC(=O)N(CCC)CC(=O)N(CC(N)=O)CC1=CN(CCCNC(=O)CCCOC2=C(C=C(C=C2C(C)(C)C)C2=NC3=CC(=CC=C3N2)N2CC[NH+](C)CC2)C(C)(C)C)N=N1)C(=O)CCCOC1=CC=CC(=C1)C1=NC2=CC(=CC=C2N1)C1=NC2=CC(=CC=C2N1)N1CC[NH+](C)CC1	GGGAGAGGGUUUACGAUUUACGAAAGUAAAUGGUGGAUCCGCAAGG	Targaprimir-96	Target_lig_627	Pri-miR-96 RNA5 (UU loop mutant to UA loop)	Target_164	5.823908740944432
1066	CCCN(CC(=O)N(CCC)CC(=O)N(CC(N)=O)CC1=CN(CCCNC(=O)CCCOC2=C(C=C(C=C2C(C)(C)C)C2=NC3=CC(=CC=C3N2)N2CC[NH+](C)CC2)C(C)(C)C)N=N1)C(=O)CCCOC1=CC=CC(=C1)C1=NC2=CC(=CC=C2N1)C1=NC2=CC(=CC=C2N1)N1CC[NH+](C)CC1	CGCGAATTCGCGTTTTCGCGAATTCGCG	Targaprimir-96	Target_lig_627	Pri-miR-96 AT-rich DNA hairpin	Target_165	4.301029995666398
1190	CC(C)(C)C1=CC(=CC(=C1OCCCC(=O)NCCCN=[N+]=[N-])C(C)(C)C)C2=NC3=C(N2)C=C(C=C3)N4CCN(CC4)C	UGGCCGAUUUUGGCACUAGCACAUUUUUGCUUGUGUCUCUCCGCUCUGAGCAAUCAUGUGCAGUGCCAAUAUGGGAAA	Benzimidazole 1 (2014)	Target_lig_678	5'UUU/3'AUA, miR-96 Precursor Processing Site	Target_202	5.886056647693316
1191	CC(C)(C)C1=CC(=CC(=C1OCCCC(=O)NCCCN=[N+]=[N-])C(C)(C)C)C2=NC3=C(N2)C=C(C=C3)N4CCN(CC4)C	UGGCCGAUUUUGGCACUAGCACAUUUUUGCUUGUGUCUCUCCGCUCUGAGCAAUCAUGUGCAGUGCCAAUAUGGGAAA	Benzimidazole 1 (2014)	Target_lig_678	5'CGAUUU/3'GGUAUA, Expanded miR-96 Precursor Processing Site	Target_203	5.468521082957774
1271	CN1CCN(CC1)C2=CC3=C(C=C2)N=C(N3)C4=CC5=C(C=C4)N=C(N5)C6=CC(=CC=C6)OCCCC(=O)NCCCN=[N+]=[N-]	AGCCCCUGCCCACCGCACACUGCGCUGCCCCAGACCCACUGUGCGUGUGACAGCGGCUGA	Targaprimir-210	Target_lig_709	Pre-miR-210	Target_227	6.179142010560 3
1331	COC1=CC=C(C=C1)NCC(CN2C3=C(C=C(C=C3)Br)C4=C2C=CC(=C4)Br)O	GGGUUGACUGUUGAAUCUCAUGGCAACCC	Aniline_analog_2	Target_lig_726	miR-21 hairpin	Target_265	6.154901959985574
1332	COC1=CC(=C(C=C1)NCC(CN2C3=C(C=C(C=C3)Br)C4=C2C=CC(=C4)Br)O)OC	GGGUUGACUGUUGAAUCUCAUGGCAACCC	Aniline_analog_3	Target_lig_727	miR-21 hairpin	Target_265	5.522878745280 34
1333	COC1=C(C=C(C=C1)NCC(CN2C3=C(C=C(C=C3)Br)C4=C2C=CC(=C4)Br)O)OC	GGGUUGACUGUUGAAUCUCAUGGCAACCC	Aniline_analog_4	Target_lig_728	miR-21 hairpin	Target_265	5.853871964321 76
1334	CCOc1ccc(cn1)NCC(Cn1c2ccc(cc2c2c1ccc(c2)Br)Br)O	GGGUUGACUGUUGAAUCUCAUGGCAACCC	Aniline_analog_5	Target_lig_729	miR-21 hairpin	Target_265	5.318758762624 41
1335	CCCOc1ccc(cc1)NCC(Cn1c2ccc(cc2c2c1ccc(c2)Br)Br)O	GGGUUGACUGUUGAAUCUCAUGGCAACCC	Aniline_analog_6	Target_lig_730	miR-21 hairpin	Target_265	5.657577319177779
1336	OC(Cn1c2ccc(cc2c2c1ccc(c2)Br)Br)CNc1ccc(cc1)N1CCOCC1	GGGUUGACUGUUGAAUCUCAUGGCAACCC	Aniline_analog_7	Target_lig_731	miR-21 hairpin	Target_265	5.677780705266608

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
1338	CCOc1ccc(cc1Cl)NCC(Cn1c2ccc(cc2c2c1ccc(c2)Br)Br)O	GGGUUGACUGUUGAAUCUCAUGGCAACCC	Aniline_analog_9	Target_lig_733	miR-21 hairpin	Target_265	5.537602002101104
1339	C1=CC=C(C=C1)NCC(CN2C3=C(C=C(C=C3)Br)C4=C2C=CC(=C4)Br)O	GGGUUGACUGUUGAAUCUCAUGGCAACCC	Aniline_analog_10	Target_lig_734	miR-21 hairpin	Target_265	5.677780705266608
1342	CCOC1=CC=C(C=C1)NCC(CN2C3=C(C=C(C=C3)Br)C4=C2C=CC(=C4)Br)O	GGGUUGACUGUUGAAUCUCAUGGCAACCC	Aniline_analog_13	Target_lig_737	miR-21 hairpin	Target_265	5.920818753955238
1350	CCOC1=CC=C(C=C1)NCC(CN2C3=C(C=C(C=C3)Cl)C4=C2C=CC(=C4)Cl)O	GGGUUGACUGUUGAAUCUCAUGGCAACCC	Carbazole_analog_23	Target_lig_745	miR-21 hairpin	Target_265	5.494850021689009
1351	CCOc1ccc(cc1)NCC(Cn1c2ccc(cc2c(c1C)C)Br)O	GGGUUGACUGUUGAAUCUCAUGGCAACCC	Carbazole_analog_24	Target_lig_746	miR-21 hairpin	Target_265	5
1352	CCOc1ccc(cc1)NCC(CN(c1ccc(cc1)Br)c1ccc(cc1)Br)O	GGGUUGACUGUUGAAUCUCAUGGCAACCC	Carbazole_analog_25	Target_lig_747	miR-21 hairpin	Target_265	5.638272163982241
1355	CC1=CC=CC=C1NCC(CN2C3=C(C=C(C=C3)Br)C4=C2C=CC(=C4)Br)O	GGGUUGACUGUUGAAUCUCAUGGCAACCC	Aniline_analog_1	Target_lig_725	miR-21 hairpin	Target_265	5.638272163982241
1362	CC1=C(C=CC=C1Cl)NCC(CN2C3=C(C=C(C=C3)Br)C4=C2C=CC(=C4)Br)O	GGGUUGACUGUUGAAUCUCAUGGCAACCC	Aniline_analog_8	Target_lig_732	miR-21 hairpin	Target_265	5.494850021689009
1365	C1=CC(=CC(=C1)Cl)NCC(CN2C3=C(C=C(C=C3)Br)C4=C2C=CC(=C4)Br)O	GGGUUGACUGUUGAAUCUCAUGGCAACCC	Aniline_analog_11	Target_lig_735	miR-21 hairpin	Target_265	5.920818753955238
1366	OC(Cn1c2ccc(cc2c2c1ccc(c2)Br)Br)CNc1ccc2c(c1)cccc2	GGGUUGACUGUUGAAUCUCAUGGCAACCC	Aniline_analog_12	Target_lig_736	miR-21 hairpin	Target_265	6.096910013000806
1368	CC1=CC(=C(C=C1)NCC(CN2C3=C(C=C(C=C3)Br)C4=C2C=CC(=C4)Br)O)C	GGGUUGACUGUUGAAUCUCAUGGCAACCC	Aniline_analog_14	Target_lig_738	miR-21 hairpin	Target_265	5.292429823900206
1369	C1=CC=C(C=C1)NCC(CN2C3=CC=CC=C3C4=CC=CC=C42)O	GGGUUGACUGUUGAAUCUCAUGGCAACCC	Carbazole_analog_17	Target_lig_739	miR-21 hairpin	Target_265	5.080921907623932
1370	CCOC1=CC=C(C=C1)NCC(CN2C3=C(C=C(C=C3)Br)C4=CC=CC=C42)O	GGGUUGACUGUUGAAUCUCAUGGCAACCC	Carbazole_analog_18	Target_lig_740	miR-21 hairpin	Target_265	5.698970004336602
1371	OC(Cn1c2ccc(cc2c2c1cccc2)Br)CNc1ccc(cc1)N1CCOCC1	GGGUUGACUGUUGAAUCUCAUGGCAACCC	Carbazole_analog_19	Target_lig_741	miR-21 hairpin	Target_265	5.494850021689009
1372	CCOc1ccc(cc1)NCC(Cn1c2cc(Br)ccc2c2c1cc(Br)cc2)O	GGGUUGACUGUUGAAUCUCAUGGCAACCC	Carbazole_analog_20	Target_lig_742	miR-21 hairpin	Target_265	6
1373	OC(Cn1c2cc(Br)ccc2c2c1cc(Br)cc2)CNc1ccc(cc1)N1CCOCC1	GGGUUGACUGUUGAAUCUCAUGGCAACCC	Carbazole_analog_21	Target_lig_743	miR-21 hairpin	Target_265	5.677780705266608
1374	OC(Cn1c2cc(Br)ccc2c2c1cc(Br)cc2)CNc1ccccc1C	GGGUUGACUGUUGAAUCUCAUGGCAACCC	Carbazole_analog_22	Target_lig_744	miR-21 hairpin	Target_265	5.568636235844101
1378	OC(CN(c1ccc(cc1)Br)c1ccc(cc1)Br)CNc1ccc(cc1)N1CCOCC1	GGGUUGACUGUUGAAUCUCAUGGCAACCC	Carbazole_analog_26	Target_lig_748	miR-21 hairpin	Target_265	5.443697499232271
1379	OC(CN(c1ccc(cc1)Br)c1ccc(cc1)Br)CNc1ccc	GGGUUGACUGUUGAAUCUCAUGGCAA	Carbazole_analog_27	Target_lig_749	miR-21 hairpin	Target_265	5.356547323513381

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	ccc1C	CCC					
1380	CNC(=O)C1=NC=CC(=C1)OC2=CC(=C(C=C2)NC(=O)NC3=CC(=C(C=C3)Cl)C(F)(F)F)F	GGGUUGACUGUUGAAUCUCAUGGCAACCC	Regorafenib	Target_lig_750	miR-21 hairpin	Target_265	6.136677139887954
1381	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	GUGGGCCUCAAAUGUGGAGCACUAUUCUGAUGUCCAAGUGGAAAGUGCUGCGACAUUUGAGCGUCAC	Neomycin	Target_lig_4	Pre-miR-372	Target_266	2.130768280269026
1382	NCC1OC(OC2C(Cn3nnc(c3)Cn3cnc4c3ncnc4N)OC(C2O)OC2C(O)C(N)CC(C2OC2OC(CN)C(C(C2N)O)O)N)C(C(C1O)O)N	GUGGGCCUCAAAUGUGGAGCACUAUUCUGAUGUCCAAGUGGAAAGUGCUGCGACAUUUGAGCGUCAC	Neomycin_nucleobase_3a	Target_lig_751	Pre-miR-372	Target_266	3.314258261397774
1383	NCC1OC(OC2C(Cn3nnc(c3)Cn3ccc(=O)[nH]c3=O)OC(C2O)OC2C(O)C(N)CC(C2OC2OC(CN)C(C(C2N)O)O)N)C(C(C1O)O)N	GUGGGCCUCAAAUGUGGAGCACUAUUCUGAUGUCCAAGUGGAAAGUGCUGCGACAUUUGAGCGUCAC	Neomycin_nucleobase_3b	Target_lig_752	Pre-miR-372	Target_266	2.978810700930006
1384	NCC1OC(OC2C(Cn3nnc(c3)Cn3ccc(nc3=O)N)OC(C2O)OC2C(O)C(N)CC(C2OC2OC(CN)C(C(C2N)O)O)N)C(C(C1O)O)N	GUGGGCCUCAAAUGUGGAGCACUAUUCUGAUGUCCAAGUGGAAAGUGCUGCGACAUUUGAGCGUCAC	Neomycin_nucleobase_3c	Target_lig_753	Pre-miR-372	Target_266	3.224025668870637
1385	NCC1OC(OC2C(Cn3nnc(c3)Cn3cnc4c3[nH]c(N)nc4=O)OC(C2O)OC2C(O)C(N)CC(C2OC2OC(CN)C(C(C2N)O)O)N)C(C(C1O)O)N	GUGGGCCUCAAAUGUGGAGCACUAUUCUGAUGUCCAAGUGGAAAGUGCUGCGACAUUUGAGCGUCAC	Neomycin_nucleobase_3d	Target_lig_754	Pre-miR-372	Target_266	3.838631997765503
1386	NCC1OC(OC2C(Cn3nnc(c3)CCCC(=O)Nc3cccc(c3)c3ncc(s3)NC(=O)C)OC(C2O)OC2C(O)C(N)CC(C2OC2OC(CN)C(C(C2N)O)O)N)C(C(C1O)O)N	GUGGGCCUCAAAUGUGGAGCACUAUUCUGAUGUCCAAGUGGAAAGUGCUGCGACAUUUGAGCGUCAC	Neomycin_nucleobase_3e	Target_lig_755	Pre-miR-372	Target_266	4.795880017344408
1387	NCC1OC(OC2C(Cn3nnc(c3)Cc3nc4c(o3)ccc(c4)NC(=O)Nc3ccccc3)OC(C2O)OC2C(O)C(N)CC(C2OC2OC(CN)C(C(C2N)O)O)N)C(C(C1O)O)N	GUGGGCCUCAAAUGUGGAGCACUAUUCUGAUGUCCAAGUGGAAAGUGCUGCGACAUUUGAGCGUCAC	Neomycin_nucleobase_3f	Target_lig_756	Pre-miR-372	Target_266	4.856985199774591
1388	CCCCNC(=O)Nc1ccc2c(c1)nc(o2)Cc1nnn(c1)CC1OC(C(C1OC1OC(CN)C(C(C1N)O)O)O)OC1C(O)C(N)CC(C1OC1OC(CN)C(C(C1N)O)O)N	GUGGGCCUCAAAUGUGGAGCACUAUUCUGAUGUCCAAGUGGAAAGUGCUGCGACAUUUGAGCGUCAC	Neomycin_nucleobase_3g	Target_lig_757	Pre-miR-372	Target_266	4.705533773838841
1389	NCC1OC(OC2C(Cn3nnc(c3)Cn3cnc(c3)c3ccc(c3)NC(=O)c3ccccc3)OC(C2O)OC2C(O)C(N)CC(C2OC2OC(CN)C(C(C2N)O)O)N)C(C(C1O)O)N	GUGGGCCUCAAAUGUGGAGCACUAUUCUGAUGUCCAAGUGGAAAGUGCUGCGACAUUUGAGCGUCAC	Neomycin_nucleobase_3h	Target_lig_758	Pre-miR-372	Target_266	4.723538195826676
1390	CCCCNC(=O)Nc1ccc(c1)c1ncn(c1)Cc1nnn(c1)CC1OC(C(C1OC1	GUGGGCCUCAAAUGUGGAGCACUAUUCUGAUGUCCAAGU	Neomycin_nucleobase_3i	Target_lig_759	Pre-miR-372	Target_266	4.336299074610351

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	OC(CN)C(C(C1N)O)O)O)OC1C(O)C(N)CC(C1OC1OC(CN)C(C(C1N)O)O)N	GGAAAGUGCUGCGACAUUUGAGCGUCAC					
1391	NCC1OC(OC2C(Cn3nnc(c3)CCC(=O)NCC(=O)Nc3nc4c([nH]3)cccc4)OC(C2O)OC2C(O)C(N)CC(C2OC2OC(CN)C(C(C2N)O)O)N)C(C(C1O)O)N	GUGGGCCUCAAAUGUGGAGCACUAUUCUGAUGUCCAAGUGGAAAGUGCUGCGACAUUUGAGCGUCAC	Neomycin_nucleobase_3j	Target_lig_760	Pre-miR-372	Target_266	4.829738284 60504
1392	NCC1OC(OC2C(Cn3nnc(c3)CCC(=O)Nc3ccc(c3)c3csc(n3)NC(=O)C)OC(C2O)OC2C(O)C(N)CC(C2OC2OC(CN)C(C(C2N)O)O)N)C(C(C1O)O)N	GUGGGCCUCAAAUGUGGAGCACUAUUCUGAUGUCCAAGUGGAAAGUGCUGCGACAUUUGAGCGUCAC	Neomycin-S	Target_lig_761	Pre-miR-372	Target_266	4.795880017 34408
1393	NCC1OC(OC2C(Cn3nnc(c3)CCC(=O)Nc3ccc(c3)c3csc(n3)NC(=O)c3ccc(cc3)C)OC(C2O)OC2C(O)C(N)CC(C2OC2OC(CN)C(C(C2N)O)O)N)C(C(C1O)O)N	GUGGGCCUCAAAUGUGGAGCACUAUUCUGAUGUCCAAGUGGAAAGUGCUGCGACAUUUGAGCGUCAC	Neomycin-3a	Target_lig_762	Pre-miR-372	Target_266	4.279840696 59404
1394	NCC1OC(OC2C(Cn3nnc(c3)CCC(=O)Nc3ccc(c3)c3csc(n3)NC(=O)c3ccc(cc3)Cl)OC(C2O)OC2C(O)C(N)CC(C2OC2OC(CN)C(C(C2N)O)O)N)C(C(C1O)O)N	GUGGGCCUCAAAUGUGGAGCACUAUUCUGAUGUCCAAGUGGAAAGUGCUGCGACAUUUGAGCGUCAC	Neomycin-3b	Target_lig_763	Pre-miR-372	Target_266	4.300162274 13275
1395	NCC1OC(OC2C(Cn3nnc(c3)CCC(=O)Nc3ccc(c3)c3csc(n3)NC(=O)c3ccc(cc3)F)OC(C2O)OC2C(O)C(N)CC(C2OC2OC(CN)C(C(C2N)O)O)N)C(C(C1O)O)N	GUGGGCCUCAAAUGUGGAGCACUAUUCUGAUGUCCAAGUGGAAAGUGCUGCGACAUUUGAGCGUCAC	Neomycin-3c	Target_lig_764	Pre-miR-372	Target_266	4.647817481 88864
1396	NCC1OC(OC2C(Cn3nnc(c3)CCC(=O)Nc3ccc(c3)c3csc(n3)NC(=O)c3ccc(cc3)N)OC(C2O)OC2C(O)C(N)CC(C2OC2OC(CN)C(C(C2N)O)O)N)C(C(C1O)O)N	GUGGGCCUCAAAUGUGGAGCACUAUUCUGAUGUCCAAGUGGAAAGUGCUGCGACAUUUGAGCGUCAC	Neomycin-3d	Target_lig_765	Pre-miR-372	Target_266	4.568636235 84101
1397	NCC1OC(OC2C(Cn3nnc(c3)CCCCC(=O)Nc3cccc(c3)c3csc(n3)NC(=O)C)OC(C2O)OC2C(O)C(N)CC(C2OC2OC(CN)C(C(C2N)O)O)N)C(C(C1O)O)N	GUGGGCCUCAAAUGUGGAGCACUAUUCUGAUGUCCAAGUGGAAAGUGCUGCGACAUUUGAGCGUCAC	Neomycin-4a	Target_lig_766	Pre-miR-372	Target_266	4.560667306 16974
1398	NCC1OC(OC2C(Cn3nnc(c3)CCCCCC(=O)Nc3cccc(c3)c3csc(n3)NC(=O)C)OC(C2O)OC2C(O)C(N)CC(C2OC2OC(CN)C(C(C2N)O)O)N)C(C(C1O)O)N	GUGGGCCUCAAAUGUGGAGCACUAUUCUGAUGUCCAAGUGGAAAGUGCUGCGACAUUUGAGCGUCAC	Neomycin-4b	Target_lig_767	Pre-miR-372	Target_266	4.586700235 91875
1399	NCC1OC(OC2C(Cn3nnc(c3)c3ccc(cc3)C(=O)Nc3cccc(c3)c3csc(n3)NC(=O)C)OC(C2O)OC2C(O)C(N)CC(C2	GUGGGCCUCAAAUGUGGAGCACUAUUCUGAUGUCCAAGUGGAAAGUGCUGCGACAUUUGAGCGUC	Neomycin-4c	Target_lig_768	Pre-miR-372	Target_266	4.471083299 72235

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	OC2OC(CN)C(C(C2N)O)O)N)C(C(C1O)O)N	AC					
1400	NCC1OC(OC2C(Cn3nnc(c3)c3cccc(c3)C(=O)Nc3cccc(c3)c3csc(n3)NC(=O)C)OC(C2O)OC2C(O)C(N)CC(C2OC2OC(CN)C(C(C2N)O)O)N)C(C(C1O)O)N	GUGGGCCUCAAAUGUGGAGCACUAUUCUGAUGUCCAAGUGGAAAGUGCUGCGACAUUUGAGCGUCAC	Neomycin-4d	Target_lig_769	Pre-miR-372	Target_266	4.39254497678533
1401	NCC1OC(OC2C(Cn3nnc(c3)Oc3ccc(cc3)C(=O)Nc3cccc(c3)c3csc(n3)NC(=O)C)OC(C2O)OC2C(O)C(N)CC(C2OC2OC(CN)C(C(C2N)O)O)N)C(C(C1O)O)N	GUGGGCCUCAAAUGUGGAGCACUAUUCUGAUGUCCAAGUGGAAAGUGCUGCGACAUUUGAGCGUCAC	Neomycin-4e	Target_lig_770	Pre-miR-372	Target_266	4.4907974776689
1402	NCC1OC(OC2C(Cn3nnc(c3)Oc3cccc(c3)C(=O)Nc3cccc(c3)c3csc(n3)NC(=O)C)OC(C2O)OC2C(O)C(N)CC(C2OC2OC(CN)C(C(C2N)O)O)N)C(C(C1O)O)N	GUGGGCCUCAAAUGUGGAGCACUAUUCUGAUGUCCAAGUGGAAAGUGCUGCGACAUUUGAGCGUCAC	Neomycin-4f	Target_lig_771	Pre-miR-372	Target_266	4.630784142589986
1403	CNC1C(OC2OC(Cn3nnc(c3)CCC(=O)Nc3ccc(c3)c3csc(n3)NC(=O)C)C(C(C2O)O)N)OC2C(C1O)OC(C(C2)N)OC1C(N)CC(C(C1O)O)N	GUGGGCCUCAAAUGUGGAGCACUAUUCUGAUGUCCAAGUGGAAAGUGCUGCGACAUUUGAGCGUCAC	Apramycin-6a	Target_lig_772	Pre-miR-372	Target_266	3.681936665037724
1404	NCC1OC(OC2C(N)CC(C(C2O)O)N)C(C(C1OCn1nnc(c1)CC(=O)Nc1cccc(c1)c1csc(n1)NC(=O)C)O)N	GUGGGCCUCAAAUGUGGAGCACUAUUCUGAUGUCCAAGUGGAAAGUGCUGCGACAUUUGAGCGUCAC	Neamine-6b	Target_lig_773	Pre-miR-372	Target_266	3.494850021680009
1405	O=C(Cc1nnn(c1)COC1C(N)CC(C(C1O)O)N)Nc1cccc(c1)c1csc(n1)NC(=O)C	GUGGGCCUCAAAUGUGGAGCACUAUUCUGAUGUCCAAGUGGAAAGUGCUGCGACAUUUGAGCGUCAC	2-DOS-6c	Target_lig_774	Pre-miR-372	Target_266	3.168770306133294
1406	NCC1OC(OC2C(Cn3nnc(c3)CCC(=O)Nc3ccc(c3)c3csc(n3)NC(=O)C)OC(C2O)OC2C(O)C(N)CC(C2OC2OC(CN)C(C(C2N)O)O)N)C(C(C1O)O)N	GGGAUACUCAAAAUGGGGGCGCUUUCCUUUUUGUCUGUACUGGGAAGUGCUUCGAUUUUGGGGUGUCCC	Neomycin-S	Target_lig_761	Pre-miR-373	Target_267	4.950781977329982
1407	NCC1OC(OC2C(Cn3nnc(c3)CCC(=O)Nc3ccc(c3)c3csc(n3)NC(=O)c3ccc(cc3)C)OC(C2O)OC2C(O)C(N)CC(C2OC2OC(CN)C(C(C2N)O)O)N)C(C(C1O)O)N	GGGAUACUCAAAAUGGGGGCGCUUUCCUUUUUGUCUGUACUGGGAAGUGCUUCGAUUUUGGGGUGUCCC	Neomycin-3a	Target_lig_762	Pre-miR-373	Target_267	4.366531544442041
1408	NCC1OC(OC2C(Cn3nnc(c3)CCC(=O)Nc3ccc(c3)c3csc(n3)NC(=O)c3ccc(cc3)Cl)OC(C2O)OC2C(O)C(N)CC(C2OC2OC(CN)C(C(C2N)O)O)N)C(C(C1O)O)N	GGGAUACUCAAAAUGGGGGCGCUUUCCUUUUUGUCUGUACUGGGAAGUGCUUCGAUUUUGGGGUGUCCC	Neomycin-3b	Target_lig_763	Pre-miR-373	Target_267	4.459670525220913

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
1409	NCC1OC(OC2C(Cn3nnc(c3)CCC(=O)Nc3ccc(c3)c3csc(n3)NC(=O)c3ccc(cc3)F)OC(C2O)OC2C(O)C(N)CC(C2OC2OC(CN)C(C(C2N)O)O)N)C(C(C1O)O)N	GGGAUACUCAAAAUGGGGGCGCUUUCCUUUUUGUCUGUACUGGGAAGUGCUUCGAUUUUGGGGUGUCCC	Neomycin-3c	Target_lig_764	Pre-miR-373	Target_267	4.4723700991 2866
1410	NCC1OC(OC2C(Cn3nnc(c3)CCC(=O)Nc3ccc(c3)c3csc(n3)NC(=O)c3ccc(cc3)N)OC(C2O)OC2C(O)C(N)CC(C2OC2OC(CN)C(C(C2N)O)O)N)C(C(C1O)O)N	GGGAUACUCAAAAUGGGGGCGCUUUCCUUUUUGUCUGUACUGGGAAGUGCUUCGAUUUUGGGGUGUCCC	Neomycin-3d	Target_lig_765	Pre-miR-373	Target_267	4.3233063903 7513
1411	NCC1OC(OC2C(Cn3nnc(c3)CCCCC(=O)Nc3cccc(c3)c3csc(n3)NC(=O)C)OC(C2O)OC2C(O)C(N)CC(C2OC2OC(CN)C(C(C2N)O)O)N)C(C(C1O)O)N	GGGAUACUCAAAAUGGGGGCGCUUUCCUUUUUGUCUGUACUGGGAAGUGCUUCGAUUUUGGGGUGUCCC	Neomycin-4a	Target_lig_766	Pre-miR-373	Target_267	4.6363880201 0786
1412	NCC1OC(OC2C(Cn3nnc(c3)CCCCCC(=O)Nc3cccc(c3)c3csc(n3)NC(=O)C)OC(C2O)OC2C(O)C(N)CC(C2OC2OC(CN)C(C(C2N)O)O)N)C(C(C1O)O)N	GGGAUACUCAAAAUGGGGGCGCUUUCCUUUUUGUCUGUACUGGGAAGUGCUUCGAUUUUGGGGUGUCCC	Neomycin-4b	Target_lig_767	Pre-miR-373	Target_267	4.3746875490 3833
1413	NCC1OC(OC2C(Cn3nnc(c3)c3ccc(cc3)C(=O)Nc3cccc(c3)c3csc(n3)NC(=O)C)OC(C2O)OC2C(O)C(N)CC(C2OC2OC(CN)C(C(C2N)O)O)N)C(C(C1O)O)N	GGGAUACUCAAAAUGGGGGCGCUUUCCUUUUUGUCUGUACUGGGAAGUGCUUCGAUUUUGGGGUGUCCC	Neomycin-4c	Target_lig_768	Pre-miR-373	Target_267	4.4762535331 8844
1414	NCC1OC(OC2C(Cn3nnc(c3)c3cccc(c3)C(=O)Nc3cccc(c3)c3csc(n3)NC(=O)C)OC(C2O)OC2C(O)C(N)CC(C2OC2OC(CN)C(C(C2N)O)O)N)C(C(C1O)O)N	GGGAUACUCAAAAUGGGGGCGCUUUCCUUUUUGUCUGUACUGGGAAGUGCUUCGAUUUUGGGGUGUCCC	Neomycin-4d	Target_lig_769	Pre-miR-373	Target_267	4.4634415574 2847
1415	NCC1OC(OC2C(Cn3nnc(c3)Oc3ccc(cc3)C(=O)Nc3cccc(c3)c3csc(n3)NC(=O)C)OC(C2O)OC2C(O)C(N)CC(C2OC2OC(CN)C(C(C2N)O)O)N)C(C(C1O)O)N	GGGAUACUCAAAAUGGGGGCGCUUUCCUUUUUGUCUGUACUGGGAAGUGCUUCGAUUUUGGGGUGUCCC	Neomycin-4e	Target_lig_770	Pre-miR-373	Target_267	4.4248121550 7234
1416	NCC1OC(OC2C(Cn3nnc(c3)Oc3cccc(c3)C(=O)Nc3cccc(c3)c3csc(n3)NC(=O)C)OC(C2O)OC2C(O)C(N)CC(C2OC2OC(CN)C(C(C2N)O)O)N)C(C(C1O)O)N	GGGAUACUCAAAAUGGGGGCGCUUUCCUUUUUGUCUGUACUGGGAAGUGCUUCGAUUUUGGGGUGUCCC	Neomycin-4f	Target_lig_771	Pre-miR-373	Target_267	4.4736607226 1016
1417	CNC1C(OC2OC(Cn3nnc(c3)CCC(=O)Nc3ccc(c3)c3csc(n3)NC(=O)C)C(C(C2O)O)N)OC2C(C1O)OC(C(C2)N)OC1C(N)CC(C(C1O)O)N	GGGAUACUCAAAAUGGGGGCGCUUUCCUUUUUGUCUGUACUGGGAAGUGCUUCGAUUUUGGGGUGUCCC	Apramycin-6a	Target_lig_772	Pre-miR-373	Target_267	3.9956786262 1736

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
1418	NCC1OC(OC2C(N)CC(C(C2O)O)N)C(C(C1OCn1nnc(c1)CC(=O)Nc1cccc(c1)c1csc(n1)NC(=O)C)O)N	GGGAUACUCAAAAUGGGGGCGCUUUCCUUUUUGUCUGUACUGGGAAGUGCUUCGAUUUUGGGGUGUCCC	Neamine-6b	Target_lig_773	Pre-miR-373	Target_267	3.97469413473523
1419	O=C(Cc1nnn(c1)COC1C(N)CC(C(C1O)O)N)Nc1cccc(c1)c1csc(n1)NC(=O)C	GGGAUACUCAAAAUGGGGGCGCUUUCCUUUUUGUCUGUACUGGGAAGUGCUUCGAUUUUGGGGUGUCCC	2-DOS-6c	Target_lig_774	Pre-miR-373	Target_267	2.50307035192679
1420	CC1(C(C2=CC=CC=C2NC1=NCCCNCCCCNCCCN)N(C)C3=CC=CC=C3)C	GUGGGCCUCAAAUGUGGAGCACUAUUCUGAUGUCCAAGUGGAAAGUGCUGCGACAUUUGAGCGUCAC	PA-1	Target_lig_775	Pre-miR-372	Target_266	6.823908740944432
1421	C(CCNCCCCNCCCCN)CN	GUGGGCCUCAAAUGUGGAGCACUAUUCUGAUGUCCAAGUGGAAAGUGCUGCGACAUUUGAGCGUCAC	PA-2	Target_lig_776	Pre-miR-372	Target_266	6.275724130399921
1422	NCCCCN/C(=C/1\C(=O)C=C2C(C1=O)(C)c1c(O)c(C)c(c(c1O2)C(=O)C)O)/C	GUGGGCCUCAAAUGUGGAGCACUAUUCUGAUGUCCAAGUGGAAAGUGCUGCGACAUUUGAGCGUCAC	PA-3	Target_lig_777	Pre-miR-372	Target_266	5.939302159644639
1423	CN1CCN(CC1)C2=CC3=C(C=C2)N=C(N3)C4=CC5=C(C=C4)N=C(N5)C6=CC(=CC=C6)OCCCC(=O)NCCCN=[N+]=[N-]	AGCCCCUGCCCACCGCACACUGCGCUGCCCCAGACCCACUGUGCGUGUGACAGCGGCUGA	Targapremir-210	Target_lig_1262	Pre-miR-210	Target_227	6.795880017344408
1424	CN1CCN(CC1)C2=CC3=C(C=C2)N=C(N3)C4=CC5=C(C=C4)N=C(N5)C6=CC(=CC=C6)OCCCC(=O)NCCCN=[N+]=[N-]	AGCCCCUGCCCACCGCACACUGCGCUGCCCCAGACCCACUGUGCGUGUGACAGCGGCUGA	Targapremir-210-RL	Target_lig_1263	Pre-miR-210	Target_227	6.721246399047717
1425	N=[N+]=NCCCNC(=O)CCCOc1c(cc(cc1C(C)(C)C)c1nc2c([nH]1)ccc(c2)c1nc2c([nH]1)ccc(cc2)N1CCN(CC1)C)C(C)(C)C	GGGAGAGGGUUUAAUUCUUACGAAAGUAAUAAUUGGAUCCGCAAGG	Targapremir-515/885	Target_lig_778	Pri-miR-515 drosha site (RNA 1)	Target_268	5.045757490560068
1426	N=[N+]=NCCCNC(=O)CCCOc1c(cc(cc1C(C)(C)C)c1nc2c([nH]1)ccc(c2)c1nc2c([nH]1)ccc(cc2)N1CCN(CC1)C)C(C)(C)C	GGGAGAGGGUUUAAUUUCUACGAAAGUAGCGAUUGGAUCCGCAAGG	Targapremir-515/885	Target_lig_778	Pri-miR-885 drosha site (RNA 2)	Target_269	4.920818753955238
1427	N=[N+]=NCCCNC(=O)CCCOc1c(cc(cc1C(C)(C)C)c1nc2c([nH]1)ccc(c2)c1nc2c([nH]1)ccc(cc2)N1CCN(CC1)C)C(C)(C)C	GGGAGAGGGUUUAAUUCAUACGAAAGUAUUAAUUGGAUCCGCAAGG	Targapremir-515/885	Target_lig_778	Pri-miR-515 (RNA 3)	Target_270	5.1249387366083
1432	N=[N+]=NCCCNC(=O)CCCOc1c(cc(cc1C(C)(C)C)c1nc2c([nH]1)ccc(c2)c1nc2c([nH]1)ccc(cc2)N1CCN(CC1)C)C	GGGAGAGGGUUUAAUUCAUUCUACGAAAGUAGCGUUAAUUGGAUCCGCAAGG	Targapremir-515	Target_lig_778	Pri-miR-515 and the adjacent RNA motif (RNA 4)	Target_271	7.221848749661636

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	(C)(C)C						
1433	CCCN(C(=O)CN(C(=O)CNCc1nnn(c1)N=[N+]=N)CCC)CC(=O)N(CC(=O)N(CC(=O)N(CC(=O)N)CCC)CCC)CCC	GGGAGAGGGUUUAAUUCAUUCUACGAAAGUAGCGUUAAUUGGAUCCGCAAGG	Compound 1a	Target_lig_780	Pri-miR-515 and the adjacent RNA motif (RNA 4)	Target_271	4.744727494889669
1434	CCCN(C(=O)CNCc1nnn(c1)N=[N+]=Nn1nnc(c1)CO)CC(=O)N(CC(=O)N(CC(=O)N(CC(=O)N(CC(=O)N)C)CCC)CCC)CCC	GGGAGAGGGUUUAAUUCAUUCUACGAAAGUAGCGUUAAUUGGAUCCGCAAGG	Compound 1b	Target_lig_781	Pri-miR-515 and the adjacent RNA motif (RNA 4)	Target_271	4.698970004336 02
1576	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	CCGACUGAUGUUGACUGUUGAAUCUCAUGGCAACACCAGUCGG	Neomycin	Target_lig_4	Oligonucleotide 3	Target_282	5.397940008667204
1577	CC1(COC(C(C1NC)O)OC2C(CC(C(C2O)OC3C(CC=C(O3)CN)N)N)N)O	CCGACUGAUGUUGACUGUUGAAUCUCAUGGCAACACCAGUCGG	Sisomycin	Target_lig_1269	Oligonucleotide 3	Target_282	5.397940008667204
1578	[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	CCGACUGAUGUUGACUGUUGAAUCUCAUGGCAACACCAGUCGG	Tobramycin	Target_lig_540	Oligonucleotide 3	Target_282	5.096910013008806
1579	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	CCGACUGAUGUUGACUGUUGAAUCUCAUGGCAACACCAGUCGG	Amikacin	Target_lig_175	Oligonucleotide 3	Target_282	4.823908740944432
1580	CC(C1CCC(C(O1)OC2C(CC(C(C2O)OC3C(C(C(CO3)(C)O)NC)O)N)N)N)NC	CCGACUGAUGUUGACUGUUGAAUCUCAUGGCAACACCAGUCGG	Gentamycin	Target_lig_1270	Oligonucleotide 3	Target_282	4.795880017344408
1581	CNC1C(OC2OC(Cn3nnc(c3)CCC(=O)Nc3ccc(c3)c3csc(n3)NC(=O)C)C(C(C2O)O)N)OC2C(C1O)OC(C(C2)N)OC1C(N)CC(C(C1O)O)N	CCGACUGAUGUUGACUGUUGAAUCUCAUGGCAACACCAGUCGG	Apramycin	Target_lig_772	Oligonucleotide 3	Target_282	4.657577319177779
1582	CCNC1CC(C(C(C1OC2C(C(C(CO2)(C)O)NC)O)O)OC3C(CC=C(O3)CN)N)N	CCGACUGAUGUUGACUGUUGAAUCUCAUGGCAACACCAGUCGG	Netilmicin	Target_lig_1271	Oligonucleotide 3	Target_282	4.455931955649972
1583	C1C(C(C(C(C1N)OC2C(C(C(C(O2)CN)O)O)O)OC3C(C(C(C(O3)CO)O)N)O)N	CCGACUGAUGUUGACUGUUGAAUCUCAUGGCAACACCAGUCGG	Kanamycin-A	Target_lig_1272	Oligonucleotide 3	Target_282	4.356547323513 81
1584	C1C(C(C(C(C1N)OC2C(C(C(C(O2)CN)O)O)N)OC3C(C(C(O3)CO)O)O)O)N	CCGACUGAUGUUGACUGUUGAAUCUCAUGGCAACACCAGUCGG	Ribostamycin	Target_lig_1273	Oligonucleotide 3	Target_282	4.045757490560 68
1585	CC(C1C(C(C(C(O1)OC2C(CC(C(C2O)OC3C(C(C(CO3)(C)O)NC)O)N)N)N)O)O)O	CCGACUGAUGUUGACUGUUGAAUCUCAUGGCAACACCAGUCGG	Geneticin	Target_lig_140	Oligonucleotide 3	Target_282	3.995678626217 36

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
1586	CC1C(C(C(O1)OC2C(C(C(C2O)O)N=C(N)N)O)N=C(N)N)OC3C(C(C(C(O3)CO)O)O)NC)(C=O)O	CCGACUGAUGUUGACUGUUGAAUCUCAUGGCAACACCAGUCGG	Streptomycin	Target_lig_63	Oligonucleotide 3	Target_282	3.872895201635 19
1587	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	CCGACUGAUGUUGACUGUUGAAUCUCAUGGCAACACCAGUCGG	Hygromycin	Target_lig_3	Oligonucleotide 3	Target_282	3.583359492 66172
1588	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	CCGACUGAUGUUGAXUGUUGAAUYUCAUGGCAACACCAGUCGG	Neomycin	Target_lig_4	Oligonucleotide 4	Target_283	5.522878745 28034
1589	CC1(COC(C(C1NC)O)OC2C(CC(C(C2O)OC3C(CC=C(O3)CN)N)N)N)O	CCGACUGAUGUUGAXUGUUGAAUYUCAUGGCAACACCAGUCGG	Sisomycin	Target_lig_1269	Oligonucleotide 4	Target_283	5.397940008 67204
1590	[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	CCGACUGAUGUUGAXUGUUGAAUYUCAUGGCAACACCAGUCGG	Tobramycin	Target_lig_540	Oligonucleotide 4	Target_283	5.096910013 00806
1591	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	CCGACUGAUGUUGAXUGUUGAAUYUCAUGGCAACACCAGUCGG	Amikacin	Target_lig_175	Oligonucleotide 4	Target_283	4.853871964 32176
1592	CC(C1CCC(C(O1)OC2C(CC(C(C2O)OC3C(C(C(CO3)(C)O)NC)O)N)N)N)NC	CCGACUGAUGUUGAXUGUUGAAUYUCAUGGCAACACCAGUCGG	Gentamycin	Target_lig_1270	Oligonucleotide 4	Target_283	4.886056647 69316
1593	CNC1C(OC2OC(Cn3nnc(c3)CCC(=O)Nc3ccc(c3)c3csc(n3)NC(=O)C)C(C(C2O)O)N)OC2C(C1O)OC(C(C2)N)OC1C(N)CC(C(C1O)O)N	CCGACUGAUGUUGAXUGUUGAAUYUCAUGGCAACACCAGUCGG	Apramycin	Target_lig_772	Oligonucleotide 4	Target_283	4.638272163 98241
1594	CCNC1CC(C(C(C1OC2C(C(C(CO2)(C)O)NC)O)O)OC3C(CC=C(O3)CN)N)N	CCGACUGAUGUUGAXUGUUGAAUYUCAUGGCAACACCAGUCGG	Netilmicin	Target_lig_1271	Oligonucleotide 4	Target_283	4.468521082 95774
1595	C1C(C(C(C(C1N)OC2C(C(C(C(O2)CN)O)O)O)OC3C(C(C(C(O3)CO)O)N)O)N	CCGACUGAUGUUGAXUGUUGAAUYUCAUGGCAACACCAGUCGG	Kanamycin-A	Target_lig_1272	Oligonucleotide 4	Target_283	4.346787486 22466
1596	C1C(C(C(C(C1N)OC2C(C(C(C(O2)CN)O)O)N)OC3C(C(C(O3)CO)O)O)O)N	CCGACUGAUGUUGAXUGUUGAAUYUCAUGGCAACACCAGUCGG	Ribostamycin	Target_lig_1273	Oligonucleotide 4	Target_283	4.107905397 30952
1597	CC(C1C(C(C(C(O1)OC2C(CC(C(C2O)OC3C(C(C(CO3)(C)O)NC)O)N)N)N)O)O)O	CCGACUGAUGUUGAXUGUUGAAUYUCAUGGCAACACCAGUCGG	Geneticin	Target_lig_140	Oligonucleotide 4	Target_283	4.026872146 4003
1598	CC1C(C(C(O1)OC2C(C(C(C2O)O)N=C(N)N)O)N=C(N)N)OC3C(C(C(C(O3)CO)O)	CCGACUGAUGUUGAXUGUUGAAUYUCAUGGCAACACCAGUCGG	Streptomycin	Target_lig_63	Oligonucleotide 4	Target_283	3.939302159 64639

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	O)NC)(C=O)O						
1599	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	CCGACUGAUGUUGAXUGUUGAAUYUCAUGGCAACACCAGUCGG	Hygromycin	Target_lig_3	Oligonucleotide 4	Target_283	3.536107011014 09
1729	N=[N+]=NCCCNC(=O)CCCOc1ccc(cc1)c1nc2c([nH]1)cc(cc2)c1ccc(cc1)N1CCN(CC1)C	AGCCCCUGCCCACCGCACACUGCGCUGCCCCAGACCCACUGUGCGUGUGACAGCGGCUGA	Compound1	Target_lig_965	Pre-miR-21	Target_227	4.744727494889669
1730	CN1CCN(CC1)c1ccc(cc1)c1ccc2c(c1)[nH]c(n2)c1ccc(cc1)OCCCC(=O)N1CCN(CC1)c1nncc2c1ccs2	AGCCCCUGCCCACCGCACACUGCGCUGCCCCAGACCCACUGUGCGUGUGACAGCGGCUGA	Compound9	Target_lig_966	Pre-miR-21	Target_227	6
1731	CN1CCN(CC1)c1ccc(cc1)c1ccc2c(c1)[nH]c(n2)c1ccc(cc1)OCCCC(=O)N(Cc1ccncc1)CCNC(=O)c1ccc(c(c1)C)F	AGCCCCUGCCCACCGCACACUGCGCUGCCCCAGACCCACUGUGCGUGUGACAGCGGCUGA	Compound7	Target_lig_967	Pre-miR-21	Target_227	6.892790030335213
1732	Coc1ccc(cc1OCC1=NC2N(C1)C=CC=C2)NC(=O)CCCOc1ccc(cc1)c1[nH]c2c(n1)ccc(c2)c1ccc(cc1)N1CCN(CC1)C	AGCCCCUGCCCACCGCACACUGCGCUGCCCCAGACCCACUGUGCGUGUGACAGCGGCUGA	Compound8	Target_lig_968	Pre-miR-21	Target_227	6.570247719999759
1733	CN1CCN(CC1)c1ccc(cc1)c1ccc2c(c1)[nH]c(n2)c1ccc(cc1)OCCCC(=O)N1CCN(CC1)c1nncc2c1ccs2	GUUGACUGUUGAAUCUCAUGGCAAC	Compound9	Target_lig_966	miR-21 WT	Target_301	6.473660722610 16
1734	CN1CCN(CC1)c1ccc(cc1)c1ccc2c(c1)[nH]c(n2)c1ccc(cc1)OCCCC(=O)N1CCN(CC1)c1nncc2c1ccs2	GUUGACUGUUGAAUCUCAAUGGUCAAC	Compound9	Target_lig_966	miR-21 BP	Target_302	5
1735	CN1CCN(CC1)c1ccc(cc1)c1ccc2c(c1)[nH]c(n2)c1ccc(cc1)OCCCC(=O)N1CCN(CC1)c1nncc2c1ccs2	GUUGACUGUUGAAUCUCAAUGGUCAAC	Compound9	Target_lig_966	miR-21 A bulge	Target_303	6.638272163982 41
1736	CN1CCN(CC1)c1ccc(cc1)c1ccc2c(c1)[nH]c(n2)c1ccc(cc1)OCCCC(=O)N1CCN(CC1)c1nncc2c1ccs2	GUUGACUGUUGAAUCUCAUGGUCAAC	Compound9	Target_lig_966	miR-21 U bulge	Target_304	5
1737	CN1CCN(CC1)c1ccc(cc1)c1ccc2c(c1)[nH]c(n2)c1ccc(cc1)OCCCC(=O)N1CCN(CC1)c1nncc2c1ccs2	GUUGACUGUUGAAUCUCAUAGCAAC	Compound9	Target_lig_966	miR-21 G-A	Target_305	5.481486060122211
1775	C1=CC(=CC(=C1)C2=NC3=C(N2)C=C(C=C3)N)C4=NC5=C(N4)C=C(C=C5)N	GCAGAGGUUGCCCUUGGUGAAUUCGCUUUAUUUAUGUUGAAUCACACAAAGGCAACUUUUGU	Compound C1	Target_lig_994	Pre-miR-377 dicer processing site	Target_312	4.537602002101 04
1776	CN1CCN(CC1)c1cc(Nc2nccc(c2)Nc2ccc3c(n2)cccc3)nc(n1)C	GCAGAGGUUGCCCUUGGUGAAUUCGCUUUAUUUAUGUUGAAUCACACAAAGGCAACUUUUGU	Compound C2	Target_lig_995	Pre-miR-377 5′-G_G/3′-CAC bulge	Target_313	5.522878745280 34
1777	CCOC(=O)CCCOC1=CC(=CC(=C1)C2=NC3=C(N2)C=C(C=C3)N)C4=NC5=C(N4)C=	GCAGAGGUUGCCCUUGGUGAAUUCGCUUUAUUUAUGUUGAAUCACACAAAGG	Compound C1-COOEt	Target_lig_996	Pre-miR-377 dicer processing site	Target_312	6.096910013008 06

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	C(C=C5)N	CAACUUUUGU					
1778	C#CCc1nc(Nc2nccc(c2)Nc2ccc3c(n2)cccc3)cc(n1)N1CCN(CC1)C	GCAGAGGUUGCCCUUGGUGAAUUCGCUUUAUUUAUGUUGAAUCACACAAAGGCAACUUUUGU	Compound C2-Ak	Target_lig_997	Pre-miR-377 5′-G_G/3′-CAC bulge	Target_313	5.795880017344408
1779	CCCN(C(=O)CN(C(=O)CN(C(=O)CN(C(=O)CCCOc1cc(cc(c1)c1[nH]c2c(n1)cc(cc2)N)c1[nH]c2c(n1)ccc(c2)N)CCC)CCC)CCC)CC(=O)N(CC(=O)N)CCCn1cnc(c1)CN1CCN(CC1)c1nc(CC)nc(c1)Nc1nccc(c1)Nc1ccc2c(n1)cccc2	GCAGAGGUUGCCCUUGGUGAAUUCGCUUUAUUUAUGUUGAAUCACACAAAGGCAACUUUUGU	Targapremir-377	Target_lig_998	Pre-miR-377	Target_312	6.721246399047717
1794	N=[N+]=NCCCNC(=O)CCCOc1ccc(cc1)c1nc2c([nH]1)ccc(c2)c1ccc(cc1)N1CCN(CC1)C	AGCCCCUGCCCACCGCACACUGCGCUGCCCCAGACCCACUGUGCGUGUGACAGCGGCUGA	miR-21 binder compound 1	Target_lig_1008	miR-21	Target_227	4.698970004336 02
1795	CCCN(C(=O)CN(C(=O)NCc1nnn(c1)CCCNC(=O)CCCOc1ccc(cc1)c1nc2c([nH]1)ccc(c2)c1ccc(cc1)N1CCN(CC1)C)CCC)CC(=O)N(CC(=O)N(Cc1nnn(c1)CCCNC(=O)CCCOc1ccc(cc1)c1nc2c([nH]1)ccc(c2)c1ccc(cc1)N1CCN(CC1)C)CC(=O)N)CCC	AGCCCCUGCCCACCGCACACUGCGCUGCCCCAGACCCACUGUGCGUGUGACAGCGGCUGA	miR-21 binder compound 2	Target_lig_1009	miR-21	Target_227	6.008773924300751
1797	NC(=[NH2+])C1=CC=C(NC2=CC=C(C=C2)C2=CC3=CC=C(C=C3N2)C(N)=[NH2+])C=C1	GUGCAGGUAGUGAUAUGUGCAUCUACUGCAC	Compound 2	Target_lig_676	miR-17 Dicer site	Target_316	6.920818753955238
1798	NC(=[NH2+])C1=CC=C(NC2=CC=C(C=C2)C2=CC3=CC=C(C=C3N2)C(N)=[NH2+])C=C1	GUGCAGGUAGUGAUAUGUGCAUCUACUGCAC	Compound 2	Target_lig_676	miR-17 G-bulge	Target_317	4.823908740944432
1799	NC(=[NH2+])C1=CC=C(NC2=CC=C(C=C2)C2=CC3=CC=C(C=C3N2)C(N)=[NH2+])C=C1	GUGCAGGUAGUGAUAUGUGCAUCUACCUGCAC	Compound 2	Target_lig_676	miR-17 U-bulge	Target_318	4.721246399047717
1800	NC(=[NH2+])C1=CC=C(NC2=CC=C(C=C2)C2=CC3=CC=C(C=C3N2)C(N)=[NH2+])C=C1	GUGCAGGUAGAUGAUAUGUGCAUCUACCUGCAC	Compound 2	Target_lig_676	miR-17 Base pairing control	Target_319	4
1801	NC(=[NH2+])C1=CC=C(NC2=CC=C(C=C2)C2=CC3=CC=C(C=C3N2)C(N)=[NH2+])C=C1	UGCAGAUAGUGAAGUAGAUAGGCAUCUACUGCA	Compound 2	Target_lig_676	miR-18a Dicer site	Target_320	6.906578314833777
1809	NCCCC(=O)NCCCN1Cc2ccc3c(n2)nc(cc3)NC(=O)OCC/C=C/CCOC(=O)Nc2nc3nc(C1)ccc3cc2	GCUGAUUUCUUUUGGUGUUCAGAGGGGUCGGUGGUGGUGGUGGUGGUGGUUCUAGCACCAUCUGAAAUCGGUUA	CMBL-3aL	Target_lig_1018	R-Seq1	Target_321	6.661543506 3954
1810	NCCCC(=O)NCCCN1Cc2ccc3c(n2)nc(cc3)NC(=O)OCC/C=C/	GCUGAUUUCUUUUGGUGUUCAGAGUGGUCGGUGGUUGGU	CMBL-3aL	Target_lig_1018	R-Seq2	Target_322	5.882728704344424

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	CCOC(=O)Nc2nc3nc(C1)ccc3cc2	GGUGGGUGGUGGUUCUAGCACCAUCUGAAAUCGGUUA					
1811	NCCCC(=O)NCCCN1Cc2ccc3c(n2)nc(cc3)NC(=O)OCC/C=C/CCOC(=O)Nc2nc3nc(C1)ccc3cc2	GCUGAUUUCUUUUGGUGUUCAGAGAGGUCGGUGGUUGGUGGUGGGUGGUGGUUCUAGCACCAUCUGAAAUCGGUUA	CMBL-3aL	Target_lig_1018	R-Seq3	Target_323	6.16621562534352
1812	NCCCC(=O)NCCCN1Cc2ccc3c(n2)nc(cc3)NC(=O)OCC/C=C/CCOC(=O)Nc2nc3nc(C1)ccc3cc2	GCUGAUUUCUUUUGGUGUUCAGAGUGGGGUGAGCUUUCUAGCACCAUCUGAAAUCGGUUA	CMBL-3aL	Target_lig_1018	R-Seq4	Target_324	6.869666231500499
1813	NCCCC(=O)NCCCN1Cc2ccc3c(n2)nc(cc3)NC(=O)OCC/C=C/CCOC(=O)Nc2nc3nc(C1)ccc3cc2	GUGCAUUGUAGUUGCAUUGCAUGUUCUGGUGGUACCCAUCGAAUGUUUCCACAGUGCAUCAC	CMBL-3aL	Target_lig_1018	Pre-miR-33a	Target_325	8.860120913559876
1814	NCCCC(=O)NCCCN1Cc2ccc3c(n2)nc(cc3)NC(=O)OCC/C=C/CCOC(=O)Nc2nc3nc(C1)ccc3cc2	GUGCAUUGUAGUUGCAUUGCAUGUUCUGGUAGUACCCAUCGAAUGUUUCCACAGUGCAUCAC	CMBL-3aL	Target_lig_1018	Pre-miR-33a-G31A	Target_326	8.649751981666584
1815	NCCCC(=O)NCCCN1Cc2ccc3c(n2)nc(cc3)NC(=O)OCC/C=C/CCOC(=O)Nc2nc3nc(C1)ccc3cc2	GUGCAUUGUAGUUGCAUUGCAUGUUCUGGUGAUACCCAUCGAAUGUUUCCACAGUGCAUCAC	CMBL-3aL	Target_lig_1018	Pre-miR-33a-G32A	Target_327	8.593459819566604
1816	NCCCC(=O)NCCCN1Cc2ccc3c(n2)nc(cc3)NC(=O)OCC/C=C/CCOC(=O)Nc2nc3nc(C1)ccc3cc2	UGCCUACUGAGCUGAAACACAGUUGGUUUGUGUACACUGGCUCAGUUCAGCAGGAACAG	CMBL-3aL	Target_lig_1018	Pre-miR-24-2	Target_328	8.690369832574 1
1820	N=[N+]=NCCCNC(=O)CCCOc1cccc(c1)c1nc2c([nH]1)ccc(c2)c1nc2c([nH]1)cc(cc2)N1CCN(CC1)C	AGCCCCUGCCCACCGCACACUGCGCUGCCCCAGACCCACUGUGCGUGUGACAGCGGCUGA	SMB1	Target_lig_1278	Pre-miR-210	Target_227	6.795880017344408
1821	CCCN(C(=O)NCc1nnn(c1)CCCCC(=O)CCCOc1c(cc(cc1C(C)(C)C)c1[nH]c2c(n1)cc(cc2)N1CCN(CC1)C)C(C)(C)C)CC(=O)N(C(=O)CCCOc1ccc(cc1)c1[nH]c2c(n1)cc(cc2)N1CCN(CC1)C)CCC	GGGAGAGGGUUUAAUUACGAAAGUAAUUGGAUCCGCAAGG	SMB2	Target_lig_1022	Pri-miR-96	Target_159	7.698970004333602
1822	CCCN(C(=O)CN(C(=O)NCc1nnn(c1)CCCCC(=O)CCCOc1ccc(cc1)c1nc2c([nH]1)ccc(c2)c1ccc(cc1)N1CCN(CC1)C)CCC)CC(=O)N(CC(=O)N(Cc1nnn(c1)CCCCC(=O)CCCOc1ccc(cc1)c1nc2c([nH]1)ccc(c2)c1ccc(cc1)N1CCN(CC1)C)CC(=O)N)CCC	AGCCCCUGCCCACCGCACACUGCGCUGCCCCAGACCCACUGUGCGUGUGACAGCGGCUGA	SMB3	Target_lig_1023	Pre-miR-21	Target_227	6.008773924300751
1823	CCCN(C(=O)CN(C(=O)NCc1nnn(c1)CCCCC(=O)CCCOc1c(cc(cc1C(C)(C)C)c1nc2c([nH]1)ccc(c2)c1ccc(cc1)N1CCN(CC1)C)C(C)(C)C)CCC)CC(=O)N(	UAGCUUAUCAGACUGAUGUUGACUGUUGAAUCUCAUGGCAACACCAGUCGAUGGGCUGU	SMB4	Target_lig_1279	Pre-miR-17/18a/20a	Target_331	6.920818753955238

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	CC(=O)N(Cc1nnn(c1)CCCCC(=O)CCCOc1c(cc(cc1C(C)(C)C)c1nc2c([nH]1)ccc(c2)c1ccc(cc1)N1CCN(CC1)C)C(C)(C)C)CC(=O)N)CCC						
1824	OC(COP(=O)(OC1C(O)C(OC1n1cnc2c1ncnc2N)COP(=O)(OC1C(O)C(OC1n1cnc2c1ncnc2N)COP(=O)(OC1C(O)C(OC1n1cnc2c1ncnc2N)COP(=O)(OC1C(O)C(OC1n1cnc2c1ncnc2N)COP(=O)(O)O)O)O)O)O)COCCCNC(=O)CCCOc1ccc(c1)c1nc2c([nH]1)ccc(c2)c1nc2c([nH]1)cc(cc2)N1CCN(CC1)C	AGCCCCUGCCCACCGCACACUGCGCUGCCCCAGACCCACUGUGCGUGUGACAGCGGCUGA	SMC1	Target_lig_1024	Pre-miR-210	Target_227	6.721246399047717
1825	CCCN(C(=O)N(Cc1nnn(c1)CCCCC(=O)CCCOc1c(cc(cc1C(C)(C)C)c1nc2c([nH]1)ccc(c2)N1CCN(CC1)C)C(C)(C)C)CCOCCOCCOP(=O)(OC1C(O)C(OC1n1cnc2c1ncnc2N)COP(=O)(OC1C(O)C(OC1n1cnc2c1ncnc2N)COP(=O)(OC1C(O)C(OC1n1cnc2c1ncnc2N)COP(=O)(OC1C(O)C(OC1n1cnc2c1ncnc2N)COP(=O)(O)O)O)O)O)O)CC(=O)N(C(=O)CCCOc1ccc(cc1)c1nc2c([nH]1)ccc(c2)N1CCN(CC1)C)CCC	GGGAGAGGGUUUAAUUACGAAAGUAAUUGGAUCCGCAAGG	SMC2	Target_lig_1025	Pri-miR-96	Target_159	7.075720713913812
1826	CCCN(C(=O)N(Cc1nnn(c1)CCCCC(=O)CCCOc1c(cc(cc1C(C)(C)C)c1nc2c([nH]1)ccc(c2)N1CCN(CC1)C)C(C)(C)C)CC(=O)NCCCCNCCCNC(=O)c1csc(n1)c1csc(n1)CCNC(=O)C(C(O)C)NC(=O)C(C(C(NC(=O)C(C(c1ncc[nH]1)OC1OC(CO)C(C(C1OC1OC(CO)C(C(C1O)OC(=O)N)O)O)O)NC(=O)c1nc(nc(c1C)N)C(CC(=O)N)NCC(C(=O)N)N)C)O)C)CC(=O)N(C(=O)CCCOc1ccc(cc1)c1nc2c([nH]1)ccc(c2)N1CCN(CC1)C)CCC	GGGAGAGGGUUUAAUUACGAAAGUAAUUGGAUCCGCAAGG	SMC2-2	Target_lig_1026	Pri-miR-96	Target_159	7.193820026016111