

**“Viral RNA” model test dataset curated from the ROBIN repository (Yazdani et al., 2022)**

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
1	<chem>CCOC(=O)c1ccc2nc(C(F)(F)F)nc(NC3ccc(Cl)cc3)c2c1</chem>	Neg_lig_19	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
2	<chem>O=C(Nc1ccc(-c2nc3cccc3[nH]2)cc1)C1CCN(C(=O)CO)CC1</chem>	Neg_lig_26	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
3	<chem>Cc1ccc2nc(Nc3ccc(C(=O)[O-])cc3)c3nnn3c2c1</chem>	Neg_lig_40	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
4	<chem>BrC1ccc(-c2ccc(CNC[C@H]3CCCOC3)oc2)cc1</chem>	Neg_lig_76	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
5	<chem>Cc1ccc(-c2noc(-c3nnn(-c4cc(C)ccc4C)c3N)n2)cc1</chem>	Neg_lig_103	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
6	<chem>CCOc1cccc(-c2nnn2-c2nonc2N)c1</chem>	Neg_lig_144	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
7	<chem>CCOC(=O)c1enn(-c2cc(C)nc3c(-c4ccc(Cl)cc4)c(C(F)(F)F)nn23)c1N</chem>	Neg_lig_156	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
8	<chem>Cc1ccc2[nH]c(SC[C@H](O)c3cccc3)nc2c1</chem>	Neg_lig_159	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
9	<chem>COc1ccc(C(=O)c2c(N)[nH+]c3n2CCCC3)cc1OC</chem>	Neg_lig_167	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
10	<chem>Nc1ccnc(N2CCc3onc(-c4cccc4)c3C2)n1</chem>	Neg_lig_195	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
11	<chem>COc1cc(C(=O)N2C[C@@H](C[NH+]3CCCC3)[C@H](CO)C2)c2cccc2n1</chem>	Neg_lig_198	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
12	<chem>CC[C@H](Nc1ccc(Br)cc1)C(=O)N/N=C/c1c[nH]c2cccc12</chem>	Neg_lig_201	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
13	<chem>CN(Cc1c[nH]nc1-c1ccc(F)cc1)C(=O)[C@H](N)Cc1cccc1</chem>	Neg_lig_306	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
14	<chem>COc1ccc(Cl)cc1[N-]c1c(-c2cccc2)c(=O)c1=O</chem>	Neg_lig_317	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
15	<chem>COc1nc(NCc2ccnc2)nc(N2CCSCC2)n1</chem>	Neg_lig_292	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
16	<chem>OCC[C@H]1CCCN1Cc1cc2cc3c(cc2nc1-c1ccc(Cl)cc1)OCO3</chem>	Neg_lig_359	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
17	<chem>O=C(CN1CCC[C@H](O)C1)NCc1cc2n(n1)CCC(N(C(=O)C1CCC1)C2</chem>	Neg_lig_466	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
18	<chem>Cc1cccc(OC[C@H](O)Cn2c(=N)n(CC[NH+]3CCOCC3)c3cccc32)c1</chem>	Neg_lig_525	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
19	<chem>CCc1cnc(NC[C@H]2C[C@@H](CO)[N@H+](C)[C@H]2c2cccc2F)nc1</chem>	Neg_lig_600	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
20	<chem>Cc1sc(-n2cccc2CNc2ccc(F)cc2)c</chem>	Neg_lig_604	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG	0

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	<chem>(C(=O)[O-])c1C</chem>				UGGCUUUGGGGCAUGGACC	
21	<chem>CC(C)Oc1ccccc1[C@H]1C(C#N)=C(N)Oc2c1oc(CO)cc2=O</chem>	Neg_lig_613	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
22	<chem>C[C@@H]1CCC[N@H+](C[C@H](O)COc2ccc3c(c2)OCO3)C1</chem>	Neg_lig_615	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
23	<chem>O=C(c1cn[nH]c1C1CCCCC1)N1Cc2cnn(CCO)c2C1</chem>	Neg_lig_619	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
24	<chem>C/C(=N/NC(=S)N1CCC1)c1cccn1</chem>	Neg_lig_729	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
25	<chem>[NH3+]CC[C@H]1CCCN(Cc2ccccc2C(F)(F)F)C1</chem>	Neg_lig_758	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
26	<chem>Cc1ccc2[nH]c(Cc3ccc4nc(N)sc4c3)nc2c1</chem>	Neg_lig_784	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
27	<chem>C[C@@H](Cn1cnc2ccccc2c1=O)NCc1noc(-c2ccco2)n1</chem>	Neg_lig_821	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
28	<chem>C[C@@H]1O[C@H](Nc2cc(C(=O)[O-])cc([N+](=O)[O-])c2)[C@H](O)[C@H](O)[C@H]1O</chem>	Neg_lig_850	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
29	<chem>OCC#CCN1CCCC[C@H]1c1cccn1</chem>	Neg_lig_885	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
30	<chem>Cn1nnnc1SCC[NH2+]C1CCN(c2nnc3[nH]cnc23)CC1</chem>	Neg_lig_886	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
31	<chem>CN(C)c1c([NH3+])c(=O)oc2ccccc12</chem>	Neg_lig_970	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
32	<chem>CCc1ccc(C(=O)N2CC[C@]3(CCCN(CCO)C3=O)C2)[nH]1</chem>	Neg_lig_984	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
33	<chem>Cc1cc(NCCN2CCOCC2)n2nc(-c3ccccc3)c(C)c2[nH+]1</chem>	Neg_lig_988	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
34	<chem>CCOC(=O)c1ccccc1Nc1nc2ccc(C)cc2n2cnc12</chem>	Neg_lig_1038	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
35	<chem>Nc1nonc1C(=O)N1CCN(C(=O)Nc2ccc(F)c(Cl)c2)CC1</chem>	Neg_lig_1046	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
36	<chem>O[C@@]1(CNc2nnc3cccn23)CCC[NH2+]C1</chem>	Neg_lig_64	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
37	<chem>CC[C@@]1(C)Cc2c(sc3nc(SC)nc(NCC[NH+](C)C)c23)CO1</chem>	Neg_lig_1105	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
38	<chem>O=C([C@@H](c1cccn1)N1CCOCC1)N1CCC(O)(CO)CC1</chem>	Neg_lig_1137	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
39	<chem>CCS(=O)(=O)CCNC(=O)c1ccc([C@H]2CCC[NH2+]C2)cc1</chem>	Neg_lig_1161	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
40	<chem>CCO[C@H]1C[C@@H](O)C12CC[NH+](Cc1nnc(C3CC3)o1)CC2</chem>	Neg_lig_1163	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0

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41	<chem>Cc1ccc2[nH]c(C)c([C@@H](O)C[NH+])3CCCC3)c2c1</chem>	Neg_lig_794	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
42	<chem>C[C@H](Nc1cc(=O)oc2ccccc12)c1ccccc1</chem>	Neg_lig_1195	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
43	<chem>CCc1cc(C[NH2+])C2CCN(c3cc(C)nc(-c4ccccc4)n3)CC2)on1</chem>	Neg_lig_228	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
44	<chem>OCC1(Cc2ccc(Cl)cc2)CCN(c2nccccc2F)CC1</chem>	Neg_lig_1236	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
45	<chem>CCOC(=O)c1sc2nc(Cc3ccccc3)nc(NC[C@H]3CCCCO3)c2c1C</chem>	Neg_lig_1244	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
46	<chem>COc1ccccc1OC[C@@H](O)Cn1nc(C)cc1C</chem>	Neg_lig_1258	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
47	<chem>[NH3+]CCN1CCOCC1</chem>	Neg_lig_1282	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
48	<chem>C[N@H+]1CC[C@@]2(O)OCCC[C@H]2C1</chem>	Neg_lig_1299	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
49	<chem>Nc1nonc1C(=O)N1CCCN(C(=O)Nc2ccc(F)cc2)CC1</chem>	Neg_lig_1306	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
50	<chem>CC(=O)CC[N+](C)(C)C</chem>	Neg_lig_1307	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
51	<chem>COc1ccc(Nc2nc(N)nc(CSc3nnn3C)n2)cc1</chem>	Neg_lig_580	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
52	<chem>CCn1nc(C(=O)O)c2c1CC[C@H](Nc1cc(C)oc1C(F)(F)F)C2</chem>	Neg_lig_1337	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
53	<chem>O=C1N[C@@](CCc2ccccc2)(C2CC[NH2+])CC2)C(=O)N1Cc1ccncc1</chem>	Neg_lig_1339	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
54	<chem>CCc1ccccc1OC2CN(C(=O)[C@@H](O)C(C)C)C2)c1</chem>	Neg_lig_1342	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
55	<chem>Cn1cc(CC(=O)N2CCCC[C@@H]([NH3+])C2)c2ccccc21</chem>	Neg_lig_1368	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
56	<chem>Nc1cc(C(=O)N2CCCC(c3cc(Cc4ccccc4)n[nH]3)CC2)cn1</chem>	Neg_lig_1393	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
57	<chem>CC1(C)CC(O)=C(Br)/C(=N/Cc2ccccc2)C1</chem>	Neg_lig_1425	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
58	<chem>CC(C)c1cc(C(=O)NC(C)(CO)CO)n(C)n1</chem>	Neg_lig_1428	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
59	<chem>O=C(c1ccc2c(c1)CCC2)N1CCC2(CC1)OCCC[C@@H]2O</chem>	Neg_lig_1439	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
60	<chem>Cc1[nH]nc2c1[C@H](c1ccc(Cl)c(Cl)c1)C(C#N)=C(N)O2</chem>	Neg_lig_1447	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
61	<chem>CCCCCNC(=O)n1cc(F)c</chem>	Neg_lig_354	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA	0

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	(=O)[n-]c1=O				GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	
62	CC(C)Nc1nc(N2CCCC2)n c(N2C[C@@H]3C[C@H] (C2)c2cccc(=O)n2C3)n1	Neg_lig_1469	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
63	Cc1nc(N2CCC([NH2+][C] C@H] (O)c3ccc(O)cc3)CC2)c2cc sc2n1	Neg_lig_1474	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
64	COc1cccc1CCNc1nc(N)c 2cccc2n1	Neg_lig_1485	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
65	CNC(=O)c1cc(COc2nnc(N c3ccc(Cl)cc3)c3ccoc23)cc n1	Neg_lig_1553	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
66	Cn1c(=O)c(NC2CCCCC2) c2c3c(cccc31)C(=O)c1ccc cc1-2	Neg_lig_1556	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
67	Cc1cccc(N2CCC([NH2+] CCc3nc(- c4ccc[nH+][c4]n[nH]3)CC2 )c1C	Neg_lig_1560	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
68	COc1ccc(-c2c(- c3cc(OC)c4c(c3OC)OCO4 )noc2N)cc1	Neg_lig_1603	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
69	CC(=O)C1=C(O)C(=O)N( CCO)[C@@H]1c1cccc1	Neg_lig_1628	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
70	Cc1ccc([C@@H]2C[C@H] ] (c3ccc(OCc4cccc4)cc3)n3 nc(N)nc3N2)cc1	Neg_lig_1633	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
71	Cc1nnsc1C(=O)Nc1c(F)c ccc1Cl	Neg_lig_1642	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
72	CC[NH2+][C1(C(N)=O)CC N(c2nnc3c2nc(- c2cccc2Cl)n3- c2ccc(Cl)cc2)CC1	Neg_lig_1650	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
73	O=C(O)CN1CCC2(CC1)C CN(c1cc[nH+][c1]C[C@ @H]2CO	Neg_lig_1675	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
74	CN(C)C(=O)c1ccc(- c2cccc3c2CC[NH2+][C3]o 1	Neg_lig_1714	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
75	C=CCN(Cc1nc(- c2cccc2)no1)C(=O)CC1= CC[NH2+][CC1	Neg_lig_1750	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
76	Cc1cc2oc(=O)cc(C)c2cc1 N	Neg_lig_1751	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
77	CCCCn1nc(C2CC2)nc1- c1ccc(N)[nH+][c1	Neg_lig_1752	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
78	Cc1nc2cc(CNc3cc(C(C)C) [nH+][c(N)n3)ccc2[nH]1	Neg_lig_1766	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
79	Cc1ccc2c(CNCCc3ccco3)c (C(=O)O)n(C)c2c1	Neg_lig_1770	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
80	CC(=O)c1cccc(Nc2cc(- c3ccc(C)cc3) [nH+][c(C)n2)c1	Neg_lig_1786	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0

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81	<chem>Clc1cccc(Nc2nc3nonc3nc2N2CCCC2)c1</chem>	Neg_lig_1816	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
82	<chem>CC[NH+](CC)CCNc1cc(C)[nH+]c2cc(-c3ccc(OC)c(OC)c3)nn12</chem>	Neg_lig_1830	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
83	<chem>O=C(O)[C@@H]1CC2(CCN(S(=O)(=O)N3CCCC3)CC2)CN1</chem>	Neg_lig_1843	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
84	<chem>NC(=O)c1ccc(-c2ccccc2CO)nc1</chem>	Neg_lig_1912	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
85	<chem>O=C(NCCCCc1ccccl)c1nn(-c2ccc(Cl)cc2)nc1CO</chem>	Neg_lig_1228	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
86	<chem>Cc1ccc(-c2nc3nc(C)cc(N4CCN(CC(O)CC4)n3n2)cc1</chem>	Neg_lig_2045	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
87	<chem>Cc1cc(C)c(NC(=O)c2sc3nc(C)c(C)c(C)c3c2N)c(C)c1</chem>	Neg_lig_2060	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
88	<chem>COc1ccc(C(=O)CN2CC[NH2+]CC2)cc1</chem>	Neg_lig_2120	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
89	<chem>CCN(CC)c1ccc(Nc2cc(C)nc3nccn23)c(C)c1</chem>	Neg_lig_2148	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
90	<chem>Nc1cc(C(=O)c2ccccc2C(=O)[O-])ccc1Cl</chem>	Neg_lig_2228	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
91	<chem>Cc1cccc1[C@@H]1C(C#N)=C(N)Oc2c1c(=O)n(C)c1cccc21</chem>	Neg_lig_44	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
92	<chem>Cc1ncc2c(c1CNC(=O)c1ccc(SCCO)cc1)CC[NH2+]C2</chem>	Neg_lig_2283	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
93	<chem>CC1(C)CC(=O)C2=C(C1)OC(N)=C(C#N)[C@H]2c1cccc1</chem>	Neg_lig_2326	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
94	<chem>C=CCOC(=O)C1=C(N)OC(C)=C(C(=O)OC)[C@]12C(=O)Nc1cccc12</chem>	Neg_lig_2267	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
95	<chem>CCOC(=O)Cc1ccc(NCCC(=O)c2ccccc2)cc1</chem>	Neg_lig_2352	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
96	<chem>N#CC1=C(N)Oc2cc(O)ccc2[C@H]1c1ccc(OCc2ccccc2)cc1</chem>	Neg_lig_2369	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
97	<chem>COc1ccc(-c2c(C#N)c(N)nc3c2CCCC3)cc1OC</chem>	Neg_lig_2401	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
98	<chem>C1CCc2[nH]nc(C[NH2+]C3CSCCSC3)c2CC1</chem>	Neg_lig_2405	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
99	<chem>Cc1c/c(=N\c2ccc(Cl)c(C(F)(F)F)c2)n2[nH]c[nH+]c2n1</chem>	Neg_lig_2420	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
100	<chem>Cc1cccc1CSc1nc(N)cc(N(C)CCC(N)=O)n1</chem>	Neg_lig_2454	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
101	<chem>Cc1ccc2nc(N3CCC[C@H](O)C3)c(CN(C)Cc3nnc(C)o3)cc2c1</chem>	Neg_lig_2455	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
102	<chem>Nc1nnc(CCCn2c(=O)oc3c cccc32)s1</chem>	Neg_lig_2478	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
103	<chem>COc1ccccc1- n1cc(C(=O)NC[C@H]2 C[C@H](F)CN2)cn1</chem>	Neg_lig_2481	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
104	<chem>NS(=O) (=O)c1ccc(NC2=CC(=O)c 3ccccc3C2=O)cc1</chem>	Neg_lig_2543	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
105	<chem>O=C([O-])c1cccn1</chem>	Neg_lig_2571	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
106	<chem>O=C1CCc2nc(Nc3ccc(F) cc3)ncc21</chem>	Neg_lig_2575	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
107	<chem>Cc1cc(C)cc(Nc2c(- c3cccc(O)c3)n3nccn23)c 1</chem>	Neg_lig_2576	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
108	<chem>COc1cc(N2CC(=O)C(c3nc (C)c(C)s3)=C2N)cc(OC)c1 OC</chem>	Neg_lig_2590	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
109	<chem>Cc1nc(N)ncc1- c1nc(N2CCOCC2)c2sc(C( C)(C)O)cc2[nH+]1</chem>	Neg_lig_2596	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
110	<chem>O[C@H] (CN1CCCc2ccccc21)Cn1c 2ccccc2c2ccccc21</chem>	Neg_lig_2614	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
111	<chem>Cn1nnnc1SCC[NH2+]Cc1 nc(-c2ccco2)no1</chem>	Neg_lig_2627	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
112	<chem>Cc1ccc(Nc2nc(C(=O)N3C CN(Cc4ccccc4)CC3)cs2)c c1</chem>	Neg_lig_2647	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
113	<chem>Nc1c(C(=O)Nc2ccccc2F)s c2ncccc12</chem>	Neg_lig_2691	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
114	<chem>O=C(N[C@@H] (COc1ccc2[nH]c(=O) [nH]c2c1)c1ccccc1)c1cccn (Cc2ccc(F)c(F)c2)c1=O</chem>	Neg_lig_2708	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
115	<chem>CCOC(=O) [C@H]1CCC2=C1c1c(ccc 3ccccc13)N[C@H]2c1cc c(Br)cc1</chem>	Neg_lig_2718	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
116	<chem>C[C@H]1CN(S(=O) (=O)c2ccc(C(=O)N3CC[C @H] ([NH3+])C3)cc2)CC[NH2 +])1</chem>	Neg_lig_2639	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
117	<chem>C[C@H]1C[C@H] (Nc2ccccc2)c2ccccc2N1C( =O)c1cccc(Br)c1</chem>	Neg_lig_2773	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
118	<chem>Nc1nnc(SCC(=O)NCc2c[n H]nc2-c2ccc(F)cc2)s1</chem>	Neg_lig_2812	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
119	<chem>[NH3+]CCn1cc(C(=O)NC Cc2cc(N3CCCC3)ncn2)nn 1</chem>	Neg_lig_2813	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
120	<chem>CCOC(=O)c1ccc2ncc(C(=O) OCC)c(Nc3ccc(N4CCOCC4) cc3)c2c1</chem>	Neg_lig_2712	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
121	<chem>CCCn1cc(S(=O)(=O)N2C[C@H]3C[C@H](O)[C@@H](O)C[C@H]3C2)cn1</chem>	Neg_lig_2850	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
122	<chem>Cc1nnc2c3cccc3nc(Nc3ccc(C(=O)[O-])c3)n12</chem>	Neg_lig_2864	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
123	<chem>c1ccc(C[C@H](CC[NH2+])Cc2ccco2)c2ccco2)cc1</chem>	Neg_lig_2909	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
124	<chem>CCOc1ccc(-c2nccn2C2CCCC2)cc1CO</chem>	Neg_lig_2931	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
125	<chem>Cc1ccc(C)c(NCCOc2ccccc2)c1</chem>	Neg_lig_2933	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
126	<chem>[NH3+][C@]([H])(C(=O)NCCc2ccccc2)(F)F)c2F)C1</chem>	Neg_lig_2974	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
127	<chem>O=C(CCc1nc2ccccc2[nH]c1=O)N1C[C@H](O)CO1</chem>	Neg_lig_3053	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
128	<chem>CCCC(=O)N1c2c(C)cccc2[C@]([H])(Ne2ccccc2C)C[C@H]1C</chem>	Neg_lig_3064	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
129	<chem>COc1ccc(NCCN2C(=O)[C@H]3CC=C(C)C[C@H]3C2=O)cc1</chem>	Neg_lig_3089	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
130	<chem>NC(N)=[NH+]CCO</chem>	Neg_lig_3100	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
131	<chem>O=C([O-])C[C@H](O)C[C@H](O)C=C/c1c(C2CC2)nc2ccccc2c1-c1ccc(F)cc1</chem>	Neg_lig_3120	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
132	<chem>CCNc1nc(Oc2ccc(=O)[nH]n2)nc(N(C)C)n1</chem>	Neg_lig_3182	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
133	<chem>CNc1cc(C)[nH+]c2c(-c3ccc(F)cc3)cnn12</chem>	Neg_lig_1774	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
134	<chem>Cn1cc(-c2c(C#N)c(N)nc3c2C[C@]([H])([NH3+])CC3)c(-c2ccccc2)n1</chem>	Neg_lig_3208	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
135	<chem>Cc1c(C#N)c(N)n(CCC[NH+])(C)C)c1C</chem>	Neg_lig_3209	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
136	<chem>N#Cc1c2c(c(NCCC[NH+]3CCOCC3)n3c1nc1cccc13)CCC2</chem>	Neg_lig_3210	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
137	<chem>Cc1cc(C)nc(Nc2ncc(O)n2-c2ccc(Cl)cc2)n1</chem>	Neg_lig_3265	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
138	<chem>Cc1ccc(C2(O)CCN(C(=O)[C@]([H])(N)CC3CCCC3)CC2)nc1</chem>	Neg_lig_3330	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
139	<chem>COc1ccc(-c2cc3c(C)nc(N)nc3n([C@H]3CC[C@]([H])(OCCO)CC3)c2=O)cn1</chem>	Neg_lig_1364	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
140	<chem>Nc1ccc(-c2nccc(CCC(F)(F)F)n2)c[nH+]1</chem>	Neg_lig_3349	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
					UGGCUUUGGGGCAUGGACC	
141	<chem>O=C(C[C@H]1CCc2ccccc21)NCC1CC[NH2+][C]C1</chem>	Neg_lig_3398	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
142	<chem>Cc1cc(N2CCN(CCO)CC2)n2nc(-c3ccccc(Cl)c3)c(C)c2[nH+]1</chem>	Neg_lig_3403	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
143	<chem>COC(=O)c1[nH]c2ccccc2c1NCc1ccccc1</chem>	Neg_lig_11	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	0
144	<chem>CCCCNc1oc(-c2ccccc2)nc1S(=O)(=O)c1ccc(Cl)cc1</chem>	Neg_lig_71	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
145	<chem>CCN1c2ccccc2C2=C([C@H](c3ccccc3OC)C(C#N)=C(N)O2)S1(=O)=O</chem>	Neg_lig_142	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
146	<chem>C[N@@H+]([C@H](CCCNC1CNC2Onc(-c3ccc(Cl)cc3)c12)Cc1ccccc1</chem>	Neg_lig_149	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
147	<chem>COc1cccc(OC[C@@H](O)CN2CCN(c3ccccc3)CC2)c1</chem>	Neg_lig_215	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
148	<chem>CC(C)NC(=O)[C@@H]1C[C@H]([NH3+])CN1C(=O)C1(S(=O)(=O)c2ccccc2)CC1</chem>	Neg_lig_236	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
149	<chem>Fe1ccc(Nc2c3c([nH+][c4ccccc24)CCC3)cc1</chem>	Neg_lig_241	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
150	<chem>Cc1nc([C@H]2CCC[NH2+][C2]cc(N2CCC(C(=O)NCc3ccccc3)CC2)n1</chem>	Neg_lig_255	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
151	<chem>Cc1ncc(CO)c2c1Oc1[nH]c(-c3ccccc(Cl)c3)nc(=S)c1C2</chem>	Neg_lig_272	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
152	<chem>CC(C)(C)c1nnc(N2CCC3(CC2)CNC2ccccc23)o1</chem>	Neg_lig_276	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
153	<chem>CCOC(=O)C1CCN(c2c(NC3CCCCC3)c(=O)c2=O)CC1</chem>	Neg_lig_279	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
154	<chem>Cc1cc(C)c(NC(=O)Cn2nnc(C(=O)NCc3ccccc3Cl)c2N)c(C)c1</chem>	Neg_lig_291	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
155	<chem>CC(C)c1cc(NCc2ccc(O)cc2)nc(N)[nH+]1</chem>	Neg_lig_300	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
156	<chem>CN(C)c1ccc(CNc2ccc3c(c2)ncn3-c2ccccc2)cc1</chem>	Neg_lig_348	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
157	<chem>COc1cc(F)c(C(C)C)cc1-c1ccc(C(F)(F)F)cc1CN1C(=O)O[C@H](c2cc(C(F)(F)F)cc(C(F)(F)F)c2)[C@@H]1C</chem>	Neg_lig_380	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
158	<chem>CCOC(=O)c1c(N)sc(C(=O)Nc2ccccc2)c1C</chem>	Neg_lig_409	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
159	<chem>O=S1(=O)N=C(NCCCCO)c2ccccc21</chem>	Neg_lig_421	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
160	<chem>COc1ccccc1OC[C@@H](O)Cn1c([C@H]2CC(=O)N(c3ccccc3)C2)nc2ccccc21</chem>	Neg_lig_482	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0



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161	<chem>CCOc1ccc(NC(=O)c2cnn(C(=O)c3ccccc3)c2N)cc1</chem>	Neg_lig_484	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
162	<chem>CS[C@H]1SC[C@@H]2C(=O)N(C)[C@H](C(C)C)C(=O)OC[C@H](NC(=O)c3cnc4ccccc4n3)C(=O)N[C@H](C)C(=O)N(C)[C@@H]1C(=O)N(C)[C@H](C(C)C)C(=O)OC[C@H](NC(=O)c1cnc3ccccc3n1)C(=O)N[C@H](C)C(=O)N2C</chem>	Neg_lig_486	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
163	<chem>CCc1[nH+]ccn1CCNC(=O)[C@H]1C[NH2+][C][C@H](C(=O)N2CCCC2)C1</chem>	Neg_lig_506	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
164	<chem>C=CCSc1n[nH]c(-c2cccs2)n1</chem>	Neg_lig_531	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
165	<chem>O=C(c1ccc2c(c1)n(CC1C1)c(=O)n2C1CCCCC1)N1C[C@@H]2C[NH2+][C][C@@H]2C1</chem>	Neg_lig_177	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
166	<chem>C1c1ccc(-c2noc3ncnc(NC[C@H]4C CCO4)c23)cc1</chem>	Neg_lig_547	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
167	<chem>COCCNc1nc2c(c(=O)n(Cc3cccc(Cl)c3)c(=O)n2C)n1C</chem>	Neg_lig_642	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
168	<chem>Cc1cnc(C)c(N2CC[C@H](N3CCN(CC4ccccc4)CC3)[C@H](O)C2)n1</chem>	Neg_lig_694	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
169	<chem>CCCc1nc(-c2cc3cccc(C)c3[nH+][c2N Cc2ccc(OC)c(OC)c2)no1</chem>	Neg_lig_696	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
170	<chem>Cc1cccc(-c2noc(CCc3cnn3CCO)n2)c1</chem>	Neg_lig_700	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
171	<chem>CC(C)=NNc1[nH]cnc2cnc1-2</chem>	Neg_lig_744	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
172	<chem>Cc1n[nH]c(C)c1CCNc1nc cc(N2CCC(O)CC2)n1</chem>	Neg_lig_752	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
173	<chem>CN1CCN2c3ncccc3Cc3ccc3[C@H]2C1</chem>	Neg_lig_764	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
174	<chem>Cc1cc(C)c2c(n1)sc1c(N3C CN(CCO)CC3)ncnc12</chem>	Neg_lig_808	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
175	<chem>O=C(Cn1ccc(N2CCCC2)c c1=O)N1CCN[C@H](c2ccccc2)C1</chem>	Neg_lig_855	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
176	<chem>C[NH+]1CCC(N(CCc2ccc c2)C(=O)CN2CCC[C@H](O)C2)CC1</chem>	Neg_lig_882	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
177	<chem>COCC[C@]1(CO)CCCN(C(=O)COc2ccc(C)cc2)C1</chem>	Neg_lig_888	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
178	<chem>NCC1nc2c(nnn2Cc2ccccc2)c(=O)[nH]1</chem>	Neg_lig_914	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
179	<chem>Cc1nc(CNS(=O)(=O)c2ccc(C(=O)N[C@H]3CC[NH2+][C3]cc2)no1</chem>	Neg_lig_930	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
180	<chem>CCCc1cc(C(=O)NC[C@H](O)C[NH+])2CCCCC2)n[</chem>	Neg_lig_986	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	<chem>nH]1</chem>					
181	<chem>COc1ccc(-c2nn3c(NCc4ccnc4)cc(C)[nH+]c3c2C)cc1OC</chem>	Neg_lig_999	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
182	<chem>NC(=O)c1ccc(N2CCN(Cc3c[nH]nn3)C[C@H](O)C2)nc1</chem>	Neg_lig_282	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
183	<chem>O[C@@]1(CNCc2nnc3ccc[n23])C[NH2+]CCOC1</chem>	Neg_lig_1148	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
184	<chem>COCc1ccc(C(=O)N2CCC3(CC2)[C@@H](OCC[NH3+])C[C@H]3O)s1</chem>	Neg_lig_1175	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
185	<chem>CSc1ccc(CC(=O)N2C[C@@H](C[NH+]3CCN(C)CC3)[C@@H](CO)C2)cc1</chem>	Neg_lig_1179	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
186	<chem>CCC[C@H]1CN(c2ccc(C#N)cn2)C[C@@H]1NC(=O)CCO</chem>	Neg_lig_1263	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
187	<chem>NC1=C(c2nc3ccccc3s2)C(=O)CN1c1cccc2ccccc12</chem>	Neg_lig_1281	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
188	<chem>C=CCn1cc(C[NH2+]CCCNS(=O)(=O)c2ccc(C)cc2)c(C)n1</chem>	Neg_lig_1283	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
189	<chem>CC(C)C1=C/C(=C(/O)N2Cc3ccc(C[NH+]4CCN(C)CC4)cc3C2)(C(=O)C=C1O</chem>	Neg_lig_1318	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
190	<chem>O=C1CC[C@@]2(CCCN(C(=O)c3ccc(CO)cc3)C2)CN1Cc1ccncc1</chem>	Neg_lig_1383	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
191	<chem>CC(C)C(=O)Nc1cc(NC(=O)N2CCOC[C@@H](O)C2)ccc1F</chem>	Neg_lig_1389	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
192	<chem>O=C([O-])CNc1ccc([As](=O)([O-])[O-])cc1</chem>	Neg_lig_1410	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
193	<chem>Cc1c(CO)c2ccccc2n1Cc1ccc(Br)cc1</chem>	Neg_lig_1418	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
194	<chem>COCc1cc(C)nc2sc(C(=O)Oc3ccccc3)c(N)c12</chem>	Neg_lig_1449	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
195	<chem>Oc1nccc(SCc2ccc(Cl)cc2Cl)n1</chem>	Neg_lig_1470	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
196	<chem>O=C(c1ccc(-n2cnnc2)nc1)N1CCCC[C@@](O)(CO)CC1</chem>	Neg_lig_1484	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
197	<chem>O=C(Nc1cccc2c1CCC2)c1ccc(CN2CCOC[C@@H]2CO)cc1</chem>	Neg_lig_1518	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
198	<chem>C[C@@H](CC(F)(F)F)[NH2+]CCNc1ccncc1</chem>	Neg_lig_1558	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
199	<chem>Cc1nc2c(c(NCCC[NH+](C)C)n1)CCC2</chem>	Neg_lig_1563	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
200	<chem>CC(C)C[C@@H](NC[C@@H](O)Cn1c2ccccc2c2ccccc21)C(=O)O</chem>	Neg_lig_1620	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
201	<chem>CCOC(=O)c1c(C)oc2ncnc(Nc3ccccc3)c12</chem>	Neg_lig_1648	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
202	<chem>COc1ccc([C@H]2C(C#N)=C(N)Oc3c2oc(CO)cc3=O)cc1Br</chem>	Neg_lig_1653	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
203	<chem>CCc1nc(N2CCN(CCO)CC2)c2cc(C)sc2n1</chem>	Neg_lig_1669	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
204	<chem>CCOC(=O)c1ccc(C)c(N)c1</chem>	Neg_lig_1649	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
205	<chem>CC(C)c1cc(C(=O)N[C@H]2CC[C@H]2[NH3+])on1</chem>	Neg_lig_1699	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
206	<chem>Cc1ccc2c(c1)c1c(n2C[C@H](O)C[NH+]2CCC(C)CC2)CCCC1</chem>	Neg_lig_1735	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
207	<chem>Cc1c(C)n(C[C@H](O)C[NH2+])C(C)(C)C)c2ccccc12</chem>	Neg_lig_1799	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
208	<chem>Nc1nc(CCC(=O)N2CCC[C@H]2CO)cs1</chem>	Neg_lig_1811	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
209	<chem>COC(=O)c1ccc(COc2ccc(CN[C@@H](C)C(N)=O)cc2)o1</chem>	Neg_lig_1817	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
210	<chem>COc1cc(Nc2nc3ccccc3nc2[N-]S(=O)(=O)c2ccc(NC(=O)c3ccc(C)c(OC)c3)cc2)cc(OC)c1</chem>	Neg_lig_1875	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
211	<chem>C#CCn1c(CCCO)nc2ccccc21</chem>	Neg_lig_1934	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
212	<chem>Cc1ccc([N-]S(=O)(=O)c2cc(Br)enc2N)cc1Cl</chem>	Neg_lig_1954	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
213	<chem>Cc1[nH]cnc1CN(CCO)C[C@]12C[C@H]3C[C@H](C[C@H](C3)C1)C2</chem>	Neg_lig_1964	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
214	<chem>Cc1ccc(-c2cnn3c(NCCOCCO)cc(C)[nH+]c23)cc1</chem>	Neg_lig_1974	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
215	<chem>CCn1c(=[NH2+])n(C[C@H](O)c2ccco2)c2ccccc21</chem>	Neg_lig_1990	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
216	<chem>CO[C@@]12[C@H](COC(N)=O)C3=C(C(=O)C(C)=C(N)C3=O)N1C[C@H]1[C@@H]2N1C</chem>	Neg_lig_1996	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
217	<chem>CCC[C@H](O)c1nc2ccccc2n1Cc1ccc(F)cc1</chem>	Neg_lig_1196	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
218	<chem>CCOc1c(C[NH2+])CCCn2cnc2cc(Cl)cc1OC</chem>	Neg_lig_574	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
219	<chem>COc1cc(C(C)=O)ccc1OC[C@@H](O)CN1CCN(S(=O)(=O)N(C)C)CC1</chem>	Neg_lig_2110	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
220	<chem>CC(=O)c1ccc(NC(=O)c2sc3nc(N4CCCC4)c4c(c3c2N)CCCC4)cc1</chem>	Neg_lig_2146	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
221	<chem>CC[C@H]1OC(=O)[C@H](C)[C@@H](O[C@H]2C[C@@](C)(OC)[C@@H](O)[C@H](C)O2)[C@H](C)[C@@H](O[C@@H]2O[C@H](C)C[C@H]([NH+](C)C)[C@@H]2O)[C@](C)(O)C[C@@H](C)C(=O)[C@H](C)[C@@H](O)[C@]1(C)O</chem>	Neg_lig_2149	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
222	<chem>Cc1cc(N)n(-c2ccc(S(=O)(=O)[O-])cc2)n1</chem>	Neg_lig_2201	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0

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223	<chem>COc1ccccc1-c1c(C)nn2c(N)c(-c3ccccc3)c[nH+]c12</chem>	Neg_lig_2202	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
224	<chem>Cc1ccnc([N-]S(=O)(=O)c2ccc(NC(=O)Nc3ccc(S(=O)(=O)[N-]c4nccc(C)n4)cc3)cc2)n1</chem>	Neg_lig_2215	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
225	<chem>CCc1nc(NCCO)c(C#N)c2c1CCCC2</chem>	Neg_lig_2227	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
226	<chem>CCOC(=O)N1CCC(Nc2c(N3CCN(C)CC3)c(=O)c2=O)CC1</chem>	Neg_lig_2231	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
227	<chem>CC[C@@H](C(=O)N1CCC2(CCC(=O)N(CCO)C2)CC1)n1cccn1</chem>	Neg_lig_2238	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
228	<chem>Cc1cc(N2C[C@H](C3CC3)[C@@H](NC(=O)CO)C2)cc(C)[nH+]1</chem>	Neg_lig_2254	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
229	<chem>O=C1CC[C@H]2C[N@H+](CCC(F)(F)F)CC[C@H]2N1CCCCO</chem>	Neg_lig_2270	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
230	<chem>COc1ccccc1[C@H]1C[C@@H](c2ccc(Cl)cc2)Nc2nc(N)nn21</chem>	Neg_lig_2273	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
231	<chem>Cc1ccc([C@H](C(=O)NCCCC[NH3+])[NH+](C)C)cc1</chem>	Neg_lig_2368	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
232	<chem>CC(C)c1ccc(CNc2ccc(N3CCOCC3)c(C(=O)[O-])c2)cc1</chem>	Neg_lig_2416	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
233	<chem>Cc1cc(NCCC[NH+](C)C)n2ncc(-c3ccc(Cl)cc3)c2[nH+]1</chem>	Neg_lig_2452	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
234	<chem>Cc1cc(NCc2ccccc2)n2nc(-c3ccccc3)c(C)c2[nH+]1</chem>	Neg_lig_2456	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
235	<chem>COC(=O)c1cc2n(n1)CCCN(C(=O)c1ccc(N)nc1)C2</chem>	Neg_lig_2460	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
236	<chem>Nc1nnnn1CC(=O)N(Cc1cc(F)cc1)C[C@H]1CCCCO1</chem>	Neg_lig_2537	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
237	<chem>O=S(=O)(c1ccc(F)cc1)c1nc(-c2ccc(F)cc2)oc1Nc1ccco1</chem>	Neg_lig_2559	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
238	<chem>CCCOC(=O)c1ccccc1(Nc2nc(C(=O)OCC)nc3ccccc23)c1</chem>	Neg_lig_2573	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
239	<chem>COc1ccc(CCNCC(=O)Nc2cccc(C)c2C)cc1</chem>	Neg_lig_2616	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
240	<chem>[NH3+][CCN1C(=O)CC[C@H]2CN(C(=O)c3ccccc4ncnc34)CC[C@H]21</chem>	Neg_lig_2625	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
241	<chem>CCN(C(=O)c1ccccc1F)[C@@H]1CCN(c2ccnc(N)n2)[C@H]1O</chem>	Neg_lig_2636	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
242	<chem>CCCCNc1cc(C)[nH+]c2c(-c3ccccc3OC)cnn12</chem>	Neg_lig_2663	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
243	<chem>COc1ccc(-c2[nH]nc3c2[C@]2(C(=O)Nc4ccc(C)c(Br)c42)C(C#</chem>	Neg_lig_2669	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	<chem>N)=C(N)O3)cc1</chem>					
244	<chem>CS(=O)(=O)c1cnc(NCCn2cccn2)n c1[C@H]1CCC[NH2+]C1</chem>	Neg_lig_2685	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
245	<chem>COc1cc(OC)c(Nc2[nH+]c3ccccc3c3nnn23)cc1Cl</chem>	Neg_lig_2709	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
246	<chem>N#Cc1c(N)c2c(c3c1CCCC3)CCCC2</chem>	Neg_lig_2713	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
247	<chem>NC(=O)N1c2ccccc2CC(=O)c2ccccc21</chem>	Neg_lig_2775	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
248	<chem>O=C(c1ccccc1)c1ccc(Sc2ccc([N+](=O)[O-])cc2)cc1</chem>	Neg_lig_2797	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
249	<chem>OCCN1CCN(CCCN2c3ccccc3Sc3ccc(C(F)(F)F)cc32)CC1</chem>	Neg_lig_126	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
250	<chem>COc1c(N)cc(C(=O)[O-])cc1Br</chem>	Neg_lig_2914	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
251	<chem>COc1ccccc1OCc1nc(C#N)c(NCc2ccc(C)cc2)o1</chem>	Neg_lig_2917	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
252	<chem>Clc1ccccc1-c1nncc2sc(Nc3ccccc3)nn12</chem>	Neg_lig_2920	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
253	<chem>O=C(c1ccccc1-n1cncn1)N1CCN[C@H](c2ccccc2)C1</chem>	Neg_lig_2934	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
254	<chem>Cc1cnn(CC[NH2+]C2CCN(c3ncnc4sc(C)cc34)CC2)c1</chem>	Neg_lig_2941	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
255	<chem>Cc1cn2c3c(=O)n(C)c(=O)n(C)c3nc2n1CCO</chem>	Neg_lig_2970	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
256	<chem>COc1ccccc1N1CCN(C(=O)[C@H](O)c2ccccc2)CC1=O</chem>	Neg_lig_2972	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
257	<chem>C#CCN1C(=O)[C@@]2(C(C(=O)OC)=C(N)OC(c3ccccc3)=C2C(=O)OCC)c2ccccc21</chem>	Neg_lig_2979	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
258	<chem>C[C@H](O)c1nc2ccccc2[nH]1</chem>	Neg_lig_2993	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
259	<chem>COc1ccccc1-n1nncc(-c2nc(-c3ccc(F)cc3)no2)c1N</chem>	Neg_lig_1645	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
260	<chem>CCCNc1c([N-]S(=O)(=O)c2ccccc2)c(=O)oc2ccccc12</chem>	Neg_lig_2997	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
261	<chem>Cc1csc(C2=C(N)N(CC[NH+]3CCOCC3)CC2=O)n1</chem>	Neg_lig_3031	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
262	<chem>Nc1nc(CCC(=O)N2CC(c3ccnc3)C2)cs1</chem>	Neg_lig_3058	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
263	<chem>c1ccc(-n2nnnc2SCC[NH2+]Cc2ccc(O)c2)cc1</chem>	Neg_lig_163	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
264	<chem>O=C1CSC(=O)N1C[C@@H](O)COc1ccc(OC[C@H](O)CN2C(=O)CSC2=O)cc1</chem>	Neg_lig_3119	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
265	<chem>Cc1ccc(NCc2ccccc2C[NH+]1C[C@@H]2CCCO2)C3)c1C</chem>	Neg_lig_3134	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
266	<chem>O=C(CCc1cc2n(n1)CCC[NH2+]C2)N1CCN[C@H]2CS(=O)(=O)C[C@H]21</chem>	Neg_lig_3158	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0

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267	<chem>COc1cc(N2C(=O)C[C@H](N3CCCC[C@H]3CCO)C2=O)cc(OC)c1OC</chem>	Neg_lig_3172	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
268	<chem>CCN(CC)C(=O)Cn1ccc(NC(C)=O)nc1=O</chem>	Neg_lig_3193	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
269	<chem>Nc1nonc1-c1nc2ccccc2n1Cc1cccc(C(F)(F)F)c1</chem>	Neg_lig_3194	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
270	<chem>CCOc1ccc(Cl)cc1C[NH2+]CCNC(=O)c1nonc1N</chem>	Neg_lig_3212	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
271	<chem>COc1cccc1C(=O)Oc1ccc(Cl)cc1[N-]C1=NS(=O)(=O)c2ccccc21</chem>	Neg_lig_3214	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
272	<chem>O=C([O-])c1sc2ccccc2c1Nc1ccccc1</chem>	Neg_lig_3218	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
273	<chem>CC1=N/C(=C(/O)NCC(=O)[O-])C(=O)c2ccc(Oc3cccc3)cc21</chem>	Neg_lig_3224	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
274	<chem>COc1cc(C(=O)N2CC[NH2+]CC2)cc(OC)c1OC</chem>	Neg_lig_3239	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
275	<chem>CSCC(=O)N1CCC2(CC[NH+](Cc3cn(C)nc3C)CC2)[C@@H](CO)C1</chem>	Neg_lig_3249	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
276	<chem>COC(=O)c1ccc(Nc2nc3cccc3c3nnc(C)n23)cc1</chem>	Neg_lig_3262	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
277	<chem>O=C1SC(c2ccccc2)=C/C1=C/Nc1nc(-c2ccccc2)es1</chem>	Neg_lig_3274	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
278	<chem>CCSC1=C(C#N)[C@@H](c2ccccc2Cl)C(C#N)=C(N)N1</chem>	Neg_lig_3277	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
279	<chem>C[NH+](C)CCCNC1oc(/C=C/c2ccc(F)cc2)nc1C#N</chem>	Neg_lig_3289	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
280	<chem>CCOC(=O)CSc1nc(N)nc(C)c1Br</chem>	Neg_lig_3306	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
281	<chem>Clc1ccc(C[NH2+])Cc2ccco2)cc1</chem>	Neg_lig_827	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
282	<chem>C[C@H]1CN(c2ccccc2Cl)C(=O)CN1C(=O)c1cnc(N)c1</chem>	Neg_lig_2745	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
283	<chem>OCCSc1nnc(Cc2ccccc2)n1Cc1ccccc1</chem>	Neg_lig_3354	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
284	<chem>COCCNc1cc(C)[nH+][c2c(C)c(-c3ccccc3)nn12</chem>	Neg_lig_3356	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
285	<chem>CCOc1ccccc1NC(=O)c1sc2nc3c(cc2c1N)CN(Cc1cccc1)CC3</chem>	Neg_lig_3395	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	0
286	<chem>Cc1ccccc1Nc1nc([C@]2(C)C[C@@]3(C)[C@H](COCC(C)C)OC3=O)C(=O)O2)es1</chem>	Neg_lig_10	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGCUGACGGUACA	0
287	<chem>CC(=O)Nc1c(N)c2ccccc2oc1=O</chem>	Neg_lig_20	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGCUGACGGUACA	0
288	<chem>Cc1ccc(C(=O)[C@@H](NC(=O)c2cccs2)Nc2ccccc2Br)cc1</chem>	Neg_lig_43	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGCUGACGGUACA	0
289	<chem>Cc1ccccc1CN1c2ccccc2C2=C([C@@H](c3ccc(Cl)cc3)C(C#N)=C(N)O2)S1(=O)=O</chem>	Neg_lig_55	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGCUGACGGUACA	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
290	<chem>COc1ccc([C@@H](O)[C@@H](C)O)c2ccc([C@@H]3O[C@@H](c4ccc(O[C@H](C)[C@H](O)c5ccc(OC)c(OC)c5)c(OC)c4)[C@H](C)[C@H]3C)cc2OC)cc1OC</chem>	Neg_lig_66	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
291	<chem>Cc1ccc(-c2noc(CNC3CCCC3)n2)cc1</chem>	Neg_lig_108	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
292	<chem>CCOc1ccc(-c2noc(-c3nnn(-c4cccc(OC)c4)c3N)n2)cc1</chem>	Neg_lig_118	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
293	<chem>O=C1CCC2(CC[NH+](Cc3ccoc3)CC2)CN1CCC O</chem>	Neg_lig_121	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
294	<chem>COc1cccc(CNc2ccc3c(c2)ncn3C(C)(C)C)c1OC</chem>	Neg_lig_138	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
295	<chem>NC(=O)c1ccc2c(c1SCCO)C(=O)c1cccc1C2=O</chem>	Neg_lig_208	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
296	<chem>CCCCNc1nc2c(-c3cccc(F)c3)nnn2c2cccc12</chem>	Neg_lig_218	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
297	<chem>Clc1ccc(-c2nc(-c3cc4cc(Cl)ccc4o3)cs2)cc1</chem>	Neg_lig_230	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
298	<chem>COc1cccc1-c1nc2c(OC)ccc(OC)c2cc1CN1CC[C@@H](O)C1</chem>	Neg_lig_262	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
299	<chem>O=C(CCc1nc(-c2ccc[nH+](c2)no1)N1CCC[C@@H](O)(CO)C1</chem>	Neg_lig_303	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
300	<chem>O=C(CCSc1nnc(-c2ccncc2)o1)N1CCOC[C@@H](O)C1</chem>	Neg_lig_304	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
301	<chem>C=CCNc1nc(-c2cccc2)nc(-n2cnc2)n1</chem>	Neg_lig_311	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
302	<chem>Fe1ccc(C[NH2+])CC[C@H](Cc2cccc2)c2ccco2)cc1</chem>	Neg_lig_315	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
303	<chem>Cc1cc(C)n(-c2nc3cccc3nc2Nc2ccc(Cl)cc2)n1</chem>	Neg_lig_362	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
304	<chem>C[C@]1(Cc2ccc3c(c2)OC O3)CCC[N@@H+](Cc2ccncc2N)C1</chem>	Neg_lig_382	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
305	<chem>CCc1c(N[C@H](c2ncccc2C)C2CC2)nc(N)[nH+](c1C</chem>	Neg_lig_399	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
306	<chem>Cc1c(C(=O)N2CCCCC2)nnn1-c1nonc1N</chem>	Neg_lig_407	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
307	<chem>Cc1ccc(C(=O)c2sc3nc(C)cc3c2N)cc1</chem>	Neg_lig_414	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
308	<chem>Nc1cc(C(=O)N2CCCC(c3ncn3Cc3ccncc3)CC2)ccn1</chem>	Neg_lig_462	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
309	<chem>CC[n+](c1nc(C[C@H](O)COCc2cccc2)c2cccc21</chem>	Neg_lig_488	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
310	<chem>O[C@H](COCc1cccc1)CN1CCc2cccc2C1</chem>	Neg_lig_489	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
311	<chem>Cc1cccc1C(=O)/N=C1\SC2=C(C[C@H](C(C)(C)C)C2)\C1=C(O)NCCO</chem>	Neg_lig_530	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
312	<chem>O=C(CCC1CCN(C(=O)C[C@H]2COCC[NH2+])C(C1)NCc1ccc(F)cc1</chem>	Neg_lig_539	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
313	<chem>Cn1c(=O)c2cccc(N)c2c(=O)n1C</chem>	Neg_lig_558	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
314	<chem>C=C1CC2(OC1=O)c1cccc1CCc1cccc12</chem>	Neg_lig_578	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
315	<chem>Cc1c(Cl)cccc1-n1nnc(-c2nc(-c3cccn3)no2)c1N</chem>	Neg_lig_592	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
316	<chem>CCOC(=O)N1CCN(c2ncnc3sc4c(c23)CCN4)CC1</chem>	Neg_lig_603	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
317	<chem>O=C(NC1CC1)[C@@H]1CNCCN1C(=O)c1cc2c(s1)CCCC2</chem>	Neg_lig_640	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
318	<chem>Cc1cc2c(c(=O)o1)[C@@]1(C(=O)Nc3ccc(C)c(Br)c31)C(C#N)=C(N)O2</chem>	Neg_lig_667	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
319	<chem>C1C[C@H](C[NH2+])Cc1cccc1cc1</chem>	Neg_lig_686	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
320	<chem>COc1ccc([C@@H]2C=C(c3ccc(C)cc3)[NH+]=C3NC(CCCO)=[NH+])N32)cc1</chem>	Neg_lig_692	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
321	<chem>COCc1cc(C)nc2sc(C(=O)Nc3ccc(F)cc3F)c(N)c12</chem>	Neg_lig_695	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
322	<chem>NC(=O)C1=C(NCCc2cccc2)c2cccc2S1(=O)=O</chem>	Neg_lig_743	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
323	<chem>CCCCc1nc2sc(C(=O)OCC)c(N)c2c2c1COC(C)(C)C2</chem>	Neg_lig_816	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
324	<chem>CC[C@H](O)Cn1nc(-c2ccc(O)cc2)nc1CCc1ccn1c1</chem>	Neg_lig_829	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
325	<chem>Oc1ccc(C2CCN(c3cc[nH+]c4cccc34)CC2)cc1O</chem>	Neg_lig_861	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
326	<chem>CC1(C)[C@@H]2CC[C@H](C/N=C(\N)CSS(=O)(=O)O)[C@H]1C2</chem>	Neg_lig_884	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
327	<chem>COc1ccc2cc(-c3cc(N)cc[nH+]3)[nH]c2c1</chem>	Neg_lig_904	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
328	<chem>CC(C)c1nc(CN(C)C(=O)CCc2nc(N)n[nH]2)no1</chem>	Neg_lig_911	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
329	<chem>Cn1c(=O)c2c(nc(Sc3ccc(N)cc3)n2C)n(C)c1=O</chem>	Neg_lig_305	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
330	<chem>Oc1c(CN2CCN(c3cccc3)CC2)cc(Br)c2ccn1c12</chem>	Neg_lig_945	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
331	<chem>CCN(CC)S(=O)(=O)c1ccc(Nc2ncnc3c2nc2n3CCCC2)cc1</chem>	Neg_lig_958	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
332	<chem>CS(=O)(=O)N1CCN(c2ccc(N=c3\c4c(nc5[nH+]c[nH]n35)C(C4)cc2)CC1</chem>	Neg_lig_963	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
333	<chem>O=S(=O)(c1ccc(F)cc1)N1CCC[C@H](CO)C1</chem>	Neg_lig_966	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
334	<chem>Cc1cc(OC[C@H](O)Cn2c(C)nc3cccc32)cc1Cl</chem>	Neg_lig_973	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0



Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
335	<chem>[NH3+][CC1CCN(c2cnn(Cc3noc(-c4ccccc4)n3)c(=O)c2)CC1</chem>	Neg_lig_983	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
336	<chem>C1[C@@H]2[C@@H]3/C(=N\N=C4/[C@H]5[C@H]6C[C@@H]4C[C@H]65)[C@H]1C[C@H]23</chem>	Neg_lig_1004	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
337	<chem>COC(=O)c1ccccc1Nc1c(-c2cc(Br)ccc2O)nc2cncn12</chem>	Neg_lig_1024	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
338	<chem>Cc1sc2nc(CC[NH2+][C3CSCCSC3][nH]c(=O)c2c1C</chem>	Neg_lig_1027	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
339	<chem>CCOC(=O)c1ccc2nccc(C(=O)OCC)c(NCc3ccco3)c2c1</chem>	Neg_lig_1028	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
340	<chem>CCOC(=O)c1c(Nc2ccc(Cl)cc2)cc(C)nc1C</chem>	Neg_lig_1047	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
341	<chem>Cc1nnc(-n2ccccc2)s1</chem>	Neg_lig_1064	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
342	<chem>CC(C)c1nc(CN(C)c2nc(C[C@H]3[NH3+])c2c1c[nH+]c3ccccc23)es1</chem>	Neg_lig_1074	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
343	<chem>FC(F)(F)c1nnc2c3ccccc3c(NC3CC3)nn12</chem>	Neg_lig_1079	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
344	<chem>C[C@@H](CO)NC(=O)c1cc2ccccc2oc1=O</chem>	Neg_lig_1089	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
345	<chem>CC1=[NH+]C[C@H](C)c2ccccc21</chem>	Neg_lig_998	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
346	<chem>CN(C(=O)c1ccccc1S(=O)(=O)N(C)c2ccccc2c1)[C@@H]1CCCC[C@H]1O</chem>	Neg_lig_1131	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
347	<chem>Nc1nc(NCCc2n[nH]c3c2C(CCC3)cc(N2CCOCC2)n1</chem>	Neg_lig_1143	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
348	<chem>COc1ccccc1Nc1cc(C)nc2nc(C)nn12</chem>	Neg_lig_1181	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
349	<chem>CCOc1cc([C@@H]2c3c(n[nH]c3-c3ccccc3O)C(=O)N2CCC(O)ccc1O</chem>	Neg_lig_36	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
350	<chem>CC1=C(C(=O)N=C2\C=C=CC3=NN=CC3=C2)NN(c2ccccc2)[N-]1</chem>	Neg_lig_1222	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
351	<chem>O=C(NCCCCc1ccccc1)c1nn(-c2ccc(Cl)cc2)nc1CO</chem>	Neg_lig_1228	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
352	<chem>Cc1ccc(OCc2nc(N)nc(N(C)C)n2)cc1C</chem>	Neg_lig_1260	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
353	<chem>O=C([O-])c1ccccc1Nc2c(-c3ccccc3O)c3nc3cncn23)c1</chem>	Neg_lig_1274	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
354	<chem>C=CCn1cc(C[NH2+][Cc2nncn2CCc2ccccc2)c(C)n1</chem>	Neg_lig_1325	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
355	<chem>CCC(=O)O[C@]1(C(=O)SCF)[C@H](C)C[C@H]2[C@@H]3[C@H]C[C@H](F)C4=CC(=O)C=C[C@]4(C)[C@@]3(F)[C@@H](O)C[C@]21C</chem>	Neg_lig_1346	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
356	<chem>C[C@@H](CCc1ccccc1)</chem>	Neg_lig_1354	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	[NH2+][CCSc1c[nH]nn1				UGACGGUACA	
357	O=S1(=O)N=C(/N=c2\cccc[nH]2)c2cccc21	Neg_lig_1562	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
358	CN(C)c1cccc(C(=O)N2CC C([C@@H] (O)CCc3cccc3)CC2)c1	Neg_lig_1586	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
359	COC(=O)CN1CCC([NH2+] [C@H]2CCNC2(C)C)CC1	Neg_lig_1680	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
360	[NH3+] [C@H]1CCN(C(=O)c2ccc c(-c3ncc[nH]3)c2)C1	Neg_lig_1192	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
361	Cc1cc2nc(CN3CC[C@H]4 C[NH2+][C@H]43)cc(=O)n2[nH]1	Neg_lig_1711	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
362	COc1ccc(CC=NN3C([C @@H])(Cc4cccc4) [C@@H](C)O)=[NH+] [C@H](C) [C@@H]3C(=O)N2)cc1O C	Neg_lig_1723	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
363	Cc1cccc(-n2nnc(-c3nc(- c4ccc(F)cc4)no3)c2N)c1	Neg_lig_1781	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
364	Cn1c(=O)c2c(nc(N3CCOC C3)n2CC[NH3+])n(C)c1=O	Neg_lig_1833	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
365	CN(C)c1ccc(C(=O)NC(C) (C)c2nnc(N)s2)cn1	Neg_lig_1856	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
366	Cc1ccc(N2C(=O)C(=CN)C (=O)N(c3ccc(C)cc3)C2=O )cc1	Neg_lig_1873	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
367	Cc1cccc(NCCC(=O)c2ccc 3cccc3c2)c1	Neg_lig_570	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
368	CC[C@H](O)Cn1ncnc1- c1ccc(C#N)cc1	Neg_lig_1956	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
369	Cc1ccc(NC(=O)c2ccc(CN 3CC[NH+] (C)CC3)cc2)cc1Nc1nc(- c2ccnc2)cs1	Neg_lig_1962	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
370	CC[C@@]1(C)CC(=O)c2c c(NC(=O)CCc3cc4n(n3)C CC[NH2+][C4]ccc2O1	Neg_lig_1199	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
371	O=[N+] ([O-])c1ccc(Cl)cc1NCCN1 CCOCC1	Neg_lig_2004	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
372	COCCNc1oc(- c2ccc(S(=O) (=O)N3CCCCC3)cc2)nc1 C#N	Neg_lig_2049	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
373	Nc1nc(CSCCO)nc(Nc2ccc c2)n1	Neg_lig_2058	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
374	[NH3+][C@H]1CN(/ C(O)=C2/ C=NC(C3CC3)=NC2=O)C [C@@H]1C1CC1	Neg_lig_2102	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
375	O=C1C=C(NCCC[NH+])2 CCOCC2)C2(CCCC2)O 1	Neg_lig_2112	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
376	CC(C) (C)c1[nH]nc2c1[C@@H] (c1cc(Br)ccc1F)C(C#N)=C (N)O2	Neg_lig_2156	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
377	COc1cccc(-	Neg_lig_2179	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	<chem>c2cc(=O)c3ccccc3o2)c1N</chem>				UGACGGUACA	
378	<chem>Clc1cccc1C[NH2+]Cc1ccncl</chem>	Neg_lig_2200	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
379	<chem>c1ccc(-c2ccc(C[NH2+])Cc3cccs3)o2)cc1</chem>	Neg_lig_2235	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
380	<chem>COc1ccc(C2=NC(=O)/C(=C/O)N3CC[C@H]4C[NH2+]C[C@H]43)C=C2)cc1</chem>	Neg_lig_2265	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
381	<chem>O=c1[nH]cc(l)cc1I</chem>	Neg_lig_2331	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
382	<chem>Cc1nsc1CCC(=O)N[C@H](CO)C1CCSCC1</chem>	Neg_lig_2333	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
383	<chem>c1cc2c(cc1Nc1nc(N3CCC(CC3)nc(N3CCCC3)n1)OCO2</chem>	Neg_lig_2346	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
384	<chem>CCOC(=O)c1enc2c(C)cc(C)cc2c1Nc1ccc(N(C)C)cc1</chem>	Neg_lig_2379	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
385	<chem>Cc1cccc(Nc2c(-c3ccc(O)cc3)nc3nccn23)c1</chem>	Neg_lig_2422	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
386	<chem>O=C1C[C@H](Nc2ccc(N3CCOCC3)cc2)C(=O)N1c1cccc2ccccc12</chem>	Neg_lig_2488	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
387	<chem>NS(=O)(=O)c1ccc(Cl)cc1[N+](=O)[O-]</chem>	Neg_lig_2518	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
388	<chem>C=C1C(=O)O[C@@H]2C[C@]3(C)O[C@H]3CCC(C)=C[C@H](OC(C)=O)[C@@H]12</chem>	Neg_lig_2557	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
389	<chem>Cc1cc(C(c2cc(C)c(N)c(C)c2)c2ccco2)cc(C)c1N</chem>	Neg_lig_2565	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
390	<chem>Cn1nc(C(=O)N2CCC3(CC2)[C@@H](OCC[NH3+])C[C@H]3O)cc1-c1ccccc1</chem>	Neg_lig_2567	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
391	<chem>c1cncc([C@@H]2CCCCN2c2ncnc3sc4c(c23)CCNC4)c1</chem>	Neg_lig_2652	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
392	<chem>COc1ccc(N2CC(=O)C(c3nc(C)c(C)s3)=C2N)cc1</chem>	Neg_lig_2682	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
393	<chem>O=C(C[C@@H]1Nc2cccc2NC1=O)Nc1cccc1SC(F)(F)C(F)(F)C(F)(F)F</chem>	Neg_lig_2694	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
394	<chem>Cc1ccc(OC[C@@H](O)C[NH+]2CCCCC2)c(C)c1</chem>	Neg_lig_2728	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
395	<chem>Cc1nc(CN2CCN(C(=O)c3ccccc3[C@H]3CC[NH2+]C3)CC2)no1</chem>	Neg_lig_2736	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
396	<chem>CC(C)n1cc(C#N)c(N)n1</chem>	Neg_lig_2738	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
397	<chem>O=C([O-])c1cccc1-c1cccc1C(=O)Nc1ccc2oc(=O)c3ccccc3c2c1</chem>	Neg_lig_2799	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
398	<chem>CC1CC[NH+](Cc2ccc(C(=O)N3CCO[C@]4(C[NH2+])CCOC4)C3)o2)CC1</chem>	Neg_lig_2815	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
399	<chem>O=C1Nc2ccccc2/C1=C/Nc2ccccc2C1=O</chem>	Neg_lig_2818	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
400	<chem>Cc1c(C(=O)N2CCO[C@]3(C[NH2+][CCOC3]C2)sc2ccccc12</chem>	Neg_lig_2819	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
401	<chem>CCc1ccc(CNC(=O)c2nn(-c3ccc(C)c(C)c3)nc2CO)cc1</chem>	Neg_lig_2824	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
402	<chem>C[C@]12CC[C@H]3c4cc(O)cc4CC[C@H]3[C@H]1[C@H](O)[C@H](O)[C@H]2O</chem>	Neg_lig_2832	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
403	<chem>CCn1c(N)c(C(=O)N2CCC(CC2)sc1=S</chem>	Neg_lig_2893	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
404	<chem>Cc1c/c(=N/C2=NS(=O)(=O)c3ccccc32)[n-]o1</chem>	Neg_lig_2908	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
405	<chem>O=C(c1ccc(Cn2ccnc2)o1)N1CC[C@@]2(CCCN(CCOC2=O)C1</chem>	Neg_lig_2952	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
406	<chem>O=C1C[C@H]([NH+]2CCCCC2)C=C1Nc1ccccc1</chem>	Neg_lig_2981	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
407	<chem>CO[C@H]1CN(C(=O)COc2ccc(C)c2C)CC[C@H]1[NH3+]</chem>	Neg_lig_2998	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
408	<chem>Cc1cccc(OC2CCN(Cc3c(CO)enc(C)c3O)CC2)c1</chem>	Neg_lig_2999	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
409	<chem>Cc1nc(CC(=O)N[C@H](c2nnc3n2CC[NH2+][CC3]C(C)C)c(C)s1</chem>	Neg_lig_3029	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
410	<chem>COC(=O)c1cc(/N=C2C(=C(N)[O-])/S(=O)(=O)c3ccccc3/2)ccc1Cl</chem>	Neg_lig_3032	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
411	<chem>O=C(c1ccc(Nc2nc(-c3ccccc3)c3cc(Br)ccc3n2)cc1)N1CCOCC1</chem>	Neg_lig_3033	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
412	<chem>Cn1ccnc1[C@H](O)c1ccc(N)cc1</chem>	Neg_lig_3106	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
413	<chem>CN(C)C(=O)c1cccc(COc2ccc(N3C(=N)NC(N)=[NH+]C3(C)C)cc2Cl)c1</chem>	Neg_lig_3124	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
414	<chem>O=C([C@@H]1C[C@@H](O)C[NH2+]1)N1CCC(c2[nH+]ccn2CC2CC2)CC1</chem>	Neg_lig_3142	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
415	<chem>O=C([O-])[C@H](Cc1ccccc1)Nc1ncnc2c1oc1ccccc12</chem>	Neg_lig_3164	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
416	<chem>CC(C)CNe1nc2c(c(=O)n(Cc3ccccc3)c(=O)n2C)n1C</chem>	Neg_lig_3181	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
417	<chem>COc1ccc(-c2c(C)nn3c(NCC[NH+]4CCCC4)cc(C)[nH+]c23)cc1OC</chem>	Neg_lig_3185	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
418	<chem>Fe1ccc(CNc2ccc(N3CCN(Cc4ccccc4)CC3)cc2)cc1</chem>	Neg_lig_1778	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
419	<chem>O=C1C[C@H](Nc2ccc3c(c2)OCO3)C(=O)N1c1ccccc1</chem>	Neg_lig_2168	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
420	<chem>C[N@H+]1CCc2[nH]nc(C(=O)N(C/C=C\c3ccccc3)CCO)c2C1</chem>	Neg_lig_3342	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
421	<chem>CC(=O)O[C@]1(C(C)=O)CC[C@@H]2[C@@H]3C[C@H](C)C4=CC(=O)CC[C@]4(C)[C@H]3CC[C@@]21C</chem>	Neg_lig_3360	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
422	<chem>Cn1c(N2CC[C@H](O)C2)nc2cc(C(=O)N[C@H]3CCc4ccccc43)ccc21</chem>	Neg_lig_3373	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
423	<chem>CCc1ccc(NC(=O)c2nnn(C(=O)Nc3ccccc3c2N)cc1</chem>	Neg_lig_3423	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	0
424	<chem>O=C1CCC2(CCN(Cc3nnc(c4ccccc4)o3)CC2)CN1CCO</chem>	Neg_lig_1	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
425	<chem>COc1ccc(C(=O)c2sc3nc4c(c(C(F)F)c3c2N)CCCC4)cc1</chem>	Neg_lig_51	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
426	<chem>Cc1ccn(CO)n1</chem>	Neg_lig_57	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
427	<chem>Cc1cc(N[C@H]2CC(=O)N(Cc3ccccc3C(F)(F)F)C2)nc(N)n1</chem>	Neg_lig_65	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
428	<chem>O=C(Nc1cccc(Cn2cncn2)c1)N1CCN[C@H]2CS(=O)(=O)C[C@H]21</chem>	Neg_lig_146	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
429	<chem>Cn1cc[nH+]c1CN1CCN(C[C@]2(O)CC[NH2+]C2)CC1</chem>	Neg_lig_190	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
430	<chem>CC(C)N(CCCc1ccccc1)C(=O)C1(N)CC1</chem>	Neg_lig_224	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
431	<chem>C[NH+](C)CCc1c[nH]c2ccc(CS(=O)(=O)N3CCCC3)cc12</chem>	Neg_lig_244	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
432	<chem>CN(C)c1n/c(=N/Cc2ccc2)ss1</chem>	Neg_lig_246	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
433	<chem>O=C(C1CCC1)N1C[C@H](O)[C@@H](N2CCN(c3cncn3)CC2)C1</chem>	Neg_lig_258	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
434	<chem>C[NH2+][C][C@H](O)c1cccc(OC(=O)c2ccccc2)c1</chem>	Neg_lig_265	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
435	<chem>CC1=CC(=O)C(=C(\C)O)/C(=N/c2ccc3c(c2)OCO3)O1</chem>	Neg_lig_281	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
436	<chem>CCc1c(C)nn(CCN2cc(-c3ccc(CO)o3)nn2)c1C</chem>	Neg_lig_50	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
437	<chem>COc1cccc(C[NH2+])CCO)c1OCc1ccc(Cl)cc1</chem>	Neg_lig_309	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
438	<chem>O=C(CC[NH2+][C][C@H](O)c1ccccc1Cl)NCc1cccs1</chem>	Neg_lig_319	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
439	<chem>Cc1cccc(NC(=O)c2nnn(Cc3ccc(C(C)C)cc3c2N)c1</chem>	Neg_lig_336	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
440	<chem>C[C@@H]1CCO[C@H]2CN3C=C(C(=O)[N-]C4ccc(F)cc4F)C(=O)C(=O)C3=C(O)N21</chem>	Neg_lig_376	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
441	<chem>CSc1c(CC(=O)NCCO)n(C)c2ccccc12</chem>	Neg_lig_377	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
442	<chem>O=C(CCc1nc(-c2ccccc2)no1)N1C[C@H]2CCC[C@@]2(CO)C1</chem>	Neg_lig_564	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
443	<chem>COc1ccc(CNCc2ccc(-c3ccc(OC)c(Cl)c3)o2)cc1</chem>	Neg_lig_582	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
444	<chem>N#CC1=C(N)N(c2c(F)ccc2F)C2=C(C(=O)CCC2)[C@@H]1c1ccccc1F</chem>	Neg_lig_627	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
445	<chem>CCN(CC)S(=O)(=O)c1ccc(Nc2nc3ccc(Cl)c3n3cnnc23)cc1</chem>	Neg_lig_644	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
446	<chem>COc1ccc(C(=O)c2sc3nc(C)cc(C(F)(F)F)c3c2N)cc1OC</chem>	Neg_lig_647	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
447	<chem>Cc1cc(Nc2ccccc2F)n2nc(-c3ccccc3)nc2n1</chem>	Neg_lig_697	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
448	<chem>C[N@H+]1CCN(c2ccnc(N)n2)C[C@H]12CCC(=O)N(CC1CC1)CC2</chem>	Neg_lig_720	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
449	<chem>Cc1cc2ncn(C[C@H](O)COc3ccccc(Cl)c3)c2cc1C</chem>	Neg_lig_807	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
450	<chem>CCc1ccc([C@H]2N[C@@](CC(C)C)(C(=O)OC)[C@H]3C(=O)N(C)C(=O)[C@H]23)nc1</chem>	Neg_lig_870	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
451	<chem>CCOC(=O)c1sc2nc(C)cc(C(F)(F)F)c2c1N</chem>	Neg_lig_871	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
452	<chem>CCOC(=O)CN[C@H]1CC(=O)N(c2ccc(Br)cc2)C1=O</chem>	Neg_lig_883	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
453	<chem>Cc1ccccc1-c1ccccc1C(=O)N1CC[C@H](CO)[C@H](O)C1</chem>	Neg_lig_898	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
454	<chem>C[NH2+]CC(=O)N1C[C@H]2C[C-]1C(=O)N2c1cc(-c2ccccc2)ccc1OC</chem>	Neg_lig_940	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
455	<chem>CCc1nc(NC[C@H]2CCC(O2)c(C#N)c2c1COC(C)(C)C2</chem>	Neg_lig_944	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
456	<chem>C=CCn1c(=N)n(C[C@H](O)c2ccc(C)cc2)c2ccccc21</chem>	Neg_lig_960	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
457	<chem>Cc1cc(C)n(-c2nc(NCCC[NH+](C)C)c3c4c(sc3n2)COC(C)(C)C4)n1</chem>	Neg_lig_974	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
458	<chem>CC[C@H](O)Cn1nc(-c2cncnc2)nc1C1(N2CCCC2)CCCC1</chem>	Neg_lig_39	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
459	<chem>[NH3+]C[C@H](c1ccccc1)C1CCCC1</chem>	Neg_lig_993	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
460	<chem>CN(C[C@H]1CC(=O)N(C(C)C)C1)c1nccc(N2CCCC(O)CC2)n1</chem>	Neg_lig_1006	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
461	<chem>Oc1cc(C[NH2+]C2CCCC2)c(O)cc1C[NH2+]C1CCC1</chem>	Neg_lig_1041	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
462	<chem>CCOc1ccc(CN2CCN(c3cc(Cl)n3)CC2)cc1CO</chem>	Neg_lig_1066	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
463	<chem>COCc1noc(CCN2cnc3sc4c(c3c2=O)CCNC4)n1</chem>	Neg_lig_1092	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
464	<chem>COC(=O)c1ccc(OC[C@H](O)CN2C(=O)NC(C)(C)C2=O)cc1</chem>	Neg_lig_1102	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
465	<chem>O=C1OC2(CC[NH2+](CC2)CN1CC(=O)N1CC[C@H]1c1cccs1</chem>	Neg_lig_1144	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
466	<chem>O=S1(=O)C[C@H](NCCc2ccccc2F)[C@@H](S(=O)(=O)c2ccc(F)cc2)C1</chem>	Neg_lig_1212	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
467	<chem>Clc1ccc(CCNC2ncnc3c2ncn3CCCC2)cc1</chem>	Neg_lig_1253	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
468	<chem>COc1ccc(CC[N@H+](C)[C@H]2CCCN(c3ccnc(N)n3)C2)cc1OC</chem>	Neg_lig_1262	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
469	<chem>CC(C)[C@]1(O)CN(c2nc3ccccc3n2CCO)C[C@H]1C</chem>	Neg_lig_1269	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
470	<chem>Cc1n[nH]c(C)c1[C@@H]([NH3+])C(=O)NCc1cc(C(C)C)no1</chem>	Neg_lig_1291	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
471	<chem>Nc1nc2c3ccccc3[nH+]c(Cc3ccccc3)n2n1</chem>	Neg_lig_1317	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
472	<chem>CC1=N/C(=N/Nc2ccccc2)N=C1/N=N/c1ccccc1</chem>	Neg_lig_1343	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
473	<chem>C/C(=N\NC(=O)c1cc(C)n[nH]1)c1ccc(N)cc1</chem>	Neg_lig_1357	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
474	<chem>Cc1ccc([C@H](CN)CC(=O)O)cc1</chem>	Neg_lig_1455	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
475	<chem>Cc1cc(NC(=O)Nc2cc(F)cc2F)no1</chem>	Neg_lig_1476	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
476	<chem>COc1ccc(CC[NH2+](Cc2ccc2C1)cc1</chem>	Neg_lig_1532	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
477	<chem>O=C1/C(=C\NCCO)Nc2ccccc21</chem>	Neg_lig_1568	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
478	<chem>CNc1nc(N2CCOCC2)nc(-n2cnc(SCc3ccccc3)n2)n1</chem>	Neg_lig_1573	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
479	<chem>Cc1ccc(Nc2cc(-c3cccc(N4C(=O)c5ccccc5C4=O)c3)ncn2)cc1NS(C)(=O)=O</chem>	Neg_lig_1584	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
480	<chem>Clc1ccc(-c2noc(-c3ccnc3NC3CCCC3)n2)cc1</chem>	Neg_lig_1597	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
481	<chem>Cc1ccc(-c2cc(C(=O)NCCCNc3cccn3)[nH]n2)o1</chem>	Neg_lig_1660	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
482	<chem>CCc1ccc([C@H]2NCCc3[nH]c[nH+](c32)nc1</chem>	Neg_lig_1687	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
483	<chem>Cc1nc2scn2c1C(=O)NCCc1nnc2n1CC[NH2+](CC2</chem>	Neg_lig_1718	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
484	<chem>Cc1ccc(-c2nc(N(C)Cc3ncn3C)nc2-c2ccc(N)nc2)cc1</chem>	Neg_lig_1780	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
485	<chem>Cc1cccc(OC[C@H](O)CNC(=O)c2ccccc2C(=O)[O-])c1</chem>	Neg_lig_1760	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
486	<chem>Cc1nc(C(C)C)sc1C(=O)N1CCCN([C@H]2COC[C@H]2O)CC1</chem>	Neg_lig_1783	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
487	<chem>Cc1ccc(Nc2cc(-c3cccc(O)cc3)nc3nccn23)c(C)c1</chem>	Neg_lig_1798	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
488	<chem>COc1ccc(CCnc2cc(C)[nH+]c3cc(-c4ccccc4OC)nn23)cc1OC</chem>	Neg_lig_1823	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
489	<chem>CCCCN1CCNC1=S</chem>	Neg_lig_1872	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
490	<chem>COc1cc(C[NH2+](CCO)cc1OCc1ccc2c(c1)n(C)c(=O)n2C</chem>	Neg_lig_796	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
491	<chem>c1csc(-c2nc3cncn3c2Nc2ccc3c(c2)OCCO3)c1</chem>	Neg_lig_1892	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
492	<chem>CC1(C)CC(=O)C2=C(C1)OC(N)=C(C#N)[C@H]2c1cc(Br)ccc1F</chem>	Neg_lig_1963	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
493	<chem>Nc1nonc1C(=O)NCCNCC#Cc1cccc1</chem>	Neg_lig_1973	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
494	<chem>COc1cccc(Nc2cc(C)nc3nc(Cc4ccccc4)nn23)c1</chem>	Neg_lig_1980	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
495	<chem>Nc1c(C(=O)c2ccc(Br)cc2)sc2ncccc12</chem>	Neg_lig_1981	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
496	<chem>CCCCNc1nc2c(c(=O)n(Cc3ccccc3)c(=O)n2C)n1C</chem>	Neg_lig_2042	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
497	<chem>Cc1nnsc1CNCc1nc(-c2ccco2)no1</chem>	Neg_lig_2092	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
498	<chem>Nc1ncnc(Nc2ccc3c(c2)OC(=O)n1</chem>	Neg_lig_2095	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
499	<chem>[NH3+](CCNC(=O)c1nc(-c2ccccc2)no1</chem>	Neg_lig_1619	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
500	<chem>OCc1nc2cccc2n1Cc1cccc1Cl</chem>	Neg_lig_2106	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
501	<chem>CC[C@]1(C)OC(=O)N(CCO)[C@]1(C)O</chem>	Neg_lig_2107	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
502	<chem>C[C@H]1CCc2c(sc3nnc(N4CCN(CCO)CC4)c23)C1</chem>	Neg_lig_2123	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
503	<chem>O=C(OCCNC1=NS(=O)(=O)c2ccccc21)c1ccco1</chem>	Neg_lig_2124	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
504	<chem>CCC[C@H]1C[N@H+]([C@H]1C(=O)C(=O)Cn1cc(C)cn1</chem>	Neg_lig_2206	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
505	<chem>O=C(C[S@@](=O)Cc1ccco1)NC/C=C/COc1cc(C[NH+]2CCCCC2)ccn1</chem>	Neg_lig_2251	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
506	<chem>CC(=O)c1ccc(NC(=O)c2sc3nc(N4CCCC4)c4c(c3c2N)CCCC4)cc1</chem>	Neg_lig_2146	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
507	<chem>COc1ccc2c(c1)nc(SC[C@H](C)O)n2C</chem>	Neg_lig_2330	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
508	<chem>C[NH+](C)CCNc1cc(C(C)(C)[nH+]c2cc(-c3ccccc3)ccn12</chem>	Neg_lig_2344	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
509	<chem>Cc1cc(NC(=O)Nc2cccc3ccc23)no1</chem>	Neg_lig_1654	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
510	<chem>Cn1c(=O)n(C)c2cc(C[NH2+](Cc3cccn3)ccc21</chem>	Neg_lig_2390	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
511	<chem>CCOc1cccc1Nc1cc(-c2ccccc2)[nH+]c(C)n1</chem>	Neg_lig_2425	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
512	<chem>C[NH+](C)CC([NH+])=C1\ C=C(O)CC(C)(C)C1</chem>	Neg_lig_2443	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0



Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
513	<chem>C1c1cc(N=c2\c3c(nc4[nH+][c[nH]n24)C(CC3)ccc1N1CCOCC1</chem>	Neg_lig_2447	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
514	<chem>COc1ccc(C(=O)c2sc3nc4c(c(-c5ccncc5)c3c2N)CCCC4)cc1</chem>	Neg_lig_2491	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
515	<chem>C[C@H](O)CN1CC2(CCC1=O)CCN(S(=O)(=O)N1CCCC1)CC2</chem>	Neg_lig_2589	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
516	<chem>O=C(Nc1cccc1)C1=C(Nc2ccccc2)CSC1</chem>	Neg_lig_2610	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
517	<chem>Nc1ncnc2ccc(-c3cccc(C(=O)N4CCCC4)c3)cc12</chem>	Neg_lig_2626	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
518	<chem>CCOC(=O)N1CCC([NH2+][C@H]2CC[C@H]2N(C(=O)c2nc(C)oc2C)CC1</chem>	Neg_lig_2630	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
519	<chem>c1ccc([C@H]2[NH2+][C]Cc3nc[nH]c32)cc1</chem>	Neg_lig_2631	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
520	<chem>Fe1ccccc1Nc1nc(-c2ccncc2)cs1</chem>	Neg_lig_2633	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
521	<chem>O=S1(=O)CC[C@H](CNc2cc(O)c3cccc(F)c3n2)C1</chem>	Neg_lig_2680	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
522	<chem>Cc1cccc(OCCCCn2c([C@H](C)O)nc3cccc32)cc1</chem>	Neg_lig_2707	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
523	<chem>c1ccc([C@H]2CC[NH2+][C2CCSCC2]c2ccc2)cc1</chem>	Neg_lig_2722	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
524	<chem>COc1cc(CC(=O)C(=O)[O-])oc(=O)c1</chem>	Neg_lig_2757	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
525	<chem>Cc1ccc([C@H]2C(C#N)=C(N)OC3=C2S(=O)(=O)N(Cc2ccc(F)cc2)c2ccc23)cc1</chem>	Neg_lig_2762	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
526	<chem>Cc1sc(C2=C(N)N(c3cccc(Br)c3)CC2=O)n1</chem>	Neg_lig_2763	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
527	<chem>COC(=O)[C@@H](Nc1nc(C2CCCC2)nc2c1cnn2C)[C@H](C)O</chem>	Neg_lig_2793	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
528	<chem>Cc1cccc(-c2ncc(CNCCCN3CCOCC3)cn2)cc1</chem>	Neg_lig_2825	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
529	<chem>Cn1c(=O)c2nc(N3CC[NH+](CCO)CC3)[nH]c2n(C)c1=O</chem>	Neg_lig_2840	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
530	<chem>Cc1nc(N)nc(C)c1CC(=O)N[C@@H]1CC[C@H]1([NH3+])C1</chem>	Neg_lig_2853	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
531	<chem>O=C(Nc1cccc1)c1ccc(S(=O)(=O)N2CCC[NH2+][C]2)cc1</chem>	Neg_lig_2858	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
532	<chem>CN1CC[NH+](C[C@@H]2CN(C(=O)CCc3cccs3)C[C@@H]2CO)C1</chem>	Neg_lig_2861	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
533	<chem>CCc1ccc(-n2nc(CO)c(C(=O)NCc3cccn3)n2)cc1</chem>	Neg_lig_2863	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
534	<chem>CN1CCN([C@H]2CCN(Cc3ccnc3N)C[C@H]2CCC(=O)O)CC1</chem>	Neg_lig_2887	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
535	<chem>C[N@@H+](CCNc1ncnc2onc(-c3ccc(Cl)cc3)c12)C1CCC(CC1</chem>	Neg_lig_2925	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
536	<chem>CCN(C(=O)Nc1cccc1C[NH+])1CCCCC1[C@H]1COC[C@@H]1O</chem>	Neg_lig_2930	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
537	<chem>O=C(c1ccc(-n2cnnc2)cc1)N1C[C@@H](C[NH+]2CCCC2)C[C@@H](CO)C1</chem>	Neg_lig_2995	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
538	<chem>Cc1nn2c(N3CCN(CCO)C3)cc(-c3cccc3)[nH+]c2c1-c1ccc(Cl)cc1</chem>	Neg_lig_3005	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
539	<chem>COc1cccc1Nc1ncnc2ccc(Br)cc12</chem>	Neg_lig_3027	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
540	<chem>CCc1ccc(NC(=O)c2nnn(CC(=O)Nc3cccc3C)c2N)cc1</chem>	Neg_lig_3040	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
541	<chem>CC1(C)CC(=O)C2=C(C1)OC(N)=C(C#N)[C@H]2c1c(F)cccc1Cl</chem>	Neg_lig_3073	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
542	<chem>Fe1cccc1Nc1nc2nnc2nc1N1CCOCC1</chem>	Neg_lig_3082	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
543	<chem>CNC(=O)[C@@H]1C[C@H]([NH3+])CN1S(=O)(=O)CCc1ccncc1</chem>	Neg_lig_3083	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
544	<chem>Cc1c(C(=O)NCCO)nnn1-c1ccc2noc(-c3ccc(Br)cc3)c2c1</chem>	Neg_lig_3088	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
545	<chem>Cc1ccc(C)c(NCCOc2ccccc2)c1</chem>	Neg_lig_2933	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
546	<chem>c1ccc(NN(Cc2cncc2)c2ccc2)cc1</chem>	Neg_lig_3245	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
547	<chem>Cc1cc(C)c2c(N)c(C(=O)c3ccc4c(c3)OCO4)sc2n1</chem>	Neg_lig_3278	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
548	<chem>Oc1ccc(-c2nc3ncccn3c2Nc2ccc(Cl)cc2)cc1</chem>	Neg_lig_3307	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
549	<chem>Cc1cc(-c2[nH]nc3c2[C@@H](c2ccc(F)cc2)C(C#N)=C(N)O3)c(C)s1</chem>	Neg_lig_3309	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
550	<chem>c1cn(CCC[NH2+])Cc2ccc3c(c2)OCO3)cn1</chem>	Neg_lig_1498	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
551	<chem>CCc1ccc([C@H]2C(C#N)=C(N)Oc3n[nH]c(COC)c32)cc1</chem>	Neg_lig_3322	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
552	<chem>CN(C)c1ccc(N[C@H]2CC(=O)N(c3ccc(N4CCOCC4)cc3)C2=O)cc1</chem>	Neg_lig_3353	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
553	<chem>CCOC(=O)c1sc(Nc2ccc(C)cc2C)nc1C</chem>	Neg_lig_1721	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
554	<chem>Cc1ccc2[nH]c(C)c([C@@H](O)C[NH+]3CCCCC3)c2c1</chem>	Neg_lig_794	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	0
555	<chem>C=CCN[C@H]1CC(=O)N</chem>	Neg_lig_21	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	<chem>(c2ccc(Oc3ccccc3)cc2)C1=O</chem>				ACUCUGGGAGA	
556	<chem>O=C(N[C@H]1CC[C@H]1[NH2+])C1CCOCC1)c1ccc1-c1ccccc1F</chem>	Neg_lig_27	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
557	<chem>Cc1ccc(NCc2nnc(-c3ccccc3)o2)c(C)c1</chem>	Neg_lig_79	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
558	<chem>Cc1[nH]nc2c1[C@H](c1ccc3c(c1)OCO3)C(C#N)=C(N)O2</chem>	Neg_lig_81	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
559	<chem>OC[C@H](CNc1ccc(-c2cccn2)n1)Cc1ccsc1</chem>	Neg_lig_90	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
560	<chem>CO[C@@H]1C[C@H]2/C=C(C)/C=C/C=C/C(=O)N[C@H](c3ccccc3)/C=C/C(CC[C@H](O)CC(=O)C2=C1O</chem>	Neg_lig_91	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
561	<chem>Cc1nc(C2=C(N)N(C[C@H](C)O)CC2=O)sc1C</chem>	Neg_lig_162	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
562	<chem>CNC(=O)[C@H]1C[C@H]([NH3+])CN1C(=O)c1c(-c2ccccc2)ccn1C</chem>	Neg_lig_216	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
563	<chem>CCOCCn1c(=O)[nH]c2cc(C(=O)NCc3nc(N)n[nH]3)ccc21</chem>	Neg_lig_225	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
564	<chem>Nc1ccc(S(=O)(=O)N=c2nccc[n-]2)cc1</chem>	Neg_lig_310	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
565	<chem>Cc1ccc([C@H](C(=O)NCCOCCO)N(C)C)cc1</chem>	Neg_lig_322	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
566	<chem>Cc1ccccc1N[C@H]1c2ccccc2C(=O)N1Cc1ccccc1</chem>	Neg_lig_324	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
567	<chem>Cc1ccc(NC(=O)CNC[C@H](C)c2ccccc2)c(C)c1</chem>	Neg_lig_339	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
568	<chem>O=c1[nH]c2ccccc2c(=O)n1CCO</chem>	Neg_lig_340	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
569	<chem>CCOC(=O)c1ccc(Nc2c(-c3ccc(C(C)C)cc3)c(=O)c2=O)cc1</chem>	Neg_lig_342	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
570	<chem>CC(C)c1[nH]nc2c1[C@@]1(C(=O)Nc3ccccc31)C(C#N)=C(N)O2</chem>	Neg_lig_356	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
571	<chem>Nc1ccc(S(=O)(=O)N2CCCC2)c1</chem>	Neg_lig_371	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
572	<chem>Cc1[nH]nc2c1[C@@]1(C(=O)Nc3ccccc31)C(C#N)=C(N)O2</chem>	Neg_lig_424	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
573	<chem>CCCCn1c(N)c(C#N)c2nc3ccccc3nc21</chem>	Neg_lig_463	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
574	<chem>Cc1ccc(-c2nc3ncccn3c2Nc2ccccc2)cc1</chem>	Neg_lig_475	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
575	<chem>COc1cc([C@H]2C(C#N)=C(N)Oc3c2c(=O)[nH]c2ccccc32)ccc1OC(C)C</chem>	Neg_lig_520	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
576	<chem>Nc1nc(N2CCN(C(=O)c3cccs3)CC2)c2c([nH+])1CCC2</chem>	Neg_lig_532	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
577	<chem>COc1ccc(Nc2nc(N)nc(CSc</chem>	Neg_lig_580	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	<chem>3nnnc3C)n2)cc1</chem>				ACUCUGGGAGA	
578	<chem>Nc1nonc1C(=O)N1CCN(C(=O)COc2ccccc2)CC1</chem>	Neg_lig_589	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
579	<chem>C[NH+] (C)CCCNc1ncnc2c1sc1nc 3c(cc12)COC(C)(C)C3</chem>	Neg_lig_635	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
580	<chem>COC(=O)c1cnc(Nc2ccc(Cl) cc2OC)c2ccccc12</chem>	Neg_lig_645	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
581	<chem>COc1ccc(N2C(=O)C[C@H] (n3c(CO)nc4ccccc43)C2=O) cc1</chem>	Neg_lig_671	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
582	<chem>COCCNc1nc2c(c(=O)n(C) c(=O)n2C)n1Cc1ccccc1F</chem>	Neg_lig_687	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
583	<chem>Cc1cc(F)cc(- c2ccccc3c(N)cc[nH+]c23)c 1</chem>	Neg_lig_690	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
584	<chem>CCc1[nH]nc2c1[C@H] (c1c(F)cccc1Cl)C(C#N)=C (N)O2</chem>	Neg_lig_714	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
585	<chem>Cc1cn([C@H]2C[C@H] (N=[N+]=[N-])[C@H] (CO)O2)c(=O)[nH]c1=O</chem>	Neg_lig_719	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
586	<chem>Cc1ccc(Nc2cc(N3CCN(C(=O) C(C)C)CC3) [nH+]c(C)n2)cc1</chem>	Neg_lig_761	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
587	<chem>COc1ccc2oc(- c3ccc(C)c(N)c3)nc2c1</chem>	Neg_lig_790	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
588	<chem>COc1cc(C[NH2+])C(C)C)c cc1OCc1ccc2c(c1)n(C)c(=O) n2C</chem>	Neg_lig_792	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
589	<chem>O=C([O-])c1ccc(Nc2cnc3c cccc3n2)cc1</chem>	Neg_lig_819	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
590	<chem>Nc1nonc1C(=O)NCC[NH2+] ]Cc1ccc(F)cc1</chem>	Neg_lig_825	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
591	<chem>CC[C@]1(CO)CCCN(C(=O) N)Cc2ccc(Cl)cc2)C1</chem>	Neg_lig_962	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
592	<chem>CO[C@H]1CN(C(=O)c2cc cc(C(=O)O)c2)CC[C@H]1 N</chem>	Neg_lig_981	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
593	<chem>Cc1cc(N)c(O)c(Br)c1</chem>	Neg_lig_996	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
594	<chem>O[C@H] (CN1CCOCC1)Cn1cnc2cc ccc21</chem>	Neg_lig_1017	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
595	<chem>OC1CCN(Cc2cc3cc4c(cc3 nc2-c2cccs2)CCC4)CC1</chem>	Neg_lig_1033	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
596	<chem>CCOC(=O)[C@H] (CCc1ccccc1)N[C@H]1C Cc2ccccc2N(CC(=O) [O-])C1=O</chem>	Neg_lig_1044	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
597	<chem>CCCN1cnnc1C[NH2+])C1C CN(c2ccccc2C)CC1</chem>	Neg_lig_1060	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
598	<chem>COc1ccc(OC)c(C(=O)c2oc 3ccc(N)cc3c2C)c1</chem>	Neg_lig_1062	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
599	<chem>CCOC(=O)c1cnc2ccc(C)cc 2c1Nc1ccc(C(=O)[O-])cc1</chem>	Neg_lig_1095	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
600	<chem>c1cc2c(cc1Nc1nc(N3CCO CC3)nc(N3CCOCC3)n1)O CO2</chem>	Neg_lig_1112	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
601	<chem>CCOC(=O)c1cnc2c(C)cc(</chem>	Neg_lig_1152	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	<chem>C)cc2c1Nc1ccc(C(=O)[O-])cc1</chem>				ACUCUGGGAGA	
602	<chem>CS[C@H]1SC[C@@H]2C(=O)N(C)[C@H](C(C)C)C(=O)OC[C@H](NC(=O)c3cnc4ccccc4n3)C(=O)N[C@H](C)C(=O)N(C)[C@@H]1C(=O)N(C)[C@H](C(C)C)C(=O)OC[C@H](NC(=O)c1cnc3ccccc3n1)C(=O)N[C@H](C)C(=O)N2C</chem>	Neg_lig_486	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
603	<chem>CN(C[C@H]1CCC[N@@H+](CCc2ccc(Cl)cc2)C1)C(=O)c1cc(CO)ccn1</chem>	Neg_lig_1177	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
604	<chem>CCn1ccnc1CN(C)C(=O)c1ccc([C@H]2CC[NH2+]C2)cc1</chem>	Neg_lig_1200	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
605	<chem>Cc1ccsc1CC[NH2+][C@@H](C)C(=O)NC1CCCC1</chem>	Neg_lig_1210	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
606	<chem>Nc1c(-c2nc(-c3ccc4c(c3)OCO4)no2)nnn1-c1ccc(Br)cc1F</chem>	Neg_lig_1232	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
607	<chem>O=C(NC[C@H]1(O)CC[NH2+]C1)C1CCN(C(=O)c2cccn2)CC1</chem>	Neg_lig_1288	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
608	<chem>CC(=O)OCC(=O)[C@@H]1(O)CC[C@H]2[C@@H]3CCC4=CC(=O)C=C[C@H]4(C)[C@@H]3[C@@H](O)C[C@@H]21C</chem>	Neg_lig_1292	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
609	<chem>N/C(=N/N=C\c1ccccc1)c1nonc1N</chem>	Neg_lig_1294	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
610	<chem>Cc1c(CCC#N)c(N2CC[NH+](CCO)CC2)n2c(nc3ccccc32)c1C#N</chem>	Neg_lig_1347	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
611	<chem>O=c1ccccc1n1C[C@H]1C[C@@H]2C[N@H+]2CCC[C@H]12</chem>	Neg_lig_1416	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
612	<chem>COc1ccccc1N1CCN(c2nc(-c3nonc3N)no2)CC1</chem>	Neg_lig_1437	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
613	<chem>COc1ccc(Nc2nc(-c3ccccc3)cs2)cc1</chem>	Neg_lig_1457	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
614	<chem>Cc1cc(C)n(C[C@H](C)NCC(=O)Nc2ccc(Cl)cc2F)n1</chem>	Neg_lig_1468	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
615	<chem>O[C@@H](C)Nc1ncnc2ccccc(F)c12)c1ccco1</chem>	Neg_lig_1487	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
616	<chem>C=CCC1(Nc2ccccc2)CCC1</chem>	Neg_lig_1490	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
617	<chem>CCOCCCNc1nc2c(-c3ccccc3)nnn2c2ccccc12</chem>	Neg_lig_1500	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
618	<chem>COc1ccc(N2CC(=O)C(c3nc(C)c(C)s3)=C2N)c(OC)c1</chem>	Neg_lig_1545	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
619	<chem>CCCCCNc1cc(C)[nH+]c2c(C)c(-c3ccccc3)nn12</chem>	Neg_lig_1548	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
620	<chem>Cc1nc2cc(C(=O)N(CCO)C3nccn3C)ccc2s1</chem>	Neg_lig_1575	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
621	<chem>C[C@@H](Cc1cccc1F)[NH2+]CC1(Cn2ccn2)CC1</chem>	Neg_lig_1589	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
622	<chem>[NH3+]CCNC(=O)c1nc(-c2cccc2)no1</chem>	Neg_lig_1619	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
623	<chem>CCn1cnc1C[NH2+]CCC(=O)Nc1nccs1</chem>	Neg_lig_1644	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
624	<chem>COc1cccc1-c1cccc(-c2c(O)nc3cc(Cl)c(C#N)cc3c2O)c1</chem>	Neg_lig_1665	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
625	<chem>CCOc1cccc1N[C@H]1OC(=O)c2ccccc21</chem>	Neg_lig_1601	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
626	<chem>Cc1ccc(N[C@H](O)C[NH+]2CCCCC2)S(=O)(=O)c2ccc(C)cc2cc1</chem>	Neg_lig_1679	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
627	<chem>O=c1n(Cc2nccn2)nc([C@H]2CCC[NH2+]C2)n1-c1cccc1</chem>	Neg_lig_1706	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
628	<chem>CCOc1cnc1Cn1cc(-c2ccc(CO)o2)nn1</chem>	Neg_lig_1748	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
629	<chem>O=C(c1ccc2ncsc2c1)N1C[C@@H]2c3cccc3OC[C@]2(CO)C1</chem>	Neg_lig_1810	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
630	<chem>CC[C@H]1C[C@@](C)(c2csc(Nc3cccc3)n2)OC1=O</chem>	Neg_lig_1831	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
631	<chem>c1ccc(-c2noc(CNC3CCCC3)n2)cc1</chem>	Neg_lig_1867	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
632	<chem>CC1=C(C(=O)OC(C)(C)C[C@H](c2ccc(Cl)cc2Cl)C(C#N)=C(N)O1</chem>	Neg_lig_1874	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
633	<chem>OCc1cnc(-c2cccc(C(F)(F)F)c2)c1</chem>	Neg_lig_1877	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
634	<chem>Cn1c(=O)c2c(-c3cccc(Br)c3)n(CCO)cc2n(C)c1=O</chem>	Neg_lig_1897	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
635	<chem>N#CC1=C(N)N(c2c(F)ccc2F)C2=C(C(=O)CCC2)[C@@H]1c1cccc1</chem>	Neg_lig_1924	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
636	<chem>COc1ccc2nccc(/C=C/c3ccnc4ccc(OC)cc34)c2c1</chem>	Neg_lig_1940	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
637	<chem>Cc1c[nH+]c(Nc2ccc(N3CC[NH+]3)CC3)cc2nc1Nc1cccc(S(=O)(=O)NC(C)(C)C)c1</chem>	Neg_lig_1945	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
638	<chem>Cc1nc(C(=O)N2CCN[C@H](c3cccc3)C2)cs1</chem>	Neg_lig_1182	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
639	<chem>[NH3+][C@H]1CN(C(=O)c2cccn2)C[C@H]1c1cccc1</chem>	Neg_lig_1948	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
640	<chem>N#CC1=C(N)Oc2c(oc(CO)cc2=O)[C@H]1c1cccc1C(F)(F)F</chem>	Neg_lig_1950	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
641	<chem>CC1(C)Cc2c(c(N3CCOCC3)nc3sc(C(=O)NCCc4cccc4)c(N)c23)CO1</chem>	Neg_lig_1978	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
642	<chem>N#Cc1cc2c(=O)n(Cc3(CO)CCCC3)ccc2[n-]c1=O</chem>	Neg_lig_1991	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
643	<chem>CCc1cccc1N[C@@H]1c2cccc2C(=O)N1c1ccc(Cl)c1n1</chem>	Neg_lig_2003	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
644	<chem>CCCc1nn2c(NCc3cccc3)nc3cccc3c2[nH+]1</chem>	Neg_lig_2011	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
645	<chem>Cc1cc(Nc2cccc(Cl)c2C)c2cccc2[nH+]1</chem>	Neg_lig_2022	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
646	<chem>CC[N@@H+](CCO)C[C@@H]1CN(C(=O)Cc2csc(C)n2)C[C@@H]1CO</chem>	Neg_lig_2025	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
647	<chem>CCNC(=O)[C@@H]1C[C@H]([NH3+])CN1Cc1ccc(Oc2nccn2)cc1</chem>	Neg_lig_2026	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
648	<chem>COc1cccc(C[NH2+]C(C)(C)CO)c1OCc1ccc(Cl)cc1</chem>	Neg_lig_2034	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
649	<chem>O=C(NC1CC1)[C@@H]1CNCCN1C(=O)C1=Cc2cccc2OC=C1</chem>	Neg_lig_2039	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
650	<chem>Cc1cc(Nc2ccc(F)cc2)n2nc(Cc3cccc3)n2n1</chem>	Neg_lig_2051	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
651	<chem>C[NH+](C)CCNc1ncnc2c1sc1nc3c(cc12)COC(C)(C)C3</chem>	Neg_lig_2064	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
652	<chem>CN(C)c1ccc(/C=N/NC(=O)c2cnc3cccc3c2)cc1</chem>	Neg_lig_2080	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
653	<chem>COc1ccc(-c2cc3[nH+]c(C)cc(NCC(C)C)n3n2)cc1OC</chem>	Neg_lig_2087	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
654	<chem>Nc1cccc(-n2ncc3c(Cl)cccc32)n1</chem>	Neg_lig_2088	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
655	<chem>O=C(CCCO)NCCc1nc2ccc2n1Cc1c(F)cccc1Cl</chem>	Neg_lig_2127	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
656	<chem>COC(=O)c1sc(-c2ccc(Cl)cc2)cc1N</chem>	Neg_lig_2268	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
657	<chem>Cc1cc(C2CCC2)nc(N2CC3(C(C2)Nc2cccc2NC3=O)n1</chem>	Neg_lig_2314	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
658	<chem>CCCCNc1nc(Oc2ccc(=O)n(-c3cccc3)n2)nc(N(C)C)n1</chem>	Neg_lig_2374	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
659	<chem>CCOC(=O)c1nc2c(-c3cccc(Cl)c3)c(COC)nn2c1N</chem>	Neg_lig_2391	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
660	<chem>N#CC1=C(N)Oc2[nH]nc(-c3cccn3)c2[C@H]1c1c(F)cccc1Cl</chem>	Neg_lig_2417	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
661	<chem>CNC(=O)[C@](C)(Nc1ccc(C)cc1)c1cccc1</chem>	Neg_lig_2489	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
662	<chem>O=C1C[C@H](Nc2ccc(N3CCOCC3)cc2)C(=O)N1c1cccc1Cl</chem>	Neg_lig_2492	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
663	<chem>CCCc1c(C)nc2nenn2c1Nc1ccc(CC)cc1</chem>	Neg_lig_2493	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
664	<chem>c1nccc(-c2nn3c(NC4CCCC4)nc4cccc4c3[nH+]2)c1</chem>	Neg_lig_2594	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
665	<chem>O=C(CN1CC2(CC[NH2+]CC2)OC1=O)N1CCN(c2nccs2)CC1</chem>	Neg_lig_2603	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
666	<chem>O=c1cc(CN2CCC[C@](O)(CO)C2)nc2ccc(Cl)cn12</chem>	Neg_lig_2613	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
667	<chem>N#Cc1cnn2c(NC3CCCCC3)c(-c3ccc(Br)cc3)[nH]c12</chem>	Neg_lig_2637	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
668	<chem>COc1ccc(CN2CCN(C[C@](O)Cn3c4ccccc4c4ccccc43)CC2)cc1</chem>	Neg_lig_2667	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
669	<chem>CCOC(=O)c1ccccc1NC(=O)N1CCC[C@](2(CC[NH2+])C2)C1</chem>	Neg_lig_2676	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
670	<chem>COc1cc2ncnc(Nc3cccc(Cl)c3)c2cc1OC</chem>	Neg_lig_2688	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
671	<chem>COC(=O)CCCNc1cc(C)nc2nc(-c3ccc(OC)cc3)nn12</chem>	Neg_lig_2702	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
672	<chem>COc1ccc2[nH]cc(CCNC(C)=O)c2c1</chem>	Neg_lig_2717	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
673	<chem>CN1CCOc2cc(C(=O)N3CC[C@](H)(c4ccc5c(c4)OCO5)[C@H](O)C3)ccc21</chem>	Neg_lig_2743	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
674	<chem>COc1ccc(Cl)cc1Nc1ncnc2sc(C)c(C)c12</chem>	Neg_lig_2801	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
675	<chem>COc1ccccc1Nc1cc(C)[nH+]e2ccc(Cl)cc12</chem>	Neg_lig_2808	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
676	<chem>Cc1ccccc1Nc1nc([C@](2(C)C)[C@](H)(C(C)C)C(=O)O2)cs1</chem>	Neg_lig_2869	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
677	<chem>OCCNc1nc(N2CCOCC2)nc(N2CCOCC2)n1</chem>	Neg_lig_2878	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
678	<chem>Cc1nc2sc(C(=O)Nc3cnc4cccc4c3)c(N)c2c(C)c1C</chem>	Neg_lig_2905	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
679	<chem>Nc1nonc1C(=O)N1CCN(C(=O)Nc2ccccc2F)CC1</chem>	Neg_lig_2927	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
680	<chem>COc1ccccc1[C@](H)(CC[NH2+])Cc1ccccc1F)c1ccco1</chem>	Neg_lig_2948	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
681	<chem>Cc1nn2cc(CCNc3cccc(N4CCC[C@](O)C4)n3)nc2s1</chem>	Neg_lig_2976	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
682	<chem>CC(C)([C@](H)1NCCc2[nH]c[nH+]c21)N1CCOCC1</chem>	Neg_lig_3003	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
683	<chem>CC1(C)CC(=O)C2=C(C1)OC(N)=C(C#N)C21CCCCC1</chem>	Neg_lig_2348	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
684	<chem>NC1=C(c2nc3cccc3[nH]2)C(=O)CN1c1ccc(Cl)cc1C1</chem>	Neg_lig_3099	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
685	<chem>Cc1ccc(COc2ccc(C[NH2+])C(C)C)cc2cc1</chem>	Neg_lig_3107	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
686	<chem>O=C1c2ccccc2ccc(c23)C(=O)N1CCNCCO</chem>	Neg_lig_330	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
687	<chem>CCOC(=O)N1CCN(c2c(NCCC[N@H+]3CCC[C@](H)(C)C3)c(=O)c2=O)CC1</chem>	Neg_lig_3131	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
688	<chem>O=C(CNc1ccc2c(c1)OCO2)N/N=C/c1ccccc1C1</chem>	Neg_lig_3175	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
689	<chem>COc1ccc(-c2cc(Nc3ccccc3Br)nc(C)</chem>	Neg_lig_3197	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0



Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	[nH+]2)cc1					
690	Cc1cccc(N(CC(=O)NCc2cc3n(n2)CC[NH2+][C3])S(C)(=O)=O)c1	Neg_lig_3207	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
691	CC(C)OC(=O)c1n[nH]c(N)n1	Neg_lig_3269	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
692	C=CCNC(=O)c1sc(N(CC)CC)nc1N	Neg_lig_3319	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
693	CC(C)c1cc(NC2CC2)n2nc(-c3cccnc3)nc2n1	Neg_lig_3324	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
694	CC(=O)N1C(=O)[C@]2(C(C#N)=C(N)Oc3n[nH]c(-c4ccc(F)cc4)c32)c2cccc21	Neg_lig_3365	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
695	COc1ccc(-c2c(Nc3ccc(OC)c(OC)c3)c(=O)c2=O)cc1	Neg_lig_3371	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
696	[NH3+][C@H](c1cccc1)c1ccccc1	Neg_lig_3385	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
697	C[C@H]1CCc2sc3ncnc(NCCN4CCOCC4)c3c2C1	Neg_lig_3391	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
698	C[C@H](O)C#Cc1ccccc1	Neg_lig_3392	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	0
699	COc1ccc(NC(=O)N2C[C@H](O)[C@H](N3CCOCC3)C2)cc1C#N	Neg_lig_16	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
700	COc1ccc([C@H](O)Cn2c(=[NH2+])n(C)c3cccc32)cc1	Neg_lig_47	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
701	CS(=O)(=O)c1cc(F)cc2c3c(n(Cc4cc(Cl)cc4)c12)[C@H](CC(=O)[O-])CC3	Neg_lig_89	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
702	Cc1ccc(Cl)cc1N[C@@H]1c2ncccc2C(=O)N1Cc1cccs1	Neg_lig_94	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
703	Cc1cccc(-c2nc3nc(C)cc(N(C)CCO)n3n2)c1	Neg_lig_168	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
704	O=C(c1ccc2c(c1)n(CC1C1)c(=O)n2C1CCCC1)N1C[C@@H]2C[NH2+][C@H]1C2C1	Neg_lig_177	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
705	COc1cc(Cl)c(C[N@H+]2CC[C@](C)(O)[C@H](O)C2)c(Cl)c1OC	Neg_lig_203	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
706	O=C(COc1cccc(Cl)c1)NC[C@@H]1C[C@H](F)C[NH2+]1	Neg_lig_212	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
707	COc1ccc(-c2oc3cc(OC)ccc3c2C(=O)c2ccc(C#N)cc2)cc1	Neg_lig_220	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
708	Nc1[nH+]c2n(c1C(=O)c1cc(Br)cc1)CCCC2	Neg_lig_242	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
709	Nc1cccc1-c1nn2cnnc2s1	Neg_lig_308	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
710	CC1(C)C[C@H]([C@H](CC[NH3+])c2cccc2)CCO1	Neg_lig_314	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
711	Nc1nnnn1NCc1cccc1F	Neg_lig_385	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
712	CCc1sc(CNCc2nc(-	Neg_lig_410	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	c3ccccc3C)no2)n1					
713	Cc1ccc(N[C@@H](CNS(=O)(=O)c2ccccc2)c2ccccc2)cc1	Neg_lig_434	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCCGGUGUGGGGAA	0
714	Nc1cc2c(cc1C(=O)c1ccccc1Br)OCCO2	Neg_lig_438	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCCGGUGUGGGGAA	0
715	C=CCNc1nc2c(c([O-])nc(=O)n2C)n1C[C@H](O)CO	Neg_lig_453	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCCGGUGUGGGGAA	0
716	Cc1nnc([N-]C(=O)c2cccc(N)c2)s1	Neg_lig_471	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCCGGUGUGGGGAA	0
717	O=C1CCCN1CCC[NH2+]Cc1cccc2ccccc12	Neg_lig_483	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCCGGUGUGGGGAA	0
718	CCOc1ccc(N[C@H](c2ccccc2)c2nnc(-c3ccccc3)o2)cc1	Neg_lig_515	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCCGGUGUGGGGAA	0
719	Cc1ccc(OC2(C(=O)NCCc3nc(C)(C)s3)CC[NH2+]C2)cc1	Neg_lig_548	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCCGGUGUGGGGAA	0
720	C[C@H](C[NH2+]Cc1cccn1)Oc1cccn1	Neg_lig_579	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCCGGUGUGGGGAA	0
721	Cn1nc(C(C)(C)C)cc1NC(=O)NCc1ccc(CO)cc1	Neg_lig_622	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCCGGUGUGGGGAA	0
722	c1ccc(NCCn2cc([C@H]3CC[NH2+]C3)nn2)cc1	Neg_lig_634	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCCGGUGUGGGGAA	0
723	Nc1nc(Cl)nc2c1ncn2[C@@H]1O[C@H](CO)[C@@H](O)[C@H]1F	Neg_lig_650	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCCGGUGUGGGGAA	0
724	Cc1cc(C)c(OC[C@H](O)C[N@H+]2CCCC[C@H]2C)c(C)c1	Neg_lig_831	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCCGGUGUGGGGAA	0
725	N#Cc1c(N(CC(=O)[O-])CC(=O)[O-])sc(C(=O)[O-])c1CC(=O)[O-]	Neg_lig_867	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCCGGUGUGGGGAA	0
726	CCc1cccc(-c2c(-c3ccccc3)nn2CC2(CO)C COCC2)n1	Neg_lig_876	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCCGGUGUGGGGAA	0
727	Cc1nc2ccccc2n1C[C@H](O)COc1ccc(C(C)C)cc1	Neg_lig_903	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCCGGUGUGGGGAA	0
728	Cc1ccc(C(=O)OCCCCNC2=NS(=O)(=O)c3ccccc32)cc1	Neg_lig_934	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCCGGUGUGGGGAA	0
729	CC(C)C[C@H](O)C(=O)N1CCC(c2nccn2Cc2cnc2)CC1	Neg_lig_964	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCCGGUGUGGGGAA	0
730	C[C@H](C(=O)NCc1ccccc1)N1C(=O)NC2(CC[NH2+]CC2)C1=O	Neg_lig_1000	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCCGGUGUGGGGAA	0
731	OCCCCc1nc2ccccc2n1CCC Oc1ccccc1	Neg_lig_1043	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCCGGUGUGGGGAA	0
732	CSCCc1nc([C@@H](N)[C@H](C)O)n(CC(=O)O)n1	Neg_lig_1120	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCCGGUGUGGGGAA	0
733	CCOC(=O)N1CCN(Cc2c(O)ccc3ccccc23)CC1	Neg_lig_1122	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCCGGUGUGGGGAA	0
734	CC[C@H](CO)n1cc2c(c1-c1ccc(Cl)cc1)c(=O)n(C)c	Neg_lig_1147	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCCGGUGUGGGGAA	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	=O)n2C					
735	CC1(C)CCC(=O)c2nnn(-c3nonc3N)c21	Neg_lig_1149	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
736	Cn1c(N2CC[C@H](O)C2)nc2cc(C(=O)NCCCn3cncn3)ccc21	Neg_lig_1156	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
737	CC(C)=NNc1[nH]cnc2ncn c1-2	Neg_lig_744	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
738	O=c1[nH]cnc2c1ncn2[C@H]1CC[C@H](CO)O1	Neg_lig_1164	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
739	Nc1cccc(S(=O)(=O)NC[C@H]2CCCCO2)c1	Neg_lig_1271	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
740	Nc1ccc2c(C(F)(F)F)cc(=O)oc2c1	Neg_lig_1302	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
741	OCOCc1cccc(C[NH+]2CCN([C@H]3CCc4cccc4C3)CC2)c1	Neg_lig_1305	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
742	Cc1ccc(-n2nc(CO)c(C(=O)NCc3ccnc3)n2)cc1C	Neg_lig_1381	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
743	Cc1ccc2nc(Nc3nc(C)c4ccc cc4n3)nc(O)c2c1	Neg_lig_87	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
744	O=S1(=O)C(=C(/O)Nc2cccc2)/C(=N/Cc2ccco2)c2ccccc21	Neg_lig_1535	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
745	CCc1c(C)nc2nnnc2c1NCc1ccc(Cl)cc1	Neg_lig_1551	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
746	N#Cc1c(-c2ccc(C[NH+]3CCCC3)s2)cc(-c2ccc[nH]2)nc1N	Neg_lig_1557	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
747	COc1ccc(F)c(CNC(=O)c2cc3nc(CO)[nH]c3c2)c1F	Neg_lig_1574	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
748	Cc1nc2[nH+]c[nH]n2c(=O)c1Oc1ccc(N)cc1	Neg_lig_1577	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
749	Cc1ccc(Nc2nc(C)cc(N3CCN(C(=O)C4CCCC4)CC3)n2)cc1	Neg_lig_1578	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
750	[NH3+][C@H]1CN(C(=O)CCCOc2ccccc2)C[C@@H]1C1CC1	Neg_lig_1582	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
751	O=C1CCC2(CCN(C(=O)c3ccc4occc4c3)CC2)CN1C CCO	Neg_lig_1618	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
752	NS(=O)(=O)c1ccc(N/N=C2/C(=O)C(C(=O)[O-])=Cc3ccccc32)cc1	Neg_lig_1651	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
753	C[C@](O)(CS(=O)(=O)c1ccc(F)cc1)C(=O)[N-]c1ccc(C#N)c(C(F)(F)F)c1	Neg_lig_1662	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
754	Nc1c(C(=O)NCCc2c[nH]c3ccccc23)sc2nc3c(cc12)C CC3	Neg_lig_1694	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
755	CCc1[nH]nc2c1C1(C(C#N)=C(N)O2)c2ccccc2-c2ccccc21	Neg_lig_1701	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
756	OCOCc1nc2ccccc2n1CCCC1CCCCC1	Neg_lig_1733	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
757	C[NH+]	Neg_lig_1736	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	(C)CCNC[C@@H] (O)Cn1c2cccc2c2cccc21					
758	CC[NH+] (CC)CCN1CC(=O)C(c2nc 3cccc3[nH]2)=C1N	Neg_lig_1741	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
759	COc1ccc(- c2ccc(C[NH2+])CCc3ccc(S (N)(=O)=O)cc3)o2cc1Cl	Neg_lig_1749	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
760	CNc1cc(C)[nH+]c2c(- c3ccc(F)cc3)cnn12	Neg_lig_1774	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
761	Cc1ccc([C@H]2C(C#N)= C(N)Oc3c2oc(CO)cc3=O) o1	Neg_lig_1275	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
762	Cc1cccc(CN2CCN(C(=O) CCn3cncn3)C[C@@H]2C CO)n1	Neg_lig_1835	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
763	COc1ccc(N2CCN([C@H] 3CCCN(C(=O)CO)C3)CC 2)cc1	Neg_lig_1836	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
764	Cc1nc(N)nc(C)c1CC(=O) N1CCC2(CCC(=O)N(C)C C2)CC1	Neg_lig_1880	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
765	O=C1c2cccc2C(=O)c2cc( S(=O) (=O)N(CCO)Cc3cccc3)cc c21	Neg_lig_1881	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
766	c1ccc(- c2nnc3nc(N4CCCCC4)nc( N4CCCCC4)n23)cc1	Neg_lig_1886	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
767	CN(Cc1nc(N)nc1)C(=O) Nc1cccc1C[N@@H+] (C)C1CCCCC1	Neg_lig_1902	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
768	O=C(NCC(c1cccc1)c1ccc cc1)c1nn(- c2ccc(F)cc2)nc1CO	Neg_lig_1915	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
769	Cc1c(S(=O) (=O)c2cccc2)c(N)n(CCC[ NH+])(C)C)c1C	Neg_lig_1969	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
770	CNc1oc(- c2ccc(F)cc2)nc1S(=O) (=O)c1ccc(Cl)cc1	Neg_lig_2027	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
771	O=C1c2cccc3cccc(c23)C( =O)N1CC1CC[NH+] (C)[C@H] (O)COc2ccc(F)cc2)CC1	Neg_lig_2029	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
772	CC(C) (O)CCc1ccc(C(=O)N2CC CC[C@@H]2CO)cc1	Neg_lig_2030	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
773	Cn1ncc2c(=O) [nH]c(CN3CCNC[C@H] (C(=O)O)C3)nc21	Neg_lig_187	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
774	COc1ccc(- c2nc3ncccn3c2Nc2cccc(C( F)(F)F)c2)cc1	Neg_lig_2094	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
775	O=C1C[C@H] (Nc2ccc3c(c2)OCO3)C(= O)N1c1cccc1	Neg_lig_2168	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
776	Cc1ccc(C)c(S(=O) (=O)N2CCC[C@H] (Cn3cc(CCO)nn3)C2)c1	Neg_lig_2210	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
777	Cc1ccc(- c2c(Nc3ccc(Br)c(C)c3)c(= O)c2=O)cc1C	Neg_lig_2291	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
778	<chem>Cc1cnc(N)nc1N[C@H](C[NH+])1CCCC1c1cccc1</chem>	Neg_lig_2328	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
779	<chem>Cc1cc(-c2[nH]nc3c2[C@@H](c2ccnc2)C(C#N)=C(N)O3)c(C)s1</chem>	Neg_lig_2345	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
780	<chem>COC(=O)[C@@H]1CCCCN1C(=O)CCc1cc2n(n1)CCC[NH2+]C2</chem>	Neg_lig_2373	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
781	<chem>N=c1[nH]c2c(s1)[C@@H](c1ccc(F)cc1F)CC(=O)N2</chem>	Neg_lig_2434	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
782	<chem>CSc1ncc(C(=O)NC(C)C)c(N)n1</chem>	Neg_lig_2501	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
783	<chem>COc1cc2nc(N3C[C@@H](C)[C@](O)(C4CC4)C3)nc(N)c2cc1O</chem>	Neg_lig_2520	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
784	<chem>CC(C)=CC[C@]1(CO)CCCN(C(=O)CCn2cnnc2)C1</chem>	Neg_lig_2526	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
785	<chem>COc1ccc([C@H]2C(C#N)=C(N)OC3=C2S(=O)(=O)N(Cc2cccc2C)c2cccc23)cc1</chem>	Neg_lig_2528	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
786	<chem>C[C@H](O)c1c(O)ccc2ccc(=O)oc12</chem>	Neg_lig_2534	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
787	<chem>CCCCNc1nc2c(c(=O)n(Cc3cccc3)c(=O)n2C)n1C</chem>	Neg_lig_2042	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
788	<chem>O=C(CCCO)NCCc1nc2ccc2n1Cc1ccc(Cl)cc1</chem>	Neg_lig_2611	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
789	<chem>COc1cccc(-c2cc(C(=O)N3CC=C[C@@H]3CO)n[nH]2)c1</chem>	Neg_lig_2612	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
790	<chem>COc1cccc(Nc2c(S(=O)(=O)c3cccc3)nc3cccc23)c1</chem>	Neg_lig_2648	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
791	<chem>Cc1c(C)n(Cc2ccnc2)c2[nH+]e3c(c(N)c12)CCc1cccc1-3</chem>	Neg_lig_2673	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
792	<chem>Cc1cc([C@@H]2CCCCN2C(=O)CCc2cc3n(n2)CCC[NH2+])C3)no1</chem>	Neg_lig_2703	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
793	<chem>N#Cc1c(N)nc(SCc2cccc2)c(C#N)c1-c1cccs1</chem>	Neg_lig_2726	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
794	<chem>Cc1cc(F)ccc1CC(=O)N1CCNC[C@H]1C(=O)Nc1ccc(F)cc1</chem>	Neg_lig_2754	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
795	<chem>Nc1nc2c(c(-c3ccc[nH+]c3)n1)CN(C(=O)c1secc1Cl)C2</chem>	Neg_lig_2777	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
796	<chem>COc1ccc(-c2noc(CNc3ccc(F)c(Cl)c3)n2)cc1</chem>	Neg_lig_2802	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
797	<chem>Cc1n[nH]cc1N</chem>	Neg_lig_593	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
798	<chem>C[C@@]1(CO)CN(c2cc(C(=O)Nc3ccc4c(c3)-c3c(c(C(N)=O)nn3-c3ccc(F)cc3)CC4)c(Cl)cn2)C[C@]1(C)CO</chem>	Neg_lig_2842	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
799	<chem>CCOCCCNc1c(C(=O)O)n(Cc2ccc(C)cc2)c2cccc12</chem>	Neg_lig_2916	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
800	<chem>Cc1ccc(NC(=O)CSc2nc3nc[nH]c(N)c-3n2)cc1</chem>	Neg_lig_2918	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
801	<chem>CC(C)Cc1ccc(C[N@H+](C)CCC[C@H](Nc3cccc(N)n3)C2)cc1</chem>	Neg_lig_2951	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
802	<chem>OCCN(CCO)c1nc(N2CCC(CC2)c2nc(N(CCO)CCO)nc(N3CCCCC3)c2n1</chem>	Neg_lig_2955	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
803	<chem>Nc1nc(Cl)nc2c1ncn2[C@H]1C[C@H](O)[C@@H](CO)O1</chem>	Neg_lig_2959	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
804	<chem>Cc1cc(NC[C@@H]2C[C@H](F)C[NH2+](2)nc(-c2ccccc2O)n1</chem>	Neg_lig_2971	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
805	<chem>C[N@@H+](CCNc1ncnc2onc(-c3ccc(Cl)cc3)c12)C1CCC(CC1</chem>	Neg_lig_2925	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
806	<chem>C[NH+](C)CCNc1ncnc2c1c(-c1ccccc1)cn2-c1ccc(Cl)cc1</chem>	Neg_lig_3014	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
807	<chem>CC(C)c1nn(-c2c(Cl)cccc2Cl)c2nc(Cc3ccc(OCCO)cc3)[nH]c(=O)c12</chem>	Neg_lig_3066	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
808	<chem>CC(C)(O)CCc1ccc(C(=O)NC[C@H](O)c2cccn2)cc1</chem>	Neg_lig_3069	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
809	<chem>Cc1c(F)cccc1NC(=O)CNC(Cc1cccn1</chem>	Neg_lig_3075	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
810	<chem>CCn1nc(CO)c2c1CCN(C(C(=O)c1cc(-c3cccn3C)n[nH]1)C2</chem>	Neg_lig_3103	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
811	<chem>c1ccc(OCCN2CCN(C[C@H]3CCC[NH2+](3)CC2)c1</chem>	Neg_lig_3133	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
812	<chem>COc1cccc2c1OC[C@@H](C(=O)N(C)Cc1nc(N)nc1)C2</chem>	Neg_lig_3135	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
813	<chem>N#CC1=C(N)Oc2[nH]nc(-c3cccs3)c2[C@H]1c1ccc(C(F)(F)F)cc1</chem>	Neg_lig_3234	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
814	<chem>COc1ccc(C(=O)c2sc3nc(C)c(Cl)c(C)c3c2N)cc1</chem>	Neg_lig_3271	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
815	<chem>C[N@@H+](C)C[C@@H](c2ccccc2)CC2(CCN(C(=O)c3ccc(CO)cc3)CC2)C1</chem>	Neg_lig_3295	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
816	<chem>C=C(C)CC[C@H](C)[NH2+](C)CC(=O)Nc1cccc1C</chem>	Neg_lig_3303	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
817	<chem>O=C(/C=C/c1cccc(S(=O)(=O)Nc2ccccc2)c1)NO</chem>	Neg_lig_2342	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
818	<chem>C=CCN1C(=O)[C@]2(C(C#N)=C(N)Oc3n[nH]c(C)c32)c2ccccc21</chem>	Neg_lig_3369	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
819	<chem>Cc1cccc1NC1=NS(=O)(=O)c2ccccc21</chem>	Neg_lig_3386	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
820	<chem>N#CC1=C(N)OC2=C(C(=O)CCC2)[C@@H]1c1ccc(Cl)cc1</chem>	Neg_lig_3397	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	0
821	<chem>Cc1cc(ccc1N)I</chem>	0325-0381	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAGGCCUCCAAGCUGUGCCUUGGGUGGCUUUGGGGCAUGGACC	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
822	<chem>CC(NS(c(cc1)cc2c1sc(C)n2)(=O)=O)=O</chem>	122385	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	1
823	<chem>CC(C) (CCc1ccc(cc1)C(N(C)CC1 (CCCC1)CO)=O)O</chem>	14466464	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	1
824	<chem>CC1CCC(C(C)C)C(C1)OC C(CN1CCN(CC1)c1ccccc 1)O</chem>	1502-1032	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	1
825	<chem>Cc1cc(C)c2c(c1)c(cc(C)n2 )C(N[C@H]1CN[C@H]1OC)=O</chem>	19537511	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	1
826	<chem>COc1ccc(cc1OC)c1nncc(N) o1</chem>	2158-0021	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	1
827	<chem>C1CCN(CC1)Cc1ccccc(c1) n1ccnc1c1cc2CNCCn2n1</chem>	26875627	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	1
828	<chem>O=C(N(CC1OC1)C(N1CC 2OC2)=O)N(CC2OC2)C1 =O</chem>	296934	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	1
829	<chem>CCOC/C(/ C1=CSC2=NNC(C) (C)N12)=N(O)=O</chem>	299968	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	1
830	<chem>CC1=CC2C(CC1N)C2(C) C</chem>	3295-0018	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	1
831	<chem>Cc1cc(c2cc(ccc2n1) [Cl])Nc1ccc(cc1)C(O)=O</chem>	4358-1525	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	1
832	<chem>CSC(NC(Cl)=C1)=NC1=O</chem>	45719	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	1
833	<chem>CCOC(c1ccc2c(c1)c(c(cn2 )C(=O)OCC)Nc1ccc(cc1) N(C)C)=O</chem>	4593-3030	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	1
834	<chem>C1CN(CC=C1)c1c2CCN( CCc2nc(c2ccco2)n1)C(CN )=O</chem>	47825811	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	1
835	<chem>CCOC(c1cnc2ccc(cc2c1Nc 1ccc(cc1)N(C)C)[Br])=O</chem>	4789-4367	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	1
836	<chem>CCOC(c1cnc2ccc(C)cc2c1 Nc1ccc(cc1)N(C)C)=O</chem>	4790-1159	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	1
837	<chem>Cc1cccc2c(cc(C)nc12)Nc1 ccc(cc1)N(C)C</chem>	4790-1400	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	1
838	<chem>C(CN)CN1C(CC[C@H]2 CN(CC[C@@H]12)C(CCc 1ccco1)=O)=O</chem>	48226996	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	1
839	<chem>C1CCc2c(C1)c1c3c(c(NCc 4ccco4)ncn3)sc1nc2N1CC OCC1</chem>	5504-0167	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	1
840	<chem>CN1C(N(Cc2ccccc2)C(c2c 1nc(NCCc1ccccc1)n2C)= O)=O</chem>	7282-5801	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	1
841	<chem>CCC1CCCCN1S(c1ccc(cc 1)NC1c2ccccc2S(N=1) (=O)=O)(=O)=O</chem>	7380-0010	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	1
842	<chem>CC1=CC2=C(C(C(C#N)= C(N)O2)c2ccccc2OC)C(N 1Cc1ccc2c(c1)OCO2)=O</chem>	7706-1226	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
843	<chem>CCOC(C1=C(C)OC(=C(C(=O)OCC)C12C(Nc1cccc12)=O)N)=O</chem>	8003-0370	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	1
844	<chem>CC1=C(C(C)=O)C2(C(C#N)=C(N)O1)C(Nc1ccc(cc12)[Cl])=O</chem>	8004-9533	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	1
845	<chem>Cc1ccc(cc1C)Nc1nc(cs1)c1ccc(c(c1)F)OC</chem>	8005-2731	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	1
846	<chem>c1ccc(cc1)C(c1c(c(C(Nc2ccccc2)=O)c2cccn12)N)=O</chem>	8018-2439	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	1
847	<chem>C1CCC(C1)(CN)c1ccc(cc1)[Cl]</chem>	8018-9306	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	1
848	<chem>CCC12CN3CC(CC)(CN(C1)C3C(C)(C)CO)C2=O</chem>	8019-5964	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	1
849	<chem>c1cc(N)nc2c1ccc(n2)O</chem>	8019-7722	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	1
850	<chem>COc1cc(cc(c1O)OC)C1CC(Nc2c1[se]c(N)n2)=O</chem>	8020-1898	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	1
851	<chem>c1cnccc1c1nc2ncnc(N)n2n1</chem>	8020-2786	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	1
852	<chem>Cc1c(c2ccc(c(c2)OC)OC)c2ncc(c3ccc(c(c3)OC)OC)c(N)n2n1</chem>	8104-10716	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	1
853	<chem>CCCCNc1c(C#N)c2CC(C)(C)OCc2c(c2ccccc2)n1</chem>	8640-0572	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	1
854	<chem>COc1ccc(cc1)c1cc(C(F)(F)F)nc(NCc2ccccc2)n1</chem>	C130-0241	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	1
855	<chem>Cc1ccccc1)NCc1nc2ccccc2n1C</chem>	C147-0043	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	1
856	<chem>c1ccc(cc1)Nc1c(c2c[nH]c3ccccc23)nc2cncn12</chem>	C169-0283	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	1
857	<chem>CCCCn1cnc2cc(ccc12)NCc1ccc(c1)OC</chem>	C215-0084	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	1
858	<chem>Cc1ccc2nc(c3c[nH]c4ccccc34)c(NC3CCCC3)n2c1</chem>	C239-0079	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	1
859	<chem>C1COc2cc(ccc2O1)Nc1c(c2cccs2)nc2cccn12</chem>	C273-0461	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	1
860	<chem>CC(C)C(N1CCN(CC1)c1ccc(cc1)Nc1cc(C)nc2nc(c3ccc3)nn12)=O</chem>	C301-7288	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	1
861	<chem>Cc1ccc(C)c(c1)NC(Cn1c(c(C(NCc2ccc(cc2)F)=O)nn1)N)=O</chem>	C368-0754	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	1
862	<chem>CCOc1ccccc1NC(c1c(CO)ncn1)=O</chem>	C612-0892	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	1
863	<chem>CCOC(c1ccc(cc1)NC1c2c(cccn2)C(N1c1ccc(C)cc1)=O)=O</chem>	C999-1176	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	1



Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
864	<chem>C(C(c1cccc1)Nc1ccc(cc1)[Br])NS(c1ccc(cc1)[Cl])(=O)=O</chem>	D030-0079	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	1
865	<chem>C(CNc1cc(c2cccc2)nc2nncn12)c1ccc(cc1)[Cl]</chem>	D150-0174	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	1
866	<chem>C=CCNc1nc(cs1)c1c[nH]c2cccc12</chem>	D231-0019	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	1
867	<chem>Cc1nc(cc(Nc2ccc(cc2)N2C COCC2)n1)c1cccc1</chem>	D278-0547	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	1
868	<chem>[H]N(Cc1cccc1)c1c2c(csc2nnc1)c1ccc(C)cc1</chem>	D341-0419	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	1
869	<chem>CC(C)c1cc(Nc2ccc(cc2)N(C)C)n2c(n1)nc(c1ccnc1)n2</chem>	D494-0293	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	1
870	<chem>CCOC(c1nc2c(c3ccc(cc3)[Br])c(C)nn2c1N)=O</chem>	D718-0691	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	1
871	<chem>CC1CCCC(C1C)Nc1c(c2ccc(cc2)[Cl])[nH]c2c(C#N)cnn12</chem>	E002-1096	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	1
872	<chem>CCN(CC)c1ccc(c(C)c1)N C1C(C)=C(c2ccc(C)cc2)S(N=1)(=O)=O</chem>	E013-0189	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	1
873	<chem>C1CN1P(N1CC1)(N1CC1)=S</chem>	NCGC0009504 2-08	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	1
874	<chem>CC(C)n1ene2c(Nc3cccc(c3)NC(C=C)=O)nc(NC3CCC(CC3)N(C)C)nc12</chem>	NCGC0034696 4-01	HBV	Hairpin	GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC	1
875	<chem>CC(C)(C)NCc1ccc(cc1)[Cl]</chem>	0167-0173	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
876	<chem>c1ccc(c(c1)N)I</chem>	0325-0348	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
877	<chem>c1ccc2c(c1)nc(Sc1ccc(cc1)[Cl])N)s2</chem>	0375-0604	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
878	<chem>Cc1c(C)sc(N)n1</chem>	0462-0328	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
879	<chem>C(=Cc1nc2cccc2o1)c1ccc(cc1)N</chem>	0632-0836	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
880	<chem>c1ccc2C(c3c(ccc(C(c4cccc5cccc45)=O)c3N)C(c2c1)=O)=O</chem>	0658-0270	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
881	<chem>C(c1nc2cccc2[nH]1)OC(c1ccc(cc1)N)=O</chem>	0717-0954	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
882	<chem>C(=Cc1nc2ccc(ccc2[nH]1)N)c1cccc1</chem>	0717-0957	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
883	<chem>CCN(CC)CCOC(c1ccc2c(c1)sc(NC(c1ccc(cc1)N)=O)n2)=O</chem>	0812-1025	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
884	<chem>Cc1c(C)c(C)nc2c1c(c(C(c1ccc(cc1)[Cl])=O)s2)N</chem>	0892-0702	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
885	<chem>CNc1ccc(cc1C(c1cccc1[Cl])=O)[Br]</chem>	0922-0021	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
886	<chem>c1ccc(cc1)N1C(C(Nc2cccc2C(O)=O)SC1=O)=O</chem>	1159-0328	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
887	<chem>CC1=CC(C)=NC(N1CCN C(C1CC2(CCNCC2)CN1C)=O)=O</chem>	12499963	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
888	<chem>C1CCN(C1)Cc1cc(c2c(c3c</chem>	12577678	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	<chem>cccc3)ncn2CCO)sc1</chem>					
889	<chem>C1CN(CCC1c1cc(Cc2cccc2)n[nH]1)C(C1CNCCO1)=O</chem>	12893837	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
890	<chem>C1C(CN1Cc1cccc(cc1)OCO)Oe1cccc1[Cl]</chem>	13202927	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
891	<chem>Cc1c(C)c(-c2c(CC#N)ccc(C)c2C)c(C(C#N)cc1</chem>	135412	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
892	<chem>C1CNc2cccc(c3ccc(c(c3)F)O)c12</chem>	13724969	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
893	<chem>CC(C)CCOc1cccc(CCNC(C2CC3(CCNCC3)CN2)=O)c1</chem>	14325308	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
894	<chem>CCCc1cccc(cc1)OCC(CN1CCC(C)CC1)O</chem>	1502-1054	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
895	<chem>C(c1nnnn1c1cccc1)n1ccnc1c1cccc(CO)o1</chem>	15028125	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
896	<chem>CCSc1nc2cccc2n1CCO</chem>	1535-0016	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
897	<chem>[H]OCCNC1=C(C)NC(NC1=O)=O</chem>	1545-0174	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
898	<chem>C1=C(C(=O)Oe2ccc(cc12)[Br])c1csc(N)n1</chem>	1570-0014	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
899	<chem>C1CNCCC12CN(Cc1cc3c(cc1[Cl])OCO3)C(=O)O2</chem>	15869527	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
900	<chem>C(CN)c1cccc(c1)c1ccc(cc1[Cl])F</chem>	16088353	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
901	<chem>Cc1c(C(C(NCCNc2ccccc2)=O)N)c(C)[nH]n1</chem>	16899791	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
902	<chem>C=Cc1ccc(nc1)N1CCN(C(C1)O)Cc1cccc1</chem>	17524156	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
903	<chem>CC(c1cccc(c1)C(N1CCC2(CC1)[C@H](C[C@H]2O)OCCN)=O)=O</chem>	17694000	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
904	<chem>CCNC([C@@H]1C[C@@H](CN1S(N1CCN(CC)CC1)(=O)=O)N)=O</chem>	17965244	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
905	<chem>COc1cccc(cc1)C1C(C#N)=C(N)OC2CCCC(C1=2)=O</chem>	1852-0324	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
906	<chem>C1CC2=C(C(C(C#N)=C(N)O2)c2ccc(c(c2)O)O)C(C1)=O</chem>	1852-0330	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
907	<chem>Cc1cccc1C1C(C#N)=C(N)OC2=C1C(=O)Oe1cccc12</chem>	1866-0050	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
908	<chem>CC1=CC2=C(C(C(C#N)=C(N)O2)c2ccc(cc2)[Cl])C(=O)O1</chem>	1866-0097	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
909	<chem>Cc1cc2CN(Cc2cc1C)c1ccc(c1)C(NC[C@@H]1C[C@@H](CN1)F)=O</chem>	18859448	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
910	<chem>Cc1cc(C)c2c(c1)c(cc(C)n2)C(N[C@H]1CNCC[C@@H]1OC)=O</chem>	19537511	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
911	<chem>Cc1ccc2c(c1)c(c1cccc(cc1)N)nc(c1cccc1)n2</chem>	2202-0913	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
912	<chem>CC(C)(C)C(CN1C(=N)N(CCN2CCCC2)c2cccc12)O</chem>	2226-0439	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1

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913	<chem>CCCCN1C(=N)N(CC(c2cc c(cc2)OC)O)c2ccccc12</chem>	2226-0445	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
914	<chem>CCCN1C(=N)N(CC(c2ccc cc2)O)c2ccccc12</chem>	2226-0453	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
915	<chem>CCCCN1C(=N)N(CC(c2cc ccc2)O)c2ccccc12</chem>	2226-0454	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
916	<chem>COc1cc(cc(c1OC)OC)c1n nc(N)s1</chem>	2237-2233	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
917	<chem>C(CO)N1C(c2cccc3c(ccc C1=O)c23)C(c1cccc1)=O )=O</chem>	2248-8147	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
918	<chem>COc1ccc(cc1)C(c1c(c2c(cc c3ccccc3)nc2s1)C(F) (F)F)N)=O</chem>	2434-0155	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
919	<chem>C1COc2cc(ccc2C1=O)c1c c2CC(CN)Oc2c(c1)[Cl]</chem>	26642358	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
920	<chem>C(CC(c1c(c2cc(ccc2o1) [Cl]))N=O)C(O)=O</chem>	2686-0069	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
921	<chem>Cc1nc(C2CCCN2)n(c2ccc c3ccccc23)n1</chem>	26991482	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
922	<chem>c1cc(c2cccc(c2e1) [Br])c1nc2cc(ccc2o1)N</chem>	2810-4224	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
923	<chem>Cc1cc2c(cc1C)oc(c1ccc(cc 1)N)n2</chem>	2810-4334	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
924	<chem>Cc1cc2c(cc1C)oc(c1ccc(C) c(c1)N)n2</chem>	2810-4335	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
925	<chem>CCc(cc(C(C) (C)CCC1(C)C)c1c1)c1- c1csc(C/C(N)=N/O)n1</chem>	310354	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
926	<chem>CC1=CC2=C(C(=O)O1)C 1(C(C#N)=C(N)O2)C(Nc2 ccc(cc12)[Br])=O</chem>	3132-1299	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
927	<chem>C(c1ccc(cc1) [Br])Sc1nc2ccc(cc2s1)N</chem>	3167-0427	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
928	<chem>C(c1ccc(cc1)F)Sc1nc2ccc (cc2s1)N</chem>	3167-0429	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
929	<chem>C(c1ccccc1[Cl])Sc1nc2ccc (cc2s1)N</chem>	3167-0436	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
930	<chem>C(C(c1ccccc1)=O)Sc1nc2c cc(cc2s1)N</chem>	3167-0470	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
931	<chem>Cc1ccc(CNCCc2ccc(c(c2) OC)OC)c(C)c1</chem>	3169-1196	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
932	<chem>Cc1ccc(cc1)n1nc(c1C(c1c cc(cc1)[Br])=O)N</chem>	3228-0090	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
933	<chem>C(CNC1CCN(CC1)c1nnc (c2ccccc2)s1)Cn1ccnn1</chem>	32364121	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
934	<chem>Cc1nc2c(ccc2[nH]1)C(N1 CCCC2(CCNC2)C1)=O</chem>	32365391	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
935	<chem>CNc1ccccc1C(=O)OCC(c1 ccccc1)=O</chem>	3257-1030	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
936	<chem>C(C(c1ccc(cc1) [Br])=O)OC(c1c(N)non1)= O</chem>	3257-3204	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
937	<chem>CC(C)c(cc1)ccc1- c1nc(cccc2)c2s1</chem>	33010	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
938	<chem>Cc1c(CCN(C)Cc2ccc(CO) o2)scn1</chem>	33883850	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
939	<chem>C1CNc2cc(CCC(NC(CC n3enen3)c3ccccc3)=O)nn2</chem>	35350604	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1

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	C1					
940	<chem>Cc1cc(ccc1[Br])c1nc2cc(cc2o1)N</chem>	3617-0633	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
941	<chem>C1CN(CCN1CC(COc1ccc(cc1)[Br])O)c1cccc1</chem>	3672-0047	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
942	<chem>COc1cccc(CNCc2cccc(c2)F)c1OC</chem>	3702-1553	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
943	<chem>c1ccc2c(c1)nc(c1ccc(cc1)N)s2</chem>	3729-2175	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
944	<chem>CCOCCSc1nc(c2c3CC(C)(C)OCc3sc2n1)N</chem>	3807-1214	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
945	<chem>CCc1ccc(c2c3CCCCc3nc(c2C#N)N)s1</chem>	3830-0877	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
946	<chem>C1C(=CNC2ccccc2)C(OC=1c1ccccc1)=S</chem>	3897-0025	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
947	<chem>Cc1cc(C)c(c(C)c1)c1cc(CN)ccc1F</chem>	40126718	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
948	<chem>Cc1c(cccc1N)c1nc2cc(ccc2o1)[Cl]</chem>	4269-3141	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
949	<chem>CS(c1c(c2c(cc(c3ccccc3)nc2s1)c1ccccc1N)(=O)=O</chem>	4378-0113	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
950	<chem>CCN(CC(Cn1c2cccc2c2c2ccc12)O)S(c1ccc(cc1)[Cl])(=O)=O</chem>	4390-0105	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
951	<chem>CC(C)(C)c1ccc(cc1)c1nc(c2ccccc2n1)NCc1cccn1</chem>	4491-1513	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
952	<chem>CSC(NC(Cl)=C1)=NC1=O</chem>	45719	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
953	<chem>CCN1C(NC(C12CCN(CC2)Cc1cc2CNCCCn2n1)=O)=O</chem>	47670564	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
954	<chem>C1CN(CC=C1)c1c2CCN(CCc2nc(c2ccco2)n1)C(CN)=O</chem>	47825811	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
955	<chem>CCOC(c1nc2ccc(cc2c1Nc1ccc(cc1)N(C)C)[Br])=O</chem>	4789-4367	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
956	<chem>C(CN)CN1C(CC[C@H]2CN(CC[C@H]12)C(CCc1ccco1)=O)=O</chem>	48226996	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
957	<chem>CCCCCCCCNc1ccc(c1)[Br]</chem>	5117451	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
958	<chem>Cc1nc2cc(c(cc2n1CCCO)[Cl])[Cl]</chem>	5119828	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
959	<chem>c1cc(ccc1c1c(c2ccc(cc2)F)nc2cc(ccc2n1)Oc1ccc(cc1)N)F</chem>	5174475	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
960	<chem>CCCCCc1ccc(cc1)c1ccc(c1)c1ncc(cn1)N</chem>	5213078	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
961	<chem>c1ccc2c(ccc(c2c1)Oc1ccc(cc1[Cl])N)[Cl]</chem>	5215844	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
962	<chem>CCOC(CNc1ccc(cc1)Oc1cc(cc1)Oc1ccc(cc1)NCC(=O)OCC)=O</chem>	5224153	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
963	<chem>C1CCN(CC1)CC(Cn1c2cc(c(cc2c2cc(ccc12)[Cl])[Cl])O</chem>	5236854	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
964	<chem>c1ccc2c(c1)ccc(c2[Cl])Sc1ccc(cc1[Cl])N</chem>	5250905	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
965	<chem>c1cc(ccc1c1cc(C(NN)=O)c</chem>	5350878	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1

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	<chem>2cc(ccc2n1)[Br])N</chem>					
966	<chem>C(C(Cn1c2ccccc2c2ccccc12)O)N(Cc1cccc1)S(c1cccc1)F(=O)=O</chem>	5614-0038	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
967	<chem>C(c1cccc1)Nc1cccc(c1)[Cl]</chem>	5689-0133	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
968	<chem>C(=Cc1ccc(cc1[Cl])[Cl])C(c1cccc(c1)N)=O</chem>	5689908	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
969	<chem>CCOc1cc(CO)cc(c1OCc1ccc(cc1)C(O)=O)[Br]</chem>	6415-0035	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
970	<chem>CCOC(c1cnn(C(=O)OC)c1N)=O</chem>	7395-3020	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
971	<chem>CCOC(c1ccc(cc1)N1C(CC(C1=O)NC1CCCC1)=O)=O</chem>	7627-0150	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
972	<chem>C1COCCN1S(c1ccc(cc1)c1csc(Nc2ccc(cc2)[Br])n1)(=O)=O</chem>	8004-5092	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
973	<chem>C1CCN(CC1)S(c1ccc(cc1)c1csc(Nc2ccc(cc2)F)n1)(=O)=O</chem>	8004-9292	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
974	<chem>C1CC2=C(C(C1)=O)C1(C(C#N)=C(N)O2)C(Nc2ccc(cc12)F)=O</chem>	8004-9557	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
975	<chem>C=Cc1ccc(cc1)c1csc(N)n1</chem>	8005-0366	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
976	<chem>CC[Ge](CC)(CC)c1c(CNc2ccccc2)[nH]nn1</chem>	8005-7257	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
977	<chem>C1C(C(F)(F)F)=NN(C(c2ccc(cc2)N)=O)C1(c1ccc(cc1)[Br])O</chem>	8006-7761	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
978	<chem>Cc1cc(C)c2c(c1)nc(c1ccc(cc1O)N)o2</chem>	8007-0773	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
979	<chem>C(C1C(c2ccsc2)c2ccc3ccc3c2OC=1N)#N</chem>	8007-1084	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
980	<chem>C(C(c1ccc(cc1)[Cl])=O)Sc1nc2ccc(cc2s1)N</chem>	8007-4809	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
981	<chem>CC(c1ccc(cc1)NC(CSc1nnc(N)s1)=O)=O</chem>	8008-3900	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
982	<chem>CCOC(c1c2ccc(c(c2sc1NC(C)=O)OCC(CN1CCCC1)O)[Br])=O</chem>	8008-4440	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
983	<chem>Cc1c(C(O)=O)c(c(CO)s1)Sc1ccccc1</chem>	8008-4457	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
984	<chem>COc1ccc(c(c1)NC(CSc1nc2ccc(cc2s1)N)=O)OC</chem>	8009-2885	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
985	<chem>C(C(CSc1nc2ccccc2o1)O)Oc1ccccc1</chem>	8009-3200	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
986	<chem>C(C(c1ccc(cc1)F)=O)Sc1nc2ccc(cc2s1)N</chem>	8009-5501	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
987	<chem>CC(C)c1c2C(C(C#N)=C(N)O)c2[nH]n1c1ccc(c(c1)[Br])F</chem>	8011-1991	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
988	<chem>C(c1ccccc1)n1c(c(C(Nc2ccc(cc2)Oc2ccccc2)=O)nn1)N</chem>	8011-6606	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
989	<chem>Cn1cnncc1c1cccc(c1)N</chem>	8011-8021	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
990	<chem>CC1CC(NCc2ccccc2)N(C(C)=O)N1c1ccccc1</chem>	8012-7012	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
991	<chem>CCOC(c1c(c2c(C)c(c(C)nc2s1)[Cl])N)=O</chem>	8012-7125	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
992	<chem>CN(C)CCNCc1ccc2c(c1)c1CCCCc1[nH]2</chem>	8013-3043	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
993	<chem>Nc(cc1)cc(Cc2c3)c1-c2cc(Cl)c3Cl</chem>	80141	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
994	<chem>CC1(C)Cc2c(ccc3cccc23)C(=N1)Sc1ccc(cc1)N</chem>	8015-2089	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
995	<chem>Cc1cc(C)nc2c1c(c(C(NCc1cccc1[Cl])=O)s2)N</chem>	8015-4156	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
996	<chem>CCc1ccc2c(c1)nc(c1ccc(cc1O)N)o2</chem>	8018-2852	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
997	<chem>c1cc2c(cc1N)nc(c1ccc(cc1[Cl])[Br])o2</chem>	8018-2966	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
998	<chem>C(c1ccc2c(c1)OCO2)Nc1c(c[nH]n1)C(N)=O</chem>	8018-4095	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
999	<chem>C(c1ccc2c(c1)OCO2)Nc1ccc2ccc3c(c2)OCO3)no1</chem>	8018-4194	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
1000	<chem>Cc1cc(C)nc2c1c(c(c1ccc3ccc4c(c3)OCO4)no1)s2)N</chem>	8018-6772	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
1001	<chem>Cc1cc(COC)c2c3c(C(N(CCO)C(c4cccc4OC)=N3)=O)sc2n1</chem>	8018-6812	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
1002	<chem>c1ccc(cc1)c1cc2cccc(c2o1)N</chem>	8019-4318	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
1003	<chem>c1ccc(cc1)c1cc2cc(ccc2o1)N</chem>	8019-4319	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
1004	<chem>CC(=O)OCc1cc(ccc1O)c1csc(N)n1</chem>	8019-4503	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
1005	<chem>CCNC[C@@H]1CCN(CC)[C@H]1c1cccc1OC</chem>	8019-4504	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
1006	<chem>COc1cc(C2C(C#N)=C(N)OC3CCCC(C2=3)=O)c(c2c1OCO2)OC</chem>	8019-7050	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
1007	<chem>c1cc(N)nc2c1ccc(n2)O</chem>	8019-7722	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
1008	<chem>[H]N(Cc1ccncc1)c1ccc(C(O)=O)(c1)[Cl]</chem>	8019-7876	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
1009	<chem>C(c1cccc1)c1cc(ccc1OCCN)[Cl]</chem>	8019-8811	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
1010	<chem>C1CN(C(CN)c2cccc2)N=C1c1cccc1</chem>	8019-9361	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
1011	<chem>c1cc(ccc1c1cn[nH]c1)N</chem>	8020-2683	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
1012	<chem>Cc1c2[nH]c(cccc3)c3c2ccc1CCN</chem>	81703	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
1013	<chem>C(c1cccc1)[C@@H](c1nncc(o1)SCc1cccc2ccccc12)N</chem>	8388-0720	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
1014	<chem>C(CN)c1nncc(o1)SCc1ccc(c1[Cl])[Cl]</chem>	8388-1008	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
1015	<chem>CSc1nc2ncc(c3cccc3)c(N)n2n1</chem>	8562-00102	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
1016	<chem>S=C1Oc(ccc(-c2cccc2)c2)c2N1</chem>	93817	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
1017	<chem>c1ccc(cc1)S(n1c(cc(n1)OC(c1ccc(o1)=O)N)(=O)=O</chem>	C050-0221	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
1018	<chem>C(c1nc2cccc2n1Cc1ccc(c1)[Cl])Nc1ccc(cc1)C(O)=O</chem>	C147-0025	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
1019	<chem>Cc1cccc(c1)NCc1nc2cccc2n1C</chem>	C147-0043	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
1020	<chem>CSc1c(c(N)n(Cc2ccccc2)n1)S(c1cccc1)(=O)=O</chem>	C200-4138	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
1021	<chem>Cc1ccc2nc(c(Nc3ccccc3)n2c1)c1cccc1</chem>	C239-0048	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
1022	<chem>Cc1ccn2c(c(c3ccccc3)nc2c1)NC1CCCCC1</chem>	C273-0219	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
1023	<chem>c1ccc(cc1)S(n1c(cc(c2cccc(c2)F)n1)N)(=O)=O</chem>	C665-0183	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
1024	<chem>Cc1ccc2c(c1)C(C1=C(C(N(CCCO)C13C(N(CC=C)c1cccc13)=O)=O)O2)=O</chem>	D063-1068	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
1025	<chem>Cc1ccc2c(c1)C(C1=C(C(N(CCO)C13C(N(CC=C)c1cccc13)=O)=O)O2)=O</chem>	D063-1117	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
1026	<chem>Cc1cc(NC(C(=O)OC)c2cccc2)n2c(n1)nc(Cc1cccc1)n2</chem>	D245-0574	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
1027	<chem>C1CCC2(CC1)Cc1cccc1C1=C2C(N(Cc2ccco2)C(=N1)SCCO)=O</chem>	D325-0603	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
1028	<chem>[H]N(Cc1cccc1)c1c2c(esc2ncn1)c1ccc(C)cc1</chem>	D341-0419	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
1029	<chem>COc1ccc(cc1)c1nc(C(NCCO)=O)nn1c1cccc1[Cl]</chem>	D351-2816	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
1030	<chem>C1CCC2=C(C1)N1C(=NC=C(C(NCCCO)=O)C1=O)S2</chem>	D358-0437	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
1031	<chem>CC(c1cccc(c1)Nc1cc(c2ccc(cc2)OC)nc(C)n1)=O</chem>	D482-2054	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
1032	<chem>CCCCCNC1cc(c2ccccc2)nc2nc(c3ccccc3)nn12</chem>	D494-0421	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
1033	<chem>CN(C)c1ccc(cc1)c1c(Nc2cccc(c2)[Cl])n2cnc2n1</chem>	D600-0313	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
1034	<chem>[H]N(CCc1ccc(cc1)S(N)(=O)=O)Cc1ccc(c2ccc(cc2)[Cl])o1</chem>	D665-0262	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
1035	<chem>Cc1ccc2c(c1)cc(c(NC1ccc(cc1F)F)n2)c1nc(C)on1</chem>	D704-0959	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
1036	<chem>CCOC(c1nc2c(c3cccc(c3)[Br])c(C)nn2c1N)=O</chem>	D718-0691	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
1037	<chem>COC(c1ccc(cc1)NS(c1ccc(nc1N)[Br])(=O)=O)=O</chem>	E138-2198	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
1038	<chem>CCC(C)(C)NC1=C(C(C1=O)=O)c1ccc(C)cc1</chem>	E470-0146	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
1039	<chem>CCN(CC)c1ccc(c(C)c1)NC1=C(C(C1=O)=O)c1ccc(C)c(C)c1</chem>	E470-0720	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
1040	<chem>CCC(C)NC1=C(C(C1=O)=O)c1ccc(cc1)C(C)C</chem>	E511-0764	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
1041	<chem>CC(C)c1ccc(cc1)C1=C(C(C1=O)=O)NC1CCCCC1</chem>	E511-0774	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
1042	<chem>CC(C)c1ccc(cc1)C1=C(C(C1=O)=O)NC1CCCCC1</chem>	E511-0775	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
1043	<chem>CC(C)c1ccc(cc1)C1=C(C(C1=O)=O)NCc1cccc1OC</chem>	E511-0865	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
1044	<chem>Cc1ccc(C)c(c1)Nc1nc2cccc2c2nnc(C)n12</chem>	E881-0025	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1

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1045	<chem>C(C(Cn1cncn1)(c1ccc(cc1F)F)O)n1cncn1</chem>	NCGC0009508 9-11	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
1046	<chem>CC(=O)OC[C@@H]1[C@H]([C@@H])([C@H]([C@@H](O1)S[Au])OC(C)=O)OC(C)=O)OC(C)=O</chem>	NCGC0016039 1-02	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
1047	<chem>C1C(N=C2Nc3ccc(c(c3CN12)[Cl])[Cl])=O</chem>	NCGC0016140 8-02	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
1048	<chem>Cc1ccc(cc1)S(=O)(=O)OCC(Nc1ccc(C(O)=O)c(c1)O)=O</chem>	NCGC0026264 1-02	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
1049	<chem>C(C(Nc1ccc(cc1)n1c(cc(C(F)F)n1)c1ccc2c(ccc3ccccc23)c1=O)N</chem>	NCGC0034649 0-01	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
1050	<chem>CC(C)n1cnc2c(Nc3ccccc3)NC(C=C)=O)nc(NC3CCC(CC3)N(C)C)nc12</chem>	NCGC0034696 4-01	HIV_SL3	Hairpin	GACUAGCGGAGGCUAGAA	1
1051	<chem>c1ccc(cc1)c1nc2cc(ccc2o1)N</chem>	0109-0002	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1052	<chem>c1ccc2c(c1)nc(c1ccc(cc1)N)o2</chem>	0109-0045	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1053	<chem>Cc1nc2cccc(CCO)cc2s1</chem>	0133-0036	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1054	<chem>c1ccc(c(c1)N)I</chem>	0325-0348	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1055	<chem>c1ccc(cc1)c1nc2ccccc2c2nc(N)nn12</chem>	0345-0104	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1056	<chem>Cc1c(cc(c(c1[Br])N)[Br])[Br]</chem>	0357-0017	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1057	<chem>CC(Nc1nc2ccc(cc2s1)N)=O</chem>	0478-0670	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1058	<chem>C(C1COc2cccc2O1)O</chem>	0507-0170	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1059	<chem>Cc(cccc1)c1NC(NCCN1C1)=O</chem>	101266	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1060	<chem>c(cc1)ccc1-n1c(cccc2)c2c2c1cccc2</chem>	10416	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1061	<chem>CCC(C)N(C(C)=C1)N(C(C)CC)C1=O</chem>	120844	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1062	<chem>C1CN(Cc2ccccc12)c1c2CNCc2nc(c2ccnc2)n1</chem>	12634687	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1063	<chem>C1C(CN)Oc2c1cc(cc2F)c1ccc2c(cco2)c1</chem>	12766557	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1064	<chem>C(c1ccc(c(c1)c1ccccc2cenn12)F)N</chem>	13150762	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1065	<chem>C1C(CN1Cc1ccc(cc1)OC(CO)Oc1ccccc1[Cl])</chem>	13202927	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1066	<chem>CC(Cn1cncn1)NC1CCN(C1)c1nc2ccc(cc2s1)[Cl]</chem>	13410217	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1067	<chem>C1CC(CCc2ccccc2C(F)(F)F)CN(C1)C(CN)=O</chem>	13741411	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1068	<chem>C1CN(Cc2cnc(NCc3ccccc3)nc2)C[C@@H]([C@H]1CO)O</chem>	14588562	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1069	<chem>C1CN(CCC1C1CCN(CCc2ccccc2)C1)c1cnc(N)n1</chem>	14604674	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1070	<chem>C1CN(CCN(C1)C(Cc1ccsc(N)n1)=O)Cc1ccc(cc1)F</chem>	14610180	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1



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1071	<chem>Cc1cc(NCCCCO)n2c3cccc3nc2c1C#N</chem>	1486-0661	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1072	<chem>Cc1c(cc(cc1[Cl])C(NCC(Cc1cccc1)CO)=O)[Cl]</chem>	15537048	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1073	<chem>CCCCSc1nc(cc(n1)N1CCCN(CC1)Cc1ccncc1)N</chem>	15986801	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1074	<chem>Cc1cccc(c1)n1cccc1CN1CCOC(CN)C1</chem>	16946825	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1075	<chem>COc1cccc(c1)c1c(CN2CC(C(CC2)O)cc2cc(c(cc2n1)OC)OC</chem>	16959688	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1076	<chem>CN(CC1CCN(CC1)CCc1cccc(c1)F)C([C@H](Cc1c[nH]cn1)N)=O</chem>	17007774	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1077	<chem>C=Cc1ccc(nc1)N1CCN(C(C1)O)Cc1cccc1</chem>	17524156	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1078	<chem>CCCc1c(CC)c(c(C#N)c(N)n1)c1cccc1</chem>	1756-0136	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1079	<chem>C1CNCCc2cccc(c3cccc4c3cc[nH]4)c12</chem>	17741735	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1080	<chem>CCNC([C@H]1C[C@@H](CN1S(N1CCN(CC)CC1)(=O)=O)N)=O</chem>	17965244	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1081	<chem>C1CN(CCC1(c1cccc1)c1cccc1)C(c1cn(CCN)nn1)=O</chem>	18373450	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1082	<chem>Cc1c2c(nc(CCN)nc2sc1C)N1C[C@H]2CC[C@H]1C2</chem>	18808730	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1083	<chem>C(CN)c1cccc(CN2CCN(C2)Cc2ccc(cc2)[Cl])c1</chem>	19565794	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1084	<chem>C(CNC1CCC2(CC1)CCNCC2)CNc1ccncc1</chem>	19786268	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1085	<chem>Cc1cccc2c(cn(C)c12)c1c(c2cccc2)ncn1CCN</chem>	20224956	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1086	<chem>Cc1cc(cc(c1CNc1e2CCNCc2nc(C)n1)[Cl])[Cl]</chem>	20278440	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1087	<chem>CCc1ccc2c(c1)c(CC(N1CCC3(CC1)[C@H](C[C@H]3O)OCCN)=O)c2</chem>	21565883	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1088	<chem>COc1ccc(cc1OC)c1nncc(N)o1</chem>	2158-0021	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1089	<chem>C1CNC[C@H]([C@H]1CNS(c1cccc2cccc12)(=O)=O)O</chem>	21873168	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1090	<chem>CCOc1ccc(cc1)C(CN1C(=N)N(CCN2CCCCC2)c2cccc12)O</chem>	2226-0435	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1091	<chem>c1ccc2c(c1)ccc1c2nc(c2cc(c(cc2)N)[nH]1</chem>	2252-1548	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1092	<chem>C1CCCN(CC1)C[C@H]1CN(C[C@H]1CO)C(c1cc(N)[nH]n1)=O</chem>	22664850	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1093	<chem>Cc1cc2c(cc1N)nc(NC(c1ccc(cc1)C(=O)OC)=O)s2</chem>	2284-1574	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1094	<chem>c1ccc(c(c1)c1nc2cc(ccc2s1)N)O</chem>	2372-3111	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1095	<chem>C1CN(Cc2c(c3cccc4cccc34)noc12)C(c1cc(N)</chem>	26633940	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	[nH]n1)=O					
1096	C1COc2cc(ccc2C1=O)c1c c2CC(CN)Oc2c(c1)[Cl]	26642358	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1097	C1CCN(CC1)Cc1cccc(c1) n1ccnc1c1cc2CNCCn2n1	26875627	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1098	Cc1c2c(NCc3ccc(C(NC)= O)o3)nc(CCN)nc2sc1C	27312861	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1099	Cc1cc2c(cc1C)oc(c1ccc(cc 1O)N)n2	2783-3499	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1100	c1cc(cc(c1) [Cl])n1nc2ccc(cc2n1)N	2810-4198	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1101	c1cc(c2cccc(c2c1) [Br])c1nc2cc(ccc2o1)N	2810-4224	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1102	COc1ccc(cc1[Cl])c1nc2cc( ccc2o1)N	2810-4228	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1103	c1ccc(cc1)n1nc2ccc(cc2n1 )N	2810-4237	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1104	Cc1ccc2c(c1)nc(c1cc(ccc1 [Cl])N)o2	2810-4326	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1105	Cc1ccc2c(c1)oc(c1cc(ccc1 [Cl])N)n2	2810-4327	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1106	Cc1cc2c(cc1C)oc(c1ccc(C) c(c1)N)n2	2810-4335	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1107	C(c1ccc(cc1)c1nc(c2ccc(c c2)F)F)nn1CCO)N	31242301	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1108	Cc1cccc(c1)Nc1nc(CN2C CCC2c2ccc(cc2)F)nc(N)n1	31279636	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1109	COCCOC(C1C(C2=C(CC CC2=O)OC=1N)c1ccnc1) =O	3132-0534	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1110	Cc1nc(CCN)cc(n1)N1CC N(CC1)c1ccc(C#N)cn1	31455775	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1111	C(c1ccccc1[Cl])Sc1nc2ccc (cc2s1)N	3167-0436	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1112	Cc1c[nH]c(CN(C)C(c2ccc c(c2)C2CCCN2)=O)n1	31699168	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1113	Cc1nnc2c(Nc3ccc(cc3) [Cl])nc3c(non3)n12	3175-0679	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1114	C(Cc1nc(c2ccccc2)no1)C( N[C@H]1Cc2ccccc2[C@ @H]1N)=O	31852539	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1115	CCc1nc(C)nc1N1CCC(C C1)NC1CCc2ccccc2C1	32780540	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1116	c1ccc(cc1)C(c1ccc2c(c1)n c(c1ccccc1)N)[nH]2)=O	3289-6683	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1117	C1CC1[C@H]1CN(C[C@ @H]1N)C(c1ccc2c(ccn2) c1)=O	32894310	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1118	COc(cc12)ccc2nc(cc(cc2) Cl)c2c1C#N	33173	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1119	CC(=C)Cn1c2C(NC(N(C)c 2nc1NCCO)=O)=O	3329-2956	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1120	C(C12C3C(C(c4ccccc14)c 1ccccc12)C(N(C3=O)c1cc c(cc1)F)=O)O	3406-0971	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1121	CCOc1ccccc1c1nc(COc2c ccnc2N)c(C)o1	34120503	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1122	Cc1c2cc(cc(CNC([C@H] (Cc3c[nH]en3)N)=O)c2[n	34268481	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	<chem>H]c1c1cccc1)[Cl]</chem>					
1123	<chem>C(C1C(c2cccc(c2)[Br])c2c(c3cccc3)n[nH]c2OC=1N)#N</chem>	3448-2674	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1124	<chem>CC1=CC(NC(NCCNC2CC3(CC2)CCNCC3)=N1)=O</chem>	35107446	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1125	<chem>C1CNc2cc(CCC(NC(CCn3cnen3)c3cccc3)=O)nn2C1</chem>	35350604	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1126	<chem>Cc1cc(ccc1[Br])c1nc2cc(cc2o1)N</chem>	3617-0633	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1127	<chem>C(C1C(c2cccc(c2)c(c3cc4cccc4c3)n[nH]c2OC=1N)#N</chem>	3629-0271	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1128	<chem>Cc1cc2c(cc1C)oc(c1cccc(c1C)N)n2</chem>	3639-0494	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1129	<chem>C1C(C(=C(N)N1c1ccc(cc1[Cl])[Cl])C1NC(c2cccc2N=1)=O)=O</chem>	3643-1572	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1130	<chem>Cc1ccc(c(CC=C)c1)OCC(Cn1c2cccc2nc1CO)O</chem>	3672-0031	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1131	<chem>Cc1cc(CNCc2ccc(c(c2)OC)OC)ccc1OC</chem>	3702-1752	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1132	<chem>Cc1ccc(cc1)S(N(CC(CN1CCCC1)O)c1cccc2cccc12)(=O)=O</chem>	3772-6707	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1133	<chem>CCc1ccc(c2c3CCCCc3nc(c2C#N)N)s1</chem>	3830-0877	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1134	<chem>CC1c2cccc2C(N(CC(NC(Cc2nnc(N)s2)=O)N=1)=O</chem>	40021826	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1135	<chem>c1ccnc(c1)c1sc(Nc2ccc(c2)C(O)=O)n1</chem>	4112-3301	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1136	<chem>CCC(CO)N(Cc1cccc1C)Cc1cccc1C(O)=O</chem>	41419156	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1137	<chem>CC1CC2(CC(C)(c3csc(NCC=C)n3)OC2=O)C(=O)O1</chem>	4159-0008	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1138	<chem>C(Cn1cc(C(NCc2nc(c3ccc4c(c3)OCO4)on2)=O)nn1)N</chem>	42165233	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1139	<chem>C1CNc2c1c1c(NCc3cc(c4ccco4)on3)ncnc1s2</chem>	42424648	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1140	<chem>C(CNCC1(CCNC1)O)CNc1ccnc1</chem>	42558291	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1141	<chem>Cc1nc2CNc2c(NCCCN2CCCC2=O)n1</chem>	42605975	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1142	<chem>C(c1cccc1)NC(Cn1c2ccc2nc1c1c(N)non1)=O</chem>	4281-0225	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1143	<chem>CC(c1cccc(c1)Nc1nc(cs1)c1ccc(cc1)[Cl])=O</chem>	4469-0430	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1144	<chem>CC(C)(C)c1ccc(cc1)c1nc(c2cccc2n1)NCc1ccnc1</chem>	4491-1513	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1145	<chem>CSC(NC(Cl)=C1)=NC1=O</chem>	45719	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1146	<chem>C(CNc1ccnc1)CNc1c2ccc2nc(CCN)n1</chem>	47488116	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
1147	<chem>CCN1C(NC(C12CCN(CC2)Cc1cc2CNCCc1n1)=O)=O</chem>	47670564	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1148	<chem>C1CN(CC=C1)c1c2CCN(CCC2nc(c2ccc1n1)C(CN)=O</chem>	47825811	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1149	<chem>C(CN)CN1C(CC[C@H]2CN(CC[C@@H]12)C(CCc1ccc1)=O)=O</chem>	48226996	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1150	<chem>Cc1nc2cc(c(cc2n1CCCO)[Cl])[Cl]</chem>	5119828	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1151	<chem>c1ccc(cc1)C(C(c1cccc1)=NNC(c1cccc1)[Cl])=O)O</chem>	5210270	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1152	<chem>CCCCCc1ccc(cc1)c1ccc(c1)c1ccc(c1)N</chem>	5213078	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1153	<chem>c1ccc2c(ccc(c2c1)O)c1ccc(cc1[Cl])N[Cl]</chem>	5215844	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1154	<chem>Cc1ccc(cc1NC1c2ccccc2C(=O)O1)[Cl]</chem>	5227-1352	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1155	<chem>C1CCC2C(C1)=C(C#N)c1nc3ccccc3n1C=2NCCOCCO</chem>	5228-5336	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1156	<chem>c1cc(ccc1c1cc(C(NN)=O)c2cc(ccc2n1)[Br])N</chem>	5350878	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1157	<chem>[H]N([H])c1nc(n[nH]1)SCCCCCC</chem>	5655427	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1158	<chem>C(=Cc1ccc(cc1[Cl])[Cl])C(c1cccc(c1)N)=O</chem>	5689908	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1159	<chem>C(Cc1ccccc1)C(N1Cc2nn(CCO)c2C1)=O</chem>	57806214	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1160	<chem>CCNC(Cc1ccc(cc1)c1cc2C(C(N)Oc2c(c1)[Cl])=O</chem>	57980040	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1161	<chem>C(c1ccc(cc1)c1ccccc1)NC([C@@]12CN[C@H]2CNC1)=O</chem>	58024175	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1162	<chem>C1Oc2ccc(cc2O1)c1cc(c(C#N)c(N)n1)c1ccc1</chem>	58070293	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1163	<chem>Cc1ccc(cc1)c1nc(CNc2ccc(c2)[Cl])on1</chem>	5927-0146	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1164	<chem>C(=Cc1nc(c2ccccc2O)nc(N)n1)c1ccc(cc1)[Br]</chem>	6043-0005	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1165	<chem>[H][N+](CCO)=C1C=C(c2ccccc2)Oc2ccc(C)cc12</chem>	6197-4999	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1166	<chem>C(CC(N1c2ccccc2Sc2ccc(c12)=O)CN</chem>	6640-0077	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1167	<chem>O=C(c(cc1)cc(C(Nc(cc2)cc2C2=NCCN2)=O)c1Cl)Nc(cc1)ccc1C1=NCCN1</chem>	67436	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1168	<chem>CC1(C)Cc2c(CO1)c(c1ccco1)nc1c2c2c(c(NC3CCCCC3)ncn2)s1</chem>	6940-0105	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1169	<chem>CN(C)c1ccc(cc1)Nc1nc(cs1)c1cccs1</chem>	7100-1263	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1170	<chem>Cc1ccc(c(c1)C(O)=O)Nc1nc(C)cc(C)n1</chem>	7170-3463	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1171	<chem>CC1(C)CC(=CC(C1)=O)Nc1cc(c2ccc(cc2)[Cl])n[nH]1</chem>	7428-3079	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1172	<chem>C1C(C(N(C1=O)c1ccc(cc1</chem>	7627-0033	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	<chem>)</chem> <chem>[Cl]=O)Nc1ccc(cc1)Oc1c</chem> <chem>cccc1</chem>				UGACGGUACA	
1173	<chem>CC(c1ccc(cc1)OCC(Cn1c2</chem> <chem>cccc2nc1CO)O)=O</chem>	7661-0040	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1174	<chem>Cn1c(cnc1NCc1cccc(c1)</chem> <chem>[Br])c1ccc(cc1)OC</chem>	7756-0365	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1175	<chem>Cn1c(cnc1NCc1cc(ccc1F)</chem> <chem>[Br])c1cccc(c1)OC</chem>	7756-0752	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1176	<chem>CCOC(C1C(C(C#N)=C(N)</chem> <chem>OC=1C)c1c(C)c(C)cc(C)c</chem> <chem>1C)=O</chem>	8003-8202	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1177	<chem>Cc1ccc(cc1C)Nc1nc(cs1)c</chem> <chem>1ccc(c(c1)F)OC</chem>	8005-2731	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1178	<chem>CC[Ge](CC)</chem> <chem>(CC)c1c(CNc2ccccc2)</chem> <chem>[nH]nn1</chem>	8005-7257	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1179	<chem>CN1C2=C(C(C(C#N)=C(N)</chem> <chem>O2)c2ccccc2F)C(N(C)C</chem> <chem>1=O)=O</chem>	8006-4741	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1180	<chem>C(C(c1ccc(cc1)</chem> <chem>[Cl])=O)Sc1nc2ccc(cc2s1)</chem> <chem>N</chem>	8007-4809	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1181	<chem>C1C(C(N(C1=O)c1ccc(c(c</chem> <chem>1)[Cl])</chem> <chem>[Cl])=O)Nc1ccc(cc1)F</chem>	8007-5006	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1182	<chem>CCOC(c1c2ccc(c(c2sc1NC</chem> <chem>(C)=O)OCC(CN1CCCCC1</chem> <chem>)O)[Br])=O</chem>	8008-4440	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1183	<chem>C(C(c1ccc(cc1)F)=O)Sc1n</chem> <chem>c2ccc(cc2s1)N</chem>	8009-5501	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1184	<chem>c1ccc2c(c1)nc(Sc1ccc(cc1</chem> <chem>N)C(F)(F)F)s2</chem>	8010-6075	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1185	<chem>CCN(CC)c1ccc(cc1)NCc1</chem> <chem>ccc2c(c1)OCO2</chem>	8011-7548	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1186	<chem>Cc1c(CNCCc2c3cc(c3c[n</chem> <chem>H]c2C)OC)c(n(C)n1)[Cl]</chem>	8013-0585	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1187	<chem>C1CCC(CCNC2CC(N(C2</chem> <chem>=O)c2ccc(cc2)F)=O)=CC1</chem>	8013-1383	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1188	<chem>CCCCc1ccc(cc1)n1nc2cc(</chem> <chem>C)c(cc2n1)N</chem>	8014-1852	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1189	<chem>CC(C)Nc1nc(nc(n1)n1cnc</chem> <chem>1)N(C)c1cccc1</chem>	8014-9111	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1190	<chem>CC1(C)Cc2c(ccc3ccccc23)</chem> <chem>C(=N1)Sc1ccc(cc1)N</chem>	8015-2089	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1191	<chem>c1cc(cc(c1)NC(c1c(csn1)N</chem> <chem>)=O)C(F)(F)F</chem>	8016-2265	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1192	<chem>Cc1c2c(NCCc3c4ccccc4[n</chem> <chem>H]c3C)ncnc2sc1C</chem>	8016-2589	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1193	<chem>c1cnc(c1)Sc1ccc(cc1[Cl])</chem> <chem>N</chem>	8016-2974	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1194	<chem>CCN1C(c2ccc(CN)c3cccc</chem> <chem>1c23)=O</chem>	8016-6735	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1195	<chem>CCc1ccc2c(c1)nc(c1ccc(cc</chem> <chem>1O)N)o2</chem>	8018-2852	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1196	<chem>c1ccc(cc1)c1ccc(cc1)c1nc2</chem> <chem>cc(ccc2o1)N</chem>	8018-2965	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1197	<chem>COc1ccc(cc1)c1cc(CNCC</chem> <chem>2CC(Cc3cc4c(c(c3OC)OC</chem> <chem>)OCO4)ON=2)on1</chem>	8019-1863	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
1198	<chem>COc1cc(C2C(C#N)=C(N)OC3CCCC(C2=3)=O)c(c2c1OCO2)OC</chem>	8019-7050	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1199	<chem>c1cc(N)nc2c1ccc(n2)O</chem>	8019-7722	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1200	<chem>C(c1cn[nH]c1c1ccc(cc1)F)N</chem>	8020-0151	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1201	<chem>C1CN(CCC1N)Cc1ccccc1)O</chem>	8020-1707	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1202	<chem>C(c1ccccc1)Nc1c(C(Nc2ccc(c2)C(F)(F)F)=O)c(N)[nH]n1</chem>	8020-3093	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1203	<chem>c1cc(cc(c1)[Cl])c1nc(c2ccc(cc2)N)n[nH]1</chem>	8020-5002	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1204	<chem>C(c1ccccc1)[C@@H](c1nncc(o1)SCc1ccccc2ccccc12)N</chem>	8388-0720	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1205	<chem>C(COc1ccc2c(c1)c1ccccc1o2)N.[Cl]</chem>	9188721	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1206	<chem>CC(C)CCc1ccc(nc(N)n1)[Cl]</chem>	9225768	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1207	<chem>c1ccc2c(c1)nc(c1ccc(cc1[Cl])N)s2</chem>	C066-5322	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1208	<chem>Cc1ccccc1)NCc1nc2ccccc2n1C</chem>	C147-0043	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1209	<chem>CSc1c(c(N)n(Cc2ccccc2)n1)S(c1ccccc1)(=O)=O</chem>	C200-4138	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1210	<chem>C1CCN(CC1)c1cc(Nc2ccc(cc2)[Br])ncn1</chem>	C301-6154	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1211	<chem>c1cc(ccc1c1cc[nH]n1)N</chem>	C430-1098	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1212	<chem>Cc1cc(Nc2ccccc2)nc2cc(cc12)O</chem>	C614-0105	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1213	<chem>C1CCCN(CC1)CCCNc1nc2ccccc2c2nc(c3ccccc3)nn12</chem>	C736-0159	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1214	<chem>C1Oc2ccc(cc2O1)Nc1c(cnc2ccc(cc12)F)S(c1ccccc1)(=O)=O</chem>	C769-2045	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1215	<chem>Cc1ccc(cc1F)NC(CCc1c(C)nc2nc(CN)nn2c1C)=O</chem>	C908-0521	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1216	<chem>Cc1c(CCC(Nc2ccccc2)[Br])=O)c(C)n2c(n1)nc(CN)n2</chem>	C908-0523	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1217	<chem>Cc1c(CCC(Nc2ccccc2OC)=O)c(C)n2c(n1)nc(CN)n2</chem>	C908-0524	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1218	<chem>Cc1c(CCC(NCC2CCN(CC2)Cc2ccccc2F)=O)c(C)n2c(n1)nc(CN)n2</chem>	C908-0547	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1219	<chem>Cc1ccc2c(c1)C(C1=C(C(N(CCCO)C13C(N(CC=C)c1ccccc13)=O)=O)O2)=O</chem>	D063-1068	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1220	<chem>Cc1ccc2c(c1)C(C1=C(C(N(CCO)C13C(N(CC=C)c1ccccc13)=O)=O)O2)=O</chem>	D063-1117	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1221	<chem>CCCNc1cc(C)nc2nc(c3ccc(C)cc3)nn12</chem>	D245-0069	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1222	<chem>CN(C)S(c1ccc(cc1)c1nc(C#N)c(NC2CCCCC2)o1)(=O)=O</chem>	D434-0560	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
1223	<chem>CCNc1c(C#N)nc(c2cccc(cc2)S(N2CCOCC2)(=O)=O)ol</chem>	D434-0668	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1224	<chem>C(CO)NC(C1C=COc2cccc2C=1)=O</chem>	D443-0135	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1225	<chem>C(CNc1c2c(en(c3cccc3[C l])c2ncn1)c1cccc1)CN1C COCC1</chem>	D447-0372	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1226	<chem>CC(c1cccc1)N[C@H]1C S(C[C@H]1S(c1ccc(cc1)F)(=O)=O)(=O)=O</chem>	D470-1919	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1227	<chem>C1CC1N[C@H]1CS(C[C@H]1S(c1ccc(cc1)[Cl])(=O)=O)(=O)=O</chem>	D470-2169	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1228	<chem>COCCN[C@H]1CS(C[C@H]1S(c1ccc(cc1)[Cl])(=O)=O)(=O)=O</chem>	D470-2180	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1229	<chem>CC(c1cccc(c1)Nc1cc(c2cc c(cc2)OC)nc(C)n1)=O</chem>	D482-2054	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1230	<chem>CCCCCNC1cc(c2cccc2)nc2nc(c3cccn3)nn12</chem>	D494-0421	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1231	<chem>Cc1ccc2cc(c(NCc3ccc(cc(c3)F)F)nc2c1)c1nc(C)on1</chem>	D704-0962	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1232	<chem>CC(Nc1ccc(cc1)N1CC(C(=C1N)c1nc(C)c(C)s1)=O)=O</chem>	D715-1790	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1233	<chem>COc1ccc(cc1)c1csc(C2=C(N)N(CC2=O)c2cccc2[Cl])n1</chem>	D715-1943	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1234	<chem>CCC(C)(C)NC1=C(C(C1=O)=O)c1ccc(C)cc1</chem>	E470-0146	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1235	<chem>CCN(CC)c1ccc(c(C)c1)NC1=C(C(C1=O)=O)c1ccc(C)c(C)c1</chem>	E470-0720	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1236	<chem>CCC(C)NC1=C(C(C1=O)=O)c1ccc(cc1)C(C)C</chem>	E511-0764	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1237	<chem>CC(C)c1ccc(cc1)C1=C(C(C1=O)=O)NCc1cccc1OC</chem>	E511-0865	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1238	<chem>CC(C)c1ccc(cc1)C1=C(C(C1=O)=O)NCc1ccc(cc1)N(C)C</chem>	E511-0981	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1239	<chem>C1CCc2c(C1)c(CO)cs2</chem>	E540-0003	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1240	<chem>CC1Cc2cc(ccc2N1C(C1C C1=O)S(N(CCO)Cc1cccc1)(=O)=O</chem>	E570-0206	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1241	<chem>Cc1cccc(c1)C1C(C#N)=C(N)OC2=C1S(N(Cc1cccc1C)c1cccc12)(=O)=O</chem>	E738-0440	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1242	<chem>C(C(Cn1ncn1)(c1ccc(cc1F)F)O)n1ncn1</chem>	NCGC0009508 9-11	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1243	<chem>CC(C)(C)c1ccc(cc1)C(CC(c1ccc(cc1)OC)=O)=O</chem>	NCGC0009511 2-04	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1244	<chem>C1C(N=C2Nc3ccc(c(c3CN12)[Cl])[Cl])=O</chem>	NCGC0016140 8-02	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1
1245	<chem>CC(C)c1cc(cc2c1C(N(CO C1=CC(N3C=CC=C(C3=N1)OCCN1CCCC1)=O)S2(=O)=O)=O)OC</chem>	NCGC0016775 1-03	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGC UGACGGUACA	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
1246	<chem>CCc1ccc(C=C2C(NC(=S)S2)=O)cc1</chem>	NCGC00185994-02	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGCUGACGGUACA	1
1247	<chem>C(CCN1CCCC1)CNC(Nc1c(C(N)=O)c(ns1)OCc1c(c(cc1F)[Br])F)=O</chem>	NCGC00263100-01	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGCUGACGGUACA	1
1248	<chem>C1CC1NCc1cccc(c1)NC1=CC(=c2ccc(cc2)=C2C=C(C(C=C2O)=O)NN1</chem>	NCGC00346954-01	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGCUGACGGUACA	1
1249	<chem>CC(C)n1enc2c(Nc3cccc(c3)NC(C=C)=O)nc(NC3CCC(CC3)N(C)C)nc12</chem>	NCGC00346964-01	RRE2B	Hairpin	UGGGCGCAGUGUCAUUGACGCUGACGGUACA	1
1250	<chem>C(CO)NC(C1=Cc2ccccc2OC1=O)=O</chem>	0096-0280	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A)CGCUG(m6A)CGGUACA	1
1251	<chem>c1ccc2c(c1)nc(Sc1ccc(cc1)N)s2</chem>	0375-0603	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A)CGCUG(m6A)CGGUACA	1
1252	<chem>c1cc2c(cc(c(c2nc1N)[Br])[Br]</chem>	0422-0091	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A)CGCUG(m6A)CGGUACA	1
1253	<chem>c1nnc(N)s1</chem>	0488-0194	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A)CGCUG(m6A)CGGUACA	1
1254	<chem>C(C1COc2cccc2O1)O</chem>	0507-0170	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A)CGCUG(m6A)CGGUACA	1
1255	<chem>CN(C)c1ccc(C=Cc2nc3cc(ccc3[nH]2)N)cc1</chem>	0632-0897	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A)CGCUG(m6A)CGGUACA	1
1256	<chem>Cc1c(C)c(C)nc2c1c(c(C(c1ccc(cc1)[Cl])=O)s2)N</chem>	0892-0702	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A)CGCUG(m6A)CGGUACA	1
1257	<chem>Cc(cccc1)c1NC(NCCN1C C1)=O</chem>	101266	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A)CGCUG(m6A)CGGUACA	1
1258	<chem>O=C(NCCCN1CC1)Nc1ccc2ccccc12</chem>	101298	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A)CGCUG(m6A)CGGUACA	1
1259	<chem>CC[N+]1C(C)CSC=1C=C Nc1ccccc1</chem>	1147-0135	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A)CGCUG(m6A)CGGUACA	1
1260	<chem>CCC(C)N(C(C)=C1)N(C(C)CC)C1=O</chem>	120844	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A)CGCUG(m6A)CGGUACA	1
1261	<chem>CN(CCCc1ncn1C)c1c2CNCc2nc(c2cnc2)n1</chem>	12244291	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A)CGCUG(m6A)CGGUACA	1
1262	<chem>CC(C)Oc1cc(nc(N)n1)N1CCC(CC1)c1cc(nc(C)n1)O</chem>	12360715	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A)CGCUG(m6A)CGGUACA	1
1263	<chem>Cc1ccccc2c(c[nH]c12)c1ccc c(CCN)c1</chem>	12888021	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A)CGCUG(m6A)CGGUACA	1
1264	<chem>C1CNCCC12CC(C(N1CC N(CC1)c1cccc(c1[Cl])[Cl])=O)NC2</chem>	12921403	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A)CGCUG(m6A)CGGUACA	1
1265	<chem>CC(C)c1cc(Nc(c2c3)c(ccc(Cl)c4)nc2ccc3OC)c(C)c c1O</chem>	13051	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A)CGCUG(m6A)CGGUACA	1
1266	<chem>C1C(CN1Cc1ccc(cc1)OC CO)Oc1ccccc1[Cl]</chem>	13202927	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A)CGCUG(m6A)CGGUACA	1
1267	<chem>CN1C(C=C(C=N1)N1CC C(CC1)CNC([C@H](Cc1c[nH]cn1)N)=O)=O</chem>	13216682	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A)CGCUG(m6A)CGGUACA	1
1268	<chem>CN(C)c1nc2CNCCc2c(NC c2cc(COC)[nH]n2)n1</chem>	13478828	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A)CGCUG(m6A)CGGUACA	1
1269	<chem>CN(CCO)C[C@H]1CN(Cc2ccccc3c4ccccc4sc23)C[C@H]1CO</chem>	13609905	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A)CGCUG(m6A)CGGUACA	1
1270	<chem>C1C(Cc2ccccc12)N1CC[C @H](c2ccc3c(c2)OCO3)[C@H](C1)O</chem>	13694326	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A)CGCUG(m6A)CGGUACA	1
1271	<chem>C1CC(CCc2ccccc2C(F)(F)F)CN(C1)C(CN)=O</chem>	13741411	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A)CGCUG(m6A)CGGUACA	1



Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
1272	<chem>CC(C)c1ccc(c2nc(c3cccc(cc3)n3c(cc(C)n3)N)no2)no1</chem>	14063694	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1273	<chem>NCC(Nc(ccc(Cl)c1)c1C(c1ccc[nH]1)=O)=O</chem>	140873	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1274	<chem>Cc1nc(CCN)cc(NCCC2CCCN2C)n1</chem>	14159297	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1275	<chem>Clc1nc(Oc2cccc2)nc(-c(c2c3cccc2)cn3-c2cccc2)n1</chem>	142335	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1276	<chem>CC(C)CCOc1cccc(CCN(C(C2CC3(CCNCC3)CN2)=O)c1</chem>	14325308	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1277	<chem>C1C[C@H]2CCNC[C@H]1N2c1c2CNc2nc(c2ccnc2)n1</chem>	14601902	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1278	<chem>CN(C)c1nc2CNCCc2c(NC2cc(c3cccc3)n[nH]2)n1</chem>	15510936	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1279	<chem>Cc1c(cc(cc1[Cl])C(NCC(Cc1cccc1)CO)=O)[Cl]</chem>	15537048	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1280	<chem>CCC[C@H]1CN(C[C@H]1)NC(c1nc(N)nc1C)=O)S(C)(=O)=O</chem>	15820090	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1281	<chem>C1CC(CCc2ccc(cc2)F)CN(C1)C(c1cn(CCN)nn1)=O</chem>	15955175	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1282	<chem>Cc1ccc(c(c1)NC(NCC(CN1CCCC1)O)=O)[Cl]</chem>	16657809	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1283	<chem>C=Cc1ccc(nc1)N1CCN(C(C1)O)Cc1cccc1</chem>	17524156	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1284	<chem>C1CC(c2cccc(c2)c2cc(N)nc3c2cc[nH]3)NC1</chem>	18100777	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1285	<chem>C1=C(C(=O)O)c2cc(ccc12)O)c1nnc(Nc2ccc(cc2)F)s1</chem>	1814-2026	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1286	<chem>COc1c(cccn1)C(N1[C@H]([C@H]1)O)N1CCOCC1=O</chem>	18173626	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1287	<chem>C1CN(CCC1(c1cccc1)c1cccc1)C(c1cn(CCN)nn1)=O</chem>	18373450	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1288	<chem>Cc1c2c(nc(CCN)nc2sc1C)N1C[C@H]2CC[C@H]1C2</chem>	18808730	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1289	<chem>CC(c1ccc2c(cc[nH]2)c1)NC1CCN(CC1)c1c2c(ncn1)[nH]cn2</chem>	18958506	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1290	<chem>C1CCCN(CC1)CC(CNC(c1cn(CCN)nn1)=O)O</chem>	19036853	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1291	<chem>O=C(Nc(cc1)ccc1Br)Nc(ccc1)c1Cl</chem>	190501	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1292	<chem>C(CN)c1cccc(CN2CCN(C2)Cc2ccc(cc2)[Cl])c1</chem>	19565794	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1293	<chem>C1Cc2c(CC1N)c(c1nc(c3ccco3)nc1)c(C#N)c(N)n2</chem>	19707907	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1294	<chem>Cc1cc(cc(c1CNc1c2CCNC2nc(C)n1)[Cl])[Cl]</chem>	20278440	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1295	<chem>C(c1ccc(cc1)[Cl])n1c2cccc2nc1c1c(N)non1</chem>	2039-0584	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1296	<chem>CCOC(c1nc2ccc(cccc3)c3c2c(OCC)c1)=O</chem>	204939	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1297	<chem>Cc1cccc(c1)c1nc(CN2C=N</chem>	21839710	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A)	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	<chem>c3c(C=O)c2CCNCc2s3)on1</chem>				CGCUG(m6A)CGGUACA	
1298	<chem>C1CCN(CC1)C(CNC(Cc1cc2CNCCn2n1)=O)c1ccnc1</chem>	21900063	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A)CGCUG(m6A)CGGUACA	1
1299	<chem>CC(c1cccc(n1)N1CCc2c(C1)c1cccc(c1[nH]2)[Cl])O</chem>	22241597	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A)CGCUG(m6A)CGGUACA	1
1300	<chem>c1ccc2c(c1)ccc1c2nc(c2cc(c(cc2)N)[nH])1</chem>	2252-1548	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A)CGCUG(m6A)CGGUACA	1
1301	<chem>C1CNCc2cc(c3nccn3CCNC(c3ccc(cc3)F)=O)nn2C1</chem>	22582668	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A)CGCUG(m6A)CGGUACA	1
1302	<chem>Cc1cc2c(cc1N)nc(NC(c1ccc(cc1)C(=O)OC)=O)s2</chem>	2284-1574	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A)CGCUG(m6A)CGGUACA	1
1303	<chem>CC1OC1c(cc1)ccc1-c1ccc(C2OC2C)cc1</chem>	22881	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A)CGCUG(m6A)CGGUACA	1
1304	<chem>C1CCN(CC1)CC1(CCN(Cc2cccc(CCN)c2)C1)O</chem>	22896979	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A)CGCUG(m6A)CGGUACA	1
1305	<chem>c1ccc(c(c1)c1nc2cc(ccc2s1)N)O</chem>	2372-3111	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A)CGCUG(m6A)CGGUACA	1
1306	<chem>CC(C)OC(C1=C(C)OC(=C(C#N)C12C(Nc1ccccc12)=O)N)=O</chem>	2435-0085	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A)CGCUG(m6A)CGGUACA	1
1307	<chem>CC(C)Cn1c2C(NC(N(C)c2nc1NCCCO)=O)=O</chem>	2516-4245	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A)CGCUG(m6A)CGGUACA	1
1308	<chem>C1CN(Cc2c3ccc(ccc3[nH]c12)[Cl])c1c2c(nc(N)n1)[nH]cn2</chem>	25604160	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A)CGCUG(m6A)CGGUACA	1
1309	<chem>Cc1cc2c(cc1C)n(CC(COc1cccc1C)O)cn2</chem>	2582-0009	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A)CGCUG(m6A)CGGUACA	1
1310	<chem>CC(C)(C1CC2(C)CC1)C2OC(c(c1ccc1)c1C(O)=O)=O</chem>	26349	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A)CGCUG(m6A)CGGUACA	1
1311	<chem>C1COc2cc(ccc2C1=O)c1c2CC(CN)Oc2c(c1)[Cl]</chem>	26642358	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A)CGCUG(m6A)CGGUACA	1
1312	<chem>Cc1c2c(NCc3ccc(C(NC)=O)o3)nc(CCN)nc2sc1C</chem>	27312861	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A)CGCUG(m6A)CGGUACA	1
1313	<chem>CNC([C@@H]1C[C@H](CN1S(c1ccc(c2cno2)s1)(=O)=O)N)=O</chem>	27338263	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A)CGCUG(m6A)CGGUACA	1
1314	<chem>c1cc(cc(c1)[Cl])n1nc2ccc(cc2n1)N</chem>	2810-4198	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A)CGCUG(m6A)CGGUACA	1
1315	<chem>c1cc(c2cccc(c2c1)[Br])c1nc2cc(ccc2o1)N</chem>	2810-4224	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A)CGCUG(m6A)CGGUACA	1
1316	<chem>COc1ccc(cc1[Br])c1nc2cc(ccc2o1)N</chem>	2810-4227	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A)CGCUG(m6A)CGGUACA	1
1317	<chem>COc1ccc(cc1[Cl])c1nc2cc(ccc2o1)N</chem>	2810-4228	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A)CGCUG(m6A)CGGUACA	1
1318	<chem>c1ccc(cc1)n1nc2ccc(cc2n1)N</chem>	2810-4237	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A)CGCUG(m6A)CGGUACA	1
1319	<chem>Cc1cc2c(cc1C)oc(c1ccc(cc1)N)n2</chem>	2810-4334	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A)CGCUG(m6A)CGGUACA	1
1320	<chem>Cc1cc2c(cc1C)oc(c1ccc(C)c(c1)N)n2</chem>	2810-4335	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A)CGCUG(m6A)CGGUACA	1
1321	<chem>Cc(cc(cc1)-c(cc2)cc(C)c2N(C(C23CCC3)=O)C2=O)c1N(C(C(C12CCCC2)=O)C1=O</chem>	308835	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A)CGCUG(m6A)CGGUACA	1
1322	<chem>Nc1ccc(Cn(ccc2c34)c2ccc4nc(N)nc3N)cc1.Cl</chem>	309401	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A)CGCUG(m6A)CGGUACA	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
1323	<chem>Cc1ccc(cc1c1cccc(CCN)c1)F</chem>	31003354	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1324	<chem>C(c1ccc(cc1)c1nc(c2ccc(c(c2)F)F)nn1CCO)N</chem>	31242301	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1325	<chem>C(C(c1cccc1)=O)Sc1nc2ccc(cc2s1)N</chem>	3167-0470	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1326	<chem>C(Cc1nc(c2cccc2)no1)C(N[C@H]1Cc2cccc2[C@@H]1N)=O</chem>	31852539	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1327	<chem>COc1c(cnc(n1)OC)c1cc2CC(CN)Oc2c(c1)[Cl]</chem>	32090306	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1328	<chem>C(CNC1CCN(CC1)c1nnc(c2cccc2)s1)Cn1ccnn1</chem>	32364121	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1329	<chem>CC(Cc1ccsc1)NC(c1cccc(c1C)NCc1cccc1)=O</chem>	32552149	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1330	<chem>NNC(CNC(Nc1nnc(S)s1)=O)=O</chem>	327693	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1331	<chem>CCc1cnc(C)nc1N1CCC(C1)NC1CCc2cccc2C1</chem>	32780540	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1332	<chem>C=CCN1C(=Nc2c(C1=O)c1CCCCc1s2)SCC(NCCCO)=O</chem>	3334-5625	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1333	<chem>CN1C(c2c(nc(NCCN)n2Cc2ccc(cc2)F)N(C)C1=O)=O</chem>	3346-2730	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1334	<chem>Cc1c2c(NCCSCc3nnc(C)s3)nc(CCN)nc2sc1C</chem>	33667724	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1335	<chem>Cc1cc2c(C)nc(Nc3nc(C)cc(n3)O)nc2cc1C</chem>	3389-2554	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1336	<chem>CN(CCOC)C[C@@H]1CN(Cc2cccc3c4cccc4oc23)C[C@@H]1CO</chem>	34159790	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1337	<chem>Cc1c2cc(cc(CNC([C@H](Cc3c[nH]cn3)N)=O)c2[nH]c1c1cccc1)[Cl]</chem>	34268481	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1338	<chem>CN1CCC(CC1)N(CCOC)C(Nc1cccc(CN)c1)=O</chem>	34373109	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1339	<chem>C1CNCCc2cc(CCC(NC(CCn3cncn3)c3cccc3)=O)nn2C1</chem>	35350604	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1340	<chem>Cc1cc(ccc1[Br])c1nc2cc(cc2o1)N</chem>	3617-0633	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1341	<chem>CCCCc1ccc(cc1)n1nc2ccc(cc2n1)N</chem>	3738-4868	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1342	<chem>CCC(CC)(C(N)=O)SCC=C</chem>	37883	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1343	<chem>C(C(c1ccc(cc1)N)=O)C1(C(N(Cc2ccc(cc2)[Cl])c2cccc12)=O)O</chem>	3817-0057	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1344	<chem>CCc1ccc(c2c3CCCCc3nc(c2C#N)N)s1</chem>	3830-0877	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1345	<chem>CCOC(c1c(C)c2c(Nc3ccc(cc3)F)nc(C)nc2s1)=O</chem>	3909-7545	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1346	<chem>Cc1ncn1Cc1cccc1n1ccn1c1cc2CNCCn2n1</chem>	39520902	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1347	<chem>C1CNCCc2cccc(c3cncnc3)c12</chem>	39696086	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1348	<chem>COc1cccc1OC1CCN(CC1)Cc1cccc(CCN)c1</chem>	39780332	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
1349	<chem>Cc(cc1)ccc1C1=CSSC1=S</chem>	40467	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1350	<chem>CN(C)c1ccc(cc1)Nc1nc(cs1)c1ccc(cc1)OC</chem>	4112-3682	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1351	<chem>Cc1nc2CNCCc2c(NCCc2csc(c3ccnc3)n2)n1</chem>	41602213	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1352	<chem>Cc1ccc(C)c2c1c(cc(CNCCN1CCNC1=O)n2)O</chem>	41769850	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1353	<chem>C1CC(CC2CC2)(CN(C1)C1CSCCSC1)CO</chem>	42006513	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1354	<chem>COc1ccc2cc(ccc2c1)C1CN(CCO1)C(c1cc(N)[nH]n1)=O</chem>	42028139	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1355	<chem>C(Cn1cc(C(NCc2nc(c3ccc4c(c3)OCO4)on2)=O)nn1)N</chem>	42165233	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1356	<chem>Cc1ccc(cc1[Cl])c1nc2cc(cc2o1)N</chem>	4269-3090	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1357	<chem>Cc1cc(C)c2c(c1)c(cc(C)n2)Nc1ccc(cc1)C(=O)OC</chem>	4358-4481	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1358	<chem>Cc1c(c2csc(Nc3ccccc3)n2)n2ccnc2n1</chem>	4469-0267	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1359	<chem>Cc1c(cccc1[Cl])Nc1nc(cs1)c1c(C)nc(N)s1</chem>	4469-0741	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1360	<chem>Cc(cc1)cc(S(N)(=O)=O)c1/N=N/c(cc1)c(C)cc1N</chem>	45527	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1361	<chem>C(CNc1ccnc1)CNc1c2cccce2nc(CCN)n1</chem>	47488116	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1362	<chem>Cc1ccsc1CN(CCN(C)C)C(CN)=O</chem>	47645371	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1363	<chem>CCN1C(NC(C12CCN(CC2)Cc1cc2CNCCCN2n1)=O)=O</chem>	47670564	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1364	<chem>C1CN(CC=C1)c1c2CCN(CCc2nc(c2ccco2)n1)C(CN)=O</chem>	47825811	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1365	<chem>C(CCNc1c2c3CCCCc3sc2nnc1)CCO</chem>	4789-3834	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1366	<chem>CC(C)Cc1ccc(cc1)c1c2C(C(C#N)=C(N)Oc2[nH]n1)c1ccco1</chem>	4817-0239	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1367	<chem>C(CN)CN1C(CC[C@H]2CN(CC[C@H]12)C(CCC1ccco1)=O)=O</chem>	48226996	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1368	<chem>CCCCCCCCNc1cccc(c1)[Br]</chem>	5117451	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1369	<chem>Cc1nc2cc(c(cc2n1CCCO)[Cl])[Cl]</chem>	5119828	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1370	<chem>c1cc(c(cc1c1ccc(c(c1)N)N)N)N.O.O.[Cl].[Cl].[Cl].[Cl]</chem>	5140900	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1371	<chem>c1cc(ccc1c1c(c2ccc(cc2)F)nc2cc(ccc2n1)Oc1ccc(cc1)N)F</chem>	5174475	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1372	<chem>CCCCCc1ccc(cc1)c1ccc(c1)c1ncc(en1)N</chem>	5213078	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1373	<chem>c1ccc2c(ccc(c2c1)Oc1ccc(cc1[Cl])N)[Cl]</chem>	5215844	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1374	<chem>c1cc(ccc1c1cc(C(NN)=O)c</chem>	5350878	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A)	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	<chem>2cc(ccc2n1)[Br])N</chem>				CGCUG(m6A)CGGUACA	
1375	<chem>Nc(cc1)ccc1NC(c(cc1)ccc1C(Nc(cc1)ccc1N)=O)=O</chem>	55152	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1376	<chem>COc(cn1)c(Nc(cc2)ccc2C#N)nc1SC</chem>	55453	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1377	<chem>Br(c(cc1)ccc1-c1csc(/N=C2/SC=C(c(cc3)ccc3Br)N2)n1</chem>	55691	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1378	<chem>CCc1ccc(cc1)c1ccc(cc1)C(N1CCC(CN)C1)=O</chem>	56240352	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1379	<chem>[H]N([H])c1nc(n[nH]1)SCCCCCCCC</chem>	5655427	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1380	<chem>C(=Cc1ccc(cc1)[Cl])[Cl])C(c1cccc(c1)N)=O</chem>	5689908	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1381	<chem>CCNC(Cc1ccc(cc1)c1cc2C(C(N)O)c2c(c1)[Cl])=O</chem>	57980040	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1382	<chem>C(c1ccc(cc1)c1cccc1)NC([C@@]12CNC([C@H]2CNC1)=O</chem>	58024175	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1383	<chem>Cc1nc2CNCCc2c(NCCOCc2ccc(cc2)[Cl])n1</chem>	58315365	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1384	<chem>C(c1c(cc(c2ccc(cc2)F)nc1N)c1ccnc1)#N</chem>	6233-1975	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1385	<chem>C(c1c(cc(c2ccc(cc2)[Br])nc1N)c1ccco1)#N</chem>	6233-2517	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1386	<chem>CCOc1cc(CO)cc(c1OCc1ccc(cc1)C(O)=O)[Br]</chem>	6415-0035	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1387	<chem>C(c1cc(ccc1OCc1ccc(cc1)C(O)=O)[Cl])O</chem>	6415-0097	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1388	<chem>Cc1cccc2c1c(ccc(C(C=C1)=O)c3C1=O)c3n2C</chem>	645330	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1389	<chem>O=C(c(cc1)cc(C(Nc(cc2)ccc2C2=NCCN2)=O)c1Cl)Nc(cc1)ccc1C1=NCCN1</chem>	67436	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1390	<chem>CC(c1cnc(Nc2nc(C)c3cccc(C)c3n2)nc1C)=O</chem>	6809-0295	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1391	<chem>CC1(C)Cc2c(CO1)c(c1ccco1)nc1c2c2c(c(NC3CCCCC3)ncn2)s1</chem>	6940-0105	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1392	<chem>Nc1cc(N=[N+](c2c(C3ccc(N)c2)[O-])c3cc1</chem>	70534	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1393	<chem>COc1ccc(cc1OC)c1cc(c2nnc(N)o2)no1</chem>	7213-0562	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1394	<chem>C(c1cccs1)Nc1ccc2c(c1)nc(c1ccc(cc1)[Cl])o2</chem>	7629-1287	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1395	<chem>C1CC2=C(C(C1)=O)C1(C(C#N)=C(N)O2)C(Nc2ccc(c12)=O</chem>	8003-4618	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1396	<chem>CC[Ge](CC)(CC)c1c(CNCc2cccc2)[nH]nn1</chem>	8004-6298	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1397	<chem>CC[Ge](CC)(CC)c1c(CNc2cccc2)[nH]nn1</chem>	8005-7257	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1398	<chem>C(C(c1ccc(cc1)[Cl])=O)Sc1nc2ccc(cc2s1)N</chem>	8007-4809	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1399	<chem>C1CCC(CCNC2CC(N(C2=O)c2ccc(cc2)F)=O)=CC1</chem>	8013-1383	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
1400	<chem>Nc(cc1)cc(Cc2c3)c1-c2cc(Cl)c3Cl</chem>	80141	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1401	<chem>CC1(C)Cc2c(ccc3cccc23)C(=N1)Sc1ccc(cc1)N</chem>	8015-2089	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1402	<chem>C(c1ccc2c(c1)OCO2)Nc1c(c[nH]n1)C(N)=O</chem>	8018-4095	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1403	<chem>CC(C1(CCCCC1)N)=O</chem>	8018-6357	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1404	<chem>c1cc(N)nc2c1ccc(n2)O</chem>	8019-7722	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1405	<chem>C(c1en[nH]c1c1ccc(cc1)F)N</chem>	8020-0151	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1406	<chem>c1cc(cc(c1)[Cl])c1nc(c2ccc(cc2)N)n[nH]1</chem>	8020-5002	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1407	<chem>Cc1c2[nH]c(cccc3)c3c2ccc1CCN</chem>	81703	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1408	<chem>C(CN)c1nnc(o1)SCc1c(ccc1[Cl])[Cl]</chem>	8388-1008	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1409	<chem>[H]N([H])c1c2c3CC(C)(C)OCc3sc2nc(n1)SCc1ccc1[Cl]</chem>	8640-0360	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1410	<chem>O=C1ONC(C(C(F)(F)F)(F)F)(F)F)=N1</chem>	88349	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1411	<chem>C1CN(CCN1Cc1cccc1)C1CS(CC1O)(=O)=O</chem>	9195475	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1412	<chem>S=C1Oc(ccc(-c2cccc2)c2)c2N1</chem>	93817	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1413	<chem>CCOC(c1nc2c(ccc2c1Nc1ccc(C)cc1[Br])OC)=O</chem>	C053-0427	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1414	<chem>CSc1c(c(N)n(Cc2cccc2)n1)S(c1cccc1)(=O)=O</chem>	C200-4138	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1415	<chem>CCOc1ccc(c(c1)Nc1cc(C)nc2nc(C)nn12)OCC</chem>	C301-0909	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1416	<chem>Cc1ccc(c(c1)Nc1nc2cccc2c2nnc12)OC</chem>	C301-5171	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1417	<chem>CCOC(N1CCC(CC1)N1C(c2cccc2C1=O)Nc1cc(cc(c1)C(=O)OC)C(=O)OC)=O</chem>	C429-0358	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1418	<chem>Cc1cc(NCc2ccc(cc2)F)n2c(c(c3ccc(c(c3)OC)OC)c(C)n2)n1</chem>	C535-0529	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1419	<chem>CCOc1cccc1NC(c1c(CO)ncn1)=O</chem>	C612-0892	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1420	<chem>c1ccc2C(N(C(c2c1)Nc1ccc1F)c1ccc(cc1)[Cl])=O</chem>	C614-0363	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1421	<chem>CCOC(C1CCN(CC1)C1=C(C(C1=O)=O)NC(C)c1ccc1)=O</chem>	C667-0210	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1422	<chem>C1CCCN(CC1)CCCNc1nc2cccc2c2nc(c3cccc3)nn12</chem>	C736-0159	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1423	<chem>C1CC(N(C1)CCCNc1nc2cccc2c2nc(c3cccn3)nn12)=O</chem>	C736-0199	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1424	<chem>Cc1cc(C)n(CCc2nc3c4ccc4cc4nc(NC4CCN(CC4)Cc4cccc4)n3n2)n1</chem>	C736-0369	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1425	<chem>C1Oc2ccc(cc2O1)Nc1c(cnc2ccc(cc12)F)S(c1cccc1)</chem>	C769-2045	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	(=O)=O					
1426	C(CNCc1ccc(C(O)=O)s1)c1ccc(cc1)[Cl]	C863-0011	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1427	Cc1c(CCC(Nc2cccc(c2)C(F)F)=O)c(C)n2c(n1)nc(CN)n2	C908-0403	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1428	Cc1c(CCC(Nc2cccc(cc2)[Br])=O)c(C)n2c(n1)nc(CN)n2	C908-0436	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1429	Cc1c(CCC(Nc2cccc(c2)[Cl])F)=O)c(C)n2c(n1)nc(CN)n2	C908-0501	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1430	Cc1c(CCC(Nc2cccc(CN3CCCC3)cc2)=O)c(C)n2c(n1)nc(CN)n2	C908-0509	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1431	Cc1c(CCC(Nc2cccc(c2)[Br])=O)c(C)n2c(n1)nc(CN)n2	C908-0523	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1432	Cc1c(CCC(Nc2cccc2OC)=O)c(C)n2c(n1)nc(CN)n2	C908-0524	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1433	Cc1c(CCC(NCC2CCN(CC2)Cc2cccc2F)=O)c(C)n2c(n1)nc(CN)n2	C908-0547	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1434	c1ccn2c(C(c3ccc(cc3)[Cl])=O)c(c(C(Nc3cccc(c3)F)=O)c2c1)N	D033-0008	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1435	CC(C)c1ccc(CNc2nc3nc(C)c(c(C)n3n2)[Cl])cc1	D043-0278	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1436	Cc1ccc2c(c1)C(C1=C(C(N(CCCO)C13C(N(CC=C)c1cccc13)=O)=O)O2)=O	D063-1068	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1437	Cc1ccc2c(c1)C(C1=C(C(N(CCO)C13C(N(CC=C)c1cccc13)=O)=O)O2)=O	D063-1117	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1438	C=CCN1CC(C(=C1N)c1nc2cccc2[nH]1)=O	D086-0388	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1439	CC(c1ccc(cc1)Nc1cc(c2ccc2)nc(C)n1)=O	D278-0527	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1440	[H]N(Cc1cccc1)c1c2c(csc2ncn1)c1ccc(C)cc1	D341-0419	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1441	Cc1ccc2c(c1)cc(c(NC1ccc1)n2)c1nc(C)on1	D420-1964	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1442	CCNc1c(C#N)nc(c2cccc2)S(N2CCOCC2)(=O)=O)o1	D434-0668	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1443	C(CO)NC(C1C=COc2ccc(cc2C=1)[Br])=O	D443-0435	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1444	CCCCCNc1cc(c2cccc2)nc2nc(c3cccn3)nn12	D494-0421	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1445	C1CCC(C1)Nc1cc(c2cccc2)nc2nc(c3cccn3)nn12	D494-0439	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1446	Cc1cc(NCC(N2CCN(CC2)c2cccc2)F)=O)n2c(n1)nc(c1cccn1)n2	D494-0506	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1447	Cc1ccc(cc1C)S(N1CCN(C1)c1cc(C)nc(NC2CCCC2)n1)(=O)=O	D637-0036	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1448	[H]N(CCc1ccc(cc1)S(N)(=O)=O)Cc1ccc(c2ccc(cc2)[Cl])o1	D665-0262	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
1449	<chem>[H]N(Cc1cccc1)Cc1ccc(c2cccc(c2)[Cl])o1</chem>	D665-0395	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1450	<chem>CCC(CO)NCc1ccc(c(c1)O)C)OCc1ccc2c(c1)N(C)C(N2C)=O</chem>	D666-0065	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1451	<chem>Cc1cccc(CNc2c(cc3cccc(C)c3n2)c2nc(C)on2)c1</chem>	D704-0068	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1452	<chem>Cc1ccc2c(c1)cc(c(NCc1ccc(cc1F)F)n2)c1nc(C)on1</chem>	D704-0959	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1453	<chem>Cc1ccc2c(c1)cc(c(NCc1ccc(c(cc1[Cl])F)n2)c1nc(C)on1</chem>	D704-0989	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1454	<chem>COc1ccc(cc1)c1csc(C2=C(N)N(CC2=O)C2CCCCC2)n1</chem>	D715-1979	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1455	<chem>CCOC(c1cnc2c(c3cccc(cc3)[Br])c(C)nn2c1N)=O</chem>	D718-0691	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1456	<chem>CCc1cccc(C)c1NS(c1ccc(cnc1N)[Br])(=O)=O</chem>	E138-2120	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1457	<chem>COC(c1ccc(cc1)NS(c1ccc(cnc1N)[Br])(=O)=O)=O</chem>	E138-2198	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1458	<chem>CCC(C)NC1=C(C(C1=O)=O)c1ccc(cc1)C(C)C</chem>	E511-0764	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1459	<chem>CC(C)c1ccc(cc1)C1=C(C(C1=O)=O)NCc1cccc1OC</chem>	E511-0865	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1460	<chem>CC(C)c1ccc(cc1)C1=C(C(C1=O)=O)NCc1ccc(cc1)N(C)C</chem>	E511-0981	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1461	<chem>CCSc1c2Cc3c(CO)cnc(C)c3Oc2nc(c2cccc(c2)[Cl])n1</chem>	E544-0227	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1462	<chem>CC1Cc2cc(ccc2N1C(C1C1)=O)S(N(CCO)Cc1cccc(c1)(=O)=O</chem>	E570-0206	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1463	<chem>CC(C)c1ccc(cc1)n1c(c(c2nc(c3cccc(cc3)[Cl])no2)nn1)N</chem>	E595-0345	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1464	<chem>COc1ccc(c(c1)c1nc(Nc2ccc(cc2F)F)on1)OC</chem>	E679-0017	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1465	<chem>CCCN1=C(C(C1=O)=O)c1ccc(C)c(C)cc1C</chem>	E882-0500	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1466	<chem>CCOC(Nc1ccc(NCc2ccc(c(c2)F)nc1N)=O</chem>	NCGC0001545 1-06	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1467	<chem>C(CCCN=C(N)N=C(N)Nc1ccc(cc1)[Cl])CCN=C(N)N=C(N)Nc1ccc(cc1)[Cl]</chem>	NCGC0001624 6-12	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1468	<chem>Cc1c(C(c2ccc(cc2)OC)=O)c2ccc(cc2n1CCN1CCOCC1)I</chem>	NCGC0002501 2-02	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1469	<chem>C1CN1P(N1CC1)(N1CC1)=S</chem>	NCGC0009504 2-08	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1470	<chem>C(C(Cn1cncn1)(c1ccc(cc1F)F)O)n1cncn1</chem>	NCGC0009508 9-11	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1471	<chem>CC(C)=CC[C@H](C1=CC(c2c(ccc(c2C1=O)O)O)=O)O</chem>	NCGC0016348 9-04	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1472	<chem>C(C(O)=O)O.[N-].[N-].[Pt++]</chem>	NCGC0018115 2-01	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1
1473	<chem>C1CCN(C1)CCOc1ccc2cc1COC/C=C\CCOc1cccc(c1)c1ccnc(N2)n1</chem>	NCGC0024934 6-02	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA	1



Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
1474	<chem>Cc1c2cc(ccc2n[nH]1)c1cc(cnc1)OC[C@H](Cc1ccccc1)N</chem>	NCGC00263147-01	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A)CGCUG(m6A)CGGUACA	1
1475	<chem>C(C(Nc1ccc(cc1)n1c(cc(C(F)(F)F)n1)c1ccc2c(ccc3ccccc23)c1)=O)N</chem>	NCGC00346490-01	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A)CGCUG(m6A)CGGUACA	1
1476	<chem>C([C@@H]1[C@@H]([C@H]([C@H]([C@H]([C@H]2[C@@H]([C@H]([C@H]([C@H]([C@H](O[C@@H](C#N)c3ccccc3)O2)O)O)O)O1)O)O)O)O</chem>	NCGC00346583-01	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A)CGCUG(m6A)CGGUACA	1
1477	<chem>CC1(C)CC(c2c(C(F)(F)F)nn(c3ccc(C(N)=O)c(c3)NC3CCC(CC3)OC(CN)=O)c2C1)=O</chem>	NCGC00346640-01	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A)CGCUG(m6A)CGGUACA	1
1478	<chem>C1CCN(C1)C(Nc1cccc(c1)Nc1ncc(c(NC2c2nc[nH]2)n1)[Br])=O</chem>	NCGC00346687-01	RRE2B_MeA	Hairpin	UGGGCGCAGUGUCAUUG(m6A)CGCUG(m6A)CGGUACA	1
1479	<chem>CCN(CC)CCOC(c1ccc2c(c1)sc(NC(c1ccc(cc1)N)=O)n2)=O</chem>	0812-1025	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAGACUCUGGGAGA	1
1480	<chem>O=C(NCCCN1CC1)Nc1ccc2ccccc12</chem>	101298	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAGACUCUGGGAGA	1
1481	<chem>CC(NS(c(cc1)cc2c1sc(C)n2)(=O)=O)=O</chem>	122385	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAGACUCUGGGAGA	1
1482	<chem>COc1ccc(CC(N2CCC(CC2)C(Cc2ccccc2)O)=O)c(c1)OC</chem>	12362879	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAGACUCUGGGAGA	1
1483	<chem>Cc1esc2c(ncnc12)N1CCC(CC1)NCC1=CNC(NC1=O)=O</chem>	12466595	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAGACUCUGGGAGA	1
1484	<chem>Cc1cc(cc2c(ccnc12)N1C[C@H](C2CC2)[C@H](C1)N)[Cl]</chem>	12605761	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAGACUCUGGGAGA	1
1485	<chem>C1CN(Cc2ccccc12)c1c2CNCc2nc(c2ccnc2)n1</chem>	12634687	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAGACUCUGGGAGA	1
1486	<chem>C1C(CN1Cc1ccc(cc1)OC(CO)Oc1ccccc1[Cl])</chem>	13202927	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAGACUCUGGGAGA	1
1487	<chem>CC(COC)NCc1cc(c2ccc(c2)OC)on1</chem>	14208909	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAGACUCUGGGAGA	1
1488	<chem>CNC=C1C=C(c2ccccc2)N(C)C1=S</chem>	1457-0011	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAGACUCUGGGAGA	1
1489	<chem>C1CN(Cc2enc(NCc3ccccc3)nc2)C[C@H]([C@H]1CO)O</chem>	14588562	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAGACUCUGGGAGA	1
1490	<chem>CC(C)(C)c1cc(CN(C)c2c3CCNCc3nc(c3ccnc3)n2)[nH]n1</chem>	14923635	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAGACUCUGGGAGA	1
1491	<chem>Cc1ccccc1C(N1CCOC2(CNCCOC2)C1)=O</chem>	15132958	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAGACUCUGGGAGA	1
1492	<chem>C1CCN(C1)Cc1cc(c2cn(Cc3ccc(cc3)O)O)n2)sc1</chem>	15805022	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAGACUCUGGGAGA	1
1493	<chem>C=Cc1ccc(nc1)N1CCN(C(C1)O)Cc1ccccc1</chem>	17524156	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAGACUCUGGGAGA	1
1494	<chem>CN(Cc1ccc2c(c1)ncn2)C(c1cn(CCN2CCNCC2)nn1)=O</chem>	17862547	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAGACUCUGGGAGA	1
1495	<chem>C1CC(CNC1)c1cc(c2ccc(c2)[Cl])[Cl]nc(c1C#N)N</chem>	17917068	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAGACUCUGGGAGA	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
1496	<chem>C(COC1ccc(cc1)c1cc(c2cc[nH]2)nc(c1C#N)N)n1ccn1</chem>	18432747	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1497	<chem>C1CN(CCN1Cc1ccc(cc1)C(O)=O)Cc1ccccc1CO</chem>	19125330	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1498	<chem>Cc1cc(C)c2c(c1)c(cc(C)n2)C(N[C@H]1CNCC[C@@H]1OC)=O</chem>	19537511	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1499	<chem>O=C1OCC/C1=C\NCCCCCCC/C=C\CCO1)/C1=O</chem>	197008	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1500	<chem>CNCCN1C(CC[C@H]2CN(CC[C@H]12)C1cnn(C)c1)=O</chem>	19798067	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1501	<chem>CN(Cc1cnn(c1)c1ccc(cc1)F)C(C(c1ccc(cc1)F)O)=O</chem>	19840417	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1502	<chem>CC1(CCNCC1)C(N1CCc2c(C1)c(c1ccc(cc1)[Cl])n[nH]2)=O</chem>	20251729	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1503	<chem>Cn1cnc1c1ccc2CC(CN)Oc12</chem>	21885438	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1504	<chem>C1CCN(CC1)C(CNC(CCc1cc2NCCn2n1)=O)c1ccn1</chem>	21900063	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1505	<chem>C1CCCN(CC1)C[C@@H]1CN(C[C@@H]1CO)C(c1cc(N)[nH]n1)=O</chem>	22664850	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1506	<chem>CSCC1nc([C@H]2C[C@H](CN2)O)n(c2ccc(c2)[Cl])[Cl])n1</chem>	22714385	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1507	<chem>C1CCN(CC1)Cc1cccc(c1)n1cnc1c1cc2NCCCN2n1</chem>	26875627	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1508	<chem>Cc1ccc(C)c(c1)Nc1cc(cc1OC)[Br]</chem>	2910-2364	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1509	<chem>O=C(N(CC1OC1)C(N1CC2OC2)=O)N(CC2OC2)C1=O</chem>	296934	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1510	<chem>CCOC/C(/C1=CSC2=NNC(C)(C)N12)=N/O)=O</chem>	299968	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1511	<chem>C1CCCN(CCC1)CC(N1C[C@H](c2ccccc2)[C@H](C1)N)=O</chem>	31891223	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1512	<chem>CN(C)c1c2CCN(Cc2nc(c2ccnc2)n1)C(C1(CCC1)N)=O</chem>	32350946	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1513	<chem>COCc1nc(CCNC(CCc2cc3CNCCn3n2)=O)on1</chem>	32552243	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1514	<chem>Cc1nc(CN)cc(n1)N1CCC(CC1)C(c1cncn1C)O</chem>	32807865	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1515	<chem>Cc1cc(cnc1n1enne1)c1ccc2CNCCc12</chem>	34452990	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1516	<chem>COc1ccc2ccc(cc2c1)OCc1nc(co1)C(NCc1ccnc1N)=O</chem>	35061195	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1517	<chem>Cc1ccccc1)Nc1nc(CN2C[C@@H]3CC[C@H](C2)N(C)C3=O)nc(N)n1</chem>	35485871	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1518	<chem>COc1ccc(CNCc2ccc(cc2)F)cc1</chem>	3702-0995	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
1519	<chem>COc1ccccc1CNc1ccc(cc1)C(F)(F)F</chem>	3702-1158	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1520	<chem>COc1cccc(CNCc2ccccc2C(F)(F)F)c1OC</chem>	3702-1702	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1521	<chem>Cc1c2ccccc2n(CC(CNc2ccc(cc2)[Br])O)c1C</chem>	3744-0008	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1522	<chem>Cc1ccc(C)c(c1)NCC(Cn1c(C)c(C)c2ccccc12)O</chem>	3744-0052	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1523	<chem>CCC(CO)NCC(CN1c2cccc(c2)Sc2ccccc12)O</chem>	3746-0114	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1524	<chem>CC(Nc1cccc(c1)c1ccc(c(c1)F)NC(CN)=O)=O</chem>	40118252	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1525	<chem>Cc1ccc(cc1)S(N(CC(CN1CCCC1)O)c1ccccc1OC)(=O)=O</chem>	4013-2178	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1526	<chem>Cc1c(c2sc(Nc3ccc(cc3)[Cl])n2)n2ccccc2n1</chem>	4112-3380	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1527	<chem>Cc(cc1)cc(S(N)(=O)=O)c1/N=N/c(cc1)c(C)cc1N</chem>	45527	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1528	<chem>CSC(NC(Cl)=C1)=NC1=O</chem>	45719	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1529	<chem>[H]N(c1ccccc1[Cl])c1nc(C)c(C(=O)OCC)s1</chem>	4576-0043	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1530	<chem>COc1ccc(c(c1)OC)c1sc(NCC=C)n1</chem>	4640-0152	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1531	<chem>Cc1nc(N)nc1NCC[C@@H]1C[C@H]2C[C@@H]1C=C2</chem>	47913504	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1532	<chem>Cc1nc2cc(c(cc2n1CCCO)[Cl])[Cl]</chem>	5119828	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1533	<chem>CCN(CC(COc1ccc2ccccc2c1)O)S([O-])(=O)=O.[K+]</chem>	5173055	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1534	<chem>CCOC(c1nc2ccccc2c1Nc1ccc(cc1)N1CCOCC1)=O</chem>	5174-4348	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1535	<chem>C1CCN(CC1)Cc1c(CN2CCCC2)n(c2c(N)non2)nn1</chem>	5175780	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1536	<chem>C(CCN=Cc1ccccc1N)CN=Cc1ccccc1N</chem>	5233844	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1537	<chem>c1ccc2c(c1)ccc(c2[Cl])Sc1ccc(cc1[Cl])N</chem>	5250905	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1538	<chem>C1CC[N+](CC1)CCCCSc1ccc(cc1)O.[O-][Cl](=O)=O</chem>	5251615	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1539	<chem>Cc1cc(C)n(c2cc(NCCO)ncn2)n1</chem>	5256691	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1540	<chem>COc1ccc(cc1)OCC(CN1CCN(CC1)c1ccccc1)O.[Cl].[Cl]</chem>	5257916	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1541	<chem>C1CC(N(CNc2ccc(c(c2)[Cl])[Cl])Cl=O)=O</chem>	5271658	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1542	<chem>CC(C)(C)NCC(Nc1c2CCCCc2nc2CCCC12)=O.C(O)=O.C(C(O)=O)(O)=O</chem>	5284047	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1543	<chem>COc1c(c(c(c1F)F)c1sc(N)n1)F)F</chem>	5300-0134	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1544	<chem>CCCCOc1ccc(CSCCN)cc1.[Cl]</chem>	5343258	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
1545	<chem>C(C(NN)=O)Nc1ccc(cc1[Br])[Cl]</chem>	5345379	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1546	<chem>Cc1cc(ccc1NCC(NN)=O)I</chem>	5346837	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1547	<chem>Cc1cc(ccc1NCC(NN)=O)[Cl]</chem>	5347228	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1548	<chem>CCOC(CNc1ccc(cc1C)[Cl])=O</chem>	5350316	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1549	<chem>CCCCNc1c2c(c3c4CCCCc4c(nc3s2)N2CCOCC2)nnn1</chem>	5504-0161	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1550	<chem>CCOc1cc(CNCCc2cccc(c2)F)ccc1OC</chem>	5571711	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1551	<chem>C1CCc2c(C#N)c(N)sc2CC1</chem>	5574569	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1552	<chem>COc1ccc(cc1CN1CCC(CC1)N1CCN(CC1)CCO)[Br]</chem>	5607-0223	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1553	<chem>C=CCC(CC=C)(c1ccc(cc1)C(CC=C)(CC=C)N)N</chem>	5654685	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1554	<chem>C(C(Cn1c2cccc2c2cccc12)O)NNC(c1cccc1)=O</chem>	5718973	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1555	<chem>COC(CCCCC1C(C(CS1)N)N)=O.[Br].[Br]</chem>	5728434	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1556	<chem>Cc1cc(ccc1OCCNCCCOC)[Cl].C(C(O)=O)(O)=O</chem>	5734342	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1557	<chem>C(CN1CCOCC1)C(Nc1cc(c(cc1C(c1cccc1)NCC(NN)=O)[Br])=O</chem>	5808034	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1558	<chem>CC1(C)CC(CCO1)C(CCNc1ccc(cc1)N(C)C)c1cccc1</chem>	5936315	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1559	<chem>Cc1ccc(c(C)c1)OCC(CN1CCN(CCN1C(c2cccc3cccc(C1=O)c23)=O)O.[Cl].[Cl]</chem>	6044718	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1560	<chem>c1ccc2c(c1)cc1cnc3c(c(N)n[nH]3)c1n2</chem>	6051011	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1561	<chem>OC(Cc(sc(O)n1)c1O)=O</chem>	60548	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1562	<chem>CN(C)c1ccc(CNC2CCCC2)cc1</chem>	6117-0178	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1563	<chem>CCCOC(c1c(csc1N)c1ccc(c(c1)OC)OC)=O</chem>	6131187	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1564	<chem>C1CCCCC2c(CCCC1)c(C(N)=O)c(N)s2</chem>	6132195	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1565	<chem>CCSCCC(C(O)=O)NC1C(C(C)C)CC(C=1)=O</chem>	6254-0021	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1566	<chem>CCOC(C(C(c(ccc1)c1N1)C1=O)=O)=O</chem>	646976	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1567	<chem>CCOc1ccc(cc1)NCc1nc2cccc2n1C</chem>	6524406	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1568	<chem>O=C(c(c1)cc(C(Nc(cc2)cc2C2=NCCN2)=O)c1Cl)Nc(cc1)ccc1C1=NCCN1</chem>	67436	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1569	<chem>CCC1CCCCN1S(c1ccc(cc1)NC1c2cccc2S(N=1)(=O)=O)(=O)=O</chem>	7380-0010	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1570	<chem>Cn1c(cnc1NCc1ccc(cc1)[Br])c1cccc(c1)OC</chem>	7756-0390	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
1571	<chem>Cn1c(cnc1NCc1cccc1[Cl])c1cccc(c1)OC</chem>	7756-0396	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1572	<chem>Cn1c(cnc1NCc1cccc1OC)c1cccc1</chem>	7756-0545	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1573	<chem>CCOc1ccc(cc1)c1cnc(NCc2cccc2OC)n1C</chem>	7756-0840	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1574	<chem>CC(CNCCNCc1cc(c(c1)[Br])OC)OC.O.[Cl].[Cl]</chem>	7971888	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1575	<chem>C(CN)CN1CCN(CC1)c1cccc1</chem>	7974015	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1576	<chem>Cc1ccc(cc1C)Nc1nc(cs1)c1ccc(c(c1)F)OC</chem>	8005-2731	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1577	<chem>Cc1ccc(C)c(c1)c1csc(Nc2cccc2OC)n1</chem>	8006-1580	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1578	<chem>Cc1ccc(cc1)C1C(C#N)=C(N)Oe2ccc3cccc3c12</chem>	8008-9298	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1579	<chem>[H]Nc1nnc(COc2cc(C)cc(C)c2s1</chem>	8009-2828	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1580	<chem>[H]Nc1nnc(COc2ccc(cc2)C2CCCC2)s1</chem>	8009-2831	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1581	<chem>COc1ccc(c(c1)NC(CSc1nc2ccc(cc2s1)N)=O)OC</chem>	8009-2885	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1582	<chem>C1CCN(CC1)c1ccc2C(N(CCO)C(c3cccc1c23)=O)=O</chem>	8010-2208	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1583	<chem>CC1=CC(N(C)C(N1CCCCCNC(CO)=O)=O</chem>	8012-3983	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1584	<chem>Cc1c(CCNc2c(cc(cc2OC)OC)OC)c2cc(ccc2[nH]1)OC</chem>	8013-0022	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1585	<chem>Cc1c(CCNc2ccc(C#N)cc2)c2cc(ccc2[nH]1)OC</chem>	8013-2954	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1586	<chem>COc1nc(NCCCCCCCCC=2)nc(n1)N1CC2CC(C1)C1=CC=CC(N1C2)=O</chem>	8014-8886	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1587	<chem>CC(C)C1(CCNc2ccc(cc2)OC)CCOC(C)(C)C1</chem>	8018-1266	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1588	<chem>CC(C)C1(CCNc2cccc3c2OCO3)CCOC(C)(C)C1</chem>	8018-1268	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1589	<chem>COCc1nc(c2c(N)non2)no1</chem>	8018-8577	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1590	<chem>C(CS(N1CCNCC1)(=O)=O)N</chem>	8018-8721	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1591	<chem>c1cc(N)nc2c1ccc(n2)O</chem>	8019-7722	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1592	<chem>CCOC(C1=C(c2cccc2S1(=O)=O)N)=O</chem>	8019-8616	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1593	<chem>c1cnccec1c1nc2ncnc(N)n2n1</chem>	8020-2786	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1594	<chem>CN1CCCc2ccc(cc12)N</chem>	8020-4281	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1595	<chem>C[C@]1(C)Cc2c(CO1)c(c1ccco1)nc1c2c2c(c(NCCC(C)C)n2)s1</chem>	8640-0613	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1596	<chem>COc(cc1)cc(N2)c1NP2(Oc1cccc1)=S</chem>	88402	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1597	<chem>CCC(C)C(c1nnc(o1)SCC(c1ccc(cc1)[Cl])=O)N.[Cl]</chem>	9134179	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1598	<chem>C(c1ccnc1)Nc1cccc(c1)c1</chem>	9142557	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	<chem>nc2cccc2[nH]1</chem>				ACUCUGGGAGA	
1599	<chem>C1CN(CCC1c1nc2cccc2s1)C1CS(CC1O)(=O)=O</chem>	9195478	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1600	<chem>Cc1ccc2c(N)n[nH]c2n1</chem>	9195712	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1601	<chem>Cn1c(c2c(c3ccccc3s2)N)nnc1S</chem>	9221247	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1602	<chem>CCN1CCCC1CNCc1cccc(c1)OCc1ccc(cc1)[Cl]</chem>	9312203	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1603	<chem>c1ccc2c(c1)nc(c1ccc(cc1[Cl])N)s2</chem>	C066-5322	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1604	<chem>Cc1cccc(c1)NCc1nc2cccc2n1C</chem>	C147-0043	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1605	<chem>CC1CCN(CC1)c1nc(c(C(=O)OC)s1)N</chem>	C201-1740	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1606	<chem>CCc1nc2nc(C)cc(Nc3cc(cc3C)[Cl])n2n1</chem>	C301-3944	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1607	<chem>Cc1cc(C)n2c(c(c3ccc(C)s3)nc2n1)Nc1ccc2c(c1)OCCO2</chem>	C325-0312	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1608	<chem>CCOC(C1CCN(CC1)C1=C(C(C1=O)=O)NCCCN1CCCC1)=O</chem>	C667-0368	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1609	<chem>Cc1c(CCC(Nc2cccc(c2)C(F)F)=O)c(C)n2c(n1)nc(CN)n2</chem>	C908-0403	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1610	<chem>CCOC(c1ccc(cc1)NC1c2c(cccn2)C(N1c1ccc(C)cc1)=O)=O</chem>	C999-1176	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1611	<chem>CC(C)c1ccc(C)cc1OCCCN1c2cccc2nc1C(C)O</chem>	D011-5386	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1612	<chem>COC(CCc1c(c2ccc(cc2)O)C)nc(Nc2cccc2s1)=O</chem>	D041-0023	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1613	<chem>[H]c1ccc(cc1)S(c1c(NCCOC)oc(c2cccc2)n1)(=O)=O</chem>	D072-0501	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1614	<chem>COCCNc1c(nc(c2ccc(cc2)[Cl])o1)S(c1cccc1)(=O)=O</chem>	D072-1517	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1615	<chem>CN1C(c2c(cn(c3cccc(c3)N)c2c2ccc(cc2)[Cl])N(C)C1=O)=O</chem>	D077-0219	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1616	<chem>Cc1ccc2c(c1)[nH]c(C1=C(N)N(CC1=O)c1ccc(cc1)F)n2</chem>	D086-0081	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1617	<chem>CCCOc1cccc(c1)C1c2c(c3cc(C)ccc3O)n[nH]c2C(N1CCCO)=O</chem>	D126-0083	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1618	<chem>C(CNc1c(C#N)nc(C=Cc2cc(cc2)F)o1)CN1CCOCC1</chem>	D151-0242	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1619	<chem>C1CC(CNc2c(C#N)nc(C=Cc3ccc(cc3)F)o2)OC1</chem>	D151-0248	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1620	<chem>Cc1cccc(Cn2c3ccccc3nc2CCNC(CCCO)=O)c1</chem>	D186-0280	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1621	<chem>Cc1cc(N(CCO)CCO)n2c(n1)nc(Cc1cccc1)n2</chem>	D245-0529	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1622	<chem>CN1C(N(C)c2cc(ccc12)C(CO)c1ccc(CNCCc2ccc(cc2)F)cc1O)=O</chem>	D300-0304	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
1623	<chem>CC1(C)CC(CCO1)CNCCN(C)C</chem>	D324-0105	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1624	<chem>CCN(CC)CCNCC1CCOC(C)(C)C1</chem>	D324-0106	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1625	<chem>CC1(C)CC(CCO1)CNCCCN(C)C</chem>	D324-0107	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1626	<chem>CCN(CC)CCNCC1CCOC(C)(C)C1</chem>	D324-0108	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1627	<chem>[H]N(Cc1cccc(c1)OC)c1c2c(csc2nnc1)c1cccc1</chem>	D341-0323	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1628	<chem>[H]N(Cc1cccc1)c1c2c(csc2nnc1)c1cccc(C)cc1</chem>	D341-0419	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1629	<chem>CCCC(c1nc2cccc2n1CCOe1cccc(c1)[Cl])O</chem>	D347-4130	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1630	<chem>CC(C)CNc1nc(nc(n1)n1nc(n1)SCe1cccc1)N(C)C</chem>	D385-0105	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1631	<chem>C1CCN(CC1)C(c1cccc(c1)Nc1c(c2cccc2)nc2cncn12)=O</chem>	D401-0331	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1632	<chem>Cc1ccc(cc1)Nc1cc(nc(C)n1)N1CCN(CC1)C(c1cccs1)=O</chem>	D430-0262	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1633	<chem>CC1(C)CC(CCNc2ccc3c(c2)OCO3)(CCO1)c1cccc1OC</chem>	D442-0097	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1634	<chem>Cc1cccc(c1)c1cc(Nc2ccc(c2)C(F)(F)F)nc(C)n1</chem>	D482-1812	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1635	<chem>[H]C([H])(CC)c1cc(NCCCC)n2c(n1)nc(c1ccnc1)n2</chem>	D494-0181	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1636	<chem>COe1ccc(Cc2nc3cccc3n2CC(COe2cccc2O)cc1</chem>	D510-0832	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1637	<chem>Cc1cccc(C)c1OCC(Cn1c2cccc2nc1C1CCN(C1)c1cccc(c1)OC)=O)O</chem>	D510-0970	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1638	<chem>CCNc1nc(C)cc(n1)N1CCN(CC1)S(c1ccc(cc1)[Cl])(=O)=O</chem>	D575-0012	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1639	<chem>[H]N(CCN(CC)CC)Cc1ccc(c2cccc2)o1</chem>	D665-0049	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1640	<chem>Cc1ccc2cc(c(NCc3ccc(cc3F)F)nc2c1)c1nc(C)on1</chem>	D704-0252	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1641	<chem>Cc1nn2c(Nc3cccc(c3)C(F)(F)F)nc3cccc3n12</chem>	E208-0090	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1642	<chem>COe1ccc2c(CNCc3cccc3)c(C(O)=O)[nH]c2c1</chem>	E518-1228	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1643	<chem>CCOc1ccc(cc1)c1nc(c2c(N)n(c3cccc3[Cl])nn2)on1</chem>	E595-0516	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1644	<chem>C1CN1P(N1CC1)(N1CC1)=S</chem>	NCGC0009504 2-08	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1645	<chem>C(C(Cn1cncn1)(c1ccc(cc1F)F)O)n1cncn1</chem>	NCGC0009508 9-11	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1646	<chem>Cn1cc(cn1)c1cnn2c(c(c([C@H]3CCCN3)nc12)[Br])N</chem>	NCGC0034665 3-01	Zika_NS5	G-quadruplex	GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA	1
1647	<chem>CCCCCOe(cc1)ccc1N(C(C(C)CN1)=O)C1=S</chem>	121908	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1648	<chem>C1CCN(C1)C([C@H]1C[C@H](CNC1)C(N1CCN(CC1)c1</chem>	12190856	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	<chem>ccncc1=O)=O</chem>					
1649	<chem>O=C(C1C2)N(CC3)C2C3(c(cccc2)c2N23)C3=C1C=CC2=O</chem>	122253	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1650	<chem>CC(NS(c(cc1)cc2c1sc(C)n2)(=O)=O)=O</chem>	122385	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1651	<chem>CC[C@H](C)[C@@H](C(N1CCC(CC1)Cn1cc(C2CCCC2)nn1)=O)N</chem>	12353320	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1652	<chem>Cc1c(C)nc(nc1N1C[C@@H](CN2CCCC2)[C@H](C1)CO)N1CCCC1</chem>	12918323	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1653	<chem>CCOC(N(CCc(cc1OC)c2c(c3c4)c1OC)c2cc3cc(OC)c4OC)=O</chem>	143241	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1654	<chem>C1C[C@@H](C)2CCNC[C@H]1N2c1c2CNCc2nc(c2ccnc2)n1</chem>	14601902	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1655	<chem>CCNC([C@@H]1C[C@@H](CN1C(CN1CCCCC1)=O)N)=O</chem>	15077405	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1656	<chem>Cc1cc(CNc2nccc(n2)N2C(CC(C2)O)c2c(c1)c(C)c(C)[nH]2</chem>	15700744	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1657	<chem>Cc1c(C(C(NCCNc2ccccc2)=O)N)c(C)[nH]n1</chem>	16899791	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1658	<chem>CC1=CC(=O)Oc2cc(CN3CCC(CC3)N3CCC(CC3)O)ccc12</chem>	18402936	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1659	<chem>CN1CCC2(CC1)CCN(C2)C(C1CNC1)=O</chem>	18597939	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1660	<chem>C(CN)c1ccc(CN2CCC(CC2)(c2ccccc2)C(F)(F)F)O)cc1</chem>	18809502	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1661	<chem>CC(Cc1cc(C)n[nH]1)NCc1ccc(c(c1)OC)OCCN1CCCC1</chem>	19048916	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1662	<chem>CC(C)N[C@@H]1CC[C@@H]1NC(CCc1ccc(c2ccc(cc2)[Cl])[nH]1)=O</chem>	19264424	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1663	<chem>Cc1ccc(cc1)SCCN(C)C([C@H](CCCCN)N)=O</chem>	19395269	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1664	<chem>Cc1ccc(cc1[C1])N1CCC(C1)N[C@@H]1CC[C@H](C1)N</chem>	19498560	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1665	<chem>Cc1cc(C)c2c(c1)c(cc(C)n2)C(N[C@H]1CNC[C@@H]1OC)=O</chem>	19537511	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1666	<chem>C1CN(CCNC([C@@H]2C[C@H](CNC2)C(N2CCOCC2)=O)=O)c2ccccc12</chem>	19807864	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1667	<chem>Cc1cc(NC)nc(n1)N1CCN(CC(C1)O)CC(NC)=O</chem>	20331307	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1668	<chem>C1CNCc2c1c(NCC1COc3ccccc3O1)nc(c1ccccc1)n2</chem>	20674759	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1669	<chem>Cc1c(CN2CCC3(CC2)[C@H](C[C@H]3O)OCCN)nc2ccccc2n1</chem>	21179623	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1670	<chem>C1CN(CC1n1ccnc1)c1c2C</chem>	21581365	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1



Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	CNCCc2nc(c2cccn2)n1					
1671	CCOC(CSc([nH]1)nc(nc2C1)c1nc2C1)=O	217913	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1672	Cc1ccc(c2cc(C(N3CCc4c(C3)sc(N)n4)=O)[nH]n2)s1	21799165	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1673	Cn1cnc1c1cccc2CC(CN)Oe12	21885438	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1674	C1CCN(CC1)C(CNC(CCc1cc2CNCCn2n1)=O)c1cccn1	21900063	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1675	C1CC2(CCNC2)CCN(C1)Cc1cnc2cccc12	22793936	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1676	C1CN(CC(CN1Cc1cccc2c[nH]c12)O)c1cnc1	22927120	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1677	CC(C)(C)c1cc(C=C(C#N)C#N)cc(C(C)(C)C)c1O	242557	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1678	CCC[C@H]1CN(Cc2ccc(CCN)cc2)C[C@H]1NC(C)=O	26972514	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1679	c1cc(c2cccc(c2c1)[Br])c1nc2ccc(ccc2o1)N	2810-4224	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1680	Cc1ccc(C)c(c1)NCc1cc(cc1OC)[Br]	2910-2364	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1681	O=C(N(CC1OC1)C(N1CC2OC2)=O)N(CC2OC2)C1=O	296934	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1682	CCOC(C/C1=CSC2=NNC(C)(C)N12)=N/O)=O	299968	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1683	Cc1nc(CCN)cc(n1)N1CCN(CC1)c1ccc(C#N)cn1	31455775	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1684	C(CNCc1ccc2c(c1)OCO2)c1ccc(cc1)F	3169-1371	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1685	C1CN(CC1CN)Cc1ccc(c2cccc2C#N)o1	31727519	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1686	C1CCCN(CCC1)CC(N1C[C@H](c2cccc2)[C@H](C1)N)=O	31891223	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1687	O=C(c(c(F)ccc1c1F)Nc1nnc(C(F)(F)F)s1	319424	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1688	COc1ccc(CN2CC[C@@H]3[C@@H](CCC(N3CCN)=O)C2)cc1CC=C	32030907	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1689	C1CN(CCN(C1)c1cccc(N)n1)Cc1cccc1F	32148102	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1690	Sc1ncn1-c(c(Cl)ccc1)c1Cl	321506	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1691	COc1ccc(cc1OC)c1nc2cc(ccc2o1)N	3370-0370	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1692	CCOc1cc(CNCCc2cccc2)ccc1OC	3381-1215	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1693	Cc1cccc(c1)Nc1nc(CN2C[C@@H]3CC[C@H](C2)N(C)C3=O)nc(N)n1	35485871	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1694	Cc1cc2c(ncnc2s1)N1CCC(CC1)NCCNc1cccn1	35687952	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1695	Cc1ccc(CNCc2ccc(c(c2)OC)cc1	3701-0037	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
1696	<chem>COc1cc(CNCc2ccc(cc2)F)cc(c1OC)OC</chem>	3702-0961	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1697	<chem>COc1ccc(CNCc2ccc(cc2)F)cc1</chem>	3702-0995	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1698	<chem>CCc1c(cc(c2c3CCCCc3nc(c2C#N)N)s1)[Br]</chem>	3830-0879	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1699	<chem>CC(C1COc2ccccc2O1)NCc1ccccc1</chem>	3875-0321	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1700	<chem>Cn1c(CCNc2c3CCNCCc3nc(c3ccccc3)n2)nen1</chem>	39769570	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1701	<chem>Cc1ccc(cc1)S(N(CC(CN1CCCC1)O)c1ccccc1OC)(=O)=O</chem>	4013-2178	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1702	<chem>C[As](c1cc(C(O)=O)ccc1)(O)=O</chem>	402843	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1703	<chem>Cc1c(c2csc(Nc3ccc(cc3)[Cl]))n2ccccc2n1</chem>	4112-3380	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1704	<chem>Cc1c(C(OC)=O)nc(-c(nc2C(C(N)=C3OC)=O)c cc2C3=O)c(N)c1-c(ccc(OC)c1OC)c1O</chem>	45384	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1705	<chem>CSC(NC(Cl)=C1)=NC1=O</chem>	45719	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1706	<chem>Cc1ccsc1CN(CCN(C)C)C(CN)=O</chem>	47645371	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1707	<chem>Cc1cnc(N)nc1NCC[C@@H]1C[C@H]2C[C@H]1C=C2</chem>	47913504	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1708	<chem>C(CNCc1ccc2ccccc2c1)c1c[nH]e2ccccc12</chem>	4964-5069	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1709	<chem>CCOc1cc(CNCCc2ccccc2)[Cl]ccc1OC</chem>	4964-5102	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1710	<chem>CCN(CC)CC(COc1ccc2c(C(=O)OCC)c(NC(C)=O)sc12)[Br])O</chem>	5130027	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1711	<chem>c1ccc2C(N=C(c2c1)N)=NN</chem>	5140994	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1712	<chem>C(C(CN=Cc1ccccc1O)O)N=Cc1ccccc1O</chem>	5172847	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1713	<chem>CCOC(c1ene2ccccc2e1Nc1ccc(cc1)N1CCOCC1)=O</chem>	5174-4348	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1714	<chem>C1CCN(CC1)Cc1c(CN2CCCC2)n(c2c(N)non2)nn1</chem>	5175780	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1715	<chem>C1C2CC3CC1CC(C2)(C3)N1CCNCC1</chem>	5236741	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1716	<chem>COc1ccc(cc1)OCC(CN1CCN(CC1)c1ccccc1O).[Cl].[Cl]</chem>	5257916	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1717	<chem>CCCCCOC(C1CN1C(C)(C)CO)=O</chem>	5259604	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1718	<chem>C1CN(CCC1O)Cc1ccccc1[N+](=[O-])=O</chem>	5269563	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1719	<chem>Cc1ccc2c(c1)c1CCCC3c1n2CCCN3</chem>	5271325	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1720	<chem>C1CC(N(CNe2ccc(c(c2)[Cl]))[Cl])C1=O)=O</chem>	5271658	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1721	<chem>c1cc(c(cc1[Cl]))[Cl]c1nnc(N)s1</chem>	5313490	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1722	<chem>Cc1ccc(cc1)c1csc(N)n1</chem>	5341867	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1723	<chem>Cc1cc(ccc1NCC(NN)=O)</chem>	5347228	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	[Cl]					
1724	CCCCNc1c2c(c3c4CCCCc4c(nc3s2)N2CCOCC2)nnn1	5504-0161	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1725	C(c1cnn(c2ccc3ccccc3c2)c1N)#N	5628157	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1726	C1CCC(C1)NCC(COe1ccc(cc1)OCC(CNC1CCCC1)O)O	5648415	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1727	C(C(Cn1c2ccccc2nn1)O)n1c2ccc(cc2c2cc(ccc12)[Cl])[Cl]	5654532	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1728	CCOC(c1cnc2c(C)c(ccc2c1NCCN(C)C)[Cl])=O	5695-1044	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1729	COC(CCCCC1C(C(CS1)N)N)=O.[Br].[Br]	5728434	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1730	Cc1cc(ccc1OCCNCCCCOC)[Cl].C(C(O)=O)(O)=O	5734342	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1731	CC1=Ne2ccccc2C(N1CCNc1cccc2ccccc12)=O	5789137	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1732	C(CNC(c1cn(CCN)nn1)=O)c1csc(c2ccnc2)n1	58419779	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1733	CCCCCn1c(NC(N)=NC2=S)c2nc1	58907	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1734	CC(C)CCn1c(CNC(C2CC3(CCNCC3)CN2)=O)nc2ccnc12	59041258	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1735	c1cc(ccc1c1cn2ccsc2n1)N	5968142	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1736	Cc1ccc2c(c1)c1CCCC3c1n2CCN3CC(CN1CCCCC1)O	5989-2455	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1737	CC(C)CN1CCC(CC1)NCNc1cnc1C	60244866	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1738	CCOC(C1=CNC(SCC)=NC1=O)=O	60266	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1739	O=C(c(c1)cc(Cl)c1C(Nc(cc1)ccc1C1=NCCN1)=O)Nc(cc1)ccc1C1=NCCN1	60339	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1740	CCN1CCN(CC1)CC(COe1ccc(CC=C)cc1OC)O.[Cl].[Cl]	6043920	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1741	Cc1ccc(c(C)c1)OCC(CN1CCN(CC1)CCN1C(c2ccccc2ccc(C1=O)c23)=O)O.[Cl].[Cl]	6044718	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1742	COe1cc(CC=C)ccc1OCC(CN1CCC(CC1)Cc1ccccc1)O.[Cl]	6046571	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1743	CCCOc1ccc(cc1)c1cnc(nc1N)S	6431640	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1744	C(c1ccc1)NC1C(c2ccccc2ccc1c23)NS(c1ccc(cc1)[Cl])(=O)=O	6432111	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1745	CCOC(C(C(c(ccc1)c1N1)C1=O)=O)=O	646976	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1746	C1CNCCC1C(N1CCN(CC1)c1ccccc1F)=O.C(C(O)=O)(O)=O	6579417	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1747	Cc1ccc(cc1)OCCN1CCN(CC1)CC(Cn1c2ccccc2c2ccc12)O.C(C(O)=O)(O)=O	6612808	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
1748	<chem>Cc1nc2ccccc2n1CC(COc1ccc(cc1)C1CCC=C1)O</chem>	6682831	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1749	<chem>O=C(c(cc1)cc(C(Nc(cc2)ccc2C2=NCCN2)=O)c1Cl)Nc(cc1)ccc1C1=NCCN1</chem>	67436	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1750	<chem>CCC1CCCCN1S(c1ccc(cc1)NC1c2ccccc2S(N=1)(=O)=O)(=O)=O</chem>	7380-0010	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1751	<chem>Cc1ccc(cc1)c1cnc(NCc2ccc(cc2)[Cl])n1C</chem>	7756-0705	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1752	<chem>Cc1ccc(cc1C)c1cnc(NCc2ccc(cc2)F)n1C</chem>	7756-0829	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1753	<chem>Cc1c(CCC2OCCO2)c(Cl)n c(N)n1</chem>	77596	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1754	<chem>CC(C)OC(C1C(C2=C(CC(C)CC2=O)OC=1N)c1ccc(cc1)[Cl])=O</chem>	8003-3608	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1755	<chem>C(c1ccccc1)Nc1nc(nc(n1)[Cl])N1CCOCC1</chem>	8006-8438	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1756	<chem>Cc1ccc(cc1)C1C(C#N)=C(N)Oe2ccc3ccccc3c12</chem>	8008-9298	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1757	<chem>C1CCC(CC1)NC(c1c2CC Cc2sc1N)=O</chem>	8009-1776	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1758	<chem>[H]Nc1nnc(COe2ccc(cc2)C2CCCC2)s1</chem>	8009-2831	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1759	<chem>C1CNC(CN)c2ccccc12</chem>	8009-3719	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1760	<chem>C1CCN(CC1)c1ccc2C(N(CCO)C(c3ccccc3)=O)=O</chem>	8010-2208	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1761	<chem>CN1C(c2c(nc(N3CCCC3)n2CCN)N(C)C1=O)=O</chem>	8012-0524	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1762	<chem>CC1=CC(N(C)C(N1CCCCCNC(=O)=O)=O</chem>	8012-3983	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1763	<chem>Cc1c(CCNc2c(cc(cc2OC)OC)OC)c2cc(ccc2[nH]1)OC</chem>	8013-0022	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1764	<chem>CC(Cc1ccc2c(c1)OCO2)CNCCc1c2cc(ccc2[nH]c1C)OC</chem>	8013-0190	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1765	<chem>CCCCc1nc(CNCCc2c3cc(ccc3[nH]c2C)OC)c[nH]1</chem>	8013-0624	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1766	<chem>C(CNCc1ccc2c(c1)c1ccccc1[nH]2)NCCO</chem>	8013-0978	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1767	<chem>Cc1c(CCNc2ccc(C#N)cc2)c2cc(ccc2[nH]1)OC</chem>	8013-2954	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1768	<chem>CN(C)CCCNc1ccc2c(c1)c1CCCCc1[nH]2</chem>	8013-3043	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1769	<chem>CC(C)C1(CCNc2ccc(cc2)OC)CCOC(C)(C)C1</chem>	8018-1266	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1770	<chem>CC(C)C1(CCNc2ccccc3c2OCO3)CCOC(C)(C)C1</chem>	8018-1268	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1771	<chem>C(C(c1nc2ccccc2[nH]1)N)c1ccc(cc1)O</chem>	8018-4464	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1772	<chem>c1cc(c2nnc3n2nc(Nc2ccc(cc2)[Cl])s3)sc1</chem>	8018-8096	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1773	<chem>C(CS(N1CCNCC1)(=O)=O)N</chem>	8018-8721	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1774	<chem>Cc1c(c(N)n(CCN2CCOCC</chem>	8019-0360	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	2)c1C)S(c1ccc(cc1)F)(=O)=O					
1775	CN1CCC(CC1)Oc1ccc(cc1)N	8019-4291	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCCGGUGUGGGGAA	1
1776	CCNC[C@@H]1CCN(CC)[C@H]1c1ccccc1OC	8019-4504	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCCGGUGUGGGGAA	1
1777	CC(Cc1cc2c(c(c1OC)OC)OCO2)N	8019-6342	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCCGGUGUGGGGAA	1
1778	C1CCN(CC1)c1nc(CN2C(N(c3ccccc3[Cl])N=N2)=O)nc(N)n1	8019-8781	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCCGGUGUGGGGAA	1
1779	C1CN(CCC1N)Cc1ccccc1O	8020-1707	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCCGGUGUGGGGAA	1
1780	C(COc1ccccc1)NCc1ccccc1	8020-2902	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCCGGUGUGGGGAA	1
1781	CCNCc1cc(CC=C)c(c(c1)OC)OCC	8020-2907	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCCGGUGUGGGGAA	1
1782	COc(cc1)cc(N2)c1NP2(Oc1ccccc1)=S	88402	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCCGGUGUGGGGAA	1
1783	COc1ccc(ccc1OCCCN1CCCCC1)N.[Cl].[Cl]	9122829	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCCGGUGUGGGGAA	1
1784	C1CC2=C(C(c3ccccc3)c3c(N)nc(N)nc3N2)C(C1)=O	9129209	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCCGGUGUGGGGAA	1
1785	CCN1CCCC1CNCc1ccc(C)s1.[Cl].[Cl]	9131777	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCCGGUGUGGGGAA	1
1786	C(c1ccccc1)Nc1ccccc1)c1nc2ccccc2[nH]1	9142557	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCCGGUGUGGGGAA	1
1787	Cc1ccc(cc1N)c1ccc(nn1)[Cl]	9221590	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCCGGUGUGGGGAA	1
1788	Cc1ccc2c(c1)c(C)nc(NC1NCN(CCO)CN=1)n2	9243143	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCCGGUGUGGGGAA	1
1789	Cc1cc(c2cc(ccc2n1)C(O)=O)N	9243351	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCCGGUGUGGGGAA	1
1790	CSc1ccc(cc1)OCCN	9254473	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCCGGUGUGGGGAA	1
1791	CCN1CCCC1CNCc1ccccc1)OCc1ccc(cc1)[Cl]	9312203	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCCGGUGUGGGGAA	1
1792	Cc1ccc(c(C)c1)NC(Cn1c(c(C(=O)OC)nn1)N)=O	C200-1530	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCCGGUGUGGGGAA	1
1793	CCc1nc2nc(C)cc(Nc3cc(cc3C)[Cl])n2n1	C301-3944	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCCGGUGUGGGGAA	1
1794	CCc1nc2nc(C)cc(Nc3ccccc3C)n2n1	C301-4042	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCCGGUGUGGGGAA	1
1795	Cc1ccc(cc1C)Nc1nc2ccccc2c2nnen12	C301-5182	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCCGGUGUGGGGAA	1
1796	CCN(CC)CCCNCc1ccccc2nc(c2nnc(c3ccc(C)cc3)o2)n1	C660-1575	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCCGGUGUGGGGAA	1
1797	CC(C)c1ccc(cc1)S(c1c2nc(c3ccccc3n2nn1)N)(=O)=O	C718-0270	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCCGGUGUGGGGAA	1
1798	Cc1ccccc1NC(CNS(c1ccc(cc1)[Cl])(=O)=O)c1ccccc1	D030-0069	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCCGGUGUGGGGAA	1
1799	C(CNc1nc(es1)c1c[nH]c2ccccc12)c1ccccc1	D041-0019	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCCGGUGUGGGGAA	1
1800	COC(CCc1c(c2ccc(cc2)O)C)nc(Nc2ccccc2s1)=O	D041-0023	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCCGGUGUGGGGAA	1
1801	Cc1ccccc1CNCc2nc3nc(C)cc(C)n3n2)c1	D043-0228	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCCGGUGUGGGGAA	1
1802	CCCN1C(C2(C3=C(C(N2	D063-1103	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCCGGUGUGGGGAA	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	<chem>CCO)=O)Oc2ccc(C)cc2C3=O)c2ccccc12)=O</chem>					
1803	<chem>Cc1cc2C(C3=C(C(N(CCO)C34C(N(C)c3ccccc34)=O)=O)Oc2cc1C)=O</chem>	D063-1142	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1804	<chem>[H]c1ccc(cc1)S(c1c(NCCC N(C)C)oc(c2ccccc2)n1)(=O)=O</chem>	D072-0521	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1805	<chem>CCC(c1nc2ccccc2n1CCC Oc1ccccc1C)O</chem>	D186-0091	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1806	<chem>Cc1ccc(c(c1)NC1c2ccccc2 S(N=1)(=O)=O)OC</chem>	D257-0773	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1807	<chem>Cc1ccccc1c1nc(c2ccnc2N C2CCCC2)on1</chem>	D349-3758	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1808	<chem>COc1ccc(cc1)c1nc(c2cccn c2NC2CCCC2)on1</chem>	D349-4050	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1809	<chem>CC1(C)CC(CCNCCCN(C)C)(CCO1)c1ccc(c1)C(F)(F)F</chem>	D442-0364	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1810	<chem>CC1(C)CC(CCNc2ccccc2)(CCO1)c1ccc(c1)C(F)(F)F</chem>	D442-0374	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1811	<chem>CN(C)c1ccc(cc1)c1c(Nc2ccc(cc2)[Br])n2ccncc2n1</chem>	D600-0307	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1812	<chem>CCOC(c1nc2c(c3ccc(cc3)[Br])c(C)nn2c1N)=O</chem>	D718-0691	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1813	<chem>COc1ccc2c(CNCCc3ccccc3)c(C(O)=O)n(Cc3ccccc3F)c2c1</chem>	E518-0633	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1814	<chem>Cc1cc(C)n(c2c(NCc3ccccc3)nc3ccc(cc3n2)[Cl])n1</chem>	E701-0030	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1815	<chem>C1C2CC3CC1CC(C2)(C3)N</chem>	NCGC00015036-08	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1816	<chem>C(C(c1ccc(cc1)[Cl])[Cl])OCc1ccc(cc1)[Cl])n1ccnc1</chem>	NCGC00018258-09	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1817	<chem>CCOC([C@H](CCc1ccccc1)N[C@@H](C)C(N1CCC[C@@H]1C(O)=O)=O)=O</chem>	NCGC00021569-08	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1818	<chem>CS(=O)(=O)OCCCCOS(C)(=O)=O</chem>	NCGC00090905-11	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1819	<chem>CCC(C)CCCC(N[C@@H](CCN)C(NC(C(N[C@H](CCN)C(N[C@@H]1CCNC(C([C@@H](C)O)NC([C@@H](CCN)NC([C@@H](CCN)NC([C@@H](CC(C)C)NC([C@H](Cc2ccccc2)NC([C@H](CCN)NC1=O)=O)=O)=O)=O)=O)=O)=O)[C@@H](C)O)=O</chem>	NCGC00094763-03	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1820	<chem>C1CN1P(N1CC1)(N1CC1)=S</chem>	NCGC00095042-08	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1821	<chem>CCOC(N1CCN(CC1)[N+](=NOc1ccc(cc1)[N+](O-)=O)[N+](O-)=O)[O-]=O</chem>	NCGC00165815-05	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1
1822	<chem>CCN(CC)CCN1C(C(Cc2c</chem>	NCGC0018604	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCGGUGUGGGGAA	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	<chem>cc(cc2OC)=Nc2cccc12)=O</chem>	6-02				
1823	<chem>C1CCN[C@@H](C1)[C@H](c1cccc1)NC(c1cccc(c1[C@H])C(F)(F)F)=O</chem>	NCGC0024795 4-02	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCCGUGUGGGGAA	1
1824	<chem>CC1C=C(C2=NC(=CC(N2C=1)=O)N1CCOCC1)[C@@H](C)Nc1cccc1C(O)=O</chem>	NCGC0026315 4-01	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCCGUGUGGGGAA	1
1825	<chem>[H][C@@]12CC([C@H]([C@@](C)(n3c4cccc4c4c5C(NC(c5c5c6cccc6n1c5c34)=O)=O)O2)OC)N(C)C(c1cccc1)=O</chem>	NCGC0034508 3-01	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCCGUGUGGGGAA	1
1826	<chem>Cn1cc(cn1)c1cnn2c(c(c([C@H]3CCCNC3)nc12)[Br])N</chem>	NCGC0034665 3-01	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCCGUGUGGGGAA	1
1827	<chem>CC(C)S(c1cccc1Nc1c(c(N)nc(Nc2ccc(cc2OC)N2C(C(C2)C(N)=O)n1)[Cl])(=O)=O</chem>	NCGC0034695 7-01	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCCGUGUGGGGAA	1
1828	<chem>C(C(=C1NC(c2ccc(cc2N1)[Cl])=O)C(c1ccc(cc1[Cl])[Cl])=O)#N</chem>	NCGC0034794 2-01	Zika3PrimeUTR	G-quadruplex	GCGGCGGCCCGUGUGGGGAA	1