

“Riboswitch” 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>Cc1onc(-c2ccccc2Cl)c1C(=O)NCc1cc2n(n1)CC[NH2+]C2</chem>	Neg_lig_68	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
2	<chem>OCCn1nc(CC2CC2)nc1-c1ccccc1-n1cccn1</chem>	Neg_lig_117	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
3	<chem>CN1CCC(n2[nH]c(-c3ccccc3)c(Cc3ccc3)c2=O)CC1</chem>	Neg_lig_123	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
4	<chem>C[C@H]1CN(C[C@H](O)COc2ccc(Cl)cc2)[C@H](C)O1</chem>	Neg_lig_128	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
5	<chem>c1cncc(NCC[NH2+][C@H]2CCSC2)c1</chem>	Neg_lig_169	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
6	<chem>Cc1ccc(C(=O)/N=C2\SC3=C(CC[C@H](C(C)(C)C)C3)\C2=C(/O)NCCO)cc1</chem>	Neg_lig_178	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
7	<chem>Cc1cc(C)cc(NC(=O)c2nnn(CC(=O)Nc3c(C)cc(C)cc3Cc2N)c1</chem>	Neg_lig_185	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
8	<chem>Cn1ncc2c(=O)[nH]c(CN3CCNC[C@H](C(=O)O)C3)nc21</chem>	Neg_lig_187	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
9	<chem>COc1cc(-c2nc3ncccn3c2Nc2cc(C)ccc2C)ccc1O</chem>	Neg_lig_223	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
10	<chem>CN(C)c1ccc(-c2nc3ncccn3c2Nc2ccccc2)cc1</chem>	Neg_lig_239	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
11	<chem>O=C(CCc1cc2n(n1)CCC[NH2+]C2)N1CCCN(c2cc[nH+]cc2)CC1</chem>	Neg_lig_269	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
12	<chem>Nc1nonc1C(=O)N1CCN(C(=O)Nc2ccc(C(F)(F)F)c2)CC1</chem>	Neg_lig_274	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
13	<chem>COCC[C@]1(C(=O)[O-])CCCN(C(=O)c2ccc3c2NCCC3)C1</chem>	Neg_lig_320	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
14	<chem>Cn1c(=O)c2c(ncn2CCOC(=O)C(C)(C)Oc2ccc(Cl)cc2)n(C)c1=O</chem>	Neg_lig_411	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
15	<chem>CCOc1ccc(S(=O)(=O)c2ccc(C)cc2)c2c1no[n+]2[O-]</chem>	Neg_lig_418	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
16	<chem>COc1ccc(-c2nc3nc(C)cc(Nc4cc(Cl)ccc4OC)n3n</chem>	Neg_lig_430	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	2)cc1					
17	<chem>C[NH+] (C)CCOc1ccc(-c2nc(=C3C=CNC=C3)/c(=c3/ccc4c(c3)CCC=4N=O)[nH]2)cc1</chem>	Neg_lig_461	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
18	<chem>Cc1cccc(N2C(N)=C(C#N)[C@@H](c3ccsc3)C3=C2C(C)(C)CC3=O)c1</chem>	Neg_lig_498	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
19	<chem>O=C([O-])c1ccc(OCc2ccccc2)cc1</chem>	Neg_lig_499	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
20	<chem>CCCC(C)(C)[C@H](O)/C=C\[C@@H]1[C@H](C/C=C/CCCC(=O)[O-])C(=O)C[C@H]1O</chem>	Neg_lig_508	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
21	<chem>COCc1nn2c(N)c(C#N)nn2c1-c1ccc(OC)cc1</chem>	Neg_lig_511	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
22	<chem>CSc1ccc(CCNe2ncnc3c2nc2n3CCC2)cc1</chem>	Neg_lig_514	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
23	<chem>O=C(NCc1ccc1)N1CC[C@@H](c2ccc3ccc3c2)[C@H](O)C1</chem>	Neg_lig_587	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
24	<chem>CCn1nc(CO)c2c1CCN(C(=O)c1enc(-c3ccc[nH+](c3)nc1)C2</chem>	Neg_lig_612	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
25	<chem>COc1ccc2c(c1)[C@]13CC[N@@H+](C)[C@H](C2)[C@@H]1CCCC1(C3)OCCO1</chem>	Neg_lig_618	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
26	<chem>C=CCOc1ccc([C@@H]2C(C#N)=C(N)Oc3cc4c(cc32)OCO4)cc1OC</chem>	Neg_lig_629	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
27	<chem>Cc1nc(CC(=O)N2CC[C@H](Cc3ccc(CO)cc3)C2)cs1</chem>	Neg_lig_646	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
28	<chem>CC(C)[C@H]1CC[C@@H](C)[C@@H]1O[C@@H](O)[C@H]1CCCCC1</chem>	Neg_lig_648	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
29	<chem>C[NH+]1CCN(CCNCn2nc(CO)nc3ccc23)CC1</chem>	Neg_lig_649	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
30	<chem>Nc1c(Br)cc(Br)cc1Br</chem>	Neg_lig_664	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
31	<chem>CCOC(=O)c1nc2ccc(C(=O)OC)cc2c1NCc1ccnc1</chem>	Neg_lig_679	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
32	<chem>O=C(c1ccc(C[NH+]2CCCCC2)cc1)N1CCN[C@H](c2ccccc2)C1</chem>	Neg_lig_685	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
33	<chem>C[N@H+]1C[C@H]2C[NH2+]C[C@@@]2(C(=O)NCCS(=O)(=O)c2ccc(F)cc2)C1</chem>	Neg_lig_713	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
34	<chem>CCCc1cc(Nc2cccc(C(=O)N3CCCCC3)c2)n2nc(-c3ccnc3)n2n1</chem>	Neg_lig_874	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
35	<chem>O=C(c1nn(-c2ccccc2)c(=O)cc1[O-])N1CCOC[C@@H](CO)C1</chem>	Neg_lig_806	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
36	<chem>Nc1ccc2ncc(C(=O)[O-])c(O)c2c1</chem>	Neg_lig_877	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
37	<chem>COc1cc(N[C@@H]2c3ccccc3C(=O)N2c2ccnc2)cc(O)C1OC</chem>	Neg_lig_896	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
38	<chem>O=c1[n-]cc(F)c(=O)[nH]1</chem>	Neg_lig_941	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
39	<chem>Nc1ncnc2ccccc12</chem>	Neg_lig_985	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
40	<chem>Cc1cc(NCc2ccccc2)nc(N2CCOCC2)[nH+]1</chem>	Neg_lig_1012	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
41	<chem>COCc1cc(C)nc2sc(-c3cccn3)c(N)c12</chem>	Neg_lig_1116	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
42	<chem>CC(=O)c1sc(Nc2ccc(C)cc2)nc1C</chem>	Neg_lig_1127	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
43	<chem>OCC1(O)CCN(Cc2noc(-c3ccccc3)n2)CC1</chem>	Neg_lig_1129	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
44	<chem>Cc1cccc(CCNC2cc(C)nc3nc(C)nn23)c1</chem>	Neg_lig_1159	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
45	<chem>Cc1cc(C)cc(Nc2cc(C)nc3nnn23)c1</chem>	Neg_lig_1197	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
46	<chem>CCCCNc1nc(Oc2cc(OCC)nn2)nc(N2CCOCC2)n1</chem>	Neg_lig_1219	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
47	<chem>CCC(=O)N1CCN(c2cc(Nc3ccc(C)cc3)nc(C)[nH+]2)CC1</chem>	Neg_lig_1221	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
48	<chem>Cc1ncn1C[C@H]1CCc2c(c3ccccc3n2)C1=O</chem>	Neg_lig_1223	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
49	<chem>CCOC(=O)C1=C(C)N(CCO)C(=O)N[C@H]1c1ccc(OCC)cc1</chem>	Neg_lig_1310	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
50	<chem>COc1ccc(Cl)cc1Nc1cc(C)nc2nc(-</chem>	Neg_lig_1341	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	c3cccc3)nn12				CUGAAGCAACGCGCCUC	
51	CCCNc1cc(C)nc2nc(-c3cccc(C)c3)nn12	Neg_lig_1448	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
52	CCOC(=O)c1cnc(NCc2ccccc2F)nc1C	Neg_lig_1453	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
53	O=C(Nc1ccc2[nH]nc(-c3ccccc3)c2c1)[C@@H]1CCN(C(=O)N2CCN(c3ccc(-c4ncccc4)cc3)CC2)C1	Neg_lig_1462	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
54	COC(=O)C1=C(C)OC(N)=C(C#N)[C@H]1c1ccsc1	Neg_lig_1496	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
55	Cc1ccsc1CNc1ccc(C(=O)N(C)CCN2CCCC2=O)cc1	Neg_lig_1506	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
56	CC(C)OC(=O)C1=C(N)Oc2c(oc(CO)cc2=O)[C@H]1c1cccc(F)c1	Neg_lig_1508	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
57	COCc1ccc(C(=O)N2CCC3(CC2)[C@@H](OCC[NH3+])C[C@H]3O)s1	Neg_lig_1175	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
58	Cc1ccc([C@@H]2C=C(c3ccc(F)cc3)N=C3NC(CCO)=[NH+]N32)cc1	Neg_lig_1570	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
59	COc1ccc(-c2cc(-c3sc4nc(C)c(Cl)c(C)c4c3N)on2)cc1	Neg_lig_979	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
60	O[C@@H](CN1CCN(c2ccc(Cl)cc2)CC1)c1ccc2cc[nH]c2c1	Neg_lig_1688	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
61	O=C(N[C@@H]1CCN(Cc2ccc3cccc(F)c3n2)C[C@H]1O)c1ccncc1	Neg_lig_1719	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
62	COC(=O)c1cccc(Nc2nccc3ccc(Br)cc23)c1	Neg_lig_1732	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
63	N/C(O)=C1\N=CN([C@@H]2O[C@H](CO)[C@@H](O)[C@H]2O)C1=O	Neg_lig_1758	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
64	Cc1cccc(OC[C@@H](O)CNC(=O)c2ccc(cc2C(=O)[O-])c1	Neg_lig_1760	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
65	O=C(N=c1/cn[nH]s1)c1cccc(C[N@H+]2[C@H]3CC[C@@H]2C[C@H](O)C3)c1	Neg_lig_1772	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
66	NC1(C(=O)O)CCOCC1	Neg_lig_1809	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
					CUGAAGCAACGCGCCUC	
67	<chem>CCOc1ccc(NC(=O)c2sc3nc4c(cc3c2N)CCCC4)cc1</chem>	Neg_lig_1821	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
68	<chem>C=C1CC[C@@H]2[C@](C)(CO)[C@@H](O)CC[C@]2(C)[C@H]1C/C=C1/C(=O)OC[C@H]1O</chem>	Neg_lig_1851	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
69	<chem>CCOC(=O)c1snc(-c2ccc(Cl)cc2)c1N</chem>	Neg_lig_1860	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
70	<chem>O=C(O)c1c(CNCc2ccco2)c2ccccc2n1Cc1ccccc1</chem>	Neg_lig_1901	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
71	<chem>COc1cc(O)cc/c(=N/C(=O)CCl)c1</chem>	Neg_lig_1939	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
72	<chem>CCCCCNc1cc(C(C)C)nc2nc(-c3ccccc3)nn12</chem>	Neg_lig_982	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
73	<chem>CCN(CC)c1ccc(C[NH2+])CCNC(=O)c2nonc2N)cc1</chem>	Neg_lig_1970	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
74	<chem>Cn1c(=[NH2+])n(C[C@H](O)c2ccccc2)c2cccc21</chem>	Neg_lig_1972	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
75	<chem>Cn1c(=O)n(C)c2cc(C[NH2+])CCc3cc(F)cc3)ccc21</chem>	Neg_lig_1979	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
76	<chem>Nc1ccc2oc(Cc3ccc(Cl)cc3)nc2c1</chem>	Neg_lig_1997	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
77	<chem>COc1ccccc1N1C[C@@H](c2nc3ccccc3n2C[C@@H](O)COc2ccccc2Cl)CC1=O</chem>	Neg_lig_722	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
78	<chem>COc1cc([C@@H]2CC(=O)Nc3c2ccc2ccccc32)ccc1OC=O</chem>	Neg_lig_2007	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
79	<chem>Cc1ccc(NC(=O)Cn2nnc(C(=O)NCCc3ccccc3)c2N)cc1</chem>	Neg_lig_2041	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
80	<chem>O=S(=O)(c1ccc(Cl)cc1)c1nc(-c2ccccc2)oc1NC[C@H]1CCCCO1</chem>	Neg_lig_2044	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
81	<chem>Cn1cc[nH+]c1CN1CCN(C(=O)[C@H]2C[NH2+]C[C@H](C(=O)N3CCOCC3)C2)CC1</chem>	Neg_lig_2050	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
82	<chem>CC(C)(C)NC(=O)c1ccc(C(=O)NC(C)(C)C)cc1</chem>	Neg_lig_2069	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
83	<chem>Cc1ccc(NC(=O)c2</chem>	Neg_lig_2098	Glutamine_RS	Three-way	UAAUCGUUGGCCCAGUUUAUCU	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	<chem>nnn(Cc3ccc(F)cc3Cl)c2N)cc1C</chem>			junction	GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	
84	<chem>COc1cccc(CNC(=NS(=O)=O)C(c3ccc(C(C)C)cc3)=C2C)c1</chem>	Neg_lig_2105	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
85	<chem>[NH3+][C@H]1CC[C@H](Nc2nc(Nc3ccc(C(=O)N4CCCC4)c(c3)c3ncn(-c4cccc(F)c4)c3n2)CC1</chem>	Neg_lig_2205	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
86	<chem>O=C1[C@@H]2C[C@H](O)CCN2C(=O)C1Cc1cccc2[nH]c1cc12</chem>	Neg_lig_2221	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
87	<chem>N#C/N=C/N1CC=C(c2ccc(Cl)cc2)CC1</chem>	Neg_lig_2225	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
88	<chem>COc1ccc(-c2cccc2)cc1NC(=O)NCC[N@H+][C]CCCC[C@@H]1CO</chem>	Neg_lig_2258	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
89	<chem>CCCc1cc(NCC(C)C)n2ncc(-c3cccc3)c2[nH+]1</chem>	Neg_lig_2262	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
90	<chem>Cc1cc(C)cc(Nc2c(-c3ccc(O)cc3)nc3nccn23)c1</chem>	Neg_lig_2277	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
91	<chem>Nc1cccc(-c2csnn2)c1</chem>	Neg_lig_2339	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
92	<chem>COc1ccc(Cl)cc1Nc1[nH+]c2cccc2n2cnc12</chem>	Neg_lig_2411	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
93	<chem>CCOC[C@H](O)CS(=O)(=O)c1ccccn1</chem>	Neg_lig_2474	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
94	<chem>CC[C@H](O)c1nc2cccc2n1CCCOc1c(C)cccc1C</chem>	Neg_lig_2480	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
95	<chem>COc1ccc2c(CNCc3cccs3)c(C(=O)O)n(Cc3cccc3F)c2c1</chem>	Neg_lig_2495	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
96	<chem>O=C([O-])CCn1c2c(c3cccc31)C[C@H](NS(=O)=O)c1ccc(F)cc1)CC2</chem>	Neg_lig_2506	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
97	<chem>C#CCOc1ccc([C@H]2C(C#N)=C(N)Oc3cc4c(cc32)OCO4)cc1OCC</chem>	Neg_lig_2512	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
98	<chem>Nc1nc(-c2cccc2)c(-c2cccc2)s1</chem>	Neg_lig_2548	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
99	<chem>Nc1nnc(CCN2cnc3sc4c(c3c2=O)CCN</chem>	Neg_lig_872	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	C4)s1				CUGAAGCAACGCGCCUC	
100	COc1c(C)cnc(CN(C)C(=O)c2cn(CC[NH3+])nn2)c1C	Neg_lig_2607	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
101	Nc1nnc(SCC(=O)N2CCc3[nH]cnc3C2)s1	Neg_lig_2618	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
102	COCc1cc(C)cnc2sc(C(=O)OC)c(N)c12	Neg_lig_2622	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
103	CCn1c(N)nc2cc(C(=O)NCc3cnn4ccccnc34)cnc21	Neg_lig_2655	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
104	CCc1[nH+]ccn1C CCNC[C@]1(O)C CC[N@H+]2CCC[C@H]21	Neg_lig_2678	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
105	CCCOc1ccc(Oc2nc(NC(C)(C)C)nc(N(C)C)n2)nn1	Neg_lig_2681	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
106	C=CCn1cc(C[NH2+])[C@@H](C)CCc2ccc2)c(C)n1	Neg_lig_2704	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
107	Cc1cccc(NC(=O)N2CCN(C(=O)c3nnc3N)CC2)c1	Neg_lig_2716	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
108	COc1ccc2c(c1)[C@@]13CCCC[C@H]1[C@@H](C2)[N@H+](C)CC3	Neg_lig_2724	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
109	Cn1cc(C2=C(c3nc(C4CC[NH+](Cc5cccn5)CC4)c4cccc34)C(=O)NC2=O)c2cccc21	Neg_lig_2730	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
110	Cc1nc([C@@H]2CCCN2S(=O)(=O)c2ccc(F)cc2)n(CCO)n1	Neg_lig_2739	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
111	Cc1ccnc1CCn1nc(-c2cccc2)c1-clccc(CO)o1	Neg_lig_2753	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
112	CCNC(=O)[C@@H]1C[C@@H]1([NH3+])CN1Cc1ccn1-clnccn1	Neg_lig_2767	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
113	O=C(CSc1nc2cccc2s1)N1CCN(CCOC)C1	Neg_lig_2780	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
114	CN(C)c1ccc(/C=N/C[C@@H](O)C/N=C/c2ccc(N(C)C)cc2)cc1	Neg_lig_2872	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
115	Cc1cc(C)n2nc(NC c3ccc(C(C)C)cc3)nc2n1	Neg_lig_2879	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
116	O=NC1=C(c2cccc([N+](=O)[O-])c2)Nc2cccc2S1	Neg_lig_2881	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
117	<chem>COc1ccc([C@@H]2C(C#N)=C(N)Oc3n[nH]c(C)c32)c(OC)c1OC</chem>	Neg_lig_2884	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
118	<chem>COc1ccc(-c2noc(-c3ccnc3NCc3cccnc3)n2)cc1</chem>	Neg_lig_2899	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
119	<chem>C=CCN1CC[NH+]1(Cc2cccc(OC[C@@H](O)C[N@H+](C)C3CCCC3)c2)CC1</chem>	Neg_lig_2904	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
120	<chem>O=C(Cn1c(=O)oc2ccccc21)N1CC[C@H](Cc2cccc(CO)c2)C1</chem>	Neg_lig_404	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
121	<chem>Cc1ncc1CN1CC[N@H+](C)[C@]2(CCC(=O)N(CCO)CC2)C1</chem>	Neg_lig_2964	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
122	<chem>CC(=O)c1ccc(OC[C@@H](O)C[N@H+][2CC[C@H](C)C2)cc1</chem>	Neg_lig_3046	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
123	<chem>Cc1ccc(CN(CCCO)C(=O)c2[nH]nc2Cs1</chem>	Neg_lig_3081	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
124	<chem>C[C@]1(O)CCN(C(=O)CNC(=O)c2cc(Cl)ccc2Cl)[C@@H]1O</chem>	Neg_lig_3123	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
125	<chem>CCN1CCN(CCCC(CO)[C@H]2CS(=O)(=O)C[C@H]21</chem>	Neg_lig_3130	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
126	<chem>COc1ccc(-c2csc(C3=C(N)N(C4CCCC4)CC3=O)n2)cc1OC</chem>	Neg_lig_3136	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
127	<chem>COc1ccc([N+](=O)[O-])cc1NC(=O)N(C)Cc1ccco1</chem>	Neg_lig_3184	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
128	<chem>Cc1cccc(Nc2c(-c3ccc4c(c3)OCC(=O)N4)c(=O)c2=O)c1C</chem>	Neg_lig_3195	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
129	<chem>CCSC[C@H](C)[NH2+]CCN(C)S(C)(=O)=O</chem>	Neg_lig_3286	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
130	<chem>CCCCNc1ncccc1-c1nc(-c2ccccc2C)no1</chem>	Neg_lig_3315	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
131	<chem>CCOC(=O)c1ccc2ncc(C(=O)OCC)c(Nc3ccc(C(=O)[O-])cc3)c2c1</chem>	Neg_lig_3336	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
132	<chem>CC[N@H+][1CCc2ccccc2C1</chem>	Neg_lig_3363	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
133	<chem>Cc1nc(C2CCN(C(=O)CCc3csc(N)n3)CC2)cc(=O)[nH]1</chem>	Neg_lig_3364	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
134	<chem>COc1cc(C[NH2+] CCSc2nnnn2C)ccc 1OCC(=O)N1CCc 2ccccc21</chem>	Neg_lig_3368	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	0
135	<chem>COC(C) (C)C[C@H](C) [NH2+][Cc1nnn1 C1CCCCC1</chem>	Neg_lig_29	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA	0
136	<chem>Cc1cccc(OCc2ccc(- c3nc(C#N)c(NCC[NH+] (C)C)o3)o2)c1</chem>	Neg_lig_111	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA	0
137	<chem>O=C(Cn1cccc1)N 1CCc2ncnc(NC[C @H] (O)CO)c2CC1</chem>	Neg_lig_136	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA	0
138	<chem>CCc1c(C)nc2ncnn 2c1Nc1ccc(N2CC N(S(C) (=O)=O)CC2)cc1</chem>	Neg_lig_140	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA	0
139	<chem>Cc1ncccc1Oc1nnc c(N2CC[N@@H+])(C)C[C@H] (O)C2)c1C</chem>	Neg_lig_145	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA	0
140	<chem>COCCCNc1nc2c(c (=O)n(C)c(=O)n2 C)n1Cc1cccc(Cl)c 1</chem>	Neg_lig_160	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA	0
141	<chem>OC[C@H]1CCCC [N@@H+]1Cc1cc c(-c2ccccc2)cc1</chem>	Neg_lig_207	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA	0
142	<chem>CNC(=O)c1nc(N2 CCCCC2)sc1N</chem>	Neg_lig_231	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA	0
143	<chem>Cc1cc2nc(O)c(=O) [nH]c2cc1N</chem>	Neg_lig_250	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA	0
144	<chem>CCOC(=O)C1=C(C)OC(N)=C(C#N) [C@H]1c1ccsc1</chem>	Neg_lig_263	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA	0
145	<chem>Nc1nc(- c2ccc3ccccc3c2)cs 1</chem>	Neg_lig_288	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA	0
146	<chem>CCOC(=O)c1ccc(Nc2c(- c3cc(Br)ccc3O)nc 3cncn23)cc1</chem>	Neg_lig_297	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA	0
147	<chem>c1nccc(- c2nc(NC[C@@H] 3CCCO3)c3c([nH +])2)CNCC3)c1</chem>	Neg_lig_299	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA	0
148	<chem>O=C(NCC(F)F)c1 ccc(S(=O) (=O)N[C@@H]2C [NH2+][C[C@H]2 O)cc1</chem>	Neg_lig_321	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA	0
149	<chem>CN1CCN(C(=O)c 2nc(N3CCCC3)n c2)CC12CC[NH2 +])CC2</chem>	Neg_lig_323	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA	0
150	<chem>O=C(NC1CC1)c1c ccc(-c2ccc3/c(=N\ C(=O)C4CC4) [nH][nH]c3c2)c1</chem>	Neg_lig_341	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA	0
151	<chem>Cc1ccn2c(C(=O)N 3CCC4(CC3)Nc3c</chem>	Neg_lig_364	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	<chem>cccc3NC4=O)nnc2n1</chem>					
152	<chem>O=C([O-])c1cc(=O)[nH]c(=O)[nH]1</chem>	Neg_lig_366	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAACUAA	0
153	<chem>CO[C@H]1C[C@@H]2CC[C@H](C)[C@@](O)(O2)C(=O)C(=O)N2CCCC[C@H]2C(=O)O[C@H]([C@H](C)C[C@H]2CC[C@H](OP(C)(C=O)[C@H](OC)C2)CC(=O)[C@H](C)/C=C/[C@H](O)[C@@H](OC)C(=O)[C@H](C)C[C@H](C)/C=C/C=C/C=C\1C</chem>	Neg_lig_368	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAACUAA	0
154	<chem>Cc1ccc2nc(-c3cccn3)c(Nc3ccc3)n2c1</chem>	Neg_lig_375	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAACUAA	0
155	<chem>CCC[C@](C)(COC(N)=O)COC(=O)NC(C)C</chem>	Neg_lig_403	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAACUAA	0
156	<chem>Cc1cccc1N1CCN(C(=O)c2cn(C3CC[NH2+][CC3]nn2)[C@@H](C)C1</chem>	Neg_lig_423	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAACUAA	0
157	<chem>Clc1ccc(-c2cn3nc(CNc4ccc4)n4c3c2CCCC4)cc1</chem>	Neg_lig_496	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAACUAA	0
158	<chem>CC(C)(C)n1cnc2cc(NCc3cccs3)ccc21</chem>	Neg_lig_502	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAACUAA	0
159	<chem>O=C(NCCc1cccs1)N1CCC2(CC1)[C@@H](O)C[C@H]2O</chem>	Neg_lig_540	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAACUAA	0
160	<chem>CC(C)NC(=O)c1ccc(-c2cccc(N3CC[NH2+][CC3]c2)s1</chem>	Neg_lig_542	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAACUAA	0
161	<chem>CC(C)(C)COc1ccc(-n2cc(C(=O)[O-])cn2)cc1C#N</chem>	Neg_lig_577	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAACUAA	0
162	<chem>COc1cccc1CNc1[nH+]cccc1-c1nc(C)no1</chem>	Neg_lig_614	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAACUAA	0
163	<chem>O=C(CCn1cnn1)N1CCC2(CC1)c1cccc1C[C@@H]2O</chem>	Neg_lig_616	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAACUAA	0
164	<chem>Cc1ccc(Nc2c(-c3ccc(N(C)C)cc3)nc3cncn23)cc1</chem>	Neg_lig_657	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAACUAA	0
165	<chem>Cc1nc(C)c(CC(=O)N2CC[C@H](c3secc3C)[C@H](O)C2)c(=O)[nH]1</chem>	Neg_lig_659	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAACUAA	0
166	<chem>Nc1[nH+]c2n(c1C(=O)c1ccc(Cl)cc1)CCC2</chem>	Neg_lig_661	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAACUAA	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
167	<chem>CCc1oc2ccccc2c1-c1c(-c2ccccc2)ncn1C(CO)CO</chem>	Neg_lig_678	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	0
168	<chem>O=C(Nc1csnn1)c1csnn1</chem>	Neg_lig_698	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	0
169	<chem>CCOC(=O)c1cnc2ccccc2c1Nc1ccc(Cl)cc1</chem>	Neg_lig_767	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	0
170	<chem>Cc1cc(NCc2ccco2)c2nnn2n1</chem>	Neg_lig_771	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	0
171	<chem>CCCCOC(=O)[C@H]1CCC[C@H](C(=O)OCCCC)N1</chem>	Neg_lig_776	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	0
172	<chem>Cc1nc(C2=C(N)N(Cc3ccccc3)CC2=O)sc1C</chem>	Neg_lig_777	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	0
173	<chem>CCc1ccc([C@H]2C(C#N)=C(N)OC3=C2S(=O)(=O)N(Cc2ccccc2F)c2ccccc23)cc1</chem>	Neg_lig_787	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	0
174	<chem>C[C@H]([C@@H](O)c1ccc(O)cc1)n1cnc1-c1cc2ccccc2o1</chem>	Neg_lig_795	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	0
175	<chem>CCOC(=O)Cc1cc(O)nn(-c2ccccc2)c1=O</chem>	Neg_lig_802	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	0
176	<chem>CCc1ccccc(OCCN(C)c2nncnc3c2CC[NH2+][C3])c1</chem>	Neg_lig_815	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	0
177	<chem>O=S1(=O)N=C(Nc2ccccc2Br)c2ccccc21</chem>	Neg_lig_837	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	0
178	<chem>C/C(=N)\NC(=O)c1[nH]nc2c1CCC2)c1ccc(N)cc1</chem>	Neg_lig_849	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	0
179	<chem>C=CCc1c(C)nc(N)nc1N1CCC(CCn2cc[nH+]c2C)CC1</chem>	Neg_lig_858	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	0
180	<chem>CNc1ncccc1CN(CCO)Cc1ccc(SC)cc1</chem>	Neg_lig_924	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	0
181	<chem>CC1(C)O[C@@H]2C[C@H]3[C@@H]4CCC5=CC(=O)C=C[C@]5(C)[C@H]4[C@@H](O)C[C@]3(C)[C@@]2(C(=O)CO)O1</chem>	Neg_lig_975	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	0
182	<chem>Nc1n[nH]c(CCC(=O)N2CCC[C@H]2c2nc(-c3ccccc3)no2)n1</chem>	Neg_lig_1014	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	0
183	<chem>CC(C)(C)c1nnc(N2CC[C@@H](c3ccc4ccccc4c3)[C@H](O)C2)o1</chem>	Neg_lig_1059	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
184	<chem>Nc1nc2c(ccc3cccc2)s1</chem>	Neg_lig_1075	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUAAAAACUAA	0
185	<chem>CCOC(=O)[C@H]1CCCN(c2c(NCC[N@H+]3CCCC[C@H]3CC)c(=O)c2=O)C1</chem>	Neg_lig_1076	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUAAAAACUAA	0
186	<chem>CC(C)(C)[NH2+]Cc1cc(Br)ccc1OCc1cccs1</chem>	Neg_lig_1101	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUAAAAACUAA	0
187	<chem>CN1CC2(CC[NH2+]CC2)C[C@H]1C(=O)NCc1cnm(Cc2cccc2)c1</chem>	Neg_lig_1184	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUAAAAACUAA	0
188	<chem>Cc1cccc(Cn2c(CN)n[nH]c2=O)c1</chem>	Neg_lig_1213	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUAAAAACUAA	0
189	<chem>CC(C)(O)C#Cc1cccc(C(=O)NCc2csc(N)n2)c1</chem>	Neg_lig_1218	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUAAAAACUAA	0
190	<chem>CC(C)CNc1nc(-c2cccc2)nc2cccc12</chem>	Neg_lig_1226	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUAAAAACUAA	0
191	<chem>Cc1ccc(NC(=O)Cn2nnc(C(=O)Nc3ccc(C)c3C)c2N)cc1C</chem>	Neg_lig_1257	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUAAAAACUAA	0
192	<chem>CC(=O)O[C@H]1C[C@@H]2CC[C@@H]3[C@H](CC[C@]4(C)[C@H](OC(C)=O)[C@@H](N+)5(C)CCCC5)[C@H]34[C@@]2(C)C[C@H]1[NH+]1CCCCC1</chem>	Neg_lig_1273	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUAAAAACUAA	0
193	<chem>COCCOC(=O)C1=C(C)[NH+]C2C[C@H](c3cccc3OC)CC(O)=C2[C@H]1c1ccc(O)c1</chem>	Neg_lig_1362	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUAAAAACUAA	0
194	<chem>CC[N@H+](C)[C@H]1CN(C(=O)CCc2scnc2C)[C@H]1O</chem>	Neg_lig_1396	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUAAAAACUAA	0
195	<chem>CCn1cnnc1CC[NH2+]C1CCSCC1</chem>	Neg_lig_1445	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUAAAAACUAA	0
196	<chem>CCOC(=O)c1ccc2nc(C)cc(Nc3ccc(C(=O)OC)cc3)c2c1</chem>	Neg_lig_1502	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUAAAAACUAA	0
197	<chem>Cc1cc(OCCCc2c(C(=O)[O-])n(Cc3ccnc3)c3c(-c4c(COc5ccc(N6CCN(S(C)(=O)=O)CC6)cc5)nn(C)c4C)ccc23)cc(C)c1Cl</chem>	Neg_lig_1522	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUAAAAACUAA	0
198	<chem>Nc1ncc(C[N@@H+]2CC[C@H]3(CCCN(C(=O)CCC4CCCC4)C3)C2)cn</chem>	Neg_lig_1595	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUAAAAACUAA	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	1					
199	<chem>COc1nccc(N2CCN(Cc3ccccc3)[C@@H](CCO)C2)c1C#N</chem>	Neg_lig_1613	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	0
200	<chem>CCCc1c/c(=[NH+]\Cc2cccn2)n2[nH]c3nc(C)cc(C)c3c2n1</chem>	Neg_lig_1630	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	0
201	<chem>CCC[C@H](O)c1nc2ccccc2n1Cc1ccccc1F</chem>	Neg_lig_1637	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	0
202	<chem>Cc1cc(CN(C)c2ncc(N3CCN[C@H]4CS(=O)(=O)C[C@H]43)n2)no1</chem>	Neg_lig_1652	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	0
203	<chem>c1sc(N2CCCC2)n c1C[NH2+][C@H]1CCOC2(CCOCC2)C1</chem>	Neg_lig_1666	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	0
204	<chem>O=C1Nc2ccc(Cl)c c2[C@](C#CC2CC2)(C(F)(F)F)O1</chem>	Neg_lig_1682	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	0
205	<chem>COCC[N@@H+](C)C[C@@H]1CN(C(=O)C2=Cc3cc(Cl)ccc3OC2)C[C@@H]1CO</chem>	Neg_lig_1690	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	0
206	<chem>CC[C@]12CN3C[C@](C)(CC)(CN(C1)[C@H]3c1ccc(N)c c1)C2=O</chem>	Neg_lig_1747	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	0
207	<chem>O=C(NC[C@H](O)COC1CCCCC1)c1cnn2cc(CCO)cnc12</chem>	Neg_lig_1769	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	0
208	<chem>C[NH2+][CCN1C(=O)CC[C@H]2CN(C(C=C\c3ccc(OC)cc3)CC[C@H]21</chem>	Neg_lig_1791	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	0
209	<chem>Cc1[nH]c2ccc(Cl)cc2c1CCNc1ncnc2c1CC[NH2+]C2</chem>	Neg_lig_1807	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	0
210	<chem>CCC[C@H]1CN(Cc2nc(C(F)(F)F)no2)C[C@@H]1NC(=O)CO</chem>	Neg_lig_1829	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	0
211	<chem>CNC(=O)c1ccc(CN2CCN(c3cc(=O)[nH]cn3)C[C@@H](O)C2)o1</chem>	Neg_lig_1838	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	0
212	<chem>Cn1ccccc1-c1cc(C(=O)NC[C@@H](CO)Cc2ccsc2)[nH]n1</chem>	Neg_lig_1844	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	0
213	<chem>C=CC[C@]1(CO)CCCN(S(=O)(=O)c2ccccc2)C1</chem>	Neg_lig_1866	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	0
214	<chem>c1c[nH+]cc(-c2noc(CCNc3nenc4c3CC[NH2+])CC</chem>	Neg_lig_1905	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	4)n2)c1					
215	<chem>CCCNc1cc(C)[nH+]c2c(C)(c3cccc3)nn12</chem>	Neg_lig_1923	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUAAAAACUAA	0
216	<chem>COc1ccc(-c2nn3c(NC[C@H]4CCCO4)cc(C)[nH+]c3c2C)cc1OC</chem>	Neg_lig_1927	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUAAAAACUAA	0
217	<chem>COc1cc(/N=N/c2cccc(S(N)(=O)=O)c2)c2cccc2c1N</chem>	Neg_lig_1932	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUAAAAACUAA	0
218	<chem>CCOC(=O)c1c(N)sc(C(=O)Nc2cccc(Cl)c2C)c1C</chem>	Neg_lig_1941	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUAAAAACUAA	0
219	<chem>COc1ccc(CCNe2c(Cl)c3cccc3)nn2)cc1OC</chem>	Neg_lig_1957	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUAAAAACUAA	0
220	<chem>O=C1CCC2(CC[NH+])(Cc3ccoc3)CC2)CN1CCCO</chem>	Neg_lig_121	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUAAAAACUAA	0
221	<chem>CC(C)=CCC1=C(OCC(=O)[O-])C(=O)c2cccc2C1=O</chem>	Neg_lig_1977	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUAAAAACUAA	0
222	<chem>O=C1N(CCCc2ccc2)CCC[C@]1(O)CNCC(F)F</chem>	Neg_lig_2002	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUAAAAACUAA	0
223	<chem>Cc1ccc(NC(=O)c2cccc(CN3C[C@H](O)[C@@H](OC(C)C)C3)c2n1</chem>	Neg_lig_2009	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUAAAAACUAA	0
224	<chem>O=[N+](([O-])c1ccc(Cl)cc1NCCOCC(F)F)</chem>	Neg_lig_2014	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUAAAAACUAA	0
225	<chem>CCCCCNC(=O)c1nn(-c2ccc(F)cc2)nc1CO</chem>	Neg_lig_2028	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUAAAAACUAA	0
226	<chem>O=C(C[C@H]1C[NH2+]CCO1)N1CCC2(CC1)CC(=O)N(CCCc1cccc1)C2</chem>	Neg_lig_2036	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUAAAAACUAA	0
227	<chem>OCC(CO)(CO)c1cccn1</chem>	Neg_lig_2061	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUAAAAACUAA	0
228	<chem>O=C(c1ccc(/C=C/c2n[nH]c3cccc23)cc1)N1CC[NH2+]CC1</chem>	Neg_lig_2062	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUAAAAACUAA	0
229	<chem>O=S1(=O)C[C@H](NCc2cccn2)[C@@H](S(=O)(=O)c2cccc2)C1</chem>	Neg_lig_2068	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUAAAAACUAA	0
230	<chem>Cc1ccc(C2(O)CCN(C(=O)Cn3nc(C)cc3N)CC2)nc1</chem>	Neg_lig_2119	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUAAAAACUAA	0
231	<chem>Cc1cccc1Cn1c(CCCO)nc2cccc21</chem>	Neg_lig_2140	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUAAAAACUAA	0
232	<chem>CC[C@H]([NH2+])Cc1cc(O)</chem>	Neg_lig_56	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUAAAAACUAA	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	<chem>c2cc(C)ccc2n1)c1c cnn1C</chem>					
233	<chem>O[C@@H] (CN1C2=NCCN2c 2cccc21)c1cccc1</chem>	Neg_lig_2176	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUAAAAACUAA	0
234	<chem>O=c1[nH]c(=S)c2 ncn(- c3ccccc3)c2[nH]1</chem>	Neg_lig_2257	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUAAAAACUAA	0
235	<chem>Cn1c(=O)n(C)c2cc (CNC(=O)CCc3cc 4n(n3)CC[NH2+] C4)ccc21</chem>	Neg_lig_2294	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUAAAAACUAA	0
236	<chem>CC(C)c1ccc([C@ @H]2C(C#N)=C(N)Oc3cc4c(cc32) OCO4)cc1</chem>	Neg_lig_2335	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUAAAAACUAA	0
237	<chem>CCCCn1c(N)c(C# N)c2nc3cccc3nc2 1</chem>	Neg_lig_463	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUAAAAACUAA	0
238	<chem>Nc1c(C(=O)NCc2 cccc2)nnn1CC(= O)Nc1cccc1</chem>	Neg_lig_755	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUAAAAACUAA	0
239	<chem>Cc1ccc(C(=O)N[C @@H] (Nc2ccc(S(=O) (=O) [N-]c3nc(C)cc(C)n 3)cc2)C(Cl) (Cl)Cl)cc1</chem>	Neg_lig_2381	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUAAAAACUAA	0
240	<chem>CC[C@H]1CC[C @@]2(CC1)NC(C O)(CO)CO2</chem>	Neg_lig_2382	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUAAAAACUAA	0
241	<chem>Nc1nc2ncnc- 2c(NC[C@@H]2C Oc3cccc3C2) [nH]1</chem>	Neg_lig_2395	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUAAAAACUAA	0
242	<chem>CCCc1cncnc1N1C [C@@H] ([NH3+])C[C@H] 1C(=O)N(CC)CC</chem>	Neg_lig_1413	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUAAAAACUAA	0
243	<chem>O=[N+](O-) [C-]1[C@@H] (c2cccc2)C12c1c cccc1-c1cccc12</chem>	Neg_lig_2407	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUAAAAACUAA	0
244	<chem>CCOCCN1CCN(c 2nc(N)ncc2CC)CC 1</chem>	Neg_lig_2437	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUAAAAACUAA	0
245	<chem>Cc1c(Cl)cccc1N[C @@H]1c2cccc2C (=O)N1c1cccc1</chem>	Neg_lig_2453	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUAAAAACUAA	0
246	<chem>Cc1nnc(C[NH2+] Ce2csc([C@]34C[C@H]5C[C@H] C[C@H] (C5)C3)C4)n2)o1</chem>	Neg_lig_2471	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUAAAAACUAA	0
247	<chem>CCC[C@H]1CN(c 2nc(C)ccc2C(=O) O)C[C@@H]1N</chem>	Neg_lig_2499	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUAAAAACUAA	0
248	<chem>O=C(C[C@H] (Nc1ccc2cccc2c1)c1cccc1)c1cccc 1</chem>	Neg_lig_2504	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUAAAAACUAA	0
249	<chem>COc1ccc(- c2cc(NCCO)nc(N) [nH+])2)c2ccc(C)n</chem>	Neg_lig_2516	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUAAAAACUAA	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	c12					
250	<chem>Nc1nc2c(ncn2C2CCCC2)c(=O)[nH]1</chem>	Neg_lig_2517	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	0
251	<chem>CCc1c(C(=O)N2C[C@@H](C[N@@H+]3CCCN(C)CC3)[C@@H](CO)C2)csc1C</chem>	Neg_lig_2519	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	0
252	<chem>c1ccc2sc(N3CCCC([NH2+][C4ccsc4CC3])nc2c1</chem>	Neg_lig_2552	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	0
253	<chem>N=c1[nH]c2c(s1)[C@@H](c1cc(F)ccc1F)CC(=O)N2</chem>	Neg_lig_2621	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	0
254	<chem>Clc1ccc([C@H](Cn2ccnc2)OCc2ccc(Sc3ccccc3)cc2)c(Cl)c1</chem>	Neg_lig_2741	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	0
255	<chem>Cc1ccc(N2C(=O)c3ccnc3[C@H]2Nc2ccc(C)c(F)c2)cc1</chem>	Neg_lig_2765	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	0
256	<chem>COc1ccc(C[NH2+][CC[C@@]2(CCC(C)C)CCOC(C)(C)C2)cc1</chem>	Neg_lig_2772	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	0
257	<chem>CCc1ccc(-n2nc(CO)c(C(=O)N[C@@H](C)CC)n2)cc1</chem>	Neg_lig_2774	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	0
258	<chem>Nc1cccc1S(=O)(=O)NCC(=O)[O-]</chem>	Neg_lig_2839	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	0
259	<chem>N#C[C-]1C(=O)N=C2S/c(=C(/O)c3ccc(Br)cc3)c(N)c2C12CCCCC2</chem>	Neg_lig_2859	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	0
260	<chem>COc1ccc(C)cc1-n1nn(-c2nc(-c3ccccc3C)no2)c1N</chem>	Neg_lig_2937	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	0
261	<chem>Cc1cc(N2CCC([NH2+][C@@H]3C[C@@H](CO)N(C)C3)CC2)nc(-c2ccccc2)n1</chem>	Neg_lig_2949	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	0
262	<chem>N#Cc1ccnc1N1CCC(n2ccnc2-c2ccc(CO)o2)CC1</chem>	Neg_lig_2965	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	0
263	<chem>Cc1ccccc1CN(Cc1cc(C#CCO)cs1)CC(C)C</chem>	Neg_lig_3071	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	0
264	<chem>COC(=O)c1c(N)(-c2cccc(C(F)(F)F)c2)c2nc3ccccc3nc12</chem>	Neg_lig_3092	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	0
265	<chem>Cc1ccccc1CNC(=O)1nn(-c2ccccc2)nc1CO</chem>	Neg_lig_3161	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	0
266	<chem>C[NH2+][CCN1C(=O)CC[C@H]2CN(C(=O)c3cnc(N(C)C)nc3C)CC[C@</chem>	Neg_lig_1717	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	H]21					
267	<chem>CO[C@H]1C[C@@H](O)C12CC[NH+](Cc1cc3c(cc1C)OCCO3)CC2</chem>	Neg_lig_3253	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAACAAACUAA	0
268	<chem>COc1ccc2c(c1)CCN(C(=O)c1ccc(N)nc1)CC2</chem>	Neg_lig_847	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAACAAACUAA	0
269	<chem>O=C1c2ccccc2C(=O)N1C[C@H](O)CN1c2ccccc2Sc2ccccc21</chem>	Neg_lig_3280	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAACAAACUAA	0
270	<chem>COc1cc2c(N3CCN(C(=O)Nc4ccc(O)C(C)C)cc4)CC3)nc[nH+]c2cc1OCC[C[NH+]]1CCCCC1</chem>	Neg_lig_3298	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAACAAACUAA	0
271	<chem>Cc1ccc(S(=O)(=O)NC[C@H](O)Cn2c3ccccc3c3ccccc32)cc1</chem>	Neg_lig_3316	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAACAAACUAA	0
272	<chem>CN1CC(=O)N2CCN(Cc3ccc(C#CCO)s3)C[C@H]2C1=O</chem>	Neg_lig_3318	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAACAAACUAA	0
273	<chem>O[C@H]1CN(c2nc3ccccc3s2)C[C@H]1N1CCOCC1</chem>	Neg_lig_3346	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAACAAACUAA	0
274	<chem>O=C(Nc1cccc(Cl)c1)NC(CO)(CO)CO</chem>	Neg_lig_3372	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAACAAACUAA	0
275	<chem>CCCC1(C[NH2+])C2CCN(C(=O)c3cncn3)CC2)CCC1</chem>	Neg_lig_2103	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAACAAACUAA	0
276	<chem>CCOc1cccc1CNc1ccc2c(c1)ncn2C(C)(C)C</chem>	Neg_lig_3410	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAACAAACUAA	0
277	<chem>N#Cc1c(-c2cccn2S(=O)(=O)c2ccccc2)cc(-c2cc[nH]c2)nc1N</chem>	Neg_lig_31	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
278	<chem>C[C@H](O)CCC(=O)NCCc1nc2ccccc2n1Cc1ccc(Br)cc1</chem>	Neg_lig_52	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
279	<chem>COC[C@H](NC(C)=O)C(=O)NCc1cccc1</chem>	Neg_lig_59	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
280	<chem>COc1ccc(Cn2c(CN)nc3ccccc32)cc1</chem>	Neg_lig_69	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
281	<chem>Cc1nc(N2CCCCC2)nc1C(=O)N1C[C@H](c2ccccc2)[C@@H]([NH3+])C1</chem>	Neg_lig_139	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
282	<chem>COc1ccc(C(=O)n2ncc(C(=O)Nc3ccc(cc3)c2N)cc1</chem>	Neg_lig_194	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
283	<chem>[NH3+][CCNC(=O)c1nc(Cn2c(C(F)(F)F)nc3ccccc32)no1</chem>	Neg_lig_205	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
284	<chem>Nc1ncccc1CN1CC</chem>	Neg_lig_234	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	<chem>[C@H](C2cccc(C(=O)O)c2)C1</chem>				CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	
285	<chem>N[C@@H](Cc1cnc[nH]1)C(=O)N1CCCN(Cc2ccc(F)cc2)CC1</chem>	Neg_lig_295	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
286	<chem>O=C1C[C@H](Nc2ccc(F)cc2)C(=O)N1c1ccc(Br)cc1</chem>	Neg_lig_361	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
287	<chem>COc1ccc(Nc2cc(C)[nH+]c3c(-c4ccc(F)cc4)c(C)n23)cc1</chem>	Neg_lig_405	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
288	<chem>Fc1ccc(Nc2nc(-c3cccs3)cs2)cc1</chem>	Neg_lig_416	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
289	<chem>Cc1ccc(Nc2cc(N3CCN(S(C)(=O)=O)CC3)[nH+]c(C)n2)cc1</chem>	Neg_lig_457	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
290	<chem>Cc1cc(C)c(NC(=O)Cn2nnc(C(=O)Nc3cccc(C)c3C)c2N)c(C)c1</chem>	Neg_lig_473	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
291	<chem>O[C@H](CN1CCN(Cc2ccc(cc2)CC1)Cn1c2c(c3ccccc31)CCCC2</chem>	Neg_lig_479	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
292	<chem>Cc1ccc(-c2c(NCc3ccc4c(c3)OCO4)c(=O)c2=O)cc1</chem>	Neg_lig_485	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
293	<chem>O=C(c1ccc2ccc(c1)N1CCc2nnc(NCCO)c2CC1</chem>	Neg_lig_494	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
294	<chem>COC(=O)c1cc(Nc2cc(C)c3c(O)cccc3n2)cc(C(=O)OC)c1</chem>	Neg_lig_504	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
295	<chem>N#Cc1c(-c2cccn2-c2cnc2)cc(-c2ccc[nH]2)nc1N</chem>	Neg_lig_561	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
296	<chem>COc1cc(C[NH2+])Cc2cccn2)cc(Br)c1OCc1ccccc1Cl</chem>	Neg_lig_590	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
297	<chem>Cc1ccc([C@H](NC(=O)CCc2cc3n(n2)CCC[NH2+]C3)c2cccn2)cc1C</chem>	Neg_lig_639	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
298	<chem>O=C(c1ccccc1-c1ncc[nH]1)N1CC[C@H](Cc2cccc(CO)c2)C1</chem>	Neg_lig_662	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
299	<chem>CCCCN(Cc1cccn1)C(=O)c1ccccc1[C@H]1CC[NH2+]C1</chem>	Neg_lig_666	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
300	<chem>Cc1nc(N)sc1-c1sc(Nc2nccn2)n1</chem>	Neg_lig_689	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
301	<chem>CC(=O)c1sc(Nc2cc(Cl)c(Cl)c2)nc1</chem>	Neg_lig_693	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	C				AAAAAGGG	
302	<chem>Cc1ccc(CN2c3cccc3C3=C([C@@H](c4cccc(Cl)c4)C(C#N)=C(N)O3)S2(=O)=O)cc1</chem>	Neg_lig_707	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
303	<chem>CCn1enne1CCn1cnc1-c1cc2n(n1)CC[NH2+]C2</chem>	Neg_lig_772	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
304	<chem>Cc1ccccc1N[C@@H]1c2ccccc2C(=O)N1Cc1ccc2c(c1)OCO2</chem>	Neg_lig_778	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
305	<chem>COc1cc(C[NH2+]CCO)ccc1OCc1cc2c(c1)n(C)c(=O)n2C</chem>	Neg_lig_796	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
306	<chem>C=CCn1cccc1C(=O)NCCC(=O)Nc1cccc1CC</chem>	Neg_lig_820	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
307	<chem>O=C([O-])c1cccc(Nc2nc3ccc(Cl)cc3n3enne23)c1</chem>	Neg_lig_824	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
308	<chem>Cc1ccc(NC(=O)c2nnn(Cc3cccc(Br)c3)c2N)cc1C</chem>	Neg_lig_854	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
309	<chem>CC(=O)N1CCN(c2ccc(Nc3cc(C)nc4nc(-c5ccccc5)nn34)cc2Cl)CC1</chem>	Neg_lig_865	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
310	<chem>CCCCOCCCN1CC(=O)C(c2nc3cccc3s2)=C1N</chem>	Neg_lig_878	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
311	<chem>Cn1c(=O)n(C)c2cc(CNc3ccc(N4CCOCC4)cc3)ccc21</chem>	Neg_lig_889	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
312	<chem>O=C1O[C@H](Nc2ccc(Cl)c(C(F)(F)F)c2)c2ccccc21</chem>	Neg_lig_915	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
313	<chem>Cc1cccc(N[C@@H](c2nnc(-c3ccccc3)o2)c2ccc(cc2F)c1</chem>	Neg_lig_927	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
314	<chem>CC[NH+](CC)CCNc1ncnc2c1sc1nc3c(cc12)COC(C)(C)C3</chem>	Neg_lig_950	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
315	<chem>CN1CCC[N@+](C[C@@H]2CN(C(=O)C3CCOCC3)C[C@@H]2CO)CC1</chem>	Neg_lig_672	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
316	<chem>Cc1ccc(Nc2nc3nonc3nc2N2CCCC2)cc1C</chem>	Neg_lig_976	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
317	<chem>O=c1cc(N2CCNC2)enn1Cc1noc(-c2ccc2)n1</chem>	Neg_lig_1078	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
318	<chem>COc1ccccc1CN2CC(C[C@@H](O)(CNCCS(C)</chem>	Neg_lig_1118	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	(=O)=O)C2=O)c1					
319	Cn1c(N2CCOCC2)nc2cc(C(=O)N3COC[C@H](O)C3)ccc21	Neg_lig_1169	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
320	CCc1ccc2nc(C)cc(C(=O)NC[C@H](O)c3ccco3)c2c1	Neg_lig_30	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
321	CCc1ccc(NC(=O)c2nnn(CC(=O)Nc3cccc3CC)c2N)cc1	Neg_lig_1204	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
322	COc1ccc([C@H](Cc2ccccc2)N[C@@H]2C[NH+](C2CC3)cc1	Neg_lig_1270	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
323	O=C(N[C@@H]1CC[N@H+](Cc2cc3ccccc3o2)C[C@H]1O)c1ccncc1	Neg_lig_1309	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
324	CC(C)CNC(=O)/C=C/C(=O)[O-]	Neg_lig_1338	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
325	O=C1c2n[nH]c(-c3ccccc3O)c2[C@@H](c2ccc(F)cc2)N1C	Neg_lig_1356	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
326	CCc1ccccc1NC(=O)c1nnn(CC(=O)Nc2ccc(C)cc2C)c1N	Neg_lig_1371	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
327	CC1(C)S[C@H]2[C@H](NC(=O)[C@@H](N)c3ccc(O)cc3)C(=O)N2[C@H]1C(=O)[O-]	Neg_lig_1397	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
328	O=C(c1ccc(OCc2ccccc2F)cc1)N1CCOC[C@H](CO)C1	Neg_lig_1401	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
329	C=CCNc1nc2c(c([O-])nc(=O)n2C)n1C[C@H](O)CO	Neg_lig_453	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
330	CCN(C/C=C\c1ccccc1)C(=O)[C@H]1CC[NH2+]C1	Neg_lig_1412	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
331	C#CCN1C(=O)[C@@]2(C(C#N)=C(N)OC3=C2C(=O)CC(C)(C)C3)c2ccccc21	Neg_lig_1454	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
332	COCCc1nc(-c2nc(C3CC3)nc2)n(CCO)n1	Neg_lig_1479	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
333	Cc1nn(C)c(C)c1NC(=O)NC[C@H](O)c1ccco1	Neg_lig_1488	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
334	CC[C@H](O)c1nc2ccccc2n1CCCOc1ccccc1O	Neg_lig_1499	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
335	CCOc1ccc(NC(=O	Neg_lig_1527	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	<chem>jc2cnn(C(=O)c3cc(OC)cc3)c2N)cc1</chem>				CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	
336	<chem>Cc1cc(C)c2c(N)c(S(=O)(=O)Cc3ccc(Cl)cc3)sc2n1</chem>	Neg_lig_1540	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
337	<chem>CCOC(=O)c1cc(CN[C@H]2CCS(=O)(=O)C2)on1</chem>	Neg_lig_1565	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
338	<chem>Cc1nc(C)c(CC(=O)N2CC[C@H](c3secc3C)[C@H](O)C2)c(=O)[nH]1</chem>	Neg_lig_659	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
339	<chem>Cc1ccc(NC(=O)c2nnn(Cc3ccc(Br)cc3F)c2N)c(Cl)c1</chem>	Neg_lig_1641	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
340	<chem>Cc1cc(NC(=O)Nc2cccc3ccccc23)no1</chem>	Neg_lig_1654	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
341	<chem>Cc1nn(CCO)cc1C[N@H+]1CCC[C@H](c2nnnc(C[NH+](C)C)n2C)C1</chem>	Neg_lig_1705	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
342	<chem>O=C(CN1CCCCC1)OCCNC1=NS(=O)(=O)c2ccccc21</chem>	Neg_lig_1708	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
343	<chem>CCCCCCCn1c(CO)nc2ccccc21</chem>	Neg_lig_1533	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
344	<chem>Cc1ccc(C)c(OC[C@H](O)Cn2c([C@@H]3CC(=O)N(Cc4ccc4)C3)nc3ccccc32)c1</chem>	Neg_lig_1788	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
345	<chem>Cc1ccccc1NCC(=O)c1ccc(Br)cc1</chem>	Neg_lig_1803	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
346	<chem>N#CC1=C(N)OC2=C(C(=O)CCC2)[C@@@H]1c1ccccc1c1</chem>	Neg_lig_1847	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
347	<chem>O=C(O)c1cn(-c2ccc(F)cc2)c2cc(N3CCNCC3)c(F)c2c1=O</chem>	Neg_lig_1889	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
348	<chem>Cc1nc([NH+]=C(\N)N(C)C)nc(O)c1C</chem>	Neg_lig_1918	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
349	<chem>CC1=C(C(=O)OC(C)C)[C@]2(C(=O)N(C)c3ccccc32)C(C#N)=C(N)O1</chem>	Neg_lig_1942	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
350	<chem>CC(C)[NH2+][C@H]1CC[C@H]1NC(=O)c1ccc(-c2ccccc2)c1</chem>	Neg_lig_1976	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
351	<chem>CCOc1ccc(Cl)cc1C[NH2+]CCSc1nnn1C</chem>	Neg_lig_53	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
352	<chem>C[C@@]1(C2CC[NH2+])CC2)NC(=O)NC1=O</chem>	Neg_lig_2008	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
353	<chem>CC[C@H]</chem>	Neg_lig_2037	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	(O)CNS(=O) (=O)c1ccc(C(=O) NCc2ncc[nH]2)cc 1				CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	
354	Cc1cc2c(cc1CC(=O)c1sccc1S(=O)(=O)/N=c1/o[n-]c(C)c1Cl)OC O2	Neg_lig_2055	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
355	Cc1cc2c(c(=O)o1)[C@@]1(C(=O)Nc3ccc(C)c(Br)c31)C(C#N)=C(N)O2	Neg_lig_667	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
356	CCOc1cc(C[NH2+]]CCc2ccccc2F)ccc IOC	Neg_lig_2113	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
357	Cn1cc(- c2ccccc2OC[C@ @H] (O)CN2CCOCC2) cn1	Neg_lig_2155	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
358	Cc1nn(CCO)cc1C[N@H+]1C[C@@H](c2ccc(F)cc2)[C@@H]2[C@H]1C1CCN2CC1	Neg_lig_2160	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
359	COC(=O)CNc1cc(Cnc2nc(-c3ccc(C)c3)nn12	Neg_lig_2162	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
360	C=C(C)CC[C@H](C)[NH2+]]Cc1n[nH]c2c1CCCC2	Neg_lig_2171	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
361	CNc1ccccc1C(=O)NC[C@H]1CC[N@H+](Cc2ccc(O)c2)C1	Neg_lig_2194	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
362	Cc1c(NCc2cccn2)ccc1C(=O)N[C@@H](C)CCn1ccn1	Neg_lig_2195	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
363	COC(=O)c1c(C)sc2c1OC(N)=C(C#N)[C@@H]2c1ccccc1	Neg_lig_2203	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
364	CC(C)Nc1ccc(-c2cc(N)nc3[nH]cc23)nn1	Neg_lig_2263	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
365	CCOCCn1nc(C)cc1C(=O)N1C[C@H](c2ccc(C)o2)[C@@H]([NH3+])C1	Neg_lig_1975	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
366	CN(CCC#N)c1ccc(/C=C\C#N)c2ccc(C(F)(F)F)c2cc1	Neg_lig_739	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
367	Cc1nn(CCO)cc1C[N@H+]1CCCC(c2ccccc2)(c2ccccc2)C1	Neg_lig_2350	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
368	C[C@](O)(c1ccccc1)[C@@H](c1ccccc1)[C@@H]1CCCC[Neg_lig_2355	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	NH2+][1					
369	CN(Cc1cnc(N)nc1)C(=O)Nc1cccc1C[N@@H+](C)C1CCCC1	Neg_lig_1902	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
370	OCCCNc1nc2sc3c(c2c2ncnn12)CCC3	Neg_lig_2359	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
371	OC[C@@H](O)Cn1c(COc2cccc2)nc2cccc21	Neg_lig_2370	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
372	Cn1c(CN2CC[C@@H](NC(=O)c3ccccc3)[C@H](O)C2)nc2cccc21	Neg_lig_2387	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
373	CC(=O)c1cc2c(cc1N)OCCO2	Neg_lig_2393	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
374	Cc1ccc([C@@H]2C(C#N)=C(N)OC3=C2C(=O)CC(C)(C)C3)cc1	Neg_lig_2394	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
375	Clc1ccc(-c2ccc(CNC[C@@H]3CCCCO3)o2)cc1	Neg_lig_2406	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
376	Cc1cc(NC2CCCC2)n2nc(C(F)(F)F)nc2n1	Neg_lig_2435	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
377	O[C@H]1CN[C@H](c2nnnn2-c2cccc3c2CCC3)C1	Neg_lig_2449	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
378	Cc1cc(Nc2ccc(Cl)cc2)c2cccc2[nH+]1	Neg_lig_2507	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
379	COC(=O)c1c(-c2ccc(Br)cc2)csc1N	Neg_lig_2549	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
380	CCc1cc(C[NH2+])Cc2cc(O)c3cc(C)cc3n2)on1	Neg_lig_2578	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
381	Cc1ccc(CNc2ccc3c(c2)[nH+]c(C)n3C)cc1	Neg_lig_2562	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
382	Cc1ncc(CO)c(CN2C[C@H]([NH3+])C[C@H]2C(=O)NC(C)C)IO	Neg_lig_2670	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
383	Nc1nncc(-c2cccc(Cl)c2Cl)c(N)n1	Neg_lig_2671	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
384	Cc1c(C[N@H+](C)C2CCC3(CC[NH2+])CC3)CC2)cn1C	Neg_lig_2674	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
385	CCc1nc(N)sc1C(=O)N1CCN(c2cccc2OC)C(C)(C)C1	Neg_lig_2727	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
386	O=C(Nc1ncc(-c2cc(C(F)F)nn2-c2c(Cl)cccc2Cl)s1)C1CC1	Neg_lig_2734	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
387	<chem>COc1cccc(-c2nc3c([nH]2)CCN(C(=O)[C@@H](O)Cc2cccc2)C3)c1</chem>	Neg_lig_2764	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
388	<chem>O[C@@H](CN1CC=C(/C=C\c2ccc(Br)cc2)CC1)c1cccc1</chem>	Neg_lig_2768	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
389	<chem>COCCCC[C@H]1CCCCN1C(=O)c1ccc(N)nc1</chem>	Neg_lig_2779	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
390	<chem>Cc1nc2nc(C[NH3+])nn2c(C)c1CCC(=O)Nc1cccc1</chem>	Neg_lig_2798	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
391	<chem>CCNc1nc(N(C)C)nc(-n2cnc(SC)n2)n1</chem>	Neg_lig_2860	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
392	<chem>CCOC(=O)[C@]12CCCC[NH2+][C@@H]1CCN(C(=O)c1ccn3nnnc3c1)C2</chem>	Neg_lig_2935	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
393	<chem>CN1CC[NH+](CCCNc2c([NH3+])c(=O)oc3cccc23)CC1</chem>	Neg_lig_2942	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
394	<chem>C[C@H]1CN(c2ccc2Cl)C(=O)CN1C(=O)c1ccnc(N)c1</chem>	Neg_lig_2745	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
395	<chem>Cc1cnn(Cc2ccc(Cl)cc2)c1NC(=O)N(CCO)CCO</chem>	Neg_lig_682	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
396	<chem>O=C1c2cccc2-[n+]2ccc3c([nH]4)cccc43)c21</chem>	Neg_lig_3002	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
397	<chem>O=C1c2n[nH]c(-c3cccc3O)c2[C@@H](c2ccc(Cl)cc2)N1CCO</chem>	Neg_lig_3013	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
398	<chem>COc1ccc2c(Oc3cc(NC(=O)c4c(C)n(CC(C)C)O)n(-c5cccc5)c4=O)nc3)ccnc2c1</chem>	Neg_lig_3028	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
399	<chem>COc1cccc([C@@H]2c3c(n[nH]c3-c3c(C)cc(C)cc3O)C(=O)N2CCCCO)c1</chem>	Neg_lig_3076	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
400	<chem>Cc1ccc(CN(C)CC(=O)N[C@H]2CC[C@H]2[NH2+])C(C)C)cc1</chem>	Neg_lig_3111	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
401	<chem>Nc1cnc(-n2ccc(-c3cc(Cl)ccc3O)n2)c1</chem>	Neg_lig_3151	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
402	<chem>C[NH+](C)CCCNc1c([NH3+])c(=O)oc2cccc12</chem>	Neg_lig_3157	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
403	<chem>N#CC1=C(N)N2C(=C(C#N)[C@@H]1c1ccc(C</chem>	Neg_lig_947	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	l)cc1)Sc1cccc12					
404	<chem>Nc1cc(-c2nc3cccc3o2)cc1Br</chem>	Neg_lig_3187	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
405	<chem>Cc1c2oc3c(C)ccc(C(=O)N[C@H]4C(=O)N[C@@H](C(C)C)C(=O)N5CCC[C@H]5C(=O)N(C)CC(=O)N(C)[C@@H](C(C)C)C(=O)O[C@H]4C)c3nc2c(C(=O)N[C@H]2C(=O)N[C@@H](C(C)C)C(=O)N3CCC[C@H]3C(=O)N(C)CC(=O)N(C)[C@H](C(C)C)C(=O)O[C@@H]2C)c(N)c1=O</chem>	Neg_lig_3226	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
406	<chem>CCc1cccc1N[C@@H]1c2cccc2C(=O)N1c1ccc(Cl)cn1</chem>	Neg_lig_2003	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
407	<chem>O=C(NCC(c1cccc1)c1cccc1)c1nn(-c2ccc(Cl)cc2)nc1CO</chem>	Neg_lig_3376	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
408	<chem>CCn1c(C2CCN(C(=O)CC3=CC[NH2+][CC3]CC2)n[nH]c1=O</chem>	Neg_lig_3405	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
409	<chem>CC(C)N1cc(C[NH2+])Cc2nn(CCC(N)=O)c3cccc23)cn1</chem>	Neg_lig_3420	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	0
410	<chem>COC(=O)c1[nH]c2cccc2c1NCc1ccnc1</chem>	Neg_lig_11	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
411	<chem>C=CCNc1oc(-c2ccc(F)cc2)nc1S(=O)(=O)c1ccc(Cl)cc1</chem>	Neg_lig_33	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
412	<chem>COc1ccc(C(=O)Oc2cccc(Nc3nnc4cccc34)c2)cc1</chem>	Neg_lig_67	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
413	<chem>CC(C)C[C@@H](CO)n1cc(-c2nn(C)c3cccc(Cl)c23)nn1</chem>	Neg_lig_100	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
414	<chem>CC(C)N[C@H](C(=O)O)c1c[nH]c2ccc(Br)cc12</chem>	Neg_lig_147	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
415	<chem>CCCOc1ccc(Oc2nc(NCC(C)C)nc(N3CCOCC3)n2)nn1</chem>	Neg_lig_165	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
416	<chem>CN1c2cc(O)c(/N=N/C(N)=O)cc2[C@@H]1S(=O)(=O)[O-]</chem>	Neg_lig_175	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
417	<chem>CC(C)NC(=O)c1c</chem>	Neg_lig_219	TPP	Three-way	CAGUACUCGGGGUGCCCUUCUG	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	<chem>cccc1-c1cc(Cl)c2c(c1)C[C@H](CN)O2</chem>			junction	CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	
418	<chem>Cc1ccc(NC(=O)CNC(=O)c2cn(C[C@H]3CCC[NH2+]C3)nn2)c(F)c1</chem>	Neg_lig_307	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
419	<chem>C[C@]12CN3CN(C1)C[C@](C)(C3)[C@H]2[NH3+]</chem>	Neg_lig_346	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
420	<chem>C[C@@H](c1nccs1)N(C)Cc1nnc(CC2CC[NH2+]CC2)n1C</chem>	Neg_lig_373	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
421	<chem>CCNe1ncc(C(=O)N2C[C@H](C[NH+]3CCCCC3)[C@H](CO)C2)cn1</chem>	Neg_lig_388	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
422	<chem>O=C1OCCN1CCn1ccn1-c1cc2n(n1)CC[NH2+]C2</chem>	Neg_lig_390	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
423	<chem>COc1ccc(-c2noc(-c3nnn(-c4ccc(C)cc4C)c3N)n2)cc1</chem>	Neg_lig_394	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
424	<chem>OC[C@H]1CCCN1Cc1ccc(-c2nc(O)cc(-c3cccc3Cl)n2)cc1</chem>	Neg_lig_422	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
425	<chem>COc1ccc(C2=C(C)C([N-]c3cc(F)ccc3F)=NS2(=O)=O)cc1</chem>	Neg_lig_435	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
426	<chem>O=S(=O)(N[C@H]1CCC[C@H]1Nc1ccc(Br)cc1)c1ccc(Cl)cc1</chem>	Neg_lig_439	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
427	<chem>CN(CC(=O)N1CC[C@H](Cc2ccc(CO)c2)C1)C1CC[NH+] (C)CC1</chem>	Neg_lig_454	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
428	<chem>Cn1c(C(=O)c2ccncc2)cc2cccc21</chem>	Neg_lig_476	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
429	<chem>CN(C)c1ccc2[nH+]c3ccc(=[N+](C)C)cc-3sc2c1</chem>	Neg_lig_529	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
430	<chem>N#CC1=C(Nc2ccc(cc2Cl)S[C@H](c2cccc2O)NC1=O</chem>	Neg_lig_608	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
431	<chem>CC(=O)N[C@H]1CCN(c2cc(N3CCOCC3)nc(N)n2)C1</chem>	Neg_lig_624	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
432	<chem>CC(C)OC(=O)Nc1ccc2c(c1)N(C(=O)CCN1CCN(CCO)CC1)c1cccc1CC2</chem>	Neg_lig_626	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
433	<chem>CCCCn1nc2cc(NC3cccc(OC)c3OC)ccc21</chem>	Neg_lig_628	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUACCCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
434	<chem>CC(C)c1ccc(CN2CCC[C@@](O)(CNCC3ccc[nH]c3=O)C2=O)cc1</chem>	Neg_lig_643	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUACCCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
435	<chem>CN1CCC[N@+](C[C@@H]2CN(C(=O)C3CCOCC3)C[C@@H]2CO)CC1</chem>	Neg_lig_672	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUACCCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
436	<chem>O=S(=O)C[C@@H]2[C@H](C1)N(CCCCOc1cccc1)CCN2CCO</chem>	Neg_lig_688	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUACCCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
437	<chem>Cc1[nH]c2c(F)ccc2c1CC(=O)NCC[N@H+]1CCCC[C@@H]1CO</chem>	Neg_lig_724	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUACCCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
438	<chem>C[C@@H]1C(C#N)=C(N)OC2=C1C(=O)C[C@H](c1cccc1)C2</chem>	Neg_lig_751	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUACCCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
439	<chem>CCOC(=O)c1c(N)n(C2CCCC2)c2nc3cccc3nc12</chem>	Neg_lig_760	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUACCCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
440	<chem>Cn1c(=O)c2c(nc3n2CC(c2ccc(F)cc2)=NN3CCO)n(C)c1=O</chem>	Neg_lig_811	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUACCCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
441	<chem>Cc1c[nH+]c(N)nc1NCc1cc(C(C)(C)C)[nH]n1</chem>	Neg_lig_848	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUACCCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
442	<chem>[NH3+][C@H]1CC[C@@H](n2cc(C(=O)NCc3nc(-c4cccn4)no3)nn2)CC1</chem>	Neg_lig_863	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUACCCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
443	<chem>O=S(=O)(c1ccc2cccc2c1)N(C[C@H](O)COCc1ccco1c1cccc1</chem>	Neg_lig_196	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUACCCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
444	<chem>Cc1[nH+]c2n(c1C(=O)N(C)C)CCN(C[C@]1(O)CCC[NH2+][C1]C2</chem>	Neg_lig_899	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUACCCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
445	<chem>CCCCCN1CC(=O)C(c2nc3cccc3s2)=C1N</chem>	Neg_lig_919	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUACCCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
446	<chem>O=C(NCc1ccoc1)[C@@]12C[NH2+][C[C@@H]1C[N@@H+](Cc1ccccc1)C2</chem>	Neg_lig_953	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUACCCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
447	<chem>Cc1ccc(Nc2nc3ccc3c3nnc(C)n23)c1F</chem>	Neg_lig_1048	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUACCCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
448	<chem>O=C(NCc1cc(-c2ccco2)on1)c1cn(CCN2CC[NH2+]C2)nn1</chem>	Neg_lig_1058	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
449	<chem>C[C@@H]1C[C@@H](Nc2ccccc2)c2ccc(cc2N1C(=O)Cc1cc(F)cc1</chem>	Neg_lig_1109	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
450	<chem>OCCN1C[C@H](O)[C@@H](O)[C@H](O)[C@H]1CO</chem>	Neg_lig_1128	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
451	<chem>CCCCOC(=O)c1ccc(Nc2nc3ccccc3nn3cnc23)cc1</chem>	Neg_lig_1214	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
452	<chem>CC[C@]1(CO)CC(C[N@@H+](CCC(=O)N2CCc3ccccc3C2)C1</chem>	Neg_lig_1235	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
453	<chem>CC[C@@H](CO)[NH2+]C[C@@H](O)Cn1c(C)c(C)c2ccccc21</chem>	Neg_lig_1242	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
454	<chem>CC[C@]1(CO)CC(C[N@@H+](CCC(=O)NC2ccc(Cl)c2)C1</chem>	Neg_lig_1259	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
455	<chem>COc1ccc(C(=O)c2sc3nc(-c4ccc(OC)cc4)ccc3c2N)cc1</chem>	Neg_lig_1311	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
456	<chem>CC(C)C[C@]1(CO)CCCN(Cc2[nH]cc[nH+]2)C1</chem>	Neg_lig_1352	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
457	<chem>c1ncn(-c2ccc([C@H]3[NH2+]CCc4nc[nH]c43)cc2)n1</chem>	Neg_lig_1394	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
458	<chem>OCC[NH2+]CCC[NH2+]Cc1ccccc1</chem>	Neg_lig_1402	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
459	<chem>c1sc(Cc2nc(Cn3cc[nH+]c3-c3cc4n(n3)CC[NH2+]C4no2)c1</chem>	Neg_lig_1444	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
460	<chem>COc1ccc(S(=O)(=O)N2CCN(c3ccc(C)nc(Nc4ccc(C)cc4)n3)CC2)cc1C</chem>	Neg_lig_1512	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
461	<chem>OCc1ccc(CN(Cc2ccncc2)Cc2ccc(F)cc2)o1</chem>	Neg_lig_1517	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
462	<chem>CC(=O)c1ccccc1NC(=O)c2sc3nc4c(cc3c2N)CCCC4)c1</chem>	Neg_lig_1531	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
463	<chem>CC(C)(CO)NC(=O)[C@@H]1CC(c2ccccc2O)=NO1</chem>	Neg_lig_1534	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
464	<chem>COc1ccc2[nH]c([S</chem>	Neg_lig_1541	TPP	Three-way	CAGUACUCGGGGUGCCCUUCUG	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	<chem>[@] (=O)Cc3ncc(C)c(OC)c3C)nc2c1</chem>			junction	CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	
465	<chem>O=C(Cc1ccc(O)cc 1)N1CCN(Cc2ccc cc2CO)CC1</chem>	Neg_lig_1646	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
466	<chem>Cc1ccn(C)c(=[NH 2+])c1</chem>	Neg_lig_1655	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
467	<chem>CCOc1cccc1Nc1 cc(C) [nH+]c2ccc(Cl)cc1 2</chem>	Neg_lig_1659	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
468	<chem>COCCCNc1oc(- c2cccc2F)nc1S(= O)(=O)c1cccc1</chem>	Neg_lig_1704	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
469	<chem>O=S(=O) (c1cccc1)c1nc(- c2ccc2)oc1NCC CN1CCOCC1</chem>	Neg_lig_1720	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
470	<chem>CCNC(=O) [C@H]1C[C@H] 1 ([NH3+])CN1C(= O)c1cc(C2CC2)nc 2cccc12</chem>	Neg_lig_1727	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
471	<chem>CCOC(=O)c1cccc(NS(=O) (=O)c2cc(Br)enc2 N)c1</chem>	Neg_lig_1740	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
472	<chem>O=C(c1ccc(Cl)nc1 c1cccs1</chem>	Neg_lig_1745	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
473	<chem>COc1nc2c(cc1C[N H2+] [C@H]1CCSC1)C (=O)N(C1CCCC1) C2</chem>	Neg_lig_1761	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
474	<chem>O=C1O[C@H] (Nc2nc(- c3cccc(Br)c3)cs2) c2cccc21</chem>	Neg_lig_1784	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
475	<chem>COc1cc(C[C@H]2 CC(CO)=NO2)cc2 c1OCO2</chem>	Neg_lig_1865	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
476	<chem>Cc1enccc1Cn1ccn c1- c1cn(C2CC[NH2+]CC2)nn1</chem>	Neg_lig_1885	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
477	<chem>O=C(NCc1ccc2no nc2c1) [C@@]12C[NH2+]][C[C@@H]1C[N @@H+] (C1CCCC1)C2</chem>	Neg_lig_1910	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
478	<chem>O=C(NCCCO)c1n nc(Cc2ccc3c(c2)O CO3)o1</chem>	Neg_lig_1914	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
479	<chem>Cc1ccc(Nc2nc(C)c 3nc(C)n(- c4ccc(C)cc4)c3n2)</chem>	Neg_lig_1943	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	cc1				CAGCGUAGGGAAGUGCUG	
480	<chem>Cn1c(=O)c2c(nc3n2CC(c2ccc(Cl)cc2)=NN3CCO)n(C)c1=O</chem>	Neg_lig_1968	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUAACCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
481	<chem>COc1ccc(N)cc1-n1nnnc1-n1cccn1</chem>	Neg_lig_1995	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUAACCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
482	<chem>COCc1nn(-c2ccccc2)c(N)c1-c1ccc(OC)c(OC)c1</chem>	Neg_lig_2047	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUAACCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
483	<chem>Cc1ncc(CO)c(CN(C)CC[NH+])2CCC(CCC2)c1O</chem>	Neg_lig_42	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUAACCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
484	<chem>O=C(NCCO)c1cnc2sc3c(n2c1=O)CC(C)C3</chem>	Neg_lig_2075	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUAACCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
485	<chem>NC(=O)C1=C(NC(c2ccc3c(c2)OCO3)c2ccccc2S1(=O)=O</chem>	Neg_lig_2081	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUAACCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
486	<chem>Nc1nonc1C(=O)NCC[NH2+]Cc1ccc(OCc2ccccc2Cl)cc1</chem>	Neg_lig_2090	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUAACCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
487	<chem>CC[C@H](C)Nc1c([NH3+])c(=O)oc2ccccc12</chem>	Neg_lig_2109	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUAACCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
488	<chem>CC[C@H](C(N)=O)N1CCC(C1=O</chem>	Neg_lig_2116	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUAACCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
489	<chem>CCCCCOC(=O)[N-]c1nc(=O)n([C@@H]2O[C@H](C)[C@@H](O)[C@H]2O)cc1F</chem>	Neg_lig_2126	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUAACCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
490	<chem>Cc1cc(NC2CCCC2)n2nc(C)c(-c3ccc(F)cc3)c2[nH+]1</chem>	Neg_lig_2170	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUAACCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
491	<chem>Cn1c(=O)c2nc(N)[nH]c2n(C)c1=O</chem>	Neg_lig_2196	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUAACCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
492	<chem>CNc1oc(-c2ccccc2Cl)nc1S(=O)(=O)c1ccc(F)cc1</chem>	Neg_lig_2230	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUAACCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
493	<chem>C[C@H](Cn1cnc2ccccc2c1=O)[NH2+][CC1=CCC(CC1</chem>	Neg_lig_2247	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUAACCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
494	<chem>COc1cccc(C2=NN(CCO)c3nc4c(c(=O)n(C)c(=O)n4C)n3C2)c1</chem>	Neg_lig_2284	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUAACCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
495	<chem>COc1ccc(-c2noc(Nc3ccc(C)c(C)c3)n2)cc1OC</chem>	Neg_lig_2299	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUAACCG UAUCACCUGAUCUGGAUAAUGC	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
					CAGCGUAGGGAAGUGCUG	
496	<chem>Nc1ccn(C[C@@H](CO)OC(=O)([O-])[O-])c(=O)n1</chem>	Neg_lig_2325	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
497	<chem>O=C([O-])C[C@@H](C(=O)[O-])N1C(=O)/C(=C2/C(=O)Nc3ccc(Br)cc3)SC1=S</chem>	Neg_lig_2351	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
498	<chem>CCOC(=O)c1cnc2c(-c3ccc(F)cc3)c(C)n2c1N</chem>	Neg_lig_2385	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
499	<chem>CCc1nnc2c(Nc3ccc3OC)nc3ccccc3n12</chem>	Neg_lig_2400	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
500	<chem>CC(C)(C)N1C[C@@H](C(=O)N(CCO)Cc2nccs2)CC1=O</chem>	Neg_lig_2423	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
501	<chem>O=C(NCCO)c1c2c(nc3ccccc13)CCC2</chem>	Neg_lig_2441	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
502	<chem>COc1ccc(OCCN[C@@H]2CS(=O)(=O)C[C@@H]2S(=O)(=O)c2ccccc2)cc1</chem>	Neg_lig_2468	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
503	<chem>CC(C)C[NH+]1CC(C([NH2+])Cc2cc(-n3cncn3)cc2)CC1</chem>	Neg_lig_2500	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
504	<chem>Cc1ccc(C)c(NC(=O)c2nnn(Cc3ccccc3C)c2N)c1</chem>	Neg_lig_2502	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
505	<chem>CCOC(=O)N1CCN(Cc2c(O)ccc3ccc23)CC1</chem>	Neg_lig_1122	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
506	<chem>C=CCn1c(N)c(C(=O)NC2CCCC2)s c1=S</chem>	Neg_lig_2513	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
507	<chem>Cc1nc2cc[nH]n2c(=O)c1CCc1ccccc1</chem>	Neg_lig_2523	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
508	<chem>Cc1ccnc(NCCNc2ncnc3c2CC[NH2+]CC3)c1</chem>	Neg_lig_2554	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
509	<chem>Cc1ccccc1[C@@H]1CN(Cc2ccnc2N)C[C@H]1C(=O)O</chem>	Neg_lig_2558	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
510	<chem>CO[C@@H]12[C@H](COC(N)=O)C3=C(C(=O)C(C)=C(N)C3=O)N1C[C@@H]1N[C@@H]12</chem>	Neg_lig_2587	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
511	<chem>COc1ccc(S(=O)(=O)c2nc3ccc(C)cc3n2)cc1</chem>	Neg_lig_2624	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
512	<chem>COc1ccccc1Nc1nc(-c2sc(N)nc2C)cs1</chem>	Neg_lig_2660	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
513	<chem>CCOC(=O)c1c(C)oc2ncnc(Nc3ccccc3)c12</chem>	Neg_lig_1648	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
514	<chem>c1nc(-c2nc(Cn3cc([C@H]4CCC[NH2+]C4)nn3)cs2)nc1</chem>	Neg_lig_2723	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
515	<chem>Cc1onc(-c2ccccc2Cl)c1C(=O)N[C@@H]1C(=O)N2[C@@H](C(=O)[O-])C(C)(C)S[C@H]12</chem>	Neg_lig_2725	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
516	<chem>O=C(Cc1ccccc1)N1CCC(C(=O)N2COC[C@@H](O)C2)CC1</chem>	Neg_lig_2751	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
517	<chem>COCc1ncnc1CC[NH2+][C]1cc(O)c2cc(C)cc(C)c2n1</chem>	Neg_lig_2756	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
518	<chem>C=CCOCC[NH+](CC)CC</chem>	Neg_lig_2761	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
519	<chem>OCCn1nc(C2CCC2)nc1CCc1nc(-c2ccccc2F)no1</chem>	Neg_lig_2810	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
520	<chem>CCc1c(C(=O)C(N)=O)c2c(OCC(=O)[O-])cccc2n1Cc1c1cccc1</chem>	Neg_lig_2831	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
521	<chem>Oc1ccccc1-c1nn(CNc2ccc(I)c2)c(=S)o1</chem>	Neg_lig_2843	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
522	<chem>CCOc1ccc(Cc2cc([C@@H]3O[C@H](CO)[C@H](O)[C@H]3O)ccc2Cl)cc1</chem>	Neg_lig_2855	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
523	<chem>Cc1ccsc1C[NH+]1CCC2(CC1)Nc1ccc1NC2=O</chem>	Neg_lig_2866	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
524	<chem>COc1ccc(-c2ccc3c(N)c(C(=O)c4ccc(OC)c(OC)c4)sc3n2)cc1</chem>	Neg_lig_2889	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
525	<chem>Nc1nc(-c2cc3c(ccc4cccc43)oc2=O)cs1</chem>	Neg_lig_2929	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
526	<chem>Cc1ccccc1-c1cc(O)c2c(c1)CN(C(=O)c1cc(N)</chem>	Neg_lig_2938	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	[nH]n1)CCO2				CAGCGUAGGGAAGUGCUG	
527	COc1ccccc1Nc1nc(-c2c(C)nc3cccn23)cs1	Neg_lig_2940	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUAACCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
528	Cn1c(-c2ccc(F)cc2)c[nH+]]c1NCc1cc(Br)cc1F	Neg_lig_2945	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUAACCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
529	C=CCc1c(C)nc(N)nc1NC[C@@H](c1ccc(F)cc1)[NH+]1CCCC1	Neg_lig_2978	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUAACCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
530	CCOC(=O)c1c(N)nn(C(=O)c2ccc(Br)cc2)c1-c1ccc(OC)cc1	Neg_lig_2794	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUAACCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
531	CCCCCNc1ncc(-c2c[nH]c3ccccc23)s1	Neg_lig_2994	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUAACCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
532	N#CC1=C(N)Oc2n[nH]c(-c3ccccc3)c2[C@H]1c1cccn1	Neg_lig_3015	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUAACCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
533	OCCn1nc(Cc2c(Cl)cccc2Cl)nc1C1CCC1	Neg_lig_3086	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUAACCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
534	CS(=O)(=O)N1CCCN(C(=O)c2ccccc2[C@H]2CC[NH2+]C2)CC1	Neg_lig_3132	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUAACCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
535	O=c1c2ccccc2nc(CNc2ccccc2)n1-c1ccccc1F	Neg_lig_3156	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUAACCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
536	NC1=C(c2nc3ccccc3s2)C(=O)CN1c1ccccc1Cl	Neg_lig_3159	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUAACCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
537	COc1ccc(CN2CCN(c3nccc(N)n3)C2=O)cc1	Neg_lig_3192	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUAACCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
538	CCC[C@@H](NC(=O)[C@@H]1[C@H]2CCC[C@H]2C1N1C(=O)[C@@H](NC(=O)[C@@H](NC(=O)c1ncn1)C1CCCC1)C(C)(C)C(=O)C(=O)NC1CC1	Neg_lig_3204	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUAACCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
539	COc1cc2[nH]c(Nc3ccc(Cl)cc3)c([N+](=O)[O-])c2cc1OC	Neg_lig_3236	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUAACCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
540	O[C@@H](Cn1cc[nH+]]c1-c1cnc(C2CCCC2)nc1)c1ccccc1	Neg_lig_3256	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUAACCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
541	Cc1cc(NCc2ccncc2)n2nc(C(F)(F)F)c(-	Neg_lig_3259	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUAACCG UAUCACCUGAUCUGGAUAAUGC	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	c3ccc(Cl)cc3)c2n1				CAGCGUAGGGAAGUGCUG	
542	Cn1c(=O)n(C)c2cc(CNc3ccc4c(c3)OCO4)ccc21	Neg_lig_3290	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
543	Cc1ccccc1Cn1c([C@H](C)O)nc2ccccc21	Neg_lig_3297	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
544	CNC(=O)c1cc(Oc2ccc(NC(=O)Nc3cc(C(C)(C)C)nn3-c3ccc4ncccc4c3)c(F)c2)ccn1	Neg_lig_440	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
545	N#CC1=C(N)N(c2ccccc2)C2=C(C(=O)CCC2)[C@H]1c1ccc(O)cc1	Neg_lig_2809	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
546	C[C@H]1[C@H]2CC[C@H](C)[C@H]3CC[C@H]4(C)OO[C@H]23[C@H](O[C@H]1C[C@H](C[C@H]1O[C@H]2O[C@H]3(C)CC[C@H]5[C@H](C)CC[C@H]([C@H]1C)[C@H]25OO3)CS(=O)(=O)c1ccc(COC(=O)N(C)C)cc1)O4	Neg_lig_3339	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
547	Cc1ccccc1Nnc(C(=O)Nc3ccc(C)c3)c2N)c1	Neg_lig_3359	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
548	Cc1cc(N[C@H]2C(C(=O)N(Cc3ccccc3C(F)(F)F)C2)nc(N)n1	Neg_lig_65	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	0
549	Cc1ccc(C[NH2+])C2ccc3c(c2)n(C)c(=O)n3C)cc1	Neg_lig_8	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
550	COc1ccccc2c(O)c(NC(=O)N3CCC(CO)CC3)cn12	Neg_lig_9	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
551	COc1ccccc1OCC[NH2+][C@H](O)COc1ccccc2[nH]c3ccccc3c12	Neg_lig_48	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
552	COCC[N@H+](C)[C@H]1CN(C(=O)C2N=c3ccccc3=NC2=O)C[C@H]1CO	Neg_lig_54	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
553	O=C(Nc1nc2ccccc3ccc(CN4CCS(=O)(=O)CC4)cc3)n2n1)C1CC1	Neg_lig_62	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
554	<chem>O=C([O-])c1[n-]c(=O)[nH](c=O)c1F</chem>	Neg_lig_85	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
555	<chem>O=S(=O)(N[C@@H]1CCC[C@H]1Nc1ccc(Cl)cc1)c1ccccc1</chem>	Neg_lig_99	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
556	<chem>COc1ccc(C(=O)[O-])cc1Nc1cccn1</chem>	Neg_lig_116	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
557	<chem>Cc1ccc(Nc2cc(C)nc3nc(-c4ccnc4)nn23)cc1</chem>	Neg_lig_182	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
558	<chem>CN(C)c1ccc2c(c1)OC(N)=C(C#N)[C@H]2c1cccc(F)c1</chem>	Neg_lig_186	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
559	<chem>CN(C)C(=O)c1ccc2c(c1)N(C)[C@@H](CC(=O)NCCO)CO2</chem>	Neg_lig_189	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
560	<chem>O=S(=O)(c1ccc2ccccc2c1)N(C)[C@H](O)COCc1ccc(O)c1ccccc1</chem>	Neg_lig_196	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
561	<chem>COc1ccc(-c2nn3c(NCCN4C(=O)COC4)cc(C)[nH+]c3c2C)cc1O</chem>	Neg_lig_197	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
562	<chem>C[C@@H]1CN(c2cc(Sc3ccc(F)cc3)n(C)N2)C[C@]1(C)O</chem>	Neg_lig_214	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
563	<chem>Cc1cc(S(=O)(=O)[C@H]2CS(=O)(=O)C[C@H]2NCCc2c[nH]c3ccccc23)ccc1F</chem>	Neg_lig_247	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
564	<chem>O=C(C[C@H]1C[NH2+][CCO]1N1C(=O)C2ccccc2C(F)(F)F)c2CC1</chem>	Neg_lig_249	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
565	<chem>CC1(C)NC(=O)N(C[C@H](O)COC2ccc(F)cc2)C1=O</chem>	Neg_lig_289	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
566	<chem>Cc1cc(Nc2ccccc2)n2ncc(-c3ccc(Cl)cc3)c2[nH+]1</chem>	Neg_lig_296	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
567	<chem>Nc1ccc(-c2ccc(N)cc2S(=O)(=O)[O-])c(S(=O)(=O)[O-])c1</chem>	Neg_lig_347	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
568	<chem>COc1ccccc1Nc2c(-c3ccc(O)cc3)nc3ccn23)c1</chem>	Neg_lig_363	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
569	<chem>Cc1ccc(C[NH2+][Cc2ccccc2Cl])s1</chem>	Neg_lig_374	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
					GUCUGGGCGAACA	
570	<chem>Cc1nc(N2CCCCC2)ncc1C(=O)N1C[C@H](c2ccccc2)[C@@H]([NH3+])C1</chem>	Neg_lig_139	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
571	<chem>CCCN(CCC)CC(=O)N1CC(=O)Nc2ccccc21</chem>	Neg_lig_391	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
572	<chem>Cc1cc(N)cc[nH+]1</chem>	Neg_lig_417	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
573	<chem>CCOC(=O)N1CCN(C[C@H](O)COCc2ccc(Cl)cc2)CC1</chem>	Neg_lig_481	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
574	<chem>Cc1cc(NC(=O)CS2nnc(N)s2)no1</chem>	Neg_lig_524	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
575	<chem>CC(C)(C)c1cc(C[N@@H+]2CCOC[C@@H]2CC(=O)Nc2ccc(CO)c2)n[nH]1</chem>	Neg_lig_528	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
576	<chem>NC(=O)c1ccc2c(c1)SCCO)C(=O)c1cccc1C2=O</chem>	Neg_lig_208	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
577	<chem>COC(=O)CNc1cc(C)nc2nc(-c3ccccc3)nn12</chem>	Neg_lig_545	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
578	<chem>c1ccc([C@H](Cn2ccnc2)NC2Cc3ccccc3C2)cc1</chem>	Neg_lig_567	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
579	<chem>O=C(c1nc(-c2ccccc2)n(-c2ccccc2)Cl)c2n1N1CCN(CCO)CC1</chem>	Neg_lig_611	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
580	<chem>CN(C[C@H](O)CO)C(=O)Nc1ccc(SCc2ccco2)cc1</chem>	Neg_lig_620	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
581	<chem>Cc1cc(NCc2cccn2)n2ncc(-c3ccc(Cl)cc3)c2[nH+]1</chem>	Neg_lig_637	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
582	<chem>COCc1cc(C)nc2sc(-c3nc(Cc4ccccc4)no3)c(N)c12</chem>	Neg_lig_675	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
583	<chem>CC[N@@H+]1CC(C[C@H]1Cn1cnc(-c2ccccc2)c1-c1ccc(C#CCO)s1</chem>	Neg_lig_677	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
584	<chem>Fc1cccc1C[NH2+]CCc1c[nH]c2ccccc12</chem>	Neg_lig_748	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
585	<chem>NC1=C(c2nc(-c3ccc(Cl)cc3)cs2)C(=O)CN1C[C@</chem>	Neg_lig_765	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	H]1CCCO1				GUCUGGGCGAACA	
586	Cc1ccsc1[C@@H]1CC[N@H+](Cc2ccc3c(C)cc(=O)oc3c2)C[C@H]1O	Neg_lig_782	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
587	Cc1ccc(-c2nc3ccccc(C)n3c2Nc2ccc3c(c2)OCCO3)o1	Neg_lig_828	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
588	COCC[C@]1(CO)CCC[N@H+](Cc2nc[nH]c2C)C1	Neg_lig_890	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
589	c1cc2c(c(-c3ncncn3)c1)CC[NH2+]C2	Neg_lig_926	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
590	Nc1cccc(C(=O)C[C@@]2(O)C(=O)N(Cc3ccccc3)c3ccccc32)c1	Neg_lig_932	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
591	O=C(Cc1cn2ccsc2n1)N1CCC2(CC1)c1ccccc1C[C@@H]2O	Neg_lig_937	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
592	CCCCOC[C@@H]1(O)Cn1c(Cc2ccccc2)nc2ccccc21	Neg_lig_965	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
593	Cn1c(=O)c2c(nc3n2CC(c2ccccc2)=N3CCO)n(C)c1=O	Neg_lig_978	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
594	CCCCCNc1cc(C(C)C)nc2nc(-c3ccccc3)nn12	Neg_lig_982	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
595	N#CC1=C(N)N(c2c(F)cccc2F)C2=C(C(=O)CCC2)[C@H]1c1ccccc1F	Neg_lig_627	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
596	Cc1ccsc1CN(CCO)C(=O)CCN1cnc2ccccc2c1=O	Neg_lig_1026	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
597	Nc1cc(N2CCC[C@H](c3n[nH]cc3Cc3ccccc3)C2)ncn1	Neg_lig_1082	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
598	Clc1ccccc1Nc1nc2ccccc2o1	Neg_lig_1096	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
599	COCCN[C@H]1CS(=O)(=O)C[C@H]1S(=O)(=O)c1ccc(C)cc1	Neg_lig_1103	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
600	CC(C)(C)c1nnc2[c-]1C(=O)c1ccccc1-2	Neg_lig_1108	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
601	CCOP(=O)(OCC)/C(C#N)=C/	Neg_lig_1114	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	<chem>c1c[nH]c2ccccc12</chem>				UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	
602	<chem>COc1ccc(-c2c[nH+]c3cc(-c4ccc(Cl)cc4)nn3c2N)cc1OC</chem>	Neg_lig_1121	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
603	<chem>CCCc1nc(-c2cc3ccccc(C)c3[nH+]c2N[C@H](C)c2ccccc2)no1</chem>	Neg_lig_1201	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
604	<chem>CNC(=O)[C@H]1C[C@H]([NH3+])CN1C(=O)c1ccc(CSc2ncccn2)o1</chem>	Neg_lig_1246	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
605	<chem>CCCCNc1ncnc2sc3c(c12)CCCC3</chem>	Neg_lig_1251	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
606	<chem>CC[C@]1(CO)CCCN(C(=O)c2ccc(N3CC[NH+](C)CC3)cc2)C1</chem>	Neg_lig_1255	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
607	<chem>COc1ccc(C(=O)c2sc3nc4c(c(-c5ccccc5)c3c2N)C(CCC4)cc1OC</chem>	Neg_lig_1272	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
608	<chem>Cc1ccc(S(=O)(=O)[C@H]2CS(=O)(=O)C[C@H]2N(Cc2ccccc2Cl)cc1</chem>	Neg_lig_1296	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
609	<chem>Cn1c(=O)n(C)c2cc([C@H](O)COc3ccc(C[NH2+])Cc4ccco4)cc3)ccc21</chem>	Neg_lig_1323	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
610	<chem>Cc1cc(C)nc(Nc2cc(S(=O)(=O)/N=c3\ccccc[nH]3)cc2)n1</chem>	Neg_lig_1327	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
611	<chem>COc1cc(F)c(CN2CCN(c3ncc(C#N)c(N)n3)CC2)c(F)c1</chem>	Neg_lig_1359	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
612	<chem>CCOC(=O)c1cnc2c(-c3ccc(OC)c(OC)c3c(CC)nn2c1N</chem>	Neg_lig_1372	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
613	<chem>CCC[N@H+]1CCc2[nH+]c[nH]c2C12CCN(C(=O)CCc1nc(N)n[nH]1)C2</chem>	Neg_lig_1390	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
614	<chem>CC1CC[NH+](C[C@H](O)CN2c3ccccc3Sc3ccccc32)CC1</chem>	Neg_lig_1423	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
615	<chem>Cc1cc(O)c2c(C)cc(C)C2n1</chem>	Neg_lig_1467	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
616	<chem>NC(=O)[C@H]1CCCc2c1[nH]c1ccc(Cl)cc21</chem>	Neg_lig_1481	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
617	<chem>C[C@H](Nc1nc(N)[nH+]c2c1CC[NH2+](CC2)c1cn2ccsc2n1</chem>	Neg_lig_1482	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
618	<chem>Cc1ccc(S(=O)(=O)c2nc3ccccc3nc2NCc2ccco2)cc1</chem>	Neg_lig_1491	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
619	<chem>COCCC[NH2+](Cc1ccc(-c2ccc([C@H](C)O)cc2)o1</chem>	Neg_lig_1507	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
620	<chem>O=C(C(CNC(=O)[C@]12C[NH2+][C[C@H]1C[NH2+](C2)Nc1cc(F)ccc1F</chem>	Neg_lig_1510	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
621	<chem>O=C1CCCN1CCC(Nc1ncnc2onc(-c3ccc(Cl)cc3)c12</chem>	Neg_lig_1515	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
622	<chem>O=c1[nH]cc(CC[NH2+][C@H]2CCOC3(CCOCC3)C2)c(=O)[nH]1</chem>	Neg_lig_1526	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
623	<chem>CCOC(=O)C1CC([NH+](Cc2oc(CO)cc(=O)c2O)CC1</chem>	Neg_lig_137	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
624	<chem>COc1cc2nccc(Oc3ccc(NC(=O)Nc4cc(C)on4)c(Cl)c3)c2cc1OC</chem>	Neg_lig_1295	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
625	<chem>CCOc1ccc(-c2noc(-c3nnn(-c4ccccc4F)c3N)n2)cc1</chem>	Neg_lig_1611	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
626	<chem>OCc1cc(-c2ccccc2OCCn2ccnc2)ccc1F</chem>	Neg_lig_1626	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
627	<chem>C[NH+](C)[C@@H]1C[C@](C)(CO)N(C(=O)Nc2ccc(Cl)c3ncccc23)C1</chem>	Neg_lig_1663	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
628	<chem>Cc1nc(C)c(-c2cc(C)c3c(C)nc(C)nc3[nH+]2)c(N)n1</chem>	Neg_lig_1673	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
629	<chem>CCc1ccccc1NC(=O)c1nnn(CC(=O)Nc2c(C)cc(C)cc2C)c1N</chem>	Neg_lig_1681	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
630	<chem>Cc1ccc(-c2ccc3[nH]c(CO)n3c2)c(-n2cccn2)c1</chem>	Neg_lig_1703	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
631	<chem>CNC(=O)c1ccc(N2C(=S)N(c3cnc(C#N)c(C(F)(F)F)c3)C(=O)C23CCC3)cc1F</chem>	Neg_lig_1737	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
632	<chem>CCOC(=O)c1c(N)</chem>	Neg_lig_1754	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	<chem>nn(C(C)=O)c1-c1cccc1</chem>				ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	
633	<chem>NS(=O)(=O)c1ccc(CN[C@H]2CC(=O)N(c3ccc(Cl)cc3)C2=O)cc1</chem>	Neg_lig_1764	ZTP	Pseudoknot	UAUCAGUUAU AUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
634	<chem>OCC#CCSc1ncnn1-c1cccc1</chem>	Neg_lig_1768	ZTP	Pseudoknot	UAUCAGUUAU AUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
635	<chem>CS(=O)(=O)n1nc(OC(=O)c2cccc2Cl)cc1N</chem>	Neg_lig_1777	ZTP	Pseudoknot	UAUCAGUUAU AUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
636	<chem>COC(=O)[C@@H]1C[C@@H](O)CN1C(=O)c1cc(OCc2cccc(F)c2)cn1</chem>	Neg_lig_1802	ZTP	Pseudoknot	UAUCAGUUAU AUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
637	<chem>O=C1CC[C@@]2(CCCN(C(=O)Cc3ccc(Cl)cc3)C2)CN1CCO</chem>	Neg_lig_1818	ZTP	Pseudoknot	UAUCAGUUAU AUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
638	<chem>CCc1c(C)nc2ncnn2c1Nc1cccc1N1C CN(C(=O)C(C)C)CC1</chem>	Neg_lig_1841	ZTP	Pseudoknot	UAUCAGUUAU AUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
639	<chem>Nc1ccc2c(c1)OC1(CCCCC1)O2</chem>	Neg_lig_1863	ZTP	Pseudoknot	UAUCAGUUAU AUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
640	<chem>CCSC[C@H](N)C(=O)NCc1cnn2cccc12</chem>	Neg_lig_1879	ZTP	Pseudoknot	UAUCAGUUAU AUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
641	<chem>C[NH+](C)[C@@H](CCOc1cccc2cccc12)c1cccc1</chem>	Neg_lig_1887	ZTP	Pseudoknot	UAUCAGUUAU AUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
642	<chem>Cc1c(Cl)cc(C(=O)N2CCC[C@H]2CCO)cc1Cl</chem>	Neg_lig_1909	ZTP	Pseudoknot	UAUCAGUUAU AUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
643	<chem>CC[C@H](O)c1nc2cccc2n1Cc1cccc1Cl</chem>	Neg_lig_1921	ZTP	Pseudoknot	UAUCAGUUAU AUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
644	<chem>Cc1ccc(C[NH+]2CCC(C(=O)N(CCOCc3cccc3)CC2)O)cc1</chem>	Neg_lig_566	ZTP	Pseudoknot	UAUCAGUUAU AUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
645	<chem>Cc1n[nH]c(N)c1-c1cccc1</chem>	Neg_lig_2056	ZTP	Pseudoknot	UAUCAGUUAU AUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
646	<chem>C=CCn1c(-c2c(-c3cccc3)nn2CCO)nc2cccc21</chem>	Neg_lig_2071	ZTP	Pseudoknot	UAUCAGUUAU AUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
647	<chem>CC[C@H](O)C[N@H+]1CCc2[nH]nc(-c3ccc4c(c3)OCO4)cc2C1</chem>	Neg_lig_2086	ZTP	Pseudoknot	UAUCAGUUAU AUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
648	<chem>O=c1c2c(Cl)cccc2ncc1CCN1CCC[C@H](O)C1</chem>	Neg_lig_2099	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
649	<chem>Cc1ccc(Nc2nc(C)c(N3CCN(S(=O)(=O)c4c(C)noc4C)CC3)n2)cc1</chem>	Neg_lig_2114	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
650	<chem>OCc1nccc(-c2ccccc2)s1</chem>	Neg_lig_2151	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
651	<chem>COc1ccc(-c2nc(N)c3c4c(sc3n2)CCCC4)cc1</chem>	Neg_lig_2164	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
652	<chem>COc1ccc(-c2nc3nc(C)cc(Nc4ccc(Br)cc4)n3n2)cc1</chem>	Neg_lig_2178	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
653	<chem>Cc1ccc(OC[C@@H](O)C[N@@H+](2C(CCC[C@H]2C)c(C)c1</chem>	Neg_lig_2199	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
654	<chem>CCCC(=O)Nc1ccc(C(=O)NC[C@H]2CCCC[NH2+](2)c1</chem>	Neg_lig_2208	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
655	<chem>CCSC[C@H](C)[NH2+](C1CCN(S(C)(=O)=O)CC1</chem>	Neg_lig_2266	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
656	<chem>Cc1cc(Nc2ccccc2F)n2nc(-c3ccnc3)nc2n1</chem>	Neg_lig_2276	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
657	<chem>Cc1ccc(-c2c(C(F)(F)F)nn3c(N4CCN(CCO)CC4)cc(C)n23)cc1</chem>	Neg_lig_2285	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
658	<chem>CCCOc1cc(Cl)c(CN2CC[NH2+][C@H](C(=O)NC3CC3)C2)cc1OC</chem>	Neg_lig_2288	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
659	<chem>Cc1ccc([C@H]2CN(C(=O)Cn3nc(C)c4ccccc4c3=O)C[C@H]2[NH3+])o1</chem>	Neg_lig_2317	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
660	<chem>CC[C@H]([NH2+])Cc1cc(N2CCOCC2)ncn1)C(=O)NC1CCCC1</chem>	Neg_lig_2323	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
661	<chem>Cc1ccc(N2C(=O)c3ccccc3[C@H]2Nc2ccccc2)nc1</chem>	Neg_lig_2341	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
662	<chem>N#CC1=C(N)N2C(=C(C#N)[C@H]1c1ccc(Cl)cc1)Se1ccccc12</chem>	Neg_lig_947	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
663	<chem>O=C(N=C1\SC2=C(CCCC2)\C1=C(\O)NC[C@H]</chem>	Neg_lig_2410	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	(O)CO)c1cccc1					
664	C[C@H] (O)CCNS(=O) (=O)c1ccc2c(c1)C CN(C(=O)c1ccc[n H]1)C2	Neg_lig_2476	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
665	COc1ccc(- n2c3c(c(S[C@H] (N)c4cccc5cccc4 5)nc2=O)CCC3)c1	Neg_lig_2511	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
666	COc1ccc(Cl)cc1N c1nc(SC)nc2c1CC C2	Neg_lig_2527	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
667	CC(C)c1nc(CN(C) c2nc(CC[NH3+]) [nH+]c3cccc23)c s1	Neg_lig_1074	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
668	NC(=O)CCn1cc(C [NH2+])CCN2CC NC2=O)c2cccc21	Neg_lig_2546	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
669	COc1cc(OC)c([C @@H]2C(C#N)= C(N)Oc3n[nH]c(C c32)cc1OC	Neg_lig_2547	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
670	COC(=O)c1c(- c2cc(C)ccc2C)jsc 1N	Neg_lig_994	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
671	CCN(CC)S(=O) (=O)c1ccc(Nc2nc3 ccc(Cl)cc3n3nncc2 3)cc1	Neg_lig_644	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
672	CC(=O)Nc1ccc(O CCOc2ccc([N+] (=O)[O-])cc2)cc1	Neg_lig_2609	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
673	O=C(N[C@@H]1 CC[C@H] (C(=O)Nc2cccc(C O)c2)C1)c1cnc2cc cnn12	Neg_lig_2623	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
674	CCc1[nH]nc2c1[C @H] (c1ccc(Cl)cc1)C(C #N)=C(N)O2	Neg_lig_2629	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
675	CC(=O)c1ccc(N[C @H]2OC(=O)c3cc ccc32)cc1	Neg_lig_2651	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
676	Cc1nc(C(C)C)sc1 C(=O)N1CCN[C @H]2CS(=O) (=O)C[C@H]21	Neg_lig_2662	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
677	O=S1(=O)N=C(N CCCCO)c2cccc21	Neg_lig_2698	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
678	C[C@@]1(c2csc(Nc3cccc3Cl)n2)C CC(=O)O1	Neg_lig_2783	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
679	Cn1c(NCc2cccc2)nc2c1c(=O)n(Cc1 cccc1F)c(=O)n2C	Neg_lig_2792	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
					GUCUGGGCGAACA	
680	<chem>CCOc1cc(CNc2[nH+]cc(-c3cccc3)n2C)ccc1O</chem>	Neg_lig_2806	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
681	<chem>CN1CCC[N@+H](C[C@H]2CN(c3nc(C(N)=O)cs3)C[C@H]2CO)C1</chem>	Neg_lig_2814	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
682	<chem>Nc1nc2ncnc-2c(N2CCC(c3[nH+]ccn3CC3CC3)C2)[nH]1</chem>	Neg_lig_2817	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
683	<chem>CNC(=O)[C@+H]1C[C@H](NH3+)CN1C(=O)CSc1n[nH]c(-c2ccco2)n1</chem>	Neg_lig_2837	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
684	<chem>NC(=O)C1=C(NC(CO)c2cccc2S1(=O)=O</chem>	Neg_lig_2874	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
685	<chem>COc1ccc(-c2c(-c3cccc3)oc3ncnc(N)c23)cc1</chem>	Neg_lig_2883	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
686	<chem>Cc1cccc1N1CCCN(C(=O)c2ccc([C@H]3CCC[NH2+])s2)CC1</chem>	Neg_lig_2912	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
687	<chem>COc1ccc(OC[C@H](O)CSc2cccn2)cc1</chem>	Neg_lig_2924	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
688	<chem>COCC(=O)N1C[C@H]2C[NH2+][C][C@+](C(=O)N2CCC(Cn3cccn3)C2)C1</chem>	Neg_lig_2939	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
689	<chem>Cc1cc(C)c(NC(=O)c2sc3nc(C)c(C)c(C)c3c2N)c(C)c1</chem>	Neg_lig_2060	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
690	<chem>OCc1cc(-c2ccc3c(c2)OCCO3)ccn1</chem>	Neg_lig_2968	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
691	<chem>O[C@+H](Cn1cccc1)c1cccc1</chem>	Neg_lig_2982	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
692	<chem>N#Cc1nc(COc2cc(F)c2)oc1NCCCn1ccn1</chem>	Neg_lig_2991	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
693	<chem>COc1cc(NC(=O)c2ccc(-c3ccc(Cl)cc3)o2)c(O)c1</chem>	Neg_lig_3008	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
694	<chem>CC[NH+]1CCN(Cc2ccc(Nc3ncc(F)c(-c4cc(F)c5nc(C)n(C(C)C)c5c4)n3)nc</chem>	Neg_lig_3041	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	2)CC1					
695	<chem>O=C([C@@H]1CCN1Cc1cccc1)N1CCC2(CC1)[NH2+]CCNC2=O</chem>	Neg_lig_3077	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
696	<chem>Nc1c[nH+]c(Nc2ccc(Br)cc2)nc1N</chem>	Neg_lig_3094	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
697	<chem>Cc1ccc(-n2nc(C(=O)N(CCOC)CCO)nc2-c2cccc2)cc1</chem>	Neg_lig_3109	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
698	<chem>CCC[C@H]1CN(C(=O)c2cccc2C#N)C[C@H]1[NH3+]</chem>	Neg_lig_3118	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
699	<chem>CC(C)c1ccc(-c2c(NCC[N@@H+]3CCCC[C@@H]3C)c(=O)c2=O)cc1</chem>	Neg_lig_3230	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
700	<chem>CCn1nc(C)c(NC(=O)CN[C@@H](C)Cn2nc(C)cc2C)c1C</chem>	Neg_lig_3235	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
701	<chem>CCOC(=O)c1[nH]nc(N)c1-c1ccc(OC)cc1</chem>	Neg_lig_3246	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
702	<chem>Nc1c(C(=O)c2cccc2)sc2nc3c(cc12)CCCC3</chem>	Neg_lig_3292	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
703	<chem>O=S(=O)(/N=c1/[nH]c2cccc2nc1N)Cc1ccc(Cl)cc1c1cccc1</chem>	Neg_lig_3321	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
704	<chem>O=C(Nc1cccc1C(=O)NCCO)c1ccco1</chem>	Neg_lig_3351	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
705	<chem>COc1ccc([C@@H]2C(C#N)=C(N)Oc3n[nH]c(C)c32)c(OC)c1OC</chem>	Neg_lig_2884	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	0
706	<chem>c1ccc2c(c1)nc(c1ccc(cc1)N)o2</chem>	0109-0045	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	1
707	<chem>CC(C)(C)NCc1ccc(cc1)[Cl]</chem>	0167-0173	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	1
708	<chem>c1ccc(c(c1)N)I</chem>	0325-0348	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	1
709	<chem>c1ccc2c(c1)nc(Sc1ccc(cc1[Cl])N)s2</chem>	0375-0604	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	1
710	<chem>C(=Cc1nc2cccc2o1)c1ccc(cc1)N</chem>	0632-0836	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	1
711	<chem>CN(C)c1ccc(C=Cc2nc3ccc(cc3[nH]2)N)cc1</chem>	0632-0897	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	1
712	<chem>C(=Cc1nc2cc(ccc2</chem>	0717-0957	Glutamine_RS	Three-way	UAAUCGUUGGCCAGUUUAUCU	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	[nH]1)N)c1ccccc1			junction	GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	
713	CCN(CC)CCOC(c1ccc2c(c1)sc(NC(c1ccc(cc1)N)=O)n2)=O	0812-1025	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	1
714	Cc1c(C)c(C)nc2c1c(c(C(c1ccc(cc1)[Cl])=O)s2)N	0892-0702	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	1
715	C1Oc2ccc(cc2O1)c1c(C#N)c(N)n2c3cccc3nc2c1C#N	2144-0693	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	1
716	CC(C)(C)C(CN1C(=N)N(CCN2CCCC2)c2ccccc12)O	2226-0439	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	1
717	c1ccc2c(c1)ccc1c2nc(c2ccc(cc2)N)[nH]1	2252-1548	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	1
718	Cc1cc2c(cc1N)nc(NC(c1ccc(cc1)C(=O)OC)=O)s2	2284-1574	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	1
719	c1ccc(c(c1)c1nc2c(c(ccc2s1)N)O	2372-3111	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	1
720	Cc1ccc(cc1)S(N(CCO)CC(Cn1c2ccc(c2c2ccccc12)O)(=O)=O	2378-0048	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	1
721	c1cc2c(cc1N)nn(c1ccc(cc1)[Cl])n2	2810-2075	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	1
722	c1cc(ccc1)[Cl])n1nc2ccc(cc2n1)N	2810-4198	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	1
723	Cc1ccc(cc1N)c1nc2cc(ccc2o1)[Cl]	2810-4217	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	1
724	c1cc(c2cccc(c2c1)[Br])c1nc2cc(ccc2o1)N	2810-4224	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	1
725	COc1ccc(cc1[Br])c1nc2cc(ccc2o1)N	2810-4227	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	1
726	COc1ccc(cc1[Cl])c1nc2cc(ccc2o1)N	2810-4228	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	1
727	Cc1cc(C)c2c(c1)nc(c1cc(ccc1[Cl])N)o2	2810-4324	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	1
728	Cc1ccc2c(c1)nc(c1cc(ccc1[Cl])N)o2	2810-4326	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	1
729	COc1ccc(c(CNc2cc(cc2)[Br])c1)OC	2910-1869	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	1
730	C(c1ccc(cc1)[Br])Sc1nc2ccc(cc2s1)N	3167-0427	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	1
731	C(c1ccccc1[Cl])Sc1nc2ccc(cc2s1)N	3167-0436	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	1
732	C(C(c1ccccc1)=O)	3167-0470	Glutamine_RS	Three-way	UAAUCGUUGGCCAGUUUAUCU	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	<chem>Sc1nc2ccc(cc2s1)N</chem>			junction	GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	
733	<chem>CCOC(c1c2ccc(c(c2sc1N)OCc1cccc1)[Br])=O</chem>	3473-2720	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	1
734	<chem>Cc1cc(ccc1[Br])c1nc2cc(ccc2o1)N</chem>	3617-0633	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	1
735	<chem>Cc1cc2c(cc1C)oc(c1cccc(c1C)N)n2</chem>	3639-0494	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	1
736	<chem>CCOc1ccc(CNCCc2ccc3c(c2)OCO3)cc1</chem>	3701-0014	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	1
737	<chem>c1ccc2c(c1)nc(c1ccc(cc1)N)s2</chem>	3729-2175	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	1
738	<chem>CCCCc1ccc(cc1)n1nc2ccc(cc2n1)N</chem>	3738-4868	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	1
739	<chem>CCCCN1CCC(CC1)(C#N)Nc1cccc1</chem>	4237-0134	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	1
740	<chem>C1CCC2C(C1)=C(C#N)c1nc3cccc3n1C=2NCCN1CCOCC1</chem>	4852-0279	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	1
741	<chem>CCCCNc1c2c(c3c4CCCCc4c(nc3s2)N2CCOCC2)nnn1</chem>	5504-0161	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	1
742	<chem>CCOc1cc(CO)cc(c1OCc1ccc(cc1)C(O)=O)[Br]</chem>	6415-0035	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	1
743	<chem>C(C#CCSc1nnc(c2cccc(c2)[Br])o1)O</chem>	7199-0097	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	1
744	<chem>C(C(c1ccc(cc1)[Cl])=O)Sc1nc2cc(c(cc2s1)N</chem>	8007-4809	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	1
745	<chem>C(c1c(cc(c2cccc2)nc1N)c1cccc(c1)[Br])#N</chem>	8008-0679	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	1
746	<chem>C(c1cccc1)n1c(cc(c2ccc(cc2)[Br])n1)N</chem>	8008-1484	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	1
747	<chem>CC1=C(C(C(C#N)=C(N)O1)c1cccc1)C(=O)OCC=C</chem>	8008-9248	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	1
748	<chem>[H]Nc1nnc(COc2c(cc2)C2CCCC2)s1</chem>	8009-2831	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	1
749	<chem>C(c1cc(ccc1[Cl])[Cl])Sc1nnc(N)s1</chem>	8011-5554	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	1
750	<chem>C(C1C(c2c[nH]nc2c2ccc(cc2)F)c2c(c3cccc(cc3)[Cl])n[nH]c2OC=1N)#N</chem>	8011-9730	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	1
751	<chem>C1Oc2ccc(cc2O1)C1C(C#N)=C(N)Oc2c1c(c1ccc(cc1)F)n[nH]2</chem>	8012-0501	Glutamine_RS	Three-way junction	UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
752	<chem>CC1=CC(N(C)C(N1CCCCCNCCO)=O)=O</chem>	8012-3983	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	1
753	<chem>CC(C)(C)c1ccc(CSc2nnc(N)s2)cc1</chem>	8012-4068	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	1
754	<chem>Cc1c(CCNc2ccc(C#N)cc2)c2cc(ccc2[nH]1)OC</chem>	8013-2954	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	1
755	<chem>Cc1cc2NC(Nc3ccc(c(c3)[Cl])F)Sn2n1</chem>	8015-1245	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	1
756	<chem>COc1ccc(CCNc2nc(cs2)c2cccs2)cc1OC</chem>	8018-0995	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	1
757	<chem>CC(C)C1(CCNc2cccc3c2OCO3)C(COC(C)(C)C1</chem>	8018-1268	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	1
758	<chem>c1ccc(cc1)c1ccc(c(c1)c1nc2cc(ccc2o1)N</chem>	8018-2965	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	1
759	<chem>c1cc2c(cc1N)nc(c1cc(ccc1[Cl])[Br])o2</chem>	8018-2966	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	1
760	<chem>c1ccc(cc1)C(c1c(c2ccc(c3ccnc3)nc2s1)N)=O</chem>	8019-6975	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	1
761	<chem>c1cc(N)nc2c1ccc(n2)O</chem>	8019-7722	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	1
762	<chem>C(c1cccc1)c1cc(cc1OCCN)[Cl]</chem>	8019-8811	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	1
763	<chem>C(c1cccc2c1cc[nH]2)NCc1cccc2c1cc[nH]2</chem>	8019-9725	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	1
764	<chem>C(c1cn[nH]c1c1cc(c(cc1)[Cl])N</chem>	8019-9983	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	1
765	<chem>COc1ccc(CNCc2ccc3c(cc[nH]3)c2)c1</chem>	8020-0063	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	1
766	<chem>C(CNCc1ccc2c(cc[nH]2)c1)c1ccc(cc1)F</chem>	8020-0064	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	1
767	<chem>C(CN)c1csc(c2ccc(cc2)C(F)(F)F)n1</chem>	8020-2422	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	1
768	<chem>c1cc(c2c(c1)nc(N)o2)[Cl]</chem>	8020-5450	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	1
769	<chem>CN(C)c1ccc(cc1)NC1CC(N(C1=O)c1ccc(cc1)O)=O</chem>	8440-1765	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	1
770	<chem>CN(C)c1ccc(cc1)NC1CC(N(C1=O)c1ccc(cc1)F)=O</chem>	8440-1773	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	1
771	<chem>c1ccc2c(c1)nc(c1ccc(cc1[Cl])N)s2</chem>	C066-5322	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	1
772	<chem>Cc1ccc(cc1)C1NC(C2Cc3c(CO)cnc(C)c3OC=2N1)=S</chem>	C200-2788	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
773	<chem>CNc1c(c(N)[nH]n1)c1nc(c2ccc(cc2)OC)no1</chem>	C201-1012	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	1
774	<chem>CC(C)(C)c1ccc(cc1)c1cc(N)n(n1)S(c1ccc(cc1)OC)(=O)=O</chem>	C665-0270	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	1
775	<chem>c1cc(ccc1c1cc(N)n(n1)S(c1ccc(cc1)F)(=O)=O)[Br]</chem>	C665-0314	Glutamine_RS	Three-way junction	UAAUCGUUGGCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC	1
776	<chem>O=C(NCCCC1CC1)Nc1cccc2ccccc12</chem>	101298	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA	1
777	<chem>CC(C)=CCC(C(/C)=C/C(N)=O</chem>	108655	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA	1
778	<chem>Cc1cc(nc2cc(ccc12)OC)N1C[C@H](C2CC2)[C@H](C1)N</chem>	12182839	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA	1
779	<chem>C1[C@H](c2ccccc2)[C@H](CN1S(c1ccc2c(c1)NC(N2)=O)(=O)=O)N</chem>	12201213	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA	1
780	<chem>CC(NS(c(cc1)cc2c1sc(C)n2)(=O)=O)=O</chem>	122385	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA	1
781	<chem>Cc1nc(CCN)cc(n1)N(C)Cc1cccc(c1)C(F)(F)F</chem>	12267434	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA	1
782	<chem>C1CN(Cc2ccccc12)c1c2CCNCc2nc(c2ccnc2)n1</chem>	12634687	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA	1
783	<chem>C1C(CN)Oc2c1cc(cc2F)c1ccc2c(cco2)c1</chem>	12766557	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA	1
784	<chem>C(c1cc(ccc1F)c1cc(c(cc1)c1sc(N)n1)O</chem>	12892198	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA	1
785	<chem>Cc1c(C(C(N2CCC(CCCc3ccccc3)CC2)=O)N)c(C)[nH]n1</chem>	13119286	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA	1
786	<chem>C1C(CN1Cc1ccc(cc1)OCCO)Oc1ccc(c1)[Cl]</chem>	13202927	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA	1
787	<chem>C1CCC(C1)(C#N)c1ccc(cc1)c1cccc2CNCCc12</chem>	14224931	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA	1
788	<chem>CC(C)CCOc1cccc(CCNC(C2CC3(CCNCC3)CN2)=O)c1</chem>	14325308	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA	1
789	<chem>C1CN(CCC1C1CCN(CCc2ccccc2)C1)c1ccnc(N)n1</chem>	14604674	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA	1
790	<chem>Cc1cccc1c1nc(CCC(N2CCCC(CCN)C2)=O)on1</chem>	15196499	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA	1
791	<chem>CC(C)(CCCC1(C)C(OC(CO)=C2)C1=CC2=O</chem>	157940	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA	1
792	<chem>Cc1c(C(C(NCCNc</chem>	16899791	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	<chem>2cccnc2=O)N)c(C)[nH]n1</chem>				AUAAAAAACUAA	
793	<chem>C1CNCCc2c1c1C(N(C=Nc1s2)C1c2cccc2c2cccc12)=O</chem>	17311387	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA	1
794	<chem>Cc1cc2CC(CN)Oc2c(c1)c1cnc2cccc2n1</chem>	17587941	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA	1
795	<chem>C1CNCCc2cccc(c3ccc4c3ccc[nH]4)c12</chem>	17741735	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA	1
796	<chem>C1CC(CNC1)c1cc(c2ccc(c(c2)[Cl])[Cl])nc(c1C#N)N</chem>	17917068	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA	1
797	<chem>[H]N1CCCN2c(C1)cc(CNS(c1ccc(cc1)n1cccn1)(=O)=O)n2</chem>	17922447	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA	1
798	<chem>C1CC[C@H]([C@H](C1)CNCCC(Nc1cc(cc1)C(N)=O)=O)O</chem>	18391632	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA	1
799	<chem>C1CN(Cc2ccc(cc2)Oc2ccc(cc2)[Cl])C[C@H]([C@H]1CO)O</chem>	18682916	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA	1
800	<chem>Cc1cnc(CNCc2ccc(cc2)OCC(N2CCOCC2)=O)cn1</chem>	19297220	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA	1
801	<chem>Cc1cc(cc(c1CNc1c2CCNCc2nc(C)n1)[Cl])[Cl]</chem>	20278440	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA	1
802	<chem>CCCCOc(cc1)ccc1OC(Nc(cc(c1)Cl)c1OC)=O</chem>	205832	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA	1
803	<chem>Cc1cc(N)n(CC(N2C[C@H]3COc4ccc4C[C@]3(C2)C(O)=O)=O)n1</chem>	21044903	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA	1
804	<chem>C1CN(CCC1N1C(Nc2cccc12)=O)c1cc(NCCO)nc(N)n1</chem>	21582243	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA	1
805	<chem>CC1CC2(C)CC(C)C1(CO)CO2</chem>	2190-0577	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA	1
806	<chem>CNc1cc(c2ccc(cc2)c2nnc(N)s2)c2cc[nH]c2n1</chem>	25638728	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA	1
807	<chem>C1CN(Cc2c(c3ccc4cccc34)nc12)C(c1cc(N)[nH]n1)=O</chem>	26633940	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA	1
808	<chem>C1COc2cc(ccc2C1=O)c1cc2CC(CN)Oc2c(c1)[Cl]</chem>	26642358	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA	1
809	<chem>C1CNCC2=C1C(NC(NCc1nc(cs1)c1ccc(cc1)F)=N2)=O</chem>	26965809	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA	1
810	<chem>c1cc(c2cccc(c2c1)[Br])c1nc2ccc(cc2o1)N</chem>	2810-4224	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
811	<chem>COc1ccc(cc1[Br])c1nc2cc(ccc2o1)N</chem>	2810-4227	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
812	<chem>Cc1ccc(cc1c1cccc(CCN)c1)F</chem>	31003354	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
813	<chem>C(c1ccc(cc1)c1nc(c2ccc(c(c2)F)nn1CCO)N</chem>	31242301	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
814	<chem>C1CCc2c(C1)nc(C(N1[C@H]3CC[C@@H]1CCNC3)=O)s2</chem>	31575004	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
815	<chem>CN(C)CCNc1ccc2cccc2CO)c2cc[nH]c2n1</chem>	31764292	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
816	<chem>C(Cc1nc(c2cccc2)no1)C(N[C@H]1Cc2cccc2[C@@H]1N)=O</chem>	31852539	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
817	<chem>C1CNCc2cc(CC3Cc4cccc4OC3)cc12</chem>	31917501	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
818	<chem>Cc1cc(CNc2ccc3c(c2)ncs3)n[nH]1</chem>	32903475	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
819	<chem>COc1ccc2cc(ccc2c1)c1cccc1CN</chem>	33557632	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
820	<chem>C1C[C@H](C[C@@H]1N)Nc1c(cc(en1)[Cl])[Cl]</chem>	33921774	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
821	<chem>Cc1c2cc(cc(CNC([C@H](Cc3c[nH]cn3)N)=O)c2[nH]c1c1cccc1)[Cl]</chem>	34268481	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
822	<chem>CCCOc1ccc(cc1)C1C(C#N)=C(N)Oc2c1c(C(C)(C)C)n[nH]2</chem>	3448-7906	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
823	<chem>C1CC(CCOc2cccc2)(CN(C1)c1nnnn1c1cccc1)CO</chem>	34785173	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
824	<chem>c1ccc(cc1)c1c2c(N)ncnc2oc1c1cccc1</chem>	3720-2377	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
825	<chem>CCS(Nc1ccc(cc1)C(N1CC[C@@](C)([C@H](C1)O)O)=O)=O</chem>	39666518	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
826	<chem>C1CSCCN1S(c1ccc(cc1)c1ccc2c(c1)c(N)n[nH]2)(=O)=O</chem>	39837810	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
827	<chem>Cc1ccc(cc1)S(N(C(CN1CCCC1)O)c1cccc1OC)(=O)=O</chem>	4013-2178	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
828	<chem>Cc1cccc(c1OCCN(C(c1cn(CCN)nn1)=O)[Cl]</chem>	41830928	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
829	<chem>COc1ccc2cc(ccc2c1)C1CN(CCO1)C(c1cc(N)[nH]n1)=O</chem>	42028139	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
830	<chem>Cc1nc(CCN)cc(n1)N(C)Cc1cccc2ncccc12</chem>	42532169	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
831	<chem>COc1cccc(c1c1cc(CN)ccc1F)[Cl]</chem>	42929743	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
832	<chem>CC(C1C(c2ccc(cc2)[Br])N(CCO)C(C=1O)=O)=O</chem>	4616-0292	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
833	<chem>C1CCN(CC1)CCNC1=C2CCCCC2=C(C#N)c2nc3cccc3n12</chem>	4708-0071	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
834	<chem>C(CNc1cccn1)CNC1c2cccc2nc(CCN)n1</chem>	47488116	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
835	<chem>CCOC(c1nc2c(C)cccc2c1NCc1cccn1)=O</chem>	4790-1176	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
836	<chem>Cc1nc(N)nc1NC[C@@H]1C[C@H]2C[C@@H]1C=C2</chem>	47913504	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
837	<chem>C(CNCc1ccc2c(c1)OCO2)c1c[nH]c2cccc12</chem>	4964-5174	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
838	<chem>Cc1nc2cc(c(cc2n1CCCO)[Cl])[Cl]</chem>	5119828	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
839	<chem>c1ccc(cc1)Oc1ccc(cc1N)C(c1ccc(c(c1)N)Oc1cccc1)=O</chem>	5172392	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
840	<chem>CCOC(c1nc2c(C)cc(C)cc2c1NCCC(C)O)=O</chem>	5174-4431	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
841	<chem>C(C(NN=Cc1c(ccc1[Cl])[Cl])=O)Nc1cccc2cccc12</chem>	5201830	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
842	<chem>CCCCCc1ccc(cc1)c1ccc(cc1)C1nc(c1)N</chem>	5213078	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
843	<chem>CCOC(CNc1ccc(c1)Oc1ccc(cc1)Oc1ccc(cc1)NCC(=O)OCC)=O</chem>	5224153	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
844	<chem>c1ccc2c(c1)ccc(c2[Cl])Sc1ccc(cc1[C])N</chem>	5250905	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
845	<chem>c1ccc2c(c1)C(Nc1cccc(c1)OC(c1ccc1)=O)=NS2(=O)=O</chem>	5251-2481	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
846	<chem>C1CN(CCC1O)Cc1cccc1[N+](O-)=O</chem>	5269563	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
847	<chem>C1CN(CCN1CC(Cn1c2cccc2c1cccc12)O)Cc1cccc1</chem>	5320336	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
848	<chem>COc1ccc(cc1)c1nnc(N)s1</chem>	5324234	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
849	<chem>CC1(C)CC2=C(C(c3cccc3)[Br])Nc3cccc3N2</chem>	5325779	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
)C(C1)=O					
850	C(c1cccs1)=NNC(c1cccc1N)=O	5331322	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
851	C1c2ccc3ccccc3c2c2c(CN1)cccc1cccc12	5346676	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
852	Cc1cc(ccc1NCC(NN)=O)I	5346837	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
853	CC1CCCCC1=NNC(CNc1ccc(cc1C)I)=O	5347443	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
854	c1cc(ccc1c1cc(C(NN)=O)c2cc(ccc2n1)[Br])N	5350878	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
855	Cc1c2cc(CNC(c3cc(N)[nH]n3)=O)ccc2[nH]c1c1cccc1F	56075039	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
856	CCCc1ccc(cc1)c1ccc(cc1)C(N1CCC(CN)C1)=O	56240352	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
857	[H]N([H])c1nc(n[nH]1)SCCCCCC	5655427	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
858	CCOC(c1cnc2c(ccc2c1Nc1ccc(cc1)N(C)C)C(F)(F)F)=O	5695-0979	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
859	Cc1ccc(C(NCCNc2ccc(cc2[N+]([O-])=O)[Cl])=O)o1	5717805	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
860	C(C(Cn1c2ccccc2c2ccccc12)O)NNC(c1ccccc1)=O	5718973	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
861	CCNC(Cc1ccc(cc1)c1cc2CC(CN)Oc2c(c1)[Cl])=O	57980040	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
862	C(c1ccccc1)c1cccc1OCCN.[Cl]	5924771	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
863	COc1ccc(cc1)C1C2=C(C(c3c[nH]c4ccccc34)Nc3cccc3N2)C(C1)=O	6044923	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
864	C(C(N1c2ccccc2Sc2ccccc12)=O)Sc1nnc(N)s1	6134473	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
865	C(C(c1ccc(cc1)[Br])=O)Sc1nnc(N)[nH]1	6357130	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
866	CCCCSc1nc2c(c3cc(ccc3NC3(CCC3)O2)[Br])nn1	6372845	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
867	CS(c1ccc(c(c1)[N+](O-)=O)NCC(Nc1ccccc1SC(C(C(F)(F)F)(F)F)=O)(=O)=O	6786638	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
868	Cc1ccc(cc1)C(CNc1ccc(cc1)F)=O	6802876	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
869	CC(C)(C)NC(CSc1c(C#	8001-8198	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	<chem>N)cc(C#N)c(N)n1=O</chem>					
870	<chem>CC1(C)CC2=C(C(C1)=O)C1(C(C#N)=C(N)O2)C(Nc2c cc(cc12)[Br])=O</chem>	8004-9540	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA	1
871	<chem>C=Cc1ccc(cc1)c1c sc(N)n1</chem>	8005-0366	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA	1
872	<chem>Cc1cc(C)c2c(c1)nc(c1ccc(cc1O)N)o2</chem>	8007-0773	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA	1
873	<chem>C(C1C(c2ccsc2)c2ccc3cccc3c2OC=1N)#N</chem>	8007-1084	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA	1
874	<chem>Cc1ccc(cc1[Cl])Nc1nc(cs1)c1ccc(cc1)S(N1CCOCC1)(=O)=O</chem>	8007-2266	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA	1
875	<chem>CCOC(c1c2ccc(c(c2sc1NC(C)=O)OCC(CN1CCCCC1)O)[Br])=O</chem>	8008-4440	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA	1
876	<chem>COc1ccc2c(c1)SC(=N)N2CCO</chem>	8010-0067	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA	1
877	<chem>CN1C(c2c(nc(NC COCCO)n2C)N(C)C1=O)=O</chem>	8010-4817	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA	1
878	<chem>Cc1c(CCNc2ccc(C#N)cc2)c2cc(ccc2[nH]1)OC</chem>	8013-2954	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA	1
879	<chem>C1Cc2c(C(=O)OC CO)c(C#N)c(N)nc2C1</chem>	8014-7935	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA	1
880	<chem>Nc(cc1)cc(Cc2c3)c1-c2cc(Cl)c3Cl</chem>	80141	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA	1
881	<chem>COc1cc(c(c(c1OC)OC)[Br])c1nnc(N)o1</chem>	8018-2758	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA	1
882	<chem>CCc1ccc2c(c1)nc(c1ccc(cc1O)N)o2</chem>	8018-2852	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA	1
883	<chem>c1cc2c(cc1N)nc(c1cc(ccc1[Cl])[Br])o2</chem>	8018-2966	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA	1
884	<chem>C(c1ccc2c(c1)OC O2)Nc1c(c[nH]n1)C(N)=O</chem>	8018-4095	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA	1
885	<chem>C1Cc2nc(c(C(c3cc(c3)[Br])=O)n2C1)N</chem>	8018-7423	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA	1
886	<chem>COc1ccc(cc1)c1c(c2ccc(cc2)OC)sc(N)n1</chem>	8019-6726	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA	1
887	<chem>CCc1c2C(C(C#N)=C(N)Oc2n[nH]1)c1cc(c2c(c1)OCO2)OC</chem>	8019-9061	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA	1
888	<chem>C(c1cn[nH]c1c1cc(c(cc1)[Cl])N</chem>	8019-9983	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA	1
889	<chem>C(C1C(c2ccc3cccc3c2OC=1N)c1ccc s1)#N</chem>	8020-0820	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA	1
890	<chem>Cc1c2c(N)nn(Cc3ccc(cc3[Cl])</chem>	8020-1001	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	<chem>[Cl]c2nc(c2cccc2)n1</chem>					
891	<chem>c1cc(c(c1C(c1c(c2ccc(c3ccncc3)nc2s1)N)=O)F</chem>	8020-1052	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
892	<chem>c1cc(cc(c1)[Cl])c1nnc2n1nc(N)s2</chem>	8020-1571	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
893	<chem>C(COC1ccccn1)NCc1ccsc1</chem>	8020-2578	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
894	<chem>c1cc(c(c1c1cn[nH]c1)N</chem>	8020-2683	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
895	<chem>[H]N(CCNC(c1c(N)non1)=O)Cc1c(ccc2cccc12)OCc1cccc1</chem>	8104-04425	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
896	<chem>[H]N(CCNC(c1c(N)non1)=O)Cc1cc(ccc1OCc1cccc1[Cl])[Br]</chem>	8104-04684	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
897	<chem>[H]N(CCNC(c1c(N)non1)=O)Cc1cc(ccc1OCc1cccc1[Cl])</chem>	8104-04926	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
898	<chem>C(CN)c1nnc(o1)SCc1ccc(cc1[Cl])[Cl]</chem>	8388-1007	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
899	<chem>C(CN)c1nnc(o1)SCc1c(cccc1[Cl])[Cl]</chem>	8388-1008	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
900	<chem>C(COC1ccc2c(c1)c1cccc1o2)N.[Cl]</chem>	9188721	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
901	<chem>c1c(cc2c(c1[Cl])nc(N)s2)F</chem>	9190966	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
902	<chem>C(c1ccc2c(c1)OC(O2)Nc1cc(nc(N)n1)[Cl]</chem>	9205277	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
903	<chem>CCOc1ccc2c(c1)sc(NC(CSc1nc(N)n[nH]1)=O)n2</chem>	9207725	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
904	<chem>Cc1cccc(c1C)n1c(c2c(c3ccncc3s2)N)nnc1S</chem>	9209599	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
905	<chem>C(CNC(c1c(c2ccc(c3cccn3)nc2s1)N)=O)c1c[nH]c2cccc12</chem>	9212199	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
906	<chem>CCN(CCCC/C1=N/O)CCCC/C1=N/O</chem>	96491	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
907	<chem>c1ccc2c(c1)nc(c1ccc(cc1[Cl])N)s2</chem>	C066-5322	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
908	<chem>CC(C)c1ccc(cc1)Nc1c(c2cccc2O)nc2ccn12</chem>	C169-0255	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
909	<chem>COC1ccc(cc1OC)C(c1c(c2cccc2o1)N)=O</chem>	C200-2690	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
910	<chem>CSe1c(c(N)n(Cc2cccc2)n1)S(c1cccc1)(=O)=O</chem>	C200-4138	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
911	<chem>CCOC(c1c2c(nc3cccc3n2)n(Cc2ccc</chem>	C201-0688	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	<chem>c(c2)OC)c1N)=O</chem>					
912	<chem>CC1CCN(CC1)c1nc(c(C(=O)OC)s1)N</chem>	C201-1740	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
913	<chem>Cc1cccc1Nc1c(c2ccncc2)nc2ccc(en12)[Br]</chem>	C273-0281	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
914	<chem>Cc1cccc1Nc1c(c2ccc(cc2)N2CCOC2)nc2ncccn12</chem>	C273-0340	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
915	<chem>c1cc(ccc1c1cc[nH]n1)N</chem>	C430-1098	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
916	<chem>COc1ccc(cc1)c1nc(Nc2ccc(cc2F)F)on1</chem>	C749-0018	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
917	<chem>Cc1c(CCC(Nc2ccc(CN3CCCC3)cc2)=O)c(C)n2c(n1)nc(CN)n2</chem>	C908-0509	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
918	<chem>Cc1ccc(cc1C)C(c1c(c(C(Nc2cccc(c2)F)=O)c2ccccn12)N)=O</chem>	D033-0127	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
919	<chem>Cc1ccc2c(c1)C(C1=C(C(N(CCCO)C13C(N(CC=C)c1cccc13)=O)=O)O2)=O</chem>	D063-1068	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
920	<chem>Cc1ccc2c(c1)C(C1=C(C(N(CCO)C13C(N(CC=C)c1cccc13)=O)=O)O2)=O</chem>	D063-1117	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
921	<chem>CCCCC(CC)n1c(c(c1)O)N</chem>	D068-0219	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
922	<chem>CC(C)CNc1c(nc(c2cccc2)o1)S(c1ccc(cc1)[Cl])(=O)=O</chem>	D072-0403	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
923	<chem>CC(C)Nc1c2c(c(C)nn1)nnn2Cc1cccc1[Cl]</chem>	D172-0473	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
924	<chem>CC(CCC(NCCc1nc2cccc2n1Cc1c(C)c(C)cc(C)c1C)=O)O</chem>	D186-0394	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
925	<chem>Cc1cc(Nc2cccc2)n2c(n1)nc(c1ccc(c1)[Cl])n2</chem>	D245-0159	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
926	<chem>CC(c1cccc(c1)Nc1cc(c2ccc(cc2)OC)nc(C)n1)=O</chem>	D482-2054	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
927	<chem>Cc1cc(NCC(N2CCN(CC2)c2ccc(cc2)F)=O)n2c(n1)nc(c1cccn1)n2</chem>	D494-0506	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
928	<chem>Cc1ccc2cc(c(Nc3ccc(cc3)F)nc2c1)c1nc(C)on1</chem>	D704-1692	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
929	<chem>CCOC(c1cnc2c(c3ccc(cc3)[Br])c(C)nn2c1N)=O</chem>	D718-0691	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1
930	<chem>c1ccc(cc1)n1c(c(c2nc3cccc3s2)nn1)</chem>	D731-0066	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUUUUUACUAA	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	N					
931	<chem>CCC(C)(C)NC1=C(C(C1=O)=O)c1ccc(C)cc1</chem>	E470-0146	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUAAAAACUAA	1
932	<chem>CCC(C)NC1=C(C(C1=O)=O)c1ccc(cc1)C(C)C</chem>	E511-0764	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUAAAAACUAA	1
933	<chem>CCOc1ccc(cc1)c1nc(c2c(N)n(c3cccc(c3C)[Cl])nn2)on1</chem>	E595-0532	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUAAAAACUAA	1
934	<chem>COc1ccc(c(c1)c1nc(Nc2cc(ccc2OC)[Cl])on1)OC</chem>	E679-0020	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUAAAAACUAA	1
935	<chem>C[N+](C)(C)CC(O)=O</chem>	NCGC00015150-04	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUAAAAACUAA	1
936	<chem>CN(C)CCN(Cc1ccc(c1)[Cl])c1ccccn1</chem>	NCGC00016672-04	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUAAAAACUAA	1
937	<chem>C(c1cc(ccc1c1cn[nH]c1)NC(Nc1nnc(c2ccncc2)s1)=O)#N</chem>	NCGC00247866-04	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUAAAAACUAA	1
938	<chem>C(C(Nc1ccc(cc1)n1c(cc(C(F)(F)F)n1)c1ccc2c(cc3cccc23)c1)=O)N</chem>	NCGC00346490-01	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUAAAAACUAA	1
939	<chem>CC(C)n1cnc2c(Nc3cccc(c3)NC(C=C)O)nc(NC3CCC(CC3)N(C)C)nc12</chem>	NCGC00346964-01	PreQ1	Pseudoknot	AGAGGUUCUAGCUACACCCUCU AUAUAAAAACUAA	1
940	<chem>C(=Cc1nc2cccc2o1)c1ccc(cc1)N</chem>	0632-0836	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
941	<chem>Cc1ccc(cc1)NCC(c1ccc(cc1)c1cccc1)=O</chem>	0836-0042	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
942	<chem>C1c2cccc2c2ccc(cc12)c1csc(N)n1</chem>	0846-0051	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
943	<chem>Cc(cccc1)c1NC(NCCN1CC1)=O</chem>	101266	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
944	<chem>O=C(NCCCN1CC1)Nc1cccc2cccc12</chem>	101298	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
945	<chem>Nc1nc(N)nc(Nc(cc2)ccc2Br)c1/C=N/c(cc1)ccc1Br</chem>	103520	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
946	<chem>[O-][N+](c(cc1)cc(C(c2c3)=O)c1-c2cc(Br)c3/N=C(C(F)(F)F)\NO)=O</chem>	107582	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
947	<chem>C(CSc1nc(cccc2)c2s1)Nc1cccc1</chem>	117908	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
948	<chem>C1CC(CNC1)(CNCc1cccc(c1)OCc1cccc1)O</chem>	12262594	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
949	<chem>C1C(CN)Oc2c1cc(cc2F)c1ccc2c(cco2)c1</chem>	12766557	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
950	<chem>CC(c1cc(c2ccccc2)[nH]n1)N(C)C(c1cn(CCN)nn1)=O</chem>	12801231	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
951	<chem>C1C(CN)Oe2c1cc(cc2[Cl])c1ccc(cn1)C(N)=O</chem>	13047935	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
952	<chem>O=C1OC(c2ccc(-c3ccccc3)nc3ccccc23)=NN1</chem>	130847	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
953	<chem>C1C(CN1Cc1ccc(cc1)OCCO)Oc1ccc1[Cl]</chem>	13202927	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
954	<chem>Nc(ccc(Oc(cc1cc([N+](O-)=O)c1N)c1c1[N+](O-)=O</chem>	133351	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
955	<chem>CC(C)Oc1cc(NCC2=Cc3ccc(cc3NC2=O)F)nc(N)n1</chem>	13416689	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
956	<chem>CN(CCO)C[C@@H]1CN(Cc2ccccc3c4ccccc4sc23)C[C@@H]1CO</chem>	13609905	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
957	<chem>CN(Cc1cccc(c1)OCC=C)c1c2ccccc2nc(CCN)n1</chem>	13692816	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
958	<chem>C1CC(CCc2ccccc2C(F)(F)F)CN(C1)C(CN)=O</chem>	13741411	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
959	<chem>NCC(Nc(ccc(Cl)c1c1c(c1ccc[nH]1)=O)=O</chem>	140873	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
960	<chem>C1CCC(C1)(C#N)c1ccc(cc1)c1cccc2CNCCc12</chem>	14224931	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
961	<chem>Cc1cc(NC(Nc(cc2)ccc2SC)=O)nc1</chem>	142269	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
962	<chem>C1COCC(CN1)CNC(Nc1cccc(c1)c1ccc(cc1)F)=O</chem>	14244960	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
963	<chem>CN(C)c1c(enc(c2ccc3CC(CN)Oe23)n1)F</chem>	14250223	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
964	<chem>Cc1ccc(c2ccccc2C(CN)c2ccccc12</chem>	14279637	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
965	<chem>C1CNCc2cc(C(NC3c4ccccc4c4ccccc34)=O)nn2C1</chem>	15136552	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
966	<chem>Cc1c(cc(cc1[Cl])C(NCC(Cc1ccc1)CO)=O)[Cl]</chem>	15537048	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
967	<chem>C1CN(CCC1Oc1ccc(cc1)F)c1cc(NC(CO)nc(N)n1</chem>	15760058	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
968	<chem>C1CC(CN(C1)CCNC(c1ccc2c(ccs2)c1)=O)CO</chem>	15947215	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
969	<chem>CCOc1ccc(CN2C(C(C2)C(O)=O)Oc2ccccc2</chem>	16013629	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	(c2)F)cc1CO					
970	C(CN)c1cccc(c1)c1ccc(cc1[Cl])F	16088353	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
971	Cc1c(C(C(NCCNc2ccnc2)=O)N)c(C)[nH]n1	16899791	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
972	Cc1cc2CC(CN)Oe2c(c1)c1cnc2ccccc2n1	17587941	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
973	C1CC(CNC1)c1cc(c2ccc(c2)[Cl])[Cl]nc(c1C#N)N	17917068	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
974	CCCC(c1cccs1)Nc1c2CCNc2nc(c2ccnc2)n1	17936868	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
975	C1CC(c2cccc(c2)c2cc(N)nc3c2cc[nH]3)NC1	18100777	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
976	C1[C@@H](CNC(Nc2cc(ccc2[Cl])F)F)=O)NC[C@H]1F	18739450	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
977	C(CN)c1ccc(CN2CCC(CC2)(c2ccccc2)C(F)(F)F)O)cc1	18809502	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
978	CC(c1ccc2c(cc[nH]2)c1)NC1CCN(C1)c1c2c(ncn1)[nH]cn2	18958506	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
979	C1CCN(C1)C(CCc1cc2CN(CN2n1)C(C1CNCCO1)=O)=O	18969954	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
980	Cc1c(cccc1NCc1cccn1)C(Nc1cnc2CCCCn12)=O	19005272	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
981	C(CN)c1nnen1c1ccc2ccccc12	19267055	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
982	Cc1nc(CCN)cc(n1)N1CCN(C1)c1cccc1[Cl]	19416537	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
983	Cc1ccc(cc1[Cl])N1CCC(CC1)N[C@H]1CC[C@H](C1)N	19498560	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
984	C1CNCc2c1c(NC[C@@H]1C[C@H]3C[C@@H]1C=C3)nc(c1cccn1)n2	20252371	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
985	Cc1cc(cc(c1CNc1c2CCNc2nc(C)n1)[Cl])[Cl]	20278440	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
986	CCCCOc(cc1ccc1OC(Nc(cc(c1)Cl)c1OC)=O	205832	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
987	Cc1cccc(NC(Nc2nc(C)ccc2)=S)n1	20618	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
988	Cc1cccn1NC(Nc1ncccc1C)=S	20619	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
					AAAAAGGG	
989	<chem>C1CNc2c1c(NC1COc3ccccc3O1)nc(c1ccnc1)n2</chem>	20674759	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
990	<chem>CC(c1ccc(cc1)c1c cc(c(c1)F)NC(CN) =O)OC</chem>	20734365	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
991	<chem>C1CN(CCC1NCC c1c[nH]cn1)c1nc2 ccc(cc2s1)[Cl]</chem>	20802556	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
992	<chem>C1Oc2ccc(cc2O1) c1c(C#N)c(N)n2c3 ccccc3nc2c1C#N</chem>	2144-0693	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
993	<chem>COc1cccc(c1)c1cc ccc1NC(C1CCN(CC1)c1ccnc(N)n1) =O</chem>	21531690	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
994	<chem>COc(cc1)ccc1/ N=N/c1c(N) [nH]nc1N</chem>	21678	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
995	<chem>COc1ccc(CCN(Cc 2ccncc2)C(CC2C OCCN2)=O)cc1</chem>	21791855	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
996	<chem>C(CNc1ccnc1)N C(c1nc(Nc2ccccc 2)nc1)=O</chem>	22517399	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
997	<chem>Cc1c2ccc(cc2oc1C (NCCCNc1ccnc1)=O)OC</chem>	22734195	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
998	<chem>Cc1c2c(ncnc2sc1C)N1C[C@H] (c2ccc(cc2)OC) [C@H](C1)N</chem>	25720738	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
999	<chem>C1CN(Cc2c(c3ccc c4ccccc34)nc12) C(c1cc(N) [nH]n1)=O</chem>	26633940	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1000	<chem>C1CNCC1NS(c1c ccc(c1)C(NCCc1c cccc1)=O)(=O)=O</chem>	26804304	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1001	<chem>COc1ccc(CCCNc2 c3CCNCCc3nc(N) n2)cc1OC</chem>	27263777	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1002	<chem>Cc1cc2c(cc1C)oc(c1ccc(cc1O)N)n2</chem>	2783-3499	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1003	<chem>c1cc(cc(c1) [Cl])n1nc2ccc(cc2 n1)N</chem>	2810-4198	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1004	<chem>c1cc(c2ccccc2c1) [Br])c1nc2cc(ccc2 o1)N</chem>	2810-4224	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1005	<chem>CCCOc(cc1)ccc1- c1nc(- c(cc2)ccc2N)cs1</chem>	281624	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1006	<chem>Nc1ccc(Cn(ccc2c3 4)c2ccc4nc(N)nc3 N)cc1.Cl</chem>	309401	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1007	<chem>C(c1ccc(cc1)c1nc(c2ccc(c(c2)F)F)nn 1CCO)N</chem>	31242301	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1008	<chem>Cc1c(c2c(c3ccccc 3)ncn2CCCN(CC</chem>	31750799	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	O)CCO)[nH]cn1				AAAAAGGG	
1009	C1CNCC2cc(Cc3Cc4cccc4OC3)cc c12	31917501	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1010	C1CN(CCC1NCc1 nc(N) [nH]n1)c1nc2ccc(c c2s1)[Cl]	32629911	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1011	C1CC(C(C(C(N2C C(c3cccc3C2)O) =O)=C1c1cccc1) =O	32885020	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1012	C1CN(CCC1n1cc(c2cccn2)nn1)c1c 2c(nc(N)n1) [nH]cn2	33118185	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1013	Nc1n[nH]c(Nc2cc ccc2)n1	331208	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1014	COc(cc12)ccc2nc(cc(cc2)Cl)c2c1C# N	33173	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1015	Clc(ccc(- c1c(Cc2c- 3cccc2)c3n[nH]1)c 1)c1Cl	331968	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1016	C1CC(CCN(C1)C(CCc1ccc(c2ccc(cc 2)[Cl])[nH]1)=O) (CO)O	33269848	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1017	Cc1ccc(cc1)c1cc(C(N[C@@H]2CN C[C@H]2O)=O)c 2cccc2n1	33446163	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1018	COc1ccc2cc(ccc2c 1)c1cccc1CN	33557632	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1019	Cc1ccc2c(c1)c(CN c1c3CCNCc3nc(N)n1)nn2C	34365043	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1020	COc1cccc(c1)c1nc c(CNC([C@H]2C C[C@H] (C2)N)=O)s1	35144470	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1021	C(CN)C1CN(CCO 1)c1cc(c2cccc2)n c2cnn12	35432137	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1022	Cc1cc(ccc1[Br])c1 nc2cc(ccc2o1)N	3617-0633	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1023	CCCCc1ccc(cc1)n 1nc2ccc(cc2n1)N	3738-4868	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1024	CCC(CC) (C(N)=O)SCC=C	37883	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1025	CC(c1ccc(cc1)c1c cc(cc1)c1nnc(N)s1)N1CCOCC1	39723040	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1026	COc1cccc1OC1C CN(CC1)Cc1cccc(CCN)c1	39780332	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1027	C1CSCCN1S(c1cc c(cc1)c1ccc2c(c1)	39837810	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	<chem>c(N)n[nH]2(=O)=O</chem>				AAAAAGGG	
1028	<chem>Cc1cc(C)n(CC(CO)c2ccc(cc2)[Cl])O)n1</chem>	4013-0076	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1029	<chem>Cc1ccc(cc1)S(N(C(CCN1CCCCC1)O)c1ccccc1OC(=O)=O</chem>	4013-2178	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1030	<chem>NC(NC(Nc(cc1)cc1Cl)=S)=N</chem>	403374	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1031	<chem>Cc(cc1)ccc1Cl=CSSC1=S</chem>	40467	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1032	<chem>C(Cc1ccccc1)CN1CCCN(CC1)c1cc(N)nc(N)n1</chem>	41736108	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1033	<chem>Cc1cccc(c1OCCN(C(c1cn(CCN)n1)=O)[Cl]</chem>	41830928	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1034	<chem>COc1ccc2cc(ccc2c1)C1CN(CCO1)C(c1cc(N)[nH]n1)=O</chem>	42028139	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1035	<chem>CCNC(c1ccccc1)c1ccc(cc1CN)F=O</chem>	42044437	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1036	<chem>C1CNCc2c1c1c(NCc3cc(c4ccco4)on3)ncc1s2</chem>	42424648	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1037	<chem>Cc1cc(c(cc1[Cl])O)C)NC(c1ccccc1C1CCNC1)=O</chem>	45877478	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1038	<chem>C1CN(CC(C(O)=O)N1)c1nnnn1c1c(cc(cc1)Oc1ccccc1</chem>	46257953	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1039	<chem>Cc1ccsc1CN(CCN(C)C)C(CN)=O</chem>	47645371	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1040	<chem>C1CN(CCC1Nc1c2CNCC2nc(c2ccncc2)n1)Cc1ccccc1</chem>	48129446	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1041	<chem>CC[n+]1cn(CC(COc2ccccc2)OC)O)c2ccccc12</chem>	5010-0656	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1042	<chem>Cc1nc(SC)nc(N2CC2)c1Br</chem>	50199	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1043	<chem>Nc(cc1)ccc1NC(Nc1ccccc1)=S</chem>	509563	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1044	<chem>Cc1nc2cc(c(cc2n1CCCO)[Cl])[Cl]</chem>	5119828	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1045	<chem>c1ccc(cc1)Oc1ccc(cc1N)C(c1ccc(c(c1)N)Oc1ccccc1)=O</chem>	5172392	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1046	<chem>CCOC(c1enc2c(C)cc(C)cc2c1NCC(C)O)=O</chem>	5174-4431	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1047	<chem>c1ccc(cc1)C(c1cc(ccc1N)Sc1ccc(c(c</chem>	5180537	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	1)C(c1ccccc1)=O) N)=O				AAAAAGGG	
1048	C(C(NN=Cc1c(ccc c1[Cl]) [Cl])=O)Nc1ccccc2 ccccc12	5201830	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1049	CCCCCc1ccc(cc1) c1ccc(cc1)c1ncc(c n1)N	5213078	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1050	c1ccc2c(ccc(c2c1) Oc1ccc(cc1[Cl])N) [Cl]	5215844	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1051	CC(c1ccc(cc1)Oc1 ccc(cc1)N)=O	5228159	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1052	C1CCN(CC1)CC(Cn1c2ccc(cc2c2cc (ccc12)[Cl])[Cl])O	5236854	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1053	CC12CCC(CN(CC (Cn3c4ccc(cc4c4c c(ccc34)[Br]) [Br])O)C1)C2(C)C	5236945	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1054	c1ccc(cc1)c1c(en(c2ccccc2)n1)C(Nc 1cc(cc(c1)Oc1ccccc c1)N)=O	5248546	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1055	c1ccc2c(c1)ccc(c2 [Cl])Sc1ccc(cc1[C l])N	5250905	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1056	[H]N([H])c1c(C# N)c2c(nc3ccccc3n 2)n1Cc1ccccc1	5253879	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1057	C1CN(CCN1CC(Cn1c2ccccc2c2ccc cc12)O)Cc1ccccc1	5320336	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1058	CC(c1ccc(cc1)N)= NNc1nc(C)cc(c2cc ccc2)n1	5339282	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1059	C(C(NN)=O)Nc1c cc(cc1[Br])[Cl]	5345379	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1060	Cc1cc(ccc1NCC(NN)=O)I	5346837	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1061	CC1CCCCC1=NN C(CNc1ccc(cc1C)I)=O	5347443	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1062	c1cc(ccc1c1cc(C(NN)=O)c2cc(ccc2 n1)[Br])N	5350878	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1063	Cc1ccccc1Cn1c2c cccc2nc1c1c(N)no n1	5408-3036	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1064	Br(c1c1ccc1- c1sc(N=C2/ SC=C(c(cc3)ccc3 Br)N2)n1	55691	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1065	Cc1c2cc(CNC(c3c c(N) [nH]n3)=O)ccc2[n H]c1c1ccccc1F	56075039	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1066	C1CCC(C1)NCC(COc1ccc(cc1)OC C(CNC1CCCC1)	5648415	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	O)O					
1067	[H]N([H])c1nc(n[nH]1)SCCCCCC CC	5655427	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1068	C(c1ccccc1)Oe1cc c(cc1)C1Nc2cccc3 cccc(c23)N1	5661401	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1069	COe1cc(c(cc1NC(C(NCCN1CCNCC 1)=O)=O)OC)[Cl]	5688029	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1070	C(=Cc1ccc(cc1[Cl]) [Cl])C(c1ccccc(c1) N)=O	5689908	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1071	Cc1ccc(C(NCCNc 2ccc(cc2[N+] ([O-])=O) [Cl])=O)o1	5717805	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1072	C(CN1CCOCC1) C(Nc1ccc(cc1C(c1 ccccc1)NCC(NN =O)[Br])=O	5808034	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1073	C(C(Cn1c2cccc(cc2 c2cc(ccc12)[Br]) [Br])O)NCc1ccco1	5864844	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1074	[H]N(Cc1cc(c(c(c 1) [Cl])OCC(N)=O)O C)c1ccc(cc1)N1C COCC1	5868-0480	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1075	C(CN)c1nc(c2cccc c2n1)NCc1cn[nH] c1c1cccs1	58789773	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1076	C(CCO)CN(Cc1cc ccc1)c1c2cccc2nc (CCN)n1	58803915	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1077	Cc1c2c(nc(CCN)n c2sc1C)N(CCN(C) C)Cc1ccccc1	59025931	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1078	COe1cc(CC=C)cc c1OCC(CN1CCC(CC1)Cc1ccccc1)O .[Cl]	6046571	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1079	C1CCCCC2c(C(C CC1)c(C(N)=O)c(N)s2	6132195	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1080	Nc(cc1)ccc1- c(nc12)c(- c(cc3)ccc3N)nc1n c(N)nc2N	61642	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1081	C(c1c(cc(c2ccc(cc 2)F)nc1N)c1ccnc 1)#N	6233-1975	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1082	[H]N(Cc1cc(c(c(c 1) [Cl])OCc1cccs1)O CC)Cc1ccnc1	6408-0223	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1083	C(c1ccco1)NC1C(c2cccc3ccccc1c23) NS(c1ccc(cc1) [Cl])(=O)=O	6432111	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1084	O=C(c(cc1)cc(C(N c(cc2)ccc2C2=NC CN2)=O)c1Cl)Nc(cc1)ccc1C1=NCC	67436	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	N1					
1085	<chem>C(CC(=O)OC1C(Nc2ccc(cc2C(c2ccc(Cl)=N1)[Br])=O)CN.[Br]</chem>	6748287	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1086	<chem>Nc1cc(N=[N+](c2c(C3)ccc(N)c2)[O-])c3cc1</chem>	70534	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1087	<chem>CC1C=C(C)C2C(C)C1(CO)COC2c1cccc1O</chem>	8005-2272	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1088	<chem>C(c1cccc1)c1nnc(N)s1</chem>	8008-6271	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1089	<chem>C1CCc2c(C1)c(C(c1cccc1)=O)c(N)s2</chem>	8010-1935	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1090	<chem>Cc1c(CCNc2ccc(C#N)cc2)c2cc(ccc2[nH]1)OC</chem>	8013-2954	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1091	<chem>Nc(cc1)cc(Cc2c3)c1-c2cc(Cl)c3Cl</chem>	80141	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1092	<chem>Cc1c(c2csc(Nc3ccc(cc3)C(F)(F)F)n2)sc(C)n1</chem>	8015-5644	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1093	<chem>CCN1CCc2c(C1)c1c(c(C(Nc3ccc(cc3)C(F)(F)F)=O)sc1n2)N</chem>	8016-6889	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1094	<chem>C1C(c2ccc(c(c2)[Br])F)c2c(NC(=O)nc(N)s2</chem>	8019-3634	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1095	<chem>C1CN2C(=CSC2=N1)c1cccc(c1)N</chem>	8019-6474	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1096	<chem>CN1C(c2c(en(c3ccc3N)c2c2cccc2F)N(C)C1=O)=O</chem>	8019-7142	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1097	<chem>c1cc(N)nc2c1ccc(n2)O</chem>	8019-7722	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1098	<chem>COc1ccc(cc1)c1c(CN)c[nH]n1</chem>	8019-7792	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1099	<chem>c1cnccc1c1nc2ncn(c(N)n2n1</chem>	8020-2786	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1100	<chem>Cc1c2[nH]c(ccc3)c3c2ccc1CCN</chem>	81703	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1101	<chem>CCc1ccc(cc1)OCC#CCNCC=C</chem>	9118214	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1102	<chem>CCNCC#CCOc1c(cc(cc1)[Br]</chem>	9126666	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1103	<chem>Cc1ccc(c(c1)[Cl])OCC#CCNC.[Cl]</chem>	9128115	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1104	<chem>CC(c1ccc(cc1)c1c(cc(CNCCc2c[nH]c3cccc23)o1)O.</chem>	9135919	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	[Cl]					
1105	<chem>c1c(cc2c(c1[Cl])nc(N)s2)F</chem>	9190966	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1106	<chem>COc1cc(cc(c1OC)OC)c1nc(c2cccc(c2)N)n[nH]1</chem>	9204334	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1107	<chem>CCOc1ccc2c(c1)sc(NC(CSc1nc(N)n[nH]1)=O)n2</chem>	9207725	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1108	<chem>CSc1ccc(cc1)OCCN</chem>	9254473	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1109	<chem>Cn1c(c(C(C=C2=O)c(cc3)C2=O)c3c2c1cccc2</chem>	92937	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1110	<chem>S=C1Oc(ccc(-c2cccc2)c2)N1</chem>	93817	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1111	<chem>CCN(CCCC/C1=N\O)CCCC/C1=N\O</chem>	96491	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1112	<chem>c1ccc2c(c1)nc(c1ccc(cc1[Cl])N)s2</chem>	C066-5322	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1113	<chem>Cc1cccc(c1)NCc1nc2cccc2n1C</chem>	C147-0043	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1114	<chem>C(c1ccc(cc1)[Cl])N1c2cccc2C2=C(C(C(C#N)=C(N)O2)c2cccc2)S1(=O)=O</chem>	C200-3388	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1115	<chem>CSc1c(c(N)n(Cc2cccc2)n1)S(c1cccc1)(=O)=O</chem>	C200-4138	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1116	<chem>CC1CCN(CC1)c1nc(c(C(=O)OC)s1)N</chem>	C201-1740	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1117	<chem>CCN1CCc2c(C1)c1c(c(C(Nc3cccc3C)=O)sc1n2)N</chem>	C611-0673	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1118	<chem>C(CCCN=C(N)N=C(N)Nc1ccc(cc1)[Cl])CCN=C(N)N=C(N)Nc1ccc(cc1)[Cl]</chem>	NCGC00016246-12	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1119	<chem>CCN1C=C(C(O)=O)C(c2cc(c(nc12)N1CCNCC1)F)=O</chem>	NCGC00016927-10	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1120	<chem>c1cc2C(c3cc(cc3C(c2c(c1O)=O)O)C(O)=O)=O</chem>	NCGC00018199-06	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1121	<chem>[H][C@@]12CC[C@@H]([C@@]1(C)CC[C@@]1([H])[C@@]3([H])CCC(C=C3CC[C@@]12[H])=O)OC(CCc1cccc1)=O</chem>	NCGC00159356-02	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1122	<chem>CCCCN(CCCC)C(c1cc(cc2C(=Cc3ccc(cc3)</chem>	NCGC00167490-02	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	[Cl]c3cc(ccc3c12)[Cl][Cl]O					
1123	CCCCN(CCCC)C CC(c1cc2c(cc2 c2cc(ccc12)C(F) (F)F)[Cl])[Cl]O	NCGC00179250-04	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1124	CCCCCCCCCCC CCCCC(=O)O[C @H]1[C@H] ([C@H]([C@H] ([C@H]([C@H] (C) [Cl])NC([C@H] 2C[C@H] (CCC)CN2C)=O) O[C@H]1SC)O) O.[Cl]	NCGC00185773-02	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1125	Cc1ccc(cc1c1ccc2 c(c1)enc(NCCN1C COCC1)n2)C(Nc1 cccc(c1)C(F) (F)F)=O	NCGC00263206-02	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1126	C[C@H](C(C) (C)C)NCc1ccc2c(c 1)nc(NC(c1ccc(c3 cn[nH]c3)s1)=O)n 2CCc1cccc1	NCGC00344999-01	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1127	C=CC(Nc1ccc2c(c 1)c(Nc1ccc(c(c1) [Cl])OCc1cccc(c1) F)ncn2)=O	NCGC00346478-02	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1128	C(C(Nc1ccc(cc1)n 1c(cc(C(F) (F)F)n1)c1ccc2c(c cc3cccc23)c1)=O)N	NCGC00346490-01	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1129	CN1CCN(CC1)c1 ccc(cc1)Nc1ncc(c n1)Sc1cccc(c1)NC (C=C)=O)[Cl]	NCGC00346497-01	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1130	Cc1cccc1C(c1ccc (cc1[Cl])Nc1ccc(c c1N)[Br])=O	NCGC00346804-01	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1131	CCC(=C(c1ccc(cc 1)O)c1ccc(cc1)OC CNC)c1cccc1	NCGC00346806-01	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1132	C1CC1NCc1cccc (c1)NC1=CC(=c2c cc(cc2)=C2C=CC(C=C2O)=O)NN1	NCGC00346954-01	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1133	CC(C)n1cnc2c(Nc 3cccc(c3)NC(C=C)=O)nc(NC3CCC(CC3)N(C)C)n12	NCGC00346964-01	SAM_II	Pseudoknot	UCGCGCUGAUUUAAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG	1
1134	CCN(CC)CCOC(c 1ccc2c(c1)sc(NC(c 1ccc(cc1)N)=O)n2)=O	0812-1025	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAUAGC CAGCGUAGGGAAGUGCUG	1
1135	Cc(cccc1)c1NC(N CCN1CC1)=O	101266	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAUAGC CAGCGUAGGGAAGUGCUG	1
1136	O=C(NCCCN1CC 1)Nc1cccc2cccc1 2	101298	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAUAGC CAGCGUAGGGAAGUGCUG	1
1137	Nc1nc(N)nc(Nc(cc	103520	TPP	Three-way	CAGUACUCGGGGUGCCCUUCUG	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	<chem>2)ccc2Br)c1/C=N/c(cc1)ccc1Br</chem>			junction	CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	
1138	<chem>CCC(C)N(C(C)=C1)N(C(C)CC)C1=O</chem>	120844	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1139	<chem>Cc1cc(nc2cc(ccc12)OC)N1C[C@H](C2CC2)[C@H](C1)N</chem>	12182839	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1140	<chem>Cc1nc(CCN)cc(n1)N(C)Cc1cccc(c1)C(F)(F)F</chem>	12267434	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1141	<chem>C1CN(Cc2cccc12)c1c2CCNCc2nc(c2ccnc2)n1</chem>	12634687	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1142	<chem>C1C(CN)Oc2c1cc(cc2F)c1ccc2c(cco2)c1</chem>	12766557	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1143	<chem>C(c1cc(ccc1F)c1cc(c(cc1)c1csc(N)n1)O</chem>	12892198	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1144	<chem>O=C1OC(c2cc(-c3cccc3)nc3cccc23)=NN1</chem>	130847	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1145	<chem>C1C(CN1Cc1ccc(cc1)OCCO)Oc1ccc(cc1)[Cl]</chem>	13202927	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1146	<chem>C1CC(CCc2cccc2C(F)(F)F)CN(C1)C(CN)=O</chem>	13741411	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1147	<chem>C1CCC(C1)(C#N)c1ccc(cc1)c1cccc2CNCCc12</chem>	14224931	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1148	<chem>CC(C)CCOc1cccc(CCN(C2CC3(CCNCC3)CN2)=O)c1</chem>	14325308	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1149	<chem>C1CN(CCC1C1CN(Cc2cccc2)C1)c1ccnc(N)n1</chem>	14604674	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1150	<chem>Nc(cc1)ccc1C(Nc(cc1)ccc1Nc1ccnc1)=O</chem>	146770	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1151	<chem>Cc1cc(nc(N)n1)N1CCC(CC1)NCCC1CCc2cccc12</chem>	15043866	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1152	<chem>C(CN)c1cccc(c1)c1ccc(cc1[Cl])F</chem>	16088353	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1153	<chem>Cc1c(cn(C)n1)NC(NCC(Cc1cccs1)C)O=O</chem>	16859921	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
1170	<chem>C1COc2cc(ccc2C1=O)c1cc2CC(CN)Oc2c(c1)[Cl]</chem>	26642358	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1171	<chem>c1cc(cc(c1)[Cl])n1nc2ccc(cc2n1)N</chem>	2810-4198	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1172	<chem>c1cc(c2cccc(c2c1)[Br])c1nc2ccc(cc2o1)N</chem>	2810-4224	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1173	<chem>COc1ccc(CNCc2ccc(c2)OC)cc1</chem>	2910-2885	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1174	<chem>Nc1ccc(Cn(ccc2c34)c2ccc4nc(N)nc3N)cc1.Cl</chem>	309401	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1175	<chem>Cc1ccc(cc1c1cccc(CCN)c1)F</chem>	31003354	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1176	<chem>CCc(cc(C(C)(C)CCC1(C(C)c1c1)c1-c1csc(C(C(/N)=N/O)n1</chem>	310354	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1177	<chem>C(c1ccc(cc1)c1nc(c2ccc(c(c2)F)nn1CCO)N</chem>	31242301	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1178	<chem>CCC1CN(CCN1)C(c1coc(CN2CCN(CC2)c2nccn2)n1)=O</chem>	31761532	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1179	<chem>C(CNC1NC(C2CCNCC=2N=1)=O)C(c1ccc(cc1)F)c1ccc1</chem>	31828522	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1180	<chem>C1CNCc2cc(CC3Cc4cccc4OC3)ccc12</chem>	31917501	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1181	<chem>Cc1c2cc(cc(CNC([C@H](Cc3c[nH]cn3)N)=O)c2[nH]c1c1cccc1)[Cl]</chem>	34268481	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1182	<chem>Cc1ccc2c(c1)c(CNc1c3CCNCc3nc(N)n1)nn2C</chem>	34365043	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1183	<chem>COc1cccc(CNCc2cccc(c2)F)c1OC</chem>	3702-1553	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1184	<chem>Cc1ccc(cc1)S(N(C(C(N1CCCC1)O)c1cccc1OC)(=O)=O</chem>	4013-2178	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1185	<chem>Cc(cc1)ccc1C1=CSSC1=S</chem>	40467	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1186	<chem>C(c1ccc(cc1[Cl])</chem>	4052-1804	TPP	Three-way	CAGUACUCGGGGUGCCCUUCUG	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	<chem>[Cl]c1cnc(N)s1</chem>			junction	CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	
1187	<chem>Cc1cccc(c1OCCN C(c1cn(CCN)nn1) =O)[Cl]</chem>	41830928	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1188	<chem>COc1ccc2cc(ccc2c 1)C1CN(CCO1)C(c1cc(N)[nH]n1)=O</chem>	42028139	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1189	<chem>[H]c1nc2CCNCCc 2c(n1)N1CCC(C1) (c1ccccc1)O</chem>	42335780	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1190	<chem>COc1cccc(c1c1cc(CN)ccc1F)[Cl]</chem>	42929743	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1191	<chem>Cc(cc1)cc(S(N) (=O)=O)c1/N=N/ c(cc1)c(C)cc1N</chem>	45527	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1192	<chem>C(CNc1cccn1)C Nc1c2ccccc2nc(C CN)n1</chem>	47488116	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1193	<chem>Cc1ccsc1CN(CCN (C)C)C(CN)=O</chem>	47645371	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1194	<chem>Cc1cnc(N)nc1NC C[C@@H]1C[C@ H]2C[C@@H]1C =C2</chem>	47913504	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1195	<chem>CCCCCCCCNc1c ccc(c1)[Br]</chem>	5117451	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1196	<chem>Cc1nc2cc(c(cc2n1 CCCO)[Cl])[Cl]</chem>	5119828	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1197	<chem>CCCCNCC(COc1 c(ccc2c3C(N4CC CCCC4=Ne3sc12) =O)[Br])O</chem>	5124607	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1198	<chem>CCN(CC)CC(COc 1c(ccc2c(C(=O)O CC)c(NC(C)=O)sc 12)[Br])O</chem>	5130027	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1199	<chem>c1ccc(cc1)Oc1ccc(cc1N)C(c1ccc(c(c 1)N)Oc1ccccc1)= O</chem>	5172392	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1200	<chem>CCOC(c1nc2c(C) cc(C)cc2c1NCC(C)O)=O</chem>	5174-4431	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1201	<chem>c1cc(ccc1c1c(c2cc c(cc2F)nc2cc(ccc 2n1)Oc1ccc(cc1)N)F</chem>	5174475	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1202	<chem>CCCCC1ccc(cc1) c1ccc(cc1)c1nc(c n1)N</chem>	5213078	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
					CAGCGUAGGGAAGUGCUG	
1203	<chem>c1ccc2c(ccc(c2c1)O)c1ccc(cc1[C])N[C]</chem>	5215844	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1204	<chem>C1CCC2(CC1)Cc1ccccc1c1c2c(N)n c(NN)n1</chem>	5232878	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1205	<chem>C1CCN(CC1)CC(Cn1c2ccc(cc2c2cc(ccc12)[C])C1)O</chem>	5236854	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1206	<chem>CC12CCC(CN(CC(Cn3c4ccc(cc4c4c c(ccc34)[Br]))[Br])O)C1)C2(C)C</chem>	5236945	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1207	<chem>c1ccc(cc1)c1c(en(c2ccccc2n1)C(Nc1cc(cc(c1)O)c1ccccc1)N)=O</chem>	5248546	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1208	<chem>Cc1ccc(cc1)NCCC C(NN=Cc1cccs1)=O</chem>	5248916	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1209	<chem>c1ccc2c(c1)ccc(c2[C])Sc1ccc(cc1[C])N</chem>	5250905	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1210	<chem>c1cc(ccc1C(Nc1ccc(cc1)O)c1ccc(cc1)NC(c1ccc(cc1)N)=O)=O)N</chem>	5253020	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1211	<chem>[H]N([H])c1c(C#N)c2c(nc3ccccc3n2)n1Cc1ccccc1</chem>	5253879	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1212	<chem>C(C1=C(N)O)c2cc(ccc2C12C(Nc1ccc(cc12)[Br])=O)N)#N</chem>	5313703	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1213	<chem>CC1(C)CC2=C(C(c3nc4ccccc4[nH]3)Nc3ccccc3N2)C(C1)=O</chem>	5326075	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1214	<chem>c1cc(ccc1c1cc(C(NN)=O)c2cc(ccc2n1)[Br])N</chem>	5350878	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1215	<chem>CCCCOc1ccc(cc1)c1ncc(cn1)N</chem>	5365506	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1216	<chem>Br(c1ccc1-c1csc(N=C2/SC=C(c(cc3)ccc3Br)N2)n1</chem>	55691	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1217	<chem>Cc1c2cc(CNC(c3c c(N)[nH]n3)=O)ccc2[nH]c1c1ccccc1F</chem>	56075039	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1218	<chem>CCCN1c2ccccc2nc1C(c1ccc(cc1)OC)O</chem>	5652903	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
1219	<chem>CC(c1ccc(cc1)N)=NNC(c1cc(C23CC4CC(CC(C4)C3)C2)n[nH]1)=O</chem>	5791299	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1220	<chem>CCNC(Cc1ccc(cc1)c1cc2CC(CN)Oc2c(c1)[Cl])=O</chem>	57980040	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1221	<chem>C(CN1CCOCC1)C(Nc1ccc(cc1C(c1cccc1)NCC(NN)=O)[Br])=O</chem>	5808034	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1222	<chem>c1ccc2c(c1)cc1cnc3c(c(N)n[nH]3)c1n2</chem>	6051011	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1223	<chem>C1CCCCC2c(CC(C1)c(C(N)=O)c(N)s2</chem>	6132195	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1224	<chem>C(C(N1c2ccccc2Sc2ccccc12)=O)Sc1nnc(N)s1</chem>	6134473	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1225	<chem>[H]N(Cc1cc(c(c(c1)[Cl])OCc1cccs1)OCC)Cc1ccnc1</chem>	6408-0223	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1226	<chem>CC(C)c1cc(CCC2C3(C)CCCC2(C)C N)c3cc1.OC(c1cccc1)=O</chem>	65238	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1227	<chem>Cc1nc2ccccc2n1C(C(COc1ccc(cc1)C1CCC=C1)O</chem>	6682831	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1228	<chem>O=C(c(cc1)cc(C(Nc(cc2)ccc2C2=NCN2)=O)c1Cl)Nc(cc1)ccc1C1=NCCN1</chem>	67436	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1229	<chem>CS(c1ccc(c(c1)[N+])([O-])=O)NCC(Nc1ccccc1SC(C(C(F)(F)F)(F)F)(F)F)=O)(=O)=O</chem>	6786638	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1230	<chem>Cc1cc(C)c2c(c1)nc(c1ccc(cc1O)N)o2</chem>	8007-0773	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1231	<chem>CCOC(c1c2ccc(c(c2sc1NC(C)=O)OCC(CN1CCCCC1)O)[Br])=O</chem>	8008-4440	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1232	<chem>Nc(cc1)cc(Cc2c3)c1-c2cc(Cl)c3Cl</chem>	80141	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1233	<chem>CC(C)C1(CCNCc2ccccc2OC(=O)COC(C)(C)C1</chem>	8018-1268	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1234	<chem>C1CN2C(=CSC2=N1)c1cccc(c1)N</chem>	8019-6474	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
1235	<chem>Cc1c2[nH]c(cccc3)c3c2ccc1CCN</chem>	81703	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1236	<chem>C(c1cccc2c1cc[nH]2)Nc1ccc(Cn2cncn2)cc1</chem>	9189417	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1237	<chem>Cc1cccc(c1C)n1c(c2c(c3ccnc3s2)N)nnc1S</chem>	9209599	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1238	<chem>C(CNC(c1c(c2ccc(c3cccn3)nc2s1)N)=O)c1c[nH]c2ccc(cc12</chem>	9212199	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1239	<chem>C(c1cccc1)NC(C(c1cccc1)Sc1nc(N)n[nH]1)=O</chem>	9241226	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1240	<chem>C(C(N1c2cccc2Sc2cccc12)=O)Sc1nnc(N)[nH]1</chem>	9248541	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1241	<chem>Oc(ccc([As](O)(O)=O)c1c1NC(c1cccc1)=O</chem>	92892	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1242	<chem>CCN1CCCC1CN Cc1cccc(c1)OCc1ccc(cc1)[Cl]</chem>	9312203	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1243	<chem>S=C1Oc(ccc(-c2cccc2)c2)N1</chem>	93817	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1244	<chem>CC[C@](C(C=C1N2Cc3cc4cccc4nc13)=C(C(O1)C2=O)(C1=O)O</chem>	94600	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1245	<chem>CCN(CCCC/C1=N\O)CCCC/C1=N\O</chem>	96491	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1246	<chem>c1ccc2c(c1)nc(c1ccc(cc1[Cl])N)s2</chem>	C066-5322	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1247	<chem>Cc1cccc(c1)NCc1nc2cccc2n1C</chem>	C147-0043	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1248	<chem>CSc1c(c(N)n(Cc2cccc2)n1)Sc1cccc(c1)(=O)=O</chem>	C200-4138	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1249	<chem>CC1CCN(CC1)c1nc(c(C(=O)OC)s1)N</chem>	C201-1740	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1250	<chem>CCN(CC)CCCNc1c2cccc2nc(c2nnc(c3ccc(C)cc3)o2)n1</chem>	C660-1575	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1251	<chem>C1CCCN(CC1)CC</chem>	C736-0159	TPP	Three-way	CAGUACUCGGGGUGCCCUUCUG	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	<chem>CNc1nc2ccccc2c2nc(c3ccccc3)nn12</chem>			junction	CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	
1252	<chem>CCCc1nc2c3ccccc3nc(NCCCN3CCN(CC3)c3ccccc3F)n2n1</chem>	C736-0671	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1253	<chem>COc1ccc(cc1)c1nc(Nc2ccc(cc2F)F)on1</chem>	C749-0018	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1254	<chem>Cc1c(CCC(Nc2ccc(c2)C(F)(F)F)=O)c(C)n2c(n1)nc(CN)n2</chem>	C908-0403	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1255	<chem>Cc1c(CCC(Nc2ccc(c2)[Br])=O)c(C)n2c(n1)nc(CN)n2</chem>	C908-0523	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1256	<chem>Cc1c(CCC(NCC2CCN(CC2)Cc2ccc(cc2)F)=O)c(C)n2c(n1)nc(CN)n2</chem>	C908-0552	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1257	<chem>CC(c1nc2ccccc2n1CCc1ccccc1)O</chem>	D011-4242	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1258	<chem>C(Cc1nc2ccccc2n1Cc1c(cccc1[Cl])F)CO</chem>	D011-4273	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1259	<chem>c1ccn2c(C(c3ccc(c3)[Cl])=O)c(c(C(Nc3ccccc3)F)=O)c2c1)N</chem>	D033-0008	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1260	<chem>Cc1ccc(cc1C)C(c1c(c(C(Nc2ccccc2)F)=O)c2ccccc12)N)=O</chem>	D033-0127	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1261	<chem>CC(C)c1ccc(CNc2nc3nc(C)c(c(C)n3n2)[Cl])cc1</chem>	D043-0278	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1262	<chem>Cc1ccc2c(c1)C(C1=C(C(N(CCCO)C13C(N(CC=C)c1cccc13)=O)=O)O2)=O</chem>	D063-1068	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1263	<chem>Cc1ccc2c(c1)C(C1=C(C(N(CCO)C13C(N(CC=C)c1cccc13)=O)=O)O2)=O</chem>	D063-1117	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1264	<chem>[H]c1ccc(cc1)S(c1c(NCC(C)C)oc(c2ccccc2)n1)(=O)=O</chem>	D072-0402	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1265	<chem>Cc1ccc(cc1)S(c1c(NCCOC)oc(c2ccc(c(C)c2)n1)(=O)=O</chem>	D072-0517	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1266	<chem>C(CNc1c(nc(c2ccc(c2)o1)S(c1ccc(cc1)[Cl])(=O)=O)Cn1ccnc1</chem>	D072-0802	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
1267	<chem>CCOc1cccc(c1)N1CC(C(=C1N)c1nc2cccc2s1)=O</chem>	D086-0218	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1268	<chem>C(CNC(c1c(CO)n n(c2ccc(cc2)F)n1)=O)c1cccc1</chem>	D217-0409	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1269	<chem>CCOC(c1cccc(c1)Nc1cc(c2cccc2)n cn1)=O</chem>	D278-0165	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1270	<chem>Cc1nc(cc(Nc2cccc(c2)OC)n1)c1cccc1</chem>	D278-0401	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1271	<chem>CN1C(N(C)c2cc(CO)c3ccc(CNCc4ccnc4)cc3OC)ccc12)=O</chem>	D300-0082	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1272	<chem>CC1(C)CC(CCOC1)CNCCN(C)C</chem>	D324-0105	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1273	<chem>CC1(C)CC(CCNC2CCN(C)CC2)(CCO1)c1cccc(c1)C(F)(F)F</chem>	D442-0355	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1274	<chem>Cc1cccc(c1)C1(CCNCCN2CCOCC2)CCOC(C)(C)C1</chem>	D442-0384	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1275	<chem>c1cccc(c1)n1c(c(c2nc3cccc3s2)nn1)N</chem>	D731-0066	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1276	<chem>CCc1cccc1NC1C(C)=C(c2cccc2)S(N=1)(=O)=O</chem>	E013-3228	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1277	<chem>Cn1c2cccc2c2c1nc(NCCCN1CCCCC1)nn2</chem>	E205-0046	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1278	<chem>Cc1cccc(c1)C1=C(C(C1=O)=O)NCCCc1cccc1</chem>	E470-0615	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1279	<chem>CCOc1ccc(cc1)c1nc(c2c(N)n(c3cccc(c3C)[Cl])nn2)on1</chem>	E595-0532	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1280	<chem>CCCNC1=C(C(C1=O)=O)c1cc(C)c(C)cc1C</chem>	E882-0500	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1281	<chem>C(CCCN=C(N)N=C(N)Nc1ccc(cc1)[Cl])CCN=C(N)N=C(N)Nc1ccc(cc1)[Cl]</chem>	NCGC00016246-12	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1282	<chem>CCC(C)CCCC(N[C@@H](CCN)C(NC(C(N[C@@H](CCN)C(N[C@@H]1CCNC(C([C@</chem>	NCGC00094763-03	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	<chem>[C@H](C)O)NC([C@@H]1(CCN)NC([C@@H]1(CCN)NC([C@@H]1(C(C)C)NC([C@@H]1(Cc2ccccc2)NC([C@@H]1(CCN)NC1=O)=O)=O)=O)=O)=O)[C@@H](C)O)=O</chem>					
1283	<chem>CCCCN(CCCC)C(C1cc(cc2C(=Cc3ccc(cc3)[Cl])c3cc(ccc3c12)[Cl])[Cl])O</chem>	NCGC00167490-02	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1284	<chem>C(c1cc(ccc1c1en[nH]c1)NC(Nc1nnc(c2ccncc2)s1)=O)#N</chem>	NCGC00247866-04	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1285	<chem>Cc1cc(c2c3ccccc3c(Nc3ccc(cc3)Oc3(cccn3)c3ccnc(N)n3)nn2)sc1</chem>	NCGC00263094-01	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1286	<chem>C(CCN1CCCC1)CNC(Nc1c(C(N)=O)c(ns1)OCc1c(cc(c1F)[Br])F)=O</chem>	NCGC00263100-01	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1287	<chem>C[C@@H](C(C)(C)NCc1ccc2c(c1)nc(NC(c1ccc(c3cn[nH]c3)s1)=O)n2CCc1cccc1</chem>	NCGC00344999-01	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1288	<chem>C(C(Nc1ccc(cc1)n1c(cc(C(F)(F)F)n1)c1ccc2c(cc3ccccc23)c1)=O)N</chem>	NCGC00346490-01	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1289	<chem>CCCCCCCCCCCc1ccc(cc1)S(Nc1nncs1)(=O)=O</chem>	NCGC00346547-01	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1290	<chem>CC(C)n1ene2c(Nc3ccccc3)NC(C=C)=O)nc(NC3CCC(CC3)N(C)C)nc12</chem>	NCGC00346964-01	TPP	Three-way junction	CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG	1
1291	<chem>CC(c1ccc(c(c1)N)[Br])=O</chem>	0054-0090	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1292	<chem>Cc1nc2ccc(CCO)c2s1</chem>	0133-0036	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1293	<chem>c1ccc2c(c1)nc(Sc1ccc(cc1)N)s2</chem>	0375-0603	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1294	<chem>c1ccc2c(c1)nc(Sc1ccc(cc1[Cl])N)s2</chem>	0375-0604	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1295	<chem>c1cc2c(cc(c2nc1</chem>	0422-0091	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
)N)[Br]][Br]				ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	
1296	CCN(CC)CCOC(c1ccc2c(c1)sc(NC(c1ccc(cc1)N)=O)n2)=O	0812-1025	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1297	C1c2ccccc2c2ccc(cc12)c1csc(N)n1	0846-0051	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1298	c(cc1)cc2c1Nc(ccc1)c1C=C2	123458	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1299	C1CCCN(CC1)C(CCC(NC[C@@H]1CCNC[C@H]1O)=O)=O	13691493	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1300	CN(Cc1ccc(cc1)Oc1ccccc1)Cc1cc2CNCCn2n1	13915713	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1301	C1CNCc2c1c(NCc1cccn1)nc(c1ccccc1)n2	14876887	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1302	Cc1ccc(cc1)OCc1c(cco1)C(NC[C@@H]1C[C@@H](CN1)F)=O	15670813	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1303	C1C2CC3CC1CC(C2)(C3)c1nc(CNC2CS(C=C2)(=O)=O)cs1	15896825	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1304	Cc1c(C(C(NCCNc2cccn2)=O)N)c(C)[nH]n1	16899791	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1305	C1CN(C[C@H]([C@@H]1NC(c1cccn1)=O)O)C(COc1ccccc1)F)=O	17818802	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1306	C1CC(CNC1)c1cc(c2ccc(c2)[Cl])[Cl]nc(c1C#N)N	17917068	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1307	Cc1cc(c2ccc(cc2n1)F)c1nc(CCSC)n1CCO	17988292	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1308	C=CCC1(CCCN(CC(NCCc2ccc(cc2)[Cl])=O)C1)CO	18112009	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1309	C(Cn1cnc(c2ccccc2)c1c1cnc(N)nc1)c1cccs1	18838660	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1310	CC(C)N[C@@H]1CC[C@@H]1NC(CCc1ccc(c2ccc(c2)[Cl])[nH]1)=O	19264424	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1311	CC1=C(C#N)C(C2=C(CC(C)	1965-0024	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	<chem>(C)CC(=O)N1)c1c cc(c(c1)OC)OCC O</chem>				UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	
1312	<chem>C1CCN(C1)CC(C n1c2ccccc2c2ccccc12)O</chem>	1988-0087	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1313	<chem>C1CNCc2c1c(NC C[C@@H]1C[C@ H]3C[C@@H]1C =C3)nc(c1ccnc1) n2</chem>	20252371	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1314	<chem>CC(Cc1ccccc1F)N Cc1nc(C2CCCCC 2)no1</chem>	20290768	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1315	<chem>CCc1ccccc1NC(c1 cccc(c1)NC(C1C= CCN1)=O)=O</chem>	20360930	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1316	<chem>C1CNCc2c1c(NC C1COc3ccccc3O1)nc(c1ccnc1)n2</chem>	20674759	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1317	<chem>Cc1c(C(NC[C@@ H]2C[C@@H] (CN2)F)=O)c(C)o n1</chem>	20675366	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1318	<chem>Cc1c(CN2CCCC3(CC2)[C@H] (C[C@H]3O)OCC N)nc2ccccc2n1</chem>	21179623	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1319	<chem>C(Cn1cc(c2ccc(C O)o2)nn1)Nc1ccccc1</chem>	21562311	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1320	<chem>c1ccc2c(c1)ccc1c2 nc(c2ccc(cc2)N) [nH]1</chem>	2252-1548	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1321	<chem>CC1=C(C(=O)OC) C2(C(C#N)=C(N) O1)C(Nc1ccc(cc1 2)[Cl])=O</chem>	2435-0198	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1322	<chem>Cc1cc2c(cc1C)oc(c1ccc(cc1O)N)n2</chem>	2783-3499	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1323	<chem>c1cc(ccc1) [Cl])n1nc2ccc(cc2 n1)N</chem>	2810-4198	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1324	<chem>c1cc(c2cccc(c2c1) [Br])c1nc2ccc(ccc2 o1)N</chem>	2810-4224	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1325	<chem>COc1ccc(cc1[Br]) c1nc2cc(ccc2o1)N</chem>	2810-4227	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1326	<chem>COc1ccc(cc1[Cl]) c1nc2cc(ccc2o1)N</chem>	2810-4228	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1327	<chem>Cc1cc2c(cc1C)oc(c1cc(ccc1[Cl])N)n</chem>	2810-4329	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	2				UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	
1328	<chem>Cc1cc2e(cc1C)oc(c1ccc(cc1)N)n2</chem>	2810-4334	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1329	<chem>Cc1cc2e(cc1C)oc(c1ccc(C)c(c1)N)n2</chem>	2810-4335	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1330	<chem>C(c1ccc(cc1)F)Sc1nc2ccc(cc2s1)N</chem>	3167-0429	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1331	<chem>CC(N[C@@H](CCc(c(C1=CC=C2OC)c3OC)c(C=O)c(OC)c3OC)C1=CC2=O)=O</chem>	328403	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1332	<chem>C(CCNC(CSc1nnc(N)s1)=O)Cc1ccccn1</chem>	33060622	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1333	<chem>CC1CCCCN1CC(CO)c1ccc(cc1)C(C)(C)O</chem>	3343-3198	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1334	<chem>CCn1c(N)nc2cc(cnc12)C(NCCCc1c(C)ncs1)=O</chem>	33439679	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1335	<chem>Cc1ccc(cc1)c1cc(C[N][C@@H]2CN[C@H]2O)=O)c2ccccc2n1</chem>	33446163	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1336	<chem>C1CNCCC12CCN(C2)C(Nc1cccc2ccc12)=O</chem>	33552957	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1337	<chem>CCc1ccc(cc1)C1C(C#N)=C(N)Oc2c1c(c1ccc3c(c1)OC(O3)n[nH]2</chem>	3394-0298	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1338	<chem>C1CCc2e(C1)c1ccc1n2C(CSc1nnc(N)s1)=O</chem>	3535-0310	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1339	<chem>Cc1cc(ccc1[Br])c1nc2cc(ccc2o1)N</chem>	3617-0633	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1340	<chem>CCCCc1ccc(cc1)n1nc2ccc(cc2n1)N</chem>	3738-4868	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1341	<chem>C1CSCCN1S(c1ccc(cc1)c1ccc2e(c1)c(N)n[nH]2)(=O)=O</chem>	39837810	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1342	<chem>Cc1cc(C)c(c(C)c1)c1cc(CN)ccc1F</chem>	40126718	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1343	<chem>Cc1ccc(cc1)S(N(C(CN1CCCC1)O)c1cccc1OC)</chem>	4013-2178	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	(=O)=O				GUCUGGGCGAACA	
1344	Cc1cc2NC(CN3C CC4(CC3)C(Cc3c cccc34)O)=CC(n2 n1)=O	40183085	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1345	Cc1c(c2csc(Nc3cc c(cc3) [Cl])n2)n2cccc2n 1	4112-3380	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1346	Cc1c(c2csc(Nc3cc c(cc3) [Br])n2)sc(N)n1	4112-3524	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1347	C1CN(CCN(C1)c1 necc(n1)N1CCC(C 1)O)Cc1cccc(c1)F	41253715	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1348	Cc1cc(C)n(C2CN(C2)c2c3CCCCc3n c(N)n2)n1	41650554	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1349	C(C(CNc1cc(c2cc ccc2)nc2ccnn12)C O)c1ccsc1	42351021	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1350	Cc1ccc(cc1[Cl])c1 nc2cc(ccc2o1)N	4269-3090	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1351	c1ccc(c(c1)c1ne2c cc(cc2s1)N)[Br]	4432-2269	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1352	C1CC(CN(C1)c1c (ccc(c2ccc(cc2)F)n 1)C(O)=O)(CO)O	47509829	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1353	c1ccc2c(cccc2e1)c 1nc2cc(ccc2o1)N	4788-0739	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1354	[H]N1CCn2c(C1)c c(CNS(c1ccc3c(c1)N(C)C(N3C)=O) (=O)=O)n2	47926615	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1355	C1C[C@H] (CO)N(C1)Cc1ccc c(c1)C(Nc1ne2ccc cc2s1)=O	48085150	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1356	CCC(Cn1c(CN2C COc3cccc3C2)nc (c2ccc2)n1)O	48093352	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1357	C1CC(CN(C1)CC NC(Nc1cccc(c1)c1 cccc(c1) [Cl])=O)CO	48121597	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1358	Cc1ne2cc(c(cc2n1 CCCO)[Cl])[Cl]	5119828	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1359	c1ccc(cc1)Oc1ccc(cc1N)C(c1ccc(c(c 1)N)Oc1cccc1)= O	5172392	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
1360	<chem>c1cc(ccc1c1c(c2cc(c(cc2)F)nc2cc(ccc2n1)Oc1cccc(c1)N)F</chem>	5174475	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1361	<chem>c1cccc(cc1)C(c1cc(c1cc1N)Sc1ccc(c(c1)C(c1cccc1)=O)N)=O</chem>	5180537	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1362	<chem>C(C(NN=Cc1cc2cccc2nc1[Cl])=O)Nc1ccc2cccc2c1</chem>	5200786	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1363	<chem>CCCCCc1ccc(cc1)c1ccc(cc1)c1ncc(c1n1)N</chem>	5213078	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1364	<chem>c1ccc2c(ccc(c2c1)Oc1ccc(cc1[Cl])N)[Cl]</chem>	5215844	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1365	<chem>CCOC(CNc1ccc(c1)Oc1ccc(cc1)Oc1ccc(cc1)NCC(=O)OCC)=O</chem>	5224153	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1366	<chem>C1CCN(CC1)CC(Cn1c2ccc(cc2c2cc(ccc12)[Cl])[Cl])O</chem>	5236854	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1367	<chem>CC12CCC(CN(CC(Cn3c4ccc(cc4c4c(c(ccc34)[Br])[Br])O)C1)C2(C)C</chem>	5236945	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1368	<chem>c1ccc(cc1)c1c(en(c2cccc2n1)C(Nc1cc(cc1)Oc1cccc1)N)=O</chem>	5248546	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1369	<chem>c1ccc2c(c1)ccc(c2[Cl])Sc1ccc(cc1[C])N</chem>	5250905	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1370	<chem>[H]N([H])c1c(C#N)c2c(nc3cccc3n2)n1Cc1cccc1</chem>	5253879	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1371	<chem>C1CN(CCN1CC(Cn1c2cccc2c2ccc12)O)Cc1cccc1</chem>	5320336	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1372	<chem>C(C(c1cccc1)O)N=Cc1ccc(cc1)[Br]</chem>	5321062	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1373	<chem>CC(c1ccc(cc1)N)=NNc1nc(C)cc(c2cccc2)n1</chem>	5339282	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1374	<chem>c1cc(c2ccc3c(c(C(Nc4ccc(c(c4)F)F)=O)sc3n2)N)sc1</chem>	5350-0016	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1375	<chem>c1cc(cc1)F)NC(c1c2ccc(c3cnc3)nc2s1)N=O</chem>	5350-0056	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1376	<chem>c1cc(ccc1c1cc(C(NN)=O)c2cc(ccc2</chem>	5350878	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	n1)[Br])N				UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	
1377	CC1=CC(C)=NC(N1CC(Cn1c2cccc2c2cccc12)O)=O	5600837	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1378	Cc1c2cc(CNC(c3c c(N) [nH]n3)=O)ccc2[n H]c1c1cccc1F	56075039	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1379	C(c1cnn(c2ccc3cc ccc3c2)c1N)#N	5628157	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1380	[H]N([H])c1nc(n[n H]1)SCCCCCC CC	5655427	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1381	C(c1cccc1)Oc1cc c(cc1)C1Nc2cccc3 cccc(c23)N1	5661401	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1382	COc1cc(c(cc1NC(C NCCN1CCNCC 1)=O)=O)OC)[Cl]	5688029	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1383	C(C(Cn1c2cccc2 c2cccc12)O)NNC (c1cccc1)=O	5718973	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1384	C1CC1c1nc2cccc 2n1CC(NCc1cc2C NCCn2n1)=O	58209539	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1385	C(C(Cn1c2ccc(cc2 c2cc(ccc12)[Br]) [Br])O)NCc1ccco1	5864844	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1386	CCn1c2cccc2c2c c(CN3CCNCC3)c cc12	5878848	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1387	CNC(c1cc(ccc1[Cl])c1cccc1CO)=O	58975776	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1388	C(c1cccc1)c1cccc c1OCCN.[Cl]	5924771	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1389	Cc1ccc(c(C)c1)OC C(CN1CCN(CC1) CCN1C(c2cccc3cc cc(C1=O)c23)=O) O.[Cl].[Cl]	6044718	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1390	C(c1c(cc(c2ccc(cc 2) [Br])nc1N)c1ccco 1)#N	6233-2517	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1391	CCCCSc1nc2c(c3 cc(ccc3NC3(CCC C3)O2)[Br])nn1	6372845	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1392	CCOc1cc(CO)cc(c 1OCc1ccc(cc1)C(O)=O)[Br]	6415-0035	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
					GUCUGGGCGAACA	
1393	<chem>C(c1ccco1)NC1C(c2cccc3cccc1c23)NS(c1ccc(cc1)[Cl])(=O)=O</chem>	6432111	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1394	<chem>CCOC(C(C(c(ccc1)c1N1)C1=O)=O)=O</chem>	646976	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1395	<chem>C(CC(N1c2ccccc2Sc2cccc12)=O)C</chem> N	6640-0077	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1396	<chem>O=C(c(cc1)cc(C(Nc(cc2)ccc2C2=NCN2)=O)c1Cl)Nc(cc1)ccc1C1=NCCN1</chem>	67436	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1397	<chem>CN(C)c1ccc(cc1)Nc1nc(cs1)c1cccs1</chem>	7100-1263	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1398	<chem>CCC1CCCCN1S(c1ccc(cc1)NC1c2ccc2S(N=1)(=O)=O)(=O)=O</chem>	7380-0010	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1399	<chem>Cn1c(cnc1NCc1ccc1OC)c1cccc1</chem>	7756-0545	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1400	<chem>Cc1c2[nH]c(cccc3)c3c2ccc1CCN</chem>	81703	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1401	<chem>C(c1ccenc1)Nc1ccc(c1)c1nc2ccccc2[nH]1</chem>	9142557	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1402	<chem>C(COc1ccc2c(c1)c1ccccc1o2)N.[Cl]</chem>	9188721	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1403	<chem>c1c(cc2c(c1[Cl])nc(N)s2)F</chem>	9190966	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1404	<chem>C(c1ccc2c(c1)OC(O2)Nc1cc(nc(N)n1)[Cl]</chem>	9205277	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1405	<chem>Oc(ccc([As](O)(O)=O)c1)NC(c1ccccc1)=O</chem>	92892	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1406	<chem>S=C1Oc(ccc(-c2ccccc2)c2)N1</chem>	93817	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1407	<chem>CC[C@](C(C=C1N2Cc3cc4ccccc4nc13)=C(CO1)C2=O)(C1=O)O</chem>	94600	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1408	<chem>C1CCCN(CC1)CCCNc1nc2ccccc2c2nc(c3ccccc3)nn12</chem>	C736-0159	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
					GUCUGGGCGAACA	
1409	CCOC(N1CCC(C C1)NC1=C(C(C1= O)=O)N1CCCC1) =O	C748-0097	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1410	Cc1ccc(CNc2c(en c3ccc(cc23)F)S(c2 cccc2) (=O)=O)cc1	C769-1565	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1411	COc1ccc(cc1)S(c1 cnc2ccc(cc2c1NCc 1ccc(cc1)F)F) (=O)=O	C769-1653	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1412	Cc1ccc(cc1)S(c1c nc2cccc2c1Nc1cc cc(c1)OC)(=O)=O	C769-1951	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1413	Cc1c(CCC(Nc2ccc c(c2)C(F) (F)F)=O)c(C)n2c(n1)nc(CN)n2	C908-0403	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1414	Cc1cccc1NC(CN S(c1cccc1) (=O)=O)c1cccc1	D030-0007	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1415	Cc1ccc(cc1)NC(C NS(c1ccc(cc1) [Cl]) (=O)=O)c1cccc1	D030-0071	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1416	c1ccn2c(C(c3ccc(c c3) [Cl])=O)c(c(C(Nc 3cccc(c3)F)=O)c2 c1)N	D033-0008	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1417	Cc1ccc(cc1C)C(c1 c(c(C(Nc2cccc(c2) F)=O)c2ccccn12) N)=O	D033-0127	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1418	Cc1cc(C)n2c(n1)n c(NCc1ccc(cc1) [Br])n2	D043-0245	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1419	CC(C)c1ccc(CNc2 nc3nc(C)c(c(C)n3 n2)[Cl])cc1	D043-0278	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1420	Cc1ccc2c(c1)C(C1 =C(C(N(CCCO)C 13C(N(CC=C)c1ccc cccc13)=O)=O)O2)=O	D063-1068	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1421	Cc1ccc2c(c1)C(C1 =C(C(N(CCO)C13 C(N(CC=C)c1cccc c13)=O)=O)O2)= O	D063-1117	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1422	CCCCNc1c(nc(c2 cccc2)o1)S(c1ccc cc1)(=O)=O	D072-0067	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1423	CCCCNc1c(nc(c2 ccc(cc2)F)o1)S(c1 cccc1)(=O)=O	D072-0077	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1424	Cc1ccc(cc1)c1nc(c (NC2CC2)o1)S(c1	D072-0757	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	<chem>ccc(cc1)F(=O)=O</chem>				UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	
1425	<chem>COCCCN1CC(C(=C1N)c1nc2ccccc2s1)=O</chem>	D086-0291	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1426	<chem>CN1C(N(Cc2cccc2)C(c2c1nc(NCCN)n2C)=O)=O</chem>	D114-0037	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1427	<chem>C(CNc1cc(c2ccccc2)nc2nnen12)c1ccc1</chem>	D150-0146	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1428	<chem>Cc1c2c(c(NCCCN3CCOCC3)nn1)n(Cc1cccc1[Cl])nn2</chem>	D172-0423	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1429	<chem>[H]N(CCNC(c1c(N)non1)=O)Cc1ccc(c1)[Br]</chem>	D175-0122	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1430	<chem>[H]N(CCNC(c1c(N)non1)=O)Cc1ccc(ccc1OCc1ccc(cc1)F)[Br]</chem>	D175-0127	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1431	<chem>CCC(c1nc2ccccc2n1Cc1cccc1F)O</chem>	D186-0041	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1432	<chem>[H]N(Cc1cccc1)Cc1ccc2c(c1)N(C)C(N2C)=O</chem>	D272-0686	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1433	<chem>[H]N(CCCOCC)Cc1ccc2c(c1)N(C)C(N2C)=O</chem>	D272-0707	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1434	<chem>[H]N(Cc1ccc2c(c1)N(C)C(N2C)=O)C1CCCCC1</chem>	D272-0737	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1435	<chem>CN1C(N(C)c2cc(c2c12)C(COc1ccc(CNCc2cccs2)cc1)O)=O</chem>	D300-0283	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1436	<chem>CN1C(N(C)c2cc(c2c12)C(COc1ccc(CNCc2ccc(cc2)OC)cc1)O)=O</chem>	D300-0327	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1437	<chem>Cc1ccc(cc1)OCc1ccc(c2nc(C#N)c(NCCCN3CCOCC3)o2)o1</chem>	D301-0080	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1438	<chem>C(c1nnc(o1)SCc1ccc(c1)[Br])N</chem>	D334-0126	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1439	<chem>Cc1cccc(c1)c1nc(c2ccene2Nc2ccccc2OC)on1</chem>	D349-3872	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1440	<chem>Cc1cccc(c1)Nc1nc2C(CC(Cc2n1)c1ccc(c1)OC)OC)=O</chem>	D367-0429	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
1441	<chem>CN1C(c2c(en(c2c2cccc(c2)[Br])C(CO)(CO)C)C1=O)=O</chem>	D383-0064	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1442	<chem>CCNc1nc(nc(n1)n1cnc(n1)SCc1cccc1)N1CCCC1</chem>	D385-0095	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1443	<chem>CCCCNc1nc(nc(n1)n1cnc(n1)SCc1cccc1)N(C)C</chem>	D385-0102	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1444	<chem>C1CC1Nc1c(C#N)nc(c2ccc(cc2)S(N2CCOCC2)(=O)=O)o1</chem>	D434-0692	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1445	<chem>C=CCNc1c2c(en(c3cccc3[Cl])c2ncn1)c1cccc1</chem>	D447-0385	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1446	<chem>C1Cn2c3cccc3nc2CN1c1cccc(c1)N</chem>	D454-0054	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1447	<chem>C1Cn2c3cccc(cc3nc2CN1c1cccc(c1)N)[Cl]</chem>	D454-0510	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1448	<chem>CCCNc1cc(C)nc2c(C)c(c3cccc(c3)[Cl])nn12</chem>	D503-0232	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1449	<chem>[H]N(CCc1cccc(c1)S(N)(=O)=O)Cc1cccc(c2ccc(cc2)[Cl])o1</chem>	D665-0262	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1450	<chem>c1cc(c(cc1NS(c1c c(nc1N)[Br])(=O)=O)C(F)(F)F)[Cl]</chem>	E138-2000	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1451	<chem>CC(C)c1cccc(cc1)C1=C(C(C1=O)=O)NCc1cccc1OC</chem>	E511-0865	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1452	<chem>Cc1cccc(C)c1NCc1cccc(C(O)=O)s1</chem>	E536-0036	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1453	<chem>CCc1cccc(C)c1NCc1cccc(C(O)=O)s1</chem>	E536-0078	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1454	<chem>C1CCc2c(C1)c(CO)cs2</chem>	E540-0003	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1455	<chem>C(c1cccc1F)N1c2cccc2C2=C(C(C(C#N)=C(N)O2)c2ccc(cc2)F)S1(=O)=O</chem>	E738-0215	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1456	<chem>CCc1cccc(cc1)C1C(C#N)=C(N)OC2=C1S(N(Cc1cccc1C)c1cccc12)(=O)=O</chem>	E738-0441	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
1457	<chem>CCCNC1=C(C(C1=O)=O)c1cc(C)c(C)cc1C</chem>	E882-0500	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1458	<chem>C1CNCCNCCCN(CCNC1)Cc1ccc(CN2CCCNCCNCCCNCC2)cc1</chem>	NCGC00165722-02	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1
1459	<chem>CC(C)n1cnc2c(Nc3cccc(c3)NC(C=C)=O)nc(NC3CCC(CC3)N(C)C)nc12</chem>	NCGC00346964-01	ZTP	Pseudoknot	UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAAACGAUGACAAUGCCGACC GUCUGGGCGAACA	1