

**“miRNA” 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>Cc1cc(C)n(-c2nc(C)c(C(=O)N(CCO)CCO)CCO)s2)n1</chem>	Neg_lig_4	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAUUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
2	<chem>CCc1ccc2nc(C)cc(C(=O)NC[C@H](O)c3ccco3)c2c1</chem>	Neg_lig_30	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAUUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
3	<chem>c1cc(C2CCCC2)nc(N2CCO[C@]3(C[NH2+])CCOC3)C2)n1</chem>	Neg_lig_49	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAUUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
4	<chem>O=C(NCCO)c1nnc(-c2ccc3c(c2)OCO3)o1</chem>	Neg_lig_58	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAUUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
5	<chem>CN(C)c1nc(N)nc(COC2cccc3c2OC(C)(C)C3)n1</chem>	Neg_lig_83	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAUUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
6	<chem>COCC[C@]1(CO)CCCN(CC(=O)N2CCc3ccccc32)C1</chem>	Neg_lig_96	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAUUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
7	<chem>COCc1nn2c(N)c(-c3ccc(Cl)cc3)nc2c1-c1ccccc1</chem>	Neg_lig_130	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAUUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
8	<chem>O=C1N(CCO)CCC[C@@]12CC[N@H+](Cc1cccc(C(F)(F)F)c1)C2</chem>	Neg_lig_275	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAUUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
9	<chem>CS[C@@H](C)CC[NH+]1CCC2(CC1)NCCNC2=O</chem>	Neg_lig_277	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAUUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
10	<chem>Cc1ccccc1-c1ccc(CN2CC[C@](N)(C(=O)O)C2)cc1</chem>	Neg_lig_285	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAUUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
11	<chem>COc1ccc(Cl)cc1NC(=O)CCc1c(C)nc2nc(C[NH3+])nn2c1C</chem>	Neg_lig_294	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAUUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
12	<chem>CCOC(=O)c1c(N)n(-c2ccc(F)cc2)c2nc3ccccc3nc12</chem>	Neg_lig_325	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAUUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
13	<chem>[NH3+]Cc1ccc2ccccc2n1</chem>	Neg_lig_351	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAUUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
14	<chem>Cc1cccc(N2CCN(C(=O)c3ccc(CNc4c(N5CCCC5)c(=O)c4=O)cc3)CC2)c1C</chem>	Neg_lig_487	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAUUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
15	<chem>Cc1ccccc1Cn1c(C(=O)O)c(CNCc2ccco2)c2ccccc21</chem>	Neg_lig_492	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAUUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
16	<chem>COc1ccc2cc3c(N)nn(C(=O)c4cc(Cl)c4)c3nc2c1</chem>	Neg_lig_500	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAUUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0

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17	<chem>Cc1cn2c(-c3cn[nH]c3)cnc2c(Nc2ccc(C(=O)N3CC[NH2+][CC3]cc2F)n1</chem>	Neg_lig_513	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
18	<chem>CN1C[C@@]2(CCCN(c3cc(N4CC[NH+](C)CC4)nc(N)n3)C2)OC1=O</chem>	Neg_lig_549	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
19	<chem>Cc1ccc(C[NH+][2CCC(C(=O)N(CCO)Cc3ccccc3)CC2)o1</chem>	Neg_lig_566	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
20	<chem>COc1cccc(Nc2cc(C)[nH+][c3cc(-c4ccccc4OC)nn23)c1</chem>	Neg_lig_591	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
21	<chem>Cn1c(=O)n(C)c2cc(CNc3ccc(Br)cc3)ccc21</chem>	Neg_lig_621	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
22	<chem>[NH2+]=c1n(CCO)c2ccccc2n1C c1ccccc1F</chem>	Neg_lig_623	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
23	<chem>NS(=O)(=O)c1ccc(N/N=C2\C=C(CC(=O)NC2=O)cc1</chem>	Neg_lig_641	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
24	<chem>Cc1c(S(=O)(=O)c2ccc(Cl)cc2)c(N)n(Cc2cccn2)c1C</chem>	Neg_lig_718	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
25	<chem>c1ccc2cc(CN3CC[C@]4(CCC[NH2+][C4]C3)ccc2c1</chem>	Neg_lig_733	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
26	<chem>COc1ccc(-c2cc(-c3ccccc3)nc(N)n2)cc1</chem>	Neg_lig_734	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
27	<chem>C[C@H]1CC[C@@H](Nc2c(-c3ccc(Br)cc3)[nH]c3c(C#N)cnn23)CC1</chem>	Neg_lig_750	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
28	<chem>CC(=O)N1CCC([NH2+][C@@H](C)CCCC(C)(C)O)CC1</chem>	Neg_lig_774	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
29	<chem>CNc1ncnc2c1cnn2[C@@H]1CCCO1</chem>	Neg_lig_785	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
30	<chem>Cc1nc(N(C)Cc2cc(C(C)(C)[nH]n2)cc([C@H]2CCC[NH2+][C2])[nH+])1</chem>	Neg_lig_793	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
31	<chem>CN(C)c1ccc([C@@H](O)c2cccs2)cc1</chem>	Neg_lig_813	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
32	<chem>Cc1ccc(NCC(=O)n2nc(C)cc2C)c(C)c1</chem>	Neg_lig_822	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
33	<chem>Clc1ccc(C[NH2+][Cc2ccco2)cc1</chem>	Neg_lig_827	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC	0

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					UACUGCAGUGAAGGCACU UGUAG	
34	<chem>Cc1nc(N)sc1Cc1ccc(O)cc1</chem>	Neg_lig_887	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
35	<chem>CCc1[nH]nc2c1[C@@]1(C(=O)N(CC)c3ccccc31)C(C#N)=C(N)O2</chem>	Neg_lig_900	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
36	<chem>Cc1ccc(S(=O)(=O)Nc2ccccc2Cnc2ccccc2Br)cc1</chem>	Neg_lig_925	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
37	<chem>CC(C)C[C@H](O)C(=O)N1CCCN(C(=O)c2ccco2)CC1</chem>	Neg_lig_936	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
38	<chem>Cc1c(C(=O)c2ccccc23)c2ccccc2n1[C@H](CN1CCOCC1)CO3</chem>	Neg_lig_972	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
39	<chem>COc1ccc(C)c(NC(=O)N2C[C@H](CO)[C@H](CO)C2)c1</chem>	Neg_lig_989	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
40	<chem>CCCC[S@@](=O)c1sc2nc(C)cc(C)c2c1N</chem>	Neg_lig_990	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
41	<chem>Cn1c(CC(=O)NCCCC)c(Sc2ccccc2)c2ccccc21</chem>	Neg_lig_997	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
42	<chem>Nc1nonc1C(=O)N1CCN(C(=O)c2ccccc(F)c2)CC1</chem>	Neg_lig_1002	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
43	<chem>COc1ccc(C(=O)CCC(=O)N2CC[C@H](Cc3ccccc(CO)c3)C2)cc1</chem>	Neg_lig_1013	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
44	<chem>Cc1noc(-c2ccc[nH+]c2NCc2ccco2)n1</chem>	Neg_lig_1022	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
45	<chem>CCOC(=O)c1ccccc1N[C@@H]1c2ccccc2C(=O)N1c1ccc(Cl)cc1</chem>	Neg_lig_1054	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
46	<chem>C[C@@H](Cc1cn(CCc2nnc(N)s2)nn1)c1cccc1</chem>	Neg_lig_1056	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
47	<chem>COc1ccc(-c2cc(C)cc3c2O[C@@H](C[NH3+])C3)c(C)c1</chem>	Neg_lig_1100	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
48	<chem>Fc1cccc(Cl)c1Cn1ccnc1-c1cc2n(n1)CC[NH2+]C2</chem>	Neg_lig_1125	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
49	<chem>O=C(NCCCC[NH+])CCCC(O)CC1)Nc1ccccc1OCc1ccccc1</chem>	Neg_lig_1132	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0

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50	<chem>CC(C)NC(=O)c1ccc(-c2cccc(N3CC[NH2+][CC3]c2)s1</chem>	Neg_lig_542	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
51	<chem>CC(=O)c1ccc(Nc2cc(C)nc3nc(-c4ccc(Cl)cc4)nn23)cc1</chem>	Neg_lig_1151	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
52	<chem>CCN(CC)C(=O)[C@@H]1C[C@@H]([NH3+])CN1C1CCOCC1</chem>	Neg_lig_1171	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
53	<chem>CCC[C@H](N[C@@H](C)C(=O)N1[C@H](C(=O)O)C[C@H]2CCCC[C@H]21)C(=O)OCC</chem>	Neg_lig_1189	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
54	<chem>NS(=O)(=O)c1ccc(NC2(C(=O)[O-])CCCC2)cc1</chem>	Neg_lig_1191	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
55	<chem>CCC[C@H](O)c1nc2ccccc2n1Cc1ccc(F)cc1</chem>	Neg_lig_1196	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
56	<chem>CCOc1ccc([C@@H]2c3c(n[nH]c3-c3ccccc3O)C(=O)N2CCCO)cc1OC</chem>	Neg_lig_1287	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
57	<chem>Cc1cc(C)n(-c2nnc(N)nn2)n1</chem>	Neg_lig_1369	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
58	<chem>COC(=O)CNc1cc(C)nc2nc(-c3ccc(C)cc3)nn12</chem>	Neg_lig_1405	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
59	<chem>O=C(c1cn(C/C=C/c2ccccc2)nn1)N1[C@H]2CC[C@H]1CC[NH2+][C2]</chem>	Neg_lig_1408	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
60	<chem>C[NH+](C)C1CCN(C(=O)c2ccc(NC(=O)Nc3nc(N4CCOCC4)nc(N4CCOCC4)n3)cc2)CC1</chem>	Neg_lig_1440	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
61	<chem>Cc1cc(N2CCN([C@H]3CCOC4(CCOCC4)C3)CC2)nc(N)n1</chem>	Neg_lig_1451	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
62	<chem>c1cc2c(cc1[C@H]1OC[C@H]3[C@H]1CO[C@H]3c1ccc3c(c1)OCO3)OCO2</chem>	Neg_lig_1501	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
63	<chem>CCSc1ncc(-c2c(-c3ccccc3)ncn2CC[C@H](C)CO)cn1</chem>	Neg_lig_1587	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
64	<chem>COc1cc([C@H]2c3c(n[nH]c3-c3ccccc3O)C(=O)N2CCCO)ccc1O</chem>	Neg_lig_1239	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
65	<chem>O=S(=O)(NCCCNc1cccn1)NCc1ccccc1</chem>	Neg_lig_1676	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
66	<chem>Clc1nc(Cl)nc(-c2cn(-c3ccccc3)c3ccccc23)n1</chem>	Neg_lig_1712	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC	0

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					UACUGCAGUGAAGGCACU UGUAG	
67	<chem>COC(=O)c1nn(Cc2nc(N)nc(N(C)C)n2)c2ccccc12</chem>	Neg_lig_1728	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
68	<chem>CCN1CCN(C2(CNc3oc(-c4ccc(Cl)cc4)nc3C#N)CCCC2)CC1</chem>	Neg_lig_1729	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
69	<chem>CC1(C)Cc2c(C#N)c(NC3CCCCC3)nc(Cc3ccccc3)c2CO1</chem>	Neg_lig_1738	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
70	<chem>Cc1ccc([C@H]2C(C#N)=C(N)Oc3cc(O)ccc32)cc1</chem>	Neg_lig_1739	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
71	<chem>Cc1cc(C)c(Cn2c(CCCO)nc3ccccc32)c(C)c1</chem>	Neg_lig_1794	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
72	<chem>O=C1C[C@@]2(CC[N@@H+](Cc3cc4n(n3)CC[NH2+]C4)C2)Oc2ccccc21</chem>	Neg_lig_1801	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
73	<chem>CCN(CCOc1ccc(Cl)cc1)C(=O)c1ccc2c(c1)ncn2CCO</chem>	Neg_lig_1839	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
74	<chem>O=C([O-])c1ccc(-c2cc3ccnc3c(-c3ccccc4nnc4c3)n2)cc1</chem>	Neg_lig_1857	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
75	<chem>O=C(OC1CCCC1)c1ccc(NC(=O)N2CCC3(CC2)C[C@H](O)CO3)cc1</chem>	Neg_lig_1864	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
76	<chem>O=C(c1ccc2ccccc(F)c2n1)N(CCOC)c1ccccc1Cl</chem>	Neg_lig_1899	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
77	<chem>CO[C@@H](Cn1ccnc1-c1ccc(CO)o1)c1cccs1</chem>	Neg_lig_1904	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
78	<chem>COc1cc(OC)c([N-]S(=O)(=O)c2cc(Br)enc2N)cc1Cl</chem>	Neg_lig_1920	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
79	<chem>Cn1c(N2CCOCC2)nc2cc(C(=O)N3C[C@H](O)CO3)ccc21</chem>	Neg_lig_2001	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
80	<chem>Cc1ccc(Nc2cc(N3CCCCC3)ncn2)cc1C</chem>	Neg_lig_2038	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
81	<chem>COc1ccc2c(c1)OC[C@]1(CO)CN(C(=O)CSc3ccncc3)C[C@H]21</chem>	Neg_lig_2077	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
82	<chem>CCOC(=O)C1CCN(c2nc(N)c(C(=O)N3CCCC3)s2)CC1</chem>	Neg_lig_2108	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
83	<chem>O=C1N=c2ccc(Cl)cc2=C(N[C@@H]2C[NH+]3CCCC2CC3)C1=C1Nc2ccccc2N1</chem>	Neg_lig_2115	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
84	<chem>N#Cc1ccccc1C(=O)N1CC[C@@H](CNC(=O)CC2CCCC2)[C@H](O)C1</chem>	Neg_lig_2129	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
85	<chem>COc1c(N)c2c(c(OC)c1OC)COC2=O</chem>	Neg_lig_2135	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
86	<chem>C=CCOc1c(Cl)cc([C@H]2C(C#N)=C(N)Oc3cc(O)ccc32)cc1OC</chem>	Neg_lig_2141	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
87	<chem>CC(C)CNc1ncnc2c1sc1nc(-c3ccco3)c3c(c12)CC(C)(C)OC3</chem>	Neg_lig_2229	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
88	<chem>C[N@H+]1CCc2c(c3ccccc3n2C2ccc(C(=O)NO)cc2)C1</chem>	Neg_lig_2237	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
89	<chem>Cc1nc(NCCc2c(C)[nH]c3ccccc23)c2c3c(sc2n1)CC3</chem>	Neg_lig_906	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
90	<chem>NC(=O)Nc1ccc(Nc2ccccc2)cc1</chem>	Neg_lig_2261	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
91	<chem>CCCCn1c(=N)n(C[C@H](O)COc2ccccc2OC)c2ccccc21</chem>	Neg_lig_2264	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
92	<chem>C[NH+](C)CCOC(c1ccccc1)c1ccccc1</chem>	Neg_lig_2292	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
93	<chem>CCNc1ncc(C(=O)N2C[C@@H](C[NH+]3CCCC3)[C@@H](CO)C2)cn1</chem>	Neg_lig_388	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
94	<chem>CCOC(=O)c1c(N)n(-c2ccc(C)cc2)c2nc3ccccc3nc12</chem>	Neg_lig_2320	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
95	<chem>Nc1nc(SCCc2ccccc2)ns1</chem>	Neg_lig_2332	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
96	<chem>Cc1cccc(N2C[C@H](C)N(C(=O)c3ccc(SCCO)cc3)C2=O)c1</chem>	Neg_lig_2338	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
97	<chem>Cc1nc(-c2ccc[nH+]c2)ncc1-c1nc(CC(N)=O)nn1CCO</chem>	Neg_lig_2366	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
98	<chem>Fc1ccc(CNc2nc3ccc(Cl)cc3s2)cc1</chem>	Neg_lig_2375	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
99	<chem>CN(C)c1ccccc1-c1nc(CC(N)=O)nn1CCO</chem>	Neg_lig_2415	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
					UACUGCAGUGAAGGCACU UGUAG	
100	<chem>O=C(c1ccc(-c2cc[nH]n2)cc1)N1CCOC[C@H](O)C1</chem>	Neg_lig_2427	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
101	<chem>CCc1ccc(C[N@H+]2CC[C@@H](NC(=O)c3cncn3)[C@H](O)C2)cc1</chem>	Neg_lig_2542	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
102	<chem>CC(C)Nc1nc2c(-c3cccc(C(F)(F)F)c3)nnn2c2ccccc12</chem>	Neg_lig_2579	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
103	<chem>CCc1[nH+]ccn1CCCNC(=O)[C@H](CC)Nc1cccc(OC)c1</chem>	Neg_lig_2582	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
104	<chem>C[C@]12CC[C@H]3c4ccc(O)cc4CC[C@@H]3[C@H]1CCC2=O</chem>	Neg_lig_2597	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
105	<chem>Cc1cc(NC(=O)CNCCc2nc(-c3ccc[nH+]c3)n[nH]2)ccc1C1</chem>	Neg_lig_2604	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
106	<chem>C=C(C)C[C@H]1CC=C[C@@H](CC(=C)C)N1C[C@@H](O)C(F)(F)C(F)(F)C(F)(F)F</chem>	Neg_lig_2635	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
107	<chem>C=CCOC(=O)C1=C(C)OC(N)=C(C(=O)OCC)[C@@]12C(=O)N(CC=C)c1cccc12</chem>	Neg_lig_2644	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
108	<chem>Nc1cc(C(=O)N2CCCC2)ccc1C1</chem>	Neg_lig_2706	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
109	<chem>CC[NH+](CC)CCNc1ncnc2c1sc1nc(-c3ccc3)c3c(c12)CC(C)(C)OC3</chem>	Neg_lig_2828	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
110	<chem>Nc1nc(NCC[NH+]2CCCC2)c2c([nH+]1)CCCC2</chem>	Neg_lig_2835	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
111	<chem>COc1ccc(-c2csc(NCc3ccco3)n2)cc1OC</chem>	Neg_lig_2841	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
112	<chem>Oc1ccc2ccccc2c1SSc1c(O)ccc2ccccc12</chem>	Neg_lig_2844	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
113	<chem>CC1(C)CC(NC(=O)C(F)(F)F)CC(C)(C)[NH2+]1</chem>	Neg_lig_2862	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
114	<chem>C=C[C@@H]1C[N@H+]2CC[C@@H]1C[C@H]2[C@H](O)c1ccnc2ccccc12</chem>	Neg_lig_2957	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
115	<chem>CCOC(=O)[C@H]1CCCN(c2c(NCCC[NH+]3CCN(C)CC3)c(=O)c2=O)C1</chem>	Neg_lig_2967	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
116	<chem>COc1ccc(CNc2ncnc3scc(-c4ccc(C)cc4)c23)cc1</chem>	Neg_lig_2983	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
117	<chem>COc1ccc(Nc2cc(C)[nH+]c3c(C)cccc23)cc1OC</chem>	Neg_lig_3007	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
118	<chem>Cc1ccc([N-]C2=C(C(N)=O)S(=O)(=O)c3ccccc32)c(C)c1</chem>	Neg_lig_3057	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
119	<chem>Nc1cccc1Oe1c(F)c(F)c(Oc2cccc2N)c(F)c1F</chem>	Neg_lig_3068	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
120	<chem>O=C(Nc1ccc(Nc2cc[nH+]cc2)cc1)c1ccc(Nc2cnc3ccc([N+](=O)[O-])cc23)cc1[N+](=O)[O-]</chem>	Neg_lig_3116	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
121	<chem>OCCN(CC#CCC(O)(c1cccc1)c1cccc1)CCO</chem>	Neg_lig_3138	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
122	<chem>CCOC(=O)c1cccc(N2C(=O)[C@@H]3[C@@H]4C=C[C@@@](CO)(O4)[C@@H]3C2=O)c1</chem>	Neg_lig_3155	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
123	<chem>Nc1nc(CCC[NH2+])C2CCN(c3ncnc4ccsc34)CC2)cs1</chem>	Neg_lig_1266	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
124	<chem>CCOC(=O)CSc1nc(Nc#N)nc(N(CC)CC)n1</chem>	Neg_lig_3168	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
125	<chem>CCc1ccc([C@H]2C(C(=O)OC)=C(N)OC3=C2C(=O)CC(C)(C)C3)cc1</chem>	Neg_lig_3178	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
126	<chem>Cc1cccc1[C@@H]1CN(Cc2ccc(CC[NH3+])c2)C[C@H]1C(=O)O</chem>	Neg_lig_3222	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
127	<chem>Nc1cccc(-n2c(=O)[c-]3nc(c2=O)CCC3)c1</chem>	Neg_lig_3229	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
128	<chem>C=CC[NH2+]Cc1cc(O)c2cc(C(N)=O)ccc2n1</chem>	Neg_lig_3240	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
129	<chem>CN(C)S(=O)(=O)N1C[C@@H]2CC[C@H](C1)N(Cc1ccnc1N)C2</chem>	Neg_lig_3243	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
130	<chem>OCc1nc2cccc2n1CCCCOc1cccc1</chem>	Neg_lig_3260	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
131	<chem>O=C1c2cccc3cccc(c23)C(=O)N1CCN1CCN(C[C@H](O)COCc2cccc2)CC1</chem>	Neg_lig_3283	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
132	<chem>COc1ccc(-c2nc(C(=O)N3CCN(CCO)CC3))</chem>	Neg_lig_3291	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC	0



Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	<chem>nn2-c2ccccc2Cl)cc1</chem>				UACUGCAGUGAAGGCACU UGUAG	
133	<chem>Cc1nc(C)n(CCNC(=O)c2cccc([C@H]3CCCC[NH2+][C3]c2)n1</chem>	Neg_lig_3325	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
134	<chem>CCCN1ncc(C(=O)NCc2c(C)ncc3c2CC[NH2+][C3]c1C</chem>	Neg_lig_3338	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
135	<chem>Cc1ccc([N+](=O)[O-])cc1S(=O)(=O)N(C)/N=C\c1nc2ccc(Br)cn12</chem>	Neg_lig_830	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
136	<chem>Nc1nnc(SCC(=O)Nc2cccc(F)c2)s1</chem>	Neg_lig_176	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
137	<chem>COc1cccc1/N=C1C(=C(\N[O-])/S(=O)(=O)c2cccc2/1</chem>	Neg_lig_1111	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
138	<chem>Cc1nc(C(F)(F)F)nc(N2CCO[C@]3(CNCCOC3)C2)c1C</chem>	Neg_lig_3399	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
139	<chem>Cc1ccc(N[C@]([H])2c3cccc3C(=O)N2c2cccn2)c(C)c1</chem>	Neg_lig_3343	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	0
140	<chem>Cn1c(=O)n(C)c2cc(NC3=NS(=O)(=O)c4cccc43)ccc21</chem>	Neg_lig_12	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
141	<chem>CCc1c(C)nn(CCn2cc(-c3ccc(CO)o3)nn2)c1C</chem>	Neg_lig_50	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
142	<chem>CCOc1cccc1-c1nc(CN2CC[NH+](CCCO)CC2)c(C)o1</chem>	Neg_lig_60	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
143	<chem>O[C@H]1CCC[N@H+](Cc2cccc(Br)c2)C1</chem>	Neg_lig_80	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
144	<chem>O=C(CN1CCCCC1=O)NCc1cc2n(n1)CC[NH2+][C2]</chem>	Neg_lig_101	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
145	<chem>CC(C)Cc1noc([C@H](C)n2cc[nH+][c2-c2cc3n(n2)CCC[NH2+][C3]n1</chem>	Neg_lig_155	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
146	<chem>CC(=O)c1cccc(N[C@]([H])2c3ccc3C(=O)N2C2ccco2)c1</chem>	Neg_lig_235	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
147	<chem>CCOC(=O)c1cnn(-c2cc(C)[nH+][c3c(C)c(-c4cccc4)nn23)c1N</chem>	Neg_lig_238	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
148	<chem>CS/C(N)=N\S(=O)(=O)c1ccc(NC(C)=O)cc1</chem>	Neg_lig_248	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
149	<chem>CN(C)c1cccc(NC(=O)N2CC[NH2+][C@H](c3cccc3)C2)c1</chem>	Neg_lig_283	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
150	<chem>CCn1nc(C)c(NC(=O)CNC[C@H]2CN(S(C)=O)=O)CCO2)c1C</chem>	Neg_lig_334	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
151	<chem>O=C(c1ccc(CO)o1)N1CCC([C@]([H])(O)Cc2cccc2)CC1</chem>	Neg_lig_372	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
152	<chem>CCc1cccc1OC1C[NH+](C2CC[NH2+][CC2])C1</chem>	Neg_lig_441	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
153	<chem>CCOC(=O)N1CCC(N2C(=O)c3cccc3[C@H]2Nc2cc(C)cc2)C1</chem>	Neg_lig_490	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
154	<chem>COc1ccc(OC)c(N[C@@H](NC(=O)c2cccs2)C(=O)c2ccc(C)cc2)c1</chem>	Neg_lig_516	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
155	<chem>N#C[C@H]1C(=O)NC(=O)[C@H](C#N)C12CCC[C@H](C(F)(F)F)C2</chem>	Neg_lig_519	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
156	<chem>CC1=C(c2ccc(C(C)C)cc2)S(=O)(=O)N=C1Nc1cccc(Cl)c1</chem>	Neg_lig_552	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
157	<chem>Cc1cccc1OCCCCn1c(CCCO)n2cccc21</chem>	Neg_lig_553	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
158	<chem>Cc1n[nH]cc1N</chem>	Neg_lig_593	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
159	<chem>C[C@H]1CCC[C@H](Ne2ncnc3onc(-c4ccc(Cl)cc4)c23)[C@H]1C</chem>	Neg_lig_705	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
160	<chem>CCc1ccc(C[N@@H+]2CC[C@H]3[C@H](CCC(=O)N3CCCCO)C2)nc1</chem>	Neg_lig_716	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
161	<chem>COc1ccnc2[nH]cc(C(=O)C(=O)N3CCN(C(=O)c4cccc4)C[C@H]3C)c12</chem>	Neg_lig_736	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
162	<chem>COc1[n-]cn/c(=N/S(=O)(=O)c2ccc(N)cc2)c1OC</chem>	Neg_lig_746	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
163	<chem>O=C(Nc1ccc(F)cc1)Oc1ccc[nH]c1=O</chem>	Neg_lig_756	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
164	<chem>CCc1cccc1NC(=O)Cn1c(-c2none2N)nc2cccc21</chem>	Neg_lig_799	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
165	<chem>O=C(CS[C@H]1Nc2sc3c(c2C(=O)N1c1cccc1)CCC3)c1ccc(Br)cc1</chem>	Neg_lig_801	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
166	<chem>Cc1ccc(-c2noc(-c3nnn(-c4cccc(C)c4)c3N)n2)cc1</chem>	Neg_lig_834	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
167	<chem>Cc1nc(N)nc(NCCc2nc(N)n[nH]2)c1CCC(=O)[O-]</chem>	Neg_lig_835	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
168	<chem>CCCc1cc(Nc2ccc(C(=O)N3CCC(CCC3)cc2)n2nc(-c3ccnc3)nc2n1</chem>	Neg_lig_852	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
169	<chem>O=C(NC1CCOCC1)c1ccc(-c2cc(-c3c[nH]nc3-c3cccn3)ccn2)cc1</chem>	Neg_lig_869	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
170	<chem>Cc1ccc2[nH+]c(-c3cccn3)c(Nc3cccc3C)n2c1</chem>	Neg_lig_931	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
171	<chem>Cn1c(CN2CCCCC2)[nH+]e2cc(NCc3cenn3)ccc21</chem>	Neg_lig_938	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
172	<chem>OCc1nc2cc(Cc3ccc4[nH]c(CO)n4c3)ccc2[nH]1</chem>	Neg_lig_942	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
173	<chem>CCn1c(=O)c2c(nc(/C=C\c3ccc(OC)c(OC)c3)n2C)n(CC)c1=O</chem>	Neg_lig_954	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
174	<chem>Cc1ncccc1OC1(C(=O)N2CCc3c([nH]c4cccc34)C2)CC[NH2+]CC1</chem>	Neg_lig_977	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
175	<chem>COc1cc(Cl)cc(OC)c1-c1cccc2c(N)cc[nH+]c12</chem>	Neg_lig_1035	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
176	<chem>O=C(c1cccc1-c1ncc[nH]1)N1CC[C@H]([NH+]2CCCCC2)[C@H](O)C1</chem>	Neg_lig_1057	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
177	<chem>Cc1nc2ccc(C(=O)N3CC[C@H]4(CCCN(CCO)C4=O)C3)cc2s1</chem>	Neg_lig_1072	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
178	<chem>Cc1ccc(-</chem>	Neg_lig_1107	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	<chem>c2ccc3c(ccc4sc5c(c43)NC[C@@H](C)NC5=O)[nH+][2]cn1</chem>				CAUGGCAACCC	
179	<chem>OCCn1nc(COe2cccc2)nc1-c1ccc2[nH]nnc2c1</chem>	Neg_lig_1146	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
180	<chem>Cc1c(-e2cn([C@@H](C)c3nnc(N)s3)nn2)c(=O)n(-c2cccc2)n1C</chem>	Neg_lig_1178	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
181	<chem>COe1cccc1CNc1ncc2nc(-c3cccc3)oc2n1</chem>	Neg_lig_1206	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
182	<chem>CCOc1nc(NC(C)C)nc(N2C[C@@H]3C[C@H](C2)c2cccc(=O)n2C3)n1</chem>	Neg_lig_1216	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
183	<chem>[NH3+]CCn1cc(C(=O)N2CCC[C@H](c3n[nH]c(=O)n3-c3cccc3)C2)nn1</chem>	Neg_lig_1067	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
184	<chem>O=C(NC[C@H](O)c1cccc(O)c1c1cc(O)c2cccc(F)c2n1</chem>	Neg_lig_1224	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
185	<chem>CC[C@H](NC(=O)c1cn([C@H]2CC[C@H]([NH3+])CC2)nn1)c1cn2ccccn2n1</chem>	Neg_lig_1233	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
186	<chem>O=C1[N-]C(=O)C(c2cccc2[N+](=O)[O-])=C1Nc1ccc(O)c(Cl)c1</chem>	Neg_lig_1243	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
187	<chem>N[C@H]1CCCCN(c2nc(-c3cccc3)ccc2C(=O)O)C1</chem>	Neg_lig_1261	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
188	<chem>C[C@H]1C[C@H](C)C(=O)[C@H]([C@H](O)CC2CC(=O)NC(=O)C2)C1</chem>	Neg_lig_1285	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
189	<chem>Nc1c(C(=O)Nc2ccc(Cl)cc2)sc2ncccc12</chem>	Neg_lig_1301	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
190	<chem>CCc1ccc(-n2nnc(-c3nc(-c4ccc(OC)cc4)no3)c2N)cc1</chem>	Neg_lig_1348	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
191	<chem>c1cc(C[NH2+])Cc2ccc3c(c2)OC(O3)c2cc[nH]c2c1</chem>	Neg_lig_1384	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
192	<chem>COe1ccc2c3c([nH]c2c1)[C@H]1C[C@H]2[C@H](C[C@H](O)[C@H](OC)[C@H]2C(=O)O)CN1CC3</chem>	Neg_lig_1421	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
193	<chem>C[C@H]1Cc2cc(Cn3ccnc3-c3cc4n(n3)CCC[NH2+])C4)ccc2O1</chem>	Neg_lig_1450	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
194	<chem>Cn1c(CC2CC[NH2+])CC2)nn1CN1CC[C@H]([NH+](C)C)C1</chem>	Neg_lig_1464	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
195	<chem>Cc1cccc([C@H]2Nc3cccc3C(=O)N2CCe2cccc2)n1</chem>	Neg_lig_1493	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
196	<chem>COc1cc([C@@H]2C(C#N)=C(N)OC(C)=C2C(=O)OC(C)C)cc(OC)c1OC</chem>	Neg_lig_1495	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
197	<chem>Cc1nc(N)nc1C(=O)N1CCC[C@H]1c1ccc(C[NH+](C)C)cc1</chem>	Neg_lig_1503	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
198	<chem>Cc1cccc(Nc2cc(C(C)C)nc3nc(-c4cccn4)nn23)c1</chem>	Neg_lig_1528	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
199	<chem>O=C(C1c2cccc2-c2cccc21)N1CC[C@H]2[NH2+][CCC[C@]2(CO)C1</chem>	Neg_lig_1537	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
200	<chem>Cc1cc(C)n(Cc2ccc(C(=O)N3CCOC[C@@H](O)C3)c2)n1</chem>	Neg_lig_1561	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
201	<chem>Cc1nnc(SCC(=O)N2C[C@@H]</chem>	Neg_lig_1616	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	<chem>3c4ccccc4OC[C@]3(CO)C2)O1</chem>				CAUGGCAACCC	
202	<chem>CN1CCC(=C(c2ccc(Cl)cc2)c2ccn2)CC1</chem>	Neg_lig_1621	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
203	<chem>COc1ccc(C)cc1Nc1c(-c2ccc(C)c(C)c2)c(=O)c1=O</chem>	Neg_lig_1624	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
204	<chem>Cc1noc(C)c1Cn1nc([C@H]2CC[C@H](NH2+)C2)n(-c2ccccc2)c1=O</chem>	Neg_lig_1689	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
205	<chem>Cc1ccc(NC[C@H](O)Cn2c(C)c(C)c3ccccc32)cc1C</chem>	Neg_lig_1731	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
206	<chem>Cc1cccc(Nc2c(-c3ccc(N4CCOCC4)cc3)nc3ncccn23)c1</chem>	Neg_lig_1813	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
207	<chem>CCOC(=O)N1CCC([NH2+]Cc2ccccc2-n2cc[nH+]c2C)CC1</chem>	Neg_lig_1828	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
208	<chem>O=C1c2ccccc2[C@H](Nc2ccc(Cl)cc2)N1c1cccn1</chem>	Neg_lig_1840	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
209	<chem>Cc1ccc2c(c1)c1c(n2C[C@H](O)C[NH2+]c(C)(C)C)CCCC1</chem>	Neg_lig_1871	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
210	<chem>Cc1noc(N)c1C(=O)Nc1ccc2c(c1)OCCO2</chem>	Neg_lig_1888	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
211	<chem>CCOc1ccc(CNc2nc3nc(C)cc(C)n3n2)cc1</chem>	Neg_lig_1937	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
212	<chem>C[C@H]1C[C@H]2(C)Oc3ccccc3[C@H]3OC[C@H]1(CO)[C@H](C)[C@H]32</chem>	Neg_lig_1951	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
213	<chem>O=C(Nc1cccc2ccccc12)c1ccccc1</chem>	Neg_lig_2093	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
214	<chem>CCOc1ccc(CCNC2=NS(=O)(=O)C(c3ccc(OC)cc3)=C2C)cc1</chem>	Neg_lig_2096	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
215	<chem>O=C(Nc1cccc1-c1ccccc1)C(=O)Nc1cccc1-c1ccccc1</chem>	Neg_lig_2139	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
216	<chem>COCc1[nH]nc2c1[C@@H](c1c(F)cccc1Cl)C(C#N)=C(N)O2</chem>	Neg_lig_2184	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
217	<chem>CCCC[NH2+]C[C@H]1CCC O1</chem>	Neg_lig_2185	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
218	<chem>Oc1cc(-n2cccn2)c(O)cc1-n1cccn1</chem>	Neg_lig_2198	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
219	<chem>OCc1ccc(-c2ccc(-c3nc(Cc4ccc(Cl)cc4)no3)c[nH+]2)cc1</chem>	Neg_lig_2232	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
220	<chem>Cc1ccc(NC(=O)Cn2nnc(C(=O)Nc3ccccc3)c3C)c2N)c(C)c1</chem>	Neg_lig_2281	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
221	<chem>COc1ccc(C[NH2+]CC[C@]2(c3ccc(F)cc3)CCOC(C)(C)C2)cc1OC</chem>	Neg_lig_2295	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
222	<chem>COC(=O)c1ccc(NC(=O)CCN2CCN[C@H]3CS(=O)(=O)C[C@H]32)cc1</chem>	Neg_lig_2303	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
223	<chem>O=C1O[C@H](Nc2ccc(S(=O)(=O)/N=c3\ccccc[nH]3)cc2)c2ccccc21</chem>	Neg_lig_2310	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
224	<chem>CCOC(=O)c1c(N)sc2c1CCN(Cc1ccccc1)C2</chem>	Neg_lig_2356	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
225	<chem>CC(=O)N1CCN(c2nc(-c3ccccc3)nc3c2CCC3)C[C@@H](O)C1</chem>	Neg_lig_2364	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
226	<chem>COc1ccc(Cl)cc1NC(=O)c1nnn(Cc2ccc(F)cc2)c1N</chem>	Neg_lig_2377	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
227	<chem>O=C(CSCCO)Nc1nc(-c2ccccc2)cs1</chem>	Neg_lig_2413	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
228	<chem>COc1ccc(-c2cc3[nH+]c(C)cc(NC4ccccc4)n3n2)cc1OC</chem>	Neg_lig_2428	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
229	<chem>O=C(NC[C@H](O)CO)c1ccc2[nH]c3c(c2c1)CC CC3</chem>	Neg_lig_2432	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
230	<chem>Cc1cn([C@H]2C[C@H](N=[N+]=[N-])[C@@H](CO)O2)c(=O)[nH]c1=O</chem>	Neg_lig_719	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
231	<chem>CCCCCNc1cc(C)[nH+]c2c(C)c(-c3ccccc3)nn12</chem>	Neg_lig_1548	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
232	<chem>COc1cc(OC)c([N-]C2=NS(=O)(=O)C(c3ccc(C(C)C)cc3)=C2C)cc1Cl</chem>	Neg_lig_2477	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
233	<chem>CC1(C)CC(=O)C2=C(C1)OC(N)=C(C#N)[C@H]2c1ccc(Cl)c(Cl)c1</chem>	Neg_lig_2479	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
234	<chem>CCCCc1nc(-c2c(-c3ccccc3)ncn2CC2CC[NH2+])C C2)c[nH]1</chem>	Neg_lig_2551	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
235	<chem>CN(C)S(=O)(=O)c1cccc(N)c1</chem>	Neg_lig_1304	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
236	<chem>Cc1nn(Cc2ccccc2)c(N)c1-c1ccccc1</chem>	Neg_lig_2561	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
237	<chem>Cc1nc(-c2nc(CCO)n(-c3ccccc3Cl)n2)cs1</chem>	Neg_lig_2583	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
238	<chem>C#Cc1ccccc1(Nc2ncnc3cc(OC)c(OCCCCCCC(=O)NO)cc23)c1</chem>	Neg_lig_2598	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
239	<chem>Cc1ccc(OCCCCn2c([C@H](C)O)nc3ccccc32)cc1</chem>	Neg_lig_2605	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
240	<chem>Cc1ccc2nc(C[NH2+])C[C@H](C)Oc3ccccc3[nH]c2c1C</chem>	Neg_lig_2615	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
241	<chem>CC1(C)CC(Nc2nc(Cl)c(C#N)c(Cl)c2Cl)CC(C)(C)[NH2+]1</chem>	Neg_lig_2658	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
242	<chem>COCCN1C[C@@H](Cn2ccnc2-c2ccc(CO)o2)CC1=O</chem>	Neg_lig_1674	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
243	<chem>Nc1nc2c(ncn2COC(CO)CO)c(=O)[nH]1</chem>	Neg_lig_2668	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
244	<chem>COc1ccc2ccccc2c1CNc1ccncc1</chem>	Neg_lig_2705	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
245	<chem>CCOC(=O)c1ccc2nc(C(F)(F)F)nc(NCCc3ccc(OC)cc3)c2c1</chem>	Neg_lig_2711	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
246	<chem>CC(C)C[C@H](NC(=O)[C@@H](NC(=O)c1ccc(-c2ccccc2)n1)[C@@H](C)O)B(O)O</chem>	Neg_lig_2752	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
247	<chem>O=C(c1coc(CN2CCOCC2)c1)N1[C@H]2CC[C@H]1CC[NH2+]C2</chem>	Neg_lig_2782	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
248	<chem>Cn1cc(CCC(=O)N2C[C@@H](C[NH+])3CCCCC3)[C@@H](CO)C2)cn1</chem>	Neg_lig_2823	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
249	<chem>Cc1cc(NC2CCCCC2)ncn1</chem>	Neg_lig_1895	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
250	<chem>CC1=NC2=NC(C(Cl)(Cl)Cl)=NC3=CC=CC(=N1)N32</chem>	Neg_lig_2829	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
251	<chem>CCCCNc1nc(Oc2ccc(OCC)nn2)nc(N(C)C)n1</chem>	Neg_lig_2846	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
252	<chem>NC(=O)Cc1nc(-c2ccc3c(c2)NC(=O)CN3)n(-c2ccc(F)c2)n1</chem>	Neg_lig_2851	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
253	<chem>CN1CCC(=C2c3ccccc3[C-](O)c3ccccc32)CC1</chem>	Neg_lig_2892	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
254	<chem>CN(C)c1n/c(=N/c2ccc(Cl)c2)ss1</chem>	Neg_lig_2898	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
255	<chem>c1ccc2c(-c3cc(NC4CC[NH2+]CC4)nc4[nH]ccc34)ccnc2c1</chem>	Neg_lig_2901	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
256	<chem>CCCCSCc1cc(C(=O)N2CC[C@H]3C[NH2+]C[C@H]32)oc1C</chem>	Neg_lig_1994	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
257	<chem>COc1ccc2ccccc2c1[C@@H](O)c1[nH+]ccn1C</chem>	Neg_lig_2911	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
258	<chem>O=C(NCCc1nnc2n1CC[NH2+]CC2)c1ccc(-c2ccccc2)[nH]1</chem>	Neg_lig_2973	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
259	<chem>CC(C)CN1CC2(CCN(c3nccc(N4CCC[C@H](O)C4)n3)CC2)CC1=O</chem>	Neg_lig_2987	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
260	<chem>COc1cc(C[C@H](O)CO)cc2c1OCO2</chem>	Neg_lig_3001	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
261	<chem>Cc1nn(C(=O)c2ccc(C(C)(C)C)cc2)c(N)c1-c1ccccc1</chem>	Neg_lig_1967	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
262	<chem>Cc1ncc(CO)c(CN2C[C@H]([NH3+])C[C@H]2C(=O)NC(C)C)c1O</chem>	Neg_lig_2670	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
263	<chem>Cc1ccc2c(N)c(C(=O)[O-])sc2n1</chem>	Neg_lig_3010	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
264	<chem>COc1ccc(OC[C@@H](O)Cn2c(NCCc3ccc(OC)c(OC)c3)nc3c2c([O-])nc(=O)n3C)cc1</chem>	Neg_lig_3016	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
265	<chem>Cc1sc2c(N3CCC(O)(CO)CC3)nc[nH+]c12</chem>	Neg_lig_3056	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
266	<chem>COc1ccc([C@@H]2CNC(=O)C2)cc1OC1CCCC1</chem>	Neg_lig_3098	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
267	<chem>Cc1c(NCc2ccnc2)cccc1C(=O)N(C)Cc1ccoc1</chem>	Neg_lig_3121	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
268	<chem>CC1=C(C(=O)OCc2ccccc2)[C@]2(C(=O)Nc3ccccc32)C(C(=O)OCc2ccccc2)=C(N)O1</chem>	Neg_lig_2796	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
269	<chem>COCC[C@]1(CO)CCCN(C(=O)Cc2ccc(CO)cc2)C1</chem>	Neg_lig_129	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
270	<chem>Cc1cc(NC(C)C)n2nc(-c3ccc(Cl)cc3)c(C)c2[nH+]1</chem>	Neg_lig_3205	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
271	<chem>C=C[C@@H]1C[N@@H+]2CC[C@H]1C[C@@H]2[C@@H](O)c1ccnc2ccccc12</chem>	Neg_lig_3233	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
272	<chem>CCC[C@H](O)c1nc2ccccc2n1Cc1ccccc1OC</chem>	Neg_lig_3247	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
273	<chem>Cc1ccc(C)c(NCC(=O)Nc2c(C)ccc2C)c1</chem>	Neg_lig_3251	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
274	<chem>OC[C@H]1C[N@H+](C2CCN(Cc3ccccc3)CC2)C[C@H]1CN1CCCC1</chem>	Neg_lig_3252	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
275	<chem>CCC(=O)N[C@H]1CC[C@H](C(=O)N(C)C)c2ccc(-c3nc4ccccc4o3)cc2C1</chem>	Neg_lig_3258	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
276	<chem>COc1ccc(Nc2nc(-c3ccc(OC)c(OC)c3)no2)c(OC)c1</chem>	Neg_lig_3276	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
277	<chem>CCOC(=O)N1CCC(N2C(=O)c3cccc3[C@H]2Nc2cc(F)c(Cl)c2)CC1</chem>	Neg_lig_3329	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
278	<chem>CCn1c(N)nc2cc(C(=O)NCCC=CSC4=[NH+]CCCN34)cnc21</chem>	Neg_lig_3333	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
279	<chem>Cc1cc(NC[C@H]2CCCO2)n2nc(-c3ccc(Cl)cc3)c(C)c2[nH+]1</chem>	Neg_lig_3348	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
280	<chem>COc1cccc1-c1cc2[nH+]c(C)cc(NCC(C)C)n2n1</chem>	Neg_lig_3402	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
281	<chem>N#Cc1c(-c2ccccc2)cc(-c2ccc(Br)c2)c1N</chem>	Neg_lig_3413	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	0
282	<chem>CCCCc1nc(C)cc(NCCNC(=O)c2cn3c(n2)CNCC3)n1</chem>	Neg_lig_37	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
283	<chem>C=CCNC(=O)c1sc(N2CCCC2)n1N</chem>	Neg_lig_72	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
284	<chem>Cn1c(=O)c2c(nc(NC[C@H]3CCCO3)n2Cc2cc(F)cc2)n(C)c1=O</chem>	Neg_lig_110	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
285	<chem>Cc1n[nH]c(C)c1S(=O)(=O)N1CC[NH2+]CC1</chem>	Neg_lig_134	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
286	<chem>CC(C)NC(=O)[C@@H]1C[C@@H](NC(=O)c2ccon2)CN1Cc1ccnc1N</chem>	Neg_lig_253	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
287	<chem>COc1ccc(OC)c([C@H]2CCN(C(=O)C3([NH3+])CC3)C2)c1</chem>	Neg_lig_270	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
288	<chem>CCn1c([C@H]2CCCC[NH2+]C2)nn(CCCS(=O)(=O)N(C)C)c1=O</chem>	Neg_lig_406	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
289	<chem>C[C@@H]1C(C#N)=C(N)OC2=C1C(=O)CCC2</chem>	Neg_lig_448	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
290	<chem>Cc1cc(C(F)(F)F)nc(N2CCN(C[C@H]3CCC[NH2+]C3)CC2)n1</chem>	Neg_lig_497	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
291	<chem>Cc1cc(Nc2ccc(C(=O)O)cc2)c2cc(F)ccc2n1</chem>	Neg_lig_568	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
292	<chem>COc1ccc(F)cc1NC(=O)NC[C@H](O)CO</chem>	Neg_lig_630	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
293	<chem>Cc1ccc(C)c2c(O)cc(CN3C[C@H](O)[C@@H](N4CCOCC4)C3)nc12</chem>	Neg_lig_651	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
294	<chem>CCCc1ccc(C[N@H+]2CC[C@H](NC(=O)c3ccncc3)[C@H](O)C2)o1</chem>	Neg_lig_654	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
295	<chem>CC(C)n1cnc1CN(C)</chem>	Neg_lig_699	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	<chem>[C@H]1CCCC[NH2+]C1</chem>				GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	
296	<chem>N#CC1=C(N)Oe2cc(N)ccc2[C@@H]1c1ccc(Br)s1</chem>	Neg_lig_709	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
297	<chem>CCc1ccc(OC[C@@H](O)C[NH+]2CCCC(C)CC2)cc1</chem>	Neg_lig_735	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
298	<chem>Cc1cnn([C@@H](C)CNC(=O)c2cc(C[NH+]3CC(C(O)CC3)on2)c1</chem>	Neg_lig_740	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
299	<chem>O=C(NC[C@@H](CO)Cc1ccsc1)c1cnc(-c2cncce2)nc1</chem>	Neg_lig_741	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
300	<chem>Cc1c(CN2CC[C@H]3CC[C@@H](C2)[NH2+]3)c(=O)n(-c2cccc2)n1C</chem>	Neg_lig_781	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
301	<chem>O=C1N=C(C(F)(F)F)C=C/C1=C(\O)N1CC[C@H]2[NH2+]CCC[C@]2(CO)C1</chem>	Neg_lig_868	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
302	<chem>CCNc1nc(OC)nc(Oc2ccc(=O)n(C)n2)n1</chem>	Neg_lig_902	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
303	<chem>CN(CC[NH+](C)C)C(=O)c1ccc(NC(=O)Nc2ccc(-c3nc(N4CCOCC4)c4ccn(CC(F)(F)F)c4[nH+]3)cc2)cc1</chem>	Neg_lig_912	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
304	<chem>COc1cccc1-n1cc(-c2cc(-c3cnn(C)c3C)c(C#N)c(N)n2)cn1</chem>	Neg_lig_543	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
305	<chem>CC(C)(C)c1ccc(OC[C@@H](O)CN2CCOCC2)cc1</chem>	Neg_lig_1008	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
306	<chem>O=C1C=C/C(=N\Nc2ccccc2)C(C(=O)[O-])=C1</chem>	Neg_lig_1133	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
307	<chem>CCCCc1[nH]nc2c1C1(CCN(C(=O)OCC)CC1)C(C#N)=C(N)O2</chem>	Neg_lig_1138	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
308	<chem>N#Cc1c(-c2ccccc3cnccc23)cc(-c2ccco2)nc1N</chem>	Neg_lig_1245	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
309	<chem>O=C1OC2(CCN(C(=O)c3ccc(CO)o3)CC2)CN1CCOc1cccc1</chem>	Neg_lig_1279	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
310	<chem>OCc1cc(-c2ccc3c(c2)OCO3)no1</chem>	Neg_lig_1330	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
311	<chem>COc1cc(C(C)=O)ccc1OC[C@@H](O)CN1CCN(c2ccccc2F)CC1</chem>	Neg_lig_1349	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC	0



Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
					UGCUAUGCCAACAUUUG CCAUC	
312	<chem>C=CCN1C(=O) [C@]2(c3ccccc31)c1c(oc3cc(C) c(C)cc3c1=O)C(=O)N2CCCO</chem>	Neg_lig_1353	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUUUG CCAUC	0
313	<chem>CCn1cc(S(=O) (=O)N2CC[C@H](CO)[C@H] (O)C2)cn1</chem>	Neg_lig_1355	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUUUG CCAUC	0
314	<chem>CC1(C)C[C@@](C) (c2ccccc2)c2ccccc2N1C(=O)CS c1nnc(N)s1</chem>	Neg_lig_1376	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUUUG CCAUC	0
315	<chem>Cc1cc(=O)n(C)c(=O)n1CCCCO</chem>	Neg_lig_1403	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUUUG CCAUC	0
316	<chem>CC(C)Oc1ccccc1Nc1nnc2ccccc 12</chem>	Neg_lig_1411	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUUUG CCAUC	0
317	<chem>[NH3+][CCNC(=O)c1nc(Cn2cc( Br)cn2)no1</chem>	Neg_lig_1424	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUUUG CCAUC	0
318	<chem>COC(=O)c1ccc(NC(=O)N2CCO C[C@H]2CO)cc1Cl</chem>	Neg_lig_1446	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUUUG CCAUC	0
319	<chem>S=C1NC2(CCCCC2)NN1c1cc ccc1</chem>	Neg_lig_1494	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUUUG CCAUC	0
320	<chem>Cc1cc(Br)ccc1N[C@H]1OC(=O )c2ccccc21</chem>	Neg_lig_1511	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUUUG CCAUC	0
321	<chem>CCCCCCCn1c(CO)nc2ccccc21</chem>	Neg_lig_1533	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUUUG CCAUC	0
322	<chem>Cc1nc(Nc2ncc3c(n2)C[C@H] (C)CC3=O)nc2ccccc12</chem>	Neg_lig_1576	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUUUG CCAUC	0
323	<chem>O[C@@H] (CSc1nnc2[nH]cnc12)c1ccc(Cl )cc1</chem>	Neg_lig_1606	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUUUG CCAUC	0
324	<chem>CSCCc1nc(Cn2cc(Cl)c(C)n2)n( CCO)n1</chem>	Neg_lig_1609	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUUUG CCAUC	0
325	<chem>CC1(C)CC(=O)c2cc3c(N)c(C(= O)c4ccc(F)cc4)sc3nc2C1</chem>	Neg_lig_1625	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUUUG CCAUC	0
326	<chem>Nc1nc(NCCc2nc(Cc3ccccc3)no 2)c2c([nH+]1)CCCC2</chem>	Neg_lig_1629	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUUUG CCAUC	0
327	<chem>CCNC(=O) [C@@H]1C[C@H] (NC(=O)Cn2cc(Cl)cn2)CN1C(= O)CCO</chem>	Neg_lig_1685	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUUUG CCAUC	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
328	<chem>Cc1c(S(=O)(=O)c2ccc(F)cc2)c(N)n(C2CCC(CC2)c1C</chem>	Neg_lig_1692	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
329	<chem>CC(C)c1nc(N2CCC([NH2+][CCSc3nnnn3C)CC2)cc(=O)[nH]1</chem>	Neg_lig_1702	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
330	<chem>Nc1cccc(C(=O)Nc2cc([O-])n(-c3c(Cl)cc(Cl)cc3Cl)n2)c1</chem>	Neg_lig_1746	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
331	<chem>Fc1cccc(CCNCc2nc(-c3ccc[nH+][c3]nc3c2CC[NH2+][CC3)c1</chem>	Neg_lig_1792	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
332	<chem>Cc1noc(C)c1CCC(=O)NCc1cc2n(n1)CCC[NH2+][C2</chem>	Neg_lig_1925	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
333	<chem>O=c1cc(-c2cccc2)oc2ccc(O)cc12</chem>	Neg_lig_1936	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
334	<chem>Fc1cccc1CC[NH2+][Cc1cccc(Oc2ncccn2)c1</chem>	Neg_lig_1998	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
335	<chem>CN(C)c1nc(NC(C)(C)C)nc(-n2cnc(SCc3ccccc3)n2)n1</chem>	Neg_lig_2091	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
336	<chem>CSc1nc(N)nc(SCC(=O)Nc2ccc(C)cc2)c1C#N</chem>	Neg_lig_2097	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
337	<chem>O=C(c1cc(=O)[nH]c2cccc12)N1CCOC[C@@H]1CO</chem>	Neg_lig_2101	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
338	<chem>CCCC1(C[NH2+][C2CCN(C(=O)c3cncn3)CC2)CCC1</chem>	Neg_lig_2103	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
339	<chem>Cc1ccc(OC2(C(=O)NCCc3nc(C)c(C)s3)CC[NH2+][CC2)cc1</chem>	Neg_lig_548	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
340	<chem>Cc1nc(-c2cccc(-n3ccnc3-c3cc4n(n3)CC[NH2+][C4)c2)cs1</chem>	Neg_lig_2131	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
341	<chem>COc1ccc(Cn2nnc(C(=O)Nc3cc(C)ccc3OC)c2N)cc1Br</chem>	Neg_lig_2161	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
342	<chem>COc1ccc(-c2c(C)nn3c(NCc4ccc(Cl)cc4)cc(C)[nH+][c23)cc1OC</chem>	Neg_lig_2174	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
343	<chem>COC(=O)c1cc(SC#N)ccc1N</chem>	Neg_lig_2181	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
344	<chem>CO[C@H]1C[C@@H](O)C12CCN(C(=O)Cc1nc3nc(C</chem>	Neg_lig_2182	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	<chem>)cc(C)n3n1)CC2</chem>				UGCUAUGCCAACAUAUUG CCAUC	
345	<chem>O=C(O) [C@@H]1CN(Cc2ccc(OCOC)c c2)C[C@H]1c1cccc(F)c1</chem>	Neg_lig_2187	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
346	<chem>O=c1cc/c(=[NH+])\Nc2ccccc2)c(=O)/c1=N\Nc1cccc1</chem>	Neg_lig_2216	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
347	<chem>c1ccc(COC2CCN(c3nnc4c3CC[NH2+])CC4)CC2)nc1</chem>	Neg_lig_2217	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
348	<chem>c1ccc2c(CC[NH2+])Cc3ccsc3)c[nH]c2c1</chem>	Neg_lig_2218	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
349	<chem>C[C@H] ([NH2+])Cc1csc2ccc(Cl)cc12)C(=O)NC1CCCC1</chem>	Neg_lig_2252	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
350	<chem>COC(=O)c1ccc(OC[C@@H](O)Cn2nc3cc(C)c(C)cc32)cc1</chem>	Neg_lig_2271	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
351	<chem>O=C1[C@H]2[C@@H]3C=C[C@@H](C3) [C@H]2C(=O)N1c1cccc1CO</chem>	Neg_lig_2280	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
352	<chem>CC(C)c1ccc([C@@H](O)C2nc3ccccc3n2C)cc1</chem>	Neg_lig_2286	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
353	<chem>c1ccc(Cn2cnc2CNC2CCC3(CC[NH2+])CC3)CC2)cc1</chem>	Neg_lig_2309	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
354	<chem>CC(C)c1cc(N2CCc3nnc(-c4ccccc4)n3CC2)nc(N)n1</chem>	Neg_lig_2313	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
355	<chem>c1ccc(-c2nc[nH]c2-c2ccccc2)cc1</chem>	Neg_lig_2322	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
356	<chem>COc1ccc(CNc2c(-c3ccc(C)cc3)c(=O)c2=O)cc1</chem>	Neg_lig_2324	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
357	<chem>Cc1sc2nnc(NCc3ccc4c(c3)OC(=O)c2c1C</chem>	Neg_lig_2340	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
358	<chem>Nc1nc(SCC2c2ccccc2)ns1</chem>	Neg_lig_2332	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
359	<chem>C[NH+]1CCCC(N(CC2ccccc2)C(=O)CN2CCC[C@H](O)C2)CC1</chem>	Neg_lig_882	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
360	<chem>CCCC(=O)C1=C(O)CC(C)(C)C/C1=N/[C@@H](CC)CO</chem>	Neg_lig_2426	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
361	<chem>Clc1cccc1COc1cccc(C[NH2+] Cc2ccnc2)c1</chem>	Neg_lig_2429	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
362	<chem>CC(C) (C)n1cnc2cc(NCc3cccn3)ccc21</chem>	Neg_lig_2446	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
363	<chem>[NH3+][C@H]1CC[C@H] (C(=O)Nc2ccccc2OCCc2cccn2 )C1</chem>	Neg_lig_2448	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
364	<chem>CSc1nc(N)nc(SCC(=O)CC(=O) OC(C)C)c1C#N</chem>	Neg_lig_2464	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
365	<chem>CC[C@H] (c1nc(Cc2cccs2)nn1CCO)n1ccc n1</chem>	Neg_lig_2469	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
366	<chem>O[C@@]1(C[NH2+])CCCc2ccn cc2)CNCCOC1</chem>	Neg_lig_2472	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
367	<chem>CCCc1ccc(C[N@H+]2CCOC[C @@H](CO)C2)o1</chem>	Neg_lig_2530	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
368	<chem>c1ccc(- n2nnnc2SCC[NH2+])Cc2ccco2)c c1</chem>	Neg_lig_163	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
369	<chem>Cc1cc(=O)c2ccccc2n1CC[C@ H](O)c1ccccc1</chem>	Neg_lig_2653	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
370	<chem>COc1ccc(-c2noc(- c3ccnc3NCc3ccccc3Cl)n2)cc1</chem>	Neg_lig_2687	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
371	<chem>CC(C)Cc1cc(C(=O)N(CCCO)Cc 2ccnc2)n(C)n1</chem>	Neg_lig_2696	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
372	<chem>CCCCCn1c(N)c(C#N)c2nc3cccc c3nc21</chem>	Neg_lig_2820	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
373	<chem>COc1ccc(C2=C(C)NN/C2=C2\ C=CC([O-])=CC2=O)cc1</chem>	Neg_lig_2857	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
374	<chem>COC1=C2C[C@@H] (C)C[C@H](OC)[C@@H](O) [C@@H](C)/C=C/[C@H] (OC(N)=O)[C@@H](OC)/C=C\ C=C(\C)C(=O) [N-]C(=CC1=O)C2=O</chem>	Neg_lig_2903	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
375	<chem>O=C(Cc1cccc2ccccc12)N1CCO[ C@]2(C[NH2+])CCOC2)C1</chem>	Neg_lig_2922	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
376	<chem>Cc1cccc(- c2nc3nc(C)cc(Nc4ccc(N(C)C)cc 4)n3n2)c1</chem>	Neg_lig_2928	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
377	<chem>c1cnc(Oc2cccc(C[NH2+])Cc3ccc(O)c2)nc1</chem>	Neg_lig_2650	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
378	<chem>O=C(c1cnc(Br)c1)N1CCC([NH+])C2CCCC2CC1</chem>	Neg_lig_2988	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
379	<chem>Cc1cccc(C[NH+])C2CCC(n3cc(CO)nn3)CC2)c1C</chem>	Neg_lig_2996	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
380	<chem>CC[C@@H](CO)NC(=O)c1ccc(-c2nn(C)c(=O)c3ccccc23)cc1</chem>	Neg_lig_3006	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
381	<chem>CC(C)(C)n1cnc2cc(NCc3cccc4ccccc34)ccc21</chem>	Neg_lig_3072	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
382	<chem>COc1ccccc1N1CCN(C(=O)[C@H]2[C@@H]([NH3+])[C@H]3CC[C@@H]2C3)CC1=O</chem>	Neg_lig_3096	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
383	<chem>NCc1nc(-c2ccccc2)no1</chem>	Neg_lig_3154	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
384	<chem>O=S(=O)(c1ccc2c(c1)CCCN2)N1CCC[C@H]2CCCC[C@@H]21</chem>	Neg_lig_3163	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
385	<chem>COc1ccc(N2CCN(C[C@H](O)c3ccc4c(c3)CCN4)CC2)cc1</chem>	Neg_lig_3165	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
386	<chem>Cc1ccn(CO)n1</chem>	Neg_lig_57	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
387	<chem>COCc1cc(C)nc(NCCO)c1C#N</chem>	Neg_lig_3176	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
388	<chem>CC(C)Cc1nc2sc3c(NCCCO)ncnc3c2c1COC(C)(C)C2</chem>	Neg_lig_3202	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
389	<chem>CCN(CC)C(=O)[C@@H]1C[C@H]([NH3+])CN1Cc1ccc(Cl)nc1</chem>	Neg_lig_3228	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
390	<chem>Cc1nc2c(c(N3CC=CC3)n1)CCN(C(=O)c1cnc(N)c1)CC2</chem>	Neg_lig_3248	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
391	<chem>C=CCN(CC=C)C(=O)Nc1cc(OC)ccc1OC</chem>	Neg_lig_3254	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
392	<chem>COCc1nn(-c2ccccc2)c(N)c1-c1ccc(OC)c(OC)c1</chem>	Neg_lig_2047	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
393	<chem>O=C1[C@@H](CO)[C@@H](CO)[C@@H](CO)[C@@H]1CO</chem>	Neg_lig_3332	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
					UGCUAUGCCAACAUAUUG CCAUC	
394	<chem>C[C@@H](C[N@H+]1CCc2ccccc2C1)Nc1cccc(N2CCC(O)CC2)n1</chem>	Neg_lig_3374	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
395	<chem>CNc1ccc(Br)c2c1C(=O)c1ccccc1C2=O</chem>	Neg_lig_3378	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
396	<chem>CC[C@@H](CO)[NH2+][C][C@@H](O)Cn1c(C)c(C)c2ccccc21</chem>	Neg_lig_1242	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
397	<chem>CCOC(=O)c1c(-c2cccc(OC)c2)n[nH]c1N</chem>	Neg_lig_3418	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
398	<chem>Cc1ccc2nc(C(=O)[O-])cc(Nc3ccc(N(C)C)cc3)c2c1</chem>	Neg_lig_3422	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	0
399	<chem>c1ccc(cc1)N1C(C(Nc2cccc(c2)C(O)=O)SC1=O)=O</chem>	1159-0329	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	1
400	<chem>Cc1ccc([C@H]2CN(C[C@@H]2N)C(COc2ccc(cc2)n2cnnn2)=O)o1</chem>	13917927	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	1
401	<chem>C1CN(CC(c2ccccc2)N1)C(c1ccn2cnc2c1)=O</chem>	13930321	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	1
402	<chem>CNC(c1cc2CN(CCc2s1)C(C1CNCCO1)=O)=O</chem>	14100811	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	1
403	<chem>C(CCN1cc(c2ccccc2c2ccco2)nn1)CCO</chem>	14330381	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	1
404	<chem>C1[C@@H](C2(CCN(CC2)Cc2ccccc2)OCN2CCOCC2)[C@@H]1O)O</chem>	14778588	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	1
405	<chem>CN1CCCN(C)C2(CCN(CC2)C(Nc2cccc(CN)c2)=O)C1</chem>	15129370	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	1
406	<chem>COCCN(CC1CC1)C(c1ccc(cc1)C1CCCN1)=O</chem>	15822403	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	1
407	<chem>Cc1ccc(cc1)NC([C@H]1C[C@H](CN1)C(NCCN1CCCC1=O)=O)=O</chem>	17600296	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	1
408	<chem>CC(C)Cc1cc(CNC2CCN(CC2)C(C)C)no1</chem>	17766103	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	1
409	<chem>Cc1c(CNC(c2cn(CCC3CCCCN3)nn2)=O)c(C)on1</chem>	18521194	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
410	<chem>C(Cc1csc(N)n1)CNC(C1CCCN(C1)Cc1ccco1)=O</chem>	18722734	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	1
411	<chem>C(COCc1ccc(cc1)[Cl])NCC1(CNCCOC1)O</chem>	20639134	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	1
412	<chem>C1CC(CNC1)c1ccc(cc1)C(N1CCN(CC1)c1ccc(cc1)F)=O</chem>	21010099	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	1
413	<chem>CC1CC2(C)CC(C)C1(CO)CO2</chem>	2190-0577	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	1
414	<chem>Cn1c(Cn2ccnc2c2cc3CNCCn3n2)cnc1SC</chem>	22199819	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	1
415	<chem>CNc1cc(c2ccc(cc2)c2nnc(N)s2)c2cc[nH]c2n1</chem>	25638728	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	1
416	<chem>COc1cccc(CNCCc2cccc(c2)F)c1</chem>	2910-1991	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	1
417	<chem>O=C(N(CC1OC1)C(N1CC2OC2)=O)N(CC2OC2)C1=O</chem>	296934	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	1
418	<chem>C1COC2(CCOCC2)CC1NCc1nc(c2cncnc2)n[nH]1</chem>	31093015	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	1
419	<chem>Cc1c2c(NCc3nc(N)[nH]n3)nc(C)nc2on1</chem>	31495708	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	1
420	<chem>Cc1c(cccc1NC(NCCNc1ccnc1)=O)C(NC(C)(C)C)=O</chem>	31773556	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	1
421	<chem>C(CNc1c2c(csc2nnc1)c1ccc(cc1)F)c1cccs1</chem>	3230-0825	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	1
422	<chem>Cc1c(CNC(CCc2ccsc2)=O)c2CCNCCc2en1</chem>	32845432	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	1
423	<chem>CC(C)c1nc(CCNC(c2ccccc2C2CCNC2)=O)on1</chem>	33313650	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	1
424	<chem>C(Cc1nc(c2ccco2)nn1CCO)c1ccc2c(c1)OCO2</chem>	33326934	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	1
425	<chem>C1CCc2c(C1)nc(CCNCC1(CCN C1)O)s2</chem>	33880841	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	1
426	<chem>[H] [C@@@]12CCCCN2CCC[C@]1(</chem>	33884666	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	CNCCSCC)O				UACUGCAGUGAAGGCACU UGUAG	
427	CNC(C(NCc1cc2CN(CCn2n1)C (N(C)C)=O)=O)c1cccc1	34114692	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	1
428	Cc(cc1nc(ccc(N(C)C)c2c[s+] lc1)c1N.[Cl-])	36758	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	1
429	Cc1cc2NC(CN3CCC4(CC3)C(C c3ccccc34)O)=CC(n2n1)=O	40183085	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	1
430	CCC(c1ccnn1C)NCc1ccc(c(CC= C)c1)OCC	41760826	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	1
431	C1CN(Cc2cc3cc[nH]c3cn2)Cc2 cc(C(NCCO)=O)nn2C1	41857771	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	1
432	C1CCN(C1)C[C@@H]1CN(Cc 2ccc(cc2)c2nn[nH]n2)C[C@@H ]1CO	42363475	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	1
433	CCN(CCn1cccn1)C(c1ccc(cc1) C1CCCN1)=O	42585880	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	1
434	CCc1nc2cc(cnc2[nH]1)c1cc(NC CO)nc2c1cc[nH]2	46180634	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	1
435	CCC(CO)N(Cc1ccc(cc1)F)Cc1c c(c(c1)[Cl])O)OC	46503727	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	1
436	Cc1c(CC=C)c(nc(N)n1)N1CCN( CC1)c1c2c(ncn1)[nH]cn2	47603260	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	1
437	CC[n+] ]1cn(CC(COc2ccccc2)O) c2ccccc12	5010-0422	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	1
438	CCOC(c1c(C)c(C)sc1NC(CNCc 1ccccc1)=O)=O	5132485	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	1
439	CCOC(c1cnc2ccc(cc2c1Nc1ccc cc1)N1CCOCC1)[Cl])=O	5173-3862	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	1
440	CCOC(c1cnc2ccc(C)cc2c1NCC( C)O)=O	5174-4400	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	1
441	C1CCCC(C1)N[C@@H]1CC[C C@@H]1NC(c1ccccc1N1CCO CC1)=O	56098188	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	1
442	CC1=CC2=C(C(C(C#N)=C(N) O2)c2ccccc2OC)C(N1Cc1ccc2c (c1)OCO2)=O	7706-1226	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	1



Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
443	<chem>CCOC(C1=C(C)OC(=C(C(=O)OCC)C12C(Nc1cccc12)=O)N)=O</chem>	8003-0370	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	1
444	<chem>C(C1C(c2cccc2)c2c(c3cccc3)n[nH]c2OC=1N)#N</chem>	8008-9218	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	1
445	<chem>Cc1c(CCNc2ccc(C#N)cc2)c2c(c(ccc2[nH]1)OC</chem>	8013-2954	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	1
446	<chem>C(c1ccoc1C(O)=O)N</chem>	8015-0997	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	1
447	<chem>C(c1ccc(cc1)F)N1C(C2C(C#N)=C(N)N(C3COC(C2=3)=O)c2ccc2)c2cccc12)=O</chem>	8017-5050	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	1
448	<chem>C=CCOc1ccc(cc1)C1C(C#N)=C(N)OC2=C1C(c1cccc1C2=O)=O</chem>	8017-5263	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	1
449	<chem>Cc1c(C#N)c(N)n(CCCn2ccnc2)c1C</chem>	8018-7492	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	1
450	<chem>Cc1c(c2ccc(cc2)[Br])c2ncc(C#N)c(N)n2n1</chem>	8019-5330	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	1
451	<chem>c1cc(N)nc2c1ccc(n2)O</chem>	8019-7722	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	1
452	<chem>CCc1c(C)cc2c(c(C(c3cccc3)=O)sc2n1)N</chem>	8020-0635	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	1
453	<chem>c1cnccc1c1nc2nenc(N)n2n1</chem>	8020-2786	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	1
454	<chem>[H]N(CCNc(c1c(N)non1)=O)Cc1cc(ccc1OCc1ccc(cc1)[Cl])[Br]</chem>	8104-04658	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	1
455	<chem>Cc1c(c2ccc(c(c2)OC)OC)c2ncc(c3ccc(c(c3)OC)OC)c(N)n2n1</chem>	8104-10716	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	1
456	<chem>Cc1cc(Nc2ccc(cc2)N2CCOCC2)n2c(ncn2)n1</chem>	8246-0044	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	1
457	<chem>c1ccc2c(c1)nc(c1ccc(cc1[Cl])N)s2</chem>	C066-5322	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	1
458	<chem>Cn1c2cccc2nc1CNCc1cccc1</chem>	C147-0039	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	1
459	<chem>Cc1cccc(c1)NCc1nc2cccc2n1C</chem>	C147-0043	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
					UACUGCAGUGAAGGCACU UGUAG	
460	<chem>Cc1cccc(C)c1Nc1c(c2ccc(cc2)N2CCOCC2)nc2cncn12</chem>	C169-0291	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	1
461	<chem>CCCCn1cnc2cc(ccc12)NCc1ccc(c1)OC</chem>	C215-0084	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	1
462	<chem>c1ccc(cc1)C(c1nnc(c2ccccc2)o1)Nc1ccc(cc1)F</chem>	C301-5596	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	1
463	<chem>Cc1ccc(cc1)NC(Cn1c(c(C(Nc2ccc(cc2)[Br])=O)nn1)N)=O</chem>	C368-0780	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	1
464	<chem>c1ccc2C(N(C(c2c1)Nc1ccc(cc1)F)c1cccn1)=O</chem>	C430-0215	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	1
465	<chem>CCN(CC)CCCNc1c2ccccc2nc(c2nnc(c3ccc(C)cc3)o2)n1</chem>	C660-1575	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	1
466	<chem>Cc1cccc(Cn2c3ccccc3nc2CCNC(CCCO)=O)c1</chem>	D186-0280	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	1
467	<chem>Cc1cc(Nc2ccc(cc2)F)n2c(n1)nc(c1ccc(cc1)OC)n2</chem>	D245-0284	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	1
468	<chem>Cc1nc(cc(Nc2ccccc2)C(=O)OC)n1)c1ccc(cc1)OC</chem>	D482-2049	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	1
469	<chem>Cc1c(c2ccc(cc2)OC)nn2c(cc(C)n12)N1CCN(CC1)CCO</chem>	D503-0348	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	1
470	<chem>c1ccc2c(c1)C(=C(C(N)=O)S2(=O)=O)Nc1cccc(c1)C(F)(F)F</chem>	D531-0321	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	1
471	<chem>CCOc1ccc(c(c1)NC1=C(C(C1=O)=O)c1ccccc1)OCC</chem>	E470-0451	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	1
472	<chem>C(c1ccccc1)N=C(N)NC(c1c(N)nc(c(n1)[Cl])N)=O</chem>	NCGC0001514 7-09	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	1
473	<chem>CC(C)n1cnc2c(Nc3ccccc3)NC(C=C=O)nc(NC3CCC(CC3)N(C)C)n12</chem>	NCGC0034696 4-01	Pre_miR_17	Hairpin	CAAAGUGCUUACAGUGCA GGUAGUGAU AUGUGCAUC UACUGCAGUGAAGGCACU UGUAG	1
474	<chem>CC1CCN(CC1)CC(COc1ccccc1CC=C)O</chem>	1189-2046	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	1
475	<chem>C1CNc2cc(CN3CCc4nnc(c5ccc5)n4CC3)nn2C1</chem>	12129103	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	1
476	<chem>CC(NS(c(cc1)cc2c1sc(C)n2)(=O)=O)=O</chem>	122385	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	1
477	<chem>Cc1ccc([C@H]2CN(C[C@@H]</chem>	13917927	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	<chem>2N)C(COc2ccc(cc2)n2cnnc2)=O</chem> <chem>o1</chem>				CAUGGCAACCC	
478	<chem>C1CN(CC(c2ccccc2)N1)C(c1ccn2cnnc2c1)=O</chem>	13930321	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	1
479	<chem>CN1CCN(CC12CCNCC2)C(c1ccc2c1ncn2)=O</chem>	13948752	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	1
480	<chem>C(CCN1cc(c2ccccc2c2ccco2)nn1)CCO</chem>	14330381	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	1
481	<chem>C(CO)Nc1cc(c2ccc(c(c2)[Cl])O)c2cc[nH]c2n1</chem>	15290349	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	1
482	<chem>Cc1ccccc1C(NC[C@@H]1CCN(C[C@H]1O)C(Cc1ccccc1)=O)=O</chem>	16828885	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	1
483	<chem>CC(C)Cc1cc(CNC2CCN(CC2)C(C(C)C)no1</chem>	17766103	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	1
484	<chem>Cc1c(CNC(c2en(CCC3CCCCN3)nn2)=O)c(C)on1</chem>	18521194	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	1
485	<chem>C(COCc1ccc(cc1)[Cl])NCC1(CNCCOC1)O</chem>	20639134	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	1
486	<chem>CCCCN1C(=N)N(CC(c2ccc(cc2)OC)O)c2ccccc12</chem>	2226-0445	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	1
487	<chem>CN(C)[C@@H]1C[C@@H](CO)N(C1)C(c1cc2c(c3ccccc3)nn(C)c2s1)=O</chem>	22692463	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	1
488	<chem>CNc1cc(c2ccc(cc2)c2nnc(N)s2)c2cc[nH]c2n1</chem>	25638728	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	1
489	<chem>Cc1ccccc2c1nc(C1CCN(CC1)C(Cc1c(C)nc(N)nc1C)=O)[nH]2</chem>	26941110	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	1
490	<chem>COc1ccccc(CNCCc2cccc(c2)F)c1</chem>	2910-1991	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	1
491	<chem>C(CO)Nc1cc2c(c3C(c4ccccc4C(c13)=O)=O)Nc1ccccc1O2</chem>	2920-0632	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	1
492	<chem>C1CN(CC1Cc1ccc(CO)cc1)C(Cc1cn2ccsc2n1)=O</chem>	31022825	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	1
493	<chem>C1COC2(CCOCC2)CC1NCc1nc(c2cnccn2)n[nH]1</chem>	31093015	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	1
494	<chem>C(C1C(c2ccccc2[Cl])c2c[nH]c2c2ccccc2)OC=1N)#N</chem>	3132-0191	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	1
495	<chem>Cc1c(cccc1NC(NCCNc1ccccc1)=O)C(NC(C)(C)C)=O</chem>	31773556	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	1
496	<chem>C1CCN(CC1)CCN1C(=N)N(CCOC)c2ccccc12</chem>	3260-0393	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	1
497	<chem>C1Cc2cc(Cn3cc(c4ccc(C#CCO)s4)nn3)ccc2OC1</chem>	33240961	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	1
498	<chem>CC(c1cc(CC(N[C@H]2CC[C@H](CC2)N)=O)cs1)=O</chem>	33946523	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	1
499	<chem>C1CC2(CCNC2)CCN(C1)Cc1c(ne2n1ccs2)[Cl]</chem>	35729906	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	1
500	<chem>Cc(cc1nc(ccc(N(C)C)c2c2[s+][c1c1)c1N.[Cl-]</chem>	36758	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	1
501	<chem>CC(C)CC1CC(C)(c2csc(Nc3ccccc3)n2)OC1=O</chem>	4075-3209	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	1
502	<chem>CCC(c1ccnn1C)Nc1ccc(c(CC=C)c1)OCC</chem>	41760826	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	1
503	<chem>CCN(CCN1cccn1)C(c1ccc(cc1)C1CCCN1)=O</chem>	42585880	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	1
504	<chem>COc1ccc(c(c1)OC)c1esc(NCC=C)n1</chem>	4640-0152	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
505	<chem>CCC(CO)N(Cc1ccc(cc1)F)Cc1c c(c(c(c1)[Cl])O)OC</chem>	46503727	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	1
506	<chem>Cc1ccc(cc1)NC(C) (C(NCCCc1nn[nH]1)=O)c1ccc cc1</chem>	47814214	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	1
507	<chem>CCOC(c1cnc2ccc(C)cc2c1Nc1c cc(cc1)N(C)C)=O</chem>	4790-1159	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	1
508	<chem>Cc1cccc2c(cc(C)nc12)Nc1ccc(c c1)N(C)C</chem>	4790-1400	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	1
509	<chem>C(CNCc1ccc2c(c1)OCO2)c1c[n H]c2ccccc12</chem>	4964-5174	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	1
510	<chem>CC[n+1]1cn(CC(COe2ccccc2)O) c2ccccc12</chem>	5010-0422	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	1
511	<chem>Cc1c2c([nH]n1)OC(=C(C#N)C2 1C(N(C)c2ccccc12)=O)N</chem>	5066-0352	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	1
512	<chem>CCOC(c1cnc2ccc(cc2c1Nc1ccc( cc1)N1CCOCC1)[Cl])=O</chem>	5173-3862	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	1
513	<chem>CCOC(c1cnc2ccc(C)cc2c1NCC( C)O)=O</chem>	5174-4400	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	1
514	<chem>C1CCN(CC1)c1ccccc1N</chem>	5784-1967	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	1
515	<chem>C(C#CCSc1nnc(c2ccccc2) [Br]o1)O</chem>	7199-0097	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	1
516	<chem>CC(Nc1c(C(c2cccc(c2)F)N2CC N(CC2)CCO)c2CCCCc2s1)=O</chem>	7287-0672	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	1
517	<chem>CCCCN(C)S(c1ccc(cc1)NC1c2c cccc2S(N=1)(=O)=O)(=O)=O</chem>	7489-2048	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	1
518	<chem>CC(c1ccccc1OCC(Cn1c2ccccc2 nc1CO)O)=O</chem>	7661-0041	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	1
519	<chem>CC1=CC2=C(C(C(C#N)=C(N) O2)c2ccccc2OC)C(N1Cc1ccc2c (c1)OCO2)=O</chem>	7706-1226	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	1
520	<chem>Cn1c(enc1Nc1c1ccccc1OC)c1cc ccc1</chem>	7756-0545	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	1
521	<chem>CCOC(C1=C(C)OC(=C(C(=O) OCC)C12C(Nc1ccccc12)=O)N) =O</chem>	8003-0370	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	1
522	<chem>CC1=CC2=C(C(C(C#N)=C(N) O2)c2ccc(cc2)[Br])C(=O)O1</chem>	8003-0435	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	1
523	<chem>COC(C1=C(N)OC2=C(C(=O)O c3ccccc23)C12C(Nc1ccccc12)= O)=O</chem>	8005-2656	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	1
524	<chem>CN1C(C2C(C(C#N)=C(N)OC= 2c2ccccc12)c1c(ccc1[Cl])F)=O</chem>	8016-4538	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	1
525	<chem>C(c1ccc(cc1)F)N1C(C2(C(C#N) =C(N)N(C3COC(C2=3)=O)c2cc ccc2)c2ccccc12)=O</chem>	8017-5050	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	1
526	<chem>Cc1c(C#N)c(N)n(CCCn2ccnc2) c1C</chem>	8018-7492	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	1
527	<chem>c1cc(N)nc2c1ccc(n2)O</chem>	8019-7722	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	1
528	<chem>CCc1c(C)cc2c(c(C(c3ccccc3)=O )sc2n1)N</chem>	8020-0635	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	1
529	<chem>c1cnc1c1nc2ncnc(N)n2n1</chem>	8020-2786	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	1
530	<chem>Cc1c(c2ccc(c(c2)OC)OC)c2ncc( c3ccc(c(c3)OC)OC)c(N)n2n1</chem>	8104-10716	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	1
531	<chem>[H]N(Cc1ccccc1OCc1ccc(cc1) F)OC)Cc1ccccc1</chem>	8320-0678	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
532	<chem>Cc1ccc(cc1)c1cnc2c(cnn2c1N)c1cccc1</chem>	8562-00039	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	1
533	<chem>CC1=CC2=C(C(C(C#N)=C(N)O2)c2c(cccc2[Cl])[Cl])C(=O)O1</chem>	8645-0078	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	1
534	<chem>c1ccc2c(c1)nc(c1ccc(cc1[Cl])N)s2</chem>	C066-5322	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	1
535	<chem>C(CO)Nc1c2c(ncn1)[nH]cn2</chem>	C143-0023	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	1
536	<chem>Cn1c2cccc2nc1CNc1cccc1</chem>	C147-0039	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	1
537	<chem>Cc1cccc(c1)NCc1nc2cccc2n1C</chem>	C147-0043	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	1
538	<chem>Cc1cccc(C)c1Nc1c(c2ccc(cc2)N2CCOCC2)nc2cncn12</chem>	C169-0291	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	1
539	<chem>CCCCn1cnc2cc(ccc12)NCc1ccc(c1)OC</chem>	C215-0084	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	1
540	<chem>Cc1nnc2c(Nc3cccc3[Cl])nc3ccc3n12</chem>	C301-3100	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	1
541	<chem>Cc1cccc1Nc1c(c2ccc(C)o2)nc2nccn12</chem>	C325-0048	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	1
542	<chem>Cc1cccc1NC(Cn1c(c(C(NC2c(cc2)F)=O)nn1)N)=O</chem>	C368-0744	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	1
543	<chem>CCOC(N1CCN(CC1)C1=C(C(C1=O)=O)N)CCCC1CCCCC1=O</chem>	C748-1353	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	1
544	<chem>Cc1ccc(cc1)S(c1c(NCCOC)oc(c2cccc(C)c2)n1)(=O)=O</chem>	D072-0517	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	1
545	<chem>CCOC(c1cccc(c1)Nc1cc(c2cccc2)ncn1)=O</chem>	D278-0165	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	1
546	<chem>CN1C(N(C)c2cc(COc3ccc(CNC4ccccc4)cc3OC)ccc12)=O</chem>	D300-0082	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	1
547	<chem>CCC(C)Nc1nc(nc(n1)n1cnc(n1)SCc1cccc1)N(C)C</chem>	D385-0103	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	1
548	<chem>Cc1nc(cc(Nc2cccc(c2)C(=O)OC)n1)c1ccc(cc1)OC</chem>	D482-2049	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	1
549	<chem>CN(C)CCN(Cc1ccc(cc1)[Cl])c1cccc1</chem>	NCGC0001667 2-04	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	1
550	<chem>CC(C)n1cnc2c(Nc3cccc(c3)NC(C=C)=O)nc(NC3CCC(CC3)N(C)C)nc12</chem>	NCGC0034696 4-01	Pre_miR_21	Hairpin	GGGUUGACUGUUGAAUCU CAUGGCAACCC	1
551	<chem>Cc1ccc(cc1C)NCC(C(C(CO)O)O)O</chem>	0527-0256	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	1
552	<chem>c1ccc(cc1)N1C(C(Nc2cccc(c2)C(O)=O)SC1=O)=O</chem>	1159-0329	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	1
553	<chem>CC(NS(c(cc1)cc2c1sc(C)n2)(=O)=O)=O</chem>	122385	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	1
554	<chem>CCN(CC)c1ccc(/C=C/c2nc3cccc3c(-c3cccc3)c2)cc1</chem>	13487	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	1
555	<chem>C(CCN1cc(c2cccc2c2ccco2)nn1)CCO</chem>	14330381	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	1
556	<chem>C1[C@@H]</chem>	14778588	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	<chem>(C2(CCN(CC2)C2cccc(c2)OC CN2CCOCC2)[C@@H]1O)O</chem>				GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	
557	<chem>CN(C(c1cccc(c2ccccc2[Cl])o1)= O)[C@H]1COC[C@@H]1O</chem>	15922890	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	1
558	<chem>FC(c1cccc(- c([nH]2nc(nc3Cl)c2nc3Cl)c1) (F)F</chem>	177407	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	1
559	<chem>Cc1c(CNC(c2cn(CCC3CCCCN 3)nn2)=O)c(C)on1</chem>	18521194	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	1
560	<chem>Cn1c(Cn2ccnc2c2cc3CNCCn3n 2)cnc1SC</chem>	22199819	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	1
561	<chem>CCCCN1C(=N)N(CC(c2ccc(cc2 )OC)O)c2ccccc12</chem>	2226-0445	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	1
562	<chem>Cc(cc1)ccc1S(c(c1nnc11)ccc1[ N+])([O-])=O=O</chem>	228150	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	1
563	<chem>CNc1cc(c2ccc(cc2)c2nnc(N)s2)c 2cc[nH]c2n1</chem>	25638728	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	1
564	<chem>CC(C)CCCCCCCCCCCCC(NC C(NC(C(C)OC(C1O)Nc2nnc3c 2[nH]cn3)C1O)=O)=O</chem>	268251	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	1
565	<chem>CN(C)CCOc1cc(C(/C2)=C\ c(n3C)ncc3[N+] ([O-])=O)=O)c2cc1.OS(O) (=O)=O</chem>	277184	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	1
566	<chem>O=C(N(CC1OC1)C(N1CC2OC 2)=O)N(CC2OC2)C1=O</chem>	296934	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	1
567	<chem>CC1(C)C(N(CC(CN(c2ccccc2)c 2ccccc2)O)C(N1)=O)=O</chem>	2996-0044	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	1
568	<chem>C1COC2(CCOCC2)CC1NCc1n c(c2cnccn2)n[nH]1</chem>	31093015	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	1
569	<chem>C(C1C(c2ccccc2[Cl])c2c(n[nH]c 2c2ccccc2)OC=1N)#N</chem>	3132-0191	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	1
570	<chem>Cc1c(cccc1NC(NCCNc1ccnc1) =O)C(NC(C)(C)C)=O</chem>	31773556	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	1
571	<chem>C(CNc1c2c(csc2nnc1)c1ccc(cc1 )F)c1cccs1</chem>	3230-0825	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	1
572	<chem>C1CCN(CC1)CCN1C(=N)N(CC O)c2ccccc12</chem>	3260-0393	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
					CCAUC	
573	<chem>Cc1ccc(c(C)c1)NC(c1c2CCc2sc1N)=O</chem>	3261-0869	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	1
574	<chem>C(/C=C/CSelncecc1)Selncecc1</chem>	326921	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	1
575	<chem>CC1(CCNCC1)C(N1CCCC(C1)C(CCc1cccc1)=O)=O</chem>	33248227	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	1
576	<chem>C(c1c(N)nc2c3c(cc4cccc4)nc13)c1cccc1o2)#N</chem>	3331-3338	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	1
577	<chem>CN(C=C/C(N1C)=C/[N+](O-)=O)C1=O</chem>	342460	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	1
578	<chem>Cc(cc1nc(ccc(N(C)C)c2)c2[s+][c1c1)c1N.[Cl-]</chem>	36758	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	1
579	<chem>CCN(CCN1cccn1)C(c1ccc(cc1)C1CCCN1)=O</chem>	42585880	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	1
580	<chem>Cc1c(non1)OCCNCc1nnc(c2ccc(C)n2C)o1</chem>	45836039	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	1
581	<chem>COc1ccc(c(c1)OC)c1csc(NCC=C)n1</chem>	4640-0152	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	1
582	<chem>Cc1nccn1CCC1CCCCN1Cc1ccc(c(CCN)c1</chem>	47531251	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	1
583	<chem>CCOC(c1enc2ccc(C)cc2c1Nc1c(cc(cc1)N(C)C)=O</chem>	4790-1159	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	1
584	<chem>CC[n+][l]cn(CC(CO2c2cccc2)O)c2cccc12</chem>	5010-0422	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	1
585	<chem>Cc1nc(SC)nc(N2CC2)c1Br</chem>	50199	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	1
586	<chem>COc1ccc(CCNe2c3c4CCCCc4sc3n2)cc1</chem>	5067-0641	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	1
587	<chem>CCOC(c1c(C)c(C)sc1NC(CNCc1cccc1)=O)=O</chem>	5132485	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	1
588	<chem>CCOC(c1enc2ccc(cc2c1Nc1ccc(cc1)N1CCOCC1)[Cl])=O</chem>	5173-3862	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
589	<chem>CCOC(c1cnc2cccc2c1Nc1cc(cc1C)C(O)=O)=O</chem>	5174-4337	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	1
590	<chem>CCOC(c1cnc2ccc(C)cc2c1NCC(C)O)=O</chem>	5174-4400	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	1
591	<chem>C1CCC2C(C1)=C(C#N)c1nc3ccccc3n1C=2NCCOCCO</chem>	5228-5336	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	1
592	<chem>CCCCOC(C1=C(N)OC(C)=C(C(=O)OCC=C)C12C(Nc1cccc12)=O)=O</chem>	5587-0169	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	1
593	<chem>CCOC(C1=C(C)OC(=C(C(=O)OCC)C12C(Nc1cccc12)=O)N)=O</chem>	8003-0370	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	1
594	<chem>CC1(C)CC2(CC(C)(C)N1)C(C)(N(CCCO)C(=O)O2)O</chem>	8012-5768	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	1
595	<chem>C(c1ccoc1C(O)=O)N</chem>	8015-0997	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	1
596	<chem>CN1C(C2C(C(C#N)=C(N)OC=2c2cccc12)c1c(cccc1[Cl])F)=O</chem>	8016-4538	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	1
597	<chem>Cc1c(C#N)c(N)n(CCCn2ccnc2)c1C</chem>	8018-7492	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	1
598	<chem>Cc1c(c2ccc(cc2)[Br])c2ncc(C#N)c(N)n2n1</chem>	8019-5330	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	1
599	<chem>c1cc(N)nc2c1ccc(n2)O</chem>	8019-7722	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	1
600	<chem>CCc1c(C)cc2c(c(C(c3cccc3)=O)sc2n1)N</chem>	8020-0635	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	1
601	<chem>c1cnc1c1nc2nnc(N)n2n1</chem>	8020-2786	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	1
602	<chem>CCN(CC)c(cc1ccc1C(c(cc1)ccc1N(CC)CC)=C(C=C1)C=CC1=[N+](CC)CC.[Cl-])</chem>	8675	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	1
603	<chem>c1ccc2c(c1)nc(c1ccc(cc1[Cl])N)s2</chem>	C066-5322	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	1
604	<chem>C(CO)Nc1c2c(ncn1)[nH]cn2</chem>	C143-0023	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	1
605	<chem>Cc1ccc(cc1)NCc1nc2cccc2n1C</chem>	C147-0010	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC	1



Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
					UGCUAUGCCAACAUAUUG CCAUC	
606	<chem>Cn1c2ccccc2nc1CNc1ccccc1</chem>	C147-0039	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	1
607	<chem>Cc1cccc(c1)NCc1nc2ccccc2n1C</chem>	C147-0043	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	1
608	<chem>Cc1cccc(C)c1Nc1c(c2ccc(cc2)N2CCOCC2)nc2cncn12</chem>	C169-0291	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	1
609	<chem>CCCCn1enc2cc(ccc12)NCc1ccc c(c1)OC</chem>	C215-0084	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	1
610	<chem>CC(C)C(N1CCN(CC1)c1ccc(cc1) Nc1cc(C)nc2nc(c3ccco3)nn12 )=O</chem>	C301-7288	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	1
611	<chem>c1ccc2C(N(C(c2c1)Nc1ccc(cc1) F)c1cccn1)=O</chem>	C430-0215	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	1
612	<chem>c1ccc(cc1)S(n1c(cc2ccccc2)F n1)N(=O)=O</chem>	C665-0183	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	1
613	<chem>CCOC(N1CCN(CC1)C1=C(C(C 1=O)=O)NCCCN1CCCCC1)= O</chem>	C748-1353	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	1
614	<chem>COc1ccccc1CNc1ccc(C(O)=O s1</chem>	C863-0034	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	1
615	<chem>C(CN1CCOCC1)Nc1c(nc2ccc o2)o1S(c1ccc(cc1)F)(=O)=O</chem>	D072-1128	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	1
616	<chem>CCCCNc1c(nc2ccc(cc2) [Cl])o1S(c1ccccc1)(=O)=O</chem>	D072-1502	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	1
617	<chem>CN1C(c2c(cn(CCO)c2c2ccc(cc2 )[Cl])N(C)C1=O)=O</chem>	D077-0206	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	1
618	<chem>CCOC(c1cccc(c1)Nc1cc(c2ccccc2) nnc1)=O</chem>	D278-0165	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	1
619	<chem>c1ccc(cc1)c1cc(Nc2ccc(cc2) [Br])nnc1</chem>	D278-0329	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	1
620	<chem>Cc1ccccc1c1nc(c2ccnnc2NCc2c cco2)on1</chem>	D349-3751	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	1
621	<chem>CCN(CC)CCCNc1ccc2c(c1)N(C) C(N2C)=O</chem>	D664-0111	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
622	<chem>CC1CCCC(C1C)Nc1c(c2ccc(cc2)[Cl])[nH]c2c(C#N)cnn12</chem>	E002-1096	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	1
623	<chem>Cc1cc(ccc1[Br])NC1=C(C(C1=O)=O)c1ccc(cc1)[Cl]</chem>	E786-0118	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	1
624	<chem>C(c1ccccc1)N=C(N)NC(c1c(N)n c(c(n1)[Cl])N)=O</chem>	NCGC0001514 7-09	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	1
625	<chem>CCOC(Nc1ccc(NCc2ccc(cc2)F)nc1N)=O</chem>	NCGC0001545 1-06	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	1
626	<chem>C1C(C1N)c1ccccc1</chem>	NCGC0001584 8-04	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	1
627	<chem>CN(C)CCN(Cc1ccc(cc1)[Cl])c1ccccc1</chem>	NCGC0001667 2-04	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	1
628	<chem>c1cc2C(c3cc(cc(c3C(c2c(c1)O)=O)O)C(O)=O)=O</chem>	NCGC0001819 9-06	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	1
629	<chem>C([C@@H]1[C@@H]([C@@H]([C@H](N2C=CC(NC2=O)=O)O1)F)O)O</chem>	NCGC0034578 1-01	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	1
630	<chem>CC(C)n1cnc2c(Nc3ccccc3)NC(C=C)=O)nc(NC3CCC(CC3)N(C)C)nc12</chem>	NCGC0034696 4-01	Pre_miR_31	Hairpin	AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC	1