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

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 1 | Cc1cc(C)n(- c2nc(C)c(C(=O)N(CCO)CCO)s 2)n1 | Neg\_lig\_4 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 2 | CCc1ccc2nc(C)cc(C(=O)NC[C @H](O)c3ccco3)c2c1 | Neg\_lig\_30 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 3 | c1cc(C2CCCC2)nc(N2CCO[C@  ]3(C[NH2+]CCOC3)C2)n1 | Neg\_lig\_49 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 4 | O=C(NCCO)c1nnc(-  c2ccc3c(c2)OCO3)o1 | Neg\_lig\_58 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 5 | CN(C)c1nc(N)nc(COc2cccc3c2 OC(C)(C)C3)n1 | Neg\_lig\_83 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 6 | COCC[C@]1(CO)CCCN(CC(=  O)N2CCc3ccccc32)C1 | Neg\_lig\_96 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 7 | COCc1nn2c(N)c(- c3ccc(Cl)cc3)cnc2c1-c1ccccc1 | Neg\_lig\_130 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 8 | O=C1N(CCO)CCC[C@@]12C C[N@H+](Cc1cccc(C(F) (F)F)c1)C2 | Neg\_lig\_275 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 9 | CS[C@@H] (C)CC[NH+]1CCC2(CC1)NCC NC2=O | Neg\_lig\_277 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 10 | Cc1ccccc1- c1ccc(CN2CC[C@@](N) (C(=O)O)C2)cc1 | Neg\_lig\_285 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 11 | COc1ccc(Cl)cc1NC(=O)CCc1c( C)nc2nc(C[NH3+])nn2c1C | Neg\_lig\_294 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 12 | CCOC(=O)c1c(N)n(-  c2ccc(F)cc2)c2nc3ccccc3nc12 | Neg\_lig\_325 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 13 | [NH3+]Cc1ccc2ccccc2n1 | Neg\_lig\_351 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 14 | Cc1cccc(N2CCN(C(=O)c3ccc(C Nc4c(N5CCCC5)c(=O)c4=O)cc 3)CC2)c1C | Neg\_lig\_487 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 15 | Cc1ccccc1Cn1c(C(=O)O)c(CNC c2ccco2)c2ccccc21 | Neg\_lig\_492 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 16 | COc1ccc2cc3c(N)nn(C(=O)c4cc cc(Cl)c4)c3nc2c1 | Neg\_lig\_500 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 17 | Cc1cn2c(- c3cn[nH]c3)cnc2c(Nc2ccc(C(=O  )N3CC[NH2+]CC3)cc2F)n1 | Neg\_lig\_513 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 18 | CN1C[C@@]2(CCCN(c3cc(N4 CC[NH+] (C)CC4)nc(N)n3)C2)OC1=O | Neg\_lig\_549 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 19 | Cc1ccc(C[NH+]2CCC(C(=O)N(  CCO)Cc3ccccc3)CC2)o1 | Neg\_lig\_566 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 20 | COc1cccc(Nc2cc(C)[nH+]c3cc(- c4ccccc4OC)nn23)c1 | Neg\_lig\_591 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 21 | Cn1c(=O)n(C)c2cc(CNc3ccc(Br  )cc3)ccc21 | Neg\_lig\_621 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 22 | [NH2+]=c1n(CCO)c2ccccc2n1C c1ccccc1F | Neg\_lig\_623 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 23 | NS(=O)(=O)c1ccc(N/N=C2\ C=CC(=O)NC2=O)cc1 | Neg\_lig\_641 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 24 | Cc1c(S(=O)  (=O)c2ccc(Cl)cc2)c(N)n(Cc2ccc cn2)c1C | Neg\_lig\_718 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 25 | c1ccc2cc(CN3CC[C@]4(CCC[ NH2+]C4)C3)ccc2c1 | Neg\_lig\_733 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 26 | COc1ccc(-c2cc(- c3ccccc3)nc(N)n2)cc1 | Neg\_lig\_734 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 27 | C[C@H]1CC[C@@H](Nc2c(-  c3ccc(Br)cc3) [nH]c3c(C#N)cnn23)CC1 | Neg\_lig\_750 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 28 | CC(=O)N1CCC([NH2+] [C@@H](C)CCCC(C) (C)O)CC1 | Neg\_lig\_774 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 29 | CNc1ncnc2c1cnn2[C@@H]1CC CCO1 | Neg\_lig\_785 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 30 | Cc1nc(N(C)Cc2cc(C(C)(C)C)  [nH]n2)cc([C@H]2CCC[NH2+] C2)[nH+]1 | Neg\_lig\_793 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 31 | CN(C)c1ccc([C@@H] (O)c2cccs2)cc1 | Neg\_lig\_813 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 32 | Cc1ccc(NCC(=O)n2nc(C)cc2C) c(C)c1 | Neg\_lig\_822 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 33 | Clc1ccc(C[NH2+]Cc2ccco2)cc1 | Neg\_lig\_827 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  |  |  |  |  | UACUGCAGUGAAGGCACU UGUAG |  |
| 34 | Cc1nc(N)sc1Cc1ccc(O)cc1 | Neg\_lig\_887 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 35 | CCc1[nH]nc2c1[C@@]1(C(=O) N(CC)c3ccccc31)C(C#N)=C(N) O2 | Neg\_lig\_900 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 36 | Cc1ccc(S(=O) (=O)Nc2ccccc2CNc2ccccc2Br)c c1 | Neg\_lig\_925 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 37 | CC(C)C[C@H] (O)C(=O)N1CCCN(C(=O)c2ccc o2)CC1 | Neg\_lig\_936 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 38 | Cc1c(C(=O)c2cccc3ccccc23)c2c ccc3c2n1[C@H] (CN1CCOCC1)CO3 | Neg\_lig\_972 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 39 | COc1ccc(C)c(NC(=O)N2C[C@ @H](CO)[C@H](CO)C2)c1 | Neg\_lig\_989 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 40 | CCCC[S@@]  (=O)c1sc2nc(C)cc(C)c2c1N | Neg\_lig\_990 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 41 | Cn1c(CC(=O)NCCCO)c(Sc2ccc  cc2)c2ccccc21 | Neg\_lig\_997 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 42 | Nc1nonc1C(=O)N1CCN(C(=O)  c2cccc(F)c2)CC1 | Neg\_lig\_1002 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 43 | COc1ccc(C(=O)CCC(=O)N2CC  [C@H](Cc3cccc(CO)c3)C2)cc1 | Neg\_lig\_1013 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 44 | Cc1noc(- c2ccc[nH+]c2NCc2ccco2)n1 | Neg\_lig\_1022 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 45 | CCOC(=O)c1ccccc1N[C@@H] 1c2ccccc2C(=O)N1c1ccc(Cl)cc1 | Neg\_lig\_1054 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 46 | C[C@@H]  (Cc1cn(CCc2nnc(N)s2)nn1)c1cc ccc1 | Neg\_lig\_1056 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 47 | COc1ccc(- c2cc(C)cc3c2O[C@@H] (C[NH3+])C3)c(C)c1 | Neg\_lig\_1100 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 48 | Fc1cccc(Cl)c1Cn1ccnc1- c1cc2n(n1)CC[NH2+]C2 | Neg\_lig\_1125 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 49 | O=C(NCCC[NH+]1CCC(O)CC  1)Nc1ccccc1OCc1ccccc1 | Neg\_lig\_1132 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 50 | CC(C)NC(=O)c1ccc(- c2cccc(N3CC[NH2+]CC3)c2)s1 | Neg\_lig\_542 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 51 | CC(=O)c1ccc(Nc2cc(C)nc3nc(- c4ccc(Cl)cc4)nn23)cc1 | Neg\_lig\_1151 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 52 | CCN(CC)C(=O) [C@@H]1C[C@@H] ([NH3+])CN1C1CCOCC1 | Neg\_lig\_1171 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 53 | 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 | Neg\_lig\_1189 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 54 | NS(=O)(=O)c1ccc(NC2(C(=O) [O-])CCCC2)cc1 | Neg\_lig\_1191 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 55 | CCC[C@H]  (O)c1nc2ccccc2n1Cc1ccc(F)cc1 | Neg\_lig\_1196 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 56 | CCOc1ccc([C@@H]2c3c(n[nH] c3- c3ccccc3O)C(=O)N2CCCO)cc1 OC | Neg\_lig\_1287 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 57 | Cc1cc(C)n(-c2nnc(N)nn2)n1 | Neg\_lig\_1369 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 58 | COC(=O)CNc1cc(C)nc2nc(- c3ccc(C)cc3)nn12 | Neg\_lig\_1405 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 59 | O=C(c1cn(C/C=C/ c2ccccc2)nn1)N1[C@H]2CC[C @@H]1CC[NH2+]C2 | Neg\_lig\_1408 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 60 | C[NH+] (C)C1CCN(C(=O)c2ccc(NC(=O  )Nc3nc(N4CCOCC4)nc(N4CCO CC4)n3)cc2)CC1 | Neg\_lig\_1440 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 61 | Cc1cc(N2CCN([C@H]3CCOC4 (CCOCC4)C3)CC2)nc(N)n1 | Neg\_lig\_1451 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 62 | c1cc2c(cc1[C@H]1OC[C@H]3[ C@H]1CO[C@H]3c1ccc3c(c1) OCO3)OCO2 | Neg\_lig\_1501 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 63 | CCSc1ncc(-c2c(- c3ccccc3)ncn2CC[C@@H] (C)CO)cn1 | Neg\_lig\_1587 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 64 | COc1cc([C@@H]2c3c(n[nH]c3- c3ccccc3O)C(=O)N2CCCO)ccc 1O | Neg\_lig\_1239 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 65 | O=S(=O)  (NCCCNc1cccnc1)NCc1ccccc1 | Neg\_lig\_1676 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 66 | Clc1nc(Cl)nc(-c2cn(- c3ccccc3)c3ccccc23)n1 | Neg\_lig\_1712 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  |  |  |  |  | UACUGCAGUGAAGGCACU UGUAG |  |
| 67 | COC(=O)c1nn(Cc2nc(N)nc(N(C  )C)n2)c2ccccc12 | Neg\_lig\_1728 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 68 | CCN1CCN(C2(CNc3oc(-  c4ccc(Cl)cc4)nc3C#N)CCCCC2  )CC1 | Neg\_lig\_1729 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 69 | CC1(C)Cc2c(C#N)c(NC3CCCC  C3)nc(Cc3ccccc3)c2CO1 | Neg\_lig\_1738 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 70 | Cc1ccc([C@H]2C(C#N)=C(N)O  c3cc(O)ccc32)cc1 | Neg\_lig\_1739 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 71 | Cc1cc(C)c(Cn2c(CCCO)nc3cccc c32)c(C)c1 | Neg\_lig\_1794 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 72 | O=C1C[C@@]2(CC[N@@H+] (Cc3cc4n(n3)CC[NH2+]C4)C2)  Oc2ccccc21 | Neg\_lig\_1801 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 73 | CCN(CCOc1ccc(Cl)cc1)C(=O)c 1ccc2c(c1)ncn2CCO | Neg\_lig\_1839 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 74 | O=C([O-])c1ccc(-  c2cc3cccnc3c(- c3ccc4nonc4c3)n2)cc1 | Neg\_lig\_1857 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 75 | O=C(OC1CCCC1)c1ccc(NC(=O  )N2CCC3(CC2)C[C@H] (O)CO3)cc1 | Neg\_lig\_1864 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 76 | O=C(c1ccc2cccc(F)c2n1)N(CC O)Cc1ccccc1Cl | Neg\_lig\_1899 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 77 | CO[C@@H](Cn1ccnc1- c1ccc(CO)o1)c1cccs1 | Neg\_lig\_1904 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 78 | COc1cc(OC)c([N-]S(=O)  (=O)c2cc(Br)cnc2N)cc1Cl | Neg\_lig\_1920 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 79 | Cn1c(N2CCOCC2)nc2cc(C(=O) N3C[C@H](O)CO3)ccc21 | Neg\_lig\_2001 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 80 | Cc1ccc(Nc2cc(N3CCCCC3)ncn 2)cc1C | Neg\_lig\_2038 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 81 | COc1ccc2c(c1)OC[C@]1(CO)C N(C(=O)CSc3ccncc3)C[C@H]2 1 | Neg\_lig\_2077 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 82 | CCOC(=O)C1CCN(c2nc(N)c(C(  =O)N3CCCC3)s2)CC1 | Neg\_lig\_2108 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 83 | O=C1N=c2ccc(Cl)cc2=C(N[C@ @H]2C[NH+]3CCC2CC3)C1=  C1Nc2ccccc2N1 | Neg\_lig\_2115 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 84 | N#Cc1ccccc1C(=O)N1CC[C@ @H](CNC(=O)CC2CCCC2) [C@H](O)C1 | Neg\_lig\_2129 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 85 | COc1c(N)c2c(c(OC)c1OC)COC 2=O | Neg\_lig\_2135 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 86 | C=CCOc1c(Cl)cc([C@H]2C(C#  N)=C(N)Oc3cc(O)ccc32)cc1OC | Neg\_lig\_2141 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 87 | CC(C)CNc1ncnc2c1sc1nc(- c3ccco3)c3c(c12)CC(C)(C)OC3 | Neg\_lig\_2229 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 88 | C[N@H+]1CCc2c(c3ccccc3n2C c2ccc(C(=O)NO)cc2)C1 | Neg\_lig\_2237 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 89 | Cc1nc(NCCc2c(C) [nH]c3ccccc23)c2c3c(sc2n1)CC C3 | Neg\_lig\_906 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 90 | NC(=O)Nc1ccc(Nc2ccccc2)cc1 | Neg\_lig\_2261 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 91 | CCCCn1c(=N)n(C[C@H]  (O)COc2ccccc2OC)c2ccccc21 | Neg\_lig\_2264 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 92 | C[NH+]  (C)CCOC(c1ccccc1)c1ccccc1 | Neg\_lig\_2292 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 93 | CCNc1ncc(C(=O)N2C[C@@H] (C[NH+]3CCCCC3)[C@@H] (CO)C2)cn1 | Neg\_lig\_388 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 94 | CCOC(=O)c1c(N)n(-  c2ccc(C)cc2)c2nc3ccccc3nc12 | Neg\_lig\_2320 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 95 | Nc1nc(SCCc2ccccc2)ns1 | Neg\_lig\_2332 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 96 | Cc1cccc(N2C[C@H] (C)N(C(=O)c3ccc(SCCO)cc3)C C2=O)c1 | Neg\_lig\_2338 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 97 | Cc1nc(-c2ccc[nH+]c2)ncc1- c1nc(CC(N)=O)nn1CCO | Neg\_lig\_2366 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 98 | Fc1ccc(CNc2nc3ccc(Cl)cc3s2)c c1 | Neg\_lig\_2375 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 99 | CN(C)c1ccccc1- c1nc(CC(N)=O)nn1CCO | Neg\_lig\_2415 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  |  |  |  |  | UACUGCAGUGAAGGCACU UGUAG |  |
| 100 | O=C(c1ccc(- c2cc[nH]n2)cc1)N1CCOC[C@ @H](O)C1 | Neg\_lig\_2427 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 101 | CCc1ccc(C[N@H+]2CC[C@@ H](NC(=O)c3cnccn3)[C@H] (O)C2)cc1 | Neg\_lig\_2542 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 102 | CC(C)Nc1nc2c(-c3cccc(C(F) (F)F)c3)nnn2c2ccccc12 | Neg\_lig\_2579 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 103 | CCc1[nH+]ccn1CCCNC(=O)  [C@H](CC)Nc1cccc(OC)c1 | Neg\_lig\_2582 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 104 | C[C@]12CC[C@H]3c4ccc(O)cc 4CC[C@@H]3[C@H]1CCC2= O | Neg\_lig\_2597 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 105 | Cc1cc(NC(=O)CNCCc2nc(-  c3ccc[nH+]c3)n[nH]2)ccc1Cl | Neg\_lig\_2604 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 106 | 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 | Neg\_lig\_2635 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 107 | C=CCOC(=O)C1=C(C)OC(N)= C(C(=O)OCC) [C@@]12C(=O)N(CC=C)c1ccc  cc12 | Neg\_lig\_2644 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 108 | Nc1cc(C(=O)N2CCCC2)ccc1Cl | Neg\_lig\_2706 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 109 | CC[NH+]  (CC)CCNc1ncnc2c1sc1nc(- c3ccco3)c3c(c12)CC(C)(C)OC3 | Neg\_lig\_2828 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 110 | Nc1nc(NCC[NH+]2CCCC2)c2c ([nH+]1)CCCC2 | Neg\_lig\_2835 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 111 | COc1ccc(- c2csc(NCc3ccco3)n2)cc1OC | Neg\_lig\_2841 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 112 | Oc1ccc2ccccc2c1SSc1c(O)ccc2c cccc12 | Neg\_lig\_2844 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 113 | CC1(C)CC(NC(=O)C(F)  (F)F)CC(C)(C)[NH2+]1 | Neg\_lig\_2862 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 114 | C=C[C@@H]1C[N@H+]2CC[ C@@H]1C[C@H]2[C@H]  (O)c1ccnc2ccccc12 | Neg\_lig\_2957 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 115 | CCOC(=O) [C@H]1CCCN(c2c(NCCC[NH+  ]3CCN(C)CC3)c(=O)c2=O)C1 | Neg\_lig\_2967 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 116 | COc1ccc(CNc2ncnc3scc(- c4ccc(C)cc4)c23)cc1 | Neg\_lig\_2983 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 117 | COc1ccc(Nc2cc(C) [nH+]c3c(C)cccc23)cc1OC | Neg\_lig\_3007 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 118 | Cc1ccc([N-]C2=C(C(N)=O)S(=  O)(=O)c3ccccc32)c(C)c1 | Neg\_lig\_3057 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 119 | Nc1ccccc1Oc1c(F)c(F)c(Oc2ccc cc2N)c(F)c1F | Neg\_lig\_3068 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 120 | O=C(Nc1ccc(Nc2cc[nH+]cc2)cc 1)c1ccc(Nc2ccnc3ccc([N+](=O) [O-])cc23)cc1[N+](=O)[O-] | Neg\_lig\_3116 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 121 | OCCN(CC#CCC(O)  (c1ccccc1)c1ccccc1)CCO | Neg\_lig\_3138 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 122 | CCOC(=O)c1cccc(N2C(=O) [C@@H]3[C@@H]4C=C[C@ @](CO)(O4)[C@@H]3C2=O)c1 | Neg\_lig\_3155 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 123 | Nc1nc(CCC[NH2+]C2CCN(c3n  cnc4ccsc34)CC2)cs1 | Neg\_lig\_1266 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 124 | CCOC(=O)CSc1nc(NC#N)nc(N (CC)CC)n1 | Neg\_lig\_3168 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 125 | CCc1ccc([C@H]2C(C(=O)OC)= C(N)OC3=C2C(=O)CC(C) (C)C3)cc1 | Neg\_lig\_3178 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 126 | Cc1ccccc1[C@@H]1CN(Cc2cc cc(CC[NH3+])c2)C[C@H]1C(= O)O | Neg\_lig\_3222 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 127 | Nc1cccc(-n2c(=O) [c-]3n(c2=O)CCC3)c1 | Neg\_lig\_3229 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 128 | C=CC[NH2+]Cc1cc(O)c2cc(C(  N)=O)ccc2n1 | Neg\_lig\_3240 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 129 | CN(C)S(=O) (=O)N1C[C@@H]2CC[C@H]  (C1)N(Cc1cccnc1N)C2 | Neg\_lig\_3243 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 130 | OCc1nc2ccccc2n1CCCCOc1ccc cc1 | Neg\_lig\_3260 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 131 | O=C1c2cccc3cccc(c23)C(=O)N 1CCN1CCN(C[C@H]  (O)COCc2ccccc2)CC1 | Neg\_lig\_3283 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 132 | COc1ccc(- c2nc(C(=O)N3CCN(CCO)CC3) | Neg\_lig\_3291 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | nn2-c2ccccc2Cl)cc1 |  |  |  | UACUGCAGUGAAGGCACU UGUAG |  |
| 133 | Cc1nc(C)n(CCNC(=O)c2cccc([ C@H]3CCC[NH2+]C3)c2)n1 | Neg\_lig\_3325 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 134 | CCCn1ncc(C(=O)NCc2c(C)ncc3 c2CC[NH2+]C3)c1C | Neg\_lig\_3338 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 135 | Cc1ccc([N+](=O)[O-])cc1S(=O) (=O)N(C)/N=C\  c1cnc2ccc(Br)cn12 | Neg\_lig\_830 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 136 | Nc1nnc(SCC(=O)Nc2cccc(F)c2) s1 | Neg\_lig\_176 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 137 | COc1ccccc1/N=C1C(=C(\N) [O-])/S(=O)(=O)c2ccccc2/1 | Neg\_lig\_1111 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 138 | Cc1nc(C(F) (F)F)nc(N2CCO[C@]3(CNCCO C3)C2)c1C | Neg\_lig\_3399 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 139 | Cc1ccc(N[C@@H]2c3ccccc3C(  =O)N2c2cccnc2)c(C)c1 | Neg\_lig\_3343 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 0 |
| 140 | Cn1c(=O)n(C)c2cc(NC3=NS(=  O)(=O)c4ccccc43)ccc21 | Neg\_lig\_12 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 141 | CCc1c(C)nn(CCn2cc(- c3ccc(CO)o3)nn2)c1C | Neg\_lig\_50 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 142 | CCOc1ccccc1- c1nc(CN2CC[NH+] (CCCO)CC2)c(C)o1 | Neg\_lig\_60 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 143 | O[C@H]1CCC[N@H+]  (Cc2cccc(Br)c2)C1 | Neg\_lig\_80 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 144 | O=C(CN1CCCCCC1=O)NCc1c c2n(n1)CC[NH2+]C2 | Neg\_lig\_101 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 145 | CC(C)Cc1noc([C@H]  (C)n2cc[nH+]c2- c2cc3n(n2)CCC[NH2+]C3)n1 | Neg\_lig\_155 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 146 | CC(=O)c1cccc(N[C@@H]2c3cc ccc3C(=O)N2Cc2ccco2)c1 | Neg\_lig\_235 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 147 | CCOC(=O)c1cnn(-c2cc(C) [nH+]c3c(C)c(-  c4ccccc4)nn23)c1N | Neg\_lig\_238 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 148 | CS/C(N)=N\S(=O) (=O)c1ccc(NC(C)=O)cc1 | Neg\_lig\_248 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 149 | CN(C)c1cccc(NC(=O)N2CC[N  H2+][C@H](c3ccccc3)C2)c1 | Neg\_lig\_283 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 150 | CCn1nc(C)c(NC(=O)CNC[C@ H]2CN(S(C)(=O)=O)CCO2)c1C | Neg\_lig\_334 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 151 | O=C(c1ccc(CO)o1)N1CCC([C  @@H](O)Cc2ccccc2)CC1 | Neg\_lig\_372 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 152 | CCc1ccccc1OC1C[NH+] (C2CC[NH2+]CC2)C1 | Neg\_lig\_441 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 153 | CCOC(=O)N1CCC(N2C(=O)c3  ccccc3[C@H]2Nc2ccc(C)cc2)C C1 | Neg\_lig\_490 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 154 | COc1ccc(OC)c(N[C@@H] (NC(=O)c2cccs2)C(=O)c2ccc(C  )cc2)c1 | Neg\_lig\_516 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 155 | N#C[C@H]1C(=O)NC(=O) [C@H](C#N)C12CCC[C@@H] (C(F)(F)F)C2 | Neg\_lig\_519 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 156 | CC1=C(c2ccc(C(C)C)cc2)S(=O)  (=O)N=C1Nc1cccc(Cl)c1 | Neg\_lig\_552 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 157 | Cc1ccccc1OCCCCn1c(CCCO)n c2ccccc21 | Neg\_lig\_553 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 158 | Cc1n[nH]cc1N | Neg\_lig\_593 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 159 | C[C@H]1CCC[C@H]  (Nc2ncnc3onc(- c4ccc(Cl)cc4)c23)[C@H]1C | Neg\_lig\_705 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 160 | CCc1ccc(C[N@@H+]2CC[C@ @H]3[C@@H] (CCC(=O)N3CCCCO)C2)nc1 | Neg\_lig\_716 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 161 | COc1ccnc2[nH]cc(C(=O)C(=O) N3CCN(C(=O)c4ccccc4)C[C@ @H]3C)c12 | Neg\_lig\_736 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 162 | COc1[n-]cn/c(=N/S(=O) (=O)c2ccc(N)cc2)c1OC | Neg\_lig\_746 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 163 | O=C(Nc1ccc(F)cc1)Oc1ccc[nH] c1=O | Neg\_lig\_756 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 164 | CCc1ccccc1NC(=O)Cn1c(- c2nonc2N)nc2ccccc21 | Neg\_lig\_799 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 165 | O=C(CS[C@H]1Nc2sc3c(c2C(=  O)N1c1ccccc1)CCC3)c1ccc(Br) cc1 | Neg\_lig\_801 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 166 | Cc1ccc(-c2noc(-c3nnn(- c4cccc(C)c4)c3N)n2)cc1 | Neg\_lig\_834 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 167 | Cc1nc(N)nc(NCCc2nc(N)n[nH] 2)c1CCC(=O)[O-] | Neg\_lig\_835 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 168 | CCCc1cc(Nc2ccc(C(=O)N3CCC  CCC3)cc2)n2nc(- c3cccnc3)nc2n1 | Neg\_lig\_852 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 169 | O=C(NC1CCOCC1)c1ccc(-  c2cc(-c3c[nH]nc3- c3ccccn3)ccn2)cc1 | Neg\_lig\_869 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 170 | Cc1ccc2[nH+]c(- c3cccnc3)c(Nc3ccccc3C)n2c1 | Neg\_lig\_931 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 171 | Cn1c(CN2CCCCC2)  [nH+]c2cc(NCc3ccncc3)ccc21 | Neg\_lig\_938 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 172 | OCc1nc2cc(Cc3ccc4[nH]c(CO)n c4c3)ccc2[nH]1 | Neg\_lig\_942 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 173 | CCn1c(=O)c2c(nc(/C=C\ c3ccc(OC)c(OC)c3)n2C)n(CC)c 1=O | Neg\_lig\_954 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 174 | Cc1ncccc1OC1(C(=O)N2CCc3c ([nH]c4ccccc34)C2)CC[NH2+] CC1 | Neg\_lig\_977 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 175 | COc1cc(Cl)cc(OC)c1- c1cccc2c(N)cc[nH+]c12 | Neg\_lig\_1035 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 176 | O=C(c1ccccc1- c1ncc[nH]1)N1CC[C@@H] ([NH+]2CCCCCC2)[C@H] (O)C1 | Neg\_lig\_1057 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 177 | Cc1nc2ccc(C(=O)N3CC[C@@] 4(CCCN(CCO)C4=O)C3)cc2s1 | Neg\_lig\_1072 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 178 | Cc1ccc(- | Neg\_lig\_1107 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | c2ccc3c(ccc4sc5c(c43)NC[C@ @H](C)NC5=O)[nH+]2)cn1 |  |  |  | CAUGGCAACCC |  |
| 179 | OCCn1nc(COc2ccccc2)nc1- c1ccc2[nH]nnc2c1 | Neg\_lig\_1146 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 180 | Cc1c(-c2cn([C@@H] (C)c3nnc(N)s3)nn2)c(=O)n(- c2ccccc2)n1C | Neg\_lig\_1178 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 181 | COc1ccccc1CNc1ncc2nc(- c3ccccc3)oc2n1 | Neg\_lig\_1206 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 182 | CCOc1nc(NC(C)C)nc(N2C[C@ @H]3C[C@H]  (C2)c2cccc(=O)n2C3)n1 | Neg\_lig\_1216 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 183 | [NH3+]CCn1cc(C(=O)N2CCC[ C@H](c3n[nH]c(=O)n3- c3ccccc3)C2)nn1 | Neg\_lig\_1067 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 184 | O=C(NC[C@H]  (O)c1cccc(O)c1)c1cc(O)c2cccc( F)c2n1 | Neg\_lig\_1224 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 185 | CC[C@H] (NC(=O)c1cn([C@H]2CC[C@  @H] ([NH3+])CC2)nn1)c1cn2cccnc2 n1 | Neg\_lig\_1233 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 186 | O=C1[N-]C(=O)C(c2ccccc2[N+  ](=O)  [O-])=C1Nc1ccc(O)c(Cl)c1 | Neg\_lig\_1243 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 187 | N[C@H]1CCCCN(c2nc(-  c3ccccc3)ccc2C(=O)O)C1 | Neg\_lig\_1261 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 188 | C[C@H]1C[C@H](C)C(=O) [C@H]([C@H]  (O)CC2CC(=O)NC(=O)C2)C1 | Neg\_lig\_1285 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 189 | Nc1c(C(=O)Nc2ccc(Cl)cc2)sc2n cccc12 | Neg\_lig\_1301 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 190 | CCc1ccc(-n2nnc(-c3nc(- c4ccc(OC)cc4)no3)c2N)cc1 | Neg\_lig\_1348 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 191 | c1cc(C[NH2+]Cc2ccc3c(c2)OC O3)c2cc[nH]c2c1 | Neg\_lig\_1384 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 192 | COc1ccc2c3c([nH]c2c1) [C@H]1C[C@H]2[C@H] (C[C@@H](O)[C@H](OC) [C@H]2C(=O)O)CN1CC3 | Neg\_lig\_1421 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 193 | C[C@H]1Cc2cc(Cn3ccnc3- c3cc4n(n3)CCC[NH2+]C4)ccc2 O1 | Neg\_lig\_1450 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 194 | Cn1c(CC2CC[NH2+]CC2)nnc1 CN1CC[C@H]([NH+](C)C)C1 | Neg\_lig\_1464 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 195 | Cc1cccc([C@H]2Nc3ccccc3C(= O)N2CCc2ccccc2)n1 | Neg\_lig\_1493 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 196 | COc1cc([C@@H]2C(C#N)=C( N)OC(C)=C2C(=O)OC(C)C)cc( OC)c1OC | Neg\_lig\_1495 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 197 | Cc1nc(N)ncc1C(=O)N1CCC[C @H]1c1ccc(C[NH+](C)C)cc1 | Neg\_lig\_1503 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 198 | Cc1cccc(Nc2cc(C(C)C)nc3nc(- c4cccnc4)nn23)c1 | Neg\_lig\_1528 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 199 | O=C(C1c2ccccc2- c2ccccc21)N1CC[C@H]2[NH2  +]CCC[C@]2(CO)C1 | Neg\_lig\_1537 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 200 | Cc1cc(C)n(Cc2cccc(C(=O)N3C COC[C@@H](O)C3)c2)n1 | Neg\_lig\_1561 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 201 | Cc1nnc(SCC(=O)N2C[C@@H] | Neg\_lig\_1616 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | 3c4ccccc4OC[C@]3(CO)C2)o1 |  |  |  | CAUGGCAACCC |  |
| 202 | CN1CCC(=C(c2ccc(Cl)cc2)c2cc ccn2)CC1 | Neg\_lig\_1621 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 203 | COc1ccc(C)cc1Nc1c(- c2ccc(C)c(C)c2)c(=O)c1=O | Neg\_lig\_1624 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 204 | Cc1noc(C)c1Cn1nc([C@H]2CC C[NH2+]C2)n(-c2ccccc2)c1=O | Neg\_lig\_1689 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 205 | Cc1ccc(NC[C@@H] (O)Cn2c(C)c(C)c3ccccc32)cc1C | Neg\_lig\_1731 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 206 | Cc1cccc(Nc2c(- c3ccc(N4CCOCC4)cc3)nc3nccc n23)c1 | Neg\_lig\_1813 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 207 | CCOC(=O)N1CCC([NH2+]Cc2  ccccc2-n2cc[nH+]c2C)CC1 | Neg\_lig\_1828 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 208 | O=C1c2ccccc2[C@@H] (Nc2ccc(Cl)cc2)N1c1ccccn1 | Neg\_lig\_1840 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 209 | Cc1ccc2c(c1)c1c(n2C[C@H] (O)C[NH2+]C(C)(C)C)CCCC1 | Neg\_lig\_1871 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 210 | Cc1noc(N)c1C(=O)Nc1ccc2c(c1  )OCCO2 | Neg\_lig\_1888 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 211 | CCOc1ccc(CNc2nc3nc(C)cc(C) n3n2)cc1 | Neg\_lig\_1937 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 212 | C[C@@H]1C[C@@]2(C)Oc3cc ccc3[C@H]3OC[C@]1(CO) [C@H](C)[C@H]32 | Neg\_lig\_1951 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 213 | O=C(Nc1cccc2ccccc12)c1ccccc 1 | Neg\_lig\_2093 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 214 | CCOc1ccc(CCNC2=NS(=O) (=O)C(c3ccc(OC)cc3)=C2C)cc1 | Neg\_lig\_2096 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 215 | O=C(Nc1ccccc1- c1ccccc1)C(=O)Nc1ccccc1- c1ccccc1 | Neg\_lig\_2139 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 216 | COCc1[nH]nc2c1[C@@H] (c1c(F)cccc1Cl)C(C#N)=C(N)O 2 | Neg\_lig\_2184 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 217 | CCCC[NH2+]C[C@@H]1CCC O1 | Neg\_lig\_2185 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 218 | Oc1cc(-n2cccn2)c(O)cc1- n1cccn1 | Neg\_lig\_2198 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 219 | OCc1ccc(-c2ccc(- c3nc(Cc4ccc(Cl)cc4)no3)c[nH+] 2)cc1 | Neg\_lig\_2232 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 220 | Cc1ccc(NC(=O)Cn2nnc(C(=O) Nc3cccc(C)c3C)c2N)c(C)c1 | Neg\_lig\_2281 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 221 | COc1ccc(C[NH2+]CC[C@]2(c3 ccc(F)cc3)CCOC(C) (C)C2)cc1OC | Neg\_lig\_2295 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 222 | COC(=O)c1ccc(NC(=O)CCN2C CN[C@H]3CS(=O) (=O)C[C@H]32)cc1 | Neg\_lig\_2303 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 223 | O=C1O[C@H](Nc2ccc(S(=O) (=O)/N=c3\ cccc[nH]3)cc2)c2ccccc21 | Neg\_lig\_2310 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 224 | CCOC(=O)c1c(N)sc2c1CCN(C  Cc1ccccc1)C2 | Neg\_lig\_2356 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 225 | CC(=O)N1CCN(c2nc(-  c3ccccc3)nc3c2CCC3)C[C@@ H](O)C1 | Neg\_lig\_2364 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 226 | COc1ccc(Cl)cc1NC(=O)c1nnn( Cc2ccc(F)cc2)c1N | Neg\_lig\_2377 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 227 | O=C(CSCCO)Nc1nc(-  c2ccccc2)cs1 | Neg\_lig\_2413 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 228 | COc1ccc(- c2cc3[nH+]c(C)cc(NCc4ccccc4) n3n2)cc1OC | Neg\_lig\_2428 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 229 | O=C(NC[C@H]  (O)CO)c1ccc2[nH]c3c(c2c1)CC CC3 | Neg\_lig\_2432 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 230 | Cc1cn([C@H]2C[C@H] (N=[N+]=[N-])[C@@H]  (CO)O2)c(=O)[nH]c1=O | Neg\_lig\_719 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 231 | CCCCCNc1cc(C)  [nH+]c2c(C)c(-c3ccccc3)nn12 | Neg\_lig\_1548 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 232 | COc1cc(OC)c([N-]C2=NS(=O)  (=O)C(c3ccc(C(C)C)cc3)=C2C)  cc1Cl | Neg\_lig\_2477 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 233 | CC1(C)CC(=O)C2=C(C1)OC(N  )=C(C#N)  [C@H]2c1ccc(Cl)c(Cl)c1 | Neg\_lig\_2479 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 234 | CCCCc1nc(-c2c(- c3ccccc3)ncn2CC2CC[NH2+]C C2)c[nH]1 | Neg\_lig\_2551 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 235 | CN(C)S(=O)(=O)c1cccc(N)c1 | Neg\_lig\_1304 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 236 | Cc1nn(Cc2ccccc2)c(N)c1- c1ccccc1 | Neg\_lig\_2561 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 237 | Cc1nc(-c2nc(CCO)n(- c3ccccc3Cl)n2)cs1 | Neg\_lig\_2583 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 238 | C#Cc1cccc(Nc2ncnc3cc(OC)c( OCCCCCCC(=O)NO)cc23)c1 | Neg\_lig\_2598 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 239 | Cc1ccc(OCCCCn2c([C@H] (C)O)nc3ccccc32)cc1 | Neg\_lig\_2605 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 240 | Cc1ccc2nc(C[NH2+]C[C@H] (C)Oc3cccnc3)[nH]c2c1C | Neg\_lig\_2615 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 241 | CC1(C)CC(Nc2nc(Cl)c(C#N)c(  Cl)c2Cl)CC(C)(C)[NH2+]1 | Neg\_lig\_2658 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 242 | COCCN1C[C@@H](Cn2ccnc2- c2ccc(CO)o2)CC1=O | Neg\_lig\_1674 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 243 | Nc1nc2c(ncn2COC(CO)CO)c(= O)[nH]1 | Neg\_lig\_2668 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 244 | COc1ccc2ccccc2c1CNCc1ccncc 1 | Neg\_lig\_2705 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 245 | CCOC(=O)c1ccc2nc(C(F)  (F)F)nc(NCCc3ccc(OC)cc3)c2c 1 | Neg\_lig\_2711 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 246 | CC(C)C[C@H](NC(=O)  [C@@H](NC(=O)c1cccc(- c2ccccc2)n1)[C@@H] (C)O)B(O)O | Neg\_lig\_2752 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 247 | O=C(c1coc(CN2CCOCC2)c1)N 1[C@H]2CC[C@@H]1CC[NH2  +]C2 | Neg\_lig\_2782 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 248 | Cn1cc(CCC(=O)N2C[C@@H] (C[NH+]3CCCCCC3)[C@@H] (CO)C2)cn1 | Neg\_lig\_2823 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 249 | Cc1cc(NC2CCCCC2)ncn1 | Neg\_lig\_1895 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 250 | CC1=NC2=NC(C(Cl) (Cl)Cl)=NC3=CC=CC(=N1)N32 | Neg\_lig\_2829 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 251 | CCCCNc1nc(Oc2ccc(OCC)nn2) nc(N(C)C)n1 | Neg\_lig\_2846 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 252 | NC(=O)Cc1nc(- c2ccc3c(c2)NC(=O)CN3)n(-  c2cccc(F)c2)n1 | Neg\_lig\_2851 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 253 | CN1CCC(=C2c3ccccc3[C-]  (O)c3ccccc32)CC1 | Neg\_lig\_2892 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 254 | CN(C)c1n/c(=N/ c2cccc(Cl)c2)ss1 | Neg\_lig\_2898 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 255 | c1ccc2c(- c3cc(NC4CC[NH2+]CC4)nc4[n  H]ccc34)ccnc2c1 | Neg\_lig\_2901 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 256 | CCCCSCc1cc(C(=O)N2CC[C@ H]3C[NH2+]C[C@H]32)oc1C | Neg\_lig\_1994 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 257 | COc1ccc2ccccc2c1[C@@H] (O)c1[nH+]ccn1C | Neg\_lig\_2911 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 258 | O=C(NCCc1nnc2n1CC[NH2+]  CC2)c1ccc(-c2ccccc2)[nH]1 | Neg\_lig\_2973 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 259 | CC(C)CN1CC2(CCN(c3nccc(N 4CCC[C@H] (O)C4)n3)CC2)CC1=O | Neg\_lig\_2987 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 260 | COc1cc(C[C@H] (O)CO)cc2c1OCO2 | Neg\_lig\_3001 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 261 | Cc1nn(C(=O)c2ccc(C(C) (C)C)cc2)c(N)c1-c1ccccc1 | Neg\_lig\_1967 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 262 | Cc1ncc(CO)c(CN2C[C@H] ([NH3+])C[C@H]2C(=O)NC(C) C)c1O | Neg\_lig\_2670 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 263 | Cc1ccc2c(N)c(C(=O)[O-])sc2n1 | Neg\_lig\_3010 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 264 | COc1ccc(OC[C@@H] (O)Cn2c(NCCc3ccc(OC)c(OC)c 3)nc3c2c([O-])nc(=O)n3C)cc1 | Neg\_lig\_3016 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 265 | Cc1csc2c(N3CCC(O) (CO)CC3)nc[nH+]c12 | Neg\_lig\_3056 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 266 | COc1ccc([C@@H]2CNC(=O)C 2)cc1OC1CCCC1 | Neg\_lig\_3098 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 267 | Cc1c(NCc2cccnc2)cccc1C(=O) N(C)Cc1ccoc1 | Neg\_lig\_3121 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 268 | CC1=C(C(=O)OCc2ccccc2) [C@]2(C(=O)Nc3ccccc32)C(C(  =O)OCc2ccccc2)=C(N)O1 | Neg\_lig\_2796 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 269 | COCC[C@]1(CO)CCCN(C(=O)  Cc2ccc(CO)cc2)C1 | Neg\_lig\_129 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 270 | Cc1cc(NC(C)C)n2nc(- c3ccc(Cl)cc3)c(C)c2[nH+]1 | Neg\_lig\_3205 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 271 | C=C[C@@H]1C[N@@H+]2CC [C@H]1C[C@@H]2[C@@H]  (O)c1ccnc2ccccc12 | Neg\_lig\_3233 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 272 | CCC[C@H]  (O)c1nc2ccccc2n1Cc1ccccc1OC | Neg\_lig\_3247 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 273 | Cc1ccc(C)c(NCC(=O)Nc2c(C)c ccc2C)c1 | Neg\_lig\_3251 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 274 | OC[C@H]1C[N@H+] (C2CCN(Cc3ccccc3)CC2)C[C@ H]1CN1CCCC1 | Neg\_lig\_3252 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 275 | CCC(=O)N[C@H]1CC[C@H] (C(=O)N(C)c2ccc(-  c3nc4ccccc4o3)cc2)C1 | Neg\_lig\_3258 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 276 | COc1ccc(Nc2nc(- c3ccc(OC)c(OC)c3)no2)c(OC)c 1 | Neg\_lig\_3276 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 277 | CCOC(=O)N1CCC(N2C(=O)c3  ccccc3[C@H]2Nc2ccc(F)c(Cl)c 2)CC1 | Neg\_lig\_3329 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 278 | CCn1c(N)nc2cc(C(=O)NCCC3= CSC4=[NH+]CCCN34)cnc21 | Neg\_lig\_3333 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 279 | Cc1cc(NC[C@H]2CCCO2)n2nc  (-c3ccc(Cl)cc3)c(C)c2[nH+]1 | Neg\_lig\_3348 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 280 | COc1ccccc1- c1cc2[nH+]c(C)cc(NCC(C)C)n2  n1 | Neg\_lig\_3402 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 281 | N#Cc1c(-c2ccccc2)cc(- c2cccc(Br)c2)nc1N | Neg\_lig\_3413 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 0 |
| 282 | CCCCc1nc(C)cc(NCCNC(=O)c 2cn3c(n2)CNCC3)n1 | Neg\_lig\_37 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 283 | C=CCNC(=O)c1sc(N2CCCC2)n  c1N | Neg\_lig\_72 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 284 | Cn1c(=O)c2c(nc(NC[C@H]3CC  CO3)n2Cc2ccc(F)cc2)n(C)c1=O | Neg\_lig\_110 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 285 | Cc1n[nH]c(C)c1S(=O) (=O)N1CC[NH2+]CC1 | Neg\_lig\_134 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 286 | CC(C)NC(=O) [C@@H]1C[C@@H]  (NC(=O)c2ccon2)CN1Cc1cccnc 1N | Neg\_lig\_253 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 287 | COc1ccc(OC)c([C@H]2CCN(C (=O)C3([NH3+])CC3)C2)c1 | Neg\_lig\_270 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 288 | CCn1c([C@H]2CCC[NH2+]C2) nn(CCCS(=O)(=O)N(C)C)c1=O | Neg\_lig\_406 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 289 | C[C@@H]1C(C#N)=C(N)OC2  =C1C(=O)CCC2 | Neg\_lig\_448 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 290 | Cc1cc(C(F) (F)F)nc(N2CCN(C[C@H]3CCC [NH2+]C3)CC2)n1 | Neg\_lig\_497 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 291 | Cc1cc(Nc2ccc(C(=O)O)cc2)c2c c(F)ccc2n1 | Neg\_lig\_568 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 292 | COc1ccc(F)cc1NC(=O)NC[C@ H](O)CO | Neg\_lig\_630 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 293 | Cc1ccc(C)c2c(O)cc(CN3C[C@ H](O)[C@@H] (N4CCOCC4)C3)nc12 | Neg\_lig\_651 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 294 | CCCc1ccc(C[N@H+]2CC[C@  @H](NC(=O)c3ccncc3)[C@H] (O)C2)o1 | Neg\_lig\_654 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 295 | CC(C)n1cnnc1CN(C) | Neg\_lig\_699 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | [C@H]1CCC[NH2+]C1 |  |  |  | GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC |  |
| 296 | N#CC1=C(N)Oc2cc(N)ccc2[C  @@H]1c1ccc(Br)s1 | Neg\_lig\_709 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 297 | CCc1ccc(OC[C@@H] (O)C[NH+]2CCC(C)CC2)cc1 | Neg\_lig\_735 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 298 | Cc1cnn([C@@H] (C)CNC(=O)c2cc(C[NH+]3CC C(O)CC3)on2)c1 | Neg\_lig\_740 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 299 | O=C(NC[C@@H]  (CO)Cc1ccsc1)c1cnc(- c2ccncc2)nc1 | Neg\_lig\_741 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 300 | Cc1c(CN2CC[C@H]3CC[C@@ H](C2)[NH2+]3)c(=O)n(-  c2ccccc2)n1C | Neg\_lig\_781 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 301 | O=C1N=C(C(F)(F)F)C=C/ C1=C(\ O)N1CC[C@H]2[NH2+]CCC[C @]2(CO)C1 | Neg\_lig\_868 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 302 | CCNc1nc(OC)nc(Oc2ccc(=O)n( C)n2)n1 | Neg\_lig\_902 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 303 | CN(CC[NH+] (C)C)C(=O)c1ccc(NC(=O)Nc2c  cc(- c3nc(N4CCOCC4)c4ccn(CC(F) (F)F)c4[nH+]3)cc2)cc1 | Neg\_lig\_912 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 304 | COc1ccccc1-n1cc(-c2cc(- c3cnn(C)c3C)c(C#N)c(N)n2)cn1 | Neg\_lig\_543 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 305 | CC(C)(C)c1ccc(OC[C@@H] (O)CN2CCOCC2)cc1 | Neg\_lig\_1008 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 306 | O=C1C=C/C(=N\ Nc2ccccc2)C(C(=O)[O-])=C1 | Neg\_lig\_1133 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 307 | CCCc1[nH]nc2c1C1(CCN(C(= O)OCC)CC1)C(C#N)=C(N)O2 | Neg\_lig\_1138 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 308 | N#Cc1c(-c2cccc3cnccc23)cc(- c2ccco2)nc1N | Neg\_lig\_1245 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 309 | O=C1OC2(CCN(C(=O)c3ccc(C  O)o3)CC2)CN1CCOc1ccccc1 | Neg\_lig\_1279 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 310 | OCc1cc(-c2ccc3c(c2)OCO3)no1 | Neg\_lig\_1330 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 311 | COc1cc(C(C)=O)ccc1OC[C@@ H](O)CN1CCN(c2ccccc2F)CC1 | Neg\_lig\_1349 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  |  |  |  |  | UGCUAUGCCAACAUAUUG CCAUC |  |
| 312 | C=CCN1C(=O)  [C@]2(c3ccccc31)c1c(oc3cc(C) c(C)cc3c1=O)C(=O)N2CCCO | Neg\_lig\_1353 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 313 | CCn1cc(S(=O) (=O)N2CC[C@H](CO)[C@H] (O)C2)cn1 | Neg\_lig\_1355 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 314 | CC1(C)C[C@@](C)  (c2ccccc2)c2ccccc2N1C(=O)CS c1nnc(N)s1 | Neg\_lig\_1376 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 315 | Cc1cc(=O)n(C)c(=O)n1CCCCO | Neg\_lig\_1403 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 316 | CC(C)Oc1ccccc1Nc1ncnc2ccccc 12 | Neg\_lig\_1411 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 317 | [NH3+]CCNC(=O)c1nc(Cn2cc(  Br)cn2)no1 | Neg\_lig\_1424 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 318 | COC(=O)c1ccc(NC(=O)N2CCO  C[C@@H]2CO)cc1Cl | Neg\_lig\_1446 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 319 | S=C1NC2(CCCCCC2)NN1c1cc  ccc1 | Neg\_lig\_1494 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 320 | Cc1cc(Br)ccc1N[C@H]1OC(=O  )c2ccccc21 | Neg\_lig\_1511 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 321 | CCCCCCCn1c(CO)nc2ccccc21 | Neg\_lig\_1533 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 322 | Cc1nc(Nc2ncc3c(n2)C[C@H] (C)CC3=O)nc2ccccc12 | Neg\_lig\_1576 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 323 | O[C@@H]  (CSc1ncnc2[nH]cnc12)c1ccc(Cl  )cc1 | Neg\_lig\_1606 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 324 | CSCCc1nc(Cn2cc(Cl)c(C)n2)n( CCO)n1 | Neg\_lig\_1609 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 325 | CC1(C)CC(=O)c2cc3c(N)c(C(=  O)c4ccc(F)cc4)sc3nc2C1 | Neg\_lig\_1625 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 326 | Nc1nc(NCCc2nc(Cc3ccccc3)no 2)c2c([nH+]1)CCCC2 | Neg\_lig\_1629 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 327 | CCNC(=O) [C@@H]1C[C@@H] (NC(=O)Cn2cc(Cl)cn2)CN1C(= O)CCO | Neg\_lig\_1685 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 328 | Cc1c(S(=O) (=O)c2ccc(F)cc2)c(N)n(C2CCC CC2)c1C | Neg\_lig\_1692 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 329 | CC(C)c1nc(N2CCC([NH2+]CC  Sc3nnnn3C)CC2)cc(=O)[nH]1 | Neg\_lig\_1702 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 330 | Nc1cccc(C(=O)Nc2cc([O-])n(- c3c(Cl)cc(Cl)cc3Cl)n2)c1 | Neg\_lig\_1746 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 331 | Fc1cccc(CCNc2nc(- c3ccc[nH+]c3)nc3c2CC[NH2+] CC3)c1 | Neg\_lig\_1792 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 332 | Cc1noc(C)c1CCC(=O)NCc1cc2 n(n1)CCC[NH2+]C2 | Neg\_lig\_1925 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 333 | O=c1cc(- c2ccccc2)oc2ccc(O)cc12 | Neg\_lig\_1936 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 334 | Fc1ccccc1CC[NH2+]Cc1cccc(O c2ncccn2)c1 | Neg\_lig\_1998 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 335 | CN(C)c1nc(NC(C)(C)C)nc(-  n2cnc(SCc3ccccc3)n2)n1 | Neg\_lig\_2091 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 336 | CSc1nc(N)nc(SCC(=O)Nc2ccc( C)cc2)c1C#N | Neg\_lig\_2097 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 337 | O=C(c1cc(=O)  [nH]c2ccccc12)N1CCOC[C@@ H]1CO | Neg\_lig\_2101 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 338 | CCCC1(C[NH2+]C2CCN(C(=O  )c3cnccn3)CC2)CCC1 | Neg\_lig\_2103 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 339 | Cc1ccc(OC2(C(=O)NCCc3nc(C  )c(C)s3)CC[NH2+]CC2)cc1 | Neg\_lig\_548 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 340 | Cc1nc(-c2cccc(-n3ccnc3- c3cc4n(n3)CC[NH2+]C4)c2)cs1 | Neg\_lig\_2131 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 341 | COc1ccc(Cn2nnc(C(=O)Nc3cc( C)ccc3OC)c2N)cc1Br | Neg\_lig\_2161 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 342 | COc1ccc(- c2c(C)nn3c(NCc4ccc(Cl)cc4)cc( C)[nH+]c23)cc1OC | Neg\_lig\_2174 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 343 | COC(=O)c1cc(SC#N)ccc1N | Neg\_lig\_2181 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 344 | CO[C@H]1C[C@@H] (O)C12CCN(C(=O)Cc1nc3nc(C | Neg\_lig\_2182 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | )cc(C)n3n1)CC2 |  |  |  | UGCUAUGCCAACAUAUUG CCAUC |  |
| 345 | O=C(O)  [C@@H]1CN(Cc2ccc(OCCO)c c2)C[C@H]1c1cccc(F)c1 | Neg\_lig\_2187 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 346 | O=c1cc/c(=[NH+]\ Nc2ccccc2)c(=O)/c1=N\ Nc1ccccc1 | Neg\_lig\_2216 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 347 | c1ccc(COC2CCN(c3ncnc4c3CC [NH2+]CC4)CC2)nc1 | Neg\_lig\_2217 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 348 | c1ccc2c(CC[NH2+]Cc3ccsc3)c[ nH]c2c1 | Neg\_lig\_2218 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 349 | C[C@H]  ([NH2+]Cc1csc2ccc(Cl)cc12)C(  =O)NC1CCCC1 | Neg\_lig\_2252 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 350 | COC(=O)c1ccc(OC[C@@H]  (O)Cn2cnc3cc(C)c(C)cc32)cc1 | Neg\_lig\_2271 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 351 | O=C1[C@H]2[C@@H]3C=C[C @@H](C3)  [C@H]2C(=O)N1c1ccccc1CO | Neg\_lig\_2280 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 352 | CC(C)c1ccc([C@@H] (O)Cc2nc3ccccc3n2C)cc1 | Neg\_lig\_2286 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 353 | c1ccc(Cn2ccnc2CNC2CCC3(CC [NH2+]CC3)CC2)cc1 | Neg\_lig\_2309 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 354 | CC(C)c1cc(N2CCc3nnc(- c4ccccc4)n3CC2)nc(N)n1 | Neg\_lig\_2313 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 355 | c1ccc(-c2nc[nH]c2- c2ccccc2)cc1 | Neg\_lig\_2322 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 356 | COc1ccc(CNc2c(- c3ccc(C)cc3)c(=O)c2=O)cc1 | Neg\_lig\_2324 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 357 | Cc1sc2ncnc(NCc3ccc4c(c3)OC O4)c2c1C | Neg\_lig\_2340 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 358 | Nc1nc(SCCc2ccccc2)ns1 | Neg\_lig\_2332 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 359 | C[NH+]1CCC(N(CCc2ccccc2)C (=O)CN2CCC[C@H] (O)C2)CC1 | Neg\_lig\_882 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 360 | CCCC(=O)C1=C(O)CC(C) (C)C/C1=N\[C@@H](CC)CO | Neg\_lig\_2426 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 361 | Clc1ccccc1COc1cccc(C[NH2+] Cc2cccnc2)c1 | Neg\_lig\_2429 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 362 | CC(C)  (C)n1cnc2cc(NCc3ccccn3)ccc21 | Neg\_lig\_2446 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 363 | [NH3+][C@@H]1CC[C@H]  (C(=O)Nc2ccccc2OCCc2ccccn2  )C1 | Neg\_lig\_2448 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 364 | CSc1nc(N)nc(SCC(=O)CC(=O) OC(C)C)c1C#N | Neg\_lig\_2464 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 365 | CC[C@@H]  (c1nc(Cc2cccs2)nn1CCO)n1ccc n1 | Neg\_lig\_2469 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 366 | O[C@@]1(C[NH2+]CCCc2ccn cc2)CNCCOC1 | Neg\_lig\_2472 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 367 | CCCc1ccc(C[N@H+]2CCOC[C @@H](CO)C2)o1 | Neg\_lig\_2530 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 368 | c1ccc(- n2nnnc2SCC[NH2+]Cc2ccco2)c c1 | Neg\_lig\_163 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 369 | Cc1cc(=O)c2ccccc2n1CC[C@@ H](O)c1ccccc1 | Neg\_lig\_2653 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 370 | COc1ccc(-c2noc(- c3cccnc3NCc3ccccc3Cl)n2)cc1 | Neg\_lig\_2687 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 371 | CC(C)Cc1cc(C(=O)N(CCCO)Cc  2ccncc2)n(C)n1 | Neg\_lig\_2696 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 372 | CCCCCn1c(N)c(C#N)c2nc3cccc c3nc21 | Neg\_lig\_2820 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 373 | COc1ccc(C2=C(C)NN/C2=C2\ C=CC([O-])=CC2=O)cc1 | Neg\_lig\_2857 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 374 | COC1=C2C[C@@H] (C)C[C@H](OC)[C@@H](O)  [C@@H](C)/C=C(/C)[C@H]  (OC(N)=O)[C@@H](OC)/C=C\ C=C(\C)C(=O)  [N-]C(=CC1=O)C2=O | Neg\_lig\_2903 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 375 | O=C(Cc1cccc2ccccc12)N1CCO[ C@]2(C[NH2+]CCOC2)C1 | Neg\_lig\_2922 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 376 | Cc1cccc(- c2nc3nc(C)cc(Nc4ccc(N(C)C)cc 4)n3n2)c1 | Neg\_lig\_2928 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 377 | c1cnc(Oc2cccc(C[NH2+]Cc3ccc o3)c2)nc1 | Neg\_lig\_2650 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 378 | O=C(c1cncc(Br)c1)N1CCC([NH  +]2CCCC2)CC1 | Neg\_lig\_2988 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 379 | Cc1cccc(C[NH+]2CCC(n3cc(C CO)nn3)CC2)c1C | Neg\_lig\_2996 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 380 | CC[C@@H] (CO)NC(=O)c1ccc(-  c2nn(C)c(=O)c3ccccc23)cc1 | Neg\_lig\_3006 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 381 | CC(C)  (C)n1cnc2cc(NCc3cccc4ccccc34  )ccc21 | Neg\_lig\_3072 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 382 | COc1ccccc1N1CCN(C(=O) [C@H]2[C@@H]([NH3+]) [C@H]3CC[C@@H]2C3)CC1= O | Neg\_lig\_3096 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 383 | NCc1nc(-c2ccccc2)no1 | Neg\_lig\_3154 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 384 | O=S(=O) (c1ccc2c(c1)CCCN2)N1CCC[C @H]2CCCC[C@@H]21 | Neg\_lig\_3163 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 385 | COc1ccc(N2CCN(C[C@H]  (O)c3ccc4c(c3)CCN4)CC2)cc1 | Neg\_lig\_3165 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 386 | Cc1ccn(CO)n1 | Neg\_lig\_57 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 387 | COCc1cc(C)nc(NCCO)c1C#N | Neg\_lig\_3176 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 388 | CC(C)Cc1nc2sc3c(NCCCO)ncn c3c2c2c1COC(C)(C)C2 | Neg\_lig\_3202 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 389 | CCN(CC)C(=O)  [C@@H]1C[C@H] ([NH3+])CN1Cc1ccc(Cl)nc1 | Neg\_lig\_3228 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 390 | Cc1nc2c(c(N3CC=CC3)n1)CCN (C(=O)c1ccnc(N)c1)CC2 | Neg\_lig\_3248 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 391 | C=CCN(CC=C)C(=O)Nc1cc(O  C)ccc1OC | Neg\_lig\_3254 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 392 | COCc1nn(-c2ccccc2)c(N)c1- c1ccc(OC)c(OC)c1 | Neg\_lig\_2047 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 393 | O=C1[C@@H](CO)[C@@H] (CO)[C@H](CO)[C@@H]1CO | Neg\_lig\_3332 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  |  |  |  |  | UGCUAUGCCAACAUAUUG CCAUC |  |
| 394 | C[C@@H]  (C[N@@H+]1CCc2ccccc2C1)N c1nccc(N2CCC(O)CC2)n1 | Neg\_lig\_3374 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 395 | CNc1ccc(Br)c2c1C(=O)c1ccccc 1C2=O | Neg\_lig\_3378 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 396 | CC[C@@H](CO)  [NH2+]C[C@@H]  (O)Cn1c(C)c(C)c2ccccc21 | Neg\_lig\_1242 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 397 | CCOC(=O)c1c(-  c2cccc(OC)c2)n[nH]c1N | Neg\_lig\_3418 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 398 | Cc1ccc2nc(C(=O)  [O-])cc(Nc3ccc(N(C)C)cc3)c2c1 | Neg\_lig\_3422 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 0 |
| 399 | c1ccc(cc1)N1C(C(Nc2cccc(c2)C (O)=O)SC1=O)=O | 1159-0329 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 1 |
| 400 | Cc1ccc([C@H]2CN(C[C@@H] 2N)C(COc2ccc(cc2)n2cnnn2)=O  )o1 | 13917927 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 1 |
| 401 | C1CN(CC(c2ccccc2)N1)C(c1cc n2cnnc2c1)=O | 13930321 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 1 |
| 402 | CNC(c1cc2CN(CCc2s1)C(C1C NCCO1)=O)=O | 14100811 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 1 |
| 403 | C(CCn1cc(c2ccccc2c2ccco2)nn1  )CCO | 14330381 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 1 |
| 404 | C1[C@@H] (C2(CCN(CC2)Cc2cccc(c2)OC CN2CCOCC2)[C@@H]1O)O | 14778588 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 1 |
| 405 | CN1CCCN(C)C2(CCN(CC2)C(  Nc2cccc(CN)c2)=O)C1 | 15129370 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 1 |
| 406 | COCCN(CC1CC1)C(c1ccc(cc1) C1CCCNC1)=O | 15822403 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 1 |
| 407 | Cc1ccc(cc1)NC([C@H]1C[C@ H] (CNC1)C(NCCN1CCCC1=O)= O)=O | 17600296 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 1 |
| 408 | CC(C)Cc1cc(CNC2CCN(CC2)C C(C)C)no1 | 17766103 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 1 |
| 409 | Cc1c(CNC(c2cn(CCC3CCCCN  3)nn2)=O)c(C)on1 | 18521194 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 410 | C(Cc1csc(N)n1)CNC(C1CCCN(  C1)Cc1ccco1)=O | 18722734 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 1 |
| 411 | C(COCc1ccc(cc1) [Cl])NCC1(CNCCOC1)O | 20639134 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 1 |
| 412 | C1CC(CNC1)c1ccc(cc1)C(N1C CCN(CC1)c1ccc(cc1)F)=O | 21010099 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 1 |
| 413 | CC1CC2(C)CC(C)C1(CO)CO2 | 2190-0577 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 1 |
| 414 | Cn1c(Cn2ccnc2c2cc3CNCCn3n 2)cnc1SC | 22199819 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 1 |
| 415 | CNc1cc(c2ccc(cc2)c2nnc(N)s2)c 2cc[nH]c2n1 | 25638728 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 1 |
| 416 | COc1cccc(CNCCc2cccc(c2)F)c1 | 2910-1991 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 1 |
| 417 | O=C(N(CC1OC1)C(N1CC2OC 2)=O)N(CC2OC2)C1=O | 296934 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 1 |
| 418 | C1COC2(CCOCC2)CC1NCc1n  c(c2cnccn2)n[nH]1 | 31093015 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 1 |
| 419 | Cc1c2c(NCc3nc(N) [nH]n3)nc(C)nc2on1 | 31495708 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 1 |
| 420 | Cc1c(cccc1NC(NCCNc1cccnc1)  =O)C(NC(C)(C)C)=O | 31773556 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 1 |
| 421 | C(CNc1c2c(csc2ncn1)c1ccc(cc1  )F)c1cccs1 | 3230-0825 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 1 |
| 422 | Cc1c(CNC(CCc2ccsc2)=O)c2C CNCc2cn1 | 32845432 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 1 |
| 423 | CC(C)c1nc(CCNC(c2ccccc2C2 CCNC2)=O)on1 | 33313650 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 1 |
| 424 | C(Cc1nc(c2ccco2)nn1CCO)c1cc c2c(c1)OCO2 | 33326934 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 1 |
| 425 | C1CCc2c(C1)nc(CCNCC1(CCN C1)O)s2 | 33880841 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 1 |
| 426 | [H] [C@@]12CCCCN2CCC[C@]1( | 33884666 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC | 1 |

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| **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)c1ccccc1 | 34114692 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 1 |
| 428 | Cc(cc1nc(ccc(N(C)C)c2)c2[s+]c 1c1)c1N.[Cl-] | 36758 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 1 |
| 429 | Cc1cc2NC(CN3CCC4(CC3)C(C  c3ccccc34)O)=CC(n2n1)=O | 40183085 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 1 |
| 430 | CCC(c1ccnn1C)NCc1ccc(c(CC= C)c1)OCC | 41760826 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 1 |
| 431 | C1CN(Cc2cc3cc[nH]c3cn2)Cc2 cc(C(NCCO)=O)nn2C1 | 41857771 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC 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 GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 1 |
| 433 | CCN(CCn1cccn1)C(c1ccc(cc1) C1CCCNC1)=O | 42585880 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 1 |
| 434 | CCc1nc2cc(cnc2[nH]1)c1cc(NC CO)nc2c1cc[nH]2 | 46180634 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 1 |
| 435 | CCC(CO)N(Cc1ccc(cc1)F)Cc1c c(c(c(c1)[Cl])O)OC | 46503727 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 1 |
| 436 | Cc1c(CC=C)c(nc(N)n1)N1CCN(  CC1)c1c2c(ncn1)[nH]cn2 | 47603260 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 1 |
| 437 | CC[n+]1cn(CC(COc2ccccc2)O) c2ccccc12 | 5010-0422 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 1 |
| 438 | CCOC(c1c(C)c(C)sc1NC(CNCc  1ccccc1)=O)=O | 5132485 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 1 |
| 439 | CCOC(c1cnc2ccc(cc2c1Nc1ccc( cc1)N1CCOCC1)[Cl])=O | 5173-3862 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 1 |
| 440 | CCOC(c1cnc2ccc(C)cc2c1NCC( C)O)=O | 5174-4400 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 1 |
| 441 | C1CCCC(CC1)N[C@@H]1CC[  C@@H]1NC(c1ccccc1N1CCO CC1)=O | 56098188 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC 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 GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 443 | CCOC(C1=C(C)OC(=C(C(=O) OCC)C12C(Nc1ccccc12)=O)N)  =O | 8003-0370 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 1 |
| 444 | C(C1C(c2ccccc2)c2c(c3ccccc3) n[nH]c2OC=1N)#N | 8008-9218 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 1 |
| 445 | Cc1c(CCNCc2ccc(C#N)cc2)c2c c(ccc2[nH]1)OC | 8013-2954 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 1 |
| 446 | C(c1ccoc1C(O)=O)N | 8015-0997 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 1 |
| 447 | C(c1ccc(cc1)F)N1C(C2(C(C#N)  =C(N)N(C3COC(C2=3)=O)c2cc  ccc2)c2ccccc12)=O | 8017-5050 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 1 |
| 448 | C=CCOc1ccc(cc1)C1C(C#N)=C (N)OC2=C1C(c1ccccc1C2=O)= O | 8017-5263 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 1 |
| 449 | Cc1c(C#N)c(N)n(CCCn2ccnc2) c1C | 8018-7492 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 1 |
| 450 | Cc1c(c2ccc(cc2) [Br])c2ncc(C#N)c(N)n2n1 | 8019-5330 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 1 |
| 451 | c1cc(N)nc2c1ccc(n2)O | 8019-7722 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 1 |
| 452 | CCc1c(C)cc2c(c(C(c3ccccc3)=O  )sc2n1)N | 8020-0635 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 1 |
| 453 | c1cnccc1c1nc2ncnc(N)n2n1 | 8020-2786 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 1 |
| 454 | [H]N(CCNC(c1c(N)non1)=O)Cc  1cc(ccc1OCc1ccc(cc1)[Cl])[Br] | 8104-04658 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 1 |
| 455 | Cc1c(c2ccc(c(c2)OC)OC)c2ncc( c3ccc(c(c3)OC)OC)c(N)n2n1 | 8104-10716 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 1 |
| 456 | Cc1cc(Nc2ccc(cc2)N2CCOCC2) n2c(ncn2)n1 | 8246-0044 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 1 |
| 457 | c1ccc2c(c1)nc(c1ccc(cc1[Cl])N) s2 | C066-5322 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 1 |
| 458 | Cn1c2ccccc2nc1CNCc1ccccc1 | C147-0039 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 1 |
| 459 | Cc1cccc(c1)NCc1nc2ccccc2n1C | C147-0043 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  |  |  |  |  | UACUGCAGUGAAGGCACU UGUAG |  |
| 460 | Cc1cccc(C)c1Nc1c(c2ccc(cc2)N 2CCOCC2)nc2cnccn12 | C169-0291 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 1 |
| 461 | CCCCn1cnc2cc(ccc12)NCc1ccc c(c1)OC | C215-0084 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 1 |
| 462 | c1ccc(cc1)C(c1nnc(c2ccccc2)o1  )Nc1ccc(cc1)F | C301-5596 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 1 |
| 463 | Cc1ccc(cc1)NC(Cn1c(c(C(Nc2c cc(cc2)[Br])=O)nn1)N)=O | C368-0780 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 1 |
| 464 | c1ccc2C(N(C(c2c1)Nc1ccc(cc1) F)c1ccccn1)=O | C430-0215 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 1 |
| 465 | CCN(CC)CCCNc1c2ccccc2nc(c 2nnc(c3ccc(C)cc3)o2)n1 | C660-1575 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 1 |
| 466 | Cc1cccc(Cn2c3ccccc3nc2CCNC (CCCO)=O)c1 | D186-0280 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 1 |
| 467 | Cc1cc(Nc2ccc(cc2)F)n2c(n1)nc( c1ccc(cc1)OC)n2 | D245-0284 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 1 |
| 468 | Cc1nc(cc(Nc2cccc(c2)C(=O)OC  )n1)c1ccc(cc1)OC | D482-2049 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 1 |
| 469 | Cc1c(c2ccc(cc2)OC)nn2c(cc(C) nc12)N1CCN(CC1)CCO | D503-0348 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 1 |
| 470 | c1ccc2c(c1)C(=C(C(N)=O)S2(= O)=O)Nc1cccc(c1)C(F)(F)F | D531-0321 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 1 |
| 471 | CCOc1ccc(c(c1)NC1=C(C(C1=  O)=O)c1ccccc1)OCC | E470-0451 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 1 |
| 472 | C(c1ccccc1)N=C(N)NC(c1c(N)n c(c(n1)[Cl])N)=O | NCGC0001514 7-09 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 1 |
| 473 | CC(C)n1cnc2c(Nc3cccc(c3)NC( C=C)=O)nc(NC3CCC(CC3)N(C  )C)nc12 | NCGC0034696 4-01 | Pre\_miR\_17 | Hairpin | CAAAGUGCUUACAGUGCA GGUAGUGAUAUGUGCAUC UACUGCAGUGAAGGCACU UGUAG | 1 |
| 474 | CC1CCN(CC1)CC(COc1ccccc1 CC=C)O | 1189-2046 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 1 |
| 475 | C1CNCc2cc(CN3CCc4nnc(c5cc ccc5)n4CC3)nn2C1 | 12129103 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 1 |
| 476 | CC(NS(c(cc1)cc2c1sc(C)n2) (=O)=O)=O | 122385 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 1 |
| 477 | Cc1ccc([C@H]2CN(C[C@@H] | 13917927 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | 2N)C(COc2ccc(cc2)n2cnnn2)=O  )o1 |  |  |  | CAUGGCAACCC |  |
| 478 | C1CN(CC(c2ccccc2)N1)C(c1cc n2cnnc2c1)=O | 13930321 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 1 |
| 479 | CN1CCN(CC12CCNCC2)C(c1c  ccc2c1nccn2)=O | 13948752 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 1 |
| 480 | C(CCn1cc(c2ccccc2c2ccco2)nn1  )CCO | 14330381 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 1 |
| 481 | C(CO)Nc1cc(c2ccc(c(c2) [Cl])O)c2cc[nH]c2n1 | 15290349 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 1 |
| 482 | Cc1ccccc1C(NC[C@@H]1CCN (C[C@H]1O)C(Cc1ccccn1)=O)  =O | 16828885 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 1 |
| 483 | CC(C)Cc1cc(CNC2CCN(CC2)C C(C)C)no1 | 17766103 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 1 |
| 484 | Cc1c(CNC(c2cn(CCC3CCCCN  3)nn2)=O)c(C)on1 | 18521194 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 1 |
| 485 | C(COCc1ccc(cc1) [Cl])NCC1(CNCCOC1)O | 20639134 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 1 |
| 486 | CCCCN1C(=N)N(CC(c2ccc(cc2  )OC)O)c2ccccc12 | 2226-0445 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 1 |
| 487 | CN(C)[C@@H]1C[C@@H]  (CO)N(C1)C(c1cc2c(c3ccccc3)n n(C)c2s1)=O | 22692463 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 1 |
| 488 | CNc1cc(c2ccc(cc2)c2nnc(N)s2)c 2cc[nH]c2n1 | 25638728 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 1 |
| 489 | Cc1cccc2c1nc(C1CCN(CC1)C( Cc1c(C)nc(N)nc1C)=O)[nH]2 | 26941110 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 1 |
| 490 | COc1cccc(CNCCc2cccc(c2)F)c1 | 2910-1991 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 1 |
| 491 | C(CO)Nc1cc2c(c3C(c4ccccc4C( c13)=O)=O)Nc1ccccc1O2 | 2920-0632 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 1 |
| 492 | C1CN(CC1Cc1ccc(CO)cc1)C(C  c1cn2ccsc2n1)=O | 31022825 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 1 |
| 493 | C1COC2(CCOCC2)CC1NCc1n  c(c2cnccn2)n[nH]1 | 31093015 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 1 |
| 494 | C(C1C(c2ccccc2[Cl])c2c(n[nH]c 2c2ccccc2)OC=1N)#N | 3132-0191 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 1 |
| 495 | Cc1c(cccc1NC(NCCNc1cccnc1)  =O)C(NC(C)(C)C)=O | 31773556 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 1 |
| 496 | C1CCN(CC1)CCN1C(=N)N(CC  O)c2ccccc12 | 3260-0393 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 1 |
| 497 | C1Cc2cc(Cn3cc(c4ccc(C#CCO) s4)nn3)ccc2OC1 | 33240961 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 1 |
| 498 | CC(c1cc(CC(N[C@H]2CC[C@ H](CC2)N)=O)cs1)=O | 33946523 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 1 |
| 499 | C1CC2(CCNCC2)CCN(C1)Cc1  c(nc2n1ccs2)[Cl] | 35729906 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 1 |
| 500 | Cc(cc1nc(ccc(N(C)C)c2)c2[s+]c 1c1)c1N.[Cl-] | 36758 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 1 |
| 501 | CC(C)CC1CC(C)  (c2csc(Nc3ccccc3)n2)OC1=O | 4075-3209 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 1 |
| 502 | CCC(c1ccnn1C)NCc1ccc(c(CC= C)c1)OCC | 41760826 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 1 |
| 503 | CCN(CCn1cccn1)C(c1ccc(cc1) C1CCCNC1)=O | 42585880 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 1 |
| 504 | COc1ccc(c(c1)OC)c1csc(NCC= C)n1 | 4640-0152 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 505 | CCC(CO)N(Cc1ccc(cc1)F)Cc1c c(c(c(c1)[Cl])O)OC | 46503727 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 1 |
| 506 | Cc1ccc(cc1)NC(C) (C(NCCCc1nnn[nH]1)=O)c1ccc cc1 | 47814214 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 1 |
| 507 | CCOC(c1cnc2ccc(C)cc2c1Nc1c cc(cc1)N(C)C)=O | 4790-1159 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 1 |
| 508 | Cc1cccc2c(cc(C)nc12)Nc1ccc(c c1)N(C)C | 4790-1400 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 1 |
| 509 | C(CNCc1ccc2c(c1)OCO2)c1c[n H]c2ccccc12 | 4964-5174 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 1 |
| 510 | CC[n+]1cn(CC(COc2ccccc2)O) c2ccccc12 | 5010-0422 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 1 |
| 511 | Cc1c2c([nH]n1)OC(=C(C#N)C2 1C(N(C)c2ccccc12)=O)N | 5066-0352 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 1 |
| 512 | CCOC(c1cnc2ccc(cc2c1Nc1ccc( cc1)N1CCOCC1)[Cl])=O | 5173-3862 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 1 |
| 513 | CCOC(c1cnc2ccc(C)cc2c1NCC( C)O)=O | 5174-4400 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 1 |
| 514 | C1CCN(CC1)c1ccccc1N | 5784-1967 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 1 |
| 515 | C(C#CCSc1nnc(c2cccc(c2) [Br])o1)O | 7199-0097 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 1 |
| 516 | CC(Nc1c(C(c2cccc(c2)F)N2CC N(CC2)CCO)c2CCCCc2s1)=O | 7287-0672 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 1 |
| 517 | CCCCN(C)S(c1ccc(cc1)NC1c2c cccc2S(N=1)(=O)=O)(=O)=O | 7489-2048 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 1 |
| 518 | CC(c1ccccc1OCC(Cn1c2ccccc2 nc1CO)O)=O | 7661-0041 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 1 |
| 519 | CC1=CC2=C(C(C(C#N)=C(N)  O2)c2ccccc2OC)C(N1Cc1ccc2c (c1)OCO2)=O | 7706-1226 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 1 |
| 520 | Cn1c(cnc1NCc1ccccc1OC)c1cc ccc1 | 7756-0545 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 1 |
| 521 | CCOC(C1=C(C)OC(=C(C(=O) OCC)C12C(Nc1ccccc12)=O)N)  =O | 8003-0370 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 1 |
| 522 | CC1=CC2=C(C(C(C#N)=C(N) O2)c2ccc(cc2)[Br])C(=O)O1 | 8003-0435 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 1 |
| 523 | COC(C1=C(N)OC2=C(C(=O)O  c3ccccc23)C12C(Nc1ccccc12)= O)=O | 8005-2656 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 1 |
| 524 | CN1C(C2C(C(C#N)=C(N)OC=  2c2ccccc12)c1c(cccc1[Cl])F)=O | 8016-4538 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 1 |
| 525 | C(c1ccc(cc1)F)N1C(C2(C(C#N)  =C(N)N(C3COC(C2=3)=O)c2cc  ccc2)c2ccccc12)=O | 8017-5050 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 1 |
| 526 | Cc1c(C#N)c(N)n(CCCn2ccnc2) c1C | 8018-7492 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 1 |
| 527 | c1cc(N)nc2c1ccc(n2)O | 8019-7722 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 1 |
| 528 | CCc1c(C)cc2c(c(C(c3ccccc3)=O  )sc2n1)N | 8020-0635 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 1 |
| 529 | c1cnccc1c1nc2ncnc(N)n2n1 | 8020-2786 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 1 |
| 530 | Cc1c(c2ccc(c(c2)OC)OC)c2ncc( c3ccc(c(c3)OC)OC)c(N)n2n1 | 8104-10716 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 1 |
| 531 | [H]N(Cc1cccc(c1OCc1ccc(cc1) F)OC)Cc1ccco1 | 8320-0678 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 532 | Cc1ccc(cc1)c1cnc2c(cnn2c1N)c 1ccccc1 | 8562-00039 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 1 |
| 533 | CC1=CC2=C(C(C(C#N)=C(N) O2)c2c(cccc2[Cl])[Cl])C(=O)O1 | 8645-0078 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 1 |
| 534 | c1ccc2c(c1)nc(c1ccc(cc1[Cl])N) s2 | C066-5322 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 1 |
| 535 | C(CO)Nc1c2c(ncn1)[nH]cn2 | C143-0023 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 1 |
| 536 | Cn1c2ccccc2nc1CNCc1ccccc1 | C147-0039 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 1 |
| 537 | Cc1cccc(c1)NCc1nc2ccccc2n1C | C147-0043 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 1 |
| 538 | Cc1cccc(C)c1Nc1c(c2ccc(cc2)N 2CCOCC2)nc2cnccn12 | C169-0291 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 1 |
| 539 | CCCCn1cnc2cc(ccc12)NCc1ccc c(c1)OC | C215-0084 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 1 |
| 540 | Cc1nnc2c(Nc3ccccc3[Cl])nc3cc ccc3n12 | C301-3100 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 1 |
| 541 | Cc1ccccc1Nc1c(c2ccc(C)o2)nc2 ncccn12 | C325-0048 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 1 |
| 542 | Cc1ccccc1NC(Cn1c(c(C(NCc2c cc(cc2)F)=O)nn1)N)=O | C368-0744 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 1 |
| 543 | CCOC(N1CCN(CC1)C1=C(C(C 1=O)=O)NCCCN1CCCCCC1)= O | C748-1353 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 1 |
| 544 | Cc1ccc(cc1)S(c1c(NCCOC)oc(c 2cccc(C)c2)n1)(=O)=O | D072-0517 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 1 |
| 545 | CCOC(c1cccc(c1)Nc1cc(c2cccc c2)ncn1)=O | D278-0165 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 1 |
| 546 | CN1C(N(C)c2cc(COc3ccc(CNC  c4cccnc4)cc3OC)ccc12)=O | D300-0082 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 1 |
| 547 | CCC(C)Nc1nc(nc(n1)n1cnc(n1) SCc1ccccc1)N(C)C | D385-0103 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 1 |
| 548 | Cc1nc(cc(Nc2cccc(c2)C(=O)OC  )n1)c1ccc(cc1)OC | D482-2049 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 1 |
| 549 | CN(C)CCN(Cc1ccc(cc1) [Cl])c1ccccn1 | NCGC0001667 2-04 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 1 |
| 550 | CC(C)n1cnc2c(Nc3cccc(c3)NC( C=C)=O)nc(NC3CCC(CC3)N(C  )C)nc12 | NCGC0034696 4-01 | Pre\_miR\_21 | Hairpin | GGGUUGACUGUUGAAUCU CAUGGCAACCC | 1 |
| 551 | Cc1ccc(cc1C)NCC(C(C(CO)O) O)O | 0527-0256 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 1 |
| 552 | c1ccc(cc1)N1C(C(Nc2cccc(c2)C (O)=O)SC1=O)=O | 1159-0329 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 1 |
| 553 | CC(NS(c(cc1)cc2c1sc(C)n2) (=O)=O)=O | 122385 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 1 |
| 554 | CCN(CC)c1ccc(/C=C/ c2nc3ccccc3c(-c3ccccc3)c2)cc1 | 13487 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 1 |
| 555 | C(CCn1cc(c2ccccc2c2ccco2)nn1  )CCO | 14330381 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 1 |
| 556 | C1[C@@H] | 14778588 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | (C2(CCN(CC2)Cc2cccc(c2)OC CN2CCOCC2)[C@@H]1O)O |  |  |  | GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC |  |
| 557 | CN(C(c1ccc(c2ccccc2[Cl])o1)= O)[C@H]1COC[C@@H]1O | 15922890 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 1 |
| 558 | FC(c1cccc(- c([nH]2)nc(nc3Cl)c2nc3Cl)c1) (F)F | 177407 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 1 |
| 559 | Cc1c(CNC(c2cn(CCC3CCCCN  3)nn2)=O)c(C)on1 | 18521194 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 1 |
| 560 | Cn1c(Cn2ccnc2c2cc3CNCCn3n 2)cnc1SC | 22199819 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 1 |
| 561 | CCCCN1C(=N)N(CC(c2ccc(cc2  )OC)O)c2ccccc12 | 2226-0445 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 1 |
| 562 | Cc(cc1)ccc1S(c(c1nonc11)ccc1[ N+]([O-])=O)=O | 228150 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 1 |
| 563 | CNc1cc(c2ccc(cc2)c2nnc(N)s2)c 2cc[nH]c2n1 | 25638728 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 1 |
| 564 | CC(C)CCCCCCCCCCCCC(NC C(NC(C(C)OC(C1O)Nc2ncnc3c 2[nH]cn3)C1O)=O)=O | 268251 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 1 |
| 565 | CN(C)CCOc1cc(C(/C(/C2)=C\  c(n3C)ncc3[N+]  ([O-])=O)=O)c2cc1.OS(O) (=O)=O | 277184 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 1 |
| 566 | O=C(N(CC1OC1)C(N1CC2OC 2)=O)N(CC2OC2)C1=O | 296934 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 1 |
| 567 | CC1(C)C(N(CC(CN(c2ccccc2)c 2ccccc2)O)C(N1)=O)=O | 2996-0044 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 1 |
| 568 | C1COC2(CCOCC2)CC1NCc1n  c(c2cnccn2)n[nH]1 | 31093015 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 1 |
| 569 | C(C1C(c2ccccc2[Cl])c2c(n[nH]c 2c2ccccc2)OC=1N)#N | 3132-0191 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 1 |
| 570 | Cc1c(cccc1NC(NCCNc1cccnc1)  =O)C(NC(C)(C)C)=O | 31773556 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 1 |
| 571 | C(CNc1c2c(csc2ncn1)c1ccc(cc1  )F)c1cccs1 | 3230-0825 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 1 |
| 572 | C1CCN(CC1)CCN1C(=N)N(CC  O)c2ccccc12 | 3260-0393 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  |  |  |  |  | CCAUC |  |
| 573 | Cc1ccc(c(C)c1)NC(c1c2CCCc2s c1N)=O | 3261-0869 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 1 |
| 574 | C(/C=C/CSc1ncccc1)Sc1ncccc1 | 326921 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 1 |
| 575 | CC1(CCNCC1)C(N1CCCC(C1)  C(CCc1ccccc1)=O)=O | 33248227 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 1 |
| 576 | C(c1c(N)nc2c3c(cc(c4ccccc4)nc 13)c1ccccc1o2)#N | 3331-3338 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 1 |
| 577 | CN(C=C/C(/N1C)=C/[N+] ([O-])=O)C1=O | 342460 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 1 |
| 578 | Cc(cc1nc(ccc(N(C)C)c2)c2[s+]c 1c1)c1N.[Cl-] | 36758 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 1 |
| 579 | CCN(CCn1cccn1)C(c1ccc(cc1) C1CCCNC1)=O | 42585880 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 1 |
| 580 | Cc1c(non1)OCCNCc1nnc(c2ccc (C)n2C)o1 | 45836039 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 1 |
| 581 | COc1ccc(c(c1)OC)c1csc(NCC= C)n1 | 4640-0152 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 1 |
| 582 | Cc1nccn1CCC1CCCCN1Cc1ccc c(CCN)c1 | 47531251 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 1 |
| 583 | CCOC(c1cnc2ccc(C)cc2c1Nc1c cc(cc1)N(C)C)=O | 4790-1159 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 1 |
| 584 | CC[n+]1cn(CC(COc2ccccc2)O) c2ccccc12 | 5010-0422 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 1 |
| 585 | Cc1nc(SC)nc(N2CC2)c1Br | 50199 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 1 |
| 586 | COc1ccc(CCNc2c3c4CCCCc4sc 3ncn2)cc1 | 5067-0641 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 1 |
| 587 | CCOC(c1c(C)c(C)sc1NC(CNCc  1ccccc1)=O)=O | 5132485 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 1 |
| 588 | CCOC(c1cnc2ccc(cc2c1Nc1ccc( cc1)N1CCOCC1)[Cl])=O | 5173-3862 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 589 | CCOC(c1cnc2ccccc2c1Nc1cc(cc c1C)C(O)=O)=O | 5174-4337 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 1 |
| 590 | CCOC(c1cnc2ccc(C)cc2c1NCC( C)O)=O | 5174-4400 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 1 |
| 591 | C1CCC2C(C1)=C(C#N)c1nc3cc ccc3n1C=2NCCOCCO | 5228-5336 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 1 |
| 592 | CCCCOC(C1=C(N)OC(C)=C(C (=O)OCC=C)C12C(Nc1ccccc12  )=O)=O | 5587-0169 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 1 |
| 593 | CCOC(C1=C(C)OC(=C(C(=O) OCC)C12C(Nc1ccccc12)=O)N)  =O | 8003-0370 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 1 |
| 594 | CC1(C)CC2(CC(C)(C)N1)C(C) (N(CCCO)C(=O)O2)O | 8012-5768 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 1 |
| 595 | C(c1ccoc1C(O)=O)N | 8015-0997 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 1 |
| 596 | CN1C(C2C(C(C#N)=C(N)OC=  2c2ccccc12)c1c(cccc1[Cl])F)=O | 8016-4538 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 1 |
| 597 | Cc1c(C#N)c(N)n(CCCn2ccnc2) c1C | 8018-7492 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 1 |
| 598 | Cc1c(c2ccc(cc2) [Br])c2ncc(C#N)c(N)n2n1 | 8019-5330 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 1 |
| 599 | c1cc(N)nc2c1ccc(n2)O | 8019-7722 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 1 |
| 600 | CCc1c(C)cc2c(c(C(c3ccccc3)=O  )sc2n1)N | 8020-0635 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 1 |
| 601 | c1cnccc1c1nc2ncnc(N)n2n1 | 8020-2786 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 1 |
| 602 | CCN(CC)c(cc1)ccc1C(c(cc1)ccc 1N(CC)CC)=C(C=C1)C=CC1=[ N+](CC)CC.[Cl-] | 8675 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 1 |
| 603 | c1ccc2c(c1)nc(c1ccc(cc1[Cl])N) s2 | C066-5322 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 1 |
| 604 | C(CO)Nc1c2c(ncn1)[nH]cn2 | C143-0023 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 1 |
| 605 | Cc1ccc(cc1)NCc1nc2ccccc2n1C | C147-0010 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  |  |  |  |  | UGCUAUGCCAACAUAUUG CCAUC |  |
| 606 | Cn1c2ccccc2nc1CNCc1ccccc1 | C147-0039 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 1 |
| 607 | Cc1cccc(c1)NCc1nc2ccccc2n1C | C147-0043 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 1 |
| 608 | Cc1cccc(C)c1Nc1c(c2ccc(cc2)N 2CCOCC2)nc2cnccn12 | C169-0291 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 1 |
| 609 | CCCCn1cnc2cc(ccc12)NCc1ccc c(c1)OC | C215-0084 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 1 |
| 610 | CC(C)C(N1CCN(CC1)c1ccc(cc  1)Nc1cc(C)nc2nc(c3ccco3)nn12  )=O | C301-7288 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 1 |
| 611 | c1ccc2C(N(C(c2c1)Nc1ccc(cc1) F)c1ccccn1)=O | C430-0215 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 1 |
| 612 | c1ccc(cc1)S(n1c(cc(c2cccc(c2)F  )n1)N)(=O)=O | C665-0183 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 1 |
| 613 | CCOC(N1CCN(CC1)C1=C(C(C 1=O)=O)NCCCN1CCCCCC1)= O | C748-1353 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 1 |
| 614 | COc1ccccc1CNCc1ccc(C(O)=O  )s1 | C863-0034 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 1 |
| 615 | C(CN1CCOCC1)Nc1c(nc(c2ccc o2)o1)S(c1ccc(cc1)F)(=O)=O | D072-1128 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 1 |
| 616 | CCCCNc1c(nc(c2ccc(cc2) [Cl])o1)S(c1ccccc1)(=O)=O | D072-1502 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 1 |
| 617 | CN1C(c2c(cn(CCO)c2c2ccc(cc2  )[Cl])N(C)C1=O)=O | D077-0206 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 1 |
| 618 | CCOC(c1cccc(c1)Nc1cc(c2cccc c2)ncn1)=O | D278-0165 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 1 |
| 619 | c1ccc(cc1)c1cc(Nc2ccc(cc2) [Br])ncn1 | D278-0329 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 1 |
| 620 | Cc1ccccc1c1nc(c2cccnc2NCc2c cco2)on1 | D349-3751 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 1 |
| 621 | CCN(CC)CCCNCc1ccc2c(c1)N( C)C(N2C)=O | D664-0111 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 622 | CC1CCCC(C1C)Nc1c(c2ccc(cc 2)[Cl])[nH]c2c(C#N)cnn12 | E002-1096 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 1 |
| 623 | Cc1cc(ccc1[Br])NC1=C(C(C1=  O)=O)c1ccc(cc1)[Cl] | E786-0118 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 1 |
| 624 | C(c1ccccc1)N=C(N)NC(c1c(N)n c(c(n1)[Cl])N)=O | NCGC0001514 7-09 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 1 |
| 625 | CCOC(Nc1ccc(NCc2ccc(cc2)F) nc1N)=O | NCGC0001545 1-06 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 1 |
| 626 | C1C(C1N)c1ccccc1 | NCGC0001584 8-04 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 1 |
| 627 | CN(C)CCN(Cc1ccc(cc1) [Cl])c1ccccn1 | NCGC0001667 2-04 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 1 |
| 628 | c1cc2C(c3cc(cc(c3C(c2c(c1)O)= O)O)C(O)=O)=O | NCGC0001819 9-06 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 1 |
| 629 | C([C@@H]1[C@@H]  ([C@@H]([C@H] (N2C=CC(NC2=O)=O)O1)F)O) O | NCGC0034578 1-01 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 1 |
| 630 | CC(C)n1cnc2c(Nc3cccc(c3)NC( C=C)=O)nc(NC3CCC(CC3)N(C  )C)nc12 | NCGC0034696 4-01 | Pre\_miR\_31 | Hairpin | AGGCAAGAUGCUGGCAUA GCUGUUGAACUGGGAACC UGCUAUGCCAACAUAUUG CCAUC | 1 |