“Riboswitch” 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 | Cc1onc(- c2ccccc2Cl)c1C(= O)NCc1cc2n(n1)C C[NH2+]C2 | Neg\_lig\_68 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 2 | OCCn1nc(CC2CC  2)nc1-c1ccccc1- n1cccn1 | Neg\_lig\_117 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 3 | CN1CCC(n2[nH]c (-  c3ccccc3)c(Cc3ccc cc3)c2=O)CC1 | Neg\_lig\_123 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 4 | C[C@H]1CN(C[C  @H] (O)COc2ccc(Cl)cc 2)C[C@@H] (C)O1 | Neg\_lig\_128 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 5 | c1cncc(NCC[NH2  +] [C@H]2CCSC2)c 1 | Neg\_lig\_169 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 6 | Cc1ccc(C(=O)/ N=C2\ SC3=C(CC[C@H] (C(C)(C)C)C3)\ C2=C(/ O)NCCO)cc1 | Neg\_lig\_178 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 7 | Cc1cc(C)cc(NC(= O)c2nnn(CC(=O)  Nc3c(C)cc(C)cc3C  )c2N)c1 | Neg\_lig\_185 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 8 | Cn1ncc2c(=O) [nH]c(CN3CCNC[ C@H] (C(=O)O)C3)nc21 | Neg\_lig\_187 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 9 | COc1cc(- c2nc3ncccn3c2Nc 2cc(C)ccc2C)ccc1 O | Neg\_lig\_223 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 10 | CN(C)c1ccc(- c2nc3ncccn3c2Nc 2ccccc2)cc1 | Neg\_lig\_239 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 11 | O=C(CCc1cc2n(n 1)CCC[NH2+]C2) N1CCCN(c2cc[nH  +]cc2)CC1 | Neg\_lig\_269 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 12 | Nc1nonc1C(=O)N 1CCN(C(=O)Nc2c  ccc(C(F)  (F)F)c2)CC1 | Neg\_lig\_274 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 13 | COCC[C@]1(C(= O)  [O-])CCCN(C(=O)  c2cccc3c2NCCC3) C1 | Neg\_lig\_320 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 14 | Cn1c(=O)c2c(ncn2 CCOC(=O)C(C)  (C)Oc2ccc(Cl)cc2) n(C)c1=O | Neg\_lig\_411 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 15 | CCOc1ccc(S(=O)  (=O)c2ccc(C)cc2)c 2c1no[n+]2[O-] | Neg\_lig\_418 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 16 | COc1ccc(- c2nc3nc(C)cc(Nc4 cc(Cl)ccc4OC)n3n | Neg\_lig\_430 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | 2)cc1 |  |  |  |  |  |
| 17 | C[NH+]  (C)CCOc1ccc(- c2nc(=C3C=CNC  =C3)/c(=c3/ ccc4c(c3)CCC=4N  =O)[nH]2)cc1 | Neg\_lig\_461 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 18 | Cc1cccc(N2C(N)= C(C#N)[C@@H]  (c3ccsc3)C3=C2C C(C)(C)CC3=O)c1 | Neg\_lig\_498 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 19 | O=C([O-])c1ccc(O  CCOc2ccccc2)cc1 | Neg\_lig\_499 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 20 | CCCCC(C)(C)  [C@H](O)/C=C\  [C@@H]1[C@H] (C/C=C/ CCCC(=O)  [O-])C(=O)C[C@ H]1O | Neg\_lig\_508 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 21 | COCc1nn2c(N)c( C#N)nnc2c1- c1ccc(OC)cc1 | Neg\_lig\_511 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 22 | CSc1ccc(CCNc2n cnc3c2nc2n3CCC C2)cc1 | Neg\_lig\_514 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 23 | O=C(NCc1ccco1) N1CC[C@@H]  (c2ccc3ccccc3c2) [C@H](O)C1 | Neg\_lig\_587 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 24 | CCn1nc(CO)c2c1 CCN(C(=O)c1cnc(  -  c3ccc[nH+]c3)nc1  )C2 | Neg\_lig\_612 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 25 | COc1ccc2c(c1) [C@]13CC[N@@ H+](C)[C@H] (C2) [C@@H]1CCC1( C3)OCCO1 | Neg\_lig\_618 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 26 | C=CCOc1ccc([C @@H]2C(C#N)=  C(N)Oc3cc4c(cc3 2)OCO4)cc1OC | Neg\_lig\_629 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 27 | Cc1nc(CC(=O)N2 CC[C@H]  (Cc3ccc(CO)cc3)C 2)cs1 | Neg\_lig\_646 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 28 | CC(C) [C@H]1CC[C@@ H] (C)C[C@@H]1O C[C@@H] (O)C[NH+]1CCC CC1 | Neg\_lig\_648 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 29 | C[NH+]1CCN(CC  CNc2nc(CO)nc3cc ccc23)CC1 | Neg\_lig\_649 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 30 | Nc1c(Br)cc(Br)cc1 Br | Neg\_lig\_664 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 31 | CCOC(=O)c1cnc2  ccc(C(=O)OC)cc2 c1NCc1cccnc1 | Neg\_lig\_679 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 32 | O=C(c1ccc(C[NH  +]2CCCCC2)cc1) N1CCN[C@H]  (c2ccccc2)C1 | Neg\_lig\_685 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 33 | C[N@H+]1C[C@ H]2C[NH2+]C[C  @@]2(C(=O)NCC S(=O)  (=O)c2ccc(F)cc2) C1 | Neg\_lig\_713 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 34 | CCCc1cc(Nc2cccc (C(=O)N3CCCCC  C3)c2)n2nc(- c3cccnc3)nc2n1 | Neg\_lig\_874 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 35 | O=C(c1nn(- c2ccccc2)c(=O)cc 1[O-])N1CCOC[C @@H](CO)C1 | Neg\_lig\_806 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 36 | Nc1ccc2ncc(C(=O  )[O-])c(O)c2c1 | Neg\_lig\_877 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 37 | COc1cc(N[C@@ H]2c3ccccc3C(=O  )N2c2cccnc2)cc(O C)c1OC | Neg\_lig\_896 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 38 | O=c1[n-]cc(F)c(= O)[nH]1 | Neg\_lig\_941 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 39 | Nc1ncnc2ccccc12 | Neg\_lig\_985 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 40 | Cc1cc(NCc2ccccc 2)nc(N2CCOCC2) [nH+]1 | Neg\_lig\_1012 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 41 | COCc1cc(C)nc2sc (-  c3ccccn3)c(N)c12 | Neg\_lig\_1116 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 42 | CC(=O)c1sc(Nc2c cc(C)cc2)nc1C | Neg\_lig\_1127 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 43 | OCC1(O)CCN(Cc  2noc(- c3ccccc3)n2)CC1 | Neg\_lig\_1129 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 44 | Cc1cccc(CCNc2cc (C)nc3nc(C)nn23) c1 | Neg\_lig\_1159 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 45 | Cc1cc(C)cc(Nc2cc (C)nc3nncn23)c1 | Neg\_lig\_1197 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 46 | CCCCNc1nc(Oc2c cc(OCC)nn2)nc(N 2CCOCC2)n1 | Neg\_lig\_1219 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 47 | CCC(=O)N1CCN(  c2cc(Nc3ccc(C)cc 3)nc(C) [nH+]2)CC1 | Neg\_lig\_1221 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 48 | Cc1nccn1C[C@H] 1CCc2c(c3ccccc3n 2C)C1=O | Neg\_lig\_1223 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 49 | CCOC(=O)C1=C( C)N(CCO)C(=O)  N[C@H]1c1ccc(O CC)cc1 | Neg\_lig\_1310 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 50 | COc1ccc(Cl)cc1N c1cc(C)nc2nc(- | Neg\_lig\_1341 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | c3ccccc3)nn12 |  |  |  | CUGAAGCAACGCGCCUC |  |
| 51 | CCCNc1cc(C)nc2 nc(- c3cccc(C)c3)nn12 | Neg\_lig\_1448 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 52 | CCOC(=O)c1cnc(  NCc2ccccc2F)nc1 C | Neg\_lig\_1453 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 53 | O=C(Nc1ccc2[nH] nc(- c3ccncc3)c2c1) [C@@H]1CCN(C C(=O)N2CCN(c3c  cc(- c4ncccn4)cc3)CC2  )C1 | Neg\_lig\_1462 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 54 | COC(=O)C1=C(C) OC(N)=C(C#N)  [C@H]1c1ccsc1 | Neg\_lig\_1496 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 55 | Cc1ccsc1CNc1ccc (C(=O)N(C)CCN2 CCCCC2=O)cc1 | Neg\_lig\_1506 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 56 | CC(C)OC(=O)C1= C(N)Oc2c(oc(CO)  cc2=O) [C@H]1c1cccc(F) c1 | Neg\_lig\_1508 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 57 | COCc1ccc(C(=O) N2CCC3(CC2)  [C@@H] (OCC[NH3+])C[C @H]3O)s1 | Neg\_lig\_1175 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 58 | Cc1ccc([C@@H]2 C=C(c3ccc(F)cc3) N=C3NC(CCCO)  =[NH+]N32)cc1 | Neg\_lig\_1570 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 59 | COc1ccc(-c2cc(- c3sc4nc(C)c(Cl)c( C)c4c3N)on2)cc1 | Neg\_lig\_979 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 60 | O[C@@H] (CN1CCN(c2ccc(  Cl)cc2)CC1)c1ccc 2cc[nH]c2c1 | Neg\_lig\_1688 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 61 | O=C(N[C@@H]1  CCN(Cc2ccc3cccc (F)c3n2)C[C@H]1  O)c1ccncc1 | Neg\_lig\_1719 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 62 | COC(=O)c1cccc( Nc2ncnc3ccc(Br)c c23)c1 | Neg\_lig\_1732 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 63 | N/C(O)=C1\ N=CN([C@@H]2 O[C@H](CO)  [C@@H](O) [C@@H]2O)C1= O | Neg\_lig\_1758 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 64 | Cc1cccc(OC[C@ @H] (O)CNC(=O)c2ccc cc2C(=O)[O-])c1 | Neg\_lig\_1760 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 65 | O=C(/N=c1/ cn[nH]s1)c1cccc( C[N@H+]2[C@H] 3CC[C@@H]2C[ C@H](O)C3)c1 | Neg\_lig\_1772 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 66 | NC1(C(=O)O)CC OCC1 | Neg\_lig\_1809 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  |  |  |  |  | CUGAAGCAACGCGCCUC |  |
| 67 | CCOc1ccc(NC(=O  )c2sc3nc4c(cc3c2 N)CCCCC4)cc1 | Neg\_lig\_1821 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 68 | C=C1CC[C@@H] 2[C@](C)(CO)  [C@@H] (O)CC[C@]2(C) [C@H]1C/C=C1/ C(=O)OC[C@H]1 O | Neg\_lig\_1851 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 69 | CCOC(=O)c1snc(-  c2ccc(Cl)cc2)c1N | Neg\_lig\_1860 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 70 | O=C(O)c1c(CNCc  2ccco2)c2ccccc2n 1Cc1ccccc1 | Neg\_lig\_1901 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 71 | COc1cc(O)cc/ c(=N/ C(=O)CCl)c1 | Neg\_lig\_1939 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 72 | CCCCCCNc1cc(C  (C)C)nc2nc(- c3cccnc3)nn12 | Neg\_lig\_982 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 73 | CCN(CC)c1ccc(C[ NH2+]CCNC(=O)  c2nonc2N)cc1 | Neg\_lig\_1970 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 74 | Cn1c(=[NH2+])n( C[C@H]  (O)c2ccccc2)c2ccc cc21 | Neg\_lig\_1972 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 75 | Cn1c(=O)n(C)c2cc (C[NH2+]CCc3cc  c(F)cc3)ccc21 | Neg\_lig\_1979 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 76 | Nc1ccc2oc(Cc3ccc (Cl)cc3)nc2c1 | Neg\_lig\_1997 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 77 | COc1ccccc1N1C[ C@@H] (c2nc3ccccc3n2C[ C@@H] (O)COc2ccccc2Cl) CC1=O | Neg\_lig\_722 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 78 | COc1cc([C@@H] 2CC(=O)Nc3c2ccc 2ccccc32)ccc1OC CO | Neg\_lig\_2007 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 79 | Cc1ccc(NC(=O)C n2nnc(C(=O)NCC  c3ccccc3)c2N)cc1 | Neg\_lig\_2041 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 80 | O=S(=O)  (c1ccc(Cl)cc1)c1n c(- c2ccccc2)oc1NC[ C@H]1CCCO1 | Neg\_lig\_2044 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 81 | Cn1cc[nH+]c1CN 1CCN(C(=O) [C@H]2C[NH2+] C[C@H] (C(=O)N3CCOCC 3)C2)CC1 | Neg\_lig\_2050 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 82 | CC(C) (C)NC(=O)c1ccc(  C(=O)NC(C)  (C)C)cc1 | Neg\_lig\_2069 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 83 | Cc1ccc(NC(=O)c2 | Neg\_lig\_2098 | Glutamine\_RS | Three-way | UAAUCGUUGGCCCAGUUUAUCU | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | nnn(Cc3ccc(F)cc3 Cl)c2N)cc1C |  |  | junction | GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC |  |
| 84 | COc1cccc(CNC2= NS(=O) (=O)C(c3ccc(C(C) C)cc3)=C2C)c1 | Neg\_lig\_2105 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 85 | [NH3+] [C@H]1CC[C@H  ]  (Nc2nc(Nc3ccc(C(  =O)N4CCCCC4)c  c3)c3ncn(- c4cccc(F)c4)c3n2) CC1 | Neg\_lig\_2205 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 86 | O=C1[C@@H]2C [C@H] (O)CCN2C(=O)C  N1Cc1cccc2[nH]c cc12 | Neg\_lig\_2221 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 87 | N#C/N=C/  N1CC=C(c2ccc(Cl  )cc2)CC1 | Neg\_lig\_2225 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 88 | COc1ccc(- c2ccccc2)cc1NC(= O)NCC[N@H+]1 CCCC[C@@H]1C O | Neg\_lig\_2258 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 89 | CCCc1cc(NCC(C)  C)n2ncc(- c3ccccc3)c2[nH+] 1 | Neg\_lig\_2262 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 90 | Cc1cc(C)cc(Nc2c(  -  c3ccc(O)cc3)nc3n cccn23)c1 | Neg\_lig\_2277 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 91 | Nc1cccc(- c2csnn2)c1 | Neg\_lig\_2339 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 92 | COc1ccc(Cl)cc1N c1[nH+]c2ccccc2n 2cnnc12 | Neg\_lig\_2411 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 93 | CCOC[C@H] (O)CS(=O)  (=O)c1ccccn1 | Neg\_lig\_2474 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 94 | CC[C@H]  (O)c1nc2ccccc2n1 CCCOc1c(C)cccc1 C | Neg\_lig\_2480 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 95 | COc1ccc2c(CNCc 3cccs3)c(C(=O)O) n(Cc3ccccc3F)c2c 1 | Neg\_lig\_2495 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 96 | O=C([O-])CCn1c2  c(c3ccccc31)C[C @H](NS(=O)  (=O)c1ccc(F)cc1) CC2 | Neg\_lig\_2506 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 97 | C#CCOc1ccc([C @H]2C(C#N)=C(  N)Oc3cc4c(cc32) OCO4)cc1OCC | Neg\_lig\_2512 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 98 | Nc1nc(- c2ccccc2)c(- c2ccccc2)s1 | Neg\_lig\_2548 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 99 | Nc1nnc(CCn2cnc3 sc4c(c3c2=O)CCN | Neg\_lig\_872 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | C4)s1 |  |  |  | CUGAAGCAACGCGCCUC |  |
| 100 | COc1c(C)cnc(CN( C)C(=O)c2cn(CC[ NH3+])nn2)c1C | Neg\_lig\_2607 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 101 | Nc1nnc(SCC(=O)  N2CCc3[nH]cnc3 C2)s1 | Neg\_lig\_2618 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 102 | COCc1cc(C)nc2sc (C(=O)OC)c(N)c1 2 | Neg\_lig\_2622 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 103 | CCn1c(N)nc2cc(C (=O)NCc3cnn4ccc nc34)cnc21 | Neg\_lig\_2655 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 104 | CCc1[nH+]ccn1C CCNC[C@]1(O)C CC[N@H+]2CCC C[C@@H]21 | Neg\_lig\_2678 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 105 | CCCOc1ccc(Oc2n c(NC(C) (C)C)nc(N(C)C)n2  )nn1 | Neg\_lig\_2681 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 106 | C=CCn1cc(C[NH2  +][C@@H]  (C)CCc2ccco2)c(C  )n1 | Neg\_lig\_2704 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 107 | Cc1cccc(NC(=O) N2CCN(C(=O)c3n  onc3N)CC2)c1 | Neg\_lig\_2716 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 108 | COc1ccc2c(c1) [C@@]13CCCC[ C@H]1[C@@H] (C2)[N@@H+] (C)CC3 | Neg\_lig\_2724 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 109 | Cn1cc(C2=C(c3cn (C4CC[NH+]  (Cc5ccccn5)CC4)c 4ccccc34)C(=O)N C2=O)c2ccccc21 | Neg\_lig\_2730 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 110 | Cc1nc([C@@H]2 CCCN2S(=O)  (=O)c2ccc(F)cc2)n (CCO)n1 | Neg\_lig\_2739 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 111 | Cc1cccnc1CCn1cn c(-c2ccccc2)c1- c1ccc(CO)o1 | Neg\_lig\_2753 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 112 | CCNC(=O) [C@@H]1C[C@  @H] ([NH3+])CN1Cc1  cccn1-c1ncccn1 | Neg\_lig\_2767 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 113 | O=C(CSc1nc2cccc c2s1)N1CCN(CC O)CC1 | Neg\_lig\_2780 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 114 | CN(C)c1ccc(/ C=N\C[C@@H] (O)C/N=C/  c2ccc(N(C)C)cc2) cc1 | Neg\_lig\_2872 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 115 | Cc1cc(C)n2nc(NC c3ccc(C(C)C)cc3) nc2n1 | Neg\_lig\_2879 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 116 | O=NC1=C(c2cccc ([N+](=O)  [O-])c2)Nc2ccccc2 S1 | Neg\_lig\_2881 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 117 | COc1ccc([C@@H  ]2C(C#N)=C(N)O  c3n[nH]c(C)c32)c( OC)c1OC | Neg\_lig\_2884 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 118 | COc1ccc(-c2noc(- c3cccnc3NCc3ccc cn3)n2)cc1 | Neg\_lig\_2899 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 119 | C=CCN1CC[NH+  ]  (Cc2cccc(OC[C@ @H](O)C[N@H+] (C)C3CCCCC3)c2  )CC1 | Neg\_lig\_2904 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 120 | O=C(Cn1c(=O)oc  2ccccc21)N1CC[C @H] (Cc2cccc(CO)c2)C 1 | Neg\_lig\_404 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 121 | Cc1ncsc1CN1CC[ N@@H+](C) [C@]2(CCC(=O) N(CCO)CC2)C1 | Neg\_lig\_2964 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 122 | CC(=O)c1ccc(OC[  C@@H] (O)C[N@H+]2CC C[C@@H] (C)C2)cc1 | Neg\_lig\_3046 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 123 | Cc1ccc(CN(CCCO  )C(=O)c2c[nH]nc2 C)s1 | Neg\_lig\_3081 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 124 | C[C@]1(O)CCN( C(=O)CNC(=O)c2  cc(Cl)ccc2Cl)C[C @@H]1O | Neg\_lig\_3123 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 125 | CCN1CCN(CCCC CCO) [C@H]2CS(=O)  (=O)C[C@H]21 | Neg\_lig\_3130 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 126 | COc1ccc(- c2csc(C3=C(N)N( C4CCCCCC4)CC 3=O)n2)cc1OC | Neg\_lig\_3136 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 127 | COc1ccc([N+] (=O)  [O-])cc1NC(=O)N  (C)Cc1ccco1 | Neg\_lig\_3184 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 128 | Cc1cccc(Nc2c(- c3ccc4c(c3)OCC(  =O)N4)c(=O)c2= O)c1C | Neg\_lig\_3195 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 129 | CCSC[C@H](C)  [NH2+]CCN(C)S( C)(=O)=O | Neg\_lig\_3286 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 130 | CCCCNc1ncccc1- c1nc(- c2ccccc2C)no1 | Neg\_lig\_3315 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 131 | CCOC(=O)c1ccc2 ncc(C(=O)OCC)c(  Nc3ccc(C(=O) [O-])cc3)c2c1 | Neg\_lig\_3336 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 132 | CC[N@@H+]1CC  c2ccccc2C1 | Neg\_lig\_3363 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 133 | Cc1nc(C2CCN(C(  =O)CCc3csc(N)n3  )CC2)cc(=O)[nH]1 | Neg\_lig\_3364 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 134 | COc1cc(C[NH2+]  CCSc2nnnn2C)ccc 1OCC(=O)N1CCc  2ccccc21 | Neg\_lig\_3368 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 0 |
| 135 | COC(C) (C)C[C@H](C)  [NH2+]Cc1nncn1 C1CCCCC1 | Neg\_lig\_29 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 136 | Cc1cccc(OCc2ccc(  - c3nc(C#N)c(NCC[ NH+] (C)C)o3)o2)c1 | Neg\_lig\_111 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 137 | O=C(Cn1cccc1)N 1CCc2ncnc(NC[C @H] (O)CO)c2CC1 | Neg\_lig\_136 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 138 | CCc1c(C)nc2ncnn 2c1Nc1ccc(N2CC N(S(C) (=O)=O)CC2)cc1 | Neg\_lig\_140 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 139 | Cc1ncccc1Oc1ncn c(N2CC[N@@H+  ](C)C[C@H] (O)C2)c1C | Neg\_lig\_145 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 140 | COCCCNc1nc2c(c (=O)n(C)c(=O)n2  C)n1Cc1cccc(Cl)c 1 | Neg\_lig\_160 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 141 | OC[C@H]1CCCC  [N@@H+]1Cc1cc c(-c2ccccc2)cc1 | Neg\_lig\_207 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 142 | CNC(=O)c1nc(N2 CCCCC2)sc1N | Neg\_lig\_231 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 143 | Cc1cc2nc(O)c(=O) [nH]c2cc1N | Neg\_lig\_250 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 144 | CCOC(=O)C1=C( C)OC(N)=C(C#N)  [C@H]1c1ccsc1 | Neg\_lig\_263 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 145 | Nc1nc(- c2ccc3ccccc3c2)cs 1 | Neg\_lig\_288 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 146 | CCOC(=O)c1ccc(  Nc2c(- c3cc(Br)ccc3O)nc 3cnccn23)cc1 | Neg\_lig\_297 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 147 | c1cncc(- c2nc(NC[C@@H] 3CCCO3)c3c([nH  +]2)CNCC3)c1 | Neg\_lig\_299 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 148 | O=C(NCC(F)F)c1  ccc(S(=O)  (=O)N[C@@H]2C  [NH2+]C[C@H]2  O)cc1 | Neg\_lig\_321 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 149 | CN1CCN(C(=O)c 2cnc(N3CCCC3)n c2)CC12CC[NH2  +]CC2 | Neg\_lig\_323 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 150 | O=C(NC1CC1)c1c  ccc(-c2ccc3/c(=N\ C(=O)C4CC4)  [nH][nH]c3c2)c1 | Neg\_lig\_341 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 151 | Cc1ccn2c(C(=O)N 3CCC4(CC3)Nc3c | Neg\_lig\_364 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | cccc3NC4=O)nnc2 n1 |  |  |  |  |  |
| 152 | O=C([O-])c1cc(=  O)[nH]c(=O)[nH]1 | Neg\_lig\_366 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 153 | CO[C@H]1C[C@ @H]2CC[C@@H] (C)[C@@](O)  (O2)C(=O)C(=O) N2CCCC[C@@H  ]2C(=O)O[C@H] ([C@H]  (C)C[C@@H]2CC  [C@H](OP(C)  (C)=O)[C@H]  (OC)C2)CC(=O)  [C@H](C)/C=C(/  C)[C@@H](O)  [C@@H] (OC)C(=O)[C@H]  (C)C[C@H](C)/ C=C\C=C/C=C\1C | Neg\_lig\_368 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 154 | Cc1ccc2nc(- c3ccccn3)c(Nc3cc ccc3)n2c1 | Neg\_lig\_375 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 155 | CCC[C@@](C)  (COC(N)=O)COC  (=O)NC(C)C | Neg\_lig\_403 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 156 | Cc1ccccc1N1CCN (C(=O)c2cn(C3CC [NH2+]CC3)nn2) [C@@H](C)C1 | Neg\_lig\_423 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 157 | Clc1ccc(- c2cn3nc(CNc4ccc cc4)n4c3c2CCCC 4)cc1 | Neg\_lig\_496 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 158 | CC(C)  (C)n1cnc2cc(NCc 3cccs3)ccc21 | Neg\_lig\_502 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 159 | O=C(NCCc1cccs1  )N1CCC2(CC1)  [C@@H] (O)C[C@H]2O | Neg\_lig\_540 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 160 | CC(C)NC(=O)c1c  cc(- c2cccc(N3CC[NH 2+]CC3)c2)s1 | Neg\_lig\_542 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 161 | CC(C)  (C)COc1ccc(- n2cc(C(=O)  [O-])cn2)cc1C#N | Neg\_lig\_577 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 162 | COc1ccccc1CNc1[ nH+]cccc1- c1nc(C)no1 | Neg\_lig\_614 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 163 | O=C(CCn1cnnc1) N1CCC2(CC1)c1c  cccc1C[C@@H]2 O | Neg\_lig\_616 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 164 | Cc1ccc(Nc2c(- c3ccc(N(C)C)cc3) nc3cnccn23)cc1 | Neg\_lig\_657 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 165 | Cc1nc(C)c(CC(=O  )N2CC[C@@H]  (c3sccc3C)[C@H] (O)C2)c(=O)[nH]1 | Neg\_lig\_659 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 166 | Nc1[nH+]c2n(c1C (=O)c1ccc(Cl)cc1) CCC2 | Neg\_lig\_661 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 167 | CCc1oc2ccccc2c1- c1c(- c2ccccc2)ncn1C(C O)CO | Neg\_lig\_678 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 168 | O=C(Nc1csnn1)c1 csnn1 | Neg\_lig\_698 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 169 | CCOC(=O)c1cnc2  ccccc2c1Nc1ccc(C l)cc1 | Neg\_lig\_767 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 170 | Cc1cc(NCc2ccco2  )c2nncn2n1 | Neg\_lig\_771 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 171 | CCCCOC(=O) [C@H]1CCC[C@ H] (C(=O)OCCCC)N 1 | Neg\_lig\_776 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 172 | Cc1nc(C2=C(N)N(  Cc3ccccc3)CC2= O)sc1C | Neg\_lig\_777 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 173 | CCc1ccc([C@H]2 C(C#N)=C(N)OC3  =C2S(=O)  (=O)N(Cc2ccccc2 F)c2ccccc23)cc1 | Neg\_lig\_787 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 174 | C[C@H] ([C@@H]  (O)c1ccc(O)cc1)n 1ccnc1- c1cc2ccccc2o1 | Neg\_lig\_795 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 175 | CCOC(=O)Cc1cc(  O)nn(- c2ccccc2)c1=O | Neg\_lig\_802 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 176 | CCc1cccc(OCCN( C)c2ncnc3c2CC[N H2+]C3)c1 | Neg\_lig\_815 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 177 | O=S1(=O)N=C(Nc  2ccccc2Br)c2ccccc 21 | Neg\_lig\_837 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 178 | C/C(=N\ NC(=O)c1[nH]nc2  c1CCC2)c1ccc(N) cc1 | Neg\_lig\_849 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 179 | C=CCc1c(C)nc(N) nc1N1CCC(CCn2 cc[nH+]c2C)CC1 | Neg\_lig\_858 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 180 | CNc1ncccc1CN(C CO)Cc1ccc(SC)cc 1 | Neg\_lig\_924 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 181 | CC1(C)O[C@@H  ]2C[C@H]3[C@ @H]4CCC5=CC(  =O)C=C[C@]5(C)  [C@H]4[C@@H] (O)C[C@]3(C)  [C@@]2(C(=O)C O)O1 | Neg\_lig\_975 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 182 | Nc1n[nH]c(CCC(= O)N2CCC[C@H]  2c2nc(- c3ccccc3)no2)n1 | Neg\_lig\_1014 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 183 | CC(C) (C)c1nnc(N2CC[C  @@H] (c3ccc4ccccc4c3) [C@H](O)C2)o1 | Neg\_lig\_1059 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 184 | Nc1nc2c(ccc3cccc c32)s1 | Neg\_lig\_1075 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 185 | CCOC(=O) [C@H]1CCCN(c2 c(NCC[N@H+]3C CCC[C@@H]3CC  )c(=O)c2=O)C1 | Neg\_lig\_1076 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 186 | CC(C)(C) [NH2+]Cc1cc(Br)  ccc1OCc1cccs1 | Neg\_lig\_1101 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 187 | CN1CC2(CC[NH2  +]CC2)C[C@H]1 C(=O)NCc1cnn(C  c2ccccc2)c1 | Neg\_lig\_1184 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 188 | Cc1cccc(Cn2c(CN  )n[nH]c2=O)c1 | Neg\_lig\_1213 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 189 | CC(C)  (O)C#Cc1cccc(C(  =O)NCc2csc(N)n2  )c1 | Neg\_lig\_1218 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 190 | CC(C)CNc1nc(-  c2ccccc2)nc2ccccc 12 | Neg\_lig\_1226 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 191 | Cc1ccc(NC(=O)C  n2nnc(C(=O)Nc3c ccc(C)c3C)c2N)cc 1C | Neg\_lig\_1257 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 192 | CC(=O)O[C@H]1 C[C@@H]2CC[C @@H]3[C@H] (CC[C@]4(C)  [C@H](OC(C)=O)  [C@@H] ([N+]5(C)CCCCC  5)C[C@H]34)  [C@@]2(C)C[C@ H]1[NH+]1CCCC C1 | Neg\_lig\_1273 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 193 | COCCOC(=O)C1  =C(C) [NH+]=C2C[C@H  ]  (c3ccccc3OC)CC( O)=C2[C@H]1c1c  ccc(O)c1 | Neg\_lig\_1362 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 194 | CC[N@H+](C)  [C@H]1CN(C(=O  )CCc2scnc2C)C[C @@H]1O | Neg\_lig\_1396 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 195 | CCn1cnnc1CC[N H2+]C1CCSCC1 | Neg\_lig\_1445 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 196 | CCOC(=O)c1ccc2  nc(C)cc(Nc3ccc(C (=O)OC)cc3)c2c1 | Neg\_lig\_1502 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 197 | Cc1cc(OCCCc2c( C(=O)  [O-])n(Cc3cccnc3) c3c(- c4c(COc5ccc(N6C CN(S(C) (=O)=O)CC6)cc5)  nn(C)c4C)cccc23) cc(C)c1Cl | Neg\_lig\_1522 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 198 | Nc1ncc(C[N@@H  +]2CC[C@@]3(C CCN(C(=O)CCC4 CCCC4)C3)C2)cn | Neg\_lig\_1595 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | 1 |  |  |  |  |  |
| 199 | COc1nccc(N2CC N(Cc3ccccc3) [C@@H] (CCO)C2)c1C#N | Neg\_lig\_1613 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 200 | CCCc1c/ c(=[NH+]\  Cc2ccccn2)n2[nH] c3nc(C)cc(C)c3c2 n1 | Neg\_lig\_1630 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 201 | CCC[C@H]  (O)c1nc2ccccc2n1 Cc1ccccc1F | Neg\_lig\_1637 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 202 | Cc1cc(CN(C)c2nc cc(N3CCN[C@H] 4CS(=O) (=O)C[C@H]43)n  2)no1 | Neg\_lig\_1652 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 203 | c1sc(N2CCCC2)n c1C[NH2+] [C@H]1CCOC2(C COCC2)C1 | Neg\_lig\_1666 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 204 | O=C1Nc2ccc(Cl)c c2[C@] (C#CC2CC2)(C(F) (F)F)O1 | Neg\_lig\_1682 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 205 | COCC[N@@H+] (C)C[C@@H]1C N(C(=O)C2=Cc3c  c(Cl)ccc3OC2)C[ C@@H]1CO | Neg\_lig\_1690 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 206 | CC[C@]12CN3C[ C@](CC)(CN(C1)  [C@H]3c1ccc(N)c c1)C2=O | Neg\_lig\_1747 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 207 | O=C(NC[C@H] (O)COC1CCCCC  1)c1cnn2cc(CCO) cnc12 | Neg\_lig\_1769 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 208 | C[NH2+]CCN1C(  =O)CC[C@H]2C N(C/C=C\  c3ccc(OC)cc3)CC[ C@H]21 | Neg\_lig\_1791 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 209 | Cc1[nH]c2ccc(Cl) cc2c1CCNc1ncnc2 c1CC[NH2+]C2 | Neg\_lig\_1807 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 210 | CCC[C@H]1CN( Cc2nc(C(F) (F)F)no2)C[C@@ H]1NC(=O)CO | Neg\_lig\_1829 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 211 | CNC(=O)c1ccc(C N2CCN(c3cc(=O)  [nH]cn3)C[C@@  H](O)C2)o1 | Neg\_lig\_1838 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 212 | Cn1cccc1- c1cc(C(=O)NC[C  @@H] (CO)Cc2ccsc2) [nH]n1 | Neg\_lig\_1844 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 213 | C=CC[C@]1(CO) CCCN(S(=O)  (=O)c2ccccc2)C1 | Neg\_lig\_1866 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 214 | c1c[nH+]cc(- c2noc(CCNc3ncnc 4c3CC[NH2+]CC | Neg\_lig\_1905 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | 4)n2)c1 |  |  |  |  |  |
| 215 | CCCNc1cc(C) [nH+]c2c(C)c(-  c3ccccc3)nn12 | Neg\_lig\_1923 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 216 | COc1ccc(- c2nn3c(NC[C@H] 4CCCO4)cc(C)  [nH+]c3c2C)cc1O C | Neg\_lig\_1927 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 217 | COc1cc(/N=N/ c2cccc(S(N) (=O)=O)c2)c2cccc c2c1N | Neg\_lig\_1932 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 218 | CCOC(=O)c1c(N)  sc(C(=O)Nc2cccc( Cl)c2C)c1C | Neg\_lig\_1941 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 219 | COc1ccc(CCNc2c c(- c3ccccc3)ncn2)cc1 OC | Neg\_lig\_1957 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 220 | O=C1CCC2(CC[N H+]  (Cc3ccoc3)CC2)C N1CCCO | Neg\_lig\_121 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 221 | CC(C)=CCC1=C( OCC(=O)  [O-])C(=O)c2cccc c2C1=O | Neg\_lig\_1977 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 222 | O=C1N(CCCc2cc  ccc2)CCC[C@@] 1(O)CNCC(F)F | Neg\_lig\_2002 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 223 | Cc1ccc(NC(=O)c2 cccc(CN3C[C@H] (O)[C@@H] (OC(C)C)C3)c2)c  n1 | Neg\_lig\_2009 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 224 | O=[N+]  ([O-])c1ccc(Cl)cc1 NCCOCC(F)(F)F | Neg\_lig\_2014 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 225 | CCCCCNC(=O)c1  nn(- c2ccc(F)cc2)nc1C O | Neg\_lig\_2028 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 226 | O=C(C[C@H]1C[ NH2+]CCO1)N1C CC2(CC1)CC(=O)  N(CCCc1ccccc1)C 2 | Neg\_lig\_2036 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 227 | OCC(CO)  (CO)c1ccccn1 | Neg\_lig\_2061 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 228 | O=C(c1ccc(/C=C\ c2n[nH]c3ccccc23  )cc1)N1CC[NH2+  ]CC1 | Neg\_lig\_2062 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 229 | O=S1(=O)C[C@H  ](NCc2ccccn2) [C@@H](S(=O)  (=O)c2ccccc2)C1 | Neg\_lig\_2068 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 230 | Cc1ccc(C2(O)CC N(C(=O)Cn3nc(C)  cc3N)CC2)nc1 | Neg\_lig\_2119 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 231 | Cc1ccccc1Cn1c(C CCO)nc2ccccc21 | Neg\_lig\_2140 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 232 | CC[C@H] ([NH2+]Cc1cc(O) | Neg\_lig\_56 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | c2cc(C)ccc2n1)c1c cnn1C |  |  |  |  |  |
| 233 | O[C@@H] (CN1C2=NCCN2c  2ccccc21)c1ccccc1 | Neg\_lig\_2176 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 234 | O=c1[nH]c(=S)c2  ncn(- c3ccccc3)c2[nH]1 | Neg\_lig\_2257 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 235 | Cn1c(=O)n(C)c2cc (CNC(=O)CCc3cc 4n(n3)CC[NH2+]  C4)ccc21 | Neg\_lig\_2294 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 236 | CC(C)c1ccc([C@ @H]2C(C#N)=C(  N)Oc3cc4c(cc32) OCO4)cc1 | Neg\_lig\_2335 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 237 | CCCCn1c(N)c(C#  N)c2nc3ccccc3nc2 1 | Neg\_lig\_463 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 238 | Nc1c(C(=O)NCc2  ccccc2)nnn1CC(= O)Nc1ccccc1 | Neg\_lig\_755 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 239 | Cc1ccc(C(=O)N[C  @@H] (Nc2ccc(S(=O) (=O)  [N-]c3nc(C)cc(C)n 3)cc2)C(Cl)  (Cl)Cl)cc1 | Neg\_lig\_2381 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 240 | CC[C@H]1CC[C @@]2(CC1)NC(C  O)(CO)CO2 | Neg\_lig\_2382 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 241 | Nc1nc2ncnc- 2c(NC[C@@H]2C  Oc3ccccc3C2) [nH]1 | Neg\_lig\_2395 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 242 | CCCc1cncnc1N1C [C@@H] ([NH3+])C[C@H] 1C(=O)N(CC)CC | Neg\_lig\_1413 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 243 | O=[N+]([O-])  [C-]1[C@@H]  (c2ccccc2)C12c1c cccc1-c1ccccc12 | Neg\_lig\_2407 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 244 | CCOCCN1CCN(c  2nc(N)ncc2CC)CC 1 | Neg\_lig\_2437 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 245 | Cc1c(Cl)cccc1N[C @@H]1c2ccccc2C (=O)N1c1ccccn1 | Neg\_lig\_2453 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 246 | Cc1nnc(C[NH2+]  Cc2csc([C@]34C[ C@H]5C[C@H] (C[C@H] (C5)C3)C4)n2)o1 | Neg\_lig\_2471 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 247 | CCC[C@H]1CN(c  2nc(C)ccc2C(=O) O)C[C@@H]1N | Neg\_lig\_2499 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 248 | O=C(C[C@H]  (Nc1ccc2ccccc2c1  )c1ccccc1)c1ccccc 1 | Neg\_lig\_2504 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 249 | COc1ccc(- c2cc(NCCO)nc(N) [nH+]2)c2ccc(C)n | Neg\_lig\_2516 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | c12 |  |  |  |  |  |
| 250 | Nc1nc2c(ncn2C2C CCC2)c(=O)[nH]1 | Neg\_lig\_2517 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 251 | CCc1c(C(=O)N2C  [C@@H] (C[N@@H+]3CC CN(C)CC3)  [C@@H] (CO)C2)csc1C | Neg\_lig\_2519 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 252 | c1ccc2sc(N3CCC( [NH2+]Cc4ccsc4) CC3)nc2c1 | Neg\_lig\_2552 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 253 | N=c1[nH]c2c(s1) [C@@H] (c1cc(F)ccc1F)CC (=O)N2 | Neg\_lig\_2621 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 254 | Clc1ccc([C@H] (Cn2ccnc2)OCc2c cc(Sc3ccccc3)cc2) c(Cl)c1 | Neg\_lig\_2741 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 255 | Cc1ccc(N2C(=O)c 3cccnc3[C@H]2N c2ccc(C)c(F)c2)cc 1 | Neg\_lig\_2765 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 256 | COc1ccc(C[NH2+  ]CC[C@@]2(CCC  (C)C)CCOC(C) (C)C2)cc1 | Neg\_lig\_2772 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 257 | CCc1ccc(- n2nc(CO)c(C(=O) N[C@@H] (C)CC)n2)cc1 | Neg\_lig\_2774 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 258 | Nc1ccccc1S(=O) (=O)NCC(=O)[O-] | Neg\_lig\_2839 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 259 | N#C[C-]1C(=O)N  =c2s/c(=C(/ O)c3ccc(Br)cc3)c( N)c2C12CCCCC2 | Neg\_lig\_2859 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 260 | COc1ccc(C)cc1- n1nnc(-c2nc(- c3ccccc3C)no2)c1 N | Neg\_lig\_2937 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 261 | Cc1cc(N2CCC([N H2+] [C@@H]3C[C@  @H] (CO)N(C)C3)CC2  )nc(-c2ccccc2)n1 | Neg\_lig\_2949 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 262 | N#Cc1cccnc1N1C CC(n2ccnc2- c2ccc(CO)o2)CC1 | Neg\_lig\_2965 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 263 | Cc1ccccc1CN(Cc1 cc(C#CCO)cs1)C C(C)C | Neg\_lig\_3071 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 264 | COC(=O)c1c(N)n(  -c2cccc(C(F) (F)F)c2)c2nc3cccc c3nc12 | Neg\_lig\_3092 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 265 | Cc1ccccc1CNC(= O)c1nn(- c2ccccc2)nc1CO | Neg\_lig\_3161 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 266 | C[NH2+]CCN1C(  =O)CC[C@H]2C N(C(=O)c3cnc(N( C)C)nc3C)CC[C@ | Neg\_lig\_1717 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | H]21 |  |  |  |  |  |
| 267 | CO[C@H]1C[C@  @H] (O)C12CC[NH+]  (Cc1cc3c(cc1C)O CCO3)CC2 | Neg\_lig\_3253 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 268 | COc1ccc2c(c1)CC N(C(=O)c1ccc(N) nc1)CC2 | Neg\_lig\_847 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 269 | O=C1c2ccccc2C(= O)N1C[C@H]  (O)CN1c2ccccc2S c2ccccc21 | Neg\_lig\_3280 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 270 | COc1cc2c(N3CC N(C(=O)Nc4ccc(O C(C)C)cc4)CC3)n  c[nH+]c2cc1OCC C[NH+]1CCCCC1 | Neg\_lig\_3298 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 271 | Cc1ccc(S(=O) (=O)NC[C@H]  (O)Cn2c3ccccc3c3 ccccc32)cc1 | Neg\_lig\_3316 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 272 | CN1CC(=O)N2CC N(Cc3ccc(C#CCO  )s3)C[C@H]2C1= O | Neg\_lig\_3318 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 273 | O[C@H]1CN(c2n  c3ccccc3s2)C[C@ @H]1N1CCOCC1 | Neg\_lig\_3346 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 274 | O=C(Nc1cccc(Cl) c1)NC(CO) (CO)CO | Neg\_lig\_3372 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 275 | CCCC1(C[NH2+] C2CCN(C(=O)c3c nccn3)CC2)CCC1 | Neg\_lig\_2103 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 276 | CCOc1ccccc1CNc 1ccc2c(c1)ncn2C( C)(C)C | Neg\_lig\_3410 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 0 |
| 277 | N#Cc1c(-  c2cccn2S(=O) (=O)c2ccccc2)cc(- c2cc[nH]c2)nc1N | Neg\_lig\_31 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 278 | C[C@H] (O)CCC(=O)NCC  c1nc2ccccc2n1Cc1 ccc(Br)cc1 | Neg\_lig\_52 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 279 | COC[C@@H] (NC(C)=O)C(=O)  NCc1ccccc1 | Neg\_lig\_59 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 280 | COc1ccc(Cn2c(C N)nc3cccnc32)cc1 | Neg\_lig\_69 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 281 | Cc1nc(N2CCCCC 2)ncc1C(=O)N1C[  C@H](c2ccccc2) [C@@H] ([NH3+])C1 | Neg\_lig\_139 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 282 | COc1ccc(C(=O)n2 ncc(C(=O)Nc3ccc cc3)c2N)cc1 | Neg\_lig\_194 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 283 | [NH3+]CCNC(=O  )c1nc(Cn2c(C(F) (F)F)nc3ccccc32)n o1 | Neg\_lig\_205 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 284 | Nc1ncccc1CN1CC | Neg\_lig\_234 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | [C@H]  (Cc2cccc(C(=O)O) c2)C1 |  |  |  | CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG |  |
| 285 | N[C@@H]  (Cc1cnc[nH]1)C(= O)N1CCCN(Cc2c  cc(F)cc2)CC1 | Neg\_lig\_295 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 286 | O=C1C[C@H]  (Nc2ccc(F)cc2)C(  =O)N1c1ccc(Br)cc 1 | Neg\_lig\_361 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 287 | COc1ccc(Nc2cc(C  )[nH+]c3c(-  c4ccc(F)cc4)c(C)n n23)cc1 | Neg\_lig\_405 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 288 | Fc1ccc(Nc2nc(- c3cccs3)cs2)cc1 | Neg\_lig\_416 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 289 | Cc1ccc(Nc2cc(N3 CCN(S(C)  (=O)=O)CC3)  [nH+]c(C)n2)cc1 | Neg\_lig\_457 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 290 | Cc1cc(C)c(NC(=O  )Cn2nnc(C(=O)Nc 3cccc(C)c3C)c2N) c(C)c1 | Neg\_lig\_473 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 291 | O[C@H] (CN1CCN(Cc2ccc  cc2)CC1)Cn1c2c(c 3ccccc31)CCCC2 | Neg\_lig\_479 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 292 | Cc1ccc(- c2c(NCc3ccc4c(c3  )OCO4)c(=O)c2=  O)cc1 | Neg\_lig\_485 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 293 | O=C(c1ccc2occc2 c1)N1CCc2ncnc(N CCO)c2CC1 | Neg\_lig\_494 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 294 | COC(=O)c1cc(Nc  2cc(C)c3c(O)cccc 3n2)cc(C(=O)OC)  c1 | Neg\_lig\_504 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 295 | N#Cc1c(-c2cccn2- c2ccncc2)cc(- c2ccc[nH]2)nc1N | Neg\_lig\_561 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 296 | COc1cc(C[NH2+]  Cc2cccnc2)cc(Br)c 1OCc1ccccc1Cl | Neg\_lig\_590 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 297 | Cc1ccc([C@H] (NC(=O)CCc2cc3 n(n2)CCC[NH2+]  C3)c2cccnc2)cc1C | Neg\_lig\_639 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 298 | O=C(c1ccccc1- c1ncc[nH]1)N1CC [C@H]  (Cc2cccc(CO)c2)C 1 | Neg\_lig\_662 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 299 | CCCCN(Cc1cccnc 1)C(=O)c1ccccc1[ C@H]1CC[NH2+] C1 | Neg\_lig\_666 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 300 | Cc1nc(N)sc1- c1csc(Nc2ncccn2) n1 | Neg\_lig\_689 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 301 | CC(=O)c1sc(Nc2c cc(Cl)c(Cl)c2)nc1 | Neg\_lig\_693 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | C |  |  |  | AAAAAGGG |  |
| 302 | Cc1ccc(CN2c3ccc cc3C3=C([C@@H  ]  (c4cccc(Cl)c4)C(C #N)=C(N)O3)S2(= O)=O)cc1 | Neg\_lig\_707 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 303 | CCn1cnnc1CCn1c cnc1- c1cc2n(n1)CC[NH 2+]C2 | Neg\_lig\_772 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 304 | Cc1ccccc1N[C@ @H]1c2ccccc2C(= O)N1Cc1ccc2c(c1  )OCO2 | Neg\_lig\_778 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 305 | COc1cc(C[NH2+]  CCO)ccc1OCc1cc c2c(c1)n(C)c(=O)n 2C | Neg\_lig\_796 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 306 | C=CCNc1ccccc1C (=O)NCCC(=O)N  c1ccccc1CC | Neg\_lig\_820 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 307 | O=C([O-])c1cccc( Nc2nc3ccc(Cl)cc3 n3cnnc23)c1 | Neg\_lig\_824 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 308 | Cc1ccc(NC(=O)c2 nnn(Cc3cccc(Br)c 3)c2N)cc1C | Neg\_lig\_854 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 309 | CC(=O)N1CCN(c  2ccc(Nc3cc(C)nc4 nc(- c5ccccc5)nn34)cc2 Cl)CC1 | Neg\_lig\_865 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 310 | CCCCOCCCN1C  C(=O)C(c2nc3ccc cc3s2)=C1N | Neg\_lig\_878 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 311 | Cn1c(=O)n(C)c2cc (CNc3ccc(N4CCO  CC4)cc3)ccc21 | Neg\_lig\_889 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 312 | O=C1O[C@H]  (Nc2ccc(Cl)c(C(F) (F)F)c2)c2ccccc21 | Neg\_lig\_915 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 313 | Cc1cccc(N[C@@ H](c2nnc(- c3ccccc3)o2)c2ccc cc2F)c1 | Neg\_lig\_927 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 314 | CC[NH+]  (CC)CCNc1ncnc2 c1sc1nc3c(cc12)C OC(C)(C)C3 | Neg\_lig\_950 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 315 | CN1CCC[N@@H  +] (C[C@@H]2CN( C(=O)C3CCOCC3  )C[C@@H]2CO) CC1 | Neg\_lig\_672 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 316 | Cc1ccc(Nc2nc3no nc3nc2N2CCCCC 2)cc1C | Neg\_lig\_976 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 317 | O=c1cc(N2CCNC  C2)cnn1Cc1noc(- c2ccco2)n1 | Neg\_lig\_1078 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 318 | COc1cccc(CN2CC C[C@@](O)  (CNCCS(C) | Neg\_lig\_1118 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | (=O)=O)C2=O)c1 |  |  |  |  |  |
| 319 | Cn1c(N2CCOCC2  )nc2cc(C(=O)N3C COC[C@@H] (O)C3)ccc21 | Neg\_lig\_1169 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 320 | CCc1ccc2nc(C)cc( C(=O)NC[C@H]  (O)c3ccco3)c2c1 | Neg\_lig\_30 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 321 | CCc1ccc(NC(=O)c 2nnn(CC(=O)Nc3c cccc3CC)c2N)cc1 | Neg\_lig\_1204 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 322 | COc1ccc([C@H] (Cc2ccccc2)N[C@ @H]2C[NH+]3CC C2CC3)cc1 | Neg\_lig\_1270 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 323 | O=C(N[C@@H]1 CC[N@H+]  (Cc2cc3ccccc3o2) C[C@H]1O)c1ccn cc1 | Neg\_lig\_1309 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 324 | CC(C)CNC(=O)/  C=C\C(=O)[O-] | Neg\_lig\_1338 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 325 | O=C1c2n[nH]c(-  c3ccccc3O)c2[C@ @H] (c2ccc(F)cc2)N1C CCO | Neg\_lig\_1356 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 326 | CCc1ccccc1NC(= O)c1nnn(CC(=O)  Nc2ccc(C)cc2C)c1 N | Neg\_lig\_1371 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 327 | CC1(C)S[C@H]2[  C@H](NC(=O)  [C@@H] (N)c3ccc(O)cc3)C  (=O)N2[C@@H]1  C(=O)[O-] | Neg\_lig\_1397 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 328 | O=C(c1ccc(OCc2c cccc2F)cc1)N1CC OC[C@@H] (CO)C1 | Neg\_lig\_1401 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 329 | C=CCNc1nc2c(c([ O-])nc(=O)n2C)n1 C[C@H](O)CO | Neg\_lig\_453 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 330 | CCN(C/C=C\  c1ccccc1)C(=O) [C@H]1CC[NH2+  ]C1 | Neg\_lig\_1412 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 331 | C#CCN1C(=O) [C@@]2(C(C#N)  =C(N)OC3=C2C(  =O)CC(C)  (C)C3)c2ccccc21 | Neg\_lig\_1454 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 332 | COCCc1nc(- c2cnc(C3CC3)nc2  )n(CCO)n1 | Neg\_lig\_1479 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 333 | Cc1nn(C)c(C)c1N C(=O)NC[C@H]  (O)c1ccco1 | Neg\_lig\_1488 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 334 | CC[C@H]  (O)c1nc2ccccc2n1 CCCOc1ccccc1O C | Neg\_lig\_1499 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 335 | CCOc1ccc(NC(=O | Neg\_lig\_1527 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | )c2cnn(C(=O)c3cc c(OC)cc3)c2N)cc1 |  |  |  | CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG |  |
| 336 | Cc1cc(C)c2c(N)c( S(=O)  (=O)Cc3ccc(Cl)cc 3)sc2n1 | Neg\_lig\_1540 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 337 | CCOC(=O)c1cc(C N[C@H]2CCS(=O  )(=O)C2)on1 | Neg\_lig\_1565 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 338 | Cc1nc(C)c(CC(=O  )N2CC[C@@H]  (c3sccc3C)[C@H] (O)C2)c(=O)[nH]1 | Neg\_lig\_659 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 339 | Cc1ccc(NC(=O)c2 nnn(Cc3ccc(Br)cc 3F)c2N)c(Cl)c1 | Neg\_lig\_1641 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 340 | Cc1cc(NC(=O)Nc  2cccc3ccccc23)no 1 | Neg\_lig\_1654 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 341 | Cc1nn(CCO)cc1C[ N@H+]1CCC[C@ H](c2nnc(C[NH+]  (C)C)n2C)C1 | Neg\_lig\_1705 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 342 | O=C(CN1CCCCC C1)OCCNC1=NS(  =O)(=O)c2ccccc21 | Neg\_lig\_1708 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 343 | CCCCCCCn1c(C  O)nc2ccccc21 | Neg\_lig\_1533 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 344 | Cc1ccc(C)c(OC[C @H] (O)Cn2c([C@@H] 3CC(=O)N(Cc4cc  ccc4)C3)nc3ccccc 32)c1 | Neg\_lig\_1788 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 345 | Cc1ccccc1NCC(= O)c1ccc(Br)cc1 | Neg\_lig\_1803 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 346 | N#CC1=C(N)OC2  =C(C(=O)CCC2)  [C@@H]1c1cccc( I)c1 | Neg\_lig\_1847 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 347 | O=C(O)c1cn(-  c2ccc(F)cc2)c2cc( N3CCNCC3)c(F)c  c2c1=O | Neg\_lig\_1889 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 348 | Cc1nc(/[NH+]=C(\ N)N(C)C)nc(O)c1 C | Neg\_lig\_1918 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 349 | CC1=C(C(=O)OC( C)C) [C@]2(C(=O)N(C  )c3ccccc32)C(C#N  )=C(N)O1 | Neg\_lig\_1942 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 350 | CC(C)[NH2+] [C@@H]1CC[C@ @H]1NC(=O)c1cc  cc(-c2ccccc2)c1 | Neg\_lig\_1976 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 351 | CCOc1ccc(Cl)cc1 C[NH2+]CCSc1nn  nn1C | Neg\_lig\_53 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 352 | C[C@@]1(C2CC[ NH2+]CC2)NC(= O)NC1=O | Neg\_lig\_2008 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 353 | CC[C@H] | Neg\_lig\_2037 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | (O)CNS(=O)  (=O)c1ccc(C(=O)  NCc2ncc[nH]2)cc 1 |  |  |  | CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG |  |
| 354 | Cc1cc2c(cc1CC(= O)c1sccc1S(=O) (=O)/N=c1/  o[n-]c(C)c1Cl)OC O2 | Neg\_lig\_2055 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 355 | Cc1cc2c(c(=O)o1) [C@@]1(C(=O)N  c3ccc(C)c(Br)c31) C(C#N)=C(N)O2 | Neg\_lig\_667 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 356 | CCOc1cc(C[NH2+  ]CCc2ccccc2F)ccc 1OC | Neg\_lig\_2113 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 357 | Cn1cc(- c2ccccc2OC[C@ @H] (O)CN2CCOCC2)  cn1 | Neg\_lig\_2155 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 358 | Cc1nn(CCO)cc1C[ N@H+]1C[C@@  H](c2ccc(F)cc2)  [C@@H]2[C@H] 1C1CCN2CC1 | Neg\_lig\_2160 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 359 | COC(=O)CNc1cc(  C)nc2nc(- c3cccc(C)c3)nn12 | Neg\_lig\_2162 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 360 | C=C(C)CC[C@H] (C) [NH2+]Cc1n[nH]c 2c1CCCCC2 | Neg\_lig\_2171 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 361 | CNc1ccccc1C(=O) NC[C@H]1CC[N @H+]  (Cc2cccc(O)c2)C1 | Neg\_lig\_2194 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 362 | Cc1c(NCc2ccccn2  )cccc1C(=O)N[C  @@H] (C)CCn1cccn1 | Neg\_lig\_2195 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 363 | COC(=O)c1c(C)sc 2c1OC(N)=C(C#N  )  [C@@H]2c1ccccc 1 | Neg\_lig\_2203 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 364 | CC(C)Nc1ccc(- c2cc(N)nc3[nH]cc c23)nn1 | Neg\_lig\_2263 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 365 | CCOCCn1nc(C)cc 1C(=O)N1C[C@H  ](c2ccc(C)o2) [C@@H] ([NH3+])C1 | Neg\_lig\_1975 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 366 | CN(CCC#N)c1ccc (/C=C(\  C#N)c2cccc(C(F) (F)F)c2)cc1 | Neg\_lig\_739 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 367 | Cc1nn(CCO)cc1C[ N@H+]1CCCC(c2  ccccc2) (c2ccccc2)C1 | Neg\_lig\_2350 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 368 | C[C@](O)  (c1ccccc1) [C@@H] (c1ccccc1) [C@@H]1CCCC[ | Neg\_lig\_2355 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | NH2+]1 |  |  |  |  |  |
| 369 | CN(Cc1cnc(N)nc1  )C(=O)Nc1ccccc1 C[N@@H+] (C)C1CCCCC1 | Neg\_lig\_1902 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 370 | OCCCNc1nc2sc3c (c2c2ncnn12)CCC C3 | Neg\_lig\_2359 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 371 | OC[C@@H]  (O)Cn1c(COc2ccc cc2)nc2ccccc21 | Neg\_lig\_2370 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 372 | Cn1c(CN2CC[C@  @H] (NC(=O)c3cccnc3) [C@H]  (O)C2)nc2ccccc21 | Neg\_lig\_2387 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 373 | CC(=O)c1cc2c(cc 1N)OCCO2 | Neg\_lig\_2393 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 374 | Cc1ccc([C@@H]2 C(C#N)=C(N)OC3  =C2C(=O)CC(C)  (C)C3)cc1 | Neg\_lig\_2394 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 375 | Clc1ccc(- c2ccc(CNC[C@@ H]3CCCO3)o2)cc 1 | Neg\_lig\_2406 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 376 | Cc1cc(NC2CCCC C2)n2nc(C(F) (F)F)nc2n1 | Neg\_lig\_2435 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 377 | O[C@H]1CN[C@  H](c2ncnn2- c2cccc3c2CCC3)C 1 | Neg\_lig\_2449 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 378 | Cc1cc(Nc2ccc(Cl) cc2)c2ccccc2[nH+  ]1 | Neg\_lig\_2507 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 379 | COC(=O)c1c(-  c2ccc(Br)cc2)csc1 N | Neg\_lig\_2549 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 380 | CCc1cc(C[NH2+]  Cc2cc(O)c3cc(C)c cc3n2)on1 | Neg\_lig\_2578 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 381 | Cc1ccc(CNc2ccc3 c(c2) [nH+]c(C)n3C)cc1 | Neg\_lig\_2562 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 382 | Cc1ncc(CO)c(CN2 C[C@H] ([NH3+])C[C@H]  2C(=O)NC(C)C)c  1O | Neg\_lig\_2670 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 383 | Nc1nnc(- c2cccc(Cl)c2Cl)c( N)n1 | Neg\_lig\_2671 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 384 | Cc1c(C[N@H+] (C)C2CCC3(CC[N H2+]CC3)CC2)cn  n1C | Neg\_lig\_2674 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 385 | CCc1nc(N)sc1C(= O)N1CCN(c2cccc c2OC)C(C)(C)C1 | Neg\_lig\_2727 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 386 | O=C(Nc1ncc(- c2cc(C(F)F)nn2- c2c(Cl)cccc2Cl)s1  )C1CC1 | Neg\_lig\_2734 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 387 | COc1cccc(- c2nc3c([nH]2)CC N(C(=O)[C@@H]  (O)Cc2ccccc2)C3) c1 | Neg\_lig\_2764 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 388 | O[C@@H] (CN1CC=C(/C=C\  c2ccc(Br)cc2)CC1  )c1ccccc1 | Neg\_lig\_2768 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 389 | COCCC[C@H]1C CCCN1C(=O)c1cc  c(N)nc1 | Neg\_lig\_2779 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 390 | Cc1nc2nc(C[NH3  +])nn2c(C)c1CCC  (=O)Nc1ccccc1 | Neg\_lig\_2798 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 391 | CCNc1nc(N(C)C)  nc(- n2cnc(SC)n2)n1 | Neg\_lig\_2860 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 392 | CCOC(=O) [C@]12CCC[NH2  +] [C@@H]1CCN(C  (=O)c1ccn3nnnc3c 1)C2 | Neg\_lig\_2935 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 393 | CN1CC[NH+] (CCCNc2c([NH3+  ])c(=O)oc3ccccc23  )CC1 | Neg\_lig\_2942 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 394 | C[C@H]1CN(c2cc ccc2Cl)C(=O)CN1  C(=O)c1ccnc(N)c1 | Neg\_lig\_2745 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 395 | Cc1cnn(Cc2ccc(Cl  )cc2)c1NC(=O)N( CCO)CCO | Neg\_lig\_682 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 396 | O=C1c2ccccc2- [n+]2ccc3c([nH]c4 ccccc43)c21 | Neg\_lig\_3002 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 397 | O=C1c2n[nH]c(-  c3ccccc3O)c2[C@ @H] (c2ccc(Cl)cc2)N1 CCO | Neg\_lig\_3013 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 398 | COc1ccc2c(Oc3cc c(NC(=O)c4c(C)n(  CC(C)(C)O)n(-  c5ccccc5)c4=O)nc 3)ccnc2c1 | Neg\_lig\_3028 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 399 | COc1cccc([C@@ H]2c3c(n[nH]c3-  c3c(C)cc(C)cc3O) C(=O)N2CCCO)c 1 | Neg\_lig\_3076 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 400 | Cc1ccc(CN(C)CC(  =O)N[C@H]2CC[  C@H]2[NH2+]C( C)C)cc1 | Neg\_lig\_3111 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 401 | Nc1cncc(-n2ccc(- c3cc(Cl)ccc3O)n2) c1 | Neg\_lig\_3151 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 402 | C[NH+] (C)CCCNc1c([NH  3+])c(=O)oc2cccc c12 | Neg\_lig\_3157 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 403 | N#CC1=C(N)N2C (=C(C#N)  [C@@H]1c1ccc(C | Neg\_lig\_947 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | l)cc1)Sc1ccccc12 |  |  |  |  |  |
| 404 | Nc1cc(- c2nc3ccccc3o2)cc c1Br | Neg\_lig\_3187 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 405 | Cc1c2oc3c(C)ccc( C(=O)N[C@H]4C  (=O)N[C@@H] (C(C)C)C(=O)N5 CCC[C@H]5C(= O)N(C)CC(=O)N( C)[C@@H] (C(C)C)C(=O)O[C  @H]4C)c3nc- 2c(C(=O)N[C@H]  2C(=O)N[C@@H] (C(C)C)C(=O)N3 CCC[C@@H]3C(  =O)N(C)CC(=O)N  (C)[C@H] (C(C)C)C(=O)O[C @@H]2C)c(N)c1= O | Neg\_lig\_3226 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 406 | CCc1ccccc1N[C@ @H]1c2ccccc2C(= O)N1c1ccc(Cl)cn1 | Neg\_lig\_2003 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 407 | O=C(NCC(c1cccc c1)c1ccccc1)c1nn(  -  c2ccc(Cl)cc2)nc1C O | Neg\_lig\_3376 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 408 | CCn1c(C2CCN(C(  =O)CC3=CC[NH2  +]CC3)CC2)n[nH] c1=O | Neg\_lig\_3405 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 409 | CC(C)n1cc(C[NH 2+]Cc2cn(CCC(N)  =O)c3ccccc23)cn1 | Neg\_lig\_3420 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 0 |
| 410 | COC(=O)c1[nH]c  2ccccc2c1NCc1cc cnc1 | Neg\_lig\_11 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 411 | C=CCNc1oc(-  c2ccc(F)cc2)nc1S(  =O)  (=O)c1ccc(Cl)cc1 | Neg\_lig\_33 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 412 | COc1ccc(C(=O)O  c2cccc(Nc3ncnc4c cccc34)c2)cc1 | Neg\_lig\_67 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 413 | CC(C)C[C@@H]  (CO)n1cc(- c2nn(C)c3cccc(Cl) c23)nn1 | Neg\_lig\_100 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 414 | CC(C)N[C@@H] (C(=O)O)c1c[nH]c  2ccc(Br)cc12 | Neg\_lig\_147 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 415 | CCCOc1ccc(Oc2n c(NCC(C)C)nc(N3 CCOCC3)n2)nn1 | Neg\_lig\_165 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 416 | CN1c2cc(O)c(/ N=N/ C(N)=O)cc2C[C@ @H]1S(=O)(=O) [O-] | Neg\_lig\_175 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 417 | CC(C)NC(=O)c1c | Neg\_lig\_219 | TPP | Three-way | CAGUACUCGGGGUGCCCUUCUG | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | cccc1- c1cc(Cl)c2c(c1)C[ C@H](CN)O2 |  |  | junction | CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG |  |
| 418 | Cc1ccc(NC(=O)C NC(=O)c2cn(C[C @H]3CCC[NH2+]  C3)nn2)c(F)c1 | Neg\_lig\_307 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 419 | C[C@]12CN3CN( C1)C[C@@](C) (C3) [C@@H]2[NH3+] | Neg\_lig\_346 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 420 | C[C@@H]  (c1nccs1)N(C)Cc1 nnc(CC2CC[NH2  +]CC2)n1C | Neg\_lig\_373 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 421 | CCNc1ncc(C(=O) N2C[C@@H] (C[NH+]3CCCCC 3)[C@@H] (CO)C2)cn1 | Neg\_lig\_388 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 422 | O=C1OCCN1CCn  1ccnc1- c1cc2n(n1)CC[NH 2+]C2 | Neg\_lig\_390 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 423 | COc1ccc(-c2noc(- c3nnn(- c4ccc(C)cc4C)c3N  )n2)cc1 | Neg\_lig\_394 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 424 | OC[C@@H]1CC  CN1Cc1ccc(- c2nc(O)cc(- c3ccccc3Cl)n2)cc1 | Neg\_lig\_422 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 425 | COc1ccc(C2=C(C)  C([N-]c3cc(F)ccc3 F)=NS2(=O)=O)cc 1 | Neg\_lig\_435 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 426 | O=S(=O) (N[C@@H]1CCC  C[C@H]1Nc1ccc( Br)cc1)c1ccc(Cl)c c1 | Neg\_lig\_439 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 427 | CN(CC(=O)N1CC [C@H]  (Cc2cccc(CO)c2)C 1)C1CC[NH+] (C)CC1 | Neg\_lig\_454 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 428 | Cn1c(C(=O)c2ccn cc2)cc2ccccc21 | Neg\_lig\_476 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 429 | CN(C)c1ccc2[nH+  ]c3ccc(=[N+] (C)C)cc-3sc2c1 | Neg\_lig\_529 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 430 | N#CC1=C(Nc2ccc  cc2Cl)S[C@@H] (c2ccccc2O)NC1= O | Neg\_lig\_608 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 431 | CC(=O)N[C@H]1 CCN(c2cc(N3CC OCC3)nc(N)n2)C1 | Neg\_lig\_624 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 432 | CC(C)OC(=O)Nc1  ccc2c(c1)N(C(=O) CCN1CCN(CCO)  CC1)c1ccccc1CC2 | Neg\_lig\_626 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 433 | CCCCn1cnc2cc(N Cc3cccc(OC)c3O C)ccc21 | Neg\_lig\_628 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 434 | CC(C)c1ccc(CN2 CCC[C@@](O)  (CNCc3ccc[nH]c3  =O)C2=O)cc1 | Neg\_lig\_643 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 435 | CN1CCC[N@@H  +] (C[C@@H]2CN( C(=O)C3CCOCC3  )C[C@@H]2CO) CC1 | Neg\_lig\_672 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 436 | O=S1(=O)C[C@ @H]2[C@H] (C1)N(CCCCOc1c  cccc1)CCN2CCO | Neg\_lig\_688 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 437 | Cc1[nH]c2c(F)ccc c2c1CC(=O)NCC[ N@H+]1CCCC[C @@H]1CO | Neg\_lig\_724 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 438 | C[C@@H]1C(C# N)=C(N)OC2=C1 C(=O)C[C@H]  (c1ccccc1)C2 | Neg\_lig\_751 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 439 | CCOC(=O)c1c(N) n(C2CCCCC2)c2n  c3ccccc3nc12 | Neg\_lig\_760 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 440 | Cn1c(=O)c2c(nc3n 2CC(c2ccc(F)cc2)  =NN3CCO)n(C)c1  =O | Neg\_lig\_811 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 441 | Cc1c[nH+]c(N)nc 1NCc1cc(C(C) (C)C)[nH]n1 | Neg\_lig\_848 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 442 | [NH3+] [C@H]1CC[C@@ H] (n2cc(C(=O)NCc3  nc(- c4ccccn4)no3)nn2) CC1 | Neg\_lig\_863 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 443 | O=S(=O)  (c1ccc2ccccc2c1) N(C[C@H]  (O)COCc1ccco1)c 1ccccc1 | Neg\_lig\_196 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 444 | Cc1[nH+]c2n(c1C (=O)N(C)C)CCN(  C[C@]1(O)CCC[ NH2+]C1)C2 | Neg\_lig\_899 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 445 | CCCCCCN1CC(=  O)C(c2nc3ccccc3s 2)=C1N | Neg\_lig\_919 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 446 | O=C(NCc1ccoc1) [C@@]12C[NH2+  ]C[C@@H]1C[N  @@H+] (Cc1ccccc1)C2 | Neg\_lig\_953 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 447 | Cc1ccc(Nc2nc3ccc cc3c3nnc(C)n23)c c1F | Neg\_lig\_1048 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 448 | O=C(NCc1cc(-  c2ccco2)on1)c1cn( CCN2CC[NH2+]C  C2)nn1 | Neg\_lig\_1058 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 449 | C[C@@H]1C[C@  @H] (Nc2ccccc2)c2ccc cc2N1C(=O)Cc1cc c(F)cc1 | Neg\_lig\_1109 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 450 | OCCN1C[C@H] (O)[C@@H](O) [C@H](O) [C@H]1CO | Neg\_lig\_1128 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 451 | CCCCOC(=O)c1c  cc(Nc2nc3ccccc3n 3cnnc23)cc1 | Neg\_lig\_1214 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 452 | CC[C@]1(CO)CC C[N@@H+] (CCC(=O)N2CCc  3ccccc3C2)C1 | Neg\_lig\_1235 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 453 | CC[C@@H](CO)  [NH2+]C[C@@H] (O)Cn1c(C)c(C)c2  ccccc21 | Neg\_lig\_1242 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 454 | CC[C@]1(CO)CC C[N@@H+] (CCC(=O)NCc2cc  cc(Cl)c2)C1 | Neg\_lig\_1259 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 455 | COc1ccc(C(=O)c2 sc3nc(- c4ccc(OC)cc4)ccc 3c2N)cc1 | Neg\_lig\_1311 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 456 | CC(C)C[C@]1(C O)CCCN(Cc2[nH] cc[nH+]2)C1 | Neg\_lig\_1352 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 457 | c1ncn(- c2ccc([C@H]3[N H2+]CCc4nc[nH]c 43)cc2)n1 | Neg\_lig\_1394 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 458 | OCC[NH2+]CCC[  NH2+]Cc1ccccc1 | Neg\_lig\_1402 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 459 | c1csc(Cc2nc(Cn3c c[nH+]c3- c3cc4n(n3)CC[NH 2+]C4)no2)c1 | Neg\_lig\_1444 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 460 | COc1ccc(S(=O) (=O)N2CCN(c3cc(  C)nc(Nc4ccc(C)cc 4)n3)CC2)cc1C | Neg\_lig\_1512 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 461 | OCc1ccc(CN(Cc2 ccncc2)Cc2ccc(F)c c2)o1 | Neg\_lig\_1517 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 462 | CC(=O)c1cccc(NC (=O)c2sc3nc4c(cc 3c2N)CCCCC4)c1 | Neg\_lig\_1531 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 463 | CC(C) (CO)NC(=O)  [C@@H]1CC(c2c cccc2O)=NO1 | Neg\_lig\_1534 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 464 | COc1ccc2[nH]c([S | Neg\_lig\_1541 | TPP | Three-way | CAGUACUCGGGGUGCCCUUCUG | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | @] (=O)Cc3ncc(C)c( OC)c3C)nc2c1 |  |  | junction | CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG |  |
| 465 | O=C(Cc1ccc(O)cc 1)N1CCN(Cc2ccc cc2CO)CC1 | Neg\_lig\_1646 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 466 | Cc1ccn(C)c(=[NH 2+])c1 | Neg\_lig\_1655 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 467 | CCOc1ccccc1Nc1 cc(C) [nH+]c2ccc(Cl)cc1 2 | Neg\_lig\_1659 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 468 | COCCCNc1oc(-  c2ccccc2F)nc1S(= O)(=O)c1ccccc1 | Neg\_lig\_1704 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 469 | O=S(=O)  (c1ccccc1)c1nc(- c2ccco2)oc1NCC CN1CCOCC1 | Neg\_lig\_1720 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 470 | CCNC(=O) [C@@H]1C[C@H  ] ([NH3+])CN1C(=  O)c1cc(C2CC2)nc 2ccccc12 | Neg\_lig\_1727 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 471 | CCOC(=O)c1cccc( NS(=O)  (=O)c2cc(Br)cnc2 N)c1 | Neg\_lig\_1740 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 472 | O=C(c1ccc(Cl)nc1  )c1cccs1 | Neg\_lig\_1745 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 473 | COc1nc2c(cc1C[N H2+] [C@H]1CCSC1)C (=O)N(C1CCCC1) C2 | Neg\_lig\_1761 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 474 | O=C1O[C@H]  (Nc2nc(- c3cccc(Br)c3)cs2) c2ccccc21 | Neg\_lig\_1784 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 475 | COc1cc(C[C@H]2 CC(CO)=NO2)cc2 c1OCO2 | Neg\_lig\_1865 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 476 | Cc1cnccc1Cn1ccn c1- c1cn(C2CC[NH2+  ]CC2)nn1 | Neg\_lig\_1885 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 477 | O=C(NCc1ccc2no nc2c1) [C@@]12C[NH2+  ]C[C@@H]1C[N  @@H+] (C1CCCC1)C2 | Neg\_lig\_1910 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 478 | O=C(NCCCO)c1n  nc(Cc2ccc3c(c2)O CO3)o1 | Neg\_lig\_1914 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 479 | Cc1ccc(Nc2nc(C)c 3nc(C)n(- c4ccc(C)cc4)c3n2) | Neg\_lig\_1943 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | cc1 |  |  |  | CAGCGUAGGGAAGUGCUG |  |
| 480 | Cn1c(=O)c2c(nc3n 2CC(c2ccc(Cl)cc2  )=NN3CCO)n(C)c 1=O | Neg\_lig\_1968 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 481 | COc1ccc(N)cc1- n1nnnc1-n1cccn1 | Neg\_lig\_1995 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 482 | COCc1nn(- c2ccccc2)c(N)c1- c1ccc(OC)c(OC)c 1 | Neg\_lig\_2047 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 483 | Cc1ncc(CO)c(CN( C)CC[NH+]2CCC CCC2)c1O | Neg\_lig\_42 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 484 | O=C(NCCO)c1cnc  2sc3c(n2c1=O)CC CC3 | Neg\_lig\_2075 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 485 | NC(=O)C1=C(NC  c2ccc3c(c2)OCO3  )c2ccccc2S1(=O)= O | Neg\_lig\_2081 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 486 | Nc1nonc1C(=O)N CC[NH2+]Cc1ccc  (OCc2ccccc2Cl)cc 1 | Neg\_lig\_2090 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 487 | CC[C@H] (C)Nc1c([NH3+])c  (=O)oc2ccccc12 | Neg\_lig\_2109 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 488 | CC[C@H] (C(N)=O)N1CCC C1=O | Neg\_lig\_2116 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 489 | CCCCCOC(=O) [N-]c1nc(=O)n([C @@H]2O[C@H] (C)[C@@H](O)  [C@@H]2O)cc1F | Neg\_lig\_2126 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 490 | Cc1cc(NC2CCCC  2)n2nc(C)c(- c3ccc(F)cc3)c2[nH  +]1 | Neg\_lig\_2170 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 491 | Cn1c(=O)c2nc(N) [nH]c2n(C)c1=O | Neg\_lig\_2196 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 492 | CNc1oc(- c2ccccc2Cl)nc1S(  =O)  (=O)c1ccc(F)cc1 | Neg\_lig\_2230 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 493 | C[C@@H]  (Cn1cnc2ccccc2c1  =O) [NH2+]CC1=CCC CC1 | Neg\_lig\_2247 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 494 | COc1cccc(C2=NN (CCO)c3nc4c(c(= O)n(C)c(=O)n4C) n3C2)c1 | Neg\_lig\_2284 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 495 | COc1ccc(- c2noc(Nc3ccc(C)c (C)c3)n2)cc1OC | Neg\_lig\_2299 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  |  |  |  |  | CAGCGUAGGGAAGUGCUG |  |
| 496 | Nc1ccn(C[C@@H  ](CO)OCP(=O)  ([O-])  [O-])c(=O)n1 | Neg\_lig\_2325 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 497 | O=C([O-])C[C@ @H](C(=O)  [O-])N1C(=O)/ C(=C2/  C(=O)Nc3ccc(Br)c c32)SC1=S | Neg\_lig\_2351 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 498 | CCOC(=O)c1cnc2  c(- c3ccc(F)cc3)c(C)n n2c1N | Neg\_lig\_2385 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 499 | CCc1nnc2c(Nc3cc ccc3OC)nc3ccccc3 n12 | Neg\_lig\_2400 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 500 | CC(C) (C)N1C[C@@H]  (C(=O)N(CCO)Cc  2nccs2)CC1=O | Neg\_lig\_2423 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 501 | O=C(NCCO)c1c2c  (nc3ccccc13)CCC C2 | Neg\_lig\_2441 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 502 | COc1ccc(OCCN[ C@H]2CS(=O) (=O)C[C@@H]2S (=O)  (=O)c2ccccc2)cc1 | Neg\_lig\_2468 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 503 | CC(C)C[NH+]1C CC([NH2+]Cc2cc  c(- n3cncn3)cc2)CC1 | Neg\_lig\_2500 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 504 | Cc1ccc(C)c(NC(= O)c2nnn(Cc3ccccc 3C)c2N)c1 | Neg\_lig\_2502 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 505 | CCOC(=O)N1CC  N(Cc2c(O)ccc3ccc cc23)CC1 | Neg\_lig\_1122 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 506 | C=CCn1c(N)c(C(= O)NC2CCCCC2)s c1=S | Neg\_lig\_2513 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 507 | Cc1nc2cc[nH]n2c(  =O)c1CCc1ccccc1 | Neg\_lig\_2523 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 508 | Cc1ccnc(NCCNc2 ncnc3c2CC[NH2+  ]CC3)c1 | Neg\_lig\_2554 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 509 | Cc1ccccc1[C@@ H]1CN(Cc2cccnc2 N)C[C@H]1C(=O  )O | Neg\_lig\_2558 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 510 | CO[C@@]12[C@ H] (COC(N)=O)C3= C(C(=O)C(C)=C( N)C3=O)N1C[C@ @H]1N[C@@H]1 2 | Neg\_lig\_2587 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 511 | COc1ccc(S(=O) (=O)c2cnc3ccc(C) cc3c2N)cc1 | Neg\_lig\_2624 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 512 | COc1ccccc1Nc1nc (-c2sc(N)nc2C)cs1 | Neg\_lig\_2660 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 513 | CCOC(=O)c1c(C)  oc2ncnc(Nc3cccc( CC)c3)c12 | Neg\_lig\_1648 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 514 | c1cnc(- c2nc(Cn3cc([C@ H]4CCC[NH2+]C  4)nn3)cs2)nc1 | Neg\_lig\_2723 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 515 | Cc1onc(- c2ccccc2Cl)c1C(= O)N[C@@H]1C(= O)N2[C@@H] (C(=O)[O-])C(C) (C)S[C@H]12 | Neg\_lig\_2725 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 516 | O=C(Cc1ccccc1)N 1CCC(C(=O)N2C COC[C@@H] (O)C2)CC1 | Neg\_lig\_2751 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 517 | COCCn1cnnc1CC [NH2+]Cc1cc(O)c  2cc(C)cc(C)c2n1 | Neg\_lig\_2756 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 518 | C=CCOCC[NH+] (CC)CC | Neg\_lig\_2761 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 519 | OCCn1nc(C2CCC  C2)nc1CCc1nc(- c2ccccc2F)no1 | Neg\_lig\_2810 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 520 | CCc1c(C(=O)C(N)  =O)c2c(OCC(=O)  [O-])cccc2n1Cc1c cccc1 | Neg\_lig\_2831 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 521 | Oc1ccccc1- c1nn(CNc2ccc(I)c c2)c(=S)o1 | Neg\_lig\_2843 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 522 | CCOc1ccc(Cc2cc( [C@@H]3O[C@ H](CO)[C@@H]  (O)[C@H](O)  [C@@H]3O)ccc2 Cl)cc1 | Neg\_lig\_2855 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 523 | Cc1ccsc1C[NH+]1 CCC2(CC1)Nc1cc  ccc1NC2=O | Neg\_lig\_2866 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 524 | COc1ccc(- c2ccc3c(N)c(C(=O  )c4ccc(OC)c(OC)c 4)sc3n2)cc1 | Neg\_lig\_2889 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 525 | Nc1nc(- c2cc3c(ccc4ccccc4 3)oc2=O)cs1 | Neg\_lig\_2929 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 526 | Cc1ccccc1- c1cc(O)c2c(c1)CN (C(=O)c1cc(N) | Neg\_lig\_2938 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | [nH]n1)CCO2 |  |  |  | CAGCGUAGGGAAGUGCUG |  |
| 527 | COc1ccccc1Nc1nc (-  c2c(C)nc3ccccn23  )cs1 | Neg\_lig\_2940 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 528 | Cn1c(- c2ccc(F)cc2)c[nH  +]c1NCc1cc(Br)cc c1F | Neg\_lig\_2945 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 529 | C=CCc1c(C)nc(N)  nc1NC[C@@H] (c1ccc(F)cc1) [NH+]1CCCC1 | Neg\_lig\_2978 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 530 | CCOC(=O)c1c(N)  nn(C(=O)c2ccc(Br  )cc2)c1- c1ccc(OC)cc1 | Neg\_lig\_2794 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 531 | CCCCCCNc1ncc(-  c2c[nH]c3ccccc23  )s1 | Neg\_lig\_2994 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 532 | N#CC1=C(N)Oc2  n[nH]c(- c3ccccc3)c2[C@H  ]1c1cccnc1 | Neg\_lig\_3015 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 533 | OCCn1nc(Cc2c(Cl  )cccc2Cl)nc1C1C CC1 | Neg\_lig\_3086 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 534 | CS(=O) (=O)N1CCCN(C(  =O)c2ccccc2[C@ H]2CC[NH2+]C2) CC1 | Neg\_lig\_3132 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 535 | O=c1c2ccccc2nc( CNc2ccccc2)n1- c1ccccc1F | Neg\_lig\_3156 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 536 | NC1=C(c2nc3cccc c3s2)C(=O)CN1c1  ccccc1Cl | Neg\_lig\_3159 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 537 | COc1ccc(CN2CC N(c3nccc(N)n3)C C2=O)cc1 | Neg\_lig\_3192 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 538 | CCC[C@@H] (NC(=O)  [C@@H]1[C@H] 2CCC[C@@H]2C N1C(=O)[C@@H]  (NC(=O)[C@@H]  (NC(=O)c1cnccn1  )C1CCCCC1)C(C) (C)C)C(=O)C(=O) NC1CC1 | Neg\_lig\_3204 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 539 | COc1cc2[nH]c(Nc 3ccc(Cl)cc3)c([N+  ](=O)  [O-])c2cc1OC | Neg\_lig\_3236 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 540 | O[C@@H]  (Cn1cc[nH+]c1- c1cnc(C2CCCCC2  )nc1)c1ccccc1 | Neg\_lig\_3256 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 541 | Cc1cc(NCc2cccnc 2)n2nc(C(F)  (F)F)c(- | Neg\_lig\_3259 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | c3ccc(Cl)cc3)c2n1 |  |  |  | CAGCGUAGGGAAGUGCUG |  |
| 542 | Cn1c(=O)n(C)c2cc (CNc3ccc4c(c3)O CO4)ccc21 | Neg\_lig\_3290 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 543 | Cc1ccccc1Cn1c([ C@H]  (C)O)nc2ccccc21 | Neg\_lig\_3297 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 544 | CNC(=O)c1cc(Oc  2ccc(NC(=O)Nc3c c(C(C)(C)C)nn3-  c3ccc4ncccc4c3)c( F)c2)ccn1 | Neg\_lig\_440 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 545 | N#CC1=C(N)N(c2  ccccc2)C2=C(C(= O)CCC2)  [C@@H]1c1ccc(O  )cc1 | Neg\_lig\_2809 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 546 | C[C@H]1[C@@H  ]2CC[C@@H](C) [C@@H]3CC[C@ @]4(C)OO[C@@] 23[C@H] (O[C@@H]1C[C  @H] (C[C@H]1O[C@  @H]2O[C@@]3(  C)CC[C@@H]5[C  @H] (C)CC[C@@H]  ([C@H]1C) [C@@]25OO3)CS (=O) (=O)c1ccc(COC(= O)N(C)C)cc1)O4 | Neg\_lig\_3339 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 547 | Cc1cccc(Cn2nnc( C(=O)Nc3cccc(C) c3)c2N)c1 | Neg\_lig\_3359 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 548 | Cc1cc(N[C@H]2C  C(=O)N(Cc3ccccc 3C(F) (F)F)C2)nc(N)n1 | Neg\_lig\_65 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 0 |
| 549 | Cc1ccc(C[NH2+]  Cc2ccc3c(c2)n(C) c(=O)n3C)cc1 | Neg\_lig\_8 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 550 | COc1cccc2c(O)c( NC(=O)N3CCC(C O)CC3)cnc12 | Neg\_lig\_9 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 551 | COc1ccccc1OCC[ NH2+]C[C@H]  (O)COc1cccc2[nH  ]c3ccccc3c12 | Neg\_lig\_48 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 552 | COCC[N@@H+] (C)C[C@@H]1C N(/C(O)=C2\  N=c3ccccc3=NC2  =O)C[C@@H]1C O | Neg\_lig\_54 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 553 | O=C(Nc1nc2cccc(  - c3ccc(CN4CCS(= O) (=O)CC4)cc3)n2n 1)C1CC1 | Neg\_lig\_62 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 554 | O=C([O-])c1[n-]c(  =O)[nH]c(=O)c1F | Neg\_lig\_85 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 555 | O=S(=O) (N[C@@H]1CCC  C[C@H]1Nc1ccc( Cl)cc1)c1ccccc1 | Neg\_lig\_99 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 556 | COc1ccc(C(=O) [O-])cc1NCc1cccc n1 | Neg\_lig\_116 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 557 | Cc1ccc(Nc2cc(C)n c3nc(- c4cccnc4)nn23)cc 1 | Neg\_lig\_182 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 558 | CN(C)c1ccc2c(c1) OC(N)=C(C#N)  [C@H]2c1cccc(F) c1 | Neg\_lig\_186 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 559 | CN(C)C(=O)c1ccc 2c(c1)N(C)  [C@@H] (CC(=O)NCCO)C O2 | Neg\_lig\_189 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 560 | O=S(=O)  (c1ccc2ccccc2c1) N(C[C@H]  (O)COCc1ccco1)c 1ccccc1 | Neg\_lig\_196 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 561 | COc1ccc(- c2nn3c(NCCN4C COCC4)cc(C)  [nH+]c3c2C)cc1O C | Neg\_lig\_197 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 562 | C[C@@H]1CN(c2  cc(Sc3ccc(F)cc3)n c(N)n2)C[C@]1(C  )O | Neg\_lig\_214 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 563 | Cc1cc(S(=O)(=O)  [C@H]2CS(=O)  (=O)C[C@@H]2N  CCc2c[nH]c3cccc c23)ccc1F | Neg\_lig\_247 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 564 | O=C(C[C@H]1C[ NH2+]CCO1)N1C  CC(Oc2cccc(C(F) (F)F)c2)CC1 | Neg\_lig\_249 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 565 | CC1(C)NC(=O)N( C[C@H]  (O)COc2ccc(F)cc2  )C1=O | Neg\_lig\_289 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 566 | Cc1cc(Nc2ccccc2) n2ncc(- c3ccc(Cl)cc3)c2[n H+]1 | Neg\_lig\_296 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 567 | Nc1ccc(- c2ccc(N)cc2S(=O) (=O)[O-])c(S(=O) (=O)[O-])c1 | Neg\_lig\_347 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 568 | COc1cccc(Nc2c(- c3ccc(O)cc3)nc3c nccn23)c1 | Neg\_lig\_363 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 569 | Cc1ccc(C[NH2+]  Cc2ccccc2Cl)s1 | Neg\_lig\_374 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  |  |  |  |  | GUCUGGGCGAACA |  |
| 570 | Cc1nc(N2CCCCC 2)ncc1C(=O)N1C[  C@H](c2ccccc2) [C@@H] ([NH3+])C1 | Neg\_lig\_139 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 571 | CCCN(CCC)CC(= O)N1CC(=O)Nc2c  cccc21 | Neg\_lig\_391 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 572 | Cc1cc(N)cc[nH+]1 | Neg\_lig\_417 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 573 | CCOC(=O)N1CC N(C[C@H]  (O)COCc2ccc(Cl) cc2)CC1 | Neg\_lig\_481 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 574 | Cc1cc(NC(=O)CS  c2nnc(N)s2)no1 | Neg\_lig\_524 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 575 | CC(C)  (C)c1cc(C[N@@ H+]2CCOC[C@@ H]2CC(=O)Nc2cc  cc(CO)c2)n[nH]1 | Neg\_lig\_528 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 576 | NC(=O)c1ccc2c(c 1SCCO)C(=O)c1c  cccc1C2=O | Neg\_lig\_208 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 577 | COC(=O)CNc1cc(  C)nc2nc(- c3ccccc3)nn12 | Neg\_lig\_545 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 578 | c1ccc([C@H] (Cn2ccnc2)NC2Cc 3ccccc3C2)cc1 | Neg\_lig\_567 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 579 | O=C(c1nc(- c2ccccc2)n(- c2cccc(Cl)c2)n1)N 1CCN(CCO)CC1 | Neg\_lig\_611 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 580 | CN(C[C@H] (O)CO)C(=O)Nc1  ccc(SCc2ccco2)cc 1 | Neg\_lig\_620 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 581 | Cc1cc(NCc2ccccn 2)n2ncc(- c3ccc(Cl)cc3)c2[n H+]1 | Neg\_lig\_637 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 582 | COCc1cc(C)nc2sc (-  c3nc(Cc4ccccc4)n o3)c(N)c12 | Neg\_lig\_675 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 583 | CC[N@@H+]1CC CC[C@@H]1Cn1  cnc(-c2ccccc2)c1- c1ccc(C#CCO)s1 | Neg\_lig\_677 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 584 | Fc1ccccc1C[NH2+  ]CCc1c[nH]c2cccc c12 | Neg\_lig\_748 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 585 | NC1=C(c2nc(-  c3ccc(Cl)cc3)cs2) C(=O)CN1C[C@ | Neg\_lig\_765 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | H]1CCCO1 |  |  |  | GUCUGGGCGAACA |  |
| 586 | Cc1ccsc1[C@@H] 1CC[N@@H+]  (Cc2ccc3c(C)cc(= O)oc3c2)C[C@H] 1O | Neg\_lig\_782 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 587 | Cc1ccc(- c2nc3cccc(C)n3c2 Nc2ccc3c(c2)OCC O3)o1 | Neg\_lig\_828 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 588 | COCC[C@]1(CO) CCC[N@@H+]  (Cc2nc[nH]c2C)C 1 | Neg\_lig\_890 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 589 | c1cc2c(c(- c3cnccn3)c1)CC[ NH2+]C2 | Neg\_lig\_926 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 590 | Nc1cccc(C(=O)C[ C@@]2(O)C(=O)  N(Cc3ccccc3)c3cc ccc32)c1 | Neg\_lig\_932 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 591 | O=C(Cc1cn2ccsc2 n1)N1CCC2(CC1)  c1ccccc1C[C@@ H]2O | Neg\_lig\_937 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 592 | CCCCOC[C@@H  ]  (O)Cn1c(Cc2ccccc 2)nc2ccccc21 | Neg\_lig\_965 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 593 | Cn1c(=O)c2c(nc3n 2CC(c2ccccc2)=N N3CCO)n(C)c1=O | Neg\_lig\_978 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 594 | CCCCCCNc1cc(C  (C)C)nc2nc(- c3cccnc3)nn12 | Neg\_lig\_982 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 595 | N#CC1=C(N)N(c2  c(F)cccc2F)C2=C( C(=O)CCC2)  [C@@H]1c1ccccc 1F | Neg\_lig\_627 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 596 | Cc1ccsc1CN(CCO  )C(=O)CCCn1cnc  2ccccc2c1=O | Neg\_lig\_1026 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 597 | Nc1cc(N2CCC[C  @H] (c3n[nH]cc3Cc3cc ccc3)C2)ncn1 | Neg\_lig\_1082 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 598 | Clc1ccccc1Nc1nc2 ccccc2o1 | Neg\_lig\_1096 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 599 | COCCN[C@H]1C S(=O) (=O)C[C@@H]1S (=O)  (=O)c1ccc(C)cc1 | Neg\_lig\_1103 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 600 | CC(C) (C)c1nnc2[c-]1C(=  O)c1ccccc1-2 | Neg\_lig\_1108 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 601 | CCOP(=O)(OCC)/ C(C#N)=C/ | Neg\_lig\_1114 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | c1c[nH]c2ccccc12 |  |  |  | UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA |  |
| 602 | COc1ccc(- c2c[nH+]c3cc(- c4ccc(Cl)cc4)nn3c 2N)cc1OC | Neg\_lig\_1121 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 603 | CCCc1nc(- c2cc3cccc(C)c3[n H+]c2N[C@@H]  (C)c2ccccn2)no1 | Neg\_lig\_1201 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 604 | CNC(=O) [C@@H]1C[C@H  ] ([NH3+])CN1C(=  O)c1ccc(CSc2nccc n2)o1 | Neg\_lig\_1246 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 605 | CCCCNc1ncnc2sc 3c(c12)CCCC3 | Neg\_lig\_1251 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 606 | CC[C@]1(CO)CC CN(C(=O)c2ccc(N 3CC[NH+] (C)CC3)cc2)C1 | Neg\_lig\_1255 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 607 | COc1ccc(C(=O)c2 sc3nc4c(c(- c5cccnc5)c3c2N)C CCC4)cc1OC | Neg\_lig\_1272 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 608 | Cc1ccc(S(=O)(=O)  [C@H]2CS(=O)  (=O)C[C@@H]2N  Cc2ccccc2Cl)cc1 | Neg\_lig\_1296 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 609 | Cn1c(=O)n(C)c2cc ([C@@H] (O)COc3ccc(C[N  H2+]Cc4ccco4)cc 3)ccc21 | Neg\_lig\_1323 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 610 | Cc1cc(C)nc(Nc2cc c(S(=O)(=O)/  N=c3\ cccc[nH]3)cc2)n1 | Neg\_lig\_1327 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 611 | COc1cc(F)c(CN2  CCN(c3ncc(C#N)c (N)n3)CC2)c(F)c1 | Neg\_lig\_1359 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 612 | CCOC(=O)c1cnc2  c(- c3ccc(OC)c(OC)c 3)c(CC)nn2c1N | Neg\_lig\_1372 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 613 | CCC[N@H+]1CC  c2[nH+]c[nH]c2C 12CCN(C(=O)CC  c1nc(N)n[nH]1)C C2 | Neg\_lig\_1390 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 614 | CC1CC[NH+] (C[C@H]  (O)CN2c3ccccc3S c3ccccc32)CC1 | Neg\_lig\_1423 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 615 | Cc1cc(O)c2c(C)cc c(C)c2n1 | Neg\_lig\_1467 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 616 | NC(=O) [C@@H]1CCCc2  c1[nH]c1ccc(Cl)cc 21 | Neg\_lig\_1481 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 617 | C[C@H]  (Nc1nc(N) [nH+]c2c1CC[NH  2+]CC2)c1cn2ccsc 2n1 | Neg\_lig\_1482 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 618 | Cc1ccc(S(=O) (=O)c2nc3ccccc3n c2NCc2ccco2)cc1 | Neg\_lig\_1491 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 619 | COCCC[NH2+]Cc  1ccc(- c2ccc([C@H] (C)O)cc2)o1 | Neg\_lig\_1507 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 620 | O=C(CCNC(=O) [C@]12C[NH2+] C[C@H]1C[NH2+  ]C2)Nc1cc(F)ccc1 F | Neg\_lig\_1510 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 621 | O=C1CCCN1CCC  Nc1ncnc2onc(- c3ccc(Cl)cc3)c12 | Neg\_lig\_1515 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 622 | O=c1[nH]cc(CC[N H2+] [C@H]2CCOC3(C COCC3)C2)c(=O) [nH]1 | Neg\_lig\_1526 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 623 | CCOC(=O)C1CC[ NH+]  (Cc2oc(CO)cc(=O  )c2O)CC1 | Neg\_lig\_137 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 624 | COc1cc2nccc(Oc3 ccc(NC(=O)Nc4cc (C)on4)c(Cl)c3)c2 cc1OC | Neg\_lig\_1295 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 625 | CCOc1ccc(- c2noc(-c3nnn(- c4ccccc4F)c3N)n2  )cc1 | Neg\_lig\_1611 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 626 | OCc1cc(- c2ccccc2OCCn2cc nc2)ccc1F | Neg\_lig\_1626 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 627 | C[NH+](C) [C@@H]1C[C@  @H] (CO)N(C(=O)Nc2  ccc(Cl)c3ncccc23) C1 | Neg\_lig\_1663 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 628 | Cc1nc(C)c(-  c2cc(C)c3c(C)nc(  C)nc3[nH+]2)c(N)  n1 | Neg\_lig\_1673 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 629 | CCc1ccccc1NC(= O)c1nnn(CC(=O)  Nc2c(C)cc(C)cc2C  )c1N | Neg\_lig\_1681 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 630 | Cc1ccc(- c2ccc3[nH]c(CO)n c3c2)c(- n2cccn2)c1 | Neg\_lig\_1703 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 631 | CNC(=O)c1ccc(N 2C(=S)N(c3cnc(C #N)c(C(F) (F)F)c3)C(=O)C23 CCC3)cc1F | Neg\_lig\_1737 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 632 | CCOC(=O)c1c(N) | Neg\_lig\_1754 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | nn(C(C)=O)c1-  c1ccccc1 |  |  |  | ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA |  |
| 633 | NS(=O) (=O)c1ccc(CN[C @H]2CC(=O)N(c  3ccc(Cl)cc3)C2=O  )cc1 | Neg\_lig\_1764 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 634 | OCC#CCSc1ncnn 1-c1ccccc1 | Neg\_lig\_1768 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 635 | CS(=O) (=O)n1nc(OC(=O)  c2ccccc2Cl)cc1N | Neg\_lig\_1777 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 636 | COC(=O) [C@@H]1C[C@  @H] (O)CN1C(=O)c1c  oc(COc2cccc(F)c2  )n1 | Neg\_lig\_1802 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 637 | O=C1CC[C@@]2 (CCCN(C(=O)Cc3  ccc(Cl)cc3)C2)CN 1CCO | Neg\_lig\_1818 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 638 | CCc1c(C)nc2ncnn 2c1Nc1ccccc1N1C CN(C(=O)C(C)C) CC1 | Neg\_lig\_1841 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 639 | Nc1ccc2c(c1)OC1 (CCCCC1)O2 | Neg\_lig\_1863 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 640 | CCSC[C@H] (N)C(=O)NCc1cn  n2ccccc12 | Neg\_lig\_1879 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 641 | C[NH+](C)  [C@@H] (CCOc1cccc2cccc c12)c1ccccc1 | Neg\_lig\_1887 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 642 | Cc1c(Cl)cc(C(=O) N2CCC[C@@H]2  CCO)cc1Cl | Neg\_lig\_1909 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 643 | CC[C@H]  (O)c1nc2ccccc2n1 Cc1ccccc1Cl | Neg\_lig\_1921 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 644 | Cc1ccc(C[NH+]2 CCC(C(=O)N(CC  O)Cc3ccccc3)CC2  )o1 | Neg\_lig\_566 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 645 | Cc1n[nH]c(N)c1- c1ccccc1 | Neg\_lig\_2056 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 646 | C=CCn1c(-c2c(-  c3ccccc3)ncn2CC O)nc2ccccc21 | Neg\_lig\_2071 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 647 | CC[C@H] (O)C[N@H+]1CC  c2[nH]nc(- c3ccc4c(c3)OCO4  )c2C1 | Neg\_lig\_2086 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 648 | O=c1c2c(Cl)cccc2 ncn1CCN1CCC[C @H](O)C1 | Neg\_lig\_2099 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 649 | Cc1ccc(Nc2nc(C)c c(N3CCN(S(=O)  (=O)c4c(C)noc4C) CC3)n2)cc1 | Neg\_lig\_2114 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 650 | OCc1ncc(- c2ccccc2)s1 | Neg\_lig\_2151 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 651 | COc1ccc(- c2nc(N)c3c4c(sc3 n2)CCCC4)cc1 | Neg\_lig\_2164 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 652 | COc1ccc(- c2nc3nc(C)cc(Nc4 ccc(Br)cc4)n3n2)c c1 | Neg\_lig\_2178 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 653 | Cc1ccc(OC[C@@ H] (O)C[N@@H+]2C CCC[C@@H]2C)  c(C)c1 | Neg\_lig\_2199 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 654 | CCCC(=O)Nc1ccc c(C(=O)NC[C@H  ]2CCC[NH2+]2)c 1 | Neg\_lig\_2208 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 655 | CCSC[C@H](C) [NH2+]C1CCN(S( C)(=O)=O)CC1 | Neg\_lig\_2266 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 656 | Cc1cc(Nc2ccccc2 F)n2nc(- c3cccnc3)nc2n1 | Neg\_lig\_2276 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 657 | Cc1ccc(-c2c(C(F) (F)F)nn3c(N4CCN (CCO)CC4)cc(C)n  c23)cc1 | Neg\_lig\_2285 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 658 | CCCOc1cc(Cl)c(C N2CC[NH2+] [C@H] (C(=O)NC3CC3)C 2)cc1OC | Neg\_lig\_2288 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 659 | Cc1ccc([C@H]2C N(C(=O)Cn3nc(C)  c4ccccc4c3=O)C[ C@@H]2[NH3+])  o1 | Neg\_lig\_2317 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 660 | CC[C@@H] ([NH2+]Cc1cc(N2 CCOCC2)ncn1)C(  =O)NC1CCCC1 | Neg\_lig\_2323 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 661 | Cc1ccc(N2C(=O)c 3ccccc3[C@H]2N c2ccccc2)nc1 | Neg\_lig\_2341 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 662 | N#CC1=C(N)N2C (=C(C#N)  [C@@H]1c1ccc(C l)cc1)Sc1ccccc12 | Neg\_lig\_947 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 663 | O=C(/N=C1\ SC2=C(CCCC2)\ C1=C(\ O)NC[C@H] | Neg\_lig\_2410 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | (O)CO)c1ccccc1 |  |  |  |  |  |
| 664 | C[C@H] (O)CCNS(=O)  (=O)c1ccc2c(c1)C CN(C(=O)c1ccc[n H]1)C2 | Neg\_lig\_2476 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 665 | COc1cccc(- n2c3c(c(S[C@H] (N)c4cccc5ccccc4 5)nc2=O)CCC3)c1 | Neg\_lig\_2511 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 666 | COc1ccc(Cl)cc1N c1nc(SC)nc2c1CC C2 | Neg\_lig\_2527 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 667 | CC(C)c1nc(CN(C) c2nc(CC[NH3+])  [nH+]c3ccccc23)c s1 | Neg\_lig\_1074 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 668 | NC(=O)CCn1cc(C [NH2+]CCN2CC  NC2=O)c2ccccc21 | Neg\_lig\_2546 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 669 | COc1cc(OC)c([C @@H]2C(C#N)= C(N)Oc3n[nH]c(C  )c32)cc1OC | Neg\_lig\_2547 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 670 | COC(=O)c1c(-  c2cc(C)ccc2C)csc 1N | Neg\_lig\_994 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 671 | CCN(CC)S(=O)  (=O)c1ccc(Nc2nc3 ccc(Cl)cc3n3cnnc2 3)cc1 | Neg\_lig\_644 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 672 | CC(=O)Nc1ccc(O  CCOc2ccc([N+] (=O)[O-])cc2)cc1 | Neg\_lig\_2609 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 673 | O=C(N[C@@H]1 CC[C@H]  (C(=O)Nc2cccc(C O)c2)C1)c1cnc2cc cnn12 | Neg\_lig\_2623 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 674 | CCc1[nH]nc2c1[C @H] (c1ccc(Cl)cc1)C(C #N)=C(N)O2 | Neg\_lig\_2629 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 675 | CC(=O)c1ccc(N[C @H]2OC(=O)c3cc  ccc32)cc1 | Neg\_lig\_2651 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 676 | Cc1nc(C(C)C)sc1 C(=O)N1CCN[C @H]2CS(=O) (=O)C[C@H]21 | Neg\_lig\_2662 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 677 | O=S1(=O)N=C(N  CCCO)c2ccccc21 | Neg\_lig\_2698 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 678 | C[C@@]1(c2csc( Nc3ccccc3Cl)n2)C CC(=O)O1 | Neg\_lig\_2783 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 679 | Cn1c(NCc2ccccc2  )nc2c1c(=O)n(Cc1 ccccc1F)c(=O)n2C | Neg\_lig\_2792 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  |  |  |  |  | GUCUGGGCGAACA |  |
| 680 | CCOc1cc(CNc2[n H+]cc(-  c3ccccc3)n2C)ccc 1O | Neg\_lig\_2806 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 681 | CN1CCC[N@@H  +] (C[C@@H]2CN(c  3nc(C(N)=O)cs3) C[C@@H]2CO)C C1 | Neg\_lig\_2814 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 682 | Nc1nc2ncnc- 2c(N2CCC(c3[nH  +]ccn3CC3CC3)C C2)[nH]1 | Neg\_lig\_2817 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 683 | CNC(=O) [C@@H]1C[C@  @H] ([NH3+])CN1C(=  O)CSc1n[nH]c(-  c2ccco2)n1 | Neg\_lig\_2837 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 684 | NC(=O)C1=C(NC  CO)c2ccccc2S1(= O)=O | Neg\_lig\_2874 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 685 | COc1ccc(-c2c(- c3ccccc3)oc3ncnc( N)c23)cc1 | Neg\_lig\_2883 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 686 | Cc1ccccc1N1CCC N(C(=O)c2ccc([C @@H]3CCC[NH2  +]3)s2)CC1 | Neg\_lig\_2912 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 687 | COc1ccc(OC[C@ H]  (O)CSc2ccccn2)cc 1 | Neg\_lig\_2924 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 688 | COCC(=O)N1C[C @H]2C[NH2+]C[  C@@]2(C(=O)N2  CCC(Cn3cccn3)C C2)C1 | Neg\_lig\_2939 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 689 | Cc1cc(C)c(NC(=O  )c2sc3nc(C)c(C)c( C)c3c2N)c(C)c1 | Neg\_lig\_2060 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 690 | OCc1cc(- c2ccc3c(c2)OCCO 3)ccn1 | Neg\_lig\_2968 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 691 | O[C@@H]  (Cn1cccc1)c1cccc c1 | Neg\_lig\_2982 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 692 | N#Cc1nc(COc2cc c(F)cc2)oc1NCCC n1ccnc1 | Neg\_lig\_2991 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 693 | COc1cc(NC(=O)c  2ccc(- c3ccc(Cl)cc3)o2)c c(OC)c1 | Neg\_lig\_3008 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 694 | CC[NH+]1CCN(C  c2ccc(Nc3ncc(F)c(  -  c4cc(F)c5nc(C)n(  C(C)C)c5c4)n3)nc | Neg\_lig\_3041 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | 2)CC1 |  |  |  |  |  |
| 695 | O=C([C@@H]1C  CCN1Cc1ccccc1) N1CCC2(CC1) [NH2+]CCNC2=O | Neg\_lig\_3077 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 696 | Nc1c[nH+]c(Nc2c cc(Br)cc2)nc1N | Neg\_lig\_3094 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 697 | Cc1ccc(- n2nc(C(=O)N(CC O)CCO)nc2-  c2ccccc2)cc1 | Neg\_lig\_3109 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 698 | CCC[C@H]1CN(  C(=O)c2ccccc2C# N)C[C@@H]1[N H3+] | Neg\_lig\_3118 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 699 | CC(C)c1ccc(- c2c(NCC[N@@H  +]3CCCC[C@@H  ]3C)c(=O)c2=O)cc 1 | Neg\_lig\_3230 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 700 | CCn1nc(C)c(NC(= O)CN[C@@H]  (C)Cn2nc(C)cc2C) c1C | Neg\_lig\_3235 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 701 | CCOC(=O)c1[nH]  nc(N)c1- c1ccc(OC)cc1 | Neg\_lig\_3246 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 702 | Nc1c(C(=O)c2ccc cc2)sc2nc3c(cc12) CCCCC3 | Neg\_lig\_3292 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 703 | O=S(=O)(/N=c1/  [nH]c2ccccc2nc1N Cc1ccc(Cl)cc1)c1c cccc1 | Neg\_lig\_3321 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 704 | O=C(Nc1ccccc1C(  =O)NCCO)c1ccco 1 | Neg\_lig\_3351 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 705 | COc1ccc([C@@H  ]2C(C#N)=C(N)O  c3n[nH]c(C)c32)c( OC)c1OC | Neg\_lig\_2884 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 0 |
| 706 | c1ccc2c(c1)nc(c1c cc(cc1)N)o2 | 0109-0045 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 1 |
| 707 | CC(C)  (C)NCc1ccc(cc1) [Cl] | 0167-0173 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 1 |
| 708 | c1ccc(c(c1)N)I | 0325-0348 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 1 |
| 709 | c1ccc2c(c1)nc(Sc1 ccc(cc1[Cl])N)s2 | 0375-0604 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 1 |
| 710 | C(=Cc1nc2ccccc2 o1)c1ccc(cc1)N | 0632-0836 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 1 |
| 711 | CN(C)c1ccc(C=Cc 2nc3cc(ccc3[nH]2) N)cc1 | 0632-0897 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 1 |
| 712 | C(=Cc1nc2cc(ccc2 | 0717-0957 | Glutamine\_RS | Three-way | UAAUCGUUGGCCCAGUUUAUCU | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | [nH]1)N)c1ccccc1 |  |  | junction | GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC |  |
| 713 | CCN(CC)CCOC(c  1ccc2c(c1)sc(NC(c 1ccc(cc1)N)=O)n2  )=O | 0812-1025 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 1 |
| 714 | Cc1c(C)c(C)nc2c1 c(c(C(c1ccc(cc1)  [Cl])=O)s2)N | 0892-0702 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 1 |
| 715 | C1Oc2ccc(cc2O1) c1c(C#N)c(N)n2c3 ccccc3nc2c1C#N | 2144-0693 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 1 |
| 716 | CC(C) (C)C(CN1C(=N)N (CCN2CCCCC2)c  2ccccc12)O | 2226-0439 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 1 |
| 717 | c1ccc2c(c1)ccc1c2 nc(c2ccc(cc2)N) [nH]1 | 2252-1548 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 1 |
| 718 | Cc1cc2c(cc1N)nc( NC(c1ccc(cc1)C(= O)OC)=O)s2 | 2284-1574 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 1 |
| 719 | c1ccc(c(c1)c1nc2c c(ccc2s1)N)O | 2372-3111 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 1 |
| 720 | Cc1ccc(cc1)S(N(C CO)CC(Cn1c2ccc cc2c2ccccc12)O) (=O)=O | 2378-0048 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 1 |
| 721 | c1cc2c(cc1N)nn(c 1ccc(cc1)[Cl])n2 | 2810-2075 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 1 |
| 722 | c1cc(cc(c1) [Cl])n1nc2ccc(cc2 n1)N | 2810-4198 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 1 |
| 723 | Cc1ccc(cc1N)c1nc 2cc(ccc2o1)[Cl] | 2810-4217 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 1 |
| 724 | c1cc(c2cccc(c2c1) [Br])c1nc2cc(ccc2 o1)N | 2810-4224 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 1 |
| 725 | COc1ccc(cc1[Br]) c1nc2cc(ccc2o1)N | 2810-4227 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 1 |
| 726 | COc1ccc(cc1[Cl]) c1nc2cc(ccc2o1)N | 2810-4228 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 1 |
| 727 | Cc1cc(C)c2c(c1)n c(c1cc(ccc1[Cl])N  )o2 | 2810-4324 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 1 |
| 728 | Cc1ccc2c(c1)nc(c1 cc(ccc1[Cl])N)o2 | 2810-4326 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 1 |
| 729 | COc1ccc(c(CNc2c cc(cc2)[Br])c1)OC | 2910-1869 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 1 |
| 730 | C(c1ccc(cc1) [Br])Sc1nc2ccc(cc 2s1)N | 3167-0427 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 1 |
| 731 | C(c1ccccc1[Cl])Sc 1nc2ccc(cc2s1)N | 3167-0436 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 1 |
| 732 | C(C(c1ccccc1)=O) | 3167-0470 | Glutamine\_RS | Three-way | UAAUCGUUGGCCCAGUUUAUCU | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | Sc1nc2ccc(cc2s1) N |  |  | junction | GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC |  |
| 733 | CCOC(c1c2ccc(c( c2sc1N)OCc1cccc c1)[Br])=O | 3473-2720 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 1 |
| 734 | Cc1cc(ccc1[Br])c1 nc2cc(ccc2o1)N | 3617-0633 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 1 |
| 735 | Cc1cc2c(cc1C)oc( c1cccc(c1C)N)n2 | 3639-0494 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 1 |
| 736 | CCOc1ccc(CNCC c2ccc3c(c2)OCO3  )cc1 | 3701-0014 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 1 |
| 737 | c1ccc2c(c1)nc(c1c cc(cc1)N)s2 | 3729-2175 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 1 |
| 738 | CCCCc1ccc(cc1)n 1nc2ccc(cc2n1)N | 3738-4868 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 1 |
| 739 | CCCCN1CCC(CC 1)  (C#N)Nc1ccccc1 | 4237-0134 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 1 |
| 740 | C1CCC2C(C1)=C(  C#N)c1nc3ccccc3 n1C=2NCCN1CC OCC1 | 4852-0279 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 1 |
| 741 | CCCCNc1c2c(c3c 4CCCCc4c(nc3s2) N2CCOCC2)nnn1 | 5504-0161 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 1 |
| 742 | CCOc1cc(CO)cc(c 1OCc1ccc(cc1)C( O)=O)[Br] | 6415-0035 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 1 |
| 743 | C(C#CCSc1nnc(c2 cccc(c2)[Br])o1)O | 7199-0097 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 1 |
| 744 | C(C(c1ccc(cc1) [Cl])=O)Sc1nc2cc c(cc2s1)N | 8007-4809 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 1 |
| 745 | C(c1c(cc(c2ccccc2  )nc1N)c1cccc(c1) [Br])#N | 8008-0679 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 1 |
| 746 | C(c1ccccc1)n1c(cc (c2ccc(cc2) [Br])n1)N | 8008-1484 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 1 |
| 747 | CC1=C(C(C(C#N)  =C(N)O1)c1ccccc 1)C(=O)OCC=C | 8008-9248 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 1 |
| 748 | [H]Nc1nnc(COc2c cc(cc2)C2CCCCC 2)s1 | 8009-2831 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 1 |
| 749 | C(c1cc(ccc1[Cl])  [Cl])Sc1nnc(N)s1 | 8011-5554 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 1 |
| 750 | C(C1C(c2c[nH]nc 2c2ccc(cc2)F)c2c( c3ccc(cc3) [Cl])n[nH]c2OC=1 N)#N | 8011-9730 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 1 |
| 751 | C1Oc2ccc(cc2O1) C1C(C#N)=C(N)O  c2c1c(c1ccc(cc1)F  )n[nH]2 | 8012-0501 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 752 | CC1=CC(N(C)C( N1CCCCCCNCC O)=O)=O | 8012-3983 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 1 |
| 753 | CC(C)  (C)c1ccc(CSc2nnc (N)s2)cc1 | 8012-4068 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 1 |
| 754 | Cc1c(CCNCc2ccc( C#N)cc2)c2cc(ccc 2[nH]1)OC | 8013-2954 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 1 |
| 755 | Cc1cc2NC(Nc3ccc (c(c3)  [Cl])F)Sn2n1 | 8015-1245 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 1 |
| 756 | COc1ccc(CCNc2n c(cs2)c2cccs2)cc1 OC | 8018-0995 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 1 |
| 757 | CC(C)C1(CCNCc  2cccc3c2OCO3)C COC(C)(C)C1 | 8018-1268 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 1 |
| 758 | c1ccc(cc1)c1ccc(c c1)c1nc2cc(ccc2o1  )N | 8018-2965 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 1 |
| 759 | c1cc2c(cc1N)nc(c 1cc(ccc1[Cl])  [Br])o2 | 8018-2966 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 1 |
| 760 | c1ccc(cc1)C(c1c(c 2ccc(c3ccncc3)nc2 s1)N)=O | 8019-6975 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 1 |
| 761 | c1cc(N)nc2c1ccc( n2)O | 8019-7722 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 1 |
| 762 | C(c1ccccc1)c1cc(c cc1OCCN)[Cl] | 8019-8811 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 1 |
| 763 | C(c1cccc2c1cc[nH  ]2)NCc1cccc2c1cc [nH]2 | 8019-9725 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 1 |
| 764 | C(c1cn[nH]c1c1cc c(cc1)[Cl])N | 8019-9983 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 1 |
| 765 | COc1ccc(CNCc2c cc3c(cc[nH]3)c2)c c1 | 8020-0063 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 1 |
| 766 | C(CNCc1ccc2c(cc [nH]2)c1)c1ccc(cc 1)F | 8020-0064 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 1 |
| 767 | C(CN)c1csc(c2ccc (cc2)C(F)(F)F)n1 | 8020-2422 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 1 |
| 768 | c1cc(c2c(c1)nc(N) o2)[Cl] | 8020-5450 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 1 |
| 769 | CN(C)c1ccc(cc1) NC1CC(N(C1=O)  c1ccc(cc1)O)=O | 8440-1765 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 1 |
| 770 | CN(C)c1ccc(cc1) NC1CC(N(C1=O)  c1ccc(cc1)F)=O | 8440-1773 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 1 |
| 771 | c1ccc2c(c1)nc(c1c cc(cc1[Cl])N)s2 | C066-5322 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 1 |
| 772 | Cc1ccc(cc1)C1NC (C2Cc3c(CO)cnc( C)c3OC=2N=1)=S | C200-2788 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 773 | CNc1c(c(N) [nH]n1)c1nc(c2ccc (cc2)OC)no1 | C201-1012 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 1 |
| 774 | CC(C)  (C)c1ccc(cc1)c1cc (N)n(n1)S(c1ccc(c c1)OC)(=O)=O | C665-0270 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 1 |
| 775 | c1cc(ccc1c1cc(N)n (n1)S(c1ccc(cc1)F  )(=O)=O)[Br] | C665-0314 | Glutamine\_RS | Three-way junction | UAAUCGUUGGCCCAGUUUAUCU GGGUGGAAGUAAGGUCUUUGGC CUGAAGCAACGCGCCUC | 1 |
| 776 | O=C(NCCCN1CC  1)Nc1cccc2ccccc1 2 | 101298 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 777 | CC(C)=CCC/C(/ C)=C\C(N)=O | 108655 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 778 | Cc1cc(nc2cc(ccc1 2)OC)N1C[C@H]  (C2CC2)[C@H] (C1)N | 12182839 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 779 | C1[C@H]  (c2ccccc2)[C@H] (CN1S(c1ccc2c(c1  )NC(N2)=O)  (=O)=O)N | 12201213 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 780 | CC(NS(c(cc1)cc2c 1sc(C)n2)  (=O)=O)=O | 122385 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 781 | Cc1nc(CCN)cc(n1  )N(C)Cc1cccc(c1)  C(F)(F)F | 12267434 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 782 | C1CN(Cc2ccccc12  )c1c2CCNCc2nc(c 2cccnc2)n1 | 12634687 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 783 | C1C(CN)Oc2c1cc(  cc2F)c1ccc2c(cco2  )c1 | 12766557 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 784 | C(c1cc(ccc1F)c1cc c(cc1)c1csc(N)n1) O | 12892198 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 785 | Cc1c(C(C(N2CCC  (CCCc3ccccc3)CC 2)=O)N)c(C)  [nH]n1 | 13119286 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 786 | C1C(CN1Cc1ccc(  cc1)OCCO)Oc1cc ccc1[Cl] | 13202927 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 787 | C1CCC(C1)  (C#N)c1ccc(cc1)c 1cccc2CNCCc12 | 14224931 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 788 | CC(C)CCOc1cccc (CCNC(C2CC3(C CNCC3)CN2)=O)  c1 | 14325308 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 789 | C1CN(CCC1C1C  CN(CCc2ccccc2)C 1)c1ccnc(N)n1 | 14604674 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 790 | Cc1ccccc1c1nc(C CC(N2CCCC(CC N)C2)=O)on1 | 15196499 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 791 | CC(C) (CCCC1(C)C(OC CO)=C2)C1=CC2  =O | 157940 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 792 | Cc1c(C(C(NCCNc | 16899791 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | 2cccnc2)=O)N)c(C  )[nH]n1 |  |  |  | AUAAAAAACUAA |  |
| 793 | C1CNCc2c1c1C( N(C=Nc1s2)C1c2c  cccc2c2ccccc12)= O | 17311387 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 794 | Cc1cc2CC(CN)Oc  2c(c1)c1cnc2ccccc 2n1 | 17587941 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 795 | C1CNCc2cccc(c3c ccc4c3cc[nH]4)c1 2 | 17741735 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 796 | C1CC(CNC1)c1cc  (c2ccc(c(c2)[Cl])  [Cl])nc(c1C#N)N | 17917068 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 797 | [H]N1CCCn2c(C1  )cc(CNS(c1ccc(cc 1)n1cccn1) (=O)=O)n2 | 17922447 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 798 | C1CC[C@H] ([C@H] (C1)CNCCC(Nc1c cc(cc1)C(N)=O)= O)O | 18391632 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 799 | C1CN(Cc2ccc(cc2  )Oc2ccc(cc2) [Cl])C[C@H]  ([C@H]1CO)O | 18682916 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 800 | Cc1cnc(CNCc2ccc (cc2)OCC(N2CCO CC2)=O)cn1 | 19297220 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 801 | Cc1cc(cc(c1CNc1 c2CCNCc2nc(C)n 1)[Cl])[Cl] | 20278440 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 802 | CCCCOc(cc1)ccc1 OC(Nc(cc(cc1)Cl) c1OC)=O | 205832 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 803 | Cc1cc(N)n(CC(N2  C[C@H]3COc4cc ccc4C[C@]3(C2) C(O)=O)=O)n1 | 21044903 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 804 | C1CN(CCC1N1C(  Nc2ccccc12)=O)c 1cc(NCCO)nc(N)n 1 | 21582243 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 805 | CC1CC2(C)CC(C) C1(CO)CO2 | 2190-0577 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 806 | CNc1cc(c2ccc(cc2  )c2nnc(N)s2)c2cc[ nH]c2n1 | 25638728 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 807 | C1CN(Cc2c(c3ccc c4ccccc34)noc12) C(c1cc(N)  [nH]n1)=O | 26633940 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 808 | C1COc2cc(ccc2C1  =O)c1cc2CC(CN)  Oc2c(c1)[Cl] | 26642358 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 809 | C1CNCC2=C1C(  NC(NCc1nc(cs1)c 1ccc(cc1)F)=N2)= O | 26965809 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 810 | c1cc(c2cccc(c2c1) [Br])c1nc2cc(ccc2 o1)N | 2810-4224 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 811 | COc1ccc(cc1[Br]) c1nc2cc(ccc2o1)N | 2810-4227 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 812 | Cc1ccc(cc1c1cccc( CCN)c1)F | 31003354 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 813 | C(c1ccc(cc1)c1nc( c2ccc(c(c2)F)F)nn 1CCO)N | 31242301 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 814 | C1CCc2c(C1)nc(C (N1[C@H]3CC[C @@H]1CCNC3)= O)s2 | 31575004 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 815 | CN(C)CCNc1cc(c  2ccccc2CO)c2cc[n H]c2n1 | 31764292 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 816 | C(Cc1nc(c2ccccc2  )no1)C(N[C@H]1  Cc2ccccc2[C@@ H]1N)=O | 31852539 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 817 | C1CNCc2cc(CC3  Cc4ccccc4OC3)cc c12 | 31917501 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 818 | Cc1cc(CNc2ccc3c (c2)ncs3)n[nH]1 | 32903475 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 819 | COc1ccc2cc(ccc2c 1)c1ccccc1CN | 33557632 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 820 | C1C[C@H] (C[C@@H]1N)Nc  1c(cc(cn1)[Cl]) [Cl] | 33921774 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 821 | Cc1c2cc(cc(CNC([ C@H]  (Cc3c[nH]cn3)N)= O)c2[nH]c1c1cccc c1)[Cl] | 34268481 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 822 | CCCOc1ccc(cc1)C 1C(C#N)=C(N)Oc  2c1c(C(C) (C)C)n[nH]2 | 3448-7906 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 823 | C1CC(CCOc2cccc c2) (CN(C1)c1nnnn1c 1ccccc1)CO | 34785173 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 824 | c1ccc(cc1)c1c2c(N  )ncnc2oc1c1ccccc 1 | 3720-2377 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 825 | CCS(Nc1ccc(cc1) C(N1CC[C@@] (C)([C@H]  (C1)O)O)=O) (=O)=O | 39666518 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 826 | C1CSCCN1S(c1cc  c(cc1)c1ccc2c(c1) c(N)n[nH]2) (=O)=O | 39837810 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 827 | Cc1ccc(cc1)S(N(C C(CN1CCCCC1)  O)c1ccccc1OC) (=O)=O | 4013-2178 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 828 | Cc1cccc(c1OCCN C(c1cn(CCN)nn1)  =O)[Cl] | 41830928 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 829 | COc1ccc2cc(ccc2c 1)C1CN(CCO1)C(  c1cc(N)[nH]n1)=O | 42028139 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 830 | Cc1nc(CCN)cc(n1  )N(C)Cc1cccc2cnc cc12 | 42532169 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 831 | COc1cccc(c1c1cc( CN)ccc1F)[Cl] | 42929743 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 832 | CC(C1C(c2ccc(cc 2) [Br])N(CCO)C(C= 1O)=O)=O | 4616-0292 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 833 | C1CCN(CC1)CC NC1=C2CCCC2=  C(C#N)c2nc3cccc c3n12 | 4708-0071 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 834 | C(CNc1cccnc1)C Nc1c2ccccc2nc(C CN)n1 | 47488116 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 835 | CCOC(c1cnc2c(C) cccc2c1NCc1cccn c1)=O | 4790-1176 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 836 | Cc1cnc(N)nc1NC C[C@@H]1C[C@ H]2C[C@@H]1C  =C2 | 47913504 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 837 | C(CNCc1ccc2c(c1  )OCO2)c1c[nH]c2  ccccc12 | 4964-5174 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 838 | Cc1nc2cc(c(cc2n1 CCCO)[Cl])[Cl] | 5119828 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 839 | c1ccc(cc1)Oc1ccc( cc1N)C(c1ccc(c(c 1)N)Oc1ccccc1)= O | 5172392 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 840 | CCOC(c1cnc2c(C) cc(C)cc2c1NCC(C  )O)=O | 5174-4431 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 841 | C(C(NN=Cc1c(ccc c1[Cl])  [Cl])=O)Nc1cccc2 ccccc12 | 5201830 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 842 | CCCCCc1ccc(cc1) c1ccc(cc1)c1ncc(c n1)N | 5213078 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 843 | CCOC(CNc1ccc(c c1)Oc1ccc(cc1)Oc 1ccc(cc1)NCC(=O  )OCC)=O | 5224153 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 844 | c1ccc2c(c1)ccc(c2 [Cl])Sc1ccc(cc1[C l])N | 5250905 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 845 | c1ccc2c(c1)C(Nc1 cccc(c1)OC(c1ccc o1)=O)=NS2(=O)  =O | 5251-2481 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 846 | C1CN(CCC1O)Cc  1ccccc1[N+] ([O-])=O | 5269563 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 847 | C1CN(CCN1CC(  Cn1c2ccccc2c2ccc cc12)O)Cc1ccccc1 | 5320336 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 848 | COc1ccc(cc1)c1nn c(N)s1 | 5324234 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 849 | CC1(C)CC2=C(C(  c3ccc(cc3) [Br])Nc3ccccc3N2 | 5325779 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | )C(C1)=O |  |  |  |  |  |
| 850 | C(c1cccs1)=NNC( c1ccccc1N)=O | 5331322 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 851 | C1c2ccc3ccccc3c2 c2c(CN1)ccc1cccc c12 | 5346676 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 852 | Cc1cc(ccc1NCC( NN)=O)I | 5346837 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 853 | CC1CCCCC1=NN  C(CNc1ccc(cc1C)I  )=O | 5347443 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 854 | c1cc(ccc1c1cc(C( NN)=O)c2cc(ccc2 n1)[Br])N | 5350878 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 855 | Cc1c2cc(CNC(c3c c(N)  [nH]n3)=O)ccc2[n H]c1c1ccccc1F | 56075039 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 856 | CCCc1ccc(cc1)c1c cc(cc1)C(N1CCC( CN)C1)=O | 56240352 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 857 | [H]N([H])c1nc(n[n H]1)SCCCCCCC CC | 5655427 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 858 | CCOC(c1cnc2c(cc cc2c1Nc1ccc(cc1) N(C)C)C(F) (F)F)=O | 5695-0979 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 859 | Cc1ccc(C(NCCNc 2ccc(cc2[N+]  ([O-])=O) [Cl])=O)o1 | 5717805 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 860 | C(C(Cn1c2ccccc2 c2ccccc12)O)NNC (c1ccccc1)=O | 5718973 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 861 | CCNC(Cc1ccc(cc1  )c1cc2CC(CN)Oc2 c(c1)[Cl])=O | 57980040 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 862 | C(c1ccccc1)c1cccc c1OCCN.[Cl] | 5924771 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 863 | COc1ccc(cc1)C1C C2=C(C(c3c[nH]c  4ccccc34)Nc3cccc c3N2)C(C1)=O | 6044923 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 864 | C(C(N1c2ccccc2S c2ccccc12)=O)Sc1 nnc(N)s1 | 6134473 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 865 | C(C(c1ccc(cc1) [Br])=O)Sc1nnc(N  )[nH]1 | 6357130 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 866 | CCCCSc1nc2c(c3 cc(ccc3NC3(CCC C3)O2)[Br])nn1 | 6372845 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 867 | CS(c1ccc(c(c1) [N+]  ([O-])=O)NCC(Nc  1ccccc1SC(C(C(F) (F)F)(F)F)  (F)F)=O)(=O)=O | 6786638 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 868 | Cc1ccc(cc1)C(CN c1ccc(cc1)F)=O | 6802876 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 869 | CC(C) (C)NC(CSc1c(C# | 8001-8198 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | N)cc(C#N)c(N)n1)  =O |  |  |  |  |  |
| 870 | CC1(C)CC2=C(C( C1)=O)C1(C(C#N  )=C(N)O2)C(Nc2c  cc(cc12)[Br])=O | 8004-9540 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 871 | C=Cc1ccc(cc1)c1c sc(N)n1 | 8005-0366 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 872 | Cc1cc(C)c2c(c1)n c(c1ccc(cc1O)N)o 2 | 8007-0773 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 873 | C(C1C(c2ccsc2)c2 ccc3ccccc3c2OC= 1N)#N | 8007-1084 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 874 | Cc1ccc(cc1[Cl])N c1nc(cs1)c1ccc(cc 1)S(N1CCOCC1) (=O)=O | 8007-2266 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 875 | CCOC(c1c2ccc(c( c2sc1NC(C)=O)O CC(CN1CCCCC1) O)[Br])=O | 8008-4440 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 876 | COc1ccc2c(c1)SC (=N)N2CCO | 8010-0067 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 877 | CN1C(c2c(nc(NC COCCO)n2C)N(C  )C1=O)=O | 8010-4817 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 878 | Cc1c(CCNCc2ccc( C#N)cc2)c2cc(ccc 2[nH]1)OC | 8013-2954 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 879 | C1Cc2c(C(=O)OC CO)c(C#N)c(N)nc 2C1 | 8014-7935 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 880 | Nc(cc1)cc(Cc2c3) c1-c2cc(Cl)c3Cl | 80141 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 881 | COc1cc(c(c(c1OC  )OC)  [Br])c1nnc(N)o1 | 8018-2758 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 882 | CCc1ccc2c(c1)nc( c1ccc(cc1O)N)o2 | 8018-2852 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 883 | c1cc2c(cc1N)nc(c 1cc(ccc1[Cl])  [Br])o2 | 8018-2966 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 884 | C(c1ccc2c(c1)OC O2)Nc1c(c[nH]n1) C(N)=O | 8018-4095 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 885 | C1Cc2nc(c(C(c3cc c(cc3) [Br])=O)n2C1)N | 8018-7423 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 886 | COc1ccc(cc1)c1c( c2ccc(cc2)OC)sc( N)n1 | 8019-6726 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 887 | CCc1c2C(C(C#N)  =C(N)Oc2n[nH]1)  c1cc(c2c(c1)OCO 2)OC | 8019-9061 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 888 | C(c1cn[nH]c1c1cc c(cc1)[Cl])N | 8019-9983 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 889 | C(C1C(c2ccc3cccc c3c2OC=1N)c1ccc s1)#N | 8020-0820 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 890 | Cc1c2c(N)nn(Cc3 ccc(cc3[Cl]) | 8020-1001 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | [Cl])c2nc(c2ccccc 2)n1 |  |  |  |  |  |
| 891 | c1cc(ccc1C(c1c(c2 ccc(c3ccncc3)nc2s 1)N)=O)F | 8020-1052 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 892 | c1cc(cc(c1) [Cl])c1nnc2n1nc( N)s2 | 8020-1571 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 893 | C(COc1ccccn1)N Cc1ccsc1 | 8020-2578 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 894 | c1cc(ccc1c1cn[nH  ]c1)N | 8020-2683 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 895 | [H]N(CCNC(c1c(  N)non1)=O)Cc1c( ccc2ccccc12)OCc1 ccccc1 | 8104-04425 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 896 | [H]N(CCNC(c1c(  N)non1)=O)Cc1cc (ccc1OCc1ccccc1[ Cl])[Br] | 8104-04684 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 897 | [H]N(CCNC(c1c(  N)non1)=O)Cc1cc (ccc1OCc1ccccc1) [Cl] | 8104-04926 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 898 | C(CN)c1nnc(o1)S Cc1ccc(cc1[Cl]) [Cl] | 8388-1007 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 899 | C(CN)c1nnc(o1)S Cc1c(cccc1[Cl]) [Cl] | 8388-1008 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 900 | C(COc1ccc2c(c1)c 1ccccc1o2)N.[Cl] | 9188721 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 901 | c1c(cc2c(c1[Cl])nc (N)s2)F | 9190966 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 902 | C(c1ccc2c(c1)OC O2)Nc1cc(nc(N)n 1)[Cl] | 9205277 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 903 | CCOc1ccc2c(c1)sc (NC(CSc1nc(N)n[ nH]1)=O)n2 | 9207725 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 904 | Cc1cccc(c1C)n1c( c2c(c3cccnc3s2)N) nnc1S | 9209599 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 905 | C(CNC(c1c(c2ccc( c3ccccn3)nc2s1)N  )=O)c1c[nH]c2ccc cc12 | 9212199 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 906 | CCN(CCCC/ C1=N\O)CCCC/ C1=N\O | 96491 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 907 | c1ccc2c(c1)nc(c1c cc(cc1[Cl])N)s2 | C066-5322 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 908 | CC(C)c1ccc(cc1)N c1c(c2ccccc2O)nc 2cnccn12 | C169-0255 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 909 | COc1ccc(cc1OC) C(c1c(c2ccccc2o1) N)=O | C200-2690 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 910 | CSc1c(c(N)n(Cc2c cccc2)n1)S(c1cccc c1)(=O)=O | C200-4138 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 911 | CCOC(c1c2c(nc3c cccc3n2)n(Cc2ccc | C201-0688 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | c(c2)OC)c1N)=O |  |  |  |  |  |
| 912 | CC1CCN(CC1)c1 nc(c(C(=O)OC)s1) N | C201-1740 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 913 | Cc1ccccc1Nc1c(c2 ccncc2)nc2ccc(cn1 2)[Br] | C273-0281 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 914 | Cc1ccccc1Nc1c(c2 ccc(cc2)N2CCOC C2)nc2ncccn12 | C273-0340 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 915 | c1cc(ccc1c1cc[nH] n1)N | C430-1098 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 916 | COc1ccc(cc1)c1nc (Nc2ccc(cc2F)F)o n1 | C749-0018 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 917 | Cc1c(CCC(Nc2ccc (CN3CCCCC3)cc 2)=O)c(C)n2c(n1)  nc(CN)n2 | C908-0509 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 918 | Cc1ccc(cc1C)C(c1 c(c(C(Nc2cccc(c2) F)=O)c2ccccn12) N)=O | D033-0127 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 919 | Cc1ccc2c(c1)C(C1  =C(C(N(CCCO)C 13C(N(CC=C)c1c cccc13)=O)=O)O2  )=O | D063-1068 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 920 | Cc1ccc2c(c1)C(C1  =C(C(N(CCO)C13  C(N(CC=C)c1cccc c13)=O)=O)O2)= O | D063-1117 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 921 | CCCCC(CC)n1c(c c(n1)O)N | D068-0219 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 922 | CC(C)CNc1c(nc(c 2ccccc2)o1)S(c1cc c(cc1)[Cl])(=O)=O | D072-0403 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 923 | CC(C)Nc1c2c(c(C  )nn1)nnn2Cc1cccc c1[Cl] | D172-0473 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 924 | CC(CCC(NCCc1n  c2ccccc2n1Cc1c(C  )c(C)cc(C)c1C)=O  )O | D186-0394 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 925 | Cc1cc(Nc2ccccc2) n2c(n1)nc(c1ccc(c c1)[Cl])n2 | D245-0159 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 926 | CC(c1cccc(c1)Nc1 cc(c2ccc(cc2)OC) nc(C)n1)=O | D482-2054 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 927 | Cc1cc(NCC(N2C  CN(CC2)c2ccc(cc 2)F)=O)n2c(n1)nc(  c1cccnc1)n2 | D494-0506 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 928 | Cc1ccc2cc(c(Nc3c cc(cc3)F)nc2c1)c1 nc(C)on1 | D704-1692 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 929 | CCOC(c1cnc2c(c3 ccc(cc3) [Br])c(C)nn2c1N)  =O | D718-0691 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 930 | c1ccc(cc1)n1c(c(c 2nc3ccccc3s2)nn1) | D731-0066 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | N |  |  |  |  |  |
| 931 | CCC(C) (C)NC1=C(C(C1=  O)=O)c1ccc(C)cc1 | E470-0146 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 932 | CCC(C)NC1=C(C (C1=O)=O)c1ccc( cc1)C(C)C | E511-0764 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 933 | CCOc1ccc(cc1)c1 nc(c2c(N)n(c3cccc (c3C)[Cl])nn2)on1 | E595-0532 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 934 | COc1ccc(c(c1)c1n c(Nc2cc(ccc2OC) [Cl])on1)OC | E679-0020 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 935 | C[N+](C)  (C)CC(O)=O | NCGC00015150- 04 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 936 | CN(C)CCN(Cc1cc  c(cc1) [Cl])c1ccccn1 | NCGC00016672- 04 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 937 | C(c1cc(ccc1c1cn[n H]c1)NC(Nc1nnc( c2ccncc2)s1)=O)# N | NCGC00247866- 04 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 938 | C(C(Nc1ccc(cc1)n 1c(cc(C(F) (F)F)n1)c1ccc2c(c cc3ccccc23)c1)=O  )N | NCGC00346490- 01 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 939 | CC(C)n1cnc2c(Nc 3cccc(c3)NC(C=C  )=O)nc(NC3CCC( CC3)N(C)C)nc12 | NCGC00346964- 01 | PreQ1 | Pseudoknot | AGAGGUUCUAGCUACACCCUCU AUAAAAAACUAA | 1 |
| 940 | C(=Cc1nc2ccccc2 o1)c1ccc(cc1)N | 0632-0836 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 941 | Cc1ccc(cc1)NCC( c1ccc(cc1)c1ccccc 1)=O | 0836-0042 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 942 | C1c2ccccc2c2ccc( cc12)c1csc(N)n1 | 0846-0051 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 943 | Cc(cccc1)c1NC(N CCN1CC1)=O | 101266 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 944 | O=C(NCCCN1CC  1)Nc1cccc2ccccc1 2 | 101298 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 945 | Nc1nc(N)nc(Nc(cc 2)ccc2Br)c1/C=N/ c(cc1)ccc1Br | 103520 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 946 | [O-][N+]  (c(cc1)cc(C(c2c3)  =O)c1-c2cc(Br)c3/ N=C(/C(F)(F)F)\ NO)=O | 107582 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 947 | C(CSc1nc(cccc2)c 2s1)Nc1ccccc1 | 117908 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 948 | C1CC(CNC1)  (CNCc1cccc(c1)O Cc1ccccc1)O | 12262594 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 949 | C1C(CN)Oc2c1cc(  cc2F)c1ccc2c(cco2  )c1 | 12766557 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 950 | CC(c1cc(c2ccccc2  ) [nH]n1)N(C)C(c1c n(CCN)nn1)=O | 12801231 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 951 | C1C(CN)Oc2c1cc(  cc2[Cl])c1ccc(cn1) C(N)=O | 13047935 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 952 | O=C1OC(c2cc(-  c3ccccc3)nc3ccccc 23)=NN1 | 130847 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 953 | C1C(CN1Cc1ccc(  cc1)OCCO)Oc1cc ccc1[Cl] | 13202927 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 954 | Nc(ccc(Oc(cc1)cc( [N+]  ([O-])=O)c1N)c1)c  1[N+]([O-])=O | 133351 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 955 | CC(C)Oc1cc(NCC  2=Cc3ccc(cc3NC2  =O)F)nc(N)n1 | 13416689 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 956 | CN(CCO)C[C@@  H]1CN(Cc2cccc3c 4ccccc4sc23)C[C @@H]1CO | 13609905 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 957 | CN(Cc1cccc(c1)O CC=C)c1c2ccccc2 nc(CCN)n1 | 13692816 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 958 | C1CC(CCc2ccccc 2C(F) (F)F)CN(C1)C(CN  )=O | 13741411 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 959 | NCC(Nc(ccc(Cl)c 1)c1C(c1ccc[nH]1  )=O)=O | 140873 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 960 | C1CCC(C1)  (C#N)c1ccc(cc1)c 1cccc2CNCCc12 | 14224931 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 961 | Cc1cc(NC(Nc(cc2  )ccc2SC)=O)ncc1 | 142269 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 962 | C1COCC(CN1)C  NC(Nc1cccc(c1)c1 ccc(cc1)F)=O | 14244960 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 963 | CN(C)c1c(cnc(c2c ccc3CC(CN)Oc23) n1)F | 14250223 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 964 | Cc1ccc(c2ccccc2C CN)c2cccnc12 | 14279637 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 965 | C1CNCc2cc(C(N  C3c4ccccc4c4cccc c34)=O)nn2C1 | 15136552 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 966 | Cc1c(cc(cc1[Cl])C (NCC(Cc1ccco1)C O)=O)[Cl] | 15537048 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 967 | C1CN(CCC1Oc1c  cc(cc1)F)c1cc(NC CO)nc(N)n1 | 15760058 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 968 | C1CC(CN(C1)CC  NC(c1ccc2c(ccs2) c1)=O)CO | 15947215 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 969 | CCOc1ccc(CN2C CC(CC2)  (C(O)=O)Oc2cccc | 16013629 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | (c2)F)cc1CO |  |  |  |  |  |
| 970 | C(CN)c1cccc(c1)c 1ccc(cc1[Cl])F | 16088353 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 971 | Cc1c(C(C(NCCNc  2cccnc2)=O)N)c(C  )[nH]n1 | 16899791 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 972 | Cc1cc2CC(CN)Oc  2c(c1)c1cnc2ccccc 2n1 | 17587941 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 973 | C1CC(CNC1)c1cc  (c2ccc(c(c2)[Cl])  [Cl])nc(c1C#N)N | 17917068 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 974 | CCCC(c1cccs1)Nc 1c2CCNCc2nc(c2 cccnc2)n1 | 17936868 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 975 | C1CC(c2cccc(c2)c 2cc(N)nc3c2cc[nH  ]3)NC1 | 18100777 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 976 | C1[C@@H]  (CNC(Nc2cc(cc(c 2[Cl])F)F)=O)NC[ C@H]1F | 18739450 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 977 | C(CN)c1ccc(CN2 CCC(CC2)  (c2cccc(c2)C(F)  (F)F)O)cc1 | 18809502 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 978 | CC(c1ccc2c(cc[nH  ]2)c1)NC1CCN(C  C1)c1c2c(ncn1) [nH]cn2 | 18958506 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 979 | C1CCN(C1)C(CC  c1cc2CN(CCn2n1) C(C1CNCCO1)=O  )=O | 18969954 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 980 | Cc1c(cccc1NCc1c cccn1)C(Nc1cnc2 CCCCn12)=O | 19005272 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 981 | C(CN)c1nncn1c1c ccc2ccccc12 | 19267055 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 982 | Cc1nc(CCN)cc(n1  )N1CCN(CC1)c1c  cccc1[Cl] | 19416537 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 983 | Cc1ccc(cc1[Cl])N 1CCC(CC1)N[C@ @H]1CC[C@H] (C1)N | 19498560 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 984 | C1CNCc2c1c(NC C[C@@H]1C[C@ H]3C[C@@H]1C  =C3)nc(c1cccnc1) n2 | 20252371 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 985 | Cc1cc(cc(c1CNc1 c2CCNCc2nc(C)n 1)[Cl])[Cl] | 20278440 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 986 | CCCCOc(cc1)ccc1 OC(Nc(cc(cc1)Cl) c1OC)=O | 205832 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 987 | Cc1cccc(NC(Nc2n c(C)ccc2)=S)n1 | 20618 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 988 | Cc1cccnc1NC(Nc 1ncccc1C)=S | 20619 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  |  |  |  |  | AAAAAGGG |  |
| 989 | C1CNCc2c1c(NC  C1COc3ccccc3O1  )nc(c1cccnc1)n2 | 20674759 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 990 | CC(c1ccc(cc1)c1c cc(c(c1)F)NC(CN)  =O)OC | 20734365 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 991 | C1CN(CCC1NCC  c1c[nH]cn1)c1nc2 ccc(cc2s1)[Cl] | 20802556 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 992 | C1Oc2ccc(cc2O1) c1c(C#N)c(N)n2c3 ccccc3nc2c1C#N | 2144-0693 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 993 | COc1cccc(c1)c1cc ccc1NC(C1CCN(  CC1)c1ccnc(N)n1)  =O | 21531690 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 994 | COc(cc1)ccc1/ N=N/c1c(N) [nH]nc1N | 21678 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 995 | COc1ccc(CCN(Cc 2ccncc2)C(CC2C OCCN2)=O)cc1 | 21791855 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 996 | C(CNc1cccnc1)N C(c1cnc(Nc2ccccc 2)nc1)=O | 22517399 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 997 | Cc1c2ccc(cc2oc1C (NCCCNc1cccnc1  )=O)OC | 22734195 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 998 | Cc1c2c(ncnc2sc1C  )N1C[C@H]  (c2ccc(cc2)OC) [C@H](C1)N | 25720738 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 999 | C1CN(Cc2c(c3ccc c4ccccc34)noc12) C(c1cc(N)  [nH]n1)=O | 26633940 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1000 | C1CNCC1NS(c1c  ccc(c1)C(NCCc1c cccc1)=O)(=O)=O | 26804304 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1001 | COc1ccc(CCCNc2 c3CCNCCc3nc(N)  n2)cc1OC | 27263777 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1002 | Cc1cc2c(cc1C)oc( c1ccc(cc1O)N)n2 | 2783-3499 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1003 | c1cc(cc(c1) [Cl])n1nc2ccc(cc2 n1)N | 2810-4198 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1004 | c1cc(c2cccc(c2c1) [Br])c1nc2cc(ccc2 o1)N | 2810-4224 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1005 | CCCOc(cc1)ccc1- c1nc(- c(cc2)ccc2N)cs1 | 281624 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1006 | Nc1ccc(Cn(ccc2c3 4)c2ccc4nc(N)nc3 N)cc1.Cl | 309401 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1007 | C(c1ccc(cc1)c1nc( c2ccc(c(c2)F)F)nn 1CCO)N | 31242301 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1008 | Cc1c(c2c(c3ccccc 3)ncn2CCCN(CC | 31750799 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | O)CCO)[nH]cn1 |  |  |  | AAAAAGGG |  |
| 1009 | C1CNCc2cc(CC3  Cc4ccccc4OC3)cc c12 | 31917501 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1010 | C1CN(CCC1NCc1  nc(N) [nH]n1)c1nc2ccc(c c2s1)[Cl] | 32629911 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1011 | C1CC(C(CC(N2C  C(c3ccccc3C2)O)  =O)=C1c1ccccc1)  =O | 32885020 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1012 | C1CN(CCC1n1cc(  c2cccnc2)nn1)c1c 2c(nc(N)n1) [nH]cn2 | 33118185 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1013 | Nc1n[nH]c(Nc2cc ccc2)n1 | 331208 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1014 | COc(cc12)ccc2nc( cc(cc2)Cl)c2c1C# N | 33173 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1015 | Clc(ccc(- c1c(Cc2c- 3cccc2)c3n[nH]1)c 1)c1Cl | 331968 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1016 | C1CC(CCN(C1)C(  CCc1ccc(c2ccc(cc 2)[Cl])[nH]1)=O) (CO)O | 33269848 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1017 | Cc1ccc(cc1)c1cc( C(N[C@@H]2CN C[C@H]2O)=O)c  2ccccc2n1 | 33446163 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1018 | COc1ccc2cc(ccc2c 1)c1ccccc1CN | 33557632 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1019 | Cc1ccc2c(c1)c(CN c1c3CCNCc3nc(N  )n1)nn2C | 34365043 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1020 | COc1cccc(c1)c1nc c(CNC([C@H]2C C[C@H] (C2)N)=O)s1 | 35144470 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1021 | C(CN)C1CN(CCO  1)c1cc(c2ccccc2)n c2ccnn12 | 35432137 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1022 | Cc1cc(ccc1[Br])c1 nc2cc(ccc2o1)N | 3617-0633 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1023 | CCCCc1ccc(cc1)n 1nc2ccc(cc2n1)N | 3738-4868 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1024 | CCC(CC) (C(N)=O)SCC=C | 37883 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1025 | CC(c1ccc(cc1)c1c cc(cc1)c1nnc(N)s1  )N1CCOCC1 | 39723040 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1026 | COc1ccccc1OC1C CN(CC1)Cc1cccc( CCN)c1 | 39780332 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1027 | C1CSCCN1S(c1cc  c(cc1)c1ccc2c(c1) | 39837810 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | c(N)n[nH]2) (=O)=O |  |  |  | AAAAAGGG |  |
| 1028 | Cc1cc(C)n(CC(CO  c2ccc(cc2) [Cl])O)n1 | 4013-0076 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1029 | Cc1ccc(cc1)S(N(C C(CN1CCCCC1)  O)c1ccccc1OC) (=O)=O | 4013-2178 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1030 | NC(NC(Nc(cc1)cc c1Cl)=S)=N | 403374 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1031 | Cc(cc1)ccc1C1=C SSC1=S | 40467 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1032 | C(Cc1ccccc1)CN1 CCCN(CC1)c1cc(  N)nc(N)n1 | 41736108 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1033 | Cc1cccc(c1OCCN C(c1cn(CCN)nn1)  =O)[Cl] | 41830928 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1034 | COc1ccc2cc(ccc2c 1)C1CN(CCO1)C(  c1cc(N)[nH]n1)=O | 42028139 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1035 | CCNC(c1cccc(c1) c1ccc(cc1CN)F)= O | 42044437 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1036 | C1CNCc2c1c1c(N  Cc3cc(c4ccco4)on 3)ncnc1s2 | 42424648 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1037 | Cc1cc(c(cc1[Cl])O C)NC(c1ccccc1C1 CCNC1)=O | 45877478 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1038 | C1CN(CC(C(O)=  O)N1)c1nnnn1c1c cc(cc1)Oc1ccccc1 | 46257953 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1039 | Cc1ccsc1CN(CCN (C)C)C(CN)=O | 47645371 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1040 | C1CN(CCC1Nc1c  2CNCc2nc(c2cccn c2)n1)Cc1ccccc1 | 48129446 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1041 | CC[n+]1cn(CC(C  Oc2cccc(c2)OC)O  )c2ccccc12 | 5010-0656 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1042 | Cc1nc(SC)nc(N2C C2)c1Br | 50199 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1043 | Nc(cc1)ccc1NC(N c1ccccc1)=S | 509563 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1044 | Cc1nc2cc(c(cc2n1 CCCO)[Cl])[Cl] | 5119828 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1045 | c1ccc(cc1)Oc1ccc( cc1N)C(c1ccc(c(c 1)N)Oc1ccccc1)= O | 5172392 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1046 | CCOC(c1cnc2c(C) cc(C)cc2c1NCC(C  )O)=O | 5174-4431 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1047 | c1ccc(cc1)C(c1cc( ccc1N)Sc1ccc(c(c | 5180537 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | 1)C(c1ccccc1)=O) N)=O |  |  |  | AAAAAGGG |  |
| 1048 | C(C(NN=Cc1c(ccc c1[Cl])  [Cl])=O)Nc1cccc2 ccccc12 | 5201830 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1049 | CCCCCc1ccc(cc1) c1ccc(cc1)c1ncc(c n1)N | 5213078 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1050 | c1ccc2c(ccc(c2c1) Oc1ccc(cc1[Cl])N) [Cl] | 5215844 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1051 | CC(c1ccc(cc1)Oc1 ccc(cc1)N)=O | 5228159 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1052 | C1CCN(CC1)CC(  Cn1c2ccc(cc2c2cc (ccc12)[Cl])[Cl])O | 5236854 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1053 | CC12CCC(CN(CC  (Cn3c4ccc(cc4c4c c(ccc34)[Br])  [Br])O)C1)C2(C)C | 5236945 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1054 | c1ccc(cc1)c1c(cn( c2ccccc2)n1)C(Nc 1cc(cc(c1)Oc1cccc c1)N)=O | 5248546 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1055 | c1ccc2c(c1)ccc(c2 [Cl])Sc1ccc(cc1[C l])N | 5250905 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1056 | [H]N([H])c1c(C#  N)c2c(nc3ccccc3n 2)n1Cc1ccccc1 | 5253879 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1057 | C1CN(CCN1CC(  Cn1c2ccccc2c2ccc cc12)O)Cc1ccccc1 | 5320336 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1058 | CC(c1ccc(cc1)N)= NNc1nc(C)cc(c2cc ccc2)n1 | 5339282 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1059 | C(C(NN)=O)Nc1c  cc(cc1[Br])[Cl] | 5345379 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1060 | Cc1cc(ccc1NCC( NN)=O)I | 5346837 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1061 | CC1CCCCC1=NN  C(CNc1ccc(cc1C)I  )=O | 5347443 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1062 | c1cc(ccc1c1cc(C( NN)=O)c2cc(ccc2 n1)[Br])N | 5350878 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1063 | Cc1ccccc1Cn1c2c cccc2nc1c1c(N)no n1 | 5408-3036 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1064 | Brc(cc1)ccc1- c1csc(/N=C2/ SC=C(c(cc3)ccc3 Br)N2)n1 | 55691 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1065 | Cc1c2cc(CNC(c3c c(N)  [nH]n3)=O)ccc2[n H]c1c1ccccc1F | 56075039 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1066 | C1CCC(C1)NCC(  COc1ccc(cc1)OC C(CNC1CCCC1) | 5648415 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | O)O |  |  |  |  |  |
| 1067 | [H]N([H])c1nc(n[n H]1)SCCCCCCC CC | 5655427 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1068 | C(c1ccccc1)Oc1cc c(cc1)C1Nc2cccc3 cccc(c23)N1 | 5661401 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1069 | COc1cc(c(cc1NC( C(NCCN1CCNCC 1)=O)=O)OC)[Cl] | 5688029 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1070 | C(=Cc1ccc(cc1[Cl  ])  [Cl])C(c1cccc(c1) N)=O | 5689908 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1071 | Cc1ccc(C(NCCNc 2ccc(cc2[N+]  ([O-])=O) [Cl])=O)o1 | 5717805 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1072 | C(CN1CCOCC1)  C(Nc1ccc(cc1C(c1 ccccc1)NCC(NN)  =O)[Br])=O | 5808034 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1073 | C(C(Cn1c2ccc(cc2 c2cc(ccc12)[Br]) [Br])O)NCc1ccco1 | 5864844 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1074 | [H]N(Cc1cc(c(c(c 1) [Cl])OCC(N)=O)O  C)c1ccc(cc1)N1C COCC1 | 5868-0480 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1075 | C(CN)c1nc(c2cccc c2n1)NCc1cn[nH] c1c1cccs1 | 58789773 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1076 | C(CCO)CN(Cc1cc  ccc1)c1c2ccccc2nc (CCN)n1 | 58803915 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1077 | Cc1c2c(nc(CCN)n c2sc1C)N(CCN(C)  C)Cc1ccccc1 | 59025931 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1078 | COc1cc(CC=C)cc c1OCC(CN1CCC(  CC1)Cc1ccccc1)O  .[Cl] | 6046571 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1079 | C1CCCCCc2c(CC CC1)c(C(N)=O)c( N)s2 | 6132195 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1080 | Nc(cc1)ccc1- c(nc12)c(- c(cc3)ccc3N)nc1n c(N)nc2N | 61642 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1081 | C(c1c(cc(c2ccc(cc 2)F)nc1N)c1cccnc 1)#N | 6233-1975 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1082 | [H]N(Cc1cc(c(c(c 1)  [Cl])OCc1cccs1)O CC)Cc1cccnc1 | 6408-0223 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1083 | C(c1ccco1)NC1C( c2cccc3cccc1c23) NS(c1ccc(cc1) [Cl])(=O)=O | 6432111 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1084 | O=C(c(cc1)cc(C(N c(cc2)ccc2C2=NC CN2)=O)c1Cl)Nc(  cc1)ccc1C1=NCC | 67436 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | N1 |  |  |  |  |  |
| 1085 | C(CC(=O)OC1C(  Nc2ccc(cc2C(c2cc ccc2[Cl])=N1) [Br])=O)CN.[Br] | 6748287 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1086 | Nc1cc(N=[N+]  (c2c(C3)ccc(N)c2) [O-])c3cc1 | 70534 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1087 | CC1C=C(C)C2C( C)C1(CO)COC2c1  ccccc1O | 8005-2272 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1088 | C(c1ccccc1)c1nnc( N)s1 | 8008-6271 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1089 | C1CCc2c(C1)c(C(  c1ccccc1)=O)c(N) s2 | 8010-1935 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1090 | Cc1c(CCNCc2ccc( C#N)cc2)c2cc(ccc 2[nH]1)OC | 8013-2954 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1091 | Nc(cc1)cc(Cc2c3) c1-c2cc(Cl)c3Cl | 80141 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1092 | Cc1c(c2csc(Nc3cc cc(c3)C(F) (F)F)n2)sc(C)n1 | 8015-5644 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1093 | CCN1CCc2c(C1)c  c1c(c(C(Nc3ccc(cc 3)C(F) (F)F)=O)sc1n2)N | 8016-6889 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1094 | C1C(c2ccc(c(c2) [Br])F)c2c(NC1=  O)nc(N)s2 | 8019-3634 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1095 | C1CN2C(=CSC2=  N1)c1cccc(c1)N | 8019-6474 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1096 | CN1C(c2c(cn(c3cc ccc3N)c2c2ccccc2 F)N(C)C1=O)=O | 8019-7142 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1097 | c1cc(N)nc2c1ccc( n2)O | 8019-7722 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1098 | COc1ccc(cc1)c1c( CN)c[nH]n1 | 8019-7792 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1099 | c1cnccc1c1nc2ncn c(N)n2n1 | 8020-2786 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1100 | Cc1c2[nH]c(cccc3  )c3c2ccc1CCN | 81703 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1101 | CCc1ccc(cc1)OCC #CCNCC=C | 9118214 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1102 | CCNCC#CCOc1c  cc(cc1)[Br] | 9126666 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1103 | Cc1ccc(c(c1) [Cl])OCC#CCNC. [Cl] | 9128115 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1104 | CC(c1ccc(cc1)c1c cc(CNCCc2c[nH]c 3ccccc23)o1)O. | 9135919 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | [Cl] |  |  |  |  |  |
| 1105 | c1c(cc2c(c1[Cl])nc (N)s2)F | 9190966 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1106 | COc1cc(cc(c1OC) OC)c1nc(c2cccc(c 2)N)n[nH]1 | 9204334 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1107 | CCOc1ccc2c(c1)sc (NC(CSc1nc(N)n[ nH]1)=O)n2 | 9207725 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1108 | CSc1ccc(cc1)OCC N | 9254473 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1109 | Cn1c(c(C(C=C2)=  O)c(cc3)C2=O)c3c 2c1cccc2 | 92937 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1110 | S=C1Oc(ccc(- c2ccccc2)c2)c2N1 | 93817 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1111 | CCN(CCCC/ C1=N\O)CCCC/ C1=N\O | 96491 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1112 | c1ccc2c(c1)nc(c1c cc(cc1[Cl])N)s2 | C066-5322 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1113 | Cc1cccc(c1)NCc1 nc2ccccc2n1C | C147-0043 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1114 | C(c1ccc(cc1) [Cl])N1c2ccccc2C 2=C(C(C(C#N)=C  (N)O2)c2ccccc2)S 1(=O)=O | C200-3388 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1115 | CSc1c(c(N)n(Cc2c cccc2)n1)S(c1cccc c1)(=O)=O | C200-4138 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1116 | CC1CCN(CC1)c1 nc(c(C(=O)OC)s1) N | C201-1740 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1117 | CCN1CCc2c(C1)c  c1c(c(C(Nc3ccccc 3C)=O)sc1n2)N | C611-0673 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1118 | C(CCCN=C(N)N=  C(N)Nc1ccc(cc1) [Cl])CCN=C(N)N  =C(N)Nc1ccc(cc1) [Cl] | NCGC00016246- 12 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1119 | CCN1C=C(C(O)=  O)C(c2cc(c(nc12) N1CCNCC1)F)=O | NCGC00016927- 10 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1120 | c1cc2C(c3cc(cc(c3 C(c2c(c1)O)=O)O) C(O)=O)=O | NCGC00018199- 06 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1121 | [H] [C@@]12CC[C@  @H] ([C@@]1(C)CC[C  @]1([H])  [C@@]3([H])CCC (C=C3CC[C@]12[ H])=O)OC(CCc1c  cccc1)=O | NCGC00159356- 02 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1122 | CCCCN(CCCC)C  C(c1cc(cc2C(=Cc3 ccc(cc3) | NCGC00167490- 02 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | [Cl])c3cc(ccc3c12) [Cl])[Cl])O |  |  |  |  |  |
| 1123 | CCCCN(CCCC)C  CC(c1cc2c(cc(cc2 c2cc(ccc12)C(F) (F)F)[Cl])[Cl])O | NCGC00179250- 04 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1124 | CCCCCCCCCCC CCCCC(=O)O[C @@H]1[C@H] ([C@H]([C@@H]  ([C@@H]([C@H] (C) [Cl])NC([C@@H] 2C[C@@H] (CCC)CN2C)=O)  O[C@@H]1SC)O)  O.[Cl] | NCGC00185773- 02 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1125 | Cc1ccc(cc1c1ccc2 c(c1)cnc(NCCN1C COCC1)n2)C(Nc1  cccc(c1)C(F)  (F)F)=O | NCGC00263206- 02 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1126 | C[C@@H](C(C)  (C)C)NCc1ccc2c(c 1)nc(NC(c1ccc(c3 cn[nH]c3)s1)=O)n 2CCc1ccccc1 | NCGC00344999- 01 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1127 | C=CC(Nc1ccc2c(c 1)c(Nc1ccc(c(c1) [Cl])OCc1cccc(c1) F)ncn2)=O | NCGC00346478- 02 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1128 | C(C(Nc1ccc(cc1)n 1c(cc(C(F) (F)F)n1)c1ccc2c(c cc3ccccc23)c1)=O  )N | NCGC00346490- 01 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1129 | CN1CCN(CC1)c1  ccc(cc1)Nc1ncc(c( n1)Sc1cccc(c1)NC (C=C)=O)[Cl] | NCGC00346497- 01 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1130 | Cc1ccccc1C(c1ccc (cc1[Cl])Nc1ccc(c c1N)[Br])=O | NCGC00346804- 01 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1131 | CCC(=C(c1ccc(cc 1)O)c1ccc(cc1)OC CNC)c1ccccc1 | NCGC00346806- 01 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1132 | C1CC1NCc1cccc( c1)NC1=CC(=c2c cc(cc2)=C2C=CC( C=C2O)=O)NN1 | NCGC00346954- 01 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1133 | CC(C)n1cnc2c(Nc 3cccc(c3)NC(C=C  )=O)nc(NC3CCC( CC3)N(C)C)nc12 | NCGC00346964- 01 | SAM\_ll | Pseudoknot | UCGCGCUGAUUUAACCGUAUUG CAAGCGCGUGAUAAAUGUAGCU AAAAAGGG | 1 |
| 1134 | CCN(CC)CCOC(c  1ccc2c(c1)sc(NC(c 1ccc(cc1)N)=O)n2  )=O | 0812-1025 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1135 | Cc(cccc1)c1NC(N CCN1CC1)=O | 101266 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1136 | O=C(NCCCN1CC  1)Nc1cccc2ccccc1 2 | 101298 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1137 | Nc1nc(N)nc(Nc(cc | 103520 | TPP | Three-way | CAGUACUCGGGGUGCCCUUCUG | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | 2)ccc2Br)c1/C=N/ c(cc1)ccc1Br |  |  | junction | CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG |  |
| 1138 | CCC(C)N(C(C)=C  1)N(C(C)CC)C1= O | 120844 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1139 | Cc1cc(nc2cc(ccc1 2)OC)N1C[C@H]  (C2CC2)[C@H] (C1)N | 12182839 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1140 | Cc1nc(CCN)cc(n1  )N(C)Cc1cccc(c1)  C(F)(F)F | 12267434 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1141 | C1CN(Cc2ccccc12  )c1c2CCNCc2nc(c 2cccnc2)n1 | 12634687 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1142 | C1C(CN)Oc2c1cc(  cc2F)c1ccc2c(cco2  )c1 | 12766557 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1143 | C(c1cc(ccc1F)c1cc c(cc1)c1csc(N)n1) O | 12892198 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1144 | O=C1OC(c2cc(-  c3ccccc3)nc3ccccc 23)=NN1 | 130847 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1145 | C1C(CN1Cc1ccc(  cc1)OCCO)Oc1cc ccc1[Cl] | 13202927 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1146 | C1CC(CCc2ccccc 2C(F) (F)F)CN(C1)C(CN  )=O | 13741411 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1147 | C1CCC(C1)  (C#N)c1ccc(cc1)c 1cccc2CNCCc12 | 14224931 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1148 | CC(C)CCOc1cccc (CCNC(C2CC3(C CNCC3)CN2)=O)  c1 | 14325308 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1149 | C1CN(CCC1C1C  CN(CCc2ccccc2)C 1)c1ccnc(N)n1 | 14604674 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1150 | Nc(cc1)ccc1C(Nc( cc1)ccc1Nc1ccncc 1)=O | 146770 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1151 | Cc1cc(nc(N)n1)N1 CCC(CC1)NCCC  N1CCc2ccccc12 | 15043866 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1152 | C(CN)c1cccc(c1)c 1ccc(cc1[Cl])F | 16088353 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1153 | Cc1c(cn(C)n1)NC( NCC(Cc1cccs1)C O)=O | 16859921 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  |  |  |  |  | CAGCGUAGGGAAGUGCUG |  |
| 1154 | Cc1c(C(C(NCCNc  2cccnc2)=O)N)c(C  )[nH]n1 | 16899791 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1155 | C1CNCc2c1c1C( N(C=Nc1s2)C1c2c  cccc2c2ccccc12)= O | 17311387 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1156 | C=Cc1ccc(nc1)N1 CCN(CC(C1)O)Cc  1ccccc1 | 17524156 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1157 | Cc1cc2CC(CN)Oc  2c(c1)c1cnc2ccccc 2n1 | 17587941 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1158 | C1CNCc2cccc(c3c ccc4c3cc[nH]4)c1 2 | 17741735 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1159 | C1CC(CNC1)c1cc  (c2ccc(c(c2)[Cl])  [Cl])nc(c1C#N)N | 17917068 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1160 | C1CN(CCC1(c1cc  ccc1)c1ccccc1)C(c 1cn(CCN)nn1)=O | 18373450 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1161 | Cc1nc(CCN)cc(n1  )N1CCN(CC1)c1c  cccc1[Cl] | 19416537 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1162 | Cc1ccc(cc1[Cl])N 1CCC(CC1)N[C@ @H]1CC[C@H] (C1)N | 19498560 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1163 | C1CNCc2c1c(NC C[C@@H]1C[C@ H]3C[C@@H]1C  =C3)nc(c1cccnc1) n2 | 20252371 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1164 | Cc1cc(cc(c1CNc1 c2CCNCc2nc(C)n 1)[Cl])[Cl] | 20278440 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1165 | CCCCOc(cc1)ccc1 OC(Nc(cc(cc1)Cl) c1OC)=O | 205832 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1166 | Cc1cccc(NC(Nc2n c(C)ccc2)=S)n1 | 20618 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1167 | Cc1cccnc1NC(Nc 1ncccc1C)=S | 20619 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1168 | C1CNCc2c1c(NC  C1COc3ccccc3O1  )nc(c1cccnc1)n2 | 20674759 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1169 | C1CN(Cc2c(c3ccc c4ccccc34)noc12) C(c1cc(N)  [nH]n1)=O | 26633940 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 1170 | C1COc2cc(ccc2C1  =O)c1cc2CC(CN)  Oc2c(c1)[Cl] | 26642358 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1171 | c1cc(cc(c1) [Cl])n1nc2ccc(cc2 n1)N | 2810-4198 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1172 | c1cc(c2cccc(c2c1) [Br])c1nc2cc(ccc2 o1)N | 2810-4224 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1173 | COc1ccc(CNCc2c ccc(c2)OC)cc1 | 2910-2885 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1174 | Nc1ccc(Cn(ccc2c3 4)c2ccc4nc(N)nc3 N)cc1.Cl | 309401 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1175 | Cc1ccc(cc1c1cccc( CCN)c1)F | 31003354 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1176 | CCc(cc(C(C)  (C)CCC1(C)C)c1c  1)c1-c1csc(C/C(/ N)=N/O)n1 | 310354 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1177 | C(c1ccc(cc1)c1nc( c2ccc(c(c2)F)F)nn 1CCO)N | 31242301 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1178 | CCC1CN(CCN1) C(c1coc(CN2CCN  (CC2)c2ncccn2)n1  )=O | 31761532 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1179 | C(CNC1NC(C2C CNCC=2N=1)=O)  C(c1ccc(cc1)F)c1c cco1 | 31828522 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1180 | C1CNCc2cc(CC3  Cc4ccccc4OC3)cc c12 | 31917501 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1181 | Cc1c2cc(cc(CNC([ C@H]  (Cc3c[nH]cn3)N)= O)c2[nH]c1c1cccc c1)[Cl] | 34268481 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1182 | Cc1ccc2c(c1)c(CN c1c3CCNCc3nc(N  )n1)nn2C | 34365043 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1183 | COc1cccc(CNCc2 cccc(c2)F)c1OC | 3702-1553 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1184 | Cc1ccc(cc1)S(N(C C(CN1CCCCC1)  O)c1ccccc1OC) (=O)=O | 4013-2178 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1185 | Cc(cc1)ccc1C1=C SSC1=S | 40467 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1186 | C(c1ccc(cc1[Cl]) | 4052-1804 | TPP | Three-way | CAGUACUCGGGGUGCCCUUCUG | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | [Cl])c1cnc(N)s1 |  |  | junction | CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG |  |
| 1187 | Cc1cccc(c1OCCN C(c1cn(CCN)nn1)  =O)[Cl] | 41830928 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1188 | COc1ccc2cc(ccc2c 1)C1CN(CCO1)C(  c1cc(N)[nH]n1)=O | 42028139 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1189 | [H]c1nc2CCNCCc 2c(n1)N1CCC(C1)  (c1ccccc1)O | 42335780 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1190 | COc1cccc(c1c1cc( CN)ccc1F)[Cl] | 42929743 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1191 | Cc(cc1)cc(S(N) (=O)=O)c1/N=N/  c(cc1)c(C)cc1N | 45527 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1192 | C(CNc1cccnc1)C Nc1c2ccccc2nc(C CN)n1 | 47488116 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1193 | Cc1ccsc1CN(CCN (C)C)C(CN)=O | 47645371 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1194 | Cc1cnc(N)nc1NC C[C@@H]1C[C@ H]2C[C@@H]1C  =C2 | 47913504 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1195 | CCCCCCCCNc1c  ccc(c1)[Br] | 5117451 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1196 | Cc1nc2cc(c(cc2n1 CCCO)[Cl])[Cl] | 5119828 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1197 | CCCCNCC(COc1  c(ccc2c3C(N4CC CCCC4=Nc3sc12)  =O)[Br])O | 5124607 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1198 | CCN(CC)CC(COc  1c(ccc2c(C(=O)O CC)c(NC(C)=O)sc  12)[Br])O | 5130027 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1199 | c1ccc(cc1)Oc1ccc( cc1N)C(c1ccc(c(c 1)N)Oc1ccccc1)= O | 5172392 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1200 | CCOC(c1cnc2c(C) cc(C)cc2c1NCC(C  )O)=O | 5174-4431 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1201 | c1cc(ccc1c1c(c2cc c(cc2)F)nc2cc(ccc 2n1)Oc1ccc(cc1)N  )F | 5174475 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1202 | CCCCCc1ccc(cc1) c1ccc(cc1)c1ncc(c n1)N | 5213078 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  |  |  |  |  | CAGCGUAGGGAAGUGCUG |  |
| 1203 | c1ccc2c(ccc(c2c1) Oc1ccc(cc1[Cl])N) [Cl] | 5215844 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1204 | C1CCC2(CC1)Cc  1ccccc1c1c2c(N)n c(NN)n1 | 5232878 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1205 | C1CCN(CC1)CC(  Cn1c2ccc(cc2c2cc (ccc12)[Cl])[Cl])O | 5236854 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1206 | CC12CCC(CN(CC  (Cn3c4ccc(cc4c4c c(ccc34)[Br])  [Br])O)C1)C2(C)C | 5236945 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1207 | c1ccc(cc1)c1c(cn( c2ccccc2)n1)C(Nc 1cc(cc(c1)Oc1cccc c1)N)=O | 5248546 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1208 | Cc1ccc(cc1)NCCC C(NN=Cc1cccs1)= O | 5248916 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1209 | c1ccc2c(c1)ccc(c2 [Cl])Sc1ccc(cc1[C l])N | 5250905 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1210 | c1cc(ccc1C(Nc1cc c(cc1)Oc1ccc(cc1) NC(c1ccc(cc1)N)= O)=O)N | 5253020 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1211 | [H]N([H])c1c(C#  N)c2c(nc3ccccc3n 2)n1Cc1ccccc1 | 5253879 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1212 | C(C1=C(N)Oc2cc(  ccc2C12C(Nc1ccc (cc12) [Br])=O)N)#N | 5313703 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1213 | CC1(C)CC2=C(C(  c3nc4ccccc4[nH]3  )Nc3ccccc3N2)C( C1)=O | 5326075 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1214 | c1cc(ccc1c1cc(C( NN)=O)c2cc(ccc2 n1)[Br])N | 5350878 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1215 | CCCCOc1ccc(cc1) c1ncc(cn1)N | 5365506 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1216 | Brc(cc1)ccc1- c1csc(/N=C2/ SC=C(c(cc3)ccc3 Br)N2)n1 | 55691 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1217 | Cc1c2cc(CNC(c3c c(N)  [nH]n3)=O)ccc2[n H]c1c1ccccc1F | 56075039 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1218 | CCCn1c2ccccc2nc 1C(c1ccc(cc1)OC) O | 5652903 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 1219 | CC(c1ccc(cc1)N)= NNC(c1cc(C23CC 4CC(CC(C4)C3)C  2)n[nH]1)=O | 5791299 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1220 | CCNC(Cc1ccc(cc1  )c1cc2CC(CN)Oc2 c(c1)[Cl])=O | 57980040 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1221 | C(CN1CCOCC1)  C(Nc1ccc(cc1C(c1 ccccc1)NCC(NN)  =O)[Br])=O | 5808034 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1222 | c1ccc2c(c1)cc1cnc 3c(c(N)n[nH]3)c1 n2 | 6051011 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1223 | C1CCCCCc2c(CC CC1)c(C(N)=O)c( N)s2 | 6132195 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1224 | C(C(N1c2ccccc2S c2ccccc12)=O)Sc1 nnc(N)s1 | 6134473 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1225 | [H]N(Cc1cc(c(c(c 1)  [Cl])OCc1cccs1)O CC)Cc1cccnc1 | 6408-0223 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1226 | CC(C)c1cc(CCC2 C3(C)CCCC2(C)C  N)c3cc1.OC(c1ccc cc1)=O | 65238 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1227 | Cc1nc2ccccc2n1C C(COc1ccc(cc1)C 1CCC=C1)O | 6682831 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1228 | O=C(c(cc1)cc(C(N c(cc2)ccc2C2=NC CN2)=O)c1Cl)Nc(  cc1)ccc1C1=NCC N1 | 67436 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1229 | CS(c1ccc(c(c1) [N+]  ([O-])=O)NCC(Nc  1ccccc1SC(C(C(F) (F)F)(F)F)  (F)F)=O)(=O)=O | 6786638 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1230 | Cc1cc(C)c2c(c1)n c(c1ccc(cc1O)N)o 2 | 8007-0773 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1231 | CCOC(c1c2ccc(c( c2sc1NC(C)=O)O CC(CN1CCCCC1) O)[Br])=O | 8008-4440 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1232 | Nc(cc1)cc(Cc2c3) c1-c2cc(Cl)c3Cl | 80141 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1233 | CC(C)C1(CCNCc  2cccc3c2OCO3)C COC(C)(C)C1 | 8018-1268 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1234 | C1CN2C(=CSC2=  N1)c1cccc(c1)N | 8019-6474 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 1235 | Cc1c2[nH]c(cccc3  )c3c2ccc1CCN | 81703 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1236 | C(c1cccc2c1cc[nH  ]2)Nc1ccc(Cn2cnc n2)cc1 | 9189417 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1237 | Cc1cccc(c1C)n1c( c2c(c3cccnc3s2)N) nnc1S | 9209599 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1238 | C(CNC(c1c(c2ccc( c3ccccn3)nc2s1)N  )=O)c1c[nH]c2ccc cc12 | 9212199 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1239 | C(c1ccccc1)NC(C( c1ccccc1)Sc1nc(N  )n[nH]1)=O | 9241226 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1240 | C(C(N1c2ccccc2S c2ccccc12)=O)Sc1 nnc(N)[nH]1 | 9248541 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1241 | Oc(ccc([As](O)  (O)=O)c1)c1NC(c  1ccccc1)=O | 92892 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1242 | CCN1CCCC1CN  Cc1cccc(c1)OCc1 ccc(cc1)[Cl] | 9312203 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1243 | S=C1Oc(ccc(- c2ccccc2)c2)c2N1 | 93817 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1244 | CC[C@] (C(C=C1N2Cc3cc  4ccccc4nc13)=C(C O1)C2=O) (C1=O)O | 94600 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1245 | CCN(CCCC/ C1=N\O)CCCC/ C1=N\O | 96491 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1246 | c1ccc2c(c1)nc(c1c cc(cc1[Cl])N)s2 | C066-5322 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1247 | Cc1cccc(c1)NCc1 nc2ccccc2n1C | C147-0043 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1248 | CSc1c(c(N)n(Cc2c cccc2)n1)S(c1cccc c1)(=O)=O | C200-4138 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1249 | CC1CCN(CC1)c1 nc(c(C(=O)OC)s1) N | C201-1740 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1250 | CCN(CC)CCCNc1  c2ccccc2nc(c2nnc( c3ccc(C)cc3)o2)n1 | C660-1575 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1251 | C1CCCN(CC1)CC | C736-0159 | TPP | Three-way | CAGUACUCGGGGUGCCCUUCUG | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | CNc1nc2ccccc2c2 nc(c3ccccc3)nn12 |  |  | junction | CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG |  |
| 1252 | CCCc1nc2c3ccccc 3nc(NCCCN3CC  N(CC3)c3ccccc3F  )n2n1 | C736-0671 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1253 | COc1ccc(cc1)c1nc (Nc2ccc(cc2F)F)o n1 | C749-0018 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1254 | Cc1c(CCC(Nc2ccc c(c2)C(F) (F)F)=O)c(C)n2c(  n1)nc(CN)n2 | C908-0403 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1255 | Cc1c(CCC(Nc2ccc c(c2) [Br])=O)c(C)n2c(n 1)nc(CN)n2 | C908-0523 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1256 | Cc1c(CCC(NCC2 CCN(CC2)Cc2ccc (cc2)F)=O)c(C)n2  c(n1)nc(CN)n2 | C908-0552 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1257 | CC(c1nc2ccccc2n 1CCc1ccccc1)O | D011-4242 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1258 | C(Cc1nc2ccccc2n 1Cc1c(cccc1[Cl])F  )CO | D011-4273 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1259 | c1ccn2c(C(c3ccc(c c3) [Cl])=O)c(c(C(Nc  3cccc(c3)F)=O)c2 c1)N | D033-0008 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1260 | Cc1ccc(cc1C)C(c1 c(c(C(Nc2cccc(c2) F)=O)c2ccccn12) N)=O | D033-0127 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1261 | CC(C)c1ccc(CNc2 nc3nc(C)c(c(C)n3  n2)[Cl])cc1 | D043-0278 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1262 | Cc1ccc2c(c1)C(C1  =C(C(N(CCCO)C 13C(N(CC=C)c1c cccc13)=O)=O)O2  )=O | D063-1068 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1263 | Cc1ccc2c(c1)C(C1  =C(C(N(CCO)C13  C(N(CC=C)c1cccc c13)=O)=O)O2)= O | D063-1117 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1264 | [H]c1ccc(cc1)S(c1 c(NCC(C)C)oc(c2  ccccc2)n1)(=O)=O | D072-0402 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1265 | Cc1ccc(cc1)S(c1c( NCCOC)oc(c2ccc c(C)c2)n1)(=O)=O | D072-0517 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1266 | C(CNc1c(nc(c2ccc cc2)o1)S(c1ccc(cc 1)[Cl])  (=O)=O)Cn1ccnc1 | D072-0802 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 1267 | CCOc1cccc(c1)N1 CC(C(=C1N)c1nc  2ccccc2s1)=O | D086-0218 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1268 | C(CNC(c1c(CO)n  n(c2ccc(cc2)F)n1)  =O)c1ccccc1 | D217-0409 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1269 | CCOC(c1cccc(c1) Nc1cc(c2ccccc2)n cn1)=O | D278-0165 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1270 | Cc1nc(cc(Nc2cccc (c2)OC)n1)c1cccc c1 | D278-0401 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1271 | CN1C(N(C)c2cc(  COc3ccc(CNCc4c ccnc4)cc3OC)ccc1 2)=O | D300-0082 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1272 | CC1(C)CC(CCO1) CNCCN(C)C | D324-0105 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1273 | CC1(C)CC(CCNC 2CCN(C)CC2)  (CCO1)c1cccc(c1) C(F)(F)F | D442-0355 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1274 | Cc1ccc(cc1)C1(C CNCCN2CCOCC 2)CCOC(C)(C)C1 | D442-0384 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1275 | c1ccc(cc1)n1c(c(c 2nc3ccccc3s2)nn1) N | D731-0066 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1276 | CCc1ccccc1NC1C (C)=C(c2ccccc2)S (N=1)(=O)=O | E013-3228 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1277 | Cn1c2ccccc2c2c1n c(NCCCN1CCCC CC1)nn2 | E205-0046 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1278 | Cc1ccc(cc1C)C1= C(C(C1=O)=O)N  CCCc1ccccc1 | E470-0615 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1279 | CCOc1ccc(cc1)c1 nc(c2c(N)n(c3cccc (c3C)[Cl])nn2)on1 | E595-0532 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1280 | CCCNC1=C(C(C1  =O)=O)c1cc(C)c(  C)cc1C | E882-0500 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1281 | C(CCCN=C(N)N=  C(N)Nc1ccc(cc1) [Cl])CCN=C(N)N  =C(N)Nc1ccc(cc1) [Cl] | NCGC00016246- 12 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1282 | CCC(C)CCCCC(N  [C@@H] (CCN)C(NC(C(N[ C@H] (CCN)C(N[C@@  H]1CCNC(C([C@ | NCGC00094763- 03 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | @H] (C)O)NC([C@@H  ] (CCN)NC([C@@ H] (CCN)NC([C@@ H] (CC(C)C)NC([C@ H]  (Cc2ccccc2)NC([C @H] (CCN)NC1=O)=O  )=O)=O)=O)=O)= O)=O)=O)  [C@@H] (C)O)=O)=O |  |  |  |  |  |
| 1283 | CCCCN(CCCC)C  C(c1cc(cc2C(=Cc3 ccc(cc3) [Cl])c3cc(ccc3c12) [Cl])[Cl])O | NCGC00167490- 02 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1284 | C(c1cc(ccc1c1cn[n H]c1)NC(Nc1nnc( c2ccncc2)s1)=O)# N | NCGC00247866- 04 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1285 | Cc1cc(c2c3ccccc3 c(Nc3ccc(cc3)Oc3 c(cccn3)c3ccnc(N) n3)nn2)sc1 | NCGC00263094- 01 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1286 | C(CCN1CCCC1)C NC(Nc1c(C(N)=O  )c(ns1)OCc1c(cc(c c1F)[Br])F)=O | NCGC00263100- 01 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1287 | C[C@@H](C(C)  (C)C)NCc1ccc2c(c 1)nc(NC(c1ccc(c3 cn[nH]c3)s1)=O)n 2CCc1ccccc1 | NCGC00344999- 01 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1288 | C(C(Nc1ccc(cc1)n 1c(cc(C(F) (F)F)n1)c1ccc2c(c cc3ccccc23)c1)=O  )N | NCGC00346490- 01 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1289 | CCCCCCCCCCC  Cc1ccc(cc1)S(Nc1 nncs1)(=O)=O | NCGC00346547- 01 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1290 | CC(C)n1cnc2c(Nc 3cccc(c3)NC(C=C  )=O)nc(NC3CCC( CC3)N(C)C)nc12 | NCGC00346964- 01 | TPP | Three-way junction | CAGUACUCGGGGUGCCCUUCUG CGUGAAGGCUGAGAAAUACCCG UAUCACCUGAUCUGGAUAAUGC CAGCGUAGGGAAGUGCUG | 1 |
| 1291 | CC(c1ccc(c(c1)N) [Br])=O | 0054-0090 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1292 | Cc1nc2ccc(CCO)c c2s1 | 0133-0036 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1293 | c1ccc2c(c1)nc(Sc1 ccc(cc1)N)s2 | 0375-0603 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1294 | c1ccc2c(c1)nc(Sc1 ccc(cc1[Cl])N)s2 | 0375-0604 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1295 | c1cc2c(cc(c(c2nc1 | 0422-0091 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | )N)[Br])[Br] |  |  |  | ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA |  |
| 1296 | CCN(CC)CCOC(c  1ccc2c(c1)sc(NC(c 1ccc(cc1)N)=O)n2  )=O | 0812-1025 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1297 | C1c2ccccc2c2ccc( cc12)c1csc(N)n1 | 0846-0051 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1298 | c(cc1)cc2c1Nc(ccc c1)c1C=C2 | 123458 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1299 | C1CCCN(CC1)C( CCC(NC[C@@H] 1CCNC[C@H]1O  )=O)=O | 13691493 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1300 | CN(Cc1ccc(cc1)O c1ccccc1)Cc1cc2C NCCCn2n1 | 13915713 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1301 | C1CNCc2c1c(NCc  1ccccn1)nc(c1cccc c1)n2 | 14876887 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1302 | Cc1ccc(cc1)OCc1 c(cco1)C(NC[C@ @H]1C[C@@H] (CN1)F)=O | 15670813 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1303 | C1C2CC3CC1CC( C2) (C3)c1nc(CNC2C S(C=C2) (=O)=O)cs1 | 15896825 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1304 | Cc1c(C(C(NCCNc  2cccnc2)=O)N)c(C  )[nH]n1 | 16899791 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1305 | C1CN(C[C@H] ([C@@H]1NC(c1  ccccn1)=O)O)C(C Oc1cccc(c1)F)=O | 17818802 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1306 | C1CC(CNC1)c1cc  (c2ccc(c(c2)[Cl])  [Cl])nc(c1C#N)N | 17917068 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1307 | Cc1cc(c2ccc(cc2n 1)F)c1nc(CCSC)n n1CCO | 17988292 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1308 | C=CCC1(CCCN(  CC(NCCc2ccc(cc2  )[Cl])=O)C1)CO | 18112009 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1309 | C(Cn1cnc(c2ccccc 2)c1c1cnc(N)nc1)c 1cccs1 | 18838660 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1310 | CC(C)N[C@@H] 1CC[C@@H]1NC  (CCc1ccc(c2ccc(c c2)[Cl])[nH]1)=O | 19264424 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1311 | CC1=C(C#N)C(C 2=C(CC(C) | 1965-0024 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | (C)CC2=O)N1)c1c cc(c(c1)OC)OCC O |  |  |  | UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA |  |
| 1312 | C1CCN(C1)CC(C  n1c2ccccc2c2cccc c12)O | 1988-0087 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1313 | C1CNCc2c1c(NC C[C@@H]1C[C@ H]3C[C@@H]1C  =C3)nc(c1cccnc1) n2 | 20252371 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1314 | CC(Cc1ccccc1F)N Cc1nc(C2CCCCC  2)no1 | 20290768 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1315 | CCc1ccccc1NC(c1 cccc(c1)NC(C1C= CCN1)=O)=O | 20360930 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1316 | C1CNCc2c1c(NC  C1COc3ccccc3O1  )nc(c1cccnc1)n2 | 20674759 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1317 | Cc1c(C(NC[C@@ H]2C[C@@H] (CN2)F)=O)c(C)o  n1 | 20675366 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1318 | Cc1c(CN2CCC3( CC2)[C@H]  (C[C@H]3O)OCC  N)nc2ccccc2n1 | 21179623 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1319 | C(Cn1cc(c2ccc(C O)o2)nn1)Nc1cccc c1 | 21562311 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1320 | c1ccc2c(c1)ccc1c2 nc(c2ccc(cc2)N) [nH]1 | 2252-1548 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1321 | CC1=C(C(=O)OC) C2(C(C#N)=C(N)  O1)C(Nc1ccc(cc1 2)[Cl])=O | 2435-0198 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1322 | Cc1cc2c(cc1C)oc( c1ccc(cc1O)N)n2 | 2783-3499 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1323 | c1cc(cc(c1) [Cl])n1nc2ccc(cc2 n1)N | 2810-4198 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1324 | c1cc(c2cccc(c2c1) [Br])c1nc2cc(ccc2 o1)N | 2810-4224 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1325 | COc1ccc(cc1[Br]) c1nc2cc(ccc2o1)N | 2810-4227 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1326 | COc1ccc(cc1[Cl]) c1nc2cc(ccc2o1)N | 2810-4228 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1327 | Cc1cc2c(cc1C)oc( c1cc(ccc1[Cl])N)n | 2810-4329 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | 2 |  |  |  | UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA |  |
| 1328 | Cc1cc2c(cc1C)oc( c1ccc(cc1)N)n2 | 2810-4334 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1329 | Cc1cc2c(cc1C)oc( c1ccc(C)c(c1)N)n2 | 2810-4335 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1330 | C(c1ccc(cc1)F)Sc1 nc2ccc(cc2s1)N | 3167-0429 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1331 | CC(N[C@@H] (CCc(c(C1=CC=C 2OC)c3OC)c(C=O  )c(OC)c3OC)C1= CC2=O)=O | 328403 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1332 | C(CCNC(CSc1nnc  (N)s1)=O)Cc1cccc n1 | 33060622 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1333 | CC1CCCCN1CC(  COc1ccc(cc1)C(C) (C)C)O | 3343-3198 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1334 | CCn1c(N)nc2cc(c nc12)C(NCCCc1c(  C)ncs1)=O | 33439679 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1335 | Cc1ccc(cc1)c1cc( C(N[C@@H]2CN C[C@H]2O)=O)c  2ccccc2n1 | 33446163 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1336 | C1CNCCC12CCN  (C2)C(Nc1cccc2cc ccc12)=O | 33552957 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1337 | CCc1ccc(cc1)C1C (C#N)=C(N)Oc2c  1c(c1ccc3c(c1)OC O3)n[nH]2 | 3394-0298 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1338 | C1CCc2c(C1)c1cc ccc1n2C(CSc1nnc (N)s1)=O | 3535-0310 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1339 | Cc1cc(ccc1[Br])c1 nc2cc(ccc2o1)N | 3617-0633 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1340 | CCCCc1ccc(cc1)n 1nc2ccc(cc2n1)N | 3738-4868 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1341 | C1CSCCN1S(c1cc  c(cc1)c1ccc2c(c1) c(N)n[nH]2) (=O)=O | 39837810 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1342 | Cc1cc(C)c(c(C)c1) c1cc(CN)ccc1F | 40126718 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1343 | Cc1ccc(cc1)S(N(C C(CN1CCCCC1)  O)c1ccccc1OC) | 4013-2178 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | (=O)=O |  |  |  | GUCUGGGCGAACA |  |
| 1344 | Cc1cc2NC(CN3C CC4(CC3)C(Cc3c  cccc34)O)=CC(n2 n1)=O | 40183085 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1345 | Cc1c(c2csc(Nc3cc c(cc3) [Cl])n2)n2ccccc2n 1 | 4112-3380 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1346 | Cc1c(c2csc(Nc3cc c(cc3) [Br])n2)sc(N)n1 | 4112-3524 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1347 | C1CN(CCN(C1)c1  nccc(n1)N1CCC(C 1)O)Cc1cccc(c1)F | 41253715 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1348 | Cc1cc(C)n(C2CN( C2)c2c3CCCCc3n  c(N)n2)n1 | 41650554 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1349 | C(C(CNc1cc(c2cc ccc2)nc2ccnn12)C O)c1ccsc1 | 42351021 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1350 | Cc1ccc(cc1[Cl])c1 nc2cc(ccc2o1)N | 4269-3090 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1351 | c1ccc(c(c1)c1nc2c cc(cc2s1)N)[Br] | 4432-2269 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1352 | C1CC(CN(C1)c1c  (ccc(c2ccc(cc2)F)n 1)C(O)=O)(CO)O | 47509829 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1353 | c1ccc2c(cccc2c1)c 1nc2cc(ccc2o1)N | 4788-0739 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1354 | [H]N1CCn2c(C1)c  c(CNS(c1ccc3c(c1  )N(C)C(N3C)=O) (=O)=O)n2 | 47926615 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1355 | C1C[C@H] (CO)N(C1)Cc1ccc  c(c1)C(Nc1nc2ccc cc2s1)=O | 48085150 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1356 | CCC(Cn1c(CN2C  COc3ccccc3C2)nc (c2ccco2)n1)O | 48093352 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1357 | C1CC(CN(C1)CC  NC(Nc1cccc(c1)c1 cccc(c1) [Cl])=O)CO | 48121597 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1358 | Cc1nc2cc(c(cc2n1 CCCO)[Cl])[Cl] | 5119828 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1359 | c1ccc(cc1)Oc1ccc( cc1N)C(c1ccc(c(c 1)N)Oc1ccccc1)= O | 5172392 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 1360 | c1cc(ccc1c1c(c2cc c(cc2)F)nc2cc(ccc 2n1)Oc1ccc(cc1)N  )F | 5174475 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1361 | c1ccc(cc1)C(c1cc( ccc1N)Sc1ccc(c(c 1)C(c1ccccc1)=O) N)=O | 5180537 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1362 | C(C(NN=Cc1cc2c  cccc2nc1[Cl])=O) Nc1ccc2ccccc2c1 | 5200786 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1363 | CCCCCc1ccc(cc1) c1ccc(cc1)c1ncc(c n1)N | 5213078 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1364 | c1ccc2c(ccc(c2c1) Oc1ccc(cc1[Cl])N) [Cl] | 5215844 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1365 | CCOC(CNc1ccc(c c1)Oc1ccc(cc1)Oc 1ccc(cc1)NCC(=O  )OCC)=O | 5224153 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1366 | C1CCN(CC1)CC(  Cn1c2ccc(cc2c2cc (ccc12)[Cl])[Cl])O | 5236854 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1367 | CC12CCC(CN(CC  (Cn3c4ccc(cc4c4c c(ccc34)[Br])  [Br])O)C1)C2(C)C | 5236945 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1368 | c1ccc(cc1)c1c(cn( c2ccccc2)n1)C(Nc 1cc(cc(c1)Oc1cccc c1)N)=O | 5248546 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1369 | c1ccc2c(c1)ccc(c2 [Cl])Sc1ccc(cc1[C l])N | 5250905 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1370 | [H]N([H])c1c(C#  N)c2c(nc3ccccc3n 2)n1Cc1ccccc1 | 5253879 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1371 | C1CN(CCN1CC(  Cn1c2ccccc2c2ccc cc12)O)Cc1ccccc1 | 5320336 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1372 | C(C(c1ccccc1)O) N=Cc1ccc(cc1) [Br] | 5321062 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1373 | CC(c1ccc(cc1)N)= NNc1nc(C)cc(c2cc ccc2)n1 | 5339282 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1374 | c1cc(c2ccc3c(c(C( Nc4ccc(c(c4)F)F)= O)sc3n2)N)sc1 | 5350-0016 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1375 | c1cc(cc(c1)F)NC(c 1c(c2ccc(c3ccncc3  )nc2s1)N)=O | 5350-0056 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1376 | c1cc(ccc1c1cc(C( NN)=O)c2cc(ccc2 | 5350878 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | n1)[Br])N |  |  |  | UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA |  |
| 1377 | CC1=CC(C)=NC(  N1CC(Cn1c2ccccc 2c2ccccc12)O)=O | 5600837 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1378 | Cc1c2cc(CNC(c3c c(N)  [nH]n3)=O)ccc2[n H]c1c1ccccc1F | 56075039 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1379 | C(c1cnn(c2ccc3cc ccc3c2)c1N)#N | 5628157 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1380 | [H]N([H])c1nc(n[n H]1)SCCCCCCC CC | 5655427 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1381 | C(c1ccccc1)Oc1cc c(cc1)C1Nc2cccc3 cccc(c23)N1 | 5661401 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1382 | COc1cc(c(cc1NC( C(NCCN1CCNCC 1)=O)=O)OC)[Cl] | 5688029 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1383 | C(C(Cn1c2ccccc2 c2ccccc12)O)NNC (c1ccccc1)=O | 5718973 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1384 | C1CC1c1nc2ccccc 2n1CC(NCc1cc2C NCCn2n1)=O | 58209539 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1385 | C(C(Cn1c2ccc(cc2 c2cc(ccc12)[Br]) [Br])O)NCc1ccco1 | 5864844 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1386 | CCn1c2ccccc2c2c c(CN3CCNCC3)c  cc12 | 5878848 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1387 | CNC(c1cc(ccc1[Cl  ])c1ccccc1CO)=O | 58975776 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1388 | C(c1ccccc1)c1cccc c1OCCN.[Cl] | 5924771 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1389 | Cc1ccc(c(C)c1)OC C(CN1CCN(CC1)  CCN1C(c2cccc3cc cc(C1=O)c23)=O) O.[Cl].[Cl] | 6044718 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1390 | C(c1c(cc(c2ccc(cc 2)  [Br])nc1N)c1ccco 1)#N | 6233-2517 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1391 | CCCCSc1nc2c(c3 cc(ccc3NC3(CCC C3)O2)[Br])nn1 | 6372845 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1392 | CCOc1cc(CO)cc(c 1OCc1ccc(cc1)C( O)=O)[Br] | 6415-0035 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  |  |  |  |  | GUCUGGGCGAACA |  |
| 1393 | C(c1ccco1)NC1C( c2cccc3cccc1c23) NS(c1ccc(cc1) [Cl])(=O)=O | 6432111 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1394 | CCOC(C(C(c(cccc 1)c1N1)C1=O)=O)  =O | 646976 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1395 | C(CC(N1c2ccccc2 Sc2ccccc12)=O)C N | 6640-0077 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1396 | O=C(c(cc1)cc(C(N c(cc2)ccc2C2=NC CN2)=O)c1Cl)Nc(  cc1)ccc1C1=NCC N1 | 67436 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1397 | CN(C)c1ccc(cc1) Nc1nc(cs1)c1cccs 1 | 7100-1263 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1398 | CCC1CCCCN1S(c  1ccc(cc1)NC1c2cc ccc2S(N=1) (=O)=O)(=O)=O | 7380-0010 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1399 | Cn1c(cnc1NCc1cc ccc1OC)c1ccccc1 | 7756-0545 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1400 | Cc1c2[nH]c(cccc3  )c3c2ccc1CCN | 81703 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1401 | C(c1cccnc1)Nc1cc cc(c1)c1nc2ccccc2 [nH]1 | 9142557 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1402 | C(COc1ccc2c(c1)c 1ccccc1o2)N.[Cl] | 9188721 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1403 | c1c(cc2c(c1[Cl])nc (N)s2)F | 9190966 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1404 | C(c1ccc2c(c1)OC O2)Nc1cc(nc(N)n 1)[Cl] | 9205277 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1405 | Oc(ccc([As](O)  (O)=O)c1)c1NC(c  1ccccc1)=O | 92892 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1406 | S=C1Oc(ccc(- c2ccccc2)c2)c2N1 | 93817 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1407 | CC[C@] (C(C=C1N2Cc3cc  4ccccc4nc13)=C(C O1)C2=O) (C1=O)O | 94600 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1408 | C1CCCN(CC1)CC  CNc1nc2ccccc2c2 nc(c3ccccc3)nn12 | C736-0159 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  |  |  |  |  | GUCUGGGCGAACA |  |
| 1409 | CCOC(N1CCC(C C1)NC1=C(C(C1= O)=O)N1CCCC1)  =O | C748-0097 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1410 | Cc1ccc(CNc2c(cn c3ccc(cc23)F)S(c2 ccccc2) (=O)=O)cc1 | C769-1565 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1411 | COc1ccc(cc1)S(c1 cnc2ccc(cc2c1NCc 1ccc(cc1)F)F) (=O)=O | C769-1653 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1412 | Cc1ccc(cc1)S(c1c nc2ccccc2c1Nc1cc cc(c1)OC)(=O)=O | C769-1951 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1413 | Cc1c(CCC(Nc2ccc c(c2)C(F) (F)F)=O)c(C)n2c(  n1)nc(CN)n2 | C908-0403 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1414 | Cc1ccccc1NC(CN S(c1ccccc1) (=O)=O)c1ccccc1 | D030-0007 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1415 | Cc1ccc(cc1)NC(C NS(c1ccc(cc1) [Cl])  (=O)=O)c1ccccc1 | D030-0071 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1416 | c1ccn2c(C(c3ccc(c c3) [Cl])=O)c(c(C(Nc  3cccc(c3)F)=O)c2 c1)N | D033-0008 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1417 | Cc1ccc(cc1C)C(c1 c(c(C(Nc2cccc(c2) F)=O)c2ccccn12) N)=O | D033-0127 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1418 | Cc1cc(C)n2c(n1)n c(NCc1ccc(cc1) [Br])n2 | D043-0245 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1419 | CC(C)c1ccc(CNc2 nc3nc(C)c(c(C)n3  n2)[Cl])cc1 | D043-0278 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1420 | Cc1ccc2c(c1)C(C1  =C(C(N(CCCO)C 13C(N(CC=C)c1c cccc13)=O)=O)O2  )=O | D063-1068 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1421 | Cc1ccc2c(c1)C(C1  =C(C(N(CCO)C13  C(N(CC=C)c1cccc c13)=O)=O)O2)= O | D063-1117 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1422 | CCCCNc1c(nc(c2 ccccc2)o1)S(c1ccc cc1)(=O)=O | D072-0067 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1423 | CCCCNc1c(nc(c2 ccc(cc2)F)o1)S(c1 ccccc1)(=O)=O | D072-0077 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1424 | Cc1ccc(cc1)c1nc(c (NC2CC2)o1)S(c1 | D072-0757 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | ccc(cc1)F)(=O)=O |  |  |  | UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA |  |
| 1425 | COCCCN1CC(C(  =C1N)c1nc2ccccc 2s1)=O | D086-0291 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1426 | CN1C(N(Cc2cccc c2)C(c2c1nc(NCC N)n2C)=O)=O | D114-0037 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1427 | C(CNc1cc(c2ccccc 2)nc2nncn12)c1cc ccc1 | D150-0146 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1428 | Cc1c2c(c(NCCCN 3CCOCC3)nn1)n(  Cc1ccccc1[Cl])nn 2 | D172-0423 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1429 | [H]N(CCNC(c1c(  N)non1)=O)Cc1cc cc(c1)[Br] | D175-0122 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1430 | [H]N(CCNC(c1c(  N)non1)=O)Cc1cc (ccc1OCc1ccc(cc1  )F)[Br] | D175-0127 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1431 | CCC(c1nc2ccccc2 n1Cc1ccccc1F)O | D186-0041 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1432 | [H]N(Cc1ccccc1) Cc1ccc2c(c1)N(C) C(N2C)=O | D272-0686 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1433 | [H]N(CCCOCC)C  c1ccc2c(c1)N(C)C (N2C)=O | D272-0707 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1434 | [H]N(Cc1ccc2c(c1  )N(C)C(N2C)=O) C1CCCCCC1 | D272-0737 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1435 | CN1C(N(C)c2cc(c  cc12)C(COc1ccc( CNCc2cccs2)cc1) O)=O | D300-0283 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1436 | CN1C(N(C)c2cc(c  cc12)C(COc1ccc( CNCc2ccc(cc2)O C)cc1)O)=O | D300-0327 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1437 | Cc1ccc(cc1)OCc1 ccc(c2nc(C#N)c(N CCCN3CCOCC3)  o2)o1 | D301-0080 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1438 | C(c1nnc(o1)SCc1c ccc(c1)[Br])N | D334-0126 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1439 | Cc1cccc(c1)c1nc(c 2cccnc2NCc2cccc c2OC)on1 | D349-3872 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1440 | Cc1cccc(c1)Nc1nc c2C(CC(Cc2n1)c1  ccc(c(c1)OC)OC)= O | D367-0429 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 1441 | CN1C(c2c(cn(c2c 2cccc(c2) [Br])C(CO)  (CO)CO)N(C)C1= O)=O | D383-0064 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1442 | CCNc1nc(nc(n1)n 1cnc(n1)SCc1cccc c1)N1CCCC1 | D385-0095 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1443 | CCCCNc1nc(nc(n 1)n1cnc(n1)SCc1c cccc1)N(C)C | D385-0102 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1444 | C1CC1Nc1c(C#N)  nc(c2ccc(cc2)S(N2 CCOCC2) (=O)=O)o1 | D434-0692 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1445 | C=CCNc1c2c(cn(c 3ccccc3[Cl])c2ncn 1)c1ccccc1 | D447-0385 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1446 | C1Cn2c3ccccc3nc 2CN1c1cccc(c1)N | D454-0054 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1447 | C1Cn2c3ccc(cc3n c2CN1c1cccc(c1) N)[Cl] | D454-0510 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1448 | CCCNc1cc(C)nc2 c(C)c(c3cccc(c3) [Cl])nn12 | D503-0232 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1449 | [H]N(CCc1ccc(cc 1)S(N)  (=O)=O)Cc1ccc(c 2ccc(cc2)[Cl])o1 | D665-0262 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1450 | c1cc(c(cc1NS(c1c c(cnc1N)[Br]) (=O)=O)C(F)(F)F) [Cl] | E138-2000 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1451 | CC(C)c1ccc(cc1)C 1=C(C(C1=O)=O)  NCc1ccccc1OC | E511-0865 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1452 | Cc1cccc(C)c1NCc 1ccc(C(O)=O)s1 | E536-0036 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1453 | CCc1cccc(C)c1NC c1ccc(C(O)=O)s1 | E536-0078 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1454 | C1CCc2c(C1)c(C  O)cs2 | E540-0003 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1455 | C(c1ccccc1F)N1c2 ccccc2C2=C(C(C( C#N)=C(N)O2)c2  ccc(cc2)F)S1(=O)  =O | E738-0215 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1456 | CCc1ccc(cc1)C1C (C#N)=C(N)OC2=  C1S(N(Cc1ccccc1 C)c1ccccc12) (=O)=O | E738-0441 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 1457 | CCCNC1=C(C(C1  =O)=O)c1cc(C)c(  C)cc1C | E882-0500 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1458 | C1CNCCNCCCN( CCNC1)Cc1ccc(C N2CCCNCCNCC CNCC2)cc1 | NCGC00165722- 02 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |
| 1459 | CC(C)n1cnc2c(Nc 3cccc(c3)NC(C=C  )=O)nc(NC3CCC( CC3)N(C)C)nc12 | NCGC00346964- 01 | ZTP | Pseudoknot | UAUCAGUUAUAUGACUGACGGA ACGUGGAAUUAACCACAUGAAG UAUAACGAUGACAAUGCCGACC GUCUGGGCGAACA | 1 |