“Viral RNA” 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 | CCOC(=O)c1ccc2nc(C(F)  (F)F)nc(NCc3ccc(Cl)cc3)c 2c1 | Neg\_lig\_19 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 2 | O=C(Nc1ccc(- c2nc3ccccc3[nH]2)cc1)C1 CCN(C(=O)CO)CC1 | Neg\_lig\_26 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 3 | Cc1ccc2nc(Nc3ccc(C(=O) [O-])cc3)c3nncn3c2c1 | Neg\_lig\_40 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 4 | Brc1ccc(- c2ccc(CNC[C@@H]3CCC O3)o2)cc1 | Neg\_lig\_76 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 5 | Cc1ccc(-c2noc(-c3nnn(- c4cc(C)ccc4C)c3N)n2)cc1 | Neg\_lig\_103 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 6 | CCOc1cccc(-c2cnnn2- c2nonc2N)c1 | Neg\_lig\_144 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 7 | CCOC(=O)c1cnn(-  c2cc(C)nc3c(- c4ccc(Cl)cc4)c(C(F) (F)F)nn23)c1N | Neg\_lig\_156 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 8 | Cc1ccc2[nH]c(SC[C@H] (O)c3ccccc3)nc2c1 | Neg\_lig\_159 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 9 | COc1ccc(C(=O)c2c(N) [nH+]c3n2CCCC3)cc1OC | Neg\_lig\_167 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 10 | Nc1ccnc(N2CCc3onc(- c4ccccc4)c3C2)n1 | Neg\_lig\_195 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 11 | COc1cc(C(=O)N2C[C@@ H] (C[NH+]3CCCC3)C[C@  @H](CO)C2)c2ccccc2n1 | Neg\_lig\_198 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 12 | CC[C@H]  (Nc1ccc(Br)cc1)C(=O)N/ N=C/c1c[nH]c2ccccc12 | Neg\_lig\_201 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 13 | CN(Cc1c[nH]nc1- c1ccc(F)cc1)C(=O)[C@H] (N)Cc1ccccc1 | Neg\_lig\_306 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 14 | COc1ccc(Cl)cc1[N-]c1c(- c2ccccc2)c(=O)c1=O | Neg\_lig\_317 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 15 | COc1nc(NCc2cccnc2)nc(N 2CCSCC2)n1 | Neg\_lig\_292 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 16 | OCC[C@H]1CCCN1Cc1c  c2cc3c(cc2nc1- c1ccc(Cl)cc1)OCO3 | Neg\_lig\_359 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 17 | O=C(CN1CCC[C@H] (O)C1)NCc1cc2n(n1)CCC N(C(=O)C1CCC1)C2 | Neg\_lig\_466 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 18 | Cc1cccc(OC[C@@H] (O)Cn2c(=N)n(CC[NH+]3  CCOCC3)c3ccccc32)c1 | Neg\_lig\_525 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 19 | CCc1cnc(NC[C@H]2C[C @@H](CO)[N@H+](C)  [C@H]2c2ccccc2F)nc1 | Neg\_lig\_600 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 20 | Cc1sc(- n2cccc2CNCc2ccc(F)cc2)c | Neg\_lig\_604 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | (C(=O)[O-])c1C |  |  |  | UGGCUUUGGGGCAUGGACC |  |
| 21 | CC(C)Oc1ccccc1[C@H]1 C(C#N)=C(N)Oc2c1oc(C O)cc2=O | Neg\_lig\_613 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 22 | C[C@@H]1CCC[N@H+] (C[C@H] (O)COc2ccc3c(c2)OCO3) C1 | Neg\_lig\_615 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 23 | O=C(c1cn[nH]c1C1CCCC C1)N1Cc2cnn(CCO)c2C1 | Neg\_lig\_619 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 24 | C/C(=N/ NC(=S)N1CCC1)c1ccccn1 | Neg\_lig\_729 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 25 | [NH3+]CC[C@H]1CCCN( Cc2ccccc2C(F)(F)F)C1 | Neg\_lig\_758 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 26 | Cc1ccc2[nH]c(Cc3ccc4nc( N)sc4c3)nc2c1 | Neg\_lig\_784 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 27 | C[C@@H]  (Cn1cnc2ccccc2c1=O)NCc 1noc(-c2ccco2)n1 | Neg\_lig\_821 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 28 | C[C@@H]1O[C@H] (Nc2cc(C(=O)[O-])cc([N+]  (=O)[O-])c2)[C@H](O) [C@H](O)[C@H]1O | Neg\_lig\_850 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 29 | OCC#CCN1CCCC[C@H]  1c1cccnc1 | Neg\_lig\_885 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 30 | Cn1nnnc1SCC[NH2+]C1C  CN(c2ncnc3[nH]cnc23)CC 1 | Neg\_lig\_886 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 31 | CN(C)c1c([NH3+])c(=O)o  c2ccccc12 | Neg\_lig\_970 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 32 | CCc1ccc(C(=O)N2CC[C@ @]3(CCCN(CCO)C3=O)C 2)[nH]1 | Neg\_lig\_984 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 33 | Cc1cc(NCCN2CCOCC2)n  2nc(- c3ccccc3)c(C)c2[nH+]1 | Neg\_lig\_988 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 34 | CCOC(=O)c1ccccc1Nc1nc 2ccc(C)cc2n2cnnc12 | Neg\_lig\_1038 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 35 | Nc1nonc1C(=O)N1CCN(C  (=O)Nc2ccc(F)c(Cl)c2)CC 1 | Neg\_lig\_1046 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 36 | O[C@@]1(CNCc2nnc3ccc cn23)CCC[NH2+]C1 | Neg\_lig\_64 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 37 | CC[C@@]1(C)Cc2c(sc3nc (SC)nc(NCC[NH+]  (C)C)c23)CO1 | Neg\_lig\_1105 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 38 | O=C([C@@H] (c1cccnc1)N1CCOCC1)N1 CCC(O)(CO)CC1 | Neg\_lig\_1137 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 39 | CCS(=O) (=O)CCNC(=O)c1ccc([C @H]2CCC[NH2+]C2)cc1 | Neg\_lig\_1161 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 40 | CCO[C@H]1C[C@@H] (O)C12CC[NH+] (Cc1nnc(C3CC3)o1)CC2 | Neg\_lig\_1163 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |

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| 41 | Cc1ccc2[nH]c(C)c([C@@ H] (O)C[NH+]3CCCCC3)c2c 1 | Neg\_lig\_794 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 42 | C[C@H]  (Nc1cc(=O)oc2ccccc12)c1 ccccc1 | Neg\_lig\_1195 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 43 | CCc1cc(C[NH2+]C2CCN(  c3cc(C)nc(- c4ccccc4)n3)CC2)on1 | Neg\_lig\_228 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 44 | OCC1(Cc2ccc(Cl)cc2)CC N(c2ncccc2F)CC1 | Neg\_lig\_1236 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 45 | CCOC(=O)c1sc2nc(Cc3cc ccc3)nc(NC[C@H]3CCCO 3)c2c1C | Neg\_lig\_1244 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 46 | COc1ccccc1OC[C@@H] (O)Cn1nc(C)cc1C | Neg\_lig\_1258 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 47 | [NH3+]CCN1CCOCC1 | Neg\_lig\_1282 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 48 | C[N@H+]1CC[C@@]2(O  )OCCC[C@H]2C1 | Neg\_lig\_1299 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 49 | Nc1nonc1C(=O)N1CCCN( C(=O)Nc2ccc(F)cc2)CC1 | Neg\_lig\_1306 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 50 | CC(=O)CC[N+](C)(C)C | Neg\_lig\_1307 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 51 | COc1ccc(Nc2nc(N)nc(CSc 3nncn3C)n2)cc1 | Neg\_lig\_580 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 52 | CCn1nc(C(=O)O)c2c1CC[ C@H](NCc1cc(C)oc1C(F) (F)F)C2 | Neg\_lig\_1337 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 53 | O=C1N[C@@]  (CCCc2ccccc2) (C2CC[NH2+]CC2)C(=O)  N1Cc1ccncc1 | Neg\_lig\_1339 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 54 | CCc1cccc(OC2CN(C(=O) [C@@H](O)C(C)C)C2)c1 | Neg\_lig\_1342 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 55 | Cn1cc(CC(=O)N2CCCC[C  @H] ([NH3+])C2)c2ccccc21 | Neg\_lig\_1368 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 56 | Nc1cc(C(=O)N2CCC(c3cc  (Cc4ccccc4)n[nH]3)CC2)c cn1 | Neg\_lig\_1393 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 57 | CC1(C)CC(O)=C(Br)/  C(=N/Cc2ccccc2)C1 | Neg\_lig\_1425 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 58 | CC(C)c1cc(C(=O)NC(C)  (CO)CO)n(C)n1 | Neg\_lig\_1428 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 59 | O=C(c1ccc2c(c1)CCC2)N 1CCC2(CC1)OCCC[C@@ H]2O | Neg\_lig\_1439 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 60 | Cc1[nH]nc2c1[C@H] (c1ccc(Cl)c(Cl)c1)C(C#N)  =C(N)O2 | Neg\_lig\_1447 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 61 | CCCCCCNC(=O)n1cc(F)c | Neg\_lig\_354 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA | 0 |

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|  | (=O)[n-]c1=O |  |  |  | GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC |  |
| 62 | CC(C)Nc1nc(N2CCCC2)n c(N2C[C@@H]3C[C@H]  (C2)c2cccc(=O)n2C3)n1 | Neg\_lig\_1469 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 63 | Cc1nc(N2CCC([NH2+]C[ C@H]  (O)c3ccc(O)cc3)CC2)c2cc sc2n1 | Neg\_lig\_1474 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 64 | COc1ccccc1CCNc1nc(N)c 2ccccc2n1 | Neg\_lig\_1485 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 65 | CNC(=O)c1cc(COc2nnc(N c3ccc(Cl)cc3)c3ccoc23)cc n1 | Neg\_lig\_1553 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 66 | Cn1c(=O)c(NC2CCCCC2)  c2c3c(cccc31)C(=O)c1ccc cc1-2 | Neg\_lig\_1556 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 67 | Cc1cccc(N2CCC([NH2+]  CCc3nc(- c4ccc[nH+]c4)n[nH]3)CC2  )c1C | Neg\_lig\_1560 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 68 | COc1ccc(-c2c(- c3cc(OC)c4c(c3OC)OCO4  )noc2N)cc1 | Neg\_lig\_1603 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 69 | CC(=O)C1=C(O)C(=O)N(  CCO)[C@@H]1c1ccccc1 | Neg\_lig\_1628 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 70 | Cc1ccc([C@@H]2C[C@H  ]  (c3ccc(OCc4ccccc4)cc3)n3 nc(N)nc3N2)cc1 | Neg\_lig\_1633 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 71 | Cc1nnsc1C(=O)NCc1c(F)c ccc1Cl | Neg\_lig\_1642 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 72 | CC[NH2+]C1(C(N)=O)CC  N(c2ncnc3c2nc(- c2ccccc2Cl)n3- c2ccc(Cl)cc2)CC1 | Neg\_lig\_1650 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 73 | O=C(O)CN1CCC2(CC1)C  CN(c1cc[nH+]cc1)C[C@ @H]2CO | Neg\_lig\_1675 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 74 | CN(C)C(=O)c1ccc(-  c2cccc3c2CC[NH2+]C3)o 1 | Neg\_lig\_1714 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 75 | C=CCN(Cc1nc(-  c2ccccc2)no1)C(=O)CC1= CC[NH2+]CC1 | Neg\_lig\_1750 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 76 | Cc1cc2oc(=O)cc(C)c2cc1 N | Neg\_lig\_1751 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 77 | CCCCn1nc(C2CC2)nc1-  c1ccc(N)[nH+]c1 | Neg\_lig\_1752 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 78 | Cc1nc2cc(CNc3cc(C(C)C) [nH+]c(N)n3)ccc2[nH]1 | Neg\_lig\_1766 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 79 | Cc1ccc2c(CNCCc3ccco3)c (C(=O)O)n(C)c2c1 | Neg\_lig\_1770 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 80 | CC(=O)c1cccc(Nc2cc(- c3ccc(C)cc3) [nH+]c(C)n2)c1 | Neg\_lig\_1786 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |

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| 81 | Clc1cccc(Nc2nc3nonc3nc2 N2CCCCC2)c1 | Neg\_lig\_1816 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 82 | CC[NH+] (CC)CCNc1cc(C)  [nH+]c2cc(- c3ccc(OC)c(OC)c3)nn12 | Neg\_lig\_1830 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 83 | O=C(O) [C@@H]1CC2(CCN(S(= O) (=O)N3CCCC3)CC2)CN1 | Neg\_lig\_1843 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 84 | NC(=O)c1ccc(- c2ccccc2CO)nc1 | Neg\_lig\_1912 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 85 | O=C(NCCCCc1ccccc1)c1 nn(-c2ccc(Cl)cc2)nc1CO | Neg\_lig\_1228 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 86 | Cc1ccc(- c2nc3nc(C)cc(N4CCN(CC O)CC4)n3n2)cc1 | Neg\_lig\_2045 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 87 | Cc1cc(C)c(NC(=O)c2sc3n c(C)c(C)c(C)c3c2N)c(C)c1 | Neg\_lig\_2060 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 88 | COc1ccc(C(=O)CN2CC[N H2+]CC2)cc1 | Neg\_lig\_2120 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 89 | CCN(CC)c1ccc(Nc2cc(C)n c3ncnn23)c(C)c1 | Neg\_lig\_2148 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 90 | Nc1cc(C(=O)c2ccccc2C(= O)[O-])ccc1Cl | Neg\_lig\_2228 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 91 | Cc1ccccc1[C@@H]1C(C# N)=C(N)Oc2c1c(=O)n(C)c  1ccccc21 | Neg\_lig\_44 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 92 | Cc1ncc2c(c1CNC(=O)c1cc c(SCCO)cc1)CC[NH2+]C 2 | Neg\_lig\_2283 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 93 | CC1(C)CC(=O)C2=C(C1) OC(N)=C(C#N)  [C@H]2c1ccccc1 | Neg\_lig\_2326 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 94 | C=CCOC(=O)C1=C(N)O C(C)=C(C(=O)OC)  [C@]12C(=O)Nc1ccccc12 | Neg\_lig\_2267 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 95 | CCOC(=O)Cc1ccc(NCCC(  =O)c2ccccc2)cc1 | Neg\_lig\_2352 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 96 | N#CC1=C(N)Oc2cc(O)ccc  2[C@H]1c1ccc(OCc2cccc c2)cc1 | Neg\_lig\_2369 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 97 | COc1ccc(- c2c(C#N)c(N)nc3c2CCCC C3)cc1OC | Neg\_lig\_2401 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 98 | C1CCc2[nH]nc(C[NH2+] C3CSCCSC3)c2CC1 | Neg\_lig\_2405 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 99 | Cc1c/c(=N\ c2ccc(Cl)c(C(F) (F)F)c2)n2[nH]c[nH+]c2n 1 | Neg\_lig\_2420 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 100 | Cc1ccccc1CSc1nc(N)cc(N (C)CCC(N)=O)n1 | Neg\_lig\_2454 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 101 | Cc1ccc2nc(N3CCC[C@H] (O)C3)c(CN(C)Cc3nnc(C)  o3)cc2c1 | Neg\_lig\_2455 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 102 | Nc1nnc(CCCn2c(=O)oc3c cccc32)s1 | Neg\_lig\_2478 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 103 | COc1ccccc1- n1cc(C(=O)NC[C@@H]2 C[C@H](F)CN2)cn1 | Neg\_lig\_2481 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 104 | NS(=O) (=O)c1ccc(NC2=CC(=O)c  3ccccc3C2=O)cc1 | Neg\_lig\_2543 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 105 | O=C([O-])c1cccnc1 | Neg\_lig\_2571 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 106 | O=C1CCCc2nc(Nc3ccc(F) cc3)ncc21 | Neg\_lig\_2575 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 107 | Cc1cc(C)cc(Nc2c(- c3cccc(O)c3)nc3ncccn23)c 1 | Neg\_lig\_2576 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 108 | COc1cc(N2CC(=O)C(c3nc (C)c(C)s3)=C2N)cc(OC)c1 OC | Neg\_lig\_2590 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 109 | Cc1nc(N)ncc1- c1nc(N2CCOCC2)c2sc(C( C)(C)O)cc2[nH+]1 | Neg\_lig\_2596 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 110 | O[C@H]  (CN1CCCc2ccccc21)Cn1c 2ccccc2c2ccccc21 | Neg\_lig\_2614 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 111 | Cn1nnnc1SCC[NH2+]Cc1 nc(-c2ccco2)no1 | Neg\_lig\_2627 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 112 | Cc1ccc(Nc2nc(C(=O)N3C CN(Cc4ccccc4)CC3)cs2)c c1 | Neg\_lig\_2647 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 113 | Nc1c(C(=O)Nc2ccccc2F)s c2ncccc12 | Neg\_lig\_2691 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 114 | O=C(N[C@@H]  (COc1ccc2[nH]c(=O) [nH]c2c1)c1ccccc1)c1cccn (Cc2ccc(F)c(F)c2)c1=O | Neg\_lig\_2708 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 115 | CCOC(=O) [C@H]1CCC2=C1c1c(ccc 3ccccc13)N[C@@H]2c1cc c(Br)cc1 | Neg\_lig\_2718 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 116 | C[C@@H]1CN(S(=O) (=O)c2ccc(C(=O)N3CC[C  @H] ([NH3+])C3)cc2)CC[NH2  +]1 | Neg\_lig\_2639 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 117 | C[C@H]1C[C@H]  (Nc2ccccc2)c2ccccc2N1C(  =O)c1cccc(Br)c1 | Neg\_lig\_2773 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 118 | Nc1nnc(SCC(=O)NCc2c[n H]nc2-c2ccc(F)cc2)s1 | Neg\_lig\_2812 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 119 | [NH3+]CCn1cc(C(=O)NC  Cc2cc(N3CCCC3)ncn2)nn 1 | Neg\_lig\_2813 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 120 | CCOC(=O)c1ccc2ncc(C(= O)OCC)c(Nc3ccc(N4CCO  CC4)cc3)c2c1 | Neg\_lig\_2712 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 121 | CCCn1cc(S(=O) (=O)N2C[C@H]3C[C@H] (O)[C@@H]  (O)C[C@H]3C2)cn1 | Neg\_lig\_2850 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 122 | Cc1nnc2c3ccccc3nc(Nc3cc cc(C(=O)[O-])c3)n12 | Neg\_lig\_2864 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 123 | c1ccc(C[C@H] (CC[NH2+]Cc2ccco2)c2cc co2)cc1 | Neg\_lig\_2909 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 124 | CCOc1ccc(- c2nccn2C2CCCC2)cc1CO | Neg\_lig\_2931 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 125 | Cc1ccc(C)c(NCCOc2ccccc 2)c1 | Neg\_lig\_2933 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 126 | [NH3+] [C@@H]1CC[C@H] (C(=O)NCc2cccc(C(F) (F)F)c2F)C1 | Neg\_lig\_2974 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 127 | O=C(CCc1nc2ccccc2[nH]c 1=O)N1C[C@H](O)CO1 | Neg\_lig\_3053 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 128 | CCCC(=O)N1c2c(C)cccc2  [C@@H] (Nc2ccccc2C)C[C@H]1C | Neg\_lig\_3064 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 129 | COc1ccc(NCCN2C(=O) [C@H]3CC=C(Cl)C[C@H  ]3C2=O)cc1 | Neg\_lig\_3089 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 130 | NC(N)=[NH+]CCO | Neg\_lig\_3100 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 131 | O=C([O-])C[C@H]  (O)C[C@H](O)/C=C/  c1c(C2CC2)nc2ccccc2c1- c1ccc(F)cc1 | Neg\_lig\_3120 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 132 | CCNc1nc(Oc2ccc(=O) [nH]n2)nc(N(C)C)n1 | Neg\_lig\_3182 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 133 | CNc1cc(C)[nH+]c2c(- c3ccc(F)cc3)cnn12 | Neg\_lig\_1774 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 134 | Cn1cc(- c2c(C#N)c(N)nc3c2C[C@ @H]([NH3+])CC3)c(-  c2ccccc2)n1 | Neg\_lig\_3208 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 135 | Cc1c(C#N)c(N)n(CCC[NH  +](C)C)c1C | Neg\_lig\_3209 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 136 | N#Cc1c2c(c(NCCC[NH+]  3CCOCC3)n3c1nc1ccccc1 3)CCC2 | Neg\_lig\_3210 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 137 | Cc1cc(C)nc(Nc2ncc(O)n2- c2ccc(Cl)cc2)n1 | Neg\_lig\_3265 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 138 | Cc1ccc(C2(O)CCN(C(=O)  [C@@H] (N)CC3CCCC3)CC2)nc1 | Neg\_lig\_3330 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 139 | COc1ccc(- c2cc3c(C)nc(N)nc3n([C@ H]3CC[C@@H] (OCCO)CC3)c2=O)cn1 | Neg\_lig\_1364 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 140 | Nc1ccc(-c2nccc(CCC(F) (F)F)n2)c[nH+]1 | Neg\_lig\_3349 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  |  |  |  |  | UGGCUUUGGGGCAUGGACC |  |
| 141 | O=C(C[C@H]1CCc2ccccc 21)NCC1CC[NH2+]CC1 | Neg\_lig\_3398 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 142 | Cc1cc(N2CCN(CCO)CC2)  n2nc(- c3cccc(Cl)c3)c(C)c2[nH+] 1 | Neg\_lig\_3403 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 143 | COC(=O)c1[nH]c2ccccc2c 1NCc1cccnc1 | Neg\_lig\_11 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 0 |
| 144 | CCCCNc1oc(-  c2ccccc2)nc1S(=O) (=O)c1ccc(Cl)cc1 | Neg\_lig\_71 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 145 | CCN1c2ccccc2C2=C([C@ @H] (c3ccccc3OC)C(C#N)=C( N)O2)S1(=O)=O | Neg\_lig\_142 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 146 | C[N@@H+]  (CCCNc1ncnc2onc(- c3ccc(Cl)cc3)c12)Cc1cccc c1 | Neg\_lig\_149 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 147 | COc1cccc(OC[C@@H] (O)CN2CCN(c3ccccc3)CC 2)c1 | Neg\_lig\_215 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 148 | CC(C)NC(=O)  [C@@H]1C[C@H] ([NH3+])CN1C(=O)C1(S(  =O)(=O)c2ccccc2)CC1 | Neg\_lig\_236 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 149 | Fc1ccc(Nc2c3c([nH+]c4cc ccc24)CCC3)cc1 | Neg\_lig\_241 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 150 | Cc1nc([C@H]2CCC[NH2  +]C2)cc(N2CCC(C(=O)N  Cc3ccccn3)CC2)n1 | Neg\_lig\_255 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 151 | Cc1ncc(CO)c2c1Oc1[nH]c (-  c3cccc(Cl)c3)nc(=S)c1C2 | Neg\_lig\_272 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 152 | CC(C) (C)c1nnc(N2CCC3(CC2)C  Nc2ccccc23)o1 | Neg\_lig\_276 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 153 | CCOC(=O)C1CCN(c2c(N C3CCCCCC3)c(=O)c2=O) CC1 | Neg\_lig\_279 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 154 | Cc1cc(C)c(NC(=O)Cn2nnc (C(=O)NCc3ccccc3Cl)c2N  )c(C)c1 | Neg\_lig\_291 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 155 | CC(C)c1cc(NCc2ccc(O)cc 2)nc(N)[nH+]1 | Neg\_lig\_300 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 156 | CN(C)c1ccc(CNc2ccc3c(c 2)ncn3-c2ccccc2)cc1 | Neg\_lig\_348 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 157 | COc1cc(F)c(C(C)C)cc1-  c1ccc(C(F) (F)F)cc1CN1C(=O)O[C@ H](c2cc(C(F)(F)F)cc(C(F) (F)F)c2)[C@@H]1C | Neg\_lig\_380 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 158 | CCOC(=O)c1c(N)sc(C(=O  )Nc2ccccc2)c1C | Neg\_lig\_409 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 159 | O=S1(=O)N=C(NCCCCO)  c2ccccc21 | Neg\_lig\_421 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 160 | COc1ccccc1OC[C@@H] (O)Cn1c([C@H]2CC(=O)  N(c3cccc(C)c3)C2)nc2ccc cc21 | Neg\_lig\_482 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 161 | CCOc1ccc(NC(=O)c2cnn( C(=O)c3ccccc3)c2N)cc1 | Neg\_lig\_484 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 162 | CS[C@H]1SC[C@@H]2C (=O)N(C)[C@H]  (C(C)C)C(=O)OC[C@H]  (NC(=O)c3cnc4ccccc4n3) C(=O)N[C@H] (C)C(=O)N(C)  [C@@H]1C(=O)N(C) [C@H] (C(C)C)C(=O)OC[C@H]  (NC(=O)c1cnc3ccccc3n1) C(=O)N[C@H]  (C)C(=O)N2C | Neg\_lig\_486 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 163 | CCc1[nH+]ccn1CCNC(=O  ) [C@H]1C[NH2+]C[C@@ H](C(=O)N2CCCC2)C1 | Neg\_lig\_506 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 164 | C=CCSc1n[nH]c(-  c2cccs2)n1 | Neg\_lig\_531 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 165 | O=C(c1ccc2c(c1)n(CC1C C1)c(=O)n2C1CCCCC1)N 1C[C@@H]2C[NH2+]C[C @@H]2C1 | Neg\_lig\_177 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 166 | Clc1ccc(- c2noc3ncnc(NC[C@H]4C CCO4)c23)cc1 | Neg\_lig\_547 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 167 | COCCNc1nc2c(c(=O)n(Cc 3cccc(Cl)c3)c(=O)n2C)n1 C | Neg\_lig\_642 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 168 | Cc1cnc(C)c(N2CC[C@@ H] (N3CCN(CCc4ccccc4)CC 3)[C@H](O)C2)n1 | Neg\_lig\_694 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 169 | CCCc1nc(- c2cc3cccc(C)c3[nH+]c2N Cc2ccc(OC)c(OC)c2)no1 | Neg\_lig\_696 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 170 | Cc1cccc(- c2noc(CCc3ncnn3CCO)n2  )c1 | Neg\_lig\_700 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 171 | CC(C)=NNc1[nH]cnc2ncn c1-2 | Neg\_lig\_744 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 172 | Cc1n[nH]c(C)c1CCNc1nc cc(N2CCC(O)CC2)n1 | Neg\_lig\_752 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 173 | CN1CCN2c3ncccc3Cc3cc ccc3[C@@H]2C1 | Neg\_lig\_764 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 174 | Cc1cc(C)c2c(n1)sc1c(N3C CN(CCO)CC3)ncnc12 | Neg\_lig\_808 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 175 | O=C(Cn1ncc(N2CCCC2)c c1=O)N1CCN[C@H]  (c2ccccc2)C1 | Neg\_lig\_855 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 176 | C[NH+]1CCC(N(CCc2ccc cc2)C(=O)CN2CCC[C@H  ](O)C2)CC1 | Neg\_lig\_882 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 177 | COCCC[C@]1(CO)CCCN (C(=O)COc2ccc(C)cc2)C1 | Neg\_lig\_888 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 178 | NCc1nc2c(nnn2Cc2ccccc2  )c(=O)[nH]1 | Neg\_lig\_914 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 179 | Cc1nc(CNS(=O) (=O)c2ccc(C(=O)N[C@H] 3CC[NH2+]C3)cc2)no1 | Neg\_lig\_930 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 180 | CCCc1cc(C(=O)NC[C@H  ] (O)C[NH+]2CCCCCC2)n[ | Neg\_lig\_986 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | nH]1 |  |  |  |  |  |
| 181 | COc1ccc(- c2nn3c(NCc4cccnc4)cc(C) [nH+]c3c2C)cc1OC | Neg\_lig\_999 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 182 | NC(=O)c1ccc(N2CCN(Cc  3c[nH]nn3)C[C@H] (O)C2)nc1 | Neg\_lig\_282 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 183 | O[C@@]1(CNCc2nnc3ccc cn23)C[NH2+]CCOC1 | Neg\_lig\_1148 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 184 | COCc1ccc(C(=O)N2CCC3 (CC2)[C@@H] (OCC[NH3+])C[C@H]3O  )s1 | Neg\_lig\_1175 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 185 | CSc1ccc(CC(=O)N2C[C@  @H] (C[NH+]3CCN(C)CC3)  [C@@H](CO)C2)cc1 | Neg\_lig\_1179 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 186 | CCC[C@H]1CN(c2ccc(C# N)cn2)C[C@@H]1NC(=O  )CCO | Neg\_lig\_1263 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 187 | NC1=C(c2nc3ccccc3s2)C(  =O)CN1c1cccc2ccccc12 | Neg\_lig\_1281 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 188 | C=CCn1cc(C[NH2+]CCC NS(=O)  (=O)c2ccc(C)cc2)c(C)n1 | Neg\_lig\_1283 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 189 | CC(C)C1=C/C(=C(/ O)N2Cc3ccc(C[NH+]4CC N(C)CC4)cc3C2)C(=O)C= C1O | Neg\_lig\_1318 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 190 | O=C1CC[C@@]2(CCCN( C(=O)c3ccc(CO)o3)C2)C  N1Cc1ccncc1 | Neg\_lig\_1383 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 191 | CC(C)C(=O)Nc1cc(NC(= O)N2CCOC[C@@H] (O)C2)ccc1F | Neg\_lig\_1389 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 192 | O=C([O-])CNc1ccc([As]  (=O)([O-])[O-])cc1 | Neg\_lig\_1410 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 193 | Cc1c(CO)c2ccccc2n1Cc1c cc(Br)cc1 | Neg\_lig\_1418 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 194 | COCc1cc(C)nc2sc(C(=O) Oc3ccccc3)c(N)c12 | Neg\_lig\_1449 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 195 | Oc1nccc(SCc2ccc(Cl)cc2C l)n1 | Neg\_lig\_1470 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 196 | O=C(c1ccc(- n2cnnc2)nc1)N1CCC[C@ @](O)(CO)CC1 | Neg\_lig\_1484 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 197 | O=C(Nc1cccc2c1CCC2)c1 ccc(CN2CCOC[C@@H]2  CO)cc1 | Neg\_lig\_1518 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 198 | C[C@@H](CC(F)(F)F)  [NH2+]CCNc1cccnc1 | Neg\_lig\_1558 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 199 | Cc1nc2c(c(NCCC[NH+] (C)C)n1)CCC2 | Neg\_lig\_1563 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 200 | CC(C)C[C@@H]  (NC[C@@H]  (O)Cn1c2ccccc2c2ccccc21  )C(=O)O | Neg\_lig\_1620 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 201 | CCOC(=O)c1c(C)oc2ncnc( Nc3cccc(CC)c3)c12 | Neg\_lig\_1648 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 202 | COc1ccc([C@H]2C(C#N)  =C(N)Oc3c2oc(CO)cc3=O  )cc1Br | Neg\_lig\_1653 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 203 | CCc1nc(N2CCN(CCO)CC  2)c2cc(C)sc2n1 | Neg\_lig\_1669 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 204 | CCOC(=O)c1ccc(C)c(N)c1 | Neg\_lig\_1649 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 205 | CC(C)c1cc(C(=O)N[C@H  ]2CC[C@H]2[NH3+])on1 | Neg\_lig\_1699 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 206 | Cc1ccc2c(c1)c1c(n2C[C@ H] (O)C[NH+]2CCC(C)CC2) CCCC1 | Neg\_lig\_1735 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 207 | Cc1c(C)n(C[C@H]  (O)C[NH2+]C(C)  (C)C)c2ccccc12 | Neg\_lig\_1799 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 208 | Nc1nc(CCC(=O)N2CCC[  C@@H]2CO)cs1 | Neg\_lig\_1811 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 209 | COC(=O)c1ccc(COc2ccc( CN[C@@H] (C)C(N)=O)cc2)o1 | Neg\_lig\_1817 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 210 | COc1cc(Nc2nc3ccccc3nc2 [N-]S(=O)  (=O)c2ccc(NC(=O)c3ccc( C)c(OC)c3)cc2)cc(OC)c1 | Neg\_lig\_1875 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 211 | C#CCn1c(CCCO)nc2ccccc 21 | Neg\_lig\_1934 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 212 | Cc1ccc([N-]S(=O)  (=O)c2cc(Br)cnc2N)cc1Cl | Neg\_lig\_1954 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 213 | Cc1[nH]cnc1CN(CCO)C[ C@]12C[C@H]3C[C@H] (C[C@H](C3)C1)C2 | Neg\_lig\_1964 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 214 | Cc1ccc(- c2cnn3c(NCCOCCO)cc(C) [nH+]c23)cc1 | Neg\_lig\_1974 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 215 | CCn1c(=[NH2+])n(C[C@  H](O)c2ccco2)c2ccccc21 | Neg\_lig\_1990 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 216 | CO[C@@]12[C@H] (COC(N)=O)C3=C(C(=O)  C(C)=C(N)C3=O)N1C[C @H]1[C@@H]2N1C | Neg\_lig\_1996 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 217 | CCC[C@H]  (O)c1nc2ccccc2n1Cc1ccc( F)cc1 | Neg\_lig\_1196 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 218 | CCOc1c(C[NH2+]CCCn2c  cnc2)cc(Cl)cc1OC | Neg\_lig\_574 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 219 | COc1cc(C(C)=O)ccc1OC[  C@@H] (O)CN1CCN(S(=O)  (=O)N(C)C)CC1 | Neg\_lig\_2110 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 220 | CC(=O)c1ccc(NC(=O)c2sc 3nc(N4CCCC4)c4c(c3c2N  )CCCC4)cc1 | Neg\_lig\_2146 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 221 | CC[C@H]1OC(=O) [C@H](C)[C@@H]  (O[C@H]2C[C@@](C)  (OC)[C@@H](O)[C@H]  (C)O2)[C@H](C)  [C@@H] (O[C@@H]2O[C@@H] (C)C[C@H]([NH+](C)C) [C@@H]2O)[C@](C)  (O)C[C@@H](C)C(=O)  [C@H](C)[C@@H](O) [C@]1(C)O | Neg\_lig\_2149 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 222 | Cc1cc(N)n(-c2ccc(S(=O)  (=O)[O-])cc2)n1 | Neg\_lig\_2201 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 223 | COc1ccccc1- c1c(C)nn2c(N)c(- c3ccccc3)c[nH+]c12 | Neg\_lig\_2202 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 224 | Cc1ccnc([N-]S(=O)  (=O)c2ccc(NC(=O)Nc3ccc (S(=O)(=O)  [N-]c4nccc(C)n4)cc3)cc2) n1 | Neg\_lig\_2215 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 225 | CCc1nc(NCCO)c(C#N)c2c 1CCCC2 | Neg\_lig\_2227 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 226 | CCOC(=O)N1CCC(Nc2c( N3CCN(C)CC3)c(=O)c2= O)CC1 | Neg\_lig\_2231 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 227 | CC[C@@H] (C(=O)N1CCC2(CCC(=O) N(CCO)C2)CC1)n1cccn1 | Neg\_lig\_2238 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 228 | Cc1cc(N2C[C@H] (C3CC3)[C@@H] (NC(=O)CO)C2)cc(C) [nH+]1 | Neg\_lig\_2254 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 229 | O=C1CC[C@H]2C[N@H  +](CCC(F) (F)F)CC[C@H]2N1CCCC O | Neg\_lig\_2270 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 230 | COc1ccccc1[C@H]1C[C @@H] (c2ccc(Cl)cc2)Nc2nc(N)nn 21 | Neg\_lig\_2273 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 231 | Cc1ccc([C@H] (C(=O)NCCCCC[NH3+])  [NH+](C)C)cc1 | Neg\_lig\_2368 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 232 | CC(C)c1ccc(CNc2ccc(N3 CCOCC3)c(C(=O)  [O-])c2)cc1 | Neg\_lig\_2416 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 233 | Cc1cc(NCCC[NH+]  (C)C)n2ncc(- c3ccc(Cl)cc3)c2[nH+]1 | Neg\_lig\_2452 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 234 | Cc1cc(NCc2ccccc2)n2nc(- c3ccccc3)c(C)c2[nH+]1 | Neg\_lig\_2456 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 235 | COC(=O)c1cc2n(n1)CCC N(C(=O)c1ccc(N)nc1)C2 | Neg\_lig\_2460 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 236 | Nc1nnnn1CC(=O)N(Cc1cc c(F)cc1)C[C@H]1CCCO1 | Neg\_lig\_2537 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 237 | O=S(=O)  (c1ccc(F)cc1)c1nc(- c2ccc(F)cc2)oc1NCc1ccco 1 | Neg\_lig\_2559 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 238 | CCCOC(=O)c1cccc(Nc2nc (C(=O)OCC)nc3ccccc23)c 1 | Neg\_lig\_2573 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 239 | COc1ccc(CCNCC(=O)Nc2  cccc(C)c2C)cc1 | Neg\_lig\_2616 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 240 | [NH3+]CCN1C(=O)CC[C  @H]2CN(C(=O)c3cccc4nc cnc34)CC[C@H]21 | Neg\_lig\_2625 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 241 | CCN(C(=O)c1cccc(F)c1F)  [C@@H]1CCN(c2ccnc(N) n2)C[C@H]1O | Neg\_lig\_2636 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 242 | CCCCNc1cc(C)[nH+]c2c(-  c3ccccc3OC)cnn12 | Neg\_lig\_2663 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 243 | COc1ccc(- c2[nH]nc3c2[C@]2(C(=O)  Nc4ccc(C)c(Br)c42)C(C# | Neg\_lig\_2669 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | N)=C(N)O3)cc1 |  |  |  |  |  |
| 244 | CS(=O)  (=O)c1cnc(NCCn2cccn2)n c1[C@H]1CCC[NH2+]C1 | Neg\_lig\_2685 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 245 | COc1cc(OC)c(Nc2[nH+]c 3ccccc3c3nncn23)cc1Cl | Neg\_lig\_2709 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 246 | N#Cc1c(N)c2c(c3c1CCCC 3)CCCC2 | Neg\_lig\_2713 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 247 | NC(=O)N1c2ccccc2CC(= O)c2ccccc21 | Neg\_lig\_2775 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 248 | O=C(c1ccccc1)c1ccc(Sc2c cc([N+](=O)[O-])cc2)cc1 | Neg\_lig\_2797 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 249 | OCCN1CCN(CCCN2c3cc  ccc3Sc3ccc(C(F) (F)F)cc32)CC1 | Neg\_lig\_126 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 250 | COc1c(N)cc(C(=O)  [O-])cc1Br | Neg\_lig\_2914 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 251 | COc1ccccc1OCc1nc(C#N) c(NCc2ccc(C)cc2)o1 | Neg\_lig\_2917 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 252 | Clc1ccccc1- c1nnc2sc(Nc3ccccc3)nn12 | Neg\_lig\_2920 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 253 | O=C(c1ccccc1- n1cncn1)N1CCN[C@H] (c2ccccc2)C1 | Neg\_lig\_2934 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 254 | Cc1cnn(CC[NH2+]C2CC  N(c3ncnc4sc(C)cc34)CC2) c1 | Neg\_lig\_2941 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 255 | Cc1cn2c3c(=O)n(C)c(=O) n(C)c3nc2n1CCO | Neg\_lig\_2970 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 256 | COc1ccccc1N1CCN(C(=O  )[C@H]  (O)c2ccccc2)CC1=O | Neg\_lig\_2972 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 257 | C#CCN1C(=O) [C@@]2(C(C(=O)OC)=C( N)OC(c3ccccc3)=C2C(=O  )OCC)c2ccccc21 | Neg\_lig\_2979 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 258 | C[C@H]  (O)c1nc2ccccc2[nH]1 | Neg\_lig\_2993 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 259 | COc1ccccc1-n1nnc(-c2nc(- c3ccc(F)cc3)no2)c1N | Neg\_lig\_1645 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 260 | CCCNc1c([N-]S(=O)  (=O)c2cccc(Cl)c2)c(=O)oc 2ccccc12 | Neg\_lig\_2997 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 261 | Cc1csc(C2=C(N)N(CC[N H+]3CCOCC3)CC2=O)n1 | Neg\_lig\_3031 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 262 | Nc1nc(CCC(=O)N2CC(c3  cccnc3)C2)cs1 | Neg\_lig\_3058 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 263 | c1ccc(- n2nnnc2SCC[NH2+]Cc2cc co2)cc1 | Neg\_lig\_163 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 264 | O=C1CSC(=O)N1C[C@@ H](O)COc1ccc(OC[C@H] (O)CN2C(=O)CSC2=O)cc 1 | Neg\_lig\_3119 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 265 | Cc1ccc(NCc2cccc3c2C[N @H+] (C[C@@H]2CCCO2)C3)c  c1C | Neg\_lig\_3134 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 266 | O=C(CCc1cc2n(n1)CCC[ NH2+]C2)N1CCN[C@H] 2CS(=O)(=O)C[C@H]21 | Neg\_lig\_3158 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 267 | COc1cc(N2C(=O)C[C@H] (N3CCCC[C@H]3CCO)C 2=O)cc(OC)c1OC | Neg\_lig\_3172 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 268 | CCN(CC)C(=O)Cn1ccc(N C(C)=O)nc1=O | Neg\_lig\_3193 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 269 | Nc1nonc1- c1nc2ccccc2n1Cc1cccc(C( F)(F)F)c1 | Neg\_lig\_3194 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 270 | CCOc1ccc(Cl)cc1C[NH2+  ]CCNC(=O)c1nonc1N | Neg\_lig\_3212 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 271 | COc1ccccc1C(=O)Oc1ccc( Cl)cc1[N-]C1=NS(=O)  (=O)c2ccccc21 | Neg\_lig\_3214 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 272 | O=C([O-])c1sc2ccccc2c1N c1ccccc1 | Neg\_lig\_3218 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 273 | CC1=N/C(=C(/ O)NCC(=O)  [O-])C(=O)c2ccc(Oc3cccc c3)cc21 | Neg\_lig\_3224 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 274 | COc1cc(C(=O)N2CC[NH2  +]CC2)cc(OC)c1OC | Neg\_lig\_3239 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 275 | CSCC(=O)N1CCC2(CC[N H+](Cc3cn(C)nc3C)CC2) [C@@H](CO)C1 | Neg\_lig\_3249 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 276 | COC(=O)c1ccc(Nc2nc3ccc cc3c3nnc(C)n23)cc1 | Neg\_lig\_3262 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 277 | O=C1SC(c2ccccc2)=C/ C1=C/Nc1nc(- c2ccccc2)cs1 | Neg\_lig\_3274 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 278 | CCSC1=C(C#N)[C@@H]  (c2ccccc2Cl)C(C#N)=C(N  )N1 | Neg\_lig\_3277 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 279 | C[NH+](C)CCCNc1oc(/  C=C/c2ccc(F)cc2)nc1C#N | Neg\_lig\_3289 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 280 | CCOC(=O)CSc1nc(N)nc(  C)c1Br | Neg\_lig\_3306 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 281 | Clc1ccc(C[NH2+]Cc2ccco 2)cc1 | Neg\_lig\_827 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 282 | C[C@H]1CN(c2ccccc2Cl) C(=O)CN1C(=O)c1ccnc(N  )c1 | Neg\_lig\_2745 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 283 | OCCSc1nnc(Cc2ccccc2)n1 Cc1ccccc1 | Neg\_lig\_3354 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 284 | COCCNc1cc(C) [nH+]c2c(C)c(-  c3ccccc3)nn12 | Neg\_lig\_3356 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 285 | CCOc1ccccc1NC(=O)c1sc 2nc3c(cc2c1N)CN(Cc1ccc cc1)CC3 | Neg\_lig\_3395 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 0 |
| 286 | Cc1ccccc1Nc1nc([C@]2(C  )C[C@@]3(C[C@H]  (COCC(C)C)OC3=O)C(= O)O2)cs1 | Neg\_lig\_10 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 287 | CC(=O)Nc1c(N)c2ccccc2o c1=O | Neg\_lig\_20 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 288 | Cc1ccc(C(=O)[C@@H] (NC(=O)c2cccs2)Nc2ccccc 2Br)cc1 | Neg\_lig\_43 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 289 | Cc1ccccc1CN1c2ccccc2C2  =C([C@@H]  (c3ccc(Cl)cc3)C(C#N)=C( N)O2)S1(=O)=O | Neg\_lig\_55 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 290 | COc1ccc([C@@H](O) [C@@H] (C)Oc2ccc([C@H]3O[C@ H](c4ccc(O[C@H](C) [C@H]  (O)c5ccc(OC)c(OC)c5)c(O  C)c4)[C@H](C) [C@H]3C)cc2OC)cc1OC | Neg\_lig\_66 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 291 | Cc1ccc(- c2noc(CNC3CCCCC3)n2)  cc1 | Neg\_lig\_108 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 292 | CCOc1ccc(-c2noc(- c3nnn(- c4cccc(OC)c4)c3N)n2)cc1 | Neg\_lig\_118 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 293 | O=C1CCC2(CC[NH+] (Cc3ccoc3)CC2)CN1CCC O | Neg\_lig\_121 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 294 | COc1cccc(CNc2ccc3c(c2) ncn3C(C)(C)C)c1OC | Neg\_lig\_138 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 295 | NC(=O)c1ccc2c(c1SCCO)  C(=O)c1ccccc1C2=O | Neg\_lig\_208 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 296 | CCCCNc1nc2c(- c3cccc(F)c3)nnn2c2ccccc1 2 | Neg\_lig\_218 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 297 | Clc1ccc(-c2nc(- c3cc4cc(Cl)ccc4o3)cs2)cc1 | Neg\_lig\_230 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 298 | COc1ccccc1- c1nc2c(OC)ccc(OC)c2cc1 CN1CC[C@@H](O)C1 | Neg\_lig\_262 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 299 | O=C(CCc1nc(-  c2ccc[nH+]c2)no1)N1CCC [C@@](O)(CO)C1 | Neg\_lig\_303 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 300 | O=C(CCSc1nnc(-  c2ccncc2)o1)N1CCOC[C @@H](O)C1 | Neg\_lig\_304 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 301 | C=CCNc1nc(-  c2ccccc2)nc(-n2ccnc2)n1 | Neg\_lig\_311 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 302 | Fc1ccc(C[NH2+]CC[C@H  ](Cc2ccccc2)c2ccco2)cc1 | Neg\_lig\_315 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 303 | Cc1cc(C)n(- c2nc3ccccc3nc2Nc2ccc(Cl  )cc2)n1 | Neg\_lig\_362 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 304 | C[C@]1(Cc2ccc3c(c2)OC O3)CCC[N@@H+]  (Cc2cccnc2N)C1 | Neg\_lig\_382 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 305 | CCc1c(N[C@H]  (c2ncccc2C)C2CC2)nc(N) [nH+]c1C | Neg\_lig\_399 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 306 | Cc1c(C(=O)N2CCCCCC2)  nnn1-c1nonc1N | Neg\_lig\_407 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 307 | Cc1ccc(C(=O)c2sc3nc(C)c cc3c2N)cc1 | Neg\_lig\_414 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 308 | Nc1cc(C(=O)N2CCC(c3nc  cn3Cc3ccncc3)CC2)ccn1 | Neg\_lig\_462 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 309 | CC[n+]1cn(C[C@H]  (O)COCc2ccccc2)c2ccccc 21 | Neg\_lig\_488 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 310 | O[C@H]  (COCc1ccccc1)CN1CCc2c cccc2C1 | Neg\_lig\_489 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 311 | Cc1ccccc1C(=O)/N=C1\ SC2=C(CC[C@H](C(C) (C)C)C2)\C1=C(\O)NCCO | Neg\_lig\_530 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 312 | O=C(CCC1CCN(C(=O)C[ C@H]2COCC[NH2+]2)C  C1)NCc1ccc(F)cc1 | Neg\_lig\_539 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 313 | Cn1c(=O)c2cccc(N)c2c(= O)n1C | Neg\_lig\_558 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 314 | C=C1CC2(OC1=O)c1cccc  c1CCc1ccccc12 | Neg\_lig\_578 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 315 | Cc1c(Cl)cccc1-n1nnc(- c2nc(-c3ccccn3)no2)c1N | Neg\_lig\_592 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 316 | CCOC(=O)N1CCN(c2ncn c3sc4c(c23)CCNC4)CC1 | Neg\_lig\_603 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 317 | O=C(NC1CC1) [C@@H]1CNCCN1C(=O)  c1cc2c(s1)CCCCC2 | Neg\_lig\_640 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 318 | Cc1cc2c(c(=O)o1) [C@@]1(C(=O)Nc3ccc(C)  c(Br)c31)C(C#N)=C(N)O2 | Neg\_lig\_667 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 319 | ClC[C@H]  (C[NH2+]Cc1ccccc1)c1cc ccc1 | Neg\_lig\_686 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 320 | COc1ccc([C@@H]2C=C(c 3ccc(C)cc3) [NH+]=C3NC(CCCO)=[N H+]N32)cc1 | Neg\_lig\_692 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 321 | COCc1cc(C)nc2sc(C(=O) Nc3ccc(F)cc3F)c(N)c12 | Neg\_lig\_695 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 322 | NC(=O)C1=C(NCCc2cccc  c2)c2ccccc2S1(=O)=O | Neg\_lig\_743 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 323 | CCCCc1nc2sc(C(=O)OCC  )c(N)c2c2c1COC(C)(C)C2 | Neg\_lig\_816 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 324 | CC[C@H](O)Cn1nc(-  c2ccc(O)cc2)nc1CCc1cccn c1 | Neg\_lig\_829 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 325 | Oc1ccc(C2CCN(c3cc[nH+  ]c4ccccc34)CC2)cc1O | Neg\_lig\_861 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 326 | CC1(C) [C@@H]2CC[C@@H](C/ N=C(\N)CSS(=O)(=O)O) [C@H]1C2 | Neg\_lig\_884 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 327 | COc1ccc2cc(- c3cc(N)cc[nH+]3) [nH]c2c1 | Neg\_lig\_904 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 328 | CC(C)c1nc(CN(C)C(=O)C  Cc2nc(N)n[nH]2)no1 | Neg\_lig\_911 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 329 | Cn1c(=O)c2c(nc(Sc3ccc(N  )cc3)n2C)n(C)c1=O | Neg\_lig\_305 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 330 | Oc1c(CN2CCN(c3ccccc3) CC2)cc(Br)c2cccnc12 | Neg\_lig\_945 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 331 | CCN(CC)S(=O)  (=O)c1ccc(Nc2ncnc3c2nc2 n3CCCCC2)cc1 | Neg\_lig\_958 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 332 | CS(=O)  (=O)N1CCN(c2ccc(/N=c3\ c4c(nc5[nH+]c[nH]n35)C CC4)cc2)CC1 | Neg\_lig\_963 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 333 | O=S(=O)  (c1ccc(F)cc1)N1CCC[C@ H](CO)C1 | Neg\_lig\_966 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 334 | Cc1cc(OC[C@@H] (O)Cn2c(C)nc3ccccc32)cc c1Cl | Neg\_lig\_973 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 335 | [NH3+]CC1CCN(c2cnn(C  c3noc(- c4ccccc4)n3)c(=O)c2)CC1 | Neg\_lig\_983 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 336 | C1[C@@H]2[C@@H]3/ C(=N\N=C4\ [C@H]5[C@H]6C[C@@ H]4C[C@H]65) [C@H]1C[C@H]23 | Neg\_lig\_1004 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 337 | COC(=O)c1ccccc1Nc1c(- c2cc(Br)ccc2O)nc2cnccn1 2 | Neg\_lig\_1024 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 338 | Cc1sc2nc(CC[NH2+]C3C SCCSC3)[nH]c(=O)c2c1C | Neg\_lig\_1027 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 339 | CCOC(=O)c1ccc2ncc(C(= O)OCC)c(NCc3ccco3)c2c 1 | Neg\_lig\_1028 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 340 | CCOC(=O)c1c(Nc2ccc(Cl) cc2)cc(C)nc1C | Neg\_lig\_1047 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 341 | Cc1nnc(-n2cccc2)s1 | Neg\_lig\_1064 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 342 | CC(C)c1nc(CN(C)c2nc(C C[NH3+])  [nH+]c3ccccc23)cs1 | Neg\_lig\_1074 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 343 | FC(F)  (F)c1nnc2c3ccccc3c(NC3 CC3)nn12 | Neg\_lig\_1079 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 344 | C[C@@H]  (CO)NC(=O)c1cc2ccccc2o c1=O | Neg\_lig\_1089 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 345 | CC1=[NH+]C[C@H]  (C)c2ccccc21 | Neg\_lig\_998 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 346 | CN(C(=O)c1cccc(S(=O)  (=O)N(C)c2ccccc2)c1) [C@@H]1CCCC[C@H]1 O | Neg\_lig\_1131 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 347 | Nc1nc(NCCc2n[nH]c3c2C CCC3)cc(N2CCOCC2)n1 | Neg\_lig\_1143 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 348 | COc1ccccc1Nc1cc(C)nc2n c(C)nn12 | Neg\_lig\_1181 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 349 | CCOc1cc([C@@H]2c3c(n [nH]c3- c3ccccc3O)C(=O)N2CCC O)ccc1O | Neg\_lig\_36 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 350 | CC1=C(C(=O)/N=C2\ C=CC3=NN=CC3=C2)NN  (c2ccccc2)[N-]1 | Neg\_lig\_1222 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 351 | O=C(NCCCCc1ccccc1)c1 nn(-c2ccc(Cl)cc2)nc1CO | Neg\_lig\_1228 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 352 | Cc1ccc(OCc2nc(N)nc(N(C  )C)n2)cc1C | Neg\_lig\_1260 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 353 | O=C([O-])c1cccc(Nc2c(- c3cccc(O)c3)nc3cnccn23)c 1 | Neg\_lig\_1274 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 354 | C=CCn1cc(C[NH2+]Cc2n  ncn2CCc2ccccc2)c(C)n1 | Neg\_lig\_1325 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 355 | CCC(=O)O[C@]1(C(=O)S CF)[C@H] (C)C[C@H]2[C@@H]3C[ C@H] (F)C4=CC(=O)C=C[C@]4 (C)[C@@]3(F)[C@@H] (O)C[C@@]21C | Neg\_lig\_1346 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 356 | C[C@@H](CCc1ccccc1) | Neg\_lig\_1354 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | [NH2+]CCSc1c[nH]nn1 |  |  |  | UGACGGUACA |  |
| 357 | O=S1(=O)N=C(/N=c2\  cccc[nH]2)c2ccccc21 | Neg\_lig\_1562 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 358 | CN(C)c1cccc(C(=O)N2CC C([C@@H]  (O)CCc3ccccc3)CC2)c1 | Neg\_lig\_1586 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 359 | COC(=O)CN1CCC([NH2+  ] [C@H]2CCNC2(C)C)CC1 | Neg\_lig\_1680 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 360 | [NH3+] [C@H]1CCN(C(=O)c2ccc  c(-c3ncc[nH]3)c2)C1 | Neg\_lig\_1192 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 361 | Cc1cc2nc(CN3CC[C@H]4 C[NH2+]C[C@H]43)cc(= O)n2[nH]1 | Neg\_lig\_1711 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 362 | COc1ccc(CC2=NN3C([C  @@H](CCc4ccccc4) [C@@H](C)O)=[NH+] [C@H](C) [C@@H]3C(=O)N2)cc1O C | Neg\_lig\_1723 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 363 | Cc1cccc(-n2nnc(-c3nc(- c4ccc(F)cc4)no3)c2N)c1 | Neg\_lig\_1781 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 364 | Cn1c(=O)c2c(nc(N3CCOC C3)n2CC[NH3+])n(C)c1= O | Neg\_lig\_1833 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 365 | CN(C)c1ccc(C(=O)NC(C)  (C)c2nnc(N)s2)cn1 | Neg\_lig\_1856 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 366 | Cc1ccc(N2C(=O)C(=CN)C (=O)N(c3ccc(C)cc3)C2=O  )cc1 | Neg\_lig\_1873 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 367 | Cc1cccc(NCCC(=O)c2ccc 3ccccc3c2)c1 | Neg\_lig\_570 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 368 | CC[C@H](O)Cn1ncnc1- c1ccc(C#N)cc1 | Neg\_lig\_1956 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 369 | Cc1ccc(NC(=O)c2ccc(CN 3CC[NH+]  (C)CC3)cc2)cc1Nc1nc(- c2cccnc2)cs1 | Neg\_lig\_1962 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 370 | CC[C@@]1(C)CC(=O)c2c c(NC(=O)CCc3cc4n(n3)C CC[NH2+]C4)ccc2O1 | Neg\_lig\_1199 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 371 | O=[N+]  ([O-])c1ccc(Cl)cc1NCCN1 CCOCC1 | Neg\_lig\_2004 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 372 | COCCNc1oc(-  c2ccc(S(=O) (=O)N3CCCCC3)cc2)nc1 C#N | Neg\_lig\_2049 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 373 | Nc1nc(CSCCO)nc(Nc2ccc cc2)n1 | Neg\_lig\_2058 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 374 | [NH3+][C@H]1CN(/ C(O)=C2/ C=NC(C3CC3)=NC2=O)C [C@@H]1C1CC1 | Neg\_lig\_2102 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 375 | O=C1C=C(NCCC[NH+]2 CCOCC2)C2(CCCCC2)O 1 | Neg\_lig\_2112 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 376 | CC(C)  (C)c1[nH]nc2c1[C@@H] (c1cc(Br)ccc1F)C(C#N)=C (N)O2 | Neg\_lig\_2156 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 377 | COc1cccc(- | Neg\_lig\_2179 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | c2cc(=O)c3ccccc3o2)c1N |  |  |  | UGACGGUACA |  |
| 378 | Clc1ccccc1C[NH2+]Cc1cc cnc1 | Neg\_lig\_2200 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 379 | c1ccc(- c2ccc(C[NH2+]Cc3cccs3) o2)cc1 | Neg\_lig\_2235 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 380 | COc1ccc(C2=NC(=O)/ C(=C(/ O)N3CC[C@H]4C[NH2+] C[C@H]43)C=C2)cc1 | Neg\_lig\_2265 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 381 | O=c1[nH]cc(I)cc1I | Neg\_lig\_2331 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 382 | Cc1ncsc1CCC(=O)N[C@ @H](CO)C1CCSCC1 | Neg\_lig\_2333 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 383 | c1cc2c(cc1Nc1nc(N3CCC CC3)nc(N3CCCCC3)n1)O CO2 | Neg\_lig\_2346 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 384 | CCOC(=O)c1cnc2c(C)cc( C)cc2c1Nc1ccc(N(C)C)cc 1 | Neg\_lig\_2379 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 385 | Cc1cccc(Nc2c(- c3ccc(O)cc3)nc3ncccn23)c 1 | Neg\_lig\_2422 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 386 | O=C1C[C@H] (Nc2ccc(N3CCOCC3)cc2)  C(=O)N1c1cccc2ccccc12 | Neg\_lig\_2488 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 387 | NS(=O)  (=O)c1ccc(Cl)cc1[N+] (=O)[O-] | Neg\_lig\_2518 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 388 | C=C1C(=O)O[C@@H]2C [C@]3(C)O[C@H]3CCC(  C)=C[C@H](OC(C)=O) [C@@H]12 | Neg\_lig\_2557 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 389 | Cc1cc(C(c2cc(C)c(N)c(C)c 2)c2ccco2)cc(C)c1N | Neg\_lig\_2565 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 390 | Cn1nc(C(=O)N2CCC3(CC 2)[C@@H] (OCC[NH3+])C[C@H]3O  )cc1-c1ccccc1 | Neg\_lig\_2567 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 391 | c1cncc([C@@H]2CCCCN 2c2ncnc3sc4c(c23)CCNC4  )c1 | Neg\_lig\_2652 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 392 | COc1ccc(N2CC(=O)C(c3n c(C)c(C)s3)=C2N)cc1 | Neg\_lig\_2682 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 393 | O=C(C[C@@H]1Nc2cccc c2NC1=O)Nc1ccccc1SC(F  )(F)C(F)(F)C(F)(F)F | Neg\_lig\_2694 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 394 | Cc1ccc(OC[C@@H] (O)C[NH+]2CCCCC2)c(C  )c1 | Neg\_lig\_2728 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 395 | Cc1nc(CN2CCN(C(=O)c3 ccccc3[C@H]3CC[NH2+] C3)CC2)no1 | Neg\_lig\_2736 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 396 | CC(C)n1cc(C#N)c(N)n1 | Neg\_lig\_2738 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 397 | O=C([O-])c1ccccc1- c1ccccc1C(=O)Nc1ccc2oc(  =O)c3ccccc3c2c1 | Neg\_lig\_2799 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 398 | CC1CC[NH+] (Cc2ccc(C(=O)N3CCO[C @]4(C[NH2+]CCOC4)C3) o2)CC1 | Neg\_lig\_2815 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 399 | O=C1Nc2ccccc2/C1=C1/ Nc2ccccc2C1=O | Neg\_lig\_2818 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 400 | Cc1c(C(=O)N2CCO[C@]3 (C[NH2+]CCOC3)C2)sc2c  cccc12 | Neg\_lig\_2819 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 401 | CCc1ccc(CNC(=O)c2nn(- c3ccc(C)c(C)c3)nc2CO)cc 1 | Neg\_lig\_2824 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 402 | C[C@]12CC[C@@H]3c4c  cc(O)cc4CC[C@H]3[C@ H]1[C@@H](O)[C@@H] (O)[C@H]2O | Neg\_lig\_2832 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 403 | CCn1c(N)c(C(=O)N2CCC CC2)sc1=S | Neg\_lig\_2893 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 404 | Cc1c/c(=N\C2=NS(=O)  (=O)c3ccccc32)[n-]o1 | Neg\_lig\_2908 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 405 | O=C(c1ccc(Cn2ccnc2)o1) N1CC[C@@]2(CCCN(CC O)C2=O)C1 | Neg\_lig\_2952 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 406 | O=C1C[C@H] ([NH+]2CCCCC2)C=C1N  c1ccccc1 | Neg\_lig\_2981 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 407 | CO[C@H]1CN(C(=O)COc 2cccc(C)c2C)CC[C@H]1[ NH3+] | Neg\_lig\_2998 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 408 | Cc1cccc(OC2CCN(Cc3c(C O)cnc(C)c3O)CC2)c1 | Neg\_lig\_2999 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 409 | Cc1nc(CC(=O)N[C@H] (c2nnc3n2CC[NH2+]CC3) C(C)C)c(C)s1 | Neg\_lig\_3029 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 410 | COC(=O)c1cc(/ N=C2C(=C(/N)[O-])/ S(=O)  (=O)c3ccccc3/2)ccc1Cl | Neg\_lig\_3032 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 411 | O=C(c1ccc(Nc2nc(- c3ccccc3)c3cc(Br)ccc3n2) cc1)N1CCOCC1 | Neg\_lig\_3033 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 412 | Cn1ccnc1[C@H] (O)c1ccc(N)cc1 | Neg\_lig\_3106 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 413 | CN(C)C(=O)c1cccc(COc2 ccc(N3C(=N)NC(N)=[NH  +]C3(C)C)cc2Cl)c1 | Neg\_lig\_3124 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 414 | O=C([C@@H]1C[C@@H  ] (O)C[NH2+]1)N1CCC(c2[ nH+]ccn2CC2CC2)CC1 | Neg\_lig\_3142 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 415 | O=C([O-])[C@H]  (Cc1ccccc1)Nc1ncnc2c1oc 1ccccc12 | Neg\_lig\_3164 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 416 | CC(C)CNc1nc2c(c(=O)n(  Cc3ccccc3)c(=O)n2C)n1C | Neg\_lig\_3181 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 417 | COc1ccc(- c2c(C)nn3c(NCC[NH+]4C CCC4)cc(C) [nH+]c23)cc1OC | Neg\_lig\_3185 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 418 | Fc1ccc(CNc2ccc(N3CCN( Cc4ccccc4)CC3)cc2)cc1 | Neg\_lig\_1778 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 419 | O=C1C[C@H] (Nc2ccc3c(c2)OCO3)C(=  O)N1c1ccccc1 | Neg\_lig\_2168 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 420 | C[N@H+]1CCc2[nH]nc(C (=O)N(C/C=C\  c3ccccc3)CCO)c2C1 | Neg\_lig\_3342 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 421 | CC(=O)O[C@]1(C(C)=O) CC[C@@H]2[C@@H]3C [C@H] (C)C4=CC(=O)CC[C@]4( C)[C@H]3CC[C@@]21C | Neg\_lig\_3360 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 422 | Cn1c(N2CC[C@H] (O)C2)nc2cc(C(=O)N[C@  H]3CCc4ccccc43)ccc21 | Neg\_lig\_3373 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 423 | CCc1ccc(NC(=O)c2nnn(C C(=O)Nc3ccccc3)c2N)cc1 | Neg\_lig\_3423 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 0 |
| 424 | O=C1CCC2(CCN(Cc3nnc(  -  c4cccnc4)o3)CC2)CN1CC O | Neg\_lig\_1 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 425 | COc1ccc(C(=O)c2sc3nc4c (c(C(F)F)c3c2N)CCCC4)c  c1 | Neg\_lig\_51 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 426 | Cc1ccn(CO)n1 | Neg\_lig\_57 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 427 | Cc1cc(N[C@H]2CC(=O)N  (Cc3ccccc3C(F) (F)F)C2)nc(N)n1 | Neg\_lig\_65 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 428 | O=C(Nc1cccc(Cn2cncn2)c 1)N1CCN[C@H]2CS(=O) (=O)C[C@H]21 | Neg\_lig\_146 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 429 | Cn1cc[nH+]c1CN1CCN(C [C@]2(O)CC[NH2+]C2)C C1 | Neg\_lig\_190 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 430 | CC(C)N(CCCc1ccccc1)C(  =O)C1(N)CC1 | Neg\_lig\_224 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 431 | C[NH+]  (C)CCc1c[nH]c2ccc(CS(= O)(=O)N3CCCC3)cc12 | Neg\_lig\_244 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 432 | CN(C)c1n/c(=N/ Cc2ccco2)ss1 | Neg\_lig\_246 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 433 | O=C(C1CCC1)N1C[C@H  ](O)[C@@H] (N2CCN(c3cnccn3)CC2)C 1 | Neg\_lig\_258 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 434 | C[NH2+]C[C@H]  (O)c1cccc(OC(=O)c2ccccc 2C)c1 | Neg\_lig\_265 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 435 | CC1=CC(=O)C(=C(\C)O)/ C(=N/  c2ccc3c(c2)OCO3)O1 | Neg\_lig\_281 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 436 | CCc1c(C)nn(CCn2cc(- c3ccc(CO)o3)nn2)c1C | Neg\_lig\_50 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 437 | COc1cccc(C[NH2+]CCO)  c1OCc1ccc(Cl)cc1 | Neg\_lig\_309 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 438 | O=C(CC[NH2+]C[C@H]  (O)c1ccccc1Cl)NCc1cccs1 | Neg\_lig\_319 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 439 | Cc1cccc(NC(=O)c2nnn(Cc 3ccc(C(C)C)cc3)c2N)c1 | Neg\_lig\_336 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 440 | C[C@@H]1CCO[C@H]2 CN3C=C(C(=O)  [N-]Cc4ccc(F)cc4F)C(=O) C(=O)C3=C(O)N21 | Neg\_lig\_376 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 441 | CSc1c(CC(=O)NCCO)n(C  )c2ccccc12 | Neg\_lig\_377 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 442 | O=C(CCc1nc(-  c2ccccc2)no1)N1C[C@H] 2CCC[C@@]2(CO)C1 | Neg\_lig\_564 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 443 | COc1ccc(CNCc2ccc(- c3ccc(OC)c(Cl)c3)o2)cc1 | Neg\_lig\_582 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 444 | N#CC1=C(N)N(c2c(F)ccc c2F)C2=C(C(=O)CCC2)  [C@@H]1c1ccccc1F | Neg\_lig\_627 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 445 | CCN(CC)S(=O)  (=O)c1ccc(Nc2nc3ccc(Cl)c c3n3cnnc23)cc1 | Neg\_lig\_644 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 446 | COc1ccc(C(=O)c2sc3nc(C  )cc(C(F) (F)F)c3c2N)cc1OC | Neg\_lig\_647 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 447 | Cc1cc(Nc2ccccc2F)n2nc(- c3ccccc3)nc2n1 | Neg\_lig\_697 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 448 | C[N@H+]1CCN(c2ccnc(N  )n2)C[C@@]12CCC(=O) N(CC1CC1)CC2 | Neg\_lig\_720 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 449 | Cc1cc2ncn(C[C@H] (O)COc3cccc(Cl)c3)c2cc1 C | Neg\_lig\_807 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 450 | CCc1ccc([C@H]2N[C@@  ](CC(C)C)(C(=O)OC)  [C@H]3C(=O)N(C)C(=O)  [C@@H]23)nc1 | Neg\_lig\_870 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 451 | CCOC(=O)c1sc2nc(C)cc( C(F)(F)F)c2c1N | Neg\_lig\_871 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 452 | CCOC(=O)CN[C@H]1CC  (=O)N(c2ccc(Br)cc2)C1= O | Neg\_lig\_883 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 453 | Cc1ccccc1- c1ccccc1C(=O)N1CC[C@ H](CO)[C@@H](O)C1 | Neg\_lig\_898 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 454 | C[NH2+]CC(=O)N1C[C@ H]2C[C-]1C(=O)N2c1cc(-  c2ccccc2)ccc1OC | Neg\_lig\_940 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 455 | CCc1nc(NC[C@H]2CCC O2)c(C#N)c2c1COC(C) (C)C2 | Neg\_lig\_944 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 456 | C=CCn1c(=N)n(C[C@H]  (O)c2ccc(C)cc2)c2ccccc21 | Neg\_lig\_960 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 457 | Cc1cc(C)n(- c2nc(NCCC[NH+] (C)C)c3c4c(sc3n2)COC(C) (C)C4)n1 | Neg\_lig\_974 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 458 | CC[C@H](O)Cn1nc(-  c2ccncc2)nc1C1(N2CCCC 2)CCCC1 | Neg\_lig\_39 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 459 | [NH3+]C[C@H]  (c1ccccc1)C1CCCC1 | Neg\_lig\_993 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 460 | CN(C[C@H]1CC(=O)N(C (C) (C)C)C1)c1nccc(N2CCC( O)CC2)n1 | Neg\_lig\_1006 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 461 | Oc1cc(C[NH2+]C2CCCC C2)c(O)cc1C[NH2+]C1CC CCC1 | Neg\_lig\_1041 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 462 | CCOc1ccc(CN2CCN(c3cc c(Cl)cn3)CC2)cc1CO | Neg\_lig\_1066 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 463 | COCc1noc(CCn2cnc3sc4c (c3c2=O)CCNC4)n1 | Neg\_lig\_1092 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 464 | COC(=O)c1ccc(OC[C@@ H](O)CN2C(=O)NC(C) (C)C2=O)cc1 | Neg\_lig\_1102 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 465 | O=C1OC2(CC[NH2+]CC2  )CN1CC(=O)N1CC[C@H]  1c1cccs1 | Neg\_lig\_1144 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 466 | O=S1(=O)C[C@H]  (NCCc2ccccc2F)[C@@H] (S(=O)  (=O)c2ccc(F)cc2)C1 | Neg\_lig\_1212 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 467 | Clc1ccc(CCNc2ncnc3c2nc 2n3CCCC2)cc1 | Neg\_lig\_1253 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 468 | COc1ccc(CC[N@H+](C) [C@H]2CCCN(c3ccnc(N) n3)C2)cc1OC | Neg\_lig\_1262 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 469 | CC(C)  [C@]1(O)CN(c2nc3ccccc3 n2CCO)C[C@H]1C | Neg\_lig\_1269 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 470 | Cc1n[nH]c(C)c1[C@@H] ([NH3+])C(=O)NCc1cc(C C(C)C)no1 | Neg\_lig\_1291 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 471 | Nc1nc2c3ccccc3[nH+]c(C c3ccccc3)n2n1 | Neg\_lig\_1317 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 472 | CC1=N/C(=N/  Nc2ccccc2)N=C1/N=N/ c1ccccc1 | Neg\_lig\_1343 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 473 | C/C(=N\ NC(=O)c1cc(C)n[nH]1)c1  ccc(N)cc1 | Neg\_lig\_1357 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 474 | Cc1ccc([C@H] (CN)CC(=O)O)cc1 | Neg\_lig\_1455 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 475 | Cc1cc(NC(=O)Nc2cc(F)cc c2F)no1 | Neg\_lig\_1476 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 476 | COc1ccc(CC[NH2+]Cc2cc ccc2Cl)cc1 | Neg\_lig\_1532 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 477 | O=C1/C(=C\  NCCO)Nc2ccccc21 | Neg\_lig\_1568 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 478 | CNc1nc(N2CCOCC2)nc(-  n2cnc(SCc3ccccc3)n2)n1 | Neg\_lig\_1573 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 479 | Cc1ccc(Nc2cc(- c3cccc(N4C(=O)c5ccccc5 C4=O)c3)ncn2)cc1NS(C) (=O)=O | Neg\_lig\_1584 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 480 | Clc1ccc(-c2noc(- c3cccnc3NC3CCCCC3)n2  )cc1 | Neg\_lig\_1597 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 481 | Cc1ccc(- c2cc(C(=O)NCCCNc3cccn c3)[nH]n2)o1 | Neg\_lig\_1660 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 482 | CCc1ccc([C@H]2NCCc3[ nH]c[nH+]c32)nc1 | Neg\_lig\_1687 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 483 | Cc1nc2sccn2c1C(=O)NCC c1nnc2n1CC[NH2+]CC2 | Neg\_lig\_1718 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 484 | Cc1ccc(- c2nc(N(C)Cc3nccn3C)ncc 2-c2ccc(N)nc2)cc1 | Neg\_lig\_1780 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 485 | Cc1cccc(OC[C@@H] (O)CNC(=O)c2ccccc2C(= O)[O-])c1 | Neg\_lig\_1760 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 486 | Cc1nc(C(C)C)sc1C(=O)N1 CCCN([C@H]2COC[C@ @H]2O)CC1 | Neg\_lig\_1783 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 487 | Cc1ccc(Nc2c(- c3ccc(O)cc3)nc3ncccn23)c (C)c1 | Neg\_lig\_1798 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 488 | COc1ccc(CCNc2cc(C) [nH+]c3cc(- c4ccccc4OC)nn23)cc1OC | Neg\_lig\_1823 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 489 | CCCCN1CCNC1=S | Neg\_lig\_1872 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 490 | COc1cc(C[NH2+]CCO)cc  c1OCc1ccc2c(c1)n(C)c(=O  )n2C | Neg\_lig\_796 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 491 | c1csc(- c2nc3cnccn3c2Nc2ccc3c(c 2)OCCO3)c1 | Neg\_lig\_1892 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 492 | CC1(C)CC(=O)C2=C(C1) OC(N)=C(C#N)  [C@H]2c1cc(Br)ccc1F | Neg\_lig\_1963 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 493 | Nc1nonc1C(=O)NCCNCC  #Cc1ccccc1 | Neg\_lig\_1973 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 494 | COc1cccc(Nc2cc(C)nc3nc( Cc4ccccc4)nn23)c1 | Neg\_lig\_1980 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 495 | Nc1c(C(=O)c2ccc(Br)cc2) sc2ncccc12 | Neg\_lig\_1981 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 496 | CCCCNc1nc2c(c(=O)n(Cc 3ccccc3)c(=O)n2C)n1C | Neg\_lig\_2042 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 497 | Cc1nnsc1CNCc1nc(- c2ccco2)no1 | Neg\_lig\_2092 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 498 | Nc1ncnc(Nc2ccc3c(c2)OC O3)n1 | Neg\_lig\_2095 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 499 | [NH3+]CCNC(=O)c1nc(-  c2ccccc2)no1 | Neg\_lig\_1619 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 500 | OCc1nc2ccccc2n1Cc1cccc c1Cl | Neg\_lig\_2106 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 501 | CC[C@]1(C)OC(=O)N(C  CO)[C@]1(C)O | Neg\_lig\_2107 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 502 | C[C@H]1CCc2c(sc3ncnc( N4CCN(CCO)CC4)c23)C 1 | Neg\_lig\_2123 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 503 | O=C(OCCNC1=NS(=O)  (=O)c2ccccc21)c1ccco1 | Neg\_lig\_2124 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 504 | CCC[C@H]1C[N@@H+] (CCCO)C[C@@H]1NC(=  O)Cn1cc(C)cn1 | Neg\_lig\_2206 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 505 | O=C(C[S@@]  (=O)Cc1ccco1)NC/C=C/ COc1cc(C[NH+]2CCCCC  2)ccn1 | Neg\_lig\_2251 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 506 | CC(=O)c1ccc(NC(=O)c2sc 3nc(N4CCCC4)c4c(c3c2N  )CCCC4)cc1 | Neg\_lig\_2146 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 507 | COc1ccc2c(c1)nc(SC[C@ H](C)O)n2C | Neg\_lig\_2330 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 508 | C[NH+](C)CCNc1cc(C(C)  (C)C)[nH+]c2c(-  c3ccc(Cl)cc3)cnn12 | Neg\_lig\_2344 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 509 | Cc1cc(NC(=O)Nc2cccc3cc ccc23)no1 | Neg\_lig\_1654 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 510 | Cn1c(=O)n(C)c2cc(C[NH2  +]Cc3ccccn3)ccc21 | Neg\_lig\_2390 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 511 | CCOc1ccccc1Nc1cc(- c2ccccc2)[nH+]c(C)n1 | Neg\_lig\_2425 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 512 | C[NH+](C)CC/[NH+]=C1\ C=C(O)CC(C)(C)C1 | Neg\_lig\_2443 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 513 | Clc1cc(/N=c2\ c3c(nc4[nH+]c[nH]n24)C CC3)ccc1N1CCOCC1 | Neg\_lig\_2447 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 514 | COc1ccc(C(=O)c2sc3nc4c (c(-  c5ccncc5)c3c2N)CCCC4)c c1 | Neg\_lig\_2491 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 515 | C[C@H] (O)CN1CC2(CCC1=O)CC N(S(=O) (=O)N1CCCC1)CC2 | Neg\_lig\_2589 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 516 | O=C(Nc1ccccc1)C1=C(Nc 2ccccc2)CSC1 | Neg\_lig\_2610 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 517 | Nc1ncnc2ccc(- c3cccc(C(=O)N4CCCC4)c  3)cc12 | Neg\_lig\_2626 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 518 | CCOC(=O)N1CCC([NH2+  ] [C@@H]2CC[C@@H]2N C(=O)c2nc(C)oc2C)CC1 | Neg\_lig\_2630 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 519 | c1ccc([C@H]2[NH2+]CCc  3nc[nH]c32)cc1 | Neg\_lig\_2631 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 520 | Fc1ccccc1Nc1nc(- c2cccnc2)cs1 | Neg\_lig\_2633 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 521 | O=S1(=O)CC[C@H]  (CNCc2cc(O)c3cccc(F)c3n 2)C1 | Neg\_lig\_2680 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 522 | Cc1cccc(OCCCCn2c([C@ H](C)O)nc3ccccc32)c1 | Neg\_lig\_2707 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 523 | c1ccc([C@@H] (CC[NH2+]C2CCSCC2)c2  ccco2)cc1 | Neg\_lig\_2722 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 524 | COc1cc(CC(=O)C(=O) [O-])oc(=O)c1 | Neg\_lig\_2757 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 525 | Cc1ccc([C@H]2C(C#N)= C(N)OC3=C2S(=O)  (=O)N(Cc2ccc(F)cc2)c2cc ccc23)cc1 | Neg\_lig\_2762 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 526 | Cc1csc(C2=C(N)N(c3cccc (Br)c3)CC2=O)n1 | Neg\_lig\_2763 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 527 | COC(=O)[C@@H]  (Nc1nc(C2CCCC2)nc2c1c nn2C)[C@@H](C)O | Neg\_lig\_2793 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 528 | Cc1cccc(- c2ncc(CNCCCN3CCOCC  3)cn2)c1 | Neg\_lig\_2825 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 529 | Cn1c(=O)c2nc(N3CC[NH  +](CCO)CC3) [nH]c2n(C)c1=O | Neg\_lig\_2840 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 530 | Cc1nc(N)nc(C)c1CC(=O) N[C@@H]1CC[C@@H] ([NH3+])C1 | Neg\_lig\_2853 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 531 | O=C(Nc1ccccc1)c1ccc(S(= O) (=O)N2CCC[NH2+]CC2)c  c1 | Neg\_lig\_2858 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 532 | CN1CC[NH+] (C[C@@H]2CN(C(=O)CC  c3cccs3)C[C@@H]2CO)C C1 | Neg\_lig\_2861 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 533 | CCc1ccc(- n2nc(CO)c(C(=O)NCc3ccc cn3)n2)cc1 | Neg\_lig\_2863 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 534 | CN1CCN([C@H]2CCN(C  c3cccnc3N)C[C@H]2CCC (=O)O)CC1 | Neg\_lig\_2887 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 535 | C[N@@H+]  (CCNc1ncnc2onc(- c3ccc(Cl)cc3)c12)C1CCC CC1 | Neg\_lig\_2925 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 536 | CCN(C(=O)Nc1ccccc1C[ NH+]1CCCCC1) [C@H]1COC[C@@H]1O | Neg\_lig\_2930 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 537 | O=C(c1ccc(- n2cnnc2)cc1)N1C[C@@H  ] (C[NH+]2CCCC2)C[C@ @H](CO)C1 | Neg\_lig\_2995 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 538 | Cc1nn2c(N3CCN(CCO)C  C3)cc(-c3ccccc3) [nH+]c2c1-c1ccc(Cl)cc1 | Neg\_lig\_3005 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 539 | COc1ccccc1Nc1ncnc2ccc( Br)cc12 | Neg\_lig\_3027 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 540 | CCc1ccc(NC(=O)c2nnn(C C(=O)Nc3ccccc3C)c2N)cc 1 | Neg\_lig\_3040 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 541 | CC1(C)CC(=O)C2=C(C1) OC(N)=C(C#N)  [C@H]2c1c(F)cccc1Cl | Neg\_lig\_3073 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 542 | Fc1ccccc1Nc1nc2nonc2nc 1N1CCOCC1 | Neg\_lig\_3082 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 543 | CNC(=O) [C@@H]1C[C@H] ([NH3+])CN1S(=O)  (=O)CCc1ccncc1 | Neg\_lig\_3083 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 544 | Cc1c(C(=O)NCCO)nnn1-  c1ccc2noc(- c3ccc(Br)cc3)c2c1 | Neg\_lig\_3088 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 545 | Cc1ccc(C)c(NCCOc2ccccc 2)c1 | Neg\_lig\_2933 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 546 | c1ccc(NN(Cc2ccncc2)c2cc ccc2)cc1 | Neg\_lig\_3245 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 547 | Cc1cc(C)c2c(N)c(C(=O)c3 ccc4c(c3)OCO4)sc2n1 | Neg\_lig\_3278 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 548 | Oc1ccc(- c2nc3ncccn3c2Nc2ccc(Cl) cc2)cc1 | Neg\_lig\_3307 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 549 | Cc1cc(- c2[nH]nc3c2[C@@H] (c2ccc(F)cc2)C(C#N)=C(N  )O3)c(C)s1 | Neg\_lig\_3309 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 550 | c1cn(CCC[NH2+]Cc2ccc3 c(c2)OCO3)cn1 | Neg\_lig\_1498 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 551 | CCc1ccc([C@H]2C(C#N)  =C(N)Oc3n[nH]c(COC)c3  2)cc1 | Neg\_lig\_3322 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 552 | CN(C)c1ccc(N[C@H]2CC (=O)N(c3ccc(N4CCOCC4)  cc3)C2=O)cc1 | Neg\_lig\_3353 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 553 | CCOC(=O)c1sc(Nc2ccc(C  )cc2C)nc1C | Neg\_lig\_1721 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 554 | Cc1ccc2[nH]c(C)c([C@@ H] (O)C[NH+]3CCCCC3)c2c 1 | Neg\_lig\_794 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 0 |
| 555 | C=CCN[C@H]1CC(=O)N | Neg\_lig\_21 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | (c2ccc(Oc3ccccc3)cc2)C1  =O |  |  |  | ACUCUGGGAGA |  |
| 556 | O=C(N[C@H]1CC[C@H] 1[NH2+]C1CCOCC1)c1cc  ccc1-c1ccccc1F | Neg\_lig\_27 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 557 | Cc1ccc(NCc2nnc(- c3ccccc3)o2)c(C)c1 | Neg\_lig\_79 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 558 | Cc1[nH]nc2c1[C@H] (c1ccc3c(c1)OCO3)C(C#N  )=C(N)O2 | Neg\_lig\_81 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 559 | OC[C@H](CNc1nccc(- c2cccnc2)n1)Cc1ccsc1 | Neg\_lig\_90 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 560 | CO[C@@H]1C[C@@H]2  /C=C(C)/C=C/C=C/ C(=O)N[C@H]  (c3ccccc3)C/C=C/ CC[C@H] (O)CC(=O)C2=C1O | Neg\_lig\_91 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 561 | Cc1nc(C2=C(N)N(C[C@H  ](C)O)CC2=O)sc1C | Neg\_lig\_162 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 562 | CNC(=O) [C@@H]1C[C@H] ([NH3+])CN1C(=O)c1c(-  c2ccccc2)ccnc1C | Neg\_lig\_216 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 563 | CCOCCn1c(=O)  [nH]c2cc(C(=O)NCc3nc(N  )n[nH]3)ccc21 | Neg\_lig\_225 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 564 | Nc1ccc(S(=O) (=O)N=c2nccc[n-]2)cc1 | Neg\_lig\_310 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 565 | Cc1ccc([C@H] (C(=O)NCCOCCO)N(C)C  )cc1 | Neg\_lig\_322 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 566 | Cc1ccccc1N[C@@H]1c2c cccc2C(=O)N1Cc1ccccc1 | Neg\_lig\_324 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 567 | Cc1ccc(NC(=O)CNC[C@  H](C)c2ccccc2)c(C)c1 | Neg\_lig\_339 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 568 | O=c1[nH]c2ccccc2c(=O)n 1CCO | Neg\_lig\_340 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 569 | CCOC(=O)c1ccc(Nc2c(- c3ccc(C(C)C)cc3)c(=O)c2  =O)cc1 | Neg\_lig\_342 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 570 | CC(C)c1[nH]nc2c1[C@@] 1(C(=O)Nc3ccccc31)C(C# N)=C(N)O2 | Neg\_lig\_356 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 571 | Nc1cccc(S(=O) (=O)N2CCCC2)c1 | Neg\_lig\_371 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 572 | Cc1[nH]nc2c1[C@@]1(C(  =O)Nc3ccccc31)C(C#N)= C(N)O2 | Neg\_lig\_424 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 573 | CCCCn1c(N)c(C#N)c2nc3  ccccc3nc21 | Neg\_lig\_463 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 574 | Cc1ccc(- c2nc3ncccn3c2Nc2ccccc2) cc1 | Neg\_lig\_475 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 575 | COc1cc([C@@H]2C(C#N  )=C(N)Oc3c2c(=O)  [nH]c2ccccc32)ccc1OC(C) C | Neg\_lig\_520 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 576 | Nc1nc(N2CCN(C(=O)c3cc cs3)CC2)c2c([nH+]1)CCC C2 | Neg\_lig\_532 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 577 | COc1ccc(Nc2nc(N)nc(CSc | Neg\_lig\_580 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | 3nncn3C)n2)cc1 |  |  |  | ACUCUGGGAGA |  |
| 578 | Nc1nonc1C(=O)N1CCN(C  (=O)COc2ccccc2)CC1 | Neg\_lig\_589 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 579 | C[NH+]  (C)CCCNc1ncnc2c1sc1nc 3c(cc12)COC(C)(C)C3 | Neg\_lig\_635 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 580 | COC(=O)c1cnc(Nc2ccc(Cl  )cc2OC)c2ccccc12 | Neg\_lig\_645 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 581 | COc1ccc(N2C(=O)C[C@ H]  (n3c(CO)nc4ccccc43)C2= O)cc1 | Neg\_lig\_671 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 582 | COCCNc1nc2c(c(=O)n(C)  c(=O)n2C)n1Cc1ccccc1F | Neg\_lig\_687 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 583 | Cc1cc(F)cc(- c2cccc3c(N)cc[nH+]c23)c 1 | Neg\_lig\_690 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 584 | CCc1[nH]nc2c1[C@H] (c1c(F)cccc1Cl)C(C#N)=C (N)O2 | Neg\_lig\_714 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 585 | Cc1cn([C@H]2C[C@H] (N=[N+]=[N-])[C@@H]  (CO)O2)c(=O)[nH]c1=O | Neg\_lig\_719 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 586 | Cc1ccc(Nc2cc(N3CCN(C(  =O)C(C)C)CC3)  [nH+]c(C)n2)cc1 | Neg\_lig\_761 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 587 | COc1ccc2oc(- c3ccc(C)c(N)c3)nc2c1 | Neg\_lig\_790 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 588 | COc1cc(C[NH2+]C(C)C)c  cc1OCc1ccc2c(c1)n(C)c(= O)n2C | Neg\_lig\_792 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 589 | O=C([O-])c1ccc(Nc2cnc3c cccc3n2)cc1 | Neg\_lig\_819 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 590 | Nc1nonc1C(=O)NCC[NH2  +]Cc1ccc(F)cc1 | Neg\_lig\_825 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 591 | CC[C@]1(CO)CCCN(C(=  O)NCc2ccc(Cl)cc2)C1 | Neg\_lig\_962 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 592 | CO[C@H]1CN(C(=O)c2cc cc(C(=O)O)c2)CC[C@H]1 N | Neg\_lig\_981 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 593 | Cc1cc(N)c(O)c(Br)c1 | Neg\_lig\_996 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 594 | O[C@H] (CN1CCOCC1)Cn1cnc2cc ccc21 | Neg\_lig\_1017 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 595 | OC1CCN(Cc2cc3cc4c(cc3 nc2-c2cccs2)CCC4)CC1 | Neg\_lig\_1033 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 596 | CCOC(=O)[C@H]  (CCc1ccccc1)N[C@H]1C Cc2ccccc2N(CC(=O)  [O-])C1=O | Neg\_lig\_1044 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 597 | CCCn1cnnc1C[NH2+]C1C  CN(c2cccc(C)c2C)CC1 | Neg\_lig\_1060 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 598 | COc1ccc(OC)c(C(=O)c2oc 3ccc(N)cc3c2C)c1 | Neg\_lig\_1062 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 599 | CCOC(=O)c1cnc2ccc(C)cc 2c1Nc1ccc(C(=O)[O-])cc1 | Neg\_lig\_1095 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 600 | c1cc2c(cc1Nc1nc(N3CCO CC3)nc(N3CCOCC3)n1)O CO2 | Neg\_lig\_1112 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 601 | CCOC(=O)c1cnc2c(C)cc( | Neg\_lig\_1152 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | C)cc2c1Nc1ccc(C(=O) [O-])cc1 |  |  |  | ACUCUGGGAGA |  |
| 602 | CS[C@H]1SC[C@@H]2C (=O)N(C)[C@H]  (C(C)C)C(=O)OC[C@H]  (NC(=O)c3cnc4ccccc4n3) C(=O)N[C@H] (C)C(=O)N(C)  [C@@H]1C(=O)N(C) [C@H] (C(C)C)C(=O)OC[C@H]  (NC(=O)c1cnc3ccccc3n1) C(=O)N[C@H]  (C)C(=O)N2C | Neg\_lig\_486 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 603 | CN(C[C@H]1CCC[N@@ H+]  (CCc2ccc(Cl)cc2)C1)C(=O  )c1cc(CO)ccn1 | Neg\_lig\_1177 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 604 | CCn1ccnc1CN(C)C(=O)c1 ccc([C@H]2CC[NH2+]C2  )cc1 | Neg\_lig\_1200 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 605 | Cc1ccsc1CC[NH2+] [C@@H] (C)C(=O)NC1CCCC1 | Neg\_lig\_1210 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 606 | Nc1c(-c2nc(- c3ccc4c(c3)OCO4)no2)nn n1-c1ccc(Br)cc1F | Neg\_lig\_1232 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 607 | O=C(NC[C@]1(O)CC[NH 2+]C1)C1CCN(C(=O)c2cc  ccn2)CC1 | Neg\_lig\_1288 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 608 | CC(=O)OCC(=O) [C@@]1(O)CC[C@H]2[C @@H]3CCC4=CC(=O)C= C[C@]4(C)  [C@@H]3[C@@H]  (O)C[C@@]21C | Neg\_lig\_1292 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 609 | N/C(=N\N=C\  c1ccccc1)c1nonc1N | Neg\_lig\_1294 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 610 | Cc1c(CCC#N)c(N2CC[NH  +]  (CCO)CC2)n2c(nc3ccccc3 2)c1C#N | Neg\_lig\_1347 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 611 | O=c1cccc2n1C[C@H]1C[ C@@H]2C[N@H+]2CCC C[C@@H]12 | Neg\_lig\_1416 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 612 | COc1ccccc1N1CCN(c2nc(  -c3nonc3N)no2)CC1 | Neg\_lig\_1437 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 613 | COc1ccc(Nc2nc(- c3cccnc3)cs2)cc1 | Neg\_lig\_1457 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 614 | Cc1cc(C)n(C[C@H] (C)NCC(=O)Nc2ccc(Cl)cc 2F)n1 | Neg\_lig\_1468 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 615 | O[C@@H]  (CNc1ncnc2cccc(F)c12)c1 ccco1 | Neg\_lig\_1487 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 616 | C=CCC1(Nc2ccccc2)CCC CC1 | Neg\_lig\_1490 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 617 | CCOCCCNc1nc2c(-  c3ccccc3)nnn2c2ccccc12 | Neg\_lig\_1500 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 618 | COc1ccc(N2CC(=O)C(c3n c(C)c(C)s3)=C2N)c(OC)c1 | Neg\_lig\_1545 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 619 | CCCCCNc1cc(C) [nH+]c2c(C)c(-  c3ccccc3)nn12 | Neg\_lig\_1548 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 620 | Cc1nc2cc(C(=O)N(CCO)C  c3nccn3C)ccc2s1 | Neg\_lig\_1575 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 621 | C[C@@H](Cc1ccccc1F) [NH2+]CC1(Cn2ccnc2)CC 1 | Neg\_lig\_1589 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 622 | [NH3+]CCNC(=O)c1nc(-  c2ccccc2)no1 | Neg\_lig\_1619 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 623 | CCn1cncc1C[NH2+]CCC(  =O)Nc1nccs1 | Neg\_lig\_1644 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 624 | COc1ccccc1-c1cccc(- c2c(O)nc3cc(Cl)c(C#N)cc 3c2O)c1 | Neg\_lig\_1665 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 625 | CCOc1ccccc1N[C@H]1O C(=O)c2ccccc21 | Neg\_lig\_1601 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 626 | Cc1ccc(N(C[C@H] (O)C[NH+]2CCCCC2)S(=  O)(=O)c2ccc(C)cc2)cc1 | Neg\_lig\_1679 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 627 | O=c1n(Cc2ncccn2)nc([C@ H]2CCC[NH2+]C2)n1-  c1ccccc1 | Neg\_lig\_1706 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 628 | CCOc1ncccc1Cn1cc(- c2ccc(CO)o2)nn1 | Neg\_lig\_1748 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 629 | O=C(c1ccc2ncsc2c1)N1C[ C@@H]2c3ccccc3OC[C@  ]2(CO)C1 | Neg\_lig\_1810 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 630 | CC[C@H]1C[C@@](C)  (c2csc(Nc3ccccc3)n2)OC1  =O | Neg\_lig\_1831 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 631 | c1ccc(- c2noc(CNC3CCCCC3)n2)  cc1 | Neg\_lig\_1867 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 632 | CC1=C(C(=O)OC(C)(C)C) [C@H]  (c2ccc(Cl)cc2Cl)C(C#N)= C(N)O1 | Neg\_lig\_1874 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 633 | OCc1ccnc(-c2cccc(C(F) (F)F)c2)c1 | Neg\_lig\_1877 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 634 | Cn1c(=O)c2c(- c3cccc(Br)c3)n(CCO)cc2n (C)c1=O | Neg\_lig\_1897 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 635 | N#CC1=C(N)N(c2c(F)ccc c2F)C2=C(C(=O)CCC2)  [C@@H]1c1ccccc1 | Neg\_lig\_1924 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 636 | COc1ccc2nccc(/C=C/ c3ccnc4ccc(OC)cc34)c2c1 | Neg\_lig\_1940 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 637 | Cc1c[nH+]c(Nc2ccc(N3C C[NH+]  (C)CC3)cc2)nc1Nc1cccc(S (=O)(=O)NC(C)(C)C)c1 | Neg\_lig\_1945 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 638 | Cc1nc(C(=O)N2CCN[C@  H](c3ccccc3)C2)cs1 | Neg\_lig\_1182 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 639 | [NH3+] [C@H]1CN(C(=O)c2cccn n2)C[C@@H]1c1ccccc1 | Neg\_lig\_1948 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 640 | N#CC1=C(N)Oc2c(oc(CO  )cc2=O)  [C@H]1c1ccccc1C(F)(F)F | Neg\_lig\_1950 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 641 | CC1(C)Cc2c(c(N3CCOCC  3)nc3sc(C(=O)NCCc4cccc c4)c(N)c23)CO1 | Neg\_lig\_1978 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 642 | N#Cc1cc2c(=O)n(CC3(CO  )CCCC3)ccc2[n-]c1=O | Neg\_lig\_1991 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 643 | CCc1ccccc1N[C@@H]1c2 ccccc2C(=O)N1c1ccc(Cl)c n1 | Neg\_lig\_2003 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 644 | CCCc1nn2c(NCc3ccccc3) nc3ccccc3c2[nH+]1 | Neg\_lig\_2011 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 645 | Cc1cc(Nc2cccc(Cl)c2C)c2 ccccc2[nH+]1 | Neg\_lig\_2022 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 646 | CC[N@@H+] (CCO)C[C@@H]1CN(C(=  O)Cc2csc(C)n2)C[C@@H  ]1CO | Neg\_lig\_2025 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 647 | CCNC(=O) [C@@H]1C[C@H] ([NH3+])CN1Cc1ccc(Oc2  ncccn2)cc1 | Neg\_lig\_2026 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 648 | COc1cccc(C[NH2+]C(C)  (C)CO)c1OCc1ccc(Cl)cc1 | Neg\_lig\_2034 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 649 | O=C(NC1CC1) [C@@H]1CNCCN1C(=O)  C1=Cc2ccccc2OC=C1 | Neg\_lig\_2039 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 650 | Cc1cc(Nc2ccc(F)cc2)n2nc( Cc3ccccc3)nc2n1 | Neg\_lig\_2051 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 651 | C[NH+]  (C)CCNc1ncnc2c1sc1nc3c (cc12)COC(C)(C)C3 | Neg\_lig\_2064 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 652 | CN(C)c1ccc(/C=N/ NC(=O)c2cnc3ccccc3c2)cc 1 | Neg\_lig\_2080 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 653 | COc1ccc(- c2cc3[nH+]c(C)cc(NCC(C  )C)n3n2)cc1OC | Neg\_lig\_2087 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 654 | Nc1cccc(- n2ncc3c(Cl)cccc32)n1 | Neg\_lig\_2088 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 655 | O=C(CCCO)NCCc1nc2cc  ccc2n1Cc1c(F)cccc1Cl | Neg\_lig\_2127 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 656 | COC(=O)c1sc(-  c2ccc(Cl)cc2)cc1N | Neg\_lig\_2268 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 657 | Cc1cc(C2CCC2)nc(N2CC C3(CC2)Nc2ccccc2NC3= O)n1 | Neg\_lig\_2314 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 658 | CCCCNc1nc(Oc2ccc(=O)n (-  c3ccccc3)n2)nc(N(C)C)n1 | Neg\_lig\_2374 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 659 | CCOC(=O)c1cnc2c(-  c3cccc(Cl)c3)c(COC)nn2c 1N | Neg\_lig\_2391 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 660 | N#CC1=C(N)Oc2[nH]nc(-  c3ccccn3)c2[C@H]1c1c(F  )cccc1Cl | Neg\_lig\_2417 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 661 | CNC(=O)[C@](C)  (Nc1ccc(C)cc1)c1ccccc1 | Neg\_lig\_2489 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 662 | O=C1C[C@H] (Nc2ccc(N3CCOCC3)cc2)  C(=O)N1c1ccccc1Cl | Neg\_lig\_2492 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 663 | CCCc1c(C)nc2ncnn2c1Nc 1ccc(CC)cc1 | Neg\_lig\_2493 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 664 | c1cncc(- c2nn3c(NC4CCCCC4)nc4 ccccc4c3[nH+]2)c1 | Neg\_lig\_2594 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 665 | O=C(CN1CC2(CC[NH2+] CC2)OC1=O)N1CCN(c2n  ccs2)CC1 | Neg\_lig\_2603 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 666 | O=c1cc(CN2CCC[C@@] (O)  (CO)C2)nc2ccc(Cl)cn12 | Neg\_lig\_2613 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 667 | N#Cc1cnn2c(NC3CCCCC  C3)c(-c3ccc(Br)cc3) [nH]c12 | Neg\_lig\_2637 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 668 | COc1ccc(CN2CCN(C[C@  @H] (O)Cn3c4ccccc4c4ccccc43  )CC2)cc1 | Neg\_lig\_2667 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 669 | CCOC(=O)c1ccccc1NC(= O)N1CCC[C@@]2(CC[N H2+]C2)C1 | Neg\_lig\_2676 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 670 | COc1cc2ncnc(Nc3cccc(Cl) c3)c2cc1OC | Neg\_lig\_2688 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 671 | COC(=O)CCCNc1cc(C)nc  2nc(-c3ccc(OC)cc3)nn12 | Neg\_lig\_2702 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 672 | COc1ccc2[nH]cc(CCNC(C  )=O)c2c1 | Neg\_lig\_2717 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 673 | CN1CCOc2cc(C(=O)N3C C[C@@H]  (c4ccc5c(c4)OCO5) [C@H](O)C3)ccc21 | Neg\_lig\_2743 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 674 | COc1ccc(Cl)cc1Nc1ncnc2 sc(C)c(C)c12 | Neg\_lig\_2801 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 675 | COc1ccccc1Nc1cc(C) [nH+]c2ccc(Cl)cc12 | Neg\_lig\_2808 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 676 | Cc1ccccc1Nc1nc([C@@]2 (C)C[C@@H] (C(C)C)C(=O)O2)cs1 | Neg\_lig\_2869 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 677 | OCCNc1nc(N2CCOCC2)n c(N2CCOCC2)n1 | Neg\_lig\_2878 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 678 | Cc1nc2sc(C(=O)Nc3cnc4c cccc4c3)c(N)c2c(C)c1C | Neg\_lig\_2905 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 679 | Nc1nonc1C(=O)N1CCN(C  (=O)Nc2ccccc2F)CC1 | Neg\_lig\_2927 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 680 | COc1ccccc1[C@@H] (CC[NH2+]Cc1ccccc1F)c1 ccco1 | Neg\_lig\_2948 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 681 | Cc1nn2cc(CCNc3nccc(N4 CCC[C@H] (O)C4)n3)nc2s1 | Neg\_lig\_2976 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 682 | CC(C) ([C@@H]1NCCc2[nH]c[n H+]c21)N1CCOCC1 | Neg\_lig\_3003 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 683 | CC1(C)CC(=O)C2=C(C1) OC(N)=C(C#N)C21CCCC C1 | Neg\_lig\_2348 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 684 | NC1=C(c2nc3ccccc3[nH]2  )C(=O)CN1c1ccc(Cl)cc1Cl | Neg\_lig\_3099 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 685 | Cc1ccc(COc2ccc(C[NH2+  ]C(C)C)cc2)cc1 | Neg\_lig\_3107 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 686 | O=C1c2cccc3cccc(c23)C(  =O)N1CCNCCO | Neg\_lig\_330 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 687 | CCOC(=O)N1CCN(c2c(N CCC[N@H+]3CCC[C@H] (C)C3)c(=O)c2=O)CC1 | Neg\_lig\_3131 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 688 | O=C(CNc1ccc2c(c1)OCO 2)N/N=C/c1ccccc1Cl | Neg\_lig\_3175 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 689 | COc1ccc(- c2cc(Nc3ccccc3Br)nc(C) | Neg\_lig\_3197 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | [nH+]2)cc1 |  |  |  |  |  |
| 690 | Cc1cccc(N(CC(=O)NCc2c c3n(n2)CC[NH2+]C3)S(C) (=O)=O)c1 | Neg\_lig\_3207 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 691 | CC(C)OC(=O)c1n[nH]c(N  )n1 | Neg\_lig\_3269 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 692 | C=CCNC(=O)c1sc(N(CC) CC)nc1N | Neg\_lig\_3319 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 693 | CC(C)c1cc(NC2CC2)n2nc  (-c3cccnc3)nc2n1 | Neg\_lig\_3324 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 694 | CC(=O)N1C(=O) [C@]2(C(C#N)=C(N)Oc3  n[nH]c(- c4ccc(F)cc4)c32)c2ccccc2 1 | Neg\_lig\_3365 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 695 | COc1ccc(- c2c(Nc3ccc(OC)c(OC)c3)c (=O)c2=O)cc1 | Neg\_lig\_3371 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 696 | [NH3+][C@H]  (c1ccccc1)c1cccnc1 | Neg\_lig\_3385 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 697 | C[C@H]1CCc2sc3ncnc(N CCN4CCOCC4)c3c2C1 | Neg\_lig\_3391 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 698 | C[C@H](O)C#Cc1ccccn1 | Neg\_lig\_3392 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 0 |
| 699 | COc1ccc(NC(=O)N2C[C @H](O)[C@@H] (N3CCOCC3)C2)cc1C#N | Neg\_lig\_16 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 700 | COc1ccc([C@@H] (O)Cn2c(=[NH2+])n(C)c3  ccccc32)cc1 | Neg\_lig\_47 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 701 | CS(=O)  (=O)c1cc(F)cc2c3c(n(Cc4c cc(Cl)cc4)c12)[C@H]  (CC(=O)[O-])CC3 | Neg\_lig\_89 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 702 | Cc1ccc(Cl)cc1N[C@@H]1 c2ncccc2C(=O)N1Cc1cccs 1 | Neg\_lig\_94 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 703 | Cc1cccc(- c2nc3nc(C)cc(N(C)CCO)n 3n2)c1 | Neg\_lig\_168 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 704 | O=C(c1ccc2c(c1)n(CC1C C1)c(=O)n2C1CCCCC1)N 1C[C@@H]2C[NH2+]C[C @@H]2C1 | Neg\_lig\_177 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 705 | COc1cc(Cl)c(C[N@H+]2C C[C@](C)(O)[C@@H] (O)C2)c(Cl)c1OC | Neg\_lig\_203 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 706 | O=C(COc1cccc(Cl)c1)NC[ C@@H]1C[C@H] (F)C[NH2+]1 | Neg\_lig\_212 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 707 | COc1ccc(- c2oc3cc(OC)ccc3c2C(=O) c2ccc(C#N)cc2)cc1 | Neg\_lig\_220 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 708 | Nc1[nH+]c2n(c1C(=O)c1c cc(Br)cc1)CCCC2 | Neg\_lig\_242 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 709 | Nc1ccccc1-c1nn2cnnc2s1 | Neg\_lig\_308 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 710 | CC1(C)C[C@@H]([C@H] (CC[NH3+])c2ccccc2)CC O1 | Neg\_lig\_314 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 711 | Nc1nnnn1NCc1ccccc1F | Neg\_lig\_385 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 712 | CCc1csc(CNCc2nc(- | Neg\_lig\_410 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | c3ccccc3C)no2)n1 |  |  |  |  |  |
| 713 | Cc1ccc(N[C@@H] (CNS(=O)  (=O)c2ccccc2)c2ccccc2)cc 1 | Neg\_lig\_434 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 714 | Nc1cc2c(cc1C(=O)c1ccccc 1Br)OCCO2 | Neg\_lig\_438 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 715 | C=CCNc1nc2c(c([O-])nc(  =O)n2C)n1C[C@H](O)CO | Neg\_lig\_453 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 716 | Cc1nnc([N-]C(=O)c2cccc( N)c2)s1 | Neg\_lig\_471 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 717 | O=C1CCCN1CCC[NH2+]  Cc1cccc2ccccc12 | Neg\_lig\_483 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 718 | CCOc1ccc(N[C@H] (c2ccccc2)c2nnc(- c3ccccc3)o2)cc1 | Neg\_lig\_515 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 719 | Cc1ccc(OC2(C(=O)NCCc 3nc(C)c(C)s3)CC[NH2+]C  C2)cc1 | Neg\_lig\_548 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 720 | C[C@@H]  (C[NH2+]Cc1ccccn1)Oc1c cccn1 | Neg\_lig\_579 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 721 | Cn1nc(C(C) (C)C)cc1NC(=O)NCc1ccc(  CO)cc1 | Neg\_lig\_622 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 722 | c1ccc(NCCn2cc([C@H]3C CC[NH2+]C3)nn2)cc1 | Neg\_lig\_634 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 723 | Nc1nc(Cl)nc2c1ncn2[C@ @H]1O[C@H](CO)  [C@@H](O)[C@H]1F | Neg\_lig\_650 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 724 | Cc1cc(C)c(OC[C@@H] (O)C[N@H+]2CCCC[C@ H]2C)c(C)c1 | Neg\_lig\_831 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 725 | N#Cc1c(N(CC(=O) [O-])CC(=O)  [O-])sc(C(=O)  [O-])c1CC(=O)[O-] | Neg\_lig\_867 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 726 | CCc1nccc(-c2c(- c3ccccc3)ncn2CC2(CO)C COCC2)n1 | Neg\_lig\_876 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 727 | Cc1nc2ccccc2n1C[C@H] (O)COc1ccc(C(C)C)cc1 | Neg\_lig\_903 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 728 | Cc1ccc(C(=O)OCCCCNC 2=NS(=O)  (=O)c3ccccc32)cc1 | Neg\_lig\_934 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 729 | CC(C)C[C@H] (O)C(=O)N1CCC(c2nccn2  Cc2ccncc2)CC1 | Neg\_lig\_964 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 730 | C[C@@H] (C(=O)NCc1ccccc1)N1C(  =O)NC2(CC[NH2+]CC2) C1=O | Neg\_lig\_1000 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 731 | OCCCc1nc2ccccc2n1CCC Oc1ccccc1 | Neg\_lig\_1043 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 732 | CSCCc1nc([C@@H](N)  [C@@H] (C)O)n(CC(=O)O)n1 | Neg\_lig\_1120 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 733 | CCOC(=O)N1CCN(Cc2c(  O)ccc3ccccc23)CC1 | Neg\_lig\_1122 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 734 | CC[C@@H]  (CO)n1cc2c(c1- c1ccc(Cl)cc1)c(=O)n(C)c( | Neg\_lig\_1147 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | =O)n2C |  |  |  |  |  |
| 735 | CC1(C)CCC(=O)c2nnn(-  c3nonc3N)c21 | Neg\_lig\_1149 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 736 | Cn1c(N2CC[C@H] (O)C2)nc2cc(C(=O)NCCC  n3cncn3)ccc21 | Neg\_lig\_1156 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 737 | CC(C)=NNc1[nH]cnc2ncn c1-2 | Neg\_lig\_744 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 738 | O=c1[nH]cnc2c1ncn2[C@ H]1CC[C@@H](CO)O1 | Neg\_lig\_1164 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 739 | Nc1cccc(S(=O) (=O)NC[C@H]2CCCO2)c 1 | Neg\_lig\_1271 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 740 | Nc1ccc2c(C(F) (F)F)cc(=O)oc2c1 | Neg\_lig\_1302 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 741 | OCCOc1cccc(C[NH+]2CC  N([C@H]3CCc4ccccc4C3) CC2)c1 | Neg\_lig\_1305 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 742 | Cc1ccc(- n2nc(CO)c(C(=O)NCc3ccc nc3)n2)cc1C | Neg\_lig\_1381 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 743 | Cc1ccc2nc(Nc3nc(C)c4ccc cc4n3)nc(O)c2c1 | Neg\_lig\_87 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 744 | O=S1(=O)C(=C(/  O)Nc2ccccc2)/C(=N/ Cc2ccco2)c2ccccc21 | Neg\_lig\_1535 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 745 | CCc1c(C)nc2nncn2c1NCc 1ccc(Cl)cc1 | Neg\_lig\_1551 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 746 | N#Cc1c(- c2ccc(C[NH+]3CCCC3)s2  )cc(-c2ccc[nH]2)nc1N | Neg\_lig\_1557 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 747 | COc1ccc(F)c(CNC(=O)c2c cc3nc(CO)[nH]c3c2)c1F | Neg\_lig\_1574 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 748 | Cc1nc2[nH+]c[nH]n2c(=O  )c1Oc1ccc(N)cc1 | Neg\_lig\_1577 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 749 | Cc1ccc(Nc2nc(C)cc(N3CC N(C(=O)C4CCCCC4)CC3  )n2)cc1 | Neg\_lig\_1578 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 750 | [NH3+] [C@H]1CN(C(=O)CCCO  Cc2ccccc2)C[C@@H]1C1 CC1 | Neg\_lig\_1582 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 751 | O=C1CCC2(CCN(C(=O)c  3ccc4occc4c3)CC2)CN1C CCO | Neg\_lig\_1618 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 752 | NS(=O)(=O)c1ccc(N/ N=C2\C(=O)C(C(=O)  [O-])=Cc3ccccc32)cc1 | Neg\_lig\_1651 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 753 | C[C@](O)(CS(=O)  (=O)c1ccc(F)cc1)C(=O)  [N-]c1ccc(C#N)c(C(F) (F)F)c1 | Neg\_lig\_1662 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 754 | Nc1c(C(=O)NCCc2c[nH]c  3ccccc23)sc2nc3c(cc12)C CC3 | Neg\_lig\_1694 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 755 | CCc1[nH]nc2c1C1(C(C#N  )=C(N)O2)c2ccccc2- c2ccccc21 | Neg\_lig\_1701 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 756 | OCCCc1nc2ccccc2n1CCC 1CCCCC1 | Neg\_lig\_1733 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 757 | C[NH+] | Neg\_lig\_1736 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | (C)CCCNC[C@@H]  (O)Cn1c2ccccc2c2ccccc21 |  |  |  |  |  |
| 758 | CC[NH+] (CC)CCN1CC(=O)C(c2nc  3ccccc3[nH]2)=C1N | Neg\_lig\_1741 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 759 | COc1ccc(- c2ccc(C[NH2+]CCc3ccc(S (N)(=O)=O)cc3)o2)cc1Cl | Neg\_lig\_1749 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 760 | CNc1cc(C)[nH+]c2c(- c3ccc(F)cc3)cnn12 | Neg\_lig\_1774 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 761 | Cc1ccc([C@H]2C(C#N)= C(N)Oc3c2oc(CO)cc3=O)  o1 | Neg\_lig\_1275 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 762 | Cc1cccc(CN2CCN(C(=O)  CCn3cncn3)C[C@@H]2C CO)n1 | Neg\_lig\_1835 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 763 | COc1ccc(N2CCN([C@H] 3CCCN(C(=O)CO)C3)CC  2)cc1 | Neg\_lig\_1836 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 764 | Cc1nc(N)nc(C)c1CC(=O) N1CCC2(CCC(=O)N(C)C C2)CC1 | Neg\_lig\_1880 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 765 | O=C1c2ccccc2C(=O)c2cc( S(=O)  (=O)N(CCO)Cc3ccccc3)cc c21 | Neg\_lig\_1881 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 766 | c1ccc(- c2nnc3nc(N4CCCCC4)nc( N4CCCCC4)n23)cc1 | Neg\_lig\_1886 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 767 | CN(Cc1cnc(N)nc1)C(=O)  Nc1ccccc1C[N@@H+] (C)C1CCCCC1 | Neg\_lig\_1902 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 768 | O=C(NCC(c1ccccc1)c1ccc cc1)c1nn(- c2ccc(F)cc2)nc1CO | Neg\_lig\_1915 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 769 | Cc1c(S(=O)  (=O)c2ccccc2)c(N)n(CCC[ NH+](C)C)c1C | Neg\_lig\_1969 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 770 | CNc1oc(- c2ccc(F)cc2)nc1S(=O) (=O)c1ccc(Cl)cc1 | Neg\_lig\_2027 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 771 | O=C1c2cccc3cccc(c23)C(  =O)N1CC1CC[NH+] (C[C@H] (O)COc2ccc(F)cc2)CC1 | Neg\_lig\_2029 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 772 | CC(C) (O)CCc1ccc(C(=O)N2CC CC[C@@H]2CO)cc1 | Neg\_lig\_2030 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 773 | Cn1ncc2c(=O) [nH]c(CN3CCNC[C@H] (C(=O)O)C3)nc21 | Neg\_lig\_187 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 774 | COc1ccc(- c2nc3ncccn3c2Nc2cccc(C( F)(F)F)c2)cc1 | Neg\_lig\_2094 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 775 | O=C1C[C@H] (Nc2ccc3c(c2)OCO3)C(=  O)N1c1ccccc1 | Neg\_lig\_2168 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 776 | Cc1ccc(C)c(S(=O) (=O)N2CCC[C@H] (Cn3cc(CCO)nn3)C2)c1 | Neg\_lig\_2210 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 777 | Cc1ccc(- c2c(Nc3ccc(Br)c(C)c3)c(= O)c2=O)cc1C | Neg\_lig\_2291 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 778 | Cc1cnc(N)nc1N[C@H] (C[NH+]1CCCC1)c1ccccc 1 | Neg\_lig\_2328 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 779 | Cc1cc(- c2[nH]nc3c2[C@@H] (c2cccnc2)C(C#N)=C(N)O 3)c(C)s1 | Neg\_lig\_2345 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 780 | COC(=O) [C@@H]1CCCCN1C(=O) CCc1cc2n(n1)CCC[NH2+] C2 | Neg\_lig\_2373 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 781 | N=c1[nH]c2c(s1)[C@@H] (c1ccc(F)cc1F)CC(=O)N2 | Neg\_lig\_2434 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 782 | CSc1ncc(C(=O)NC(C)C)c( N)n1 | Neg\_lig\_2501 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 783 | COc1cc2nc(N3C[C@@H] (C)[C@](O) (C4CC4)C3)nc(N)c2cc1O C | Neg\_lig\_2520 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 784 | CC(C)=CC[C@]1(CO)CC CN(C(=O)CCn2cnnc2)C1 | Neg\_lig\_2526 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 785 | COc1ccc([C@H]2C(C#N)  =C(N)OC3=C2S(=O)  (=O)N(Cc2ccccc2C)c2cccc c23)cc1 | Neg\_lig\_2528 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 786 | C[C@H]  (O)c1c(O)ccc2ccc(=O)oc1 2 | Neg\_lig\_2534 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 787 | CCCCNc1nc2c(c(=O)n(Cc 3ccccc3)c(=O)n2C)n1C | Neg\_lig\_2042 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 788 | O=C(CCCO)NCCc1nc2cc  ccc2n1Cc1ccc(Cl)cc1 | Neg\_lig\_2611 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 789 | COc1cccc(- c2cc(C(=O)N3CC=C[C@ @H]3CO)n[nH]2)c1 | Neg\_lig\_2612 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 790 | COc1cccc(Nc2c(S(=O) (=O)c3ccccc3)cnc3ccccc23  )c1 | Neg\_lig\_2648 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 791 | Cc1c(C)n(Cc2cccnc2)c2[n H+]c3c(c(N)c12)CCc1cccc c1-3 | Neg\_lig\_2673 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 792 | Cc1cc([C@@H]2CCCCN 2C(=O)CCc2cc3n(n2)CCC [NH2+]C3)no1 | Neg\_lig\_2703 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 793 | N#Cc1c(N)nc(SCc2ccccc2  )c(C#N)c1-c1cccs1 | Neg\_lig\_2726 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 794 | Cc1cc(F)ccc1CC(=O)N1C CNC[C@H]1C(=O)Nc1cc  c(F)cc1 | Neg\_lig\_2754 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 795 | Nc1nc2c(c(- c3ccc[nH+]c3)n1)CN(C(= O)c1sccc1Cl)C2 | Neg\_lig\_2777 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 796 | COc1ccc(- c2noc(CNc3ccc(F)c(Cl)c3) n2)cc1 | Neg\_lig\_2802 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 797 | Cc1n[nH]cc1N | Neg\_lig\_593 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 798 | C[C@@]1(CO)CN(c2cc(C  (=O)Nc3ccc4c(c3)- c3c(c(C(N)=O)nn3-  c3ccc(F)cc3)CC4)c(Cl)cn2  )C[C@]1(C)CO | Neg\_lig\_2842 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 799 | CCOCCCNCc1c(C(=O)O)  n(Cc2ccc(C)cc2)c2ccccc12 | Neg\_lig\_2916 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 800 | Cc1ccc(NC(=O)CSc2nc3n c[nH]c(N)c-3n2)cc1 | Neg\_lig\_2918 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 801 | CC(C)Cc1ccc(C[N@H+]2 CCC[C@H]  (Nc3nccc(N)n3)C2)cc1 | Neg\_lig\_2951 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 802 | OCCN(CCO)c1nc(N2CCC CC2)c2nc(N(CCO)CCO)n c(N3CCCCC3)c2n1 | Neg\_lig\_2955 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 803 | Nc1nc(Cl)nc2c1ncn2[C@ H]1C[C@H](O)[C@@H] (CO)O1 | Neg\_lig\_2959 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 804 | Cc1cc(NC[C@@H]2C[C @H](F)C[NH2+]2)nc(-  c2ccccc2O)n1 | Neg\_lig\_2971 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 805 | C[N@@H+]  (CCNc1ncnc2onc(- c3ccc(Cl)cc3)c12)C1CCC CC1 | Neg\_lig\_2925 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 806 | C[NH+]  (C)CCNc1ncnc2c1c(- c1ccccc1)cn2-c1ccc(Cl)cc1 | Neg\_lig\_3014 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 807 | CC(C)c1nn(-  c2c(Cl)cccc2Cl)c2nc(Cc3c cc(OCCO)cc3) [nH]c(=O)c12 | Neg\_lig\_3066 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 808 | CC(C) (O)CCc1ccc(C(=O)NC[C  @H](O)c2ccccn2)cc1 | Neg\_lig\_3069 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 809 | Cc1c(F)cccc1NC(=O)CNC  Cc1ccccn1 | Neg\_lig\_3075 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 810 | CCn1nc(CO)c2c1CCN(C(  =O)c1cc(- c3cccn3C)n[nH]1)C2 | Neg\_lig\_3103 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 811 | c1ccc(OCCN2CCN(C[C@ H]3CCC[NH2+]C3)CC2)c  c1 | Neg\_lig\_3133 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 812 | COc1cccc2c1OC[C@@H] (C(=O)N(C)Cc1cnc(N)nc1  )C2 | Neg\_lig\_3135 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 813 | N#CC1=C(N)Oc2[nH]nc(-  c3cccs3)c2[C@H]1c1ccc( C(F)(F)F)cc1 | Neg\_lig\_3234 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 814 | COc1ccc(C(=O)c2sc3nc(C  )c(Cl)c(C)c3c2N)cc1 | Neg\_lig\_3271 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 815 | C[N@@H+]1C[C@@H] (c2ccccc2)CC2(CCN(C(= O)c3ccc(CO)cc3)CC2)C1 | Neg\_lig\_3295 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 816 | C=C(C)CC[C@H](C) [NH2+]CC(=O)Nc1ccccc1 C | Neg\_lig\_3303 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 817 | O=C(/C=C/c1cccc(S(=O) (=O)Nc2ccccc2)c1)NO | Neg\_lig\_2342 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 818 | C=CCN1C(=O) [C@]2(C(C#N)=C(N)Oc3  n[nH]c(C)c32)c2ccccc21 | Neg\_lig\_3369 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 819 | Cc1ccccc1NC1=NS(=O) (=O)c2ccccc21 | Neg\_lig\_3386 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 820 | N#CC1=C(N)OC2=C(C(= O)CCC2)  [C@@H]1c1ccc(Cl)cc1 | Neg\_lig\_3397 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 0 |
| 821 | Cc1cc(ccc1N)I | 0325-0381 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 822 | CC(NS(c(cc1)cc2c1sc(C)n 2)(=O)=O)=O | 122385 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 1 |
| 823 | CC(C) (CCc1ccc(cc1)C(N(C)CC1 (CCCC1)CO)=O)O | 14466464 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 1 |
| 824 | CC1CCC(C(C)C)C(C1)OC C(CN1CCN(CC1)c1ccccc 1)O | 1502-1032 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 1 |
| 825 | Cc1cc(C)c2c(c1)c(cc(C)n2  )C(N[C@H]1CNC[C@@ H]1OC)=O | 19537511 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 1 |
| 826 | COc1ccc(cc1OC)c1nnc(N) o1 | 2158-0021 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 1 |
| 827 | C1CCN(CC1)Cc1cccc(c1)  n1ccnc1c1cc2CNCCCn2n1 | 26875627 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 1 |
| 828 | O=C(N(CC1OC1)C(N1CC 2OC2)=O)N(CC2OC2)C1  =O | 296934 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 1 |
| 829 | CCOC(/C(/ C1=CSC2=NNC(C) (C)N12)=N\O)=O | 299968 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 1 |
| 830 | CC1=CC2C(CC1N)C2(C) C | 3295-0018 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 1 |
| 831 | Cc1cc(c2cc(ccc2n1) [Cl])Nc1ccc(cc1)C(O)=O | 4358-1525 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 1 |
| 832 | CSC(NC(Cl)=C1)=NC1=O | 45719 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 1 |
| 833 | CCOC(c1ccc2c(c1)c(c(cn2  )C(=O)OCC)Nc1ccc(cc1) N(C)C)=O | 4593-3030 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 1 |
| 834 | C1CN(CC=C1)c1c2CCN(  CCc2nc(c2ccco2)n1)C(CN  )=O | 47825811 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 1 |
| 835 | CCOC(c1cnc2ccc(cc2c1Nc 1ccc(cc1)N(C)C)[Br])=O | 4789-4367 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 1 |
| 836 | CCOC(c1cnc2ccc(C)cc2c1 Nc1ccc(cc1)N(C)C)=O | 4790-1159 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 1 |
| 837 | Cc1cccc2c(cc(C)nc12)Nc1 ccc(cc1)N(C)C | 4790-1400 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 1 |
| 838 | C(CN)CN1C(CC[C@H]2 CN(CC[C@@H]12)C(CCc  1ccco1)=O)=O | 48226996 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 1 |
| 839 | C1CCc2c(C1)c1c3c(c(NCc 4ccco4)ncn3)sc1nc2N1CC OCC1 | 5504-0167 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 1 |
| 840 | CN1C(N(Cc2ccccc2)C(c2c 1nc(NCCc1ccccc1)n2C)= O)=O | 7282-5801 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 1 |
| 841 | CCC1CCCCN1S(c1ccc(cc 1)NC1c2ccccc2S(N=1) (=O)=O)(=O)=O | 7380-0010 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 1 |
| 842 | CC1=CC2=C(C(C(C#N)= C(N)O2)c2ccccc2OC)C(N 1Cc1ccc2c(c1)OCO2)=O | 7706-1226 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 843 | CCOC(C1=C(C)OC(=C(C(  =O)OCC)C12C(Nc1ccccc1 2)=O)N)=O | 8003-0370 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 1 |
| 844 | CC1=C(C(C)=O)C2(C(C# N)=C(N)O1)C(Nc1ccc(cc1 2)[Cl])=O | 8004-9533 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 1 |
| 845 | Cc1ccc(cc1C)Nc1nc(cs1)c 1ccc(c(c1)F)OC | 8005-2731 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 1 |
| 846 | c1ccc(cc1)C(c1c(c(C(Nc2c cccc2)=O)c2ccccn12)N)= O | 8018-2439 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 1 |
| 847 | C1CCC(C1)  (CN)c1ccc(cc1)[Cl] | 8018-9306 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 1 |
| 848 | CCC12CN3CC(CC) (CN(C1)C3C(C) (C)CO)C2=O | 8019-5964 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 1 |
| 849 | c1cc(N)nc2c1ccc(n2)O | 8019-7722 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 1 |
| 850 | COc1cc(cc(c1O)OC)C1CC  (Nc2c1[se]c(N)n2)=O | 8020-1898 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 1 |
| 851 | c1cnccc1c1nc2ncnc(N)n2n 1 | 8020-2786 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 1 |
| 852 | Cc1c(c2ccc(c(c2)OC)OC)c 2ncc(c3ccc(c(c3)OC)OC)c (N)n2n1 | 8104-10716 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 1 |
| 853 | CCCCNc1c(C#N)c2CC(C)  (C)OCc2c(c2ccccc2)n1 | 8640-0572 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 1 |
| 854 | COc1ccc(cc1)c1cc(C(F) (F)F)nc(NCc2ccccc2)n1 | C130-0241 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 1 |
| 855 | Cc1cccc(c1)NCc1nc2ccccc 2n1C | C147-0043 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 1 |
| 856 | c1ccc(cc1)Nc1c(c2c[nH]c3 ccccc23)nc2cnccn12 | C169-0283 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 1 |
| 857 | CCCCn1cnc2cc(ccc12)NC c1cccc(c1)OC | C215-0084 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 1 |
| 858 | Cc1ccc2nc(c3c[nH]c4cccc c34)c(NC3CCCC3)n2c1 | C239-0079 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 1 |
| 859 | C1COc2cc(ccc2O1)Nc1c(c 2cccs2)nc2ccccn12 | C273-0461 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 1 |
| 860 | CC(C)C(N1CCN(CC1)c1c  cc(cc1)Nc1cc(C)nc2nc(c3c cco3)nn12)=O | C301-7288 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 1 |
| 861 | Cc1ccc(C)c(c1)NC(Cn1c(c (C(NCc2ccc(cc2)F)=O)nn1  )N)=O | C368-0754 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 1 |
| 862 | CCOc1ccccc1NC(c1c(CO) nccn1)=O | C612-0892 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 1 |
| 863 | CCOC(c1ccc(cc1)NC1c2c( cccn2)C(N1c1ccc(C)cc1)= O)=O | C999-1176 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 864 | C(C(c1ccccc1)Nc1ccc(cc1) [Br])NS(c1ccc(cc1)[Cl]) (=O)=O | D030-0079 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 1 |
| 865 | C(CNc1cc(c2ccccc2)nc2nn cn12)c1ccc(cc1)[Cl] | D150-0174 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 1 |
| 866 | C=CCNc1nc(cs1)c1c[nH]c 2ccccc12 | D231-0019 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 1 |
| 867 | Cc1nc(cc(Nc2ccc(cc2)N2C COCC2)n1)c1ccccc1 | D278-0547 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 1 |
| 868 | [H]N(Cc1ccccc1)c1c2c(csc 2ncn1)c1ccc(C)cc1 | D341-0419 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 1 |
| 869 | CC(C)c1cc(Nc2ccc(cc2)N( C)C)n2c(n1)nc(c1cccnc1)n 2 | D494-0293 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 1 |
| 870 | CCOC(c1cnc2c(c3ccc(cc3) [Br])c(C)nn2c1N)=O | D718-0691 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 1 |
| 871 | CC1CCCC(C1C)Nc1c(c2c  cc(cc2)[Cl]) [nH]c2c(C#N)cnn12 | E002-1096 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 1 |
| 872 | CCN(CC)c1ccc(c(C)c1)N C1C(C)=C(c2ccc(C)cc2)S( N=1)(=O)=O | E013-0189 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 1 |
| 873 | C1CN1P(N1CC1) (N1CC1)=S | NCGC0009504 2-08 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 1 |
| 874 | CC(C)n1cnc2c(Nc3cccc(c3  )NC(C=C)=O)nc(NC3CCC (CC3)N(C)C)nc12 | NCGC0034696 4-01 | HBV | Hairpin | GGUUCAUGUCCUACUGUUCAA GCCUCCAAGCUGUGCCUUGGG UGGCUUUGGGGCAUGGACC | 1 |
| 875 | CC(C)(C)NCc1ccc(cc1) [Cl] | 0167-0173 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 876 | c1ccc(c(c1)N)I | 0325-0348 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 877 | c1ccc2c(c1)nc(Sc1ccc(cc1[ Cl])N)s2 | 0375-0604 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 878 | Cc1c(C)sc(N)n1 | 0462-0328 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 879 | C(=Cc1nc2ccccc2o1)c1ccc (cc1)N | 0632-0836 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 880 | c1ccc2C(c3c(ccc(C(c4cccc 5ccccc45)=O)c3N)C(c2c1)  =O)=O | 0658-0270 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 881 | C(c1nc2ccccc2[nH]1)OC(c 1ccc(cc1)N)=O | 0717-0954 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 882 | C(=Cc1nc2cc(ccc2[nH]1) N)c1ccccc1 | 0717-0957 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 883 | CCN(CC)CCOC(c1ccc2c(  c1)sc(NC(c1ccc(cc1)N)=O  )n2)=O | 0812-1025 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 884 | Cc1c(C)c(C)nc2c1c(c(C(c1 ccc(cc1)[Cl])=O)s2)N | 0892-0702 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 885 | CNc1ccc(cc1C(c1ccccc1[C l])=O)[Br] | 0922-0021 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 886 | c1ccc(cc1)N1C(C(Nc2cccc c2C(O)=O)SC1=O)=O | 1159-0328 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 887 | CC1=CC(C)=NC(N1CCN C(C1CC2(CCNCC2)CN1 C)=O)=O | 12499963 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 888 | C1CCN(C1)Cc1cc(c2c(c3c | 12577678 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | cccc3)ncn2CCO)sc1 |  |  |  |  |  |
| 889 | C1CN(CCC1c1cc(Cc2cccc c2)n[nH]1)C(C1CNCCO1)  =O | 12893837 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 890 | C1C(CN1Cc1ccc(cc1)OC CO)Oc1ccccc1[Cl] | 13202927 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 891 | Cc1c(C)c(- c2c(CC#N)ccc(C)c2C)c(C C#N)cc1 | 135412 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 892 | C1CNCc2cccc(c3ccc(c(c3) F)O)c12 | 13724969 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 893 | CC(C)CCOc1cccc(CCNC( C2CC3(CCNCC3)CN2)=O  )c1 | 14325308 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 894 | CCCc1ccc(cc1)OCC(CN1 CCC(C)CC1)O | 1502-1054 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 895 | C(c1nnnn1c1ccccc1)n1ccn c1c1ccc(CO)o1 | 15028125 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 896 | CCSc1nc2ccccc2n1CCO | 1535-0016 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 897 | [H]OCCNC1=C(C)NC(NC 1=O)=O | 1545-0174 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 898 | C1=C(C(=O)Oc2ccc(cc12)  [Br])c1csc(N)n1 | 1570-0014 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 899 | C1CNCCC12CN(Cc1cc3c( cc1[Cl])OCO3)C(=O)O2 | 15869527 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 900 | C(CN)c1cccc(c1)c1ccc(cc1 [Cl])F | 16088353 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 901 | Cc1c(C(C(NCCNc2cccnc2  )=O)N)c(C)[nH]n1 | 16899791 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 902 | C=Cc1ccc(nc1)N1CCN(C C(C1)O)Cc1ccccc1 | 17524156 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 903 | CC(c1cccc(c1)C(N1CCC2( CC1)[C@H] (C[C@H]2O)OCCN)=O)= O | 17694000 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 904 | CCNC([C@@H]1C[C@@ H] (CN1S(N1CCN(CC)CC1) (=O)=O)N)=O | 17965244 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 905 | COc1ccc(cc1)C1C(C#N)= C(N)OC2CCCC(C1=2)=O | 1852-0324 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 906 | C1CC2=C(C(C(C#N)=C(N  )O2)c2ccc(c(c2)O)O)C(C1  )=O | 1852-0330 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 907 | Cc1ccccc1C1C(C#N)=C(N  )OC2=C1C(=O)Oc1ccccc1 2 | 1866-0050 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 908 | CC1=CC2=C(C(C(C#N)=  C(N)O2)c2ccc(cc2) [Cl])C(=O)O1 | 1866-0097 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 909 | Cc1cc2CN(Cc2cc1C)c1ccc c(c1)C(NC[C@@H]1C[C @@H](CN1)F)=O | 18859448 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 910 | Cc1cc(C)c2c(c1)c(cc(C)n2  )C(N[C@H]1CNC[C@@ H]1OC)=O | 19537511 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 911 | Cc1ccc2c(c1)c(c1ccc(cc1) N)nc(c1ccccc1)n2 | 2202-0913 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 912 | CC(C) (C)C(CN1C(=N)N(CCN2  CCCCC2)c2ccccc12)O | 2226-0439 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 913 | CCCCN1C(=N)N(CC(c2cc  c(cc2)OC)O)c2ccccc12 | 2226-0445 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 914 | CCCN1C(=N)N(CC(c2ccc  cc2)O)c2ccccc12 | 2226-0453 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 915 | CCCCN1C(=N)N(CC(c2cc  ccc2)O)c2ccccc12 | 2226-0454 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 916 | COc1cc(cc(c1OC)OC)c1n nc(N)s1 | 2237-2233 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 917 | C(CO)N1C(c2cccc3c(ccc( C1=O)c23)C(c1ccccc1)=O  )=O | 2248-8147 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 918 | COc1ccc(cc1)C(c1c(c2c(cc (c3ccccc3)nc2s1)C(F) (F)F)N)=O | 2434-0155 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 919 | C1COc2cc(ccc2C1=O)c1c c2CC(CN)Oc2c(c1)[Cl] | 26642358 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 920 | C(CC(c1c(c2cc(ccc2o1) [Cl])N)=O)C(O)=O | 2686-0069 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 921 | Cc1nc(C2CCCN2)n(c2ccc c3ccccc23)n1 | 26991482 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 922 | c1cc(c2cccc(c2c1) [Br])c1nc2cc(ccc2o1)N | 2810-4224 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 923 | Cc1cc2c(cc1C)oc(c1ccc(cc 1)N)n2 | 2810-4334 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 924 | Cc1cc2c(cc1C)oc(c1ccc(C) c(c1)N)n2 | 2810-4335 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 925 | CCc(cc(C(C) (C)CCC1(C)C)c1c1)c1-  c1csc(C/C(/N)=N/O)n1 | 310354 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 926 | CC1=CC2=C(C(=O)O1)C 1(C(C#N)=C(N)O2)C(Nc2  ccc(cc12)[Br])=O | 3132-1299 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 927 | C(c1ccc(cc1) [Br])Sc1nc2ccc(cc2s1)N | 3167-0427 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 928 | C(c1ccc(cc1)F)Sc1nc2ccc( cc2s1)N | 3167-0429 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 929 | C(c1ccccc1[Cl])Sc1nc2ccc (cc2s1)N | 3167-0436 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 930 | C(C(c1ccccc1)=O)Sc1nc2c cc(cc2s1)N | 3167-0470 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 931 | Cc1ccc(CNCCc2ccc(c(c2) OC)OC)c(C)c1 | 3169-1196 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 932 | Cc1ccc(cc1)n1cnc(c1C(c1c cc(cc1)[Br])=O)N | 3228-0090 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 933 | C(CNC1CCN(CC1)c1nnc(  c2ccccc2)s1)Cn1ccnn1 | 32364121 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 934 | Cc1nc2c(cccc2[nH]1)C(N1 CCCC2(CCNC2)C1)=O | 32365391 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 935 | CNc1ccccc1C(=O)OCC(c1 ccccc1)=O | 3257-1030 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 936 | C(C(c1ccc(cc1) [Br])=O)OC(c1c(N)non1)= O | 3257-3204 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 937 | CC(C)c(cc1)ccc1- c1nc(cccc2)c2s1 | 33010 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 938 | Cc1c(CCN(C)Cc2ccc(CO)  o2)scn1 | 33883850 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 939 | C1CNCc2cc(CCC(NC(CC  n3cncn3)c3ccccc3)=O)nn2 | 35350604 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | C1 |  |  |  |  |  |
| 940 | Cc1cc(ccc1[Br])c1nc2cc(c cc2o1)N | 3617-0633 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 941 | C1CN(CCN1CC(COc1ccc  (cc1)[Br])O)c1ccccc1 | 3672-0047 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 942 | COc1cccc(CNCc2cccc(c2) F)c1OC | 3702-1553 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 943 | c1ccc2c(c1)nc(c1ccc(cc1) N)s2 | 3729-2175 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 944 | CCOCCSc1nc(c2c3CC(C) (C)OCc3sc2n1)N | 3807-1214 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 945 | CCc1ccc(c2c3CCCCc3nc( c2C#N)N)s1 | 3830-0877 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 946 | C1C(=CNc2ccccc2)C(OC=  1c1ccccc1)=S | 3897-0025 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 947 | Cc1cc(C)c(c(C)c1)c1cc(C N)ccc1F | 40126718 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 948 | Cc1c(cccc1N)c1nc2cc(ccc 2o1)[Cl] | 4269-3141 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 949 | CS(c1c(c2c(cc(c3ccccc3)n c2s1)c1ccccc1)N)(=O)=O | 4378-0113 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 950 | CCN(CC(Cn1c2ccccc2c2c cccc12)O)S(c1ccc(cc1) [Cl])(=O)=O | 4390-0105 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 951 | CC(C)  (C)c1ccc(cc1)c1nc(c2ccccc 2n1)NCc1cccnc1 | 4491-1513 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 952 | CSC(NC(Cl)=C1)=NC1=O | 45719 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 953 | CCN1C(NC(C12CCN(CC 2)Cc1cc2CNCCCn2n1)=O  )=O | 47670564 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 954 | C1CN(CC=C1)c1c2CCN(  CCc2nc(c2ccco2)n1)C(CN  )=O | 47825811 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 955 | CCOC(c1cnc2ccc(cc2c1Nc 1ccc(cc1)N(C)C)[Br])=O | 4789-4367 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 956 | C(CN)CN1C(CC[C@H]2 CN(CC[C@@H]12)C(CCc  1ccco1)=O)=O | 48226996 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 957 | CCCCCCCCNc1cccc(c1) [Br] | 5117451 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 958 | Cc1nc2cc(c(cc2n1CCCO) [Cl])[Cl] | 5119828 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 959 | c1cc(ccc1c1c(c2ccc(cc2)F) nc2cc(ccc2n1)Oc1ccc(cc1) N)F | 5174475 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 960 | CCCCCc1ccc(cc1)c1ccc(c c1)c1ncc(cn1)N | 5213078 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 961 | c1ccc2c(ccc(c2c1)Oc1ccc( cc1[Cl])N)[Cl] | 5215844 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 962 | CCOC(CNc1ccc(cc1)Oc1c cc(cc1)Oc1ccc(cc1)NCC(= O)OCC)=O | 5224153 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 963 | C1CCN(CC1)CC(Cn1c2cc  c(cc2c2cc(ccc12)[Cl]) [Cl])O | 5236854 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 964 | c1ccc2c(c1)ccc(c2[Cl])Sc1 ccc(cc1[Cl])N | 5250905 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 965 | c1cc(ccc1c1cc(C(NN)=O)c | 5350878 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | 2cc(ccc2n1)[Br])N |  |  |  |  |  |
| 966 | C(C(Cn1c2ccccc2c2ccccc1 2)O)N(Cc1ccco1)S(c1ccc( cc1)F)(=O)=O | 5614-0038 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 967 | C(c1ccco1)Nc1cccc(c1) [Cl] | 5689-0133 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 968 | C(=Cc1ccc(cc1[Cl]) [Cl])C(c1cccc(c1)N)=O | 5689908 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 969 | CCOc1cc(CO)cc(c1OCc1c cc(cc1)C(O)=O)[Br] | 6415-0035 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 970 | CCOC(c1cnn(C(=O)OC)c1 N)=O | 7395-3020 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 971 | CCOC(c1ccc(cc1)N1C(CC (C1=O)NC1CCCCC1)=O)  =O | 7627-0150 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 972 | C1COCCN1S(c1ccc(cc1)c 1csc(Nc2ccc(cc2)[Br])n1) (=O)=O | 8004-5092 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 973 | C1CCN(CC1)S(c1ccc(cc1)  c1csc(Nc2ccc(cc2)F)n1) (=O)=O | 8004-9292 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 974 | C1CC2=C(C(C1)=O)C1(C (C#N)=C(N)O2)C(Nc2ccc( cc12)F)=O | 8004-9557 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 975 | C=Cc1ccc(cc1)c1csc(N)n1 | 8005-0366 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 976 | CC[Ge](CC)  (CC)c1c(CNc2ccccc2) [nH]nn1 | 8005-7257 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 977 | C1C(C(F) (F)F)=NN(C(c2ccc(cc2)N)  =O)C1(c1ccc(cc1)[Br])O | 8006-7761 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 978 | Cc1cc(C)c2c(c1)nc(c1ccc( cc1O)N)o2 | 8007-0773 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 979 | C(C1C(c2ccsc2)c2ccc3ccc cc3c2OC=1N)#N | 8007-1084 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 980 | C(C(c1ccc(cc1) [Cl])=O)Sc1nc2ccc(cc2s1) N | 8007-4809 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 981 | CC(c1ccc(cc1)NC(CSc1nn c(N)s1)=O)=O | 8008-3900 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 982 | CCOC(c1c2ccc(c(c2sc1NC (C)=O)OCC(CN1CCCCC1  )O)[Br])=O | 8008-4440 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 983 | Cc1c(C(O)=O)c(c(CO)s1)  Sc1ccccc1 | 8008-4457 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 984 | COc1ccc(c(c1)NC(CSc1nc 2ccc(cc2s1)N)=O)OC | 8009-2885 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 985 | C(C(CSc1nc2ccccc2o1)O) Oc1ccccc1 | 8009-3200 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 986 | C(C(c1ccc(cc1)F)=O)Sc1n c2ccc(cc2s1)N | 8009-5501 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 987 | CC(C)c1c2C(C(C#N)=C(N  )Oc2[nH]n1)c1ccc(c(c1) [Br])F | 8011-1991 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 988 | C(c1ccccc1)n1c(c(C(Nc2c cc(cc2)Oc2ccccc2)=O)nn1  )N | 8011-6606 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 989 | Cn1cnnc1c1cccc(c1)N | 8011-8021 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 990 | CC1CC(NCc2ccccc2)N(C(  C)=O)N1c1ccccc1 | 8012-7012 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 991 | CCOC(c1c(c2c(C)c(c(C)nc  2s1)[Cl])N)=O | 8012-7125 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 992 | CN(C)CCCNCc1ccc2c(c1) c1CCCCc1[nH]2 | 8013-3043 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 993 | Nc(cc1)cc(Cc2c3)c1- c2cc(Cl)c3Cl | 80141 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 994 | CC1(C)Cc2c(ccc3ccccc23) C(=N1)Sc1ccc(cc1)N | 8015-2089 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 995 | Cc1cc(C)nc2c1c(c(C(NCc 1ccccc1[Cl])=O)s2)N | 8015-4156 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 996 | CCc1ccc2c(c1)nc(c1ccc(cc 1O)N)o2 | 8018-2852 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 997 | c1cc2c(cc1N)nc(c1cc(ccc1 [Cl])[Br])o2 | 8018-2966 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 998 | C(c1ccc2c(c1)OCO2)Nc1c (c[nH]n1)C(N)=O | 8018-4095 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 999 | C(c1ccc2c(c1)OCO2)NCc 1cc(c2ccc3c(c2)OCO3)no1 | 8018-4194 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 1000 | Cc1cc(C)nc2c1c(c(c1cc(c3 ccc4c(c3)OCO4)no1)s2)N | 8018-6772 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 1001 | Cc1cc(COC)c2c3c(C(N(C CO)C(c4ccccc4OC)=N3)=  O)sc2n1 | 8018-6812 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 1002 | c1ccc(cc1)c1cc2cccc(c2o1) N | 8019-4318 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 1003 | c1ccc(cc1)c1cc2cc(ccc2o1) N | 8019-4319 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 1004 | CC(=O)OCc1cc(ccc1O)c1 csc(N)n1 | 8019-4503 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 1005 | CCNC[C@@H]1CCN(CC  )[C@H]1c1ccccc1OC | 8019-4504 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 1006 | COc1cc(C2C(C#N)=C(N) OC3CCCC(C2=3)=O)c(c2 c1OCO2)OC | 8019-7050 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 1007 | c1cc(N)nc2c1ccc(n2)O | 8019-7722 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 1008 | [H]N(Cc1cccnc1)c1ccc(C( O)=O)c(c1)[Cl] | 8019-7876 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 1009 | C(c1ccccc1)c1cc(ccc1OCC N)[Cl] | 8019-8811 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 1010 | C1CN(C(CN)c2ccccc2)N=  C1c1ccccc1 | 8019-9361 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 1011 | c1cc(ccc1c1cn[nH]c1)N | 8020-2683 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 1012 | Cc1c2[nH]c(cccc3)c3c2ccc 1CCN | 81703 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 1013 | C(c1ccccc1)[C@@H] (c1nnc(o1)SCc1cccc2ccccc 12)N | 8388-0720 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 1014 | C(CN)c1nnc(o1)SCc1c(ccc c1[Cl])[Cl] | 8388-1008 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 1015 | CSc1nc2ncc(c3ccccc3)c(N  )n2n1 | 8562-00102 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 1016 | S=C1Oc(ccc(- c2ccccc2)c2)c2N1 | 93817 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 1017 | c1ccc(cc1)S(n1c(cc(n1)OC (c1ccco1)=O)N)(=O)=O | C050-0221 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 1018 | C(c1nc2ccccc2n1Cc1ccc(c c1) [Cl])Nc1ccc(cc1)C(O)=O | C147-0025 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 1019 | Cc1cccc(c1)NCc1nc2ccccc 2n1C | C147-0043 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 1020 | CSc1c(c(N)n(Cc2ccccc2)n 1)S(c1ccccc1)(=O)=O | C200-4138 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 1021 | Cc1ccc2nc(c(Nc3ccccc3)n 2c1)c1ccco1 | C239-0048 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 1022 | Cc1ccn2c(c(c3ccccn3)nc2c 1)NC1CCCCC1 | C273-0219 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 1023 | c1ccc(cc1)S(n1c(cc(c2cccc (c2)F)n1)N)(=O)=O | C665-0183 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 1024 | Cc1ccc2c(c1)C(C1=C(C(N (CCCO)C13C(N(CC=C)c1 ccccc13)=O)=O)O2)=O | D063-1068 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 1025 | Cc1ccc2c(c1)C(C1=C(C(N (CCO)C13C(N(CC=C)c1c cccc13)=O)=O)O2)=O | D063-1117 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 1026 | Cc1cc(NC(C(=O)OC)c2cc  ccc2)n2c(n1)nc(Cc1ccccc1  )n2 | D245-0574 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 1027 | C1CCC2(CC1)Cc1ccccc1 C1=C2C(N(Cc2ccco2)C(= N1)SCCO)=O | D325-0603 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 1028 | [H]N(Cc1ccccc1)c1c2c(csc 2ncn1)c1ccc(C)cc1 | D341-0419 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 1029 | COc1ccc(cc1)c1nc(C(NCC O)=O)nn1c1ccccc1[Cl] | D351-2816 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 1030 | C1CCC2=C(C1)N1C(=NC  =C(C(NCCCO)=O)C1=O) S2 | D358-0437 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 1031 | CC(c1cccc(c1)Nc1cc(c2cc c(cc2)OC)nc(C)n1)=O | D482-2054 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 1032 | CCCCCCNc1cc(c2ccccc2) nc2nc(c3cccnc3)nn12 | D494-0421 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 1033 | CN(C)c1ccc(cc1)c1c(Nc2c ccc(c2)[Cl])n2ccncc2n1 | D600-0313 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 1034 | [H]N(CCc1ccc(cc1)S(N)  (=O)=O)Cc1ccc(c2ccc(cc2  )[Cl])o1 | D665-0262 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 1035 | Cc1ccc2c(c1)cc(c(NCc1cc c(cc1F)F)n2)c1nc(C)on1 | D704-0959 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 1036 | CCOC(c1cnc2c(c3ccc(cc3) [Br])c(C)nn2c1N)=O | D718-0691 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 1037 | COC(c1ccc(cc1)NS(c1cc(c nc1N)[Br])(=O)=O)=O | E138-2198 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 1038 | CCC(C) (C)NC1=C(C(C1=O)=O)c  1ccc(C)cc1 | E470-0146 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 1039 | CCN(CC)c1ccc(c(C)c1)N C1=C(C(C1=O)=O)c1ccc( C)c(C)c1 | E470-0720 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 1040 | CCC(C)NC1=C(C(C1=O)  =O)c1ccc(cc1)C(C)C | E511-0764 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 1041 | CC(C)c1ccc(cc1)C1=C(C( C1=O)=O)NC1CCCCCC1 | E511-0774 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 1042 | CC(C)c1ccc(cc1)C1=C(C( C1=O)=O)NC1CCCCC1 | E511-0775 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 1043 | CC(C)c1ccc(cc1)C1=C(C( C1=O)=O)NCc1ccccc1OC | E511-0865 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 1044 | Cc1ccc(C)c(c1)Nc1nc2ccc cc2c2nnc(C)n12 | E881-0025 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 1045 | C(C(Cn1cncn1) (c1ccc(cc1F)F)O)n1cncn1 | NCGC0009508 9-11 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 1046 | CC(=O)OC[C@@H]1[C@ H]([C@@H]([C@H] ([C@@H] (O1)S[Au])OC(C)=O)OC( C)=O)OC(C)=O | NCGC0016039 1-02 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 1047 | C1C(N=C2Nc3ccc(c(c3CN 12)[Cl])[Cl])=O | NCGC0016140 8-02 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 1048 | Cc1ccc(cc1)S(=O) (=O)OCC(Nc1ccc(C(O)=O  )c(c1)O)=O | NCGC0026264 1-02 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 1049 | C(C(Nc1ccc(cc1)n1c(cc(C( F)  (F)F)n1)c1ccc2c(ccc3ccccc 23)c1)=O)N | NCGC0034649 0-01 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 1050 | CC(C)n1cnc2c(Nc3cccc(c3  )NC(C=C)=O)nc(NC3CCC (CC3)N(C)C)nc12 | NCGC0034696 4-01 | HIV\_SL3 | Hairpin | GACUAGCGGAGGCUAGAA | 1 |
| 1051 | c1ccc(cc1)c1nc2cc(ccc2o1  )N | 0109-0002 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1052 | c1ccc2c(c1)nc(c1ccc(cc1) N)o2 | 0109-0045 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1053 | Cc1nc2ccc(CCO)cc2s1 | 0133-0036 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1054 | c1ccc(c(c1)N)I | 0325-0348 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1055 | c1ccc(cc1)c1nc2ccccc2c2n c(N)nn12 | 0345-0104 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1056 | Cc1c(cc(c(c1[Br])N)[Br]) [Br] | 0357-0017 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1057 | CC(Nc1nc2ccc(cc2s1)N)= O | 0478-0670 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1058 | C(C1COc2ccccc2O1)O | 0507-0170 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1059 | Cc(cccc1)c1NC(NCCN1C C1)=O | 101266 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1060 | c(cc1)ccc1- n1c(cccc2)c2c2c1cccc2 | 10416 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1061 | CCC(C)N(C(C)=C1)N(C( C)CC)C1=O | 120844 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1062 | C1CN(Cc2ccccc12)c1c2C CNCc2nc(c2cccnc2)n1 | 12634687 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1063 | C1C(CN)Oc2c1cc(cc2F)c1 ccc2c(cco2)c1 | 12766557 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1064 | C(c1ccc(c(c1)c1cccc2ccnn 12)F)N | 13150762 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1065 | C1C(CN1Cc1ccc(cc1)OC CO)Oc1ccccc1[Cl] | 13202927 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1066 | CC(Cn1cncn1)NC1CCN(C  C1)c1nc2ccc(cc2s1)[Cl] | 13410217 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1067 | C1CC(CCc2ccccc2C(F) (F)F)CN(C1)C(CN)=O | 13741411 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1068 | C1CN(Cc2cnc(NCc3ccccc 3)nc2)C[C@@H]  ([C@H]1CO)O | 14588562 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1069 | C1CN(CCC1C1CCN(CCc  2ccccc2)C1)c1ccnc(N)n1 | 14604674 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1070 | C1CN(CCN(C1)C(CCc1cs  c(N)n1)=O)Cc1ccc(cc1)F | 14610180 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 1071 | Cc1cc(NCCCO)n2c3ccccc 3nc2c1C#N | 1486-0661 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1072 | Cc1c(cc(cc1[Cl])C(NCC(C c1ccco1)CO)=O)[Cl] | 15537048 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1073 | CCCCSc1nc(cc(n1)N1CC CN(CC1)Cc1ccncc1)N | 15986801 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1074 | Cc1cccc(c1)n1cccc1CN1C COC(CN)C1 | 16946825 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1075 | COc1cccc(c1)c1c(CN2CC C(CC2)O)cc2cc(c(cc2n1)O C)OC | 16959688 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1076 | CN(CC1CCN(CC1)CCc1c  ccc(c1)F)C([C@H] (Cc1c[nH]cn1)N)=O | 17007774 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1077 | C=Cc1ccc(nc1)N1CCN(C C(C1)O)Cc1ccccc1 | 17524156 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1078 | CCCc1c(CC)c(c(C#N)c(N)  n1)c1ccco1 | 1756-0136 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1079 | C1CNCc2cccc(c3cccc4c3c c[nH]4)c12 | 17741735 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1080 | CCNC([C@@H]1C[C@@ H] (CN1S(N1CCN(CC)CC1) (=O)=O)N)=O | 17965244 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1081 | C1CN(CCC1(c1ccccc1)c1 ccccc1)C(c1cn(CCN)nn1)= O | 18373450 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1082 | Cc1c2c(nc(CCN)nc2sc1C) N1C[C@H]2CC[C@H]1C 2 | 18808730 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1083 | C(CN)c1cccc(CN2CCN(C  C2)Cc2ccc(cc2)[Cl])c1 | 19565794 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1084 | C(CNC1CCC2(CC1)CCN  CC2)CNc1cccnc1 | 19786268 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1085 | Cc1cccc2c(cn(C)c12)c1c(c 2ccccc2)ncn1CCN | 20224956 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1086 | Cc1cc(cc(c1CNc1c2CCNC c2nc(C)n1)[Cl])[Cl] | 20278440 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1087 | CCc1ccc2c(c1)c(CC(N1C CC3(CC1)[C@H] (C[C@H]3O)OCCN)=O)c  o2 | 21565883 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1088 | COc1ccc(cc1OC)c1nnc(N) o1 | 2158-0021 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1089 | C1CNC[C@H]  ([C@@H]1CNS(c1cccc2c cccc12)(=O)=O)O | 21873168 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1090 | CCOc1ccc(cc1)C(CN1C(= N)N(CCN2CCCCC2)c2cc  ccc12)O | 2226-0435 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1091 | c1ccc2c(c1)ccc1c2nc(c2cc c(cc2)N)[nH]1 | 2252-1548 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1092 | C1CCCN(CC1)C[C@@H] 1CN(C[C@@H]1CO)C(c1 cc(N)[nH]n1)=O | 22664850 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1093 | Cc1cc2c(cc1N)nc(NC(c1cc c(cc1)C(=O)OC)=O)s2 | 2284-1574 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1094 | c1ccc(c(c1)c1nc2cc(ccc2s1  )N)O | 2372-3111 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1095 | C1CN(Cc2c(c3cccc4ccccc 34)noc12)C(c1cc(N) | 26633940 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | [nH]n1)=O |  |  |  |  |  |
| 1096 | C1COc2cc(ccc2C1=O)c1c c2CC(CN)Oc2c(c1)[Cl] | 26642358 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1097 | C1CCN(CC1)Cc1cccc(c1)  n1ccnc1c1cc2CNCCCn2n1 | 26875627 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1098 | Cc1c2c(NCc3ccc(C(NC)= O)o3)nc(CCN)nc2sc1C | 27312861 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1099 | Cc1cc2c(cc1C)oc(c1ccc(cc 1O)N)n2 | 2783-3499 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1100 | c1cc(cc(c1) [Cl])n1nc2ccc(cc2n1)N | 2810-4198 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1101 | c1cc(c2cccc(c2c1) [Br])c1nc2cc(ccc2o1)N | 2810-4224 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1102 | COc1ccc(cc1[Cl])c1nc2cc( ccc2o1)N | 2810-4228 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1103 | c1ccc(cc1)n1nc2ccc(cc2n1  )N | 2810-4237 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1104 | Cc1ccc2c(c1)nc(c1cc(ccc1 [Cl])N)o2 | 2810-4326 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1105 | Cc1ccc2c(c1)oc(c1cc(ccc1 [Cl])N)n2 | 2810-4327 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1106 | Cc1cc2c(cc1C)oc(c1ccc(C) c(c1)N)n2 | 2810-4335 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1107 | C(c1ccc(cc1)c1nc(c2ccc(c( c2)F)F)nn1CCO)N | 31242301 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1108 | Cc1cccc(c1)Nc1nc(CN2C CCC2c2ccc(cc2)F)nc(N)n1 | 31279636 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1109 | COCCOC(C1C(C2=C(CC CC2=O)OC=1N)c1cccnc1)  =O | 3132-0534 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1110 | Cc1nc(CCN)cc(n1)N1CC N(CC1)c1ccc(C#N)cn1 | 31455775 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1111 | C(c1ccccc1[Cl])Sc1nc2ccc (cc2s1)N | 3167-0436 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1112 | Cc1c[nH]c(CN(C)C(c2ccc c(c2)C2CCCNC2)=O)n1 | 31699168 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1113 | Cc1nnc2c(Nc3ccc(cc3) [Cl])nc3c(non3)n12 | 3175-0679 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1114 | C(Cc1nc(c2ccccc2)no1)C( N[C@H]1Cc2ccccc2[C@ @H]1N)=O | 31852539 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1115 | CCc1cnc(C)nc1N1CCC(C C1)NC1CCc2ccccc2C1 | 32780540 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1116 | c1ccc(cc1)C(c1ccc2c(c1)n c(c1cccc(c1)N)[nH]2)=O | 3289-6683 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1117 | C1CC1[C@H]1CN(C[C@  @H]1N)C(c1ccc2c(cccn2) c1)=O | 32894310 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1118 | COc(cc12)ccc2nc(cc(cc2) Cl)c2c1C#N | 33173 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1119 | CC(=C)Cn1c2C(NC(N(C)c 2nc1NCCO)=O)=O | 3329-2956 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1120 | C(C12C3C(C(c4ccccc14)c 1ccccc12)C(N(C3=O)c1cc c(cc1)F)=O)O | 3406-0971 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1121 | CCOc1ccccc1c1nc(COc2c ccnc2N)c(C)o1 | 34120503 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1122 | Cc1c2cc(cc(CNC([C@H] (Cc3c[nH]cn3)N)=O)c2[n | 34268481 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | H]c1c1ccccc1)[Cl] |  |  |  |  |  |
| 1123 | C(C1C(c2cccc(c2) [Br])c2c(c3ccccc3)n[nH]c2 OC=1N)#N | 3448-2674 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1124 | CC1=CC(NC(NCCNC2CC C3(CC2)CCNCC3)=N1)= O | 35107446 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1125 | C1CNCc2cc(CCC(NC(CC  n3cncn3)c3ccccc3)=O)nn2 C1 | 35350604 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1126 | Cc1cc(ccc1[Br])c1nc2cc(c cc2o1)N | 3617-0633 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1127 | C(C1C(c2ccccc2)c2c(c3cc c4ccccc4c3)n[nH]c2OC=1 N)#N | 3629-0271 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1128 | Cc1cc2c(cc1C)oc(c1cccc(c 1C)N)n2 | 3639-0494 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1129 | C1C(C(=C(N)N1c1ccc(cc1 [Cl])  [Cl])C1NC(c2ccccc2N=1)  =O)=O | 3643-1572 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1130 | Cc1ccc(c(CC=C)c1)OCC(  Cn1c2ccccc2nc1CO)O | 3672-0031 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1131 | Cc1cc(CNCc2ccc(c(c2)OC  )OC)ccc1OC | 3702-1752 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1132 | Cc1ccc(cc1)S(N(CC(CN1  CCCCC1)O)c1cccc2ccccc 12)(=O)=O | 3772-6707 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1133 | CCc1ccc(c2c3CCCCc3nc( c2C#N)N)s1 | 3830-0877 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1134 | CC1c2ccccc2C(N(CC(NC CCc2nnc(N)s2)=O)N=1)= O | 40021826 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1135 | c1ccnc(c1)c1csc(Nc2ccc(c c2)C(O)=O)n1 | 4112-3301 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1136 | CCC(CO)N(Cc1ccccc1C) Cc1ccccc1C(O)=O | 41419156 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1137 | CC1CC2(CC(C) (c3csc(NCC=C)n3)OC2=O  )C(=O)O1 | 4159-0008 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1138 | C(Cn1cc(C(NCc2nc(c3ccc 4c(c3)OCO4)on2)=O)nn1) N | 42165233 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1139 | C1CNCc2c1c1c(NCc3cc(c 4ccco4)on3)ncnc1s2 | 42424648 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1140 | C(CNCC1(CCNC1)O)CNc  1cccnc1 | 42558291 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1141 | Cc1nc2CNCc2c(NCCCN2 CCCC2=O)n1 | 42605975 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1142 | C(c1ccccc1)NC(Cn1c2ccc cc2nc1c1c(N)non1)=O | 4281-0225 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1143 | CC(c1cccc(c1)Nc1nc(cs1)c 1ccc(cc1)[Cl])=O | 4469-0430 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1144 | CC(C)  (C)c1ccc(cc1)c1nc(c2ccccc 2n1)NCc1cccnc1 | 4491-1513 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1145 | CSC(NC(Cl)=C1)=NC1=O | 45719 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1146 | C(CNc1cccnc1)CNc1c2ccc cc2nc(CCN)n1 | 47488116 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 1147 | CCN1C(NC(C12CCN(CC 2)Cc1cc2CNCCCn2n1)=O  )=O | 47670564 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1148 | C1CN(CC=C1)c1c2CCN(  CCc2nc(c2ccco2)n1)C(CN  )=O | 47825811 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1149 | C(CN)CN1C(CC[C@H]2 CN(CC[C@@H]12)C(CCc  1ccco1)=O)=O | 48226996 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1150 | Cc1nc2cc(c(cc2n1CCCO) [Cl])[Cl] | 5119828 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1151 | c1ccc(cc1)C(C(c1ccccc1)= NNC(c1cccc(c1)[Cl])=O)O | 5210270 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1152 | CCCCCc1ccc(cc1)c1ccc(c c1)c1ncc(cn1)N | 5213078 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1153 | c1ccc2c(ccc(c2c1)Oc1ccc( cc1[Cl])N)[Cl] | 5215844 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1154 | Cc1ccc(cc1NC1c2ccccc2C (=O)O1)[Cl] | 5227-1352 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1155 | C1CCC2C(C1)=C(C#N)c1  nc3ccccc3n1C=2NCCOCC O | 5228-5336 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1156 | c1cc(ccc1c1cc(C(NN)=O)c 2cc(ccc2n1)[Br])N | 5350878 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1157 | [H]N([H])c1nc(n[nH]1)SC CCCCCCCC | 5655427 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1158 | C(=Cc1ccc(cc1[Cl]) [Cl])C(c1cccc(c1)N)=O | 5689908 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1159 | C(Cc1cccnc1)C(N1Cc2cnn (CCO)c2C1)=O | 57806214 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1160 | CCNC(Cc1ccc(cc1)c1cc2C C(CN)Oc2c(c1)[Cl])=O | 57980040 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1161 | C(c1ccc(cc1)c1ccccc1)NC( [C@@]12CNC[C@H]2C NC1)=O | 58024175 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1162 | C1Oc2ccc(cc2O1)c1cc(c(C #N)c(N)n1)c1ccco1 | 58070293 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1163 | Cc1ccc(cc1)c1nc(CNc2ccc c(c2)[Cl])on1 | 5927-0146 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1164 | C(=Cc1nc(c2ccccc2O)nc( N)n1)c1ccc(cc1)[Br] | 6043-0005 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1165 | [H][N+] (CCO)=C1C=C(c2ccccc2)  Oc2ccc(C)cc12 | 6197-4999 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1166 | C(CC(N1c2ccccc2Sc2cccc c12)=O)CN | 6640-0077 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1167 | O=C(c(cc1)cc(C(Nc(cc2)c cc2C2=NCCN2)=O)c1Cl)  Nc(cc1)ccc1C1=NCCN1 | 67436 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1168 | CC1(C)Cc2c(CO1)c(c1ccc o1)nc1c2c2c(c(NC3CCCC C3)ncn2)s1 | 6940-0105 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1169 | CN(C)c1ccc(cc1)Nc1nc(cs 1)c1cccs1 | 7100-1263 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1170 | Cc1ccc(c(c1)C(O)=O)Nc1 nc(C)cc(C)n1 | 7170-3463 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1171 | CC1(C)CC(=CC(C1)=O)N  c1cc(c2ccc(cc2) [Cl])n[nH]1 | 7428-3079 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1172 | C1C(C(N(C1=O)c1ccc(cc1 | 7627-0033 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | )  [Cl])=O)Nc1ccc(cc1)Oc1c cccc1 |  |  |  | UGACGGUACA |  |
| 1173 | CC(c1ccc(cc1)OCC(Cn1c2 ccccc2nc1CO)O)=O | 7661-0040 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1174 | Cn1c(cnc1NCc1cccc(c1) [Br])c1ccc(cc1)OC | 7756-0365 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1175 | Cn1c(cnc1NCc1cc(ccc1F) [Br])c1cccc(c1)OC | 7756-0752 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1176 | CCOC(C1C(C(C#N)=C(N) OC=1C)c1c(C)c(C)cc(C)c 1C)=O | 8003-8202 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1177 | Cc1ccc(cc1C)Nc1nc(cs1)c 1ccc(c(c1)F)OC | 8005-2731 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1178 | CC[Ge](CC)  (CC)c1c(CNc2ccccc2) [nH]nn1 | 8005-7257 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1179 | CN1C2=C(C(C(C#N)=C( N)O2)c2ccccc2F)C(N(C)C 1=O)=O | 8006-4741 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1180 | C(C(c1ccc(cc1) [Cl])=O)Sc1nc2ccc(cc2s1) N | 8007-4809 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1181 | C1C(C(N(C1=O)c1ccc(c(c 1)[Cl])  [Cl])=O)Nc1ccc(cc1)F | 8007-5006 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1182 | CCOC(c1c2ccc(c(c2sc1NC (C)=O)OCC(CN1CCCCC1  )O)[Br])=O | 8008-4440 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1183 | C(C(c1ccc(cc1)F)=O)Sc1n c2ccc(cc2s1)N | 8009-5501 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1184 | c1ccc2c(c1)nc(Sc1ccc(cc1 N)C(F)(F)F)s2 | 8010-6075 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1185 | CCN(CC)c1ccc(cc1)NCc1 ccc2c(c1)OCO2 | 8011-7548 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1186 | Cc1c(CNCCc2c3cc(ccc3[n H]c2C)OC)c(n(C)n1)[Cl] | 8013-0585 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1187 | C1CCC(CCNC2CC(N(C2  =O)c2ccc(cc2)F)=O)=CC1 | 8013-1383 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1188 | CCCCc1ccc(cc1)n1nc2cc( C)c(cc2n1)N | 8014-1852 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1189 | CC(C)Nc1nc(nc(n1)n1ccnc 1)N(C)c1ccccc1 | 8014-9111 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1190 | CC1(C)Cc2c(ccc3ccccc23) C(=N1)Sc1ccc(cc1)N | 8015-2089 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1191 | c1cc(cc(c1)NC(c1c(csn1)N  )=O)C(F)(F)F | 8016-2265 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1192 | Cc1c2c(NCCc3c4ccccc4[n H]c3C)ncnc2sc1C | 8016-2589 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1193 | c1ccnc(c1)Sc1ccc(cc1[Cl]) N | 8016-2974 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1194 | CCN1C(c2ccc(CN)c3cccc 1c23)=O | 8016-6735 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1195 | CCc1ccc2c(c1)nc(c1ccc(cc 1O)N)o2 | 8018-2852 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1196 | c1ccc(cc1)c1ccc(cc1)c1nc2 cc(ccc2o1)N | 8018-2965 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1197 | COc1ccc(cc1)c1cc(CNCC 2CC(Cc3cc4c(c(c3OC)OC  )OCO4)ON=2)on1 | 8019-1863 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 1198 | COc1cc(C2C(C#N)=C(N) OC3CCCC(C2=3)=O)c(c2 c1OCO2)OC | 8019-7050 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1199 | c1cc(N)nc2c1ccc(n2)O | 8019-7722 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1200 | C(c1cn[nH]c1c1ccc(cc1)F) N | 8020-0151 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1201 | C1CN(CCC1N)Cc1cccc(c 1)O | 8020-1707 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1202 | C(c1ccccc1)Nc1c(C(Nc2cc cc(c2)C(F)(F)F)=O)c(N)  [nH]n1 | 8020-3093 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1203 | c1cc(cc(c1) [Cl])c1nc(c2ccc(cc2)N)n[n H]1 | 8020-5002 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1204 | C(c1ccccc1)[C@@H] (c1nnc(o1)SCc1cccc2ccccc 12)N | 8388-0720 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1205 | C(COc1ccc2c(c1)c1ccccc1 o2)N.[Cl] | 9188721 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1206 | CC(C)CCc1cc(nc(N)n1) [Cl] | 9225768 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1207 | c1ccc2c(c1)nc(c1ccc(cc1[ Cl])N)s2 | C066-5322 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1208 | Cc1cccc(c1)NCc1nc2ccccc 2n1C | C147-0043 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1209 | CSc1c(c(N)n(Cc2ccccc2)n 1)S(c1ccccc1)(=O)=O | C200-4138 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1210 | C1CCN(CC1)c1cc(Nc2ccc (cc2)[Br])ncn1 | C301-6154 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1211 | c1cc(ccc1c1cc[nH]n1)N | C430-1098 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1212 | Cc1cc(Nc2ccccc2)nc2cc(c cc12)O | C614-0105 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1213 | C1CCCN(CC1)CCCNc1nc  2ccccc2c2nc(c3ccccc3)nn1 2 | C736-0159 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1214 | C1Oc2ccc(cc2O1)Nc1c(cn c2ccc(cc12)F)S(c1ccccc1) (=O)=O | C769-2045 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1215 | Cc1ccc(cc1F)NC(CCc1c(C  )nc2nc(CN)nn2c1C)=O | C908-0521 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1216 | Cc1c(CCC(Nc2cccc(c2) [Br])=O)c(C)n2c(n1)nc(C N)n2 | C908-0523 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1217 | Cc1c(CCC(Nc2ccccc2OC)  =O)c(C)n2c(n1)nc(CN)n2 | C908-0524 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1218 | Cc1c(CCC(NCC2CCN(CC  2)Cc2ccccc2F)=O)c(C)n2c (n1)nc(CN)n2 | C908-0547 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1219 | Cc1ccc2c(c1)C(C1=C(C(N (CCCO)C13C(N(CC=C)c1 ccccc13)=O)=O)O2)=O | D063-1068 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1220 | Cc1ccc2c(c1)C(C1=C(C(N (CCO)C13C(N(CC=C)c1c cccc13)=O)=O)O2)=O | D063-1117 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1221 | CCCNc1cc(C)nc2nc(c3ccc (C)cc3)nn12 | D245-0069 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1222 | CN(C)S(c1ccc(cc1)c1nc(C #N)c(NC2CCCCC2)o1) (=O)=O | D434-0560 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 1223 | CCNc1c(C#N)nc(c2ccc(cc 2)S(N2CCOCC2) (=O)=O)o1 | D434-0668 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1224 | C(CO)NC(C1C=COc2cccc c2C=1)=O | D443-0135 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1225 | C(CNc1c2c(cn(c3ccccc3[C l])c2ncn1)c1ccccc1)CN1C COCC1 | D447-0372 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1226 | CC(c1ccccc1)N[C@H]1C S(C[C@@H]1S(c1ccc(cc1  )F)(=O)=O)(=O)=O | D470-1919 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1227 | C1CC1N[C@H]1CS(C[C  @@H]1S(c1ccc(cc1)[Cl])  (=O)=O)(=O)=O | D470-2169 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1228 | COCCN[C@H]1CS(C[C@  @H]1S(c1ccc(cc1)[Cl])  (=O)=O)(=O)=O | D470-2180 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1229 | CC(c1cccc(c1)Nc1cc(c2cc c(cc2)OC)nc(C)n1)=O | D482-2054 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1230 | CCCCCCNc1cc(c2ccccc2) nc2nc(c3cccnc3)nn12 | D494-0421 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1231 | Cc1ccc2cc(c(NCc3cc(cc(c 3)F)F)nc2c1)c1nc(C)on1 | D704-0962 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1232 | CC(Nc1ccc(cc1)N1CC(C(  =C1N)c1nc(C)c(C)s1)=O)  =O | D715-1790 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1233 | COc1ccc(cc1)c1csc(C2=C( N)N(CC2=O)c2ccccc2[Cl]  )n1 | D715-1943 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1234 | CCC(C) (C)NC1=C(C(C1=O)=O)c  1ccc(C)cc1 | E470-0146 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1235 | CCN(CC)c1ccc(c(C)c1)N C1=C(C(C1=O)=O)c1ccc( C)c(C)c1 | E470-0720 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1236 | CCC(C)NC1=C(C(C1=O)  =O)c1ccc(cc1)C(C)C | E511-0764 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1237 | CC(C)c1ccc(cc1)C1=C(C( C1=O)=O)NCc1ccccc1OC | E511-0865 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1238 | CC(C)c1ccc(cc1)C1=C(C( C1=O)=O)NCc1ccc(cc1)N (C)C | E511-0981 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1239 | C1CCc2c(C1)c(CO)cs2 | E540-0003 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1240 | CC1Cc2cc(ccc2N1C(C1C C1)=O)S(N(CCO)Cc1cccc c1)(=O)=O | E570-0206 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1241 | Cc1cccc(c1)C1C(C#N)=C( N)OC2=C1S(N(Cc1ccccc1  C)c1ccccc12)(=O)=O | E738-0440 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1242 | C(C(Cn1cncn1) (c1ccc(cc1F)F)O)n1cncn1 | NCGC0009508 9-11 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1243 | CC(C)  (C)c1ccc(cc1)C(CC(c1ccc( cc1)OC)=O)=O | NCGC0009511 2-04 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1244 | C1C(N=C2Nc3ccc(c(c3CN 12)[Cl])[Cl])=O | NCGC0016140 8-02 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1245 | CC(C)c1cc(cc2c1C(N(CO C1=CC(N3C=CC=C(C3= N1)OCCN1CCCCC1)=O) S2(=O)=O)=O)OC | NCGC0016775 1-03 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 1246 | CCc1ccc(C=C2C(NC(=S)S 2)=O)cc1 | NCGC0018599 4-02 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1247 | C(CCN1CCCC1)CNC(Nc  1c(C(N)=O)c(ns1)OCc1c(c  c(cc1F)[Br])F)=O | NCGC0026310 0-01 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1248 | C1CC1NCc1cccc(c1)NC1  =CC(=c2ccc(cc2)=C2C=C C(C=C2O)=O)NN1 | NCGC0034695 4-01 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1249 | CC(C)n1cnc2c(Nc3cccc(c3  )NC(C=C)=O)nc(NC3CCC (CC3)N(C)C)nc12 | NCGC0034696 4-01 | RRE2B | Hairpin | UGGGCGCAGUGUCAUUGACGC UGACGGUACA | 1 |
| 1250 | C(CO)NC(C1=Cc2ccccc2 OC1=O)=O | 0096-0280 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1251 | c1ccc2c(c1)nc(Sc1ccc(cc1) N)s2 | 0375-0603 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1252 | c1cc2c(cc(c(c2nc1)N)[Br]) [Br] | 0422-0091 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1253 | c1nnc(N)s1 | 0488-0194 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1254 | C(C1COc2ccccc2O1)O | 0507-0170 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1255 | CN(C)c1ccc(C=Cc2nc3cc( ccc3[nH]2)N)cc1 | 0632-0897 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1256 | Cc1c(C)c(C)nc2c1c(c(C(c1 ccc(cc1)[Cl])=O)s2)N | 0892-0702 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1257 | Cc(cccc1)c1NC(NCCN1C C1)=O | 101266 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1258 | O=C(NCCCN1CC1)Nc1cc  cc2ccccc12 | 101298 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1259 | CC[N+]1C(C)CSC=1C=C  Nc1ccccc1 | 1147-0135 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1260 | CCC(C)N(C(C)=C1)N(C( C)CC)C1=O | 120844 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1261 | CN(CCCc1nccn1C)c1c2C CNCc2nc(c2ccncc2)n1 | 12244291 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1262 | CC(C)Oc1cc(nc(N)n1)N1 CCC(CC1)c1cc(nc(C)n1)O | 12360715 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1263 | Cc1cccc2c(c[nH]c12)c1ccc c(CCN)c1 | 12888021 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1264 | C1CNCCC12CC(C(N1CC  N(CC1)c1cccc(c1[Cl]) [Cl])=O)NC2 | 12921403 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1265 | CC(C)c1cc(Nc(c2c3)c(ccc( Cl)c4)c4nc2ccc3OC)c(C)c c1O | 13051 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1266 | C1C(CN1Cc1ccc(cc1)OC CO)Oc1ccccc1[Cl] | 13202927 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1267 | CN1C(C=C(C=N1)N1CC C(CC1)CNC([C@H] (Cc1c[nH]cn1)N)=O)=O | 13216682 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1268 | CN(C)c1nc2CNCCc2c(NC  c2cc(COC)[nH]n2)n1 | 13478828 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1269 | CN(CCO)C[C@@H]1CN(  Cc2cccc3c4ccccc4sc23)C[ C@@H]1CO | 13609905 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1270 | C1C(Cc2ccccc12)N1CC[C  @@H](c2ccc3c(c2)OCO3) [C@@H](C1)O | 13694326 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1271 | C1CC(CCc2ccccc2C(F) (F)F)CN(C1)C(CN)=O | 13741411 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 1272 | CC(C)c1cc(c2nc(c3ccc(cc3  )n3c(cc(C)n3)N)no2)no1 | 14063694 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1273 | NCC(Nc(ccc(Cl)c1)c1C(c1 ccc[nH]1)=O)=O | 140873 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1274 | Cc1nc(CCN)cc(NCCC2CC CN2C)n1 | 14159297 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1275 | Clc1nc(Oc2ccccc2)nc(- c(c2c3cccc2)cn3- c2ccccc2)n1 | 142335 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1276 | CC(C)CCOc1cccc(CCNC( C2CC3(CCNCC3)CN2)=O  )c1 | 14325308 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1277 | C1C[C@@H]2CCNC[C@  H]1N2c1c2CNCc2nc(c2cc cnc2)n1 | 14601902 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1278 | CN(C)c1nc2CNCCc2c(NC  c2cc(c3ccccc3)n[nH]2)n1 | 15510936 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1279 | Cc1c(cc(cc1[Cl])C(NCC(C c1ccco1)CO)=O)[Cl] | 15537048 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1280 | CCC[C@H]1CN(C[C@@ H]1NC(c1cnc(N)nc1C)=O) S(C)(=O)=O | 15820090 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1281 | C1CC(CCc2ccc(cc2)F)CN (C1)C(c1cn(CCN)nn1)=O | 15955175 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1282 | Cc1ccc(c(c1)NC(NCC(CN 1CCCC1)O)=O)[Cl] | 16657809 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1283 | C=Cc1ccc(nc1)N1CCN(C C(C1)O)Cc1ccccc1 | 17524156 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1284 | C1CC(c2cccc(c2)c2cc(N)n c3c2cc[nH]3)NC1 | 18100777 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1285 | C1=C(C(=O)Oc2cc(ccc12)  O)c1nnc(Nc2ccc(cc2)F)s1 | 1814-2026 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1286 | COc1c(cccn1)C(N1C[C@ @H]([C@H] (C1)O)N1CCOCC1)=O | 18173626 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1287 | C1CN(CCC1(c1ccccc1)c1 ccccc1)C(c1cn(CCN)nn1)= O | 18373450 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1288 | Cc1c2c(nc(CCN)nc2sc1C) N1C[C@H]2CC[C@H]1C 2 | 18808730 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1289 | CC(c1ccc2c(cc[nH]2)c1)N C1CCN(CC1)c1c2c(ncn1)  [nH]cn2 | 18958506 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1290 | C1CCCN(CC1)CC(CNC(c 1cn(CCN)nn1)=O)O | 19036853 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1291 | O=C(Nc(cc1)ccc1Br)Nc(cc cc1)c1Cl | 190501 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1292 | C(CN)c1cccc(CN2CCN(C  C2)Cc2ccc(cc2)[Cl])c1 | 19565794 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1293 | C1Cc2c(CC1N)c(c1cnc(c3 ccco3)nc1)c(C#N)c(N)n2 | 19707907 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1294 | Cc1cc(cc(c1CNc1c2CCNC c2nc(C)n1)[Cl])[Cl] | 20278440 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1295 | C(c1ccc(cc1) [Cl])n1c2ccccc2nc1c1c(N) non1 | 2039-0584 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1296 | CCOC(c1nc2ccc(cccc3)c3 c2c(OCC)c1)=O | 204939 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1297 | Cc1cccc(c1)c1nc(CN2C=N | 21839710 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | c3c(C2=O)c2CCNCc2s3)o  n1 |  |  |  | CGCUG(m6A)CGGUACA |  |
| 1298 | C1CCN(CC1)C(CNC(CCc  1cc2CNCCn2n1)=O)c1ccc nc1 | 21900063 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1299 | CC(c1cccc(n1)N1CCc2c(C 1)c1cccc(c1[nH]2)[Cl])O | 22241597 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1300 | c1ccc2c(c1)ccc1c2nc(c2cc c(cc2)N)[nH]1 | 2252-1548 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1301 | C1CNCc2cc(c3nccn3CCN C(c3ccc(cc3)F)=O)nn2C1 | 22582668 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1302 | Cc1cc2c(cc1N)nc(NC(c1cc c(cc1)C(=O)OC)=O)s2 | 2284-1574 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1303 | CC1OC1c(cc1)ccc1- c1ccc(C2OC2C)cc1 | 22881 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1304 | C1CCN(CC1)CC1(CCN(C  c2cccc(CCN)c2)C1)O | 22896979 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1305 | c1ccc(c(c1)c1nc2cc(ccc2s1  )N)O | 2372-3111 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1306 | CC(C)OC(C1=C(C)OC(=C (C#N)C12C(Nc1ccccc12)= O)N)=O | 2435-0085 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1307 | CC(C)Cn1c2C(NC(N(C)c2 nc1NCCCO)=O)=O | 2516-4245 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1308 | C1CN(Cc2c3cc(ccc3[nH]c 12)[Cl])c1c2c(nc(N)n1) [nH]cn2 | 25604160 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1309 | Cc1cc2c(cc1C)n(CC(COc1 ccccc1C)O)cn2 | 2582-0009 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1310 | CC(C) (C1CC2(C)CC1)C2OC(c(c ccc1)c1C(O)=O)=O | 26349 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1311 | C1COc2cc(ccc2C1=O)c1c c2CC(CN)Oc2c(c1)[Cl] | 26642358 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1312 | Cc1c2c(NCc3ccc(C(NC)= O)o3)nc(CCN)nc2sc1C | 27312861 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1313 | CNC([C@@H]1C[C@H]  (CN1S(c1ccc(c2ccno2)s1) (=O)=O)N)=O | 27338263 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1314 | c1cc(cc(c1) [Cl])n1nc2ccc(cc2n1)N | 2810-4198 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1315 | c1cc(c2cccc(c2c1) [Br])c1nc2cc(ccc2o1)N | 2810-4224 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1316 | COc1ccc(cc1[Br])c1nc2cc( ccc2o1)N | 2810-4227 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1317 | COc1ccc(cc1[Cl])c1nc2cc( ccc2o1)N | 2810-4228 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1318 | c1ccc(cc1)n1nc2ccc(cc2n1  )N | 2810-4237 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1319 | Cc1cc2c(cc1C)oc(c1ccc(cc 1)N)n2 | 2810-4334 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1320 | Cc1cc2c(cc1C)oc(c1ccc(C) c(c1)N)n2 | 2810-4335 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1321 | Cc(cc(cc1)- c(cc2)cc(C)c2N(C(CC23C CCC3)=O)C2=O)c1N(C(C C12CCCC2)=O)C1=O | 308835 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1322 | Nc1ccc(Cn(ccc2c34)c2ccc 4nc(N)nc3N)cc1.Cl | 309401 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 1323 | Cc1ccc(cc1c1cccc(CCN)c1  )F | 31003354 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1324 | C(c1ccc(cc1)c1nc(c2ccc(c( c2)F)F)nn1CCO)N | 31242301 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1325 | C(C(c1ccccc1)=O)Sc1nc2c cc(cc2s1)N | 3167-0470 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1326 | C(Cc1nc(c2ccccc2)no1)C( N[C@H]1Cc2ccccc2[C@ @H]1N)=O | 31852539 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1327 | COc1c(cnc(n1)OC)c1cc2C C(CN)Oc2c(c1)[Cl] | 32090306 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1328 | C(CNC1CCN(CC1)c1nnc(  c2ccccc2)s1)Cn1ccnn1 | 32364121 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1329 | CC(Cc1ccsc1)NC(c1cccc(c 1C)NCc1ccccn1)=O | 32552149 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1330 | NNC(CNC(Nc1nnc(S)s1)= O)=O | 327693 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1331 | CCc1cnc(C)nc1N1CCC(C C1)NC1CCc2ccccc2C1 | 32780540 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1332 | C=CCN1C(=Nc2c(C1=O)c 1CCCCc1s2)SCC(NCCCO  )=O | 3334-5625 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1333 | CN1C(c2c(nc(NCCN)n2C c2ccc(cc2)F)N(C)C1=O)= O | 3346-2730 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1334 | Cc1c2c(NCCCSc3nnc(C)s 3)nc(CCN)nc2sc1C | 33667724 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1335 | Cc1cc2c(C)nc(Nc3nc(C)cc (n3)O)nc2cc1C | 3389-2554 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1336 | CN(CCOC)C[C@@H]1C  N(Cc2cccc3c4ccccc4oc23) C[C@@H]1CO | 34159790 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1337 | Cc1c2cc(cc(CNC([C@H] (Cc3c[nH]cn3)N)=O)c2[n H]c1c1ccccc1)[Cl] | 34268481 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1338 | CN1CCC(CC1)N(CCOC)  C(Nc1cccc(CN)c1)=O | 34373109 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1339 | C1CNCc2cc(CCC(NC(CC  n3cncn3)c3ccccc3)=O)nn2 C1 | 35350604 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1340 | Cc1cc(ccc1[Br])c1nc2cc(c cc2o1)N | 3617-0633 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1341 | CCCCc1ccc(cc1)n1nc2ccc (cc2n1)N | 3738-4868 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1342 | CCC(CC) (C(N)=O)SCC=C | 37883 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1343 | C(C(c1ccc(cc1)N)=O)C1(  C(N(Cc2ccc(cc2) [Cl])c2ccccc12)=O)O | 3817-0057 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1344 | CCc1ccc(c2c3CCCCc3nc( c2C#N)N)s1 | 3830-0877 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1345 | CCOC(c1c(C)c2c(Nc3ccc( cc3)F)nc(C)nc2s1)=O | 3909-7545 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1346 | Cc1nccn1Cc1ccccc1n1ccn c1c1cc2CNCCn2n1 | 39520902 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1347 | C1CNCc2cccc(c3cncnc3)c 12 | 39696086 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1348 | COc1ccccc1OC1CCN(CC 1)Cc1cccc(CCN)c1 | 39780332 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 1349 | Cc(cc1)ccc1C1=CSSC1=S | 40467 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1350 | CN(C)c1ccc(cc1)Nc1nc(cs 1)c1ccc(cc1)OC | 4112-3682 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1351 | Cc1nc2CNCCc2c(NCCc2c sc(c3cccnc3)n2)n1 | 41602213 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1352 | Cc1ccc(C)c2c1c(cc(CNCC N1CCNC1=O)n2)O | 41769850 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1353 | C1CC(CC2CC2) (CN(C1)C1CSCCSC1)CO | 42006513 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1354 | COc1ccc2cc(ccc2c1)C1CN (CCO1)C(c1cc(N) [nH]n1)=O | 42028139 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1355 | C(Cn1cc(C(NCc2nc(c3ccc 4c(c3)OCO4)on2)=O)nn1) N | 42165233 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1356 | Cc1ccc(cc1[Cl])c1nc2cc(c cc2o1)N | 4269-3090 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1357 | Cc1cc(C)c2c(c1)c(cc(C)n2  )Nc1ccc(cc1)C(=O)OC | 4358-4481 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1358 | Cc1c(c2csc(Nc3ccccc3)n2) n2cccnc2n1 | 4469-0267 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1359 | Cc1c(cccc1[Cl])Nc1nc(cs1  )c1c(C)nc(N)s1 | 4469-0741 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1360 | Cc(cc1)cc(S(N) (=O)=O)c1/N=N/  c(cc1)c(C)cc1N | 45527 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1361 | C(CNc1cccnc1)CNc1c2ccc cc2nc(CCN)n1 | 47488116 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1362 | Cc1ccsc1CN(CCN(C)C)C( CN)=O | 47645371 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1363 | CCN1C(NC(C12CCN(CC 2)Cc1cc2CNCCCn2n1)=O  )=O | 47670564 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1364 | C1CN(CC=C1)c1c2CCN(  CCc2nc(c2ccco2)n1)C(CN  )=O | 47825811 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1365 | C(CCNc1c2c3CCCCc3sc2 ncn1)CCO | 4789-3834 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1366 | CC(C)Cc1ccc(cc1)c1c2C( C(C#N)=C(N)Oc2[nH]n1)  c1ccco1 | 4817-0239 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1367 | C(CN)CN1C(CC[C@H]2 CN(CC[C@@H]12)C(CCc  1ccco1)=O)=O | 48226996 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1368 | CCCCCCCCNc1cccc(c1) [Br] | 5117451 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1369 | Cc1nc2cc(c(cc2n1CCCO) [Cl])[Cl] | 5119828 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1370 | c1cc(c(cc1c1ccc(c(c1)N)N  )N)N.O.O.[Cl].[Cl].[Cl]. [Cl] | 5140900 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1371 | c1cc(ccc1c1c(c2ccc(cc2)F) nc2cc(ccc2n1)Oc1ccc(cc1) N)F | 5174475 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1372 | CCCCCc1ccc(cc1)c1ccc(c c1)c1ncc(cn1)N | 5213078 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1373 | c1ccc2c(ccc(c2c1)Oc1ccc( cc1[Cl])N)[Cl] | 5215844 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1374 | c1cc(ccc1c1cc(C(NN)=O)c | 5350878 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | 2cc(ccc2n1)[Br])N |  |  |  | CGCUG(m6A)CGGUACA |  |
| 1375 | Nc(cc1)ccc1NC(c(cc1)ccc 1C(Nc(cc1)ccc1N)=O)=O | 55152 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1376 | COc(cn1)c(Nc(cc2)ccc2C# N)nc1SC | 55453 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1377 | Brc(cc1)ccc1-c1csc(/ N=C2/  SC=C(c(cc3)ccc3Br)N2)n1 | 55691 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1378 | CCCc1ccc(cc1)c1ccc(cc1) C(N1CCC(CN)C1)=O | 56240352 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1379 | [H]N([H])c1nc(n[nH]1)SC CCCCCCCC | 5655427 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1380 | C(=Cc1ccc(cc1[Cl]) [Cl])C(c1cccc(c1)N)=O | 5689908 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1381 | CCNC(Cc1ccc(cc1)c1cc2C C(CN)Oc2c(c1)[Cl])=O | 57980040 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1382 | C(c1ccc(cc1)c1ccccc1)NC( [C@@]12CNC[C@H]2C NC1)=O | 58024175 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1383 | Cc1nc2CNCCc2c(NCCOC  c2ccc(cc2)[Cl])n1 | 58315365 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1384 | C(c1c(cc(c2ccc(cc2)F)nc1 N)c1cccnc1)#N | 6233-1975 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1385 | C(c1c(cc(c2ccc(cc2) [Br])nc1N)c1ccco1)#N | 6233-2517 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1386 | CCOc1cc(CO)cc(c1OCc1c cc(cc1)C(O)=O)[Br] | 6415-0035 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1387 | C(c1cc(ccc1OCc1ccc(cc1) C(O)=O)[Cl])O | 6415-0097 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1388 | Cc1cccc2c1c(ccc(C(C=C1)  =O)c3C1=O)c3n2C | 645330 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1389 | O=C(c(cc1)cc(C(Nc(cc2)c cc2C2=NCCN2)=O)c1Cl)  Nc(cc1)ccc1C1=NCCN1 | 67436 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1390 | CC(c1cnc(Nc2nc(C)c3cccc (C)c3n2)nc1C)=O | 6809-0295 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1391 | CC1(C)Cc2c(CO1)c(c1ccc o1)nc1c2c2c(c(NC3CCCC C3)ncn2)s1 | 6940-0105 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1392 | Nc1cc(N=[N+]  (c2c(C3)ccc(N)c2) [O-])c3cc1 | 70534 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1393 | COc1ccc(cc1OC)c1cc(c2n nc(N)o2)no1 | 7213-0562 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1394 | C(c1cccs1)Nc1ccc2c(c1)nc (c1ccc(cc1)[Cl])o2 | 7629-1287 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1395 | C1CC2=C(C(C1)=O)C1(C (C#N)=C(N)O2)C(Nc2ccc cc12)=O | 8003-4618 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1396 | CC[Ge](CC)  (CC)c1c(CNCc2ccccc2) [nH]nn1 | 8004-6298 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1397 | CC[Ge](CC)  (CC)c1c(CNc2ccccc2) [nH]nn1 | 8005-7257 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1398 | C(C(c1ccc(cc1) [Cl])=O)Sc1nc2ccc(cc2s1) N | 8007-4809 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1399 | C1CCC(CCNC2CC(N(C2  =O)c2ccc(cc2)F)=O)=CC1 | 8013-1383 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 1400 | Nc(cc1)cc(Cc2c3)c1- c2cc(Cl)c3Cl | 80141 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1401 | CC1(C)Cc2c(ccc3ccccc23) C(=N1)Sc1ccc(cc1)N | 8015-2089 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1402 | C(c1ccc2c(c1)OCO2)Nc1c (c[nH]n1)C(N)=O | 8018-4095 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1403 | CC(C1(CCCCC1)N)=O | 8018-6357 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1404 | c1cc(N)nc2c1ccc(n2)O | 8019-7722 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1405 | C(c1cn[nH]c1c1ccc(cc1)F) N | 8020-0151 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1406 | c1cc(cc(c1) [Cl])c1nc(c2ccc(cc2)N)n[n H]1 | 8020-5002 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1407 | Cc1c2[nH]c(cccc3)c3c2ccc 1CCN | 81703 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1408 | C(CN)c1nnc(o1)SCc1c(ccc c1[Cl])[Cl] | 8388-1008 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1409 | [H]N([H])c1c2c3CC(C)  (C)OCc3sc2nc(n1)SCc1cc ccc1[Cl] | 8640-0360 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1410 | O=C1ONC(C(C(C(F)(F)F)  (F)F)(F)F)=N1 | 88349 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1411 | C1CN(CCN1Cc1ccccc1)C 1CS(CC1O)(=O)=O | 9195475 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1412 | S=C1Oc(ccc(- c2ccccc2)c2)c2N1 | 93817 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1413 | CCOC(c1cnc2c(cccc2c1Nc 1ccc(C)cc1[Br])OC)=O | C053-0427 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1414 | CSc1c(c(N)n(Cc2ccccc2)n 1)S(c1ccccc1)(=O)=O | C200-4138 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1415 | CCOc1ccc(c(c1)Nc1cc(C) nc2nc(C)nn12)OCC | C301-0909 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1416 | Cc1ccc(c(c1)Nc1nc2ccccc 2c2nncn12)OC | C301-5171 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1417 | CCOC(N1CCC(CC1)N1C(  c2ccccc2C1=O)Nc1cc(cc(c 1)C(=O)OC)C(=O)OC)=O | C429-0358 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1418 | Cc1cc(NCc2ccc(cc2)F)n2c (c(c3ccc(c(c3)OC)OC)c(C) n2)n1 | C535-0529 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1419 | CCOc1ccccc1NC(c1c(CO) nccn1)=O | C612-0892 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1420 | c1ccc2C(N(C(c2c1)Nc1ccc cc1F)c1ccc(cc1)[Cl])=O | C614-0363 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1421 | CCOC(C1CCN(CC1)C1= C(C(C1=O)=O)NC(C)c1cc  ccc1)=O | C667-0210 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1422 | C1CCCN(CC1)CCCNc1nc  2ccccc2c2nc(c3ccccc3)nn1 2 | C736-0159 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1423 | C1CC(N(C1)CCCNc1nc2c  cccc2c2nc(c3cccnc3)nn12)  =O | C736-0199 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1424 | Cc1cc(C)n(CCc2nc3c4ccc cc4nc(NC4CCN(CC4)Cc4  ccccc4)n3n2)n1 | C736-0369 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1425 | C1Oc2ccc(cc2O1)Nc1c(cn c2ccc(cc12)F)S(c1ccccc1) | C769-2045 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | (=O)=O |  |  |  |  |  |
| 1426 | C(CNCc1ccc(C(O)=O)s1)c  1ccc(cc1)[Cl] | C863-0011 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1427 | Cc1c(CCC(Nc2cccc(c2)C( F) (F)F)=O)c(C)n2c(n1)nc(C N)n2 | C908-0403 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1428 | Cc1c(CCC(Nc2ccc(cc2) [Br])=O)c(C)n2c(n1)nc(C N)n2 | C908-0436 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1429 | Cc1c(CCC(Nc2ccc(c(c2) [Cl])F)=O)c(C)n2c(n1)nc( CN)n2 | C908-0501 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1430 | Cc1c(CCC(Nc2ccc(CN3C CCCC3)cc2)=O)c(C)n2c(n 1)nc(CN)n2 | C908-0509 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1431 | Cc1c(CCC(Nc2cccc(c2) [Br])=O)c(C)n2c(n1)nc(C N)n2 | C908-0523 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1432 | Cc1c(CCC(Nc2ccccc2OC)  =O)c(C)n2c(n1)nc(CN)n2 | C908-0524 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1433 | Cc1c(CCC(NCC2CCN(CC  2)Cc2ccccc2F)=O)c(C)n2c (n1)nc(CN)n2 | C908-0547 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1434 | c1ccn2c(C(c3ccc(cc3) [Cl])=O)c(c(C(Nc3cccc(c3  )F)=O)c2c1)N | D033-0008 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1435 | CC(C)c1ccc(CNc2nc3nc(C  )c(c(C)n3n2)[Cl])cc1 | D043-0278 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1436 | Cc1ccc2c(c1)C(C1=C(C(N (CCCO)C13C(N(CC=C)c1 ccccc13)=O)=O)O2)=O | D063-1068 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1437 | Cc1ccc2c(c1)C(C1=C(C(N (CCO)C13C(N(CC=C)c1c cccc13)=O)=O)O2)=O | D063-1117 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1438 | C=CCN1CC(C(=C1N)c1n  c2ccccc2[nH]1)=O | D086-0388 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1439 | CC(c1ccc(cc1)Nc1cc(c2cc ccc2)nc(C)n1)=O | D278-0527 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1440 | [H]N(Cc1ccccc1)c1c2c(csc 2ncn1)c1ccc(C)cc1 | D341-0419 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1441 | Cc1ccc2c(c1)cc(c(NCc1cc ccc1)n2)c1nc(C)on1 | D420-1964 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1442 | CCNc1c(C#N)nc(c2ccc(cc 2)S(N2CCOCC2) (=O)=O)o1 | D434-0668 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1443 | C(CO)NC(C1C=COc2ccc( cc2C=1)[Br])=O | D443-0435 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1444 | CCCCCCNc1cc(c2ccccc2) nc2nc(c3cccnc3)nn12 | D494-0421 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1445 | C1CCC(C1)Nc1cc(c2ccccc 2)nc2nc(c3cccnc3)nn12 | D494-0439 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1446 | Cc1cc(NCC(N2CCN(CC2)  c2ccc(cc2)F)=O)n2c(n1)nc (c1cccnc1)n2 | D494-0506 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1447 | Cc1ccc(cc1C)S(N1CCN(C C1)c1cc(C)nc(NC2CCCC C2)n1)(=O)=O | D637-0036 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1448 | [H]N(CCc1ccc(cc1)S(N)  (=O)=O)Cc1ccc(c2ccc(cc2  )[Cl])o1 | D665-0262 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 1449 | [H]N(Cc1ccco1)Cc1ccc(c2 cccc(c2)[Cl])o1 | D665-0395 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1450 | CCC(CO)NCc1ccc(c(c1)O C)OCc1ccc2c(c1)N(C)C(N 2C)=O | D666-0065 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1451 | Cc1cccc(CNc2c(cc3cccc(C  )c3n2)c2nc(C)on2)c1 | D704-0068 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1452 | Cc1ccc2c(c1)cc(c(NCc1cc c(cc1F)F)n2)c1nc(C)on1 | D704-0959 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1453 | Cc1ccc2c(c1)cc(c(NCc1cc c(cc1[Cl])F)n2)c1nc(C)on1 | D704-0989 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1454 | COc1ccc(cc1)c1csc(C2=C( N)N(CC2=O)C2CCCCCC C2)n1 | D715-1979 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1455 | CCOC(c1cnc2c(c3ccc(cc3) [Br])c(C)nn2c1N)=O | D718-0691 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1456 | CCc1cccc(C)c1NS(c1cc(cn c1N)[Br])(=O)=O | E138-2120 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1457 | COC(c1ccc(cc1)NS(c1cc(c nc1N)[Br])(=O)=O)=O | E138-2198 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1458 | CCC(C)NC1=C(C(C1=O)  =O)c1ccc(cc1)C(C)C | E511-0764 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1459 | CC(C)c1ccc(cc1)C1=C(C( C1=O)=O)NCc1ccccc1OC | E511-0865 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1460 | CC(C)c1ccc(cc1)C1=C(C( C1=O)=O)NCc1ccc(cc1)N (C)C | E511-0981 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1461 | CCSc1c2Cc3c(CO)cnc(C)c 3Oc2nc(c2cccc(c2)[Cl])n1 | E544-0227 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1462 | CC1Cc2cc(ccc2N1C(C1C C1)=O)S(N(CCO)Cc1cccc c1)(=O)=O | E570-0206 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1463 | CC(C)c1ccc(cc1)n1c(c(c2n c(c3ccc(cc3) [Cl])no2)nn1)N | E595-0345 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1464 | COc1ccc(c(c1)c1nc(Nc2cc c(cc2F)F)on1)OC | E679-0017 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1465 | CCCNC1=C(C(C1=O)=O)  c1cc(C)c(C)cc1C | E882-0500 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1466 | CCOC(Nc1ccc(NCc2ccc(c c2)F)nc1N)=O | NCGC0001545 1-06 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1467 | C(CCCN=C(N)N=C(N)Nc  1ccc(cc1) [Cl])CCN=C(N)N=C(N)N  c1ccc(cc1)[Cl] | NCGC0001624 6-12 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1468 | Cc1c(C(c2ccc(cc2)OC)=O) c2ccc(cc2n1CCN1CCOCC 1)I | NCGC0002501 2-02 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1469 | C1CN1P(N1CC1) (N1CC1)=S | NCGC0009504 2-08 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1470 | C(C(Cn1cncn1) (c1ccc(cc1F)F)O)n1cncn1 | NCGC0009508 9-11 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1471 | CC(C)=CC[C@H] (C1=CC(c2c(ccc(c2C1=O) O)O)=O)O | NCGC0016348 9-04 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1472 | C(C(O)=O)O.[N-].[N-]. [Pt++] | NCGC0018115 2-01 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1473 | C1CCN(C1)CCOc1ccc2cc 1COC/C=C\  CCOc1cccc(c1)c1ccnc(N2) n1 | NCGC0024934 6-02 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 1474 | Cc1c2cc(ccc2n[nH]1)c1cc( cnc1)OC[C@H] (Cc1ccccc1)N | NCGC0026314 7-01 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1475 | C(C(Nc1ccc(cc1)n1c(cc(C( F)  (F)F)n1)c1ccc2c(ccc3ccccc 23)c1)=O)N | NCGC0034649 0-01 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1476 | C([C@@H]1[C@@H] ([C@H]([C@H]([C@H] (OC[C@@H]2[C@@H] ([C@H]([C@H]([C@H] (O[C@@H] (C#N)c3ccccc3)O2)O)O)O  )O1)O)O)O)O | NCGC0034658 3-01 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1477 | CC1(C)CC(c2c(C(F)  (F)F)nn(c3ccc(C(N)=O)c(c 3)NC3CCC(CC3)OC(CN)  =O)c2C1)=O | NCGC0034664 0-01 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1478 | C1CCN(C1)C(Nc1cccc(c1  )Nc1ncc(c(NCCc2cnc[nH] 2)n1)[Br])=O | NCGC0034668 7-01 | RRE2B\_MeA | Hairpin | UGGGCGCAGUGUCAUUG(m6A) CGCUG(m6A)CGGUACA | 1 |
| 1479 | CCN(CC)CCOC(c1ccc2c(  c1)sc(NC(c1ccc(cc1)N)=O  )n2)=O | 0812-1025 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1480 | O=C(NCCCN1CC1)Nc1cc  cc2ccccc12 | 101298 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1481 | CC(NS(c(cc1)cc2c1sc(C)n 2)(=O)=O)=O | 122385 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1482 | COc1ccc(CC(N2CCC(CC2  )C(Cc2ccccc2)O)=O)c(c1) OC | 12362879 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1483 | Cc1csc2c(ncnc12)N1CCC( CC1)NCC1=CNC(NC1=O  )=O | 12466595 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1484 | Cc1cc(cc2c(ccnc12)N1C[C @H](C2CC2)[C@H]  (C1)N)[Cl] | 12605761 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1485 | C1CN(Cc2ccccc12)c1c2C CNCc2nc(c2cccnc2)n1 | 12634687 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1486 | C1C(CN1Cc1ccc(cc1)OC CO)Oc1ccccc1[Cl] | 13202927 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1487 | CC(COC)NCc1cc(c2ccc(c c2)OC)on1 | 14208909 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1488 | CNC=C1C=C(c2ccccc2)N( C)C1=S | 1457-0011 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1489 | C1CN(Cc2cnc(NCc3ccccc 3)nc2)C[C@@H]  ([C@H]1CO)O | 14588562 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1490 | CC(C) (C)c1cc(CN(C)c2c3CCNC  c3nc(c3cccnc3)n2)[nH]n1 | 14923635 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1491 | Cc1ccccc1C(N1CCOC2(C NCCOC2)C1)=O | 15132958 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1492 | C1CCN(C1)Cc1cc(c2cn(C  C(c3ccc(cc3)O)O)nn2)sc1 | 15805022 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1493 | C=Cc1ccc(nc1)N1CCN(C C(C1)O)Cc1ccccc1 | 17524156 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1494 | CN(Cc1ccc2c(c1)nccn2)C( c1cn(CCN2CCNCC2)nn1)  =O | 17862547 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1495 | C1CC(CNC1)c1cc(c2ccc(c (c2)[Cl])[Cl])nc(c1C#N)N | 17917068 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 1496 | C(COc1ccc(cc1)c1cc(c2cc c[nH]2)nc(c1C#N)N)n1ccn c1 | 18432747 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1497 | C1CN(CCN1Cc1ccc(cc1) C(O)=O)Cc1ccccc1CO | 19125330 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1498 | Cc1cc(C)c2c(c1)c(cc(C)n2  )C(N[C@H]1CNC[C@@ H]1OC)=O | 19537511 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1499 | O=C1OCC/C1=C\ NCCCCCCCCN/C=C(\ CCO1)/C1=O | 197008 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1500 | CNCCN1C(CC[C@H]2C N(CC[C@@H]12)Cc1cnn( C)c1)=O | 19798067 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1501 | CN(Cc1cnn(c1)c1ccc(cc1) F)C(C(c1ccc(cc1)F)O)=O | 19840417 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1502 | CC1(CCNCC1)C(N1CCc2  c(C1)c(c1ccc(cc1) [Cl])n[nH]2)=O | 20251729 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1503 | Cn1cncc1c1cccc2CC(CN) Oc12 | 21885438 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1504 | C1CCN(CC1)C(CNC(CCc  1cc2CNCCn2n1)=O)c1ccc nc1 | 21900063 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1505 | C1CCCN(CC1)C[C@@H] 1CN(C[C@@H]1CO)C(c1 cc(N)[nH]n1)=O | 22664850 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1506 | CSCCc1nc([C@@H]2C[C  @H] (CN2)O)n(c2ccc(c(c2)[Cl]) [Cl])n1 | 22714385 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1507 | C1CCN(CC1)Cc1cccc(c1)  n1ccnc1c1cc2CNCCCn2n1 | 26875627 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1508 | Cc1ccc(C)c(c1)NCc1cc(cc c1OC)[Br] | 2910-2364 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1509 | O=C(N(CC1OC1)C(N1CC 2OC2)=O)N(CC2OC2)C1  =O | 296934 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1510 | CCOC(/C(/ C1=CSC2=NNC(C) (C)N12)=N\O)=O | 299968 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1511 | C1CCCN(CCC1)CC(N1C[  C@H](c2ccccc2)[C@H] (C1)N)=O | 31891223 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1512 | CN(C)c1c2CCN(Cc2nc(c2 cccnc2)n1)C(C1(CCC1)N)  =O | 32350946 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1513 | COCc1nc(CCNC(CCc2cc3 CNCCn3n2)=O)on1 | 32552243 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1514 | Cc1nc(CN)cc(n1)N1CCC(  CC1)C(c1nccn1C)O | 32807865 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1515 | Cc1cc(cnc1n1cnnc1)c1ccc c2CNCCc12 | 34452990 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1516 | COc1ccc2ccc(cc2c1)OCc1 nc(co1)C(NCc1cccnc1N)= O | 35061195 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1517 | Cc1cccc(c1)Nc1nc(CN2C[ C@@H]3CC[C@H] (C2)N(C)C3=O)nc(N)n1 | 35485871 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1518 | COc1ccc(CNCc2ccc(cc2)F  )cc1 | 3702-0995 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 1519 | COc1ccccc1CNCc1ccc(cc 1)C(F)(F)F | 3702-1158 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1520 | COc1cccc(CNCc2ccccc2C (F)(F)F)c1OC | 3702-1702 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1521 | Cc1c2ccccc2n(CC(CNc2cc c(cc2)[Br])O)c1C | 3744-0008 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1522 | Cc1ccc(C)c(c1)NCC(Cn1c (C)c(C)c2ccccc12)O | 3744-0052 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1523 | CCC(CO)NCC(CN1c2cccc  c2Sc2ccccc12)O | 3746-0114 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1524 | CC(Nc1cccc(c1)c1ccc(c(c1  )F)NC(CN)=O)=O | 40118252 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1525 | Cc1ccc(cc1)S(N(CC(CN1 CCCCC1)O)c1ccccc1OC) (=O)=O | 4013-2178 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1526 | Cc1c(c2csc(Nc3ccc(cc3) [Cl])n2)n2ccccc2n1 | 4112-3380 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1527 | Cc(cc1)cc(S(N) (=O)=O)c1/N=N/  c(cc1)c(C)cc1N | 45527 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1528 | CSC(NC(Cl)=C1)=NC1=O | 45719 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1529 | [H]N(c1ccccc1[Cl])c1nc(C  )c(C(=O)OCC)s1 | 4576-0043 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1530 | COc1ccc(c(c1)OC)c1csc(N CC=C)n1 | 4640-0152 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1531 | Cc1cnc(N)nc1NCC[C@@ H]1C[C@H]2C[C@@H]1 C=C2 | 47913504 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1532 | Cc1nc2cc(c(cc2n1CCCO) [Cl])[Cl] | 5119828 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1533 | CCN(CC(COc1ccc2ccccc2 c1)O)S([O-])(=O)=O.[K+] | 5173055 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1534 | CCOC(c1cnc2ccccc2c1Nc 1ccc(cc1)N1CCOCC1)=O | 5174-4348 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1535 | C1CCN(CC1)Cc1c(CN2C  CCCC2)n(c2c(N)non2)nn1 | 5175780 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1536 | C(CCN=Cc1ccccc1N)CN= Cc1ccccc1N | 5233844 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1537 | c1ccc2c(c1)ccc(c2[Cl])Sc1 ccc(cc1[Cl])N | 5250905 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1538 | C1CC[N+] (CC1)CCCCCSc1ccc(cc1) O.[O-][Cl](=O)(=O)=O | 5251615 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1539 | Cc1cc(C)n(c2cc(NCCO)nc n2)n1 | 5256691 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1540 | COc1ccc(cc1)OCC(CN1C CN(CC1)c1ccccc1)O.[Cl]. [Cl] | 5257916 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1541 | C1CC(N(CNc2ccc(c(c2) [Cl])[Cl])C1=O)=O | 5271658 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1542 | CC(C) (C)NCC(Nc1c2CCCCc2nc 2CCCc12)=O.C(O)=O.C(C (O)=O)(O)=O | 5284047 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1543 | COc1c(c(c(c(c1F)F)c1csc( N)n1)F)F | 5300-0134 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1544 | CCCCOc1ccc(CSCCN)cc1  .[Cl] | 5343258 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 1545 | C(C(NN)=O)Nc1ccc(cc1[ Br])[Cl] | 5345379 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1546 | Cc1cc(ccc1NCC(NN)=O)I | 5346837 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1547 | Cc1cc(ccc1NCC(NN)=O) [Cl] | 5347228 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1548 | CCOC(CNc1ccc(cc1C) [Cl])=O | 5350316 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1549 | CCCCNc1c2c(c3c4CCCCc 4c(nc3s2)N2CCOCC2)nnn 1 | 5504-0161 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1550 | CCOc1cc(CNCCc2cccc(c2  )F)ccc1OC | 5571711 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1551 | C1CCc2c(C#N)c(N)sc2CC 1 | 5574569 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1552 | COc1ccc(cc1CN1CCC(CC 1)N1CCN(CC1)CCO)[Br] | 5607-0223 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1553 | C=CCC(CC=C)  (c1ccc(cc1)C(CC=C) (CC=C)N)N | 5654685 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1554 | C(C(Cn1c2ccccc2c2ccccc1 2)O)NNC(c1ccccc1)=O | 5718973 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1555 | COC(CCCCC1C(C(CS1)N  )N)=O.[Br].[Br] | 5728434 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1556 | Cc1cc(ccc1OCCNCCCOC  )[Cl].C(C(O)=O)(O)=O | 5734342 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1557 | C(CN1CCOCC1)C(Nc1cc  c(cc1C(c1ccccc1)NCC(NN  )=O)[Br])=O | 5808034 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1558 | CC1(C)CC(CCO1)C(CCN  Cc1ccc(cc1)N(C)C)c1cccc c1 | 5936315 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1559 | Cc1ccc(c(C)c1)OCC(CN1 CCN(CC1)CCN1C(c2cccc 3cccc(C1=O)c23)=O)O. [Cl].[Cl] | 6044718 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1560 | c1ccc2c(c1)cc1cnc3c(c(N) n[nH]3)c1n2 | 6051011 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1561 | OC(Cc(sc(O)n1)c1O)=O | 60548 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1562 | CN(C)c1ccc(CNC2CCCC  C2)cc1 | 6117-0178 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1563 | CCCOC(c1c(csc1N)c1ccc( c(c1)OC)OC)=O | 6131187 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1564 | C1CCCCCc2c(CCCC1)c( C(N)=O)c(N)s2 | 6132195 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1565 | CCSCCC(C(O)=O)NC1C C(C)(C)CC(C=1)=O | 6254-0021 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1566 | CCOC(C(C(c(cccc1)c1N1) C1=O)=O)=O | 646976 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1567 | CCOc1ccc(cc1)NCc1nc2cc ccc2n1C | 6524406 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1568 | O=C(c(cc1)cc(C(Nc(cc2)c cc2C2=NCCN2)=O)c1Cl)  Nc(cc1)ccc1C1=NCCN1 | 67436 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1569 | CCC1CCCCN1S(c1ccc(cc 1)NC1c2ccccc2S(N=1) (=O)=O)(=O)=O | 7380-0010 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1570 | Cn1c(cnc1NCc1ccc(cc1) [Br])c1cccc(c1)OC | 7756-0390 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 1571 | Cn1c(cnc1NCc1ccccc1[Cl]  )c1cccc(c1)OC | 7756-0396 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1572 | Cn1c(cnc1NCc1ccccc1OC  )c1ccccc1 | 7756-0545 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1573 | CCOc1ccc(cc1)c1cnc(NCc 2ccccc2OC)n1C | 7756-0840 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1574 | CC(CNCCNCc1cc(c(c(c1) [Br])OC)OC)O.[Cl].[Cl] | 7971888 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1575 | C(CN)CN1CCN(CC1)c1cc  ccc1 | 7974015 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1576 | Cc1ccc(cc1C)Nc1nc(cs1)c 1ccc(c(c1)F)OC | 8005-2731 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1577 | Cc1ccc(C)c(c1)c1csc(Nc2c cccc2OC)n1 | 8006-1580 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1578 | Cc1ccc(cc1)C1C(C#N)=C(  N)Oc2ccc3ccccc3c12 | 8008-9298 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1579 | [H]Nc1nnc(COc2cc(C)cc( C)c2)s1 | 8009-2828 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1580 | [H]Nc1nnc(COc2ccc(cc2) C2CCCCC2)s1 | 8009-2831 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1581 | COc1ccc(c(c1)NC(CSc1nc 2ccc(cc2s1)N)=O)OC | 8009-2885 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1582 | C1CCN(CC1)c1ccc2C(N( CCO)C(c3cccc1c23)=O)= O | 8010-2208 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1583 | CC1=CC(N(C)C(N1CCCC CCNCCO)=O)=O | 8012-3983 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1584 | Cc1c(CCNCc2c(cc(cc2OC  )OC)OC)c2cc(ccc2[nH]1) OC | 8013-0022 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1585 | Cc1c(CCNCc2ccc(C#N)cc 2)c2cc(ccc2[nH]1)OC | 8013-2954 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1586 | COc1nc(NCCC2CCCCC= 2)nc(n1)N1CC2CC(C1)C1  =CC=CC(N1C2)=O | 8014-8886 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1587 | CC(C)C1(CCNCc2ccc(cc2  )OC)CCOC(C)(C)C1 | 8018-1266 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1588 | CC(C)C1(CCNCc2cccc3c2 OCO3)CCOC(C)(C)C1 | 8018-1268 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1589 | COCc1nc(c2c(N)non2)no1 | 8018-8577 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1590 | C(CS(N1CCNCC1) (=O)=O)N | 8018-8721 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1591 | c1cc(N)nc2c1ccc(n2)O | 8019-7722 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1592 | CCOC(C1=C(c2ccccc2S1(  =O)=O)N)=O | 8019-8616 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1593 | c1cnccc1c1nc2ncnc(N)n2n 1 | 8020-2786 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1594 | CN1CCCc2ccc(cc12)N | 8020-4281 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1595 | C[C@]1(C)Cc2c(CO1)c(c  1ccco1)nc1c2c2c(c(NCCC N(C)C)ncn2)s1 | 8640-0613 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1596 | COc(cc1)cc(N2)c1NP2(Oc 1ccccc1)=S | 88402 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1597 | CCC(C)C(c1nnc(o1)SCC(c  1ccc(cc1)[Cl])=O)N.[Cl] | 9134179 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1598 | C(c1cccnc1)Nc1cccc(c1)c1 | 9142557 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | nc2ccccc2[nH]1 |  |  |  | ACUCUGGGAGA |  |
| 1599 | C1CN(CCC1c1nc2ccccc2s 1)C1CS(CC1O)(=O)=O | 9195478 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1600 | Cc1ccc2c(N)n[nH]c2n1 | 9195712 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1601 | Cn1c(c2c(c3cccnc3s2)N)n nc1S | 9221247 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1602 | CCN1CCCC1CNCc1cccc(  c1)OCc1ccc(cc1)[Cl] | 9312203 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1603 | c1ccc2c(c1)nc(c1ccc(cc1[ Cl])N)s2 | C066-5322 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1604 | Cc1cccc(c1)NCc1nc2ccccc 2n1C | C147-0043 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1605 | CC1CCN(CC1)c1nc(c(C(= O)OC)s1)N | C201-1740 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1606 | CCc1nc2nc(C)cc(Nc3cc(cc c3C)[Cl])n2n1 | C301-3944 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1607 | Cc1cc(C)n2c(c(c3ccc(C)s3  )nc2n1)Nc1ccc2c(c1)OCC O2 | C325-0312 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1608 | CCOC(C1CCN(CC1)C1= C(C(C1=O)=O)NCCCN1C CCCC1)=O | C667-0368 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1609 | Cc1c(CCC(Nc2cccc(c2)C( F) (F)F)=O)c(C)n2c(n1)nc(C N)n2 | C908-0403 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1610 | CCOC(c1ccc(cc1)NC1c2c( cccn2)C(N1c1ccc(C)cc1)= O)=O | C999-1176 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1611 | CC(C)c1ccc(C)cc1OCCCn 1c2ccccc2nc1C(C)O | D011-5386 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1612 | COC(CCc1c(c2ccc(cc2)O C)nc(Nc2ccccc2)s1)=O | D041-0023 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1613 | [H]c1ccc(cc1)S(c1c(NCC OC)oc(c2ccccc2)n1) (=O)=O | D072-0501 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1614 | COCCNc1c(nc(c2ccc(cc2) [Cl])o1)S(c1ccccc1) (=O)=O | D072-1517 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1615 | CN1C(c2c(cn(c3cccc(c3)N  )c2c2ccc(cc2) [Cl])N(C)C1=O)=O | D077-0219 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1616 | Cc1ccc2c(c1) [nH]c(C1=C(N)N(CC1=O)  c1ccc(cc1)F)n2 | D086-0081 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1617 | CCCOc1cccc(c1)C1c2c(c3 cc(C)ccc3O)n[nH]c2C(N1 CCCO)=O | D126-0083 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1618 | C(CNc1c(C#N)nc(C=Cc2c cc(cc2)F)o1)CN1CCOCC1 | D151-0242 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1619 | C1CC(CNc2c(C#N)nc(C=  Cc3ccc(cc3)F)o2)OC1 | D151-0248 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1620 | Cc1cccc(Cn2c3ccccc3nc2 CCNC(CCCO)=O)c1 | D186-0280 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1621 | Cc1cc(N(CCO)CCO)n2c(n  1)nc(Cc1ccccc1)n2 | D245-0529 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1622 | CN1C(N(C)c2cc(ccc12)C(  COc1ccc(CNCCc2ccc(cc2) F)cc1)O)=O | D300-0304 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 1623 | CC1(C)CC(CCO1)CNCC N(C)C | D324-0105 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1624 | CCN(CC)CCNCC1CCOC( C)(C)C1 | D324-0106 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1625 | CC1(C)CC(CCO1)CNCC CN(C)C | D324-0107 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1626 | CCN(CC)CCCNCC1CCO C(C)(C)C1 | D324-0108 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1627 | [H]N(Cc1ccc(cc1)OC)c1c2 c(csc2ncn1)c1ccccc1 | D341-0323 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1628 | [H]N(Cc1ccccc1)c1c2c(csc 2ncn1)c1ccc(C)cc1 | D341-0419 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1629 | CCCC(c1nc2ccccc2n1CC Oc1ccc(cc1)[Cl])O | D347-4130 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1630 | CC(C)CNc1nc(nc(n1)n1cn c(n1)SCc1ccccc1)N(C)C | D385-0105 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1631 | C1CCN(CC1)C(c1cccc(c1)  Nc1c(c2ccccc2)nc2cnccn1 2)=O | D401-0331 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1632 | Cc1ccc(cc1)Nc1cc(nc(C)n 1)N1CCN(CC1)C(c1cccs1  )=O | D430-0262 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1633 | CC1(C)CC(CCNCc2ccc3c (c2)OCO3)  (CCO1)c1ccccc1OC | D442-0097 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1634 | Cc1cccc(c1)c1cc(Nc2cccc( c2)C(F)(F)F)nc(C)n1 | D482-1812 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1635 | [H]C([H]) (CC)c1cc(NCCCC)n2c(n1)  nc(c1cccnc1)n2 | D494-0181 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1636 | COc1ccc(Cc2nc3ccccc3n2 CC(COc2ccccc2)O)cc1 | D510-0832 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1637 | Cc1cccc(C)c1OCC(Cn1c2 ccccc2nc1C1CC(N(C1)c1c ccc(c1)OC)=O)O | D510-0970 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1638 | CCNc1nc(C)cc(n1)N1CC N(CC1)S(c1ccc(cc1)[Cl]) (=O)=O | D575-0012 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1639 | [H]N(CCN(CC)CC)Cc1cc  c(c2ccccc2)o1 | D665-0049 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1640 | Cc1ccc2cc(c(NCc3cc(ccc3 F)F)nc2c1)c1nc(C)on1 | D704-0252 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1641 | Cc1nnc2c(Nc3cccc(c3)C(F  )(F)F)nc3ccccc3n12 | E208-0090 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1642 | COc1ccc2c(CNCc3ccccc3) c(C(O)=O)[nH]c2c1 | E518-1228 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1643 | CCOc1ccc(cc1)c1nc(c2c(N  )n(c3ccccc3[Cl])nn2)on1 | E595-0516 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1644 | C1CN1P(N1CC1) (N1CC1)=S | NCGC0009504 2-08 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1645 | C(C(Cn1cncn1) (c1ccc(cc1F)F)O)n1cncn1 | NCGC0009508 9-11 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1646 | Cn1cc(cn1)c1cnn2c(c(c([C @H]3CCCNC3)nc12) [Br])N | NCGC0034665 3-01 | Zika\_NS5 | G-quadruplex | GUGGAGGUGGGACGGGAGAG ACUCUGGGAGA | 1 |
| 1647 | CCCCCOc(cc1)ccc1N(C( C(C)CN1)=O)C1=S | 121908 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1648 | C1CCN(C1)C([C@@H]1 C[C@H] (CNC1)C(N1CCN(CC1)c1 | 12190856 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | ccncc1)=O)=O |  |  |  |  |  |
| 1649 | O=C(C1C2)N(CC3)C2C3( c(cccc2)c2N23)C3=C1C= CC2=O | 122253 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1650 | CC(NS(c(cc1)cc2c1sc(C)n 2)(=O)=O)=O | 122385 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1651 | CC[C@H](C)[C@@H] (C(N1CCC(CC1)Cn1cc(C 2CCCC2)nn1)=O)N | 12353320 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1652 | Cc1c(C)nc(nc1N1C[C@@ H](CN2CCCCC2)[C@H] (C1)CO)N1CCCC1 | 12918323 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1653 | CCOC(N(CCc(cc1OC)c2c(  c3c4)c1OC)c2cc3cc(OC)c 4OC)=O | 143241 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1654 | C1C[C@@H]2CCNC[C@  H]1N2c1c2CNCc2nc(c2cc cnc2)n1 | 14601902 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1655 | CCNC([C@@H]1C[C@@ H] (CN1C(CN1CCCCCCC1)  =O)N)=O | 15077405 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1656 | Cc1cc(CNc2nccc(n2)N2C CC(CC2)O)c2c(c1)c(C)c( C)[nH]2 | 15700744 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1657 | Cc1c(C(C(NCCNc2cccnc2  )=O)N)c(C)[nH]n1 | 16899791 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1658 | CC1=CC(=O)Oc2cc(CN3 CCC(CC3)N3CCC(CC3)O  )ccc12 | 18402936 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1659 | CN1CCC2(CC1)CCN(C2) C(C1CNC1)=O | 18597939 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1660 | C(CN)c1ccc(CN2CCC(CC  2)(c2cccc(c2)C(F) (F)F)O)cc1 | 18809502 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1661 | CC(Cc1cc(C)n[nH]1)NCc1 ccc(c(c1)OC)OCCN1CCC C1 | 19048916 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1662 | CC(C)N[C@@H]1CC[C@  @H]1NC(CCc1ccc(c2ccc( cc2)[Cl])[nH]1)=O | 19264424 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1663 | Cc1ccc(cc1)SCCN(C)C([C @H](CCCCN)N)=O | 19395269 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1664 | Cc1ccc(cc1[Cl])N1CCC(C C1)N[C@@H]1CC[C@H] (C1)N | 19498560 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1665 | Cc1cc(C)c2c(c1)c(cc(C)n2  )C(N[C@H]1CNC[C@@ H]1OC)=O | 19537511 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1666 | C1CN(CCNC([C@@H]2C [C@H] (CNC2)C(N2CCOCC2)=O  )=O)c2ccccc12 | 19807864 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1667 | Cc1cc(NC)nc(n1)N1CCN( CC(C1)O)CC(NC)=O | 20331307 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1668 | C1CNCc2c1c(NCC1COc3  ccccc3O1)nc(c1cccnc1)n2 | 20674759 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1669 | Cc1c(CN2CCC3(CC2) [C@H] (C[C@H]3O)OCCN)nc2cc  ccc2n1 | 21179623 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1670 | C1CN(CC1n1ccnc1)c1c2C | 21581365 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | CNCCc2nc(c2ccccn2)n1 |  |  |  |  |  |
| 1671 | CCOC(CSc([nH]1)nc(nc2  Cl)c1nc2Cl)=O | 217913 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1672 | Cc1ccc(c2cc(C(N3CCc4c( C3)sc(N)n4)=O)[nH]n2)s1 | 21799165 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1673 | Cn1cncc1c1cccc2CC(CN) Oc12 | 21885438 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1674 | C1CCN(CC1)C(CNC(CCc  1cc2CNCCn2n1)=O)c1ccc nc1 | 21900063 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1675 | C1CC2(CCNCC2)CCN(C  1)Cc1ccnc2ccccc12 | 22793936 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1676 | C1CN(CC(CN1Cc1cccc2c c[nH]c12)O)c1ccncc1 | 22927120 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1677 | CC(C) (C)c1cc(C=C(C#N)C#N)cc (C(C)(C)C)c1O | 242557 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1678 | CCC[C@@H]1CN(Cc2ccc (CCN)cc2)C[C@H]1NC(C  )=O | 26972514 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1679 | c1cc(c2cccc(c2c1) [Br])c1nc2cc(ccc2o1)N | 2810-4224 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1680 | Cc1ccc(C)c(c1)NCc1cc(cc c1OC)[Br] | 2910-2364 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1681 | O=C(N(CC1OC1)C(N1CC 2OC2)=O)N(CC2OC2)C1  =O | 296934 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1682 | CCOC(/C(/ C1=CSC2=NNC(C) (C)N12)=N\O)=O | 299968 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1683 | Cc1nc(CCN)cc(n1)N1CC N(CC1)c1ccc(C#N)cn1 | 31455775 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1684 | C(CNCc1ccc2c(c1)OCO2)  c1ccc(cc1)F | 3169-1371 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1685 | C1CN(CC1CN)Cc1ccc(c2  ccccc2C#N)o1 | 31727519 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1686 | C1CCCN(CCC1)CC(N1C[  C@H](c2ccccc2)[C@H] (C1)N)=O | 31891223 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1687 | O=C(c(c(F)ccc1)c1F)Nc1n nc(C(F)(F)F)s1 | 319424 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1688 | COc1ccc(CN2CC[C@@H  ]3[C@@H] (CCC(N3CCN)=O)C2)cc1 CC=C | 32030907 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1689 | C1CN(CCN(C1)c1nccc(N)  n1)Cc1ccccc1F | 32148102 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1690 | Sc1nccn1- c(c(Cl)ccc1)c1Cl | 321506 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1691 | COc1ccc(cc1OC)c1nc2cc( ccc2o1)N | 3370-0370 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1692 | CCOc1cc(CNCCc2ccccc2) ccc1OC | 3381-1215 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1693 | Cc1cccc(c1)Nc1nc(CN2C[ C@@H]3CC[C@H] (C2)N(C)C3=O)nc(N)n1 | 35485871 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1694 | Cc1cc2c(ncnc2s1)N1CCC( CC1)NCCNc1cccnc1 | 35687952 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1695 | Cc1ccc(CNCc2ccc(c(c2)O C)OC)cc1 | 3701-0037 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 1696 | COc1cc(CNCc2ccc(cc2)F) cc(c1OC)OC | 3702-0961 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1697 | COc1ccc(CNCc2ccc(cc2)F  )cc1 | 3702-0995 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1698 | CCc1c(cc(c2c3CCCCc3nc( c2C#N)N)s1)[Br] | 3830-0879 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1699 | CC(C1COc2ccccc2O1)NC c1ccccc1 | 3875-0321 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1700 | Cn1c(CCNc2c3CCNCCc3  nc(c3ccccn3)n2)ncn1 | 39769570 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1701 | Cc1ccc(cc1)S(N(CC(CN1 CCCCC1)O)c1ccccc1OC) (=O)=O | 4013-2178 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1702 | C[As](c1cc(C(O)=O)ccc1) (O)=O | 402843 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1703 | Cc1c(c2csc(Nc3ccc(cc3) [Cl])n2)n2ccccc2n1 | 4112-3380 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1704 | Cc1c(C(OC)=O)nc(- c(nc2C(C(N)=C3OC)=O)c cc2C3=O)c(N)c1-  c(ccc(OC)c1OC)c1O | 45384 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1705 | CSC(NC(Cl)=C1)=NC1=O | 45719 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1706 | Cc1ccsc1CN(CCN(C)C)C( CN)=O | 47645371 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1707 | Cc1cnc(N)nc1NCC[C@@ H]1C[C@H]2C[C@@H]1 C=C2 | 47913504 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1708 | C(CNCc1ccc2ccccc2c1)c1 c[nH]c2ccccc12 | 4964-5069 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1709 | CCOc1cc(CNCCc2cccc(c2  )[Cl])ccc1OC | 4964-5102 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1710 | CCN(CC)CC(COc1c(ccc2 c(C(=O)OCC)c(NC(C)=O) sc12)[Br])O | 5130027 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1711 | c1ccc2C(N=C(c2c1)N)=N N | 5140994 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1712 | C(C(CN=Cc1ccccc1O)O) N=Cc1ccccc1O | 5172847 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1713 | CCOC(c1cnc2ccccc2c1Nc 1ccc(cc1)N1CCOCC1)=O | 5174-4348 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1714 | C1CCN(CC1)Cc1c(CN2C  CCCC2)n(c2c(N)non2)nn1 | 5175780 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1715 | C1C2CC3CC1CC(C2) (C3)N1CCNCC1 | 5236741 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1716 | COc1ccc(cc1)OCC(CN1C CN(CC1)c1ccccc1)O.[Cl]. [Cl] | 5257916 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1717 | CCCCCCOC(C1CN1C(C) (C)CO)=O | 5259604 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1718 | C1CN(CCC1O)Cc1ccccc1 [N+]([O-])=O | 5269563 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1719 | Cc1ccc2c(c1)c1CCCC3c1n 2CCCN3 | 5271325 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1720 | C1CC(N(CNc2ccc(c(c2) [Cl])[Cl])C1=O)=O | 5271658 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1721 | c1cc(c(cc1[Cl])  [Cl])c1nnc(N)s1 | 5313490 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1722 | Cc1ccc(cc1)c1csc(N)n1 | 5341867 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1723 | Cc1cc(ccc1NCC(NN)=O) | 5347228 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | [Cl] |  |  |  |  |  |
| 1724 | CCCCNc1c2c(c3c4CCCCc 4c(nc3s2)N2CCOCC2)nnn 1 | 5504-0161 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1725 | C(c1cnn(c2ccc3ccccc3c2)c 1N)#N | 5628157 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1726 | C1CCC(C1)NCC(COc1ccc (cc1)OCC(CNC1CCCC1) O)O | 5648415 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1727 | C(C(Cn1c2ccccc2nn1)O)n 1c2ccc(cc2c2cc(ccc12) [Cl])[Cl] | 5654532 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1728 | CCOC(c1cnc2c(C)c(ccc2c 1NCCN(C)C)[Cl])=O | 5695-1044 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1729 | COC(CCCCC1C(C(CS1)N  )N)=O.[Br].[Br] | 5728434 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1730 | Cc1cc(ccc1OCCNCCCOC  )[Cl].C(C(O)=O)(O)=O | 5734342 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1731 | CC1=Nc2ccccc2C(N1CCN c1cccc2ccccc12)=O | 5789137 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1732 | C(CNC(c1cn(CCN)nn1)=  O)c1csc(c2cccnc2)n1 | 58419779 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1733 | CCCCCn1c(NC(N)=NC2=  S)c2nc1 | 58907 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1734 | CC(C)CCn1c(CNC(C2CC 3(CCNCC3)CN2)=O)nc2c  ccnc12 | 59041258 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1735 | c1cc(ccc1c1cn2ccsc2n1)N | 5968142 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1736 | Cc1ccc2c(c1)c1CCCC3c1n 2CCN3CC(CN1CCCCC1) O | 5989-2455 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1737 | CC(C)CN1CCC(CC1)NC  CNc1ccncc1C | 60244866 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1738 | CCOC(C1=CNC(SCC)=N C1=O)=O | 60266 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1739 | O=C(c(cc1)cc(Cl)c1C(Nc( cc1)ccc1C1=NCCN1)=O)  Nc(cc1)ccc1C1=NCCN1 | 60339 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1740 | CCN1CCN(CC1)CC(COc 1ccc(CC=C)cc1OC)O.[Cl]. [Cl] | 6043920 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1741 | Cc1ccc(c(C)c1)OCC(CN1 CCN(CC1)CCN1C(c2cccc 3cccc(C1=O)c23)=O)O. [Cl].[Cl] | 6044718 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1742 | COc1cc(CC=C)ccc1OCC( CN1CCC(CC1)Cc1ccccc1) O.[Cl] | 6046571 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1743 | CCCOc1ccc(cc1)c1cnc(nc 1N)S | 6431640 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1744 | C(c1ccco1)NC1C(c2cccc3 cccc1c23)NS(c1ccc(cc1) [Cl])(=O)=O | 6432111 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1745 | CCOC(C(C(c(cccc1)c1N1) C1=O)=O)=O | 646976 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1746 | C1CNCCC1C(N1CCN(CC 1)c1ccccc1F)=O.C(C(O)= O)(O)=O | 6579417 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1747 | Cc1ccc(cc1)OCCN1CCN( CC1)CC(Cn1c2ccccc2c2cc ccc12)O.C(C(O)=O)(O)=O | 6612808 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 1748 | Cc1nc2ccccc2n1CC(COc1 ccc(cc1)C1CCC=C1)O | 6682831 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1749 | O=C(c(cc1)cc(C(Nc(cc2)c cc2C2=NCCN2)=O)c1Cl)  Nc(cc1)ccc1C1=NCCN1 | 67436 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1750 | CCC1CCCCN1S(c1ccc(cc 1)NC1c2ccccc2S(N=1) (=O)=O)(=O)=O | 7380-0010 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1751 | Cc1ccc(cc1)c1cnc(NCc2cc cc(c2)[Cl])n1C | 7756-0705 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1752 | Cc1ccc(cc1C)c1cnc(NCc2 ccc(cc2)F)n1C | 7756-0829 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1753 | Cc1c(CCC2OCCO2)c(Cl)n  c(N)n1 | 77596 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1754 | CC(C)OC(C1C(C2=C(CC( C) (C)CC2=O)OC=1N)c1ccc( cc1)[Cl])=O | 8003-3608 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1755 | C(c1cccnc1)Nc1nc(nc(n1) [Cl])N1CCOCC1 | 8006-8438 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1756 | Cc1ccc(cc1)C1C(C#N)=C(  N)Oc2ccc3ccccc3c12 | 8008-9298 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1757 | C1CCC(CC1)NC(c1c2CC CCc2sc1N)=O | 8009-1776 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1758 | [H]Nc1nnc(COc2ccc(cc2) C2CCCCC2)s1 | 8009-2831 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1759 | C1CNC(CN)c2ccccc12 | 8009-3719 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1760 | C1CCN(CC1)c1ccc2C(N( CCO)C(c3cccc1c23)=O)= O | 8010-2208 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1761 | CN1C(c2c(nc(N3CCCCC3  )n2CCN)N(C)C1=O)=O | 8012-0524 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1762 | CC1=CC(N(C)C(N1CCCC CCNCCO)=O)=O | 8012-3983 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1763 | Cc1c(CCNCc2c(cc(cc2OC  )OC)OC)c2cc(ccc2[nH]1) OC | 8013-0022 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1764 | CC(Cc1ccc2c(c1)OCO2)C  NCCc1c2cc(ccc2[nH]c1C) OC | 8013-0190 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1765 | CCCCc1nc(CNCCc2c3cc( ccc3[nH]c2C)OC)c[nH]1 | 8013-0624 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1766 | C(CNCc1ccc2c(c1)c1ccccc 1[nH]2)NCCO | 8013-0978 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1767 | Cc1c(CCNCc2ccc(C#N)cc 2)c2cc(ccc2[nH]1)OC | 8013-2954 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1768 | CN(C)CCCNCc1ccc2c(c1) c1CCCCc1[nH]2 | 8013-3043 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1769 | CC(C)C1(CCNCc2ccc(cc2  )OC)CCOC(C)(C)C1 | 8018-1266 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1770 | CC(C)C1(CCNCc2cccc3c2 OCO3)CCOC(C)(C)C1 | 8018-1268 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1771 | C(C(c1nc2ccccc2[nH]1)N) c1ccc(cc1)O | 8018-4464 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1772 | c1cc(c2nnc3n2nc(Nc2ccc( cc2)[Cl])s3)sc1 | 8018-8096 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1773 | C(CS(N1CCNCC1) (=O)=O)N | 8018-8721 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1774 | Cc1c(c(N)n(CCN2CCOCC | 8019-0360 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | 2)c1C)S(c1ccc(cc1)F) (=O)=O |  |  |  |  |  |
| 1775 | CN1CCC(CC1)Oc1ccc(cc 1)N | 8019-4291 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1776 | CCNC[C@@H]1CCN(CC  )[C@H]1c1ccccc1OC | 8019-4504 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1777 | CC(Cc1cc2c(c(c1OC)OC) OCO2)N | 8019-6342 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1778 | C1CCN(CC1)c1nc(CN2C(  N(c3ccccc3[Cl])N=N2)=O  )nc(N)n1 | 8019-8781 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1779 | C1CN(CCC1N)Cc1cccc(c 1)O | 8020-1707 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1780 | C(COc1ccccn1)NCc1ccccn 1 | 8020-2902 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1781 | CCNCc1cc(CC=C)c(c(c1) OC)OCC | 8020-2907 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1782 | COc(cc1)cc(N2)c1NP2(Oc 1ccccc1)=S | 88402 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1783 | COc1cc(ccc1OCCCN1CC CCC1)N.[Cl].[Cl] | 9122829 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1784 | C1CC2=C(C(c3ccccc3)c3c (N)nc(N)nc3N2)C(C1)=O | 9129209 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1785 | CCN1CCCC1CNCc1ccc(C  )s1.[Cl].[Cl] | 9131777 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1786 | C(c1cccnc1)Nc1cccc(c1)c1 nc2ccccc2[nH]1 | 9142557 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1787 | Cc1ccc(cc1N)c1ccc(nn1) [Cl] | 9221590 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1788 | Cc1ccc2c(c1)c(C)nc(NC1 NCN(CCO)CN=1)n2 | 9243143 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1789 | Cc1cc(c2cc(ccc2n1)C(O)= O)N | 9243351 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1790 | CSc1ccc(cc1)OCCN | 9254473 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1791 | CCN1CCCC1CNCc1cccc(  c1)OCc1ccc(cc1)[Cl] | 9312203 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1792 | Cc1ccc(c(C)c1)NC(Cn1c(c (C(=O)OC)nn1)N)=O | C200-1530 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1793 | CCc1nc2nc(C)cc(Nc3cc(cc c3C)[Cl])n2n1 | C301-3944 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1794 | CCc1nc2nc(C)cc(Nc3cccc( C)c3C)n2n1 | C301-4042 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1795 | Cc1ccc(cc1C)Nc1nc2ccccc 2c2nncn12 | C301-5182 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1796 | CCN(CC)CCCNc1c2ccccc 2nc(c2nnc(c3ccc(C)cc3)o2  )n1 | C660-1575 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1797 | CC(C)c1ccc(cc1)S(c1c2nc( c3ccccc3n2nn1)N)(=O)=O | C718-0270 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1798 | Cc1ccccc1NC(CNS(c1ccc( cc1)[Cl])(=O)=O)c1ccccc1 | D030-0069 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1799 | C(CNc1nc(cs1)c1c[nH]c2c cccc12)c1ccccc1 | D041-0019 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1800 | COC(CCc1c(c2ccc(cc2)O C)nc(Nc2ccccc2)s1)=O | D041-0023 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1801 | Cc1cccc(CNc2nc3nc(C)cc( C)n3n2)c1 | D043-0228 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1802 | CCCN1C(C2(C3=C(C(N2 | D063-1103 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | CCO)=O)Oc2ccc(C)cc2C3  =O)c2ccccc12)=O |  |  |  |  |  |
| 1803 | Cc1cc2C(C3=C(C(N(CCO  )C34C(N(C)c3ccccc34)=O  )=O)Oc2cc1C)=O | D063-1142 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1804 | [H]c1ccc(cc1)S(c1c(NCCC N(C)C)oc(c2ccccc2)n1) (=O)=O | D072-0521 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1805 | CCC(c1nc2ccccc2n1CCC Oc1ccccc1C)O | D186-0091 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1806 | Cc1ccc(c(c1)NC1c2ccccc2 S(N=1)(=O)=O)OC | D257-0773 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1807 | Cc1ccccc1c1nc(c2cccnc2N C2CCCCC2)on1 | D349-3758 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1808 | COc1ccc(cc1)c1nc(c2cccn c2NC2CCCC2)on1 | D349-4050 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1809 | CC1(C)CC(CCNCCCN(C) C)(CCO1)c1cccc(c1)C(F) (F)F | D442-0364 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1810 | CC1(C)CC(CCNCc2cccnc 2)(CCO1)c1cccc(c1)C(F) (F)F | D442-0374 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1811 | CN(C)c1ccc(cc1)c1c(Nc2c cc(cc2)[Br])n2ccncc2n1 | D600-0307 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1812 | CCOC(c1cnc2c(c3ccc(cc3) [Br])c(C)nn2c1N)=O | D718-0691 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1813 | COc1ccc2c(CNCCc3ccco3  )c(C(O)=O)n(Cc3ccccc3F) c2c1 | E518-0633 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1814 | Cc1cc(C)n(c2c(NCc3ccccc 3)nc3ccc(cc3n2)[Cl])n1 | E701-0030 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1815 | C1C2CC3CC1CC(C2) (C3)N | NCGC0001503 6-08 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1816 | C(C(c1ccc(cc1[Cl]) [Cl])OCc1ccc(cc1) [Cl])n1ccnc1 | NCGC0001825 8-09 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1817 | CCOC([C@H]  (CCc1ccccc1)N[C@@H] (C)C(N1CCC[C@@H]1C( O)=O)=O)=O | NCGC0002156 9-08 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1818 | CS(=O) (=O)OCCCCOS(C) (=O)=O | NCGC0009090 5-11 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1819 | CCC(C)CCCCC(N[C@@ H] (CCN)C(NC(C(N[C@H] (CCN)C(N[C@@H]1CCN C(C([C@@H] (C)O)NC([C@@H]  (CCN)NC([C@@H]  (CCN)NC([C@@H]  (CC(C)C)NC([C@H]  (Cc2ccccc2)NC([C@H] (CCN)NC1=O)=O)=O)=O  )=O)=O)=O)=O)=O)  [C@@H](C)O)=O)=O | NCGC0009476 3-03 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1820 | C1CN1P(N1CC1) (N1CC1)=S | NCGC0009504 2-08 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1821 | CCOC(N1CCN(CC1)[N+]  (=NOc1ccc(cc1[N+] ([O-])=O)[N+]([O-])=O)  [O-])=O | NCGC0016581 5-05 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1822 | CCN(CC)CCN1C(C(Cc2c | NCGC0018604 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |

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| --- | --- | --- | --- | --- | --- | --- |
| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | cc(cc2)OC)=Nc2ccccc12)= O | 6-02 |  |  |  |  |
| 1823 | C1CCN[C@@H](C1) [C@H]  (c1ccccc1)NC(c1cccc(c1[C l])C(F)(F)F)=O | NCGC0024795 4-02 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1824 | CC1C=C(C2=NC(=CC(N2 C=1)=O)N1CCOCC1)  [C@@H] (C)Nc1ccccc1C(O)=O | NCGC0026315 4-01 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1825 | [H][C@@]12CC([C@H]  ([C@@](C)  (n3c4ccccc4c4c5C(NC(c5c 5c6ccccc6n1c5c34)=O)=O  )O2)OC)N(C)C(c1ccccc1)  =O | NCGC0034508 3-01 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1826 | Cn1cc(cn1)c1cnn2c(c(c([C @H]3CCCNC3)nc12) [Br])N | NCGC0034665 3-01 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1827 | CC(C)S(c1ccccc1Nc1c(c( N)nc(Nc2ccc(cc2OC)N2C CC(CC2)C(N)=O)n1)[Cl]) (=O)=O | NCGC0034695 7-01 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |
| 1828 | C(C(=C1NC(c2ccc(cc2N1)  [Cl])=O)C(c1ccc(cc1[Cl]) [Cl])=O)#N | NCGC0034794 2-01 | Zika3PrimeUTR | G-quadruplex | GCGGCGGCCGGUGUGGGGAA | 1 |