“Aptamers” 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 | Cc1nc2c(c(=O)n1C) CN(C[C@]1(O)CCC [NH2+]C1)C2 | Neg\_lig\_7 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 2 | CN(Cc1nccn1Cc1ccc cc1)C(=O)C[C@H]1 COCC[NH2+]1 | Neg\_lig\_34 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 3 | COc1ccc([C@@H]2 C[C@H]  (c3ccc(C(C)C)cc3)n3 nc(N)nc3N2)cc1 | Neg\_lig\_104 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 4 | CCCOc1ccc(Oc2nc( NC)nc(N3CCOCC3)  n2)nn1 | Neg\_lig\_107 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 5 | CC(C)[N@H+] (C[C@H]1O[C@@H  ](n2cnc3c(N)ncnc32) [C@H](O)  [C@@H]1O)  [C@H]1C[C@@H]  (CCc2[nH]c3ccc(C(C  )(C)C)cc3[nH+]2)C1 | Neg\_lig\_109 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 6 | CCn1cnnc1CCNc1nc (C2CCCC2)nc2c1C[ NH2+]C2 | Neg\_lig\_92 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 7 | CCCCOC(=O)N1CC CC2(CC[NH2+]CC2) CC1 | Neg\_lig\_206 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 8 | Nc1nonc1- c1nc2ccccc2n1CC(= O)Nc1ccc(F)c(Cl)c1 | Neg\_lig\_211 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 9 | CNS(=O) (=O)c1ccc(CN2C[C @H](O)[C@@H] (N3CC[NH+] (C)CC3)C2)cc1 | Neg\_lig\_229 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 10 | NC1(C(=O)N2CCC[ C@H]  (c3[nH]ncc3Cc3cccc c3)C2)CC1 | Neg\_lig\_261 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 11 | CC[C@@]1(O)CC[N  @H+](Cc2ccc(C(F)  (F)F)nc2)C[C@H]1O | Neg\_lig\_271 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 12 | COc1cc(N)c(C#N)cc 1OC | Neg\_lig\_331 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 13 | Fc1ccc(- c2noc3ncnc(NCCN4 CCOCC4)c23)cc1 | Neg\_lig\_378 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 14 | Cc1cc2c(c(=O)o1) [C@H] (c1cccs1)C(C#N)=C( N)O2 | Neg\_lig\_392 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 15 | O=C1S[C@H]  (Nc2ccccc2F)C(=O) N1c1ccccc1 | Neg\_lig\_397 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 16 | Cc1ccc(Nc2nc(N3CC OCC3)c3ccccc3[nH+  ]2)cc1 | Neg\_lig\_437 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 17 | C=C(C)  [C@@H]1CC[C@@  ]2(C)CC[C@]3(C) [C@H] (CC[C@@H]4[C@  @]5(C)CC[C@@H] | Neg\_lig\_469 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | (O)C(C)(C) [C@H]5CC[C@]43C  )[C@@H]12 |  |  |  |  |  |
| 18 | CCNc1nc(C)cc(N2C CN(S(=O)  (=O)c3ccc(OC)c(C)c 3C)CC2)n1 | Neg\_lig\_509 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 19 | COCCOC(=O)C1=C(  N)Oc2c(oc(CO)cc2= O)  [C@H]1c1cccc(F)c1 | Neg\_lig\_510 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 20 | NNC(=O)c1ccncc1 | Neg\_lig\_526 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 21 | CCOc1ccccc1CCNC(  =O)[C@H] ([NH3+])c1c(C)n[nH  ]c1C | Neg\_lig\_533 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 22 | Nc1ccc(S(=O) (=O)Nc2ccc(F)cc2)cc 1 | Neg\_lig\_565 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 23 | CCOc1ccc(-c2noc(- c3nnn(- c4cc(Cl)ccc4OC)c3N  )n2)cc1 | Neg\_lig\_573 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 24 | Cc1ccc(C)c(N[C@@ H](CNS(=O)  (=O)c2ccccc2)c2cccc c2)c1 | Neg\_lig\_597 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 25 | COc1cccc(- c2nccn2C[C@H] (O)c2cccnc2)c1OC | Neg\_lig\_601 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 26 | Cc1cc(C(=O)NCc2cc 3n(n2)CC[NH2+]C3)  c(-c2ccccc2)o1 | Neg\_lig\_632 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 27 | COC(=O)C1=C(N)O  c2c(oc(CO)cc2=O) [C@H]1c1ccc(F)cc1 F | Neg\_lig\_633 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 28 | O=c1cc([O-])  [nH]cc1Cl | Neg\_lig\_665 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 29 | Cc1cccc(- n2cc(C[N@@H+]3C [C@H] (N(C)C)C[C@H]3C  O)cn2)c1 | Neg\_lig\_704 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 30 | [NH3+]C[C@H]1CC N(C(=O)c2ccc(NCc3  ccncc3)cc2)C1 | Neg\_lig\_710 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 31 | COc1ccccc1OC[C@ @H] (O)C[NH+]1CCC(C) CC1 | Neg\_lig\_725 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 32 | COC(=O)c1ccc2c(/ C(=N/ c3ccc(N(C)C(=O)CN 4CC[NH+]  (C)CC4)cc3)c3ccccc 3)c(O)[nH]c2c1 | Neg\_lig\_753 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 33 | Cc1cc(Nc2ccccc2Cl) n2nc(C)nc2n1 | Neg\_lig\_768 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 34 | Cc1ccc2[nH]c(C)c([ C@@H] (O)C[NH+]3CCCCC  3)c2c1 | Neg\_lig\_794 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 35 | Cc1ccc([C@H](C) [NH2+]Cc2cn(CCC( | Neg\_lig\_798 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | N)=O)c3ccccc23)cc1 C |  |  |  |  |  |
| 36 | CC[N@@H+] (CCO)C[C@@H]1C N(c2noc(C(C)C)n2)C [C@@H]1CO | Neg\_lig\_804 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 37 | [NH3+]C1(C(=O)N2  CC[C@@H]3[C@@ H] (CCC(=O)N3CCc3cc ccn3)C2)CCC1 | Neg\_lig\_814 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 38 | CCc1nc2c(N3CCC([ NH2+]Cc4cc(C(C) (C)C)  [nH]n4)CC3)ncnc2o1 | Neg\_lig\_818 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 39 | CCn1c(N)nc2cc(C(= O)N3CCc4nc(C)  [nH]c(=O)c4CC3)cnc 21 | Neg\_lig\_838 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 40 | Nc1nnc(CCn2cnc3sc 4c(c3c2=O)CCNC4)s  1 | Neg\_lig\_872 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 41 | CC(C)(C)c1ccc(- c2nc(NCCCN3CCO  CC3)c3ccccc3[nH+]2  )cc1 | Neg\_lig\_875 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 42 | O[C@H]1CN(c2cc(C (F) (F)F)nc(N3CCCC3)n  2)Cc2ccccc21 | Neg\_lig\_920 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 43 | CN(Cc1ncc[nH]1) [C@H]1CN(C(=O)c2  cc(-c3ccsc3) [nH]n2)C[C@@H]1 O | Neg\_lig\_929 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 44 | CN1CCC(=C2c3cccc c3CCc3sccc32)CC1 | Neg\_lig\_935 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 45 | Cc1csc(N2CCC([NH  +]3CCC(O)CC3)CC2  )n1 | Neg\_lig\_967 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 46 | Cc1ccc(N)c(-c2nnc(- c3ccncc3)o2)c1 | Neg\_lig\_1086 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 47 | CC[C@H]  (Nc1cccc(OC)c1)C(= O)NCCOc1ccccc1 | Neg\_lig\_1124 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 48 | Cn1c(=O)c2c(nc(NC CCCO)n2Cc2ccccc2 Cl)n(C)c1=O | Neg\_lig\_1172 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 49 | CCOC(=O) [C@H]1CCCN(C(=O  )c2ccc(CNc3c(N4CC C(C)CC4)c(=O)c3=O  )cc2)C1 | Neg\_lig\_1225 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 50 | CCCc1cc(C(=O)N[C  @@H] (C)c2nnc(N)s2)n[nH] 1 | Neg\_lig\_1249 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 51 | [NH3+]  [C@@H]1c2ccccc2C 2(CCN(c3cnc4ccccc4 n3)CC2)[C@H]1O | Neg\_lig\_1252 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 52 | Cc1cccc2nc(CNc3ccc (Cl)c(Cl)c3)cn12 | Neg\_lig\_1267 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 53 | Nc1cc(OC(=O)c2ccc cc2)nn1S(=O) | Neg\_lig\_1315 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | (=O)c1ccccc1 |  |  |  |  |  |
| 54 | COc1ccc(S(=O) (=O)N2CCN(c3cc(C)  nc(Nc4ccc(C)cc4)n3) CC2)cc1 | Neg\_lig\_1385 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 55 | CSc1nnc(CC2CCN(c 3[nH]c(N)nc4ncnc3- 4)CC2)n1C | Neg\_lig\_1404 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 56 | CCCc1cncnc1N1C[C @@H] ([NH3+])C[C@H]1C (=O)N(CC)CC | Neg\_lig\_1413 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 57 | CCOC(=O)[C@@H] (O)C(C) (C)CN1C(=O)c2cccc c2C1=O | Neg\_lig\_1415 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 58 | N#Cc1nc(- c2ccc(S(=O) (=O)N3CCCC3)cc2) oc1NC1CCCCC1 | Neg\_lig\_1434 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 59 | CN(C)c1cncc(N2CC[ C@](C)(O)[C@@H] (O)C2)n1 | Neg\_lig\_1486 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 60 | Cc1cc(C(=O)N2C[C @@H](CO)C[C@H] (CN3CCC[N@@H+] (C)CC3)C2)c(C)o1 | Neg\_lig\_1504 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 61 | CCOC(=O)c1cccc(N C2=NS(=O)  (=O)C(c3ccc(Cl)cc3)  =C2C)c1 | Neg\_lig\_1520 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 62 | CN1CC[NH+] ([C@H]2CCN(C(=O)  Cn3cc4ccccc4n3)C[C @H]2CCCO)CC1 | Neg\_lig\_1580 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 63 | CCOc1ccccc1N[C@ H]1OC(=O)c2ccccc2 1 | Neg\_lig\_1601 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 64 | c1cnc2c([C@H]3[N H2+]CCc4[nH+]c[nH  ]c43)cnn2c1 | Neg\_lig\_1605 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 65 | COC(=O)c1cc(-  c2cccc(N)c2)nc2cccc c12 | Neg\_lig\_1643 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 66 | Nc1c(Br)cc(Cl)c2c1C (=O)c1ccccc1C2=O | Neg\_lig\_1657 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 67 | CCOC(=O)c1c(N)n(-  c2cc(C)ccc2C)c2nc3c cccc3nc12 | Neg\_lig\_1698 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 68 | C[NH2+]CCN1C(=O  )CC[C@H]2CN(C(=  O)c3cnc(N(C)C)nc3 C)CC[C@H]21 | Neg\_lig\_1717 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 69 | Nc1ccc(N2C(=O) [C@H]3[C@@H]4C C[C@@H](C4) [C@H]3C2=O)cc1 | Neg\_lig\_1724 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 70 | COc1cc([C@@H]2c 3c(n[nH]c3- c3ccccc3O)C(=O)N2 CCCO)cc(Br)c1O | Neg\_lig\_1800 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 71 | COc1ccc(Nc2cc(Cl)c cc2C(=O)[O-])cn1 | Neg\_lig\_1824 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 72 | COc1cccc(OC[C@@ | Neg\_lig\_1837 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | H] (O)CNC(=O)CCC(= O)NC2CCCC2)c1 |  |  |  |  |  |
| 73 | Cn1ccc(=[NH+]c2ccc (NC(=O)c3ccc(/ N=c4\ ccn(C)c5ccc([N+] (=O)  [O-])cc45)cc3)cc2)cc 1 | Neg\_lig\_1849 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 74 | CSCC(=O)N1CCC2( CC1)[C@@H] (OCC[NH3+])C[C@ H]2O | Neg\_lig\_1906 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 75 | COC(=O)[C@H]  (Nc1cc(C)nc2nc(- c3ccccc3C)nn12)c1cc ccc1 | Neg\_lig\_1913 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 76 | CCc1c(C)nc2nncn2c 1Nc1ccc(Cl)cc1 | Neg\_lig\_1935 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 77 | C1Cc2[nH]nc(- c3nn[n-]n3)c2C1 | Neg\_lig\_1993 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 78 | COc1ccc(CCN(C)CC C[C@@](C#N)  (c2ccc(OC)c(OC)c2) C(C)C)cc1OC | Neg\_lig\_2033 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 79 | CO/N=C(\ C(=O)N[C@@H]1C(  =O)N2C(C(=O)OCO C(=O)C(C)(C)C)=C(/ C=C\  c3scnc3C)CS[C@H] 12)c1csc(N)n1 | Neg\_lig\_2117 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 80 | Nc1cc(=O)n2c(n1)SC CC2 | Neg\_lig\_2125 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 81 | CCOC(=O)c1ccc(Nc 2ncnc3ccc(Br)cc23)c c1 | Neg\_lig\_2150 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 82 | COC[C@@H] (N)C(=O)N1CCN(Cc  2cccc(F)c2)CC1 | Neg\_lig\_2159 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 83 | CCOC(=O)c1ccccc1 N[C@@H]1c2ccccc2 C(=O)N1c1ccc(Cl)cc 1 | Neg\_lig\_1054 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 84 | COc1ccc(Nc2[nH+]c 3ccccc3c3nncn23)c( OC)c1 | Neg\_lig\_606 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 85 | COCCc1nc(- c2cnc(C3CC3)nc2)n( CCO)n1 | Neg\_lig\_1479 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 86 | Cn1c(=O)n(C)c2cc(C Nc3ccc(N4CCOCC4) c(C(=O)  [O-])c3)ccc21 | Neg\_lig\_2241 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 87 | O=C(c1ccccc1- n1cncn1)N1C[C@@ H]2CNC[C@]2(C(= O)O)C1 | Neg\_lig\_2250 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 88 | CCC(C) (C)C(=O)O[C@H]1C  [C@@H] (C)C=C2C=C[C@H] (C)[C@H] (CC[C@@H]3C[C@ @H](O)CC(=O)O3) | Neg\_lig\_2260 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | [C@H]21 |  |  |  |  |  |
| 89 | COc1cc(C[NH2+]C(  C)C)ccc1OCc1ccc2c( c1)n(C)c(=O)n2C | Neg\_lig\_792 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 90 | COc1ccccc1- c1nnc(SCC#CCO)o1 | Neg\_lig\_2365 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 91 | COc1ccccc1CC[NH2  +]Cc1ccccc1C | Neg\_lig\_2402 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 92 | COC(=O)c1ccccc1N[ C@H] (NC(=O)c1ccco1)C(=  O)c1ccccc1 | Neg\_lig\_2431 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 93 | [NH3+]CCc1ccc(S(= O) (=O)N2CCOCC2)cc1 | Neg\_lig\_2436 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 94 | OCCCc1nc2ccccc2n1 CCCOc1ccccc1 | Neg\_lig\_1043 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 95 | O=C([N-]OC[C@@ H]  (O)CO)c1cc(Br)c(F)c (F)c1Nc1ccc(I)cc1F | Neg\_lig\_2657 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 96 | CCOc1ccc(CCNc2nc 3ccccc3nc2C(=O)OC  )cc1OCC | Neg\_lig\_2731 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 97 | Cc1ccc2[nH]c(C3=C( N)N(C4CCCCCC4)C C3=O)nc2c1 | Neg\_lig\_2732 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 98 | C=CCNc1cc(C)nc2nc (-c3cccnc3)nn12 | Neg\_lig\_2744 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 99 | COc1ccc(CCNc2ncn c3sc(C)c(C)c23)cc1 | Neg\_lig\_2755 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 100 | Cn1cc(NC(=O)NCC  CNc2cccnc2)cn1 | Neg\_lig\_2781 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 101 | COc1cccc([C@H]2C [C@@H] (c3ccc(Cl)cc3)Nc3nc (N)nn32)c1 | Neg\_lig\_2873 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 102 | Cc1ccc(- c2nccn2CCCO)c(Cl) c1Cl | Neg\_lig\_2875 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 103 | Nc1ccc(C(=O)c2cccs 2)cn1 | Neg\_lig\_2915 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 104 | COc1cccc(- c2ncc(CN3CCO[C@  ]4(CNCCOC4)C3)s2)  c1 | Neg\_lig\_1458 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 105 | O=C1CCCN1c1ccc( C[NH2+]C2CCC3(C C[NH2+]CC3)CC2)c  c1 | Neg\_lig\_2950 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 106 | COc1ccc(-c2nc(- c3ccc(N)cc3)n[nH]2) cc1 | Neg\_lig\_2960 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 107 | O=C(NCCO)c1nnn(-  c2ccc(Cl)cc2)c1- c1ccco1 | Neg\_lig\_2975 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 108 | CC[C@H] (C)Nc1cc(C(C)C)c(C  #N)c2nc3ccccc3n12 | Neg\_lig\_2989 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 109 | CCOC(=O)c1nnn(-  c2nonc2N)c1CN1CC Cc2ccccc21 | Neg\_lig\_674 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 110 | CCSCCn1cnc(- c2ccccc2)c1- c1ccc(CO)o1 | Neg\_lig\_3022 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 111 | C[C@@]12C(=O)OC (=O)[C@@]1(C) [C@H]1CC[C@@H] 2O1 | Neg\_lig\_3045 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 112 | Cc1ccccc1OCCCn1c( CCCO)nc2ccccc21 | Neg\_lig\_3122 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 113 | COc1ccc(CN2C(=O)  O[C@@H]3C[N@@ H+] (C(CO)CO)C[C@@ H]32)cc1OC | Neg\_lig\_3126 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 114 | CCn1c(SCc2ccccc2C  )nc2c(cnn2CCO)c1= O | Neg\_lig\_3127 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 115 | Cc1cc(C(=O)N[C@H  ]  (CO)c2ccccc2)c2cccc (C)c2n1 | Neg\_lig\_3141 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 116 | N#CC1=C(N)OC2=C  ([C@H]1c1ccc(Cl)cc 1)S(=O)  (=O)N(Cc1ccccc1F)c 1ccccc12 | Neg\_lig\_3152 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 117 | C[C@@H] ([NH2+]CCCc1cccc( C(F)  (F)F)c1)c1cccc2ccccc 12 | Neg\_lig\_3216 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 118 | CC1=C(c2ccc(Cl)cc2  )S(=O) (=O)N=C1NC1CC[N  H+](Cc2ccccc2)CC1 | Neg\_lig\_3231 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 119 | Cc1ccc([C@H]2C(C #N)=C(N)Oc3c2oc(C O)cc3=O)o1 | Neg\_lig\_1275 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 120 | CCCOC(=O)c1cccc( Nc2nc(-c3cccnc3) [nH+]c3ccccc23)c1 | Neg\_lig\_3281 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 121 | Cn1ccnc1-c1c(- c2ccccc2)ncn1C[C@ H]1C[NH2+]CCO1 | Neg\_lig\_3285 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 122 | CCN(CC)C(=O)c1cn (C2CCN(C(=O)C3([ NH3+])CCCC3)CC2)  nn1 | Neg\_lig\_3312 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 123 | COc1cc(C)c(N)cc1C( C)C | Neg\_lig\_3340 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 124 | CCCCn1cnc2cc(NCc 3cccc(Br)c3)ccc21 | Neg\_lig\_3358 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 125 | O=C(CSc1nc2ccccc2 s1)N1CCN(CCO)CC 1 | Neg\_lig\_2780 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 126 | CC[C@@H]  (CO)N(Cc1cccnc1)C(  =O)CCCc1cccs1 | Neg\_lig\_3367 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 127 | Cc1nc(CC[NH2+]C2  CCN(c3ncccn3)CC2) sc1C | Neg\_lig\_3380 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 0 |
| 128 | Cc1cccc(CN2c3ccccc 3C3=C([C@@H]  (c4cccc(F)c4)C(C#N)  =C(N)O3)S2(=O)=O) | Neg\_lig\_3 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | c1 |  |  |  |  |  |
| 129 | COC(=O)Nc1ccc(-  c2cnn(CCO)c2)cc1 | Neg\_lig\_5 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 130 | Cn1nc(CO)c2c1CCN (C(=O)c1cnc(Nc3ccc cc3)nc1)C2 | Neg\_lig\_13 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 131 | C[NH2+]CCN1C(=O  )CC[C@H]2CN(C(= O)CCCc3cn[nH]c3)C C[C@H]21 | Neg\_lig\_24 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 132 | Cc1cc(C)cc(NC(=O)c 2nnn(Cc3ccc(Cl)cc3) c2N)c1 | Neg\_lig\_112 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 133 | COc1ccc([C@H]2C( C#N)=C(N)Oc3c2sc2  ccccc32)cc1OC | Neg\_lig\_113 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 134 | O[C@H] (C#CCN1CCOCC1)c  1ccccc1 | Neg\_lig\_148 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 135 | C[C@@H]  (CNc1nc2ccc(Cl)cc2 n2cnnc12)c1ccccc1 | Neg\_lig\_245 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 136 | Cc1ccccc1- n1nc(CO)c(C(=O)NC  c2cccs2)n1 | Neg\_lig\_267 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 137 | COc1nc(NCc2cccnc2  )nc(N2CCSCC2)n1 | Neg\_lig\_292 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 138 | C=CCOc1c(Cl)cc([C @@H]2C(C#N)=C(  N)Oc3cc4c(cc32)OC O4)cc1OCC | Neg\_lig\_293 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 139 | CSc1nc2c(c(Nc3ccc( C)cc3)n1)CCC2 | Neg\_lig\_395 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 140 | Cc1nc(Nc2ncc3c(n2) CCCC3=O)nc2ccccc 12 | Neg\_lig\_419 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 141 | Cc1ccc2c(N)c(C(=O) c3ccc(- c4ccccc4)cc3)sc2n1 | Neg\_lig\_429 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 142 | Cc1cc(NCCCn2ccnc 2)n2nc(- c3ccccc3)c(C)c2[nH+  ]1 | Neg\_lig\_447 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 143 | C#CCOc1ccc([C@H] 2CC(=O)Nc3[nH]c(=  N)sc32)cc1OC | Neg\_lig\_501 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 144 | CSCC[C@@H] (CO)NC(=O)c1cc(C)  nc2cc(F)ccc12 | Neg\_lig\_512 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 145 | Cc1ccc(- n2nc(CO)c(C(=O)NC  c3ccncc3)n2)cc1C | Neg\_lig\_544 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 146 | Cc1c(S(=O)  (=O)c2ccccc2)c(N)n( Cc2ccccn2)c1C | Neg\_lig\_584 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 147 | O[C@H]  (Cn1c(Cc2ccccc2)nc 2ccccc21)Cn1c2ccc( Cl)cc2c2cc(Cl)ccc21 | Neg\_lig\_636 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 148 | COc1ccccc1N1CCC( [N@@H+]2CCN[C  @H] (C(=O)NC3CC3)C2) | Neg\_lig\_712 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | CC1 |  |  |  |  |  |
| 149 | CCc1ccc(C[NH2+]C  Cc2ccc(OC)c(OC)c2) cc1 | Neg\_lig\_721 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 150 | OC[C@H]1CCN(Cc  2cc(O)c3cccc(Cl)c3n 2)C[C@@H]1O | Neg\_lig\_780 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 151 | O=C([O-])c1cc2cc(O  Cc3ccccc3)ccc2[nH] 1 | Neg\_lig\_921 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 152 | O=C1c2ccccc2C(=O) N1OC[C@H] (O)COc1ccc([N+]  (=O)[O-])cc1 | Neg\_lig\_928 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 153 | Cc1c(- c2ccccc2)n(CCO)c2n c3c(c(=O)n(C)c(=O)n 3C)n12 | Neg\_lig\_956 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 154 | CCCc1cc(N2CCC([N  H2+]Cc3cnn(- c4ccccc4)c3)CC2)nc( C)n1 | Neg\_lig\_1009 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 155 | Cn1c(N)c(C(=O)C[N H2+]C2CCCCC2)c(= O)n(C)c1=O | Neg\_lig\_1030 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 156 | Cc1cc(C)n2c(Nc3ccc cc3C)c(- c3cccs3)nc2n1 | Neg\_lig\_1051 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 157 | Cc1cccc2nc(CCN3C(  =O)NC4(CC[NH2+] CC4)C3=O)[nH]c12 | Neg\_lig\_1063 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 158 | COCCOC(=O)C1=C( N)OC2=C(C(=O)CC(  C)(C)C2)  [C@H]1c1ccc(F)cc1 | Neg\_lig\_1126 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 159 | COc1ccc(- c2csc(NCCc3ccc(OC  )c(OC)c3)n2)cc1 | Neg\_lig\_1153 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 160 | NS(=O) (=O)N1CCN(C(=O)c 2cn(C[C@H]3CCC[ NH2+]C3)nn2)CC1 | Neg\_lig\_1183 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 161 | O=C1N[C@@]  (CCc2ccccc2) (C2CC[NH2+]CC2)C (=O)N1CCO | Neg\_lig\_1215 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 162 | O=C(Nc1cccc(OC(F) (F)F)c1)N1C[C@H] (O)[C@@H] (N2CCOCC2)C1 | Neg\_lig\_1229 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 163 | OCC[NH2+]Cc1ccc(  OCc2ccc3c(c2)OCC O3)cc1 | Neg\_lig\_1277 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 164 | Cc1nc(O)nc(C)c1CC C(=O)N1CCCC[C@ H]([NH3+])C1 | Neg\_lig\_1284 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 165 | N#CC1=C(N)N(c2cc ccc2)C2=C(C(=O)O C2) [C@@]12C(=O)N(C  c1ccccc1)c1ccccc12 | Neg\_lig\_1313 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 166 | CC(C)NC(=O)  [C@@H]1C[C@@H  ] ([NH3+])CN1C(=O)c | Neg\_lig\_1322 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | 1cc(-c2ccc(F)cc2) [nH]n1 |  |  |  |  |  |
| 167 | O=C(/C=C\  c1cccnc1)NCCCCC1 CCN(C(=O)c2ccccc2  )CC1 | Neg\_lig\_1329 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 168 | CCOc1ccc(-c2noc(- c3nnn(- c4ccccc4)c3N)n2)cc1 | Neg\_lig\_1335 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 169 | CC(C)c1[nH+]ccn1C c1cc(C(=O)NC2CC( C)(C)[NH2+]C(C)  (C)C2)n[nH]1 | Neg\_lig\_1365 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 170 | C=CCOC(=O)C1=C( C)OC(N)=C(C#N)  [C@H]1c1cccs1 | Neg\_lig\_1387 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 171 | Cc1cccc(- c2nn3c(NCC(C)C)cc( C)[nH+]c3c2C)c1 | Neg\_lig\_1398 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 172 | Cc1ccc(N)c(C(=O)C CCCC(=O)[O-])c1 | Neg\_lig\_1409 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 173 | COc1ccc([C@@H]2c 3c(n[nH]c3- c3cc(C)ccc3O)C(=O) N2CCO)cc1OC | Neg\_lig\_1441 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 174 | c1cn(CCC[NH2+]Cc  2ccc3c(c2)OCO3)cn1 | Neg\_lig\_1498 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 175 | CN(C)c1ccc2[nH+]c 3ccc(=[N+](C)C)cc-  3sc2c1 | Neg\_lig\_529 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 176 | Nc1nonc1- c1nc2ccccc2n1Cc1cc c(Br)cc1 | Neg\_lig\_1635 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 177 | C[C@H]  (O)c1cccc(N2CCC(c 3[nH+]ccn3Cc3cccnc 3)CC2)n1 | Neg\_lig\_1658 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 178 | COCCN1C[C@@H]  (Cn2ccnc2- c2ccc(CO)o2)CC1=O | Neg\_lig\_1674 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 179 | [NH3+]CCN1C(=O) CC[C@H]2CN(C(=O  )c3nc4ccccn4c3F)CC [C@H]21 | Neg\_lig\_1700 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 180 | CCCc1c/c(=[NH+]\ CCN2CCOCC2)n2[n  H]c3nc(C)cc(C)c3c2 n1 | Neg\_lig\_1753 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 181 | Cc1cncc(C(=O)N2C CNC[C@H]2C(=O)  NCc2ccncc2)c1 | Neg\_lig\_1756 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 182 | O=C(NCc1ccncn1)c1 cn(CC[C@H]2CCCC [NH2+]2)nn1 | Neg\_lig\_1757 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 183 | COC(=O)N[C@H] (C(=O)N1CCC[C@H  ]1c1nc(-c2ccc(- c3ccc(- c4c[nH]c([C@H]5C CCN5C(=O)  [C@@H] (NC(=O)OC)C(C)C)  n4)cc3)cc2)c[nH]1)C (C)C | Neg\_lig\_1759 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 184 | NS(=O) | Neg\_lig\_1771 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | (=O)c1ccc(NC(=S)N  C(=O)c2ccco2)cc1 |  |  |  |  |  |
| 185 | C[NH+] (C)C[C@H]1C[C@  @H] (CO)CN(C(=O)CNc2  nc3ccccc3s2)C1 | Neg\_lig\_1812 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 186 | Cc1ccccc1[C@H]1C( C#N)=C(N)OC2=C1 S(=O)  (=O)N(C)c1ccccc12 | Neg\_lig\_1876 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 187 | COc1ccc(N2CCN([C @H]3CCCN(C(=O)C O)C3)CC2)cc1 | Neg\_lig\_1836 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 188 | O=C(c1cccc(- c2ncc[nH]2)c1)N1C CC2(CC1)[C@@H] (OCCO)C[C@H]2O | Neg\_lig\_1966 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 189 | CCOC(=O)c1c(N)sc(  C(=O)Nc2ccc(C)c(Cl  )c2)c1C | Neg\_lig\_1465 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 190 | C=CCNC(=S)NCC | Neg\_lig\_1986 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 191 | CO/C(O)=C1/ C2=C(CCC2)S/ C1=N\C(=O)NCCCO | Neg\_lig\_1989 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 192 | Cc1cc(C)c2oc(- c3ccc(C)c(N)c3)nc2c 1 | Neg\_lig\_2005 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 193 | O=C(c1cn[nH]c1C1C CCCC1)N1CCOc2cc c(CO)cc2C1 | Neg\_lig\_2035 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 194 | CCOc1ccc(-c2noc(- c3nnn(- c4ccccc4C)c3N)n2)c c1 | Neg\_lig\_2084 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 195 | O[C@@H]  (Cc1ccc2ccccc2n1)C( Cl)(Cl)Cl | Neg\_lig\_2134 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 196 | CCCCCN(CC[C@]1 2C[C@H]3C[C@H] (C[C@H] (C3)C1)C2)C(=O)NC  CCc1ccncc1 | Neg\_lig\_2169 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 197 | O=C(CCCCCCNC(=  O)c1cnc(N(c2ccccc2) c2ccccc2)nc1)NO | Neg\_lig\_2175 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 198 | CCOc1ncccc1C(=O) N1C[C@@H]2c3ccc cc3OC[C@]2(CO)C1 | Neg\_lig\_2193 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 199 | Cc1cccc(-c2noc(- c3cccnc3NCc3ccccc3  )n2)c1 | Neg\_lig\_2244 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 200 | Cc1ccc(C(=O)c2sc3n c4c(cc3c2N)C(=O)C C(C)(C)C4)cc1 | Neg\_lig\_2253 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 201 | CCCc1nc2nc(C)cc(N c3ccc(C)c(F)c3)n2n1 | Neg\_lig\_2256 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 202 | Cn1c(=O)n(C)c2cc(C [NH2+]CCc3ccc(Cl)c c3)ccc21 | Neg\_lig\_2319 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 203 | O=C1CCC2(CCN(Cc  3nnc(- c4cccnc4)o3)CC2)C N1CCO | Neg\_lig\_1 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 204 | Cc1nc(N2CCN(C(=O  )CN3CC(=O)NC3=O  )C[C@H](O)C2)no1 | Neg\_lig\_2362 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 205 | O=C(CN1CCCC1)Nc  1nc(- c2ccc(Cl)cc2)cs1 | Neg\_lig\_2392 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 206 | COc1ccccc1- n1nc(C)c(- c2ccccc2)c1N | Neg\_lig\_2397 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 207 | CCc1cnc(NC[C@H] (O)c2cccc(O)c2)nc1 | Neg\_lig\_2408 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 208 | CN(CC1(CO)CC1)C(  =O)Nc1ccc(-c2nnc(- c3ccco3)o2)cc1 | Neg\_lig\_2418 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 209 | CCCc1c(C)nc2ncnn2 c1Nc1ccc(N2CCOC C2)cc1 | Neg\_lig\_2440 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 210 | CC[C@@H]  (CO)N(Cc1cccnc1)C c1nn(C)c2cccc(Cl)c1 2 | Neg\_lig\_2510 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 211 | CCOC(=O)c1c(N)n(-  c2cc(C)ccc2C)c2nc3c cccc3nc12 | Neg\_lig\_1698 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 212 | CCCc1nc(C(=O)N2C C[C@@H]  (c3sccc3C)[C@H] (O)C2)cs1 | Neg\_lig\_2531 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 213 | CNC(=O)c1sc(N2CC CC2)nc1N | Neg\_lig\_2545 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 214 | CC(=O)N1CCN(Cc2  ccccc2C(=O)  [O-])C[C@H](O)C1 | Neg\_lig\_2560 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 215 | Nc1nnnn1CC(=O)N1 CCC2(CCC(=O)N(C[ C@H]3CCCO3)C2) CC1 | Neg\_lig\_2566 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 216 | Cc1ccc(N[C@@H]2c 3ccccc3C(=O)N2c2c cccc2C)cc1 | Neg\_lig\_2574 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 217 | CCOC(=O)c1ccc(- n2c(N)c(C(=O)OC)c  3nc4ccccc4nc32)cc1 | Neg\_lig\_2600 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 218 | O=C(OCc1ccccc1)c1 nc2ccccc2nc1NCc1cc ccc1 | Neg\_lig\_2620 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 219 | O=C(NC[C@H]  (O)c1ccccc1C(F) (F)F)c1c[nH]nc1- c1ccccc1 | Neg\_lig\_2649 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 220 | Oc1cccc(Nc2cc(- c3ccccc3)ncn2)c1 | Neg\_lig\_2719 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 221 | O=C(c1ccccc1[C@H  ]1CC[NH2+]C1)N1C  Cc2[nH]c3ccccc3c2C 1 | Neg\_lig\_2769 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 222 | Cc1ccc2nc(C[NH2+] C[C@H]  (C)Oc3cccnc3) [nH]c2c1C | Neg\_lig\_2615 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 223 | Cc1ccc(Nc2nc3ccccc 3c3nnc(C)n23)cc1F | Neg\_lig\_1048 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 224 | C=CCOc1ccc(- | Neg\_lig\_2885 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | n2ccnc2)cc1CO |  |  |  |  |  |
| 225 | N#Cc1c(-  c2cccc(O)c2)c(C#N)c 2nc3ccccc3n2c1N | Neg\_lig\_2890 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 226 | Cc1nc(N(C)Cc2nc3c c(F)ccc3[nH]2)cc(CC  [NH3+])[nH+]1 | Neg\_lig\_2919 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 227 | CSc1nc(- c2ccc(Cl)cc2)c(C#N) c(N2CCN(CCO)CC2  )n1 | Neg\_lig\_2926 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 228 | CC(=O)c1cccc(Nc2c cnc3ccc(F)cc23)c1 | Neg\_lig\_2954 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 229 | O=C(CCNc1ccc(Br)c c1)c1cccc([N+](=O) [O-])c1 | Neg\_lig\_2985 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 230 | CCCCCCC[C@]1(C) NC(=O)NC1=O | Neg\_lig\_3020 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 231 | CCOc1ncccc1C(=O) N1CC[C@@H]  (c2sccc2C)[C@H] (O)C1 | Neg\_lig\_3047 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 232 | Nc1c(C(=O)c2ccccc2  )sc2nc3c(cc12)C(=O) CCC3 | Neg\_lig\_3054 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 233 | Nc1c(C(=O)NCc2ccc cc2Cl)nnn1Cc1ccc(B r)cc1 | Neg\_lig\_3055 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 234 | CCC(=O)O[C@]1(C(  =O)CCl)[C@@H]  (C)C[C@H]2[C@@ H]3CCC4=CC(=O)C  =C[C@]4(C) [C@@]3(F)[C@@H] (O)C[C@@]21C | Neg\_lig\_3102 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 235 | Cc1cc(C)c(C#N)c(Sc 2nc(C)c([N+](=O)  [O-])c(C)c2C#N)n1 | Neg\_lig\_3114 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 236 | CCOc1ccc2oc(- c3ccccc3)c(C(=O)N3 CCN(CCO)CC3)c2c1 | Neg\_lig\_3125 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 237 | COc1ccc(CC(=O)n2n c(N)c3cc4ccc(OC)cc 4nc32)cc1 | Neg\_lig\_3169 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 238 | NC1=C([O-])c2ccccc 2C(=O)/C1=N\  c1ccc(Br)cc1 | Neg\_lig\_3225 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 239 | CCCCS(=O) (=O)CCCCCO | Neg\_lig\_3227 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 240 | O[C@H]  (COc1ccc2ccccc2c1) C[NH+]1CCCCC1 | Neg\_lig\_3287 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 241 | CCc1nc(N2C[C@H] (C3CC3)[C@@H] (NC(=O)CO)C2)ncc1 C | Neg\_lig\_3366 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 242 | N#CC1=C(N)OC2=C (C(=O)CCC2)  [C@@H]1c1ccc(F)cc 1 | Neg\_lig\_3375 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 243 | C[NH+] (C)C[C@H]1C[C@H  ] (CO)CN(C(=O)c2ccc | Neg\_lig\_3393 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | (-c3cnco3)cc2)C1 |  |  |  |  |  |
| 244 | Cc1cccc(CN2c3ccccc 3C3=C([C@@H]  (c4cccc(F)c4)C(C#N)  =C(N)O3)S2(=O)=O)  c1 | Neg\_lig\_3 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 245 | COC(=O)Nc1ccc(-  c2cnn(CCO)c2)cc1 | Neg\_lig\_5 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 246 | Cn1nc(CO)c2c1CCN (C(=O)c1cnc(Nc3ccc cc3)nc1)C2 | Neg\_lig\_13 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 247 | C[NH2+]CCN1C(=O  )CC[C@H]2CN(C(= O)CCCc3cn[nH]c3)C C[C@H]21 | Neg\_lig\_24 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 248 | Cc1cc(C)cc(NC(=O)c 2nnn(Cc3ccc(Cl)cc3) c2N)c1 | Neg\_lig\_112 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 249 | COc1ccc([C@H]2C( C#N)=C(N)Oc3c2sc2  ccccc32)cc1OC | Neg\_lig\_113 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 250 | O[C@H] (C#CCN1CCOCC1)c  1ccccc1 | Neg\_lig\_148 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 251 | C[C@@H]  (CNc1nc2ccc(Cl)cc2 n2cnnc12)c1ccccc1 | Neg\_lig\_245 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 252 | Cc1ccccc1- n1nc(CO)c(C(=O)NC  c2cccs2)n1 | Neg\_lig\_267 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 253 | COc1nc(NCc2cccnc2  )nc(N2CCSCC2)n1 | Neg\_lig\_292 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 254 | C=CCOc1c(Cl)cc([C @@H]2C(C#N)=C(  N)Oc3cc4c(cc32)OC O4)cc1OCC | Neg\_lig\_293 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 255 | CSc1nc2c(c(Nc3ccc( C)cc3)n1)CCC2 | Neg\_lig\_395 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 256 | Cc1nc(Nc2ncc3c(n2) CCCC3=O)nc2ccccc 12 | Neg\_lig\_419 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 257 | Cc1ccc2c(N)c(C(=O) c3ccc(- c4ccccc4)cc3)sc2n1 | Neg\_lig\_429 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 258 | Cc1cc(NCCCn2ccnc 2)n2nc(- c3ccccc3)c(C)c2[nH+  ]1 | Neg\_lig\_447 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 259 | C#CCOc1ccc([C@H] 2CC(=O)Nc3[nH]c(=  N)sc32)cc1OC | Neg\_lig\_501 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 260 | CSCC[C@@H] (CO)NC(=O)c1cc(C)  nc2cc(F)ccc12 | Neg\_lig\_512 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 261 | Cc1ccc(- n2nc(CO)c(C(=O)NC  c3ccncc3)n2)cc1C | Neg\_lig\_544 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 262 | Cc1c(S(=O)  (=O)c2ccccc2)c(N)n( Cc2ccccn2)c1C | Neg\_lig\_584 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 263 | O[C@H]  (Cn1c(Cc2ccccc2)nc 2ccccc21)Cn1c2ccc( | Neg\_lig\_636 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | Cl)cc2c2cc(Cl)ccc21 |  |  |  |  |  |
| 264 | COc1ccccc1N1CCC( [N@@H+]2CCN[C  @H] (C(=O)NC3CC3)C2) CC1 | Neg\_lig\_712 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 265 | CCc1ccc(C[NH2+]C  Cc2ccc(OC)c(OC)c2) cc1 | Neg\_lig\_721 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 266 | OC[C@H]1CCN(Cc  2cc(O)c3cccc(Cl)c3n 2)C[C@@H]1O | Neg\_lig\_780 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 267 | O=C([O-])c1cc2cc(O  Cc3ccccc3)ccc2[nH] 1 | Neg\_lig\_921 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 268 | O=C1c2ccccc2C(=O) N1OC[C@H] (O)COc1ccc([N+]  (=O)[O-])cc1 | Neg\_lig\_928 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 269 | Cc1c(- c2ccccc2)n(CCO)c2n c3c(c(=O)n(C)c(=O)n 3C)n12 | Neg\_lig\_956 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 270 | CCCc1cc(N2CCC([N  H2+]Cc3cnn(- c4ccccc4)c3)CC2)nc( C)n1 | Neg\_lig\_1009 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 271 | Cn1c(N)c(C(=O)C[N H2+]C2CCCCC2)c(= O)n(C)c1=O | Neg\_lig\_1030 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 272 | Cc1cc(C)n2c(Nc3ccc cc3C)c(- c3cccs3)nc2n1 | Neg\_lig\_1051 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 273 | Cc1cccc2nc(CCN3C(  =O)NC4(CC[NH2+] CC4)C3=O)[nH]c12 | Neg\_lig\_1063 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 274 | COCCOC(=O)C1=C( N)OC2=C(C(=O)CC(  C)(C)C2)  [C@H]1c1ccc(F)cc1 | Neg\_lig\_1126 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 275 | COc1ccc(- c2csc(NCCc3ccc(OC  )c(OC)c3)n2)cc1 | Neg\_lig\_1153 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 276 | NS(=O) (=O)N1CCN(C(=O)c 2cn(C[C@H]3CCC[ NH2+]C3)nn2)CC1 | Neg\_lig\_1183 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 277 | O=C1N[C@@]  (CCc2ccccc2) (C2CC[NH2+]CC2)C (=O)N1CCO | Neg\_lig\_1215 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 278 | O=C(Nc1cccc(OC(F) (F)F)c1)N1C[C@H] (O)[C@@H] (N2CCOCC2)C1 | Neg\_lig\_1229 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 279 | OCC[NH2+]Cc1ccc(  OCc2ccc3c(c2)OCC O3)cc1 | Neg\_lig\_1277 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 280 | Cc1nc(O)nc(C)c1CC C(=O)N1CCCC[C@ H]([NH3+])C1 | Neg\_lig\_1284 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 281 | N#CC1=C(N)N(c2cc ccc2)C2=C(C(=O)O C2) [C@@]12C(=O)N(C | Neg\_lig\_1313 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | c1ccccc1)c1ccccc12 |  |  |  |  |  |
| 282 | CC(C)NC(=O)  [C@@H]1C[C@@H  ] ([NH3+])CN1C(=O)c  1cc(-c2ccc(F)cc2) [nH]n1 | Neg\_lig\_1322 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 283 | O=C(/C=C\  c1cccnc1)NCCCCC1 CCN(C(=O)c2ccccc2  )CC1 | Neg\_lig\_1329 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 284 | CCOc1ccc(-c2noc(- c3nnn(- c4ccccc4)c3N)n2)cc1 | Neg\_lig\_1335 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 285 | CC(C)c1[nH+]ccn1C c1cc(C(=O)NC2CC( C)(C)[NH2+]C(C)  (C)C2)n[nH]1 | Neg\_lig\_1365 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 286 | C=CCOC(=O)C1=C( C)OC(N)=C(C#N)  [C@H]1c1cccs1 | Neg\_lig\_1387 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 287 | Cc1cccc(- c2nn3c(NCC(C)C)cc( C)[nH+]c3c2C)c1 | Neg\_lig\_1398 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 288 | Cc1ccc(N)c(C(=O)C CCCC(=O)[O-])c1 | Neg\_lig\_1409 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 289 | COc1ccc([C@@H]2c 3c(n[nH]c3- c3cc(C)ccc3O)C(=O) N2CCO)cc1OC | Neg\_lig\_1441 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 290 | c1cn(CCC[NH2+]Cc  2ccc3c(c2)OCO3)cn1 | Neg\_lig\_1498 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 291 | CN(C)c1ccc2[nH+]c 3ccc(=[N+](C)C)cc-  3sc2c1 | Neg\_lig\_529 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 292 | Nc1nonc1- c1nc2ccccc2n1Cc1cc c(Br)cc1 | Neg\_lig\_1635 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 293 | C[C@H]  (O)c1cccc(N2CCC(c 3[nH+]ccn3Cc3cccnc 3)CC2)n1 | Neg\_lig\_1658 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 294 | COCCN1C[C@@H]  (Cn2ccnc2- c2ccc(CO)o2)CC1=O | Neg\_lig\_1674 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 295 | [NH3+]CCN1C(=O) CC[C@H]2CN(C(=O  )c3nc4ccccn4c3F)CC [C@H]21 | Neg\_lig\_1700 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 296 | CCCc1c/c(=[NH+]\ CCN2CCOCC2)n2[n  H]c3nc(C)cc(C)c3c2 n1 | Neg\_lig\_1753 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 297 | Cc1cncc(C(=O)N2C CNC[C@H]2C(=O)  NCc2ccncc2)c1 | Neg\_lig\_1756 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 298 | O=C(NCc1ccncn1)c1 cn(CC[C@H]2CCCC [NH2+]2)nn1 | Neg\_lig\_1757 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 299 | COC(=O)N[C@H] (C(=O)N1CCC[C@H  ]1c1nc(-c2ccc(- c3ccc(- c4c[nH]c([C@H]5C CCN5C(=O) | Neg\_lig\_1759 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | [C@@H] (NC(=O)OC)C(C)C)  n4)cc3)cc2)c[nH]1)C (C)C |  |  |  |  |  |
| 300 | NS(=O) (=O)c1ccc(NC(=S)N  C(=O)c2ccco2)cc1 | Neg\_lig\_1771 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 301 | C[NH+] (C)C[C@H]1C[C@  @H] (CO)CN(C(=O)CNc2  nc3ccccc3s2)C1 | Neg\_lig\_1812 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 302 | Cc1ccccc1[C@H]1C( C#N)=C(N)OC2=C1 S(=O)  (=O)N(C)c1ccccc12 | Neg\_lig\_1876 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 303 | COc1ccc(N2CCN([C @H]3CCCN(C(=O)C O)C3)CC2)cc1 | Neg\_lig\_1836 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 304 | O=C(c1cccc(- c2ncc[nH]2)c1)N1C CC2(CC1)[C@@H] (OCCO)C[C@H]2O | Neg\_lig\_1966 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 305 | CCOC(=O)c1c(N)sc(  C(=O)Nc2ccc(C)c(Cl  )c2)c1C | Neg\_lig\_1465 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 306 | C=CCNC(=S)NCC | Neg\_lig\_1986 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 307 | CO/C(O)=C1/ C2=C(CCC2)S/ C1=N\C(=O)NCCCO | Neg\_lig\_1989 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 308 | Cc1cc(C)c2oc(- c3ccc(C)c(N)c3)nc2c 1 | Neg\_lig\_2005 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 309 | O=C(c1cn[nH]c1C1C CCCC1)N1CCOc2cc c(CO)cc2C1 | Neg\_lig\_2035 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 310 | CCOc1ccc(-c2noc(- c3nnn(- c4ccccc4C)c3N)n2)c c1 | Neg\_lig\_2084 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 311 | O[C@@H]  (Cc1ccc2ccccc2n1)C( Cl)(Cl)Cl | Neg\_lig\_2134 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 312 | CCCCCN(CC[C@]1 2C[C@H]3C[C@H] (C[C@H] (C3)C1)C2)C(=O)NC  CCc1ccncc1 | Neg\_lig\_2169 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 313 | O=C(CCCCCCNC(=  O)c1cnc(N(c2ccccc2) c2ccccc2)nc1)NO | Neg\_lig\_2175 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 314 | CCOc1ncccc1C(=O) N1C[C@@H]2c3ccc cc3OC[C@]2(CO)C1 | Neg\_lig\_2193 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 315 | Cc1cccc(-c2noc(- c3cccnc3NCc3ccccc3  )n2)c1 | Neg\_lig\_2244 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 316 | Cc1ccc(C(=O)c2sc3n c4c(cc3c2N)C(=O)C C(C)(C)C4)cc1 | Neg\_lig\_2253 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 317 | CCCc1nc2nc(C)cc(N c3ccc(C)c(F)c3)n2n1 | Neg\_lig\_2256 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 318 | Cn1c(=O)n(C)c2cc(C [NH2+]CCc3ccc(Cl)c | Neg\_lig\_2319 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | c3)ccc21 |  |  |  |  |  |
| 319 | O=C1CCC2(CCN(Cc  3nnc(- c4cccnc4)o3)CC2)C N1CCO | Neg\_lig\_1 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 320 | Cc1nc(N2CCN(C(=O  )CN3CC(=O)NC3=O  )C[C@H](O)C2)no1 | Neg\_lig\_2362 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 321 | O=C(CN1CCCC1)Nc  1nc(- c2ccc(Cl)cc2)cs1 | Neg\_lig\_2392 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 322 | COc1ccccc1- n1nc(C)c(- c2ccccc2)c1N | Neg\_lig\_2397 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 323 | CCc1cnc(NC[C@H] (O)c2cccc(O)c2)nc1 | Neg\_lig\_2408 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 324 | CN(CC1(CO)CC1)C(  =O)Nc1ccc(-c2nnc(- c3ccco3)o2)cc1 | Neg\_lig\_2418 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 325 | CCCc1c(C)nc2ncnn2 c1Nc1ccc(N2CCOC C2)cc1 | Neg\_lig\_2440 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 326 | CC[C@@H]  (CO)N(Cc1cccnc1)C c1nn(C)c2cccc(Cl)c1 2 | Neg\_lig\_2510 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 327 | CCOC(=O)c1c(N)n(-  c2cc(C)ccc2C)c2nc3c cccc3nc12 | Neg\_lig\_1698 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 328 | CCCc1nc(C(=O)N2C C[C@@H]  (c3sccc3C)[C@H] (O)C2)cs1 | Neg\_lig\_2531 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 329 | CNC(=O)c1sc(N2CC CC2)nc1N | Neg\_lig\_2545 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 330 | CC(=O)N1CCN(Cc2  ccccc2C(=O)  [O-])C[C@H](O)C1 | Neg\_lig\_2560 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 331 | Nc1nnnn1CC(=O)N1 CCC2(CCC(=O)N(C[ C@H]3CCCO3)C2) CC1 | Neg\_lig\_2566 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 332 | Cc1ccc(N[C@@H]2c 3ccccc3C(=O)N2c2c cccc2C)cc1 | Neg\_lig\_2574 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 333 | CCOC(=O)c1ccc(- n2c(N)c(C(=O)OC)c  3nc4ccccc4nc32)cc1 | Neg\_lig\_2600 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 334 | O=C(OCc1ccccc1)c1 nc2ccccc2nc1NCc1cc ccc1 | Neg\_lig\_2620 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 335 | O=C(NC[C@H]  (O)c1ccccc1C(F) (F)F)c1c[nH]nc1- c1ccccc1 | Neg\_lig\_2649 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 336 | Oc1cccc(Nc2cc(- c3ccccc3)ncn2)c1 | Neg\_lig\_2719 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 337 | O=C(c1ccccc1[C@H  ]1CC[NH2+]C1)N1C  Cc2[nH]c3ccccc3c2C 1 | Neg\_lig\_2769 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 338 | Cc1ccc2nc(C[NH2+] C[C@H] | Neg\_lig\_2615 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | (C)Oc3cccnc3) [nH]c2c1C |  |  |  |  |  |
| 339 | Cc1ccc(Nc2nc3ccccc 3c3nnc(C)n23)cc1F | Neg\_lig\_1048 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 340 | C=CCOc1ccc(- n2ccnc2)cc1CO | Neg\_lig\_2885 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 341 | N#Cc1c(-  c2cccc(O)c2)c(C#N)c 2nc3ccccc3n2c1N | Neg\_lig\_2890 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 342 | Cc1nc(N(C)Cc2nc3c c(F)ccc3[nH]2)cc(CC  [NH3+])[nH+]1 | Neg\_lig\_2919 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 343 | CSc1nc(- c2ccc(Cl)cc2)c(C#N) c(N2CCN(CCO)CC2  )n1 | Neg\_lig\_2926 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 344 | CC(=O)c1cccc(Nc2c cnc3ccc(F)cc23)c1 | Neg\_lig\_2954 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 345 | O=C(CCNc1ccc(Br)c c1)c1cccc([N+](=O) [O-])c1 | Neg\_lig\_2985 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 346 | CCCCCCC[C@]1(C) NC(=O)NC1=O | Neg\_lig\_3020 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 347 | CCOc1ncccc1C(=O) N1CC[C@@H]  (c2sccc2C)[C@H] (O)C1 | Neg\_lig\_3047 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 348 | Nc1c(C(=O)c2ccccc2  )sc2nc3c(cc12)C(=O) CCC3 | Neg\_lig\_3054 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 349 | Nc1c(C(=O)NCc2ccc cc2Cl)nnn1Cc1ccc(B r)cc1 | Neg\_lig\_3055 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 350 | CCC(=O)O[C@]1(C(  =O)CCl)[C@@H]  (C)C[C@H]2[C@@ H]3CCC4=CC(=O)C  =C[C@]4(C) [C@@]3(F)[C@@H] (O)C[C@@]21C | Neg\_lig\_3102 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 351 | Cc1cc(C)c(C#N)c(Sc 2nc(C)c([N+](=O)  [O-])c(C)c2C#N)n1 | Neg\_lig\_3114 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 352 | CCOc1ccc2oc(- c3ccccc3)c(C(=O)N3 CCN(CCO)CC3)c2c1 | Neg\_lig\_3125 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 353 | COc1ccc(CC(=O)n2n c(N)c3cc4ccc(OC)cc 4nc32)cc1 | Neg\_lig\_3169 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 354 | NC1=C([O-])c2ccccc 2C(=O)/C1=N\  c1ccc(Br)cc1 | Neg\_lig\_3225 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 355 | CCCCS(=O) (=O)CCCCCO | Neg\_lig\_3227 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 356 | O[C@H]  (COc1ccc2ccccc2c1) C[NH+]1CCCCC1 | Neg\_lig\_3287 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 357 | CCc1nc(N2C[C@H] (C3CC3)[C@@H] (NC(=O)CO)C2)ncc1 C | Neg\_lig\_3366 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 358 | N#CC1=C(N)OC2=C (C(=O)CCC2) | Neg\_lig\_3375 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | [C@@H]1c1ccc(F)cc 1 |  |  |  |  |  |
| 359 | C[NH+] (C)C[C@H]1C[C@H  ] (CO)CN(C(=O)c2ccc  (-c3cnco3)cc2)C1 | Neg\_lig\_3393 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 0 |
| 360 | CCC(=O)OCCNc1nc (-  c2ccccc2)nc2ccccc12 | Neg\_lig\_2 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 361 | CC1(C)CC(=O)C2=C (C1)OC(N)=C(C#N)  [C@H]2c1ccccc1OC (=O)N1CCOCC1 | Neg\_lig\_73 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 362 | COc1ccc(CN2C(=O)  c3cccnc3[C@H]2Nc 2cc(Cl)ccc2OC)cc1 | Neg\_lig\_78 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 363 | COCC[N@H+] (C)C[C@@H]1CN(c  2ncc(C)c(N(C)C)n2) C[C@@H]1CO | Neg\_lig\_84 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 364 | Cn1c(=[NH2+])n(CC  O)c2ccccc21 | Neg\_lig\_86 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 365 | CCN(CC)C(=O)  [C@@H]1C[C@@H  ] ([NH3+])CN1C(=O)c  1csc(-c2cccs2)n1 | Neg\_lig\_95 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 366 | COCC[C@]1(CO)C CCN(C(=O)Cc2ccc( CO)cc2)C1 | Neg\_lig\_129 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 367 | CCCc1cncnc1N1CC C([NH2+]C2CCN(C(  =O)OCC)CC2)CC1 | Neg\_lig\_131 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 368 | COc1ccc(/C=C/ CN2CC[C@@H]  (NC(=O)c3cccnc3) [C@H](O)C2)cc1 | Neg\_lig\_141 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 369 | CCn1c(CC2CC[NH2  +]CC2)nn(CC(=O)N  Cc2ccccc2)c1=O | Neg\_lig\_150 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 370 | CCOc1ccccc1NC(=O  )c1nnn(-c2cccc(C(F) (F)F)c2)c1N | Neg\_lig\_157 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 371 | NC[C@H]1CC[N@ H+](Cc2ccc(C(F)  (F)F)cc2)C1 | Neg\_lig\_158 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 372 | Cc1ccc2c(c1)c(- c1ccccc1)c(- c1ccccc1)n2C[C@H] (O)C[NH+]1CCCCC 1 | Neg\_lig\_181 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 373 | COc1ccc(- c2ccc3c(N4CCOCC4  )nc(N4C[C@H]  (C)O[C@H] (C)C4)nc3[nH+]2)cc 1CO | Neg\_lig\_209 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 374 | N#CC1=C(N)OC2=C (C(=O)CCC2)  [C@@H]1c1cc(C[N H+]2CCOCC2)cs1 | Neg\_lig\_280 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 375 | NC(=O)c1ccc(N2CC N(Cc3c[nH]nn3)C[C @H](O)C2)nc1 | Neg\_lig\_282 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 376 | COC(OC) [C@]1(C)NC(=O)c2c  cccc2N1 | Neg\_lig\_328 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 377 | Nc1cc(OC(=O)c2ccc cc2F)nn1S(=O) (=O)c1ccccc1 | Neg\_lig\_335 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 378 | CC[C@H]  (C)c1ccc(OCc2nnc(N  )s2)cc1 | Neg\_lig\_365 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 379 | CCC[C@H]  (O)c1nc2ccccc2n1Cc 1ccccc1Cl | Neg\_lig\_367 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 380 | Nc1cc(- c2ccc3c(c2)OCO3)cc n1 | Neg\_lig\_369 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 381 | C[C@@H](c1ccc(- c2nc3ccccc3n2CCO) cc1)N1CCOCC1 | Neg\_lig\_384 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 382 | COCc1cc(C)nc2sc(- c3nnc(- c4ccccc4)o3)c(N)c12 | Neg\_lig\_398 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 383 | [NH3+]CCn1cc(C(=  O)NCCc2noc(- c3ccccc3)n2)nn1 | Neg\_lig\_408 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 384 | C[C@@H]1C[C@H] 2[C@@H]3CCC4=C C(=O)C=C[C@]4(C)  [C@@]3(F)[C@@H]  (O)C[C@]2(C)  [C@@]1(O)C(=O)C O | Neg\_lig\_425 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 385 | COc1ccc([C@@H]2 C(C#N)=C(N)OC3= C2C(=O)CC(C) (C)C3)cc1OC | Neg\_lig\_436 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 386 | C[NH+]  (C)CCc1c[nH]c2ccc( CS(=O) (=O)N3CCCC3)cc12 | Neg\_lig\_244 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 387 | OCCSc1nnc(COc2cc c(Cl)cc2)n1-c1ccccc1 | Neg\_lig\_468 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 388 | O=C(CCCCCCC(=O  )Nc1ccc([C@@H]2O [C@H]  (c3ccc(CO)cc3)C[C @H](CSc3nc(- c4ccccc4)c(- c4ccccc4)o3)O2)cc1) NO | Neg\_lig\_517 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 389 | CO[C@H]1C[C@@ H] (O)C12CCN(C(=O)C  [NH+]1CCC(C(N)=O  )CC1)CC2 | Neg\_lig\_594 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 390 | CC1=C(CCN2CC[C  @@H] (NC(=O)c3ccncc3) [C@H](O)C2)C(C) (C)CCC1 | Neg\_lig\_668 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 391 | O=[N+]  ([O-])c1ccc2c(c1) [S@](=O)c1ccccc1-2 | Neg\_lig\_702 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 392 | CC1(C)CC(NC(=O)C  CCOc2ccc(Cl)cc2Cl) CC(C)(C)[NH2+]1 | Neg\_lig\_726 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 393 | O[C@@]1(C[NH+]2  CCC3(C=Cc4ccccc4 3)CC2)CNCCOC1 | Neg\_lig\_732 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 394 | COc1ccccc1N1CCN( C[C@H] (O)COc2ccc([C@]34 C[C@H]5C[C@H]  (C[C@H] (C5)C3)C4)cc2)CC1 | Neg\_lig\_742 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 395 | Cc1ccc(C)c(-n2c(- c3ccc(Br)cc3)cs/ c2=N\ C(=O)c2ccccc2F)c1 | Neg\_lig\_745 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 396 | CCO/C(O)=C1/ C(C)=[NH+]C(=O)N  [C@H]1c1ccc(OCC O)c(OC)c1 | Neg\_lig\_803 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 397 | CC(C)c1cc(NCc2nc( N)nc(N(C)C)n2)n2nc cc2[nH+]1 | Neg\_lig\_809 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 398 | COc1ccc(C)cc1- n1nnc(-c2nc(- c3ccccc3Cl)no2)c1N | Neg\_lig\_841 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 399 | Cc1ccc2nc(CNCc3cs c(- c4ncccn4)n3)cc(O)c2 c1 | Neg\_lig\_866 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 400 | Cc1[nH]c(/C=C2/ C(=O)Nc3ccccc32)c( C)c1CCC(=O)[O-] | Neg\_lig\_873 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 401 | CC(=O)N1CCN(c2cc  c(NCc3ccc(F)cc3)cc2  )CC1 | Neg\_lig\_943 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 402 | Cc1cc(C)n(C[C@H]  (C)O)c(=O)c1C#N | Neg\_lig\_969 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 403 | COc1cc(OC)c(OC)cc 1C=O | Neg\_lig\_1061 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 404 | C=CCNc1ncnc2c1sc 1nc3c(cc12)COC(C) (C)C3 | Neg\_lig\_1087 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 405 | S=C1SCN(CCc2cccc c2)CN1CCc1ccccc1 | Neg\_lig\_1099 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 406 | Cn1nccc1- c1ccccc1OC[C@@H  ] (O)C[NH+]1CCCCC 1 | Neg\_lig\_1123 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 407 | CCOC(=O)c1ccccc1 N[C@H]1OC(=O)c2  ccccc21 | Neg\_lig\_1135 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 408 | CCN(CC1CCOCC1)  C(=O)c1ccc(C[C@H  ]2CCC[NH2+]C2)cc 1 | Neg\_lig\_1158 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 409 | COc1ccc2c(c1) [C@]13CC[N@@H+  ](C)[C@H](C2) [C@@H]1CCC1(C3) OCCO1 | Neg\_lig\_618 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 410 | [NH3+] [C@H]1CCN(C(=O)  c2cccc(- c3ncc[nH]3)c2)C1 | Neg\_lig\_1192 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 411 | COc1cccc(C[NH2+] Cc2cccnc2)c1OCc1c | Neg\_lig\_1237 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | cc(F)cc1 |  |  |  |  |  |
| 412 | O=C1C[C@H] (NC2CCCC2)C(=O)  N1c1ccc(Cl)cc1 | Neg\_lig\_1248 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 413 | COc1ccc(- n2nc3ccc(N)cc3n2)cc 1 | Neg\_lig\_1290 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 414 | Nc1ncnc2c1ncn2[C @@H]1O[C@@H] (CO)[C@@H](O) [C@@H]1N | Neg\_lig\_1319 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 415 | Cn1c(=O)n(C)c2cc(C [NH2+]Cc3cccnc3)cc c21 | Neg\_lig\_1358 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 416 | OC[C@H]1C[N@H+  ] (Cc2cnc(N3CCCCC3  )nc2)C[C@H]1CN1C COCC1 | Neg\_lig\_1399 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 417 | CNc1ncnc2c1c(- c1ccccc1)cn2- c1cccc(Cl)c1 | Neg\_lig\_1420 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 418 | CC[C@H]  (O)c1nc2ccccc2n1CC COc1cccc(C)c1C | Neg\_lig\_1426 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 419 | O=C(CCCc1cn[nH]c 1)N1CCC2(CC1)Nc1  ccccc1NC2=O | Neg\_lig\_1430 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 420 | CC[C@@]1(c2ccc(N  )cc2)CCC(=O)NC1= O | Neg\_lig\_1442 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 421 | O=C([O-])c1ccccc1C N1CCN(C(=O)c2ccc o2)C[C@@H](O)C1 | Neg\_lig\_1443 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 422 | COc1cc(C)nc(N(CC O)CCO)n1 | Neg\_lig\_1472 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 423 | CS(=O)(=O)  [N-]c1ccc(- c2ccc(N)cc2)cc1[N+] (=O)[O-] | Neg\_lig\_1505 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 424 | COC(=O)c1ccc(-  c2c(C#N)c(N)nc3c2C CCCC3)cc1 | Neg\_lig\_1554 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 425 | COc1ccc(CN[C@H] 2CS(=O) (=O)C[C@@H]2S(= O)  (=O)c2ccc(OC)cc2)c c1 | Neg\_lig\_1583 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 426 | O=C(c1cccc(OC2CC N(Cc3ccncc3)CC2)c 1)N1CCC[NH2+]CC  1 | Neg\_lig\_1593 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 427 | CC(C)[NH2+]  [C@@H]1CC[C@@ H]1NC(=O)CCSCc1c  cccc1 | Neg\_lig\_1598 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 428 | Cc1ccc(F)c(Cn2ccnc 2-  c2ccc(C#CCO)s2)c1 F | Neg\_lig\_1607 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 429 | Cc1[nH+]ccn1- c1ccc(C[NH2+] [C@@H](C)CO)cc1 | Neg\_lig\_1610 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 430 | C=CCn1cc(C[NH2+]  Cc2cc3cc(OC)ccc3[n H]2)c(C)n1 | Neg\_lig\_1678 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 431 | O=C1CC[C@]2(CC C[N@H+]  (CCOc3ccc(Cl)cc3)C 2)CN1CCO | Neg\_lig\_1744 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 432 | COCc1cc([C@H]2N[  C@](CO)(c3ccccc3) [C@H]3C[N@H+]  (C)C[C@@H]23)ccc 1OC | Neg\_lig\_1762 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 433 | COc1ccc(C2=NC(=O  )N[C@@H]2c2ccc(O C)cc2)cc1 | Neg\_lig\_1776 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 434 | CCCn1cnc2cc(NCc3 ccc(Br)cc3)ccc21 | Neg\_lig\_1806 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 435 | NC1=C(c2nc3ccccc3 s2)C(=O)CN1c1ccc( N2CCCCC2)cc1 | Neg\_lig\_1846 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 436 | Cc1ccc(CC[NH2+]C  c2cc(O)c3cccc(Cl)c3 n2)s1 | Neg\_lig\_1853 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 437 | Cc1nnc2c(NCCCN3 CCN(c4cccc(Cl)c4)C C3)nc3ccccc3n12 | Neg\_lig\_1858 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 438 | COc1ccc2c(CNCCc3 ccccc3OC)c(C(=O)O  )n(C)c2c1 | Neg\_lig\_1894 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 439 | O=c1c2c(nc(NCCCO  )n1-c1ccccc1)- c1ccccc1CC21CCCC 1 | Neg\_lig\_1958 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 440 | CCSc1ccc(C(=O)N2 CCC3(CC2)  [C@@H] (O)C[C@H]3O)s1 | Neg\_lig\_1960 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 441 | Cc1ccc([C@H]2C[C @@H](C(F) (F)F)n3ncc(C(=O)Nc  4ccc([C@@H] (C)O)cc4)c3N2)cc1 | Neg\_lig\_1971 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 442 | CN(C)c1nc(-  c2ccccc2)nc2c1CCN( C(=O)c1ccc(N)nc1)C 2 | Neg\_lig\_2010 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 443 | C[C@H](O)Cc1n/  c(=N/ C(=O)c2ccc(C(C)  (C)C)cc2)s[nH]1 | Neg\_lig\_2013 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 444 | COc1ccc(- c2c(NCc3ccccc3Cl)c(  =O)c2=O)cc1 | Neg\_lig\_2021 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 445 | CCc1[nH]nc2c1C1(C (C#N)=C(N)O2)c2cc  ccc2-c2ccccc21 | Neg\_lig\_1701 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 446 | Cc1nc(C2=C(N)N(C[ C@H] (C)O)CC2=O)sc1C | Neg\_lig\_162 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 447 | Cc1ccc(- c2noc(CNc3cccc(C)c 3)n2)cc1 | Neg\_lig\_2128 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 448 | CC1=C(c2ccccc2)S(= O)  (=O)N=C1Nc1ccccc1 | Neg\_lig\_2132 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | Br |  |  |  |  |  |
| 449 | Cc1cc(NC2CCCC2)n  c2ccccc12 | Neg\_lig\_2138 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 450 | Nc1nnc(CC(=O)N2C CC(Cc3noc(C4CC4) n3)CC2)s1 | Neg\_lig\_2142 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 451 | C=CCNc1c(O)cc2c( O)c1C[C@@H] (C)C[C@H](OC) [C@@H](O)  [C@@H](C)/C=C(/  C)[C@H](OC(N)=O) [C@@H](OC)/C=C\ C=C(\C)C(=O)N2 | Neg\_lig\_2147 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 452 | COc1ccc(CNc2[nH+] c3ccc(C)cc3cc2- c2noc(C)n2)cc1OC | Neg\_lig\_2189 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 453 | CC[n+]1cn(C[C@H]  (O)COc2ccccc2)c2cc (C)c(C)cc21 | Neg\_lig\_2279 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 454 | O=C(/C=C/  c1cccc(S(=O) (=O)Nc2ccccc2)c1)N O | Neg\_lig\_2342 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 455 | CCN1c2ccccc2C2=C ([C@@H]  (c3ccc(Br)cc3)C(C# N)=C(N)O2)S1(=O)= O | Neg\_lig\_2347 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 456 | Cc1cc(C)nc([N-]S(= O)  (=O)c2ccc(NCc3nc4c cccc4n3C)cc2)n1 | Neg\_lig\_2380 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 457 | CC1=NC(C) (C)C[C@H]2CC[C@  @H](O)[C@@H]12 | Neg\_lig\_2433 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 458 | Cn1c(=O)nc([O-])c2c 1nc(NCCO)n2Cc1ccc (Cl)cc1 | Neg\_lig\_2219 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 459 | OCCSc1nnc(COc2cc c(Br)cc2)n1-c1ccccc1 | Neg\_lig\_2442 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 460 | Cc1ccc(S(=O)(=O)  [C@H]2CS(=O) (=O)C[C@@H]2NC  Cc2ccc(F)cc2)cc1 | Neg\_lig\_2458 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 461 | Cc1nc(N)nc(N2CC[C  @@]3(CC(=O)c4ccc cc4O3)C2)c1C | Neg\_lig\_2483 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 462 | CC1=C(c2ccc(C(C)C  )cc2)S(=O)  (=O)N=C1NCc1cccc c1F | Neg\_lig\_2529 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 463 | CS(=O)  (=O)N(Cc1ccccc1)c1 ccc(C(=O)N[C@@H  ]2CCCC[C@@H]2O  )cc1 | Neg\_lig\_2570 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 464 | NC(=O)CN1CC2(CC C1=O)CCN(C(=O) [C@@H]1C[NH2+] CCO1)CC2 | Neg\_lig\_2586 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 465 | Cc1ccc2nc(- c3ccsc3)c(Nc3ccccc3  )n2c1 | Neg\_lig\_2591 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 466 | CC(=O)c1cccc(- | Neg\_lig\_2666 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | c2nc(CC3CC[NH+] (C)CC3)nn2CCO)c1 |  |  |  | GG |  |
| 467 | Nc1nn2c(- c3ccncc3)nnc2s1 | Neg\_lig\_2697 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 468 | Cn1ncc2c(Nc3ccccc3 Cl)nc(Nc3ccccc3Cl)n c21 | Neg\_lig\_2710 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 469 | Cc1ccccc1Cn1c(NCC O)nc2c1c(=O)n(C)c(  =O)n2C | Neg\_lig\_2721 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 470 | CNC(=O)  [C@@H]1C[C@@H  ]([NH3+])CN1C(=O)  [C@@H] (OC)c1ccccc1 | Neg\_lig\_2729 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 471 | O[C@H]  (c1ccccc1)c1nn(C[N H+]2CCOCC2)c(=S)  n1-c1ccccc1 | Neg\_lig\_2740 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 472 | CC(=O)c1sc(NC(C)C  )nc1N | Neg\_lig\_2795 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 473 | CCn1c(N)nc2cc(C(= O)N(C)Cc3noc(-  c4ccccc4)n3)cnc21 | Neg\_lig\_2816 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 474 | Nc1ccc2ncc(=O) [nH]c2c1 | Neg\_lig\_2830 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 475 | Cc1ccc(NC(=O)N2C CN(C(=O)c3nonc3N)  CC2)cc1Cl | Neg\_lig\_2833 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 476 | CCCCCCCCc1ccc(C CC([NH3+]) (CO)CO)cc1 | Neg\_lig\_2868 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 477 | C[C@H](/ N=C1C(=C(\N)O)/ S(=O)  (=O)c2ccccc2/1)c1cc ccc1 | Neg\_lig\_2882 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 478 | Cc1cc(Nc2cc(N3CC[ NH+](C)CC3)nc(/  C=C/c3ccccc3)n2) [nH]n1 | Neg\_lig\_2886 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 479 | CCOC(=O)c1sc2nc3c (cc2c1N)CO[C@H] (C(C)C)C3 | Neg\_lig\_2888 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 480 | CCOC(=O)Cn1nc2oc (=O)c(CCN3CCN(c4  ccccc4OC)CC3)c(C)c 2c1C | Neg\_lig\_2947 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 481 | Cc1ccc(NC(C) (C)C(=O)N2CC[C@  H](C[NH3+])C2)cc1 | Neg\_lig\_3004 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 482 | CSCCc1nc(-c2ccc(- c3cc[nH]n3)cc2)n(C CO)n1 | Neg\_lig\_3025 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 483 | Cc1ccc2[nH]c3c(c2c 1)CCC[C@@H]3[N H2+]CCCOc1ccc(F)c  c1 | Neg\_lig\_3042 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 484 | COc1ccc(C(=O)NC2 CC2)cc1NC(=O)N[C  @@H] (C)c1nnc(N)s1 | Neg\_lig\_3049 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 485 | Nc1c(-c2nc(- c3ccccc3)no2)nnn1- | Neg\_lig\_2907 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | c1ccc(F)cc1F |  |  |  |  |  |
| 486 | CCCc1c(C(=O)OCC) sc(N)c1C#N | Neg\_lig\_3112 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 487 | CC[N@H+]1C[C@ @H]2[C@H](C1)  [C@H]1CC[C@]2(C  )O1 | Neg\_lig\_3117 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 488 | CC1CCN(C(=O)c2cc cc(NC(=O)N[C@@H  ]  (CO)c3ccccc3)c2)CC 1 | Neg\_lig\_3139 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 489 | O=C(O) [C@@H]1CC2(CCN (C(=O)CCCn3ccnc3) CC2)CN1 | Neg\_lig\_3149 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 490 | c1ccc2c(c1)nc(Nc1cc c(N3CCOCC3)cc1)n  1cnnc21 | Neg\_lig\_3215 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 491 | COc1ccc(-c2noc(- c3nnn(- c4cc(C)ccc4C)c3N)n 2)cc1 | Neg\_lig\_3221 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 492 | COCc1cc(CN2CC3( CC[NH2+]CC3)C[C @H]2C(=O)O)ccc1O C | Neg\_lig\_3241 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 493 | Cc1nc(C(=O)N2CC[ C@H] ([NH+]3CCN(C)CC3  )[C@H] (CCCO)C2)cs1 | Neg\_lig\_3282 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 494 | C/C1=C2/N=C(/ C=C3\N=C(/ C(C)=C4\N[C@@] (C) ([C@@H]5N=C1[C @](C) (CCC(=O)NC[C@H]  (C)O[P@](=O)  ([O-])O[C@@H]1[C @@H](CO)O[C@H]  (n6cnc7cc(C)c(C)cc7 6)[C@@H]1O)  [C@H]5CC(N)=O)  [C@@](C)  (CC(N)=O) [C@@H]4CCC(N)= O)[C@@](C)  (CC(N)=O) [C@@H]3CCC(N)= O)C(C)(C) [C@@H]2CCC(N)= O.O.[Co+] | Neg\_lig\_3314 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 495 | Cc1ccccc1N1CCN(C (=O)c2cn(C3CC[NH 2+]CC3)nn2) [C@@H](C)C1 | Neg\_lig\_423 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 496 | O=C(c1ccc2c(c1)CC C2)N1CCC2(CC1)O CCC[C@@H]2O | Neg\_lig\_1439 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 497 | [NH3+] [C@@H]1CC[C@H]  (C(=O)NCc2ccc3c(c2  )CCCC3)C1 | Neg\_lig\_1992 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 0 |
| 498 | COc1cccc(OCc2cc([ C@H]3Nc4ccccc4C(  =O)N3Cc3ccccc3)ccc | Neg\_lig\_18 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | 2OC)c1 |  |  |  |  |  |
| 499 | O=C([O-])c1cc(NC2  =NS(=O)  (=O)c3ccccc32)ccc1 O | Neg\_lig\_75 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 500 | Cc1cc2c(c(=O)o1) [C@H]  (c1ccc(Cl)c(Cl)c1)C( C#N)=C(N)O2 | Neg\_lig\_102 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 501 | COc1ccccc1Nc1nc(N  )nc(CSc2nc3ccccc3s2  )n1 | Neg\_lig\_161 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 502 | Nc1nnc(SCC(=O)Nc 2cccc(F)c2)s1 | Neg\_lig\_176 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 503 | COCC[C@]1(CO)C CCN(C(=O)CCN2C CCCCC2=O)C1 | Neg\_lig\_179 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 504 | O=C(CNCc1ccccc1) N1c2ccccc2Sc2ccc(C (F)(F)F)cc21 | Neg\_lig\_227 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 505 | C[NH+]1CCN(c2nc( N)cc(=O)[nH]2)CC1 | Neg\_lig\_233 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 506 | Nc1ncccc1C[NH+]1 CCC2(CC1)CN(CCO  c1ccccc1)C(=O)O2 | Neg\_lig\_237 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 507 | CC(=O)C1=C(O)C[C  @H](c2ccccc2)C/ C1=N\CCc1c(C)  [nH]c2ccccc12 | Neg\_lig\_251 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 508 | Cc1ccnc(-n2cccc2- c2cc(- c3cn(C)nc3C)nc(N)c 2C#N)c1 | Neg\_lig\_254 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 509 | CSc1ccc([C@@H]2 C(C#N)=C(N)OC3= C2C(=O)CC(C)  (C)C3)cc1 | Neg\_lig\_387 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 510 | CO[C@H]1/C=C\ O[C@@]2(C)Oc3c(C  )c(O)c4c(c3C2=O)C(  =O)/C(=C\ NN2CCN(C3CCCC3  )CC2)C(=C4O)NC(= O)/C(C)=C\C=C/ [C@H](C)[C@H](O) [C@@H](C)  [C@@H](O) [C@@H](C)[C@H]  (OC(C)=O)[C@H]1C | Neg\_lig\_415 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 511 | O=C(CN1CCC(c2ccc  cc2)CC1)NCc1cc2n( n1)CC[NH2+]C2 | Neg\_lig\_465 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 512 | [NH3+]  [C@@H]1CCN(c2nc 3c(c(C(F) (F)F)n2)CCCC3)C[C @H]1O | Neg\_lig\_507 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 513 | Nc1cc(=O) [nH]c(CCNC(=O)c2c  n(-c3ccccc3)nn2)n1 | Neg\_lig\_534 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 514 | CSc1nc(NCCC[NH+] (C)C)c(C#N)c(-  c2ccc(Cl)cc2)n1 | Neg\_lig\_546 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 515 | CCOC(=O)NC[C@ @H]1CCN(C(=O)c2 | Neg\_lig\_557 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | nc3cc(F)ccc3[nH]2)C [C@H]1O |  |  |  |  |  |
| 516 | Nc1c(-c2nc(- c3ccc(Br)cc3)no2)nn n1-c1ccccc1F | Neg\_lig\_569 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 517 | O=c1[nH]  [nH]c(CNc2ccc(Cl)cc 2)[nH+]1 | Neg\_lig\_576 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 518 | C=CC[NH2+]Cc1ccc cc1C(F)(F)F | Neg\_lig\_588 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 519 | O[C@@H](Cn1cnc(- c2ccccc2)c1- c1ccc2nonc2c1)c1ccc nc1 | Neg\_lig\_605 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 520 | CN(C) [C@@H]1C(O)=C(C  (N)=O)C(=O)  [C@]2(O)C(O)=C3C  (=O)c4c(O)cccc4[C @@](C)(O)  [C@H]3[C@H](O) [C@@H]12 | Neg\_lig\_684 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 521 | Nc1nc(- c2ccc(Cl)c(Cl)c2)nc2 c1c(=O)oc1ccccc12 | Neg\_lig\_708 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 522 | CCOC(=O)c1cnoc1N | Neg\_lig\_754 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 523 | Cc1cccc(-n2nnc(- c3nc(- c4ccc(Br)cc4)no3)c2 N)c1C | Neg\_lig\_789 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 524 | Cc1cc(C)c(- c2c(N[C@H]3CC[C  @@H] (C)CC3)c(=O)c2=O)  cc1C | Neg\_lig\_791 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 525 | COc1ccc(CN[C@H] 2CS(=O) (=O)C[C@@H]2S(= O)  (=O)c2ccc(F)cc2)cc1 OC | Neg\_lig\_897 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 526 | Cc1ccc(-c2cc(- c3ccc(OC(C)C)c(CO)  c3)c(C#N)c(N)n2)nc 1 | Neg\_lig\_908 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 527 | CCN(CC)C(=O)  [C@H]1C(=O)N(CC O) [C@@]2(C)C[C@@  H]1c1ccccc1O2 | Neg\_lig\_933 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 528 | CC(=O)C[NH2+]C(C  )(C)C | Neg\_lig\_946 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 529 | Cc1ccc(OCCNC[C@  ]2(O)CCC[NH2+]C2  )cc1C | Neg\_lig\_1003 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 530 | Cc1cc(N[C@H]2CC  Cc3nc(- c4ccccc4)ncc32)nc(N  )n1 | Neg\_lig\_1025 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 531 | Nc1c(-c2nc(- c3ccc(F)cc3)no2)nnn 1-c1ccccc1 | Neg\_lig\_1045 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 532 | CC1=C(C(=O)OC(C) (C)C) [C@]2(C(=O)Nc3ccc | Neg\_lig\_1077 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | cc32)C(C(=O)OC(C)  (C)C)=C(N)O1 |  |  |  |  |  |
| 533 | O=C(NCc1cn2c([nH  +]1)SCC2)c1cn(C[C @H]2CCC[NH2+]C2  )nn1 | Neg\_lig\_1104 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 534 | COCC[N@@H+] (C)C[C@H]1C[C@H  ] (CO)CN(C(=O)C=C( C)C)C1 | Neg\_lig\_1141 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 535 | C#CCSc1nnnn1- c1ccc(Br)c(C)c1 | Neg\_lig\_1220 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 536 | COCCCN[C@H]1CS (=O) (=O)C[C@@H]1S(=  O)(=O)c1ccc(C)cc1 | Neg\_lig\_1240 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 537 | Nc1nc(CCC[NH2+]C  2CCN(c3ncnc4ccsc3 4)CC2)cs1 | Neg\_lig\_1266 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 538 | COc1cc2nccc(Oc3cc c(NC(=O)Nc4cc(C)o  n4)c(Cl)c3)c2cc1OC | Neg\_lig\_1295 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 539 | CSCC[C@H]  (O)c1nc(C)nn1- c1ccc2c(c1)OCO2 | Neg\_lig\_1360 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 540 | Cc1[nH]nc2c1[C@@ H]  (c1ccncc1)C(C#N)=C (N)O2 | Neg\_lig\_1367 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 541 | O=C([C@H]1CCOc2  ccccc2C1)N1CCOc2 ccc(CO)cc2C1 | Neg\_lig\_1395 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 542 | CC(C)OCC[NH2+]C CC(=O)NC1CCCCC 1 | Neg\_lig\_1406 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 543 | CC(C)  (C)c1ccc(OC[C@H] (O)CSCc2ccc(Cl)cc2  )cc1 | Neg\_lig\_1477 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 544 | COC(C)(C)C[C@H] (C)  [NH2+]Cc1nncn1C1 CCCCC1 | Neg\_lig\_29 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 545 | C=CCn1cc(C[NH2+] C2CCN(S(C) (=O)=O)CC2)c(C)n1 | Neg\_lig\_1539 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 546 | COCCCNc1nc2c(c(= O)n(C)c(=O)n2C)n1  Cc1ccccc1Cl | Neg\_lig\_1567 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 547 | COc1ccccc1OC[C@ @H] (O)Cn1cnc2cc(C)c(C  )cc21 | Neg\_lig\_1579 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 548 | C=CC[C@]1(CO)CC CN(C(=O)COCc2ccc  cc2)C1 | Neg\_lig\_1596 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 549 | CC(=O)OCC(=O)  [C@]12OC(C)  (C)O[C@H]1C[C@H  ]1[C@@H]3C[C@H  ] (F)C4=CC(=O)C=C[  C@]4(C)[C@@]3(F)  [C@@H] | Neg\_lig\_1612 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | (O)C[C@@]12C |  |  |  |  |  |
| 550 | C=CC[C@@H] (CC)C(=O)NC(=O)N  1CCCc2ccccc21 | Neg\_lig\_1664 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 551 | COc1ccc(C2=C(Nc3c cccc3)c3ccccc3C2=O  )cc1 | Neg\_lig\_1697 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 552 | COc1ccc(- c2csc(Nc3cccc(C(C)  =O)c3)n2)cc1 | Neg\_lig\_127 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 553 | CC1(C)C[C@]2(C)O  [C@@H]2[C@]2(C1  )N=N/C(=N/  c1ccccc1)O2 | Neg\_lig\_1763 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 554 | O=C1[C@H]  (Cc2ccc(O)cc2)N2C(  =O)CCN(C(=O)NCc  3ccccc3) [C@H]2CN1Cc1cccc 2ccccc12 | Neg\_lig\_1815 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 555 | CCSc1nc([O-])cc(O)  n1 | Neg\_lig\_1832 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 556 | Cc1cc(NC2CCCCC2  )ncn1 | Neg\_lig\_1895 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 557 | Cc1n[nH]c([C@H]  (C)[N-]S(=O) (=O)c2sc3c(c2C(=O) [O-])CCNC3)n1 | Neg\_lig\_1903 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 558 | Nc1nnc(SCC(=O)N2 CCC[C@H] (CCC(=O)N3CCOC C3)C2)s1 | Neg\_lig\_1564 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 559 | COc1ccccc1N[C@H] (c1ccccc1)c1nnc(- c2ccccc2F)o1 | Neg\_lig\_2144 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 560 | CN(C)S(=O) (=O)c1ccc(CN2CC3( CC[NH2+]CC3)CCC 2=O)cc1 | Neg\_lig\_2180 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 561 | O=C([O-])c1ccccc1O C[C@@H]  (O)Cn1cnc2ccccc21 | Neg\_lig\_2207 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 562 | CC[NH+]  (CC)CCCCNc1ncc2c c(- c3cc(OC)cc(OC)c3)c (NC(=O)NC(C) (C)C)nc2n1 | Neg\_lig\_2214 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 563 | Cn1c(=O)nc([O-])c2c 1nc(NCCO)n2Cc1ccc (Cl)cc1 | Neg\_lig\_2219 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 564 | COc1ccc(N2CC(=O) C(c3nc(C)c(C)s3)=C 2N)c(OC)c1 | Neg\_lig\_1545 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 565 | COc1ccccc1C(=O) [C@H]  (O)c1ccccc1OC | Neg\_lig\_2233 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 566 | N#Cc1c(N)nc2c(c1- c1cnc(N3CCCC3)nc1  )COCC2 | Neg\_lig\_2234 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 567 | CN(C)C(=O)C(CC[N H+]1CCC(O)  (c2ccc(Cl)cc2)CC1) (c1ccccc1)c1ccccc1 | Neg\_lig\_2240 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 568 | O=C([C@H]  (O)c1ccc(F)cc1)N1C CC(c2ncc[nH]2)CC1 | Neg\_lig\_2243 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 569 | O=C1c2ccccc2[C@ @H] (Nc2ccccc2)N1Cc1cc c2c(c1)OCO2 | Neg\_lig\_2249 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 570 | Cc1cc(C)c2c3c(sc2n1  )C1(CCSCC1)C(C#N  )=C(N)O3 | Neg\_lig\_2278 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 571 | Nc1c(C(=O)Nc2ccc( F)c(F)c2)nnn1Cc1ccc (F)cc1 | Neg\_lig\_2311 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 572 | O=c1cc[nH]c2c(Cl)c ccc12 | Neg\_lig\_2371 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 573 | CC[C@@H](C) [C@H]  (Nc1ncnc2sc3c(c12) CCC3)C(=O)[O-] | Neg\_lig\_2396 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 574 | COC(=O) [C@@H]1CC2=CC(  =O)CC[C@]2(C) [C@@]23O[C@@H] 2C[C@@]2(C)  [C@@H] (CC[C@@]24CCC(= O)O4)[C@@H]13 | Neg\_lig\_2473 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 575 | COc1cccc([C@@H]2 c3c(n[nH]c3- c3cc(C)ccc3O)C(=O) N2CCO)c1 | Neg\_lig\_2484 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 576 | COC(=O) [C@@H]1CCCCN1 C(=O)CCc1cc2n(n1) CCC[NH2+]C2 | Neg\_lig\_2373 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 577 | O=C(CCc1cc(Cl)no1  )N1C[C@@H] (C[NH+]2CCOCC2) [C@@H](CO)C1 | Neg\_lig\_2524 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 578 | O=C(Nc1ccc2ncccc2 c1)Nc1ccc2ncccc2c1 | Neg\_lig\_2581 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 579 | COc1cc([C@@H]2C (C#N)=C(N)OC3=C2 C(=O)CC(C) (C)C3)ccc1O | Neg\_lig\_2601 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 580 | Cc1ccc([N-]S(=O)  (=O)c2cc(Br)cnc2N)c (Cl)c1 | Neg\_lig\_1227 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 581 | O=C(NCCN1CCOC1  =O)c1ccc([C@H]2C CC[NH2+]C2)cc1 | Neg\_lig\_2606 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 582 | CCOc1ccc(NC(=O)c 2sc3nc4c(cc3c2N)CN (C)CC4)cc1 | Neg\_lig\_2654 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 583 | O=C(Cn1ncc(N2CC NCC2)cc1=O)NCCc  1ccc(F)cc1 | Neg\_lig\_2661 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 584 | CCCCn1c2nc3ccccc3 nc2c2c(N)ncnc21 | Neg\_lig\_2165 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 585 | CCOc1ccccc1-c1nc(- c2nonc2N)no1 | Neg\_lig\_2737 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 586 | O=C(CCc1cn[nH]c1)  N(CCO)Cc1ccccc1Cl | Neg\_lig\_2758 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 587 | CC[C@H] | Neg\_lig\_2784 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | (C)Nc1nc(N(C)C)nc(  -n2cnc(SC)n2)n1 |  |  |  |  |  |
| 588 | Nc1nonc1C(=O)NCC [NH2+]Cc1cccc(OCc 2ccccc2F)c1 | Neg\_lig\_2800 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 589 | Nc1c(C(=O)NCc2ccc cc2Cl)nnn1Cc1ccc(F) cc1 | Neg\_lig\_2595 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 590 | Cc1cc(Nc2ccc(N3CC N(C(=O)c4ccccc4F) CC3)cc2)n2ncnc2n1 | Neg\_lig\_2849 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 591 | Cc1nc(N)sc1- c1csc(Nc2ncccn2)n1 | Neg\_lig\_689 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 592 | OCc1cc2cc3c(cc2nc1 Cl)CCC3 | Neg\_lig\_2854 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 593 | C[C@@H]1CC[C@ @]2(C(=O)  [O-])CC[C@]3(C)C(  =CC[C@@H]4[C@ @]5(C)C[C@@H]  (O)[C@H](O)  [C@@](C)(CO) [C@H]5CC[C@]43C  ) [C@H]2[C@@H]1C | Neg\_lig\_2876 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 594 | N#Cc1cccc(C[N@H  +]2CC[C@H] (CNC(=O)C3CC[NH 2+]CC3)C2)c1 | Neg\_lig\_2943 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 595 | Cn1c(N2CCOCC2)nc 2cc(C(=O)N3C[C@ H](O)CO3)ccc21 | Neg\_lig\_2001 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 596 | c1ccc(Cc2noc(CC[N H2+] [C@H]3CCOC4(CC OCC4)C3)n2)cc1 | Neg\_lig\_3011 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 597 | Fc1ccc(OCCC[NH+]  2CCN(c3ncnc4c3CC[ NH2+]C4)CC2)cc1 | Neg\_lig\_2076 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 598 | CO[C@H]1CC[C@H  ](O[C@H]2C[C@H]  ([C@]3(C)CC[C@]4( C[C@H](O)  [C@@H](C)  [C@@H]([C@@H]  (C)/C=C(\C)C(=O)  [C@H](C)C[C@H] (C)C(=O)  [O-])O4)O3)O[C@]3 (O[C@@H] ([C@H]4O[C@@]  (O)(CO)[C@H]  (C)C[C@H]4C)C[C @H]3C) [C@H]2C)O[C@H]1 C | Neg\_lig\_3017 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 599 | Nc1ccccc1NC(=O)c1 ccc(CNc2nccc(- c3cccnc3)n2)cc1 | Neg\_lig\_3052 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 600 | c1cn(Cc2ccc3nonc3c 2)c(- c2cc3n(n2)CCC[NH2  +]C3)n1 | Neg\_lig\_3087 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 601 | CSc1cccc(NC(=O)c2 cc3c(CO)cnc(C)c3oc 2=O)c1 | Neg\_lig\_3101 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 602 | CC1(C)CC2(CC(C) | Neg\_lig\_3108 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | (C) [NH2+]1)OC(=O)N( C[C@@H]  (O)c1ccccc1) [C@]2(C)O |  |  |  |  |  |
| 603 | Cc1cc(=O)n2[nH]c(- c3ccc(C(C) (C)C)cc3)cc2n1 | Neg\_lig\_3145 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 604 | CSC(C)(C)C[C@H] (C)  [NH2+]Cc1ccc2c(c1) n(C)c(=O)n2C | Neg\_lig\_3147 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 605 | Nc1nc(N)nc(- c2cc(Cl)ccc2Cl)n1 | Neg\_lig\_3160 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 606 | Cc1nc2nc(O)cc(N)n2 n1 | Neg\_lig\_3173 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 607 | Cc1ccc(-c2c(C(F) (F)F)nn3c(NCc4cccc n4)cc(C)nc23)cc1 | Neg\_lig\_3244 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 608 | CCCc1nc2c(C)cc(- c3nc4ccccc4n3C)cc2 n1Cc1ccc(- c2ccccc2C(=O)O)cc1 | Neg\_lig\_3250 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 609 | CCCCN[C@H]1CS(  =O) (=O)C[C@@H]1S(=  O)(=O)c1ccc(Cl)cc1 | Neg\_lig\_3266 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 610 | CCN(CC)C(=O)Cn1c (-  c2nonc2N)nc2ccccc2 1 | Neg\_lig\_3270 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 611 | C[C@@H](CC(C#N)  (c1ccccc1)c1ccccc1) [NH+]1CCCCC1 | Neg\_lig\_3272 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 612 | COc1cccc(NC(=S)Nc 2ccc(O)cc2)c1 | Neg\_lig\_3294 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 613 | O[C@H]  (COc1ccccc1)C[NH+  ]1CCCCCC1 | Neg\_lig\_2646 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 614 | Cc1cnccc1Cn1ccnc1- c1cn(C2CC[NH2+]C  C2)nn1 | Neg\_lig\_1885 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 615 | Cc1ccc(N[C@@H]2c 3ccccc3C(=O)N2c2c ccnc2)c(C)c1 | Neg\_lig\_3343 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 616 | CCc1ncc(C(=O)N[C  @@H](c2ccccc2) [C@H]  (O)c2ccccc2)cn1 | Neg\_lig\_3350 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 617 | O=C(c1ccccc1) [C@@H]1[C-]([N+]  (=O)[O-])  [C@@H]1c1ccccc1 | Neg\_lig\_3357 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 618 | CC[C@H]1C(c2cccc c2)=NN(CCO)c2nc3c (c(=O)n(C)c(=O)n3C  )n21 | Neg\_lig\_3048 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 619 | N#CC1=C(N)Oc2c(c  (=O)oc3ccccc23) [C@@H]1CCc1cccc c1 | Neg\_lig\_3396 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 620 | OCCCc1nc2ccccc2n1 CCOc1ccc(Cl)cc1 | Neg\_lig\_3406 | TERRA | G-quadruplex | GGGUUAGGGU | 0 |
| 621 | Cc1nc(CCN)n[nH]1 | 0342-0285 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 622 | CSCCC(C(O)=O)Nc  1c2c3CCCCc3sc2ncn 1 | 0866-0023 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 623 | O=C(NCCCN1CC1)  Nc1cccc2ccccc12 | 101298 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 624 | CC(c1ccc(cc1)NC1c2 ccc(c(c2C(=O)O1)O C)OC)=O | 1080-0649 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 625 | O=C(C(C(N1)=O)=C  c2csc3c2cccc3)NC1= O | 108783 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 626 | NC(NC(c1nccnc1C( O)=O)=O)=O | 117922 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 627 | Cc1cc(nc2cc(ccc12) OC)N1C[C@H] (C2CC2)[C@H] (C1)N | 12182839 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 628 | CC(NS(c(cc1)cc2c1s c(C)n2)(=O)=O)=O | 122385 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 629 | CC1=CC(C)=NC(N1 CCNC(C1CC2(CCN CC2)CN1C)=O)=O | 12499963 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 630 | CN1CCN(CC1) [C@H]1CCN(C[C@ H]1CCCO)C(c1cccc2  c1ccn2C)=O | 12576044 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 631 | C1CCN(C1)Cc1cc(C N2CCC(Cc3ccc(CO)  cc3)C2)sc1 | 12617773 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 632 | C1CC2(CCN(CC2)C C(C(F) (F)F)O)CN(CC(N)= O)C1=O | 13525118 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 633 | CN(Cc1ccc(cc1)n1cc cn1)Cc1cccc(CCN)c1 | 13860811 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 634 | Cc1nc(CCN)cc(NCC C2CCCN2C)n1 | 14159297 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 635 | CCN(CC)Cc1cnc2c(c nn2c1)C(NCc1ccc(C N)cc1)=O | 14229566 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 636 | CCc1nc2CCNCCc2c( NCc2nc(c3ncccn3)no 2)n1 | 14445071 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 637 | C1CN(CCC1C1CCN  (CCc2ccccc2)C1)c1c cnc(N)n1 | 14604674 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 638 | CCc1cc(nc(n1)N1CC CC1)N1C[C@@H] (C[C@H]1C(N(CC) CC)=O)N | 15018109 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 639 | Cc1cc(nc(N)n1)N1C CC(CC1)NCCCN1C  Cc2ccccc12 | 15043866 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 640 | CCNC([C@@H]1C[  C@@H] (CN1C(CN1CCCCC CC1)=O)N)=O | 15077405 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 641 | Clc(c(NC1CCCCC1)  nnc1Cl)c1Cl | 154127 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 642 | COc1ccc(cc1)OC1C CN(CC1)C([C@@H] 1C[C@H] (CN1)O)=O | 15579241 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 643 | C(CN)c1cccc(CN2C COCC(C2)CO)c1 | 15684586 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 644 | COCCCN1C(CC[C @H]2CN(CC[C@@  H]12)c1c2cn[nH]c2n c(N)n1)=O | 15765444 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 645 | Cc1ccc(cc1)c1csc(Nc 2ccc(C)cc2) [n+]1CC=C | 1611-2955 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 646 | COc1ccc(cc1)N1C(C 2C3c4ccccc4C(CO) (C2C1=O)c1ccccc13)  =O | 1657-0369 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 647 | CCc1nnc(NCC2CCC CCN2)o1 | 16631339 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 648 | Cc1c(C(C(NCCNc2c  ccnc2)=O)N)c(C) [nH]n1 | 16899791 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 649 | CN(CC1CCN(CC1)C  Cc1cccc(c1)F)C([C@ H] (Cc1c[nH]cn1)N)=O | 17007774 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 650 | C1CCN(CCCNC(c2c  ccc(c2)c2cn[nH]c2)= O)C(C1)CO | 17250805 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 651 | C=Cc1ccc(nc1)N1CC N(CC(C1)O)Cc1cccc  c1 | 17524156 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 652 | CCn1cncc1CNc1c2C CNCc2nc(c2ccncc2)n 1 | 18384397 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 653 | CN(C)CCC1CCCCN  1Cc1ccc(CCN)cc1 | 18585072 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 654 | C1CN(CCC12c1cccc c1[C@H] ([C@@H]2O)N)Cc1  c[nH]nc1c1ccccc1 | 18741551 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 655 | Cc1nccn1CC1CCN( CC1)c1c2CCNCc2nc n1 | 19035660 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 656 | C1CCCN(CC1)CC(C NC(c1cn(CCN)nn1)= O)O | 19036853 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 657 | C1CN(CC1c1ccccc1 F)Cc1ccc(CCN)cc1 | 19080499 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 658 | C1CCN(CC1)c1ccc(c  c1)c1cc(c2cccnc2)c( C#N)c(N)n1 | 19252160 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 659 | Cc1cc2c(cc1CN1C[C @@H] (CN3CCCCCC3) [C@H] (C1)CO)OCCO2 | 19474966 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 660 | Cc1ccc(cc1[Cl])N1C CC(CC1)N[C@@H] 1CC[C@H](C1)N | 19498560 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 661 | Cc1cc(C)c2c(c1)c(cc( C)n2)C(N[C@H]1C NC[C@@H]1OC)=O | 19537511 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 662 | C(CN)c1cccc(CN2C CN(CC2)Cc2ccc(cc2  )[Cl])c1 | 19565794 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 663 | O=C1OCC/C1=C\ | 197008 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | NCCCCCCCCN/ C=C(\CCO1)/C1=O |  |  |  |  |  |
| 664 | C(CNC1CCC2(CC1)  CCNCC2)CNc1cccnc 1 | 19786268 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 665 | CN(Cc1cnn(c1)c1ccc (cc1)F)C(C(c1ccc(cc 1)F)O)=O | 19840417 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 666 | C(CN)C1CN(CCO1)  c1c2CCNCc2nc(c2cc ccc2)n1 | 19916102 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 667 | C1C[C@@H]2CCN(  Cc3ccccn3)C[C@H] 1N2 | 20138450 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 668 | Cn1c2c(cn1)c(nc(c1c cncc1)n2)N1CCCC2( CCNCC2)CC1 | 20352833 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 669 | C1CNCc2c1c(NCC1  COc3ccccc3O1)nc(c1 cccnc1)n2 | 20674759 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 670 | Cc1nccn1c1ccc(CNC (CCc2cc3CNCCCn3  n2)=O)cc1 | 20920311 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 671 | C1[C@@H] (C2(CCN(CC2)Cc2n  cc[nH]2) [C@@H]1O)O | 21540130 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 672 | C1CCN(CC1)C(CNC  (CCc1cc2CNCCn2n1  )=O)c1cccnc1 | 21900063 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 673 | COc1ccc(cc1)c1c(CN 2CCC3(CC2)[C@H] (C[C@H]3O)OCCN)  c[nH]n1 | 22516313 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 674 | CN(C[C@@H]1CC[  C@@H] (CC1)N)CC1(CCCC 1)CO | 22559794 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 675 | C1CCCN(CC1)C[C  @@H]1CN(C[C@@ H]1CO)C(c1cc(N) [nH]n1)=O | 22664850 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 676 | C1CCN(CC1)C[C@ @H]1CN(C[C@@H]  1CO)C(c1cn2cc(cnc2 n1)[Cl])=O | 22667725 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 677 | Cc1cc(C)cc(CN2CC C3(CCNCC3)C2)c1 | 22860169 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 678 | C1CCN(CC1)CC1(C  CN(Cc2cccc(CCN)c2  )C1)O | 22896979 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 679 | C(c1c(c2cccc(c2) [Cl])c(C#N)c2nc3ccc cc3n2c1N)#N | 2367-1144 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 680 | CC1CCCC(C)N1CC(  COc1c(C)cccc1C)O | 2388-0120 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 681 | CN(C)S(Nc1cccc(Br) c1)(=O)=O | 241621 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 682 | CN1CCN(CC1)c1cc( nc(N)n1)N1CCCC(C N2CCCCC2)C1 | 25666870 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 683 | C1CCN(CC1)Cc1ccc  c(c1)n1ccnc1c1cc2C | 26875627 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | NCCCn2n1 |  |  |  |  |  |
| 684 | CN(C)CCOc1cc(C(/ C(/C2)=C\  c(n3C)ncc3[N+] ([O-])=O)=O)c2cc1.  OS(O)(=O)=O | 277184 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 685 | O=C(Nc1ccccc1)OC 1=CC=CNC1=O | 277806 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 686 | CCOc1ccc(CNCCc2c cc(cc2)F)cc1 | 2910-0686 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 687 | COc1ccc(c(CNc2ccc( cc2)[Br])c1)OC | 2910-1869 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 688 | O=C(N(CC1OC1)C( N1CC2OC2)=O)N(C C2OC2)C1=O | 296934 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 689 | Cc1ccc(cc1)N1C(CC (C1=O)NCCc1ccc(cc 1)OC)=O | 3076-0323 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 690 | COCCOC(C1C(C2=  C(c3ccccc3OC2=O) OC=1N)c1ccncc1)=O | 3132-1032 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 691 | Cc1nc(CCN)cc(n1)N 1CCN(CC1)c1ccc(C#  N)cn1 | 31455775 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 692 | COc1ccc(CCNCc2cc cc(c2)C(F)(F)F)cc1 | 3169-1283 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 693 | C(CNCc1ccc2c(c1)O CO2)c1ccc(cc1)F | 3169-1371 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 694 | C1CN(CC1CN)Cc1c  cc(c2ccccc2C#N)o1 | 31727519 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 695 | CCN(CC)Cc(c(OC)c  1)cc2c1c1cnc(cc(cc3) Cl)c3c1[nH]2 | 317605 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 696 | Cc1cccc(NC(SC(c(cc 2)cc(OC)c2O)NC2= O)=C2C#N)c1 | 319435 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 697 | [H]Nc1nnc(C(CC)c2  ccccc2)s1 | 3202-0205 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 698 | CN(C)CCNc1nc2c(C (N(C)C(N2C)=O)=O)  n1Cc1ccccc1[Cl] | 3238-0121 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 699 | COCc1nc(CCNC(CC  c2cc3CNCCn3n2)=O  )on1 | 32552243 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 700 | O=C(NC(N1c2ccccc 2)=C2NC1=S)NC2= S | 33182 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 701 | CN1C(c2c(nc(NCCN  )n2Cc2ccc(cc2)F)N( C)C1=O)=O | 3346-2730 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 702 | CCN(CCN)c1ccc2C( NNC(c2c1)=O)=O | 3367-1212 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 703 | COc1ccc(cc1OC)c1n c2cc(ccc2o1)N | 3370-0370 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 704 | C1CC(N(C1)CCC1C  CN(CC1)Cc1cccc(C CN)c1)=O | 34485551 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 705 | CC(C) (CO1)COP1(OC(C= NN(C1CCCCC1)C1= O)=C1OC)=S | 350187 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 706 | CC1=CC(NC(NCCN C2CCC3(CC2)CCN CC3)=N1)=O | 35107446 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 707 | Cc1cccc(c1)Nc1nc(C N2C[C@@H]3CC[C  @H] (C2)N(C)C3=O)nc(N  )n1 | 35485871 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 708 | COc1cccc(CNCc2ccc c(c2)F)c1OC | 3702-1553 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 709 | COc1cccc(CCNCc2c cc(cc2)C(F)(F)F)c1 | 3702-1570 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 710 | C(c1ccncc1)NCc1ccc 2c(c1)OCO2 | 3702-1584 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 711 | CSC(N1NC(c(cc2)cc c2Cl)N=C11)=NC=C 1C#N | 379538 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 712 | Cc1c(C(NN/C(/ SC)=N/S(c2ccccc2) (=O)=O)=O)c(-  c(c(Cl)ccc2)c2Cl)no1 | 379696 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 713 | N#CC1=C(Nc(cccc2)  c2Cl)SC(c2ccncc2)N C1=O | 379697 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 714 | COc1ccccc1OC1CC N(CC1)Cc1cccc(CC N)c1 | 39780332 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 715 | CC(Nc1cccc(c1)c1cc c(c(c1)F)NC(CN)=O)  =O | 40118252 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 716 | Cc1ccc(cc1)S(N(CC( CN1CCCCC1)O)c1c cccc1OC)(=O)=O | 4013-2178 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 717 | CC(C)CC1CC(C)  (c2csc(Nc3ccccc3)n2  )OC1=O | 4075-3209 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 718 | C1CN(CCN(C1)c1nc cc(n1)N1CCC(C1)O)  Cc1cccc(c1)F | 41253715 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 719 | Cc1nc2CNCCc2c(N CCc2csc(c3cccnc3)n 2)n1 | 41602213 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 720 | CC(C)  [C@@H]1CN(Cc2cc cc(CCN)c2)C[C@H] 1N(C)C | 42043717 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 721 | CC1CCc2c(C(Nc3cc ccc3C)=O)c(N)sc2C1 | 4488-1595 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 722 | CC(c1cccc(c1)Nc1cc (C)nc2ccc(C)cc12)= O | 4491-0985 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 723 | Cc1ccc2c(c1)c(c1CC Cc1n2)Nc1cccc(c1)O | 4491-1565 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 724 | CCOC(c1ccc2c(c1)c( cc(C)n2)Nc1ccc(cc1) N(C)C)=O | 4593-2976 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 725 | CCOC(c1ccc2c(c1)c( cc(C)n2)Nc1cccc(c1) O)=O | 4593-2992 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 726 | Cc1c2ccccc2n(CC(C n2c(C)c(c(C)n2) [Br])O)c1C | 4593-8144 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 727 | Cc1c(CN2CC3(CCN | 46066918 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | CC3)OC2=O)nc2ccc cc2n1 |  |  |  |  |  |
| 728 | COc1ccc(c(c1)OC)c1 csc(NCC=C)n1 | 4640-0152 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 729 | CCC1CN(CCN1C(C)  C)Cc1cccc(CCN)c1 | 46449375 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 730 | C(CNc1cccnc1)CNc1 c2ccccc2nc(CCN)n1 | 47488116 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 731 | Cc1nccn1CCC1CCC CN1Cc1cccc(CCN)c 1 | 47531251 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 732 | Cc1ccsc1CN(CCN(C  )C)C(CN)=O | 47645371 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 733 | Cc1cnc(N)nc1NCC[ C@@H]1C[C@H]2 C[C@@H]1C=C2 | 47913504 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 734 | CCOc1cc(CNCCc2cc cc(c2)OC)ccc1OC | 4964-4425 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 735 | C(CNCc1ccc2ccccc2 c1)c1c[nH]c2ccccc12 | 4964-5069 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 736 | C(c1ccc(cc1)F)NCc1 ccc2c(c1)OCO2 | 4964-5172 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 737 | [O-][N+](c(cc(cc1)  [As](c(cc2)cc([N+]  ([O-])=O)c2O) (O)=O)c1O)=O | 49852 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 738 | Cc1nc(SC)nc(N2CC2  )c1Br | 50199 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 739 | CCOC(c1c2c(nc3ccc cc3n2)n(c2cccc(c2) [Cl])c1N)=O | 5122-1932 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 740 | C1CCC(CCNc2c(NS  (c3ccccc3) (=O)=O)nc3ccccc3n2  )=CC1 | 5122-2566 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 741 | CCOC(c1cnc2c(C)cc (C)cc2c1NCC(C)O)= O | 5174-4431 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 742 | C(Cc1nc2NC(=CC(c  3ccc(cc3) [Cl])n2n1)c1ccccc1) CO | 5228-4308 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 743 | C(CCN=Cc1ccccc1N  )CN=Cc1ccccc1N | 5233844 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 744 | COc1ccc(cc1)OCC(C N1CCN(CC1)c1cccc c1)O.[Cl].[Cl] | 5257916 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 745 | CC(C) (C)NCC(Nc1c2CCC Cc2nc2CCCc12)=O. C(O)=O.C(C(O)=O) (O)=O | 5284047 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 746 | CCCCOC(C1=C(N) OC2CC(C) (C)CC(C=2C12C(Nc 1ccccc12)=O)=O)=O | 5587-0160 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 747 | C=CCC(CC=C)  (c1ccc(cc1)C(CC=C) (CC=C)N)N | 5654685 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 748 | CC(c1ccccc1)NC(CC (C)=C)c1ccco1 | 5689-0049 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 749 | CC(=C)CC(c1ccc(cc | 5689-0111 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | 1)OC)NCc1ccco1 |  |  |  |  |  |
| 750 | Cc1ccc(c(c1) [Cl])OCCNC(C)  (C)C.[Cl] | 5729988 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 751 | CCCCNCCOc1ccccc 1F.C(C(O)=O)(O)=O | 5734218 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 752 | CCCOc1ccccc1Nc1c 2ccccc2nc(C(=O)OC C)n1 | 5847-0398 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 753 | c1cc(ccc1c1cn2ccsc2 n1)N | 5968142 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 754 | CC(C)CN1CCC(CC1  )NCCNc1ccncc1C | 60244866 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 755 | CCN1CCN(CC1)CC(  COc1ccc(CC=C)cc1 OC)O.[Cl].[Cl] | 6043920 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 756 | Cc1cc(N)n(c2ccc(c(c 2)S(O)  (=O)=O)Oc2ccccc2)n 1 | 6075116 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 757 | C1CCCN(CC1)CC(C  Oc1ccccc1)O | 6228-0261 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 758 | O=C(c(cc1)cc(C(Nc( cc2)ccc2C2=NCCN2  )=O)c1Cl)Nc(cc1)ccc 1C1=NCCN1 | 67436 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 759 | O=C(C(C(C=C(c1ccc cc1)O1)=O)C1=O)c1  ccccc1 | 6844 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 760 | Cc1cccc(c1C)NC(CS c1nnc(C(c2ccccc2)O) n1c1ccccc1)=O | 6960143 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 761 | C1CCN(CC1)CC(Cn  1ccc2ccccc12)O | 7230-0020 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 762 | Cc1cc(nc(N)n1)Oc1c cc(cc1)C(=O)OC | 7796-0682 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 763 | C(CN)CN1CCN(CC1  )c1ccccc1 | 7974015 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 764 | C(C1C(C2=C(NC(N C2=O)=O)OC=1N)c1  ccccc1)#N | 8002-4077 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 765 | Cc1ccc(cc1C)Nc1nc( cs1)c1ccc(c(c1)F)OC | 8005-2731 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 766 | Cc1ccc(cc1C)Nc1nc( cs1)c1ccccc1 | 8005-2768 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 767 | Cc1ccc(C)c(c1)c1csc (Nc2ccccc2OC)n1 | 8006-1580 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 768 | Cc1ccc(cc1)C1C(C# N)=C(N)Oc2ccc3ccc cc3c12 | 8008-9298 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 769 | CC1=C(C(C(C#N)=C  (N)O1)c1ccccc1)n1c 2ccccc2nn1 | 8009-2467 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 770 | COc1ccc(c(c1)NC(C Sc1nc2ccc(cc2s1)N)= O)OC | 8009-2885 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 771 | C1CCc2c(C1)c(C(c1  ccccc1)=O)c(N)s2 | 8010-1935 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 772 | CN1C(c2c(ncn2CCN  )N(C)C1=O)=O | 8012-1255 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 773 | CC1=CC(N(C)C(N1 | 8012-3983 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | CCCCCCNCCO)=O)  =O |  |  |  |  |  |
| 774 | Cc1cc(C)c2c(c1)c(C CN)c(C)[nH]2 | 8012-5803 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 775 | Cc1ccc(C)c2c1c(CC N)c(C)[nH]2 | 8012-5804 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 776 | Cc1c(CCNCc2c(cc(c c2OC)OC)OC)c2cc(c cc2[nH]1)OC | 8013-0022 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 777 | CCCCc1nc(CNCCc2  c3cc(ccc3[nH]c2C)O C)c[nH]1 | 8013-0624 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 778 | Cc1c(CCNCc2ccc(C #N)cc2)c2cc(ccc2[nH  ]1)OC | 8013-2954 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 779 | CN1CCC(CC1) (CN)N1CCN(CC1)c1  ccccc1 | 8017-3009 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 780 | C=CCOc1ccc(cc1)C1 C(C#N)=C(N)OC2=  C1C(c1ccccc1C2=O)  =O | 8017-5263 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 781 | COc1ccc(CCNc2nc(c s2)c2cccs2)cc1OC | 8018-0995 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 782 | CC(C)C1(CCNCc2cc c(c(c2)OC)OC)CCO  C(C)(C)C1 | 8018-1267 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 783 | CC(C)C1(CCNCc2cc cc3c2OCO3)CCOC( C)(C)C1 | 8018-1268 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 784 | Cc1c(C#N)c(N)n(CC  Cn2ccnc2)c1C | 8018-7492 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 785 | Cc1c(c(N)n(CCOC)c  1C)S(c1ccc(cc1)[Cl]) (=O)=O | 8019-0265 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 786 | Cc1c(c(N)n(CCCN(C  )C)c1C)S(c1ccc(cc1) F)(=O)=O | 8019-0616 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 787 | CN1CCC(CC1)Oc1c  cc(cc1)N | 8019-4291 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 788 | c1cc(N)nc2c1ccc(n2) O | 8019-7722 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 789 | COc1c(cc2c(c1OC)O CO2)C1C(C#N)=C( N)OC2CCCC(C1=2)  =O | 8019-9373 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 790 | CCNCc1cc(CC=C)c( c(c1)OC)OCC | 8020-2907 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 791 | CN1CCCc2ccc(cc12) N | 8020-4281 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 792 | OC(/C=C\  C(Nc1nccs1)=O)=O | 80807 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 793 | C1C(NCC2)N3C2NC CC3NC1 | 81462 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 794 | C1CCN(C1)c1ccccc1 NC1c2ccccc2S(N=1) (=O)=O | 8209-0032 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 795 | CCCCNc1c(C#N)c2 CC(C)  (C)OCc2c(c2ccccc2) n1 | 8640-0572 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 796 | CCNCC#CCOc1ccc(  cc1)[Br] | 9126666 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 797 | CC(c1ccc(cc1)c1ccc( CNCCc2c[nH]c3cccc c23)o1)O.[Cl] | 9135919 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 798 | C1CCC(CCNCc2ccc cn2)=CC1.[Cl] | 9137483 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 799 | O=C(C(C(N1)=O)=C  c2cc3ccccc3cc2)NC1  =O | 95909 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 800 | CCN(CCCC/C1=N\ O)CCCC/C1=N\O | 96491 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 801 | Cc1cccc(c1)NCc1nc2 ccccc2n1C | C147-0043 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 802 | C1COc2cc(ccc2O1)N c1c(c2ccco2)nc2ccc( cn12)[Cl] | C177-0188 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 803 | CC1CCN(CC1)c1nc( c(C(=O)OC)s1)N | C201-1740 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 804 | Cc1cc(Nc2ccccc2)nc 2cc(ccc12)O | C614-0105 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 805 | CCOC(C1CCN(CC1) C1=C(C(C1=O)=O)N CCCN1CCCCC1)=O | C667-0368 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 806 | C1CCCN(CC1)CCC  Nc1nc2ccccc2c2nc(c 3ccccc3)nn12 | C736-0159 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 807 | CCOC(N1CCN(CC1) C1=C(C(C1=O)=O)N CCCN1CCCCCC1)= O | C748-1353 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 808 | Cc1c(CCC(Nc2ccc(c c2) [Cl])=O)c(C)n2c(n1)  nc(CN)n2 | C908-0503 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 809 | Cc1c(CCC(Nc2ccc(C N3CCCCC3)cc2)=O)  c(C)n2c(n1)nc(CN)n 2 | C908-0509 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 810 | CCc1cccc(c1)NC(CC c1c(C)nc2nc(CN)nn2 c1C)=O | C908-0512 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 811 | Cc1ccc(c(C)c1)NC(C Cc1c(C)nc2nc(CN)nn 2c1C)=O | C908-0520 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 812 | Cc1c(CCC(Nc2cccc( c2) [Br])=O)c(C)n2c(n1)  nc(CN)n2 | C908-0523 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 813 | Cc1c(CCC(NCC2CC  N(CC2)Cc2ccccc2F)  =O)c(C)n2c(n1)nc(C N)n2 | C908-0547 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 814 | Cc1c(CCC(NCC2CC  N(CC2)Cc2ccccc2O C)=O)c(C)n2c(n1)nc( CN)n2 | C908-0549 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 815 | Cc1c(CCC(NCC2CC  N(CC2)Cc2ccc(cc2)F  )=O)c(C)n2c(n1)nc(C N)n2 | C908-0552 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 816 | C(CNc1c(nc(c2ccccc 2F)o1)S(c1ccccc1) | D072-1643 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | (=O)=O)Cn1ccnc1 |  |  |  |  |  |
| 817 | C=CCNc1cc(c2ccccc 2)nc2nncn12 | D150-0143 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 818 | CCOC(c1cccc(c1)NC 1c2ccccc2S(N=1) (=O)=O)=O | D257-0714 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 819 | CCN(CC)CCCNCC1 CCOC(C)(C)C1 | D324-0108 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 820 | Cc1cc(NC2CCCCC2  )n2c(cc(c3ccc(c(c3)O C)OC)n2)n1 | D393-0160 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 821 | Cc1cccc(c1C)N1CC N(CC1)CC(c1c[nH]c  2ccccc12)O | D424-0008 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 822 | CC1(C)CC(CCNCc2  ccc3c(c2)OCO3) (CCO1)c1ccccc1OC | D442-0097 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 823 | COc1ccc(Cc2nc3cccc c3n2CC(COc2ccccc2  )O)cc1 | D510-0832 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 824 | CCC(CO)NCc1ccc(c(  c1)OC)OCc1ccc2c(c 1)N(C)C(N2C)=O | D666-0065 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 825 | CCOC(c1cnc2c(c3cc c(cc3) [Br])c(C)nn2c1N)=O | D718-0691 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 826 | CCc1ccc(cc1)NC1C( C)=C(c2ccc(cc2)OC) S(N=1)(=O)=O | E013-1594 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 827 | Cc1cc(ccc1[Br])NC1  =C(C(C1=O)=O)c1cc  c(cc1)[Cl] | E786-0118 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 828 | C(c1ccccc1)N=C(N) NC(c1c(N)nc(c(n1) [Cl])N)=O | NCGC00015147- 09 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 829 | CCN1C=C(C(O)=O)  C(c2cc(c(nc12)N1CC NCC1)F)=O | NCGC00016927- 10 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 830 | C1CN=C(c2ccc(cc2) NC(C=Cc2ccc(C=CC  (Nc3ccc(cc3)C3NCC N=3)=O)cc2)=O)N1 | NCGC00165782- 02 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 831 | C(CCOc1ccc(cc1)C( Nc1cccc2C(C=C(c3n n[nH]n3)Oc12)=O)=  O)Cc1ccccc1 | NCGC00181765- 01 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 832 | C1CNCCC1n1cc(cn1  )c1cnc2cccc(c3cc(c( CN4CCOCC4)c(c3)F  )F)c2n1 | NCGC00263202- 01 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 833 | C[C@@H](C(C)  (C)C)NCc1ccc2c(c1) nc(NC(c1ccc(c3cn[n H]c3)s1)=O)n2CCc1  ccccc1 | NCGC00344999- 01 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 834 | C([C@@H]1[C@@ H]([C@@H]([C@H] (N2C=CC(NC2=O)= O)O1)F)O)O | NCGC00345781- 01 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 835 | COc1cc(C[C@@H] (CO)[C@@H]  (Cc2ccc(c(c2)OC)O) CO)ccc1O | NCGC00346838- 01 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 836 | CC(C)n1cnc2c(Nc3c ccc(c3)NC(C=C)=O) nc(NC3CCC(CC3)N( C)C)nc12 | NCGC00346964- 01 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 837 | CC(c1ccc2c(c1)OCC O2)N[C@H]1C[C@  H]1c1ccccc1 | NCGC00347951- 01 | AKTIP | G-quadruplex | GGGGUGGGGCGGGGCGGGG | 1 |
| 838 | CCN(CC)CCOC(c1c  cc2c(c1)sc(NC(c1ccc (cc1)N)=O)n2)=O | 0812-1025 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 839 | CSCCC(C(O)=O)Nc  1c2c3CCCCc3sc2ncn 1 | 0866-0023 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 840 | Cc(cc(cc1)- n2c(NC=NC3=O)c3n  c2)c1N | 100120 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 841 | CC1CCN(CC1)CC(C  Oc1ccccc1CC=C)O | 1189-2046 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 842 | CC(NS(c(cc1)cc2c1s c(C)n2)(=O)=O)=O | 122385 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 843 | CN(CCCc1nccn1C)c 1c2CCNCc2nc(c2ccn cc2)n1 | 12244291 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 844 | CN(CC(N1C[C@@H  ](CN2CCCCCC2) [C@H] (C1)CO)=O)Cc1cccc  c1F | 12553104 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 845 | CN1CCN(CC1) [C@H]1CCN(C[C@ H]1CCCO)C(c1cccc2  c1ccn2C)=O | 12576044 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 846 | CN1CCCN(CC1)C[C  @@H]1CN(C[C@@ H]1CO)C(c1ccnc2cc ccc12)=O | 13336906 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 847 | CN(Cc1cccc(c1)OCC  =C)c1c2ccccc2nc(CC N)n1 | 13692816 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 848 | Cc1cnc(nc1N)N1C[C @H]2[C@@H] (C1)OC(N2CCCN1C COCC1)=O | 13797550 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 849 | C1CNCCC12c1ccccc 1[C@H]  ([C@@H]2OCc1ccc nc1)NC(c1cc[nH]n1)  =O | 14122667 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 850 | Cc1nc(CCN)cc(NCC C2CCCN2C)n1 | 14159297 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 851 | Cc1ccc(cn1)NC([C@ H]1C[C@H] (CNC1)C(NCCc1c[n H]cn1)=O)=O | 14326970 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 852 | CCc1cc(nc(n1)N1CC CC1)N1C[C@@H] (C[C@H]1C(N(CC) CC)=O)N | 15018109 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 853 | Cc1cc(nc(N)n1)N1C CC(CC1)NCCCN1C  Cc2ccccc12 | 15043866 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 854 | CCNC([C@@H]1C[  C@@H] (CN1C(CN1CCCCC CC1)=O)N)=O | 15077405 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 855 | CN(CCc1cn[nH]c1)C ([C@H]1CC[C@H] (C1)N)=O | 15410184 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 856 | CCCC=Cc1ccc2c(c1) nc(C(C)O)[nH]2 | 15802636 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 857 | CCc1nnc(NCC2CCC CCN2)o1 | 16631339 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 858 | Cc1c(cn(C)n1)NC(N CC(Cc1cccs1)CO)=O | 16859921 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 859 | Cn1ccnc1CCC1CCC CN1C(c1cn(CCN)nn 1)=O | 16896468 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 860 | Cc1c(C(C(NCCNc2c  ccnc2)=O)N)c(C) [nH]n1 | 16899791 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 861 | C=Cc1ccc(nc1)N1CC N(CC(C1)O)Cc1cccc  c1 | 17524156 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 862 | Cc1cc2CC(CN)Oc2c(  c1)c1cnc2ccccc2n1 | 17587941 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 863 | NC(NCCCS(Nc(cc1)  ccc1Nc1c(cccc2)c2nc 2cc([N+]  ([O-])=O)ccc12) (=O)=O)=N.Cl | 177365 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 864 | OC(C(Nc1n[nH]cn1)  =O)=O | 177952 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 865 | CCc1cnc(N)nc1NCC C(C)N(C)CC | 18668112 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 866 | C(CN)c1ccc(CN2CC C(CC2)  (c2cccc(c2)C(F)  (F)F)O)cc1 | 18809502 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 867 | C(Cn1cc(C(NCCOc2  cccc3cccnc23)=O)nn 1)N | 18917752 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 868 | CC(Cc1cc(C)n[nH]1)  NCc1ccc(c(c1)OC)O CCN1CCCC1 | 19048916 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 869 | CC(C)n1cnnc1CN(C)  c1cc(CCN)nc(C)n1 | 19341804 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 870 | C1CN(Cc2c1c(ncn2) N1CCOCC1)C([C@ H]  (Cc1ccc(cc1)O)N)=O | 19595168 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 871 | Cc1nc2cc(CNC(c3cn (CCN)nn3)=O)ccc2n 1C | 20202809 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 872 | Cc1cc(N)n(CC(N2C[  C@@H] (CN3CCCCCC3) [C@H] (C2)CO)=O)n1 | 20853195 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 873 | CCc1cc(nc(C)n1)N1 CCC(CC1)NCCNc1c  cncc1C | 20968889 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 874 | Cc1cnc(nc1N(C)C)N 1CCN(CC1)Cc1cn(C CO)nc1C | 21083372 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 875 | C1CC2(CCNCC2)C  CN(C1)Cc1ccnc2ccc cc12 | 22793936 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 876 | C1CCN(CC1)CC1(C | 22896979 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | CN(Cc2cccc(CCN)c2  )C1)O |  |  |  |  |  |
| 877 | CNc1cc(c2ccc(cc2)c2 nnc(N)s2)c2cc[nH]c2 n1 | 25638728 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 878 | C1CC(CN(C1)Cc1cc  cc(CCN)c1)C(Cc1ccc cc1)=O | 27037369 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 879 | C1CC(CN(C1)Cc1cc  cc(c1)O)NC(c1cn(CC N)nn1)=O | 27067624 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 880 | COc1ccc(CCNCc2cc c(cc2)[Cl])cc1 | 2910-0536 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 881 | CCc1ccc(CNCCc2cc ccc2OC)cc1 | 2910-0568 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 882 | CCOc1ccc(CNCCc2c cc(cc2)[Cl])cc1 | 2910-0651 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 883 | CCOc1ccc(CNCCc2c cc(cc2)F)cc1 | 2910-0686 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 884 | COc1cc(CNCc2cc(cc c2OC)[Br])cc(c1)OC | 2910-1798 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 885 | Cc1ccc(C)c(c1)NCc1 cc(ccc1OC)[Br] | 2910-2364 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 886 | O=C(N(CC1OC1)C( N1CC2OC2)=O)N(C C2OC2)C1=O | 296934 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 887 | CCOC(/C(/ C1=CSC2=NNC(C) (C)N12)=N\O)=O | 299968 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 888 | Cc1cc2c(C)c(C)cc(N) c2nc1 | 304902 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 889 | Nc1ccc(Cn(ccc2c34) c2ccc4nc(N)nc3N)cc 1.Cl | 309401 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 890 | Cc1c(COC)c(C(NCc  2ccc(CN)cc2)=O)no1 | 31033192 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 891 | CC(C)Oc1cc(nc(N)n 1)N1CCCN(CC1)c1c  cncc1C | 31256092 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 892 | Cc1nc(CCN)cc(n1)N 1CCN(CC1)c1ccc(C#  N)cn1 | 31455775 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 893 | Cc1c2c(NCc3nc(N) [nH]n3)nc(C)nc2on1 | 31495708 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 894 | COc1ccc(CCNCc2cc cc(c2)C(F)(F)F)cc1 | 3169-1283 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 895 | C(CNCc1ccc2c(c1)O CO2)c1ccc(cc1)F | 3169-1371 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 896 | Cc(c(Sc(cc1)c2cc1O) c1C2=O)ccc1NCCN( C)C.I | 317003 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 897 | C1CN(CC1CN)Cc1c  cc(c2ccccc2C#N)o1 | 31727519 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 898 | CNCC(N1CCn2c(C1  )cc(CN1CCN(CC1)c  1ncccn1)n2)=O | 31916172 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 899 | CN(C)CCNc1nc2c(C (N(C)C(N2C)=O)=O)  n1Cc1ccccc1[Cl] | 3238-0121 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 900 | C1CCN(CC1)CCN1 C(=N)N(CCO)c2cccc | 3260-0393 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | c12 |  |  |  |  |  |
| 901 | C(/C=C/  CSc1ncccc1)Sc1nccc c1 | 326921 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 902 | Cc1ccc2cc(ccc2n1)C 1(CCN(CC1)C([C@ H] (Cc1c[nH]cn1)N)=O) O | 32773903 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 903 | C1CC1C(N1C[C@H  ]2CN(Cc3ccc(C#CC O)cc3)C[C@]2(C1)C (O)=O)=O | 32890291 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 904 | C1[C@@H] (C2(CCN(CC2)Cc2c  cc3c(c2)nsn3) [C@@H]1O)OCCN | 33199582 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 905 | C1CCCN(CC1)C[C  @@H]1CN(C[C@@ H]1CO)C(C1=CN=C 2C=CC=CN2C1=O)  =O | 33208201 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 906 | CCc1c(C)c(NCC(CN (C)C)O)nc(N)n1 | 33322598 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 907 | C1CN(CCN1)Cc1ccc  (cc1)c1cccc(CN2CC OCC2)c1 | 33356104 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 908 | Cc1ccc(cc1) [C@H]1CN(C(c2cc(  N)[nH]n2)=O) [C@@H]2C3CCN(C C3)[C@H]12 | 33481810 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 909 | COc1cccc(CCNCc2c (cccc2F)F)c1 | 3381-1346 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 910 | COc1cc(CNC2CCCc  3ccccc23)cc(c1OC)O C | 3381-1370 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 911 | CCc1cnc(N)nc1NCC CNc1ccc(C)cn1 | 33868270 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 912 | C(c1c[nH]cn1) [C@@H] (C(N1CCN(CC1)Cc1  ccc(cc1)[Cl])=O)N | 34469220 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 913 | Cc1c2c(N[C@H] (Cc3ccccc3)CO)nc(c 3ccncc3)nc2n(C)n1 | 34522202 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 914 | C1CC(CN(C1)CCc1c  cccc1)Nc1nccc(N)n1 | 34987857 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 915 | Cc1c2ccccc2n(CC(C n2c(C)cc(C)n2)O)c1 C | 3573-0009 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 916 | CCCCOCC(CN1CC N(CC1)C(C)=O)O | 3672-0063 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 917 | COc1ccc(CNCc2ccc( cc2)[Cl])cc1OC | 3701-0030 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 918 | COc1ccc(CNCc2ccc( cc2)[Br])cc1 | 3702-1263 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 919 | COc1cccc(CNCc2c(c ccc2F)F)c1OC | 3702-1409 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 920 | COc1ccccc1CNCc1c cc(c(c1)[Br])OC | 3702-1457 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 921 | COc1ccc(CCNCc2cc c(cc2)C(F) | 3702-1472 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | (F)F)cc1OC |  |  |  |  |  |
| 922 | COc1ccc(CNCc2cc(c cc2OC)[Br])cc1 | 3702-1485 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 923 | COc1cccc(CNCc2ccc c(c2)F)c1OC | 3702-1553 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 924 | COc1cccc(CCNCc2c cc(cc2)C(F)(F)F)c1 | 3702-1570 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 925 | C(c1ccncc1)NCc1ccc 2c(c1)OCO2 | 3702-1584 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 926 | CCC(CO)NCC(CN1c  2ccccc2Sc2ccccc12) O | 3746-0114 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 927 | CC(C1COc2ccccc2O 1)NCc1ccccc1 | 3875-0321 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 928 | Cc1ccc(cc1)S(N(CC( CN1CCCCC1)O)c1c cccc1OC)(=O)=O | 4013-2178 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 929 | CC1=CC(C)=NC(N1 CCNC1CCC2(CC1) CCNCC2)=O | 41200051 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 930 | C1COC(CNCc2ccccc 2)c2ccccc12 | 4192-0361 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 931 | CC1=CC(C)=NC(N1  CCNc1nccc(n1)N1C CC(C1)O)=O | 42681157 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 932 | Cc1cc(COC)c2c(c(C( Nc3ccccc3[Cl])=O)sc 2n1)N | 4281-0203 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 933 | CCOC(c1cnc2c(C)cc (C)cc2c1NCCCN1C COCC1)=O | 4358-4469 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 934 | Cc(cc1)cc(S(N) (=O)=O)c1/N=N/  c(cc1)c(C)cc1N | 45527 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 935 | C(CNc1cccnc1)CNc1 c2ccccc2nc(CCN)n1 | 47488116 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 936 | Cc1ccsc1CN(CCN(C  )C)C(CN)=O | 47645371 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 937 | CCN(CC)CCCNc1c2  c3CCCCc3sc2ncn1 | 4789-3782 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 938 | Cc1cnc(N)nc1NCC[ C@@H]1C[C@H]2 C[C@@H]1C=C2 | 47913504 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 939 | CCOc1cc(CNCCc2cc cc(c2)OC)ccc1OC | 4964-4425 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 940 | C(CNCc1cccnc1)c1c[ nH]c2ccccc12 | 4964-4666 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 941 | COc1ccccc1CCNCc1 ccc(cc1)C(F)(F)F | 4964-4708 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 942 | CSc1ccc(CNCCc2c[n H]c3ccccc23)cc1 | 4964-4965 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 943 | COc1cc(CNCCc2c[n H]c3ccccc23)cc(c1)O C | 4964-5192 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 944 | Cc1nc(SC)nc(N2CC2  )c1Br | 50199 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 945 | O=C(C=C(c1nnn[nH] 1)N1)NC1=O | 51093 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 946 | CCOC(c1c2c(nc3ccc cc3n2)n(c2cccc(c2) | 5122-1932 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | [Cl])c1N)=O |  |  |  |  |  |
| 947 | C1CCC(CCNc2c(NS  (c3ccccc3) (=O)=O)nc3ccccc3n2  )=CC1 | 5122-2566 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 948 | C(CC(O)=O)CNc1cc c(cc1)S(O)(=O)=O | 5137336 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 949 | C(C(CN=Cc1ccccc1 O)O)N=Cc1ccccc1O | 5172847 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 950 | C(CN1CCN(CC1)CC  O)C(N1c2ccccc2Sc2 ccc(cc12)C(F) (F)F)=O.[Cl].[Cl] | 5216181 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 951 | CCCCc1c(CCC)c(c2  ccccc2n1)NC(CNC(C  ) (C)C)=O.C(C(O)=O) (O)=O | 5229954 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 952 | C(CCN=Cc1ccccc1N  )CN=Cc1ccccc1N | 5233844 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 953 | C1CN(CCN1CC=Cc  1ccccc1)CC(Cn1c2cc ccc2c2ccccc12)O | 5236683 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 954 | Cc1cc(C)n(c2cc(NC CO)ncn2)n1 | 5256691 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 955 | COc1ccc(cc1)OCC(C N1CCN(CC1)c1cccc c1)O.[Cl].[Cl] | 5257916 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 956 | C1CC(CN(C1)Cc1cc cc(c1)[N+]  ([O-])=O)O | 5260879 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 957 | C1CN(CCC1O)Cc1c cccc1[N+]([O-])=O | 5269563 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 958 | CC(C) (C)NCC(Nc1c2CCC Cc2nc2CCCc12)=O. C(O)=O.C(C(O)=O) (O)=O | 5284047 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 959 | Cc1cccc(C)c1OCC(C N(c1ccccc1OC)S(c1c cccc1)(=O)=O)O | 5500-1497 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 960 | CCOc1cc(CNCCc2cc cc(c2)F)ccc1OC | 5571711 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 961 | CCCNC(c1c2CCCC Cc2sc1N)=O | 5577437 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 962 | CCCCOC(C1=C(N) OC2CC(C) (C)CC(C=2C12C(Nc 1ccccc12)=O)=O)=O | 5587-0160 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 963 | COc1cccc(CN2CCC( CC2)N2CCN(CC2)C CO)c1 | 5607-0221 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 964 | COc1ccc(cc1CN1CC C(CC1)N1CCN(CC1  )CCO)[Br] | 5607-0223 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 965 | CCn1c2ccccc2c2cc(C N3CCC(CC3)N3CC N(CC3)CCO)ccc12 | 5607-0247 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 966 | CC1CC2(CC(C)  (c3csc(Nc4ccccc4C)n 3)OC2=O)C(=O)O1 | 5613-0424 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 967 | C=CCC(CC=C)  (c1ccc(cc1)C(CC=C) | 5654685 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | (CC=C)N)N |  |  |  |  |  |
| 968 | CC(=C)CC(c1ccc(cc 1)OC)NCc1ccco1 | 5689-0111 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 969 | CN1CCc2c(c3ccccc3 nc12)NC(CNCCc1cc c(c(c1)OC)OC)=O.C(  C(O)=O)(O)=O | 5705994 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 970 | COC(CCCCC1C(C( CS1)N)N)=O.[Br]. [Br] | 5728434 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 971 | CCCCNCCOc1ccccc 1OCC.C(C(O)=O) (O)=O | 5728614 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 972 | CC(C)  (C)NCCOc1ccc(cc1) [Br].[Cl] | 5728895 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 973 | Cc1ccc(c(c1) [Cl])OCCNC(C)  (C)C.[Cl] | 5729988 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 974 | CCCCNCCOc1ccccc 1F.C(C(O)=O)(O)=O | 5734218 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 975 | C(CN1CCOCC1)C(N  c1ccc(cc1C(c1ccccc1  )NCC(NN)=O)  [Br])=O | 5808034 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 976 | C(CN)c1nc(c2ccccc2 n1)NCc1cn[nH]c1c1c ccs1 | 58789773 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 977 | C(CCO)CN(Cc1cccc c1)c1c2ccccc2nc(CC N)n1 | 58803915 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 978 | COc1c(cc(cc1[Cl])c1 cn(CCN2CCNCC2)n n1)F | 58951723 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 979 | c1cc(ccc1c1cn2ccsc2 n1)N | 5968142 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 980 | CC(C)CN1CCC(CC1  )NCCNc1ccncc1C | 60244866 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 981 | O=C(c(cc1)cc(Cl)c1 C(Nc(cc1)ccc1C1=N CCN1)=O)Nc(cc1)cc c1C1=NCCN1 | 60339 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 982 | C1CCCCCc2c(CCC C1)c(C(N)=O)c(N)s2 | 6132195 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 983 | CCC(CO)NCC(Cn1c nc2c1C(N(C)C(N2C)  =O)=O)O | 6212-0073 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 984 | C(CNCC(CN1c2cccc c2Sc2ccccc12)O)c1c cccc1.C(C(O)=O) (O)=O | 6401418 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 985 | Cc1c2ccccc2n(CC(C NCCCO)O)c1C.C(C(  O)=O)(O)=O | 6401887 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 986 | C1CN(CCN1CC(CN  1c2ccccc2Sc2ccccc1 2)O)Cc1ccccc1.C(C( O)=O)(O)=O | 6409737 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 987 | C1Cc2ccc(cc2C1)NC (CCN1CCN(CC1)CC O)=O.[Cl] | 6544961 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 988 | O=C(c(cc1)cc(C(Nc( cc2)ccc2C2=NCCN2 | 67436 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | )=O)c1Cl)Nc(cc1)ccc 1C1=NCCN1 |  |  |  |  |  |
| 989 | C1CCN(CC1)CC(Cn  1ccc2ccccc12)O | 7230-0020 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 990 | [H]N(CCCN(C)C)Cc  1cccn1C | 7465-0190 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 991 | COc1cccc(CNc2ccc3 c(c2)ncn3C2CCCCC 2)c1 | 7491-0191 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 992 | C1CCN(C1)c1ccc(cc 1[Cl])NC1c2ccccc2S (N=1)(=O)=O | 7641-0012 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 993 | CCOc1ccccc1CNc1n cc(c2cccc(c2) [Cl])n1C | 7756-0249 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 994 | Cn1c(cnc1NCc1ccc(c (c1)OC)OC)c1ccc(cc 1)[Br] | 7756-0269 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 995 | CCOc1ccc(CNc2ncc( c3ccc(cc3) [Br])n2C)cc1 | 7756-0277 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 996 | Cn1c(cnc1NCc1cccc( c1) [Cl])c1cccc(c1)OC | 7756-0392 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 997 | CCc1ccc(CNc2ncc(c 3cccc(c3)OC)n2C)cc 1 | 7756-0420 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 998 | Cn1c(cnc1NCc1ccc(c c1)F)c1ccc(cc1)[Cl] | 7756-0612 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 999 | Cn1c(cnc1NCc1cccc c1F)c1ccc(cc1)[Cl] | 7756-0619 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1000 | Cn1c(cnc1NCc1cccc c1F)c1cccc(c1)[Br] | 7756-0646 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1001 | Cn1c(cnc1NCc1cccc( c1)F)c1cccc(c1)[Br] | 7756-0657 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1002 | Cn1c(cnc1NCc1c(ccc c1[Cl])F)c1ccc(cc1)O C | 7756-0741 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1003 | CCOc1ccc(cc1)c1cnc (NCc2ccccc2OC)n1C | 7756-0840 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1004 | CC(CNCCCSc1ccc( C)cc1)O.C(C(O)=O) (O)=O | 7969636 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1005 | C=CCc1cc(ccc1OCC NCCN1CCOCC1) [Cl].C(C(O)=O) (O)=O | 7969784 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1006 | C(CCOc1cccc(c1)C( F) (F)F)CNCCN1CCOC C1.C(C(O)=O)(O)=O | 7970451 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1007 | C(CN)CN1CCN(CC1  )c1ccccc1 | 7974015 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1008 | COc1ccc(c(c1)NC1C CN(CC1)Cc1ccc(cc1  )[Br])OC.C(C(F) (F)F)(O)=O | 7974260 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1009 | CCOC(C1C(C(C#N)  =C(N)OC=1C)c1ccc( cc1)SC)=O | 8003-3604 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1010 | CC(C)OC(C1C(C2= C(CC(C) | 8003-3608 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | (C)CC2=O)OC=1N)c  1ccc(cc1)[Cl])=O |  |  |  |  |  |
| 1011 | Cc1ccc(cc1C)Nc1nc( cs1)c1ccc(cc1)S(N1C COCC1)(=O)=O | 8004-5090 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1012 | C1COCCN1S(c1ccc(  cc1)c1csc(Nc2ccc(cc 2)[Cl])n1)(=O)=O | 8004-5091 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1013 | CCN(CC)S(c1ccc(cc 1)c1csc(Nc2cccc(c2) OC)n1)(=O)=O | 8005-1875 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1014 | CCOC(C1=C(C)OC(  =C(C#N)C12C(Nc1c  cc(cc12) [Br])=O)N)=O | 8005-2600 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1015 | Cc1ccc(cc1C)Nc1nc( cs1)c1ccccc1 | 8005-2768 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1016 | CCOC(C1=C(N)OC( C)=C(C(=O)OCc2ccc  cc2)C12C(Nc1ccccc1 2)=O)=O | 8006-8591 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1017 | CC1=C(C(=O)OCc2c cccc2)C2(C(=C(N)O 1)C(=O)OC(C)  (C)C)C(Nc1ccccc12)  =O | 8006-8595 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1018 | CCCC1=C(C(=O)OC C)C2(C(C#N)=C(N)  O1)C(Nc1ccc(C)cc12  )=O | 8008-1721 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1019 | [H]Nc1nnc(COc2ccc( cc2)C2CCCCC2)s1 | 8009-2831 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1020 | [H]Nc1nnc(COc2cc( C)ccc2C)s1 | 8009-6459 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1021 | C1CCc2c(C1)c(C(c1  ccccc1)=O)c(N)s2 | 8010-1935 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1022 | Cc1c2c(n(c3cccc(c3) [Cl])n1)OC(=C(C#N)  C21C(N(CC(=O)OC)  c2ccccc12)=O)N | 8012-0517 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1023 | CC1CCc2c(C1)c(c1c  cc(cc1)F)c(C#N)c(N) n2 | 8012-3332 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1024 | COc1ccc(CCNCc2cc ccn2)cc1OC | 8012-7793 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1025 | Cc1c(CCNCc2ccc(C #N)cc2)c2cc(ccc2[nH  ]1)OC | 8013-2954 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1026 | CCn1c2C(N(C)C(N(  C)c2nc1NCc1ccccn1)  =O)=O | 8013-6370 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1027 | C(CO)n1c(cn2c(c3cc ccc3)c(c3ccccc3)nc1 2)c1ccccc1 | 8014-9053 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1028 | CCOc1ccc(CC(C2=C (CCCC2=O)NC(C)C( O)=O)=O)cc1OCC | 8015-5677 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1029 | CC(C)C(c1cc2c(cc1 N)OCCO2)=O | 8016-5460 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1030 | C=CCN1C(C2(C(C# N)=C(N)N(C3COC(  C2=3)=O)c2cccc(c2) C(F) | 8017-5296 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | (F)F)c2ccccc12)=O |  |  |  |  |  |
| 1031 | C(c1ccc(cc1)F)N1C( C2(C(C#N)=C(N)N( C3COC(C2=3)=O)c2  ccc(cc2)F)c2ccccc12)  =O | 8017-5304 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1032 | C(c1cccc(c1)F)N1C( C2(C(C#N)=C(N)N( C3COC(C2=3)=O)c2  ccc(cc2)F)c2ccccc12)  =O | 8017-5320 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1033 | COc1ccc(CCNc2nc(c s2)c2cccs2)cc1OC | 8018-0995 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1034 | CC(C)C(CCNCc1ccc (cc1)OC)C1CCOC(C  )(C)C1 | 8018-1265 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1035 | CC(C)C1(CCNCc2cc c(cc2)OC)CCOC(C) (C)C1 | 8018-1266 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1036 | CC(C)C1(CCNCc2cc cc3c2OCO3)CCOC( C)(C)C1 | 8018-1268 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1037 | CC1=CC(C)=NC(N1 CCN)=O | 8018-1719 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1038 | C1CC(c2cnn(c3ccccn 3)c2C1)N | 8018-2974 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1039 | Cc1c(C#N)c(N)n(CC  Cn2ccnc2)c1C | 8018-7492 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1040 | C#CC1(CCCCC1)N | 8018-8549 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1041 | C1CC1(CN)c1ccc(cc 1)[Cl] | 8018-9305 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1042 | CCc1ccc(cc1)OCCn1 c2ccccc2nc1CO | 8019-2262 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1043 | C1C(c2ccc(cc2)C(F) (F)F)c2c(NC1=O)nc( N)s2 | 8019-3691 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1044 | COc1cc(ccc1OC1CC CC1)C1CC(Nc2c1sc( N)n2)=O | 8019-3694 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1045 | C(COc1cccc(c1) [Cl])N | 8019-3866 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1046 | Cn1c(cc(c2ccc(cc2)F  )n1)N | 8019-7127 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1047 | CCn1cc(CNCC2CC(  Cc3cc(c4c(c3)OCO4) OC)ON=2)c(C)n1 | 8019-7189 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1048 | C1CCC2=C(C1)C(C  #N)=C(Nc1ccccc1)n1 cnnc12 | 8019-7543 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1049 | C(c1cn[nH]c1c1ccc(c c1)[Cl])N | 8019-9983 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1050 | [H]N(CCNCCO)Cc1  cc(c(c(c1)  [Br])OC)OC | 8020-1349 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1051 | C(c1cn2cc(sc2n1) [Cl])N | 8020-2315 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1052 | C1C(NCC2)N3C2NC CC3NC1 | 81462 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1053 | COc1cc(ccc1OCCCN 1CCCCC1)N.[Cl]. [Cl] | 9122829 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 1054 | CCNCC#CCOc1ccc(  cc1)[Br] | 9126666 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1055 | CCN1CCCC1CNCc1  ccc(C)s1.[Cl].[Cl] | 9131777 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1056 | CC(c1ccc(cc1)c1ccc( CNCCc2c[nH]c3cccc c23)o1)O.[Cl] | 9135919 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1057 | CSc1ccc(cc1)OCCN | 9254473 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1058 | CCN1CCCC1CNCc1  cccc(c1)OCc1ccc(cc1  )[Cl] | 9312203 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1059 | O=C(C(C(N1)=O)=C  c2cc3ccccc3cc2)NC1  =O | 95909 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1060 | CCN(CCCC/C1=N\ O)CCCC/C1=N\O | 96491 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1061 | S=C1Nc(cccc2)c2- c2c1cccc2 | 98857 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1062 | C(c1nc2ccccc2n1CC Oc1ccccc1)Nc1ccccc 1 | C147-0115 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1063 | CCOC(N1CCC(CC1)  Nc1nc2ccccc2c2nnc( C)n12)=O | C301-4817 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1064 | CCc1nnc2c3ccccc3nc (Nc3ccccc3OCC)n12 | C301-5148 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1065 | Cc1cc(NCCC2CCCC  C=2)n2c(c(c3ccc(c(c 3)OC)OC)c(C)n2)n1 | C535-0544 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1066 | Cc1ccc2cc3c(N)nn(C (c4cccc(c4) [Cl])=O)c3nc2c1 | C619-0133 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1067 | C1CCC(CCNc2c3ccc cc3c(Cc3cccnc3)nn2)  =CC1 | C696-0004 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1068 | C1CCCN(CC1)CCC  Nc1nc2ccccc2c2nc(c 3ccccc3)nn12 | C736-0159 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1069 | CCOC(N1CCN(CC1) C1=C(C(C1=O)=O)N CCCN1CCCCCC1)= O | C748-1353 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1070 | CCOC(N1CCN(CC1) C1=C(C(C1=O)=O)N CCN1CCCCCC1)=O | C748-1355 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1071 | COc1ccc(CCNCc2cc c(C(O)=O)s2)cc1OC | C863-0014 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1072 | Cc1c(CCC(Nc2ccc(c c2)OC)=O)c(C)n2c(n 1)nc(CN)n2 | C908-0409 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1073 | Cc1cc(ccc1NC(CCc1 c(C)nc2nc(CN)nn2c1 C)=O)F | C908-0490 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1074 | Cc1cccc(c1)NC(CCc 1c(C)nc2nc(CN)nn2c 1C)=O | C908-0492 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1075 | Cc1c(CCC(NCC2CC  N(CC2)Cc2ccccc2F)  =O)c(C)n2c(n1)nc(C N)n2 | C908-0547 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1076 | Cc1c(CCC(NCC2CC  N(CC2)Cc2ccccc2O | C908-0549 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | C)=O)c(C)n2c(n1)nc( CN)n2 |  |  |  |  |  |
| 1077 | Cc1ccc(cc1)S(NCC(c 1ccccc1)Nc1cc(C)ccc 1C)(=O)=O | D030-0042 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1078 | Cc1cc(C)n2c(n1)nc( NCc1cccc(c1)[Cl])n2 | D043-0239 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1079 | Cn1c2ccccc2nc1CN | D047-0045 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1080 | CCCCNc1c(nc(c2ccc cc2)o1)S(c1ccccc1) (=O)=O | D072-0067 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1081 | COCCCNc1c(nc(c2c cccc2)o1)S(c1ccccc1) (=O)=O | D072-0340 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1082 | [H]c1ccc(cc1)S(c1c( NCC(C)C)oc(c2ccc(c c2)F)n1)(=O)=O | D072-0411 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1083 | C(CNc1c(nc(c2ccc(c c2) [Cl])o1)S(c1ccc(cc1) F)(=O)=O)Cn1ccnc1 | D072-1602 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1084 | COCCNc1c(nc(c2ccc cc2F)o1)S(c1ccc(cc1) F)(=O)=O | D072-1707 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1085 | CCN(CC)CC(CN1C  Cn2c3C1CCCc3c1cc (C)ccc12)O | D090-0003 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1086 | CN1C(N(Cc2ccccc2) C(c2c1nc(NCCN)n2 C)=O)=O | D114-0037 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1087 | CCc1c(C)nc2nncn2c 1NCc1ccc(cc1)OC | D150-0320 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1088 | c1ccc(cc1)c1cc(Nc2c cc(cc2)C(O)=O)ncn1 | D278-0137 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1089 | CCOC(c1cccc(c1)Nc 1cc(c2ccccc2)ncn1)= O | D278-0165 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1090 | CSc1nc2CCCc2c(Nc 2cccc(c2)O)n1 | D278-0388 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1091 | CN1C(N(C)c2cc(CO  c3ccc(CNCc4cccnc4) cc3OC)ccc12)=O | D300-0082 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1092 | CCN(CC)CCCNCC1 CCOC(C)(C)C1 | D324-0108 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1093 | C(c1nnc(o1)SCc1ccc c(c1)[Br])N | D334-0126 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1094 | CCCNc1cc(C)nc2cc( c3ccccc3OC)nn12 | D393-0453 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1095 | CC1(C)CC(CCNC2C CN(C)CC2)  (CCO1)c1cccc(c1)C( F)(F)F | D442-0355 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1096 | CC1(C)CC(CCNCc2  cccnc2) (CCO1)c1cccc(c1)C( F)(F)F | D442-0374 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1097 | Cc1ccc(cc1)C1(CCN CCN2CCOCC2)CCO C(C)(C)C1 | D442-0384 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1098 | C1Cn2c3ccc(cc3nc2 CN1c1cccc(c1)N) [Cl] | D454-0510 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 1099 | CCCNc1cc(C(C)C)nc  2nc(c3cccnc3)nn12 | D494-0272 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1100 | Cc1cc(NCC(N2CCN(  CC2)c2ccccc2)=O)n2 c(n1)nc(c1cccnc1)n2 | D494-0459 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1101 | Cc1cc(C)cc(c1)OCC( Cn1c2ccccc2nc1C)O | D510-0556 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1102 | Cc1ccc(cc1)Nc1nc(C  )cc(n1)N1CCN(CC1)  C(c1ccco1)=O | D573-0288 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1103 | [H]N(Cc1cccnc1)Cc1 ccc(c2ccccc2)o1 | D665-0016 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1104 | Cc1ccc(CNc2c(cc3cc cc(C)c3n2)c2nc(C)on 2)cc1 | D704-1168 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1105 | Cc1c(C)nc2c(cnn2c1 NCC1CCCO1)c1cccc c1 | D724-0815 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1106 | c1cc2c(nc1)nc(c1cc(c cc1O)N)o2 | D725-0184 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1107 | CCOC(c1ccc(cc1)NC 1C(C)=C(c2ccc(C)c( C)c2)S(N=1)  (=O)=O)=O | E013-0432 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1108 | CC(C)c1ccc(cc1)C1= C(C)C(NCCc2ccccc2  )=NS1(=O)=O | E013-2935 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1109 | Cc1ccc(C)c(c1)Nc1n c2ccccc2c2nnc(C)n1 2 | E881-0025 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1110 | C(CCNCCCN)CN | NCGC00015937- 02 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1111 | C(CCCN=C(N)N=C(  N)Nc1ccc(cc1) [Cl])CCN=C(N)N=C  (N)Nc1ccc(cc1)[Cl] | NCGC00016246- 12 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1112 | CN(C)CCN(Cc1ccc(c  c1)[Cl])c1ccccn1 | NCGC00016672- 04 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1113 | CS(=O) (=O)OCCCCOS(C) (=O)=O | NCGC00090905- 11 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1114 | CCC(C)CCCCC(N[C  @@H] (CCN)C(NC(C(N[C  @H] (CCN)C(N[C@@H]1  CCNC(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 | NCGC00094763- 03 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1115 | C([C@H] (C(O)=O)N)SC(c1cc  ccc1) (c1ccccc1)c1ccccc1 | NCGC00159541- 02 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1116 | C1C(CN1)Nc1cccc(c 2cnc3ccc(cn23) [Cl])n1 | NCGC00241410- 01 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1117 | CC(C)c1cnn2c(cc(N | NCGC00346553- | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | CCCCCCN)nc12)NC  c1ccccc1 | 01 |  |  |  |  |
| 1118 | Cc1cc(ccc1Oc1ccn2c (c1)ncn2)Nc1c2cc(cc c2ncn1)c1ccc(CNCC S(C)(=O)=O)o1 | NCGC00346672- 01 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1119 | C1C(C(O)=O)N=C(C  =C1C=CN1C(Cc2cc( c(cc12)O)OC1C(C(C (C(CO)O1)O)O)O)C( O)=O)C(O)=O | NCGC00346734- 01 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1120 | C[C@@H]  (c1ccccc1)NC(c1c(cc s1)OCc1ccc(cc1) [Cl])=O | NCGC00346882- 01 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1121 | CC(C)n1cnc2c(Nc3c ccc(c3)NC(C=C)=O) nc(NC3CCC(CC3)N( C)C)nc12 | NCGC00346964- 01 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1122 | CC(C)=CCCC(C)=C CNCCNC1[C@H]2C [C@H]3C[C@@H]1 C[C@H](C3)C2 | NCGC00348216- 02 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1123 | CCN(CC)CCOC(c1c  cc2c(c1)sc(NC(c1ccc (cc1)N)=O)n2)=O | 0812-1025 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1124 | CSCCC(C(O)=O)Nc  1c2c3CCCCc3sc2ncn 1 | 0866-0023 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1125 | Cc(cc(cc1)- n2c(NC=NC3=O)c3n  c2)c1N | 100120 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1126 | CC1CCN(CC1)CC(C  Oc1ccccc1CC=C)O | 1189-2046 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1127 | CC(NS(c(cc1)cc2c1s c(C)n2)(=O)=O)=O | 122385 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1128 | CN(CCCc1nccn1C)c 1c2CCNCc2nc(c2ccn cc2)n1 | 12244291 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1129 | CN(CC(N1C[C@@H  ](CN2CCCCCC2) [C@H] (C1)CO)=O)Cc1cccc  c1F | 12553104 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1130 | CN1CCN(CC1) [C@H]1CCN(C[C@ H]1CCCO)C(c1cccc2  c1ccn2C)=O | 12576044 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1131 | CN1CCCN(CC1)C[C  @@H]1CN(C[C@@ H]1CO)C(c1ccnc2cc ccc12)=O | 13336906 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1132 | CN(Cc1cccc(c1)OCC  =C)c1c2ccccc2nc(CC N)n1 | 13692816 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1133 | Cc1cnc(nc1N)N1C[C @H]2[C@@H] (C1)OC(N2CCCN1C COCC1)=O | 13797550 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1134 | C1CNCCC12c1ccccc 1[C@H]  ([C@@H]2OCc1ccc nc1)NC(c1cc[nH]n1)  =O | 14122667 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1135 | Cc1nc(CCN)cc(NCC | 14159297 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | C2CCCN2C)n1 |  |  |  |  |  |
| 1136 | Cc1ccc(cn1)NC([C@ H]1C[C@H] (CNC1)C(NCCc1c[n H]cn1)=O)=O | 14326970 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1137 | CCc1cc(nc(n1)N1CC CC1)N1C[C@@H] (C[C@H]1C(N(CC) CC)=O)N | 15018109 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1138 | Cc1cc(nc(N)n1)N1C CC(CC1)NCCCN1C  Cc2ccccc12 | 15043866 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1139 | CCNC([C@@H]1C[  C@@H] (CN1C(CN1CCCCC CC1)=O)N)=O | 15077405 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1140 | CN(CCc1cn[nH]c1)C ([C@H]1CC[C@H] (C1)N)=O | 15410184 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1141 | CCCC=Cc1ccc2c(c1) nc(C(C)O)[nH]2 | 15802636 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1142 | CCc1nnc(NCC2CCC CCN2)o1 | 16631339 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1143 | Cc1c(cn(C)n1)NC(N CC(Cc1cccs1)CO)=O | 16859921 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1144 | Cn1ccnc1CCC1CCC CN1C(c1cn(CCN)nn 1)=O | 16896468 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1145 | Cc1c(C(C(NCCNc2c  ccnc2)=O)N)c(C) [nH]n1 | 16899791 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1146 | C=Cc1ccc(nc1)N1CC N(CC(C1)O)Cc1cccc  c1 | 17524156 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1147 | Cc1cc2CC(CN)Oc2c(  c1)c1cnc2ccccc2n1 | 17587941 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1148 | NC(NCCCS(Nc(cc1)  ccc1Nc1c(cccc2)c2nc 2cc([N+]  ([O-])=O)ccc12) (=O)=O)=N.Cl | 177365 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1149 | OC(C(Nc1n[nH]cn1)  =O)=O | 177952 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1150 | CCc1cnc(N)nc1NCC C(C)N(C)CC | 18668112 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1151 | C(CN)c1ccc(CN2CC C(CC2)  (c2cccc(c2)C(F)  (F)F)O)cc1 | 18809502 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1152 | C(Cn1cc(C(NCCOc2  cccc3cccnc23)=O)nn 1)N | 18917752 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1153 | CC(Cc1cc(C)n[nH]1)  NCc1ccc(c(c1)OC)O CCN1CCCC1 | 19048916 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1154 | CC(C)n1cnnc1CN(C)  c1cc(CCN)nc(C)n1 | 19341804 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1155 | C1CN(Cc2c1c(ncn2) N1CCOCC1)C([C@ H]  (Cc1ccc(cc1)O)N)=O | 19595168 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1156 | Cc1nc2cc(CNC(c3cn (CCN)nn3)=O)ccc2n | 20202809 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | 1C |  |  |  |  |  |
| 1157 | Cc1cc(N)n(CC(N2C[  C@@H] (CN3CCCCCC3) [C@H] (C2)CO)=O)n1 | 20853195 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1158 | CCc1cc(nc(C)n1)N1 CCC(CC1)NCCNc1c  cncc1C | 20968889 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1159 | Cc1cnc(nc1N(C)C)N 1CCN(CC1)Cc1cn(C CO)nc1C | 21083372 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1160 | C1CC2(CCNCC2)C  CN(C1)Cc1ccnc2ccc cc12 | 22793936 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1161 | C1CCN(CC1)CC1(C  CN(Cc2cccc(CCN)c2  )C1)O | 22896979 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1162 | CNc1cc(c2ccc(cc2)c2 nnc(N)s2)c2cc[nH]c2 n1 | 25638728 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1163 | C1CC(CN(C1)Cc1cc  cc(CCN)c1)C(Cc1ccc cc1)=O | 27037369 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1164 | C1CC(CN(C1)Cc1cc  cc(c1)O)NC(c1cn(CC N)nn1)=O | 27067624 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1165 | COc1ccc(CCNCc2cc c(cc2)[Cl])cc1 | 2910-0536 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1166 | CCc1ccc(CNCCc2cc ccc2OC)cc1 | 2910-0568 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1167 | CCOc1ccc(CNCCc2c cc(cc2)[Cl])cc1 | 2910-0651 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1168 | CCOc1ccc(CNCCc2c cc(cc2)F)cc1 | 2910-0686 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1169 | COc1cc(CNCc2cc(cc c2OC)[Br])cc(c1)OC | 2910-1798 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1170 | Cc1ccc(C)c(c1)NCc1 cc(ccc1OC)[Br] | 2910-2364 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1171 | O=C(N(CC1OC1)C( N1CC2OC2)=O)N(C C2OC2)C1=O | 296934 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1172 | CCOC(/C(/ C1=CSC2=NNC(C) (C)N12)=N\O)=O | 299968 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1173 | Cc1cc2c(C)c(C)cc(N) c2nc1 | 304902 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1174 | Nc1ccc(Cn(ccc2c34) c2ccc4nc(N)nc3N)cc 1.Cl | 309401 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1175 | Cc1c(COC)c(C(NCc  2ccc(CN)cc2)=O)no1 | 31033192 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1176 | CC(C)Oc1cc(nc(N)n 1)N1CCCN(CC1)c1c  cncc1C | 31256092 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1177 | Cc1nc(CCN)cc(n1)N 1CCN(CC1)c1ccc(C#  N)cn1 | 31455775 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1178 | Cc1c2c(NCc3nc(N) [nH]n3)nc(C)nc2on1 | 31495708 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1179 | COc1ccc(CCNCc2cc | 3169-1283 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | cc(c2)C(F)(F)F)cc1 |  |  |  |  |  |
| 1180 | C(CNCc1ccc2c(c1)O CO2)c1ccc(cc1)F | 3169-1371 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1181 | Cc(c(Sc(cc1)c2cc1O) c1C2=O)ccc1NCCN( C)C.I | 317003 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1182 | C1CN(CC1CN)Cc1c  cc(c2ccccc2C#N)o1 | 31727519 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1183 | CNCC(N1CCn2c(C1  )cc(CN1CCN(CC1)c  1ncccn1)n2)=O | 31916172 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1184 | CN(C)CCNc1nc2c(C (N(C)C(N2C)=O)=O)  n1Cc1ccccc1[Cl] | 3238-0121 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1185 | C1CCN(CC1)CCN1 C(=N)N(CCO)c2cccc  c12 | 3260-0393 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1186 | C(/C=C/  CSc1ncccc1)Sc1nccc c1 | 326921 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1187 | Cc1ccc2cc(ccc2n1)C 1(CCN(CC1)C([C@ H] (Cc1c[nH]cn1)N)=O) O | 32773903 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1188 | C1CC1C(N1C[C@H  ]2CN(Cc3ccc(C#CC O)cc3)C[C@]2(C1)C (O)=O)=O | 32890291 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1189 | C1[C@@H] (C2(CCN(CC2)Cc2c  cc3c(c2)nsn3) [C@@H]1O)OCCN | 33199582 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1190 | C1CCCN(CC1)C[C  @@H]1CN(C[C@@ H]1CO)C(C1=CN=C 2C=CC=CN2C1=O)  =O | 33208201 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1191 | CCc1c(C)c(NCC(CN (C)C)O)nc(N)n1 | 33322598 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1192 | C1CN(CCN1)Cc1ccc  (cc1)c1cccc(CN2CC OCC2)c1 | 33356104 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1193 | Cc1ccc(cc1) [C@H]1CN(C(c2cc(  N)[nH]n2)=O) [C@@H]2C3CCN(C C3)[C@H]12 | 33481810 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1194 | COc1cccc(CCNCc2c (cccc2F)F)c1 | 3381-1346 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1195 | COc1cc(CNC2CCCc  3ccccc23)cc(c1OC)O C | 3381-1370 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1196 | CCc1cnc(N)nc1NCC CNc1ccc(C)cn1 | 33868270 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1197 | C(c1c[nH]cn1) [C@@H] (C(N1CCN(CC1)Cc1  ccc(cc1)[Cl])=O)N | 34469220 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1198 | Cc1c2c(N[C@H] (Cc3ccccc3)CO)nc(c 3ccncc3)nc2n(C)n1 | 34522202 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1199 | C1CC(CN(C1)CCc1c | 34987857 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | cccc1)Nc1nccc(N)n1 |  |  |  |  |  |
| 1200 | Cc1c2ccccc2n(CC(C n2c(C)cc(C)n2)O)c1 C | 3573-0009 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1201 | CCCCOCC(CN1CC N(CC1)C(C)=O)O | 3672-0063 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1202 | COc1ccc(CNCc2ccc( cc2)[Cl])cc1OC | 3701-0030 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1203 | COc1ccc(CNCc2ccc( cc2)[Br])cc1 | 3702-1263 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1204 | COc1cccc(CNCc2c(c ccc2F)F)c1OC | 3702-1409 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1205 | COc1ccccc1CNCc1c cc(c(c1)[Br])OC | 3702-1457 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1206 | COc1ccc(CCNCc2cc c(cc2)C(F) (F)F)cc1OC | 3702-1472 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1207 | COc1ccc(CNCc2cc(c cc2OC)[Br])cc1 | 3702-1485 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1208 | COc1cccc(CNCc2ccc c(c2)F)c1OC | 3702-1553 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1209 | COc1cccc(CCNCc2c cc(cc2)C(F)(F)F)c1 | 3702-1570 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1210 | C(c1ccncc1)NCc1ccc 2c(c1)OCO2 | 3702-1584 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1211 | CCC(CO)NCC(CN1c  2ccccc2Sc2ccccc12) O | 3746-0114 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1212 | CC(C1COc2ccccc2O 1)NCc1ccccc1 | 3875-0321 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1213 | Cc1ccc(cc1)S(N(CC( CN1CCCCC1)O)c1c cccc1OC)(=O)=O | 4013-2178 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1214 | CC1=CC(C)=NC(N1 CCNC1CCC2(CC1) CCNCC2)=O | 41200051 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1215 | C1COC(CNCc2ccccc 2)c2ccccc12 | 4192-0361 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1216 | CC1=CC(C)=NC(N1  CCNc1nccc(n1)N1C CC(C1)O)=O | 42681157 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1217 | Cc1cc(COC)c2c(c(C( Nc3ccccc3[Cl])=O)sc 2n1)N | 4281-0203 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1218 | CCOC(c1cnc2c(C)cc (C)cc2c1NCCCN1C COCC1)=O | 4358-4469 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1219 | Cc(cc1)cc(S(N) (=O)=O)c1/N=N/  c(cc1)c(C)cc1N | 45527 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1220 | C(CNc1cccnc1)CNc1 c2ccccc2nc(CCN)n1 | 47488116 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1221 | Cc1ccsc1CN(CCN(C  )C)C(CN)=O | 47645371 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1222 | CCN(CC)CCCNc1c2  c3CCCCc3sc2ncn1 | 4789-3782 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1223 | Cc1cnc(N)nc1NCC[ C@@H]1C[C@H]2 C[C@@H]1C=C2 | 47913504 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1224 | CCOc1cc(CNCCc2cc | 4964-4425 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | cc(c2)OC)ccc1OC |  |  |  |  |  |
| 1225 | C(CNCc1cccnc1)c1c[ nH]c2ccccc12 | 4964-4666 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1226 | COc1ccccc1CCNCc1 ccc(cc1)C(F)(F)F | 4964-4708 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1227 | CSc1ccc(CNCCc2c[n H]c3ccccc23)cc1 | 4964-4965 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1228 | COc1cc(CNCCc2c[n H]c3ccccc23)cc(c1)O C | 4964-5192 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1229 | Cc1nc(SC)nc(N2CC2  )c1Br | 50199 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1230 | O=C(C=C(c1nnn[nH] 1)N1)NC1=O | 51093 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1231 | CCOC(c1c2c(nc3ccc cc3n2)n(c2cccc(c2) [Cl])c1N)=O | 5122-1932 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1232 | C1CCC(CCNc2c(NS  (c3ccccc3) (=O)=O)nc3ccccc3n2  )=CC1 | 5122-2566 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1233 | C(CC(O)=O)CNc1cc c(cc1)S(O)(=O)=O | 5137336 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1234 | C(C(CN=Cc1ccccc1 O)O)N=Cc1ccccc1O | 5172847 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1235 | C(CN1CCN(CC1)CC  O)C(N1c2ccccc2Sc2 ccc(cc12)C(F) (F)F)=O.[Cl].[Cl] | 5216181 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1236 | CCCCc1c(CCC)c(c2  ccccc2n1)NC(CNC(C  ) (C)C)=O.C(C(O)=O) (O)=O | 5229954 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1237 | C(CCN=Cc1ccccc1N  )CN=Cc1ccccc1N | 5233844 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1238 | C1CN(CCN1CC=Cc  1ccccc1)CC(Cn1c2cc ccc2c2ccccc12)O | 5236683 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1239 | Cc1cc(C)n(c2cc(NC CO)ncn2)n1 | 5256691 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1240 | COc1ccc(cc1)OCC(C N1CCN(CC1)c1cccc c1)O.[Cl].[Cl] | 5257916 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1241 | C1CC(CN(C1)Cc1cc cc(c1)[N+]  ([O-])=O)O | 5260879 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1242 | C1CN(CCC1O)Cc1c cccc1[N+]([O-])=O | 5269563 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1243 | CC(C) (C)NCC(Nc1c2CCC Cc2nc2CCCc12)=O. C(O)=O.C(C(O)=O) (O)=O | 5284047 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1244 | Cc1cccc(C)c1OCC(C N(c1ccccc1OC)S(c1c cccc1)(=O)=O)O | 5500-1497 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1245 | CCOc1cc(CNCCc2cc cc(c2)F)ccc1OC | 5571711 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1246 | CCCNC(c1c2CCCC Cc2sc1N)=O | 5577437 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 1247 | CCCCOC(C1=C(N) OC2CC(C) (C)CC(C=2C12C(Nc 1ccccc12)=O)=O)=O | 5587-0160 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1248 | COc1cccc(CN2CCC( CC2)N2CCN(CC2)C CO)c1 | 5607-0221 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1249 | COc1ccc(cc1CN1CC C(CC1)N1CCN(CC1  )CCO)[Br] | 5607-0223 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1250 | CCn1c2ccccc2c2cc(C N3CCC(CC3)N3CC N(CC3)CCO)ccc12 | 5607-0247 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1251 | CC1CC2(CC(C)  (c3csc(Nc4ccccc4C)n 3)OC2=O)C(=O)O1 | 5613-0424 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1252 | C=CCC(CC=C)  (c1ccc(cc1)C(CC=C) (CC=C)N)N | 5654685 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1253 | CC(=C)CC(c1ccc(cc 1)OC)NCc1ccco1 | 5689-0111 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1254 | CN1CCc2c(c3ccccc3 nc12)NC(CNCCc1cc c(c(c1)OC)OC)=O.C(  C(O)=O)(O)=O | 5705994 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1255 | COC(CCCCC1C(C( CS1)N)N)=O.[Br]. [Br] | 5728434 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1256 | CCCCNCCOc1ccccc 1OCC.C(C(O)=O) (O)=O | 5728614 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1257 | CC(C)  (C)NCCOc1ccc(cc1) [Br].[Cl] | 5728895 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1258 | Cc1ccc(c(c1) [Cl])OCCNC(C)  (C)C.[Cl] | 5729988 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1259 | CCCCNCCOc1ccccc 1F.C(C(O)=O)(O)=O | 5734218 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1260 | C(CN1CCOCC1)C(N  c1ccc(cc1C(c1ccccc1  )NCC(NN)=O)  [Br])=O | 5808034 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1261 | C(CN)c1nc(c2ccccc2 n1)NCc1cn[nH]c1c1c ccs1 | 58789773 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1262 | C(CCO)CN(Cc1cccc c1)c1c2ccccc2nc(CC N)n1 | 58803915 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1263 | COc1c(cc(cc1[Cl])c1 cn(CCN2CCNCC2)n n1)F | 58951723 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1264 | c1cc(ccc1c1cn2ccsc2 n1)N | 5968142 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1265 | CC(C)CN1CCC(CC1  )NCCNc1ccncc1C | 60244866 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1266 | O=C(c(cc1)cc(Cl)c1 C(Nc(cc1)ccc1C1=N CCN1)=O)Nc(cc1)cc c1C1=NCCN1 | 60339 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1267 | C1CCCCCc2c(CCC C1)c(C(N)=O)c(N)s2 | 6132195 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1268 | CCC(CO)NCC(Cn1c | 6212-0073 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | nc2c1C(N(C)C(N2C)  =O)=O)O |  |  |  |  |  |
| 1269 | C(CNCC(CN1c2cccc c2Sc2ccccc12)O)c1c cccc1.C(C(O)=O) (O)=O | 6401418 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1270 | Cc1c2ccccc2n(CC(C NCCCO)O)c1C.C(C(  O)=O)(O)=O | 6401887 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1271 | C1CN(CCN1CC(CN  1c2ccccc2Sc2ccccc1 2)O)Cc1ccccc1.C(C( O)=O)(O)=O | 6409737 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1272 | C1Cc2ccc(cc2C1)NC (CCN1CCN(CC1)CC O)=O.[Cl] | 6544961 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1273 | O=C(c(cc1)cc(C(Nc( cc2)ccc2C2=NCCN2  )=O)c1Cl)Nc(cc1)ccc 1C1=NCCN1 | 67436 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1274 | C1CCN(CC1)CC(Cn  1ccc2ccccc12)O | 7230-0020 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1275 | [H]N(CCCN(C)C)Cc  1cccn1C | 7465-0190 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1276 | COc1cccc(CNc2ccc3 c(c2)ncn3C2CCCCC 2)c1 | 7491-0191 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1277 | C1CCN(C1)c1ccc(cc 1[Cl])NC1c2ccccc2S (N=1)(=O)=O | 7641-0012 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1278 | CCOc1ccccc1CNc1n cc(c2cccc(c2) [Cl])n1C | 7756-0249 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1279 | Cn1c(cnc1NCc1ccc(c (c1)OC)OC)c1ccc(cc 1)[Br] | 7756-0269 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1280 | CCOc1ccc(CNc2ncc( c3ccc(cc3) [Br])n2C)cc1 | 7756-0277 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1281 | Cn1c(cnc1NCc1cccc( c1) [Cl])c1cccc(c1)OC | 7756-0392 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1282 | CCc1ccc(CNc2ncc(c 3cccc(c3)OC)n2C)cc 1 | 7756-0420 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1283 | Cn1c(cnc1NCc1ccc(c c1)F)c1ccc(cc1)[Cl] | 7756-0612 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1284 | Cn1c(cnc1NCc1cccc c1F)c1ccc(cc1)[Cl] | 7756-0619 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1285 | Cn1c(cnc1NCc1cccc c1F)c1cccc(c1)[Br] | 7756-0646 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1286 | Cn1c(cnc1NCc1cccc( c1)F)c1cccc(c1)[Br] | 7756-0657 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1287 | Cn1c(cnc1NCc1c(ccc c1[Cl])F)c1ccc(cc1)O C | 7756-0741 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1288 | CCOc1ccc(cc1)c1cnc (NCc2ccccc2OC)n1C | 7756-0840 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1289 | CC(CNCCCSc1ccc( C)cc1)O.C(C(O)=O) (O)=O | 7969636 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1290 | C=CCc1cc(ccc1OCC | 7969784 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | NCCN1CCOCC1) [Cl].C(C(O)=O) (O)=O |  |  |  |  |  |
| 1291 | C(CCOc1cccc(c1)C( F) (F)F)CNCCN1CCOC C1.C(C(O)=O)(O)=O | 7970451 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1292 | C(CN)CN1CCN(CC1  )c1ccccc1 | 7974015 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1293 | COc1ccc(c(c1)NC1C CN(CC1)Cc1ccc(cc1  )[Br])OC.C(C(F) (F)F)(O)=O | 7974260 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1294 | CCOC(C1C(C(C#N)  =C(N)OC=1C)c1ccc( cc1)SC)=O | 8003-3604 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1295 | CC(C)OC(C1C(C2= C(CC(C) (C)CC2=O)OC=1N)c  1ccc(cc1)[Cl])=O | 8003-3608 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1296 | Cc1ccc(cc1C)Nc1nc( cs1)c1ccc(cc1)S(N1C COCC1)(=O)=O | 8004-5090 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1297 | C1COCCN1S(c1ccc(  cc1)c1csc(Nc2ccc(cc 2)[Cl])n1)(=O)=O | 8004-5091 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1298 | CCN(CC)S(c1ccc(cc 1)c1csc(Nc2cccc(c2) OC)n1)(=O)=O | 8005-1875 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1299 | CCOC(C1=C(C)OC(  =C(C#N)C12C(Nc1c  cc(cc12) [Br])=O)N)=O | 8005-2600 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1300 | Cc1ccc(cc1C)Nc1nc( cs1)c1ccccc1 | 8005-2768 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1301 | CCOC(C1=C(N)OC( C)=C(C(=O)OCc2ccc  cc2)C12C(Nc1ccccc1 2)=O)=O | 8006-8591 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1302 | CC1=C(C(=O)OCc2c cccc2)C2(C(=C(N)O 1)C(=O)OC(C)  (C)C)C(Nc1ccccc12)  =O | 8006-8595 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1303 | CCCC1=C(C(=O)OC C)C2(C(C#N)=C(N)  O1)C(Nc1ccc(C)cc12  )=O | 8008-1721 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1304 | [H]Nc1nnc(COc2ccc( cc2)C2CCCCC2)s1 | 8009-2831 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1305 | [H]Nc1nnc(COc2cc( C)ccc2C)s1 | 8009-6459 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1306 | C1CCc2c(C1)c(C(c1  ccccc1)=O)c(N)s2 | 8010-1935 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1307 | Cc1c2c(n(c3cccc(c3) [Cl])n1)OC(=C(C#N)  C21C(N(CC(=O)OC)  c2ccccc12)=O)N | 8012-0517 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1308 | CC1CCc2c(C1)c(c1c  cc(cc1)F)c(C#N)c(N) n2 | 8012-3332 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1309 | COc1ccc(CCNCc2cc ccn2)cc1OC | 8012-7793 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 1310 | Cc1c(CCNCc2ccc(C #N)cc2)c2cc(ccc2[nH  ]1)OC | 8013-2954 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1311 | CCn1c2C(N(C)C(N(  C)c2nc1NCc1ccccn1)  =O)=O | 8013-6370 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1312 | C(CO)n1c(cn2c(c3cc ccc3)c(c3ccccc3)nc1 2)c1ccccc1 | 8014-9053 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1313 | CCOc1ccc(CC(C2=C (CCCC2=O)NC(C)C( O)=O)=O)cc1OCC | 8015-5677 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1314 | CC(C)C(c1cc2c(cc1 N)OCCO2)=O | 8016-5460 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1315 | C=CCN1C(C2(C(C# N)=C(N)N(C3COC(  C2=3)=O)c2cccc(c2) C(F)  (F)F)c2ccccc12)=O | 8017-5296 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1316 | C(c1ccc(cc1)F)N1C( C2(C(C#N)=C(N)N( C3COC(C2=3)=O)c2  ccc(cc2)F)c2ccccc12)  =O | 8017-5304 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1317 | C(c1cccc(c1)F)N1C( C2(C(C#N)=C(N)N( C3COC(C2=3)=O)c2  ccc(cc2)F)c2ccccc12)  =O | 8017-5320 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1318 | COc1ccc(CCNc2nc(c s2)c2cccs2)cc1OC | 8018-0995 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1319 | CC(C)C(CCNCc1ccc (cc1)OC)C1CCOC(C  )(C)C1 | 8018-1265 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1320 | CC(C)C1(CCNCc2cc c(cc2)OC)CCOC(C) (C)C1 | 8018-1266 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1321 | CC(C)C1(CCNCc2cc cc3c2OCO3)CCOC( C)(C)C1 | 8018-1268 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1322 | CC1=CC(C)=NC(N1 CCN)=O | 8018-1719 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1323 | C1CC(c2cnn(c3ccccn 3)c2C1)N | 8018-2974 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1324 | Cc1c(C#N)c(N)n(CC  Cn2ccnc2)c1C | 8018-7492 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1325 | C#CC1(CCCCC1)N | 8018-8549 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1326 | C1CC1(CN)c1ccc(cc 1)[Cl] | 8018-9305 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1327 | CCc1ccc(cc1)OCCn1 c2ccccc2nc1CO | 8019-2262 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1328 | C1C(c2ccc(cc2)C(F) (F)F)c2c(NC1=O)nc( N)s2 | 8019-3691 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1329 | COc1cc(ccc1OC1CC CC1)C1CC(Nc2c1sc( N)n2)=O | 8019-3694 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1330 | C(COc1cccc(c1) [Cl])N | 8019-3866 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1331 | Cn1c(cc(c2ccc(cc2)F  )n1)N | 8019-7127 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1332 | CCn1cc(CNCC2CC( | 8019-7189 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | Cc3cc(c4c(c3)OCO4) OC)ON=2)c(C)n1 |  |  |  |  |  |
| 1333 | C1CCC2=C(C1)C(C  #N)=C(Nc1ccccc1)n1 cnnc12 | 8019-7543 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1334 | C(c1cn[nH]c1c1ccc(c c1)[Cl])N | 8019-9983 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1335 | [H]N(CCNCCO)Cc1  cc(c(c(c1)  [Br])OC)OC | 8020-1349 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1336 | C(c1cn2cc(sc2n1) [Cl])N | 8020-2315 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1337 | C1C(NCC2)N3C2NC CC3NC1 | 81462 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1338 | COc1cc(ccc1OCCCN 1CCCCC1)N.[Cl]. [Cl] | 9122829 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1339 | CCNCC#CCOc1ccc(  cc1)[Br] | 9126666 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1340 | CCN1CCCC1CNCc1  ccc(C)s1.[Cl].[Cl] | 9131777 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1341 | CC(c1ccc(cc1)c1ccc( CNCCc2c[nH]c3cccc c23)o1)O.[Cl] | 9135919 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1342 | CSc1ccc(cc1)OCCN | 9254473 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1343 | CCN1CCCC1CNCc1  cccc(c1)OCc1ccc(cc1  )[Cl] | 9312203 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1344 | O=C(C(C(N1)=O)=C  c2cc3ccccc3cc2)NC1  =O | 95909 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1345 | CCN(CCCC/C1=N\ O)CCCC/C1=N\O | 96491 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1346 | S=C1Nc(cccc2)c2- c2c1cccc2 | 98857 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1347 | C(c1nc2ccccc2n1CC Oc1ccccc1)Nc1ccccc 1 | C147-0115 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1348 | CCOC(N1CCC(CC1)  Nc1nc2ccccc2c2nnc( C)n12)=O | C301-4817 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1349 | CCc1nnc2c3ccccc3nc (Nc3ccccc3OCC)n12 | C301-5148 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1350 | Cc1cc(NCCC2CCCC  C=2)n2c(c(c3ccc(c(c 3)OC)OC)c(C)n2)n1 | C535-0544 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1351 | Cc1ccc2cc3c(N)nn(C (c4cccc(c4) [Cl])=O)c3nc2c1 | C619-0133 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1352 | C1CCC(CCNc2c3ccc cc3c(Cc3cccnc3)nn2)  =CC1 | C696-0004 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1353 | C1CCCN(CC1)CCC  Nc1nc2ccccc2c2nc(c 3ccccc3)nn12 | C736-0159 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1354 | CCOC(N1CCN(CC1) C1=C(C(C1=O)=O)N CCCN1CCCCCC1)= O | C748-1353 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1355 | CCOC(N1CCN(CC1) C1=C(C(C1=O)=O)N | C748-1355 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | CCN1CCCCCC1)=O |  |  |  |  |  |
| 1356 | COc1ccc(CCNCc2cc c(C(O)=O)s2)cc1OC | C863-0014 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1357 | Cc1c(CCC(Nc2ccc(c c2)OC)=O)c(C)n2c(n 1)nc(CN)n2 | C908-0409 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1358 | Cc1cc(ccc1NC(CCc1 c(C)nc2nc(CN)nn2c1 C)=O)F | C908-0490 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1359 | Cc1cccc(c1)NC(CCc 1c(C)nc2nc(CN)nn2c 1C)=O | C908-0492 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1360 | Cc1c(CCC(NCC2CC  N(CC2)Cc2ccccc2F)  =O)c(C)n2c(n1)nc(C N)n2 | C908-0547 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1361 | Cc1c(CCC(NCC2CC  N(CC2)Cc2ccccc2O C)=O)c(C)n2c(n1)nc( CN)n2 | C908-0549 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1362 | Cc1ccc(cc1)S(NCC(c 1ccccc1)Nc1cc(C)ccc 1C)(=O)=O | D030-0042 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1363 | Cc1cc(C)n2c(n1)nc( NCc1cccc(c1)[Cl])n2 | D043-0239 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1364 | Cn1c2ccccc2nc1CN | D047-0045 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1365 | CCCCNc1c(nc(c2ccc cc2)o1)S(c1ccccc1) (=O)=O | D072-0067 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1366 | COCCCNc1c(nc(c2c cccc2)o1)S(c1ccccc1) (=O)=O | D072-0340 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1367 | [H]c1ccc(cc1)S(c1c( NCC(C)C)oc(c2ccc(c c2)F)n1)(=O)=O | D072-0411 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1368 | C(CNc1c(nc(c2ccc(c c2) [Cl])o1)S(c1ccc(cc1) F)(=O)=O)Cn1ccnc1 | D072-1602 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1369 | COCCNc1c(nc(c2ccc cc2F)o1)S(c1ccc(cc1) F)(=O)=O | D072-1707 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1370 | CCN(CC)CC(CN1C  Cn2c3C1CCCc3c1cc (C)ccc12)O | D090-0003 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1371 | CN1C(N(Cc2ccccc2) C(c2c1nc(NCCN)n2 C)=O)=O | D114-0037 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1372 | CCc1c(C)nc2nncn2c 1NCc1ccc(cc1)OC | D150-0320 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1373 | c1ccc(cc1)c1cc(Nc2c cc(cc2)C(O)=O)ncn1 | D278-0137 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1374 | CCOC(c1cccc(c1)Nc 1cc(c2ccccc2)ncn1)= O | D278-0165 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1375 | CSc1nc2CCCc2c(Nc 2cccc(c2)O)n1 | D278-0388 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1376 | CN1C(N(C)c2cc(CO  c3ccc(CNCc4cccnc4) cc3OC)ccc12)=O | D300-0082 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1377 | CCN(CC)CCCNCC1 CCOC(C)(C)C1 | D324-0108 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 1378 | C(c1nnc(o1)SCc1ccc c(c1)[Br])N | D334-0126 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1379 | CCCNc1cc(C)nc2cc( c3ccccc3OC)nn12 | D393-0453 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1380 | CC1(C)CC(CCNC2C CN(C)CC2)  (CCO1)c1cccc(c1)C( F)(F)F | D442-0355 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1381 | CC1(C)CC(CCNCc2  cccnc2) (CCO1)c1cccc(c1)C( F)(F)F | D442-0374 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1382 | Cc1ccc(cc1)C1(CCN CCN2CCOCC2)CCO C(C)(C)C1 | D442-0384 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1383 | C1Cn2c3ccc(cc3nc2 CN1c1cccc(c1)N) [Cl] | D454-0510 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1384 | CCCNc1cc(C(C)C)nc  2nc(c3cccnc3)nn12 | D494-0272 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1385 | Cc1cc(NCC(N2CCN(  CC2)c2ccccc2)=O)n2 c(n1)nc(c1cccnc1)n2 | D494-0459 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1386 | Cc1cc(C)cc(c1)OCC( Cn1c2ccccc2nc1C)O | D510-0556 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1387 | Cc1ccc(cc1)Nc1nc(C  )cc(n1)N1CCN(CC1)  C(c1ccco1)=O | D573-0288 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1388 | [H]N(Cc1cccnc1)Cc1 ccc(c2ccccc2)o1 | D665-0016 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1389 | Cc1ccc(CNc2c(cc3cc cc(C)c3n2)c2nc(C)on 2)cc1 | D704-1168 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1390 | Cc1c(C)nc2c(cnn2c1 NCC1CCCO1)c1cccc c1 | D724-0815 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1391 | c1cc2c(nc1)nc(c1cc(c cc1O)N)o2 | D725-0184 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1392 | CCOC(c1ccc(cc1)NC 1C(C)=C(c2ccc(C)c( C)c2)S(N=1)  (=O)=O)=O | E013-0432 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1393 | CC(C)c1ccc(cc1)C1= C(C)C(NCCc2ccccc2  )=NS1(=O)=O | E013-2935 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1394 | Cc1ccc(C)c(c1)Nc1n c2ccccc2c2nnc(C)n1 2 | E881-0025 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1395 | C(CCNCCCN)CN | NCGC00015937- 02 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1396 | C(CCCN=C(N)N=C(  N)Nc1ccc(cc1) [Cl])CCN=C(N)N=C  (N)Nc1ccc(cc1)[Cl] | NCGC00016246- 12 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1397 | CN(C)CCN(Cc1ccc(c  c1)[Cl])c1ccccn1 | NCGC00016672- 04 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1398 | CS(=O) (=O)OCCCCOS(C) (=O)=O | NCGC00090905- 11 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1399 | CCC(C)CCCCC(N[C  @@H] (CCN)C(NC(C(N[C  @H] | NCGC00094763- 03 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | (CCN)C(N[C@@H]1  CCNC(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 |  |  |  |  |  |
| 1400 | C([C@H] (C(O)=O)N)SC(c1cc  ccc1) (c1ccccc1)c1ccccc1 | NCGC00159541- 02 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1401 | C1C(CN1)Nc1cccc(c 2cnc3ccc(cn23) [Cl])n1 | NCGC00241410- 01 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1402 | CC(C)c1cnn2c(cc(N CCCCCCN)nc12)NC  c1ccccc1 | NCGC00346553- 01 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1403 | Cc1cc(ccc1Oc1ccn2c (c1)ncn2)Nc1c2cc(cc c2ncn1)c1ccc(CNCC S(C)(=O)=O)o1 | NCGC00346672- 01 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1404 | C1C(C(O)=O)N=C(C  =C1C=CN1C(Cc2cc( c(cc12)O)OC1C(C(C (C(CO)O1)O)O)O)C( O)=O)C(O)=O | NCGC00346734- 01 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1405 | C[C@@H]  (c1ccccc1)NC(c1c(cc s1)OCc1ccc(cc1) [Cl])=O | NCGC00346882- 01 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1406 | CC(C)n1cnc2c(Nc3c ccc(c3)NC(C=C)=O) nc(NC3CCC(CC3)N( C)C)nc12 | NCGC00346964- 01 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1407 | CC(C)=CCCC(C)=C CNCCNC1[C@H]2C [C@H]3C[C@@H]1 C[C@H](C3)C2 | NCGC00348216- 02 | EWSR1 | G-quadruplex | GGGGCAGGGGAAGAGGGGG | 1 |
| 1408 | CC1CCN(CC1)CC(C  Oc1ccccc1CC=C)O | 1189-2046 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1409 | CN(CCCc1nccn1C)c 1c2CCNCc2nc(c2ccn cc2)n1 | 12244291 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1410 | Cc1c(CCN(C)c2c3C CNCc3nc(n2)N(C)C)  scn1 | 12498605 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1411 | CN1CCN(CC1) [C@H]1CCN(C[C@ H]1CCCO)C(c1cccc2  c1ccn2C)=O | 12576044 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1412 | CCN1CC(CC1=O)Nc  1c2CNCc2nc(c2ccnc c2)n1 | 14924624 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1413 | CCc1nnc(NCC2CCC CCN2)o1 | 16631339 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1414 | COc1ccc(cc1)NC1CS (C=C1)(=O)=O | 1683-5965 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1415 | C(CN)c1nc(c2ccccc2 n1)NCc1ccccc1n1cnc n1 | 17428082 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 1416 | CCn1cncc1CNc1c2C CNCc2nc(c2ccncc2)n 1 | 18384397 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1417 | C1CN(CCC12c1cccc c1[C@H] ([C@@H]2O)N)Cc1  c[nH]nc1c1ccccc1 | 18741551 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1418 | C(CN)C1CN(CCO1)  c1c2CCNCc2nc(c2cc ccc2)n1 | 19916102 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1419 | Cn1c2c(cn1)c(nc(c1c cncc1)n2)N1CCCC2( CCNCC2)CC1 | 20352833 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1420 | CC1CC2(C)CC(C)C1 (CO)CO2 | 2190-0577 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1421 | C1CCCN(CC1)C[C  @@H]1CN(C[C@@ H]1CO)C(c1cc(N) [nH]n1)=O | 22664850 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1422 | C1CCN(CC1)CC1(C  CN(Cc2cccc(CCN)c2  )C1)O | 22896979 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1423 | CCOC(C1=C(C)OC(  =C(C(=O)OCc2ccccc 2)C12C(Nc1ccccc12)  =O)N)=O | 2435-0117 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1424 | Cc1cc2cc(CNC([C@ @H]3C[C@H] (CN3)NC(c3cccc(C# N)c3)=O)=O)ccc2[n H]1 | 26878527 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1425 | CCOc1ccc(CNCCc2c cc(cc2)[Cl])cc1 | 2910-0651 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1426 | CCOc1ccc(CNCCc2c cc(cc2)F)cc1 | 2910-0686 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1427 | COc1cc(CNCc2cc(cc c2OC)[Br])cc(c1)OC | 2910-1798 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1428 | COc1ccc(c(CNc2ccc( cc2)[Br])c1)OC | 2910-1869 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1429 | COc1ccccc1CCNCc1 cccc(c1)C(F)(F)F | 2910-1902 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1430 | COc1ccc(CNCc2cccc (c2)OC)cc1 | 2910-2885 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1431 | Cc1nc(CCN)cc(n1)N 1CCN(CC1)c1ccc(C#  N)cn1 | 31455775 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1432 | COc1ccc(CCNCc2cc cc(c2)C(F)(F)F)cc1 | 3169-1283 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1433 | C(CNCc1ccc2c(c1)O CO2)c1ccc(cc1)F | 3169-1371 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1434 | C1CCN(CC1)CCN1 C(=N)N(CCO)c2cccc  c12 | 3260-0393 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1435 | CCOc1cc(CNCCc2cc c(cc2)F)ccc1OC | 3381-1809 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1436 | C1CC(N(C1)CCC1C  CN(CC1)Cc1cccc(C CN)c1)=O | 34485551 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1437 | Cc1ccsc1S(N1C[C@ H] (C[C@H]1C(NC)=O) N)(=O)=O | 35026530 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 1438 | COc1ccc(CNCc2cc(c cc2OC)[Br])cc1 | 3702-1485 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1439 | COc1cccc(CNCc2ccc c(c2)F)c1OC | 3702-1553 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1440 | COc1cccc(CCNCc2c cc(cc2)C(F)(F)F)c1 | 3702-1570 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1441 | COc1cc(CNCc2ccc(c (c2) [Br])OC)cc(c1)OC | 3702-1693 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1442 | COc1cccc(CNCc2ccc cc2C(F)(F)F)c1OC | 3702-1702 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1443 | CN(C)c1ccc(cc1)Nc1 nc(cs1)c1ccc(cc1)OC | 4112-3682 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1444 | CC1=CC(C)=NC(N1 CCNC1CCC2(CC1) CCNCC2)=O | 41200051 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1445 | C1CN(CCN(C1)c1cc  c(cc1)F)C([C@@H] (Cc1ccccc1)N)=O | 41213525 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1446 | Cc1cnccc1NCCn1ccn c1c1cc2CNCCn2n1 | 41482306 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1447 | COC(c1cccc(c1)Nc1c 2ccccc2nc(c2ccccc2 O)n1)=O | 4229-0068 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1448 | COc1ccc(c(c1)OC)c1 csc(NCC=C)n1 | 4640-0152 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1449 | C(CNc1cccnc1)CNc1 c2ccccc2nc(CCN)n1 | 47488116 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1450 | CCOc1cc(CNCCc2cc cc(c2)OC)ccc1OC | 4964-4425 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1451 | C(c1ccc(cc1)F)NCc1 ccc2c(c1)OCO2 | 4964-5172 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1452 | COc1ccc(cc1CN1CC C(CC1)N1CCN(CC1  )CCO)[Br] | 5607-0223 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1453 | CC(=C)CC(c1ccc(cc 1)OC)NCc1ccco1 | 5689-0111 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1454 | COc1cc(CNc2nccs2) cc(c1OCc1ccc(cc1)F) [Br] | 5868-0785 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1455 | Cc1c2c(nc(CCN)nc2s c1C)N(CCN(C)C)Cc  1ccccc1 | 59025931 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1456 | C1CCN(C1)c1ccc(cc 1[Cl])NC1c2ccccc2S (N=1)(=O)=O | 7641-0012 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1457 | CC(C) (C)NC(CSc1c(C#N)c c(C#N)c(N)n1)=O | 8001-8198 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1458 | CCOC(C1=C(C)OC(  =C(C(=O)OCC)C12  C(Nc1ccccc12)=O)N  )=O | 8003-0370 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1459 | CCN(CC)S(c1ccc(cc 1)c1csc(Nc2ccccc2O C)n1)(=O)=O | 8004-5097 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1460 | CC1=C(C(C(C#N)=C  (N)O1)c1ccccc1)C(C  )=O | 8004-7491 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1461 | Cc1ccc(cc1C)Nc1nc( cs1)c1ccccc1 | 8005-2768 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 1462 | CN1C2=C(C(C(C#N)  =C(N)O2)c2ccc(cc2) [Cl])C(N(C)C1=O)= O | 8006-4483 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1463 | C(c1ccccc1)c1nnc(N) s1 | 8008-6271 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1464 | Cc1ccc(cc1)C1C(C# N)=C(N)Oc2ccc3ccc cc3c12 | 8008-9298 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1465 | Cc1ccc(cc1)C1C(C# N)=C(N)Oc2c1c(C(F  )(F)F)n[nH]2 | 8009-1517 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1466 | [H]Nc1nnc(COc2ccc( cc2)C2CCCCC2)s1 | 8009-2831 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1467 | C1CCc2c(C1)c(C(c1  ccccc1)=O)c(N)s2 | 8010-1935 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1468 | CC(C) (C)c1c2C(C(C#N)=C  (N)Oc2[nH]n1)c1c[n H]nc1c1ccc(cc1)F | 8011-9128 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1469 | CC1=CC(N(C)C(N1 CCCCCCNCCO)=O)  =O | 8012-3983 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1470 | Cc1cc(C)c2c(c1)c(C CN)c(C)[nH]2 | 8012-5803 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1471 | Cc1c(CCNCc2ccc(cc 2F)F)c2ccccc2[nH]1 | 8012-8388 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1472 | Cc1c(CCNCc2ccc(C #N)cc2)c2cc(ccc2[nH  ]1)OC | 8013-2954 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1473 | CCN1C(c2ccc(CN)c3  cccc1c23)=O | 8016-6735 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1474 | COc1ccc(CCNc2nc(c s2)c2cccs2)cc1OC | 8018-0995 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1475 | CC(C)C(CCNCc1ccc (cc1)OC)C1CCOC(C  )(C)C1 | 8018-1265 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1476 | CC(C)C1(CCNCc2cc c(cc2)OC)CCOC(C) (C)C1 | 8018-1266 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1477 | CC(C)C1(CCNCc2cc cc3c2OCO3)CCOC( C)(C)C1 | 8018-1268 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1478 | CC1=CC(C)=NC(N1 CCN)=O | 8018-1719 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1479 | C#CC1(CCCCC1)N | 8018-8549 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1480 | Cc1c(c(N)n(CCC2C CCCC=2)c1C)S(c1cc c(cc1)[Cl])(=O)=O | 8019-0262 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1481 | COc1cc(ccc1OC1CC CC1)C1CC(Nc2c1sc( N)n2)=O | 8019-3694 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1482 | C1CN2C(=CSC2=N1  )c1cccc(c1)N | 8019-6474 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1483 | c1cc(N)nc2c1ccc(n2) O | 8019-7722 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1484 | COc1ccc(cc1)c1c(CN  )c[nH]n1 | 8019-7792 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1485 | CCOc1c(CC=C)cc(C NCCO)cc1OC | 8020-0299 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 1486 | c1cnccc1c1nc2ncnc( N)n2n1 | 8020-2786 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1487 | c1ccc2c(c1)nc(c1ccc( cc1[Cl])N)s2 | C066-5322 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1488 | Cc1cccc(c1)NCc1nc2 ccccc2n1C | C147-0043 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1489 | CCc1nnc2c3ccccc3nc (Nc3ccccc3OCC)n12 | C301-5148 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1490 | CCN(CC)CCCNc1c2  ccccc2nc(c2nnc(c3cc c(C)cc3)o2)n1 | C660-1575 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1491 | CCOC(N1CCN(CC1) C1=C(C(C1=O)=O)N CCCN1CCCCCC1)= O | C748-1353 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1492 | C(c1ccccc1)Nc1c(cnc 2ccc(cc12) [Cl])S(c1ccccc1) (=O)=O | C769-1518 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1493 | Cc1ccc(cc1)S(c1c(N CCOC)oc(c2cccc(C)c 2)n1)(=O)=O | D072-0517 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1494 | CN1C(N(Cc2ccccc2) C(c2c1nc(NCCN)n2 C)=O)=O | D114-0037 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1495 | CCc1ccc(cc1)n1nc(C O)c(C(NCCc2ccccc2  )=O)n1 | D217-0759 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1496 | CCOC(c1cccc(c1)Nc 1cc(c2ccccc2)ncn1)= O | D278-0165 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1497 | CSc1nc2CCCc2c(Nc 2cccc(c2)O)n1 | D278-0388 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1498 | CN1C(N(C)c2cc(CO  c3ccc(CNCc4cccnc4) cc3OC)ccc12)=O | D300-0082 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1499 | Cc1ccccc1c1nc(c2ccc nc2NCc2ccco2)on1 | D349-3751 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1500 | Cc1ccccc1c1nc(c2ccc nc2NC2CCCCC2)on 1 | D349-3758 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1501 | COc1ccc(cc1)c1nc(c 2cccnc2NCC2CCCO 2)on1 | D349-4034 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1502 | CCCNc1cc(C)nc2cc( c3ccc(c(c3)OC)OC)n n12 | D393-0193 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1503 | Cc1cc(C)n2c(n1)nc( CNc1cccc(c1)[Cl])n2 | D433-0351 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1504 | CC1(C)CC(CCNC2C CN(C)CC2)  (CCO1)c1cccc(c1)C( F)(F)F | D442-0355 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1505 | Cc1ccc(cc1)C1(CCN CCN2CCOCC2)CCO C(C)(C)C1 | D442-0384 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1506 | CN1C(N(C)c2cc(CN  c3ccc(c(c3)C(O)=O) [Cl])ccc12)=O | D664-0087 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1507 | Cn1c2ccccc2c2c1nc( NCCCN1CCCCCC1)  nn2 | E205-0046 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 1508 | C(CNc1c2c(c3ccc(cc 3)F)noc2ncn1)c1ccsc 1 | E899-0297 | NRAS | G-quadruplex | UGUGGGAGGGGCGGGUCUG GG | 1 |
| 1509 | CC1CCN(CC1)CC(C  Oc1ccccc1CC=C)O | 1189-2046 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1510 | CN(CCCc1nccn1C)c 1c2CCNCc2nc(c2ccn cc2)n1 | 12244291 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1511 | CNC(C1CCCN(C1)c  1c2CCNCCc2nc(c2c cco2)n1)=O | 13043417 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1512 | CCN(CC)Cc1cnc2c(c nn2c1)C(NCc1ccc(C N)cc1)=O | 14229566 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1513 | CCNC([C@@H]1C[  C@@H] (CN1C(CN1CCCCC CC1)=O)N)=O | 15077405 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1514 | COc1ccc(cc1)OC1C CN(CC1)C([C@@H] 1C[C@H] (CN1)O)=O | 15579241 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1515 | CCc1nnc(NCC2CCC CCN2)o1 | 16631339 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1516 | COc1ccc(cc1)NC1CS (C=C1)(=O)=O | 1683-5965 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1517 | C=Cc1ccc(nc1)N1CC N(CC(C1)O)Cc1cccc  c1 | 17524156 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1518 | CCn1cncc1CNc1c2C CNCc2nc(c2ccncc2)n 1 | 18384397 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1519 | C=CCN1CCC(CNCc  2c[nH]nc2c2ccc(cc2) F)C1 | 18501966 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1520 | C1CN(CCC12c1cccc c1[C@H] ([C@@H]2O)N)Cc1  c[nH]nc1c1ccccc1 | 18741551 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1521 | C1CCN(CC1)c1ccc(c  c1)c1cc(c2cccnc2)c( C#N)c(N)n1 | 19252160 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1522 | C(CN)C1CN(CCO1)  c1c2CCNCc2nc(c2cc ccc2)n1 | 19916102 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1523 | C1C[C@@H]2CCN(  Cc3ccccn3)C[C@H] 1N2 | 20138450 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1524 | Cn1c2c(cn1)c(nc(c1c cncc1)n2)N1CCCC2( CCNCC2)CC1 | 20352833 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1525 | COc1cccc(c1)c1cn[n H]c1C1CCN(CC1)c1  ccnc(N)n1 | 21608058 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1526 | CN(C[C@@H]1CC[  C@@H] (CC1)N)CC1(CCCC 1)CO | 22559794 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1527 | C1CCCN(CC1)C[C  @@H]1CN(C[C@@ H]1CO)C(c1cc(N) [nH]n1)=O | 22664850 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1528 | Cc1cc2c(cc1N)nc(N | 2284-1574 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | C(c1ccc(cc1)C(=O)O C)=O)s2 |  |  |  |  |  |
| 1529 | C1CCN(CC1)CC1(C  CN(Cc2cccc(CCN)c2  )C1)O | 22896979 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1530 | C1CC(CN(C1)Cc1cc  cc(CCN)c1)C(Cc1ccc cc1)=O | 27037369 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1531 | CCOc1ccc(CNCCc2c cc(cc2)[Cl])cc1 | 2910-0651 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1532 | CCOc1ccc(CNCCc2c cc(cc2)F)cc1 | 2910-0686 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1533 | COc1cc(CNCc2cc(cc c2OC)[Br])cc(c1)OC | 2910-1798 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1534 | CC(COC)NCc1c(ccc c1F)F | 2910-2353 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1535 | Cc1nc(CCN)cc(n1)N 1CCN(CC1)c1ccc(C#  N)cn1 | 31455775 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1536 | C1CCCN(CCC1)CC( N1C[C@H]  (c2ccccc2)[C@H] (C1)N)=O | 31891223 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1537 | COCc1nc(CCNC(CC  c2cc3CNCCn3n2)=O  )on1 | 32552243 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1538 | C1CCN(CC1)CCN1 C(=N)N(CCO)c2cccc  c12 | 3260-0393 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1539 | C(CC(N1CCOC(CN)  C1)=O)CN1Cc2ccccc 2C1 | 32832871 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1540 | C1CC(N(C1)CCC1C  CN(CC1)Cc1cccc(C CN)c1)=O | 34485551 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1541 | Cc1cccc(c1)Nc1nc(C N2C[C@@H]3CC[C  @H] (C2)N(C)C3=O)nc(N  )n1 | 35485871 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1542 | COc1ccc(CNCc2ccc( cc2)F)c(c1)OC | 3702-0980 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1543 | COc1cccc(CCNCc2c cc(cc2)C(F)(F)F)c1 | 3702-1570 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1544 | COc1cc(CNCc2ccc(c (c2) [Br])OC)cc(c1)OC | 3702-1693 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1545 | Cc1ccc(c(CC=C)c1) OCC(Cn1c2ccccc2nc 1C)O | 3915-0002 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1546 | CN(C)CCNc1c2cccc c2nc(c2cccnc2)n1 | 3993-3579 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1547 | CC(Nc1cccc(c1)c1cc c(c(c1)F)NC(CN)=O)  =O | 40118252 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1548 | CC(C)CC1CC(C)  (c2csc(Nc3ccccc3)n2  )OC1=O | 4075-3209 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1549 | CN(C)c1ccc(cc1)Nc1 nc(cs1)c1ccc(cc1)OC | 4112-3682 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1550 | C1CN(CCN(C1)c1cc  c(cc1)F)C([C@@H] | 41213525 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | (Cc1ccccc1)N)=O |  |  |  |  |  |
| 1551 | CC1CCc2c(C(Nc3cc ccc3C)=O)c(N)sc2C1 | 4488-1595 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1552 | COc1ccc(c(c1)OC)c1 csc(NCC=C)n1 | 4640-0152 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1553 | C(CNc1cccnc1)CNc1 c2ccccc2nc(CCN)n1 | 47488116 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1554 | CCN(CC)CCCNc1c2  c3CCCCc3sc2ncn1 | 4789-3782 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1555 | Cc1cnc(N)nc1NCC[ C@@H]1C[C@H]2 C[C@@H]1C=C2 | 47913504 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1556 | C(CN)CN1C(CC[C @H]2CN(CC[C@@ H]12)C(CCc1ccco1)  =O)=O | 48226996 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1557 | c1ccc2C(N=C(c2c1) N)=NN | 5140994 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1558 | C(CCN=Cc1ccccc1N  )CN=Cc1ccccc1N | 5233844 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1559 | C1CC(N(CNc2ccc(c( c2)[Cl])  [Cl])C1=O)=O | 5271658 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1560 | CCOc1cc(CNCCc2cc cc(c2)F)ccc1OC | 5571711 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1561 | C1CCC(C1)NCC(CO  c1ccc(cc1)OCC(CNC 1CCCC1)O)O | 5648415 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1562 | CCCCNCCOc1ccccc 1OCC.C(C(O)=O) (O)=O | 5728614 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1563 | Cc1ccc(c(c1) [Cl])OCCNC(C)  (C)C.[Cl] | 5729988 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1564 | CCCCNCCOc1ccccc 1F.C(C(O)=O)(O)=O | 5734218 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1565 | Cc1ccc(cc1)NC1CS( C=C1)(=O)=O | 5769-0121 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1566 | [H]N([H])c1c(C#N)c  (C(=Cc2cc3ccccc3nc 2N2CCCCC2)C#N)n  n1c1ccccc1 | 5796654 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1567 | Cc1c2c(nc(CCN)nc2s c1C)N(CCN(C)C)Cc  1ccccc1 | 59025931 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1568 | Cc1ccc2c(c1)c1CCC C(c1n2CC(CN1CCC CCC1)O)=O | 5926-0040 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1569 | CCN1C(=C(C(NCC= C)=O)SC1=S)N | 6000-2112 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1570 | c1ccc2c(c1)cc1cnc3c (c(N)n[nH]3)c1n2 | 6051011 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1571 | Cc1cc(N)n(c2ccc(c(c 2)S(O)  (=O)=O)Oc2ccccc2)n 1 | 6075116 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1572 | Cc1ccc2c(c1)SC(=Cc 1ccc[n+] (CCO)c1)N2C | 6253-0703 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1573 | C1CNCCC1C(N1CC  N(CC1)c1ccccc1F)= | 6579417 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | O.C(C(O)=O)(O)=O |  |  |  |  |  |
| 1574 | Cc1nc2ccccc2n1CC( COc1ccc(cc1)C1CC C=C1)O | 6682831 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1575 | COc1ccc(CCNCC(C  Oc2ccc(cc2) [Cl])O)cc1OC.[Cl] | 6945348 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1576 | C=CCNCCOCCOc1c  ccc(c1) [Br].C(C(O)=O) (O)=O | 7002064 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1577 | C1CCN(C1)c1ccc(cc 1[Cl])NC1c2ccccc2S (N=1)(=O)=O | 7641-0012 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1578 | Cn1c(cnc1NCc1cccc( c1) [Cl])c1cccc(c1)OC | 7756-0392 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1579 | Cn1c(cnc1NCc1c(ccc c1[Cl])F)c1ccc(cc1)O C | 7756-0741 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1580 | C=CCc1cc(ccc1OCC NCCN1CCOCC1) [Cl].C(C(O)=O) (O)=O | 7969784 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1581 | C(CN)CN1CCN(CC1  )c1ccccc1 | 7974015 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1582 | CC(C) (C)NC(CSc1c(C#N)c c(C#N)c(N)n1)=O | 8001-8198 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1583 | CCN(CC)S(c1ccc(cc 1)c1csc(Nc2ccccc2O C)n1)(=O)=O | 8004-5097 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1584 | CC1=C(C(C(C#N)=C  (N)O1)c1ccccc1)C(C  )=O | 8004-7491 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1585 | CCN(CC)S(c1ccc(cc 1)c1csc(Nc2cccc(c2) OC)n1)(=O)=O | 8005-1875 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1586 | Cc1ccc(cc1C)Nc1nc( cs1)c1ccccc1 | 8005-2768 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1587 | COCC1=C(C(C(C#N  )=C(N)O1)c1cccc(c1)  [Br])C(=O)OC | 8007-0167 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1588 | C(c1ccccc1)c1nnc(N) s1 | 8008-6271 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1589 | Cc1ccc(cc1)C1C(C# N)=C(N)Oc2ccc3ccc cc3c12 | 8008-9298 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1590 | Cc1ccc(cc1)C1C(C# N)=C(N)Oc2c1c(C(F  )(F)F)n[nH]2 | 8009-1517 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1591 | C1CCc2c(C1)c(C(c1  ccccc1)=O)c(N)s2 | 8010-1935 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1592 | CC1=CC(N(C)C(N1 CCCCCCNCCO)=O)  =O | 8012-3983 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1593 | Cc1c(CCNCc2ccc(cc 2F)F)c2ccccc2[nH]1 | 8012-8388 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1594 | Cc1c(CCNCc2ccc(C #N)cc2)c2cc(ccc2[nH  ]1)OC | 8013-2954 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1595 | COc1ccc(CCNc2nc(c | 8018-0995 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
|  | s2)c2cccs2)cc1OC |  |  |  |  |  |
| 1596 | CC(C)C(CCNCc1ccc (cc1)OC)C1CCOC(C  )(C)C1 | 8018-1265 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1597 | CC(C)C1(CCNCc2cc c(cc2)OC)CCOC(C) (C)C1 | 8018-1266 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1598 | CC(C)C1(CCNCc2cc cc3c2OCO3)CCOC( C)(C)C1 | 8018-1268 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1599 | C(CS(N1CCNCC1) (=O)=O)N | 8018-8721 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1600 | Cc1c(c(N)n(CCC2C CCCC=2)c1C)S(c1cc c(cc1)[Cl])(=O)=O | 8019-0262 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1601 | C1CN2C(=CSC2=N1  )c1cccc(c1)N | 8019-6474 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1602 | c1cc(N)nc2c1ccc(n2) O | 8019-7722 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1603 | COc1ccc(cc1)c1c(CN  )c[nH]n1 | 8019-7792 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1604 | c1cnccc1c1nc2ncnc( N)n2n1 | 8020-2786 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1605 | [H]N(Cc1cc(c(c(c1) [Cl])OCc1cccs1)OC) Cc1cccnc1 | 8319-0189 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1606 | CCCCNc1c(C#N)c2 CC(C)  (C)OCc2c(c2ccccc2) n1 | 8640-0572 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1607 | COc1cc(cc(c1OC)OC  )c1nc(c2cccc(c2)N)n[ nH]1 | 9204334 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1608 | c1ccc2c(c1)nc(c1ccc( cc1[Cl])N)s2 | C066-5322 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1609 | Cc1cccc(c1)NCc1nc2 ccccc2n1C | C147-0043 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1610 | c1ccc2c(c1)c1nncn1c (Nc1ccc(cc1F) [Br])n2 | C301-5173 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1611 | CCN(CC)CCCNc1c2  ccccc2nc(c2nnc(c3cc c(C)cc3)o2)n1 | C660-1575 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1612 | C1CCCN(CC1)CCC  Nc1nc2ccccc2c2nc(c 3ccccc3)nn12 | C736-0159 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1613 | CCOC(N1CCN(CC1) C1=C(C(C1=O)=O)N CCCN1CCCCCC1)= O | C748-1353 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1614 | Cc1ccc(cc1)S(c1c(N CCOC)oc(c2cccc(C)c 2)n1)(=O)=O | D072-0517 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1615 | CCOC(c1cccc(c1)Nc 1cc(c2ccccc2)ncn1)= O | D278-0165 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1616 | CSc1nc2CCCc2c(Nc 2cccc(c2)O)n1 | D278-0388 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |
| 1617 | CN1C(N(C)c2cc(CO  c3ccc(CNCc4cccnc4) cc3OC)ccc12)=O | D300-0082 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |

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| **Entry\_ID** | **SMILES** | **Molecule\_ID** | **RNA\_target** | **SS\_type** | **RNA\_sequence** | **Class** |
| 1618 | C(CNc1c2c(c3ccc(cc 3)F)noc2ncn1)c1ccsc 1 | E899-0297 | TERRA | G-quadruplex | GGGUUAGGGU | 1 |