"Aptamers" model test dataset curated from the ROBIN repository (Yazdani et al., 2022)

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
1	Cc1nc2c(c(=O)n1C) CN(C[C@]1(O)CCC [NH2+]C1)C2	Neg_lig_7	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	0
2	CN(Cc1nccn1Cc1ccc cc1)C(=O)C[C@H]1 COCC[NH2+]1	Neg_lig_34	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	0
3	COclccc([C@@H]2 C[C@H] (c3ccc(C(C)C)cc3)n3 nc(N)nc3N2)cc1	Neg_lig_104	AKTIP	G-quadruplex	GGGGUGGGGCGGGGG	0
4	CCCOc1ccc(Oc2nc(NC)nc(N3CCOCC3) n2)nn1	Neg_lig_107	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	0
5	CC(C)[N@H+] (C[C@H]10[C@@H](n2enc3c(N)nenc32) [C@H](O) [C@H]10) [C@H]1C[C@@H] (CCc2[nH]c3ccc(C(C)(C)(C)cc3[nH+]2)C1	Neg_lig_109	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	0
6	CCn1cnnc1CCNc1nc (C2CCCC2)nc2c1C[NH2+]C2	Neg_lig_92	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	0
7	CCCCOC(=O)N1CC CC2(CC[NH2+]CC2) CC1	Neg_lig_206	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	0
8	Nc1nonc1- c1nc2cccc2n1CC(= O)Nc1ccc(F)c(Cl)c1	Neg_lig_211	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	0
9	CNS(=O) (=O)c1ccc(CN2C[C @H](O)[C@@H] (N3CC[NH+] (C)CC3)C2)cc1	Neg_lig_229	AKTIP	G-quadruplex	GGGGUGGGGCGGGGG	0
10	NC1(C(=0)N2CCC[C@H] (c3[nH]ncc3Cc3ccc c3)C2)CC1	Neg_lig_261	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	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	GGGGUGGGGGGGGGGGG	0
12	COc1cc(N)c(C#N)cc 1OC	Neg_lig_331	AKTIP	G-quadruplex	GGGGUGGGGCGGGGGGGG	0
13	Fc1ccc(- c2noc3ncnc(NCCN4 CCOCC4)c23)cc1	Neg_lig_378	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	0
14	Cc1cc2c(c(=O)o1) [C@H] (c1cccs1)C(C#N)=C(N)O2	Neg_lig_392	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	0
15	O=C1S[C@H] (Nc2cccc2F)C(=O) N1c1ccccc1	Neg_lig_397	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	0
16	Cc1ccc(Nc2nc(N3CC OCC3)c3ccccc3[nH+]2)cc1	Neg_lig_437	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	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	GGGGUGGGGGGGGGGGG	0

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	(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	GGGGUGGGGCGGGGG	0
19	COCCOC(=O)C1=C(N)Oc2c(oc(CO)cc2= O) [C@H]1c1cccc(F)c1	Neg_lig_510	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	0
20	NNC(=0)c1ccncc1	Neg_lig_526	AKTIP	G-quadruplex	GGGGUGGGGCGGGGG	0
21	CCOclecccc1CCNC(=O)[C@H] ([NH3+])c1c(C)n[nH]c1C	Neg_lig_533	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	0
22	Nc1ccc(S(=O) (=O)Nc2ccc(F)cc2)cc 1	Neg_lig_565	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	0
23	CCOc1ccc(-c2noc(- c3nnn(- c4cc(Cl)ccc4OC)c3N)n2)cc1	Neg_lig_573	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	0
24	Cc1ccc(C)c(N[C@@ H](CNS(=O) (=O)c2cccc2)c2ccc c2)c1	Neg_lig_597	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	0
25	COc1cccc(- c2nccn2C[C@H] (O)c2cccnc2)c1OC	Neg_lig_601	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	0
26	Cc1cc(C(=O)NCc2cc 3n(n2)CC[NH2+]C3) c(-c2cccc2)o1	Neg_lig_632	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	0
27	COC(=0)C1=C(N)O c2c(oc(CO)cc2=O) [C@H]1c1ccc(F)cc1 F	Neg_lig_633	AKTIP	G-quadruplex	GGGGUGGGGCGGGGG	0
28	O=c1cc([O-]) [nH]cc1Cl	Neg_lig_665	AKTIP	G-quadruplex	GGGGUGGGGCGGGGGGGG	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	GGGGUGGGGCGGGG	0
30	[NH3+]C[C@H]1CC N(C(=O)c2ccc(NCc3 ccncc3)cc2)C1	Neg_lig_710	AKTIP	G-quadruplex	GGGGUGGGGCGGGGG	0
31	COcleccc1OC[C@ @H] (O)C[NH+]1CCC(C) CC1	Neg_lig_725	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGG	0
32	COC(=0)c1ccc2c(/ C(=N/ c3ccc(N(C)C(=0)CN 4CC[NH+] (C)CC4)cc3)c3ccccc 3)c(O)[nH]c2c1	Neg_lig_753	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	0
33	Cc1cc(Nc2cccc2Cl) n2nc(C)nc2n1	Neg_lig_768	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	0
34	Ce1ccc2[nH]c(C)c([C@@H] (O)C[NH+]3CCCCC 3)c2c1	Neg_lig_794	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGG	0
35	Cc1ccc([C@H](C) [NH2+]Cc2cn(CCC(Neg_lig_798	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	0

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	N)=O)c3cccc23)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	GGGGUGGGGCGGGG	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	GGGGUGGGGCGGGGG	0
38	CCc1nc2c(N3CCC([NH2+]Cc4cc(C(C) (C)C) [nH]n4)CC3)ncnc2o1	Neg_lig_818	AKTIP	G-quadruplex	GGGGUGGGGCGGGGG	0
39	CCn1c(N)nc2cc(C(= O)N3CCc4nc(C) [nH]c(=O)c4CC3)cnc 21	Neg_lig_838	AKTIP	G-quadruplex	GGGGUGGGGCGGGGG	0
40	Nc1nnc(CCn2cnc3sc 4c(c3c2=O)CCNC4)s 1	Neg_lig_872	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	0
41	CC(C)(C)c1ccc(- c2nc(NCCCN3CCO CC3)c3ccccc3[nH+]2)cc1	Neg_lig_875	AKTIP	G-quadruplex	GGGGUGGGGCGGGGG	0
42	O[C@H]1CN(c2cc(C (F) (F)F)nc(N3CCCC3)n 2)Cc2cccc21	Neg_lig_920	AKTIP	G-quadruplex	GGGGUGGGGCGGGGG	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	GGGGUGGGGCGGGG	0
44	CN1CCC(=C2c3cccc c3CCc3sccc32)CC1	Neg_lig_935	AKTIP	G-quadruplex	GGGGUGGGGCGGGGG	0
45	Cc1csc(N2CCC([NH +]3CCC(O)CC3)CC2)n1	Neg_lig_967	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	0
46	Cc1ccc(N)c(-c2nnc(- c3cencc3)o2)c1	Neg_lig_1086	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	0
47	CC[C@H] (Nc1cccc(OC)c1)C(= O)NCCOc1ccccc1	Neg_lig_1124	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	0
48	Cn1c(=O)c2c(nc(NC CCCO)n2Cc2cccc2 Cl)n(C)c1=O	Neg_lig_1172	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	0
49	CCOC(=0) [C@H]1CCCN(C(=0))c2ccc(CNc3c(N4CC C(C)CC4)c(=0)c3=0)cc2)C1	Neg_lig_1225	AKTIP	G-quadruplex	GGGGUGGGGCGGGGG	0
50	CCCc1cc(C(=O)N[C @@H] (C)c2nnc(N)s2)n[nH] 1	Neg_lig_1249	AKTIP	G-quadruplex	GGGGUGGGGCGGGGG	0
51	[NH3+] [C@@H]1c2cccc2C 2(CCN(c3cnc4cccc4 n3)CC2)[C@H]1O	Neg_lig_1252	AKTIP	G-quadruplex	GGGGUGGGGCGGGGG	0
52	Cc1cccc2nc(CNc3ccc (Cl)c(Cl)c3)cn12	Neg_lig_1267	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	0
53	Nc1cc(OC(=O)c2ccc cc2)nn1S(=O)	Neg_lig_1315	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	0

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	(=O)c1ccccc1					
54	COc1ccc(S(=O) (=O)N2CCN(c3cc(C) nc(Nc4ccc(C)cc4)n3) CC2)cc1	Neg_lig_1385	AKTIP	G-quadruplex	GGGGUGGGGCGGGGG	0
55	CSc1nnc(CC2CCN(c 3[nH]c(N)nc4ncnc3- 4)CC2)n1C	Neg_lig_1404	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	0
56	CCCe1enene1N1C[C @@H] ([NH3+])C[C@H]1C (=O)N(CC)CC	Neg_lig_1413	AKTIP	G-quadruplex	GGGGUGGGGCGGGGG	0
57	CCOC(=O)[C@@H] (O)C(C) (C)CN1C(=O)c2cccc c2C1=O	Neg_lig_1415	AKTIP	G-quadruplex	GGGGUGGGGCGGGGG	0
58	N#Cc1nc(- c2ccc(S(=O) (=O)N3CCCC3)cc2) oc1NC1CCCCC1	Neg_lig_1434	AKTIP	G-quadruplex	GGGGUGGGGCGGGGG	0
59	CN(C)c1cncc(N2CC[C@](C)(O)[C@@H] (O)C2)n1	Neg_lig_1486	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	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	GGGGUGGGGCGGGGG	0
61	CCOC(=O)c1cccc(N C2=NS(=O) (=O)C(c3ccc(Cl)cc3) =C2C)c1	Neg_lig_1520	AKTIP	G-quadruplex	GGGGUGGGGCGGGGG	0
62	CN1CC[NH+] ([C@H]2CCN(C(=O) Cn3cc4ccccc4n3)C[C @H]2CCCO)CC1	Neg_lig_1580	AKTIP	G-quadruplex	GGGGUGGGGCGGGGG	0
63	CCOc1cccc1N[C@ H]1OC(=O)c2cccc2	Neg_lig_1601	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	0
64	c1cnc2c([C@H]3[N H2+]CCc4[nH+]c[nH]c43)cnn2c1	Neg_lig_1605	AKTIP	G-quadruplex	GGGGUGGGGCGGGGG	0
65	COC(=O)c1cc(- c2cccc(N)c2)nc2cccc c12	Neg_lig_1643	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	0
66	Nc1c(Br)cc(Cl)c2c1C (=O)c1cccc1C2=O	Neg_lig_1657	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	0
67	CCOC(=O)c1c(N)n(- c2cc(C)ccc2C)c2nc3c cccc3nc12	Neg_lig_1698	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	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	GGGGUGGGGCGGGG	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	GGGGUGGGGCGGGGG	0
70	COc1cc([C@@H]2c 3c(n[nH]c3- c3ccccc3O)C(=O)N2 CCCO)cc(Br)c1O	Neg_lig_1800	AKTIP	G-quadruplex	GGGGUGGGGCGGGGG	0
71	COc1ccc(Nc2cc(Cl)c cc2C(=O)[O-])cn1	Neg_lig_1824	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	0
72	COc1cccc(OC[C@@	Neg_lig_1837	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	0

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	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	Neg_lig_1849	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	0
74	CSCC(=O)N1CCC2(CC1)[C@@H] (OCC[NH3+])C[C@ H]2O	Neg_lig_1906	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	0
75	COC(=O)[C@H] (Nc1cc(C)nc2nc(- c3ccccc3C)nn12)c1cc ccc1	Neg_lig_1913	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	0
76	CCc1c(C)nc2nncn2c 1Nc1ccc(Cl)cc1	Neg_lig_1935	AKTIP	G-quadruplex	GGGGUGGGGCGGGGG	0
77	C1Cc2[nH]nc(- c3nn[n-]n3)c2C1	Neg_lig_1993	AKTIP	G-quadruplex	GGGGUGGGGCGGGGG	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	GGGGUGGGGGGGGGGGG	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	GGGGUGGGGCGGGG	0
80	Nc1cc(=O)n2c(n1)SC CC2	Neg_lig_2125	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	0
81	CCOC(=O)c1ccc(Nc 2ncnc3ccc(Br)cc23)c c1	Neg_lig_2150	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	0
82	COC[C@@H] (N)C(=O)N1CCN(Cc 2cccc(F)c2)CC1	Neg_lig_2159	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	0
83	CCOC(=O)c1ccccc1 N[C@@H]1c2cccc2 C(=O)N1c1ccc(Cl)cc 1	Neg_lig_1054	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	0
84	COc1ccc(Nc2[nH+]c 3cccc3c3nncn23)c(OC)c1	Neg_lig_606	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	0
85	COCCe1nc(- c2cnc(C3CC3)nc2)n(CCO)n1	Neg_lig_1479	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	0
86	Cn1c(=O)n(C)c2cc(C Nc3ccc(N4CCOCC4) c(C(=O) [O-])c3)ccc21	Neg_lig_2241	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	0
87	O=C(c1cccc1- n1cncn1)N1C[C@@ H]2CNC[C@]2(C(= O)O)C1	Neg_lig_2250	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	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	GGGGUGGGGCGGGG	0

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	[C@H]21					
89	COc1cc(C[NH2+]C(C)C)ccc1OCc1ccc2c(c1)n(C)c(=O)n2C	Neg_lig_792	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	0
90	COc1cccc1- c1nnc(SCC#CCO)o1	Neg_lig_2365	AKTIP	G-quadruplex	GGGGUGGGGCGGGGG	0
91	COc1ccccc1CC[NH2 +]Cc1ccccc1C	Neg_lig_2402	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	0
92	COC(=O)c1ccccc1N[Neg_lig_2431	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	0
93	[NH3+]CCc1ccc(S(= O) (=O)N2CCOCC2)cc1	Neg_lig_2436	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	0
94	OCCCc1nc2cccc2n1 CCCOc1ccccc1	Neg_lig_1043	AKTIP	G-quadruplex	GGGGUGGGGCGGGGGGGGG	0
95	O=C([N-]OC[C@@ H] (O)CO)c1cc(Br)c(F)c (F)c1Nc1ccc(1)cc1F	Neg_lig_2657	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	0
96	CCOc1ccc(CCNc2nc 3cccc3nc2C(=O)OC)cc1OCC	Neg_lig_2731	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	0
97	Cc1ccc2[nH]c(C3=C(N)N(C4CCCCC4)C C3=O)nc2c1	Neg_lig_2732	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	0
98	C=CCNc1cc(C)nc2nc (-c3ccnc3)nn12	Neg_lig_2744	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	0
99	COc1ccc(CCNc2ncn c3sc(C)c(C)c23)cc1	Neg_lig_2755	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	0
100	Cn1cc(NC(=O)NCC CNc2ccnc2)cn1	Neg_lig_2781	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	0
101	COc1cccc([C@H]2C [C@@H] (c3ccc(Cl)cc3)Nc3nc (N)nn32)c1	Neg_lig_2873	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	0
102	Cc1ccc(- c2nccn2CCCO)c(Cl) c1Cl	Neg_lig_2875	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	0
103	Nc1ccc(C(=O)c2cccs 2)cn1	Neg_lig_2915	AKTIP	G-quadruplex	GGGGUGGGGCGGGGGGGG	0
104	COclcccc(- c2ncc(CN3CCO[C@]]4(CNCCOC4)C3)s2) c1	Neg_lig_1458	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	0
105	O=C1CCCN1c1ccc(C[NH2+]C2CCC3(C C[NH2+]CC3)CC2)c c1	Neg_lig_2950	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	0
106	COc1ccc(-c2nc(- c3ccc(N)cc3)n[nH]2) cc1	Neg_lig_2960	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	0
107	O=C(NCCO)c1nnn(- c2ccc(Cl)cc2)c1- c1ccco1	Neg_lig_2975	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	0
108	CC[C@H] (C)Nc1cc(C(C)C)c(C #N)c2nc3ccccc3n12	Neg_lig_2989	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	0
109	CCOC(=O)c1nnn(- c2nonc2N)c1CN1CC Cc2cccc21	Neg_lig_674	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	0

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110	CCSCCn1cnc(- c2cccc2)c1- c1ccc(CO)o1	Neg_lig_3022	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	0
111	C[C@@]12C(=O)OC (=O)[C@@]1(C) [C@H]1CC[C@@H] 2O1	Neg_lig_3045	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	0
112	Cc1ccccc1OCCCn1c(CCCO)nc2ccccc21	Neg_lig_3122	AKTIP	G-quadruplex	GGGGUGGGGCGGGGG	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	GGGGUGGGGCGGGG	0
114	CCn1c(SCc2cccc2C)nc2c(cnn2CCO)c1=	Neg_lig_3127	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	0
115	Cc1cc(C(=O)N[C@H] (CO)c2cccc2)c2cccc (C)c2n1	Neg_lig_3141	AKTIP	G-quadruplex	gggguggggcgggggg	0
116	N#CC1=C(N)OC2=C ([C@H]]t1ctcc(Cl)cc 1)S(=O) (=O)N(Cc1cccc1F)c 1cccc12	Neg_lig_3152	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	0
117	C[C@@H] ([NH2+]CCCc1cccc(C(F) (F)F)c1)c1cccc2ccccc	Neg_lig_3216	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	0
118	CC1=C(c2ccc(Cl)cc2)S(=O) (=O)N=C1NC1CC[N H+](Cc2cccc2)CC1	Neg_lig_3231	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	0
119	Cc1ccc([C@H]2C(C #N)=C(N)Oc3c2oc(C O)cc3=O)o1	Neg_lig_1275	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	0
120	CCCOC(=O)c1cccc(Nc2nc(-c3ccnc3) [nH+]c3cccc23)c1	Neg_lig_3281	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	0
121	Cn1ccnc1-c1c(- c2cccc2)ncn1C[C@ H]1C[NH2+]CCO1	Neg_lig_3285	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	0
122	CCN(CC)C(=0)c1cn (C2CCN(C(=0)C3([NH3+])CCCC3)CC2) nn1	Neg_lig_3312	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	0
123	COc1cc(C)c(N)cc1C(C)C	Neg_lig_3340	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	0
124	CCCCn1cnc2cc(NCc 3cccc(Br)c3)ccc21	Neg_lig_3358	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGG	0
125	O=C(CSc1nc2cccc2 s1)N1CCN(CCO)CC 1	Neg_lig_2780	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	0
126	CC[C@@H] (CO)N(Cc1cccnc1)C(=O)CCCc1cccs1	Neg_lig_3367	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	0
127	Cc1nc(CC[NH2+]C2 CCN(c3ncccn3)CC2) sc1C	Neg_lig_3380	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	0
128	Cc1ccc(CN2c3ccccc 3C3=C([C@@H] (c4ccc(F)c4)C(C#N) =C(N)O3)S2(=O)=O)	Neg_lig_3	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	0

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 cccc32)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	GGGCAGGGGAAGAGGGG	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)nc2cccc 12	Neg_lig_419	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	0
141	Cc1ccc2c(N)c(C(=O) c3ccc(- c4cccc4)cc3)sc2n1	Neg_lig_429	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	0
142	Cc1cc(NCCCn2cenc 2)n2nc(- c3cccc3)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 c3cencc3)n2)cc1C	Neg_lig_544	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	0
146	Cc1c(S(=O) (=O)c2cccc2)c(N)n(Cc2ccccn2)c1C	Neg_lig_584	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	0
147	O[C@H] (Cn1c(Cc2cccc2)nc 2cccc21)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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	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(Ce 2cc(O)c3cccc(Cl)c3n 2)C[C@@H]1O	Neg_lig_780	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	0
151	O=C([O-])c1cc2cc(O Cc3cccc3)ccc2[nH]	Neg_lig_921	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	0
152	O=C1c2cccc2C(=O) N1OC[C@H] (O)COc1ccc([N+] (=O)[O-])cc1	Neg_lig_928	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	0
153	Cc1c(- c2cccc2)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+]C2CCCC2)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(=0)C1=C(N)OC2=C(C(=0)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@@] (CCc2cccc2) (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+]Ce1ecc(OCe2ece3e(e2)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	Neg_lig_1322	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	0
	([NH3+])CN1C(=O)c					

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	1cc(-c2ccc(F)cc2) [nH]n1					
167	O=C(/C=C\ c1cccnc1)NCCCCC1 CCN(C(=O)c2cccc2)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	EWSRI	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- c1nc2cccc2n1Cc1cc 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(NCe1cenen1)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]C(-O)[C@M]5C]C(-O)[C@M](NC(=O)OC)C(C)C)n4)cc3)cc2)c[nH]1)C	Neg_lig_1759	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	0
184	(C)C NS(=O)	Neg lig 1771	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	0

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	(=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	COclecc(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	CCOclccc(-c2noc(- c3nnn(- c4cccc4C)c3N)n2)c c1	Neg_lig_2084	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	0
195	O[C@@H] (Cc1ccc2cccc2n1)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(CCCCCNC(= O)c1cnc(N(c2cccc2) c2cccc2)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(- c3cccnc3NCc3cccc3)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	GGGCAGGGGAAGAGGGGG	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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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	COclecccl- nlnc(C)c(- c2cccc2)clN	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	CCCe1c(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 cccc2C(=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 3cccc3C(=O)N2c2c ccc2C)cc1	Neg_lig_2574	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	0
217	CCOC(=O)c1ccc(- n2c(N)c(C(=O)OC)c 3nc4cccc4nc32)cc1	Neg_lig_2600	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	0
218	O=C(OCc1cccc1)c1 nc2cccc2nc1NCc1cc ccc1	Neg_lig_2620	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	0
219	O=C(NC[C@H] (O)c1cccc1C(F) (F)F)c1c[nH]nc1- c1cccc1	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]c3cccc3c2C	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	GGGCAGGGGAAGAGGGGG	0
224	C=CCOc1ccc(-	Neg_lig_2885	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	0

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	n2cenc2)cc1CO					
225	N#Cc1c(- c2ccc(O)c2)c(C#N)c 2nc3cccc3n2c1N	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)c2cccc2)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(=0)O[C@]1(C(=0)CCl)[C@@H] (C)C[C@H]2[C@@ H]3CCC4=CC(=0)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-])c2cccc 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] (COc1ccc2cccc2c1) 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]	Neg_lig_3393	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	0
	(CO)CN(C(=O)c2ccc					

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 cccc32)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)nc2cccc 12	Neg_lig_419	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	0
257	Cc1ccc2c(N)c(C(=O) c3ccc(- c4cccc4)cc3)sc2n1	Neg_lig_429	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	0
258	Cc1cc(NCCCn2cene 2)n2nc(- c3cccc3)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)c2cccc2)c(N)n(Cc2ccccn2)c1C	Neg_lig_584	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	0
263	O[C@H] (Cn1c(Cc2cccc2)nc 2ccccc21)Cn1c2ccc(Neg_lig_636	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	0

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	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]	Neg_lig_921	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	0
268	O=C1c2cccc2C(=O) N1OC[C@H] (O)COc1ccc([N+] (=O)[O-])cc1	Neg_lig_928	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	0
269	Cc1c(- c2cccc2)n(CCO)c2n c3c(c(=O)n(C)c(=O)n 3C)n12	Neg_lig_956	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	0
270	CCCe1cc(N2CCC([N H2+]Cc3cnn(- c4cccc4)c3)CC2)nc(C)n1	Neg_lig_1009	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	0
271	Cn1c(N)c(C(=O)C[N H2+]C2CCCC2)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(=0)C1=C(N)OC2=C(C(=0)CC(C)(C)C2) [C@H]lc1ccc(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@@] (CCc2cccc2) (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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	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)c2cccc2)CC1	Neg_lig_1329	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	0
284	CCOc1ccc(-c2noc(- c3nnn(- c4cccc4)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- c1nc2cccc2n1Cc1cc 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))c3nc4cccn4c3F)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(=0)N[C@H] (C(=0)N1CCC[C@H]]lclnc(-c2ccc(- c3ccc(- c4c[nH]c([C@H]5C CCN5C(=0)	Neg_lig_1759	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	[C@@H] (NC(=0)OC)C(C)C) n4)cc3)cc2)c[nH]1)C (C)C					
300	NS(=O) (=O)c1ccc(NC(=S)N C(=O)c2ccc2)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(- c4cccc4C)c3N)n2)c c1	Neg_lig_2084	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	0
311	O[C@@H] (Cc1ccc2cccc2n1)C(Cl)(Cl)Cl	Neg_lig_2134	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	0
312	CCCCCN(CC[C@]I 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(CCCCCNC(= O)c1cnc(N(c2ccccc2) c2cccc2)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(- c3ccenc3NCc3ccccc3)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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	c3)ccc21					
319	O=C1CCC2(CCN(Cc 3nnc(- c4ccnc4)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(CN1CCC1)Nc 1nc(- c2ccc(Cl)cc2)cs1	Neg_lig_2392	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	0
322	COclccccl- nlnc(C)c(- c2cccc2)clN	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)c2ccc(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	CCCe1nc(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 cccc2C(=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 3cccc3C(=O)N2c2c ccc2C)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 nc2cccc2nc1NCc1cc ccc1	Neg_lig_2620	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	0
335	O=C(NC[C@H] (O)c1cccc1C(F) (F)F)c1c[nH]nc1- c1cccc1	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	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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	(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 2nc3cccc3n2c1N	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)c2cccc2)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(=0)O[C@]1(C(=0)CCI)[C@@H] (C)C[C@H]2[C@@ H]3CCC4=CC(=0)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-])c2cccc 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] (COc1ccc2cccc2c1) C[NH+]1CCCCC1	Neg_lig_3287	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	0
357	CCc1nc(N2C[C@H] (C3CC3)[C@@H] (NC(=0)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

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	[C@@H]1c1ccc(F)cc					
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 (- c2cccc2)nc2ccccc12	Neg_lig_2	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	0
361	CC1(C)CC(=O)C2=C (C1)OC(N)=C(C#N) [C@H]2c1cccc1OC (=O)N1CCOCC1	Neg_lig_73	NRAS	G-quadruplex	UGUGGGAGGGGCGGUCUG GG	0
362	COc1ccc(CN2C(=O) c3cccnc3[C@H]2Nc 2cc(Cl)ccc2OC)cc1	Neg_lig_78	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG 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	UGUGGGAGGGCGGGUCUG GG	0
364	Cn1c(=[NH2+])n(CC O)c2cccc21	Neg_lig_86	NRAS	G-quadruplex	UGUGGGAGGGGCGGUCUG GG	0
365	CCN(CC)C(=O) [C@@H]1C[C@@H] ([NH3+])CN1C(=O)c 1csc(-c2ccs2)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	UGUGGGAGGGCGGGUCUG GG	0
367	CCCc1cncnc1N1CC C([NH2+]C2CCN(C(=O)OCC)CC2)CC1	Neg_lig_131	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	0
368	COc1ccc(/C=C/ CN2CC[C@@H] (NC(=O)c3cccnc3) [C@H](O)C2)cc1	Neg_lig_141	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	0
369	CCn1c(CC2CC[NH2 +]CC2)nn(CC(=O)N Cc2cccc2)c1=O	Neg_lig_150	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	0
370	CCOcleccc1NC(=O)clnnn(-c2ccc(C(F) (F)F)c2)c1N	Neg_lig_157	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	0
371	NC[C@H]1CC[N@ H+](Cc2ccc(C(F) (F)F)cc2)C1	Neg_lig_158	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	0
372	Cc1ccc2c(c1)c(- c1ccccc1)c(- c1ccccc1)n2C[C@H] (O)C[NH+]ICCCCC	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	UGUGGGAGGGCGGGUCUG GG	0
374	N#CC1=C(N)OC2=C (C(=0)CCC2) [C@@H]1c1cc(C[N H+]2CCOCC2)cs1	Neg_lig_280	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	0
375	NC(=0)c1ccc(N2CC N(Cc3c[nH]nn3)C[C @H](O)C2)nc1	Neg_lig_282	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	0

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	UGUGGGAGGGCGGGUCUG GG	0
377	Nc1cc(OC(=O)c2ccc cc2F)nn1S(=O) (=O)c1cccc1	Neg_lig_335	NRAS	G-quadruplex	UGUGGGAGGGGCGGUCUG GG	0
378	CC[C@H] (C)c1ccc(OCc2nnc(N)s2)cc1	Neg_lig_365	NRAS	G-quadruplex	UGUGGGAGGGGCGGUCUG GG	0
379	CCC[C@H] (O)c1nc2cccc2n1Cc 1ccccc1Cl	Neg_lig_367	NRAS	G-quadruplex	UGUGGGAGGGGCGGUCUG GG	0
380	Nc1cc(- c2ccc3c(c2)OCO3)cc n1	Neg_lig_369	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	0
381	C[C@@H](c1ccc(- c2nc3ccccc3n2CCO) cc1)N1CCOCC1	Neg_lig_384	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	0
382	COCc1cc(C)nc2sc(- c3nnc(- c4cccc4)o3)c(N)c12	Neg_lig_398	NRAS	G-quadruplex	UGUGGGAGGGGCGGUCUG GG	0
383	[NH3+]CCn1cc(C(= O)NCCc2noc(- c3ccccc3)n2)nn1	Neg_lig_408	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG 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	Neg_lig_425	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	0
385	COclccc([C@@H]2 C(C#N)=C(N)OC3= C2C(=0)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	UGUGGGAGGGCGGGUCUG GG	0
387	OCCSc1nnc(COc2cc c(Cl)cc2)n1-c1ccccc1	Neg_lig_468	NRAS	G-quadruplex	UGUGGGAGGGGCGGUCUG GG	0
388	O=C(CCCCCC(=O)Nc1ccc([C@@H]2O [C@H] (c3ccc(CO)cc3)C[C @H](CSc3nc(- c4ccccc4)c(- c4cccc4)o3)O2)cc1) NO	Neg_lig_517	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG 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	UGUGGGAGGGCGGGUCUG 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	UGUGGGAGGGCGGGUCUG GG	0
391	O=[N+] ([O-])c1ccc2c(c1) [S@](=O)c1cccc1-2	Neg_lig_702	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	0
392	CC1(C)CC(NC(=O)C CCOc2ccc(Cl)cc2Cl) CC(C)(C)[NH2+]1	Neg_lig_726	NRAS	G-quadruplex	UGUGGGAGGGGCGGUCUG GG	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
393	O[C@@]1(C[NH+]2 CCC3(C=Cc4cccc4 3)CC2)CNCCOC1	Neg_lig_732	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG 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	UGUGGGAGGGCGGGUCUG GG	0
395	Cc1ccc(C)c(-n2c(- c3ccc(Br)cc3)cs/ c2=N\ C(=O)c2cccc2F)c1	Neg_lig_745	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG 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	UGUGGGAGGGCGGGUCUG GG	0
397	CC(C)c1cc(NCc2nc(N)nc(N(C)C)n2)n2nc cc2[nH+]1	Neg_lig_809	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	0
398	COc1ccc(C)cc1- n1nnc(-c2nc(- c3cccc3Cl)no2)c1N	Neg_lig_841	NRAS	G-quadruplex	UGUGGGAGGGGCGGUCUG GG	0
399	Cc1ccc2nc(CNCc3cs c(- c4ncccn4)n3)cc(O)c2 c1	Neg_lig_866	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	0
400	Cc1[nH]c(/C=C2/ C(=O)Nc3cccc32)c(C)c1CCC(=O)[O-]	Neg_lig_873	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	0
401	CC(=O)N1CCN(c2cc c(NCc3ccc(F)cc3)cc2)CC1	Neg_lig_943	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	0
402	Cc1cc(C)n(C[C@H] (C)O)c(=O)c1C#N	Neg_lig_969	NRAS	G-quadruplex	UGUGGGAGGGGCGGUCUG GG	0
403	COc1cc(OC)c(OC)cc 1C=O	Neg_lig_1061	NRAS	G-quadruplex	UGUGGGAGGGGCGGUCUG GG	0
404	C=CCNc1ncnc2c1sc 1nc3c(cc12)COC(C) (C)C3	Neg_lig_1087	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	0
405	S=C1SCN(CCe2cccc c2)CN1CCe1cccc1	Neg_lig_1099	NRAS	G-quadruplex	UGUGGGAGGGGCGGUCUG GG	0
406	Cn1nccc1- c1ccccc1OC[C@@H] (O)C[NH+]1CCCCC 1	Neg_lig_1123	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	0
407	CCOC(=O)c1ccccc1 N[C@H]1OC(=O)c2 cccc21	Neg_lig_1135	NRAS	G-quadruplex	UGUGGGAGGGGCGGUCUG GG	0
408	CCN(CC1CCOCC1) C(=0)c1ccc(C[C@H]2CCC[NH2+]C2)cc 1	Neg_lig_1158	NRAS	G-quadruplex	UGUGGGAGGGGCGGUCUG GG	0
409	COc1ccc2c(c1) [C@]13CC[N@@H+](C)[C@H](C2) [C@@H]1CCC1(C3) OCCO1	Neg_lig_618	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	0
410	[NH3+] [C@H]1CCN(C(=O) c2cccc(- c3ncc[nH]3)c2)C1	Neg_lig_1192	NRAS	G-quadruplex	UGUGGGAGGGGCGGUCUG GG	0
411	COc1cccc(C[NH2+] Cc2cccnc2)c1OCc1c	Neg_lig_1237	NRAS	G-quadruplex	UGUGGGAGGGGCGGUCUG GG	0

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	cc(F)cc1					
412	O=C1C[C@H] (NC2CCC2)C(=O) N1c1ccc(C1)cc1	Neg_lig_1248	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	0
413	COc1ccc(- n2nc3ccc(N)cc3n2)cc 1	Neg_lig_1290	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	0
414	Nc1ncnc2c1ncn2[C @@H]10[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+]Cc3ccnc3)cc c21	Neg_lig_1358	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	0
416	OC[C@H]1C[N@H+] (Cc2cnc(N3CCCCC3)nc2)C[C@H]1CN1C COCC1	Neg_lig_1399	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	0
417	CNc1nenc2c1c(- c1ccccc1)cn2- c1cccc(Cl)c1	Neg_lig_1420	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	0
418	CC[C@H] (O)clnc2cccc2nlCC COclccc(C)clC	Neg_lig_1426	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	0
419	O=C(CCCc1cn[nH]c 1)N1CCC2(CC1)Nc1 ccccc1NC2=O	Neg_lig_1430	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	0
420	CC[C@@]1(c2ccc(N)cc2)CCC(=O)NC1= O	Neg_lig_1442	NRAS	G-quadruplex	UGUGGGAGGGGCGGUCUG GG	0
421	O=C([O-])c1cccc1C N1CCN(C(=O)c2ccc o2)C[C@@H](O)C1	Neg_lig_1443	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	0
422	COc1cc(C)nc(N(CC O)CCO)n1	Neg_lig_1472	NRAS	G-quadruplex	UGUGGGAGGGGGGUCUG GG	0
423	CS(=O)(=O) [N-]c1ccc(- c2ccc(N)cc2)cc1[N+] (=O)[O-]	Neg_lig_1505	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	0
424	COC(=O)c1ccc(- c2c(C#N)c(N)nc3c2C CCCC3)cc1	Neg_lig_1554	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG 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	UGUGGGAGGGCGGGUCUG GG	0
427	CC(C)[NH2+] [C@@H]1CC[C@@ H]1NC(=O)CCSCc1c cccc1	Neg_lig_1598	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	0
428	Cc1ccc(F)c(Cn2ccnc 2- c2ccc(C#CCO)s2)c1	Neg_lig_1607	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	0
429	Cc1[nH+]ccn1- c1ccc(C[NH2+] [C@@H](C)CO)cc1	Neg_lig_1610	NRAS	G-quadruplex	UGUGGGAGGGGCGGUCUG GG	0

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	UGUGGGAGGGCGGGUCUG GG	0
431	O=C1CC[C@]2(CC C[N@H+] (CCOc3ccc(Cl)cc3)C 2)CN1CCO	Neg_lig_1744	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	0
432	COCc1cc([C@H]2N[C@](CO)(c3cccc3) [C@H]3C[N@H+] (C)C[C@@H]23)ccc 1OC	Neg_lig_1762	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	0
433	COc1ccc(C2=NC(=O)N[C@@H]2c2ccc(O C)cc2)cc1	Neg_lig_1776	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	0
434	CCCn1cnc2cc(NCc3 ccc(Br)cc3)ccc21	Neg_lig_1806	NRAS	G-quadruplex	UGUGGGAGGGGCGGUCUG GG	0
435	NC1=C(c2nc3ccccc3 s2)C(=O)CN1c1ccc(N2CCCCC2)cc1	Neg_lig_1846	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	0
436	Cc1ccc(CC[NH2+]C c2cc(O)c3cccc(Cl)c3 n2)s1	Neg_lig_1853	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	0
437	Cc1nnc2c(NCCCN3 CCN(c4ccc(Cl)c4)C C3)nc3cccc3n12	Neg_lig_1858	NRAS	G-quadruplex	UGUGGGAGGGGCGGUCUG GG	0
438	COc1ccc2c(CNCCc3 cccc3OC)c(C(=O)O)n(C)c2c1	Neg_lig_1894	NRAS	G-quadruplex	UGUGGGAGGGGCGGUCUG GG	0
439	O=c1c2c(nc(NCCCO))n1-c1cccc1)- c1ccccc1CC21CCCC	Neg_lig_1958	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	0
440	CCSc1ccc(C(=O)N2 CCC3(CC2) [C@@H] (O)C[C@H]3O)s1	Neg_lig_1960	NRAS	G-quadruplex	UGUGGGAGGGGCGGUCUG 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(- c2cccc2)nc2c1CCN(C(=O)c1ccc(N)nc1)C	Neg_lig_2010	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG 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	UGUGGGAGGGGCGGUCUG GG	0
444	COc1ccc(- c2c(NCc3cccc3Cl)c(=O)c2=O)cc1	Neg_lig_2021	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	0
445	CCc1[nH]nc2c1C1(C (C#N)=C(N)O2)c2cc ccc2-c2cccc21	Neg_lig_1701	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	0
446	Cc1nc(C2=C(N)N(C[C@H] (C)O)CC2=O)sc1C	Neg_lig_162	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	0
447	Cc1ccc(- c2noc(CNe3cccc(C)c 3)n2)cc1	Neg_lig_2128	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	0
448	CC1=C(c2cccc2)S(= O) (=O)N=C1Nc1cccc1	Neg_lig_2132	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	0

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	Br					
449	Cc1cc(NC2CCC2)n c2cccc12	Neg_lig_2138	NRAS	G-quadruplex	UGUGGGAGGGGGGUCUG GG	0
450	Nc1nnc(CC(=O)N2C CC(Cc3noc(C4CC4) n3)CC2)s1	Neg_lig_2142	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	0
451	C=CCNc1c(O)cc2c(O)c1C[C@@H] (C)C[C@H](OC) [C@@H](O) [C@@H](O) [C@@H](OC(N)=O) [C@@H](OC/C=C\ C=C(\C)C(=O)N2	Neg_lig_2147	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	0
452	COc1ccc(CNc2[nH+] c3ccc(C)cc3cc2- c2noc(C)n2)cc1OC	Neg_lig_2189	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	0
453	CC[n+]1cn(C[C@H] (O)COc2cccc2)c2cc (C)c(C)cc21	Neg_lig_2279	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	0
454	O=C(/C=C/ c1cccc(S(=O) (=O)Nc2cccc2)c1)N O	Neg_lig_2342	NRAS	G-quadruplex	UGUGGGAGGGGCGGGUCUG GG	0
455	CCN1c2cccc2C2=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	Ce1cc(C)nc([N-]S(= O) (=O)c2ccc(NCc3nc4c cccc4n3C)cc2)n1	Neg_lig_2380	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	0
457	CC1=NC(C) (C)C[C@H]2CC[C@ @H](O)[C@@H]12	Neg_lig_2433	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	0
458	Cn1c(=O)nc([O-])c2c 1nc(NCCO)n2Cc1ccc (Cl)cc1	Neg_lig_2219	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG 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	UGUGGGAGGGCGGGUCUG GG	0
462	CC1=C(c2ccc(C(C)C)cc2)S(=O) (=O)N=C1NCc1ccc 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(=0)CN1CC2(CC C1=0)CCN(C(=0) [C@@H]1C[NH2+] CCO1)CC2	Neg_lig_2586	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	0
465	Cc1ccc2nc(- c3ccsc3)c(Nc3cccc3)n2c1	Neg_lig_2591	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	0
466	CC(=O)c1cccc(-	Neg_lig_2666	NRAS	G-quadruplex	UGUGGGAGGGGGGUCUG	0

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	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	UGUGGGAGGGCGGGUCUG GG	0
469	Cc1cccc1Cn1c(NCC O)nc2c1c(=O)n(C)c(=O)n2C	Neg_lig_2721	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	0
470	CNC(=0) [C@@H]1C[C@@H]((NH3+])CN1C(=0) [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-c1cccc1	Neg_lig_2740	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG 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(- c4cccc4)n3)cnc21	Neg_lig_2816	NRAS	G-quadruplex	UGUGGGAGGGGCGGUCUG GG	0
474	Nc1ccc2ncc(=O) [nH]c2c1	Neg_lig_2830	NRAS	G-quadruplex	UGUGGGAGGGGCGGUCUG GG	0
475	Cc1ccc(NC(=O)N2C CN(C(=O)c3nonc3N) CC2)cc1Cl	Neg_lig_2833	NRAS	G-quadruplex	UGUGGGAGGGGCGGUCUG GG	0
476	CCCCCCclccc(C CC([NH3+]) (CO)CO)cc1	Neg_lig_2868	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	0
477	C[C@H](/ N=C1C(=C(\N)O)/ S(=O) (=O)c2cccc2/1)c1cc ccc1	Neg_lig_2882	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	0
478	Cc1cc(Nc2cc(N3CC[NH+](C)CC3)nc(/ C=C/c3cccc3)n2) [nH]n1	Neg_lig_2886	NRAS	G-quadruplex	UGUGGGAGGGGCGGUCUG GG	0
479	CCOC(=O)c1sc2nc3c (cc2c1N)CO[C@H] (C(C)C)C3	Neg_lig_2888	NRAS	G-quadruplex	UGUGGGAGGGGCGGUCUG GG	0
480	CCOC(=O)Cn1nc2oc (=O)c(CCN3CCN(c4 cccc4OC)CC3)c(C)c 2c1C	Neg_lig_2947	NRAS	G-quadruplex	UGUGGGAGGGGCGGUCUG GG	0
481	Cc1ccc(NC(C) (C)C(=0)N2CC[C@ H](C[NH3+])C2)cc1	Neg_lig_3004	NRAS	G-quadruplex	UGUGGGAGGGGCGGUCUG GG	0
482	CSCCc1nc(-c2ccc(-c3cc[nH]n3)cc2)n(C CO)n1	Neg_lig_3025	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	0
483	Cc1ccc2[nH]c3c(c2c 1)CCC[C@@H]3[N H2+]CCCOc1ccc(F)c c1	Neg_lig_3042	NRAS	G-quadruplex	UGUGGGAGGGGCGGUCUG GG	0
484	COc1ccc(C(=O)NC2 CC2)cc1NC(=O)N[C @@H] (C)c1nnc(N)s1	Neg_lig_3049	NRAS	G-quadruplex	UGUGGGAGGGGCGGUCUG GG	0
485	Nc1c(-c2nc(- c3ccccc3)no2)nnn1-	Neg_lig_2907	NRAS	G-quadruplex	UGUGGGAGGGGCGGUCUG GG	0

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	UGUGGGAGGGCGGGUCUG 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	UGUGGGAGGGCGGGUCUG GG	0
488	CC1CCN(C(=0)c2cc cc(NC(=0)N[C@@H] (CO)c3cccc3)c2)CC	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	UGUGGGAGGGCGGGUCUG 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	UGUGGGAGGGCCGGUCUG GG	0
493	Cclnc(C(=0)N2CC[C@H] ([NH+]3CCN(C)CC3)[C@H] (CCCO)C2)cs1	Neg_lig_3282	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG 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)cC)ccc7 6)[C@@H]1O) [C@H]5CC(N)=O) [C@@](C) (CC(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@@H]2CCC(N)= O.O.[Co+]	Neg_lig_3314	NRAS	G-quadruplex	UGUGGGAGGGGCGGGUCUG GG	0
495	Cc1cccce1N1CCN(C (=O)c2cn(C3CC[NH 2+]CC3)nn2) [C@@H](C)C1	Neg_lig_423	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	0
496	O=C(c1ccc2c(c1)CC C2)N1CCC2(CC1)O CCC[C@@H]2O	Neg_lig_1439	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	0
497	[NH3+] [C@@H]1CC[C@H] (C(=O)NCc2ccc3c(c2)CCCC3)C1	Neg_lig_1992	NRAS	G-quadruplex	UGUGGGAGGGGCGGUCUG GG	0
498	COc1cccc(OCc2cc([C@H]3Nc4ccccc4C(=O)N3Cc3ccccc3)ccc	Neg_lig_18	TERRA	G-quadruplex	GGGUUAGGGU	0

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	2OC)c1					
499	O=C([O-])c1cc(NC2 =NS(=O) (=O)c3cccc32)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(CSc2nc3cccc3s2)n1	Neg_lig_161	TERRA	G-quadruplex	GGGUUAGGGU	0
502	Nc1nnc(SCC(=O)Nc 2ccc(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(CNCe1eccec1) N1e2ecce2Se2ece(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](c2cccc2)C/ C1=N\CCc1c(C) [nH]c2cccc12	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](C) [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(-c3cccc3)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

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(- c2cccc2)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(C1)c(C1)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	Neg_lig_908	TERRA	G-quadruplex	GGGUUAGGGU	0
527	CCN(CC)C(=0) [C@H]1C(=0)N(CC O) [C@@]2(C)C[C@@ H]1c1cccc1O2	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(- c4cccc4)ncc32)nc(N)n1	Neg_lig_1025	TERRA	G-quadruplex	GGGUUAGGGU	0
531	Nc1c(-c2nc(- c3ccc(F)cc3)no2)nnn 1-c1cccc1	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

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 cccc2C1)N1CCOc2 ccc(CO)cc2C1	Neg_lig_1395	TERRA	G-quadruplex	GGGUUAGGGU	0
542	CC(C)OCC[NH2+]C CC(=O)NC1CCCC 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 Cc1cccc1C1	Neg_lig_1567	TERRA	G-quadruplex	GGGUUAGGGU	0
547	COclecceclOC[C@ @H] (O)Cnlcnc2cc(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(=0)OCC(=0) [C@]12OC(C) (C)O[C@H]1C[C@H]1[C@@H]3C[C@H	Neg_lig_1612	TERRA	G-quadruplex	GGGUUAGGGU	0
] (F)C4=CC(=O)C=C[C@]4(C)[C@@]3(F) [C@@H]					

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	(O)C[C@@]12C					
550	C=CC[C@@H] (CC)C(=O)NC(=O)N 1CCCc2cccc21	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/ c1cccc1)O2	Neg_lig_1763	TERRA	G-quadruplex	GGGUUAGGGU	0
554	O=C1[C@H] (Cc2ccc(O)cc2)N2C(=O)CCN(C(=O)NCc 3cccc3) [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(NC2CCCC2)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(- c2cccc2F)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)Cn1cnc2cccc21	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	COclccccc1C(=O) [C@H] (O)clccccc1OC	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

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=C1c2cccc2[C@ @H] (Nc2cccc2)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(=0) [C@@H]1CC2=CC(=0)CC[C@]2(C) [C@@]230[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)Nc1ccc2nccc2c1	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	CCOc1cccc1-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

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+]Cc1ccce(OCc 2cccc2F)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)c4cccc4F) 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(=0)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)[C@@H](C)/C=C)(C)(C=O)[C@H](C)C[C@H](C)C(C=O)[C]3(O[C@H]4O[C@]3(O)(C)[C@H](C)C(C)(C)(C)(C)(C)(C)(C)(C)(C)(C)(C)(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

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(- c2cccc2C(=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)nc2cccc2 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] (COclecccl)C[NH+]1CCCCCl	Neg_lig_2646	TERRA	G-quadruplex	GGGUUAGGGU	0
614	CelenecelCnlcenel- elen(C2CC[NH2+]C C2)nn1	Neg_lig_1885	TERRA	G-quadruplex	GGGUUAGGGU	0
615	Cc1ccc(N[C@@H]2c 3cccc3C(=O)N2c2c ccnc2)c(C)c1	Neg_lig_3343	TERRA	G-quadruplex	GGGUUAGGGU	0
616	CCc1ncc(C(=O)N[C @@H](c2cccc2) [C@H] (O)c2cccc2)cn1	Neg_lig_3350	TERRA	G-quadruplex	GGGUUAGGGU	0
617	O=C(c1ccccc1) [C@@H]1[C-]([N+] (=O)[O-]) [C@@H]1c1cccc1	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	OCCCc1nc2cccc2n1 CCOc1ccc(Cl)cc1	Neg_lig_3406	TERRA	G-quadruplex	GGGUUAGGGU	0
621	Cc1nc(CCN)n[nH]1	0342-0285	AKTIP	G-quadruplex	GGGGUGGGGCGGGGG	1

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622	CSCCC(C(O)=O)Nc 1c2c3CCCCc3sc2ncn 1	0866-0023	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	1
623	O=C(NCCCN1CC1) Nc1cccc2cccc12	101298	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
624	CC(c1ccc(cc1)NC1c2 ccc(c(c2C(=O)O1)O C)OC)=O	1080-0649	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	1
625	O=C(C(C(N1)=O)=C c2csc3c2cccc3)NC1= O	108783	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	1
626	NC(NC(c1ncenc1C(O)=O)=O)=O	117922	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
627	Ce1cc(ne2cc(ccc12) OC)N1C[C@H] (C2CC2)[C@H] (C1)N	12182839	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	1
628	CC(NS(c(cc1)cc2c1s c(C)n2)(=O)=O)=O	122385	AKTIP	G-quadruplex	GGGGUGGGGCGGGGG	1
629	CC1=CC(C)=NC(N1 CCNC(C1CC2(CCN CC2)CN1C)=O)=O	12499963	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	1
630	CN1CCN(CC1) [C@H]1CCN(C[C@ H]1CCCO)C(c1cccc2 c1ccn2C)=O	12576044	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
631	C1CCN(C1)Cc1cc(C N2CCC(Cc3ccc(CO) cc3)C2)sc1	12617773	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	1
632	C1CC2(CCN(CC2)C C(C(F) (F)F)O)CN(CC(N)= O)C1=O	13525118	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
633	CN(Cc1ccc(cc1)n1cc cn1)Cc1cccc(CCN)c1	13860811	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGG	1
634	Cc1nc(CCN)cc(NCC C2CCCN2C)n1	14159297	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
635	CCN(CC)Cc1cnc2c(c nn2c1)C(NCc1ccc(C N)cc1)=O	14229566	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
636	CCc1nc2CCNCCc2c(NCc2nc(c3ncccn3)no 2)n1	14445071	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	1
637	C1CN(CCC1C1CCN (CCc2cccc2)C1)c1c cnc(N)n1	14604674	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
638	CCc1cc(nc(n1)N1CC CC1)N1C[C@H] (C[C@H]1C(N(CC) CC)=O)N	15018109	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
639	Cc1cc(nc(N)n1)N1C CC(CC1)NCCCN1C Cc2cccc12	15043866	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	1
640	CCNC([C@@H]1C[C@@H] (CN1C(CN1CCCCC CC1)=O)N)=O	15077405	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
641	Clc(c(NC1CCCCC1) nnc1Cl)c1Cl	154127	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
642	COclecc(cc1)OC1C CN(CC1)C([C@@H] 1C[C@H] (CN1)O)=O	15579241	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1

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643	C(CN)c1cccc(CN2C COCC(C2)CO)c1	15684586	AKTIP	G-quadruplex	GGGGUGGGGCGGGGG	1
644	COCCCN1C(CC[C @H]2CN(CC[C@@ H]12)c1c2cn[nH]c2n c(N)n1)=O	15765444	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
645	Cc1ccc(cc1)c1csc(Nc 2ccc(C)cc2) [n+]1CC=C	1611-2955	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	1
646	COe1ccc(cc1)N1C(C 2C3c4cccc4C(CO) (C2C1=O)c1ccccc13) =O	1657-0369	AKTIP	G-quadruplex	GGGGUGGGGCGGGGG	1
647	CCc1nnc(NCC2CCC CCN2)o1	16631339	AKTIP	G-quadruplex	GGGGUGGGGCGGGGGGGG	1
648	Cc1c(C(C(NCCNc2c ccnc2)=O)N)c(C) [nH]n1	16899791	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	1
649	CN(CC1CCN(CC1)C Cc1cccc(c1)F)C([C@ H] (Cc1c[nH]cn1)N)=O	17007774	AKTIP	G-quadruplex	GGGGUGGGGCGGGGG	1
650	C1CCN(CCCNC(c2c ccc(c2)c2cn[nH]c2)= O)C(C1)CO	17250805	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	1
651	C=Cc1ccc(nc1)N1CC N(CC(C1)O)Cc1cccc c1	17524156	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
652	CCn1cncc1CNc1c2C CNCc2nc(c2cncc2)n	18384397	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	1
653	CN(C)CCC1CCCCN 1Cc1ccc(CCN)cc1	18585072	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
654	C1CN(CCC12c1cccc c1[C@H] ([C@@H]2O)N)Cc1 c[nH]nc1c1ccccc1	18741551	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	1
655	Cc1nccn1CC1CCN(CC1)c1c2CCNCc2nc n1	19035660	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	1
656	C1CCCN(CC1)CC(C NC(c1cn(CCN)nn1)= O)O	19036853	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	1
657	C1CN(CC1c1cccc1 F)Cc1ccc(CCN)cc1	19080499	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
658	C1CCN(CC1)c1ccc(c c1)c1cc(c2ccnc2)c(C#N)c(N)n1	19252160	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	1
659	Cc1cc2c(cc1CN1C[C @@H] (CN3CCCCCC3) [C@H] (C1)CO)OCCO2	19474966	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
660	Cc1ccc(cc1[Cl])N1C CC(CC1)N[C@@H] 1CC[C@H](C1)N	19498560	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
661	Cc1cc(C)c2c(c1)c(cc(C)n2)C(N[C@H]1C NC[C@@H]1OC)=O	19537511	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
662	C(CN)c1cccc(CN2C CN(CC2)Cc2ccc(cc2)[Cl])c1	19565794	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	1
663	O=C1OCC/C1=C\	197008	AKTIP	G-quadruplex	GGGGUGGGGCGGGGG	1

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	NCCCCCCCN/ C=C(\CCO1)/C1=O					
664	C(CNC1CCC2(CC1) CCNCC2)CNc1ccenc 1	19786268	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
665	CN(Cc1cnn(c1)c1ccc (cc1)F)C(C(c1ccc(cc 1)F)O)=O	19840417	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
666	C(CN)C1CN(CCO1) c1c2CCNCc2nc(c2cc ccc2)n1	19916102	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
667	C1C[C@@H]2CCN(Cc3ccccn3)C[C@H] 1N2	20138450	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
668	Cn1e2c(cn1)c(nc(c1c cncc1)n2)N1CCCC2(CCNCC2)CC1	20352833	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
669	C1CNCc2c1c(NCC1 COc3cccc3O1)nc(c1 cccnc1)n2	20674759	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	1
670	Cc1ncen1c1ccc(CNC (CCc2cc3CNCCCn3 n2)=O)cc1	20920311	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
671	C1[C@@H] (C2(CCN(CC2)Cc2n cc[nH]2) [C@@H]1O)O	21540130	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
672	C1CCN(CC1)C(CNC (CCc1cc2CNCCn2n1)=O)c1cccnc1	21900063	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
673	COclccc(ccl)clc(CN 2CCC3(CC2)[C@H] (C[C@H]3O)OCCN) c[nH]n1	22516313	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
674	CN(C[C@@H]1CC[C@@H] (CC1)N)CC1(CCCC 1)CO	22559794	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
675	C1CCCN(CC1)C[C @@H]1CN(C[C@@ H]1CO)C(c1cc(N) [nH]n1)=O	22664850	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
676	C1CCN(CC1)C[C@ @H]1CN(C[C@@H] 1CO)C(c1cn2cc(cnc2 n1)[C1])=O	22667725	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
677	Cc1cc(C)cc(CN2CC C3(CCNCC3)C2)c1	22860169	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
678	C1CCN(CC1)CC1(C CN(Cc2ccc(CCN)c2)C1)O	22896979	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
679	C(c1c(c2ccc(c2) [C1])c(C#N)c2nc3ccc cc3n2c1N)#N	2367-1144	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
680	CC1CCC(C)N1CC(COc1c(C)cccc1C)O	2388-0120	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
681	CN(C)S(Nc1cccc(Br) c1)(=O)=O	241621	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
682	CN1CCN(CC1)c1cc(nc(N)n1)N1CCCC(C N2CCCC2)C1	25666870	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	1
683	C1CCN(CC1)Cc1ccc c(c1)n1ccnc1c1cc2C	26875627	AKTIP	G-quadruplex	GGGGUGGGGCGGGGG	1

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	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	GGGGUGGGGCGGGG	1
685	O=C(Nc1ccccc1)OC 1=CC=CNC1=O	277806	AKTIP	G-quadruplex	GGGGUGGGGCGGGGGGGGG	1
686	CCOc1ccc(CNCCc2c cc(cc2)F)cc1	2910-0686	AKTIP	G-quadruplex	GGGGUGGGGCGGGGGGGGG	1
687	COc1ccc(c(CNc2ccc(cc2)[Br])c1)OC	2910-1869	AKTIP	G-quadruplex	GGGGUGGGGCGGGGGGGGG	1
688	O=C(N(CC1OC1)C(N1CC2OC2)=O)N(C C2OC2)C1=O	296934	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	1
689	Cc1ccc(cc1)N1C(CC (C1=O)NCCc1ccc(cc 1)OC)=O	3076-0323	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
690	COCCOC(C1C(C2= C(c3cccc3OC2=O) OC=1N)c1ccncc1)=O	3132-1032	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
691	Cc1nc(CCN)cc(n1)N 1CCN(CC1)c1ccc(C# N)cn1	31455775	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
692	COc1ccc(CCNCc2cc cc(c2)C(F)(F)F)cc1	3169-1283	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
693	C(CNCc1ccc2c(c1)O CO2)c1ccc(cc1)F	3169-1371	AKTIP	G-quadruplex	GGGGUGGGGCGGGGG	1
694	C1CN(CC1CN)Cc1c cc(c2cccc2C#N)o1	31727519	AKTIP	G-quadruplex	GGGGUGGGGCGGGGG	1
695	CCN(CC)Cc(c(OC)c 1)cc2c1c1cnc(cc(cc3) Cl)c3c1[nH]2	317605	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	1
696	Ce1cccc(NC(SC(c(cc 2)cc(OC)c2O)NC2= O)=C2C#N)c1	319435	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
697	[H]Nc1nnc(C(CC)c2 cccc2)s1	3202-0205	AKTIP	G-quadruplex	GGGGUGGGGCGGGGGGGGG	1
698	CN(C)CCNc1nc2c(C (N(C)C(N2C)=O)=O) n1Cc1cccc1[C1]	3238-0121	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	1
699	COCc1nc(CCNC(CC c2cc3CNCCn3n2)=O)on1	32552243	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
700	O=C(NC(N1c2cccc 2)=C2NC1=S)NC2= S	33182	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
701	CN1C(c2c(nc(NCCN)n2Cc2ccc(cc2)F)N(C)C1=O)=O	3346-2730	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
702	CCN(CCN)c1ccc2C(NNC(c2c1)=O)=O	3367-1212	AKTIP	G-quadruplex	GGGUGGGGCGGGG	1
703	COc1ccc(cc1OC)c1n c2cc(ccc2o1)N	3370-0370	AKTIP	G-quadruplex	GGGGUGGGGCGGGGG	1
704	C1CC(N(C1)CCC1C CN(CC1)Cc1cccc(C CN)c1)=O	34485551	AKTIP	G-quadruplex	GGGGUGGGGCGGGGG	1
705	CC(C) (CO1)COP1(OC(C= NN(C1CCCCC1)C1= O)=C1OC)=S	350187	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	1

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706	CC1=CC(NC(NCCN C2CCC3(CC2)CCN CC3)=N1)=O	35107446	AKTIP	G-quadruplex	GGGGUGGGGCGGGGG	1
707	Cc1ccc(c1)Nc1nc(C N2C[C@@H]3CC[C @H] (C2)N(C)C3=O)nc(N)n1	35485871	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
708	COc1cccc(CNCc2ccc c(c2)F)c1OC	3702-1553	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	1
709	COc1cccc(CCNCc2c cc(cc2)C(F)(F)F)c1	3702-1570	AKTIP	G-quadruplex	GGGGUGGGGCGGGGGGGG	1
710	C(c1cencc1)NCc1ccc 2c(c1)OCO2	3702-1584	AKTIP	G-quadruplex	GGGGUGGGGCGGGGGGGGG	1
711	CSC(N1NC(c(cc2)cc c2Cl)N=C11)=NC=C 1C#N	379538	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
712	Cc1c(C(NN/C(/ SC)=N/S(c2cccc2) (=O)=O)=O)c(- c(c(Cl)ccc2)c2Cl)no1	379696	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
713	N#CC1=C(Nc(cccc2) c2Cl)SC(c2ccncc2)N C1=O	379697	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	1
714	COcleccc1OC1CC N(CC1)Cc1ccc(CC N)c1	39780332	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
715	CC(Nc1cccc(c1)c1cc c(c(c1)F)NC(CN)=O) =O	40118252	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
716	Cc1ccc(cc1)S(N(CC(CN1CCCC1)O)c1c cccc1OC)(=O)=O	4013-2178	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
717	CC(C)CC1CC(C) (c2csc(Nc3ccccc3)n2)OC1=O	4075-3209	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
718	C1CN(CCN(C1)c1nc cc(n1)N1CCC(C1)O) Cc1ccc(c1)F	41253715	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	1
719	Cc1nc2CNCCc2c(N CCc2csc(c3cccnc3)n 2)n1	41602213	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	1
720	CC(C) [C@@H]1CN(Cc2cc cc(CCN)c2)C[C@H] 1N(C)C	42043717	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
721	CC1CCe2c(C(Ne3ce ccc3C)=O)c(N)sc2C1	4488-1595	AKTIP	G-quadruplex	GGGGUGGGGCGGGGG	1
722	CC(c1cccc(c1)Nc1cc (C)nc2ccc(C)cc12)= O	4491-0985	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
723	Cc1ccc2c(c1)c(c1CC Cc1n2)Nc1cccc(c1)O	4491-1565	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
724	CCOC(c1ccc2c(c1)c(cc(C)n2)Nc1ccc(cc1) N(C)C)=O	4593-2976	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	1
725	CCOC(c1ccc2c(c1)c(cc(C)n2)Nc1cccc(c1) O)=O	4593-2992	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
726	Cc1c2cccc2n(CC(C n2c(C)c(c(C)n2) [Br])O)c1C	4593-8144	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
727	Cc1c(CN2CC3(CCN	46066918	AKTIP	G-quadruplex	GGGGUGGGGCGGGGG	1

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	GGGGUGGGGCGGGG	1
729	CCC1CN(CCN1C(C) C)Cc1cccc(CCN)c1	46449375	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
730	C(CNc1cccnc1)CNc1 c2cccc2nc(CCN)n1	47488116	AKTIP	G-quadruplex	GGGGUGGGGCGGGGG	1
731	Cc1ncen1CCC1CCC CN1Cc1cccc(CCN)c 1	47531251	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
732	Cc1ccsc1CN(CCN(C)C)C(CN)=O	47645371	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
733	Cc1cnc(N)nc1NCC[C@@H]1C[C@H]2 C[C@@H]1C=C2	47913504	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
734	CCOc1cc(CNCCc2cc cc(c2)OC)ccc1OC	4964-4425	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
735	C(CNCc1ccc2ccccc2 c1)c1c[nH]c2cccc12	4964-5069	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
736	C(c1ccc(cc1)F)NCc1 ccc2c(c1)OCO2	4964-5172	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
737	[O-][N+](c(cc(cc1) [As](c(cc2)cc([N+] ([O-])=O)c2O) (O)=O)c1O)=O	49852	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
738	Cc1nc(SC)nc(N2CC2)c1Br	50199	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
739	CCOC(c1c2c(nc3ccc cc3n2)n(c2cccc(c2) [C1])c1N)=O	5122-1932	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
740	C1CCC(CCNc2c(NS (c3ccccc3) (=O)=O)nc3ccccc3n2)=CC1	5122-2566	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
741	CCOC(c1cnc2c(C)cc (C)cc2c1NCC(C)O)= O	5174-4431	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	1
742	C(Cc1nc2NC(=CC(c 3ccc(cc3) [Cl])n2n1)c1ccccc1) CO	5228-4308	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	1
743	C(CCN=Cc1ccccc1N)CN=Cc1ccccc1N	5233844	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
744	COclccc(ccl)OCC(C N1CCN(CCl)clcccc cl)O.[Cl].[Cl]	5257916	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	1
745	CC(C) (C)NCC(Nc1c2CCC Cc2nc2CCCc12)=O. C(O)=O.C(C(O)=O) (O)=O	5284047	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
746	CCCCOC(C1=C(N) OC2CC(C) (C)CC(C=2C12C(Nc 1ccccc12)=O)=O)=O	5587-0160	AKTIP	G-quadruplex	GGGGUGGGGCGGGGG	1
747	C=CCC(CC=C) (c1ccc(cc1)C(CC=C) (CC=C)N)N	5654685	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	1
748	CC(c1cccc1)NC(CC (C)=C)c1ccco1	5689-0049	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
749	CC(=C)CC(c1ccc(cc	5689-0111	AKTIP	G-quadruplex	GGGGUGGGGCGGGGG	1

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	1)OC)NCc1ccco1					
750	Cc1ccc(c(c1) [Cl])OCCNC(C) (C)C.[Cl]	5729988	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	1
751	CCCCNCCOc1ccccc 1F.C(C(O)=O)(O)=O	5734218	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	1
752	CCCOc1ccccc1Nc1c 2cccc2nc(C(=O)OC C)n1	5847-0398	AKTIP	G-quadruplex	GGGGUGGGGCGGGGG	1
753	clcc(ccclclcn2ccsc2 n1)N	5968142	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
754	CC(C)CN1CCC(CC1)NCCNc1cencc1C	60244866	AKTIP	G-quadruplex	GGGGUGGGGCGGGGG	1
755	CCN1CCN(CC1)CC(COc1ccc(CC=C)cc1 OC)O.[Cl].[Cl]	6043920	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	1
756	Cc1cc(N)n(c2ccc(c(c 2)S(O) (=O)=O)Oc2cccc2)n 1	6075116	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	1
757	C1CCCN(CC1)CC(C Oc1ccccc1)O	6228-0261	AKTIP	G-quadruplex	GGGGUGGGGCGGGGG	1
758	O=C(c(cc1)cc(C(Nc(cc2)ccc2C2=NCCN2)=O)c1Cl)Nc(cc1)ccc 1C1=NCCN1	67436	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
759	O=C(C(C(C=C(c1ccc cc1)O1)=O)C1=O)c1 ccccc1	6844	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	1
760	Cc1ccc(c1C)NC(CS c1nnc(C(c2cccc2)O) n1c1cccc1)=O	6960143	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
761	C1CCN(CC1)CC(Cn 1ccc2cccc12)O	7230-0020	AKTIP	G-quadruplex	GGGGUGGGGCGGGGG	1
762	Cc1cc(nc(N)n1)Oc1c cc(cc1)C(=O)OC	7796-0682	AKTIP	G-quadruplex	GGGGUGGGGCGGGGGGGG	1
763	C(CN)CN1CCN(CC1)c1ccccc1	7974015	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
764	C(C1C(C2=C(NC(N C2=O)=O)OC=1N)c1 ccccc1)#N	8002-4077	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
765	Cc1ccc(cc1C)Nc1nc(cs1)c1ccc(c(c1)F)OC	8005-2731	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
766	Cc1ccc(cc1C)Nc1nc(cs1)c1ccccc1	8005-2768	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
767	Cc1ccc(C)c(c1)c1csc (Nc2cccc2OC)n1	8006-1580	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
768	Cc1ccc(cc1)C1C(C# N)=C(N)Oc2ccc3ccc cc3c12	8008-9298	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
769	CC1=C(C(C(C#N)=C (N)O1)c1ccccc1)n1c 2ccccc2nn1	8009-2467	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
770	COclccc(c(c1)NC(C Sc1nc2ccc(cc2s1)N)= O)OC	8009-2885	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	1
771	C1CCc2c(C1)c(C(c1 ccccc1)=O)c(N)s2	8010-1935	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	1
772	CN1C(c2c(ncn2CCN)N(C)C1=O)=O	8012-1255	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	1
773	CC1=CC(N(C)C(N1	8012-3983	AKTIP	G-quadruplex	GGGGUGGGGCGGGGG	1

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	CCCCCCNCCO)=O) =O					
774	Cc1cc(C)c2c(c1)c(C CN)c(C)[nH]2	8012-5803	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
775	Cc1ccc(C)c2c1c(CC N)c(C)[nH]2	8012-5804	AKTIP	G-quadruplex	GGGGUGGGGCGGGGG	1
776	Cc1c(CCNCc2c(cc(c c2OC)OC)OC)oC)c2cc(c cc2[nH]1)OC	8013-0022	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	1
777	CCCCe1nc(CNCCe2 e3cc(cee3[nH]e2C)O C)c[nH]1	8013-0624	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	1
778	Cc1c(CCNCc2ccc(C #N)cc2)c2cc(ccc2[nH]1)OC	8013-2954	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	1
779	CN1CCC(CC1) (CN)N1CCN(CC1)c1 ccccc1	8017-3009	AKTIP	G-quadruplex	GGGGUGGGGCGGGGG	1
780	C=CCOc1ccc(cc1)C1 C(C#N)=C(N)OC2= C1C(c1ccccc1C2=O) =O	8017-5263	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	1
781	COc1ccc(CCNc2nc(c s2)c2ccs2)cc1OC	8018-0995	AKTIP	G-quadruplex	GGGGUGGGGCGGGGG	1
782	CC(C)C1(CCNCc2cc c(c(c2)OC)OC)CCO C(C)(C)C1	8018-1267	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	1
783	CC(C)C1(CCNCc2cc cc3c2OCO3)CCOC(C)(C)C1	8018-1268	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	1
784	Cc1c(C#N)c(N)n(CC Cn2ccnc2)c1C	8018-7492	AKTIP	G-quadruplex	GGGGUGGGGCGGGGGGGGG	1
785	Cc1c(c(N)n(CCOC)c 1C)S(c1ccc(cc1)[C1]) (=O)=O	8019-0265	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	1
786	Cc1c(c(N)n(CCCN(C)C)c1C)S(c1ccc(cc1) F)(=O)=O	8019-0616	AKTIP	G-quadruplex	GGGGUGGGGCGGGGG	1
787	CN1CCC(CC1)Oc1c cc(cc1)N	8019-4291	AKTIP	G-quadruplex	GGGGUGGGGCGGGGG	1
788	c1cc(N)nc2c1ccc(n2) O	8019-7722	AKTIP	G-quadruplex	GGGGUGGGGCGGGGGGGG	1
789	COc1c(cc2c(c1OC)O CO2)C1C(C#N)=C(N)OC2CCCC(C1=2) =O	8019-9373	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
790	CCNCc1cc(CC=C)c(c(c1)OC)OCC	8020-2907	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
791	CN1CCCc2ccc(cc12)	8020-4281	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
792	OC(/C=C\ C(Nc1nccs1)=O)=O	80807	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
793	C1C(NCC2)N3C2NC CC3NC1	81462	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
794	C1CCN(C1)c1ccccc1 NC1c2cccc2S(N=1) (=O)=O	8209-0032	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
795	CCCCNc1c(C#N)c2 CC(C) (C)OCc2c(c2cccc2) n1	8640-0572	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	1

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796	CCNCC#CCOc1ccc(cc1)[Br]	9126666	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
797	CC(e1ece(ec1)e1ece(CNCCe2e[nH]e3ecee e23)o1)O.[CI]	9135919	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	1
798	C1CCC(CCNCe2ece cn2)=CC1.[Cl]	9137483	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
799	O=C(C(C(N1)=O)=C c2cc3cccc3cc2)NC1 =O	95909	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGGG	1
800	CCN(CCCC/C1=N\ O)CCCC/C1=N\O	96491	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
801	Cc1cccc(c1)NCc1nc2 cccc2n1C	C147-0043	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
802	C1COc2cc(ccc2O1)N c1c(c2ccco2)nc2ccc(cn12)[C1]	C177-0188	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	1
803	CC1CCN(CC1)c1nc(c(C(=O)OC)s1)N	C201-1740	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
804	Cc1cc(Nc2cccc2)nc 2cc(ccc12)O	C614-0105	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
805	CCOC(C1CCN(CC1) C1=C(C(C1=O)=O)N CCCN1CCCCC1)=O	C667-0368	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	1
806	C1CCCN(CC1)CCC Nc1nc2cccc2c2nc(c 3cccc3)nn12	C736-0159	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	1
807	CCOC(N1CCN(CC1) C1=C(C(C1=O)=O)N CCCN1CCCCC1)= O	C748-1353	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
808	Cc1c(CCC(Nc2ccc(c c2) [C1])=O)c(C)n2c(n1) nc(CN)n2	C908-0503	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
809	Cc1c(CCC(Nc2ccc(C N3CCCCC3)cc2)=O) c(C)n2c(n1)nc(CN)n 2	C908-0509	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
810	CCc1cccc(c1)NC(CC c1c(C)nc2nc(CN)nn2 c1C)=O	C908-0512	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
811	Cc1ccc(c(C)c1)NC(C Cc1c(C)nc2nc(CN)nn 2c1C)=O	C908-0520	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	1
812	Cc1c(CCC(Nc2cccc(c2) [Br])=O)c(C)n2c(n1) nc(CN)n2	C908-0523	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
813	Cc1c(CCC(NCC2CC N(CC2)Cc2cccc2F) =O)c(C)n2c(n1)nc(C N)n2	C908-0547	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
814	Cc1c(CCC(NCC2CC N(CC2)Cc2cccc2O C)=O)c(C)n2c(n1)nc(CN)n2	C908-0549	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
815	Cc1c(CCC(NCC2CC N(CC2)Cc2ccc(cc2)F)=O)c(C)n2c(n1)nc(C N)n2	C908-0552	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	1
816	C(CNc1c(nc(c2ccccc 2F)o1)S(c1ccccc1)	D072-1643	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1

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	(=O)=O)Cn1ccnc1					
817	C=CCNc1cc(c2ccccc 2)nc2nncn12	D150-0143	AKTIP	G-quadruplex	GGGGUGGGGCGGGGG	1
818	CCOC(c1cccc(c1)NC 1c2cccc2S(N=1) (=O)=O)=O	D257-0714	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	1
819	CCN(CC)CCCNCC1 CCOC(C)(C)C1	D324-0108	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
820	Cc1cc(NC2CCCC2)n2c(cc(c3cc(c(c3)OC))n2)n1	D393-0160	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
821	Cc1cccc(c1C)N1CC N(CC1)CC(c1c[nH]c 2ccccc12)O	D424-0008	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	1
822	CC1(C)CC(CCNCc2 ccc3c(c2)OCO3) (CCO1)c1cccc1OC	D442-0097	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	1
823	COc1ccc(Cc2nc3cccc c3n2CC(COc2ccccc2)O)cc1	D510-0832	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
824	CCC(CO)NCc1ccc(c(c1)OC)OCc1ccc2c(c1)N(C)C(N2C)=O	D666-0065	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	1
825	CCOC(c1cnc2c(c3cc c(cc3) [Br])c(C)nn2c1N)=O	D718-0691	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	1
826	CCc1ccc(cc1)NC1C(C)=C(c2ccc(cc2)OC) S(N=1)(=O)=O	E013-1594	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	1
827	Cc1cc(ccc1[Br])NC1 =C(C(C1=O)=O)c1cc c(cc1)[Cl]	E786-0118	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
828	C(c1ccccc1)N=C(N) NC(c1c(N)nc(c(n1) [C1])N)=O	NCGC00015147- 09	AKTIP	G-quadruplex	GGGGUGGGGCGGGGG	1
829	CCN1C=C(C(O)=O) C(c2cc(c(nc12)N1CC NCC1)F)=O	NCGC00016927- 10	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	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	GGGGUGGGGCGGGGG	1
831	C(CCOclecc(cc1)C(Nc1cccc2C(C=C(c3n n[nH]n3)Oc12)=O)= O)Cc1cccc1	NCGC00181765- 01	AKTIP	G-quadruplex	GGGGUGGGGCGGGGG	1
832	C1CNCCC1n1cc(en1)c1cnc2cccc(c3cc(c(CN4CCOCC4)c(c3)F)F)c2n1	NCGC00263202- 01	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	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	GGGGUGGGGCGGGGG	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	GGGGUGGGGGGGGGGGG	1
835	COc1cc(C[C@@H] (CO)[C@@H] (Cc2ccc(c(c2)OC)O) CO)ccc1O	NCGC00346838- 01	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1

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836	CC(C)n1cnc2c(Nc3c ccc(c3)NC(C=C)=O) nc(NC3CCC(CC3)N(C)C)nc12	NCGC00346964- 01	AKTIP	G-quadruplex	GGGGUGGGGGGGGGGGG	1
837	CC(c1ccc2c(c1)OCC O2)N[C@H]1C[C@ H]1c1ccccc1	NCGC00347951- 01	AKTIP	G-quadruplex	GGGGUGGGGCGGGG	1
838	CCN(CC)CCOC(c1c cc2c(c1)sc(NC(c1cc (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 Oc1cccc1CC=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(CCCe1ncen1C)c 1c2CCNCc2nc(c2cen cc2)n1	12244291	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	1
844	CN(CC(N1C[C@@H](CN2CCCCC2) [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)c1c2cccc2nc(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 Cc2cccc12	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

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)c1cnc2cccc2n1	17587941	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	1
863	NC(NCCS(Nc(cc1) cce1Nc1c(ccec2)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] (CN3CCCCC3) [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	Cclenc(nc1N(C)C)N 1CCN(CC1)Cclen(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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	CN(Cc2ccc(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(c2cccc2C#N)o1	31727519	EWSR1	G-quadruplex	GGGCAGGGGAAGAGGGGG	1
898	CNCC(N1CCn2c(C1)cc(CN1CCN(CC1)c1ncccn1)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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	c12					
901	C(/C=C/ CSc1nccc1)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)[C1])=O)N	34469220	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	1
913	Cc1c2c(N[C@H] (Cc3cccc3)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	Cc1c2cccc2n(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	COc1ccc(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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	(F)F)cc1OC					
922	COc1ccc(CNCc2cc(c cc2OC)[Br])cc1	3702-1485	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	1
923	COclcccc(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(c1cence1)NCc1ccc 2c(c1)OCO2	3702-1584	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	1
926	CCC(CO)NCC(CN1c 2cccc2Sc2cccc12) O	3746-0114	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	1
927	CC(C1COc2cccc2O 1)NCc1cccc1	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(CNCe2ccccc 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(Nc3cccc3[C1])=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 c2cccc2nc(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 c3CCCc3sc2ncn1	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]c2cccc12	4964-4666	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	1
941	COc1cccc1CCNCc1 ccc(cc1)C(F)(F)F	4964-4708	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	1
942	CSc1ccc(CNCCc2c[n H]c3cccc23)cc1	4964-4965	EWSR1	G-quadruplex	GGGCAGGGGAAGAGGGGG	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	GGGCAGGGGAAGAGGGGG	1
946	CCOC(c1c2c(nc3ccc cc3n2)n(c2ccc(c2)	5122-1932	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	1

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	[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(N1c2cccc2Sc2 ccc(cc12)C(F) (F)F)=O.[Cl].[Cl]	5216181	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	1
951	CCCC1c(CCC)c(c2 cccc2n1)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	COclccc(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	Cc1ccc(C)c1OCC(C N(c1cccc1OC)S(c1c ccc1)(=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	COclecc(cc1CN1CC C(CC1)N1CCN(CC1)CCO)[Br]	5607-0223	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	1
965	CCn1c2cccc2c2cc(C N3CCC(CC3)N3CC N(CC3)CCO)ccc12	5607-0247	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	1
966	CC1CC2(CC(C) (c3csc(Nc4cccc4C)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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	(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(CCCC1C(C(CS1)N)N)=O.[Br]. [Br]	5728434	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	1
971	CCCCNCCOcleece 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)clnc(c2cccc2 n1)NCclcn[nH]clclc ccsl	58789773	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	1
977	C(CCO)CN(Cc1cccc c1)c1c2cccc2nc(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	clcc(ccclclcn2ccsc2 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	C1CCCCc2c(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	Cc1c2cccc2n(CC(C NCCCO)O)c1C.C(C(O)=O)(O)=O	6401887	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	1
986	C1CN(CCN1CC(CN 1c2cccc2Sc2cccc1 2)O)Cc1ccccc1.C(C(O)=O)(O)=O	6409737	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	1
987	C1Cc2ccc(cc2C1)NC (CCN1CCN(CC1)CC O)=O.[C1]	6544961	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	1
988	O=C(c(cc1)cc(C(Nc(cc2)ccc2C2=NCCN2	67436	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
)=O)c1Cl)Nc(cc1)ccc 1C1=NCCN1					
989	C1CCN(CC1)CC(Cn 1ccc2cccc12)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[C1])NC1c2cccc2S (N=1)(=O)=O	7641-0012	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	1
993	CCOe1eccee1CNe1n cc(e2ecce(e2) [Cl])n1C	7756-0249	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	1
994	Cn1e(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)[C1]	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	Cn1e(cnc1NCc1c(ccc c1[Cl])F)c1ccc(cc1)O C	7756-0741	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	1
1003	CCOclccc(ccl)clcnc (NCc2cccc2OC)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) [C1].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)c1cccc1	7974015	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	1
1008	COclecc(c(c1)NC1C CN(CC1)Cclecc(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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	(C)CC2=O)OC=1N)c 1ccc(cc1)[C1])=O					
1011	Ce1ece(ce1C)Ne1ne(es1)e1ece(ce1)S(N1C COCC1)(=O)=O	8004-5090	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	1
1012	C1COCCN1S(c1ccc(cc1)c1csc(Nc2ccc(cc2)[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(Nc1cccc1 2)=O)=O	8006-8591	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	1
1017	CC1=C(C(=O)OCc2c ccc2)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)C2CCCC2)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) c2cccc12)=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	CCOclccc(CC(C2=C (CCCC2=O)NC(C)C(O)=O)=O)cclOCC	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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	(F)F)c2cccc12)=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(c1ccc(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)c2ccs2)cc1OC	8018-0995	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	1
1034	CC(C)C(CCNCe1ece (ce1)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 c2cccc2nc1CO	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(clen[nH]clclccc(c cl)[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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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.[CI]	9135919	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	1
1057	CSc1ccc(cc1)OCCN	9254473	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	1
1058	CCN1CCC1CNCc1 cccc(c1)OCc1ccc(cc1)[C1]	9312203	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	1
1059	O=C(C(C(N1)=O)=C c2cc3cccc3cc2)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(c1nc2cccc2n1CC Oc1cccc1)Nc1ccccc 1	C147-0115	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	1
1063	CCOC(N1CCC(CC1) Nc1nc2cccc2c2nnc(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) [C1])=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 Nc1nc2cccc2c2nc(c 3ccccc3)nn12	C736-0159	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	1
1069	CCOC(N1CCN(CC1) C1=C(C(C1=O)=O)N CCCN1CCCCC1)= 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)Cc2cccc2F) =O)c(C)n2c(n1)nc(C N)n2	C908-0547	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	1
1076	Cc1c(CCC(NCC2CC N(CC2)Cc2cccc2O	C908-0549	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	1

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	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)[C1])n2	D043-0239	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	1
1079	Cn1c2cccc2nc1CN	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)) [C1])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(Cc2cccc2) C(c2c1nc(NCCN)n2 C)=O)=O	D114-0037	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	1
1087	CCe1c(C)ne2nnen2e 1NCe1cec(ce1)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(c2cccc2)ncn1)= O	D278-0165	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	1
1090	CSc1nc2CCc2c(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) [C1]	D454-0510	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	1

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1099	CCCNc1cc(C(C)C)nc 2nc(c3cccnc3)nn12	D494-0272	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	1
1100	Cc1cc(NCC(N2CCN(CC2)c2cccc2)=O)n2 c(n1)nc(c1cccnc1)n2	D494-0459	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	1
1101	Cc1cc(C)cc(c1)OCC(Cn1c2cccc2nc1C)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(c2cccc2)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(NCCc2cccc2)=NS1(=O)=O	E013-2935	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	1
1109	Cc1ccc(C)c(c1)Nc1n c2cccc2c2nnc(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) [C1])CCN=C(N)N=C (N)Nc1ccc(cc1)[C1]	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(=0) (=0)OCCCCOS(C) (=0)=0	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] (CCN)C(C[C@@H] (CO)NC([C@@H] (CCN)NC([C@@H] (CCN)NC([C@@H] (CCC)NC([C@H] (Cc2cccc2)NC([C@ H] (CCN)NC1=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

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	CCCCCCN)nc12)NC c1cccc1	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) [C1])=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 1c2c3CCCc3sc2ncn 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 Oc1cccc1CC=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(CCCe1ncen1C)c 1c2CCNCc2nc(c2cen cc2)n1	12244291	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	1
1129	CN(CC(N1C[C@@H](CN2CCCCC2) [C@H] (C1)CO)=O)Cc1cccc c1F	12553104	EWSRI	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)c1c2cccc2nc(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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	C2CCCN2C)n1					
1136	Cclccc(cn1)NC([C@ H]1C[C@H] (CNC1)C(NCCclc[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 Cc2cccc12	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(CCe1en[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)c1cnc2cccc2n1	17587941	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	1
1148	NC(NCCCS(Nc(cc1) ccc1Nc1c(cccc2)c2nc 2cc([N+] ([O-])=O)ccc12) (=O)=O)=N.C1	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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	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	Celenc(nc1N(C)C)N 1CCN(CC1)Celen(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	GGGCAGGGGAAGAGGGGG	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	GGGCAGGGGAAGAGGGGG	1
1179	COc1ccc(CCNCc2cc	3169-1283	EWSR1	G-quadruplex	GGGCAGGGGAAGAGGGG	1

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	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(c2cccc2C#N)o1	31727519	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	1
1183	CNCC(N1CCn2c(C1)cc(CN1CCN(CC1)clncccn1)n2)=O	31916172	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	1
1184	CN(C)CCNc1nc2c(C (N(C)C(N2C)=O)=O) n1Cc1cccc1[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	Cc1cc2cc(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#CCO)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]10)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)Ce1ece (cc1)e1ecec(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	GGGCAGGGGAAGAGGGGG	1
1195	COc1cc(CNC2CCCc 3ccccc23)cc(c1OC)O C	3381-1370	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	1
1196	CCclcnc(N)nc1NCC CNc1ccc(C)cn1	33868270	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	1
1197	C(c1c[nH]cn1) [C@@H] (C(N1CCN(CC1)Cc1 ccc(cc1)[C1])=O)N	34469220	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	1
1198	Cc1c2c(N[C@H] (Cc3cccc3)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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	cccc1)Nc1nccc(N)n1					
1200	Cc1c2cccc2n(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	COclccc(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(c1cencc1)NCc1ccc 2c(c1)OCO2	3702-1584	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	1
1211	CCC(CO)NCC(CN1c 2cccc2Sc2cccc12) O	3746-0114	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	1
1212	CC(C1COc2cccc2O 1)NCc1cccc1	3875-0321	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	1
1213	Cc1ccc(cc1)S(N(CC(CN1CCCC1)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(CNCc2cccc 2)c2cccc12	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(Nc3cccc3[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 c2cccc2nc(CCN)n1	47488116	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	1
1221	Cc1ccsc1CN(CCN(C)C)C(CN)=O	47645371	EWSR1	G-quadruplex	GGGCAGGGGAAGAGGGGG	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	GGGCAGGGGAAGAGGGGG	1

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	cc(c2)OC)ccc1OC					
1225	C(CNCc1cccnc1)c1c[nH]c2cccc12	4964-4666	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	1
1226	COcleccc1CCNCc1 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) [C1])c1N)=O	5122-1932	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	1
1232	C1CCC(CCNc2c(NS (c3ccccc3) (=O)=O)nc3ccccc3n2)=CC1	5122-2566	EWSRI	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(N1c2cccc2Sc2 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.[C1].[C1]	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	GGGCAGGGGAAGAGGGGG	1

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	5587-0160	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	1
1248	COc1cccc(CN2CCC(CC2)N2CCN(CC2)C CO)c1	5607-0221	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	1
1249	COclecc(cc1CN1CC C(CC1)N1CCN(CC1)CCO)[Br]	5607-0223	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	1
1250	CCn1c2cccc2c2cc(C N3CCC(CC3)N3CC N(CC3)CCO)ccc12	5607-0247	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	1
1251	CC1CC2(CC(C) (c3csc(Nc4cccc4C)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(CCCC1C(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)clnc(c2cccc2 nl)NCclcn[nH]clclc ccsl	58789773	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	1
1262	C(CCO)CN(Ce1ecce e1)e1e2ecce2ne(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)NCCNc1cencc1C	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	C1CCCCc2c(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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	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	Cc1c2cccc2n(CC(C NCCCO)O)c1C.C(C(O)=O)(O)=O	6401887	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	1
1271	C1CN(CCN1CC(CN 1c2cccc2Sc2cccc1 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 1ccc2cccc12)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[C1])NC1c2cccc2S (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	CCOe1ecc(CNe2ncc(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	GGGCAGGGGAAGAGGGGG	1
1285	Cn1c(cnc1NCc1cccc c1F)c1cccc(c1)[Br]	7756-0646	EWSR1	G-quadruplex	GGGCAGGGGAAGAGGGGG	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 (NCc2cccc2OC)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	GGGCAGGGGAAGAGGGGG	1

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	NCCN1CCOCC1) [CI].C(C(O)=O) (O)=O					
1291	C(CCOcleccc(c1)C(F) (F)F)CNCCN1CCOC C1.C(C(O)=O)(O)=O	7970451	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	1
1292	C(CN)CN1CCN(CC1)c1cccc1	7974015	EWSR1	G-quadruplex	GGGCAGGGGAAGAGGGGG	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)[C1])=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(cc2)[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	GGGCAGGGGAAGAGGGG	1
1301	CCOC(C1=C(N)OC(C)=C(C(=O)OCc2ccc cc2)C12C(Nc1cccc1 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(=0)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	GGGCAGGGGAAGAGGGGG	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) [C1])n1)OC(=C(C#N) C21C(N(CC(=O)OC) c2cccc12)=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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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(c3cccc3)nc1 2)c1cccc1	8014-9053	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	1
1313	CCOclccc(CC(C2=C (CCCC2=O)NC(C)C(O)=O)=O)cclOCC	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)c2cccc12) =O	8017-5304	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	1
1317	C(c1ccc(c1)F)N1C(C2(C(C#N)=C(N)N(C3COC(C2=3)=O)c2 ccc(cc2)F)c2cccc12) =O	8017-5320	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	1
1318	COc1ccc(CCNc2nc(c s2)c2ccs2)cc1OC	8018-0995	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	1
1319	CC(C)C(CCNCe1ecc (ce1)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 c2cccc2nc1CO	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	COe1cc(cce1OC1CC CC1)C1CC(Ne2c1sc(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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	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(clcn[nH]clclccc(c cl)[Cl])N	8019-9983	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	1
1335	[H]N(CCNCCO)Cc1 cc(c(c(1) [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	CCN1CCC1CNCc1 cccc(c1)OCc1ccc(cc1)[C1]	9312203	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	1
1344	O=C(C(C(N1)=O)=C c2cc3cccc3cc2)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(c1nc2cccc2n1CC Oc1cccc1)Nc1ccccc	C147-0115	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	1
1348	CCOC(N1CCC(CC1) Nc1nc2cccc2c2nnc(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 (c4ccc(c4) [C1])=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 Nc1nc2cccc2c2nc(c 3cccc3)nn12	C736-0159	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	1
1354	CCOC(N1CCN(CC1) C1=C(C(C1=0)=0)N CCCN1CCCCC1)= 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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	CCN1CCCCCC1)=O					
1356	COc1ccc(CCNCc2cc c(C(O)=O)s2)cc1OC	C863-0014	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	1
1357	Ce1e(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	Cc1ccc(c1)NC(CCc 1c(C)nc2nc(CN)nn2c 1C)=O	C908-0492	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	1
1360	Cc1c(CCC(NCC2CC N(CC2)Cc2cccc2F) =O)c(C)n2c(n1)nc(C N)n2	C908-0547	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	1
1361	Cc1c(CCC(NCC2CC N(CC2)Cc2cccc2O 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(NCc1ccc(c1)[Cl])n2	D043-0239	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	1
1364	Cn1c2cccc2nc1CN	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)) [C1])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 Cn2e3C1CCCc3c1cc (C)ccc12)O	D090-0003	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	1
1371	CN1C(N(Cc2cccc2) C(c2c1nc(NCCN)n2 C)=O)=O	D114-0037	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	1
1372	CCe1c(C)ne2nnen2e 1NCe1cec(ce1)OC	D150-0320	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	1
1373	c1ccc(cc1)c1cc(Nc2c cc(cc2)C(O)=O)ncn1	D278-0137	EWSR1	G-quadruplex	GGGCAGGGGAAGAGGGG	1
1374	CCOC(c1ccc(c1)Nc 1cc(c2cccc2)ncn1)= O	D278-0165	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	1
1375	CSc1nc2CCc2c(Nc 2cccc(c2)O)n1	D278-0388	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	1
1376	CN1C(N(C)c2cc(CO c3ccc(CNCc4ccnc4) cc3OC)ccc12)=O	D300-0082	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	1
1377	CCN(CC)CCCNCC1 CCOC(C)(C)C1	D324-0108	EWSR1	G-quadruplex	GGGCAGGGGAAGAGGGGG	1

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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) [C1]	D454-0510	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	1
1384	CCCNc1cc(C(C)C)nc 2nc(c3ccnc3)nn12	D494-0272	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	1
1385	Cc1cc(NCC(N2CCN(CC2)c2cccc2)=O)n2 c(n1)nc(c1ccnc1)n2	D494-0459	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	1
1386	Cc1cc(C)cc(c1)OCC(Cn1c2cccc2nc1C)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(c2cccc2)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) (=0)=0)=0	E013-0432	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	1
1393	CC(C)c1ccc(cc1)C1= C(C)C(NCCc2cccc2)=NS1(=O)=O	E013-2935	EWSR1	G-quadruplex	GGGGCAGGGGAAGAGGGGG	1
1394	Cc1ccc(C)c(c1)Nc1n c2cccc2c2nnc(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) [CI])CCN=C(N)N=C (N)Nc1ccc(cc1)[CI]	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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	(CCN)C(N[C@@H]1 CCNC(C([C@@H] (C)O)NC([C@@H] (CCN)NC([C@@H] (CCN)NC([C@H] (CCC)C)NC([C@H] (Cc2cccc2)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	Cclcc(ccclOclccn2c (c1)ncn2)Nclc2cc(cc c2ncn1)clccc(CNCC S(C)(=O)=O)ol	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) [C1])=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	UGUGGGAGGGGCGGUCUG GG	1
1409	CN(CCCc1nccn1C)c 1c2CCNCc2nc(c2ccn cc2)n1	12244291	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	1
1410	Cc1c(CCN(C)c2c3C CNCc3nc(n2)N(C)C) scn1	12498605	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG 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(c2cenc c2)n1	14924624	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	1
1413	CCc1nnc(NCC2CCC CCN2)o1	16631339	NRAS	G-quadruplex	UGUGGGAGGGGCGGUCUG GG	1
1414	COclccc(cc1)NC1CS (C=C1)(=O)=O	1683-5965	NRAS	G-quadruplex	UGUGGGAGGGGCGGGUCUG GG	1
1415	C(CN)c1nc(c2cccc2 n1)NCc1cccc1n1cnc n1	17428082	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	1

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1416	CCn1cncc1CNc1c2C CNCc2nc(c2ccncc2)n	18384397	NRAS	G-quadruplex	UGUGGGAGGGGCGGUCUG GG	1
1417	C1CN(CCC12e1ecce c1[C@H] ([C@@H]2O)N)Ce1 c[nH]ne1e1eccce1	18741551	NRAS	G-quadruplex	UGUGGGAGGGGCGGUCUG GG	1
1418	C(CN)C1CN(CCO1) c1c2CCNCc2nc(c2cc ccc2)n1	19916102	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	1
1419	Cn1c2c(cn1)c(nc(c1c cncc1)n2)N1CCCC2(CCNCC2)CC1	20352833	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	1
1420	CC1CC2(C)CC(C)C1 (CO)CO2	2190-0577	NRAS	G-quadruplex	UGUGGGAGGGGCGGUCUG GG	1
1421	C1CCCN(CC1)C[C @@H]1CN(C[C@@ H]1CO)C(c1cc(N) [nH]n1)=O	22664850	NRAS	G-quadruplex	UGUGGGAGGGGCGGUCUG GG	1
1422	C1CCN(CC1)CC1(C CN(Cc2cccc(CCN)c2)C1)O	22896979	NRAS	G-quadruplex	UGUGGGAGGGGCGGUCUG GG	1
1423	CCOC(C1=C(C)OC(=C(C(=O)OCc2cccc 2)C12C(Nc1ccccc12) =O)N)=O	2435-0117	NRAS	G-quadruplex	UGUGGGAGGGGCGGUCUG 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	UGUGGGAGGGCGGGUCUG GG	1
1425	CCOc1ccc(CNCCc2c cc(cc2)[C1])cc1	2910-0651	NRAS	G-quadruplex	UGUGGGAGGGGCGGUCUG 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	UGUGGGAGGGCGGGUCUG GG	1
1428	COc1ccc(c(CNc2ccc(cc2)[Br])c1)OC	2910-1869	NRAS	G-quadruplex	UGUGGGAGGGGCGGGUCUG GG	1
1429	COcleece1CCNCc1 cccc(c1)C(F)(F)F	2910-1902	NRAS	G-quadruplex	UGUGGGAGGGGCGGUCUG GG	1
1430	COclccc(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	UGUGGGAGGGCGGGUCUG 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	UGUGGGAGGGGCGGUCUG GG	1
1434	C1CCN(CC1)CCN1 C(=N)N(CCO)c2cccc c12	3260-0393	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	1
1435	CCOc1cc(CNCCc2cc c(cc2)F)ccc1OC	3381-1809	NRAS	G-quadruplex	UGUGGGAGGGGCGGUCUG GG	1
1436	C1CC(N(C1)CCC1C CN(CC1)Cc1cccc(C CN)c1)=O	34485551	NRAS	G-quadruplex	UGUGGGAGGGGCGGUCUG 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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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	UGUGGGAGGGCGGGUCUG GG	1
1440	COc1cccc(CCNCc2c cc(cc2)C(F)(F)F)c1	3702-1570	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	1
1441	COc1cc(CNCc2ccc(c (c2) [Br])OC)cc(c1)OC	3702-1693	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	1
1442	COc1ccc(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	UGUGGGAGGGGCGGUCUG GG	1
1444	CC1=CC(C)=NC(N1 CCNC1CCC2(CC1) CCNCC2)=O	41200051	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	1
1445	C1CN(CCN(C1)c1cc c(cc1)F)C([C@@H] (Cc1cccc1)N)=O	41213525	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	1
1446	Celencee1NCCn1cen elelce2CNCCn2n1	41482306	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	1
1447	COC(c1cccc(c1)Nc1c 2cccc2nc(c2cccc2 O)n1)=O	4229-0068	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	1
1448	COc1ccc(c(c1)OC)c1 csc(NCC=C)n1	4640-0152	NRAS	G-quadruplex	UGUGGGAGGGGCGGGUCUG GG	1
1449	C(CNc1cccnc1)CNc1 c2cccc2nc(CCN)n1	47488116	NRAS	G-quadruplex	UGUGGGAGGGGCGGGUCUG GG	1
1450	CCOc1cc(CNCCc2cc cc(c2)OC)ccc1OC	4964-4425	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG 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	UGUGGGAGGGCGGGUCUG GG	1
1453	CC(=C)CC(c1ccc(cc 1)OC)NCc1ccco1	5689-0111	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	1
1454	COc1cc(CNc2nccs2) cc(c1OCc1ccc(cc1)F) [Br]	5868-0785	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	1
1455	Cc1c2c(nc(CCN)nc2s c1C)N(CCN(C)C)Cc 1cccc1	59025931	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	1
1456	C1CCN(C1)c1ccc(cc 1[C1])NC1c2cccc2S (N=1)(=O)=O	7641-0012	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	1
1457	CC(C) (C)NC(CSc1c(C#N)c c(C#N)c(N)n1)=O	8001-8198	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	1
1458	CCOC(C1=C(C)OC(=C(C(=0)OCC)C12 C(Nc1cccc12)=O)N)=O	8003-0370	NRAS	G-quadruplex	UGUGGGAGGGGCGGGUCUG GG	1
1459	CCN(CC)S(c1ccc(cc 1)c1csc(Nc2cccc2O C)n1)(=O)=O	8004-5097	NRAS	G-quadruplex	UGUGGGAGGGGCGGUCUG GG	1
1460	CC1=C(C(C(C#N)=C (N)O1)c1ccccc1)C(C)=O	8004-7491	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	1
1461	Cc1ccc(cc1C)Nc1nc(cs1)c1ccccc1	8005-2768	NRAS	G-quadruplex	UGUGGGAGGGGCGGUCUG GG	1

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1462	CN1C2=C(C(C(C#N) =C(N)O2)c2ccc(cc2) [C1])C(N(C)C1=O)= O	8006-4483	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	1
1463	C(c1cccc1)c1nnc(N)	8008-6271	NRAS	G-quadruplex	UGUGGGAGGGGCGGUCUG GG	1
1464	Cc1ccc(cc1)C1C(C# N)=C(N)Oc2ccc3ccc cc3c12	8008-9298	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	1
1465	Cc1ccc(cc1)C1C(C# N)=C(N)Oc2c1c(C(F)(F)F)n[nH]2	8009-1517	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	1
1466	[H]Nc1nnc(COc2ccc(cc2)C2CCCC2)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	UGUGGGAGGGGCGGUCUG 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	UGUGGGAGGGCGGGUCUG GG	1
1469	CC1=CC(N(C)C(N1 CCCCCCNCCO)=O) =O	8012-3983	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	1
1470	Cc1cc(C)c2c(c1)c(C CN)c(C)[nH]2	8012-5803	NRAS	G-quadruplex	UGUGGGAGGGGCGGUCUG GG	1
1471	Cc1c(CCNCc2ccc(cc 2F)F)c2cccc2[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	UGUGGGAGGGCGGGUCUG GG	1
1473	CCN1C(c2ccc(CN)c3 cccc1c23)=O	8016-6735	NRAS	G-quadruplex	UGUGGGAGGGGCGGUCUG GG	1
1474	COc1ccc(CCNc2nc(c s2)c2ccs2)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	UGUGGGAGGGCGGGUCUG GG	1
1476	CC(C)C1(CCNCc2cc c(cc2)OC)CCOC(C) (C)C1	8018-1266	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	1
1477	CC(C)C1(CCNCc2cc cc3c2OCO3)CCOC(C)(C)C1	8018-1268	NRAS	G-quadruplex	UGUGGGAGGGGCGGUCUG GG	1
1478	CC1=CC(C)=NC(N1 CCN)=O	8018-1719	NRAS	G-quadruplex	UGUGGGAGGGGCGGUCUG 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	UGUGGGAGGGGCGGUCUG GG	1
1481	COc1cc(ccc1OC1CC CC1)C1CC(Nc2c1sc(N)n2)=O	8019-3694	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	1
1482	C1CN2C(=CSC2=N1)c1cccc(c1)N	8019-6474	NRAS	G-quadruplex	UGUGGGAGGGGCGGUCUG GG	1
1483	clcc(N)nc2clccc(n2) O	8019-7722	NRAS	G-quadruplex	UGUGGGAGGGGCGGUCUG GG	1
1484	COclecc(ccl)clc(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	UGUGGGAGGGGCGGUCUG GG	1

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	UGUGGGAGGGGCGGUCUG GG	1
1490	CCN(CC)CCCNc1c2 cccc2nc(c2nnc(c3cc c(C)cc3)o2)n1	C660-1575	NRAS	G-quadruplex	UGUGGGAGGGGCGGUCUG GG	1
1491	CCOC(N1CCN(CC1) C1=C(C(C1=O)=O)N CCCN1CCCCC1)= O	C748-1353	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	1
1492	C(c1ccccc1)Nc1c(enc 2ccc(cc12) [Cl])S(c1ccccc1) (=O)=O	C769-1518	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	1
1493	Cc1ccc(cc1)S(c1c(N CCOC)oc(c2cccc(C)c 2)n1)(=O)=O	D072-0517	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	1
1494	CN1C(N(Cc2cccc2) C(c2c1nc(NCCN)n2 C)=O)=O	D114-0037	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	1
1495	CCc1ccc(cc1)n1nc(C O)c(C(NCCc2cccc2)=O)n1	D217-0759	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	1
1496	CCOC(c1ccc(c1)Nc 1cc(c2cccc2)ncn1)= O	D278-0165	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG 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	UGUGGGAGGGCGGGUCUG GG	1
1499	Cc1ccccc1c1nc(c2ccc nc2NCc2ccco2)on1	D349-3751	NRAS	G-quadruplex	UGUGGGAGGGGCGGGUCUG GG	1
1500	Cc1cccc1c1nc(c2ccc nc2NC2CCCC2)on 1	D349-3758	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	1
1501	COc1ccc(cc1)c1nc(c 2cccnc2NCC2CCCO 2)on1	D349-4034	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	1
1502	CCCNc1cc(C)nc2cc(c3ccc(c(c3)OC)OC)n n12	D393-0193	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	1
1503	Cc1cc(C)n2c(n1)nc(CNc1cccc(c1)[Cl])n2	D433-0351	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG 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	UGUGGGAGGGCGGGUCUG GG	1
1506	CN1C(N(C)c2cc(CN c3ccc(c(c3)C(O)=O) [Cl])ccc12)=O	D664-0087	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG GG	1
1507	Cn1c2cccc2c2c1nc(NCCCN1CCCCC1) nn2	E205-0046	NRAS	G-quadruplex	UGUGGGAGGGGCGGUCUG GG	1

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
1508	C(CNc1c2c(c3ccc(cc 3)F)noc2ncn1)c1ccsc	E899-0297	NRAS	G-quadruplex	UGUGGGAGGGCGGGUCUG 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	COclecc(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	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	COcleccc(c1)clen[n H]c1C1CCN(CC1)c1 cenc(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

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)[C1])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] (c2cccc2)[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	Cc1ccc(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(Cn1c2cccc2nc 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

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	(Cc1ccccc1)N)=O					
1551	CC1CCe2c(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 c2cccc2nc(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	CCCCNCCOcleeccc 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(=Cc2cc3cccc3nc 2N2CCCC2)C#N)n n1c1cccc1	5796654	TERRA	G-quadruplex	GGGUUAGGGU	1
1567	Cc1c2c(nc(CCN)nc2s c1C)N(CCN(C)C)Cc 1cccc1	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)Oc2cccc2)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

Entry_ID	SMILES	Molecule_ID	RNA_target	SS_type	RNA_sequence	Class
	O.C(C(O)=O)(O)=O					
1574	Cc1nc2cccc2n1CC(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=CCNCCOCCoclc ccc(c1) [Br].C(C(O)=O) (O)=O	7002064	TERRA	G-quadruplex	GGGUUAGGGU	1
1577	C1CCN(C1)c1ccc(cc 1[Cl])NC1c2cccc2S (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[C1])F)c1ccc(cc1)O C	7756-0741	TERRA	G-quadruplex	GGGUUAGGGU	1
1580	C=CCe1cc(cce1OCC NCCN1CCOCC1) [C1].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(Nc2cccc2O 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(c1cccc1)c1nnc(N)	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)c2cccc2[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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	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	clcc(N)nc2clccc(n2) O	8019-7722	TERRA	G-quadruplex	GGGUUAGGGU	1
1603	COclecc(ccl)clc(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	CCCCNe1c(C#N)c2 CC(C) (C)OCc2c(c2cccc2) n1	8640-0572	TERRA	G-quadruplex	GGGUUAGGGU	1
1607	COc1cc(cc(c1OC)OC)c1nc(c2ccc(c2)N)n[nH]1	9204334	TERRA	G-quadruplex	GGGUUAGGGU	1
1608	c1ccc2c(c1)nc(c1ccc(cc1[C1])N)s2	C066-5322	TERRA	G-quadruplex	GGGUUAGGGU	1
1609	Cc1cccc(c1)NCc1nc2 cccc2n1C	C147-0043	TERRA	G-quadruplex	GGGUUAGGGU	1
1610	clccc2c(c1)clnncnlc (Nclccc(cc1F) [Br])n2	C301-5173	TERRA	G-quadruplex	GGGUUAGGGU	1
1611	CCN(CC)CCCNc1c2 cccc2nc(c2nnc(c3cc c(C)cc3)o2)n1	C660-1575	TERRA	G-quadruplex	GGGUUAGGGU	1
1612	C1CCCN(CC1)CCC Nc1nc2cccc2c2nc(c 3cccc3)nn12	C736-0159	TERRA	G-quadruplex	GGGUUAGGGU	1
1613	CCOC(N1CCN(CC1) C1=C(C(C1=O)=O)N CCCN1CCCCC1)= 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(c2cccc2)ncn1)= O	D278-0165	TERRA	G-quadruplex	GGGUUAGGGU	1
1616	CSc1nc2CCc2c(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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1618	C(CNc1c2c(c3ccc(cc 3)F)noc2ncn1)c1ccsc	E899-0297	TERRA	G-quadruplex	GGGUUAGGGU	1