Training dataset curated from R-SIM database for the “Repeats” model in RSAPred

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
754	NCCCC[C@@H](NC(=O)[C@@H](NC(=O)[C@H]1CCCN1C(=O)c1cc2c(OCO2)cc1)CSSC[C@@H](C(=O)N[C@@H](CCCCN)C(=O)NCCCN)NC(=O)[C@H]1CCCN1C(=O)c1cc2c(OCO2)cc1)C(=O)NCCCN	GCGCUGCUGCUGCUGCUGCUGCUGCUGCUGCGC	hexanamide derivative_1	Target_lig_512	r(CUG)	Target_55	5.1549019599 8574
755	CCC1=NC2=CC=CC=C2C=C1C(=O)N3CCC[C@H]3C(=O)N[C@@H](CSSC[C@@H](C(=O)N[C@@H](CCCCN)C(=O)NCCCN)NC(=O)[C@@H]4CCCN4C(=O)C5=CC6=CC=CC=C6N=C5CC)C(=O)N[C@@H](CCCCN)C(=O)NCCCN	GCGCUGCUGCUGCUGCUGCUGCUGCUGCUGCGC	hexanamide derivative_3	Target_lig_513	r(CUG)	Target_55	5
756	CCc1nc2c(cccc2)cc1C(=O)N1CCC[C@@H]1C(=O)N[C@H](CSSC[C@@H](NC(=O)[C@H](NC(=O)c1c(CC)nc2c(cccc2)c1)CC(=O)N)C(=O)N[C@@H](CCCCN)C(=O)NCCCN)C(=O)N[C@@H](CCCCN)C(=O)NCCCN	GCGCUGCUGCUGCUGCUGCUGCUGCUGCUGCGC	butanediamide derivative_1	Target_lig_514	r(CUG)	Target_55	5.2596373105 0576
757	CCc1nc2c(cccc2)cc1C(=O)N1CCC[C@@H]1C(=O)N[C@H](CSSC[C@@H](C(=O)N[C@@H](CCCCN)C(=O)NCCCN)NC(=O)[C@@H]1CCCN1C(=O)c1cc2c(OCO2)cc1)C(=O)N[C@H](CCCCN)C(=O)NCCCN	GCGCUGCUGCUGCUGCUGCUGCUGCUGCUGCGC	hexanamide derivative_2	Target_lig_515	r(CUG)	Target_55	5.1249387366 083
758	COC1=CC2=C(C3=C(C=C(C=C3)Cl)N=C2C=C1)NCCCCNC4=NC(=NC(=N4)N)N	GCGCUGCUGCUGCUGCUGCUGCUGCUGCUGCGC	triazine-2,4,6-triamine derivative	Target_lig_516	r(CUG)	Target_55	4.9586073148 4177
764	CCCNC(=O)CCCOC1=CC=CC(=C1)C2=NC3=C(N2)C=C(C=C3)C4=NC5=C(N4)C=C(C=C5)N6CCN(CC6)C	GGGAGAGGGUUUAAUCUGUACGAAAGUACUGAUUGGAUCCGCAAGG	N-propylbutanamide derivative	Target_lig_521	DM1-RNA-MBNL1	Target_110	6.8860566476 9316
765	C(CNC(=O)CCCOc1cccc(c1)c1nc2c([nH]1)cc(cc2)c1nc2cc	GGGAGAGGGUUUAAUCUGUACGAAAGUACUGAUUGGAUCC	butanamide derivative_1	Target_lig_522	DM1-RNA-MBNL1	Target_110	7

	c(cc2[nH]1)N1CCN(C)CC1)n1cc(CN(CC(=O)N)C(=O)CN(CCCC)C(=O)CN(CCC)C(=O)CN(C(=O)CN(C(=O)CN(Cc2nnn(c2)CCNC(=O)CCCOc2cccc(c2)c2nc3c([nH]2)cc(cc3)c2nc3ccc(cc3[nH]2)N2CCN(C)CC2)C)CCC)CCC)nn1	GCAAGG					
769	[C@@H]1([C@@H]([C@H]([C@H](O[C@@H]1CNC(=O)CCCC)O[C@@H]1[C@@H]([C@H]([C@H](C[C@@H]1N)N)O[C@@H]1O[C@H]([C@@H]([C@H]([C@H]1O)N)O)CO)O)O)O)O	GGGAGAGGGUUUAAUCUGUACGAAAGUACUGAUUGGAUCCGCAAGG	pentanamide derivative_1	Target_lig_523	DM1-RNA-MBNL1	Target_110	6
770	[C@H]1([C@@H]([C@H]([C@H](O[C@@H]1CNC(=O)CCCCc1nnn(CCCN(CC(=O)N(CC(=O)N(CC(=O)N)CCCn2nnc(c2)CCCCC(=O)NC[C@H]2[C@@H]([C@H]([C@@H]([C@@H](O2)O[C@@H]2[C@@H]([C@@H]([C@H](C[C@H]2N)N)O[C@@H]2O[C@@H]([C@H]([C@H]([C@H]2O)N)O)CO)O)O)O)O)CCC)CCC)C)c1)O[C@@H]1[C@H]([C@@H]([C@H](C[C@@H]1N)N)O[C@H]1O[C@H]([C@@H]([C@@H]([C@@H]1O)N)O)CO)O)O)O)O	GGGAGAGGGUUUAAUCUGUACGAAAGUACUGAUUGGAUCCGCAAGG	pentanamide derivative_2	Target_lig_524	DM1-RNA-MBNL1	Target_110	7.3010299956 6398
945	c12cc(ccc1c(c1c(n2)ccc(c1)OC)NCCCCc1c(nc(nc1N)N)N)Cl	CCUGCCUGCCUGCCUGCCUGCCUG	MBNL CCUG ligand 3	Target_lig_563	(CCUG)6	Target_62	3.5228787452 8034
1067	CCCN(CC(=O)N(CCC)CC(=O)N(CC(N)=O)CC1=CN(CCCNC(=[NH2+])C2=CC=C(C=C2)C2=CC=C(O2)C2=CC=C(C=C2)C(N)=[NH2+])N=N1)C(=O)CNCC1=CN(CCCNC(=[NH2+])C2=CC=C(C=C2)C2=CC=C(O2)C2=CC=C(C=C2)C(N)=[NH2+])N=N1	AUUCUAUUCUAUUCUAUUCUAUUCUAUUCUAUUCUAUUCUAUUCU	2-AU-2	Target_lig_628	r(AUUCU)11	Target_166	6.7328282715 9699
1069	CCCN(CC(=O)N(CCC)CC(=O)N(CC(N)=O)CC1=CN(CCCNC(=[NH2+])C2=CC=C(C=C2)C2=	CUGCUGCUGCUGCUGCUGCUGCUGCUGCUGCUG	2-AU-2	Target_lig_628	r(CUG)12	Target_167	5.3979400086 7204

	CC=C(O2)C2=CC=C(C=C2)C(N)=[NH2+])N=N1)C(=O)CNCC1=CN(CCCNC(=[NH2+])C2=CC=C(C=C2)C2=CC=C(O2)C2=CC=C(C=C2)C(N)=[NH2+])N=N1						
1079	CCCN(CC(=O)N(CCC)CC(=O)N(CCC)CC(=O)N(CCC)CC(=O)N(CC(N)=O)CC1=CN(CCCNC(=O)CCCOC2=CC=CC(=C2)C2=NC3=CC(=CC=C3N2)C2=NC3=CC(=CC=C3N2)N2CC[NH+](C)CC2)N=N1)C(=O)CNCC1=CN(CCCNC(=O)CCCOC2=CC=CC(=C2)C2=NC3=CC(=CC=C3N2)C2=NC3=CC(=CC=C3N2)N2CC[NH+](C)CC2)N=N1	CGGCGGCGGCGGCGGCGGCGGCGGCGGCGGC	2H-4	Target_lig_634	r(CGG)12	Target_169	6.6736641390 7125
1083	CCCN(CC(=O)N(CCC)CC(=O)N(CCC)CC(=O)N(CCC)CC(=O)N(CCC)CC(=O)N(CC(N)=O)CC1=CN(CCCNC(=O)CCCOC2=CC=CC(=C2)C2=NC3=CC(=CC=C3N2)C2=NC3=CC(=CC=C3N2)N2CC[NH+](C)CC2)N=N1)C(=O)CNCC1=CN(CCCNC(=O)CCCOC2=CC=CC(=C2)C2=NC3=CC(=CC=C3N2)C2=NC3=CC(=CC=C3N2)N2CC[NH+](C)CC2)N=N1	CGGCGGCGGCGGCGGCGGCGGCGGCGGCGGC	2H-5	Target_lig_635	r(CGG)12	Target_169	6.5528419686 5778
1088	C[C@H](N(C)C(=O)[C@H](C)N(C)C(=O)[C@H](C)N(C)C(=O)[C@H](C)N(C)C(=O)C[NH2+]CCCN1C=C(C[N+]2=CC3=C(C)C4=C(NC5=C4C=C(O)C=C5)C(C)=C3C=C2)N=N1)C(=O)N(CCCN1C=C(C[N+]2=CC3=C(C)C4=C(NC5=C4C=C(O)C=C5)C(C)=C3C=C2)N=N1)CC(N)=O	CGGCGGCGGCGGCGGCGGCGGCGGCGGCGGC	2HE-5NMe	Target_lig_637	r(CGG)12	Target_169	7.3010299956 6398
1097	C[C@H](N(C)C(=O)[C@H](C)N(C)C(=O)[C@H](C)N(C)C(=O)CCC	CUGCUGCUGCUGCUGCUGCUGCUGCUGCUGC	2H-K4NMeS	Target_lig_644	r(CUG)12	Target_167	7.8794260687 9415

	OC1=CC=CC(=C1)C1=NC2=CC(=CC=C2N1)C1=NC2=CC(=CC=C2N1)N1CC[NH+](C)CC1)C(=O)N(CCCCN(C)C(=O)CCCOC1=CC=CC(=C1)C1=NC2=CC(=CC=C2N1)C1=NC2=CC(=CC=C2N1)N1CC[NH+](C)CC1)CC(N)=O						
1101	NC1=NC(N)=[NH+]C(NCCCCNC2=C3C=CC=CC3=[NH+]C3=C(C=CC=C23)C(=O)NCCN(CC[NH3+])CC[NH3+])=N1	CUGCUGCUGCUG	Acridine 5	Target_lig_647	r(CUG)4	Target_172	7.0655015487 5643
1102	NC1=NC(NCCCCNC2=C3C=CC=C(C(=O)NCCC[NH2+]CCC[NH2+]CCCNC(=O)C4=C5[NH+]=C6C=CC=CC6=C(NCCCCNC6=NC(N)=[NH+]C(N)=N6)C5=CC=C4)C3=[NH+]C3=CC=CC=C23)=[NH+]C(N)=N1	CUGCUGCUGCUGCUGCUG	Acridine 9	Target_lig_648	r(CUG)6	Target_173	6.4948500216 8009
1104	NC1=NC(N)=[NH+]C(NCCCCNC(=[NH2+])C2=CC=C(C=C2)C(=[NH2+])NCCCCNC2=[NH+]C(N)=NC(N)=N2)=N1	CUGCUGCUGCUGCUGCUGCUGCUGCUGCUGCUG	Bisamidinium 2	Target_lig_649	r(CUG)12-MBNL1 complex	Target_167	5.0969100130 0806
1108	NC1=NC(N)=[NH+]C(NCCCCNC(=[NH2+])C2=CC=C(C=C2)C(=[NH2+])NCCCCNC2=[NH+]C(N)=NC(N)=N2)=N1	CCUGCCUGCCUGCCUGCCUGCCUGCCUGCCUG	Bisamidinium 2	Target_lig_649	r(CCUG)8]	Target_174	3.6989700043 3602
1109	NC1=NC(N)=[NH+]C(NCCCCNC(=[NH2+])C2=CC=C(C=C2)C(=[NH2+])NCCCCNC2=[NH+]C(N)=NC(N)=N2)=N1	CUGCUGCUGCUG	Bisamidinium 2	Target_lig_649	r(CUG)4	Target_172	7.0655015487 5643
1110	NC1=NC(N)=[NH+]C(NCCCCNC(=[NH2+])C2=CC=C(C=C2)C(=[NH2+])NCCCCNC2=NC(NCC3=CN(CCCNC4=[NH+]C(N)=[NH+]C(NCCCCNC(=[NH2+])C5=CC=C(C=C5)C(=[NH2+])NCCCCNC5=NC(N)=[NH+]C(N)=N5)=N4)N=N3)=NC(N)=[NH+]2)=N1	CUGCUGCUGCUGCUGCUGCUGCUGCUGCUGCUGCUGCUG	Bisamidinium 2a	Target_lig_650	r(CUG16)-MBNL1 complex	Target_175	7.6020599913 2796
1111	NC1=NC(NCCN(CC[NH3+])CC[NH3+])=NC(NCCCCNC(=[NH2+])C2=CC=C(C=C2)C(=[NH2+])NCCCCNC2=N	CUGCUGCUGCUGCUGCUGCUGCUGCUGCUG	Bisamidinium 9	Target_lig_651	r(CUG)12	Target_167	5.2218487496 1636

	C(NCCN(CC[NH3+])CC[NH3+])=NC(N)=[NH+]2)=[NH+]1						
1112	NC1=NC(NCCN(CC[NH3+])CC[NH3+])=NC(NCCCCNC(=[NH2+])C2=CC=C(C=C2)C(=[NH2+])NCCCCNC2=NC(NCCN(CC[NH3+])CC[NH3+])=NC(N)=[NH+]2)=[NH+]1	CTGCTGCTGCTGCTGCTGCTGCTGCTGCTGCTG	Bisamidinium 9	Target_lig_651	d(CTG)12	Target_176	5.3010299956 6398
1113	CCC1=C(C=C2C=C3C=CC=CC3=CC2=N1)C(=O)N1CCC[C@H]1C(=O)N[C@@H](C\C=C/C[C@H](NC(=O)[C@@H]1CCCN1C(=O)C1=C(CC)N=C2C=C3C=CC=CC3=CC2=C1)C(=O)N[C@@H](CCCC[NH3+])C(=O)NCCC[NH3+])C(=O)N[C@@H](CCCC[NH3+])C(=O)NCCC[NH3+]	CCCGCUGCUGCGG	DCC 4 (2012)	Target_lig_652	r(CUG)2	Target_177	7.4948500216 8009
1114	CCC1=C(C=C2C=C3C=CC=CC3=CC2=N1)C(=O)N1CCC[C@H]1C(=O)N[C@@H](C\C=C/C[C@H](NC(=O)[C@@H]1CCCN1C(=O)C1=C(CC)N=C2C=C3C=CC=CC3=CC2=C1)C(=O)N[C@@H](CCCC[NH3+])C(=O)NCCC[NH3+])C(=O)N[C@@H](CCCC[NH3+])C(=O)NCCC[NH3+]	CUGCUGCUGCUG	DCC 4 (2012)	Target_lig_652	r(CUG)4	Target_172	7.6478174818 8864
1116	CCC1=C(C=C2C=C3C=CC=CC3=CC2=N1)C(=O)N1CCC[C@H]1C(=O)N[C@@H](C\C=C/C[C@H](NC(=O)[C@@H]1CCCN1C(=O)C1=C(CC)N=C2C=C3C=CC=CC3=CC2=C1)C(=O)N[C@@H](CCCC[NH3+])C(=O)NCCC[NH3+])C(=O)N[C@@H](CCCC[NH3+])C(=O)NCCC[NH3+]	CCCGCCUGCCUGCCUGCCUGCCUGCCUGCCUGCCUGCCUGCGG	DCC 4 (2012)	Target_lig_652	r(CCUG)10	Target_179	7.4089353929 735
1117	CCC1=C(C=C2C=C3C=CC=CC3=CC2=N1)C(=O)N1CCC[C@H]1C(=O)N[C@@H](C\C=C/C[C@H](NC(=O)[C@@H]1CCCN1C(=O)C1=C(CC)N=C2C=C3C=CC=CC3=CC2=C1)C(=O)N[C@@H](CCCC[NH3+])C(=O)NCCC[NH3+])C	CCCGCAGCAGCAGCAGCAGCAGCAGCAGCAGCGG	DCC 4 (2012)	Target_lig_652	r(CAG)10	Target_180	7.3098039199 7149

	(=O)N[C@@H](CCCC[NH3+])C(=O)NCCC[NH3+]						
1121	CCC1=C(C=C2C=C3C=CC=CC3=CC2=N1)C(=O)N1CCC[C@H]1C(=O)N[C@@H](CCC\C=C\CCC[C@H](NC(=O)[C@@H]1CCCN1C(=O)C1=C(CC)N=C2C=C3C=CC=CC3=CC2=C1)C(=O)N[C@@H](CCCC[NH3+])C(=O)NCCC[NH3+])C(=O)N[C@@H](CCCC[NH3+])C(=O)NCCC[NH3+]	CCCGCUGCUGCGG	DCC 11 (2012)	Target_lig_653	r(CUG)2	Target_177	6.1752235375 2445
1122	CCC1=C(C=C2C=C3C=CC=CC3=CC2=N1)C(=O)N1CCC[C@H]1C(=O)N[C@@H](CCC\C=C\CCC[C@H](NC(=O)[C@@H]1CCCN1C(=O)C1=C(CC)N=C2C=C3C=CC=CC3=CC2=C1)C(=O)N[C@@H](CCCC[NH3+])C(=O)NCCC[NH3+])C(=O)N[C@@H](CCCC[NH3+])C(=O)NCCC[NH3+]	CUGCUGCUGCUG	DCC 11 (2012)	Target_lig_653	r(CUG)4	Target_172	7.2218487496 1636
1125	CCC1=C(C=C2C=C3C=CC=CC3=CC2=N1)C(=O)N1CCC[C@H]1C(=O)N[C@@H](CCC\C=C\CCC[C@H](NC(=O)[C@@H]1CCCN1C(=O)C1=C(CC)N=C2C=C3C=CC=CC3=CC2=C1)C(=O)N[C@@H](CCCC[NH3+])C(=O)NCCC[NH3+])C(=O)N[C@@H](CCCC[NH3+])C(=O)NCCC[NH3+]	CCCGCAGCAGCAGCAGCAGCAGCAGCAGCAGCGG	DCC 11 (2012)	Target_lig_653	(CAG)10	Target_180	6.0644927341 7529
1128	CCC1=C(C=C2C=C3C=CC=CC3=CC2=N1)C(=O)N1CCC[C@H]1C(=O)N[C@@H](CCC\C=C\CCC[C@H](NC(=O)[C@@H]1CCCN1C(=O)C1=C(CC)N=C2C=C3C=CC=CC3=CC2=C1)C(=O)N[C@@H](CCCC[NH3+])C(=O)NCCC[NH3+])C(=O)N[C@@H](CCCC[NH3+])C(=O)NCCC[NH3+]	CCCGCCUGCCUGCCUGCCUGCCUGCCUGCCUGCCUGCCUGCGG	DCC 11 (2012)	Target_lig_653	r(CCUG)10	Target_179	7.1331221856 625
1184	NC(=[NH2+])C1=CC=C(NC2=CC=C(C=C2)C2=CC3=CC=C(C=C3N2)C(N	CCGCCGCCGCCGCCGCCGCCGCCGCCGCCGCCG	Compound 2	Target_lig_676	r(CCG)12	Target_181	5

	)=[NH2+])C=C1						
1185	NC(=[NH2+])C1=CC=C(NC2=CC=C(C=C2)C2=CC3=CC=C(C=C3N2)C(N)=[NH2+])C=C1	GGCCGGCCGGCCGGCC	Compound 2	Target_lig_676	r(GGCC)4	Target_182	5.1426675035 6873
1187	NC(=[NH2+])C1=CC=C(NC2=CC=C(C=C2)C2=CC3=CC=C(C=C3N2)C(N)=[NH2+])C=C1	GGGGCCGGGGCCGGGGCCGGGGCCGGGGCCGGGGCC	Compound 2	Target_lig_676	Hairpin Conformation of r(GGGGCC)8	Target_183	4.8239087409 4432
1188	NC(=[NH2+])C1=CC=C(NC2=CC=C(C=C2)C2=CC3=CC=C(C=C3N2)C(N)=[NH2+])C=C1	GGGGCCGGGGCCGGGGCCGGGGCCGGGGCCGGGGCC	Compound 2	Target_lig_676	G-Quadruplex Conformation of r(GGGGCC)8	Target_184	4
1192	C1=CC(=CC=C1C(=O)OC2=CC=C(C=C2)[NH+]=C(N)N)[NH+]=C(N)N	GGGAGAGGGUUUAAUAUCAGUAUACGAAAGUAUACAGAUAUUGGAUCCGCAAGG	D6	Target_lig_679	5'CAG/3'GAC	Target_204	7.2218487496 1636
1195	CC1=C2C=C[N+](CC[NH+]3CCCCC3)=CC2=C(C)C2=C1NC1=C2C=C(O)C=C1	CGGCGGCGGCGGCGGCGGCGGCGGCGGCGGC	Hydroxyellipticine 1a	Target_lig_680	r(CGG)12	Target_169	6.0969100130 0806
1197	CC1=C2C=C[N+](CC[NH+]3CCCCC3)=CC2=C(C)C2=C1NC1=C2C=C(O)C=C1	CGGCGGCGGCGGCGGCGGCGGCGGCGGCGGC	Hydroxyellipticine 1a	Target_lig_680	5'CGG/3'GGC Loop	Target_205	7.11918640771 921
1199	CC1=C2C=C[N+](CC[NH+]3CCCCC3)=CC2=C(C)C2=C1NC1=C2C=C(O)C=C1	GGCCGGCCGGCCGGCC	Hydroxyellipticine 1a	Target_lig_680	r(GGCC)4	Target_182	5.0757207139 3812
1200	CC1=C2C=C[N+](CC[NH+]3CCCCC3)=CC2=C(C)C2=C1NC1=C2C=C(O)C=C1	GGGGCCGGGGCCGGGGCCGGGGCCGGGGCCGGGGCC	Hydroxyellipticine 1a	Target_lig_680	Hairpin	Target_183	4.3010299956 6398
1202	CC1=C2C=C[N+](CC[NH+]3CCCCC3)=CC2=C(C)C2=C1NC1=C2C=C(O)C=C1	GGGGCCGGGGCCGGGGCCGGGGCCGGGGCCGGGGCC	Hydroxyellipticine 1a	Target_lig_680	G-Quadruplex Conformation of r(GGGGCC)8	Target_184	4.0861861476 1628
1207	C1=CC(=CC(=C1)N)C2=NC3=C(N2)C=C(C=C3)C4=CC5=C(C=C4)N=C(N5)C6=CC(=CC=C6)N	GGGAGAGGGUUUAAUCUGUACGAAAGUACUGAUUGGAUCCGCAAGG	H1	Target_lig_684	5'CUG/3'GUC, DM1 Motif	Target_206	7.1549019599 8574
1215	C1CCN(C1)C2=NC(=C3C(=C2)C(=C(N=C3N)N4CCCC4)C#N)N	CUGCUGCUGCUGCUGCUGCUGCUGCUGCUG	Naphthyridine 2	Target_lig_686	r(CUG)12	Target_167	6.9030899869 9194
1216	C1CCN(C1)C2=NC(=C3C(=C2)C(=C(N=C3N)N4CCCC4)C#N)N	GGGAGAGGGUUUAAUCAGCAGCAGCAGCAGCAGUACGAAAGUACAGCAGCAGCAGCAGCAGAUUGGAUCCGCAAGG	Naphthyridine 2	Target_lig_686	r(CAG)12	Target_186	5.8538719643 2176
1219	C1=CC(=CC=C1C(=O)NC2=NC=C(C=C2)NC(=O)C3=CC=NC=C3)F	GGGAGAGGGUUUAAUCUGUACGAAAGUACUGAUUGGAUCCGCAAG	p7	Target_lig_687	5' CUG/3' GUC Internal Loop	Target_210	5.3372421683 1843
1248	C1=CC(=CC=C1C2=CC=C(O2)C3=CC=C(C=C3)C(=[N	GGCAGCAGCAGCAGCAGCAGCAGCAGCAGCAGCAGCAGC	DB75	Target_lig_697	HTT exon1 RNA, 18 repeats	Target_215	4.2225731776 1069

	H2+])N)C(=[NH2+])N	AGCAGCAGCAGCAGCC					
1249	C1=CC(=CC=C1C2=CC=C(O2)C3=CC=C(C=C3)C(=[NH2+])N)C(=[NH2+])N	GGCAGCAGCAGCAGCAGCAGCAGCAGCAGCAGCAGCAGCAGCAGCAGCC	DB75	Target_lig_697	HTT exon1 RNA, 48 repeats	Target_216	3.7958800173 4407
1556	C1=CC(=CC=C1C2=CC=C(O2)C3=CC=C(C=C3)C(=N)N)C(=N)N	AUUCUAUUCUAUUCUAUUCUAUUCUAUUCUAUUCUAUUCUAUUCUAUUCUAUUCU	Compound_2	Target_lig_850	r(AUUCU)11	Target_166	6.5228787452 8034
1557	N=[N+]=NCCCNC(=N)c1ccc(cc1)c1ccc(o1)c1ccc(cc1)C(=N)N	AUUCUAUUCUAUUCUAUUCUAUUCUAUUCUAUUCUAUUCUAUUCUAUUCUAUUCU	AU-azide	Target_lig_851	r(AUUCU)11	Target_166	6.4259687322 7228
1558	CCCN(C(=O)CN(C(=O)CNCc1nnn(c1)CCCNC(=N)c1ccc(cc1)c1ccc(o1)c1ccc(cc1)C(=N)N)CCC)CC(=O)N(Cc1nnn(c1)CCCNC(=N)c1ccc(cc1)c1ccc(o1)c1ccc(cc1)C(=N)N)CC(=O)N	AUUCUAUUCUAUUCUAUUCUAUUCUAUUCUAUUCUAUUCUAUUCUAUUCUAUUCU	2AU-2	Target_lig_1266	r(AUUCU)11	Target_166	6.7328282715 9699
1559	C1=CC(=CC=C1C2=CC=C(O2)C3=CC=C(C=C3)C(=N)N)C(=N)N	CUGCUGCUGCUGCUGCUGCUGCUGCUGCUGCUGCUGCUGCUGCUGCUGCUG	Compound_2	Target_lig_850	r(CUG)12	Target_167	5.3979400086 7204
1560	N=[N+]=NCCCNC(=N)c1ccc(cc1)c1ccc(o1)c1ccc(cc1)C(=N)N	CUGCUGCUGCUGCUGCUGCUGCUGCUGCUGCUGCUGCUGCUGCUGCUGCUG	AU-azide	Target_lig_851	r(CUG)12	Target_167	5.3010299956 6398
1561	CCCN(C(=O)CN(C(=O)CNCc1nnn(c1)CCCNC(=N)c1ccc(cc1)c1ccc(o1)c1ccc(cc1)C(=N)N)CCC)CC(=O)N(Cc1nnn(c1)CCCNC(=N)c1ccc(cc1)c1ccc(o1)c1ccc(cc1)C(=N)N)CC(=O)N	CUGCUGCUGCUGCUGCUGCUGCUGCUGCUGCUGCUGCUGCUGCUGCUGCUG	2AU-2	Target_lig_1266	r(CUG)12	Target_167	5.3979400086 7204
1562	C1=CC(=CC=C1C2=CC=C(O2)C3=CC=C(C=C3)C(=N)N)C(=N)N	CGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGG	Compound_2	Target_lig_850	r(CGG)12	Target_169	5.6989700043 3602
1563	N=[N+]=NCCCNC(=N)c1ccc(cc1)c1ccc(o1)c1ccc(cc1)C(=N)N	CGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGG	AU-azide	Target_lig_851	r(CGG)12	Target_169	5.5228787452 8034
1564	CCCN(C(=O)CN(C(=O)CNCc1nnn(c1)CCCNC(=N)c1ccc(cc1)c1ccc(o1)c1ccc(cc1)C(=N)N)CCC)CC(=O)N(Cc1nnn(c1)CCCNC(=N)c1ccc(cc1)c1ccc(o1)c1ccc(cc1)C(=N)N)CC(=O)N	CGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGG	2AU-2	Target_lig_1266	r(CGG)12	Target_169	5.3979400086 7204
1565	C1=CC(=CC=C1C2=CC=C(O2)C3=CC=C(C=C3)C(=N)N)C(=N)N	GGGAGAGGGUUUAAUCCUGCCUGCCUGCCUGCCUGCCUGUACGAAAGUACCUGCCUGCCUGCCUGCCUGCCUGAUUGGAUCCGCAAGG	Compound_2	Target_lig_850	r(CCUG)12	Target_185	5.3979400086 7204
1566	N=[N+]=NCCCNC(=N)c1ccc(cc1)c1cc	GGGAGAGGGUUUAAUCCUGCCUGCCUG	AU-azide	Target_lig_851	r(CCUG)12	Target_185	5.3010299956

	c(o1)c1ccc(cc1)C(=N)N	CCUGCCUGCCUGUACGAAAGUACCUGCCUGCCUGCCUGCCUGCCUGAUUGGAUCCGCAAGG					6398
1567	CCCN(C(=O)CN(C(=O)CNCc1nnn(c1)CCCNC(=N)c1ccc(cc1)c1ccc(o1)c1ccc(cc1)C(=N)N)CCC)CC(=O)N(Cc1nnn(c1)CCCNC(=N)c1ccc(cc1)c1ccc(o1)c1ccc(cc1)C(=N)N)CC(=O)N	GGGAGAGGGUUUAAUCCUGCCUGCCUGCCUGCCUGUACGAAAGUACCUGCCUGCCUGCCUGCCUGCCUGAUUGGAUCCGCAAGG	2AU-2	Target_lig_1266	r(CCUG)12	Target_185	5.3979400086 7204
1573	COc1ccc2c(c1)c(NCCCCNc1nc(N)nc(n1)N)c1c(n2)cc(cc1)Cl	GGGCUGCUGCUGCUGCUGCUGCUGCUGCUGCUGCUGCUGCUGCUGCUGCUGCCC	DM1_compound1	Target_lig_1267	r(CUG)16	Target_281	6.4089353929 735
1574	[NH2+]=C(c1ccc(cc1)C(=[NH2+])NCCCCNc1nc(N)nc(n1)N)NCCCCNc1nc(N)nc(n1)N	GGGCUGCUGCUGCUGCUGCUGCUGCUGCUGCUGCUGCUGCUGCUGCUGCUGCCC	DM1_compound3	Target_lig_1268	r(CUG)16	Target_281	5.0969100130 0806
1575	CN(CCCNc1nc(NCCCCCCNC(=O)CC2=CCC(=N2)NC(=O)CC2=CCC(=N2)NC(=O)CCCCCCNc2nc(N)nc(n2)N)nc(n1)N)C	GGGCUGCUGCUGCUGCUGCUGCUGCUGCUGCUGCUGCUGCUGCUGCUGCUGCCC	DM1_compound5	Target_lig_857	r(CUG)16	Target_281	4.2596373105 0576
1738	Oc1ccc2c(c1)c1c(C)c3c[n+](CCN4CCCCC4)ccc3c(c1[nH]2)C	GGGGCCGGGGCCGGGGCCGGGGCCGGGGCCGGGGCCGGGGCCGGGGCCGGGGCC	Compound1a	Target_lig_1274	r(GGGGCC)8	Target_183	5.0132282657 3376
1739	NC(=N)c1ccc(cc1)Nc1ccc(cc1)c1cc2c([nH]1)cc(cc2)C(=N)N	GGGGCCGGGGCCGGGGCCGGGGCCGGGGCCGGGGCCGGGGCCGGGGCCGGGGCC	Compound2	Target_lig_1275	r(GGGGCC)8	Target_183	5
1740	CCN(CC)CCNC(=O)C1=CC2=C(N1)C=CC(=C2)NC(=O)C3=CC4=C(N3)C=CC(=C4)N	GGGGCCGGGGCCGGGGCCGGGGCCGGGGCCGGGGCCGGGGCCGGGGCCGGGGCC	Compound3	Target_lig_969	r(GGGGCC)8	Target_183	4.7958800173 4408
1870	NC(=[NH2+])C1=CC=C(N=C1)C1=CC=C(O1)C1=CC=C(O1)C1=NC=C(C=C1)C(N)=[NH2+]	GGGAGAGGGUUUAAUUCGGCGGCGGCGGCGGCGGUACGAAAGUACGGCGGCGGCGGCGGCGGAUUGGAUCCGCAAGG	B1	Target_lig_716	(5'CGG/3'GGC)x6	Target_347	6.7212463990 4717
1871	CC(C)C1=CC2=C(C=C1)N=C3C=CC(=CN3C2=O)C(=O)NCCN(C)C	GGGAGAGGGUUUAAUUCGGCGGCGGCGGCGGCGGUACGAAAGUACGGCGGCGGCGGCGGCGGAUUGGAUCCGCAAGG	B4	Target_lig_1035	(5'CGG/3'GGC)x6	Target_347	6.5086383061 6573
1872	C1C[NH+]=C(N1)C2=CC=C(C=C2)C3=CC=C(O3)C4=CC=C(C=C4)C5=[NH+]CCN5	GGGAGAGGGUUUAAUUCGGCGGCGGCGGCGGCGGUACGAAAGUACGGCGGCGGCGGCGGCGGAUUGGAUCCGCAAGG	B6	Target_lig_696	(5'CGG/3'GGC)x6	Target_347	6.0604807473 8138
1873	C1=CC(=CC=C1C2=CC=C(O2)C3=CC=C(C=C3)C(=[NH2+])N)C(=[NH2+])N	GGGAGAGGGUUUAAUUCGGCGGCGGCGGCGGCGGUACGAAAGUACGGCGGCGGCGGCGGCGGAUUGGAUCCGCAAGG	B7	Target_lig_697	(5'CGG/3'GGC)x6	Target_347	5.9355420107 7308
1874	C1COCCN1CCNC2=C3C(=C(C=C2)	GGGAGAGGGUUUAAUUCGGCGGCGGCG	B11	Target_lig_1042	(5'CGG/3'GGC)x6	Target_347	6.4436974992

	NCCN4CCOCC4)C(=O)C5=CC=CC=C5C3=O	GCGGCGGUACGAAAGUACGGCGGCGGCGGCGGCGGAUUGGAUCCGCAAGG					3271
1875	NC(=[NH2+])C1=CC=C(N=C1)C1=CC=C(O1)C1=CC=C(O1)C1=NC=C(C=C1)C(N)=[NH2+]	GGGAGAGGGUUUAAUUCAGCAGCAGCAGCAGCAGUACGAAAGUACUGCUGCUGCUGCUGCUGAUUGGAUCCGCAAGG	B1	Target_lig_716	(5'CAG/3'GUC)x6	Target_348	5.16749108729376
1876	CC(C)C1=CC2=C(C=C1)N=C3C=CC(=CN3C2=O)C(=O)NCCN(C)C	GGGAGAGGGUUUAAUUCAGCAGCAGCAGCAGCAGUACGAAAGUACUGCUGCUGCUGCUGCUGAUUGGAUCCGCAAGG	B4	Target_lig_1035	(5'CAG/3'GUC)x6	Target_348	5.3767507096021
1877	C1C[NH+]=C(N1)C2=CC=C(C=C2)C3=CC=C(O3)C4=CC=C(C=C4)C5=[NH+]CCN5	GGGAGAGGGUUUAAUUCAGCAGCAGCAGCAGCAGUACGAAAGUACUGCUGCUGCUGCUGCUGAUUGGAUCCGCAAGG	B6	Target_lig_696	(5'CAG/3'GUC)x6	Target_348	5.55284196865778
1878	C1=CC(=CC=C1C2=CC=C(O2)C3=CC=C(C=C3)C(=[NH2+])N)C(=[NH2+])N	GGGAGAGGGUUUAAUUCAGCAGCAGCAGCAGCAGUACGAAAGUACUGCUGCUGCUGCUGCUGAUUGGAUCCGCAAGG	B7	Target_lig_697	(5'CAG/3'GUC)x6	Target_348	5.88605664769316
1879	C1COCCN1CCNC2=C3C(=C(C=C2)NCCN4CCOCC4)C(=O)C5=CC=CC=C5C3=O	GGGAGAGGGUUUAAUUCAGCAGCAGCAGCAGCAGUACGAAAGUACUGCUGCUGCUGCUGCUGAUUGGAUCCGCAAGG	B11	Target_lig_1042	(5'CAG/3'GUC)x6	Target_348	5.2839966563652
1880	NC(=[NH2+])C1=CC=C(N=C1)C1=CC=C(O1)C1=CC=C(O1)C1=NC=C(C=C1)C(N)=[NH2+]	GGGAGAGGGUUUAAUUCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGUACGAAAGUACGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGAUUGGAUCCGCAAGG	B1	Target_lig_716	(5'CGG/3'GGC)x20	Target_349	7.01772876696043
1881	CC(C)C1=CC2=C(C=C1)N=C3C=CC(=CN3C2=O)C(=O)NCCN(C)C	GGGAGAGGGUUUAAUUCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGUACGAAAGUACGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGAUUGGAUCCGCAAGG	B4	Target_lig_1035	(5'CGG/3'GGC)x20	Target_349	6.76955107862173
1882	C1COCCN1CCNC2=C3C(=C(C=C2)NCCN4CCOCC4)C(=O)C5=CC=CC=C5C3=O	GGGAGAGGGUUUAAUUCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGUACGAAAGUACGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGAUUGGAUCCGCAAGG	B11	Target_lig_1042	(5'CGG/3'GGC)x20	Target_349	6.67778070526608
1883	NC(=[NH2+])C1=CC=C(N=C1)C1=C	GGGAGAGGGUUUAAUUCGGCGGCGGCG	B1	Target_lig_716	(5'CGG/3'GGC)x40	Target_350	7.0555173278

	C=C(O1)C1=CC=C(O1)C1=NC=C(C=C1)C(N)=[NH2+]	GCGGCGGCGGCGGC GGCGGCGGCGGCGG CGGCGGCGGCGGCG GCGGCGGCGGCGGC GGCGGCGGCGGCGG CGGCGGCGGCGGCG GCGGCGGCGGCGGC GGCGGCGGCGGUAC GAAAGUACGGCGGC GGCGGCGGCGGCGG CGGCGGCGGCGGCG GCGGCGGCGGCGGC GGCGGCGGCGGCGG CGGCGGCGGCGGCG GCGGCGGCGGCGGC GGCGGCGGCGGCGG CGGCGGCGGCGGCG GAUUGGAUCCGCAA GG				4983
1884	CC(C)C1=CC2=C(C=C1)N=C3C=CC(=CN3C2=O)C(=O)NCCN(C)C	GGGAGAGGGUUUA AUUCGGCGGCGGCG GCGGCGGCGGCGGC GGCGGCGGCGGCGG CGGCGGCGGCGGCG GCGGCGGCGGCGGC GGCGGCGGCGGCGG CGGCGGCGGCGGCG GCGGCGGCGGCGGC GGCGGCGGCGGUAC GAAAGUACGGCGGC GGCGGCGGCGGCGG CGGCGGCGGCGGCG GCGGCGGCGGCGGC GGCGGCGGCGGCGG CGGCGGCGGCGGCG GCGGCGGCGGCGGC GGCGGCGGCGGCGG CGGCGGCGGCGGCG GAUUGGAUCCGCAA GG	B4	Target_lig_1035	(5'CGG/3'GGC) x40	Target_350	6.9586073148 4177
1885	C1COCCN1CCNC2=C3C(=C(C=C2)NCCN4CCOCC4)C(=O)C5=CC=CC=C5C3=O	GGGAGAGGGUUUA AUUCGGCGGCGGCG GCGGCGGCGGCGGC GGCGGCGGCGGCGG CGGCGGCGGCGGCG GCGGCGGCGGCGGC GGCGGCGGCGGCGG CGGCGGCGGCGGCG GCGGCGGCGGCGGC GGCGGCGGCGGUAC GAAAGUACGGCGGC GGCGGCGGCGGCGG CGGCGGCGGCGGCG GCGGCGGCGGCGGC GGCGGCGGCGGCGG CGGCGGCGGCGGCG GAUUGGAUCCGCAA GG	B11	Target_lig_1042	(5'CGG/3'GGC) x40	Target_350	6.7212463990 4717
1886	NC(=[NH2+])C1=CC=C(N=C1)C1=CC=C(O1)C1=CC=C(O1)C1=NC=C(C=C1)C(N)=[NH2+]	GGGAGAGGGUUUA AUUCGGCGGCGGCG GCGGCGGCGGCGGC GGCGGCGGCGGCGG CGGCGGCGGCGGCG GCGGCGGCGGCGGC GGCGGCGGCGGCGG CGGCGGCGGCGGCG GCGGCGGCGGCGGC GGCGGCGGCGGCGG CGGCGGCGGCGGCG GCGGCGGCGGCGGC GGCGGCGGCGGCGG CGGCGGCGGCGGCG GUACGAAAGUACG	B1	Target_lig_716	(5'CGG/3'GGC) x60	Target_351	7.1487416512 8092

		GCGGCGGCGGCGGC GGCGGCGGCGGCGG CGGCGGCGGCGGCG GCGGCGGCGGCGGC GGCGGCGGCGGCGG CGGCGGCGGCGGCG GCGGCGGCGGCGGC GGCGGCGGCGGCGG CGGCGGCGGCGGCG GCGGCGGCGGCGGC GGCGGCGGCGGCGG CGGCGGCGGCGGCG GCGGCGGCGGAUUG GAUCCGCAAGG					
1887	CC(C)C1=CC2=C(C=C1)N=C3C=CC(=CN3C2=O)C(=O)NCCN(C)C	GGGAGAGGGUUUA AUUCGGCGGCGGCG GCGGCGGCGGCGGC GGCGGCGGCGGCGG CGGCGGCGGCGGCG GCGGCGGCGGCGGC GGCGGCGGCGGCGG CGGCGGCGGCGGCG GCGGCGGCGGCGGC GGCGGCGGCGGCGG CGGCGGCGGCGGCG GCGGCGGCGGCGGC GGCGGCGGCGGCGG CGGCGGCGGCGGCG GUACGAAAGUACG GCGGCGGCGGCGGC GGCGGCGGCGGCGG CGGCGGCGGCGGCG GCGGCGGCGGCGGC GGCGGCGGCGGCGG CGGCGGCGGCGGCG GCGGCGGCGGCGGC GGCGGCGGCGGCGG CGGCGGCGGCGGCG GCGGCGGCGGAUUG GAUCCGCAAGG	B4	Target_lig_1035	(5'CGG/3'GGC)x60	Target_351	7
1888	C1COCCN1CCNC2=C3C(=C(C=C2)NCCN4CCOCC4)C(=O)C5=CC=CC=C5C3=O	GGGAGAGGGUUUA AUUCGGCGGCGGCG GCGGCGGCGGCGGC GGCGGCGGCGGCGG CGGCGGCGGCGGCG GCGGCGGCGGCGGC GGCGGCGGCGGCGG CGGCGGCGGCGGCG GCGGCGGCGGCGGC GGCGGCGGCGGCGG CGGCGGCGGCGGCG GCGGCGGCGGCGGC GGCGGCGGCGGCGG CGGCGGCGGCGGCG GUACGAAAGUACG GCGGCGGCGGCGGC GGCGGCGGCGGCGG CGGCGGCGGCGGCG GCGGCGGCGGCGGC GGCGGCGGCGGCGG CGGCGGCGGCGGCG GCGGCGGCGGCGGC GGCGGCGGCGGCGG CGGCGGCGGCGGCG GCGGCGGCGGAUUG GAUCCGCAAGG	B11	Target_lig_1042	(5'CGG/3'GGC)x60	Target_351	6.8538719643 2176
1954	COC1=C(C=CC(=C1)C=CC(=O)CC(=O)C=CC2=CC(=C(C=C2)O)OC)O	UUGGGCCGGGUCC	Curcumin	Target_lig_1092	r(CGGx1)	Target_354	6.9208187539 5238

1955	COC1=C(C=CC(=C1)C=CC(=O)CC(=O)C=CC2=CC(=C(C=C2)O)OC)O	UUGGGCCGGCGGGUCC	Curcumin	Target_lig_1092	r(CGGx2)	Target_355	6.8860566476 9316
1956	COC1=C(C=CC(=C1)C=CC(=O)CC(=O)C=CC2=CC(=C(C=C2)O)OC)O	UUGGGCCGGCGGCGGGUCC	Curcumin	Target_lig_1092	r(CGGx3)	Target_356	6.9208187539 5238
1957	COC1=C(C=CC(=C1)C=CC(=O)CC(=O)C=CC2=CC(=C(C=C2)O)OC)O	UUGGGCCGGCGGCGGCGGGUCC	Curcumin	Target_lig_1092	r(CGGx4)	Target_357	6.9746941347 3523
1958	COC1=C(C=CC(=C1)C=CC(=O)CC(=O)C=CC2=CC(=C(C=C2)O)OC)O	UUGGGCCGGCGGCGGCGGCGGCGGGUCC	Curcumin	Target_lig_1092	r(CGGx6)	Target_358	7.0362121726 5444
1959	COC1=C(C=CC(=C1)C=CC(=O)CC(=O)C=CC2=CC(=C(C=C2)O)OC)O	UUGGGCCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGGUCC	Curcumin	Target_lig_1092	r(CGGx20)	Target_359	7.4685210829 5774
1960	COC1=C(C=CC(=C1)C=CC(=O)CC(=O)C=CC2=CC(=C(C=C2)O)OC)O	UUGGGCCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGGUCC	Curcumin	Target_lig_1092	r(CGGx40)	Target_360	7.5376020021 0104
1961	COC1=C(C=CC(=C1)C=CC(=O)CC(=O)C=CC2=CC(=C(C=C2)O)OC)O	UUGGGCCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGGGUCC	Curcumin	Target_lig_1092	r(CGGx60)	Target_361	7.8860566476 9316
1962	COC1=C(C=CC(=C1)C=CC(=O)CC(=O)C=CC2=CC(=C(C=C2)O)OC)O	AUAUAUAUAUAU	Curcumin	Target_lig_1092	r(AUx6)	Target_362	5.6363880201 0786
1963	COC1=C(C=CC(=C1)C=CC(=O)CC(=O)C=CC2=CC(=C(C=C2)O)OC)O	UUGGGCCAGCAGCAGCAGCAGCAGGUCC	Curcumin	Target_lig_1092	r(CAGx6)	Target_363	5.7958800173 4408
1964	COC1=C(C=CC(=C1)C=CC(=O)CC(=O)C=CC2=CC(=C(C=C2)O)OC)O	UUGGGCCCGCCGCCGCCGCCGGUCC	Curcumin	Target_lig_1092	r(CCGx6)	Target_364	6.0757207139 3812
1965	COC1=C(C=CC(=C1)C=CC(=O)CC(=O)C=CC2=CC(=C(C=C2)O)OC)O	CUGCUGCUGCUGCUGCUG	Curcumin	Target_lig_1092	r(CUGx6)	Target_173	5.6575773191 7779