Training dataset curated from [R-SIM](https://web.iitm.ac.in/bioinfo2/R_SIM/) database for the “Repeats” model in [RSAPred](https://web.iitm.ac.in/bioinfo2/RSAPred/)

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| 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)c c1)CSSC[C@@H] (C(=O)N[C@@H] (CCCCN)C(=O)NC CCN)NC(=O) [C@H]1CCCN1C(  =O)c1cc2c(OCO2)c c1)C(=O)NCCCN | GCGCUGCUGCUGCU GCUGCUGCUGCUGC UGCUGCGC | hexanamide derivative\_1 | Target\_lig\_512 | r(CUG) | Target\_55 | 5.1549  019599  8574 |
| 755 | CCC1=NC2=CC=C C=C2C=C1C(=O)N 3CCC[C@H]3C(= O)N[C@@H] (CSSC[C@@H] (C(=O)N[C@@H] (CCCCN)C(=O)NC CCN)NC(=O) [C@@H]4CCCN4 C(=O)C5=CC6=CC  =CC=C6N=C5CC) C(=O)N[C@@H] (CCCCN)C(=O)NC CCN | GCGCUGCUGCUGCU GCUGCUGCUGCUGC UGCUGCGC | hexanamide derivative\_3 | Target\_lig\_513 | r(CUG) | Target\_55 | 5 |
| 756 | CCc1nc2c(cccc2)cc 1C(=O)N1CCC[C @@H]1C(=O)N[C  @H] (CSSC[C@@H] (NC(=O)[C@H]  (NC(=O)c1c(CC)nc  2c(cccc2)c1)CC(=O  )N)C(=O)N[C@@ H] (CCCCN)C(=O)NC CCN)C(=O)N[C@  @H] (CCCCN)C(=O)NC CCN | GCGCUGCUGCUGCU GCUGCUGCUGCUGC UGCUGCGC | butanediamide derivative\_1 | Target\_lig\_514 | r(CUG) | Target\_55 | 5.2596  373105  0576 |
| 757 | CCc1nc2c(cccc2)cc 1C(=O)N1CCC[C @@H]1C(=O)N[C  @H] (CSSC[C@@H] (C(=O)N[C@@H] (CCCCN)C(=O)NC CCN)NC(=O) [C@@H]1CCCN1 C(=O)c1cc2c(OCO 2)cc1)C(=O)N[C@ H] (CCCCN)C(=O)NC CCN | GCGCUGCUGCUGCU GCUGCUGCUGCUGC UGCUGCGC | hexanamide derivative\_2 | Target\_lig\_515 | r(CUG) | Target\_55 | 5.1249  387366  083 |
| 758 | COC1=CC2=C(C3  =C(C=C(C=C3)Cl) N=C2C=C1)NCCC CNC4=NC(=NC(= N4)N)N | GCGCUGCUGCUGCU GCUGCUGCUGCUGC UGCUGCGC | triazine-2,4,6- triamine derivative | Target\_lig\_516 | r(CUG) | Target\_55 | 4.9586  073148  4177 |
| 764 | CCCNC(=O)CCCO C1=CC=CC(=C1)C 2=NC3=C(N2)C=C (C=C3)C4=NC5=C (N4)C=C(C=C5)N6 CCN(CC6)C | GGGAGAGGGUUUA AUCUGUACGAAAG UACUGAUUGGAUCC GCAAGG | N-  propylbutanamide derivative | Target\_lig\_521 | DM1-RNA- MBNL1 | Target\_110 | 6.8860  566476  9316 |
| 765 | C(CNC(=O)CCCOc  1cccc(c1)c1nc2c([n H]1)cc(cc2)c1nc2cc | GGGAGAGGGUUUA AUCUGUACGAAAG UACUGAUUGGAUCC | butanamide derivative\_1 | Target\_lig\_522 | DM1-RNA- MBNL1 | Target\_110 | 7 |

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|  | c(cc2[nH]1)N1CCN (C)CC1)n1cc(CN(C  C(=O)N)C(=O)CN( CCC)C(=O)CN(CC C)C(=O)CN(C(=O) CN(C(=O)CN(Cc2n nn(c2)CCNC(=O)C  CCOc2cccc(c2)c2n c3c([nH]2)cc(cc3)c 2nc3ccc(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)C O)O)O)O)O | GGGAGAGGGUUUA AUCUGUACGAAAG UACUGAUUGGAUCC GCAAGG | 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(C CCN(CC(=O)N(CC (=O)N(CC(=O)N(C C(=O)N)CCCn2nnc (c2)CCCCC(=O)N C[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)C  O)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 | GGGAGAGGGUUUA AUCUGUACGAAAG UACUGAUUGGAUCC GCAAGG | pentanamide derivative\_2 | Target\_lig\_524 | DM1-RNA- MBNL1 | Target\_110 | 7.3010  299956  6398 |
| 945 | c12cc(ccc1c(c1c(n2  )ccc(c1)OC)NCCC  Cc1c(nc(nc1N)N)N  )Cl | CCUGCCUGCCUGCC UGCCUGCCUG | MBNL CCUG  ligand 3 | Target\_lig\_563 | (CCUG)6 | Target\_62 | 3.5228  787452  8034 |
| 1067 | CCCN(CC(=O)N(C CC)CC(=O)N(CC( N)=O)CC1=CN(CC CNC(=[NH2+])C2  =CC=C(C=C2)C2= CC=C(O2)C2=CC= C(C=C2)C(N)=[NH  2+])N=N1)C(=O)C NCC1=CN(CCCN C(=[NH2+])C2=CC  =C(C=C2)C2=CC= C(O2)C2=CC=C(C  =C2)C(N)=[NH2+]  )N=N1 | AUUCUAUUCUAUUC UAUUCUAUUCUAU UCUAUUCUAUUCUA UUCUAUUCUAUUCU | 2-AU-2 | Target\_lig\_628 | r(AUUCU)11 | Target\_166 | 6.7328  282715  9699 |
| 1069 | CCCN(CC(=O)N(C CC)CC(=O)N(CC( N)=O)CC1=CN(CC CNC(=[NH2+])C2  =CC=C(C=C2)C2= | CUGCUGCUGCUGCU GCUGCUGCUGCUGC UGCUGCUG | 2-AU-2 | Target\_lig\_628 | r(CUG)12 | Target\_167 | 5.3979  400086  7204 |

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|  | CC=C(O2)C2=CC= C(C=C2)C(N)=[NH  2+])N=N1)C(=O)C NCC1=CN(CCCN C(=[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(C CC)CC(=O)N(CCC  )CC(=O)N(CCC)C  C(=O)N(CC(N)=O) CC1=CN(CCCNC(  =O)CCCOC2=CC= CC(=C2)C2=NC3= CC(=CC=C3N2)C2  =NC3=CC(=CC=C 3N2)N2CC[NH+] (C)CC2)N=N1)C(= O)CNCC1=CN(CC CNC(=O)CCCOC2  =CC=CC(=C2)C2= NC3=CC(=CC=C3 N2)C2=NC3=CC(= CC=C3N2)N2CC[ NH+] (C)CC2)N=N1 | CGGCGGCGGCGGCG GCGGCGGCGGCGGC GGCGGCGG | 2H-4 | Target\_lig\_634 | r(CGG)12 | Target\_169 | 6.6736  641390  7125 |
| 1083 | CCCN(CC(=O)N(C CC)CC(=O)N(CCC  )CC(=O)N(CCC)C  C(=O)N(CCC)CC(  =O)N(CC(N)=O)C C1=CN(CCCNC(= O)CCCOC2=CC=C C(=C2)C2=NC3=C C(=CC=C3N2)C2= NC3=CC(=CC=C3 N2)N2CC[NH+] (C)CC2)N=N1)C(= O)CNCC1=CN(CC CNC(=O)CCCOC2  =CC=CC(=C2)C2= NC3=CC(=CC=C3 N2)C2=NC3=CC(= CC=C3N2)N2CC[ NH+] (C)CC2)N=N1 | CGGCGGCGGCGGCG GCGGCGGCGGCGGC GGCGGCGG | 2H-5 | Target\_lig\_635 | r(CGG)12 | Target\_169 | 6.5528  419686  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@H] (C)N(C)C(=O)C[N H2+]CCCN1C=C( C[N+]2=CC3=C(C) C4=C(NC5=C4C= C(O)C=C5)C(C)=C 3C=C2)N=N1)C(= O)N(CCCN1C=C( C[N+]2=CC3=C(C) C4=C(NC5=C4C= C(O)C=C5)C(C)=C 3C=C2)N=N1)CC( N)=O | CGGCGGCGGCGGCG GCGGCGGCGGCGGC GGCGGCGG | 2HE-5NMe | Target\_lig\_637 | r(CGG)12 | Target\_169 | 7.3010  299956  6398 |
| 1097 | 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)CCC | CUGCUGCUGCUGCU GCUGCUGCUGCUGC UGCUGCUG | 2H-K4NMeS | Target\_lig\_644 | r(CUG)12 | Target\_167 | 7.8794  260687  9415 |

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|  | OC1=CC=CC(=C1) C1=NC2=CC(=CC  =C2N1)C1=NC2=C C(=CC=C2N1)N1C C[NH+] (C)CC1)C(=O)N(C CCCN(C)C(=O)CC COC1=CC=CC(=C 1)C1=NC2=CC(=C C=C2N1)C1=NC2= CC(=CC=C2N1)N1 CC[NH+] (C)CC1)CC(N)=O |  |  |  |  |  |  |
| 1101 | NC1=NC(N)=[NH+  ]C(NCCCCNC2=C 3C=CC=CC3=[NH  +]C3=C(C=CC=C2 3)C(=O)NCCN(CC [NH3+])CC[NH3+]  )=N1 | CUGCUGCUGCUG | Acridine 5 | Target\_lig\_647 | r(CUG)4 | Target\_172 | 7.0655  015487  5643 |
| 1102 | NC1=NC(NCCCC NC2=C3C=CC=C( C(=O)NCCC[NH2+  ]CCC[NH2+]CCC NC(=O)C4=C5[NH  +]=C6C=CC=CC6= C(NCCCCNC6=N C(N)=[NH+]C(N)= N6)C5=CC=C4)C3  =[NH+]C3=CC=C C=C23)=[NH+]C( N)=N1 | CUGCUGCUGCUGCU GCUG | Acridine 9 | Target\_lig\_648 | r(CUG)6 | Target\_173 | 6.4948  500216  8009 |
| 1104 | NC1=NC(N)=[NH+  ]C(NCCCCNC(=[N H2+])C2=CC=C(C  =C2)C(=[NH2+])N CCCCNC2=[NH+] C(N)=NC(N)=N2)= N1 | CUGCUGCUGCUGCU GCUGCUGCUGCUGC UGCUGCUG | Bisamidinium 2 | Target\_lig\_649 | r(CUG)12-MBNL1  complex | Target\_167 | 5.0969  100130  0806 |
| 1108 | NC1=NC(N)=[NH+  ]C(NCCCCNC(=[N H2+])C2=CC=C(C  =C2)C(=[NH2+])N CCCCNC2=[NH+] C(N)=NC(N)=N2)= N1 | CCUGCCUGCCUGCC UGCCUGCCUGCCUG CCUG | Bisamidinium 2 | Target\_lig\_649 | r(CCUG)8] | Target\_174 | 3.6989  700043  3602 |
| 1109 | NC1=NC(N)=[NH+  ]C(NCCCCNC(=[N H2+])C2=CC=C(C  =C2)C(=[NH2+])N CCCCNC2=[NH+] C(N)=NC(N)=N2)= N1 | CUGCUGCUGCUG | Bisamidinium 2 | Target\_lig\_649 | r(CUG)4 | Target\_172 | 7.0655  015487  5643 |
| 1110 | NC1=NC(N)=[NH+  ]C(NCCCCNC(=[N H2+])C2=CC=C(C  =C2)C(=[NH2+])N CCCCNC2=NC(N CC3=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 | CUGCUGCUGCUGCU GCUGCUGCUGCUGC UGCUGCUGCUGCUG CUGCUG | Bisamidinium 2a | Target\_lig\_650 | r(CUG16)-MBNL1  complex | Target\_175 | 7.6020  599913  2796 |
| 1111 | NC1=NC(NCCN(C C[NH3+])CC[NH3  +])=NC(NCCCCN C(=[NH2+])C2=CC  =C(C=C2)C(=[NH2  +])NCCCCNC2=N | CUGCUGCUGCUGCU GCUGCUGCUGCUGC UGCUGCUG | Bisamidinium 9 | Target\_lig\_651 | r(CUG)12 | Target\_167 | 5.2218  487496  1636 |

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|  | C(NCCN(CC[NH3  +])CC[NH3+])=NC  (N)=[NH+]2)=[NH  +]1 |  |  |  |  |  |  |
| 1112 | NC1=NC(NCCN(C C[NH3+])CC[NH3  +])=NC(NCCCCN C(=[NH2+])C2=CC  =C(C=C2)C(=[NH2  +])NCCCCNC2=N C(NCCN(CC[NH3  +])CC[NH3+])=NC  (N)=[NH+]2)=[NH  +]1 | CTGCTGCTGCTGCT GCTGCTGCTGCTGC TGCTGCTG | Bisamidinium 9 | Target\_lig\_651 | d(CTG)12 | Target\_176 | 5.3010  299956  6398 |
| 1113 | CCC1=C(C=C2C= C3C=CC=CC3=CC 2=N1)C(=O)N1CC C[C@H]1C(=O)N[  C@@H](C\C=C/ C[C@H](NC(=O) [C@@H]1CCCN1 C(=O)C1=C(CC)N  =C2C=C3C=CC=C C3=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 | 7.4948  500216  8009 |
| 1114 | CCC1=C(C=C2C= C3C=CC=CC3=CC 2=N1)C(=O)N1CC C[C@H]1C(=O)N[  C@@H](C\C=C/ C[C@H](NC(=O) [C@@H]1CCCN1 C(=O)C1=C(CC)N  =C2C=C3C=CC=C C3=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 | 7.6478  174818  8864 |
| 1116 | CCC1=C(C=C2C= C3C=CC=CC3=CC 2=N1)C(=O)N1CC C[C@H]1C(=O)N[  C@@H](C\C=C/ C[C@H](NC(=O) [C@@H]1CCCN1 C(=O)C1=C(CC)N  =C2C=C3C=CC=C C3=CC2=C1)C(=O  )N[C@@H] (CCCC[NH3+])C(= O)NCCC[NH3+])C (=O)N[C@@H]  (CCCC[NH3+])C(= O)NCCC[NH3+] | CCCGCCUGCCUGCC UGCCUGCCUGCCUG CCUGCCUGCCUGCC UGCGG | DCC 4 (2012) | Target\_lig\_652 | r(CCUG)10 | Target\_179 | 7.4089  353929  735 |
| 1117 | CCC1=C(C=C2C= C3C=CC=CC3=CC 2=N1)C(=O)N1CC C[C@H]1C(=O)N[  C@@H](C\C=C/ C[C@H](NC(=O) [C@@H]1CCCN1 C(=O)C1=C(CC)N  =C2C=C3C=CC=C C3=CC2=C1)C(=O  )N[C@@H] (CCCC[NH3+])C(= O)NCCC[NH3+])C | CCCGCAGCAGCAGC AGCAGCAGCAGCAG CAGCAGCGG | DCC 4 (2012) | Target\_lig\_652 | r(CAG)10 | Target\_180 | 7.3098  039199  7149 |

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|  | (=O)N[C@@H]  (CCCC[NH3+])C(= O)NCCC[NH3+] |  |  |  |  |  |  |
| 1121 | CCC1=C(C=C2C= C3C=CC=CC3=CC 2=N1)C(=O)N1CC C[C@H]1C(=O)N[ C@@H](CCC\ C=C\CCC[C@H] (NC(=O) [C@@H]1CCCN1 C(=O)C1=C(CC)N  =C2C=C3C=CC=C C3=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 | 6.1752  235375  2445 |
| 1122 | CCC1=C(C=C2C= C3C=CC=CC3=CC 2=N1)C(=O)N1CC C[C@H]1C(=O)N[ C@@H](CCC\ C=C\CCC[C@H] (NC(=O) [C@@H]1CCCN1 C(=O)C1=C(CC)N  =C2C=C3C=CC=C C3=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 | 7.2218  487496  1636 |
| 1125 | CCC1=C(C=C2C= C3C=CC=CC3=CC 2=N1)C(=O)N1CC C[C@H]1C(=O)N[ C@@H](CCC\ C=C\CCC[C@H] (NC(=O) [C@@H]1CCCN1 C(=O)C1=C(CC)N  =C2C=C3C=CC=C C3=CC2=C1)C(=O  )N[C@@H] (CCCC[NH3+])C(= O)NCCC[NH3+])C (=O)N[C@@H]  (CCCC[NH3+])C(= O)NCCC[NH3+] | CCCGCAGCAGCAGC AGCAGCAGCAGCAG CAGCAGCGG | DCC 11 (2012) | Target\_lig\_653 | (CAG)10 | Target\_180 | 6.0644  927341  7529 |
| 1128 | CCC1=C(C=C2C= C3C=CC=CC3=CC 2=N1)C(=O)N1CC C[C@H]1C(=O)N[ C@@H](CCC\ C=C\CCC[C@H] (NC(=O) [C@@H]1CCCN1 C(=O)C1=C(CC)N  =C2C=C3C=CC=C C3=CC2=C1)C(=O  )N[C@@H] (CCCC[NH3+])C(= O)NCCC[NH3+])C (=O)N[C@@H]  (CCCC[NH3+])C(= O)NCCC[NH3+] | CCCGCCUGCCUGCC UGCCUGCCUGCCUG CCUGCCUGCCUGCC UGCGG | DCC 11 (2012) | Target\_lig\_653 | r(CCUG)10 | Target\_179 | 7.1331  221856  625 |
| 1184 | NC(=[NH2+])C1= CC=C(NC2=CC=C (C=C2)C2=CC3=C C=C(C=C3N2)C(N | CCGCCGCCGCCGCC GCCGCCGCCGCCGC CGCCGCCG | Compound 2 | Target\_lig\_676 | r(CCG)12 | Target\_181 | 5 |

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|  | )=[NH2+])C=C1 |  |  |  |  |  |  |
| 1185 | NC(=[NH2+])C1= CC=C(NC2=CC=C (C=C2)C2=CC3=C C=C(C=C3N2)C(N  )=[NH2+])C=C1 | GGCCGGCCGGCCGG CC | Compound 2 | Target\_lig\_676 | r(GGCC)4 | Target\_182 | 5.1426  675035  6873 |
| 1187 | NC(=[NH2+])C1= CC=C(NC2=CC=C (C=C2)C2=CC3=C C=C(C=C3N2)C(N  )=[NH2+])C=C1 | GGGGCCGGGGCCGG GGCCGGGGCCGGGG CCGGGGCCGGGGCC GGGGCC | Compound 2 | Target\_lig\_676 | Hairpin Conformation of r(GGGGCC)8 | Target\_183 | 4.8239  087409  4432 |
| 1188 | NC(=[NH2+])C1= CC=C(NC2=CC=C (C=C2)C2=CC3=C C=C(C=C3N2)C(N  )=[NH2+])C=C1 | GGGGCCGGGGCCGG GGCCGGGGCCGGGG CCGGGGCCGGGGCC GGGGCC | 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 | GGGAGAGGGUUUA AUAUCAGUAUACG AAAGUAUACAGAU AUUGGAUCCGCAAG G | D6 | Target\_lig\_679 | 5'CAG/3'GAC | Target\_204 | 7.2218  487496  1636 |
| 1195 | CC1=C2C=C[N+] (CC[NH+]3CCCCC 3)=CC2=C(C)C2= C1NC1=C2C=C(O) C=C1 | CGGCGGCGGCGGCG GCGGCGGCGGCGGC GGCGGCGG | Hydroxyellipticine 1a | Target\_lig\_680 | r(CGG)12 | Target\_169 | 6.0969  100130  0806 |
| 1197 | CC1=C2C=C[N+] (CC[NH+]3CCCCC 3)=CC2=C(C)C2= C1NC1=C2C=C(O) C=C1 | CGGCGGCGGCGGCG GCGGCGGCGGCGGC GGCGGCGG | Hydroxyellipticine 1a | Target\_lig\_680 | 5'CGG/3'GGC  Loop | Target\_205 | 7.11918  640771  921 |
| 1199 | CC1=C2C=C[N+] (CC[NH+]3CCCCC 3)=CC2=C(C)C2= C1NC1=C2C=C(O) C=C1 | GGCCGGCCGGCCGG CC | Hydroxyellipticine 1a | Target\_lig\_680 | r(GGCC)4 | Target\_182 | 5.0757  207139  3812 |
| 1200 | CC1=C2C=C[N+] (CC[NH+]3CCCCC 3)=CC2=C(C)C2= C1NC1=C2C=C(O) C=C1 | GGGGCCGGGGCCGG GGCCGGGGCCGGGG CCGGGGCCGGGGCC GGGGCC | Hydroxyellipticine 1a | Target\_lig\_680 | Hairpin | Target\_183 | 4.3010  299956  6398 |
| 1202 | CC1=C2C=C[N+] (CC[NH+]3CCCCC 3)=CC2=C(C)C2= C1NC1=C2C=C(O) C=C1 | GGGGCCGGGGCCGG GGCCGGGGCCGGGG CCGGGGCCGGGGCC GGGGCC | Hydroxyellipticine 1a | Target\_lig\_680 | G-Quadruplex Conformation of r(GGGGCC)8 | Target\_184 | 4.0861  861476  1628 |
| 1207 | C1=CC(=CC(=C1) N)C2=NC3=C(N2) C=C(C=C3)C4=CC 5=C(C=C4)N=C(N  5)C6=CC(=CC=C6  )N | GGGAGAGGGUUUA AUCUGUACGAAAG UACUGAUUGGAUCC GCAAGG | H1 | Target\_lig\_684 | 5'CUG/3'GUC,  DM1 Motif | Target\_206 | 7.1549  019599  8574 |
| 1215 | C1CCN(C1)C2=NC (=C3C(=C2)C(=C( N=C3N)N4CCCC4  )C#N)N | CUGCUGCUGCUGCU GCUGCUGCUGCUGC UGCUGCUG | Naphthyridine 2 | Target\_lig\_686 | r(CUG)12 | Target\_167 | 6.9030  899869  9194 |
| 1216 | C1CCN(C1)C2=NC (=C3C(=C2)C(=C( N=C3N)N4CCCC4  )C#N)N | GGGAGAGGGUUUA AUCAGCAGCAGCAG CAGCAGUACGAAAG UACAGCAGCAGCAG CAGCAGAUUGGAUC CGCAAGG | Naphthyridine 2 | Target\_lig\_686 | r(CAG)12 | Target\_186 | 5.8538  719643  2176 |
| 1219 | C1=CC(=CC=C1C(  =O)NC2=NC=C(C  =C2)NC(=O)C3=C C=NC=C3)F | GGGAGAGGGUUUA AUCUGUACGAAAG UACUGAUUGGAUCC GCAAG | p7 | Target\_lig\_687 | 5' CUG/3' GUC  Internal Loop | Target\_210 | 5.3372  421683  1843 |
| 1248 | C1=CC(=CC=C1C 2=CC=C(O2)C3=C C=C(C=C3)C(=[N | GGCAGCAGCAGCAG CAGCAGCAGCAGCA GCAGCAGCAGCAGC | DB75 | Target\_lig\_697 | HTT exon1 RNA, 18 repeats | Target\_215 | 4.2225  731776  1069 |

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|  | H2+])N)C(=[NH2+  ])N | AGCAGCAGCAGCAG CC |  |  |  |  |  |
| 1249 | C1=CC(=CC=C1C 2=CC=C(O2)C3=C C=C(C=C3)C(=[N H2+])N)C(=[NH2+  ])N | GGCAGCAGCAGCAG CAGCAGCAGCAGCA GCAGCAGCAGCAGC AGCAGCAGCAGCAG CC | DB75 | Target\_lig\_697 | HTT exon1 RNA, 48 repeats | Target\_216 | 3.7958  800173  4407 |
| 1556 | C1=CC(=CC=C1C 2=CC=C(O2)C3=C C=C(C=C3)C(=N) N)C(=N)N | AUUCUAUUCUAUUC UAUUCUAUUCUAU UCUAUUCUAUUCUA UUCUAUUCUAUUCU | Compound\_2 | Target\_lig\_850 | r(AUUCU)11 | Target\_166 | 6.5228  787452  8034 |
| 1557 | N=[N+]=NCCCNC  (=N)c1ccc(cc1)c1cc c(o1)c1ccc(cc1)C(= N)N | AUUCUAUUCUAUUC UAUUCUAUUCUAU UCUAUUCUAUUCUA UUCUAUUCUAUUCU | AU-azide | Target\_lig\_851 | r(AUUCU)11 | Target\_166 | 6.4259  687322  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)c1c  cc(cc1)c1ccc(o1)c1 ccc(cc1)C(=N)N)C C(=O)N | AUUCUAUUCUAUUC UAUUCUAUUCUAU UCUAUUCUAUUCUA UUCUAUUCUAUUCU | 2AU-2 | Target\_lig\_1266 | r(AUUCU)11 | Target\_166 | 6.7328  282715  9699 |
| 1559 | C1=CC(=CC=C1C 2=CC=C(O2)C3=C C=C(C=C3)C(=N) N)C(=N)N | CUGCUGCUGCUGCU GCUGCUGCUGCUGC UGCUGCUG | Compound\_2 | Target\_lig\_850 | r(CUG)12 | Target\_167 | 5.3979  400086  7204 |
| 1560 | N=[N+]=NCCCNC  (=N)c1ccc(cc1)c1cc c(o1)c1ccc(cc1)C(= N)N | CUGCUGCUGCUGCU GCUGCUGCUGCUGC UGCUGCUG | AU-azide | Target\_lig\_851 | r(CUG)12 | Target\_167 | 5.3010  299956  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)c1c  cc(cc1)c1ccc(o1)c1 ccc(cc1)C(=N)N)C C(=O)N | CUGCUGCUGCUGCU GCUGCUGCUGCUGC UGCUGCUG | 2AU-2 | Target\_lig\_1266 | r(CUG)12 | Target\_167 | 5.3979  400086  7204 |
| 1562 | C1=CC(=CC=C1C 2=CC=C(O2)C3=C C=C(C=C3)C(=N) N)C(=N)N | CGGCGGCGGCGGCG GCGGCGGCGGCGGC GGCGGCGG | Compound\_2 | Target\_lig\_850 | r(CGG)12 | Target\_169 | 5.6989  700043  3602 |
| 1563 | N=[N+]=NCCCNC  (=N)c1ccc(cc1)c1cc c(o1)c1ccc(cc1)C(= N)N | CGGCGGCGGCGGCG GCGGCGGCGGCGGC GGCGGCGG | AU-azide | Target\_lig\_851 | r(CGG)12 | Target\_169 | 5.5228  787452  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)c1c  cc(cc1)c1ccc(o1)c1 ccc(cc1)C(=N)N)C C(=O)N | CGGCGGCGGCGGCG GCGGCGGCGGCGGC GGCGGCGG | 2AU-2 | Target\_lig\_1266 | r(CGG)12 | Target\_169 | 5.3979  400086  7204 |
| 1565 | C1=CC(=CC=C1C 2=CC=C(O2)C3=C C=C(C=C3)C(=N) N)C(=N)N | GGGAGAGGGUUUA AUCCUGCCUGCCUG CCUGCCUGCCUGUA CGAAAGUACCUGCC UGCCUGCCUGCCUG CCUGAUUGGAUCCG CAAGG | Compound\_2 | Target\_lig\_850 | r(CCUG)12 | Target\_185 | 5.3979  400086  7204 |
| 1566 | N=[N+]=NCCCNC  (=N)c1ccc(cc1)c1cc | GGGAGAGGGUUUA AUCCUGCCUGCCUG | AU-azide | Target\_lig\_851 | r(CCUG)12 | Target\_185 | 5.3010  299956 |

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|  | c(o1)c1ccc(cc1)C(= N)N | CCUGCCUGCCUGUA CGAAAGUACCUGCC UGCCUGCCUGCCUG CCUGAUUGGAUCCG CAAGG |  |  |  |  | 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)c1c  cc(cc1)c1ccc(o1)c1 ccc(cc1)C(=N)N)C C(=O)N | GGGAGAGGGUUUA AUCCUGCCUGCCUG CCUGCCUGCCUGUA CGAAAGUACCUGCC UGCCUGCCUGCCUG CCUGAUUGGAUCCG CAAGG | 2AU-2 | Target\_lig\_1266 | r(CCUG)12 | Target\_185 | 5.3979  400086  7204 |
| 1573 | COc1ccc2c(c1)c(N CCCCNc1nc(N)nc( n1)N)c1c(n2)cc(cc1  )Cl | GGGCUGCUGCUGCU GCUGCUGCUGCUGC UGCUGCUGCUGCUG CUGCUGCUGCCC | DM1\_compound1 | Target\_lig\_1267 | r(CUG)16 | Target\_281 | 6.4089  353929  735 |
| 1574 | [NH2+]=C(c1ccc(c c1)C(=[NH2+])NC  CCCNc1nc(N)nc(n 1)N)NCCCCNc1nc (N)nc(n1)N | GGGCUGCUGCUGCU GCUGCUGCUGCUGC UGCUGCUGCUGCUG CUGCUGCUGCCC | DM1\_compound3 | Target\_lig\_1268 | r(CUG)16 | Target\_281 | 5.0969  100130  0806 |
| 1575 | CN(CCCNc1nc(NC CCCCCNC(=O)CC 2=CCC(=N2)NC(= O)CC2=CCC(=N2) NC(=O)CCCCCCN  c2nc(N)nc(n2)N)nc (n1)N)C | GGGCUGCUGCUGCU GCUGCUGCUGCUGC UGCUGCUGCUGCUG CUGCUGCUGCCC | DM1\_compound5 | Target\_lig\_857 | r(CUG)16 | Target\_281 | 4.2596  373105  0576 |
| 1738 | Oc1ccc2c(c1)c1c(C  )c3c[n+] (CCN4CCCCC4)cc  c3c(c1[nH]2)C | GGGGCCGGGGCCGG GGCCGGGGCCGGGG CCGGGGCCGGGGCC GGGGCC | Compound1a | Target\_lig\_1274 | r(GGGGCC)8 | Target\_183 | 5.0132  282657  3376 |
| 1739 | NC(=N)c1ccc(cc1) Nc1ccc(cc1)c1cc2c( [nH]1)cc(cc2)C(=N  )N | GGGGCCGGGGCCGG GGCCGGGGCCGGGG CCGGGGCCGGGGCC GGGGCC | 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 | GGGGCCGGGGCCGG GGCCGGGGCCGGGG CCGGGGCCGGGGCC GGGGCC | Compound3 | Target\_lig\_969 | r(GGGGCC)8 | Target\_183 | 4.7958  800173  4408 |
| 1870 | NC(=[NH2+])C1= CC=C(N=C1)C1=C C=C(O1)C1=CC=C (O1)C1=NC=C(C= C1)C(N)=[NH2+] | GGGAGAGGGUUUA AUUCGGCGGCGGCG GCGGCGGUACGAAA GUACGGCGGCGGCG GCGGCGGAUUGGA UCCGCAAGG | B1 | Target\_lig\_716 | (5'CGG/3'GGC)x6 | Target\_347 | 6.7212  463990  4717 |
| 1871 | CC(C)C1=CC2=C( C=C1)N=C3C=CC(  =CN3C2=O)C(=O) NCCN(C)C | GGGAGAGGGUUUA AUUCGGCGGCGGCG GCGGCGGUACGAAA GUACGGCGGCGGCG GCGGCGGAUUGGA UCCGCAAGG | B4 | Target\_lig\_1035 | (5'CGG/3'GGC)x6 | Target\_347 | 6.5086  383061  6573 |
| 1872 | C1C[NH+]=C(N1) C2=CC=C(C=C2)C 3=CC=C(O3)C4=C C=C(C=C4)C5=[N H+]CCN5 | GGGAGAGGGUUUA AUUCGGCGGCGGCG GCGGCGGUACGAAA GUACGGCGGCGGCG GCGGCGGAUUGGA UCCGCAAGG | B6 | Target\_lig\_696 | (5'CGG/3'GGC)x6 | Target\_347 | 6.0604  807473  8138 |
| 1873 | C1=CC(=CC=C1C 2=CC=C(O2)C3=C C=C(C=C3)C(=[N H2+])N)C(=[NH2+  ])N | GGGAGAGGGUUUA AUUCGGCGGCGGCG GCGGCGGUACGAAA GUACGGCGGCGGCG GCGGCGGAUUGGA UCCGCAAGG | B7 | Target\_lig\_697 | (5'CGG/3'GGC)x6 | Target\_347 | 5.9355  420107  7308 |
| 1874 | C1COCCN1CCNC 2=C3C(=C(C=C2) | GGGAGAGGGUUUA AUUCGGCGGCGGCG | B11 | Target\_lig\_1042 | (5'CGG/3'GGC)x6 | Target\_347 | 6.4436  974992 |

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|  | NCCN4CCOCC4)C (=O)C5=CC=CC=C 5C3=O | GCGGCGGUACGAAA GUACGGCGGCGGCG GCGGCGGAUUGGA UCCGCAAGG |  |  |  |  | 3271 |
| 1875 | NC(=[NH2+])C1= CC=C(N=C1)C1=C C=C(O1)C1=CC=C (O1)C1=NC=C(C= C1)C(N)=[NH2+] | GGGAGAGGGUUUA AUUCAGCAGCAGCA GCAGCAGUACGAAA GUACUGCUGCUGCU GCUGCUGAUUGGA UCCGCAAGG | B1 | Target\_lig\_716 | (5'CAG/3'GUC)x6 | Target\_348 | 5.1674  910872  9376 |
| 1876 | CC(C)C1=CC2=C( C=C1)N=C3C=CC(  =CN3C2=O)C(=O) NCCN(C)C | GGGAGAGGGUUUA AUUCAGCAGCAGCA GCAGCAGUACGAAA GUACUGCUGCUGCU GCUGCUGAUUGGA UCCGCAAGG | B4 | Target\_lig\_1035 | (5'CAG/3'GUC)x6 | Target\_348 | 5.3767  507096  021 |
| 1877 | C1C[NH+]=C(N1) C2=CC=C(C=C2)C 3=CC=C(O3)C4=C C=C(C=C4)C5=[N H+]CCN5 | GGGAGAGGGUUUA AUUCAGCAGCAGCA GCAGCAGUACGAAA GUACUGCUGCUGCU GCUGCUGAUUGGA UCCGCAAGG | B6 | Target\_lig\_696 | (5'CAG/3'GUC)x6 | Target\_348 | 5.5528  419686  5778 |
| 1878 | C1=CC(=CC=C1C 2=CC=C(O2)C3=C C=C(C=C3)C(=[N H2+])N)C(=[NH2+  ])N | GGGAGAGGGUUUA AUUCAGCAGCAGCA GCAGCAGUACGAAA GUACUGCUGCUGCU GCUGCUGAUUGGA UCCGCAAGG | B7 | Target\_lig\_697 | (5'CAG/3'GUC)x6 | Target\_348 | 5.8860  566476  9316 |
| 1879 | C1COCCN1CCNC 2=C3C(=C(C=C2) NCCN4CCOCC4)C (=O)C5=CC=CC=C 5C3=O | GGGAGAGGGUUUA AUUCAGCAGCAGCA GCAGCAGUACGAAA GUACUGCUGCUGCU GCUGCUGAUUGGA UCCGCAAGG | B11 | Target\_lig\_1042 | (5'CAG/3'GUC)x6 | Target\_348 | 5.2839  966563  652 |
| 1880 | NC(=[NH2+])C1= CC=C(N=C1)C1=C C=C(O1)C1=CC=C (O1)C1=NC=C(C= C1)C(N)=[NH2+] | GGGAGAGGGUUUA AUUCGGCGGCGGCG GCGGCGGCGGCGGC GGCGGCGGCGGCGG CGGCGGCGGCGGCG GCGGCGGUACGAAA GUACGGCGGCGGCG GCGGCGGCGGCGGC GGCGGCGGCGGCGG CGGCGGCGGCGGCG GCGGCGGAUUGGA UCCGCAAGG | B1 | Target\_lig\_716 | (5'CGG/3'GGC)  x20 | Target\_349 | 7.0177  287669  6043 |
| 1881 | CC(C)C1=CC2=C( C=C1)N=C3C=CC(  =CN3C2=O)C(=O) NCCN(C)C | GGGAGAGGGUUUA AUUCGGCGGCGGCG GCGGCGGCGGCGGC GGCGGCGGCGGCGG CGGCGGCGGCGGCG GCGGCGGUACGAAA GUACGGCGGCGGCG GCGGCGGCGGCGGC GGCGGCGGCGGCGG CGGCGGCGGCGGCG GCGGCGGAUUGGA UCCGCAAGG | B4 | Target\_lig\_1035 | (5'CGG/3'GGC)  x20 | Target\_349 | 6.7695  510786  2173 |
| 1882 | C1COCCN1CCNC 2=C3C(=C(C=C2) NCCN4CCOCC4)C (=O)C5=CC=CC=C 5C3=O | GGGAGAGGGUUUA AUUCGGCGGCGGCG GCGGCGGCGGCGGC GGCGGCGGCGGCGG CGGCGGCGGCGGCG GCGGCGGUACGAAA GUACGGCGGCGGCG GCGGCGGCGGCGGC GGCGGCGGCGGCGG CGGCGGCGGCGGCG GCGGCGGAUUGGA UCCGCAAGG | B11 | Target\_lig\_1042 | (5'CGG/3'GGC)  x20 | Target\_349 | 6.6777  807052  6608 |
| 1883 | NC(=[NH2+])C1= CC=C(N=C1)C1=C | GGGAGAGGGUUUA AUUCGGCGGCGGCG | B1 | Target\_lig\_716 | (5'CGG/3'GGC)  x40 | Target\_350 | 7.0555  173278 |

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|  | 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 | 6.9586  073148  4177 |
| 1885 | C1COCCN1CCNC 2=C3C(=C(C=C2) NCCN4CCOCC4)C (=O)C5=CC=CC=C 5C3=O | GGGAGAGGGUUUA AUUCGGCGGCGGCG GCGGCGGCGGCGGC GGCGGCGGCGGCGG CGGCGGCGGCGGCG GCGGCGGCGGCGGC GGCGGCGGCGGCGG CGGCGGCGGCGGCG GCGGCGGCGGCGGC GGCGGCGGCGGUAC GAAAGUACGGCGGC GGCGGCGGCGGCGG CGGCGGCGGCGGCG GCGGCGGCGGCGGC GGCGGCGGCGGCGG CGGCGGCGGCGGCG GCGGCGGCGGCGGC GGCGGCGGCGGCGG CGGCGGCGGCGGCG GAUUGGAUCCGCAA GG | B11 | Target\_lig\_1042 | (5'CGG/3'GGC)  x40 | Target\_350 | 6.7212  463990  4717 |
| 1886 | NC(=[NH2+])C1= CC=C(N=C1)C1=C C=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 | 7.1487  416512  8092 |

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|  |  | 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 GCGGCGGCGGCGGC GGCGGCGGCGGCGG CGGCGGCGGCGGCG GCGGCGGCGGAUUG GAUCCGCAAGG | B4 | Target\_lig\_1035 | (5'CGG/3'GGC)  x60 | Target\_351 | 7 |
| 1888 | C1COCCN1CCNC 2=C3C(=C(C=C2) NCCN4CCOCC4)C (=O)C5=CC=CC=C 5C3=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 GCGGCGGCGGCGGC GGCGGCGGCGGCGG CGGCGGCGGCGGCG GCGGCGGCGGAUUG GAUCCGCAAGG | B11 | Target\_lig\_1042 | (5'CGG/3'GGC)  x60 | Target\_351 | 6.8538  719643  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 | 6.9208  187539  5238 |

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| 1955 | COC1=C(C=CC(= C1)C=CC(=O)CC(  =O)C=CC2=CC(=C (C=C2)O)OC)O | UUGGGCCGGCGGGU CC | Curcumin | Target\_lig\_1092 | r(CGGx2) | Target\_355 | 6.8860  566476  9316 |
| 1956 | COC1=C(C=CC(= C1)C=CC(=O)CC(  =O)C=CC2=CC(=C (C=C2)O)OC)O | UUGGGCCGGCGGCG GGUCC | Curcumin | Target\_lig\_1092 | r(CGGx3) | Target\_356 | 6.9208  187539  5238 |
| 1957 | COC1=C(C=CC(= C1)C=CC(=O)CC(  =O)C=CC2=CC(=C (C=C2)O)OC)O | UUGGGCCGGCGGCG GCGGGUCC | Curcumin | Target\_lig\_1092 | r(CGGx4) | Target\_357 | 6.9746  941347  3523 |
| 1958 | COC1=C(C=CC(= C1)C=CC(=O)CC(  =O)C=CC2=CC(=C (C=C2)O)OC)O | UUGGGCCGGCGGCG GCGGCGGCGGGUCC | Curcumin | Target\_lig\_1092 | r(CGGx6) | Target\_358 | 7.0362  121726  5444 |
| 1959 | COC1=C(C=CC(= C1)C=CC(=O)CC(  =O)C=CC2=CC(=C (C=C2)O)OC)O | UUGGGCCGGCGGCG GCGGCGGCGGCGGC GGCGGCGGCGGCGG CGGCGGCGGCGGCG GCGGCGGCGGGUCC | Curcumin | Target\_lig\_1092 | r(CGGx20) | Target\_359 | 7.4685  210829  5774 |
| 1960 | COC1=C(C=CC(= C1)C=CC(=O)CC(  =O)C=CC2=CC(=C (C=C2)O)OC)O | UUGGGCCGGCGGCG GCGGCGGCGGCGGC GGCGGCGGCGGCGG CGGCGGCGGCGGCG GCGGCGGCGGCGGC GGCGGCGGCGGCGG CGGCGGCGGCGGCG GCGGCGGCGGCGGC GGCGGCGGCGGCGG GUCC | Curcumin | Target\_lig\_1092 | r(CGGx40) | Target\_360 | 7.5376  020021  0104 |
| 1961 | COC1=C(C=CC(= C1)C=CC(=O)CC(  =O)C=CC2=CC(=C (C=C2)O)OC)O | UUGGGCCGGCGGCG GCGGCGGCGGCGGC GGCGGCGGCGGCGG CGGCGGCGGCGGCG GCGGCGGCGGCGGC GGCGGCGGCGGCGG CGGCGGCGGCGGCG GCGGCGGCGGCGGC GGCGGCGGCGGCGG CGGCGGCGGCGGCG GCGGCGGCGGCGGC GGCGGCGGCGGCGG CGGCGGCGGCGGCG GCGGGUCC | Curcumin | Target\_lig\_1092 | r(CGGx60) | Target\_361 | 7.8860  566476  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 | 5.6363  880201  0786 |
| 1963 | COC1=C(C=CC(= C1)C=CC(=O)CC(  =O)C=CC2=CC(=C (C=C2)O)OC)O | UUGGGCCAGCAGCA GCAGCAGCAGGUCC | Curcumin | Target\_lig\_1092 | r(CAGx6) | Target\_363 | 5.7958  800173  4408 |
| 1964 | COC1=C(C=CC(= C1)C=CC(=O)CC(  =O)C=CC2=CC(=C (C=C2)O)OC)O | UUGGGCCCGCCGCC GCCGCCGCCGGUCC | Curcumin | Target\_lig\_1092 | r(CCGx6) | Target\_364 | 6.0757  207139  3812 |
| 1965 | COC1=C(C=CC(= C1)C=CC(=O)CC(  =O)C=CC2=CC(=C (C=C2)O)OC)O | CUGCUGCUGCUGCU GCUG | Curcumin | Target\_lig\_1092 | r(CUGx6) | Target\_173 | 5.6575  773191  7779 |