Training dataset curated from [R-SIM](https://web.iitm.ac.in/bioinfo2/R_SIM/) database for the “Aptamers” 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** |
| 39 | C1=CC=C2C(= C1)C(=O)C3=C (C2=O)C(=C(C  =C3NC4=CC(= C(C=C4)NC5= NC(=NC(=N5) NC6=CC=CC= C6S(=O) (=O)O)Cl)S(=O)  (=O)O)S(=O) (=O)O)N | GGGAGAATTCCCGCG GCAGAAGCCCACCT GGCTTTGAACTCTAT GTTATTGGGTGGGGG AAACTTAAGAAAACT ACCACCCTTCAACAT TACCGCCCTTCAGCC TGCCAGCGCCCTGCA GCCCGGGAAGCTT | Cibacron blue | Target\_lig\_27 | RNA\_APTAM ER\_CB\_42 | Target\_4 | 4 |
| 40 | C1=CC=C2C(= C1)C(=O)C3=C (C2=O)C(=C(C  =C3NC4=CC(= C(C=C4)S(=O) (=O)O)NC5=N C(=NC(=N5)Cl)  Cl)S(=O)  (=O)O)N | GGGAGAAUUCCCGC GGCGUUGGCCCAGG AUAAUAGGACGAAA UCCGAAAAAUCCGU ACCCAACAUGAACC CCCCAGCGCUCACA CGGACGCCCCAUUA CGGCUAACCGAACG CCUGCAGCCCGGGA AGCUU | Reactive Blue 4 | Target\_lig\_28 | RNA\_APTAM ER\_B4\_25 | Target\_5 | 3.2218487496  1636 |
| 91 | C1=NC(=C2C(= N1)N(C=N2)C3 C(C(C(O3)COP (=O)(O)OP(=O) (O)OP(=O)  (O)O)O)O)N | GGGAAGGGAAGAAA CUGCGGCUUCGGCC GGCUUCCC | ATP | Target\_lig\_65 | RNA\_Aptamer | Target\_6 | 5.3979400086  7204 |
| 92 | C1=NC(=C2C(= N1)N(C=N2)C3 C(C(C(O3)COP (=O) (O)O)O)O)N | GGGAAGGGAAGAAA CUGCGGCUUCGGCC GGCUUCCC | AMP | Target\_lig\_66 | RNA\_Aptamer | Target\_6 | 8.3010256527  4088 |
| 93 | CC1=CC2=C(C  =C1C)N(C3=N C(=O)NC(=O)C  3=N2)CC(C(C( COP(=O) (O)OP(=O)  (O)OCC4C(C(C (O4)N5C=NC6= C(N=CN=C65) N)O)O)O)O)O | GGCGUGUAGGAUAU GCUUCGGCAGAAGG ACACGCC | FAD | Target\_lig\_67 | 35 nucleotide RNA | Target\_26 | 4.6382721639  8241 |
| 94 | CC1=CC2=C(C  =C1C)N(C3=N C(=O)NC(=O)C  3=N2)CC(C(C( COP(=O) (O)O)O)O)O | GGCGUGUAGGAUAU GCUUCGGCAGAAGG ACACGCC | FMN | Target\_lig\_68 | 35 nucleotide RNA | Target\_26 | 6.3010299956  6398 |
| 95 | C1=NC(=C2C(= N1)N(C=N2)C3 C(C(C(O3)CO) O)O)N | GGCGUGUAGGAUAU GCUUCGGCAGAAGG ACACGCC | ADENOSINE | Target\_lig\_69 | 35 nucleotide RNA | Target\_26 | 2.3979400086  7204 |
| 96 | CC1=CC2=C(C  =C1C)N(C3=N C(=O)NC(=O)C  3=N2)CC(C(C(  CO)O)O)O | GGAACGAGGGAUGG AGGAGGAGUCGUUC C | riboflavin | Target\_lig\_70 | Riboflavin binding RNA aptamer | Target\_29 | - 0.4771212547  19662 |
| 97 | C1=CC(=C[N+] (=C1)C2C(C(C( O2)COP(=O) (O)  [O-])O)O)C(=O) N | GGAACCCAACUAGG CGUUUGAGGGGAUU CGGCCACGGUAACA ACCCCUC | NMN | Target\_lig\_71 | NMN binding RNA aptamer | Target\_30 | 5.6020599913  2796 |
| 98 | CC1=CC2=C(C  =C1C)N(C=N2) C3C(C(C(O3)C  O)OP(=O) | CGGGUGCGCAUAAC CACCUCAGUGCGAG CAA | cyanocobalamine | Target\_lig\_72 | cyanocobalami n 35 nt RNA aptamer | Target\_31 | 7.0604807473  8138 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA\_ID** | **pKd** |
|  | ([O-])OC(C)CN C(=O)CCC4(C(  C5C6(C(C(C(=  N6)C(=C7C(C( C(=N7)C=C8C( C(C(=N8)C(=C 4[N-]5)C)CCC(  =O)N) (C)C)CCC(=O) N) (C)CC(=O)N)C) CCC(=O)N) (C)CC(=O)N)C)  CC(=O)N)C)O.  [C-]#N.[Co+3] |  |  |  |  |  |  |
| 99 | C/C/1=C/2\ [C@@] ([C@@H] (C(=N2)/C=C\3/ C([C@@H]  (C(=N3)/C(=C\  4/[C@]([C@H]  (C([N-]4)  [C@]5([C@@] ([C@@H] (C1=N5)CCC(= O)N) (C)CC(=O)N)C) CC(=O)N)  (C)CCC(=O)NC  C(C)O)/  C)CCC(=O)N)  (C)C)CCC(=O)  N)(C)CC(=O)N.  [C-]#N.[C-]#N. [Co] | CGGGUGCGCAUAAC CACCUCAGUGCGAG CAA | cobinamide dicyanide | Target\_lig\_73 | cyanocobalami n 35 nt RNA aptamer | Target\_31 | 4.7055337738  3841 |
| 210 | CN1C2=C(C(= O)N(C1=O)C)N C=N2 | AAGUGAUACCAGCA UCGUCUUGAUGCCC UUGGCAGCACUUCA | Theophylline | Target\_lig\_15 4 | TCT8-4 RNA  Aptamer | Target\_32 | 6.4948500216  8009 |
| 211 | CN1C=NC2=C1 C(=O)N(C(=O) N2C)C | AAGUGAUACCAGCA UCGUCUUGAUGCCC UUGGCAGCACUUCA | caffeine | Target\_lig\_15 5 | TCT8-4 RNA  Aptamer | Target\_32 | 2.4559319556  4972 |
| 213 | CN1C2=C(C(= O)N(C1=O)C)N C(=O)N2 | AAGUGAUACCAGCA UCGUCUUGAUGCCC UUGGCAGCACUUCA | 1,3-dimethyluric acid | Target\_lig\_15 7 | TCT8-4 RNA  Aptamer | Target\_32 | 3 |
| 214 | CN1C=NC2=C1 C(=O)NC(=O)N 2C | AAGUGAUACCAGCA UCGUCUUGAUGCCC UUGGCAGCACUUCA | 3,7-  dimethylxanthine | Target\_lig\_15 8 | TCT8-4 RNA  Aptamer | Target\_32 | 3.3010299956  6398 |
| 215 | CN1C2=C(C(= O)NC1=O)NC= N2 | AAGUGAUACCAGCA UCGUCUUGAUGCCC UUGGCAGCACUUCA | 3-methylxanthine | Target\_lig\_15 9 | TCT8-4 RNA  Aptamer | Target\_32 | 5.6989700043  3602 |
| 216 | CN1C=NC2=C1 C(=O)NC(=O)N 2 | AAGUGAUACCAGCA UCGUCUUGAUGCCC UUGGCAGCACUUCA | 7-methylxanthine | Target\_lig\_16 0 | TCT8-4 RNA  Aptamer | Target\_32 | 3.3010299956  6398 |
| 217 | CN1C2=C(C(= O)N(C1=O)CC C(=O)O)NC=N 2 | AAGUGAUACCAGCA UCGUCUUGAUGCCC UUGGCAGCACUUCA | CP-theophylline | Target\_lig\_16 1 | TCT8-4 RNA  Aptamer | Target\_32 | 6.0315170514  4607 |
| 218 | C1=NC2=C(N1) C(=O)N=CN2 | AAGUGAUACCAGCA UCGUCUUGAUGCCC UUGGCAGCACUUCA | Hypoxanthine | Target\_lig\_16 2 | TCT8-4 RNA  Aptamer | Target\_32 | 4.3098039199  7149 |
| 219 | CN1C(=O)C2= C(NC1=O)N=C N2 | AAGUGAUACCAGCA UCGUCUUGAUGCCC UUGGCAGCACUUCA | xanthine | Target\_lig\_15 6 | TCT8-4 RNA  Aptamer | Target\_32 | 5.0705810742  8571 |
| 285 | [C@@H]1([C@ H]([C@H](O) [C@H] ([C@@H] | CGCGCGUGUGCGCG | B-12 | Target\_lig\_22 4 | RNA hairpin loop | Target\_120 | 4.6020599913  2796 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA\_ID** | **pKd** |
|  | (C1)N)O)OCCC  c1cn(nn1)Cc1cc cc(Cn2cc(nn2)C CCO[C@H]2[C  @@H] (C[C@@H] ([C@@H](O)  [C@H]2O)N)N) c1)N |  |  |  |  |  |  |
| 288 | C1C2C(C(S1)C CCCC(=O)O)N C(=O)N2 | GGAACACUAUCCGA UGGCACCGACCAUA GGCUCGGGUUGCCA GAGGUUCCACACUU UCAUCGAAAAGCCU AUGCUAGGCAAUGA CAUGGACUCCUUGG UCAUUAGGAUCG | biotin\_molecule | Target\_lig\_22 7 | Biotin aptamer | Target\_33 | 5.2438966284  149 |
| 309 | C1C(C(C(C(C1  N)OC2C(C(C(C (O2)CO)O)N)O) O)OC3C(CC(C(  O3)CN)O)N)N | GGGUCUCGAGUUUU CGAAGACCC | Ethidium bromide | Target\_lig\_6 | Bulge\_A\_RNA | Target\_121 | 5.4814860601  2211 |
| 311 | CC1=CC2=C(C  =C1C)N(C3=N C(=O)NC(=O)C  3=N2)CC(C(C( COP(=O) (O)O)O)O)O | GGCGUGUAGGAUAU GCUUCGGCAGAAGG ACACGCC | FMN | Target\_lig\_68 | FMN aptamer | Target\_34 | 8.3010299956  6398 |
| 385 | CN(C)C1=CC= C(C=C1)C(=C2 C=CC(=[N+] (C)C)C=C2)C3= CC=CC=C3.  [Cl-] | GGGAAGGGAAGAAA CUGCGGCUUCGGCC GGCUUCCC | Malachite green | Target\_lig\_30 8 | Aptamer | Target\_6 | 7.3010299956  6398 |
| 417 | CC1(C2CC3C( C(=O)C(=C(C3( C(=O)C2=C(C4  =C1C=CC=C4O  )O)O)O)C(=O) N)N(C)C)O | GGGCCUAAAACAUA CCAGAUCGCCACCC GCGCUUUAAUCUGG AGAGGUGAAGAAUA CGACACCUAGGCUC | tetracyclin | Target\_lig\_74 | Tetracycline in vitro aptamer | Target\_39 | 9.0969100130  0806 |
| 457 | CC1=C2C=CN= CC2=C(C3=C1 NC4=CC=CC= C43)C | AAAAAAAAAAAAAA AAAAAAAAAAAAAA AAAAAAAAAAAAAA AAAAAAAAAAAAAA AAAAAAAAAAAAAA AAAAAAAAAAAAAA AAAAAAAAAAAAAA AAAAAAAAAAAAAA AAAAAAAAAAAAAA AAAAAAAAAAAAAA AAAAAAAAAAAAAA AAAAAAAAAAAAAA AAAAAAAAAAAAAA AAAAAAAAAAAAAA AAAA | Ellipticine | Target\_lig\_34 2 | ss\_PolyA | Target\_40 | 5.3372421683  1843 |
| 752 | C1CN(CCN1C[ C@@H]2[C@H  ] (OC(=O)N2)CO C(=O)CC3=CC  =CC=C3)C4=C C=CC=C4 | GAGGGUGGAACCGC GCUUCGGCGUCCCU C | phenylacetate derivative | Target\_lig\_51 0 | T-box riboswitch | Target\_79 | 5.1804560644  5813 |
| 753 | CC(=O)C1=CC  =C(C=C1)NC(= O)OC[C@@H] 2[C@H] (NC(=O)O2)CN 3CCN(CC3)C4= CC=CC=C4 | GAGGGUGGAACCGC GCUUCGGCGUCCCU C | methyl N-(4- acetylphenyl)car bamate derivative | Target\_lig\_51 1 | T-box riboswitch | Target\_79 | 6.0457574905  6068 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA\_ID** | **pKd** |
| 778 | CC1C(C(C(C(O 1)OC2C3CC#C C4C(O4) (C#CC3=CC2O C(=O)C5=C(C= CC6=C5C=C(C  =C6C)OC)O)C7 COC(=O)O7)N C)O)O | GUCCGAUGCGUGUU UCACGCAGUUCGGA C | neocarzinostatin | Target\_lig\_14 8 | RNA XIII | Target\_123 | 5.9586073148  4177 |
| 779 | c12c(cccc1) [C@]1(C(=O)C  =C2)[C@@H] (O[C@@H]2[C  @@H]1c1c(C2  =O)cc2c(c1)ccc c2)O[C@@H]1[ C@H] ([C@@H] ([C@H]([C@H]  (O1)CO)O)O)N | GUCCGAUGCGUGUU UCACGCAGUUCGGA C | Neocarzinostatin  \_chromophore\_d erivative\_2 | Target\_lig\_15 0 | RNA XIII | Target\_123 | 4.6777807052  6608 |
| 780 | c12c(cccc1) [C@]1([C@@H  ] (C=C2)O[C@H] 2[C@@H] ([C@H]  ([C@@H]  ([C@@H] (O2)CO)O)O)N) C(=O)O[C@H]  2[C@@H]1c1c( C2=O)cc2c(c1)c ccc2 | GUCCGAUGCGUGUU UCACGCAGUUCGGA C | Neocarzinostatin  \_chromophore\_d erivative\_3 | Target\_lig\_15 1 | RNA XIII | Target\_123 | 4.6575773191  7779 |
| 781 | c12c(cc(cc1)OC  ) [C@@]1(C(=O) C=C2)C=C[C@ @H]2[C@@H] 1c1c([C@H]2O[ C@@H]2[C@H  ]([C@@H]  ([C@@H]  ([C@@H] (O2)C)O)O)NC)  cc2c(c1)cccc2 | GUCCGAUGCGUGUU UCACGCAGUUCGGA C | Neocarzinostatin  \_chromophore\_d erivative\_5 | Target\_lig\_15 2 | RNA XIII | Target\_123 | 5.8860566476  9316 |
| 782 | c12c(cccc1) [C@]1(C(=O)C  =C2)[C@@H] (O[C@@H]2[C  @@H]1c1c(C2  =O)cc2c(c1)ccc c2)O[C@@H]1[ C@H] ([C@@H] ([C@H]([C@H]  (O1)CO)O)O)N | GUCCGAUGCGUGUU UCACGCAGUCGGAC | Neocarzinostatin  \_chromophore\_d erivative\_2 | Target\_lig\_15 0 | RNA XIV | Target\_124 | 4.7212463990  4717 |
| 783 | c12c(cccc1) [C@]1([C@@H  ] (C=C2)O[C@H] 2[C@@H] ([C@H]  ([C@@H]  ([C@@H] (O2)CO)O)O)N) C(=O)O[C@H]  2[C@@H]1c1c( C2=O)cc2c(c1)c ccc2 | GUCCGAUGCGUGUU UCACGCAGUCGGAC | Neocarzinostatin  \_chromophore\_d erivative\_3 | Target\_lig\_15 1 | RNA XIV | Target\_124 | 4.1674910872  9376 |
| 784 | c12c(cccc1) [C@]1(C(=O)C | GUCCGAUGCGUGUU UCACGCAUCGGAC | Neocarzinostatin  \_chromophore\_d | Target\_lig\_15 0 | RNA XV | Target\_125 | 4.6989700043  3602 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA\_ID** | **pKd** |
|  | =C2)[C@@H] (O[C@@H]2[C  @@H]1c1c(C2  =O)cc2c(c1)ccc c2)O[C@@H]1[ C@H] ([C@@H] ([C@H]([C@H]  (O1)CO)O)O)N |  | erivative\_2 |  |  |  |  |
| 785 | c12c(cc(cc1)OC  ) [C@@]1(C(=O) C=C2)C=C[C@ @H]2[C@@H] 1c1c([C@H]2O[ C@@H]2[C@H  ]([C@@H] ([C@H]([C@H]  (O2)CO)O)O)N)  cc2c(c1)cccc2 | GUCCGAUGCGUGUU UCACGCAUCGGAC | Neocarzinostatin  \_chromophore\_d erivative\_4 | Target\_lig\_52 6 | RNA XV | Target\_125 | 5.3010299956  6398 |
| 786 | c12c(cc(cc1)OC  ) [C@@]1(C(=O) C=C2)C=C[C@ @H]2[C@@H] 1c1c([C@H]2O[ C@@H]2[C@H  ]([C@@H]  ([C@@H]  ([C@@H] (O2)C)O)O)NC)  cc2c(c1)cccc2 | GUCCGAUGCGUGUU UCACGCAUCGGAC | Neocarzinostatin  \_chromophore\_d erivative\_5 | Target\_lig\_15 2 | RNA XV | Target\_125 | 5.3098039199  7149 |
| 787 | c12c(cc(cc1)OC  ) [C@@]1(C(=O) C=C2)C=C[C@ H]2[C@H]1c1c( [C@@H]2O[C @@H]2[C@H] ([C@@H]  ([C@@H]  ([C@@H] (O2)C)O)O)NC)  cc2c(c1)cccc2 | GUCCGAUGCGUGUU UCACGCAUCGGAC | Neocarzinostatin  \_chromophore\_d erivative\_6 | Target\_lig\_15 3 | RNA XV | Target\_125 | 4.9208187539  5238 |
| 788 | c12c(cc(cc1)OC  ) [C@@]1(C(=O) C=C2)C=C[C@ @H]2[C@@H] 1c1c([C@H]2O[ C@@H]2[C@H  ]([C@@H]  ([C@@H]  ([C@@H] (O2)C)O)O)NC)  cc2c(c1)cccc2 | GUCCGAUGCGUGUU UUCACGCAGUUCGG AC | Neocarzinostatin  \_chromophore\_d erivative\_5 | Target\_lig\_15 2 | RNA XVII | Target\_126 | 5.7958800173  4408 |
| 789 | c12c(cc(cc1)OC  ) [C@@]1(C(=O) C=C2)C=C[C@ H]2[C@H]1c1c( [C@@H]2O[C @@H]2[C@H] ([C@@H]  ([C@@H]  ([C@@H] (O2)C)O)O)NC)  cc2c(c1)cccc2 | GUCCGAUGCGUGUU UUCACGCAGUUCGG AC | Neocarzinostatin  \_chromophore\_d erivative\_6 | Target\_lig\_15 3 | RNA XVII | Target\_126 | 5.5528419686  5778 |
| 790 | CC1C(C(C(O1)  OC2C(C(C(C(C  2O)O)N=C(N)N | GAGGGUGGAACCGC GCUUCGGCGUCCCU C | Streptomycin | Target\_lig\_63 | T box antiterminator RNA | Target\_112 | 3.1023729087  0956 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA\_ID** | **pKd** |
|  | )O)N=C(N)N)O  C3C(C(C(C(O3)  CO)O)O)NC) (C=O)O |  |  |  |  |  |  |
| 791 | C1C(C(C(C(C1  N)OC2C(C(C(C (O2)CO)O)O)N) OC3C(C(C(O3)  CO)OC4C(C(C(  C(O4)CN)O)O) N)O)O)N | GAGGGUGGAACCGC GCUUCGGCGUCCCU C | Paromomycin\_m ol\_mol | Target\_lig\_11 16 | T box antiterminator RNA | Target\_112 | 4.3010299956  6398 |
| 792 | [C@H]1([C@H] (C[C@H]  ([C@H] ([C@H]1O)O[C  @@H]1[C@@ H](C[C@@H]  ([C@@H] (O1)CN)O)N)N) N)O[C@@H]1[ C@H] ([C@@H]  ([C@H]  ([C@@H]  (O1)CNc1c2ccc cc2nc2c1cccc2) O)N)O | GAGGGUGGAACCGC GCUUCGGCGUCCCU C | Tobramycin | Target\_lig\_54 0 | T box antiterminator RNA | Target\_112 | 4.4202164033  8319 |
| 793 | C1C(C(C(C(C1  N)OC2C(C(C(C (O2)CN)O)O)O) O)OC3C(C(C(C (O3)CO)O)N)O) N | GAGGGUGGAACCGC GCUUCGGCGUCCCU C | Kanamycin A | Target\_lig\_7 | T box antiterminator RNA | Target\_112 | 3.6777807052  6608 |
| 794 | C1C(C(C(C(C1  N)OC2C(C(C(C (O2)CO)O)N)O) O)OC3C(C(C(C (O3)CN)O)O)N) N | GAGGGUGGAACCGC GCUUCGGCGUCCCU C | KANAMYCIN B | Target\_lig\_8 | T box antiterminator RNA | Target\_112 | 3.8239087409  4432 |
| 795 | C1C(C(C(C(C1  N)OC2C(C(C(C (O2)CN)O)O)N) OC3C(C(C(O3)  CO)OC4C(C(C(  C(O4)CN)O)O) N)O)O)N | GAGGGUGGAACCGC GCUUCGGCGUCCCU C | Neomycin\_B | Target\_lig\_12 46 | T box antiterminator RNA | Target\_112 | 5.0705810742  8571 |
| 796 | CC1(COC(C(C1 NC)O)OC2C(C C(C(C2O)OC3C (CCC(O3)CN)N  )N)N)O | GAGGGUGGAACCGC GCUUCGGCGUCCCU C | gentamicin\_mol\_ c | Target\_lig\_76 | T box antiterminator RNA | Target\_112 | 3.9208187539  5237 |
| 797 | C1C(C(C(C(C1  NC(=O)C(CCN)  O)OC2C(C(C(C (O2)CO)O)N)O) O)OC3C(C(C(C (O3)CN)O)O)O) N | GAGGGUGGAACCGC GCUUCGGCGUCCCU C | Amikacin | Target\_lig\_17 5 | T box antiterminator RNA | Target\_112 | 3.1191864077  1921 |
| 801 | CC1CC(=O)C2( C(O1)OC3C(C(  C(C(C3O2)NC)  O)NC)O)O | AUUUUUCCUCGAAC UUGGCGGAACGCAG AAAAAU | Spectinomycin | Target\_lig\_75 | SLI of Rep A | Target\_127 | 5.3979400086  7204 |
| 802 | CNC1CC(C(C( C1O)OC2C3C( C(C(O2)CO)O)  OC4(O3)C(C(C(  C(O4)C(CO)N)  O)O)O)O)N | AUUUUUCCUCGAAC UUGGCGGAACGCAG AAAAAU | Hygromycin\_B | Target\_lig\_3 | SLI of Rep A | Target\_127 | 5.3979400086  7204 |
| 803 | C1C(C(C(C(C1 | AUUUUUCCUCGAAC | Neomycin | Target\_lig\_4 | SLI of Rep A | Target\_127 | 7.0969100130 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA\_ID** | **pKd** |
|  | N)OC2C(C(C(C (O2)CN)O)O)N) OC3C(C(C(O3)  CO)OC4C(C(C(  C(O4)CN)O)O) N)O)O)N | UUGGCGGAACGCAG AAAAAU |  |  |  |  | 0806 |
| 804 | C1C(C(C(C(C1  N)OC2C(C(C(C (O2)CO)O)O)N) OC3C(C(C(O3)  CO)OC4C(C(C(  C(O4)CN)O)O) N)O)O)N | AUUUUUCCUCGAAC UUGGCGGAACGCAG AAAAAU | Paromomycin\_m ol\_mol | Target\_lig\_11 16 | SLI of Rep A | Target\_127 | 7.3979400086  7204 |
| 805 | [C@H]1([C@H] (C[C@H]  ([C@H] ([C@H]1O)O[C  @@H]1[C@@ H](C[C@@H]  ([C@@H] (O1)CN)O)N)N) N)O[C@@H]1[ C@H] ([C@@H]  ([C@H]  ([C@@H]  (O1)CNc1c2ccc cc2nc2c1cccc2) O)N)O | AUUUUUCCUCGAAC UUGGCGGAACGCAG AAAAAU | Tobramycin | Target\_lig\_54 0 | SLI of Rep A | Target\_127 | 7.3979400086  7204 |
| 806 | C1C(C(C(C(C1  N)OC2C(C(C(C (O2)CN)O)O)O) O)OC3C(C(C(C (O3)CO)O)N)O) N | AUUUUUCCUCGAAC UUGGCGGAACGCAG AAAAAU | Kanamycin A | Target\_lig\_7 | SLI of Rep A | Target\_127 | 6.7695510786  2173 |
| 807 | C1C(C(C(C(C1  N)OC2C(C(C(C (O2)CO)O)N)O) O)OC3C(C(C(C (O3)CN)O)O)N) N | AUUUUUCCUCGAAC UUGGCGGAACGCAG AAAAAU | KANAMYCIN B | Target\_lig\_8 | SLI of Rep A | Target\_127 | 6.9586073148  4177 |
| 808 | CC1(COC(C(C1 NC)O)OC2C(C C(C(C2O)OC3C (CC=C(O3)CN)  N)N)N)O | AUUUUUCCUCGAAC UUGGCGGAACGCAG AAAAAU | sisomicin | Target\_lig\_10 | SLI of Rep A | Target\_127 | 7.5228787452  8034 |
| 809 | C1C(C(C(C(C1  NC(=O)C(CCN)  O)OC2C(C(C(C (O2)CO)O)N)O) O)OC3C(C(C(C (O3)CN)O)O)O) N | AUUUUUCCUCGAAC UUGGCGGAACGCAG AAAAAU | Amikacin | Target\_lig\_17 5 | SLI of Rep A | Target\_127 | 7.0969100130  0806 |
| 810 | CC1(COC(C(C1 NC)O)OC2C(C C(C(C2O)OC3C (CCC(O3)CN)N  )N)N)O | AUUUUUCCUCGAAC UUGGCGGAACGCAG AAAAAU | gentamicin\_mol | Target\_lig\_76 | SLI of Rep A | Target\_127 | 7.0969100130  0806 |
| 811 | C1C(C(C(C(C1  NC(=O)C(CCN)  O)O)OC2C(C(C  (O2)CO)O)O)O  C3C(C(C(C(O3)  CN)O)O)N)N | AUUUUUCCUCGAAC UUGGCGGAACGCAG AAAAAU | Butirosin | Target\_lig\_22 0 | SLI of Rep A | Target\_127 | 6.6989700043  3602 |
| 812 | C1C(C(C(C(C1  N)OC2C(C(C(C (O2)CN)O)O)N) OC3C(C(C(O3)  CO)OC4C(C(C( | CCCCCCCGCCGCGCC AUGCCUGUGGCCGG UCGG | Neomycin | Target\_lig\_4 | Thymidylate synthase m- RNA | Target\_63 | 6.0565054840  939 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA\_ID** | **pKd** |
|  | C(O4)CN)O)O) N)O)O)N |  |  |  |  |  |  |
| 813 | C1C(C(C(C(C1  N)OC2C(C(C(C (O2)CO)O)O)N) OC3C(C(C(O3)  CO)OC4C(C(C(  C(O4)CN)O)O) N)O)O)N | CCCCCCCGCCGCGCC AUGCCUGUGGCCGG UCGG | Paromomycin\_m ol\_mol | Target\_lig\_11 16 | Thymidylate synthase m- RNA | Target\_63 | 5.6343248595  4408 |
| 814 | [C@H]1([C@H] (C[C@H]  ([C@H] ([C@H]1O)O[C  @@H]1[C@@ H](C[C@@H]  ([C@@H] (O1)CN)O)N)N) N)O[C@@H]1[ C@H] ([C@@H]  ([C@H]  ([C@@H]  (O1)CNc1c2ccc cc2nc2c1cccc2) O)N)O | CCCCCCCGCCGCGCC AUGCCUGUGGCCGG UCGG | Tobramycin | Target\_lig\_54 0 | Thymidylate synthase m- RNA | Target\_63 | 5.6929320493  387 |
| 815 | C1C(C(C(C(C1  N)OC2C(C(C(C (O2)CO)O)N)O) O)OC3C(C(C(C (O3)CN)O)O)N) N | CCCCCCCGCCGCGCC AUGCCUGUGGCCGG UCGG | KANAMYCIN B | Target\_lig\_8 | Thymidylate synthase m- RNA | Target\_63 | 5.6605485586  9356 |
| 816 | CC1(COC(C(C1 NC)O)OC2C(C C(C(C2O)OC3C (CCC(O3)CN)N  )N)N)O | CCCCCCCGCCGCGCC AUGCCUGUGGCCGG UCGG | gentamicin\_mol | Target\_lig\_76 | Thymidylate synthase m- RNA | Target\_63 | 5.5657505476  0353 |
| 817 | CC1C(C(C(O1)  OC2C(C(C(C(C  2O)O)N=C(N)N  )O)N=C(N)N)O  C3C(C(C(C(O3)  CO)O)O)NC) (C=O)O | GGCUGACCAUCAAU AAGGAAGAAGCCCU UCAGCGGCCAGUA | Streptomycin | Target\_lig\_63 | Bcr-Abl m- RNA | Target\_64 | 4.6989700043  3602 |
| 818 | CC1CC(=O)C2( C(O1)OC3C(C(  C(C(C3O2)NC)  O)NC)O)O | GGCUGACCAUCAAU AAGGAAGAAGCCCU UCAGCGGCCAGUA | Spectinomycin | Target\_lig\_75 | Bcr-Abl m- RNA | Target\_64 | 4 |
| 819 | CNC1CC(C(C( C1O)OC2C3C( C(C(O2)CO)O)  OC4(O3)C(C(C(  C(O4)C(CO)N)  O)O)O)O)N | GGCUGACCAUCAAU AAGGAAGAAGCCCU UCAGCGGCCAGUA | Hygromycin\_B | Target\_lig\_3 | Bcr-Abl m- RNA | Target\_64 | 4 |
| 820 | C1C(C(C(C(C1  N)OC2C(C(C(C (O2)CN)O)O)N) OC3C(C(C(O3)  CO)OC4C(C(C(  C(O4)CN)O)O) N)O)O)N | GGCUGACCAUCAAU AAGGAAGAAGCCCU UCAGCGGCCAGUA | Neomycin | Target\_lig\_4 | Bcr-Abl m- RNA | Target\_64 | 5.8239087409  4432 |
| 821 | C1C(C(C(C(C1  N)OC2C(C(C(C (O2)CO)O)O)N) OC3C(C(C(O3)  CO)OC4C(C(C(  C(O4)CN)O)O) N)O)O)N | GGCUGACCAUCAAU AAGGAAGAAGCCCU UCAGCGGCCAGUA | Paromomycin\_m ol\_mol | Target\_lig\_11 16 | Bcr-Abl m- RNA | Target\_64 | 5.7695510786  2173 |
| 822 | CNC1C(C2C(C C(C(O2)OC3C( | GGCUGACCAUCAAU AAGGAAGAAGCCCU | apramycin | Target\_lig\_79 | Bcr-Abl m- RNA | Target\_64 | 4.6989700043  3602 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA\_ID** | **pKd** |
|  | CC(C(C3O)O)N  )N)N)OC1OC4 C(C(C(C(O4)C  O)N)O)O)O | UCAGCGGCCAGUA |  |  |  |  |  |
| 823 | C1C(C(C(C(C1  N)OC2C(C(C(C (O2)CN)O)O)N) O)O)N | GGCUGACCAUCAAU AAGGAAGAAGCCCU UCAGCGGCCAGUA | Neamine | Target\_lig\_80 | Bcr-Abl m- RNA | Target\_64 | 4.7695510786  2173 |
| 824 | CC(C1C(C(C(C  (O1)OC2C(CC( C(C2O)OC3C(C (C(CO3) (C)O)NC)O)N) N)N)O)O)O | GGCUGACCAUCAAU AAGGAAGAAGCCCU UCAGCGGCCAGUA | Geneticin | Target\_lig\_14 0 | Bcr-Abl m- RNA | Target\_64 | 4.6989700043  3602 |
| 825 | [C@H]1([C@H] (C[C@H]  ([C@H] ([C@H]1O)O[C  @@H]1[C@@ H](C[C@@H]  ([C@@H] (O1)CN)O)N)N) N)O[C@@H]1[ C@H] ([C@@H]  ([C@H]  ([C@@H]  (O1)CNc1c2ccc cc2nc2c1cccc2) O)N)O | GGCUGACCAUCAAU AAGGAAGAAGCCCU UCAGCGGCCAGUA | Tobramycin | Target\_lig\_54 0 | Bcr-Abl m- RNA | Target\_64 | 5.4436974992  3271 |
| 826 | C1C(C(C(C(C1  N)OC2C(C(C(C (O2)CN)O)O)O) O)OC3C(C(C(C (O3)CO)O)N)O) N | GGCUGACCAUCAAU AAGGAAGAAGCCCU UCAGCGGCCAGUA | Kanamycin A | Target\_lig\_7 | Bcr-Abl m- RNA | Target\_64 | 5 |
| 827 | C1C(C(C(C(C1  N)OC2C(C(C(C (O2)CO)O)N)O) O)OC3C(C(C(C (O3)CN)O)O)N) N | GGCUGACCAUCAAU AAGGAAGAAGCCCU UCAGCGGCCAGUA | KANAMYCIN B | Target\_lig\_8 | Bcr-Abl m- RNA | Target\_64 | 5.6020599913  2796 |
| 828 | C1C(C(C(C(C1  N)OC2C(C(C(C (O2)CN)O)O)N) OC3C(C(C(O3)  CO)O)O)O)N | GGCUGACCAUCAAU AAGGAAGAAGCCCU UCAGCGGCCAGUA | ribostamycin | Target\_lig\_9 | Bcr-Abl m- RNA | Target\_64 | 4.0969100130  0806 |
| 829 | C1C(C(C(C(C1  NC(=O)C(CCN)  O)OC2C(C(C(C (O2)CO)O)N)O) O)OC3C(C(C(C (O3)CN)O)O)O) N | GGCUGACCAUCAAU AAGGAAGAAGCCCU UCAGCGGCCAGUA | Amikacin | Target\_lig\_17 5 | Bcr-Abl m- RNA | Target\_64 | 5 |
| 830 | CC1(COC(C(C1 NC)O)OC2C(C C(C(C2O)OC3C (CCC(O3)CN)N  )N)N)O | GGCUGACCAUCAAU AAGGAAGAAGCCCU UCAGCGGCCAGUA | gentamicin\_mol | Target\_lig\_76 | Bcr-Abl m- RNA | Target\_64 | 5.5228787452  8034 |
| 831 | C1C(C(C(C(C1  NC(=O)C(CCN)  O)O)OC2C(C(C  (O2)CO)O)O)O  C3C(C(C(C(O3)  CN)O)O)N)N | GGCUGACCAUCAAU AAGGAAGAAGCCCU UCAGCGGCCAGUA | Butirosin | Target\_lig\_22 0 | Bcr-Abl m- RNA | Target\_64 | 4.8239087409  4432 |
| 832 | CC1C(C(C(O1)  OC2C(C(C(C(C  2O)O)N=C(N)N  )O)N=C(N)N)O | GGAUUUAAGCAGAG UUCAAAAGCCCUUC AGCGGCCAGUAG | Streptomycin | Target\_lig\_63 | PAX3-FKHR m-RNA | Target\_65 | 4.6020599913  2796 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA\_ID** | **pKd** |
|  | C3C(C(C(C(O3)  CO)O)O)NC) (C=O)O |  |  |  |  |  |  |
| 833 | CC1CC(=O)C2( C(O1)OC3C(C(  C(C(C3O2)NC)  O)NC)O)O | GGAUUUAAGCAGAG UUCAAAAGCCCUUC AGCGGCCAGUAG | Spectinomycin | Target\_lig\_75 | PAX3-FKHR m-RNA | Target\_65 | 4 |
| 834 | CNC1CC(C(C( C1O)OC2C3C( C(C(O2)CO)O)  OC4(O3)C(C(C(  C(O4)C(CO)N)  O)O)O)O)N | GGAUUUAAGCAGAG UUCAAAAGCCCUUC AGCGGCCAGUAG | Hygromycin\_B | Target\_lig\_3 | PAX3-FKHR m-RNA | Target\_65 | 4 |
| 835 | C1C(C(C(C(C1  N)OC2C(C(C(C (O2)CN)O)O)N) OC3C(C(C(O3)  CO)OC4C(C(C(  C(O4)CN)O)O) N)O)O)N | GGAUUUAAGCAGAG UUCAAAAGCCCUUC AGCGGCCAGUAG | Neomycin | Target\_lig\_4 | PAX3-FKHR m-RNA | Target\_65 | 5.8239087409  4432 |
| 836 | C1C(C(C(C(C1  N)OC2C(C(C(C (O2)CO)O)O)N) OC3C(C(C(O3)  CO)OC4C(C(C(  C(O4)CN)O)O) N)O)O)N | GGAUUUAAGCAGAG UUCAAAAGCCCUUC AGCGGCCAGUAG | Paromomycin\_m ol\_mol | Target\_lig\_11 16 | PAX3-FKHR m-RNA | Target\_65 | 5.7447274948  9669 |
| 837 | CNC1C(C2C(C C(C(O2)OC3C(  CC(C(C3O)O)N  )N)N)OC1OC4 C(C(C(C(O4)C  O)N)O)O)O | GGAUUUAAGCAGAG UUCAAAAGCCCUUC AGCGGCCAGUAG | apramycin | Target\_lig\_79 | PAX3-FKHR m-RNA | Target\_65 | 4.6989700043  3602 |
| 838 | C1C(C(C(C(C1  N)OC2C(C(C(C (O2)CN)O)O)N) O)O)N | GGAUUUAAGCAGAG UUCAAAAGCCCUUC AGCGGCCAGUAG | Neamine | Target\_lig\_80 | PAX3-FKHR m-RNA | Target\_65 | 4.6989700043  3602 |
| 839 | CC(C1C(C(C(C  (O1)OC2C(CC( C(C2O)OC3C(C (C(CO3) (C)O)NC)O)N) N)N)O)O)O | GGAUUUAAGCAGAG UUCAAAAGCCCUUC AGCGGCCAGUAG | Geneticin | Target\_lig\_14 0 | PAX3-FKHR m-RNA | Target\_65 | 4.5228787452  8034 |
| 840 | [C@H]1([C@H] (C[C@H]  ([C@H] ([C@H]1O)O[C  @@H]1[C@@ H](C[C@@H]  ([C@@H] (O1)CN)O)N)N) N)O[C@@H]1[ C@H] ([C@@H]  ([C@H]  ([C@@H]  (O1)CNc1c2ccc cc2nc2c1cccc2) O)N)O | GGAUUUAAGCAGAG UUCAAAAGCCCUUC AGCGGCCAGUAG | Tobramycin | Target\_lig\_54 0 | PAX3-FKHR m-RNA | Target\_65 | 5.7447274948  9669 |
| 841 | C1C(C(C(C(C1  N)OC2C(C(C(C (O2)CN)O)O)O) O)OC3C(C(C(C (O3)CO)O)N)O) N | GGAUUUAAGCAGAG UUCAAAAGCCCUUC AGCGGCCAGUAG | Kanamycin A | Target\_lig\_7 | PAX3-FKHR m-RNA | Target\_65 | 4.6989700043  3602 |
| 842 | C1C(C(C(C(C1  N)OC2C(C(C(C (O2)CO)O)N)O) O)OC3C(C(C(C | GGAUUUAAGCAGAG UUCAAAAGCCCUUC AGCGGCCAGUAG | KANAMYCIN B | Target\_lig\_8 | PAX3-FKHR m-RNA | Target\_65 | 5.3010299956  6398 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA\_ID** | **pKd** |
|  | (O3)CN)O)O)N) N |  |  |  |  |  |  |
| 843 | C1C(C(C(C(C1  N)OC2C(C(C(C (O2)CN)O)O)N) OC3C(C(C(O3)  CO)O)O)O)N | GGAUUUAAGCAGAG UUCAAAAGCCCUUC AGCGGCCAGUAG | ribostamycin | Target\_lig\_9 | PAX3-FKHR m-RNA | Target\_65 | 4.0457574905  6068 |
| 844 | C1C(C(C(C(C1  NC(=O)C(CCN)  O)OC2C(C(C(C (O2)CO)O)N)O) O)OC3C(C(C(C (O3)CN)O)O)O) N | GGAUUUAAGCAGAG UUCAAAAGCCCUUC AGCGGCCAGUAG | Amikacin | Target\_lig\_17 5 | PAX3-FKHR m-RNA | Target\_65 | 4.8239087409  4432 |
| 845 | CC1(COC(C(C1 NC)O)OC2C(C C(C(C2O)OC3C (CCC(O3)CN)N  )N)N)O | GGAUUUAAGCAGAG UUCAAAAGCCCUUC AGCGGCCAGUAG | gentamicin\_mol | Target\_lig\_76 | PAX3-FKHR m-RNA | Target\_65 | 5.2218487496  1636 |
| 846 | C1C(C(C(C(C1  NC(=O)C(CCN)  O)O)OC2C(C(C  (O2)CO)O)O)O  C3C(C(C(C(O3)  CN)O)O)N)N | GGAUUUAAGCAGAG UUCAAAAGCCCUUC AGCGGCCAGUAG | Butirosin | Target\_lig\_22 0 | PAX3-FKHR m-RNA | Target\_65 | 4.6020599913  2796 |
| 871 | c12c(c(c3c(n1)c ccc3)Nc1ccc(cc 1)CNC(=O) [C@H] (C(C)C)NC(=O) [C@H] (NC(=O)CCCN)  CO)cccc2C(=O) N[C@@H] (C(=O)N)CCCN C(=N)N | GGGCGGUUUUUCGA AGCUUGAGUCUCGU AGAGGGCUUCGGCC UGGCGAAUUAGACU GACGCUC | HTP 20 | Target\_lig\_52 7 | RNA  aptamer\_1 | Target\_56 | 7.6777807052  6608 |
| 872 | c12c(c(c3c(n1)c ccc3)Nc1ccc(cc 1)CNC(=O) [C@H] (C(C)C)NC(=O) [C@H] (NC(=O)CCCN)  CO)cccc2C(=O) N[C@@H] (C(=O)N)CCCN C(=N)N | GGGCGGUUUUUCGA AGCUUGAGUCUUAC GUAGAGGGCUUCGG CCUGGCGAUAGACU GACGCUC | HTP 20 | Target\_lig\_52 7 | RNA  aptamer\_2 | Target\_57 | 6.8386319977  6503 |
| 873 | c12c(c(c3c(n1)c ccc3)Nc1ccc(cc 1)CNC(=O) [C@H] (C(C)C)NC(=O) [C@H] (NC(=O)CCCN)  CO)cccc2C(=O) N[C@@H] (C(=O)N)CCCN C(=N)N | GGGCGGUUUUUCGA AGCUUGAGUCUCUC GUAGAGGGCUUCGG CCUGGGCGCAAGAC UGACGCUC | HTP 20 | Target\_lig\_52 7 | RNA  aptamer\_3 | Target\_58 | 6.1135092748  2752 |
| 874 | c12c(c(c3c(n1)c ccc3)Nc1ccc(cc 1)CNC(=O) [C@H] (C(C)C)NC(=O) [C@H] (NC(=O)CCCN)  CO)cccc2C(=O) N[C@@H] (C(=O)N)CCCN C(=N)N | GGGCGGUUUUUCGA AGCUUGAGUCUCGU AGAGGGCUUCGGCC UGGCGUAGACUGAC GCUC | HTP 20 | Target\_lig\_52 7 | RNA  aptamer\_4 | Target\_59 | 7.0457574905  6068 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA\_ID** | **pKd** |
| 901 | COC1=CC=C(C  =C1)N2[C@@ H]([C@H] (OC2=O)COC(= O)CC3=CC=CC  =C3)CC4=CC= CC=C4 | GAGGGUGGAACCGC GCUUCGGCGUCCCU C | Oxazolidinone 2 | Target\_lig\_54 3 | T-box RNA | Target\_113 | 5.4685210829  5774 |
| 902 | C1=CC=C(C=C 1)C[C@@H]2[ C@H] (OC(=O)N2)CO C(=O)CC3=CC  =CC=C3 | GAGGGUGGAACCGC GCUUCGGCGUCCCU C | Oxazolidinone 6 | Target\_lig\_54 4 | T-box RNA | Target\_113 | 5.0457574905  6068 |
| 903 | COC1=CC=C(C  =C1)N2[C@@ H]([C@H] (OC2=O)COC(= O)CC3=CC=CC  =C3)CC4=CC= CC=C4 | GAGGGUGGAAUCGC GCUUCGGCGUCCCU C | Oxazolidinone 2 | Target\_lig\_54 3 | T-box C11U | Target\_114 | 4.6020599913  2796 |
| 904 | C1=CC=C(C=C 1)C[C@@H]2[ C@H] (OC(=O)N2)CO C(=O)CC3=CC  =CC=C3 | GAGGGUGGAAUCGC GCUUCGGCGUCCCU C | Oxazolidinone 6 | Target\_lig\_54 4 | T-box C11U | Target\_114 | 3.9030899869  9194 |
| 905 | COC(=O)C1C( CCC2C1CC3C4  =C(CCN3C2)C5  =CC=CC=C5N4  )O | UUCCUGCUUCAACA GUGCUUGGACGGAA | Yohimbine | Target\_lig\_19 3 | fIIRE | Target\_132 | 5.4089353929  735 |
| 906 | COC(=O)C1C( CCC2C1CC3C4  =C(CCN3C2)C5  =CC=CC=C5N4  )O | ACAUUACCGGGAGC AGUGUCUUCUGUAA UGU | Yohimbine | Target\_lig\_19 3 | TfR\_IRE | Target\_133 | 5.1366771398  7954 |
| 907 | COC(=O)C1C( CCC2C1CC3C4  =C(CCN3C2)C5  =CC=CC=C5N4  )O | ACAUUACCGGGAGC AGUGUCUUCUGUAA UGU | Yohimbine | Target\_lig\_19 3 | TfR\_IRE\_C24 U | Target\_134 | 5.2291479883  5786 |
| 909 | COC(=O)C1C( CCC2C1CC3C4  =C(CCN3C2)C5  =CC=CC=C5N4  )O | GGGCGAAUUGGGUA CCGGGCCCCCCC | Yohimbine | Target\_lig\_19 3 | Yohimbine\_XII  \_RNA | Target\_135 | 5.0362121726  5444 |
| 910 | C1[C@@H](N)  [C@@H](O) [C@H] ([C@@H]  ([C@H]1N)OCS  c1ccnc2c1ccc(c 2)C(F)(F)F)O | CGCGCGUGUGCGCG | DOS | Target\_lig\_38 3 | RNA\_XIX | Target\_136 | 3 |
| 911 | [C@H]1([C@H] (OCCCCCCCC CCCCO[C@H] 2[C@@H] (C[C@H](N)  [C@@H](O)  [C@H]2O)N)  [C@H](O) [C@H] ([C@@H]  (C1)N)O)N | CGCGCGUGUGCGCG | DOS\_der\_1 | Target\_lig\_54 6 | RNA\_XIX | Target\_136 | 4.4685210829  5774 |
| 912 | [C@H]1([C@H]  (OCc2ccc(cc2)C Cc2ccc(cc2)CO[ C@H]2[C@@H  ](C[C@H](N) | CGCGCGUGUGCGCG | DOS\_der\_2 | Target\_lig\_54 7 | RNA\_XIX | Target\_136 | 4.7958800173  4408 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA\_ID** | **pKd** |
|  | [C@@H](O)  [C@@H]2O)N)  [C@@H](O)  [C@@H] ([C@H]  (C1)N)O)N |  |  |  |  |  |  |
| 913 | [C@H]1([C@@ H]([C@H](O)  [C@H]([C@H]  (C1)N#N)O)OC  c1ccc(cc1)c1ccc (cc1)CO[C@H] 1[C@H] (C[C@@H] ([C@@H](O) [C@@H]1O)N# N)N#N)N#N | CGCGCGUGUGCGCG | DOS\_der\_3 | Target\_lig\_54 8 | RNA\_XIX | Target\_136 | 3.6020599913  2796 |
| 914 | OCc1ccc(cc1)C Cc1ccc(cc1)CO[ C@H]1[C@@H  ](C[C@H](N) [C@@H](O) [C@@H]1O)N | CGCGCGUGUGCGCG | DOS\_der\_4 | Target\_lig\_54 9 | RNA\_XIX | Target\_136 | 3 |
| 915 | C1[C@@H](N)  [C@@H](O) [C@H] ([C@@H]  ([C@H]1N)OCS  c1ccnc2c1ccc(c 2)C(F)(F)F)O | CGCGCAGUGUAGCG CG | DOS | Target\_lig\_38 3 | RNA\_XX | Target\_137 | 3 |
| 916 | [C@H]1([C@H] (OCCCCCCCC CCCCO[C@H] 2[C@@H] (C[C@H](N)  [C@@H](O)  [C@H]2O)N)  [C@H](O) [C@H] ([C@@H]  (C1)N)O)N | CGCGCAGUGUAGCG CG | DOS\_der\_1 | Target\_lig\_54 6 | RNA\_XX | Target\_137 | 4.9586073148  4177 |
| 917 | [C@H]1([C@H]  (OCc2ccc(cc2)C Cc2ccc(cc2)CO[ C@H]2[C@@H  ](C[C@H](N) [C@@H](O)  [C@@H]2O)N)  [C@@H](O)  [C@@H] ([C@H]  (C1)N)O)N | CGCGCAGUGUAGCG CG | DOS\_der\_2 | Target\_lig\_54 7 | RNA\_XX | Target\_137 | 5.2218487496  1636 |
| 918 | [C@H]1([C@@ H]([C@H](O)  [C@H]([C@H]  (C1)N#N)O)OC  c1ccc(cc1)c1ccc (cc1)CO[C@H] 1[C@H] (C[C@@H] ([C@@H](O) [C@@H]1O)N# N)N#N)N#N | CGCGCAGUGUAGCG CG | DOS\_der\_3 | Target\_lig\_54 8 | RNA\_XX | Target\_137 | 3.6020599913  2796 |
| 919 | OCc1ccc(cc1)C Cc1ccc(cc1)CO[ C@H]1[C@@H  ](C[C@H](N) [C@@H](O) [C@@H]1O)N | CGCGCAGUGUAGCG CG | DOS\_der\_4 | Target\_lig\_54 9 | RNA\_XX | Target\_137 | 3 |
| 920 | C1[C@@H](N) | CGCGCAGUAGUAGC | DOS | Target\_lig\_38 | RNA\_XXI | Target\_138 | 3 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA\_ID** | **pKd** |
|  | [C@@H](O) [C@H] ([C@@H]  ([C@H]1N)OCS  c1ccnc2c1ccc(c 2)C(F)(F)F)O | GCG |  | 3 |  |  |  |
| 921 | [C@H]1([C@H] (OCCCCCCCC CCCCO[C@H] 2[C@@H] (C[C@H](N)  [C@@H](O)  [C@H]2O)N)  [C@H](O) [C@H] ([C@@H]  (C1)N)O)N | CGCGCAGUAGUAGC GCG | DOS\_der\_1 | Target\_lig\_54 6 | RNA\_XXI | Target\_138 | 4.9586073148  4177 |
| 922 | [C@H]1([C@H]  (OCc2ccc(cc2)C Cc2ccc(cc2)CO[ C@H]2[C@@H  ](C[C@H](N) [C@@H](O)  [C@@H]2O)N)  [C@@H](O)  [C@@H] ([C@H]  (C1)N)O)N | CGCGCAGUAGUAGC GCG | DOS\_der\_2 | Target\_lig\_54 7 | RNA\_XXI | Target\_138 | 5.2218487496  1636 |
| 923 | [C@H]1([C@@ H]([C@H](O)  [C@H]([C@H]  (C1)N#N)O)OC  c1ccc(cc1)c1ccc (cc1)CO[C@H] 1[C@H] (C[C@@H] ([C@@H](O) [C@@H]1O)N# N)N#N)N#N | CGCGCAGUAGUAGC GCG | DOS\_der\_3 | Target\_lig\_54 8 | RNA\_XXI | Target\_138 | 3.6020599913  2796 |
| 924 | OCc1ccc(cc1)C Cc1ccc(cc1)CO[ C@H]1[C@@H  ](C[C@H](N) [C@@H](O) [C@@H]1O)N | CGCGCAGUAGUAGC GCG | DOS\_der\_4 | Target\_lig\_54 9 | RNA\_XXI | Target\_138 | 3 |
| 925 | C1[C@@H](N)  [C@@H](O) [C@H] ([C@@H]  ([C@H]1N)OCS  c1ccnc2c1ccc(c 2)C(F)(F)F)O | CGCGCAGUCAGUAG CGCG | DOS | Target\_lig\_38 3 | RNA\_XXII | Target\_139 | 3 |
| 926 | [C@H]1([C@H] (OCCCCCCCC CCCCO[C@H] 2[C@@H] (C[C@H](N)  [C@@H](O)  [C@H]2O)N)  [C@H](O) [C@H] ([C@@H]  (C1)N)O)N | CGCGCAGUCAGUAG CGCG | DOS\_der\_1 | Target\_lig\_54 6 | RNA\_XXII | Target\_139 | 5.0969100130  0806 |
| 927 | [C@H]1([C@H]  (OCc2ccc(cc2)C Cc2ccc(cc2)CO[ C@H]2[C@@H  ](C[C@H](N) [C@@H](O)  [C@@H]2O)N)  [C@@H](O) | CGCGCAGUCAGUAG CGCG | DOS\_der\_2 | Target\_lig\_54 7 | RNA\_XXII | Target\_139 | 5.2218487496  1636 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA\_ID** | **pKd** |
|  | [C@@H] ([C@H]  (C1)N)O)N |  |  |  |  |  |  |
| 928 | [C@H]1([C@@ H]([C@H](O)  [C@H]([C@H]  (C1)N#N)O)OC  c1ccc(cc1)c1ccc (cc1)CO[C@H] 1[C@H] (C[C@@H] ([C@@H](O) [C@@H]1O)N# N)N#N)N#N | CGCGCAGUCAGUAG CGCG | DOS\_der\_3 | Target\_lig\_54 8 | RNA\_XXII | Target\_139 | 3.6020599913  2796 |
| 929 | OCc1ccc(cc1)C Cc1ccc(cc1)CO[ C@H]1[C@@H  ](C[C@H](N) [C@@H](O) [C@@H]1O)N | CGCGCAGUCAGUAG CGCG | DOS\_der\_4 | Target\_lig\_54 9 | RNA\_XXII | Target\_139 | 3 |
| 930 | C1C(C(C(C(C1  N)OC2C(C(C(C (O2)CN)O)O)N) OC3C(C(C(O3)  CO)OC4C(C(C(  C(O4)CN)O)O) N)O)O)N | GGGGCGAAAGCCUU AU | Neomycin\_B | Target\_lig\_12 46 | GNRA  tetraloop construct XVIII | Target\_141 | 4.5228787452  8034 |
| 931 | C1=NC2=NC= NC(=C2N1)N | CUCGGUACCGCAAA AGCGUUUUUCGCAU ACCUAUUCGUUAUA GGUCGAUUGUACCG AG | Adenine | Target\_lig\_16 5 | Spiegelmer L- A42d RNA (58  mer) | Target\_142 | 1.7878123955  9604 |
| 932 | C1=NC(=C2C(= N1)N(C=N2) [C@H]3[C@@ H]([C@@H]  ([C@H] (O3)CO)O)O)N | CUCGGUACCGCAAA AGCGUUUUUCGCAU ACCUAUUCGUUAUA GGUCGAUUGUACCG AG | D\_Adenosine | Target\_lig\_55 1 | Spiegelmer L- A42d RNA (58  mer) | Target\_142 | 5.6575773191  7779 |
| 933 | CO[C@@H]1[C @H](O[C@H]  ([C@@H]1O)N 2C=NC3=C(N= CN=C32)N)CO | CUCGGUACCGCAAA AGCGUUUUUCGCAU ACCUAUUCGUUAUA GGUCGAUUGUACCG AG | 3-O-methyl-D- Adenosine | Target\_lig\_55 2 | Spiegelmer L- A42d RNA (58  mer) | Target\_142 | 5.8538719643  2176 |
| 934 | C1=NC2=C(N1[ C@H]3[C@@H  ]([C@@H]  ([C@H] (O3)CO)O)O)N  =C(NC2=O)N | CUCGGUACCGCAAA AGCGUUUUUCGCAU ACCUAUUCGUUAUA GGUCGAUUGUACCG AG | D-guanosine | Target\_lig\_55 3 | Spiegelmer L- A42d RNA (58  mer) | Target\_142 | 5.3187587626  2441 |
| 935 | C1[C@H] (O[C@H]  ([C@@H]1O)N 2C=NC3=C(N= CN=C32)N)CO | CUCGGUACCGCAAA AGCGUUUUUCGCAU ACCUAUUCGUUAUA GGUCGAUUGUACCG AG | 3-deoxy-D- Adenosine | Target\_lig\_55 4 | Spiegelmer L- A42d RNA (58  mer) | Target\_142 | 5.0969100130  0806 |
| 936 | C1[C@@H] ([C@H] (O[C@H]1N2C  =NC3=C(N=CN  =C32)N)CO)O | CUCGGUACCGCAAA AGCGUUUUUCGCAU ACCUAUUCGUUAUA GGUCGAUUGUACCG AG | 2-deoxy-D- Adenosine | Target\_lig\_55 5 | Spiegelmer L- A42d RNA (58  mer) | Target\_142 | 2.8538719643  2176 |
| 937 | C1=CN(C(=O)N C1=O) [C@H]2[C@@ H]([C@@H]  ([C@H]  (O2)CO)O)O | CUCGGUACCGCAAA AGCGUUUUUCGCAU ACCUAUUCGUUAUA GGUCGAUUGUACCG AG | D-uridine | Target\_lig\_55 6 | Spiegelmer L- A42d RNA (58  mer) | Target\_142 | 2.6382721639  8241 |
| 938 | C1=NC(=C2C(= N1)N(C=N2) [C@H]3[C@@ | CUCGGUACCGCAAA AGCGUUUUUCGCAU ACCUAUUCGUUAUA | D-adenosine triphosphate | Target\_lig\_55 7 | Spiegelmer L- A42d RNA (58  mer) | Target\_142 | 2.5376020021  0104 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA\_ID** | **pKd** |
|  | H]([C@@H]  ([C@H]  (O3)COP(=O)  (O)OP(=O)  (O)OP(=O)  (O)O)O)O)N | GGUCGAUUGUACCG AG |  |  |  |  |  |
| 939 | C1=CN(C(=O)N  =C1N) [C@H]2[C@@ H]([C@@H]  ([C@H]  (O2)CO)O)O | CUCGGUACCGCAAA AGCGUUUUUCGCAU ACCUAUUCGUUAUA GGUCGAUUGUACCG AG | D-Cytidine | Target\_lig\_55 8 | Spiegelmer L- A42d RNA (58  mer) | Target\_142 | 2.2076083105  0175 |
| 940 | CO[C@@H]1[C @@H]([C@H] (O[C@H]1N2C  =NC3=C(N=CN  =C32)N)CO)O | CUCGGUACCGCAAA AGCGUUUUUCGCAU ACCUAUUCGUUAUA GGUCGAUUGUACCG AG | 2-O-methyl-D- Adenosine | Target\_lig\_55 9 | Spiegelmer L- A42d RNA (58  mer) | Target\_142 | 1.8894102897  0075 |
| 941 | C1=NC(=C2C(= N1)N(C=N2) [C@@H]3[C@ H]([C@H]  ([C@@H] (O3)CO)O)O)N | CUCGGUACCGCAAA AGCGUUUUUCGCAU ACCUAUUCGUUAUA GGUCGAUUGUACCG AG | L\_Adenosine | Target\_lig\_56 0 | Spiegelmer L- A42d RNA (58  mer) | Target\_142 | 1.6946486305  5338 |
| 942 | CN1C2=C(C(= O)N(C1=O)C)N C=N2 | GGUGAUACCAGCCG AAAGGCCCUUGGCA GCACC | Theophylline | Target\_lig\_15 4 | T alpha aptamer | Target\_60 | 6.8239087409  4432 |
| 943 | N=C1N[C@@H  ]2CS[C@@H] ([C@H]2N1)CC CCC(=O)NCCO CCOCCNC(=O) CCCC[C@H]1[ C@@H]2NC(= N)N[C@H]2CS 1 | GGACCGUCAGAGGA CACGGUUAAAAAGU CCUCU | biotin dimer | Target\_lig\_56 1 | B alpha aptamer | Target\_61 | 5.6777807052  6608 |
| 944 | N=C1N[C@H]2 CS[C@H] ([C@@H]2N1) CCCCC(=O)NC COCCOCCN | GGACCGUCAGAGGA CACGGUUAAAAAGU CCUCU | biotin PEO Amine | Target\_lig\_56 2 | B alpha aptamer | Target\_61 | 4.8538719643  2176 |
| 947 | c12cc(ccc1c(c1c (n2)ccc(c1)OC) NCCCCc1c(nc( nc1N)N)N)Cl | CUGGCCUGGCGCGC CUGCCCAG | MBNL CCUG  ligand 3 | Target\_lig\_56 3 | RNA B | Target\_144 | 4.5850266520  2918 |
| 948 | c12cc(ccc1c(c1c (n2)ccc(c1)OC) NCCCCc1c(nc( nc1N)N)N)Cl | CUGGCUGCGCGCGC CGCCAG | MBNL CCUG  ligand 3 | Target\_lig\_56 3 | RNA C | Target\_145 | 3.7825160557  8609 |
| 970 | C1(=O)O[C@H  ]([C@H] (N1)CN1CCN(  CC1)c1ccccc1) COC(=O)Cc1cc  ccc1 | GAGGGUGGAACCGC GCUUCGGCGUCCCU C | racemic\_oxazoli dinones | Target\_lig\_58 5 | Antiterminator model RNA AM1A | Target\_147 | 4.8860566476  9316 |
| 971 | C1(=O)O[C@H  ]([C@H] (N1)CN1CCN(  CC1)c1ccccc1) COC(=O)Nc1cc c(cc1)C(=O)C | GAGGGUGGAACCGC GCUUCGGCGUCCCU C | racemic\_oxazoli dinones\_2 | Target\_lig\_58 6 | Antiterminator model RNA AM1A | Target\_147 | 5.3979400086  7204 |
| 1006 | COC1=C(C=C( C=C1)NCC2=C C=C(S2)[N+] (=O)[O-])OC | AUCACCUCCUUAUA AGGAGGUGAU | SL3  RNA\_ligand4 | Target\_lig\_60 7 | Double stranded RNA seq | Target\_149 | 5.4948500216  8009 |
| 1007 | C1=CC=C2C=C (C=CC2=C1)/  C=C/3\ C(=O)NC(=S)N | AUCACCUCCUUAUA AGGAGGUGAU | SL3  RNA\_ligand5 | Target\_lig\_60 8 | Double stranded RNA seq | Target\_149 | 5.0861861476  1628 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA\_ID** | **pKd** |
|  | 3 |  |  |  |  |  |  |
| 1008 | C1=CC=C(C=C 1)C[N+]2=CC= C(C=C2)C(=O)  N/N=C\ C3=CC=C(C=C 3)Br | AUCACCUCCUUAUA AGGAGGUGAU | SL3  RNA\_ligand6 | Target\_lig\_60 9 | Double stranded RNA seq | Target\_149 | 5.0809219076  2393 |
| 1009 | CC1CCN(CC1) C2=CC=C(C=C 2)N | AUCACCUCCUUAUA AGGAGGUGAU | SL3  RNA\_ligand7 | Target\_lig\_61 0 | Double stranded RNA seq | Target\_149 | 3.7235381958  2676 |
| 1010 | C1=CC2=C(C= CC(=C2N=C1)S CCO)[N+](=O) [O-] | AUCACCUCCUUAUA AGGAGGUGAU | SL3  RNA\_ligand9 | Target\_lig\_61 2 | Double stranded RNA seq | Target\_149 | 5.6595558851  5988 |
| 1011 | C1=CC=C(C(= C1)/C=C\2/ C(=O)N(C(=O) N2)/C=C/3\ C(=O)C4=CC= CC=C4OC3=O) O | AUCACCUCCUUAUA AGGAGGUGAU | SL3  RNA\_ligand10 | Target\_lig\_61 3 | Double stranded RNA seq | Target\_149 | 5.2924298239  0206 |
| 1012 | C1=CC=C2C(= C1)C(=O)C3=C (C2=O)C(=C(C  =C3NC4=CC=C (C=C4)S(=O)  (=O)N)S(=O) (=O)O)N | AUCACCUCCUUAUA AGGAGGUGAU | SL3  RNA\_ligand11 | Target\_lig\_61 4 | Double stranded RNA seq | Target\_149 | 4.9507819773  2982 |
| 1013 | c12ccccc1C(=O) [C@H]1[C@H] (C2=O)C(=CC= C1NCCO)NCC O | AUCACCUCCUUAUA AGGAGGUGAU | SL3  RNA\_ligand12 | Target\_lig\_61 5 | Double stranded RNA seq | Target\_149 | 5.0757207139  3812 |
| 1014 | CC1=CC=CN2 C1=NC3=C(C2  =O)C=C(C(=N) N3CCCO)C(=O  )NC | AUCACCUCCUUAUA AGGAGGUGAU | SL3  RNA\_ligand13 | Target\_lig\_61 6 | Double stranded RNA seq | Target\_149 | 4.9208187539  5238 |
| 1015 | CN1CCN(CC1) CCCN2C3=CC  =CC=C3SC4=C 2C=C(C=C4)C( F)(F)F | AUCACCUCCUUAUA AGGAGGUGAU | SL3  RNA\_ligand17 | Target\_lig\_62 0 | Double stranded RNA seq | Target\_149 | 2.9550684538  5084 |
| 1016 | COC1=C(C=C( C=C1)NCC2=C C=C(S2)[N+] (=O)[O-])OC | AUCACCUCCUUA | SL3  RNA\_ligand4 | Target\_lig\_60 7 | single stranded RNA seq | Target\_150 | 5.6575773191  7779 |
| 1017 | C1=CC=C2C=C (C=CC2=C1)/  C=C/3\ C(=O)NC(=S)N 3 | AUCACCUCCUUA | SL3  RNA\_ligand5 | Target\_lig\_60 8 | single stranded RNA seq | Target\_150 | 5.0222763947  1115 |
| 1018 | C1=CC=C(C=C 1)C[N+]2=CC= C(C=C2)C(=O)  N/N=C\ C3=CC=C(C=C 3)Br | AUCACCUCCUUA | SL3  RNA\_ligand6 | Target\_lig\_60 9 | single stranded RNA seq | Target\_150 | 4.9281179926  9388 |
| 1019 | CC1CCN(CC1) C2=CC=C(C=C 2)N | AUCACCUCCUUA | SL3  RNA\_ligand7 | Target\_lig\_61 0 | single stranded RNA seq | Target\_150 | 3.5528419686  5778 |
| 1020 | C1=CC2=C(C= CC(=C2N=C1)S CCO)[N+](=O) [O-] | AUCACCUCCUUA | SL3  RNA\_ligand9 | Target\_lig\_61 2 | single stranded RNA seq | Target\_150 | 5.6989700043  3602 |
| 1021 | C1=CC=C(C(= | AUCACCUCCUUA | SL3 | Target\_lig\_61 | single stranded | Target\_150 | 5.3872161432 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA\_ID** | **pKd** |
|  | C1)/C=C\2/ C(=O)N(C(=O) N2)/C=C/3\ C(=O)C4=CC= CC=C4OC3=O) O |  | RNA\_ligand10 | 3 | RNA seq |  | 8026 |
| 1022 | C1=CC=C2C(= C1)C(=O)C3=C (C2=O)C(=C(C  =C3NC4=CC=C (C=C4)S(=O)  (=O)N)S(=O) (=O)O)N | AUCACCUCCUUA | SL3  RNA\_ligand11 | Target\_lig\_61 4 | single stranded RNA seq | Target\_150 | 5.0506099933  5509 |
| 1023 | c12ccccc1C(=O) [C@H]1[C@H] (C2=O)C(=CC= C1NCCO)NCC O | AUCACCUCCUUA | SL3  RNA\_ligand12 | Target\_lig\_61 5 | single stranded RNA seq | Target\_150 | 4.8538719643  2176 |
| 1024 | CC1=CC=CN2 C1=NC3=C(C2  =O)C=C(C(=N) N3CCCO)C(=O  )NC | AUCACCUCCUUA | SL3  RNA\_ligand13 | Target\_lig\_61 6 | single stranded RNA seq | Target\_150 | 5.1249387366  083 |
| 1025 | CN1CCN(CC1) CCCN2C3=CC  =CC=C3SC4=C 2C=C(C=C4)C( F)(F)F | AUCACCUCCUUA | SL3  RNA\_ligand17 | Target\_lig\_62 0 | single stranded RNA seq | Target\_150 | 3.2189630613  7887 |
| 1030 | O1COc2c1cc(C(  =O)N1[C@H] (C(=O)N[C@H]  (C(=O)N[C@@ H] (C(=O)NCCCN) CCCCN)CSSC[ C@H](NC(=O) [C@@H]3CCC N3C(=O)c3cc4 OCOc4cc3)C(= O)N[C@H]  (C(=O)NCCCN) CCCCN)CCC1)  cc2 | CCGCUGCUGCUGCU GCGG | ligand 3-3 | Target\_lig\_62 1 | RNA seq A | Target\_151 | 5.2676062401  7703 |
| 1031 | n1c2c(cc(C(=O) N3[C@H] (C(=O)N[C@H]  (C(=O)N[C@@ H] (C(=O)NCCCN) CCCCN)CSSC[ C@H](NC(=O) [C@@H]4CCC  N4C(=O)c4cc5c (nc4CC)cccc5)C (=O)N[C@@H]  (C(=O)NCCCN) CCCCN)CCC3)  c1CC)cccc2 | CCGCUGCUGCUGCU GCGG | ligand 4-4 | Target\_lig\_62 2 | RNA seq A | Target\_151 | 5.1739251972  9917 |
| 1032 | n1c2c(cc(C(=O) N[C@H] (C(=O)N[C@@ H] (C(=O)N[C@H]  (C(=O)NCCCN) CCCCN)CSSC[ C@H](NC(=O) [C@@H]3CCC  N3C(=O)c3cc4c (nc3CC)cccc4)C (=O)N[C@@H]  (C(=O)NCCCN) | CCGCUGCUGCUGCU GCGG | ligand 2-4 | Target\_lig\_62 3 | RNA seq A | Target\_151 | 5.3467874862  2466 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA\_ID** | **pKd** |
|  | CCCCN)CC(=O  )N)c1CC)cccc2 |  |  |  |  |  |  |
| 1033 | O1COc2c1cc(C(  =O)N1[C@H] (C(=O)N[C@@ H] (C(=O)N[C@H]  (C(=O)NCCCN) CCCCN)CSSC[ C@H](NC(=O) [C@@H]3CCC  N3C(=O)c3cc4c (nc3CC)cccc4)C (=O)N[C@@H]  (C(=O)NCCCN) CCCCN)CCC1)  cc2 | CCGCUGCUGCUGCU GCGG | ligand 3-4 | Target\_lig\_62 4 | RNA seq A | Target\_151 | 5.3872161432  8026 |
| 1034 | O1COc2c1cc(C(  =O)N1[C@H] (C(=O)N[C@H]  (C(=O)N[C@@ H] (C(=O)NCCCN) CCCCN)CSSC[ C@H](NC(=O) [C@@H]3CCC N3C(=O)c3cc4 OCOc4cc3)C(= O)N[C@H]  (C(=O)NCCCN) CCCCN)CCC1)  cc2 | CCGCUGCUGCUGCU GCGG | ligand 3-3 | Target\_lig\_62 1 | RNA seq A (20 x t-RNA) | Target\_152 | 4.8538719643  2176 |
| 1035 | n1c2c(cc(C(=O) N3[C@H] (C(=O)N[C@H]  (C(=O)N[C@@ H] (C(=O)NCCCN) CCCCN)CSSC[ C@H](NC(=O) [C@@H]4CCC  N4C(=O)c4cc5c (nc4CC)cccc5)C (=O)N[C@@H]  (C(=O)NCCCN) CCCCN)CCC3)  c1CC)cccc2 | CCGCUGCUGCUGCU GCGG | ligand 4-4 | Target\_lig\_62 2 | RNA seq A (20 x t-RNA) | Target\_152 | 4.7447274948  9669 |
| 1036 | n1c2c(cc(C(=O) N[C@H] (C(=O)N[C@@ H] (C(=O)N[C@H]  (C(=O)NCCCN) CCCCN)CSSC[ C@H](NC(=O) [C@@H]3CCC  N3C(=O)c3cc4c (nc3CC)cccc4)C (=O)N[C@@H]  (C(=O)NCCCN) CCCCN)CC(=O  )N)c1CC)cccc2 | CCGCUGCUGCUGCU GCGG | ligand 2-4 | Target\_lig\_62 3 | RNA seq A (20 x t-RNA) | Target\_152 | 5 |
| 1037 | O1COc2c1cc(C(  =O)N1[C@H] (C(=O)N[C@@ H] (C(=O)N[C@H]  (C(=O)NCCCN) CCCCN)CSSC[ C@H](NC(=O) [C@@H]3CCC  N3C(=O)c3cc4c | CCGCUGCUGCUGCU GCGG | ligand 3-4 | Target\_lig\_62 4 | RNA seq A (20 x t-RNA) | Target\_152 | 5.0177287669  6043 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA\_ID** | **pKd** |
|  | (nc3CC)cccc4)C (=O)N[C@@H]  (C(=O)NCCCN) CCCCN)CCC1)  cc2 |  |  |  |  |  |  |
| 1038 | O1COc2c1cc(C(  =O)N1[C@H] (C(=O)N[C@H]  (C(=O)N[C@@ H] (C(=O)NCCCN) CCCCN)CSSC[ C@H](NC(=O) [C@@H]3CCC N3C(=O)c3cc4 OCOc4cc3)C(= O)N[C@H]  (C(=O)NCCCN) CCCCN)CCC1)  cc2 | GGGCUGCUGCUGCU GCUGGGG | ligand 3-3 | Target\_lig\_62 1 | RNA seq B | Target\_153 | 5.6020599913  2796 |
| 1039 | n1c2c(cc(C(=O) N3[C@H] (C(=O)N[C@H]  (C(=O)N[C@@ H] (C(=O)NCCCN) CCCCN)CSSC[ C@H](NC(=O) [C@@H]4CCC  N4C(=O)c4cc5c (nc4CC)cccc5)C (=O)N[C@@H]  (C(=O)NCCCN) CCCCN)CCC3)  c1CC)cccc2 | GGGCUGCUGCUGCU GCUGGGG | ligand 4-4 | Target\_lig\_62 2 | RNA seq B | Target\_153 | 5.6777807052  6608 |
| 1040 | n1c2c(cc(C(=O) N[C@H] (C(=O)N[C@@ H] (C(=O)N[C@H]  (C(=O)NCCCN) CCCCN)CSSC[ C@H](NC(=O) [C@@H]3CCC  N3C(=O)c3cc4c (nc3CC)cccc4)C (=O)N[C@@H]  (C(=O)NCCCN) CCCCN)CC(=O  )N)c1CC)cccc2 | GGGCUGCUGCUGCU GCUGGGG | ligand 2-4 | Target\_lig\_62 3 | RNA seq B | Target\_153 | 5.6777807052  6608 |
| 1041 | O1COc2c1cc(C(  =O)N1[C@H] (C(=O)N[C@@ H] (C(=O)N[C@H]  (C(=O)NCCCN) CCCCN)CSSC[ C@H](NC(=O) [C@@H]3CCC  N3C(=O)c3cc4c (nc3CC)cccc4)C (=O)N[C@@H]  (C(=O)NCCCN) CCCCN)CCC1)  cc2 | GGGCUGCUGCUGCU GCUGGGG | ligand 3-4 | Target\_lig\_62 4 | RNA seq B | Target\_153 | 5.7212463990  4717 |
| 1042 | O1COc2c1cc(C(  =O)N1[C@H] (C(=O)N[C@H]  (C(=O)N[C@@ H] (C(=O)NCCCN) CCCCN)CSSC[ | CCGCUGGGCAACCU GCGG | ligand 3-3 | Target\_lig\_62 1 | RNA seq C | Target\_154 | 5.0315170514  4607 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA\_ID** | **pKd** |
|  | C@H](NC(=O) [C@@H]3CCC N3C(=O)c3cc4 OCOc4cc3)C(= O)N[C@H]  (C(=O)NCCCN) CCCCN)CCC1)  cc2 |  |  |  |  |  |  |
| 1043 | n1c2c(cc(C(=O) N3[C@H] (C(=O)N[C@H]  (C(=O)N[C@@ H] (C(=O)NCCCN) CCCCN)CSSC[ C@H](NC(=O) [C@@H]4CCC  N4C(=O)c4cc5c (nc4CC)cccc5)C (=O)N[C@@H]  (C(=O)NCCCN) CCCCN)CCC3)  c1CC)cccc2 | CCGCUGGGCAACCU GCGG | ligand 4-4 | Target\_lig\_62 2 | RNA seq C | Target\_154 | 5.1487416512  8092 |
| 1044 | n1c2c(cc(C(=O) N[C@H] (C(=O)N[C@@ H] (C(=O)N[C@H]  (C(=O)NCCCN) CCCCN)CSSC[ C@H](NC(=O) [C@@H]3CCC  N3C(=O)c3cc4c (nc3CC)cccc4)C (=O)N[C@@H]  (C(=O)NCCCN) CCCCN)CC(=O  )N)c1CC)cccc2 | CCGCUGGGCAACCU GCGG | ligand 2-4 | Target\_lig\_62 3 | RNA seq C | Target\_154 | 5.1938200260  1611 |
| 1045 | O1COc2c1cc(C(  =O)N1[C@H] (C(=O)N[C@@ H] (C(=O)N[C@H]  (C(=O)NCCCN) CCCCN)CSSC[ C@H](NC(=O) [C@@H]3CCC  N3C(=O)c3cc4c (nc3CC)cccc4)C (=O)N[C@@H]  (C(=O)NCCCN) CCCCN)CCC1)  cc2 | CCGCUGGGCAACCU GCGG | ligand 3-4 | Target\_lig\_62 4 | RNA seq C | Target\_154 | 5.3279021420  6428 |
| 1046 | O1COc2c1cc(C(  =O)N1[C@H] (C(=O)N[C@H]  (C(=O)N[C@@ H] (C(=O)NCCCN) CCCCN)CSSC[ C@H](NC(=O) [C@@H]3CCC N3C(=O)c3cc4 OCOc4cc3)C(= O)N[C@H]  (C(=O)NCCCN) CCCCN)CCC1)  cc2 | CGCGCUGCUGCGCG | ligand 3-3 | Target\_lig\_62 1 | RNA seq D | Target\_155 | 5.1249387366  083 |
| 1047 | n1c2c(cc(C(=O) N3[C@H] (C(=O)N[C@H]  (C(=O)N[C@@ | CGCGCUGCUGCGCG | ligand 4-4 | Target\_lig\_62 2 | RNA seq D | Target\_155 | 5.0705810742  8571 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA\_ID** | **pKd** |
|  | H] (C(=O)NCCCN) CCCCN)CSSC[ C@H](NC(=O) [C@@H]4CCC  N4C(=O)c4cc5c (nc4CC)cccc5)C (=O)N[C@@H]  (C(=O)NCCCN) CCCCN)CCC3)  c1CC)cccc2 |  |  |  |  |  |  |
| 1048 | n1c2c(cc(C(=O) N[C@H] (C(=O)N[C@@ H] (C(=O)N[C@H]  (C(=O)NCCCN) CCCCN)CSSC[ C@H](NC(=O) [C@@H]3CCC  N3C(=O)c3cc4c (nc3CC)cccc4)C (=O)N[C@@H]  (C(=O)NCCCN) CCCCN)CC(=O  )N)c1CC)cccc2 | CGCGCUGCUGCGCG | ligand 2-4 | Target\_lig\_62 3 | RNA seq D | Target\_155 | 5.3372421683  1843 |
| 1049 | O1COc2c1cc(C(  =O)N1[C@H] (C(=O)N[C@@ H] (C(=O)N[C@H]  (C(=O)NCCCN) CCCCN)CSSC[ C@H](NC(=O) [C@@H]3CCC  N3C(=O)c3cc4c (nc3CC)cccc4)C (=O)N[C@@H]  (C(=O)NCCCN) CCCCN)CCC1)  cc2 | CGCGCUGCUGCGCG | ligand 3-4 | Target\_lig\_62 4 | RNA seq D | Target\_155 | 5.2218487496  1636 |
| 1050 | O1COc2c1cc(C(  =O)N1[C@H] (C(=O)N[C@H]  (C(=O)N[C@@ H] (C(=O)NCCCN) CCCCN)CSSC[ C@H](NC(=O) [C@@H]3CCC N3C(=O)c3cc4 OCOc4cc3)C(= O)N[C@H]  (C(=O)NCCCN) CCCCN)CCC1)  cc2 | CCAGCUGGCAACAG CUGG | ligand 3-3 | Target\_lig\_62 1 | RNA seq E | Target\_156 | 4.6777807052  6608 |
| 1051 | n1c2c(cc(C(=O) N3[C@H] (C(=O)N[C@H]  (C(=O)N[C@@ H] (C(=O)NCCCN) CCCCN)CSSC[ C@H](NC(=O) [C@@H]4CCC  N4C(=O)c4cc5c (nc4CC)cccc5)C (=O)N[C@@H]  (C(=O)NCCCN) CCCCN)CCC3)  c1CC)cccc2 | CCAGCUGGCAACAG CUGG | ligand 4-4 | Target\_lig\_62 2 | RNA seq E | Target\_156 | 4.3979400086  7204 |
| 1052 | n1c2c(cc(C(=O) | CCAGCUGGCAACAG | ligand 2-4 | Target\_lig\_62 | RNA seq E | Target\_156 | 4.7099653886 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA\_ID** | **pKd** |
|  | N[C@H] (C(=O)N[C@@ H] (C(=O)N[C@H]  (C(=O)NCCCN) CCCCN)CSSC[ C@H](NC(=O) [C@@H]3CCC  N3C(=O)c3cc4c (nc3CC)cccc4)C (=O)N[C@@H]  (C(=O)NCCCN) CCCCN)CC(=O  )N)c1CC)cccc2 | CUGG |  | 3 |  |  | 3748 |
| 1053 | O1COc2c1cc(C(  =O)N1[C@H] (C(=O)N[C@@ H] (C(=O)N[C@H]  (C(=O)NCCCN) CCCCN)CSSC[ C@H](NC(=O) [C@@H]3CCC  N3C(=O)c3cc4c (nc3CC)cccc4)C (=O)N[C@@H]  (C(=O)NCCCN) CCCCN)CCC1)  cc2 | CCAGCUGGCAACAG CUGG | ligand 3-4 | Target\_lig\_62 4 | RNA seq E | Target\_156 | 4.6777807052  6608 |
| 1054 | O1COc2c1cc(C(  =O)N1[C@H] (C(=O)N[C@H]  (C(=O)N[C@@ H] (C(=O)NCCCN) CCCCN)CSSC[ C@H](NC(=O) [C@@H]3CCC N3C(=O)c3cc4 OCOc4cc3)C(= O)N[C@H]  (C(=O)NCCCN) CCCCN)CCC1)  cc2 | GGCCUUCCCACAAG GGAAGGCC | ligand 3-3 | Target\_lig\_62 1 | RNA seq F | Target\_157 | 4.3872161432  8026 |
| 1055 | n1c2c(cc(C(=O) N3[C@H] (C(=O)N[C@H]  (C(=O)N[C@@ H] (C(=O)NCCCN) CCCCN)CSSC[ C@H](NC(=O) [C@@H]4CCC  N4C(=O)c4cc5c (nc4CC)cccc5)C (=O)N[C@@H]  (C(=O)NCCCN) CCCCN)CCC3)  c1CC)cccc2 | GGCCUUCCCACAAG GGAAGGCC | ligand 4-4 | Target\_lig\_62 2 | RNA seq F | Target\_157 | 4.6197887582  8839 |
| 1056 | n1c2c(cc(C(=O) N[C@H] (C(=O)N[C@@ H] (C(=O)N[C@H]  (C(=O)NCCCN) CCCCN)CSSC[ C@H](NC(=O) [C@@H]3CCC  N3C(=O)c3cc4c (nc3CC)cccc4)C (=O)N[C@@H]  (C(=O)NCCCN) CCCCN)CC(=O | GGCCUUCCCACAAG GGAAGGCC | ligand 2-4 | Target\_lig\_62 3 | RNA seq F | Target\_157 | 4.6575773191  7779 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA\_ID** | **pKd** |
|  | )N)c1CC)cccc2 |  |  |  |  |  |  |
| 1057 | O1COc2c1cc(C(  =O)N1[C@H] (C(=O)N[C@@ H] (C(=O)N[C@H]  (C(=O)NCCCN) CCCCN)CSSC[ C@H](NC(=O) [C@@H]3CCC  N3C(=O)c3cc4c (nc3CC)cccc4)C (=O)N[C@@H]  (C(=O)NCCCN) CCCCN)CCC1)  cc2 | GGCCUUCCCACAAG GGAAGGCC | ligand 3-4 | Target\_lig\_62 4 | RNA seq F | Target\_157 | 4.7958800173  4408 |
| 1058 | [NH3+]CCCC[ C@H] ([NH3+])C(=O) NC1=CC2=C(C  =C1)C1C3=CC  =C(NC(=O)  [C@@H] ([NH3+])CCCC [NH3+])C=C3C 2C2=C1C=CC( NC(=O)  [C@@H] ([NH3+])CCCC [NH3+])=C2 | AUCGAUUGAGAGGA UUUGAAUGACUGAC AAAAUGCAAAGUUU AGCUUUAGCCCCAG UUGGCAACGCAGCU AACGCGUGGCCGAU GUUGUCGGCUGACG AGGAGCGGGCGCUG GCUGAAAAGCUGCA UUACCAUGGCGCAC CUGCGGUUUGUUGU UCAUAUUGCUCGUA AUUAUGCGGGCUAU GGC | Triptycene 1 | Target\_lig\_62 5 | RpoH σ32mRNA  factor | Target\_158 | 5.6020599913  2796 |
| 1059 | NC(=[NH2+])N CCC[C@H] ([NH3+])C(=O) NC1=CC2=C(C  =C1)C1C3=CC  =C(NC(=O)  [C@@H] ([NH3+])CCCN  C(N)=[NH2+])C  =C3C2C2=C1C  =CC(NC(=O)  [C@@H] ([NH3+])CCCN  C(N)=[NH2+])= C2 | AUCGAUUGAGAGGA UUUGAAUGACUGAC AAAAUGCAAAGUUU AGCUUUAGCCCCAG UUGGCAACGCAGCU AACGCGUGGCCGAU GUUGUCGGCUGACG AGGAGCGGGCGCUG GCUGAAAAGCUGCA UUACCAUGGCGCAC CUGCGGUUUGUUGU UCAUAUUGCUCGUA AUUAUGCGGGCUAU GGC | Triptycene 2 | Target\_lig\_62 6 | RpoH σ32mRNA  factor | Target\_158 | 5.8239087409  4432 |
| 1118 | CCC1=C(C=C2 C=C3C=CC=C C3=CC2=N1)C(  =O)N1CCC[C@ H]1C(=O)N[C  @@H](C\C=C/ C[C@H] (NC(=O) [C@@H]1CCC N1C(=O)C1=C( CC)N=C2C=C3 C=CC=CC3=C C2=C1)C(=O)N  [C@@H] (CCCC[NH3+]) C(=O)NCCC[N H3+])C(=O)N[C  @@H] (CCCC[NH3+]) C(=O)NCCC[N H3+] | AAAAAAAAAAAAAA AAAAAAAAAAAAAA AAAAAAUUUUUUUU UUUUUUUUUUUUUU UUUUUUUUUUUU | DCC 4 (2012) | Target\_lig\_65 2 | RNA duplex | Target\_2 | 7.1739251972  9917 |
| 1173 | C[N+]1=C(C=C C2=CC=CC=C2 1)/C=C/ C3=CC4=CC=C C=C4N3 | UGGGGGACGGGUAG GGGCGGGAGGUAGG GG | Methylquinoliniu m 15 | Target\_lig\_67 0 | A10-RNA-WT  QGRS in ADAM10 mRNA | Target\_196 | 5.4685210829  5774 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA\_ID** | **pKd** |
| 1174 | CCN1C2=C(C= C(C=C2)/C=C/ C3=[N+] (C4=CC=CC=C 4C=C3)C)C5=C C=CC=C51 | UGGGGGACGGGUAG GGGCGGGAGGUAGG GG | Methylquinoliniu m 16 | Target\_lig\_67 1 | A10-RNA-WT  QGRS in ADAM10 mRNA | Target\_196 | 4.7166987712  9645 |
| 1175 | C[NH+]1CCN( CC1)C1=C2C= CC=CC2=[N+] (C)C(C=CC2=C C=C(C=C2)N2 CCOCC2)=C1 | UGGGGGACGGGUAG GGGCGGGAGGUAGG GG | Methylquinoliniu m 22 | Target\_lig\_67 2 | A10-RNA-WT  QGRS in ADAM10 mRNA | Target\_196 | 5.5850266520  2918 |
| 1176 | C[NH+]1CCN( CC1)C1=C2C= CC=CC2=[N+] (C)C(C=CC2=C C3=CC=CC=C3 N2)=C1 | UGGGGGACGGGUAG GGGCGGGAGGUAGG GG | Methylquinoliniu m 23 | Target\_lig\_67 3 | A10-RNA-WT  QGRS in ADAM10 mRNA | Target\_196 | 5.7447274948  9669 |
| 1178 | CCN1C2=C(C= CC=C2)C2=C1 C=CC(C=CC1= CC(N3CC[NH+  ] (C)CC3)=C3C= CC=CC3=[N+]1  C)=C2 | UGGGGGACGGGUAG GGGCGGGAGGUAGG GG | Methylquinoliniu m 24 | Target\_lig\_67 4 | A10-RNA-WT  QGRS in ADAM10  mRNA Mutant | Target\_197 | 0.1549019599  85743 |
| 1179 | CCN1C2=C(C= CC=C2)C2=C1 C=CC(C=CC1= CC(N3CC[NH+  ] (C)CC3)=C3C= CC=CC3=[N+]1  C)=C2 | UGGGGGACGGGUAG GGGCGGGAGGUAGG GG | Methylquinoliniu m 24 | Target\_lig\_67 4 | A10-RNA-WT  QGRS in ADAM10 mRNA | Target\_196 | 5.3098039199  7149 |
| 1180 | NC1=CC=C(C= C1)C1=CC2=C C=C(C=C2N1) C1=[NH+]CCN 1 | GGCAGUGUGAGUAC CUUCAUACGUC | Compound 1 | Target\_lig\_67 5 | DDPAC MAPT  A Bulge | Target\_198 | 5 |
| 1181 | NC(=[NH2+])C 1=CC=C(NC2= CC=C(C=C2)C2  =CC3=CC=C(C  =C3N2)C(N)=[ NH2+])C=C1 | GGCAGUGUGAGUAC CUUCAUACGUC | Compound 2 | Target\_lig\_67 6 | DDPAC MAPT  A Bulge | Target\_198 | 4.8538719643  2176 |
| 1182 | NC(=[NH2+])C 1=CC=C(NC2= CC=C(C=C2)C2  =CC3=CC=C(C  =C3N2)C(N)=[ NH2+])C=C1 | GGCAGUGUGAGUAC CUUCAUACGUC | Compound 2 | Target\_lig\_67 6 | DDPAC + I17T  Mutant | Target\_199 | 4 |
| 1183 | NC(=[NH2+])C 1=CC=C(NC2= CC=C(C=C2)C2  =CC3=CC=C(C  =C3N2)C(N)=[ NH2+])C=C1 | GGCAGUGUGAGUAC CUUCAUACGUC | Compound 2 | Target\_lig\_67 6 | MAPT A WT | Target\_200 | 4.8538719643  2176 |
| 1208 | C1=CC(=CC(= C1)N)C2=NC3= C(N2)C=C(C=C 3)C4=CC5=C(C  =C4)N=C(N5)C 6=CC(=CC=C6) N | GGGAGAGGGUUUAA UUAAAAGUCGACGA AAGUCGUCGCUAAU UGGAUCCGCAAGG | H1 | Target\_lig\_68 4 | Fully Paired RNA | Target\_207 | 6.7212463990  4717 |
| 1217 | C1CCN(C1)C2= NC(=C3C(=C2) C(=C(N=C3N)N 4CCCC4)C#N) N | CGCUGCGGAAACGC UGCG | Naphthyridine 2 | Target\_lig\_68 6 | 1 X 1 UU  Hairpin | Target\_208 | 6.2757241303  9921 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA\_ID** | **pKd** |
| 1218 | C1CCN(C1)C2= NC(=C3C(=C2) C(=C(N=C3N)N 4CCCC4)C#N) N | CGCAGCGGAAACGC UGCG | Naphthyridine 2 | Target\_lig\_68 6 | AU stem | Target\_209 | 4.6020599913  2796 |
| 1220 | C1=CC(=CC=C 1C(=O)NC2=N C=C(C=C2)NC(  =O)C3=CC=NC  =C3)F | GCGCGCGCGAAAGC GCGCGC | p7 | Target\_lig\_68 7 | GC Stem Loop | Target\_211 | 4.5228787452  8034 |
| 1221 | C1=CC(=CC=C 1C(=O)NC2=N C=C(C=C2)NC(  =O)C3=CC=NC  =C3)F | CGCGAATTCGCGTTT TCGCGAATTCGCG | p7 | Target\_lig\_68 7 | AT Hairpin DNA | Target\_212 | 4.3010299956  6398 |
| 1263 | CCN(CC)CCOC 1=CC=C(C=C1) NC2=NC(=NC3  =CC=CC=C32) C4=CC=CC=C4 NC(=O)CCN5C CN(CC5)C | CGCGAATTCGCGTTT TCGCGAATTCGCG | Compound 1  (2017) | Target\_lig\_70 7 | Hairpin DNA | Target\_212 | 4.6736641390  7125 |
| 1267 | C[NH+]1CCN( CC1)C1=CC=C( C=C1)C1=CC= C2NC(=NC2=C 1)C1=CC(=C(O CCCC(=O)NCC CN=[N+]=[N-]) C(=C1)C(C) (C)C)C(C)(C)C | GGGAGAGGGUUUAU GACGAAAGUCUAUG GAUCCGCAAGG | Targaprimir-18a | Target\_lig\_70 8 | G\_U/CUA  Bulge in miR- 18a | Target\_223 | 4.5228787452  8034 |
| 1268 | C[NH+]1CCN( CC1)C1=CC=C( C=C1)C1=CC= C2NC(=NC2=C 1)C1=CC(=C(O CCCC(=O)NCC CN=[N+]=[N-]) C(=C1)C(C) (C)C)C(C)(C)C | GGGAGAGGGUUUAU AGACGAAAGUCUAU GGAUCCGCAAGG | Targaprimir-18a | Target\_lig\_70 8 | GAU/CUA  Stem Mutant | Target\_224 | 4 |
| 1269 | C[NH+]1CCN( CC1)C1=CC=C( C=C1)C1=CC= C2NC(=NC2=C 1)C1=CC(=C(O CCCC(=O)NCC CN=[N+]=[N-]) C(=C1)C(C) (C)C)C(C)(C)C | GGGAGAGGGUUUAG AUACGAAAGUACUG GAUCCGCAAGG | Targaprimir-18a | Target\_lig\_70 8 | GAU/A\_C  Bulge in miR- 18a | Target\_225 | 4.4948500216  8009 |
| 1270 | C[NH+]1CCN( CC1)C1=CC=C( C=C1)C1=CC= C2NC(=NC2=C 1)C1=CC(=C(O CCCC(=O)NCC CN=[N+]=[N-]) C(=C1)C(C) (C)C)C(C)(C)C | GGGAGAGGGUUUAG GUACGAAAGUACUG GAUCCGCAAGG | Targaprimir-18a | Target\_lig\_70 8 | GGU/A\_C  Bulge Mutant | Target\_226 | 4.3979400086  7204 |
| 1287 | NC(=[NH2+])C 1=CC=C(N=C1) C1=CC=C(O1) C1=CC=C(O1) C1=NC=C(C=C 1)C(N)=[NH2+] | GGGGCCGGGGCCGG GGCCGGGGCCGGGG CCGGGGCCGGGGCC GGGGCCGGGGCCGG GGCCGGGGCCGGGG CCGGGGCCGGGGCC GGGGCCGGGGCCGG GGCCGGGGCCGGGG CCGGGGCCGGGGCC GGGGCCGGGGCCGG GGCCGGGGCCGGGG CCGGGGCCGGGGCC | DB1246 | Target\_lig\_71 6 | G4C2 repeat G- quadruplex RNA | Target\_232 | 6.3872161432  8026 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA\_ID** | **pKd** |
|  |  | GGGGCCGGGGCCGG GGCCGGGGCCGGGG CCGGGGCCGGGGCC GGGGCC |  |  |  |  |  |
| 1288 | NC(=[NH2+])C 1=CC=C(N=C1) C1=CC=C(S1)C 1=CC=C(S1)C1  =NC=C(C=C1) C(N)=[NH2+] | GGGGCCGGGGCCGG GGCCGGGGCCGGGG CCGGGGCCGGGGCC GGGGCCGGGGCCGG GGCCGGGGCCGGGG CCGGGGCCGGGGCC GGGGCCGGGGCCGG GGCCGGGGCCGGGG CCGGGGCCGGGGCC GGGGCCGGGGCCGG GGCCGGGGCCGGGG CCGGGGCCGGGGCC GGGGCCGGGGCCGG GGCCGGGGCCGGGG CCGGGGCCGGGGCC GGGGCC | DB1247 | Target\_lig\_71 7 | G4C2 repeat G- quadruplex RNA | Target\_232 | 6.5883802940  3677 |
| 1291 | C1=C(C=C(C(= C1O)O)O)C2=C (C(=O)C3=C(C  =C(C=C3O2)O) O)O | GGAGAGGGUUUAAU CAGUACGAAAGUAG ACAUUGGAUCCGCA AGG | Myricetin | Target\_lig\_71 8 | 5′CAG/3′GAC  x 2 repeat RNA | Target\_235 | 7.1958605676  6465 |
| 1292 | C1=C(C=C(C(= C1O)O)O)C2=C (C(=O)C3=C(C  =C(C=C3O2)O) O)O | GGAGAGGGUUUAAU CAGUACGAAAGUAG ACAUUGGAUCCGCA AGG | Myricetin | Target\_lig\_71 8 | 5′CAG/3′GAC  x 3 repeat RNA | Target\_236 | 8.2365720064  3706 |
| 1293 | C1=C(C=C(C(= C1O)O)O)C2=C (C(=O)C3=C(C  =C(C=C3O2)O) O)O | GGAGAGGGUUUAAU CAGUACGAAAGUAG ACAUUGGAUCCGCA AGG | Myricetin | Target\_lig\_71 8 | 5′CAG/3′GAC  x 4 repeat RNA | Target\_237 | 7.3861581781  2393 |
| 1294 | C1=C(C=C(C(= C1O)O)O)C2=C (C(=O)C3=C(C  =C(C=C3O2)O) O)O | GGAGAGGGUUUAAU CAGUACGAAAGUAG ACAUUGGAUCCGCA AGG | Myricetin | Target\_lig\_71 8 | 5′CAG/3′GAC  x 5 repeat RNA | Target\_238 | 7.2441251443  2751 |
| 1295 | C1=C(C=C(C(= C1O)O)O)C2=C (C(=O)C3=C(C  =C(C=C3O2)O) O)O | GGAGAGGGUUUAAU CAGUACGAAAGUAG UCAUUGGAUCCGCA AGG | Myricetin | Target\_lig\_71 8 | 5'CAG/3'GUC  x 6 repeat RNA | Target\_234 | 7.1366771398  7954 |
| 1296 | C1=C(C=C(C(= C1O)O)O)C2=C (C(=O)C3=C(C  =C(C=C3O2)O) O)O | GGAGAGGGUUUAAU CAGUACGAAAGUAG ACAUUGGAUCCGCA AGG | Myricetin | Target\_lig\_71 8 | 5′CAG/3′GAC  x 33 repeat RNA | Target\_239 | 8.7695510786  2173 |
| 1297 | C1=C(C=C(C(= C1O)O)O)C2=C (C(=O)C3=C(C  =C(C=C3O2)O) O)O | GGAGAGGGUUUAAU CAGUACGAAAGUAG ACAUUGGAUCCGCA AGG | Myricetin | Target\_lig\_71 8 | 5′CAG/3′GAC  internal loop | Target\_240 | 6.6020599913  2796 |
| 1298 | C1=C(C=C(C(= C1O)O)O)C2=C (C(=O)C3=C(C  =C(C=C3O2)O) O)O | GGAGAGGGUUUAAU CAGUACGAAAGUAG UCAUUGGAUCCGCA AGG | Myricetin | Target\_lig\_71 8 | 5'CAG/3'GUC  internal loop | Target\_241 | 3.6946486305  5338 |
| 1299 | [NH3+]CCNC1  =C2OC=CC2=C (NCC[NH3+])C 2=C1C(=O)C1= CC=CC=C1C2= O | GCGGCGGCGGAGGC A | Anthrafurandion e 2a | Target\_lig\_71 9 | KRAS RNA G-  quadruplex utr- 1 | Target\_242 | 7.1249387366  083 |
| 1300 | [NH3+]CCNC1  =C2OC=CC2=C | GGCGGCGGCAGUGG CGGCGG | Anthrafurandion e 2a | Target\_lig\_71 9 | KRAS RNA G-  quadruplex utr- | Target\_243 | 6.6003262785  1896 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA\_ID** | **pKd** |
|  | (NCC[NH3+])C 2=C1C(=O)C1= CC=CC=C1C2= O |  |  |  | z |  |  |
| 1301 | [NH3+]CCNC1  =C2OC=CC2=C (NCC[NH3+])C 2=C1C(=O)C1= CC=CC=C1C2= O | CAGCAGCGGCGGCG GCAGUGG | Anthrafurandion e 2a | Target\_lig\_71 9 | KRAS RNA G-  quadruplex utr- 4 | Target\_244 | 7.0177287669  6043 |
| 1302 | [NH3+]CCNC1  =C2OC=CC2=C (NCC[NH3+])C 2=C1C(=O)C1= CC=CC=C1C2= O | CCGCCGCAGUGGCG GCGG | Anthrafurandion e 2a | Target\_lig\_71 9 | RNA Hairpin | Target\_245 | 6.2890368810  0472 |
| 1304 | [NH3+]CCNC1  =C2SC=CC2=C (NCC[NH3+])C 2=C1C(=O)C1= CC=CC=C1C2= O | GCGGCGGCGGAGGC A | Anthrathiophene dione 2b | Target\_lig\_72 0 | KRAS RNA G-  quadruplex utr- 1 | Target\_242 | 7.0409586076  7891 |
| 1305 | [NH3+]CCNC1  =C2SC=CC2=C (NCC[NH3+])C 2=C1C(=O)C1= CC=CC=C1C2= O | GGCGGCGGCAGUGG CGGCGG | Anthrathiophene dione 2b | Target\_lig\_72 0 | KRAS RNA G-  quadruplex utr- z | Target\_243 | 6.5316526695  8784 |
| 1306 | [NH3+]CCNC1  =C2SC=CC2=C (NCC[NH3+])C 2=C1C(=O)C1= CC=CC=C1C2= O | CAGCAGCGGCGGCG GCAGUGG | Anthrathiophene dione 2b | Target\_lig\_72 0 | KRAS RNA G-  quadruplex utr- 4 | Target\_244 | 7.0809219076  2393 |
| 1307 | [NH3+]CCNC1  =C2SC=CC2=C (NCC[NH3+])C 2=C1C(=O)C1= CC=CC=C1C2= O | CCGCCGCAGUGGCG GCGG | Anthrathiophene dione 2b | Target\_lig\_72 0 | RNA Hairpin | Target\_245 | 6.3169529617  6115 |
| 1310 | CC[NH+]1CCN (C[C@@H]1C) C1=CC=C2C=C (C3=CN4C=C( C)N=C(C)C4=N 3)C(=O)OC2=C  1 | AGAAGGAAGGUGCU C | SMN-C2 | Target\_lig\_72 2 | Oligo-4, an AGGAAG-  containing RNA 15-mer | Target\_248 | 4.7958800173  4408 |
| 1311 | CC[NH+]1CCN (C[C@@H]1C) C1=CC=C2C=C (C3=CN4C=C( C)N=C(C)C4=N 3)C(=O)OC2=C  1 | AAUUAAGGAGUAAG U | SMN-C2 | Target\_lig\_72 2 | Oligo-7, an AAGGAG-  containing RNA 15-mer | Target\_249 | 4.3372421683  1843 |
| 1312 | CC[NH+]1CCN (C[C@@H]1C) C1=CC=C2C=C (C3=CN4C=C( C)N=C(C)C4=N 3)C(=O)OC2=C  1 | CUUCCUUUAUUUUC C | SMN-C2 | Target\_lig\_72 2 | Oligo-1, a pyrimidine-rich RNA 15-mer | Target\_250 | 3.7958800173  4407 |
| 1313 | CC[NH+]1CCN (C[C@@H]1C) C1=CC=C2C=C (C3=CN4C=C( C)N=C(C)C4=N 3)C(=O)OC2=C  1 | GGUUUUAGACAAAA U | SMN-C2 | Target\_lig\_72 2 | Oligo-2, an RNA 15-mer | Target\_251 | 3.7958800173  4407 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA\_ID** | **pKd** |
| 1314 | CC[NH+]1CCN (C[C@@H]1C) C1=CC=C2C=C (C3=CN4C=C( C)N=C(C)C4=N 3)C(=O)OC2=C  1 | AAAAUCAAAAAGAA G | SMN-C2 | Target\_lig\_72 2 | Oligo-3, a purine-rich RNA 15-mer | Target\_252 | 3.7958800173  4407 |
| 1315 | CC[NH+]1CCN (C[C@@H]1C) C1=CC=C2C=C (C3=CN4C=C( C)N=C(C)C4=N 3)C(=O)OC2=C  1 | UGCUCACAUUCCUU A | SMN-C2 | Target\_lig\_72 2 | Oligo-5, an RNA 15-mer | Target\_253 | 3.7958800173  4407 |
| 1316 | CC[NH+]1CCN (C[C@@H]1C) C1=CC=C2C=C (C3=CN4C=C( C)N=C(C)C4=N 3)C(=O)OC2=C  1 | CCUUAAAUUAAGGA G | SMN-C2 | Target\_lig\_72 2 | Oligo-6, an RNA 15-mer | Target\_254 | 3.7958800173  4407 |
| 1318 | C(CN1C=C(CN C2=C3C=CC=C C3=[NH+]C3=C 2OC2=C3C=CC  =C2)N=N1)C[N H+]1CCCCC1 | GGGUUAGGGU | Quindoline CK1- 14 | Target\_lig\_72 3 | Telomeric DNA G-  quadruplex (HTG22) | Target\_256 | 4.7798919119  5995 |
| 1319 | C(CN1C=C(CN C2=C3C=CC=C C3=[NH+]C3=C 2OC2=C3C=CC  =C2)N=N1)C[N H+]1CCCCC1 | CGCGAATTCGCGTTT TCGCGAATTCGCG | Quindoline CK1- 14 | Target\_lig\_72 3 | Hairpin DNA | Target\_212 | 0.4672456210  07502 |
| 1320 | C(CN1C=C(CN C2=C3C=CC=C C3=[NH+]C3=C 2OC2=C3C=CC  =C2)N=N1)C[N H+]1CCCCC1 | AGGGUUAGGGUUAG GGUUAGGG | Quindoline CK1- 14 | Target\_lig\_72 3 | TERRA G-  quadruplex (TERRA22) | Target\_255 | 6.6575773191  7779 |
| 1323 | C(CN1C=C(CN C2=C3C=CC=C C3=[NH+]C3=C 2OC2=C3C=CC  =C2)N=N1)C[N H+]1CCCCC1 | AGGGGGCCGUGGGG UGGGAGCUGGGG | Quindoline CK1- 14 | Target\_lig\_72 3 | BCL2 RNA G-  quadruplex | Target\_258 | 5.5301779840  2184 |
| 1324 | C(CN1C=C(CN C2=C3C=CC=C C3=[NH+]C3=C 2OC2=C3C=CC  =C2)N=N1)C[N H+]1CCCCC1 | UGUGGGAGGGGCGG GUCUGGG | Quindoline CK1- 14 | Target\_lig\_72 3 | NRAS RNA G-  quadruplex | Target\_259 | 6.3565473235  1381 |
| 1325 | C(CN1C=C(CN C2=C3C=CC=C C3=[NH+]C3=C 2OC2=C3C=CC  =C2)N=N1)C[N H+]1CCCCC1 | TGAGGGTGGGTAGG GTGGGTAA | Quindoline CK1- 14 | Target\_lig\_72 3 | Pu22 DNA G-  quadruplex | Target\_260 | 5.1487416512  8092 |
| 1326 | C(CN1C=C(CN C2=C3C=CC=C C3=[NH+]C3=C 2OC2=C3C=CC  =C2)N=N1)C[N H+]1CCCCC1 | GGGUUAGGGU | Quindoline CK1- 14 | Target\_lig\_72 3 | TRF2:Telomeri c duplex DNA (hTELO-dup) | Target\_261 | 7.2317319835  4845 |
| 1327 | C(CN1C=C(CN C2=C3C=CC=C C3=[NH+]C3=C 2OC2=C3C=CC  =C2)N=N1)C[N H+]1CCCCC1 | GGGUUAGGGU | Quindoline CK1- 14 | Target\_lig\_72 3 | TRF2:TERRA  G-quadruplex (TERRA22):Te  lomeric duplex DNA (hTELO-  dup) | Target\_262 | 6.2727841790  9151 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA\_ID** | **pKd** |
| 1505 | O=c1n2Cc3nc4s cc(c4c(=O)n3Cc 2nc2c1c(cs2)c1c coc1)c1ccco1 | AGGGUUAGGGUUAG GGUUAGGG | RGB-1 | Target\_lig\_81 5 | TERRA G-  quadruplex | Target\_255 | 5.2291479883  5786 |
| 1517 | C1=CC(=CC=C  1/C=N/ N=C(N)N)C2=C C3=C(S2)C=C( C=C3)/C=N/ N=C(N)N | GGCAGUGUGAGUAC CUUCAUACGUC | Compound 3 | Target\_lig\_82 3 | DDPAC hairpin A-bulge | Target\_198 | 5.1249387366  083 |
| 1518 | CCC1=C(C=C2 C=C3C=CC=C C3=CC2=N1)C(  =O)N(C)  [C@@H](C\ C=C\C[C@H] (N(C)C(=O)C1= C(CC)N=C2C= C3C=CC=CC3= CC2=C1)C(=O) N1CCC[C@H]1 C(=O)N(C)  [C@@H] (CC1=CC=CC= C1)C(=O)NCC C[NH3+])C(=O) N1CCC[C@H]1 C(=O)N(C)  [C@@H] (CC1=CC=CC= C1)C(=O)NCC C[NH3+] | GGCAGUGUGAGUAC CUUCAUACGUC | Compound 4 | Target\_lig\_65 4 | DDPAC hairpin A-bulge | Target\_198 | 5.4436974992  3271 |
| 1519 | Cn1c(NCc2cccc (c2)C(=O)C)ncc  1c1ccc(cc1)C(= O)C | GGCAGUGUGAGUAC CUUCAUACGUC | Compound 5 | Target\_lig\_81 3 | DDPAC hairpin A-bulge | Target\_198 | 4.7851561519  523 |
| 1520 | OC1CN(C1)Cc1  ccc(cc1)C1CCN (CC1)C(=O)c1c  n(c2c1cccc2)C | GGCAGUGUGAGUAC CUUCAUACGUC | Compound 6 | Target\_lig\_82 6 | DDPAC hairpin A-bulge | Target\_198 | 4.8181564120  5523 |
| 1521 | OC1CN(C1)Cc1  ccc(cc1)C1CCN (CC1)C(=O)c1c  (C)nc2n1ccs2 | GGCAGUGUGAGUAC CUUCAUACGUC | Compound 7 | Target\_lig\_82 7 | DDPAC hairpin A-bulge | Target\_198 | 4.7721132953  8633 |
| 1522 | Oc1ccc2c(c1)c1 c(C)c3c[n+] (CCN4CCCCC4  )ccc3c(c1[nH]2) C | GGCAGUGUGAGUAC CUUCAUACGUC | Compound 8 | Target\_lig\_12 65 | DDPAC hairpin A-bulge | Target\_198 | 5.3187587626  2441 |
| 1600 | CC[NH+]1CCN (C[C@@H]1C) C1=CC=C2C=C (C3=CN4C=C( C)N=C(C)C4=N 3)C(=O)OC2=C  1 | AAAAGAAGGAAGUG CUCACAUUCCUUAA AUUAAGGAGUAAGU CUGC | SMN-C2 | Target\_lig\_72 2 | SMN2 pre- mRNA GA-  rich sequence | Target\_284 | 5.2676062401  7703 |
| 1601 | CC1=CN2C=C( C=C(C2=N1)F) C3=CC(=O)N4 C=C(C=CC4=N 3)N5CCN(CC5) C | AAAAGAAGGAAGUG CUCACAUUCCUUAA AUUAAGGAGUAAGU CUGC | SMN-C5 | Target\_lig\_85 8 | SMN2 pre- mRNA GA-  rich sequence | Target\_284 | 5.0969100130  0806 |
| 1602 | C[C@H]1CN(C CN1)C2=CC3= C(C=C2)C=C(C (=O)O3)C4=CN 5C=C(N=C(C5= N4)C)C | AAAAGAAGGAAGUG CUCACAUUCCUUAA AUUAAGGAGUAAGU CUGC | SMN2\_compoun d\_1 | Target\_lig\_85 9 | SMN2 pre- mRNA GA-  rich sequence | Target\_284 | 4.7328282715  9699 |
| 1603 | O=C(OC(C) | AAAAGAAGGAAGUG | SMN2\_compoun | Target\_lig\_86 | SMN2 pre- | Target\_284 | 4.2924298239 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA\_ID** | **pKd** |
|  | (C)C)NCCN1C CN(C[C@@H]1  C)c1ccc2c(c1)oc (=O)c(c2)c1cn2 c(n1)c(C)nc(c2) C | CUCACAUUCCUUAA AUUAAGGAGUAAGU CUGC | d\_2 | 0 | mRNA GA-  rich sequence |  | 0206 |
| 1604 | CN1CCN(CC1)  c1ccc2c(c1)oc(= O)c(c2)c1ccccc1 Cl | AAAAGAAGGAAGUG CUCACAUUCCUUAA AUUAAGGAGUAAGU CUGC | SMN2\_compoun d\_3 | Target\_lig\_86 1 | SMN2 pre- mRNA GA-  rich sequence | Target\_284 | 4 |
| 1605 | CN1CCN(CC1)  c1ccc2c(c1)oc(= O)c(c2)c1cccc(c 1)Cl | AAAAGAAGGAAGUG CUCACAUUCCUUAA AUUAAGGAGUAAGU CUGC | SMN2\_compoun d\_4 | Target\_lig\_86 2 | SMN2 pre- mRNA GA-  rich sequence | Target\_284 | 4.4449055514  2168 |
| 1606 | CN1CCN(CC1)  c1ccc2c(c1)oc(= O)c(c2)c1ccc(cc 1)Cl | AAAAGAAGGAAGUG CUCACAUUCCUUAA AUUAAGGAGUAAGU CUGC | SMN2\_compoun d\_5 | Target\_lig\_86 3 | SMN2 pre- mRNA GA-  rich sequence | Target\_284 | 4.5142785735  1842 |
| 1607 | CN1CCN(CC1)  c1cc(F)c2c(c1)o c(=O)c(c2)c1ccc c(c1)Cl | AAAAGAAGGAAGUG CUCACAUUCCUUAA AUUAAGGAGUAAGU CUGC | SMN2\_compoun d\_6 | Target\_lig\_86 4 | SMN2 pre- mRNA GA-  rich sequence | Target\_284 | 4.4841261562  8832 |
| 1608 | CN1CCN(CC1)  c1cc(F)c2c(c1)o c(=O)c(c2)c1ccc (cc1)Cl | AAAAGAAGGAAGUG CUCACAUUCCUUAA AUUAAGGAGUAAGU CUGC | SMN2\_compoun d\_7 | Target\_lig\_86 5 | SMN2 pre- mRNA GA-  rich sequence | Target\_284 | 4.5100415205  7517 |
| 1609 | CN1CCN(CC1)  c1ccc2c(c1)oc(= O)c(c2C)c1cccc (c1)Cl | AAAAGAAGGAAGUG CUCACAUUCCUUAA AUUAAGGAGUAAGU CUGC | SMN2\_compoun d\_8 | Target\_lig\_86 6 | SMN2 pre- mRNA GA-  rich sequence | Target\_284 | 4 |
| 1610 | CN1CCN(CC1)  c1ccc2c(c1)oc(= O)c(c2C)c1ccc( cc1)Cl | AAAAGAAGGAAGUG CUCACAUUCCUUAA AUUAAGGAGUAAGU CUGC | SMN2\_compoun d\_9 | Target\_lig\_86 7 | SMN2 pre- mRNA GA-  rich sequence | Target\_284 | 4 |
| 1611 | C1CN(CCN1)C 2=CC3=C(C=C   1. C=C(C(=O)O 2. C4=CN5C=C C=CC5=N4 | AAAAGAAGGAAGUG CUCACAUUCCUUAA AUUAAGGAGUAAGU CUGC | SMN2\_compoun d\_10 | Target\_lig\_86 8 | SMN2 pre- mRNA GA-  rich sequence | Target\_284 | 4.8386319977  6503 |
| 1612 | COc1ncc2n(c1)c c(n2)c1cc2ccc(c c2oc1=O)N1CC NCC1 | AAAAGAAGGAAGUG CUCACAUUCCUUAA AUUAAGGAGUAAGU CUGC | SMN2\_compoun d\_11 | Target\_lig\_86 9 | SMN2 pre- mRNA GA-  rich sequence | Target\_284 | 4.9430951486  6353 |
| 1613 | CC[NH+]1CCN (C[C@@H]1C) C1=CC=C2C=C (C3=CN4C=C( C)N=C(C)C4=N 3)C(=O)OC2=C  1 | UGAAGGAAGGUUUC GACCUUCCUUCA | SMN-C2 | Target\_lig\_72 2 | Seq20 | Target\_285 | 4 |
| 1614 | CC[NH+]1CCN (C[C@@H]1C) C1=CC=C2C=C (C3=CN4C=C( C)N=C(C)C4=N 3)C(=O)OC2=C  1 | GCGCCGACUGAAGG AAGGAGUCGGCGC | SMN-C2 | Target\_lig\_72 2 | Seq21 | Target\_286 | 5.3372421683  1843 |
| 1615 | CC[NH+]1CCN (C[C@@H]1C) C1=CC=C2C=C (C3=CN4C=C( C)N=C(C)C4=N 3)C(=O)OC2=C  1 | GTGCCAGTTCGCTGG CACTGAAGGAAGGT | SMN-C2 | Target\_lig\_72 2 | Seq22 | Target\_287 | 4.9586073148  4177 |
| 1616 | CC[NH+]1CCN (C[C@@H]1C) C1=CC=C2C=C | GCCAGGCGCACUUU CGAGUGCGCGAAGG AAGGCUGGC | SMN-C2 | Target\_lig\_72 2 | Seq23 | Target\_288 | 5.2518119729  938 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA\_ID** | **pKd** |
|  | (C3=CN4C=C( C)N=C(C)C4=N 3)C(=O)OC2=C  1 |  |  |  |  |  |  |
| 1765 | [C@H]1([C@H] (C[C@H]  ([C@H] ([C@H]1O)O[C  @@H]1[C@@ H](C[C@@H]  ([C@@H] (O1)CN)O)N)N) N)O[C@@H]1[ C@H] ([C@@H]  ([C@H]  ([C@@H]  (O1)CNc1c2ccc cc2nc2c1cccc2) O)N)O | GGCUUAGUAUAGCG AGGUUUAGCUACAC UCGUGCUGAGCC | Tobramycin | Target\_lig\_54 0 | J6f1 RNA | Target\_307 | 8.2881927709  5881 |
| 1766 | OCC1OC(OC2 C(N)CC(C(C2O  )OC2OC(CNC(  =O)c3ccc(c(c3) C(=O)O)c3c4cc c(=[N+]  (C)C)cc4oc4c3c cc(c4)N(C)C)C( CC2N)O)N)C(C  (C1O)N)O | GGCUUAGUAUAGCG AGGUUUAGCUACAC UCGUGCUGAGCC | Tobramycin-CRT | Target\_lig\_99 3 | J6f1 RNA | Target\_307 | 6.7153437172  1148 |
| 1767 | [C@H]1([C@H] (C[C@H]  ([C@H] ([C@H]1O)O[C  @@H]1[C@@ H](C[C@@H]  ([C@@H] (O1)CN)O)N)N) N)O[C@@H]1[ C@H] ([C@@H]  ([C@H]  ([C@@H]  (O1)CNc1c2ccc cc2nc2c1cccc2) O)N)O | GGCUUAGUAUAGCU AGGUUUAGCUACAC UCGUGCUGAGCC | Tobramycin | Target\_lig\_54 0 | J6fd6 RNA | Target\_308 | 6.8297382846  0504 |
| 1768 | OCC1OC(OC2 C(N)CC(C(C2O  )OC2OC(CNC(  =O)c3ccc(c(c3) C(=O)O)c3c4cc c(=[N+]  (C)C)cc4oc4c3c cc(c4)N(C)C)C( CC2N)O)N)C(C  (C1O)N)O | GGCUUAGUAUAGCU AGGUUUAGCUACAC UCGUGCUGAGCC | Tobramycin-CRT | Target\_lig\_99 3 | J6fd6 RNA | Target\_308 | 7.4685210829  5774 |
| 1769 | [C@H]1([C@H] (C[C@H]  ([C@H] ([C@H]1O)O[C  @@H]1[C@@ H](C[C@@H]  ([C@@H] (O1)CN)O)N)N) N)O[C@@H]1[ C@H] ([C@@H]  ([C@H]  ([C@@H]  (O1)CNc1c2ccc cc2nc2c1cccc2) O)N)O | GGCUUAGUAUAGCG AGGUUUGGCUACAC UCGUGCUGAGCC | Tobramycin | Target\_lig\_54 0 | J6f15 RNA | Target\_309 | 7.7447274948  9669 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA\_ID** | **pKd** |
| 1770 | OCC1OC(OC2 C(N)CC(C(C2O  )OC2OC(CNC(  =O)c3ccc(c(c3) C(=O)O)c3c4cc c(=[N+]  (C)C)cc4oc4c3c cc(c4)N(C)C)C( CC2N)O)N)C(C  (C1O)N)O | GGCUUAGUAUAGCG AGGUUUGGCUACAC UCGUGCUGAGCC | Tobramycin-CRT | Target\_lig\_99 3 | J6f15 RNA | Target\_309 | 6.3707943428  977 |
| 1771 | [C@H]1([C@H] (C[C@H]  ([C@H] ([C@H]1O)O[C  @@H]1[C@@ H](C[C@@H]  ([C@@H] (O1)CN)O)N)N) N)O[C@@H]1[ C@H] ([C@@H]  ([C@H]  ([C@@H]  (O1)CNc1c2ccc cc2nc2c1cccc2) O)N)O | GGCUUAGUAUAGCG AGGUUUAACUACAC UCGUGCUGAGCC | Tobramycin | Target\_lig\_54 0 | J6f16 RNA | Target\_310 | 8.5934598195  6604 |
| 1772 | OCC1OC(OC2 C(N)CC(C(C2O  )OC2OC(CNC(  =O)c3ccc(c(c3) C(=O)O)c3c4cc c(=[N+]  (C)C)cc4oc4c3c cc(c4)N(C)C)C( CC2N)O)N)C(C  (C1O)N)O | GGCUUAGUAUAGCG AGGUUUAACUACAC UCGUGCUGAGCC | Tobramycin-CRT | Target\_lig\_99 3 | J6f16 RNA | Target\_310 | 7.2218487496  1636 |
| 1773 | [C@H]1([C@H] (C[C@H]  ([C@H] ([C@H]1O)O[C  @@H]1[C@@ H](C[C@@H]  ([C@@H] (O1)CN)O)N)N) N)O[C@@H]1[ C@H] ([C@@H]  ([C@H]  ([C@@H]  (O1)CNc1c2ccc cc2nc2c1cccc2) O)N)O | GGCUUAGUAUAGCG AGGUUUAGUUACAC UCGUGCUGAGCC | Tobramycin | Target\_lig\_54 0 | J6f17 RNA | Target\_311 | 7.7447274948  9669 |
| 1774 | OCC1OC(OC2 C(N)CC(C(C2O  )OC2OC(CNC(  =O)c3ccc(c(c3) C(=O)O)c3c4cc c(=[N+]  (C)C)cc4oc4c3c cc(c4)N(C)C)C( CC2N)O)N)C(C  (C1O)N)O | GGCUUAGUAUAGCG AGGUUUAGUUACAC UCGUGCUGAGCC | Tobramycin-CRT | Target\_lig\_99 3 | J6f17 RNA | Target\_311 | 6.3763372926  438 |
| 1835 | C1CN=C(N1)N N=CC2=C3C=C C=CC3=C(C4= CC=CC=C42)C  =NNC5=NCCN 5 | GGGAGAGGGUUUAA UUCAGUACGAAAGU ACGGAUUGGAUCCG CAAGG | Bisantrene | Target\_lig\_10 31 | (5'CAG/ 3'GGC) x 1 | Target\_334 | 5.3979400086  7204 |
| 1836 | C1CN=C(N1)N N=CC2=C3C=C C=CC3=C(C4= | GGGAGAGGGUUUAA UUCCGUACGAAAGU ACAGAUUGGAUCCG | Bisantrene | Target\_lig\_10 31 | (5'CCG/ 3'GAC) x 1 | Target\_335 | 5.9208187539  5238 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA\_ID** | **pKd** |
|  | CC=CC=C42)C  =NNC5=NCCN 5 | CAAGG |  |  |  |  |  |
| 1837 | C1CN=C(N1)N N=CC2=C3C=C C=CC3=C(C4= CC=CC=C42)C  =NNC5=NCCN 5 | GGGAGAGGGUUUAA UUCGGUACGAAAGU ACAGAUUGGAUCCG CAAGG | Bisantrene | Target\_lig\_10 31 | (5'CGG/ 3'GAC) x 1 | Target\_336 | 5.2218487496  1636 |
| 1838 | C1CN=C(N1)N N=CC2=C3C=C C=CC3=C(C4= CC=CC=C42)C  =NNC5=NCCN 5 | GGGAGAGGGUUUAA UUCCGUACGAAAGU ACUGAUUGGAUCCG CAAGG | Bisantrene | Target\_lig\_10 31 | (5'CCG/ 3'GUC) x 1 | Target\_337 | 5.3372421683  1843 |
| 1839 | C1CN=C(N1)N N=CC2=C3C=C C=CC3=C(C4= CC=CC=C42)C  =NNC5=NCCN 5 | GGGAGAGGGUUUAA UUCAGUACGAAAGU ACCGAUUGGAUCCG CAAGG | Bisantrene | Target\_lig\_10 31 | (5'CAG/ 3'GCC) x 1 | Target\_338 | 5.9586073148  4177 |
| 1840 | C1CN=C(N1)N N=CC2=C3C=C C=CC3=C(C4= CC=CC=C42)C  =NNC5=NCCN 5 | GGGAGAGGGUUUAA UUCUGUACGAAAGU ACCGAUUGGAUCCG CAAGG | Bisantrene | Target\_lig\_10 31 | (5'CUG/ 3'GCC) x 1 | Target\_339 | 5.9208187539  5238 |
| 1841 | C1CN=C(N1)N N=CC2=C3C=C C=CC3=C(C4= CC=CC=C42)C  =NNC5=NCCN 5 | GGGAGAGGGUUUAA UUCGGUACGAAAGU ACGGAUUGGAUCCG CAAGG | Bisantrene | Target\_lig\_10 31 | (5'CGG/ 3'GCC) x 1 | Target\_340 | 6.4685210829  5774 |
| 1842 | C1CN=C(N1)N N=CC2=C3C=C C=CC3=C(C4= CC=CC=C42)C  =NNC5=NCCN 5 | GGGAGAGGGUUUAA UUCAGUACGAAAGU ACAGAUUGGAUCCG CAAGG | Bisantrene | Target\_lig\_10 31 | (5'CAG/ 3'GAC) x 1 | Target\_341 | 5.7958800173  4408 |
| 1843 | C1CN=C(N1)N N=CC2=C3C=C C=CC3=C(C4= CC=CC=C42)C  =NNC5=NCCN 5 | GGGAGAGGGUUUAA UUCCGUACGAAAGU ACGGAUUGGAUCCG CAAGG | Bisantrene | Target\_lig\_10 31 | (5'CCG/ 3'GGC) x 1 | Target\_342 | 5.5376020021  0104 |
| 1844 | C1CN=C(N1)N N=CC2=C3C=C C=CC3=C(C4= CC=CC=C42)C  =NNC5=NCCN 5 | GGGAGAGGGUUUAA UUCUGUACGAAAGU ACUGAUUGGAUCCG CAAGG | Bisantrene | Target\_lig\_10 31 | (5'CUG/ 3'GUC) x 1 | Target\_343 | 5.4317982759  3301 |
| 1845 | C1CN=C(N1)N N=CC2=C3C=C C=CC3=C(C4= CC=CC=C42)C  =NNC5=NCCN 5 | GGGAGAGGGUUUAA UUCAGUACGAAAGU ACUGAUUGGAUCCG CAAGG | Bisantrene | Target\_lig\_10 31 | (5'CAG/ 3'CUG) x 1 | Target\_344 | 5.5528419686  5778 |
| 1846 | NC(=[NH2+])C 1=CC=C(N=C1) C1=CC=C(O1) C1=CC=C(O1) C1=NC=C(C=C 1)C(N)=[NH2+] | GGGAGAGGGUUUAA UUCGGUACGAAAGU ACGGAUUGGAUCCG CAAGG | B1 | Target\_lig\_71 6 | (5'CGG/ 3'GGC) x1 | Target\_345 | 6.6197887582  8839 |
| 1847 | C[NH+] (C)CCC[NH+]= C(C1=CC=C(C  =C1)C(=[NH+] CCC[NH+] | GGGAGAGGGUUUAA UUCGGUACGAAAGU ACGGAUUGGAUCCG CAAGG | B2 | Target\_lig\_69 3 | (5'CGG/ 3'GGC) x1 | Target\_345 | 5.9586073148  4177 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA\_ID** | **pKd** |
|  | (C)C)N)N |  |  |  |  |  |  |
| 1848 | CN(C)CCCN=C (C1=CC=C(C= C1)C2=CC=C( O2)C3=NC4=C( N3)C=C(C=C4) C(=NCCCN(C) C)N)N | GGGAGAGGGUUUAA UUCGGUACGAAAGU ACGGAUUGGAUCCG CAAGG | B3 | Target\_lig\_24 6 | (5'CGG/ 3'GGC) x1 | Target\_345 | 5.4559319556  4972 |
| 1849 | CC(C)C1=CC2= C(C=C1)N=C3 C=CC(=CN3C2  =O)C(=O)NCC N(C)C | GGGAGAGGGUUUAA UUCGGUACGAAAGU ACGGAUUGGAUCCG CAAGG | B4 | Target\_lig\_10 35 | (5'CGG/ 3'GGC) x1 | Target\_345 | 6.4814860601  2211 |
| 1850 | COC1=CC(=CC (=C1O)OC)C2= NC3=C(N2)C= C4C(=C3)NC(= O)N4 | GGGAGAGGGUUUAA UUCGGUACGAAAGU ACGGAUUGGAUCCG CAAGG | B5 | Target\_lig\_95 7 | (5'CGG/ 3'GGC) x1 | Target\_345 | 5.8538719643  2176 |
| 1851 | C1C[NH+]=C(N 1)C2=CC=C(C= C2)C3=CC=C( O3)C4=CC=C( C=C4)C5=[NH+  ]CCN5 | GGGAGAGGGUUUAA UUCGGUACGAAAGU ACGGAUUGGAUCCG CAAGG | B6 | Target\_lig\_69 6 | (5'CGG/ 3'GGC) x1 | Target\_345 | 6.4089353929  735 |
| 1852 | C1=CC(=CC=C 1C2=CC=C(O2) C3=CC=C(C=C 3)C(=[NH2+])N  )C(=[NH2+])N | GGGAGAGGGUUUAA UUCGGUACGAAAGU ACGGAUUGGAUCCG CAAGG | B7 | Target\_lig\_69 7 | (5'CGG/ 3'GGC) x1 | Target\_345 | 6.5686362358  4101 |
| 1853 | C1N(C2=CC=C C=C2N(C1)C(= O)/C=C/ C3=CC=CC=C3  )C(=O)/C=C/ C4=CC=CC=C4 | GGGAGAGGGUUUAA UUCGGUACGAAAGU ACGGAUUGGAUCCG CAAGG | B8 | Target\_lig\_10 39 | (5'CGG/ 3'GGC) x1 | Target\_345 | 5.8538719643  2176 |
| 1854 | CCN(CC)CC(= O)NC1=CC=CC 2=C1C(=O)C3= C(C4=CC=CC= C4C(=C3C2=O) O)O | GGGAGAGGGUUUAA UUCGGUACGAAAGU ACGGAUUGGAUCCG CAAGG | B9 | Target\_lig\_10 40 | (5'CGG/ 3'GGC) x1 | Target\_345 | 5.6382721639  8241 |
| 1855 | C1CC2=C(CC1 C(=O)O)C(=NC (=N2)NCC3=C C=CC=C3)NCC 4=CC=CC=C4 | GGGAGAGGGUUUAA UUCGGUACGAAAGU ACGGAUUGGAUCCG CAAGG | B10 | Target\_lig\_10 41 | (5'CGG/ 3'GGC) x1 | Target\_345 | 5.2757241303  9921 |
| 1856 | C1COCCN1CC NC2=C3C(=C( C=C2)NCCN4C COCC4)C(=O) C5=CC=CC=C5 C3=O | GGGAGAGGGUUUAA UUCGGUACGAAAGU ACGGAUUGGAUCCG CAAGG | B11 | Target\_lig\_10 42 | (5'CGG/ 3'GGC) x1 | Target\_345 | 6.4436974992  3271 |
| 1858 | NC(=[NH2+])C 1=CC=C(N=C1) C1=CC=C(O1) C1=CC=C(O1) C1=NC=C(C=C 1)C(N)=[NH2+] | GGGAGAGGGUUUAA UUCAGUACGAAAGU ACUGAUUGGAUCCG CAAGG | B1 | Target\_lig\_71 6 | (5'CAG/ 3'GUC) x1 | Target\_346 | 5.4436974992  3271 |
| 1859 | C[NH+] (C)CCC[NH+]= C(C1=CC=C(C  =C1)C(=[NH+] CCC[NH+] (C)C)N)N | GGGAGAGGGUUUAA UUCAGUACGAAAGU ACUGAUUGGAUCCG CAAGG | B2 | Target\_lig\_69 3 | (5'CAG/ 3'GUC) x1 | Target\_346 | 6.4317982759  3301 |
| 1860 | CN(C)CCCN=C (C1=CC=C(C= C1)C2=CC=C( O2)C3=NC4=C( | GGGAGAGGGUUUAA UUCAGUACGAAAGU ACUGAUUGGAUCCG CAAGG | B3 | Target\_lig\_24 6 | (5'CAG/ 3'GUC) x1 | Target\_346 | 5.8538719643  2176 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA\_ID** | **pKd** |
|  | N3)C=C(C=C4) C(=NCCCN(C) C)N)N |  |  |  |  |  |  |
| 1861 | CC(C)C1=CC2= C(C=C1)N=C3 C=CC(=CN3C2  =O)C(=O)NCC N(C)C | GGGAGAGGGUUUAA UUCAGUACGAAAGU ACUGAUUGGAUCCG CAAGG | B4 | Target\_lig\_10 35 | (5'CAG/ 3'GUC) x1 | Target\_346 | 5.3098039199  7149 |
| 1862 | COC1=CC(=CC (=C1O)OC)C2= NC3=C(N2)C= C4C(=C3)NC(= O)N4 | GGGAGAGGGUUUAA UUCAGUACGAAAGU ACUGAUUGGAUCCG CAAGG | B5 | Target\_lig\_95 7 | (5'CAG/ 3'GUC) x1 | Target\_346 | 5.8239087409  4432 |
| 1863 | C1C[NH+]=C(N 1)C2=CC=C(C= C2)C3=CC=C( O3)C4=CC=C( C=C4)C5=[NH+  ]CCN5 | GGGAGAGGGUUUAA UUCAGUACGAAAGU ACUGAUUGGAUCCG CAAGG | B6 | Target\_lig\_69 6 | (5'CAG/ 3'GUC) x1 | Target\_346 | 5.8860566476  9316 |
| 1864 | C1=CC(=CC=C 1C2=CC=C(O2) C3=CC=C(C=C 3)C(=[NH2+])N  )C(=[NH2+])N | GGGAGAGGGUUUAA UUCAGUACGAAAGU ACUGAUUGGAUCCG CAAGG | B7 | Target\_lig\_69 7 | (5'CAG/ 3'GUC) x1 | Target\_346 | 5.7212463990  4717 |
| 1865 | C1N(C2=CC=C C=C2N(C1)C(= O)/C=C/ C3=CC=CC=C3  )C(=O)/C=C/ C4=CC=CC=C4 | GGGAGAGGGUUUAA UUCAGUACGAAAGU ACUGAUUGGAUCCG CAAGG | B8 | Target\_lig\_10 39 | (5'CAG/ 3'GUC) x1 | Target\_346 | 6.1549019599  8574 |
| 1866 | CCN(CC)CC(= O)NC1=CC=CC 2=C1C(=O)C3= C(C4=CC=CC= C4C(=C3C2=O) O)O | GGGAGAGGGUUUAA UUCAGUACGAAAGU ACUGAUUGGAUCCG CAAGG | B9 | Target\_lig\_10 40 | (5'CAG/ 3'GUC) x1 | Target\_346 | 5.3187587626  2441 |
| 1867 | C1CC2=C(CC1 C(=O)O)C(=NC (=N2)NCC3=C C=CC=C3)NCC 4=CC=CC=C4 | GGGAGAGGGUUUAA UUCAGUACGAAAGU ACUGAUUGGAUCCG CAAGG | B10 | Target\_lig\_10 41 | (5'CAG/ 3'GUC) x1 | Target\_346 | 5.3872161432  8026 |
| 1868 | C1COCCN1CC NC2=C3C(=C( C=C2)NCCN4C COCC4)C(=O) C5=CC=CC=C5 C3=O | GGGAGAGGGUUUAA UUCAGUACGAAAGU ACUGAUUGGAUCCG CAAGG | B11 | Target\_lig\_10 42 | (5'CAG/ 3'GUC) x1 | Target\_346 | 5.2676062401  7703 |
| 1903 | C1CCN(CC1)C 2CCN(CC2)CC CNC3=NC(=NC 4=CC=CC=C43  )C5=NN=C(O5) C6=CC=CC=C6 | UGUGGGAGGGGCGG GUCUGGG | NRAS SAR 1 | Target\_lig\_10 53 | NRAS G4  motif | Target\_259 | 5.9208187539  5238 |
| 1904 | Fc1ccc(cc1)c1n nc(o1)c1nc(NC Cc2ccco2)c2c(n 1)cccc2 | UGUGGGAGGGGCGG GUCUGGG | NRAS SAR 2 | Target\_lig\_10 54 | NRAS G4  motif | Target\_259 | 6.5850266520  2918 |
| 1905 | C1CCC(CC1)N C2=NC(=NC3= CC=CC=C32)C 4=NN=C(O4)C5  =CC=C(C=C5)F | UGUGGGAGGGGCGG GUCUGGG | NRAS SAR 3 | Target\_lig\_10 55 | NRAS G4  motif | Target\_259 | 6.3665315444  2041 |
| 1906 | CCCSCCCNC1  =NC(=NC2=CC  =CC=C21)C3= NN=C(O3)C4= CC=CC=C4 | UGUGGGAGGGGCGG GUCUGGG | NRAS SAR 6 | Target\_lig\_10 56 | NRAS G4  motif | Target\_259 | 6.1307682802  6902 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA\_ID** | **pKd** |
| 1907 | C1=CC=C(C=C 1)C2=NN=C(O2  )C3=NC4=CC= CC=C4C(=N3) NCCC5=CC=C S5 | UGUGGGAGGGGCGG GUCUGGG | NRAS SAR 7 | Target\_lig\_10 57 | NRAS G4  motif | Target\_259 | 6.4436974992  3271 |
| 1908 | Clc1ccc(cc1)c1n nc(o1)c1nc2cccc c2c(n1)c1ccc(cc 1)N(C)C | UGUGGGAGGGGCGG GUCUGGG | NRAS SAR 8 | Target\_lig\_10 58 | NRAS G4  motif | Target\_259 | 5.5228787452  8034 |
| 1909 | CC1=CC(=CC= C1)C2=NN=C( O2)C3=NC4=C C=CC=C4C(=N 3)NCCC5=CN= CN5 | UGUGGGAGGGGCGG GUCUGGG | NRAS SAR 10 | Target\_lig\_10 59 | NRAS G4  motif | Target\_259 | 6.3187587626  2441 |
| 1910 | CC1=CC(=CC= C1)C2=NN=C( O2)C3=NC4=C C=CC=C4C(=N 3)NCCN5CCO CC5 | UGUGGGAGGGGCGG GUCUGGG | NRAS SAR 12 | Target\_lig\_10 60 | NRAS G4  motif | Target\_259 | 6.5228787452  8034 |
| 1911 | CC1=CC(=CC= C1)C2=NN=C( O2)C3=NC4=C C=CC=C4C(=N 3)NCCC5=C(O N=C5C)C | UGUGGGAGGGGCGG GUCUGGG | NRAS SAR 14 | Target\_lig\_10 61 | NRAS G4  motif | Target\_259 | 6.5528419686  5778 |
| 1912 | CC1=CC=C(C= C1)C2=NN=C( O2)C3=NC4=C C=CC=C4C(=N 3)N5CCCCC5 | UGUGGGAGGGGCGG GUCUGGG | NRAS SAR 16 | Target\_lig\_10 62 | NRAS G4  motif | Target\_259 | 6.4559319556  4972 |
| 1913 | Cc1ccc(cc1)c1n nc(o1)c1nc(NCc 2cccc3c2OCO3) c2c(n1)cccc2 | UGUGGGAGGGGCGG GUCUGGG | NRAS SAR 17 | Target\_lig\_10 63 | NRAS G4  motif | Target\_259 | 6.2518119729  938 |
| 1914 | CC1=CC=C(C= C1)C2=NN=C( O2)C3=NC4=C C=CC=C4C(=N 3)NCCC5=CC= C(C=C5)S(=O) (=O)N | UGUGGGAGGGGCGG GUCUGGG | NRAS SAR 18 | Target\_lig\_10 64 | NRAS G4  motif | Target\_259 | 6.6020599913  2796 |
| 1915 | CC1=CC=C(C= C1)C2=NN=C( O2)C3=NC4=C C=CC=C4C(=N 3)NCCN5CCCC  5 | UGUGGGAGGGGCGG GUCUGGG | NRAS SAR 24 | Target\_lig\_10 65 | NRAS G4  motif | Target\_259 | 6.3010299956  6398 |
| 1916 | CC1=CC=C(C= C1)C2=NN=C( O2)C3=NC4=C C=CC=C4C(=N 3)NCCCN5CCC  6=CC=CC=C6C  5 | UGUGGGAGGGGCGG GUCUGGG | NRAS SAR 25 | Target\_lig\_10 66 | NRAS G4  motif | Target\_259 | 6.0222763947  1115 |
| 1917 | C1CCN(CC1)C 1CCN(CC1)CC  CCNc1nc(nc2c1 cccc2)c1nnc(o1) c1ccccc1 | UGUGGGAGGGGCGG GUCUGGG | NRAS  compound 1 | Target\_lig\_10 52 | NRAS G4  motif | Target\_259 | 6.3467874862  2466 |
| 1918 | C1COCC1C2= NOC(=N2)C3= CC(=CC(=C3)C N)NC(=O)C4=C C=CC=N4 | UGUGGGAGGGGCGG GUCUGGG | Hit S1 | Target\_lig\_10 67 | NRAS G4  motif | Target\_259 | 4.9625735020  5938 |
| 1919 | CC1=CN=C(C= | UGUGGGAGGGGCGG | Hit S2 | Target\_lig\_10 | NRAS G4 | Target\_259 | 4.5951662833 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA\_ID** | **pKd** |
|  | C1)NCCCNC(= O)C2=CN(N=N 2)CCN | GUCUGGG |  | 68 | motif |  | 8006 |
| 1920 | C1CN2CCC1C( C2)NCC3=C(N  =CC=C3)OC4= CC(=C(C=C4)F  )F | UGUGGGAGGGGCGG GUCUGGG | Hit S3 | Target\_lig\_10 69 | NRAS G4  motif | Target\_259 | 4.8416375079  0475 |
| 1921 | CN1C2=C(C(= CC=C2)Cl)C(= N1)CN3CCCCC (C3)N | UGUGGGAGGGGCGG GUCUGGG | Hit S4 | Target\_lig\_10 70 | NRAS G4  motif | Target\_259 | 4.5543957967  264 |
| 1922 | C1CN(CCC1N2 CCC(CC2)O)C3  =NC=NC(=C3) CCN | UGUGGGAGGGGCGG GUCUGGG | Hit S5 | Target\_lig\_10 71 | NRAS G4  motif | Target\_259 | 4.4089353929  735 |
| 1923 | CC1=CC(=NC(  =N1)N)N2CCN( CC2)C(=O)CCC 3=NN4CCNCC  4=C3 | UGUGGGAGGGGCGG GUCUGGG | Hit S6 | Target\_lig\_10 72 | NRAS G4  motif | Target\_259 | 4.0315170514  4607 |
| 1924 | CC(CCC1=CC= CO1)NC2CCC3 (CC2)CCNCC3 | UGUGGGAGGGGCGG GUCUGGG | Hit S7 | Target\_lig\_10 73 | NRAS G4  motif | Target\_259 | 4.0177287669  6043 |
| 1925 | COC1=C(C=C( C=C1)CN2CCC (CC2)N3CCN(C C3)CCO)OCC4  =CC=CC=C4 | UGUGGGAGGGGCGG GUCUGGG | Hit S8 | Target\_lig\_10 74 | NRAS G4  motif | Target\_259 | 4 |
| 1926 | C1=CN=CC=C1 C2=NC(=NC=C 2)NCCCC3=NN  =C(S3)N | UGUGGGAGGGGCGG GUCUGGG | Hit S9 | Target\_lig\_10 75 | NRAS G4  motif | Target\_259 | 4.3178549236  2617 |
| 1927 | CC(C)OC(=O)C 1=CC=C(C=C1) NC2=NC3=CC= CC=C3C4=NN= CN42 | UGUGGGAGGGGCGG GUCUGGG | Hit S11 | Target\_lig\_10 76 | NRAS G4  motif | Target\_259 | 4 |
| 1928 | C1CCCN(CC1) CC2=NC(=NC(  =N2)NC3=CC= C(C=C3)F)N | UGUGGGAGGGGCGG GUCUGGG | Hit S12 | Target\_lig\_10 77 | NRAS G4  motif | Target\_259 | 4 |
| 1943 | COC1=C(C=CC (=C1)C=CC(=O  )CC(=O)C=CC2  =CC(=C(C=C2) O)OC)O | GGGAGAGGGUUUAA UUCAGUACGAAAGU ACGGAUUGGAUCCG CAAGG | Curcumin | Target\_lig\_10 92 | (5'CAG/ 3'GGC) x 1 | Target\_334 | 6.1249387366  083 |
| 1944 | COC1=C(C=CC (=C1)C=CC(=O  )CC(=O)C=CC2  =CC(=C(C=C2) O)OC)O | GGGAGAGGGUUUAA UUCCGUACGAAAGU ACAGAUUGGAUCCG CAAGG | Curcumin | Target\_lig\_10 92 | (5'CCG/ 3'GAC) x 1 | Target\_335 | 5.9788107009  3006 |
| 1945 | COC1=C(C=CC (=C1)C=CC(=O  )CC(=O)C=CC2  =CC(=C(C=C2) O)OC)O | GGGAGAGGGUUUAA UUCGGUACGAAAGU ACAGAUUGGAUCCG CAAGG | Curcumin | Target\_lig\_10 92 | (5'CGG/ 3'GAC) x 1 | Target\_336 | 6.2441251443  2751 |
| 1946 | COC1=C(C=CC (=C1)C=CC(=O  )CC(=O)C=CC2  =CC(=C(C=C2) O)OC)O | GGGAGAGGGUUUAA UUCCGUACGAAAGU ACUGAUUGGAUCCG CAAGG | Curcumin | Target\_lig\_10 92 | (5'CCG/ 3'GUC) x 1 | Target\_337 | 6.1079053973  0952 |
| 1947 | COC1=C(C=CC (=C1)C=CC(=O  )CC(=O)C=CC2  =CC(=C(C=C2) | GGGAGAGGGUUUAA UUCAGUACGAAAGU ACCGAUUGGAUCCG CAAGG | Curcumin | Target\_lig\_10 92 | (5'CAG/ 3'GCC) x 1 | Target\_338 | 6.3565473235  1381 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA\_ID** | **pKd** |
|  | O)OC)O |  |  |  |  |  |  |
| 1948 | COC1=C(C=CC (=C1)C=CC(=O  )CC(=O)C=CC2  =CC(=C(C=C2) O)OC)O | GGGAGAGGGUUUAA UUCUGUACGAAAGU ACCGAUUGGAUCCG CAAGG | Curcumin | Target\_lig\_10 92 | (5'CUG/ 3'GCC) x 1 | Target\_339 | 6.1804560644  5813 |
| 1949 | COC1=C(C=CC (=C1)C=CC(=O  )CC(=O)C=CC2  =CC(=C(C=C2) O)OC)O | GGGAGAGGGUUUAA UUCGGUACGAAAGU ACGGAUUGGAUCCG CAAGG | Curcumin | Target\_lig\_10 92 | (5'CGG/ 3'GCC) x 1 | Target\_340 | 6.9208187539  5238 |
| 1950 | COC1=C(C=CC (=C1)C=CC(=O  )CC(=O)C=CC2  =CC(=C(C=C2) O)OC)O | GGGAGAGGGUUUAA UUCAGUACGAAAGU ACAGAUUGGAUCCG CAAGG | Curcumin | Target\_lig\_10 92 | (5'CAG/ 3'GAC) x 1 | Target\_341 | 6.2518119729  938 |
| 1951 | COC1=C(C=CC (=C1)C=CC(=O  )CC(=O)C=CC2  =CC(=C(C=C2) O)OC)O | GGGAGAGGGUUUAA UUCCGUACGAAAGU ACGGAUUGGAUCCG CAAGG | Curcumin | Target\_lig\_10 92 | (5'CCG/ 3'GGC) x 1 | Target\_342 | 6.0655015487  5643 |
| 1952 | COC1=C(C=CC (=C1)C=CC(=O  )CC(=O)C=CC2  =CC(=C(C=C2) O)OC)O | GGGAGAGGGUUUAA UUCUGUACGAAAGU ACUGAUUGGAUCCG CAAGG | Curcumin | Target\_lig\_10 92 | (5'CUG/ 3'GUC) x 1 | Target\_343 | 6.1307682802  6902 |
| 1953 | COC1=C(C=CC (=C1)C=CC(=O  )CC(=O)C=CC2  =CC(=C(C=C2) O)OC)O | GGGAGAGGGUUUAA UUCAGUACGAAAGU ACUGAUUGGAUCCG CAAGG | Curcumin | Target\_lig\_10 92 | (5'CAG/ 3'CUG) x 1 | Target\_344 | 5.6777807052  6608 |
| 2042 | CC1=CC2=C(C  =C1C)N(C=N2) C3C(C(C(O3)C  O)OP(=O) ([O-])OC(C)CN C(=O)CCC4(C(  C5C6(C(C(C(=  N6)C(=C7C(C( C(=N7)C=C8C( C(C(=N8)C(=C 4[N-]5)C)CCC(  =O)N) (C)C)CCC(=O) N) (C)CC(=O)N)C) CCC(=O)N) (C)CC(=O)N)C)  CC(=O)N)C)O.  [C-]#N.[Co+3] | CCGGTGCGCATAACC ACCTCAGTGCGAGC AACGATGGCC | cyanocobalamine | Target\_lig\_72 | B12.9 | Target\_372 | 6.4948500216  8009 |
| 2043 | C/C/1=C/2\ [C@@] ([C@@H] (C(=N2)/C=C\3/ C([C@@H]  (C(=N3)/C(=C\  4/[C@]([C@H]  (C([N-]4)  [C@]5([C@@] ([C@@H] (C1=N5)CCC(= O)N) (C)CC(=O)N)C) CC(=O)N)  (C)CCC(=O)NC  C(C)O)/  C)CCC(=O)N)  (C)C)CCC(=O)  N)(C)CC(=O)N.  [C-]#N.[C-]#N. | CCGGTGCGCATAACC ACCTCAGTGCGAGC AACGATGGCC | cobinamide dicyanide | Target\_lig\_73 | B12.9 | Target\_372 | 5.0555173278  4983 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA\_ID** | **pKd** |
|  | [Co] |  |  |  |  |  |  |
| 2062 | N[C@@H]1C[C @H](N)[C@H] ([C@H] ([C@H]1OCCC  c1nnn(c1)Cc1cc c(cc1)Cn1nnc(c 1)CCCO[C@@ H]1[C@H]  (N)C[C@H]  ([C@@H] ([C@H]1O)O)N  )O)O | CGCGCGAAAGCGCG | B-11 | Target\_lig\_11 37 | RNA hairpin loop I | Target\_375 | 5.2418453780  3261 |
| 2063 | N[C@@H]1C[C @H](N)[C@H] ([C@H] ([C@H]1OCCC  c1nnn(c1)Cc1c( C)cc(c(c1C)Cn1 nnc(c1)CCCO[C @@H]1[C@H] (N)C[C@H]  ([C@@H] ([C@H]1O)O)N  )C)O)O | CGCGCGAAAGCGCG | B-13 | Target\_lig\_11 38 | RNA hairpin loop I | Target\_375 | 6.2006594505  4642 |
| 2064 | N[C@@H]1C[C @H](N)[C@H] ([C@H] ([C@H]1OCCC  c1nnn(c1)Cc1cc cc(n1)Cn1nnc(c 1)CCCO[C@@ H]1[C@H]  (N)C[C@H]  ([C@@H] ([C@H]1O)O)N  )O)O | CGCGCGAAAGCGCG | B-14 | Target\_lig\_11 39 | RNA hairpin loop I | Target\_375 | 5.2958494831  602 |
| 2066 | [C@@H]1([C@ H]([C@H](O) [C@H] ([C@@H]  (C1)N)O)OCCC  c1cn(nn1)Cc1cc cc(Cn2cc(nn2)C CCO[C@H]2[C  @@H] (C[C@@H] ([C@@H](O)  [C@H]2O)N)N) c1)N | CGCGCGAAAGCGCG | B-12 | Target\_lig\_22 4 | RNA hairpin loop Ia | Target\_375 | 5.8664610916  2978 |
| 2069 | N[C@@H]1C[C @H](N)[C@H] ([C@H] ([C@H]1OCCC  c1nnn(c1)Cc1cc c(cc1)Cn1nnc(c 1)CCCO[C@@ H]1[C@H]  (N)C[C@H]  ([C@@H] ([C@H]1O)O)N  )O)O | CGCGCUUCGGCGCG | B-11 | Target\_lig\_11 37 | RNA hairpin loop Ib | Target\_376 | 5.1992829217  1762 |
| 2070 | [C@@H]1([C@ H]([C@H](O) [C@H] ([C@@H]  (C1)N)O)OCCC  c1cn(nn1)Cc1cc cc(Cn2cc(nn2)C CCO[C@H]2[C  @@H] | CGCGCUUCGGCGCG | B-12 | Target\_lig\_22 4 | RNA hairpin loop Ib | Target\_376 | 5.8124792791  6354 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA\_ID** | **pKd** |
|  | (C[C@@H] ([C@@H](O)  [C@H]2O)N)N) c1)N |  |  |  |  |  |  |
| 2071 | N[C@@H]1C[C @H](N)[C@H] ([C@H] ([C@H]1OCCC  c1nnn(c1)Cc1c( C)cc(c(c1C)Cn1 nnc(c1)CCCO[C @@H]1[C@H] (N)C[C@H]  ([C@@H] ([C@H]1O)O)N  )C)O)O | CGCGCUUCGGCGCG | B-13 | Target\_lig\_11 38 | RNA hairpin loop Ib | Target\_376 | 6.0757207139  3812 |
| 2072 | N[C@@H]1C[C @H](N)[C@H] ([C@H] ([C@H]1OCCC  c1nnn(c1)Cc1cc cc(n1)Cn1nnc(c 1)CCCO[C@@ H]1[C@H]  (N)C[C@H]  ([C@@H] ([C@H]1O)O)N  )O)O | CGCGCUUCGGCGCG | B-14 | Target\_lig\_11 39 | RNA hairpin loop Ib | Target\_376 | 5.1034737825  1045 |
| 2073 | N[C@@H]1C[C @H](N)[C@H] ([C@H] ([C@H]1OCCC  c1nnn(c1)Cc1cc c(cc1)Cn1nnc(c 1)CCCO[C@@ H]1[C@H]  (N)C[C@H]  ([C@@H] ([C@H]1O)O)N  )O)O | CGCGCAGUGUAGCG CG | B-11 | Target\_lig\_11 37 | RNA hairpin loop II | Target\_377 | 5.6840296545  4308 |
| 2074 | [C@@H]1([C@ H]([C@H](O) [C@H] ([C@@H]  (C1)N)O)OCCC  c1cn(nn1)Cc1cc cc(Cn2cc(nn2)C CCO[C@H]2[C  @@H] (C[C@@H] ([C@@H](O)  [C@H]2O)N)N) c1)N | CGCGCAGUGUAGCG CG | B-12 | Target\_lig\_22 4 | RNA hairpin loop II | Target\_377 | 4.9986990669  7958 |
| 2075 | N[C@@H]1C[C @H](N)[C@H] ([C@H] ([C@H]1OCCC  c1nnn(c1)Cc1c( C)cc(c(c1C)Cn1 nnc(c1)CCCO[C @@H]1[C@H] (N)C[C@H]  ([C@@H] ([C@H]1O)O)N  )C)O)O | CGCGCAGUGUAGCG CG | B-13 | Target\_lig\_11 38 | RNA hairpin loop II | Target\_377 | 6.2218487496  1636 |
| 2076 | N[C@@H]1C[C @H](N)[C@H] ([C@H] ([C@H]1OCCC  c1nnn(c1)Cc1cc cc(n1)Cn1nnc(c | CGCGCAGUGUAGCG CG | B-14 | Target\_lig\_11 39 | RNA hairpin loop II | Target\_377 | 5.3400837999  3015 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA\_ID** | **pKd** |
|  | 1)CCCO[C@@ H]1[C@H]  (N)C[C@H]  ([C@@H] ([C@H]1O)O)N  )O)O |  |  |  |  |  |  |
| 2077 | N[C@@H]1C[C @H](N)[C@H] ([C@H] ([C@H]1OCCC  c1nnn(c1)Cc1cc c(cc1)Cn1nnc(c 1)CCCO[C@@ H]1[C@H]  (N)C[C@H]  ([C@@H] ([C@H]1O)O)N  )O)O | CGCGCAGUAGUAGC GCG | B-11 | Target\_lig\_11 37 | RNA hairpin loop III | Target\_378 | 5.8446639625  3494 |
| 2078 | [C@@H]1([C@ H]([C@H](O) [C@H] ([C@@H]  (C1)N)O)OCCC  c1cn(nn1)Cc1cc cc(Cn2cc(nn2)C CCO[C@H]2[C  @@H] (C[C@@H] ([C@@H](O)  [C@H]2O)N)N) c1)N | CGCGCAGUAGUAGC GCG | B-12 | Target\_lig\_22 4 | RNA hairpin loop III | Target\_378 | 5.0056828473  3036 |
| 2079 | N[C@@H]1C[C @H](N)[C@H] ([C@H] ([C@H]1OCCC  c1nnn(c1)Cc1c( C)cc(c(c1C)Cn1 nnc(c1)CCCO[C @@H]1[C@H] (N)C[C@H]  ([C@@H] ([C@H]1O)O)N  )C)O)O | CGCGCAGUAGUAGC GCG | B-13 | Target\_lig\_11 38 | RNA hairpin loop III | Target\_378 | 5.5934598195  6604 |
| 2080 | N[C@@H]1C[C @H](N)[C@H] ([C@H] ([C@H]1OCCC  c1nnn(c1)Cc1cc cc(n1)Cn1nnc(c 1)CCCO[C@@ H]1[C@H]  (N)C[C@H]  ([C@@H] ([C@H]1O)O)N  )O)O | CGCGCAGUAGUAGC GCG | B-14 | Target\_lig\_11 39 | RNA hairpin loop III | Target\_378 | 5.8961962790  4404 |
| 2081 | N[C@@H]1C[C @H](N)[C@H] ([C@H] ([C@H]1OCCC  c1nnn(c1)Cc1cc c(cc1)Cn1nnc(c 1)CCCO[C@@ H]1[C@H]  (N)C[C@H]  ([C@@H] ([C@H]1O)O)N  )O)O | CGCGCACAAGUAGC GCG | B-11 | Target\_lig\_11 37 | RNA hairpin loop IIIa | Target\_379 | 5.5638373529  5924 |
| 2082 | [C@@H]1([C@ H]([C@H](O) [C@H] ([C@@H] | CGCGCACAAGUAGC GCG | B-12 | Target\_lig\_22 4 | RNA hairpin loop IIIa | Target\_379 | 5.6516951369  5184 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA\_ID** | **pKd** |
|  | (C1)N)O)OCCC  c1cn(nn1)Cc1cc cc(Cn2cc(nn2)C CCO[C@H]2[C  @@H] (C[C@@H] ([C@@H](O)  [C@H]2O)N)N) c1)N |  |  |  |  |  |  |
| 2083 | N[C@@H]1C[C @H](N)[C@H] ([C@H] ([C@H]1OCCC  c1nnn(c1)Cc1c( C)cc(c(c1C)Cn1 nnc(c1)CCCO[C @@H]1[C@H] (N)C[C@H]  ([C@@H] ([C@H]1O)O)N  )C)O)O | CGCGCACAAGUAGC GCG | B-13 | Target\_lig\_11 38 | RNA hairpin loop IIIa | Target\_379 | 6.3565473235  1381 |
| 2084 | N[C@@H]1C[C @H](N)[C@H] ([C@H] ([C@H]1OCCC  c1nnn(c1)Cc1cc cc(n1)Cn1nnc(c 1)CCCO[C@@ H]1[C@H]  (N)C[C@H]  ([C@@H] ([C@H]1O)O)N  )O)O | CGCGCACAAGUAGC GCG | B-14 | Target\_lig\_11 39 | RNA hairpin loop IIIa | Target\_379 | 5.4559319556  4972 |
| 2085 | N[C@@H]1C[C @H](N)[C@H] ([C@H] ([C@H]1OCCC  c1nnn(c1)Cc1cc c(cc1)Cn1nnc(c 1)CCCO[C@@ H]1[C@H]  (N)C[C@H]  ([C@@H] ([C@H]1O)O)N  )O)O | CGCGCACAACAAGC GCG | B-11 | Target\_lig\_11 37 | RNA hairpin loop IIIb | Target\_380 | 5.6925039620  8679 |
| 2086 | [C@@H]1([C@ H]([C@H](O) [C@H] ([C@@H]  (C1)N)O)OCCC  c1cn(nn1)Cc1cc cc(Cn2cc(nn2)C CCO[C@H]2[C  @@H] (C[C@@H] ([C@@H](O)  [C@H]2O)N)N) c1)N | CGCGCACAACAAGC GCG | B-12 | Target\_lig\_22 4 | RNA hairpin loop IIIb | Target\_380 | 5.6216020990  5186 |
| 2087 | N[C@@H]1C[C @H](N)[C@H] ([C@H] ([C@H]1OCCC  c1nnn(c1)Cc1c( C)cc(c(c1C)Cn1 nnc(c1)CCCO[C @@H]1[C@H] (N)C[C@H]  ([C@@H] ([C@H]1O)O)N  )C)O)O | CGCGCACAACAAGC GCG | B-13 | Target\_lig\_11 38 | RNA hairpin loop IIIb | Target\_380 | 6.3279021420  6428 |
| 2088 | N[C@@H]1C[C | CGCGCACAACAAGC | B-14 | Target\_lig\_11 | RNA hairpin | Target\_380 | 5.4659738939 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA\_ID** | **pKd** |
|  | @H](N)[C@H] ([C@H] ([C@H]1OCCC  c1nnn(c1)Cc1cc cc(n1)Cn1nnc(c 1)CCCO[C@@ H]1[C@H]  (N)C[C@H]  ([C@@H] ([C@H]1O)O)N  )O)O | GCG |  | 39 | loop IIIb |  | 4387 |
| 2089 | N[C@@H]1C[C @H](N)[C@H] ([C@H] ([C@H]1OCCC  c1nnn(c1)Cc1cc c(cc1)Cn1nnc(c 1)CCCO[C@@ H]1[C@H]  (N)C[C@H]  ([C@@H] ([C@H]1O)O)N  )O)O | CGCGCAGUCAGUAG CGCG | B-11 | Target\_lig\_11 37 | RNA hairpin loop IV | Target\_381 | 5.5114492834  9956 |
| 2090 | [C@@H]1([C@ H]([C@H](O) [C@H] ([C@@H]  (C1)N)O)OCCC  c1cn(nn1)Cc1cc cc(Cn2cc(nn2)C CCO[C@H]2[C  @@H] (C[C@@H] ([C@@H](O)  [C@H]2O)N)N) c1)N | CGCGCAGUCAGUAG CGCG | B-12 | Target\_lig\_22 4 | RNA hairpin loop IV | Target\_381 | 6.4948500216  8009 |
| 2091 | N[C@@H]1C[C @H](N)[C@H] ([C@H] ([C@H]1OCCC  c1nnn(c1)Cc1c( C)cc(c(c1C)Cn1 nnc(c1)CCCO[C @@H]1[C@H] (N)C[C@H]  ([C@@H] ([C@H]1O)O)N  )C)O)O | CGCGCAGUCAGUAG CGCG | B-13 | Target\_lig\_11 38 | RNA hairpin loop IV | Target\_381 | 6.3872161432  8026 |
| 2092 | N[C@@H]1C[C @H](N)[C@H] ([C@H] ([C@H]1OCCC  c1nnn(c1)Cc1cc cc(n1)Cn1nnc(c 1)CCCO[C@@ H]1[C@H]  (N)C[C@H]  ([C@@H] ([C@H]1O)O)N  )O)O | CGCGCAGUCAGUAG CGCG | B-14 | Target\_lig\_11 39 | RNA hairpin loop IV | Target\_381 | 5.5228787452  8034 |
| 2093 | N[C@@H]1C[C @H](N)[C@H] ([C@H] ([C@H]1OCCC  c1nnn(c1)Cc1cc c(cc1)Cn1nnc(c 1)CCCO[C@@ H]1[C@H]  (N)C[C@H]  ([C@@H] ([C@H]1O)O)N  )O)O | CGCGCUUGCGAGUG CGCG | B-11 | Target\_lig\_11 37 | RNA hairpin loop Iva | Target\_382 | 5.6925039620  8679 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA\_ID** | **pKd** |
| 2094 | [C@@H]1([C@ H]([C@H](O) [C@H] ([C@@H]  (C1)N)O)OCCC  c1cn(nn1)Cc1cc cc(Cn2cc(nn2)C CCO[C@H]2[C  @@H] (C[C@@H] ([C@@H](O)  [C@H]2O)N)N) c1)N | CGCGCUUGCGAGUG CGCG | B-12 | Target\_lig\_22 4 | RNA hairpin loop Iva | Target\_382 | 6.8239087409  4432 |
| 2095 | N[C@@H]1C[C @H](N)[C@H] ([C@H] ([C@H]1OCCC  c1nnn(c1)Cc1c( C)cc(c(c1C)Cn1 nnc(c1)CCCO[C @@H]1[C@H] (N)C[C@H]  ([C@@H] ([C@H]1O)O)N  )C)O)O | CGCGCUUGCGAGUG CGCG | B-13 | Target\_lig\_11 38 | RNA hairpin loop Iva | Target\_382 | 6.3187587626  2441 |
| 2096 | N[C@@H]1C[C @H](N)[C@H] ([C@H] ([C@H]1OCCC  c1nnn(c1)Cc1cc cc(n1)Cn1nnc(c 1)CCCO[C@@ H]1[C@H]  (N)C[C@H]  ([C@@H] ([C@H]1O)O)N  )O)O | CGCGCUUGCGAGUG CGCG | B-14 | Target\_lig\_11 39 | RNA hairpin loop Iva | Target\_382 | 5.6497519816  6584 |
| 2112 | CN(C)C1=CC2  =C(C=C1)C(=C 3C=CC(=[N+] (C)C)C=C3O2) C4=CC=CC=C4 | GGGAAGGGAAGAAA CUGCGGCUUCGGCC GGCUUCCC | Tetramethylrosa mine (TMR) | Target\_lig\_11 51 | Aptamer | Target\_6 | 7.3010299956  6398 |
| 2113 | CN(C)C1=CC2  =C(C=C1)C=C3 C=CC(=[N+] (C)C)C=C3O2.  [Cl-] | GGGAAGGGAAGAAA CUGCGGCUUCGGCC GGCUUCCC | Pyronin Y | Target\_lig\_11 52 | Aptamer | Target\_6 | 6.6478174818  8864 |
| 2114 | CN(C)C1=CC2  =C(C=C1)C(=C 3C=CC(=[N+] (C)C)C=C3O2) C4=CC=CC=C4 | GGUACCCGACUGGC GAGAGCCAGGCAAC GAAUGGUACC | Tetramethylrosa mine (TMR) | Target\_lig\_11 51 | Aptamer mutant C25 | Target\_383 | 6.4341521813  2648 |
| 2115 | CN(C)C1=CC2  =C(C=C1)C(=C 3C=CC(=[N+] (C)C)C=C3O2) C4=CC=CC=C4 | GGUACCCGACUGGC GAGAGCCAGGGAAC GAAUGGUACC | Tetramethylrosa mine (TMR) | Target\_lig\_11 51 | Aptamer mutant G25 | Target\_384 | 5.7212463990  4717 |
| 2116 | CN(C)C1=CC2  =C(C=C1)C(=C 3C=CC(=[N+] (C)C)C=C3O2) C4=CC=CC=C4 | GGUACCCGACUGGC GAGAGCCAGGAAAC GAAUGGUACC | Tetramethylrosa mine (TMR) | Target\_lig\_11 51 | Aptamer mutant A25 | Target\_385 | 5.2596373105  0576 |
| 2117 | CN(C)C1=CC2  =C(C=C1)C(=C 3C=CC(=[N+] (C)C)C=C3O2) C4=CC=CC=C4 | GGUACCCGCCUGGC GAGAGCCAGGUAAC GAAUGGUACC | Tetramethylrosa mine (TMR) | Target\_lig\_11 51 | Aptamer mutant C9 | Target\_386 | 5.5376020021  0104 |
| 2118 | CN(C)C1=CC2  =C(C=C1)C(=C | GGUACCCGGCUGGC GAGAGCCAGGUAAC | Tetramethylrosa mine (TMR) | Target\_lig\_11 51 | Aptamer mutant G9 | Target\_387 | 7.1938200260  1611 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA\_ID** | **pKd** |
|  | 3C=CC(=[N+] (C)C)C=C3O2) C4=CC=CC=C4 | GAAUGGUACC |  |  |  |  |  |
| 2119 | CN(C)C1=CC2  =C(C=C1)C(=C 3C=CC(=[N+] (C)C)C=C3O2) C4=CC=CC=C4 | GGUACCCGUCUGGC GAGAGCCAGGUAAC GAAUGGUACC | Tetramethylrosa mine (TMR) | Target\_lig\_11 51 | Aptamer mutant U9 | Target\_388 | 6.8538719643  2176 |
| 2120 | CN(C)C1=CC2  =C(C=C1)C(=C 3C=CC(=[N+] (C)C)C=C3O2) C4=CC=CC=C4 | GGUACCCGACUGGC GAGAGCCAGGUAAC GGAUGGUACC | Tetramethylrosa mine (TMR) | Target\_lig\_11 51 | Aptamer mutant G30 | Target\_389 | 5.7958800173  4408 |
| 2121 | CN(C)C1=CC2  =C(C=C1)C(=C 3C=CC(=[N+] (C)C)C=C3O2) C4=CC=CC=C4 | GGUACCCGACUGGC GAGAGCCAGGUAAC GCAUGGUACC | Tetramethylrosa mine (TMR) | Target\_lig\_11 51 | Aptamer mutant C30 | Target\_390 | 6.3010299956  6398 |
| 2122 | CN(C)C1=CC2  =C(C=C1)C(=C 3C=CC(=[N+] (C)C)C=C3O2) C4=CC=CC=C4 | GGUACCCGACUGGC GAGAGCCAGGUAAC GUAUGGUACC | Tetramethylrosa mine (TMR) | Target\_lig\_11 51 | Aptamer mutant U30 | Target\_391 | 5.3372421683  1843 |
| 2123 | CN(C)C1=CC2  =C(C=C1)C(=C 3C=CC(=[N+] (C)C)C=C3O2) C4=CC=CC=C4 | GGUACCCGACUGGC GAGAGCCAGGUACC GAAUGGUACC | Tetramethylrosa mine (TMR) | Target\_lig\_11 51 | Aptamer mutant C27 | Target\_392 | 5.3968556273  7982 |
| 2124 | CN(C)C1=CC2  =C(C=C1)C(=C 3C=CC(=[N+] (C)C)C=C3O2) C4=CC=CC=C4 | GGUACCCGACUGGC GAGAGCCAGGUAGC GAAUGGUACC | Tetramethylrosa mine (TMR) | Target\_lig\_11 51 | Aptamer mutant G27 | Target\_393 | 5.4555598626  8231 |
| 2125 | CN(C)C1=CC2  =C(C=C1)C(=C 3C=CC(=[N+] (C)C)C=C3O2) C4=CC=CC=C4 | GGUACCCGACUGGC GAGAGCCAGGUAUC GAAUGGUACC | Tetramethylrosa mine (TMR) | Target\_lig\_11 51 | Aptamer mutant U27 | Target\_394 | 5.1249387366  083 |
| 2126 | CN(C)C1=CC2  =C(C=C1)C(=C 3C=CC(=[N+] (C)C)C=C3O2) C4=CC=CC=C4 | GGUACCCGAGUGGC GAGAGCCACGUAAC GAAUGGUACC | Tetramethylrosa mine (TMR) | Target\_lig\_11 51 | Aptamer mutant G10C23 | Target\_395 | 6.4710832997  2235 |
| 2127 | CN(C)C1=CC2  =C(C=C1)C(=C 3C=CC(=[N+] (C)C)C=C3O2) C4=CC=CC=C4 | GGUACCCGACUGGC GAGAGCCAGGUGAC GAAUGGUACC | Tetramethylrosa mine (TMR) | Target\_lig\_11 51 | Aptamer mutant G26 | Target\_396 | 5.0705810742  8571 |
| 2128 | CN(C)C1=CC2  =C(C=C1)C(=C 3C=CC(=[N+] (C)C)C=C3O2) C4=CC=CC=C4 | GGUACCCGACUGGC GAGAGCCAGGUUAC GAAUGGUACC | Tetramethylrosa mine (TMR) | Target\_lig\_11 51 | Aptamer mutant U26 | Target\_397 | 5.3467874862  2466 |
| 2129 | CN(C)C1=CC2  =C(C=C1)C(=C 3C=CC(=[N+] (C)C)C=C3O2) C4=CC=CC=C4 | GGUACCCGACUGGC GAGAGCCAGGUCAC GAAUGGUACC | Tetramethylrosa mine (TMR) | Target\_lig\_11 51 | Aptamer mutant C26 | Target\_398 | 5.2218487496  1636 |
| 2130 | CN(C)C1=CC2  =C(C=C1)C(=C 3C=CC(=[N+] (C)C)C=C3O2) C4=CC=CC=C4 | GGUACCCGACAGGC GAGAGCCUGGUAAC GAAUGGUACC | Tetramethylrosa mine (TMR) | Target\_lig\_11 51 | Aptamer mutant A11U22 | Target\_399 | 7.3187587626  2441 |
| 2131 | CN(C)C1=CC2  =C(C=C1)C(=C 3C=CC(=[N+] (C)C)C=C3O2) | GGUACCCGACUGGC GAGAGCCAGCUAAC GAAUGGUACC | Tetramethylrosa mine (TMR) | Target\_lig\_11 51 | Aptamer mutant C24 | Target\_400 | 6.2907300390  2417 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA\_ID** | **pKd** |
|  | C4=CC=CC=C4 |  |  |  |  |  |  |
| 2132 | CN(C)C1=CC2  =C(C=C1)C(=C 3C=CC(=[N+] (C)C)C=C3O2) C4=CC=CC=C4 | GGUACCCGACUGGC GAGAGCCAGGUAAC GAGUGGUACC | Tetramethylrosa mine (TMR) | Target\_lig\_11 51 | Aptamer mutant G31 | Target\_401 | 5.1426675035  6873 |
| 2133 | CN(C)C1=CC2  =C(C=C1)C(=C 3C=CC(=[N+] (C)C)C=C3O2) C4=CC=CC=C4 | GGUACCCGACUGGC GAGAGCCAGGUAAC GACUGGUACC | Tetramethylrosa mine (TMR) | Target\_lig\_11 51 | Aptamer mutant C31 | Target\_402 | 5.9208187539  5238 |
| 2134 | CN(C)C1=CC2  =C(C=C1)C(=C 3C=CC(=[N+] (C)C)C=C3O2) C4=CC=CC=C4 | GGUACCCGACUGGC GAGAGCCAGGUAAC GAUUGGUACC | Tetramethylrosa mine (TMR) | Target\_lig\_11 51 | Aptamer mutant U31 | Target\_403 | 5.7099653886  3748 |
| 2135 | CN(C)C1=CC2  =C(C=C1)C(=C 3C=CC(=[N+] (C)C)C=C3O2) C4=CC=CC=C4 | GGUACCCCACUGGC GAGAGCCAGGUAAG GAAUGGUACC | Tetramethylrosa mine (TMR) | Target\_lig\_11 51 | Aptamer mutant C8G28 | Target\_404 | 5.2596373105  0576 |
| 2170 | CC1(COC(C(C1 NC)O)OC2C(C C(C(C2O)OC3C (CC=C(O3)CN)  N)N)N)O | GAAGACAGCCGCUU CUACGAGCAU | sisomicin | Target\_lig\_10 | E. coli transglycosidas  e mRNA | Target\_407 | 4.9208187539  5238 |
| 2171 | [C@H]1([C@H] (C[C@H]  ([C@H] ([C@H]1O)O[C  @@H]1[C@@ H](C[C@@H]  ([C@@H] (O1)CN)O)N)N) N)O[C@@H]1[ C@H] ([C@@H]  ([C@H]  ([C@@H]  (O1)CNc1c2ccc cc2nc2c1cccc2) O)N)O | GAAGACAGCCGCUU CUACGAGCAU | Tobramycin | Target\_lig\_54 0 | E. coli transglycosidas  e mRNA | Target\_407 | 4.7212463990  4717 |
| 2172 | C1C(C(C(C(C1  N)OC2C(C(C(C (O2)CN)O)O)N) OC3C(C(C(O3)  CO)OC4C(C(C(  C(O4)CN)O)O) N)O)O)N | GAAGACAGCCGCUU CUACGAGCAU | Neomycin B | Target\_lig\_12 51 | E. coli transglycosidas  e mRNA | Target\_407 | 5.5528419686  5778 |
| 2173 | NCC1OC(OC2 C(N)CC(C(C2O  )OC2OC(CN)C(  C(C2O)O)N)N) C(CC1O)N | GAAGACAGCCGCUU CUACGAGCAU | Compd 32 | Target\_lig\_11 55 | E. coli transglycosidas  e mRNA | Target\_407 | 4.9586073148  4177 |
| 2174 | NCC1OC(OC2 C(N)CC(C(C2O  )OC2OC(CN)C(  CC2N)O)N)C(C (C1OC1OC(CO  )C(C(C1O)O)N) N)O | GAAGACAGCCGCUU CUACGAGCAU | Compd 33 | Target\_lig\_11 56 | E. coli transglycosidas  e mRNA | Target\_407 | 5.7447274948  9669 |
| 2175 | NCC1OC(OC2 C(N)CC(C(C2O  )OC2OC(CN)C(  CC2N)O)N)C(C (C1OC1OC(CO  )C(C(C1O)N)O) O)N | GAAGACAGCCGCUU CUACGAGCAU | Compd 34 | Target\_lig\_11 57 | E. coli transglycosidas  e mRNA | Target\_407 | 6.2076083105  0175 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA\_ID** | **pKd** |
| 2176 | NCC1OC(OC2 C(N)CC(C(C2O  )OC2OC(CN)C(  C(C2O)N)O)N) C(CC1O)N | GAAGACAGCCGCUU CUACGAGCAU | Compd 35 | Target\_lig\_11 58 | E. coli transglycosidas  e mRNA | Target\_407 | 5.3098039199  7149 |
| 2177 | NCC1OC(OC2 C(N)CC(C(C2O  )OC2OC(COC3 OC(CO)C(C(C3  N)O)O)C(C(C2  N)O)O)N)C(CC 1O)N | GAAGACAGCCGCUU CUACGAGCAU | Compd 36 | Target\_lig\_11 63 | E. coli transglycosidas  e mRNA | Target\_407 | 5.2757241303  9921 |
| 2178 | NCC1OC(OC2 C(N)CC(C(C2O  )OC2OC(CN)C(  CC2N)O)N)C(C (C1O)OC1OC( CO)C(C(C1O)O  )N)O | GAAGACAGCCGCUU CUACGAGCAU | Compd 37 | Target\_lig\_11 59 | E. coli transglycosidas  e mRNA | Target\_407 | 4.8538719643  2176 |
| 2179 | NCC1OC(OC2 C(N)CC(C(C2O  )OC2OC(CN)C(  CC2N)O)N)C(C (C1OC1OC(CO  )C(C(C1N)O)O) N)O | GAAGACAGCCGCUU CUACGAGCAU | Compd 38 | Target\_lig\_11 60 | E. coli transglycosidas  e mRNA | Target\_407 | 6 |
| 2180 | NCC1OC(OC2 C(N)CC(C(C2O  )OC2OC(COC3 OC(CN)C(C(C3  O)O)O)C(C(C2  N)O)N)N)C(CC 1O)N | GAAGACAGCCGCUU CUACGAGCAU | Compd 39 | Target\_lig\_11 61 | E. coli transglycosidas  e mRNA | Target\_407 | 6.3767507096  021 |
| 2181 | NCC1OC(OC2 C(N)CC(C(C2O  )OC2OC(COC3 OC(CN)C(C(C3  O)O)O)C(C(C2  N)O)N)N)C(CC 1O)N | GAAGACAGCCGCUU CUACGAGCAU | Compd 40 | Target\_lig\_12 81 | E. coli transglycosidas  e mRNA | Target\_407 | 5.0969100130  0806 |
| 2182 | NCC1OC(OC2 C(N)CC(C(C2O  )OC2OC(CN)C(  CC2N)O)N)C(C (C1O)OC1OC( CO)C(C(C1N)O  )O)N | GAAGACAGCCGCUU CUACGAGCAU | Compd 41 | Target\_lig\_11 62 | E. coli transglycosidas  e mRNA | Target\_407 | 6.1739251972  9917 |
| 2183 | NCC1OC(OC2 C(N)CC(C(C2O  )OC2OC(CN)C(  CC2N)O)N)C(C (C1O)OC1OC( CO)C(C(C1N)O  )O)N | GAAGACAGCCGCUU CUACGAGCAU | Compd 42 | Target\_lig\_12 82 | E. coli transglycosidas  e mRNA | Target\_407 | 5.6020599913  2796 |
| 2184 | NCC1OC(OC2 C(N)CC(C(C2O  )OC2OC(CN)C(  CC2N)O)N)C(C (C1OC1OC(CO  )C(C(C1N)O)O) N)O | GAAGACAGCCGCUU CUACGAGCAU | Compd 43 | Target\_lig\_12 83 | E. coli transglycosidas  e mRNA | Target\_407 | 5.7695510786  2173 |
| 2245 | CC1(COC(C(C1 NC)O)OC2C(C C(C(C2O)OC3C (CC=C(O3)CN)  N)N)N)O | GCCAACCCACCUAA CUACGGAAAACCUG AUCCC | sisomicin | Target\_lig\_10 | human tyrosine sulfotransferase mRNA | Target\_410 | 4.4317982759  3301 |
| 2246 | [C@H]1([C@H] (C[C@H]  ([C@H] | GCCAACCCACCUAA CUACGGAAAACCUG AUCCC | Tobramycin | Target\_lig\_54 0 | human tyrosine sulfotransferase mRNA | Target\_410 | 4.1870866433  5714 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA\_ID** | **pKd** |
|  | ([C@H]1O)O[C  @@H]1[C@@ H](C[C@@H]  ([C@@H] (O1)CN)O)N)N) N)O[C@@H]1[ C@H] ([C@@H]  ([C@H]  ([C@@H]  (O1)CNc1c2ccc cc2nc2c1cccc2) O)N)O |  |  |  |  |  |  |
| 2247 | C1C(C(C(C(C1  N)OC2C(C(C(C (O2)CN)O)O)N) OC3C(C(C(O3)  CO)OC4C(C(C(  C(O4)CN)O)O) N)O)O)N | GCCAACCCACCUAA CUACGGAAAACCUG AUCCC | Neomycin B | Target\_lig\_12 51 | human tyrosine sulfotransferase mRNA | Target\_410 | 6.5228787452  8034 |
| 2248 | NCC1OC(OC2 C(N)CC(C(C2O  )OC2OC(CN)C(  C(C2O)O)N)N) C(CC1O)N | GCCAACCCACCUAA CUACGGAAAACCUG AUCCC | Compd 32 | Target\_lig\_11 55 | human tyrosine sulfotransferase mRNA | Target\_410 | 4.6020599913  2796 |
| 2249 | NCC1OC(OC2 C(N)CC(C(C2O  )OC2OC(CN)C(  CC2N)O)N)C(C (C1OC1OC(CO  )C(C(C1O)O)N) N)O | GCCAACCCACCUAA CUACGGAAAACCUG AUCCC | Compd 33 | Target\_lig\_11 56 | human tyrosine sulfotransferase mRNA | Target\_410 | 5.7958800173  4408 |
| 2250 | NCC1OC(OC2 C(N)CC(C(C2O  )OC2OC(CN)C(  CC2N)O)N)C(C (C1OC1OC(CO  )C(C(C1O)N)O) O)N | GCCAACCCACCUAA CUACGGAAAACCUG AUCCC | Compd 34 | Target\_lig\_11 57 | human tyrosine sulfotransferase mRNA | Target\_410 | 5.0268721464  003 |
| 2251 | NCC1OC(OC2 C(N)CC(C(C2O  )OC2OC(CN)C(  C(C2O)N)O)N) C(CC1O)N | GCCAACCCACCUAA CUACGGAAAACCUG AUCCC | Compd 35 | Target\_lig\_11 58 | human tyrosine sulfotransferase mRNA | Target\_410 | 5.0915149811  2135 |
| 2252 | NCC1OC(OC2 C(N)CC(C(C2O  )OC2OC(CN)C(  CC2N)O)N)C(C (C1O)OC1OC( CO)C(C(C1O)O  )N)O | GCCAACCCACCUAA CUACGGAAAACCUG AUCCC | Compd 37 | Target\_lig\_11 59 | human tyrosine sulfotransferase mRNA | Target\_410 | 4.2839966563  652 |
| 2253 | NCC1OC(OC2 C(N)CC(C(C2O  )OC2OC(CN)C(  CC2N)O)N)C(C (C1OC1OC(CO  )C(C(C1N)O)O) N)O | GCCAACCCACCUAA CUACGGAAAACCUG AUCCC | Compd 38 | Target\_lig\_11 60 | human tyrosine sulfotransferase mRNA | Target\_410 | 4.8538719643  2176 |
| 2254 | NCC1OC(OC2 C(N)CC(C(C2O  )OC2OC(COC3 OC(CN)C(C(C3  O)O)O)C(C(C2  N)O)N)N)C(CC 1O)N | GCCAACCCACCUAA CUACGGAAAACCUG AUCCC | Compd 39 | Target\_lig\_11 61 | human tyrosine sulfotransferase mRNA | Target\_410 | 5.0177287669  6043 |
| 2255 | NCC1OC(OC2 C(N)CC(C(C2O  )OC2OC(COC3 OC(CN)C(C(C3 | GCCAACCCACCUAA CUACGGAAAACCUG AUCCC | Compd 40 | Target\_lig\_12 81 | human tyrosine sulfotransferase mRNA | Target\_410 | 4.8860566476  9316 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA\_ID** | **pKd** |
|  | O)O)O)C(C(C2  N)O)N)N)C(CC 1O)N |  |  |  |  |  |  |
| 2256 | NCC1OC(OC2 C(N)CC(C(C2O  )OC2OC(CN)C(  CC2N)O)N)C(C (C1O)OC1OC( CO)C(C(C1N)O  )O)N | GCCAACCCACCUAA CUACGGAAAACCUG AUCCC | Compd 41 | Target\_lig\_11 62 | human tyrosine sulfotransferase mRNA | Target\_410 | 5.0268721464  003 |
| 2257 | NCC1OC(OC2 C(N)CC(C(C2O  )OC2OC(CN)C(  CC2N)O)N)C(C (C1O)OC1OC( CO)C(C(C1N)O  )O)N | GCCAACCCACCUAA CUACGGAAAACCUG AUCCC | Compd 42 | Target\_lig\_12 82 | human tyrosine sulfotransferase mRNA | Target\_410 | 5.4089353929  735 |
| 2258 | NCC1OC(OC2 C(N)CC(C(C2O  )OC2OC(CN)C(  CC2N)O)N)C(C (C1OC1OC(CO  )C(C(C1N)O)O) N)O | GCCAACCCACCUAA CUACGGAAAACCUG AUCCC | Compd 43 | Target\_lig\_12 83 | human tyrosine sulfotransferase mRNA | Target\_410 | 5.2924298239  0206 |
| 2398 | Coc1ccc2c(c1)c( Nc1ccc(c(c1)CN 1CCN(CC1)C)O  )c1c(n2)cc(cc1) Cl | AUCACCUCCUUA | Acridine\_derivati ve\_2 (AD2) | Target\_lig\_12 31 | Duplex RNA | Target\_436 | 6.0604807473  8138 |
| 2399 | CCOC(=O)C1= C2C=CC=CN2 C3=C1C(=O)C4  =CC=CC=C4C3  =O | AUCACCUCCUUA | NSC119236 | Target\_lig\_12 32 | Duplex RNA | Target\_436 | 5.5228787452  8034 |
| 2400 | C[N+] (CCN[N+]1(C)  CCCc2c1cccc2) (C)C | AUCACCUCCUUA | SL3\_compound\_ 6 | Target\_lig\_12 33 | Duplex RNA | Target\_436 | 5.2146701649  8923 |
| 2401 | CC1=NC2=NC(  =NN2C(=C1)N3 CCN(CC3)C)C4  =CC=C(C=C4)  Cl | AUCACCUCCUUA | methylpiperazine derivative | Target\_lig\_49 8 | Duplex RNA | Target\_436 | 4.1611509092  6274 |
| 2402 | CC1=C(C(=O)C 2=C(C1=O)N3C [C@H]4[C@@ H] (C3=C2COC(= O)N)N4C)OC | AUCACCUCCUUA | methyl\_carbamat e derivative | Target\_lig\_49 9 | Duplex RNA | Target\_436 | 3.4621809049  2673 |
| 2403 | Coc1ccc2c(c1)c( Nc1ccc(c(c1)CN 1CCN(CC1)C)O  )c1c(n2)cc(cc1) Cl | AUCACCUCCUUA | Acridine\_derivati ve\_2 (AD2) | Target\_lig\_12 31 | Single\_strande d\_RNA | Target\_437 | 5.5228787452  8034 |
| 2404 | CCOC(=O)C1= C2C=CC=CN2 C3=C1C(=O)C4  =CC=CC=C4C3  =O | AUCACCUCCUUA | NSC119236 | Target\_lig\_12 32 | Single\_strande d\_RNA | Target\_437 | 5.6382721639  8241 |
| 2405 | C[N+] (CCN[N+]1(C)  CCCc2c1cccc2) (C)C | AUCACCUCCUUA | SL3\_compound\_ 6 | Target\_lig\_12 33 | Single\_strande d\_RNA | Target\_437 | 5.1079053973  0952 |
| 2406 | CC1=NC2=NC(  =NN2C(=C1)N3 CCN(CC3)C)C4  =CC=C(C=C4)  Cl | AUCACCUCCUUA | methylpiperazine derivative | Target\_lig\_49 8 | Single\_strande d\_RNA | Target\_437 | 3.5590909179  3478 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA\_ID** | **pKd** |
| 2407 | CC1=C(C(=O)C 2=C(C1=O)N3C [C@H]4[C@@ H] (C3=C2COC(= O)N)N4C)OC | AUCACCUCCUUA | methyl\_carbamat e derivative | Target\_lig\_49 9 | Single\_strande d\_RNA | Target\_437 | 2.3098039199  7149 |
| 2408 | C[N+] (CCN[N+]1(C)  CCCc2c1cccc2) (C)C | GGACUAGCGCUAGU CC | SL3\_compound\_ 6 | Target\_lig\_12 33 | SL3\_duplex\_R NA | Target\_438 | 4.8538719643  2176 |
| 2409 | CC1=NC2=NC(  =NN2C(=C1)N3 CCN(CC3)C)C4  =CC=C(C=C4)  Cl | GGACUAGCGCUAGU CC | methylpiperazine derivative | Target\_lig\_49 8 | SL3\_duplex\_R NA | Target\_438 | 4.2365720064  3706 |
| 2410 | CC1=C(C(=O)C 2=C(C1=O)N3C [C@H]4[C@@ H] (C3=C2COC(= O)N)N4C)OC | GGUGCGAGAGCGUC | methyl\_carbamat e derivative | Target\_lig\_49 9 | SL4 RNA | Target\_439 | 4.1023729087  0956 |
| 2411 | CC1=NC2=NC(  =NN2C(=C1)N3 CCN(CC3)C)C4  =CC=C(C=C4)  Cl | GGCGACUGGUGAGU ACGCC | methylpiperazine derivative | Target\_lig\_49 8 | SL2 RNA | Target\_440 | 4.3372421683  1843 |
| 2412 | CC1=NC2=NC(  =NN2C(=C1)N3 CCN(CC3)C)C4  =CC=C(C=C4)  Cl | GGUGCGAGAGCGUC | methylpiperazine derivative | Target\_lig\_49 8 | SL4 RNA | Target\_439 | 4.1549019599  8574 |
| 2413 | CC(=[NH+]CC CC[C@@H] (C(=O)[O-]) [NH3+])N | GAGGGUGGAACCGC GCUUCGGCGUCCCU C | N6-1-  Iminoethyl-L- lysine | Target\_lig\_12 35 | T-box riboswitch | Target\_79 | 4.9586073148  4177 |
| 2414 | C1C(C(C(C(C1  NC(=O)C(CCN)  O)O)OC2C(C(C  (O2)CO)O)O)O  C3C(C(C(C(O3)  CN)O)O)N)N | AUUUUUCCUCGAAC CCGGCGGAACGCAG AAAAAU | Butirosin | Target\_lig\_22 0 | U15C,U16C  SLI\_mutant | Target\_441 | 6.6989700043  3602 |
| 2415 | C1C(C(C(C(C1  NC(=O)C(CCN)  O)OC2C(C(C(C (O2)CO)O)N)O) O)OC3C(C(C(C (O3)CN)O)O)O) N | AUUUUUCCUCGAAC CCGGCGGAACGCAG AAAAAU | Amikacin | Target\_lig\_17 5 | U15C,U16C  SLI\_mutant | Target\_441 | 7.1549019599  8574 |
| 2416 | C1C(C(C(C(C1  N)OC2C(C(C(C (O2)CN)O)O)N) OC3C(C(C(O3)  CO)OC4C(C(C(  C(O4)CN)O)O) N)O)O)N | AUUUUUCCUCGAAC CCGGCGGAACGCAG AAAAAU | Neomycin | Target\_lig\_4 | U15C,U16C  SLI\_mutant | Target\_441 | 7.1549019599  8574 |
| 2417 | C1C(C(C(C(C1  N)OC2C(C(C(C (O2)CO)O)N)O) O)OC3C(C(C(C (O3)CN)O)O)N) N | AUUUUUCCUCGAAC CCGGCGGAACGCAG AAAAAU | KANAMYCIN B | Target\_lig\_8 | U15C,U16C  SLI\_mutant | Target\_441 | 6.9586073148  4177 |
| 2418 | C1C(C(C(C(C1  N)OC2C(C(C(C (O2)CN)O)O)O) O)OC3C(C(C(C (O3)CO)O)N)O) N | AUUUUUCCUCGAAC CCGGCGGAACGCAG AAAAAU | Kanamycin A | Target\_lig\_7 | U15C,U16C  SLI\_mutant | Target\_441 | 6.5376020021  0104 |
| 2419 | CC1(COC(C(C1 | AUUUUUCCUCGAAC | gentamicin\_mol | Target\_lig\_76 | U15C,U16C | Target\_441 | 7.2218487496 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA\_ID** | **pKd** |
|  | NC)O)OC2C(C C(C(C2O)OC3C (CCC(O3)CN)N  )N)N)O | CCGGCGGAACGCAG AAAAAU |  |  | SLI\_mutant |  | 1636 |
| 2420 | [C@H]1([C@H] (C[C@H]  ([C@H] ([C@H]1O)O[C  @@H]1[C@@ H](C[C@@H]  ([C@@H] (O1)CN)O)N)N) N)O[C@@H]1[ C@H] ([C@@H]  ([C@H]  ([C@@H]  (O1)CNc1c2ccc cc2nc2c1cccc2) O)N)O | AUUUUUCCUCGAAC CCGGCGGAACGCAG AAAAAU | Tobramycin | Target\_lig\_54 0 | U15C,U16C  SLI\_mutant | Target\_441 | 7.0457574905  6068 |
| 2421 | CC1(COC(C(C1 NC)O)OC2C(C C(C(C2O)OC3C (CC=C(O3)CN)  N)N)N)O | AUUUUUCCUCGAAC CCGGCGGAACGCAG AAAAAU | sisomicin | Target\_lig\_10 | U15C,U16C  SLI\_mutant | Target\_441 | 7.3979400086  7204 |
| 2422 | C1C(C(C(C(C1  N)OC2C(C(C(C (O2)CO)O)O)N) OC3C(C(C(O3)  CO)OC4C(C(C(  C(O4)CN)O)O) N)O)O)N | AUUUUUCCUCGAAC CCGGCGGAACGCAG AAAAAU | Paromomycin\_m ol\_mol | Target\_lig\_11 16 | U15C,U16C  SLI\_mutant | Target\_441 | 7.3979400086  7204 |
| 2423 | C1C(C(C(C(C1  NC(=O)C(CCN)  O)O)OC2C(C(C  (O2)CO)O)O)O  C3C(C(C(C(O3)  CN)O)O)N)N | AUUUUUCCUCGAAC UUAACGGAACGCAG AAAAAU | Butirosin | Target\_lig\_22 0 | G17A,G18A  SLI\_mutant | Target\_442 | 6.6989700043  3602 |
| 2424 | C1C(C(C(C(C1  NC(=O)C(CCN)  O)OC2C(C(C(C (O2)CO)O)N)O) O)OC3C(C(C(C (O3)CN)O)O)O) N | AUUUUUCCUCGAAC UUAACGGAACGCAG AAAAAU | Amikacin | Target\_lig\_17 5 | G17A,G18A  SLI\_mutant | Target\_442 | 6.8860566476  9316 |
| 2425 | C1C(C(C(C(C1  N)OC2C(C(C(C (O2)CN)O)O)N) OC3C(C(C(O3)  CO)OC4C(C(C(  C(O4)CN)O)O) N)O)O)N | AUUUUUCCUCGAAC UUAACGGAACGCAG AAAAAU | Neomycin | Target\_lig\_4 | G17A,G18A  SLI\_mutant | Target\_442 | 7.3010299956  6398 |
| 2426 | C1C(C(C(C(C1  N)OC2C(C(C(C (O2)CO)O)N)O) O)OC3C(C(C(C (O3)CN)O)O)N) N | AUUUUUCCUCGAAC UUAACGGAACGCAG AAAAAU | KANAMYCIN B | Target\_lig\_8 | G17A,G18A  SLI\_mutant | Target\_442 | 7 |
| 2427 | C1C(C(C(C(C1  N)OC2C(C(C(C (O2)CN)O)O)O) O)OC3C(C(C(C (O3)CO)O)N)O) N | AUUUUUCCUCGAAC UUAACGGAACGCAG AAAAAU | Kanamycin A | Target\_lig\_7 | G17A,G18A  SLI\_mutant | Target\_442 | 6.9208187539  5238 |
| 2428 | CC1(COC(C(C1 NC)O)OC2C(C C(C(C2O)OC3C (CCC(O3)CN)N  )N)N)O | AUUUUUCCUCGAAC UUAACGGAACGCAG AAAAAU | gentamicin\_mol | Target\_lig\_76 | G17A,G18A  SLI\_mutant | Target\_442 | 7 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA\_ID** | **pKd** |
| 2429 | [C@H]1([C@H] (C[C@H]  ([C@H] ([C@H]1O)O[C  @@H]1[C@@ H](C[C@@H]  ([C@@H] (O1)CN)O)N)N) N)O[C@@H]1[ C@H] ([C@@H]  ([C@H]  ([C@@H]  (O1)CNc1c2ccc cc2nc2c1cccc2) O)N)O | AUUUUUCCUCGAAC UUAACGGAACGCAG AAAAAU | Tobramycin | Target\_lig\_54 0 | G17A,G18A  SLI\_mutant | Target\_442 | 7.5228787452  8034 |
| 2430 | CC1(COC(C(C1 NC)O)OC2C(C C(C(C2O)OC3C (CC=C(O3)CN)  N)N)N)O | AUUUUUCCUCGAAC UUAACGGAACGCAG AAAAAU | sisomicin | Target\_lig\_10 | G17A,G18A  SLI\_mutant | Target\_442 | 7.3979400086  7204 |
| 2431 | C1C(C(C(C(C1  N)OC2C(C(C(C (O2)CO)O)O)N) OC3C(C(C(O3)  CO)OC4C(C(C(  C(O4)CN)O)O) N)O)O)N | AUUUUUCCUCGAAC UUAACGGAACGCAG AAAAAU | Paromomycin\_m ol\_mol | Target\_lig\_11 16 | G17A,G18A  SLI\_mutant | Target\_442 | 7.3010299956  6398 |
| 2432 | C1C(C(C(C(C1  NC(=O)C(CCN)  O)O)OC2C(C(C  (O2)CO)O)O)O  C3C(C(C(C(O3)  CN)O)O)N)N | AUUUUUCCUCGAAC UUGGUAGAACGCAG AAAAAU | Butirosin | Target\_lig\_22 0 | C19U,G20A  SLI\_mutant | Target\_443 | 6.8239087409  4432 |
| 2433 | C1C(C(C(C(C1  NC(=O)C(CCN)  O)OC2C(C(C(C (O2)CO)O)N)O) O)OC3C(C(C(C (O3)CN)O)O)O) N | AUUUUUCCUCGAAC UUGGUAGAACGCAG AAAAAU | Amikacin | Target\_lig\_17 5 | C19U,G20A  SLI\_mutant | Target\_443 | 7.1549019599  8574 |
| 2434 | C1C(C(C(C(C1  N)OC2C(C(C(C (O2)CN)O)O)N) OC3C(C(C(O3)  CO)OC4C(C(C(  C(O4)CN)O)O) N)O)O)N | AUUUUUCCUCGAAC UUGGUAGAACGCAG AAAAAU | Neomycin | Target\_lig\_4 | C19U,G20A  SLI\_mutant | Target\_443 | 7.3010299956  6398 |
| 2435 | C1C(C(C(C(C1  N)OC2C(C(C(C (O2)CO)O)N)O) O)OC3C(C(C(C (O3)CN)O)O)N) N | AUUUUUCCUCGAAC UUGGUAGAACGCAG AAAAAU | KANAMYCIN B | Target\_lig\_8 | C19U,G20A  SLI\_mutant | Target\_443 | 7 |
| 2436 | C1C(C(C(C(C1  N)OC2C(C(C(C (O2)CN)O)O)O) O)OC3C(C(C(C (O3)CO)O)N)O) N | AUUUUUCCUCGAAC UUGGUAGAACGCAG AAAAAU | Kanamycin A | Target\_lig\_7 | C19U,G20A  SLI\_mutant | Target\_443 | 6.5228787452  8034 |
| 2437 | CC1(COC(C(C1 NC)O)OC2C(C C(C(C2O)OC3C (CCC(O3)CN)N  )N)N)O | AUUUUUCCUCGAAC UUGGUAGAACGCAG AAAAAU | gentamicin\_mol | Target\_lig\_76 | C19U,G20A  SLI\_mutant | Target\_443 | 7.1549019599  8574 |
| 2438 | [C@H]1([C@H] (C[C@H]  ([C@H] ([C@H]1O)O[C | AUUUUUCCUCGAAC UUGGUAGAACGCAG AAAAAU | Tobramycin | Target\_lig\_54 0 | C19U,G20A  SLI\_mutant | Target\_443 | 7.2218487496  1636 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA\_ID** | **pKd** |
|  | @@H]1[C@@ H](C[C@@H]  ([C@@H] (O1)CN)O)N)N) N)O[C@@H]1[ C@H] ([C@@H]  ([C@H]  ([C@@H]  (O1)CNc1c2ccc cc2nc2c1cccc2) O)N)O |  |  |  |  |  |  |
| 2439 | CC1(COC(C(C1 NC)O)OC2C(C C(C(C2O)OC3C (CC=C(O3)CN)  N)N)N)O | AUUUUUCCUCGAAC UUGGUAGAACGCAG AAAAAU | sisomicin | Target\_lig\_10 | C19U,G20A  SLI\_mutant | Target\_443 | 7.5228787452  8034 |
| 2440 | C1C(C(C(C(C1  N)OC2C(C(C(C (O2)CO)O)O)N) OC3C(C(C(O3)  CO)OC4C(C(C(  C(O4)CN)O)O) N)O)O)N | AUUUUUCCUCGAAC UUGGUAGAACGCAG AAAAAU | Paromomycin\_m ol\_mol | Target\_lig\_11 16 | C19U,G20A  SLI\_mutant | Target\_443 | 7.3010299956  6398 |
| 2441 | C1C(C(C(C(C1  NC(=O)C(CCN)  O)O)OC2C(C(C  (O2)CO)O)O)O  C3C(C(C(C(O3)  CN)O)O)N)N | AUUUUUCCUCGAAC UUGGCGAGACGCAG AAAAAU | Butirosin | Target\_lig\_22 0 | G21A,A22G  SLI\_mutant | Target\_444 | 6.5850266520  2918 |
| 2442 | C1C(C(C(C(C1  NC(=O)C(CCN)  O)OC2C(C(C(C (O2)CO)O)N)O) O)OC3C(C(C(C (O3)CN)O)O)O) N | AUUUUUCCUCGAAC UUGGCGAGACGCAG AAAAAU | Amikacin | Target\_lig\_17 5 | G21A,A22G  SLI\_mutant | Target\_444 | 6.9208187539  5238 |
| 2443 | C1C(C(C(C(C1  N)OC2C(C(C(C (O2)CN)O)O)N) OC3C(C(C(O3)  CO)OC4C(C(C(  C(O4)CN)O)O) N)O)O)N | AUUUUUCCUCGAAC UUGGCGAGACGCAG AAAAAU | Neomycin | Target\_lig\_4 | G21A,A22G  SLI\_mutant | Target\_444 | 7.5228787452  8034 |
| 2444 | C1C(C(C(C(C1  N)OC2C(C(C(C (O2)CO)O)N)O) O)OC3C(C(C(C (O3)CN)O)O)N) N | AUUUUUCCUCGAAC UUGGCGAGACGCAG AAAAAU | KANAMYCIN B | Target\_lig\_8 | G21A,A22G  SLI\_mutant | Target\_444 | 6.8860566476  9316 |
| 2445 | C1C(C(C(C(C1  N)OC2C(C(C(C (O2)CN)O)O)O) O)OC3C(C(C(C (O3)CO)O)N)O) N | AUUUUUCCUCGAAC UUGGCGAGACGCAG AAAAAU | Kanamycin A | Target\_lig\_7 | G21A,A22G  SLI\_mutant | Target\_444 | 6.6197887582  8839 |
| 2446 | CC1(COC(C(C1 NC)O)OC2C(C C(C(C2O)OC3C (CCC(O3)CN)N  )N)N)O | AUUUUUCCUCGAAC UUGGCGAGACGCAG AAAAAU | gentamicin\_mol | Target\_lig\_76 | G21A,A22G  SLI\_mutant | Target\_444 | 7.0457574905  6068 |
| 2447 | [C@H]1([C@H] (C[C@H]  ([C@H] ([C@H]1O)O[C  @@H]1[C@@ H](C[C@@H]  ([C@@H] (O1)CN)O)N)N) | AUUUUUCCUCGAAC UUGGCGAGACGCAG AAAAAU | Tobramycin | Target\_lig\_54 0 | G21A,A22G  SLI\_mutant | Target\_444 | 7.1549019599  8574 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA\_ID** | **pKd** |
|  | N)O[C@@H]1[ C@H] ([C@@H]  ([C@H]  ([C@@H]  (O1)CNc1c2ccc cc2nc2c1cccc2) O)N)O |  |  |  |  |  |  |
| 2448 | CC1(COC(C(C1 NC)O)OC2C(C C(C(C2O)OC3C (CC=C(O3)CN)  N)N)N)O | AUUUUUCCUCGAAC UUGGCGAGACGCAG AAAAAU | sisomicin | Target\_lig\_10 | G21A,A22G  SLI\_mutant | Target\_444 | 7.2218487496  1636 |
| 2449 | C1C(C(C(C(C1  N)OC2C(C(C(C (O2)CO)O)O)N) OC3C(C(C(O3)  CO)OC4C(C(C(  C(O4)CN)O)O) N)O)O)N | AUUUUUCCUCGAAC UUGGCGAGACGCAG AAAAAU | Paromomycin\_m ol\_mol | Target\_lig\_11 16 | G21A,A22G  SLI\_mutant | Target\_444 | 7.3010299956  6398 |
| 2450 | CC(C)CC(C(=O  )NC(CC1=CNC 2=CC=CC=C21  )C(=O)N3CCC C3C(=O)O)NC(  =O)C(CCC(=O) N)NC(=O)C4C CCN4C(=O)C( CCCCN)N | CCCCCCCGCCGCGCC AUGCCUGUGGCCGG UCGG | CRP | Target\_lig\_14 7 | Thymidylate synthase m- RNA | Target\_63 | 6.1348960253  5887 |
| 2451 | CNC1C(O)C(O CC1(C)O)OC1C (N)CC(C(C1O) OC1OC(CCC1 N)C(CCNC(=O)  c1ccc(c(c1)C(= O)O)c1c2ccc(=[ N+]  (C)C)cc2oc2c1c cc(c2)N(C)C)C) N | CCCCCCCGCCGCGCC AUGCCUGUGGCCGG UCGG | CRG | Target\_lig\_12 36 | Thymidylate synthase m- RNA | Target\_63 | 6.0710923097  5605 |
| 2452 | OCC1OC(OC2 C(N)CC(C(C2O  )OC2OC(CNC(  =O)c3ccc(c(c3) C(=O)O)c3c4cc c(=[N+]  (C)C)cc4oc4c3c cc(c4)N(C)C)C( CC2N)O)N)C(C  (C1O)N)O | CCCCCCCGCCGCGCC AUGCCUGUGGCCGG UCGG | CRT | Target\_lig\_99 3 | Thymidylate synthase m- RNA | Target\_63 | 6.0888423912  6002 |
| 2453 | OCC1OC(OC2 C(N)CC(C(C2O  )OC2OC(CNC(  =O)c3ccc(c(c3) C(=O)O)c3c4cc c(=[N+]  (C)C)cc4oc4c3c cc(c4)N(C)C)C(  C(C2N)O)O)N)  C(C(C1O)N)O | CCCCCCCGCCGCGCC AUGCCUGUGGCCGG UCGG | CRK | Target\_lig\_12 38 | Thymidylate synthase m- RNA | Target\_63 | 6.0236500209  9673 |
| 2454 | C1C(C(C(C(C1  N)OC2C(C(C(C (O2)CN)O)O)N) OC3C(C(C(O3)  CO)OC4C(C(C(  C(O4)CN)O)O) N)O)O)N | CCCCCCCGCCGCGCC AUGCCUGUGGCCGG GGGG | Neomycin | Target\_lig\_4 | TS mRNA  Construct\_4 | Target\_445 | 6.0101054362  8123 |
| 2455 | C1C(C(C(C(C1  N)OC2C(C(C(C (O2)CO)O)O)N) | CCCCCCCGCCGCGCC AUGCCUGUGGCCGG GGGG | Paromomycin\_m ol\_mol | Target\_lig\_11 16 | TS mRNA  Construct\_4 | Target\_445 | 5.7297871451  0376 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA\_ID** | **pKd** |
|  | OC3C(C(C(O3)  CO)OC4C(C(C(  C(O4)CN)O)O) N)O)O)N |  |  |  |  |  |  |
| 2456 | CC1(COC(C(C1 NC)O)OC2C(C C(C(C2O)OC3C (CCC(O3)CN)N  )N)N)O | CCCCCCCGCCGCGCC AUGCCUGUGGCCGG GGGG | gentamicin\_mol | Target\_lig\_76 | TS mRNA  Construct\_4 | Target\_445 | 5.5944828930  2362 |
| 2457 | [C@H]1([C@H] (C[C@H]  ([C@H] ([C@H]1O)O[C  @@H]1[C@@ H](C[C@@H]  ([C@@H] (O1)CN)O)N)N) N)O[C@@H]1[ C@H] ([C@@H]  ([C@H]  ([C@@H]  (O1)CNc1c2ccc cc2nc2c1cccc2) O)N)O | CCCCCCCGCCGCGCC AUGCCUGUGGCCGG GGGG | Tobramycin | Target\_lig\_54 0 | TS mRNA  Construct\_4 | Target\_445 | 5.6397853867  0465 |
| 2458 | C1C(C(C(C(C1  N)OC2C(C(C(C (O2)CO)O)N)O) O)OC3C(C(C(C (O3)CN)O)O)N) N | CCCCCCCGCCGCGCC AUGCCUGUGGCCGG GGGG | KANAMYCIN B | Target\_lig\_8 | TS mRNA  Construct\_4 | Target\_445 | 5.6147513175  9678 |
| 2459 | CC(C)CC(C(=O  )NC(CC1=CNC 2=CC=CC=C21  )C(=O)N3CCC C3C(=O)O)NC(  =O)C(CCC(=O) N)NC(=O)C4C CCN4C(=O)C( CCCCN)N | CCCCCCCGCCGCGCC AUGCCUGUGGCCGG GGGG | CRP | Target\_lig\_14 7 | TS mRNA  Construct\_4 | Target\_445 | 6.1463017882  2383 |
| 2460 | CNC1C(O)C(O CC1(C)O)OC1C (N)CC(C(C1O) OC1OC(CCC1 N)C(CCNC(=O)  c1ccc(c(c1)C(= O)O)c1c2ccc(=[ N+]  (C)C)cc2oc2c1c cc(c2)N(C)C)C) N | CCCCCCCGCCGCGCC AUGCCUGUGGCCGG GGGG | CRG | Target\_lig\_12 36 | TS mRNA  Construct\_4 | Target\_445 | 6.0366844886  1389 |
| 2461 | OCC1OC(OC2 C(N)CC(C(C2O  )OC2OC(CNC(  =O)c3ccc(c(c3) C(=O)O)c3c4cc c(=[N+]  (C)C)cc4oc4c3c cc(c4)N(C)C)C( CC2N)O)N)C(C  (C1O)N)O | CCCCCCCGCCGCGCC AUGCCUGUGGCCGG GGGG | CRT | Target\_lig\_99 3 | TS mRNA  Construct\_4 | Target\_445 | 6.0570004066  3396 |
| 2462 | OCC1OC(OC2 C(N)CC(C(C2O  )OC2OC(CNC(  =O)c3ccc(c(c3) C(=O)O)c3c4cc c(=[N+]  (C)C)cc4oc4c3c cc(c4)N(C)C)C(  C(C2N)O)O)N)  C(C(C1O)N)O | CCCCCCCGCCGCGCC AUGCCUGUGGCCGG GGGG | CRK | Target\_lig\_12 38 | TS mRNA  Construct\_4 | Target\_445 | 5.9558523791  2128 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA\_ID** | **pKd** |
| 2463 | C1C(C(C(C(C1  N)OC2C(C(C(C (O2)CN)O)O)N) OC3C(C(C(O3)  CO)OC4C(C(C(  C(O4)CN)O)O) N)O)O)N | CCCCCGCCACCUUCG GGUGGCCGGGG | Neomycin | Target\_lig\_4 | TS mRNA  Construct\_5 | Target\_446 | 5.8392314381  3887 |
| 2464 | C1C(C(C(C(C1  N)OC2C(C(C(C (O2)CO)O)O)N) OC3C(C(C(O3)  CO)OC4C(C(C(  C(O4)CN)O)O) N)O)O)N | CCCCCGCCACCUUCG GGUGGCCGGGG | Paromomycin\_m ol\_mol | Target\_lig\_11 16 | TS mRNA  Construct\_5 | Target\_446 | 5.6495581434  6494 |
| 2465 | CC1(COC(C(C1 NC)O)OC2C(C C(C(C2O)OC3C (CCC(O3)CN)N  )N)N)O | CCCCCGCCACCUUCG GGUGGCCGGGG | gentamicin\_mol | Target\_lig\_76 | TS mRNA  Construct\_5 | Target\_446 | 5.5477534254  7956 |
| 2466 | [C@H]1([C@H] (C[C@H]  ([C@H] ([C@H]1O)O[C  @@H]1[C@@ H](C[C@@H]  ([C@@H] (O1)CN)O)N)N) N)O[C@@H]1[ C@H] ([C@@H]  ([C@H]  ([C@@H]  (O1)CNc1c2ccc cc2nc2c1cccc2) O)N)O | CCCCCGCCACCUUCG GGUGGCCGGGG | Tobramycin | Target\_lig\_54 0 | TS mRNA  Construct\_5 | Target\_446 | 5.4778166823  8131 |
| 2467 | C1C(C(C(C(C1  N)OC2C(C(C(C (O2)CO)O)N)O) O)OC3C(C(C(C (O3)CN)O)O)N) N | CCCCCGCCACCUUCG GGUGGCCGGGG | KANAMYCIN B | Target\_lig\_8 | TS mRNA  Construct\_5 | Target\_446 | 5.4569257649  6647 |
| 2468 | CC(C)CC(C(=O  )NC(CC1=CNC 2=CC=CC=C21  )C(=O)N3CCC C3C(=O)O)NC(  =O)C(CCC(=O) N)NC(=O)C4C CCN4C(=O)C( CCCCN)N | CCCCCGCCACCUUCG GGUGGCCGGGG | CRP | Target\_lig\_14 7 | TS mRNA  Construct\_5 | Target\_446 | 5.9519468268  8439 |
| 2469 | CNC1C(O)C(O CC1(C)O)OC1C (N)CC(C(C1O) OC1OC(CCC1 N)C(CCNC(=O)  c1ccc(c(c1)C(= O)O)c1c2ccc(=[ N+]  (C)C)cc2oc2c1c cc(c2)N(C)C)C) N | CCCCCGCCACCUUCG GGUGGCCGGGG | CRG | Target\_lig\_12 36 | TS mRNA  Construct\_5 | Target\_446 | 5.9048306485  6825 |
| 2470 | OCC1OC(OC2 C(N)CC(C(C2O  )OC2OC(CNC(  =O)c3ccc(c(c3) C(=O)O)c3c4cc c(=[N+]  (C)C)cc4oc4c3c cc(c4)N(C)C)C( CC2N)O)N)C(C  (C1O)N)O | CCCCCGCCACCUUCG GGUGGCCGGGG | CRT | Target\_lig\_99 3 | TS mRNA  Construct\_5 | Target\_446 | 5.8830603534  4924 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA\_ID** | **pKd** |
| 2471 | OCC1OC(OC2 C(N)CC(C(C2O  )OC2OC(CNC(  =O)c3ccc(c(c3) C(=O)O)c3c4cc c(=[N+]  (C)C)cc4oc4c3c cc(c4)N(C)C)C(  C(C2N)O)O)N)  C(C(C1O)N)O | CCCCCGCCACCUUCG GGUGGCCGGGG | CRK | Target\_lig\_12 38 | TS mRNA  Construct\_5 | Target\_446 | 5.8291517963  5669 |
| 2497 | O=C(Cc1ccccc1  )OC[C@H]1OC (=O)NC1CN1C  CN(CC1)c1cccc c1 | GAGGGUGGAACCGC GCUUCGGCGUCCCU C | Compound (4R,5S)-1 | Target\_lig\_12 39 | Antiterminator model RNA AM1A | Target\_147 | 4.9208187539  5238 |
| 2498 | O=C(Cc1ccccc1  )OCC1OC(=O) N[C@H]1CN1C  CN(CC1)c1cccc c1 | GAGGGUGGAACCGC GCUUCGGCGUCCCU C | Compound (4S,5R)-1 | Target\_lig\_12 40 | Antiterminator model RNA AM1A | Target\_147 | 4.7958800173  4408 |
| 2499 | O=C(Nc1ccc(cc 1)C(=O)C)OC[ C@H]1OC(=O) NC1CN1CCN(  CC1)c1ccccc1 | GAGGGUGGAACCGC GCUUCGGCGUCCCU C | Compound (4R,5S)-2 | Target\_lig\_12 41 | Antiterminator model RNA AM1A | Target\_147 | 5.5228787452  8034 |
| 2500 | O=C(Nc1ccc(cc 1)C(=O)C)OCC  1OC(=O)N[C@ H]1CN1CCN(C  C1)c1ccccc1 | GAGGGUGGAACCGC GCUUCGGCGUCCCU C | Compound (4S,5R)-2 | Target\_lig\_12 42 | Antiterminator model RNA AM1A | Target\_147 | 5.7958800173  4408 |
| 2501 | O=C(Nc1ccc(cc 1)C(=O)C)OC[ C@H]1OC(=O) N[C@H]1CN1C  CN(CC1)c1cccc c1 | GAGGGUGGAACCGC GCUUCGGCGUCCCU C | Compound cis-2 | Target\_lig\_12 43 | Antiterminator model RNA AM1A | Target\_147 | 5.7447274948  9669 |