Training dataset curated from [R-SIM](https://web.iitm.ac.in/bioinfo2/R_SIM/) database for the “Riboswitch” 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** |
| 221 | C1=NC2=NC=NC(=C2 N1)N | GGACAUAUAAUCGC GUGGAUAUGGCACG CAAGUUUCUACCGG GCACCGUAAAUGUC CGAUUAUGUCC | Adenine | Target\_lig\_165 | ADENINE RIBOSWITCH | Target\_69 | 6.3979  400086  7204 |
| 222 | C1=C2C(=NC(=N1)N) N=CN2 | GGACAUAUAAUCGC GUGGAUAUGGCACG CAAGUUUCUACCGG GCACCGUAAAUGUC CGAUUAUGUCC | 2-aminopurine | Target\_lig\_166 | ADENINE RIBOSWITCH | Target\_69 | 5.7891  466346  8511 |
| 223 | C1=C(N=C(N=C1N)N) N | GGACAUAUAAUCGC GUGGAUAUGGCACG CAAGUUUCUACCGG GCACCGUAAAUGUC CGAUUAUGUCC | 2,4,6-  triaminopyrimidine | Target\_lig\_167 | ADENINE RIBOSWITCH | Target\_69 | 4.6989  700043  3602 |
| 224 | C1=NC2=NC(=NC(=C 2N1)N)N | GGACAUAUAAUCGC GUGGAUAUGGCACG CAAGUUUCUACCGG GCACCGUAAAUGUC CGAUUAUGUCC | 2,6- diaminopurine | Target\_lig\_168 | ADENINE RIBOSWITCH | Target\_69 | 7.6989  700043  3602 |
| 225 | C1=NC(=NC2(C1=NC  =N2)N)N | GGACAUAUAAUCGC GUGGAUAUGGCACG CAAGUUUCUACCGG GCACCGUAAAUGUC CGAUUAUGUCC | 2,4-diaminopurine | Target\_lig\_169 | ADENINE RIBOSWITCH | Target\_69 | 8.3979  400086  7204 |
| 231 | CC1=CC2=C(C=C1C) N(C=N2)C3C(C(C(O3) CO)OP(=O)  ([O-])OC(C)CNC(=O) CCC4(C(C5C6(C(C(C(  =N6)C(=C7C(C(C(=N 7)C=C8C(C(C(=N8)C(  =C4[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.  [CH2-]C1C(C(C(O1)N 2C=NC3=C(N=CN=C3  2)N)O)O.[Co+3] | GCCGGUCCUGUGAG UUAAUAGGGAAUCC AGUGCGAAUCUGGA GCUGACGCGCAGCG GUAAGGAAAGGUGC GAUGAUUGCGUUAU GCGGACACUGCCAU UCGGUGGGAAGUCA UCAUCUCUUAGUAU CUUAGAUACCCCUC CAAGCCCGAAGACC UGCCGGCCAACGUC GCAUCUGGUUCUCA UCAUCGCGUAAUAU UGAUGA | deoxy\_adenosylcob alamin | Target\_lig\_173 | Riboswitch | Target\_70 | 6.5228  787452  8034 |
| 315 | C1=NC2=NC=NC(=C2 N1)N | GGACAUAUAAUCGC GUGGAUAUGGCACG CAAGUUUCUACCGG GCACCGUAAAUGUC CGACUAUGUCC | Adenine | Target\_lig\_165 | Guanine riboswitch | Target\_74 | 6.3288  271572  8492 |
| 316 | C1=NC2=C(N1)C(=O) N=CN2 | GGACAUAUAAUCGC GUGGAUAUGGCACG CAAGUUUCUACCGG GCACCGUAAAUGUC CGACUAUGUCC | Hypoxanthine | Target\_lig\_162 | Guanine riboswitch | Target\_74 | 7.3010  299956  6398 |
| 317 | C1=NC2=C(N1)C(=O) NC(=N2)N | GGACAUAUAAUCGC GUGGAUAUGGCACG CAAGUUUCUACCGG GCACCGUAAAUGUC CGACUAUGUCC | GUANINE | Target\_lig\_248 | Guanine riboswitch | Target\_74 | 8.3010  299956  6398 |
| 318 | C1=NC(=NC2(C1=NC  =N2)N)N | GGACAUAUAAUCGC GUGGAUAUGGCACG CAAGUUUCUACCGG GCACCGUAAAUGUC CGACUAUGUCC | 2,4-diaminopurine | Target\_lig\_169 | Guanine riboswitch | Target\_74 | 7.7695  510786  2173 |
| 319 | C1=NC2=C(N1)C(=N C(=N2)N)NO | GGACAUAUAAUCGC GUGGAUAUGGCACG CAAGUUUCUACCGG GCACCGUAAAUGUC CGACUAUGUCC | 2-AMINO-N6- HYDROXYADENI NE | Target\_lig\_249 | Guanine riboswitch | Target\_74 | 7.6989  700043  3602 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA\_ ID** | **pKd** |
| 320 | C1(=C(N=C(NC1=O)N  )N)N | GGACAUAUAAUCGC GUGGAUAUGGCACG CAAGUUUCUACCGG GCACCGUAAAUGUC CGACUAUGUCC | 2,5,6-TRIAMINO- PYRIMIDINE-4- ONE | Target\_lig\_250 | Guanine riboswitch | Target\_74 | 7 |
| 392 | C[S+](CCC(C(=O) [O-])N)CC1C(C(C(O1) N2C=NC3=C(N=CN=  C32)N)O)O | GGCUUAUCAAGAGA GGUGGAGGGACUGG CCCGAUGAAACCCG GCAACCAGAAAUGG UGCCAAUUCCUGCA GCGGAAACGUUGAA AGAUGAGCCA | S-adenosyl methionine | Target\_lig\_314 | S\_Adenosyl\_m ethionine\_ribos witch | Target\_71 | 8 |
| 398 | CC1=C(SC=[N+]1CC2  =CN=C(N=C2N)C)CC OP(=O)(O)OP(=O)(O) [O-] | GGACUCGGGGUGCC CUUCUGCGUGAAGG CUGAGAAAUACCCG UAUCACCUGAUCUG GAUAAUGCCAGCGU AGGGAAGUUC | Thiamine\_Pyrophos phate(TPP) | Target\_lig\_318 | thiamine\_BOX  \_Riboswitch | Target\_72 | 6.2218  487496  1636 |
| 410 | C1=NC2=NC=NC(=C2 N1)N | GGAAUAAUUGUAUA ACCUCAAUAAUAUG GUUUGAGGGUGUCU ACCAGGAACCGUAA AAUCCUGAUUACAA | Adenine | Target\_lig\_165 | B\_subtilis\_pbu E \_Adenine riboswitch | Target\_73 | 6.2358  238676  0967 |
| 412 | CC1=CC2=C(C=C1C) N(C3=NC(=O)NC(=O) C3=N2)CC(C(C(COP(  =O)(O)O)O)O)O | GGCGUGUAGGAUAU GCUUCGGCAGAAGG ACACGCC | FMN | Target\_lig\_68 | FMN RIBOSWITCH APTAMER | Target\_36 | 8.9208  187539  5238 |
| 413 | C1=C(C2=C(N1)N=C( NC2=O)N)CN | AGUAGAUGUGCUAG CAAAACAUCUUUAA AAAACUAGACUUGG GGUGCAAGUCCCCU UUUUUAUUGCUUAA AUUU | preQ1 (7- Aminomethyl-7- deazaguanine) | Target\_lig\_331 | PreQ1\_riboswit ch\_Fusobacteri um | Target\_75 | 6.5482  135644  7571 |
| 414 | CC1=C(SC=[N+]1CC2  =CN=C(N=C2N)C)CC OP(=O)(O)OP(=O)(O) [O-] | GGUAACCACUAGGG GUGUCCUUCAUAAG GGCUGAGAUAAAAG UGUGACUUUUAGAC CCUCAUAACUUGAA CAGGUUCAGACCUG CGUAGGGAAGUGGA GC | Thiamine\_Pyrophos phate(TPP) | Target\_lig\_318 | TPP RIBOSWITCH APTAMER | Target\_37 | 6.3053  948010  6643 |
| 415 | C[S+](CCC(C(=O) [O-])N)CC1C(C(C(O1) N2C=NC3=C(N=CN=  C32)N)O)O | GGCUUAUCAAGAGA GGUGGAGGGACUGG CCCGAUGAAACCCG GCAACCAGAAAUGG UGCCAAUUCCUGCA GCGGAAACGUUGAA AGAUGAGCCA | SAM | Target\_lig\_124 8 | S\_Adenosyl\_m ethionine | Target\_71 | 5.8696  662315  0499 |
| 416 | C(CCN)C[C@@H]  (C(=O)O)N | GAAGAUAGAGGUGC GAACUUCAAGAGUA UGCCUUUGGAGAAA GAUGGAUUCUGUGA AAAAGGCUGAAAGG GGAGCGUCGCCGAA GCAAAUAAAACCCC AUCGGUAUUAUUUG CUGGCCGUGCAUUG AAUAAAUGUAAGGC UGUCAAGAAAUCAU UUUCUUGGAGGGCU AUCUCGUUGUUCAU AAUCAUUUAUGAUG AUUAAUUGAUAAGC AAUGAGAGUAUUCC UCUCAUUGCUUUUU U | lysine | Target\_lig\_31 | LYSINE RIBOSWITCH APTAMER | Target\_38 | 5.7447  274948  9669 |
| 739 | CC1=C(SC=[N+]1CC2  =CN=C(N=C2N)C)CC OP(=O)(O)OP(=O)(O) | GGUAACCACUAGGG GUGUCCUUCAUAAG GGCUGAGAUAAAAG | Thiamine\_Pyrophos phate(TPP) | Target\_lig\_318 | B.subtilis tenA TPP riboswitch | Target\_76 | 7.3010  299956  6398 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA\_ ID** | **pKd** |
|  | [O-] | UGUGACUUUUAGAC CCUCAUAACUUGAA CAGGUUCAGACCUG CGUAGGGAAGUGGA GC |  |  |  |  |  |
| 740 | CC1=C(SC=[N+]1CC2  =CN=C(N=C2N)C)CC O | GGUAACCACUAGGG GUGUCCUUCAUAAG GGCUGAGAUAAAAG UGUGACUUUUAGAC CCUCAUAACUUGAA CAGGUUCAGACCUG CGUAGGGAAGUGGA GC | Thiamine\_mol | Target\_lig\_502 | B.subtilis tenA TPP riboswitch | Target\_76 | 4.3010  299956  6398 |
| 741 | CC1=C(C=CC=[N+]1 CC2=CN=C(N=C2N)C  )CCO.Br.[Br-] | GGUAACCACUAGGG GUGUCCUUCAUAAG GGCUGAGAUAAAAG UGUGACUUUUAGAC CCUCAUAACUUGAA CAGGUUCAGACCUG CGUAGGGAAGUGGA GC | Pyrithiamine\_mol | Target\_lig\_503 | B.subtilis tenA TPP riboswitch | Target\_76 | 5.2218  487496  1636 |
| 742 | n1c(ncc(c1N)CN1=CC  =CC(=C1)CCO[P@@] (=O)(O)P(=O)(O)O)C | GGUAACCACUAGGG GUGUCCUUCAUAAG GGCUGAGAUAAAAG UGUGACUUUUAGAC CCUCAUAACUUGAA CAGGUUCAGACCUG CGUAGGGAAGUGGA GC | Pyrithiamine  \_Pyrophosphate\_de r | Target\_lig\_504 | B.subtilis tenA TPP riboswitch | Target\_76 | 6.7958  800173  4408 |
| 743 | CC1=CC2=C(C=C1C) N(C3=NC(=O)NC(=O) C3=N2)CC(C(C(COP(  =O)(O)O)O)O)O | GGAAGGACAAAUGA AUAAAGAUUGUAUC CUUCGGGGCAGGGU GGAAAUCCCGACCG GCGGUAGUAAAGCA CAUUUGCUUUAGAG CCCGUGACCCGUGU GCAAUAGCACGCGG UGGAUUCAGUUUAA GCUGAAGCCGACAG UGAAAGUCUGGAUG GGAGAAGGAUG | FMN | Target\_lig\_68 | B.subtilis tenA FMN  riboswitch | Target\_77 | 8.3010  299956  6398 |
| 744 | CC1=CC2=C(C=C1C) N(C3=NC(=O)NC(=O) C3=N2)CC(C(C(CO)O  )O)O | GGAAGGACAAAUGA AUAAAGAUUGUAUC CUUCGGGGCAGGGU GGAAAUCCCGACCG GCGGUAGUAAAGCA CAUUUGCUUUAGAG CCCGUGACCCGUGU GCAAUAGCACGCGG UGGAUUCAGUUUAA GCUGAAGCCGACAG UGAAAGUCUGGAUG GGAGAAGGAUG | riboflavin | Target\_lig\_70 | B.subtilis tenA FMN  riboswitch | Target\_77 | 5.5228  787452  8034 |
| 745 | CC1=CC2=C(C=C1N( C)C)N(C3=NC(=O)NC (=O)C3=N2)CC(C(C(C O)O)O)O | GGAAGGACAAAUGA AUAAAGAUUGUAUC CUUCGGGGCAGGGU GGAAAUCCCGACCG GCGGUAGUAAAGCA CAUUUGCUUUAGAG CCCGUGACCCGUGU GCAAUAGCACGCGG UGGAUUCAGUUUAA GCUGAAGCCGACAG UGAAAGUCUGGAUG GGAGAAGGAUG | Roseoflavin | Target\_lig\_505 | B.subtilis tenA FMN  riboswitch | Target\_77 | 7 |
| 746 | C(CCN=C(N)N)C[C@  @H](C(=O)O)N | GAAGAUAGAGGUGC GAACUUCAAGAGUA UGCCUUUGGAGAAA GAUGGAUUCUGUGA AAAAGGCUGAAAGG GGAGCGUCGCCGAA | L-homoarginine | Target\_lig\_57 | B.subtilis lysine riboswitch | Target\_78 | 5.1549  019599  8574 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | GCAAAUAAAACCCC AUCGGUAUUAUUUG CUGGCCGUGCAUUG AAUAAAUGUAAGGC UGUCAAGAAAUCAU UUUCUUGGAGGGCU AUCUCGUUGUUCAU AAUCAUUUAUGAUG AUUAAUUGAUAAGC AAUGAGAGUAUUCC UCUCAUUGCUUUUU U |  |  |  |  |  |
| 747 | C(CCN)C[C@@H]  (C(=O)O)N | GAAGAUAGAGGUGC GAACUUCAAGAGUA UGCCUUUGGAGAAA GAUGGAUUCUGUGA AAAAGGCUGAAAGG GGAGCGUCGCCGAA GCAAAUAAAACCCC AUCGGUAUUAUUUG CUGGCCGUGCAUUG AAUAAAUGUAAGGC UGUCAAGAAAUCAU UUUCUUGGAGGGCU AUCUCGUUGUUCAU AAUCAUUUAUGAUG AUUAAUUGAUAAGC AAUGAGAGUAUUCC UCUCAUUGCUUUUU U | lysine | Target\_lig\_31 | B.subtilis lysine riboswitch | Target\_78 | 6.4436  974992  3271 |
| 748 | C(COC[C@@H] (C(=O)O)N)N | GAAGAUAGAGGUGC GAACUUCAAGAGUA UGCCUUUGGAGAAA GAUGGAUUCUGUGA AAAAGGCUGAAAGG GGAGCGUCGCCGAA GCAAAUAAAACCCC AUCGGUAUUAUUUG CUGGCCGUGCAUUG AAUAAAUGUAAGGC UGUCAAGAAAUCAU UUUCUUGGAGGGCU AUCUCGUUGUUCAU AAUCAUUUAUGAUG AUUAAUUGAUAAGC AAUGAGAGUAUUCC UCUCAUUGCUUUUU U | L-4 L\_4\_Oxalysine | Target\_lig\_506 | B.subtilis lysine riboswitch | Target\_78 | 4.8860  566476  9316 |
| 749 | CCC1CC1(C(=O)O)N | GAAGAUAGAGGUGC GAACUUCAAGAGUA UGCCUUUGGAGAAA GAUGGAUUCUGUGA AAAAGGCUGAAAGG GGAGCGUCGCCGAA GCAAAUAAAACCCC AUCGGUAUUAUUUG CUGGCCGUGCAUUG AAUAAAUGUAAGGC UGUCAAGAAAUCAU UUUCUUGGAGGGCU AUCUCGUUGUUCAU AAUCAUUUAUGAUG AUUAAUUGAUAAGC AAUGAGAGUAUUCC UCUCAUUGCUUUUU U | AEC | Target\_lig\_507 | B.subtilis lysine riboswitch | Target\_78 | 4.5228  787452  8034 |
| 750 | C(CS(=O) (=O)C[C@@H](C(=O)  [O-])[NH3+])[NH3+] | GAAGAUAGAGGUGC GAACUUCAAGAGUA UGCCUUUGGAGAAA GAUGGAUUCUGUGA AAAAGGCUGAAAGG GGAGCGUCGCCGAA GCAAAUAAAACCCC | L-3-[(2- AMINOETHYL)- SULFONYL]- ALANINE | Target\_lig\_508 | B.subtilis lysine riboswitch | Target\_78 | 5.6020  599913  2796 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | AUCGGUAUUAUUUG CUGGCCGUGCAUUG AAUAAAUGUAAGGC UGUCAAGAAAUCAU UUUCUUGGAGGGCU AUCUCGUUGUUCAU AAUCAUUUAUGAUG AUUAAUUGAUAAGC AAUGAGAGUAUUCC UCUCAUUGCUUUUU U |  |  |  |  |  |
| 751 | C(/C=C/ C[NH3+])C(C(=O)  [O-])[NH3+] | GAAGAUAGAGGUGC GAACUUCAAGAGUA UGCCUUUGGAGAAA GAUGGAUUCUGUGA AAAAGGCUGAAAGG GGAGCGUCGCCGAA GCAAAUAAAACCCC AUCGGUAUUAUUUG CUGGCCGUGCAUUG AAUAAAUGUAAGGC UGUCAAGAAAUCAU UUUCUUGGAGGGCU AUCUCGUUGUUCAU AAUCAUUUAUGAUG AUUAAUUGAUAAGC AAUGAGAGUAUUCC UCUCAUUGCUUUUU U | DL-TRANS-2,6- DIAMINO-4- HEXENOIC ACID | Target\_lig\_509 | B.subtilis lysine riboswitch | Target\_78 | 6.0132  282657  3376 |
| 1157 | CC(CCN1C2=CC(C)= C(C)C=C2N=C2C(=O) [N-]C(=O)N=C12)C1= CC=C(F)C=C1 | GGAAGGACAAAUGA AUAAAGAUUGUAUC CUUCGGGGCAGGGU GGAAAUCCCGACCG GCGGUAGUAAAGCA CAUUUGCUUUAGAG CCCGUGACCCGUGU GCAAUAGCACGCGG UGGAUUCAGUUUAA GCUGAAGCCGACAG UGAAAGUCUGGAUG GGAGAAGGAUG | 5FDQD | Target\_lig\_662 | 165 ribD FMN Riboswitch Aptamer, B. subtilis | Target\_189 | 8.1249  387366  083 |
| 1159 | CNC1=NC=C(C=N1)C N2CCC[C@@H] (C2)C3=NC(=CC(=O) N3)C4=CC=CS4 | GGAUCUUCGGGGCA GGGUGAAAUUCCCG ACCGGUGGUAUAGU CCACGAAAGUAUUU GCUUUGAUUUGGUG AAAUUCCAAAACCG ACAGUAGAGUCUGG AUGAGAGAAGAUUC | Ribocil-B | Target\_lig\_663 | FMN  Riboswitch Aptamer, E. Coli | Target\_190 | 8.1804  560644  5813 |
| 1160 | C1C[C@@H] (CN(C1)CC2=CN(C= N2)C3=NC=CC=N3)C 4=NC(=CC(=O)N4)C5  =CC=CS5 | GGAUCUUCGGGGCA GGGUGAAAUUCCCG ACCGGUGGUAUAGU CCACGAAAGUAUUU GCUUUGAUUUGGUG AAAUUCCAAAACCG ACAGUAGAGUCUGG AUGAGAGAAGAUUC | Ribocil-C | Target\_lig\_664 | FMN  Riboswitch Aptamer, E. Coli | Target\_190 | 9 |
| 1161 | C1C[C@@H] (CN(C1)CC2=CN(C= N2)C3=NC=CC=N3)C 4=NC(=CC(=O)N4)C5  =CC=CS5 | UAAUUCUUUCGGGG CAGGGUGAAAUUCC CAACCGGCAGUAAA UAAAGCCUGCGACC UGCUAAUAUGUUUC AUAUUAGUGGCUGA UCUAGUGAGAUUCU AGAGCCGACAGUUA AAGUCUGGAUGGGA GAAAGAAUGUUAAU UAUCGACAAAGAUA AUGUAGCGUAUUUG UAAAAAUGUGUACA AAUAGGCUUAUUUA ACGAUAAAUUUUUC | Ribocil-C | Target\_lig\_664 | FMN  Riboswitch Aptamer SA1,  S. Aureus | Target\_191 | 7.2365  720064  3706 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | UCCUUGCAUCUUAA UUCAUGAUGUGAGG AUU |  |  |  |  |  |
| 1162 | C1C[C@@H] (CN(C1)CC2=CN(C= N2)C3=NC=CC=N3)C 4=NC(=CC(=O)N4)C5  =CC=CS5 | AUUCAUCUUCGGGG UCGGGUGUAAUUCC CAACCGGCAGUAAA UAAAGCCUGCGACC UGCUAGUAUGUAUC AUAUUAGUGGCUGA UCUAGUGAGAUUCU AGAGCCGACAGUAU AGUCUGGAUGGGAG AAGAUGGAGGUUUU UUGUUGUGCAAUAA UCCUCCUAUUCUUA CGAGAUGAAUGGAA GGAGAAAAUU | Ribocil-C | Target\_lig\_664 | FMN  Riboswitch Aptamer SA2,  S. Aureus | Target\_192 | 7.4814  860601  2211 |
| 1163 | CC1=CC2=C(C=C1N( C)C)N(C3=NC(=O)NC (=O)C3=N2)CC(C(C(C O)O)O)O | GGUACCAGAAGCAG CGCACUCCGGGGUC GGUGAAAGUCCGAA CCGGCGGUUACAGU CCGCGACCCGACCG CUUCCAGCGGCCGG UUGACCAGGUGAAA UUCCUGGACCGACG GUUAAAGUCCGGAU GGGAGGCAGUGCGC GCGGCGGGCGG | Roseoflavin | Target\_lig\_505 | FMN  Riboswitch, S. Davawensis | Target\_193 | 8 |
| 1164 | NC1=NC(N)=C2NC= NC2=N1 | GGAAUAAUUGUAUA ACCUCAAUAAUAUG GUUUGAGGGUGUCU ACCAGGAACCGUAA AAUCCUGAUUACAA | 2,6-Diaminopurine | Target\_lig\_125 4 | PbuE Riboswitch | Target\_73 | 7.6020  599913  2796 |
| 1165 | CC1=C(C=CC=[N+]1 CC2=CN=C(N=C2N)C  )CCO.Br.[Br-] | GGUAACCACUAGGG GUGUCCUUCAUAAG GGCUGAGAUAAAAG UGUGACUUUUAGAC CCUCAUAACUUGAA CAGGUUCAGACCUG CGUAGGGAAGUGGA GC | Pyrithiamine | Target\_lig\_503 | TPP  Riboswitch, B. Subtilis | Target\_194 | 5.2218  487496  1636 |
| 1166 | C1=NC2=C(N1)C(=N C(=N2)N)NO | GGACAUAUAAUCGC GUGGAUAUGGCACG CAAGUUUCUACCGG GCACCGUAAAUGUC CGACUAUGUCC | 2-Amino-N6- Hydroxyadenine | Target\_lig\_665 | xpt-pbuX Guanine Riboswitch, B. Subtilis | Target\_74 | 7.6989  700043  3602 |
| 1167 | NC1=NC(=O)C(N)=C( N)N1 | GGACAUAUAAUCGC GUGGAUAUGGCACG CAAGUUUCUACCGG GCACCGUAAAUGUC CGACUAUGUCC | PC1 | Target\_lig\_125 5 | Guanine Riboswitch | Target\_74 | 7 |
| 1168 | C[N+]1=C2C(=C3C=C C(=C(C3=C1)OC)OC) C=CC4=CC5=C(C=C4 2)OCO5 | GUAUAUGGUAAACU AUGAAAAAACACGA UUCGGUUGGUAGUC CGGAUGCAUGAUUG AGAAUGUCAGUAAC CUUCCCCUCCUCGG GAUGUCCAUCAUUC UUUAAUAUCU | Chelerythrine | Target\_lig\_666 | 108 nt yjdF Riboswitch Construct, B. subtilis, Mutant 1 | Target\_195 | 8.6197  887582  8839 |
| 1169 | CC1=[N+] (C2=CC=CC=C2C(=C 1)N)CCCCCCCCCC[N  +]3=C(C=C(C4=CC=C C=C43)N)C | GUAUAUGGUAAACU AUGAAAAAACACGA UUCGGUUGGUAGUC CGGAUGCAUGAUUG AGAAUGUCAGUAAC CUUCCCCUCCUCGG GAUGUCCAUCAUUC UUUAAUAUCU | Dequalinium | Target\_lig\_667 | 108 nt yjdF Riboswitch Construct, B. subtilis, Mutant 1 | Target\_195 | 8 |
| 1170 | CC1=NC=CC2=C1NC 3=CC=CC=C23 | GUAUAUGGUAAACU AUGAAAAAACACGA | Harmane | Target\_lig\_668 | 108 nt yjdF Riboswitch | Target\_195 | 7 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | UUCGGUUGGUAGUC CGGAUGCAUGAUUG AGAAUGUCAGUAAC CUUCCCCUCCUCGG GAUGUCCAUCAUUC UUUAAUAUCU |  |  | Construct, B. subtilis, Mutant 1 |  |  |
| 1171 | C1=CC(=CC2=NC3=C (C=CC(=C3)N)C=C21) N | GUAUAUGGUAAACU AUGAAAAAACACGA UUCGGUUGGUAGUC CGGAUGCAUGAUUG AGAAUGUCAGUAAC CUUCCCCUCCUCGG GAUGUCCAUCAUUC UUUAAUAUCU | Proflavin | Target\_lig\_336 | 108 nt yjdF Riboswitch Construct, B. subtilis, Mutant 1 | Target\_195 | 8.2146  701649  8923 |
| 1172 | C[C@@]12[C@@H] ([C@@H](C[C@@H] (O1)N3C4=CC=CC=C 4C5=C6C(=C7C8=CC  =CC=C8N2C7=C53)C NC6=O)NC)OC | GUAUAUGGUAAACU AUGAAAAAACACGA UUCGGUUGGUAGUC CGGAUGCAUGAUUG AGAAUGUCAGUAAC CUUCCCCUCCUCGG GAUGUCCAUCAUUC UUUAAUAUCU | Staurosporine | Target\_lig\_669 | 108 nt yjdF Riboswitch Construct, B. subtilis, Mutant 1 | Target\_195 | 7 |
| 1279 | C1CCC(CC1)NC2=NC 3=C(C(=O)N2)NC=N3 | GGAUCAUAUAAUCG CGUGGAUAUGGCAC GCAAGUUUCUACCG GGCACCGUAAAUGU CCGACUAUGGUC | Guanine Analog 25f | Target\_lig\_714 | C. difficile guaA  riboswitch | Target\_228 | 5.1870  866433  5714 |
| 1280 | [NH3+]CCS(=O)  (=O)C[C@H] ([NH3+])C([O-])=O | GAAGAUAGAGGUGC GAACUUCAAGAGUA UGCCUUUGGAGAAA GAUGGAUUCUGUGA AAAAGGCUGAAAGG GGAGCGUCGCCGAA GCAAAUAAAACCCC AUCGGUAUUAUUUG CUGGCCGUGCAUUG AAUAAAUAUAAGGC UGUCAAGAAAUCAU UUUCUUGGAGGGCU AUCUCGUUGUUCAU AAUCAUUUAUGAUG AUUAAUUGAUAAGC AAUGAGAGUAUUCC UCUCAUUGCUUUUU U | Lysine Analog 8 | Target\_lig\_126 0 | lysC riboswitch | Target\_229 | 5.6020  599913  2796 |
| 1282 | [NH3+]CCS(=O)  (=O)C[C@H] ([NH3+])C([O-])=O | GAAGAUAGAGGUGC GAACUUCAAGAGUA UGCCUUUGGAGAAA GAUGGAUUCUGUGA AAAAGGCUGAAGGG GAGCGUCGCCGAAG CAAAUAAAACCCCA UCGGUAUUAUUUGC UGGCCGUGCAUUGA AUAAAUGUAAGGCU GUCAAGAAAUCAUU UUCUUGGAGGGCUA UCUCGUUGUUCAUA AUCAUUUAUGAUGA UUAAUUGAUAAGCA AUGAGAGUAUUCCU CUCAUUGCUUUUUU | Lysine Analog 8 | Target\_lig\_126 0 | lysC riboswitch mutant 1 (M2) | Target\_230 | 4.6197  887582  8839 |
| 1283 | [NH3+]CCOC[C@H] ([NH3+])C([O-])=O | GAAGAUAGAGGUGC GAACUUCAAGAGUA UGCCUUUGGAGAAA GAUGGAUUCUGUGA AAAAGGCUGAAAGG GGAGCGUCGCCGAA GCAAAUAAAACCCC AUCGGUAUUAUUUG CUGGCCGUGCAUUG | Lysine Analog 9 | Target\_lig\_126 1 | lysC riboswitch | Target\_229 | 4.8860  566476  9316 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | AAUAAAUAUAAGGC UGUCAAGAAAUCAU UUUCUUGGAGGGCU AUCUCGUUGUUCAU AAUCAUUUAUGAUG AUUAAUUGAUAAGC AAUGAGAGUAUUCC UCUCAUUGCUUUUU U |  |  |  |  |  |
| 1285 | [NH3+]CCOC[C@H] ([NH3+])C([O-])=O | GAAGAUAGAGGUGC GAACUUCAAGAGUA UGCCUUUGGAGAAA GAUGGAUUCUGUGA AAAAGGCUGAAGGG GAGCGUCGCCGAAG CAAAUAAAACCCCA UCGGUAUUAUUUGC UGGCCGUGCAUUGA AUAAAUGUAAGGCU GUCAAGAAAUCAUU UUCUUGGAGGGCUA UCUCGUUGUUCAUA AUCAUUUAUGAUGA UUAAUUGAUAAGCA AUGAGAGUAUUCCU CUCAUUGCUUUUUU | Lysine Analog 9 | Target\_lig\_126 1 | lysC riboswitch mutant 1 (M2) | Target\_230 | 4.1249  387366  083 |
| 1889 | C1=NC(=C(N1C2C(C( C(O2)COP(=O) (O)O)O)O)N)C(=O)N | UAUCAGUUAUAUGA CUGACGGAACGUGG AAUUAACCACAUGA AGUAUAACGAUGAC AAUGCCGACCGUCU GGGCG | AIZA analog 1 | Target\_lig\_104 4 | Fusibacterium ulcerans ZTP riboswitch | Target\_352 | 6.4948  500216  8009 |
| 1890 | Ccn1c2ccc(cc2c2c1ccc c2)N1CCNCC1 | UAUCAGUUAUAUGA CUGACGGAACGUGG AAUUAACCACAUGA AGUAUAACGAUGAC AAUGCCGACCGUCU GGGCG | AIZA analog 2 | Target\_lig\_104 5 | Fusibacterium ulcerans ZTP riboswitch | Target\_352 | 4.3872  161432  8026 |
| 1891 | C1=NC(=C(N1C2C(C( C(O2)CO)O)O)N)C(= O)N | UAUCAGUUAUAUGA CUGACGGAACGUGG AAUUAACCACAUGA AGUAUAACGAUGAC AAUGCCGACCGUCU GGGCG | AIZA analog 5 | Target\_lig\_104 6 | Fusibacterium ulcerans ZTP riboswitch | Target\_352 | 5.6382  721639  8241 |
| 1892 | C1=CN=CC=C1N2C= NC(=C2N)C(=O)N | UAUCAGUUAUAUGA CUGACGGAACGUGG AAUUAACCACAUGA AGUAUAACGAUGAC AAUGCCGACCGUCU GGGCG | AIZA analog 7 | Target\_lig\_104 7 | Fusibacterium ulcerans ZTP riboswitch | Target\_352 | 5.8538  719643  2176 |
| 1893 | C1CNCCC1N2C=NC(  =C2N)C(=O)N | UAUCAGUUAUAUGA CUGACGGAACGUGG AAUUAACCACAUGA AGUAUAACGAUGAC AAUGCCGACCGUCU GGGCG | AIZA analog 8 | Target\_lig\_104 8 | Fusibacterium ulcerans ZTP riboswitch | Target\_352 | 5.0604  807473  8138 |
| 1894 | C1=NC(=C(N1CCO)N  )C(=O)N | UAUCAGUUAUAUGA CUGACGGAACGUGG AAUUAACCACAUGA AGUAUAACGAUGAC AAUGCCGACCGUCU GGGCG | AIZA analog 10 | Target\_lig\_104 9 | Fusibacterium ulcerans ZTP riboswitch | Target\_352 | 3.8239  087409  4432 |
| 1895 | NC(=O)c1ncn(c1N)c1c cccn1 | UAUCAGUUAUAUGA CUGACGGAACGUGG AAUUAACCACAUGA AGUAUAACGAUGAC AAUGCCGACCGUCU GGGCG | AIZA analog 12 | Target\_lig\_105 0 | Fusibacterium ulcerans ZTP riboswitch | Target\_352 | 5.25181  197299  38 |
| 1896 | C1=CC(=CN=C1)N2C | UAUCAGUUAUAUGA | AIZA analog 13 | Target\_lig\_105 | Fusibacterium | Target\_352 | 6.2218 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA\_ ID** | **pKd** |
|  | =NC(=C2N)C(=O)N | CUGACGGAACGUGG AAUUAACCACAUGA AGUAUAACGAUGAC AAUGCCGACCGUCU GGGCG |  | 1 | ulcerans ZTP riboswitch |  | 487496  1636 |
| 2044 | C1(=C(N=C(N=C1N)N  )N)N | GGACAUAUAAUCGC GUGGAUAUGGCACG CAAGUUUCUACCGG GCACCGUAAAUGUC CGAUUAUGUCC | 2,4,5,6-  tetraaminopyrimidi ne | Target\_lig\_112 1 | ADENINE RIBOSWITCH | Target\_69 | 4.6989  700043  3602 |
| 2045 | C1=CN=C(N=C1N)N | GGACAUAUAAUCGC GUGGAUAUGGCACG CAAGUUUCUACCGG GCACCGUAAAUGUC CGAUUAUGUCC | 2,4-  diaminopyrimidine | Target\_lig\_112 2 | ADENINE RIBOSWITCH | Target\_69 | 3 |
| 2046 | Nc1nc(N)nc(n1)N | GGACAUAUAAUCGC GUGGAUAUGGCACG CAAGUUUCUACCGG GCACCGUAAAUGUC CGAUUAUGUCC | 2,4,6-triamino- 1,3,5-triazine | Target\_lig\_112 3 | ADENINE RIBOSWITCH | Target\_69 | 4.6989  700043  3602 |
| 2136 | C[S+](CCC(C(=O) [O-])N)CC1C(C(C(O1) N2C=NC3=C(N=CN=  C32)N)O)O | GGUACAAUCUAAAA ACUUAUCAAGAGCG GCUGAGGGACUGGA CCUAUGAAGCCCGG CAACCUGCAUAGUU UGUAAGGUGCUACU UCCAGCAAAAUGAA UUCCAUUUUGAAAG AUAAGGGCUGCAUG CUGUUCCUGUCUUU CUUUCCGCCGAUUG AAAGUUUUUU | S-adenosyl methionine | Target\_lig\_314 | B.subtilis cysH | Target\_405 | 6 |
| 2137 | C1=NC(=C2C(=N1)N( C=N2)C3C(C(C(O3)C SCCC(C(=O)O)N)O)O  )N | GGUACAAUCUAAAA ACUUAUCAAGAGCG GCUGAGGGACUGGA CCUAUGAAGCCCGG CAACCUGCAUAGUU UGUAAGGUGCUACU UCCAGCAAAAUGAA UUCCAUUUUGAAAG AUAAGGGCUGCAUG CUGUUCCUGUCUUU CUUUCCGCCGAUUG AAAGUUUUUU | SAH | Target\_lig\_115 3 | B.subtilis cysH | Target\_405 | 3.0969  100130  0806 |
| 2138 | C1=NC(=C2C(=N1)N( C=N2)C3C(C(C(O3)C SCC(C(=O)O)N)O)O) N | GGUACAAUCUAAAA ACUUAUCAAGAGCG GCUGAGGGACUGGA CCUAUGAAGCCCGG CAACCUGCAUAGUU UGUAAGGUGCUACU UCCAGCAAAAUGAA UUCCAUUUUGAAAG AUAAGGGCUGCAUG CUGUUCCUGUCUUU CUUUCCGCCGAUUG AAAGUUUUUU | SAC | Target\_lig\_115 4 | B.subtilis cysH | Target\_405 | 3 |
| 2139 | C[S+](CCC(C(=O) [O-])N)CC1C(C(C(O1) N2C=NC3=C(N=CN=  C32)N)O)O | GGAGCUUAUCAAGA GAAGCGGAGGGAAC UGGCCCGGCGAAGC UCGGCAACCUGCUU AUAGAAAGCAAGGU GCUAAAUCCAGCAA AAUGGAUUCCAUUU UGAAAGAUAAGGUA AAAUAUAUUACCGA ACAGUCUUUUCGAA AUGGGAAAGAUUUU UUUUAU | S-adenosyl methionine | Target\_lig\_314 | B.anthracis cysH | Target\_406 | 8 |
| 2140 | C1=NC(=C2C(=N1)N( C=N2)C3C(C(C(O3)C | GGAGCUUAUCAAGA GAAGCGGAGGGAAC | SAH | Target\_lig\_115 3 | B.anthracis cysH | Target\_406 | 5.5228  787452 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA\_ ID** | **pKd** |
|  | SCCC(C(=O)O)N)O)O  )N | UGGCCCGGCGAAGC UCGGCAACCUGCUU AUAGAAAGCAAGGU GCUAAAUCCAGCAA AAUGGAUUCCAUUU UGAAAGAUAAGGUA AAAUAUAUUACCGA ACAGUCUUUUCGAA AUGGGAAAGAUUUU UUUUAU |  |  |  |  | 8034 |
| 2141 | C1=NC(=C2C(=N1)N( C=N2)C3C(C(C(O3)C SCC(C(=O)O)N)O)O) N | GGAGCUUAUCAAGA GAAGCGGAGGGAAC UGGCCCGGCGAAGC UCGGCAACCUGCUU AUAGAAAGCAAGGU GCUAAAUCCAGCAA AAUGGAUUCCAUUU UGAAAGAUAAGGUA AAAUAUAUUACCGA ACAGUCUUUUCGAA AUGGGAAAGAUUUU UUUUAU | SAC | Target\_lig\_115 4 | B.anthracis cysH | Target\_406 | 3 |
| 2259 | CC1(C2CC3C(C(=O)C (=C(C3(C(=O)C2=C(C 4=C1C=CC=C4O)O)O  )O)C(=O)N)N(C)C)O | GGGCCUAGAACAUA CCAGAUCGCCACCC GCGCUUUAAUCUGG AGAGGUGAAGAAUA CGACCACCUAGGCU C | tetracyclin | Target\_lig\_74 | Tetracycline riboswitch A08G mutant | Target\_412 | 8.9788  107009  3006 |
| 2260 | CC1(C2CC3C(C(=O)C (=C(C3(C(=O)C2=C(C 4=C1C=CC=C4O)O)O  )O)C(=O)N)N(C)C)O | GGGCCUAAGACAUA CCAGAUCGCCACCC GCGCUUUAAUCUGG AGAGGUGAAGAAUA CGACCACCUAGGCU C | tetracyclin | Target\_lig\_74 | Tetracycline riboswitch A09G mutant | Target\_413 | 6.7904  849854  5737 |
| 2261 | CC1(C2CC3C(C(=O)C (=C(C3(C(=O)C2=C(C 4=C1C=CC=C4O)O)O  )O)C(=O)N)N(C)C)O | GGGCCUAAAACAUU CCAGAUCGCCACCC GCGCUUUAAUCUGG AGAGGUGAAGAAUA CGACCACCUAGGCU C | tetracyclin | Target\_lig\_74 | Tetracycline riboswitch A13U mutant | Target\_414 | 6.6536  470255  4936 |
| 2262 | CC1(C2CC3C(C(=O)C (=C(C3(C(=O)C2=C(C 4=C1C=CC=C4O)O)O  )O)C(=O)N)N(C)C)O | GGGCCUAAAACAUA CCAGAUCGCCACCC GCGCUUUAAUCUGG AGAGGUGAUGAAUA CGACCACCUAGGCU C | tetracyclin | Target\_lig\_74 | Tetracycline riboswitch A50U mutant | Target\_415 | 6.7077  439286  4352 |
| 2263 | CC1(C2CC3C(C(=O)C (=C(C3(C(=O)C2=C(C 4=C1C=CC=C4O)O)O  )O)C(=O)N)N(C)C)O | GGGCCUAAAACAUA CCAGAUCGCCACCC GCGCUUUAAUCUGG AGAGGUGAAUAAUA CGACCACCUAGGCU C | tetracyclin | Target\_lig\_74 | Tetracycline riboswitch G51U mutant | Target\_416 | 8.5331  323796  4589 |
| 2264 | CC1(C2CC3C(C(=O)C (=C(C3(C(=O)C2=C(C 4=C1C=CC=C4O)O)O  )O)C(=O)N)N(C)C)O | GGGCCUAAAACAUA CCAGAUCGCCACCC GCGCUUUAAUCUGG AGAGGUGAAGAAGA CGACCACCUAGGCU C | tetracyclin | Target\_lig\_74 | Tetracycline riboswitch U54G mutant | Target\_417 | 8.5800  442515  1024 |
| 2265 | CC1(C2CC3C(C(=O)C (=C(C3(C(=O)C2=C(C 4=C1C=CC=C4O)O)O  )O)C(=O)N)N(C)C)O | GGGCCUAAAACAUA CCAGAUCGCCACCC GCGCUUUAAUCUGG AGAGGUGAAGAAUG CGACCACCUAGGCU C | tetracyclin | Target\_lig\_74 | Tetracycline riboswitch A55G mutant | Target\_418 | 8.77211  329538  633 |
| 2266 | CN(C1C(=O)C(=C(C2( C1CC1C(=C(O)c3c(C1 (C)O)c(Cl)ccc3O)C2=  O)O)O)C(=O)N)C | GGGCCUAAAACAUA CCAGAUCGCCACCC GCGCUUUAAUCUGG AGAGGUGAAGAAUA CGACCACCUAGGCU | cltc | Target\_lig\_116 4 | Tetracycline riboswitch | Target\_411 | 9.2418  453780  3261 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | C |  |  |  |  |  |
| 2267 | NC(=O)C1=C(O)C2(C (CC1=O)CC1C(=C(O)  c3c(C1(C)O)cccc3O)C 2=O)O | GGGCCUAAAACAUA CCAGAUCGCCACCC GCGCUUUAAUCUGG AGAGGUGAAGAAUA CGACCACCUAGGCU C | cmt1 | Target\_lig\_116 5 | Tetracycline riboswitch | Target\_411 | 8.7055  337738  3841 |
| 2268 | NC(=O)C1=C(O)C2(C (C(C1=O)O)CC1C(=C(  O)c3c(C1(C)O)cccc3O  )C2=O)O | GGGCCUAAAACAUA CCAGAUCGCCACCC GCGCUUUAAUCUGG AGAGGUGAAGAAUA CGACCACCUAGGCU C | cmt6 | Target\_lig\_116 6 | Tetracycline riboswitch | Target\_411 | 8.5575  202309  3555 |
| 2269 | NNC1=C2C(=O)C3(O)  C(CC2C(c2c1c(O)ccc2  ) (C)O)CC(=O)C(=C3O) C(=O)N | GGGCCUAAAACAUA CCAGAUCGCCACCC GCGCUUUAAUCUGG AGAGGUGAAGAAUA CGACCACCUAGGCU C | cmt5 | Target\_lig\_116 7 | Tetracycline riboswitch | Target\_411 | 9.0043  648054  0245 |
| 2270 | N#CC1=C(O)C2(C(C( C1=O)N(C)C)CC1C(= C(O)c3c(C1(C)O)cccc3 O)C2=O)O | GGGCCUAAAACAUA CCAGAUCGCCACCC GCGCUUUAAUCUGG AGAGGUGAAGAAUA CGACCACCUAGGCU C | cmt2 | Target\_lig\_116 8 | Tetracycline riboswitch | Target\_411 | 8.0087  739243  0751 |
| 2271 | CN(C1C(=O)C(=C(C2( C1C(O)C1C(=C(O)c3c (C1(C)O)cccc3O)C2= O)O)O)C(=O)N)C | GGGCCUAAAACAUA CCAGAUCGCCACCC GCGCUUUAAUCUGG AGAGGUGAAGAAUA CGACCACCUAGGCU C | otc | Target\_lig\_116 9 | Tetracycline riboswitch | Target\_411 | 8.7495  799976  9111 |
| 2272 | C[C@H]1[C@H] ([C@H](C[C@@H]  (O1)O[C@H]2C[C@@  ] (CC3=C2C(=C4C(=C3  O)C(=O)C5=C(C4=O) C(=CC=C5)OC)O) (C(=O)CO)O)N)O | GGGCCUAAAACAUA CCAGAUCGCCACCC GCGCUUUAAUCUGG AGAGGUGAAGAAUA CGACCACCUAGGCU C | dox | Target\_lig\_496 | Tetracycline riboswitch | Target\_411 | 6.92811  799269  388 |
| 2273 | NC(=O)C1=C(O)C2(C (CC1=O)C(O)C1C(=C(  O)c3c(C1C)cccc3O)C2  =O)O | GGGCCUAAAACAUA CCAGAUCGCCACCC GCGCUUUAAUCUGG AGAGGUGAAGAAUA CGACCACCUAGGCU C | cmt8 | Target\_lig\_117 1 | Tetracycline riboswitch | Target\_411 | 6.2620  126736  6657 |
| 2274 | C[N+]1=C2C(=C3C=C C4=C(C3=C1)OCO4)C  =CC5=CC6=C(C=C52) OCO6 | GGGCCUAAAACAUA CCAGAUCGCCACCC GCGCUUUAAUCUGG AGAGGUGAAGAAUA CGACCACCUAGGCU C | san | Target\_lig\_18 | Tetracycline riboswitch | Target\_411 | 7.6536  470255  4936 |
| 2275 | CN(C1C(=O)C(=C(C2(  C1CC1C(C)c3cccc(c3 C(=C1C2=O)O)O)O)O  )C(=O)N)C | GGGCCUAAAACAUA CCAGAUCGCCACCC GCGCUUUAAUCUGG AGAGGUGAAGAAUA CGACCACCUAGGCU C | atc | Target\_lig\_117 3 | Tetracycline riboswitch | Target\_411 | 8.4559  319556  4972 |
| 2276 | CN(C1C(=O)C(=C(C2( C1C(O)C1C(=C(O)c3c (C1(C)O)cccc3O)C2= O)O)O)C(=O)N)C | GGGCCUAAGACAUA CCAGAUCGCCACCC GCGCUUUAAUCUGG AGAGGUGAAGAAUA CGACCACCUAGGCU C | otc | Target\_lig\_116 9 | Tetracycline riboswitch A09G mutant | Target\_413 | 6.3516  399890  1907 |
| 2277 | N#CC1=C(O)C2(C(C( C1=O)N(C)C)CC1C(= C(O)c3c(C1(C)O)cccc3 O)C2=O)O | GGGCCUAAGACAUA CCAGAUCGCCACCC GCGCUUUAAUCUGG AGAGGUGAAGAAUA CGACCACCUAGGCU | cmt2 | Target\_lig\_116 8 | Tetracycline riboswitch A09G mutant | Target\_413 | 5.5783  960731  3017 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | C |  |  |  |  |  |
| 2278 | C[C@H]1[C@H] ([C@H](C[C@@H]  (O1)O[C@H]2C[C@@  ] (CC3=C2C(=C4C(=C3  O)C(=O)C5=C(C4=O) C(=CC=C5)OC)O) (C(=O)CO)O)N)O | GGGCCUAAGACAUA CCAGAUCGCCACCC GCGCUUUAAUCUGG AGAGGUGAAGAAUA CGACCACCUAGGCU C | dox | Target\_lig\_496 | Tetracycline riboswitch A09G mutant | Target\_413 | 4.7520  267336  3819 |
| 2279 | CN(C1C(=O)C(=C(C2( C1C(O)C1C(=C(O)c3c (C1(C)O)cccc3O)C2= O)O)O)C(=O)N)C | GGGCCUAAAACAUU CCAGAUCGCCACCC GCGCUUUAAUCUGG AGAGGUGAAGAAUA CGACCACCUAGGCU C | otc | Target\_lig\_116 9 | Tetracycline riboswitch A13U mutant | Target\_414 | 6.2740  883677  0495 |
| 2280 | N#CC1=C(O)C2(C(C( C1=O)N(C)C)CC1C(= C(O)c3c(C1(C)O)cccc3 O)C2=O)O | GGGCCUAAAACAUU CCAGAUCGCCACCC GCGCUUUAAUCUGG AGAGGUGAAGAAUA CGACCACCUAGGCU C | cmt2 | Target\_lig\_116 8 | Tetracycline riboswitch A13U mutant | Target\_414 | 5.7695  510786  2173 |
| 2281 | C[C@H]1[C@H] ([C@H](C[C@@H]  (O1)O[C@H]2C[C@@  ] (CC3=C2C(=C4C(=C3  O)C(=O)C5=C(C4=O) C(=CC=C5)OC)O) (C(=O)CO)O)N)O | GGGCCUAAAACAUU CCAGAUCGCCACCC GCGCUUUAAUCUGG AGAGGUGAAGAAUA CGACCACCUAGGCU C | dox | Target\_lig\_496 | Tetracycline riboswitch A13U mutant | Target\_414 | 5.6161  846340  1957 |
| 2282 | CN(C1C(=O)C(=C(C2( C1C(O)C1C(=C(O)c3c (C1(C)O)cccc3O)C2= O)O)O)C(=O)N)C | GGGCCUAAAACAUA CCAGAUCGCCACCC GCGCUUUAAUCUGG AGAGGUGAUGAAUA CGACCACCUAGGCU C | otc | Target\_lig\_116 9 | Tetracycline riboswitch A50U mutant | Target\_415 | 6.2218  487496  1636 |
| 2283 | N#CC1=C(O)C2(C(C( C1=O)N(C)C)CC1C(= C(O)c3c(C1(C)O)cccc3 O)C2=O)O | GGGCCUAAAACAUA CCAGAUCGCCACCC GCGCUUUAAUCUGG AGAGGUGAUGAAUA CGACCACCUAGGCU C | cmt2 | Target\_lig\_116 8 | Tetracycline riboswitch A50U mutant | Target\_415 | 5.5900  668766  6871 |
| 2284 | C[C@H]1[C@H] ([C@H](C[C@@H]  (O1)O[C@H]2C[C@@  ] (CC3=C2C(=C4C(=C3  O)C(=O)C5=C(C4=O) C(=CC=C5)OC)O) (C(=O)CO)O)N)O | GGGCCUAAAACAUA CCAGAUCGCCACCC GCGCUUUAAUCUGG AGAGGUGAUGAAUA CGACCACCUAGGCU C | dox | Target\_lig\_496 | Tetracycline riboswitch A50U mutant | Target\_415 | 4.9788  107009  3006 |
| 2320 | CNC1=NC=C(C=N1)C N2CCC[C@@H] (C2)C3=NC(=CC(=O) N3)C4=CC=CS4 | GGCGUGUAGGAUAU GCUUCGGCAGAAGG ACACGCC | Ribocil | Target\_lig\_663 | FMN RIBOSWITCH APTAMER | Target\_36 | 7.7958  800173  4408 |
| 2321 | CNc1ncc(cn1)CN1CC C[C@H]  (C1)c1nc(O)cc(n1)c1cc cs1 | GGCGUGUAGGAUAU GCUUCGGCAGAAGG ACACGCC | Ribocil-A | Target\_lig\_118 7 | FMN RIBOSWITCH APTAMER | Target\_36 | 5 |
| 2322 | CNC1=NC=C(C=N1)C N2CCC[C@@H] (C2)C3=NC(=CC(=O) N3)C4=CC=CS4 | GGCGUGUAGGAUAU GCUUCGGCAGAAGG ACACGCC | Ribocil-B | Target\_lig\_663 | FMN RIBOSWITCH APTAMER | Target\_36 | 8.1804  560644  5813 |
| 2323 | C1C[C@@H] (CN(C1)CC2=CN(C= N2)C3=NC=CC=N3)C 4=NC(=CC(=O)N4)C5  =CC=CS5 | GGCGUGUAGGAUAU GCUUCGGCAGAAGG ACACGCC | Ribocil-C | Target\_lig\_664 | FMN RIBOSWITCH APTAMER | Target\_36 | 9 |