Training dataset curated from [R-SIM](https://web.iitm.ac.in/bioinfo2/R_SIM/) database for the “Ribosomal RNA” 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** |
| 100 | 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 | GAGCGUCACACCUU CGGGUGAAGUCGCU C | tetracyclin | Target\_lig\_74 | A-site 16S rRNA\_E\_coli (1) | Target\_3 | 5.45593195  564972 |
| 101 | CC1CC(=O)C2(C(O1) OC3C(C(C(C(C3O2)N C)O)NC)O)O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Spectinomycin | Target\_lig\_75 | A-site 16S rRNA\_E\_coli (1) | Target\_3 | 6.58502665  202918 |
| 103 | CC1(COC(C(C1NC)O) OC2C(CC(C(C2O)OC3 C(CCC(O3)CN)N)N)N  )O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | gentamicin\_mol\_ c1a | Target\_lig\_76 | A-site 16S rRNA\_E\_coli (1) | Target\_3 | 5.76955107  862173 |
| 104 | C1C(C(C(C(C1N)OC2 C(C(C(C(O2)CN)O)O)  O)O)OC3C(C(C(C(O3) CO)O)N)O)N | GAGCGUCACACCUU CGGGUGAAGUCGCU C | kanamycin | Target\_lig\_7 | A-site 16S rRNA\_E\_coli (1) | Target\_3 | 6.90308998  699194 |
| 107 | CC1C(CC(C(O1)OC2C (C(C(C(C2O)O)O)O)O  )N)N=C(C(=O)O)N | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Kasugamycin | Target\_lig\_78 | A-site 16S rRNA\_E\_coli (1) | Target\_3 | 4.82390874  094432 |
| 108 | CNC1C(C2C(CC(C(O2  )OC3C(CC(C(C3O)O) N)N)N)OC1OC4C(C(C (C(O4)CO)N)O)O)O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | apramycin | Target\_lig\_79 | A-site 16S rRNA\_E\_coli (1) | Target\_3 | 7.09691001  300806 |
| 109 | C1C(C(C(C(C1N)OC2 C(C(C(C(O2)CN)O)O) N)O)O)N | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Neamine | Target\_lig\_80 | A-site 16S rRNA\_E\_coli (1) | Target\_3 | 6.30102999  566398 |
| 110 | C1=CC=C2C(=C1)NC(  =N2)N | GAGCGUCACACCUU CGGGUGAAGUCGCU C | 1H-1,3-  benzodiazol-2- amine | Target\_lig\_81 | A-site 16S rRNA\_E\_coli (1) | Target\_3 | 3.63827216  398241 |
| 111 | CC1=CC2=C(C=C1C) N=CN2 | GAGCGUCACACCUU CGGGUGAAGUCGCU C | 5,6-dimethyl-1H- 1,3-benzodiazole | Target\_lig\_82 | A-site 16S rRNA\_E\_coli (1) | Target\_3 | 3.09151498  112135 |
| 112 | CC1=CC(=C2C(=C1)N C(=N2)N)C | GAGCGUCACACCUU CGGGUGAAGUCGCU C | 4,6-dimethyl-1H- 1,3-benzodiazol- 2-amine | Target\_lig\_83 | A-site 16S rRNA\_E\_coli (1) | Target\_3 | 3.58502665  202918 |
| 113 | CC1=CC(=NC2=CC=C C=C12)N | GAGCGUCACACCUU CGGGUGAAGUCGCU C | 4-  methylquinolin- 2-amine | Target\_lig\_84 | A-site 16S rRNA\_E\_coli (1) | Target\_3 | 4.04575749  056068 |
| 114 | CC1=CC2=C(C=C1C) N=C(N2)N | GAGCGUCACACCUU CGGGUGAAGUCGCU C | 5,6-dimethyl-1H- 1,3-benzodiazol- 2-amine | Target\_lig\_85 | A-site 16S rRNA\_E\_coli (1) | Target\_3 | 3.65757731  917779 |
| 115 | CC1=C(C2=C(C=C1)N C(=N2)N)C | GAGCGUCACACCUU CGGGUGAAGUCGCU C | 6,7-dimethyl-1H- 1,3-benzodiazol- 2-amine | Target\_lig\_86 | A-site 16S rRNA\_E\_coli (1) | Target\_3 | 3.79588001  734407 |
| 116 | CC1=CC(=NC2=C1C= CC(=C2)NC(=O)CC3= CC=NC=C3)N(C)C | GAGCGUCACACCUU CGGGUGAAGUCGCU C | dimethylamino\_ methylquinolinyl  \_pyridinyl\_aceta mide | Target\_lig\_87 | A-site 16S rRNA\_E\_coli (1) | Target\_3 | 4.74472749  489669 |
| 117 | CN(C)C1=NC2=CC=C C=C2C(=C1)NC(=O)C C3=CC=C(C=C3)O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | dimethylamino\_q uinolinyl\_pyridin yl\_acetamide | Target\_lig\_88 | A-site 16S rRNA\_E\_coli (1) | Target\_3 | 5.04575749  056068 |
| 118 | CC1=CC2=C(C=C1)C(  =CC(=N2)N)C | GAGCGUCACACCUU CGGGUGAAGUCGCU C | N,4-  dimethylquinolin  -2-amine | Target\_lig\_89 | A-site 16S rRNA\_E\_coli (1) | Target\_3 | 4.22184874  961636 |
| 119 | CC1=C(C2=C(C=C1)C (=CC(=N2)N)C)C | GAGCGUCACACCUU CGGGUGAAGUCGCU C | N,N,4-  trimethylquinolin  -2-amine | Target\_lig\_90 | A-site 16S rRNA\_E\_coli (1) | Target\_3 | 3.76955107  862173 |
| 120 | CN(C)C1=NC2=CC=C C=C2C=C1 | GAGCGUCACACCUU CGGGUGAAGUCGCU C | N,N-  dimethylquinolin  -2-amine | Target\_lig\_91 | A-site 16S rRNA\_E\_coli (1) | Target\_3 | 3.00436480  540245 |
| 121 | CC1=C(N=CC=C1)NC CN | GAGCGUCACACCUU CGGGUGAAGUCGCU | methylpyridine\_d er\_1 | Target\_lig\_92 | A-site 16S rRNA\_E\_coli | Target\_3 | 3.22184874  961636 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | C |  |  | (1) |  |  |
| 122 | CC1=CC(=NC=C1)NC CN | GAGCGUCACACCUU CGGGUGAAGUCGCU C | methylpyridine\_d er\_2 | Target\_lig\_93 | A-site 16S rRNA\_E\_coli (1) | Target\_3 | 5.52287874  528034 |
| 123 | CC1=CC(=NC=C1)NC CCN | GAGCGUCACACCUU CGGGUGAAGUCGCU C | methylpyridine\_d er\_3 | Target\_lig\_94 | A-site 16S rRNA\_E\_coli (1) | Target\_3 | 4.69897000  433602 |
| 124 | CC1=CN=C(C=C1)NC CN | GAGCGUCACACCUU CGGGUGAAGUCGCU C | methylpyridine\_d er\_4 | Target\_lig\_95 | A-site 16S rRNA\_E\_coli (1) | Target\_3 | 4.65757731  917779 |
| 125 | C1=CC(=NC=C1[N+] (=O)[O-])NCCN | GAGCGUCACACCUU CGGGUGAAGUCGCU C | methylpyridine\_d er\_5 | Target\_lig\_96 | A-site 16S rRNA\_E\_coli (1) | Target\_3 | 2 |
| 126 | CC1=NC(=CC=C1)NC CN | GAGCGUCACACCUU CGGGUGAAGUCGCU C | methylpyridine\_d er\_6 | Target\_lig\_97 | A-site 16S rRNA\_E\_coli (1) | Target\_3 | 3.97881070  093006 |
| 127 | C1=CC=NC(=C1)NCC N | GAGCGUCACACCUU CGGGUGAAGUCGCU C | methylpyridine\_d er\_7 | Target\_lig\_98 | A-site 16S rRNA\_E\_coli (1) | Target\_3 | 4.16749108  729376 |
| 128 | CC1=CC(=NC2=C1C= CC(=C2)N)N(C)C | GAGCGUCACACCUU CGGGUGAAGUCGCU C | 2-N,2-N,4-  trimethylquinolin e-2,7-diamine | Target\_lig\_99 | A-site 16S rRNA\_E\_coli (1) | Target\_3 | 4.45593195  564972 |
| 129 | CN(C)C1=NC2=CC=C C=C2C(=C1)N | GAGCGUCACACCUU CGGGUGAAGUCGCU C | 2-N,2-N-  dimethylquinolin e-2,4-diamine | Target\_lig\_10 0 | A-site 16S rRNA\_E\_coli (1) | Target\_3 | 4.22184874  961636 |
| 130 | CNC1=NC2=CC=CC= C2C=C1 | GAGCGUCACACCUU CGGGUGAAGUCGCU C | N-  methylquinolin- 2-amine | Target\_lig\_10 1 | A-site 16S rRNA\_E\_coli (1) | Target\_3 | 3.30980391  997149 |
| 132 | C1CCN(CC1)CN2CCN (C2=S)CN3CCCCC3 | GAGCGUCACACCUU CGGGUGAAGUCGCU C | 1,3-bis(piperidin- 1-  ylmethyl)imidazo lidine-2-thione | Target\_lig\_10 3 | A-site 16S rRNA\_E\_coli (1) | Target\_3 | 3.96257350  205938 |
| 133 | C1CN(CCN1CC2=CN C3=CC=CC=C32)CC4  =CNC5=CC=CC=C54 | GAGCGUCACACCUU CGGGUGAAGUCGCU C | 1,4-bis((1H-  indol-3- yl)methyl)pipera zine | Target\_lig\_10 4 | A-site 16S rRNA\_E\_coli (1) | Target\_3 | 3.66554624  884907 |
| 134 | CC1(CC(CC(N1) (C)C)NCC2=CC=CC= C2O)C | GAGCGUCACACCUU CGGGUGAAGUCGCU C | 2-((2,2,6,6-  tetramethylpiperi din-4- ylamino)methyl) phenol | Target\_lig\_10 5 | A-site 16S rRNA\_E\_coli (1) | Target\_3 | 3.68613277  963085 |
| 135 | OCC1=C=C=C(c2nc(C 3=C=NC4=C(C=C=C= C4)C3)c(C3=C=C=C= C=C3)[nH]2)C=C1O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | 2-  (hydroxymethyl)- 5-(5-phenyl-4-  (quinolin-3-yl)- 1H-imidazol-2- yl)phenol | Target\_lig\_10 6 | A-site 16S rRNA\_E\_coli (1) | Target\_3 | 3.95467702  121334 |
| 136 | CC1=CC=CC=C1OCC NC2=C(C=CC(=C2)N3 CCNCC3)[N+](=O)  [O-] | GAGCGUCACACCUU CGGGUGAAGUCGCU C | 2-nitro-5- (piperazin-1-yl)- N-(2-(o-  tolyloxy)ethyl)an iline | Target\_lig\_10 7 | A-site 16S rRNA\_E\_coli (1) | Target\_3 | 3.69036983  25741 |
| 137 | CCC1=CC2=C(C(=C1 O)CN3CCOCC3)OC= C(C2=O)C4=NC5=CC  =CC=C5N4 | GAGCGUCACACCUU CGGGUGAAGUCGCU C | 3-(1H-  benzo[d]imidazol  -2-yl)-6-ethyl-7- hydroxy-8- (morpholinometh yl)-4H-chromen- 4-one | Target\_lig\_10 8 | A-site 16S rRNA\_E\_coli (1) | Target\_3 | 3.60032627  851896 |
| 138 | CN1CCN(CC1)CCCN2 C=NC3=C(C2=O)NC4  =CC=CC=C43 | GAGCGUCACACCUU CGGGUGAAGUCGCU C | 3-(3-(4-  methylpiperazin- 1-yl)propyl)-3H- pyrimido[5,4- b]indol-4(5H)- one | Target\_lig\_10 9 | A-site 16S rRNA\_E\_coli (1) | Target\_3 | 3.37059040  089728 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
| 139 | CC1=C(C(=O)C2=CC= CC=C2N1)CN3CCCC CC3 | GAGCGUCACACCUU CGGGUGAAGUCGCU C | 3-(azepan-1- ylmethyl)-2- methylquinolin- 4-ol | Target\_lig\_110 | A-site 16S rRNA\_E\_coli (1) | Target\_3 | 3.39685562  737982 |
| 140 | CN1C2=C(C(=O)NC1= O)N(C=N2)CCN3CCC CC3 | GAGCGUCACACCUU CGGGUGAAGUCGCU C | 3-methyl-7-(2- (piperidin-1- yl)ethyl)-1H- purine- 2,6(3H,7H)-  dione | Target\_lig\_111 | A-site 16S rRNA\_E\_coli (1) | Target\_3 | 3.67366413  907125 |
| 141 | C1CCCN(CC1)CC2=C (N(N=N2)C3=NON=C 3N)CN4CCCCCC4 | GAGCGUCACACCUU CGGGUGAAGUCGCU C | 4-(4,5-  bis(azepan-1- ylmethyl)-1H- 1,2,3-triazol-1-  yl)-1,2,5-  oxadiazol-3- amine | Target\_lig\_112 | A-site 16S rRNA\_E\_coli (1) | Target\_3 | 3.53610701  101409 |
| 142 | C1CCN(C1)CCNC2=N N=C(C3=CC=CC=C32  )C4=CC=C(C=C4)Cl | GAGCGUCACACCUU CGGGUGAAGUCGCU C | 4-(4-  chlorophenyl)-N- (2-(pyrrolidin-1- yl)ethyl)phthalazi n-1-amine | Target\_lig\_113 | A-site 16S rRNA\_E\_coli (1) | Target\_3 | 3.83564714  421556 |
| 143 | CC1=CC=C(C=C1)C2  =C(C(=CC(=N2)CN3C CCCC3)CN4CCCCC4) O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | 4,6-bis(piperidin- 1-ylmethyl)-2-p- tolylpyridin-3-ol | Target\_lig\_114 | A-site 16S rRNA\_E\_coli (1) | Target\_3 | 3.84466396  253494 |
| 144 | C1CCN(CC1)CCCNC(  =O)C2=C(C3=CC=CC  =C3NC2=O)O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | 4-hydroxy-2- oxo-N-(3- (piperidin-1- yl)propyl)-1,2- dihydroquinoline  -3-carboxamide | Target\_lig\_115 | A-site 16S rRNA\_E\_coli (1) | Target\_3 | 3.61618463  401957 |
| 145 | CC1=CC2=C(C=C1)O C=C(C2=O)CN3CCCN (CC3)C | GAGCGUCACACCUU CGGGUGAAGUCGCU C | 6-methyl-3-((4- methyl-1,4- diazepan-1- yl)methyl)-4H- chromen-4-one | Target\_lig\_116 | A-site 16S rRNA\_E\_coli (1) | Target\_3 | 3.73518217  699046 |
| 146 | N1(CCCCCCC1)CCN1 C=NC=2N(C(NC(C12)  =O)=O)C | GAGCGUCACACCUU CGGGUGAAGUCGCU C | 7-(2-(azocan-1- yl)ethyl)-3- methyl-1H- purine- 2,6(3H,7H)-  dione | Target\_lig\_117 | A-site 16S rRNA\_E\_coli (1) | Target\_3 | 3.54821356  447571 |
| 147 | C(C1=CC=CC=C1)N1 C(=NC=2N(C(NC(C12  )=O)=O)C)N1CCNCC1 | GAGCGUCACACCUU CGGGUGAAGUCGCU C | 7-benzyl-3- methyl-8- (piperazin-1-yl)- 1H-purine- 2,6(3H,7H)-  dione | Target\_lig\_111 1 | A-site 16S rRNA\_E\_coli (1) | Target\_3 | 3.60906489  289662 |
| 148 | C1CN(CCN1)CCN2C= NC3=C(C2=O)NC4=C 3C=C(C=C4)Br | GAGCGUCACACCUU CGGGUGAAGUCGCU C | 8-bromo-3-(2- (piperazin-1- yl)ethyl)-3H- pyrimido[5,4- b]indol-4(5H)- one | Target\_lig\_118 | A-site 16S rRNA\_E\_coli (1) | Target\_3 | 3.57839607  313017 |
| 149 | CC1=CC2=C(C=C1)N C3=C2N=CN(C3=O)C CN4CCCC4 | GAGCGUCACACCUU CGGGUGAAGUCGCU C | 8-methyl-3-(2- (pyrrolidin-1- yl)ethyl)-3H- pyrimido[5,4- b]indol-4(5H)- one | Target\_lig\_119 | A-site 16S rRNA\_E\_coli (1) | Target\_3 | 3.46724562  10075 |
| 150 | N=C(N)CCCOC1=C=C  =C=C=C1C1=C=C=C= C=C1 | GAGCGUCACACCUU CGGGUGAAGUCGCU C | biphenyl\_derivati ve | Target\_lig\_12 0 | A-site 16S rRNA\_E\_coli (1) | Target\_3 | 4.27572413  039921 |
| 151 | C1CN(CCC1C(=O)NC CN2CCOCC2)CC3=C C=CC4=CC=CC=C43 | GAGCGUCACACCUU CGGGUGAAGUCGCU C | N-(2-  morpholinoethyl)  -1-(naphthalen-1- ylmethyl)piperidi | Target\_lig\_12 1 | A-site 16S rRNA\_E\_coli (1) | Target\_3 | 3.63264407  897398 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  |  | ne-4- carboxamide |  |  |  |  |
| 152 | CCN1CCN(CC1)CCC(  =O)NC2=CC(=C(C=C2  )Br)C | GAGCGUCACACCUU CGGGUGAAGUCGCU C | N-(4-bromo-3- methylphenyl)-3- (4-  ethylpiperazin-1- yl)propanamide | Target\_lig\_12 2 | A-site 16S rRNA\_E\_coli (1) | Target\_3 | 3.37778597  70337 |
| 153 | COC=1C=C(C2=CC(= CC=C2C1)OC)NCCCC (C)N | GAGCGUCACACCUU CGGGUGAAGUCGCU C | N1-(3,7-  dimethoxynaphth alen-1- yl)pentane-1,4- diamine | Target\_lig\_12 3 | A-site 16S rRNA\_E\_coli (1) | Target\_3 | 3.68613277  963085 |
| 154 | N=C(N)SCc1nc2C=C= C=Cc2n1CCC1=C=C= C=C=C1 | GAGCGUCACACCUU CGGGUGAAGUCGCU C | benzodiazolyl\_m ethyl\_sulfanylme thanimidamide | Target\_lig\_12 4 | A-site 16S rRNA\_E\_coli (1) | Target\_3 | 3.75696195  131371 |
| 155 | COC1=CC=CC=C1C2  =COC3=C(C2=O)C=C C(=C3CN4CCCCC4)O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | 7-hydroxy-3-(2- methoxyphenyl)- 8-(piperidin-1- ylmethyl)-4H- chromen-4-one | Target\_lig\_12 5 | A-site 16S rRNA\_E\_coli (1) | Target\_3 | 3.40340290  437354 |
| 156 | CC(=O)C1=CCC2C1(C C=C3C2CCC4=CC(=O  )C=CC43C)C | GAGCGUCACACCUU CGGGUGAAGUCGCU C | tetraene\_mol | Target\_lig\_12 6 | A-site 16S rRNA\_E\_coli (1) | Target\_3 | 4.45593195  564972 |
| 157 | O=C1NC(=O)N(C2=C  =C=C(Br)C=C2)C(=O)  /C/1=C/ NCCN1CCNCC1 | GAGCGUCACACCUU CGGGUGAAGUCGCU C | 5E1bromophenyl 52piperazin1 | Target\_lig\_12 7 | A-site 16S rRNA\_E\_coli (1) | Target\_3 | 3.86327943  284359 |
| 158 | CN1CCCN(CC1)CC2= COC3=C(C2=O)C=C( C=C3)Cl | GAGCGUCACACCUU CGGGUGAAGUCGCU C | 6-chloro-3-((4- methyl-1,4- diazepan-1- yl)methyl)-4H- chromen-4-one | Target\_lig\_12 8 | A-site 16S rRNA\_E\_coli (1) | Target\_3 | 3.80687540  164554 |
| 159 | O=C(NCCN1CCCCC1) c1c(O)c2C=C=C=Cc2[ nH]c1=O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | dihydroquinoline  -3-  carboxamide\_der ivative | Target\_lig\_12 9 | A-site 16S rRNA\_E\_coli (1) | Target\_3 | 3.65364702  554936 |
| 160 | C1CCN(CC1)CCCNC C2C3=CC=CC=C3CC O2 | GAGCGUCACACCUU CGGGUGAAGUCGCU C | N-(isochroman- 1-ylmethyl)-3- (piperidin-1- yl)propan-1- amine | Target\_lig\_13 0 | A-site 16S rRNA\_E\_coli (1) | Target\_3 | 4.74472749  489669 |
| 161 | CC1=CC=C(C=C1)C(= O)N2CCN(CC2)CCNC (=O)C(=O)NC(C)C | GAGCGUCACACCUU CGGGUGAAGUCGCU C | N1-isopropyl- N2-(2-(4-(4-  methylbenzoyl)pi perazin-1- yl)ethyl)oxalami de | Target\_lig\_13 1 | A-site 16S rRNA\_E\_coli (1) | Target\_3 | 3.51144928  349956 |
| 162 | C1CN(CCC1C(=O)NC CN2CCOCC2)CC3=C C=C(C=C3)Cl | GAGCGUCACACCUU CGGGUGAAGUCGCU C | 1-(4-  chlorobenzyl)-N- (2-  morpholinoethyl) piperidine-4- carboxamide | Target\_lig\_13 2 | A-site 16S rRNA\_E\_coli (1) | Target\_3 | 3.60205999  132796 |
| 163 | CN1CCCN(CC1)CC2= C(C=C(C=C2)OC)OC | GAGCGUCACACCUU CGGGUGAAGUCGCU C | 1-(2,4-  dimethoxybenzyl  )-4-methyl-1,4- diazepane | Target\_lig\_13 3 | A-site 16S rRNA\_E\_coli (1) | Target\_3 | 4.50863830  616573 |
| 164 | Cn1c2nc(N/N=C\3/ C4=C(C=C=C=C4)NC 3=O)n(CC3=C=C=C(C l)C=C3)c2c(=O) [nH]c1=O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | DIONE\_DERIV ATIVE | Target\_lig\_13 4 | A-site 16S rRNA\_E\_coli (1) | Target\_3 | 4.30102999  566398 |
| 165 | OC1C(C(NC=2CCCCC 12)=O)C(=O)NCCCN1 CCCCC1 | GAGCGUCACACCUU CGGGUGAAGUCGCU C | 4-hydroxy-2- oxo-N-(3- (piperidin-1- yl)propyl)- | Target\_lig\_13 5 | A-site 16S rRNA\_E\_coli (1) | Target\_3 | 4.76955107  862173 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  |  | 1,2,3,4,5,6,7,8-  octahydroquinoli ne-3- carboxamide |  |  |  |  |
| 166 | NC[C@H]1O[C@H] (O[C@H]2[C@H]  (CO)O[C@H]  (O[C@H]3[C@H]  ([C@H](N)C[C@H]  ([C@H]3O[C@H]3O[C  @H](CO)[C@@H](O) [C@H](O)  [C@@H]3N)N)O)  [C@H]2O)[C@@H]  (N)[C@H](O) [C@@H]1O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | pyran-3,4- diol\_derivative | Target\_lig\_13 6 | A-site 16S rRNA\_E\_coli (1) | Target\_3 | 4.91009488  85606 |
| 167 | C1C(C(C(C(C1N)OC2 C(C(C(C(O2)CN)O)O)   1. OC3C(C(C(O3)CO)   OC4C(C(C(C(O4)CN)   1. O)N)O)O)N | GCACCGGCUAACUC CGUGCCAGCAGCGC GGUAAUACGGAGG GUGC | Neomycin | Target\_lig\_4 | 16S  rRNA\_neom ycin | Target\_96 | 7.22184874  961636 |
| 196 | C1C(C(C(C(C1N)OC2 C(C(C(C(O2)CO)O)O)   1. OC3C(C(C(O3)CO)   OC4C(C(C(C(O4)CN)   1. O)N)O)O)N | AAAUUGAAGAGUU UGAUCAUGGCUCAG AUUGAACGCUGGCG GCAGGCCUAACACA UGCAAGUCGAACGG UAACAGGAAGAAG CUUGCUUCUUUGCU GACGAGUGGCGGAC GGGUGAGUAAUGU CUGGGAAACUGCCU GAUGGAGGGGGAU AACUACUGGAAACG GUAGCUAAUACCGC AUAACGUCGCAAGA CCAAAGAGGGGGAC CUUCGGGCCUCUUG CCAUCGGAUGUGCC CAGAUGGGAUUAG CUAGUAGGUGGGG UAACGGCUCACCUA GGCGACGAUCCCUA GCUGGUCUGAGAG GAUGACCAGCCACA CUGGAACUGAGACA CGGUCCAGACUCCU ACGGGAGGCAGCAG UGGGGAAUAUUGC ACAAUGGGCGCAAG CCUGAUGCAGCCAU GCCGCGUGUAUGAA GAAGGCCUUCGGGU UGUAAAGUACUUU CAGCGGGGAGGAA GGGAGUAAAGUUA AUACCUUUGCUCAU UGACGUUACCCGCA GAAGAAGCACCGGC UAACUCCGUGCCAG CAGCCGCGGUAAUA CGGAGGGUGCAAGC GUUAAUCGGAAUU ACUGGGCGUAAAGC GCACGCAGGCGGUU UGUUAAGUCAGAU GUGAAAUCCCCGGG CUCAACCUGGGAAC UGCAUCUGAUACUG GCAAGCUUGAGUCU CGUAGAGGGGGGU AGAAUUCCAGGUG UAGCGGUGAAAUG CGUAGAGAUCUGG | Paromomycin\_m ol\_mol | Target\_lig\_111 6 | decoding region 16SrRNA | Target\_97 | 5.73282827  159699 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | AGGAAUACCGGUG GCGAAGGCGGCCCC CUGGACGAAGACUG ACGCUCAGGUGCGA AAGCGUGGGGAGC AAACAGGAUUAGA UACCCUGGUAGUCC ACGCCGUAAACGAU GUCGACUUGGAGG UUGUGCCCUUGAGG CGUGGCUUCCGGAG CUAACGCGUUAAGU CGACCGCCUGGGGA GUACGGCCGCAAGG UUAAAACUCAAAU GAAUUGACGGGGG CCCGCACAAGCGGU GGAGCAUGUGGUU UAAUUCGAUGCAAC GCGAAGAACCUUAC CUGGUCUUGACAUC CACGGAAGUUUUCA GAGAUGAGAAUGU GCCUUCGGGAACCG UGAGACAGGUGCU GCAUGGCUGUCGUC AGCUCGUGUUGUG AAAUGUUGGGUUA AGUCCCGCAACGAG CGCAACCCUUAUCC UUUGUUGCCAGCGG UCCGGCCGGGAACU CAAAGGAGACUGCC AGUGAUAAACUGG AGGAAGGUGGGGA UGACGUCAAGUCAU CAUGGCCCUUACGA CCAGGGCUACACAC GUGCUACAAUGGCG CAUACAAAGAGAA GCGACCUCGCGAGA GCAAGCGGACCUCA UAAAGUGCGUCGU AGUCCGGAUUGGA GUCUGCAACUCGAC UCCAUGAAGUCGGA AUCGCUAGUAAUCG UGGAUCAGAAUGCC ACGGUGAAUACGU UCCCGGGCCUUGUA CACACCGCCCGUCA CACCAUGGGAGUGG GUUGCAAAAGAAG UAGGUAGCUUAACC UUCGGGAGGGCGCU UACCACUUUGUGAU UCAUGACUGGGGU GAAGUCGUAACAA GGUAACCGUAGGG GAACCUGCGGUUGG AUCACCUCCUUA |  |  |  |  |  |
| 197 | [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)CNc1c2ccccc2nc2 c1cccc2)O)N)O | AAAUUGAAGAGUU UGAUCAUGGCUCAG AUUGAACGCUGGCG GCAGGCCUAACACA UGCAAGUCGAACGG UAACAGGAAGAAG CUUGCUUCUUUGCU GACGAGUGGCGGAC GGGUGAGUAAUGU CUGGGAAACUGCCU GAUGGAGGGGGAU AACUACUGGAAACG GUAGCUAAUACCGC AUAACGUCGCAAGA | Tobramycin | Target\_lig\_54 0 | decoding region 16SrRNA | Target\_97 | 5.77211329  538633 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | CCAAAGAGGGGGAC CUUCGGGCCUCUUG CCAUCGGAUGUGCC CAGAUGGGAUUAG CUAGUAGGUGGGG UAACGGCUCACCUA GGCGACGAUCCCUA GCUGGUCUGAGAG GAUGACCAGCCACA CUGGAACUGAGACA CGGUCCAGACUCCU ACGGGAGGCAGCAG UGGGGAAUAUUGC ACAAUGGGCGCAAG CCUGAUGCAGCCAU GCCGCGUGUAUGAA GAAGGCCUUCGGGU UGUAAAGUACUUU CAGCGGGGAGGAA GGGAGUAAAGUUA AUACCUUUGCUCAU UGACGUUACCCGCA GAAGAAGCACCGGC UAACUCCGUGCCAG CAGCCGCGGUAAUA CGGAGGGUGCAAGC GUUAAUCGGAAUU ACUGGGCGUAAAGC GCACGCAGGCGGUU UGUUAAGUCAGAU GUGAAAUCCCCGGG CUCAACCUGGGAAC UGCAUCUGAUACUG GCAAGCUUGAGUCU CGUAGAGGGGGGU AGAAUUCCAGGUG UAGCGGUGAAAUG CGUAGAGAUCUGG AGGAAUACCGGUG GCGAAGGCGGCCCC CUGGACGAAGACUG ACGCUCAGGUGCGA AAGCGUGGGGAGC AAACAGGAUUAGA UACCCUGGUAGUCC ACGCCGUAAACGAU GUCGACUUGGAGG UUGUGCCCUUGAGG CGUGGCUUCCGGAG CUAACGCGUUAAGU CGACCGCCUGGGGA GUACGGCCGCAAGG UUAAAACUCAAAU GAAUUGACGGGGG CCCGCACAAGCGGU GGAGCAUGUGGUU UAAUUCGAUGCAAC GCGAAGAACCUUAC CUGGUCUUGACAUC CACGGAAGUUUUCA GAGAUGAGAAUGU GCCUUCGGGAACCG UGAGACAGGUGCU GCAUGGCUGUCGUC AGCUCGUGUUGUG AAAUGUUGGGUUA AGUCCCGCAACGAG CGCAACCCUUAUCC UUUGUUGCCAGCGG UCCGGCCGGGAACU CAAAGGAGACUGCC AGUGAUAAACUGG AGGAAGGUGGGGA UGACGUCAAGUCAU CAUGGCCCUUACGA |  |  |  |  |  |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | CCAGGGCUACACAC GUGCUACAAUGGCG CAUACAAAGAGAA GCGACCUCGCGAGA GCAAGCGGACCUCA UAAAGUGCGUCGU AGUCCGGAUUGGA GUCUGCAACUCGAC UCCAUGAAGUCGGA AUCGCUAGUAAUCG UGGAUCAGAAUGCC ACGGUGAAUACGU UCCCGGGCCUUGUA CACACCGCCCGUCA CACCAUGGGAGUGG GUUGCAAAAGAAG UAGGUAGCUUAACC UUCGGGAGGGCGCU UACCACUUUGUGAU UCAUGACUGGGGU GAAGUCGUAACAA GGUAACCGUAGGG GAACCUGCGGUUGG AUCACCUCCUUA |  |  |  |  |  |
| 198 | C1C(C(C(C(C1N)OC2 C(C(C(C(O2)CO)O)N)  O)O)OC3C(C(C(C(O3) CN)O)O)N)N | AAAUUGAAGAGUU UGAUCAUGGCUCAG AUUGAACGCUGGCG GCAGGCCUAACACA UGCAAGUCGAACGG UAACAGGAAGAAG CUUGCUUCUUUGCU GACGAGUGGCGGAC GGGUGAGUAAUGU CUGGGAAACUGCCU GAUGGAGGGGGAU AACUACUGGAAACG GUAGCUAAUACCGC AUAACGUCGCAAGA CCAAAGAGGGGGAC CUUCGGGCCUCUUG CCAUCGGAUGUGCC CAGAUGGGAUUAG CUAGUAGGUGGGG UAACGGCUCACCUA GGCGACGAUCCCUA GCUGGUCUGAGAG GAUGACCAGCCACA CUGGAACUGAGACA CGGUCCAGACUCCU ACGGGAGGCAGCAG UGGGGAAUAUUGC ACAAUGGGCGCAAG CCUGAUGCAGCCAU GCCGCGUGUAUGAA GAAGGCCUUCGGGU UGUAAAGUACUUU CAGCGGGGAGGAA GGGAGUAAAGUUA AUACCUUUGCUCAU UGACGUUACCCGCA GAAGAAGCACCGGC UAACUCCGUGCCAG CAGCCGCGGUAAUA CGGAGGGUGCAAGC GUUAAUCGGAAUU ACUGGGCGUAAAGC GCACGCAGGCGGUU UGUUAAGUCAGAU GUGAAAUCCCCGGG CUCAACCUGGGAAC UGCAUCUGAUACUG GCAAGCUUGAGUCU CGUAGAGGGGGGU AGAAUUCCAGGUG UAGCGGUGAAAUG | KANAMYCIN B | Target\_lig\_8 | decoding region 16SrRNA | Target\_97 | 5.66958622  665081 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | CGUAGAGAUCUGG AGGAAUACCGGUG GCGAAGGCGGCCCC CUGGACGAAGACUG ACGCUCAGGUGCGA AAGCGUGGGGAGC AAACAGGAUUAGA UACCCUGGUAGUCC ACGCCGUAAACGAU GUCGACUUGGAGG UUGUGCCCUUGAGG CGUGGCUUCCGGAG CUAACGCGUUAAGU CGACCGCCUGGGGA GUACGGCCGCAAGG UUAAAACUCAAAU GAAUUGACGGGGG CCCGCACAAGCGGU GGAGCAUGUGGUU UAAUUCGAUGCAAC GCGAAGAACCUUAC CUGGUCUUGACAUC CACGGAAGUUUUCA GAGAUGAGAAUGU GCCUUCGGGAACCG UGAGACAGGUGCU GCAUGGCUGUCGUC AGCUCGUGUUGUG AAAUGUUGGGUUA AGUCCCGCAACGAG CGCAACCCUUAUCC UUUGUUGCCAGCGG UCCGGCCGGGAACU CAAAGGAGACUGCC AGUGAUAAACUGG AGGAAGGUGGGGA UGACGUCAAGUCAU CAUGGCCCUUACGA CCAGGGCUACACAC GUGCUACAAUGGCG CAUACAAAGAGAA GCGACCUCGCGAGA GCAAGCGGACCUCA UAAAGUGCGUCGU AGUCCGGAUUGGA GUCUGCAACUCGAC UCCAUGAAGUCGGA AUCGCUAGUAAUCG UGGAUCAGAAUGCC ACGGUGAAUACGU UCCCGGGCCUUGUA CACACCGCCCGUCA CACCAUGGGAGUGG GUUGCAAAAGAAG UAGGUAGCUUAACC UUCGGGAGGGCGCU UACCACUUUGUGAU UCAUGACUGGGGU GAAGUCGUAACAA GGUAACCGUAGGG GAACCUGCGGUUGG AUCACCUCCUUA |  |  |  |  |  |
| 199 | C1C(C(C(C(C1N)OC2 C(C(C(C(O2)CN)O)O)   1. OC3C(C(C(O3)CO)   OC4C(C(C(C(O4)CN)   1. O)N)O)O)N | AAAUUGAAGAGUU UGAUCAUGGCUCAG AUUGAACGCUGGCG GCAGGCCUAACACA UGCAAGUCGAACGG UAACAGGAAGAAG CUUGCUUCUUUGCU GACGAGUGGCGGAC GGGUGAGUAAUGU CUGGGAAACUGCCU GAUGGAGGGGGAU AACUACUGGAAACG GUAGCUAAUACCGC | Neomycin\_B | Target\_lig\_12 46 | decoding region 16SrRNA | Target\_97 | 6.87942606  879415 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | AUAACGUCGCAAGA CCAAAGAGGGGGAC CUUCGGGCCUCUUG CCAUCGGAUGUGCC CAGAUGGGAUUAG CUAGUAGGUGGGG UAACGGCUCACCUA GGCGACGAUCCCUA GCUGGUCUGAGAG GAUGACCAGCCACA CUGGAACUGAGACA CGGUCCAGACUCCU ACGGGAGGCAGCAG UGGGGAAUAUUGC ACAAUGGGCGCAAG CCUGAUGCAGCCAU GCCGCGUGUAUGAA GAAGGCCUUCGGGU UGUAAAGUACUUU CAGCGGGGAGGAA GGGAGUAAAGUUA AUACCUUUGCUCAU UGACGUUACCCGCA GAAGAAGCACCGGC UAACUCCGUGCCAG CAGCCGCGGUAAUA CGGAGGGUGCAAGC GUUAAUCGGAAUU ACUGGGCGUAAAGC GCACGCAGGCGGUU UGUUAAGUCAGAU GUGAAAUCCCCGGG CUCAACCUGGGAAC UGCAUCUGAUACUG GCAAGCUUGAGUCU CGUAGAGGGGGGU AGAAUUCCAGGUG UAGCGGUGAAAUG CGUAGAGAUCUGG AGGAAUACCGGUG GCGAAGGCGGCCCC CUGGACGAAGACUG ACGCUCAGGUGCGA AAGCGUGGGGAGC AAACAGGAUUAGA UACCCUGGUAGUCC ACGCCGUAAACGAU GUCGACUUGGAGG UUGUGCCCUUGAGG CGUGGCUUCCGGAG CUAACGCGUUAAGU CGACCGCCUGGGGA GUACGGCCGCAAGG UUAAAACUCAAAU GAAUUGACGGGGG CCCGCACAAGCGGU GGAGCAUGUGGUU UAAUUCGAUGCAAC GCGAAGAACCUUAC CUGGUCUUGACAUC CACGGAAGUUUUCA GAGAUGAGAAUGU GCCUUCGGGAACCG UGAGACAGGUGCU GCAUGGCUGUCGUC AGCUCGUGUUGUG AAAUGUUGGGUUA AGUCCCGCAACGAG CGCAACCCUUAUCC UUUGUUGCCAGCGG UCCGGCCGGGAACU CAAAGGAGACUGCC AGUGAUAAACUGG AGGAAGGUGGGGA UGACGUCAAGUCAU |  |  |  |  |  |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | CAUGGCCCUUACGA CCAGGGCUACACAC GUGCUACAAUGGCG CAUACAAAGAGAA GCGACCUCGCGAGA GCAAGCGGACCUCA UAAAGUGCGUCGU AGUCCGGAUUGGA GUCUGCAACUCGAC UCCAUGAAGUCGGA AUCGCUAGUAAUCG UGGAUCAGAAUGCC ACGGUGAAUACGU UCCCGGGCCUUGUA CACACCGCCCGUCA CACCAUGGGAGUGG GUUGCAAAAGAAG UAGGUAGCUUAACC UUCGGGAGGGCGCU UACCACUUUGUGAU UCAUGACUGGGGU GAAGUCGUAACAA GGUAACCGUAGGG GAACCUGCGGUUGG AUCACCUCCUUA |  |  |  |  |  |
| 200 | CC1(COC(C(C1NC)O) OC2C(CC(C(C2O)OC3 C(CCC(O3)CN)N)N)N  )O | AAAUUGAAGAGUU UGAUCAUGGCUCAG AUUGAACGCUGGCG GCAGGCCUAACACA UGCAAGUCGAACGG UAACAGGAAGAAG CUUGCUUCUUUGCU GACGAGUGGCGGAC GGGUGAGUAAUGU CUGGGAAACUGCCU GAUGGAGGGGGAU AACUACUGGAAACG GUAGCUAAUACCGC AUAACGUCGCAAGA CCAAAGAGGGGGAC CUUCGGGCCUCUUG CCAUCGGAUGUGCC CAGAUGGGAUUAG CUAGUAGGUGGGG UAACGGCUCACCUA GGCGACGAUCCCUA GCUGGUCUGAGAG GAUGACCAGCCACA CUGGAACUGAGACA CGGUCCAGACUCCU ACGGGAGGCAGCAG UGGGGAAUAUUGC ACAAUGGGCGCAAG CCUGAUGCAGCCAU GCCGCGUGUAUGAA GAAGGCCUUCGGGU UGUAAAGUACUUU CAGCGGGGAGGAA GGGAGUAAAGUUA AUACCUUUGCUCAU UGACGUUACCCGCA GAAGAAGCACCGGC UAACUCCGUGCCAG CAGCCGCGGUAAUA CGGAGGGUGCAAGC GUUAAUCGGAAUU ACUGGGCGUAAAGC GCACGCAGGCGGUU UGUUAAGUCAGAU GUGAAAUCCCCGGG CUCAACCUGGGAAC UGCAUCUGAUACUG GCAAGCUUGAGUCU CGUAGAGGGGGGU AGAAUUCCAGGUG | gentamicin\_mol\_ c | Target\_lig\_76 | decoding region 16SrRNA | Target\_97 | 5.73518217  699046 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | UAGCGGUGAAAUG CGUAGAGAUCUGG AGGAAUACCGGUG GCGAAGGCGGCCCC CUGGACGAAGACUG ACGCUCAGGUGCGA AAGCGUGGGGAGC AAACAGGAUUAGA UACCCUGGUAGUCC ACGCCGUAAACGAU GUCGACUUGGAGG UUGUGCCCUUGAGG CGUGGCUUCCGGAG CUAACGCGUUAAGU CGACCGCCUGGGGA GUACGGCCGCAAGG UUAAAACUCAAAU GAAUUGACGGGGG CCCGCACAAGCGGU GGAGCAUGUGGUU UAAUUCGAUGCAAC GCGAAGAACCUUAC CUGGUCUUGACAUC CACGGAAGUUUUCA GAGAUGAGAAUGU GCCUUCGGGAACCG UGAGACAGGUGCU GCAUGGCUGUCGUC AGCUCGUGUUGUG AAAUGUUGGGUUA AGUCCCGCAACGAG CGCAACCCUUAUCC UUUGUUGCCAGCGG UCCGGCCGGGAACU CAAAGGAGACUGCC AGUGAUAAACUGG AGGAAGGUGGGGA UGACGUCAAGUCAU CAUGGCCCUUACGA CCAGGGCUACACAC GUGCUACAAUGGCG CAUACAAAGAGAA GCGACCUCGCGAGA GCAAGCGGACCUCA UAAAGUGCGUCGU AGUCCGGAUUGGA GUCUGCAACUCGAC UCCAUGAAGUCGGA AUCGCUAGUAAUCG UGGAUCAGAAUGCC ACGGUGAAUACGU UCCCGGGCCUUGUA CACACCGCCCGUCA CACCAUGGGAGUGG GUUGCAAAAGAAG UAGGUAGCUUAACC UUCGGGAGGGCGCU UACCACUUUGUGAU UCAUGACUGGGGU GAAGUCGUAACAA GGUAACCGUAGGG GAACCUGCGGUUGG AUCACCUCCUUA |  |  |  |  |  |
| 201 | CC(C)CC(C(=O)NC(C C1=CNC2=CC=CC=C 21)C(=O)N3CCCC3C(  =O)O)NC(=O)C(CCC(  =O)N)NC(=O)C4CCC N4C(=O)C(CCCCN)N | AAAUUGAAGAGUU UGAUCAUGGCUCAG AUUGAACGCUGGCG GCAGGCCUAACACA UGCAAGUCGAACGG UAACAGGAAGAAG CUUGCUUCUUUGCU GACGAGUGGCGGAC GGGUGAGUAAUGU CUGGGAAACUGCCU GAUGGAGGGGGAU AACUACUGGAAACG | CRP | Target\_lig\_14 7 | decoding region 16SrRNA | Target\_97 | 6.78251605  578609 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | GUAGCUAAUACCGC AUAACGUCGCAAGA CCAAAGAGGGGGAC CUUCGGGCCUCUUG CCAUCGGAUGUGCC CAGAUGGGAUUAG CUAGUAGGUGGGG UAACGGCUCACCUA GGCGACGAUCCCUA GCUGGUCUGAGAG GAUGACCAGCCACA CUGGAACUGAGACA CGGUCCAGACUCCU ACGGGAGGCAGCAG UGGGGAAUAUUGC ACAAUGGGCGCAAG CCUGAUGCAGCCAU GCCGCGUGUAUGAA GAAGGCCUUCGGGU UGUAAAGUACUUU CAGCGGGGAGGAA GGGAGUAAAGUUA AUACCUUUGCUCAU UGACGUUACCCGCA GAAGAAGCACCGGC UAACUCCGUGCCAG CAGCCGCGGUAAUA CGGAGGGUGCAAGC GUUAAUCGGAAUU ACUGGGCGUAAAGC GCACGCAGGCGGUU UGUUAAGUCAGAU GUGAAAUCCCCGGG CUCAACCUGGGAAC UGCAUCUGAUACUG GCAAGCUUGAGUCU CGUAGAGGGGGGU AGAAUUCCAGGUG UAGCGGUGAAAUG CGUAGAGAUCUGG AGGAAUACCGGUG GCGAAGGCGGCCCC CUGGACGAAGACUG ACGCUCAGGUGCGA AAGCGUGGGGAGC AAACAGGAUUAGA UACCCUGGUAGUCC ACGCCGUAAACGAU GUCGACUUGGAGG UUGUGCCCUUGAGG CGUGGCUUCCGGAG CUAACGCGUUAAGU CGACCGCCUGGGGA GUACGGCCGCAAGG UUAAAACUCAAAU GAAUUGACGGGGG CCCGCACAAGCGGU GGAGCAUGUGGUU UAAUUCGAUGCAAC GCGAAGAACCUUAC CUGGUCUUGACAUC CACGGAAGUUUUCA GAGAUGAGAAUGU GCCUUCGGGAACCG UGAGACAGGUGCU GCAUGGCUGUCGUC AGCUCGUGUUGUG AAAUGUUGGGUUA AGUCCCGCAACGAG CGCAACCCUUAUCC UUUGUUGCCAGCGG UCCGGCCGGGAACU CAAAGGAGACUGCC AGUGAUAAACUGG AGGAAGGUGGGGA |  |  |  |  |  |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | UGACGUCAAGUCAU CAUGGCCCUUACGA CCAGGGCUACACAC GUGCUACAAUGGCG CAUACAAAGAGAA GCGACCUCGCGAGA GCAAGCGGACCUCA UAAAGUGCGUCGU AGUCCGGAUUGGA GUCUGCAACUCGAC UCCAUGAAGUCGGA AUCGCUAGUAAUCG UGGAUCAGAAUGCC ACGGUGAAUACGU UCCCGGGCCUUGUA CACACCGCCCGUCA CACCAUGGGAGUGG GUUGCAAAAGAAG UAGGUAGCUUAACC UUCGGGAGGGCGCU UACCACUUUGUGAU UCAUGACUGGGGU GAAGUCGUAACAA GGUAACCGUAGGG GAACCUGCGGUUGG AUCACCUCCUUA |  |  |  |  |  |
| 226 | C1C(C(C(C(C1N)OC2 C(C(C(C(O2)CN)O)O)   1. OC3C(C(C(O3)CO)   OC4C(C(C(C(O4)CN)   1. O)N)O)O)N | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Neomycin | Target\_lig\_4 | A-site | Target\_3 | 7.22184874  961636 |
| 228 | CC1=CC(=NC2=C1C= CC(=C2)N)N(C)C | GAGCGUCACACCUU CGGGUGAAGUCGCU C | quinolinediamine  \_trimethyl\_der | Target\_lig\_17 0 | A-site | Target\_3 | 4.45593195  564972 |
| 229 | C1=CC=C2C(=C1)C= C(C=N2)C(=O)N | GAGCGUCACACCUU CGGGUGAAGUCGCU C | 3-  quinolinecarboxa mide | Target\_lig\_17 1 | A-site | Target\_3 | 4.76955107  862173 |
| 230 | CC1=CC(=NC2=C1C= CC(=C2)NC(=O)CC3= CC=NC=C3)N(C)C | GAGCGUCACACCUU CGGGUGAAGUCGCU C | 4-  pyridineacetamid e, N- [2-  (dimethylamino)- 4-methyl-7- quinolinyl] | Target\_lig\_17 2 | A-site | Target\_3 | 4.74472749  489669 |
| 232 | CCC1C2(C(C(C(=O)C(  CC(C(C(C(=O)C(C(=O  )O1)C)C)OC3C(C(CC(  O3)C)N(C)C)O) (C)OCC=CC4=CC5=C C=CC=C5N=C4)C)C) NC(=O)O2)C | UUGGCUACUAUGCC AGCUGGUGGAUUG CUCGGCUCAGGCGC UGAUGAAGGACGU GCCAAGCUGCGAUA AGCCAUGGGGAGCC GCACGGAGGCGAAG AACCAUGGAUUUCC GAAUGAGAAUCUC UCUAACAAUUGCUU CGCGCAAUGAGGAA CCCCGAGAACUGAA ACAUCUCAGUAUCG GGAGGAACAGAAA ACGCAAUGUGAUG UCGUUAGUAACCGC GAGUGAACGCGAU ACAGCCCAAACCGA AGCCCUCACGGGCA AUGUGGUGUCAGG GCUACCUCUCAUCA GCCGACCGUCUCGA CGAAGUCUCUUGGA ACAGAGCGUGAUAC AGGGUGACAACCCC GUACUCGAGACCAG UACGACGUGCGGUA GUGCCAGAGUAGCG GGGGUUGGAUAUC | Cethromycin | Target\_lig\_17 4 | U2609\_Ecoli  \_ribosome | Target\_99 | 8.88605664  769316 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | CCUCGCGAAUAACG CAGGCAUCGACUGC GAAGGCUAAACACA ACCUGAGACCGAUA GUGAACAAGUAGU GUGAACGAACGCUG CAAAGUACCCUCAG AAGGGAGGCGAAA UAGAGCAUGAAAU CAGUUGGCGAUCGA GCGACAGGGCAUAC AAGGUCCCUCGACG AAUGACCGACGCGC GAGCGUCCAGUAAG ACUCACGGGAAGCC GAUGUUCUGUCGU ACGUUUUGAAAAA CGAGCCAGGGAGUG UGUCUGCAUGGCAA GUCUAACCGGAGUA UCCGGGGAGGCACA GGGAAACCGACAUG GCCGCAGGGCUUUG CCCGAGGGCCGCCG UCUUCAAGGGCGGG GAGCCAUGUGGACA CGACCCGAAUCCGG ACGAUCUACGCAUG GACAAGAUGAAGC GUGCCGAAAGGCAC GUGGAAGUCUGUU AGAGUUGGUGUCC UACAAUACCCUCUC GUGAUCUAUGUGU AGGGGUGAAAGGC CCAUCGAGUCCGGC AACAGCUGGUUCCA AUCGAAACAUGUCG AAGCAUGACCUCCG CCGAGGUAGUCUGU GAGGUAGAGCGACC GAUUGGUGUGUCC GCCUCCGAGAGGAG UCGGCACACCUGUC AAACUCCAAACUUA CAGACGCCGUUUGA CGCGGGGAUUCCGG UGCGCGGGGUAAGC CUGUGUACCAGGAG GGGAACAACCCAGA GAUAGGUUAAGGU CCCCAAGUGUGGAU UAAGUGUAAUCCUC UGAAGGUGGUCUC GAGCCCUAGACAGC CGGGAGGUGAGCU UAGAAGCAGCUACC CUCUAAGAAAAGCG UAACAGCUUACCGG CCGAGGUUUGAGGC GCCCAAAAUGAUCG GGACUCAAAUCCAC CACCGAGACCUGUC CGUACCACUCAUAC UGGUAAUCGAGUA GAUUGGCGCUCUAA UUGGAUGGAAGUA GGGGUGAAAACUCC UAUGGACCGAUUA GUGACGAAAAUCCU GGCCAUAGUAGCAG CGAUAGUCGGGUG AGAACCCCGACGGC CUAAUGGAUAAGG GUUCCUCAGCACUG |  |  |  |  |  |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | CUGAUCAGCUGAGG GUUAGCCGGUCCUA AGUCAUACCGCAAC UCGACUAUGACGAA AUGGGAAACGGGU UAAUAUUCCCGUGC CACUAUGCAGUGAA AGUUGACGCCCUGG GGUCGAUCACGCUG GGCAUUCGCCCAGU CGAACCGUCCAACU CCGUGGAAGCCGUA AUGGCAGGAAGCG GACGAACGGCGGCA UAGGGAAACGUGA UUCAACCUGGGGCC CAUGAAAAGACGA GCAUAGUGUCCGUA CCGAGAACCGACAC AGGUGUCCAUGGCG GCGAAAGCCAAGGC CUGUCGGGAGCAAC CAACGUUAGGGAA UUCGGCAAGUUAG UCCCGUACCUUCGG AAGAAGGGAUGCC UGCUCCGGAACGGA GCAGGUCGCAGUGA CUCGGAAGCUCGGA CUGUCUAGUAACAA CAUAGGUGACCGCA AAUCCGCAAGGACU CGUACGGUCACUGA AUCCUGCCCAGUGC AGGUAUCUGAACAC CUCGUACAAGAGGA CGAAGGACCUGUCA ACGGCGGGGGUAAC UAUGACCCUCUUAA GGUAGCGUAGUACC UUGCCGCAUCAGUA GCGGCUUGCAUGAA UGGAUUAACCAGA GCUUCACUGUCCCA ACGUUGGGCCCGGU GAACUGUACAUUCC AGUGCGGAGUCUG GAGACACCCAGGGG GAAGCGAAGACCCU AUGGAGCUUUACU GCAGGCUGUCGCUG AGACGUGGUCGCCG AUGUGCAGCAUAG GUAGGAGACACUAC ACAGGUACCCGCGC UAGCGGGCCACCGA GUCAACAGUGAAA UACUACCCGUCGGU GACUGCGACUCUCA CUCCGGGAGGAGGA CACCGAUAGCCGGG CAGUUUGACUGGG GCGGUACGCGCUCG AAAAGAUAUCGAG CGCGCCCUAUGGCU AUCUCAGCCGGGAC AGAGACCCGGCGAA GAGUGCAAGAGCA AAAGAUAGCUUGA CAGUGUUCUUCCCA ACGAGGAACGCUGA CGCGAAAGCGUGGU CUAGCGAACCAAUU AGCCUGCUUGAUGC GGGCAAUUGAUGA |  |  |  |  |  |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | CAGAAAAGCUACCC UAGGGAUAACAGA GUCGUCACUCGCAA GAGCACAUAUCGAC CGAGUGGCUUGCUA CCUCGAUGUCGGUU CCCUCCAUCCUGCC CGUGCAGAAGCGGG CAAGGGUGAGGUU GUUCGCCUAUUAAA GGAGGUCGUGAGC UGGGUUUAGACCG UCGUGAGACAGGUC GGCUGCUAUCUACU GGGUGUGUAAUGG UGUCUGACAAGAAC GACCGUAUAGUACG AGAGGAACUACGG UUGGUGGCCACUGG UGUACCGGUUGUUC GAGAGAGCACGUGC CGGGUAGCCACGCC ACACGGGGUAAGA GCUGAACGCAUCUA AGCUCGAAACCCAC UUGGAAAAGAGAC ACCGCCGAGGUCCC GCGUACAAGACGCG GUCGAUAGACUCGG GGUGUGCGCGUCGA GGUAACGAGACGU UAAGCCCACGAGCA CUAACAGACCAAAG CCAUCAU |  |  |  |  |  |
| 282 | C1C(C(C(C(C1NC(=O)  C(CCN)O)OC2C(C(C(  C(O2)CO)O)N)O)O)O  C3C(C(C(C(O3)CN)O) O)O)N | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Amikacin | Target\_lig\_17 5 | A-site for Amikacin | Target\_3 | 7.25963731  050576 |
| 283 | CC(=O)OC1C(CNC1C C2=CC=C(C=C2)OC) O | UUGGCUACUAUGCC AGCUGGUGGAUUG CUCGGCUCAGGCGC UGAUGAAGGACGU GCCAAGCUGCGAUA AGCCAUGGGGAGCC GCACGGAGGCGAAG AACCAUGGAUUUCC GAAUGAGAAUCUC UCUAACAAUUGCUU CGCGCAAUGAGGAA CCCCGAGAACUGAA ACAUCUCAGUAUCG GGAGGAACAGAAA ACGCAAUGUGAUG UCGUUAGUAACCGC GAGUGAACGCGAU ACAGCCCAAACCGA AGCCCUCACGGGCA AUGUGGUGUCAGG GCUACCUCUCAUCA GCCGACCGUCUCGA CGAAGUCUCUUGGA ACAGAGCGUGAUAC AGGGUGACAACCCC GUACUCGAGACCAG UACGACGUGCGGUA GUGCCAGAGUAGCG GGGGUUGGAUAUC CCUCGCGAAUAACG CAGGCAUCGACUGC GAAGGCUAAACACA ACCUGAGACCGAUA GUGAACAAGUAGU GUGAACGAACGCUG | Anisomycin | Target\_lig\_22 2 | Ribosome (PTC) | Target\_99 | 7 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | CAAAGUACCCUCAG AAGGGAGGCGAAA UAGAGCAUGAAAU CAGUUGGCGAUCGA GCGACAGGGCAUAC AAGGUCCCUCGACG AAUGACCGACGCGC GAGCGUCCAGUAAG ACUCACGGGAAGCC GAUGUUCUGUCGU ACGUUUUGAAAAA CGAGCCAGGGAGUG UGUCUGCAUGGCAA GUCUAACCGGAGUA UCCGGGGAGGCACA GGGAAACCGACAUG GCCGCAGGGCUUUG CCCGAGGGCCGCCG UCUUCAAGGGCGGG GAGCCAUGUGGACA CGACCCGAAUCCGG ACGAUCUACGCAUG GACAAGAUGAAGC GUGCCGAAAGGCAC GUGGAAGUCUGUU AGAGUUGGUGUCC UACAAUACCCUCUC GUGAUCUAUGUGU AGGGGUGAAAGGC CCAUCGAGUCCGGC AACAGCUGGUUCCA AUCGAAACAUGUCG AAGCAUGACCUCCG CCGAGGUAGUCUGU GAGGUAGAGCGACC GAUUGGUGUGUCC GCCUCCGAGAGGAG UCGGCACACCUGUC AAACUCCAAACUUA CAGACGCCGUUUGA CGCGGGGAUUCCGG UGCGCGGGGUAAGC CUGUGUACCAGGAG GGGAACAACCCAGA GAUAGGUUAAGGU CCCCAAGUGUGGAU UAAGUGUAAUCCUC UGAAGGUGGUCUC GAGCCCUAGACAGC CGGGAGGUGAGCU UAGAAGCAGCUACC CUCUAAGAAAAGCG UAACAGCUUACCGG CCGAGGUUUGAGGC GCCCAAAAUGAUCG GGACUCAAAUCCAC CACCGAGACCUGUC CGUACCACUCAUAC UGGUAAUCGAGUA GAUUGGCGCUCUAA UUGGAUGGAAGUA GGGGUGAAAACUCC UAUGGACCGAUUA GUGACGAAAAUCCU GGCCAUAGUAGCAG CGAUAGUCGGGUG AGAACCCCGACGGC CUAAUGGAUAAGG GUUCCUCAGCACUG CUGAUCAGCUGAGG GUUAGCCGGUCCUA AGUCAUACCGCAAC UCGACUAUGACGAA AUGGGAAACGGGU UAAUAUUCCCGUGC |  |  |  |  |  |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | CACUAUGCAGUGAA AGUUGACGCCCUGG GGUCGAUCACGCUG GGCAUUCGCCCAGU CGAACCGUCCAACU CCGUGGAAGCCGUA AUGGCAGGAAGCG GACGAACGGCGGCA UAGGGAAACGUGA UUCAACCUGGGGCC CAUGAAAAGACGA GCAUAGUGUCCGUA CCGAGAACCGACAC AGGUGUCCAUGGCG GCGAAAGCCAAGGC CUGUCGGGAGCAAC CAACGUUAGGGAA UUCGGCAAGUUAG UCCCGUACCUUCGG AAGAAGGGAUGCC UGCUCCGGAACGGA GCAGGUCGCAGUGA CUCGGAAGCUCGGA CUGUCUAGUAACAA CAUAGGUGACCGCA AAUCCGCAAGGACU CGUACGGUCACUGA AUCCUGCCCAGUGC AGGUAUCUGAACAC CUCGUACAAGAGGA CGAAGGACCUGUCA ACGGCGGGGGUAAC UAUGACCCUCUUAA GGUAGCGUAGUACC UUGCCGCAUCAGUA GCGGCUUGCAUGAA UGGAUUAACCAGA GCUUCACUGUCCCA ACGUUGGGCCCGGU GAACUGUACAUUCC AGUGCGGAGUCUG GAGACACCCAGGGG GAAGCGAAGACCCU AUGGAGCUUUACU GCAGGCUGUCGCUG AGACGUGGUCGCCG AUGUGCAGCAUAG GUAGGAGACACUAC ACAGGUACCCGCGC UAGCGGGCCACCGA GUCAACAGUGAAA UACUACCCGUCGGU GACUGCGACUCUCA CUCCGGGAGGAGGA CACCGAUAGCCGGG CAGUUUGACUGGG GCGGUACGCGCUCG AAAAGAUAUCGAG CGCGCCCUAUGGCU AUCUCAGCCGGGAC AGAGACCCGGCGAA GAGUGCAAGAGCA AAAGAUAGCUUGA CAGUGUUCUUCCCA ACGAGGAACGCUGA CGCGAAAGCGUGGU CUAGCGAACCAAUU AGCCUGCUUGAUGC GGGCAAUUGAUGA CAGAAAAGCUACCC UAGGGAUAACAGA GUCGUCACUCGCAA GAGCACAUAUCGAC CGAGUGGCUUGCUA CCUCGAUGUCGGUU |  |  |  |  |  |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | CCCUCCAUCCUGCC CGUGCAGAAGCGGG CAAGGGUGAGGUU GUUCGCCUAUUAAA GGAGGUCGUGAGC UGGGUUUAGACCG UCGUGAGACAGGUC GGCUGCUAUCUACU GGGUGUGUAAUGG UGUCUGACAAGAAC GACCGUAUAGUACG AGAGGAACUACGG UUGGUGGCCACUGG UGUACCGGUUGUUC GAGAGAGCACGUGC CGGGUAGCCACGCC ACACGGGGUAAGA GCUGAACGCAUCUA AGCUCGAAACCCAC UUGGAAAAGAGAC ACCGCCGAGGUCCC GCGUACAAGACGCG GUCGAUAGACUCGG GGUGUGCGCGUCGA GGUAACGAGACGU UAAGCCCACGAGCA CUAACAGACCAAAG CCAUCAU |  |  |  |  |  |
| 284 | CCC1C(C(C(N(CC(CC (C(C(C(C(C(=O)O1)C) OC2CC(C(C(O2)C)O)  (C)OC)C)OC3C(C(CC(  O3)C)N(C)C)O) (C)O)C)C)C)O)(C)O | UUGGCUACUAUGCC AGCUGGUGGAUUG CUCGGCUCAGGCGC UGAUGAAGGACGU GCCAAGCUGCGAUA AGCCAUGGGGAGCC GCACGGAGGCGAAG AACCAUGGAUUUCC GAAUGAGAAUCUC UCUAACAAUUGCUU CGCGCAAUGAGGAA CCCCGAGAACUGAA ACAUCUCAGUAUCG GGAGGAACAGAAA ACGCAAUGUGAUG UCGUUAGUAACCGC GAGUGAACGCGAU ACAGCCCAAACCGA AGCCCUCACGGGCA AUGUGGUGUCAGG GCUACCUCUCAUCA GCCGACCGUCUCGA CGAAGUCUCUUGGA ACAGAGCGUGAUAC AGGGUGACAACCCC GUACUCGAGACCAG UACGACGUGCGGUA GUGCCAGAGUAGCG GGGGUUGGAUAUC CCUCGCGAAUAACG CAGGCAUCGACUGC GAAGGCUAAACACA ACCUGAGACCGAUA GUGAACAAGUAGU GUGAACGAACGCUG CAAAGUACCCUCAG AAGGGAGGCGAAA UAGAGCAUGAAAU CAGUUGGCGAUCGA GCGACAGGGCAUAC AAGGUCCCUCGACG AAUGACCGACGCGC GAGCGUCCAGUAAG ACUCACGGGAAGCC GAUGUUCUGUCGU ACGUUUUGAAAAA CGAGCCAGGGAGUG | Azithromycin | Target\_lig\_22 3 | Ribosome (PTC) | Target\_99 | 8.42021640  338319 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | UGUCUGCAUGGCAA GUCUAACCGGAGUA UCCGGGGAGGCACA GGGAAACCGACAUG GCCGCAGGGCUUUG CCCGAGGGCCGCCG UCUUCAAGGGCGGG GAGCCAUGUGGACA CGACCCGAAUCCGG ACGAUCUACGCAUG GACAAGAUGAAGC GUGCCGAAAGGCAC GUGGAAGUCUGUU AGAGUUGGUGUCC UACAAUACCCUCUC GUGAUCUAUGUGU AGGGGUGAAAGGC CCAUCGAGUCCGGC AACAGCUGGUUCCA AUCGAAACAUGUCG AAGCAUGACCUCCG CCGAGGUAGUCUGU GAGGUAGAGCGACC GAUUGGUGUGUCC GCCUCCGAGAGGAG UCGGCACACCUGUC AAACUCCAAACUUA CAGACGCCGUUUGA CGCGGGGAUUCCGG UGCGCGGGGUAAGC CUGUGUACCAGGAG GGGAACAACCCAGA GAUAGGUUAAGGU CCCCAAGUGUGGAU UAAGUGUAAUCCUC UGAAGGUGGUCUC GAGCCCUAGACAGC CGGGAGGUGAGCU UAGAAGCAGCUACC CUCUAAGAAAAGCG UAACAGCUUACCGG CCGAGGUUUGAGGC GCCCAAAAUGAUCG GGACUCAAAUCCAC CACCGAGACCUGUC CGUACCACUCAUAC UGGUAAUCGAGUA GAUUGGCGCUCUAA UUGGAUGGAAGUA GGGGUGAAAACUCC UAUGGACCGAUUA GUGACGAAAAUCCU GGCCAUAGUAGCAG CGAUAGUCGGGUG AGAACCCCGACGGC CUAAUGGAUAAGG GUUCCUCAGCACUG CUGAUCAGCUGAGG GUUAGCCGGUCCUA AGUCAUACCGCAAC UCGACUAUGACGAA AUGGGAAACGGGU UAAUAUUCCCGUGC CACUAUGCAGUGAA AGUUGACGCCCUGG GGUCGAUCACGCUG GGCAUUCGCCCAGU CGAACCGUCCAACU CCGUGGAAGCCGUA AUGGCAGGAAGCG GACGAACGGCGGCA UAGGGAAACGUGA UUCAACCUGGGGCC CAUGAAAAGACGA GCAUAGUGUCCGUA |  |  |  |  |  |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | CCGAGAACCGACAC AGGUGUCCAUGGCG GCGAAAGCCAAGGC CUGUCGGGAGCAAC CAACGUUAGGGAA UUCGGCAAGUUAG UCCCGUACCUUCGG AAGAAGGGAUGCC UGCUCCGGAACGGA GCAGGUCGCAGUGA CUCGGAAGCUCGGA CUGUCUAGUAACAA CAUAGGUGACCGCA AAUCCGCAAGGACU CGUACGGUCACUGA AUCCUGCCCAGUGC AGGUAUCUGAACAC CUCGUACAAGAGGA CGAAGGACCUGUCA ACGGCGGGGGUAAC UAUGACCCUCUUAA GGUAGCGUAGUACC UUGCCGCAUCAGUA GCGGCUUGCAUGAA UGGAUUAACCAGA GCUUCACUGUCCCA ACGUUGGGCCCGGU GAACUGUACAUUCC AGUGCGGAGUCUG GAGACACCCAGGGG GAAGCGAAGACCCU AUGGAGCUUUACU GCAGGCUGUCGCUG AGACGUGGUCGCCG AUGUGCAGCAUAG GUAGGAGACACUAC ACAGGUACCCGCGC UAGCGGGCCACCGA GUCAACAGUGAAA UACUACCCGUCGGU GACUGCGACUCUCA CUCCGGGAGGAGGA CACCGAUAGCCGGG CAGUUUGACUGGG GCGGUACGCGCUCG AAAAGAUAUCGAG CGCGCCCUAUGGCU AUCUCAGCCGGGAC AGAGACCCGGCGAA GAGUGCAAGAGCA AAAGAUAGCUUGA CAGUGUUCUUCCCA ACGAGGAACGCUGA CGCGAAAGCGUGGU CUAGCGAACCAAUU AGCCUGCUUGAUGC GGGCAAUUGAUGA CAGAAAAGCUACCC UAGGGAUAACAGA GUCGUCACUCGCAA GAGCACAUAUCGAC CGAGUGGCUUGCUA CCUCGAUGUCGGUU CCCUCCAUCCUGCC CGUGCAGAAGCGGG CAAGGGUGAGGUU GUUCGCCUAUUAAA GGAGGUCGUGAGC UGGGUUUAGACCG UCGUGAGACAGGUC GGCUGCUAUCUACU GGGUGUGUAAUGG UGUCUGACAAGAAC GACCGUAUAGUACG AGAGGAACUACGG |  |  |  |  |  |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | UUGGUGGCCACUGG UGUACCGGUUGUUC GAGAGAGCACGUGC CGGGUAGCCACGCC ACACGGGGUAAGA GCUGAACGCAUCUA AGCUCGAAACCCAC UUGGAAAAGAGAC ACCGCCGAGGUCCC GCGUACAAGACGCG GUCGAUAGACUCGG GGUGUGCGCGUCGA GGUAACGAGACGU UAAGCCCACGAGCA CUAACAGACCAAAG CCAUCAU |  |  |  |  |  |
| 289 | C1=CC(=CC=C1C(C(C O)NC(=O)C(Cl)Cl)O)  [N+](=O)[O-] | GGUUAAGCGACUA AGCGUACACGGUGG AUGCCCUGGCAGUC AGAGGCGAUGAAG GACGUGCUAAUCUG CGAUAAGCGUCGGU AAGGUGAUAUGAA CCGUUAUAACCGGC GAUUUCCGAAUGG GGAAACCCAGUGUG UUUCGACACACUAU CAUUAACUGAAUCC AUAGGUUAAUGAG GCGAACCGGGGGAA CUGAAACAUCUAAG UACCCCGAGGAAAA GAAAUCAACCGAGA UUCCCCCAGUAGCG GCGAGCGAACGGGG AGCAGCCCAGAGCC UGAAUCAGUGUGU GUGUUAGUGGAAG CGUCUGGAAAGGCG CGCGAUACAGGGUG ACAGCCCCGUACAC AAAAAUGCACAUGC UGUGAGCUCGAUG AGUAGGGCGGGAC ACGUGGUAUCCUGU CUGAAUAUGGGGG GACCAUCCUCCAAG GCUAAAUACUCCUG ACUGACCGAUAGUG AACCAGUACCGUGA GGGAAAGGCGAAA AGAACCCCGGCGAG GGGAGUGAAAAAG AACCUGAAACCGUG UACGUACAAGCAGU GGGAGCACGCUUAG GCGUGUGACUGCGU ACCUUUUGUAUAA UGGGUCAGCGACUU AUAUUCUGUAGCA AGGUUAACCGAAU AGGGGAGCCGAAG GGAAACCGAGUCUU AACUGGGCGUUAA GUUGCAGGGUAUA GACCCGAAACCCGG UGAUCUAGCCAUGG GCAGGUUGAAGGU UGGGUAACACUAAC UGGAGGACCGAACC GACUAAUGUUGAA AAAUUAGCGGAUG ACUUGUGGCUGGG GGUGAAAGGCCAA UCAAACCGGGAGAU | Chloramphenicol | Target\_lig\_22 8 | 50S subunit | Target\_100 | 5.69897000  433602 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | AGCUGGUUCUCCCC GAAAGCUAUUUAG GUAGCGCCUCGUGA AUUCAUCUCCGGGG GUAGAGCACUGUU UCGGCAAGGGGGUC ACUUACCAACCCGA UGCAAACUGCGAAU ACCGGAGAAUGUU AUCACGGGAGACAC ACGGCGGGUGCUAA CGUCCGUCGUGAAG AGGGAAACAACCCA GACCGCCAGCUAAG GUCCCAAAGUCAUG GUUAAGUGGGAAA CGAUGUGGGAAGG CCCAGACAGCCAGG AUGUUGGCUUAGA AGCAGCCAUCAUUU AAAGAAAGCGUAA UAGCUCACUGGUCG AGUCGGCCUGCGCG GAAGAUGUAACGG GGCUAAACCAUGCA CCGAAGCUGCGGCA GCGACGCUUAUGCG UUGUUGGGUAGGG GAGCGUUCUGUAA GCCUGCGAAGGUGU GCUGUGAGGCAUGC UGGAGGUAUCAGA AGUGCGAAUGCUG ACAUAAGUAACGA UAAAGCGGGUGAA AAGCCCGCUCGCCG GAAGACCAAGGGU UCCUGUCCAACGUU AAUCGGGGCAGGG UGAGUCGACCCCUA AGGCGAGGCCGAAA GGCGUAGUCGAUG GGAAACAGGUUAA UAUUCCUGUACUUG GUGUUACUGCGAA GGGGGGACGGAGA AGGCUAUGUUGGCC GGGCGACGGUUGUC CCGGUUUAAGCGUG UAGGCUGGUUUUCC AGGCAAAUCCGGAA AAUCAAGGCUGAG GCGUGAUGACGAG GCACUACGGUGCUG AAGCAACAAAUGCC CUGCUUCCAGGAAA AGCCUCUAAGCAUC AGGUAACAUCAAA UCGUACCCCAAACC GACACAGGUGGUCA GGUAGAGAAUACC AAGGCGCUUGAGA GAACUCGGGUGAA GGAACUAGGCAAA AUGGUGCCGUAACU UCGGGAGAAGGCAC GCUGAUAUGUAGG UGAGGUCCCUCGCG GAUGGAGCUGAAA UCAGUCGAAGAUAC CAGCUGGCUGCAAC UGUUUAUUAAAAA CACAGCACUGUGCA AACACGAAAGUGG ACGUAUACGGUGU |  |  |  |  |  |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | GACGCCUGCCCGGU GCCGGAAGGUUAA UUGAUGGGGUUAG CGCAAGCGAAGCUC UUGAUCGAAGCCCC GGUAAACGGCGGCC GUAACXAUAACGG UCCUAAGGUAGCGA AAUUCCUUGUCGGG UAAGUUCCGACCUG CACGAAUGGCGUAA UGAUGGCCAGGCUG UCUCCACCCGAGAC UCAGUGAAAUUGA ACUCGCUGUGAAGA UGCAGUGUACCCGC GGCAAGACGGAAA GACCCCGUGAACCU UUACUAUAGCUUG ACACUGAACAUUGA GCCUUGAUGUGUA GGAUAGGUGGGAG GCUUUGAAGUGUG GACGCCAGUCUGCA UGGAGCCGACCUUG AAAUACCACCCUUU AAUGUUUGAUGUU CUAACGUUGACCCG UAAUCCGGGUUGCG GACAGUGUCUGGU GGGUAGUUUGACU GGGGCGGUCUCCUC CUAAAGAGUAACG GAGGAGCACGAAG GUUGGCUAAUCCUG GUCGGACAUCAGGA GGUUAGUGCAAUG GCAUAAGCCAGCUU GACUGCGAGCGUGA CGGCGCGAGCAGGU GCGAAAGCAGGUCA UAGUGAUCCGGUG GUUCUGAAUGGAA GGGCCAUCGCUCAA CGGAUAAAAGGUA CUCCGGGGAUAACA GGCUGAUACCGCCC AAGAGUUCAUAUC GACGGCGGUGUUU GGCACCUCGAUGUC GGCUCAUCACAUCC UGGGGCUGAAGUA GGUCCCAAGGGUAU GGCUGUUCGCCAUU UAAAGUGGUACGC GAGCUGGGUUUAG AACGUCGUGAGACA GUUCGGUCCCUAUC UGCCGUGGGCGCUG GAGAACUGAGGGG GGCUGCUCCUAGUA CGAGAGGACCGGAG UGGACGCAUCACUG GUGUUCGGGUUGU CAUGCCAAUGGCAC UGCCCGGUAGCUAA AUGCGGAAGAGAU AAGUGCUGAAAGC AUCUAAGCACGAAA CUUGCCCCGAGAUG AGUUCUCCCUGACC CUUUAAGGGUCCUG AAGGAACGUUGAA GACGACGACGUUGA UAGGCCGGGUGUG |  |  |  |  |  |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | UAAGCGCAGCGAUG CGUUGAGCUAACCG GUACUAAUGAACCG UGAGGCUUAACCU |  |  |  |  |  |
| 290 | CC[C@@H]1C(=O)N2 CCC[C@H]2C(=O)N([ C@H] (C(=O)N3CCC(=O)C[  C@H]3C(=O)N[C@H]  (C(=O)O[C@@H] ([C@@H] (C(=O)N1)NC(=O)C4= C(C=CC=N4)O)C)C5= CC=CC=C5)CC6=CC= C(C=C6)N(C)C)C | GGUUAAGCGACUA AGCGUACACGGUGG AUGCCCUGGCAGUC AGAGGCGAUGAAG GACGUGCUAAUCUG CGAUAAGCGUCGGU AAGGUGAUAUGAA CCGUUAUAACCGGC GAUUUCCGAAUGG GGAAACCCAGUGUG UUUCGACACACUAU CAUUAACUGAAUCC AUAGGUUAAUGAG GCGAACCGGGGGAA CUGAAACAUCUAAG UACCCCGAGGAAAA GAAAUCAACCGAGA UUCCCCCAGUAGCG GCGAGCGAACGGGG AGCAGCCCAGAGCC UGAAUCAGUGUGU GUGUUAGUGGAAG CGUCUGGAAAGGCG CGCGAUACAGGGUG ACAGCCCCGUACAC AAAAAUGCACAUGC UGUGAGCUCGAUG AGUAGGGCGGGAC ACGUGGUAUCCUGU CUGAAUAUGGGGG GACCAUCCUCCAAG GCUAAAUACUCCUG ACUGACCGAUAGUG AACCAGUACCGUGA GGGAAAGGCGAAA AGAACCCCGGCGAG GGGAGUGAAAAAG AACCUGAAACCGUG UACGUACAAGCAGU GGGAGCACGCUUAG GCGUGUGACUGCGU ACCUUUUGUAUAA UGGGUCAGCGACUU AUAUUCUGUAGCA AGGUUAACCGAAU AGGGGAGCCGAAG GGAAACCGAGUCUU AACUGGGCGUUAA GUUGCAGGGUAUA GACCCGAAACCCGG UGAUCUAGCCAUGG GCAGGUUGAAGGU UGGGUAACACUAAC UGGAGGACCGAACC GACUAAUGUUGAA AAAUUAGCGGAUG ACUUGUGGCUGGG GGUGAAAGGCCAA UCAAACCGGGAGAU AGCUGGUUCUCCCC GAAAGCUAUUUAG GUAGCGCCUCGUGA AUUCAUCUCCGGGG GUAGAGCACUGUU UCGGCAAGGGGGUC ACUUACCAACCCGA UGCAAACUGCGAAU ACCGGAGAAUGUU AUCACGGGAGACAC ACGGCGGGUGCUAA CGUCCGUCGUGAAG | Streptogramin\_B | Target\_lig\_22 9 | 50S subunit | Target\_100 | 7.22914798  835786 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | AGGGAAACAACCCA GACCGCCAGCUAAG GUCCCAAAGUCAUG GUUAAGUGGGAAA CGAUGUGGGAAGG CCCAGACAGCCAGG AUGUUGGCUUAGA AGCAGCCAUCAUUU AAAGAAAGCGUAA UAGCUCACUGGUCG AGUCGGCCUGCGCG GAAGAUGUAACGG GGCUAAACCAUGCA CCGAAGCUGCGGCA GCGACGCUUAUGCG UUGUUGGGUAGGG GAGCGUUCUGUAA GCCUGCGAAGGUGU GCUGUGAGGCAUGC UGGAGGUAUCAGA AGUGCGAAUGCUG ACAUAAGUAACGA UAAAGCGGGUGAA AAGCCCGCUCGCCG GAAGACCAAGGGU UCCUGUCCAACGUU AAUCGGGGCAGGG UGAGUCGACCCCUA AGGCGAGGCCGAAA GGCGUAGUCGAUG GGAAACAGGUUAA UAUUCCUGUACUUG GUGUUACUGCGAA GGGGGGACGGAGA AGGCUAUGUUGGCC GGGCGACGGUUGUC CCGGUUUAAGCGUG UAGGCUGGUUUUCC AGGCAAAUCCGGAA AAUCAAGGCUGAG GCGUGAUGACGAG GCACUACGGUGCUG AAGCAACAAAUGCC CUGCUUCCAGGAAA AGCCUCUAAGCAUC AGGUAACAUCAAA UCGUACCCCAAACC GACACAGGUGGUCA GGUAGAGAAUACC AAGGCGCUUGAGA GAACUCGGGUGAA GGAACUAGGCAAA AUGGUGCCGUAACU UCGGGAGAAGGCAC GCUGAUAUGUAGG UGAGGUCCCUCGCG GAUGGAGCUGAAA UCAGUCGAAGAUAC CAGCUGGCUGCAAC UGUUUAUUAAAAA CACAGCACUGUGCA AACACGAAAGUGG ACGUAUACGGUGU GACGCCUGCCCGGU GCCGGAAGGUUAA UUGAUGGGGUUAG CGCAAGCGAAGCUC UUGAUCGAAGCCCC GGUAAACGGCGGCC GUAACXAUAACGG UCCUAAGGUAGCGA AAUUCCUUGUCGGG UAAGUUCCGACCUG CACGAAUGGCGUAA UGAUGGCCAGGCUG |  |  |  |  |  |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | UCUCCACCCGAGAC UCAGUGAAAUUGA ACUCGCUGUGAAGA UGCAGUGUACCCGC GGCAAGACGGAAA GACCCCGUGAACCU UUACUAUAGCUUG ACACUGAACAUUGA GCCUUGAUGUGUA GGAUAGGUGGGAG GCUUUGAAGUGUG GACGCCAGUCUGCA UGGAGCCGACCUUG AAAUACCACCCUUU AAUGUUUGAUGUU CUAACGUUGACCCG UAAUCCGGGUUGCG GACAGUGUCUGGU GGGUAGUUUGACU GGGGCGGUCUCCUC CUAAAGAGUAACG GAGGAGCACGAAG GUUGGCUAAUCCUG GUCGGACAUCAGGA GGUUAGUGCAAUG GCAUAAGCCAGCUU GACUGCGAGCGUGA CGGCGCGAGCAGGU GCGAAAGCAGGUCA UAGUGAUCCGGUG GUUCUGAAUGGAA GGGCCAUCGCUCAA CGGAUAAAAGGUA CUCCGGGGAUAACA GGCUGAUACCGCCC AAGAGUUCAUAUC GACGGCGGUGUUU GGCACCUCGAUGUC GGCUCAUCACAUCC UGGGGCUGAAGUA GGUCCCAAGGGUAU GGCUGUUCGCCAUU UAAAGUGGUACGC GAGCUGGGUUUAG AACGUCGUGAGACA GUUCGGUCCCUAUC UGCCGUGGGCGCUG GAGAACUGAGGGG GGCUGCUCCUAGUA CGAGAGGACCGGAG UGGACGCAUCACUG GUGUUCGGGUUGU CAUGCCAAUGGCAC UGCCCGGUAGCUAA AUGCGGAAGAGAU AAGUGCUGAAAGC AUCUAAGCACGAAA CUUGCCCCGAGAUG AGUUCUCCCUGACC CUUUAAGGGUCCUG AAGGAACGUUGAA GACGACGACGUUGA UAGGCCGGGUGUG UAAGCGCAGCGAUG CGUUGAGCUAACCG GUACUAAUGAACCG UGAGGCUUAACCU |  |  |  |  |  |
| 291 | CC1CC(=O)C2(C(O1) OC3C(C(C(C(C3O2)N C)O)NC)O)O | AAAUUGAAGAGUU UGAUCAUGGCUCAG AUUGAACGCUGGCG GCAGGCCUAACACA UGCAAGUCGAACGG UAACAGGAAGAAG CUUGCUUCUUUGCU GACGAGUGGCGGAC | Spectinomycin | Target\_lig\_75 | Small subunit | Target\_101 | 6.58502665  202918 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | GGGUGAGUAAUGU CUGGGAAACUGCCU GAUGGAGGGGGAU AACUACUGGAAACG GUAGCUAAUACCGC AUAACGUCGCAAGA CCAAAGAGGGGGAC CUUCGGGCCUCUUG CCAUCGGAUGUGCC CAGAUGGGAUUAG CUAGUAGGUGGGG UAACGGCUCACCUA GGCGACGAUCCCUA GCUGGUCUGAGAG GAUGACCAGCCACA CUGGAACUGAGACA CGGUCCAGACUCCU ACGGGAGGCAGCAG UGGGGAAUAUUGC ACAAUGGGCGCAAG CCUGAUGCAGCCAU GCCGCGUGUAUGAA GAAGGCCUUCGGGU UGUAAAGUACUUU CAGCGGGGAGGAA GGGAGUAAAGUUA AUACCUUUGCUCAU UGACGUUACCCGCA GAAGAAGCACCGGC UAACUCCGUGCCAG CAGCCGCGGUAAUA CGGAGGGUGCAAGC GUUAAUCGGAAUU ACUGGGCGUAAAGC GCACGCAGGCGGUU UGUUAAGUCAGAU GUGAAAUCCCCGGG CUCAACCUGGGAAC UGCAUCUGAUACUG GCAAGCUUGAGUCU CGUAGAGGGGGGU AGAAUUCCAGGUG UAGCGGUGAAAUG CGUAGAGAUCUGG AGGAAUACCGGUG GCGAAGGCGGCCCC CUGGACGAAGACUG ACGCUCAGGUGCGA AAGCGUGGGGAGC AAACAGGAUUAGA UACCCUGGUAGUCC ACGCCGUAAACGAU GUCGACUUGGAGG UUGUGCCCUUGAGG CGUGGCUUCCGGAG CUAACGCGUUAAGU CGACCGCCUGGGGA GUACGGCCGCAAGG UUAAAACUCAAAU GAAUUGACGGGGG CCCGCACAAGCGGU GGAGCAUGUGGUU UAAUUCGAUGCAAC GCGAAGAACCUUAC CUGGUCUUGACAUC CACGGAAGUUUUCA GAGAUGAGAAUGU GCCUUCGGGAACCG UGAGACAGGUGCU GCAUGGCUGUCGUC AGCUCGUGUUGUG AAAUGUUGGGUUA AGUCCCGCAACGAG CGCAACCCUUAUCC UUUGUUGCCAGCGG |  |  |  |  |  |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | UCCGGCCGGGAACU CAAAGGAGACUGCC AGUGAUAAACUGG AGGAAGGUGGGGA UGACGUCAAGUCAU CAUGGCCCUUACGA CCAGGGCUACACAC GUGCUACAAUGGCG CAUACAAAGAGAA GCGACCUCGCGAGA GCAAGCGGACCUCA UAAAGUGCGUCGU AGUCCGGAUUGGA GUCUGCAACUCGAC UCCAUGAAGUCGGA AUCGCUAGUAAUCG UGGAUCAGAAUGCC ACGGUGAAUACGU UCCCGGGCCUUGUA CACACCGCCCGUCA CACCAUGGGAGUGG GUUGCAAAAGAAG UAGGUAGCUUAACC UUCGGGAGGGCGCU UACCACUUUGUGAU UCAUGACUGGGGU GAAGUCGUAACAA GGUAACCGUAGGG GAACCUGCGGUUGG AUCACCUCCUUA |  |  |  |  |  |
| 292 | CN(C)C1C2CC3CC4= C(C=CC(=C4C(=C3C(  =O)C2(C(=C(C1=O)C(  =O)N)O)O)O)O)N(C)C | AAAUUGAAGAGUU UGAUCAUGGCUCAG AUUGAACGCUGGCG GCAGGCCUAACACA UGCAAGUCGAACGG UAACAGGAAGAAG CUUGCUUCUUUGCU GACGAGUGGCGGAC GGGUGAGUAAUGU CUGGGAAACUGCCU GAUGGAGGGGGAU AACUACUGGAAACG GUAGCUAAUACCGC AUAACGUCGCAAGA CCAAAGAGGGGGAC CUUCGGGCCUCUUG CCAUCGGAUGUGCC CAGAUGGGAUUAG CUAGUAGGUGGGG UAACGGCUCACCUA GGCGACGAUCCCUA GCUGGUCUGAGAG GAUGACCAGCCACA CUGGAACUGAGACA CGGUCCAGACUCCU ACGGGAGGCAGCAG UGGGGAAUAUUGC ACAAUGGGCGCAAG CCUGAUGCAGCCAU GCCGCGUGUAUGAA GAAGGCCUUCGGGU UGUAAAGUACUUU CAGCGGGGAGGAA GGGAGUAAAGUUA AUACCUUUGCUCAU UGACGUUACCCGCA GAAGAAGCACCGGC UAACUCCGUGCCAG CAGCCGCGGUAAUA CGGAGGGUGCAAGC GUUAAUCGGAAUU ACUGGGCGUAAAGC GCACGCAGGCGGUU UGUUAAGUCAGAU GUGAAAUCCCCGGG | Minocycline | Target\_lig\_23 0 | Small subunit | Target\_101 | 7 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | CUCAACCUGGGAAC UGCAUCUGAUACUG GCAAGCUUGAGUCU CGUAGAGGGGGGU AGAAUUCCAGGUG UAGCGGUGAAAUG CGUAGAGAUCUGG AGGAAUACCGGUG GCGAAGGCGGCCCC CUGGACGAAGACUG ACGCUCAGGUGCGA AAGCGUGGGGAGC AAACAGGAUUAGA UACCCUGGUAGUCC ACGCCGUAAACGAU GUCGACUUGGAGG UUGUGCCCUUGAGG CGUGGCUUCCGGAG CUAACGCGUUAAGU CGACCGCCUGGGGA GUACGGCCGCAAGG UUAAAACUCAAAU GAAUUGACGGGGG CCCGCACAAGCGGU GGAGCAUGUGGUU UAAUUCGAUGCAAC GCGAAGAACCUUAC CUGGUCUUGACAUC CACGGAAGUUUUCA GAGAUGAGAAUGU GCCUUCGGGAACCG UGAGACAGGUGCU GCAUGGCUGUCGUC AGCUCGUGUUGUG AAAUGUUGGGUUA AGUCCCGCAACGAG CGCAACCCUUAUCC UUUGUUGCCAGCGG UCCGGCCGGGAACU CAAAGGAGACUGCC AGUGAUAAACUGG AGGAAGGUGGGGA UGACGUCAAGUCAU CAUGGCCCUUACGA CCAGGGCUACACAC GUGCUACAAUGGCG CAUACAAAGAGAA GCGACCUCGCGAGA GCAAGCGGACCUCA UAAAGUGCGUCGU AGUCCGGAUUGGA GUCUGCAACUCGAC UCCAUGAAGUCGGA AUCGCUAGUAAUCG UGGAUCAGAAUGCC ACGGUGAAUACGU UCCCGGGCCUUGUA CACACCGCCCGUCA CACCAUGGGAGUGG GUUGCAAAAGAAG UAGGUAGCUUAACC UUCGGGAGGGCGCU UACCACUUUGUGAU UCAUGACUGGGGU GAAGUCGUAACAA GGUAACCGUAGGG GAACCUGCGGUUGG AUCACCUCCUUA |  |  |  |  |  |
| 293 | CC(C) (C)NCC(=O)NC1=CC(  =C2CC3CC4C(C(=O)C (=C(C4(C(=O)C3=C(C  2=C1O)O)O)O)C(=O)  N)N(C)C)N(C)C | AAAUUGAAGAGUU UGAUCAUGGCUCAG AUUGAACGCUGGCG GCAGGCCUAACACA UGCAAGUCGAACGG UAACAGGAAGAAG CUUGCUUCUUUGCU | Tigecycline\_mol | Target\_lig\_23 1 | Small subunit | Target\_101 | 8 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | GACGAGUGGCGGAC GGGUGAGUAAUGU CUGGGAAACUGCCU GAUGGAGGGGGAU AACUACUGGAAACG GUAGCUAAUACCGC AUAACGUCGCAAGA CCAAAGAGGGGGAC CUUCGGGCCUCUUG CCAUCGGAUGUGCC CAGAUGGGAUUAG CUAGUAGGUGGGG UAACGGCUCACCUA GGCGACGAUCCCUA GCUGGUCUGAGAG GAUGACCAGCCACA CUGGAACUGAGACA CGGUCCAGACUCCU ACGGGAGGCAGCAG UGGGGAAUAUUGC ACAAUGGGCGCAAG CCUGAUGCAGCCAU GCCGCGUGUAUGAA GAAGGCCUUCGGGU UGUAAAGUACUUU CAGCGGGGAGGAA GGGAGUAAAGUUA AUACCUUUGCUCAU UGACGUUACCCGCA GAAGAAGCACCGGC UAACUCCGUGCCAG CAGCCGCGGUAAUA CGGAGGGUGCAAGC GUUAAUCGGAAUU ACUGGGCGUAAAGC GCACGCAGGCGGUU UGUUAAGUCAGAU GUGAAAUCCCCGGG CUCAACCUGGGAAC UGCAUCUGAUACUG GCAAGCUUGAGUCU CGUAGAGGGGGGU AGAAUUCCAGGUG UAGCGGUGAAAUG CGUAGAGAUCUGG AGGAAUACCGGUG GCGAAGGCGGCCCC CUGGACGAAGACUG ACGCUCAGGUGCGA AAGCGUGGGGAGC AAACAGGAUUAGA UACCCUGGUAGUCC ACGCCGUAAACGAU GUCGACUUGGAGG UUGUGCCCUUGAGG CGUGGCUUCCGGAG CUAACGCGUUAAGU CGACCGCCUGGGGA GUACGGCCGCAAGG UUAAAACUCAAAU GAAUUGACGGGGG CCCGCACAAGCGGU GGAGCAUGUGGUU UAAUUCGAUGCAAC GCGAAGAACCUUAC CUGGUCUUGACAUC CACGGAAGUUUUCA GAGAUGAGAAUGU GCCUUCGGGAACCG UGAGACAGGUGCU GCAUGGCUGUCGUC AGCUCGUGUUGUG AAAUGUUGGGUUA AGUCCCGCAACGAG CGCAACCCUUAUCC |  |  |  |  |  |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | UUUGUUGCCAGCGG UCCGGCCGGGAACU CAAAGGAGACUGCC AGUGAUAAACUGG AGGAAGGUGGGGA UGACGUCAAGUCAU CAUGGCCCUUACGA CCAGGGCUACACAC GUGCUACAAUGGCG CAUACAAAGAGAA GCGACCUCGCGAGA GCAAGCGGACCUCA UAAAGUGCGUCGU AGUCCGGAUUGGA GUCUGCAACUCGAC UCCAUGAAGUCGGA AUCGCUAGUAAUCG UGGAUCAGAAUGCC ACGGUGAAUACGU UCCCGGGCCUUGUA CACACCGCCCGUCA CACCAUGGGAGUGG GUUGCAAAAGAAG UAGGUAGCUUAACC UUCGGGAGGGCGCU UACCACUUUGUGAU UCAUGACUGGGGU GAAGUCGUAACAA GGUAACCGUAGGG GAACCUGCGGUUGG AUCACCUCCUUA |  |  |  |  |  |
| 294 | CCC1C(C(C(C(=O)C(  CC(C(C(C(C(C(=O)O1  )C)OC2CC(C(C(O2)C) O) (C)OC)C)OC3C(C(CC(  O3)C)N(C)C)O)  (C)OC)C)C)O)(C)O | UUGGCUACUAUGCC AGCUGGUGGAUUG CUCGGCUCAGGCGC UGAUGAAGGACGU GCCAAGCUGCGAUA AGCCAUGGGGAGCC GCACGGAGGCGAAG AACCAUGGAUUUCC GAAUGAGAAUCUC UCUAACAAUUGCUU CGCGCAAUGAGGAA CCCCGAGAACUGAA ACAUCUCAGUAUCG GGAGGAACAGAAA ACGCAAUGUGAUG UCGUUAGUAACCGC GAGUGAACGCGAU ACAGCCCAAACCGA AGCCCUCACGGGCA AUGUGGUGUCAGG GCUACCUCUCAUCA GCCGACCGUCUCGA CGAAGUCUCUUGGA ACAGAGCGUGAUAC AGGGUGACAACCCC GUACUCGAGACCAG UACGACGUGCGGUA GUGCCAGAGUAGCG GGGGUUGGAUAUC CCUCGCGAAUAACG CAGGCAUCGACUGC GAAGGCUAAACACA ACCUGAGACCGAUA GUGAACAAGUAGU GUGAACGAACGCUG CAAAGUACCCUCAG AAGGGAGGCGAAA UAGAGCAUGAAAU CAGUUGGCGAUCGA GCGACAGGGCAUAC AAGGUCCCUCGACG AAUGACCGACGCGC GAGCGUCCAGUAAG ACUCACGGGAAGCC | Clarithromycin | Target\_lig\_23 2 | PTC | Target\_99 | 8.20760831  050175 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | GAUGUUCUGUCGU ACGUUUUGAAAAA CGAGCCAGGGAGUG UGUCUGCAUGGCAA GUCUAACCGGAGUA UCCGGGGAGGCACA GGGAAACCGACAUG GCCGCAGGGCUUUG CCCGAGGGCCGCCG UCUUCAAGGGCGGG GAGCCAUGUGGACA CGACCCGAAUCCGG ACGAUCUACGCAUG GACAAGAUGAAGC GUGCCGAAAGGCAC GUGGAAGUCUGUU AGAGUUGGUGUCC UACAAUACCCUCUC GUGAUCUAUGUGU AGGGGUGAAAGGC CCAUCGAGUCCGGC AACAGCUGGUUCCA AUCGAAACAUGUCG AAGCAUGACCUCCG CCGAGGUAGUCUGU GAGGUAGAGCGACC GAUUGGUGUGUCC GCCUCCGAGAGGAG UCGGCACACCUGUC AAACUCCAAACUUA CAGACGCCGUUUGA CGCGGGGAUUCCGG UGCGCGGGGUAAGC CUGUGUACCAGGAG GGGAACAACCCAGA GAUAGGUUAAGGU CCCCAAGUGUGGAU UAAGUGUAAUCCUC UGAAGGUGGUCUC GAGCCCUAGACAGC CGGGAGGUGAGCU UAGAAGCAGCUACC CUCUAAGAAAAGCG UAACAGCUUACCGG CCGAGGUUUGAGGC GCCCAAAAUGAUCG GGACUCAAAUCCAC CACCGAGACCUGUC CGUACCACUCAUAC UGGUAAUCGAGUA GAUUGGCGCUCUAA UUGGAUGGAAGUA GGGGUGAAAACUCC UAUGGACCGAUUA GUGACGAAAAUCCU GGCCAUAGUAGCAG CGAUAGUCGGGUG AGAACCCCGACGGC CUAAUGGAUAAGG GUUCCUCAGCACUG CUGAUCAGCUGAGG GUUAGCCGGUCCUA AGUCAUACCGCAAC UCGACUAUGACGAA AUGGGAAACGGGU UAAUAUUCCCGUGC CACUAUGCAGUGAA AGUUGACGCCCUGG GGUCGAUCACGCUG GGCAUUCGCCCAGU CGAACCGUCCAACU CCGUGGAAGCCGUA AUGGCAGGAAGCG GACGAACGGCGGCA UAGGGAAACGUGA |  |  |  |  |  |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | UUCAACCUGGGGCC CAUGAAAAGACGA GCAUAGUGUCCGUA CCGAGAACCGACAC AGGUGUCCAUGGCG GCGAAAGCCAAGGC CUGUCGGGAGCAAC CAACGUUAGGGAA UUCGGCAAGUUAG UCCCGUACCUUCGG AAGAAGGGAUGCC UGCUCCGGAACGGA GCAGGUCGCAGUGA CUCGGAAGCUCGGA CUGUCUAGUAACAA CAUAGGUGACCGCA AAUCCGCAAGGACU CGUACGGUCACUGA AUCCUGCCCAGUGC AGGUAUCUGAACAC CUCGUACAAGAGGA CGAAGGACCUGUCA ACGGCGGGGGUAAC UAUGACCCUCUUAA GGUAGCGUAGUACC UUGCCGCAUCAGUA GCGGCUUGCAUGAA UGGAUUAACCAGA GCUUCACUGUCCCA ACGUUGGGCCCGGU GAACUGUACAUUCC AGUGCGGAGUCUG GAGACACCCAGGGG GAAGCGAAGACCCU AUGGAGCUUUACU GCAGGCUGUCGCUG AGACGUGGUCGCCG AUGUGCAGCAUAG GUAGGAGACACUAC ACAGGUACCCGCGC UAGCGGGCCACCGA GUCAACAGUGAAA UACUACCCGUCGGU GACUGCGACUCUCA CUCCGGGAGGAGGA CACCGAUAGCCGGG CAGUUUGACUGGG GCGGUACGCGCUCG AAAAGAUAUCGAG CGCGCCCUAUGGCU AUCUCAGCCGGGAC AGAGACCCGGCGAA GAGUGCAAGAGCA AAAGAUAGCUUGA CAGUGUUCUUCCCA ACGAGGAACGCUGA CGCGAAAGCGUGGU CUAGCGAACCAAUU AGCCUGCUUGAUGC GGGCAAUUGAUGA CAGAAAAGCUACCC UAGGGAUAACAGA GUCGUCACUCGCAA GAGCACAUAUCGAC CGAGUGGCUUGCUA CCUCGAUGUCGGUU CCCUCCAUCCUGCC CGUGCAGAAGCGGG CAAGGGUGAGGUU GUUCGCCUAUUAAA GGAGGUCGUGAGC UGGGUUUAGACCG UCGUGAGACAGGUC GGCUGCUAUCUACU GGGUGUGUAAUGG |  |  |  |  |  |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | UGUCUGACAAGAAC GACCGUAUAGUACG AGAGGAACUACGG UUGGUGGCCACUGG UGUACCGGUUGUUC GAGAGAGCACGUGC CGGGUAGCCACGCC ACACGGGGUAAGA GCUGAACGCAUCUA AGCUCGAAACCCAC UUGGAAAAGAGAC ACCGCCGAGGUCCC GCGUACAAGACGCG GUCGAUAGACUCGG GGUGUGCGCGUCGA GGUAACGAGACGU UAAGCCCACGAGCA CUAACAGACCAAAG CCAUCAU |  |  |  |  |  |
| 295 | CCC1C(C(C(C(=O)C(  CC(C(C(C(C(C(=O)O1  )C)OC2CC(C(C(O2)C) O) (C)OC)C)OC3C(C(CC(  O3)C)N(C)C)O)  (C)O)C)C)O)(C)O | UUGGCUACUAUGCC AGCUGGUGGAUUG CUCGGCUCAGGCGC UGAUGAAGGACGU GCCAAGCUGCGAUA AGCCAUGGGGAGCC GCACGGAGGCGAAG AACCAUGGAUUUCC GAAUGAGAAUCUC UCUAACAAUUGCUU CGCGCAAUGAGGAA CCCCGAGAACUGAA ACAUCUCAGUAUCG GGAGGAACAGAAA ACGCAAUGUGAUG UCGUUAGUAACCGC GAGUGAACGCGAU ACAGCCCAAACCGA AGCCCUCACGGGCA AUGUGGUGUCAGG GCUACCUCUCAUCA GCCGACCGUCUCGA CGAAGUCUCUUGGA ACAGAGCGUGAUAC AGGGUGACAACCCC GUACUCGAGACCAG UACGACGUGCGGUA GUGCCAGAGUAGCG GGGGUUGGAUAUC CCUCGCGAAUAACG CAGGCAUCGACUGC GAAGGCUAAACACA ACCUGAGACCGAUA GUGAACAAGUAGU GUGAACGAACGCUG CAAAGUACCCUCAG AAGGGAGGCGAAA UAGAGCAUGAAAU CAGUUGGCGAUCGA GCGACAGGGCAUAC AAGGUCCCUCGACG AAUGACCGACGCGC GAGCGUCCAGUAAG ACUCACGGGAAGCC GAUGUUCUGUCGU ACGUUUUGAAAAA CGAGCCAGGGAGUG UGUCUGCAUGGCAA GUCUAACCGGAGUA UCCGGGGAGGCACA GGGAAACCGACAUG GCCGCAGGGCUUUG CCCGAGGGCCGCCG UCUUCAAGGGCGGG GAGCCAUGUGGACA CGACCCGAAUCCGG | Eryrthromycin | Target\_lig\_23 3 | PTC | Target\_99 | 6.00436480  540245 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | ACGAUCUACGCAUG GACAAGAUGAAGC GUGCCGAAAGGCAC GUGGAAGUCUGUU AGAGUUGGUGUCC UACAAUACCCUCUC GUGAUCUAUGUGU AGGGGUGAAAGGC CCAUCGAGUCCGGC AACAGCUGGUUCCA AUCGAAACAUGUCG AAGCAUGACCUCCG CCGAGGUAGUCUGU GAGGUAGAGCGACC GAUUGGUGUGUCC GCCUCCGAGAGGAG UCGGCACACCUGUC AAACUCCAAACUUA CAGACGCCGUUUGA CGCGGGGAUUCCGG UGCGCGGGGUAAGC CUGUGUACCAGGAG GGGAACAACCCAGA GAUAGGUUAAGGU CCCCAAGUGUGGAU UAAGUGUAAUCCUC UGAAGGUGGUCUC GAGCCCUAGACAGC CGGGAGGUGAGCU UAGAAGCAGCUACC CUCUAAGAAAAGCG UAACAGCUUACCGG CCGAGGUUUGAGGC GCCCAAAAUGAUCG GGACUCAAAUCCAC CACCGAGACCUGUC CGUACCACUCAUAC UGGUAAUCGAGUA GAUUGGCGCUCUAA UUGGAUGGAAGUA GGGGUGAAAACUCC UAUGGACCGAUUA GUGACGAAAAUCCU GGCCAUAGUAGCAG CGAUAGUCGGGUG AGAACCCCGACGGC CUAAUGGAUAAGG GUUCCUCAGCACUG CUGAUCAGCUGAGG GUUAGCCGGUCCUA AGUCAUACCGCAAC UCGACUAUGACGAA AUGGGAAACGGGU UAAUAUUCCCGUGC CACUAUGCAGUGAA AGUUGACGCCCUGG GGUCGAUCACGCUG GGCAUUCGCCCAGU CGAACCGUCCAACU CCGUGGAAGCCGUA AUGGCAGGAAGCG GACGAACGGCGGCA UAGGGAAACGUGA UUCAACCUGGGGCC CAUGAAAAGACGA GCAUAGUGUCCGUA CCGAGAACCGACAC AGGUGUCCAUGGCG GCGAAAGCCAAGGC CUGUCGGGAGCAAC CAACGUUAGGGAA UUCGGCAAGUUAG UCCCGUACCUUCGG AAGAAGGGAUGCC UGCUCCGGAACGGA |  |  |  |  |  |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | GCAGGUCGCAGUGA CUCGGAAGCUCGGA CUGUCUAGUAACAA CAUAGGUGACCGCA AAUCCGCAAGGACU CGUACGGUCACUGA AUCCUGCCCAGUGC AGGUAUCUGAACAC CUCGUACAAGAGGA CGAAGGACCUGUCA ACGGCGGGGGUAAC UAUGACCCUCUUAA GGUAGCGUAGUACC UUGCCGCAUCAGUA GCGGCUUGCAUGAA UGGAUUAACCAGA GCUUCACUGUCCCA ACGUUGGGCCCGGU GAACUGUACAUUCC AGUGCGGAGUCUG GAGACACCCAGGGG GAAGCGAAGACCCU AUGGAGCUUUACU GCAGGCUGUCGCUG AGACGUGGUCGCCG AUGUGCAGCAUAG GUAGGAGACACUAC ACAGGUACCCGCGC UAGCGGGCCACCGA GUCAACAGUGAAA UACUACCCGUCGGU GACUGCGACUCUCA CUCCGGGAGGAGGA CACCGAUAGCCGGG CAGUUUGACUGGG GCGGUACGCGCUCG AAAAGAUAUCGAG CGCGCCCUAUGGCU AUCUCAGCCGGGAC AGAGACCCGGCGAA GAGUGCAAGAGCA AAAGAUAGCUUGA CAGUGUUCUUCCCA ACGAGGAACGCUGA CGCGAAAGCGUGGU CUAGCGAACCAAUU AGCCUGCUUGAUGC GGGCAAUUGAUGA CAGAAAAGCUACCC UAGGGAUAACAGA GUCGUCACUCGCAA GAGCACAUAUCGAC CGAGUGGCUUGCUA CCUCGAUGUCGGUU CCCUCCAUCCUGCC CGUGCAGAAGCGGG CAAGGGUGAGGUU GUUCGCCUAUUAAA GGAGGUCGUGAGC UGGGUUUAGACCG UCGUGAGACAGGUC GGCUGCUAUCUACU GGGUGUGUAAUGG UGUCUGACAAGAAC GACCGUAUAGUACG AGAGGAACUACGG UUGGUGGCCACUGG UGUACCGGUUGUUC GAGAGAGCACGUGC CGGGUAGCCACGCC ACACGGGGUAAGA GCUGAACGCAUCUA AGCUCGAAACCCAC UUGGAAAAGAGAC ACCGCCGAGGUCCC |  |  |  |  |  |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | GCGUACAAGACGCG GUCGAUAGACUCGG GGUGUGCGCGUCGA GGUAACGAGACGU UAAGCCCACGAGCA CUAACAGACCAAAG CCAUCAU |  |  |  |  |  |
| 296 | CC1C=CC(=O)NCC=C C(=CC(CC(=O)CC2=N C(=CO2)C(=O)N3CCC  =C3C(=O)OC1C(C)C) O)C | UUGGCUACUAUGCC AGCUGGUGGAUUG CUCGGCUCAGGCGC UGAUGAAGGACGU GCCAAGCUGCGAUA AGCCAUGGGGAGCC GCACGGAGGCGAAG AACCAUGGAUUUCC GAAUGAGAAUCUC UCUAACAAUUGCUU CGCGCAAUGAGGAA CCCCGAGAACUGAA ACAUCUCAGUAUCG GGAGGAACAGAAA ACGCAAUGUGAUG UCGUUAGUAACCGC GAGUGAACGCGAU ACAGCCCAAACCGA AGCCCUCACGGGCA AUGUGGUGUCAGG GCUACCUCUCAUCA GCCGACCGUCUCGA CGAAGUCUCUUGGA ACAGAGCGUGAUAC AGGGUGACAACCCC GUACUCGAGACCAG UACGACGUGCGGUA GUGCCAGAGUAGCG GGGGUUGGAUAUC CCUCGCGAAUAACG CAGGCAUCGACUGC GAAGGCUAAACACA ACCUGAGACCGAUA GUGAACAAGUAGU GUGAACGAACGCUG CAAAGUACCCUCAG AAGGGAGGCGAAA UAGAGCAUGAAAU CAGUUGGCGAUCGA GCGACAGGGCAUAC AAGGUCCCUCGACG AAUGACCGACGCGC GAGCGUCCAGUAAG ACUCACGGGAAGCC GAUGUUCUGUCGU ACGUUUUGAAAAA CGAGCCAGGGAGUG UGUCUGCAUGGCAA GUCUAACCGGAGUA UCCGGGGAGGCACA GGGAAACCGACAUG GCCGCAGGGCUUUG CCCGAGGGCCGCCG UCUUCAAGGGCGGG GAGCCAUGUGGACA CGACCCGAAUCCGG ACGAUCUACGCAUG GACAAGAUGAAGC GUGCCGAAAGGCAC GUGGAAGUCUGUU AGAGUUGGUGUCC UACAAUACCCUCUC GUGAUCUAUGUGU AGGGGUGAAAGGC CCAUCGAGUCCGGC AACAGCUGGUUCCA AUCGAAACAUGUCG AAGCAUGACCUCCG | Pristinamycin IIA | Target\_lig\_23 4 | PTC | Target\_99 | 6.85387196  432176 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | CCGAGGUAGUCUGU GAGGUAGAGCGACC GAUUGGUGUGUCC GCCUCCGAGAGGAG UCGGCACACCUGUC AAACUCCAAACUUA CAGACGCCGUUUGA CGCGGGGAUUCCGG UGCGCGGGGUAAGC CUGUGUACCAGGAG GGGAACAACCCAGA GAUAGGUUAAGGU CCCCAAGUGUGGAU UAAGUGUAAUCCUC UGAAGGUGGUCUC GAGCCCUAGACAGC CGGGAGGUGAGCU UAGAAGCAGCUACC CUCUAAGAAAAGCG UAACAGCUUACCGG CCGAGGUUUGAGGC GCCCAAAAUGAUCG GGACUCAAAUCCAC CACCGAGACCUGUC CGUACCACUCAUAC UGGUAAUCGAGUA GAUUGGCGCUCUAA UUGGAUGGAAGUA GGGGUGAAAACUCC UAUGGACCGAUUA GUGACGAAAAUCCU GGCCAUAGUAGCAG CGAUAGUCGGGUG AGAACCCCGACGGC CUAAUGGAUAAGG GUUCCUCAGCACUG CUGAUCAGCUGAGG GUUAGCCGGUCCUA AGUCAUACCGCAAC UCGACUAUGACGAA AUGGGAAACGGGU UAAUAUUCCCGUGC CACUAUGCAGUGAA AGUUGACGCCCUGG GGUCGAUCACGCUG GGCAUUCGCCCAGU CGAACCGUCCAACU CCGUGGAAGCCGUA AUGGCAGGAAGCG GACGAACGGCGGCA UAGGGAAACGUGA UUCAACCUGGGGCC CAUGAAAAGACGA GCAUAGUGUCCGUA CCGAGAACCGACAC AGGUGUCCAUGGCG GCGAAAGCCAAGGC CUGUCGGGAGCAAC CAACGUUAGGGAA UUCGGCAAGUUAG UCCCGUACCUUCGG AAGAAGGGAUGCC UGCUCCGGAACGGA GCAGGUCGCAGUGA CUCGGAAGCUCGGA CUGUCUAGUAACAA CAUAGGUGACCGCA AAUCCGCAAGGACU CGUACGGUCACUGA AUCCUGCCCAGUGC AGGUAUCUGAACAC CUCGUACAAGAGGA CGAAGGACCUGUCA ACGGCGGGGGUAAC UAUGACCCUCUUAA |  |  |  |  |  |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | GGUAGCGUAGUACC UUGCCGCAUCAGUA GCGGCUUGCAUGAA UGGAUUAACCAGA GCUUCACUGUCCCA ACGUUGGGCCCGGU GAACUGUACAUUCC AGUGCGGAGUCUG GAGACACCCAGGGG GAAGCGAAGACCCU AUGGAGCUUUACU GCAGGCUGUCGCUG AGACGUGGUCGCCG AUGUGCAGCAUAG GUAGGAGACACUAC ACAGGUACCCGCGC UAGCGGGCCACCGA GUCAACAGUGAAA UACUACCCGUCGGU GACUGCGACUCUCA CUCCGGGAGGAGGA CACCGAUAGCCGGG CAGUUUGACUGGG GCGGUACGCGCUCG AAAAGAUAUCGAG CGCGCCCUAUGGCU AUCUCAGCCGGGAC AGAGACCCGGCGAA GAGUGCAAGAGCA AAAGAUAGCUUGA CAGUGUUCUUCCCA ACGAGGAACGCUGA CGCGAAAGCGUGGU CUAGCGAACCAAUU AGCCUGCUUGAUGC GGGCAAUUGAUGA CAGAAAAGCUACCC UAGGGAUAACAGA GUCGUCACUCGCAA GAGCACAUAUCGAC CGAGUGGCUUGCUA CCUCGAUGUCGGUU CCCUCCAUCCUGCC CGUGCAGAAGCGGG CAAGGGUGAGGUU GUUCGCCUAUUAAA GGAGGUCGUGAGC UGGGUUUAGACCG UCGUGAGACAGGUC GGCUGCUAUCUACU GGGUGUGUAAUGG UGUCUGACAAGAAC GACCGUAUAGUACG AGAGGAACUACGG UUGGUGGCCACUGG UGUACCGGUUGUUC GAGAGAGCACGUGC CGGGUAGCCACGCC ACACGGGGUAAGA GCUGAACGCAUCUA AGCUCGAAACCCAC UUGGAAAAGAGAC ACCGCCGAGGUCCC GCGUACAAGACGCG GUCGAUAGACUCGG GGUGUGCGCGUCGA GGUAACGAGACGU UAAGCCCACGAGCA CUAACAGACCAAAG CCAUCAU |  |  |  |  |  |
| 297 | CCC1C(=O)N2CCCC2 C(=O)N(C(C(=O)N3C C(C(=O)CC3C(=O)NC (C(=O)OC(C(C(=O)N1  )NC(=O)C4=C(C=CC= | UUGGCUACUAUGCC AGCUGGUGGAUUG CUCGGCUCAGGCGC UGAUGAAGGACGU GCCAAGCUGCGAUA | Quinupristin | Target\_lig\_23 5 | PTC | Target\_99 | 6.49485002  168009 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  | N4)O)C)C5=CC=CC= C5)CSC6CN7CCC6CC 7)CC8=CC=C(C=C8)N (C)C)C | AGCCAUGGGGAGCC GCACGGAGGCGAAG AACCAUGGAUUUCC GAAUGAGAAUCUC UCUAACAAUUGCUU CGCGCAAUGAGGAA CCCCGAGAACUGAA ACAUCUCAGUAUCG GGAGGAACAGAAA ACGCAAUGUGAUG UCGUUAGUAACCGC GAGUGAACGCGAU ACAGCCCAAACCGA AGCCCUCACGGGCA AUGUGGUGUCAGG GCUACCUCUCAUCA GCCGACCGUCUCGA CGAAGUCUCUUGGA ACAGAGCGUGAUAC AGGGUGACAACCCC GUACUCGAGACCAG UACGACGUGCGGUA GUGCCAGAGUAGCG GGGGUUGGAUAUC CCUCGCGAAUAACG CAGGCAUCGACUGC GAAGGCUAAACACA ACCUGAGACCGAUA GUGAACAAGUAGU GUGAACGAACGCUG CAAAGUACCCUCAG AAGGGAGGCGAAA UAGAGCAUGAAAU CAGUUGGCGAUCGA GCGACAGGGCAUAC AAGGUCCCUCGACG AAUGACCGACGCGC GAGCGUCCAGUAAG ACUCACGGGAAGCC GAUGUUCUGUCGU ACGUUUUGAAAAA CGAGCCAGGGAGUG UGUCUGCAUGGCAA GUCUAACCGGAGUA UCCGGGGAGGCACA GGGAAACCGACAUG GCCGCAGGGCUUUG CCCGAGGGCCGCCG UCUUCAAGGGCGGG GAGCCAUGUGGACA CGACCCGAAUCCGG ACGAUCUACGCAUG GACAAGAUGAAGC GUGCCGAAAGGCAC GUGGAAGUCUGUU AGAGUUGGUGUCC UACAAUACCCUCUC GUGAUCUAUGUGU AGGGGUGAAAGGC CCAUCGAGUCCGGC AACAGCUGGUUCCA AUCGAAACAUGUCG AAGCAUGACCUCCG CCGAGGUAGUCUGU GAGGUAGAGCGACC GAUUGGUGUGUCC GCCUCCGAGAGGAG UCGGCACACCUGUC AAACUCCAAACUUA CAGACGCCGUUUGA CGCGGGGAUUCCGG UGCGCGGGGUAAGC CUGUGUACCAGGAG GGGAACAACCCAGA GAUAGGUUAAGGU |  |  |  |  |  |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | CCCCAAGUGUGGAU UAAGUGUAAUCCUC UGAAGGUGGUCUC GAGCCCUAGACAGC CGGGAGGUGAGCU UAGAAGCAGCUACC CUCUAAGAAAAGCG UAACAGCUUACCGG CCGAGGUUUGAGGC GCCCAAAAUGAUCG GGACUCAAAUCCAC CACCGAGACCUGUC CGUACCACUCAUAC UGGUAAUCGAGUA GAUUGGCGCUCUAA UUGGAUGGAAGUA GGGGUGAAAACUCC UAUGGACCGAUUA GUGACGAAAAUCCU GGCCAUAGUAGCAG CGAUAGUCGGGUG AGAACCCCGACGGC CUAAUGGAUAAGG GUUCCUCAGCACUG CUGAUCAGCUGAGG GUUAGCCGGUCCUA AGUCAUACCGCAAC UCGACUAUGACGAA AUGGGAAACGGGU UAAUAUUCCCGUGC CACUAUGCAGUGAA AGUUGACGCCCUGG GGUCGAUCACGCUG GGCAUUCGCCCAGU CGAACCGUCCAACU CCGUGGAAGCCGUA AUGGCAGGAAGCG GACGAACGGCGGCA UAGGGAAACGUGA UUCAACCUGGGGCC CAUGAAAAGACGA GCAUAGUGUCCGUA CCGAGAACCGACAC AGGUGUCCAUGGCG GCGAAAGCCAAGGC CUGUCGGGAGCAAC CAACGUUAGGGAA UUCGGCAAGUUAG UCCCGUACCUUCGG AAGAAGGGAUGCC UGCUCCGGAACGGA GCAGGUCGCAGUGA CUCGGAAGCUCGGA CUGUCUAGUAACAA CAUAGGUGACCGCA AAUCCGCAAGGACU CGUACGGUCACUGA AUCCUGCCCAGUGC AGGUAUCUGAACAC CUCGUACAAGAGGA CGAAGGACCUGUCA ACGGCGGGGGUAAC UAUGACCCUCUUAA GGUAGCGUAGUACC UUGCCGCAUCAGUA GCGGCUUGCAUGAA UGGAUUAACCAGA GCUUCACUGUCCCA ACGUUGGGCCCGGU GAACUGUACAUUCC AGUGCGGAGUCUG GAGACACCCAGGGG GAAGCGAAGACCCU AUGGAGCUUUACU GCAGGCUGUCGCUG |  |  |  |  |  |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | AGACGUGGUCGCCG AUGUGCAGCAUAG GUAGGAGACACUAC ACAGGUACCCGCGC UAGCGGGCCACCGA GUCAACAGUGAAA UACUACCCGUCGGU GACUGCGACUCUCA CUCCGGGAGGAGGA CACCGAUAGCCGGG CAGUUUGACUGGG GCGGUACGCGCUCG AAAAGAUAUCGAG CGCGCCCUAUGGCU AUCUCAGCCGGGAC AGAGACCCGGCGAA GAGUGCAAGAGCA AAAGAUAGCUUGA CAGUGUUCUUCCCA ACGAGGAACGCUGA CGCGAAAGCGUGGU CUAGCGAACCAAUU AGCCUGCUUGAUGC GGGCAAUUGAUGA CAGAAAAGCUACCC UAGGGAUAACAGA GUCGUCACUCGCAA GAGCACAUAUCGAC CGAGUGGCUUGCUA CCUCGAUGUCGGUU CCCUCCAUCCUGCC CGUGCAGAAGCGGG CAAGGGUGAGGUU GUUCGCCUAUUAAA GGAGGUCGUGAGC UGGGUUUAGACCG UCGUGAGACAGGUC GGCUGCUAUCUACU GGGUGUGUAAUGG UGUCUGACAAGAAC GACCGUAUAGUACG AGAGGAACUACGG UUGGUGGCCACUGG UGUACCGGUUGUUC GAGAGAGCACGUGC CGGGUAGCCACGCC ACACGGGGUAAGA GCUGAACGCAUCUA AGCUCGAAACCCAC UUGGAAAAGAGAC ACCGCCGAGGUCCC GCGUACAAGACGCG GUCGAUAGACUCGG GGUGUGCGCGUCGA GGUAACGAGACGU UAAGCCCACGAGCA CUAACAGACCAAAG CCAUCAU |  |  |  |  |  |
| 298 | CCN(CC)CCSCC(=O) OC1CC(C(C(C23CCC( C1(C2C(=O)CC3)C)C) C)O)(C)C=C | UUGGCUACUAUGCC AGCUGGUGGAUUG CUCGGCUCAGGCGC UGAUGAAGGACGU GCCAAGCUGCGAUA AGCCAUGGGGAGCC GCACGGAGGCGAAG AACCAUGGAUUUCC GAAUGAGAAUCUC UCUAACAAUUGCUU CGCGCAAUGAGGAA CCCCGAGAACUGAA ACAUCUCAGUAUCG GGAGGAACAGAAA ACGCAAUGUGAUG UCGUUAGUAACCGC GAGUGAACGCGAU | Tiamulin | Target\_lig\_23 6 | PTC | Target\_99 | 6.82681373  158773 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | ACAGCCCAAACCGA AGCCCUCACGGGCA AUGUGGUGUCAGG GCUACCUCUCAUCA GCCGACCGUCUCGA CGAAGUCUCUUGGA ACAGAGCGUGAUAC AGGGUGACAACCCC GUACUCGAGACCAG UACGACGUGCGGUA GUGCCAGAGUAGCG GGGGUUGGAUAUC CCUCGCGAAUAACG CAGGCAUCGACUGC GAAGGCUAAACACA ACCUGAGACCGAUA GUGAACAAGUAGU GUGAACGAACGCUG CAAAGUACCCUCAG AAGGGAGGCGAAA UAGAGCAUGAAAU CAGUUGGCGAUCGA GCGACAGGGCAUAC AAGGUCCCUCGACG AAUGACCGACGCGC GAGCGUCCAGUAAG ACUCACGGGAAGCC GAUGUUCUGUCGU ACGUUUUGAAAAA CGAGCCAGGGAGUG UGUCUGCAUGGCAA GUCUAACCGGAGUA UCCGGGGAGGCACA GGGAAACCGACAUG GCCGCAGGGCUUUG CCCGAGGGCCGCCG UCUUCAAGGGCGGG GAGCCAUGUGGACA CGACCCGAAUCCGG ACGAUCUACGCAUG GACAAGAUGAAGC GUGCCGAAAGGCAC GUGGAAGUCUGUU AGAGUUGGUGUCC UACAAUACCCUCUC GUGAUCUAUGUGU AGGGGUGAAAGGC CCAUCGAGUCCGGC AACAGCUGGUUCCA AUCGAAACAUGUCG AAGCAUGACCUCCG CCGAGGUAGUCUGU GAGGUAGAGCGACC GAUUGGUGUGUCC GCCUCCGAGAGGAG UCGGCACACCUGUC AAACUCCAAACUUA CAGACGCCGUUUGA CGCGGGGAUUCCGG UGCGCGGGGUAAGC CUGUGUACCAGGAG GGGAACAACCCAGA GAUAGGUUAAGGU CCCCAAGUGUGGAU UAAGUGUAAUCCUC UGAAGGUGGUCUC GAGCCCUAGACAGC CGGGAGGUGAGCU UAGAAGCAGCUACC CUCUAAGAAAAGCG UAACAGCUUACCGG CCGAGGUUUGAGGC GCCCAAAAUGAUCG GGACUCAAAUCCAC CACCGAGACCUGUC |  |  |  |  |  |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | CGUACCACUCAUAC UGGUAAUCGAGUA GAUUGGCGCUCUAA UUGGAUGGAAGUA GGGGUGAAAACUCC UAUGGACCGAUUA GUGACGAAAAUCCU GGCCAUAGUAGCAG CGAUAGUCGGGUG AGAACCCCGACGGC CUAAUGGAUAAGG GUUCCUCAGCACUG CUGAUCAGCUGAGG GUUAGCCGGUCCUA AGUCAUACCGCAAC UCGACUAUGACGAA AUGGGAAACGGGU UAAUAUUCCCGUGC CACUAUGCAGUGAA AGUUGACGCCCUGG GGUCGAUCACGCUG GGCAUUCGCCCAGU CGAACCGUCCAACU CCGUGGAAGCCGUA AUGGCAGGAAGCG GACGAACGGCGGCA UAGGGAAACGUGA UUCAACCUGGGGCC CAUGAAAAGACGA GCAUAGUGUCCGUA CCGAGAACCGACAC AGGUGUCCAUGGCG GCGAAAGCCAAGGC CUGUCGGGAGCAAC CAACGUUAGGGAA UUCGGCAAGUUAG UCCCGUACCUUCGG AAGAAGGGAUGCC UGCUCCGGAACGGA GCAGGUCGCAGUGA CUCGGAAGCUCGGA CUGUCUAGUAACAA CAUAGGUGACCGCA AAUCCGCAAGGACU CGUACGGUCACUGA AUCCUGCCCAGUGC AGGUAUCUGAACAC CUCGUACAAGAGGA CGAAGGACCUGUCA ACGGCGGGGGUAAC UAUGACCCUCUUAA GGUAGCGUAGUACC UUGCCGCAUCAGUA GCGGCUUGCAUGAA UGGAUUAACCAGA GCUUCACUGUCCCA ACGUUGGGCCCGGU GAACUGUACAUUCC AGUGCGGAGUCUG GAGACACCCAGGGG GAAGCGAAGACCCU AUGGAGCUUUACU GCAGGCUGUCGCUG AGACGUGGUCGCCG AUGUGCAGCAUAG GUAGGAGACACUAC ACAGGUACCCGCGC UAGCGGGCCACCGA GUCAACAGUGAAA UACUACCCGUCGGU GACUGCGACUCUCA CUCCGGGAGGAGGA CACCGAUAGCCGGG CAGUUUGACUGGG GCGGUACGCGCUCG |  |  |  |  |  |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | AAAAGAUAUCGAG CGCGCCCUAUGGCU AUCUCAGCCGGGAC AGAGACCCGGCGAA GAGUGCAAGAGCA AAAGAUAGCUUGA CAGUGUUCUUCCCA ACGAGGAACGCUGA CGCGAAAGCGUGGU CUAGCGAACCAAUU AGCCUGCUUGAUGC GGGCAAUUGAUGA CAGAAAAGCUACCC UAGGGAUAACAGA GUCGUCACUCGCAA GAGCACAUAUCGAC CGAGUGGCUUGCUA CCUCGAUGUCGGUU CCCUCCAUCCUGCC CGUGCAGAAGCGGG CAAGGGUGAGGUU GUUCGCCUAUUAAA GGAGGUCGUGAGC UGGGUUUAGACCG UCGUGAGACAGGUC GGCUGCUAUCUACU GGGUGUGUAAUGG UGUCUGACAAGAAC GACCGUAUAGUACG AGAGGAACUACGG UUGGUGGCCACUGG UGUACCGGUUGUUC GAGAGAGCACGUGC CGGGUAGCCACGCC ACACGGGGUAAGA GCUGAACGCAUCUA AGCUCGAAACCCAC UUGGAAAAGAGAC ACCGCCGAGGUCCC GCGUACAAGACGCG GUCGAUAGACUCGG GGUGUGCGCGUCGA GGUAACGAGACGU UAAGCCCACGAGCA CUAACAGACCAAAG CCAUCAU |  |  |  |  |  |
| 299 | CC1CCC23CCC(=O)C 2C1(C(CC(C(C3C)O)  (C)C=C)OC(=O)CSC( C) (C)CNC(=O)C(C(C)C) N)C | UUGGCUACUAUGCC AGCUGGUGGAUUG CUCGGCUCAGGCGC UGAUGAAGGACGU GCCAAGCUGCGAUA AGCCAUGGGGAGCC GCACGGAGGCGAAG AACCAUGGAUUUCC GAAUGAGAAUCUC UCUAACAAUUGCUU CGCGCAAUGAGGAA CCCCGAGAACUGAA ACAUCUCAGUAUCG GGAGGAACAGAAA ACGCAAUGUGAUG UCGUUAGUAACCGC GAGUGAACGCGAU ACAGCCCAAACCGA AGCCCUCACGGGCA AUGUGGUGUCAGG GCUACCUCUCAUCA GCCGACCGUCUCGA CGAAGUCUCUUGGA ACAGAGCGUGAUAC AGGGUGACAACCCC GUACUCGAGACCAG UACGACGUGCGGUA GUGCCAGAGUAGCG GGGGUUGGAUAUC | Valnemulin | Target\_lig\_23 7 | PTC | Target\_99 | 11.3010299  95664 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | CCUCGCGAAUAACG CAGGCAUCGACUGC GAAGGCUAAACACA ACCUGAGACCGAUA GUGAACAAGUAGU GUGAACGAACGCUG CAAAGUACCCUCAG AAGGGAGGCGAAA UAGAGCAUGAAAU CAGUUGGCGAUCGA GCGACAGGGCAUAC AAGGUCCCUCGACG AAUGACCGACGCGC GAGCGUCCAGUAAG ACUCACGGGAAGCC GAUGUUCUGUCGU ACGUUUUGAAAAA CGAGCCAGGGAGUG UGUCUGCAUGGCAA GUCUAACCGGAGUA UCCGGGGAGGCACA GGGAAACCGACAUG GCCGCAGGGCUUUG CCCGAGGGCCGCCG UCUUCAAGGGCGGG GAGCCAUGUGGACA CGACCCGAAUCCGG ACGAUCUACGCAUG GACAAGAUGAAGC GUGCCGAAAGGCAC GUGGAAGUCUGUU AGAGUUGGUGUCC UACAAUACCCUCUC GUGAUCUAUGUGU AGGGGUGAAAGGC CCAUCGAGUCCGGC AACAGCUGGUUCCA AUCGAAACAUGUCG AAGCAUGACCUCCG CCGAGGUAGUCUGU GAGGUAGAGCGACC GAUUGGUGUGUCC GCCUCCGAGAGGAG UCGGCACACCUGUC AAACUCCAAACUUA CAGACGCCGUUUGA CGCGGGGAUUCCGG UGCGCGGGGUAAGC CUGUGUACCAGGAG GGGAACAACCCAGA GAUAGGUUAAGGU CCCCAAGUGUGGAU UAAGUGUAAUCCUC UGAAGGUGGUCUC GAGCCCUAGACAGC CGGGAGGUGAGCU UAGAAGCAGCUACC CUCUAAGAAAAGCG UAACAGCUUACCGG CCGAGGUUUGAGGC GCCCAAAAUGAUCG GGACUCAAAUCCAC CACCGAGACCUGUC CGUACCACUCAUAC UGGUAAUCGAGUA GAUUGGCGCUCUAA UUGGAUGGAAGUA GGGGUGAAAACUCC UAUGGACCGAUUA GUGACGAAAAUCCU GGCCAUAGUAGCAG CGAUAGUCGGGUG AGAACCCCGACGGC CUAAUGGAUAAGG GUUCCUCAGCACUG |  |  |  |  |  |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | CUGAUCAGCUGAGG GUUAGCCGGUCCUA AGUCAUACCGCAAC UCGACUAUGACGAA AUGGGAAACGGGU UAAUAUUCCCGUGC CACUAUGCAGUGAA AGUUGACGCCCUGG GGUCGAUCACGCUG GGCAUUCGCCCAGU CGAACCGUCCAACU CCGUGGAAGCCGUA AUGGCAGGAAGCG GACGAACGGCGGCA UAGGGAAACGUGA UUCAACCUGGGGCC CAUGAAAAGACGA GCAUAGUGUCCGUA CCGAGAACCGACAC AGGUGUCCAUGGCG GCGAAAGCCAAGGC CUGUCGGGAGCAAC CAACGUUAGGGAA UUCGGCAAGUUAG UCCCGUACCUUCGG AAGAAGGGAUGCC UGCUCCGGAACGGA GCAGGUCGCAGUGA CUCGGAAGCUCGGA CUGUCUAGUAACAA CAUAGGUGACCGCA AAUCCGCAAGGACU CGUACGGUCACUGA AUCCUGCCCAGUGC AGGUAUCUGAACAC CUCGUACAAGAGGA CGAAGGACCUGUCA ACGGCGGGGGUAAC UAUGACCCUCUUAA GGUAGCGUAGUACC UUGCCGCAUCAGUA GCGGCUUGCAUGAA UGGAUUAACCAGA GCUUCACUGUCCCA ACGUUGGGCCCGGU GAACUGUACAUUCC AGUGCGGAGUCUG GAGACACCCAGGGG GAAGCGAAGACCCU AUGGAGCUUUACU GCAGGCUGUCGCUG AGACGUGGUCGCCG AUGUGCAGCAUAG GUAGGAGACACUAC ACAGGUACCCGCGC UAGCGGGCCACCGA GUCAACAGUGAAA UACUACCCGUCGGU GACUGCGACUCUCA CUCCGGGAGGAGGA CACCGAUAGCCGGG CAGUUUGACUGGG GCGGUACGCGCUCG AAAAGAUAUCGAG CGCGCCCUAUGGCU AUCUCAGCCGGGAC AGAGACCCGGCGAA GAGUGCAAGAGCA AAAGAUAGCUUGA CAGUGUUCUUCCCA ACGAGGAACGCUGA CGCGAAAGCGUGGU CUAGCGAACCAAUU AGCCUGCUUGAUGC GGGCAAUUGAUGA |  |  |  |  |  |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | CAGAAAAGCUACCC UAGGGAUAACAGA GUCGUCACUCGCAA GAGCACAUAUCGAC CGAGUGGCUUGCUA CCUCGAUGUCGGUU CCCUCCAUCCUGCC CGUGCAGAAGCGGG CAAGGGUGAGGUU GUUCGCCUAUUAAA GGAGGUCGUGAGC UGGGUUUAGACCG UCGUGAGACAGGUC GGCUGCUAUCUACU GGGUGUGUAAUGG UGUCUGACAAGAAC GACCGUAUAGUACG AGAGGAACUACGG UUGGUGGCCACUGG UGUACCGGUUGUUC GAGAGAGCACGUGC CGGGUAGCCACGCC ACACGGGGUAAGA GCUGAACGCAUCUA AGCUCGAAACCCAC UUGGAAAAGAGAC ACCGCCGAGGUCCC GCGUACAAGACGCG GUCGAUAGACUCGG GGUGUGCGCGUCGA GGUAACGAGACGU UAAGCCCACGAGCA CUAACAGACCAAAG CCAUCAU |  |  |  |  |  |
| 310 | CC1C(C(CC(O1)OC2C (OC3(CC2O)OC4C(OC (C(C4(O3)C)O)OC5C( C(OC(C5OC)C)OC6C( OC(C(C6O)OC)OC7C( C8C(CO7)OC9(O8)C1 C(C(CO9)OC(=O)C2= C(C=C(C=C2C)O)O)O CO1)O)COC)O)C)C)O  C1CC(C(C(O1)C)OC)  (C)[N+](=O)  [O-])OC(=O)C1=C(C(=  C(C(=C1OC)Cl)O)Cl)C | GGUUAAGCGACUA AGCGUACACGGUGG AUGCCCUGGCAGUC AGAGGCGAUGAAG GACGUGCUAAUCUG CGAUAAGCGUCGGU AAGGUGAUAUGAA CCGUUAUAACCGGC GAUUUCCGAAUGG GGAAACCCAGUGUG UUUCGACACACUAU CAUUAACUGAAUCC AUAGGUUAAUGAG GCGAACCGGGGGAA CUGAAACAUCUAAG UACCCCGAGGAAAA GAAAUCAACCGAGA UUCCCCCAGUAGCG GCGAGCGAACGGGG AGCAGCCCAGAGCC UGAAUCAGUGUGU GUGUUAGUGGAAG CGUCUGGAAAGGCG CGCGAUACAGGGUG ACAGCCCCGUACAC AAAAAUGCACAUGC UGUGAGCUCGAUG AGUAGGGCGGGAC ACGUGGUAUCCUGU CUGAAUAUGGGGG GACCAUCCUCCAAG GCUAAAUACUCCUG ACUGACCGAUAGUG AACCAGUACCGUGA GGGAAAGGCGAAA AGAACCCCGGCGAG GGGAGUGAAAAAG AACCUGAAACCGUG UACGUACAAGCAGU GGGAGCACGCUUAG GCGUGUGACUGCGU | Evernimicin | Target\_lig\_24 7 | Bacterial 23S rRNA  hairpins 82  and 91 | Target\_102 | 4.52287874  528034 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | ACCUUUUGUAUAA UGGGUCAGCGACUU AUAUUCUGUAGCA AGGUUAACCGAAU AGGGGAGCCGAAG GGAAACCGAGUCUU AACUGGGCGUUAA GUUGCAGGGUAUA GACCCGAAACCCGG UGAUCUAGCCAUGG GCAGGUUGAAGGU UGGGUAACACUAAC UGGAGGACCGAACC GACUAAUGUUGAA AAAUUAGCGGAUG ACUUGUGGCUGGG GGUGAAAGGCCAA UCAAACCGGGAGAU AGCUGGUUCUCCCC GAAAGCUAUUUAG GUAGCGCCUCGUGA AUUCAUCUCCGGGG GUAGAGCACUGUU UCGGCAAGGGGGUC AUCCCGACUUACCA ACCCGAUGCAAACU GCGAAUACCGGAGA AUGUUAUCACGGG AGACACACGGCGGG UGCUAACGUCCGUC GUGAAGAGGGAAA CAACCCAGACCGCC AGCUAAGGUCCCAA AGUCAUGGUUAAG UGGGAAACGAUGU GGGAAGGCCCAGAC AGCCAGGAUGUUG GCUUAGAAGCAGCC AUCAUUUAAAGAA AGCGUAAUAGCUCA CUGGUCGAGUCGGC CUGCGCGGAAGAUG UAACGGGGCUAAAC CAUGCACCGAAGCU GCGGCAGCGACGCU UAUGCGUUGUUGG GUAGGGGAGCGUU CUGUAAGCCUGCGA AGGUGUGCUGUGA GGCAUGCUGGAGG UAUCAGAAGUGCG AAUGCUGACAUAA GUAACGAUAAAGC GGGUGAAAAGCCCG CUCGCCGGAAGACC AAGGGUUCCUGUCC AACGUUAAUCGGG GCAGGGUGAGUCG ACCCCUAAGGCGAG GCCGAAAGGCGUAG UCGAUGGGAAACA GGUUAAUAUUCCU GUACUUGGUGUUA CUGCGAAGGGGGG ACGGAGAAGGCUA UGUUGGCCGGGCGA CGGUUGUCCCGGUU UAAGCGUGUAGGC UGGUUUUCCAGGCA AAUCCGGAAAAUCA AGGCUGAGGCGUG AUGACGAGGCACUA CGGUGCUGAAGCAA CAAAUGCCCUGCUU CCAGGAAAAGCCUC |  |  |  |  |  |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | UAAGCAUCAGGUA ACAUCAAAUCGUAC CCCAAACCGACACU GGUGGUCAGGUAG AGAAUACCAAGGCG CUUGAGAGAACUCG GGUGAAGGAACUA GGCAAAAUGGUGCC GUAACUUCGGGAG AAGGCACGCUGAUA UGUAGGUGAGGUC CCUCGCGGAUGGAG CUGAAAUCAGUCGA AGAUACCAGCUGGC UGCAACUGUUUAU UAAAAACACAGCAC UGUGCAAACACGAA AGUGGACGUAUAC GGUGUGACGCCUGC CCGGUGCCGGAAGG UUAAUUGAUGGGG UUAGCGCAAGCGAA GCUCUUGAUCGAAG CCCCGGUAAACGGC GGCCGUAACUAUAA CGGUCCUAAGGUAG CGAAAUUCCUUGUC GGGUAAGUUCCGAC CUGCACGAAUGGCG UAAUGAUGGCCAG GCUGUCUCCACCCG AGACUCAGUGAAA UUGAACUCGCUGUG CAGAUGCAGUGUAC CCGCGGCAAGACGG AAAGACCCCGUGAA CCUUUACUAUAGCU UGACACUGAACAUU GAGCCUUGAUGUG UAGGAUAGGUGGG AGGCUUUGAAGUG UGGACGCCAGUCUG CAUGGAGCCGACCU UGAAAUACCACCCU UUAAUGUUUGAUG UUCUAACGUUGACC CGUAAUCCGGGUUG CGGACAGUGUCUGG UGGGUAGUUUGAC UGGGGCGGUCUCCU CCUAAAGAGUAACG GAGGAGCACGAAG GUUGGCUAAUCCUG GUCGGACAUCAGGA GGUUAGUGCAAUG GCAUAAGCCAGCUU GACUGCGAGCGUGA CGGCGCGAGCAGGU GCGAAAGCAGGUCA UAGUGAUCCGGUG GUUCUGAAUGGAA GGGCCAUCGCUCAA CGGAUAAAAGGUA CUCCGGGGAUAACA GGCUGAUACCGCCC AAGAGUUCAUAUC GACGGCGGUGUUU GGCACCUCGAUGUC GGCUCAUCACAUCC UGGGGCUGAAGUA GGUCCCAAGGGUAU GGCUGUUCGCCAUU UAAAGUGGUACGC GAGCUGGGUUUAG AACGUCGUGAGACA |  |  |  |  |  |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | GUUCGGUCCCUAUC UGCCGUGGGCGCUG GAGAACUGAGGGG GGCUGCUCCUAGUA CGAGAGGACCGGAG UGGACGCAUCACUG GUGUUCGGGUUGU CAUGCCAAUGGCAC UGCCCGGUAGCUAA AUGCGGAAGAGAU AAGUGCUGAAAGC AUCUAAGCACGAAA CUUGCCCCGAGAUG AGUUCUCCCUGACC CUUUAAGGGUCCUG AAGGAACGUUGAA GACGACGACGUUGA UAGGCCGGGUGUG UAAGCGCAGCGAUG CGUUGAGCUAACCG GUACUAAUGAACCG UGAGGCUUAACCUU |  |  |  |  |  |
| 321 | [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)CNc1c2ccccc2nc2 c1cccc2)O)N)O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Tobramycin | Target\_lig\_54 0 | Bacterial ribosomal A- site | Target\_3 | 7 |
| 323 | C1C(C(C(C(C1N)OC2 C(C(C(C(O2)CN)O)O)  N)OC3C(C(C(O3)CO) O)O)O)N | GAGCGUCACACCUU CGGGUGAAGUCGCU C | ribostamycin | Target\_lig\_9 | Bacterial ribosomal A- site | Target\_3 | 5.76955107  862173 |
| 324 | C1C(C(C(C(C1N)OC2 C(CC(C(O2)CO)O)N) OC3C(C(C(O3)CO)OC 4C(C(C(C(O4)CN)OC5  C(C(C(C(O5)CO)O)O) O)O)N)O)O)N | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Lividomycin A | Target\_lig\_12 47 | Bacterial ribosomal A- site | Target\_3 | 7.55284196  865778 |
| 325 | [C@@H]1([C@H]  ([C@@H]([C@H]  (O[C@@H]1CO)O[C @@H]1[C@H] ([C@@H]([C@H]  (C[C@H]1N)N)O)O[C  @H]1O[C@H]([C@H]  ([C@@H]1OCCc1cccc c1)O[C@@H]1[C@H]  ([C@@H]([C@@H] ([C@@H] (O1)N)O)O)N)CO)N)O  )O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Phenyl ether paromomycin derivative 1 | Target\_lig\_25 1 | Bacterial ribosomal A- site | Target\_3 | 5.42021640  338319 |
| 326 | [C@H]1([C@H]  ([C@@H]([C@H]  (O[C@@H]1CO)O[C @H]1[C@@H] ([C@@H]([C@@H]  (C[C@@H]1N)N)O)O[ C@@H]1OC[C@@H]  ([C@H]1OCCNc1cncc c1)O[C@@H]1[C@H]  ([C@@H](C[C@@H]  (O1)CN)O)N)N)O)O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Aminoglycoside derivative 1 | Target\_lig\_25 2 | Bacterial ribosomal A- site | Target\_3 | 6.22184874  961636 |
| 327 | [C@@H]1([C@@H]  ([C@@H]([C@@H]  (O[C@H]1CO)O[C@  @H]1[C@H]([C@@H] | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Aminoglycoside derivative 2 | Target\_lig\_25 3 | Bacterial ribosomal A- site | Target\_3 | 6.04575749  056068 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  | ([C@H] (C[C@H]1N)N)O)O[C @H]1OC[C@@H] ([C@@H]1OCCNCc1n  cccc1)O[C@@H]1[C@ H]([C@@H]  (C[C@@H] (O1)CN)O)N)N)O)O |  |  |  |  |  |  |
| 328 | [C@H]1([C@@H]  ([C@H]([C@@H]  (O[C@H]1CO)O[C@H  ]1[C@@H]([C@@H] ([C@H] (C[C@@H]1N)N)O)O[ C@@H]1OC[C@H] ([C@@H]1OCCNCCC N)O[C@H]1[C@@H]  ([C@H](C[C@H]  (O1)CN)O)N)N)O)O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Aminoglycoside derivative 3 | Target\_lig\_25 4 | Bacterial ribosomal A- site | Target\_3 | 6.39794000  867204 |
| 329 | [C@@H]1([C@@H]  ([C@H]([C@H]  (O[C@@H]1CO)O[C  @H]1[C@@H]([C@H] ([C@H] (C[C@H]1N)N)O)O[C  @@H]1OC[C@@H] ([C@H]1OCCNCCN)O [C@@H]1[C@H] ([C@@H](C[C@@H]  (O1)CN)O)N)N)O)O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Aminoglycoside derivative 4 | Target\_lig\_25 5 | Bacterial ribosomal A- site | Target\_3 | 6.15490195  998574 |
| 330 | [C@@H]1([C@@H]  ([C@H]([C@@H]  (O[C@@H]1CO)O[C @@H]1[C@H] ([C@@H]([C@H]  (C[C@@H]1N)N)O)O[ C@H]1OC[C@H] ([C@@H]1OCCN)O[C  @H]1[C@@H]([C@H] (C[C@H] (O1)CN)O)N)N)O)O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Aminoglycoside derivative 6 | Target\_lig\_25 6 | Bacterial ribosomal A- site | Target\_3 | 6.52287874  528034 |
| 331 | [C@H]1([C@H]  ([C@@H]([C@@H]  (O[C@H]1CO)O[C@ @H]1[C@@H] ([C@@H]([C@H]  (C[C@H]1N)N)O)O[C  @@H]1OC[C@@H] ([C@H]1OCCNCCNC CN)O[C@@H]1[C@@ H]([C@H](C[C@H]  (O1)CN)O)N)N)O)O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Aminoglycoside derivative 7 | Target\_lig\_25 7 | Bacterial ribosomal A- site | Target\_3 | 5.03621217  265444 |
| 332 | [C@@H]1([C@@H]  ([C@H]([C@@H]  (O[C@@H]1CO)O[C @@H]1[C@H] ([C@@H]([C@H]  (C[C@H]1N)N)O)O[C @@H]1OC[C@H] ([C@@H]1OCCNCCN 1CCNCC1)O[C@H]1[ C@H]([C@@H]  (C[C@@H] (O1)CN)O)N)N)O)O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Aminoglycoside derivative 8 | Target\_lig\_25 8 | Bacterial ribosomal A- site | Target\_3 | 5.88605664  769316 |
| 333 | [C@H]1([C@H]  ([C@@H]([C@H]  (O[C@H]1CO)O[C@H  ]1[C@@H]([C@H] ([C@@H] (C[C@@H]1N)N)O)O[ C@@H]1OC[C@H] | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Aminoglycoside derivative 9 | Target\_lig\_25 9 | Bacterial ribosomal A- site | Target\_3 | 7 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  | ([C@H]1OCCNC1CC NCC1)O[C@H]1[C@ @H]([C@H](C[C@H]  (O1)CN)O)N)N)O)O |  |  |  |  |  |  |
| 334 | [C@@H]1([C@H]  ([C@@H]([C@H]  (O[C@@H]1CO)O[C @H]1[C@@H] ([C@@H]([C@H]  (C[C@@H]1N)N)O)O[ C@H]1OC[C@H] ([C@@H]1OCCNC[C @H]1CNCCC1)O[C@ @H]1[C@@H]([C@H] (C[C@@H] (O1)CN)O)N)N)O)O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Aminoglycoside derivative 10 | Target\_lig\_26 0 | Bacterial ribosomal A- site | Target\_3 | 6.52287874  528034 |
| 335 | [C@H]1([C@H]  ([C@H]([C@@H]  (O[C@@H]1CO)O[C  @@H]1[C@@H] ([C@H]([C@@H]  (C[C@@H]1N)N)O)O[ C@@H]1OC[C@@H]  ([C@H]1OCCNc1ccnc 2c1cccc2)O[C@@H]1[ C@H]([C@@H]  (C[C@@H] (O1)CN)O)N)N)O)O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Aminoglycoside derivative 12 | Target\_lig\_26 1 | Bacterial ribosomal A- site | Target\_3 | 7 |
| 336 | [C@H]1([C@H]  ([C@@H]([C@H]  (O[C@H]1CO)O[C@  @H]1[C@H]([C@@H] ([C@H] (C[C@H]1N)N)O)O[C @H]1OC[C@H] ([C@@H]1OCCNC1C CCCC1)O[C@H]1[C@ @H]([C@H](C[C@H]  (O1)CN)O)N)N)O)O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Aminoglycoside derivative 13 | Target\_lig\_26 2 | Bacterial ribosomal A- site | Target\_3 | 7 |
| 337 | [C@@H]1([C@@H]  ([C@H]([C@H]  (O[C@@H]1CO)O[C @@H]1[C@H] ([C@@H]([C@@H]  (C[C@@H]1N)N)O)O[ C@H]1OC[C@@H] ([C@H]1OCCNCCc1c  nccc1)O[C@@H]1[C@ H]([C@@H]  (C[C@@H] (O1)CN)O)N)N)O)O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Aminoglycoside derivative 14 | Target\_lig\_26 3 | Bacterial ribosomal A- site | Target\_3 | 6.69897000  433602 |
| 338 | [C@H]1([C@H]  ([C@@H]([C@H]  (O[C@H]1CO)O[C@H  ]1[C@@H]([C@@H] ([C@@H] (C[C@H]1N)N)O)O[C @H]1OC[C@@H] ([C@H]1OCCNCCc1c  cccc1)O[C@@H]1[C@ H]([C@@H]  (C[C@@H] (O1)CN)O)N)N)O)O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Aminoglycoside derivative 15 | Target\_lig\_26 4 | Bacterial ribosomal A- site | Target\_3 | 7 |
| 339 | [C@H]1([C@@H]  ([C@H]([C@@H]  (O[C@H]1CO)O[C@H  ]1[C@@H]([C@H] ([C@@H] (C[C@@H]1N)N)O)O[ C@@H]1OC[C@@H] ([C@H]1OCCNCc1ccc | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Aminoglycoside derivative 16 | Target\_lig\_26 5 | Bacterial ribosomal A- site | Target\_3 | 7 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  | cc1)O[C@@H]1[C@H  ]([C@@H](C[C@@H]  (O1)CN)O)N)N)O)O |  |  |  |  |  |  |
| 340 | [C@H]1([C@H]  ([C@H]([C@@H]  (O[C@H]1CO)O[C@H  ]1[C@@H]([C@@H] ([C@H] (C[C@H]1N)N)O)O[C @@H]1OC[C@H]  ([C@H]1OCCNc1cccc( c1)O)O[C@@H]1[C@  @H]([C@H]  (C[C@@H] (O1)CN)O)N)N)O)O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Aminoglycoside derivative 17 | Target\_lig\_26 6 | Bacterial ribosomal A- site | Target\_3 | 6.22184874  961636 |
| 341 | [C@H]1([C@H]  ([C@@H]([C@@H]  (O[C@@H]1CO)O[C  @@H]1[C@@H] ([C@H]([C@H]  (C[C@@H]1N)N)O)O[ C@@H]1OC[C@H] ([C@H]1OCCNCc1cnc (cc1)N)O[C@@H]1[C @@H]([C@H]  (C[C@@H] (O1)CN)O)N)N)O)O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Aminoglycoside derivative 18 | Target\_lig\_26 7 | Bacterial ribosomal A- site | Target\_3 | 7 |
| 342 | [C@H]1([C@H]  ([C@@H]([C@H]  (O[C@@H]1CO)O[C  @@H]1[C@H]([C@H] ([C@@H] (C[C@H]1N)N)O)O[C @H]1OC[C@@H] ([C@H]1OCCNCc1ccn c(c1)N)O[C@H]1[C@  H]([C@@H](C[C@H]  (O1)CN)O)N)N)O)O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Aminoglycoside derivative 19 | Target\_lig\_26 8 | Bacterial ribosomal A- site | Target\_3 | 7.69897000  433602 |
| 343 | [C@H]1([C@H]  ([C@@H]([C@@H]  (O[C@H]1CO)O[C@  @H]1[C@H]([C@@H] ([C@H] (C[C@@H]1N)N)O)O[ C@H]1OC[C@@H]  ([C@@H]1OCCNc1nc ccc1)O[C@@H]1[C@ H]([C@@H]  (C[C@@H] (O1)CN)O)N)N)O)O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Aminoglycoside derivative 20 | Target\_lig\_26 9 | Bacterial ribosomal A- site | Target\_3 | 5.30102999  566398 |
| 344 | [C@@H]1([C@@H]  ([C@H]([C@H]  (O[C@H]1CO)O[C@H  ]1[C@@H]([C@H] ([C@@H] (C[C@H]1N)N)O)O[C  @@H]1OC[C@@H] ([C@H]1OCCNCCC(C  ) (C)C)O[C@H]1[C@H]  ([C@@H](C[C@@H]  (O1)CN)O)N)N)O)O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Aminoglycoside derivative 21 | Target\_lig\_27 0 | Bacterial ribosomal A- site | Target\_3 | 5.60205999  132796 |
| 345 | [C@H]1([C@H]  ([C@@H]([C@H]  (O[C@H]1CO)O[C@  @H]1[C@H]([C@H] ([C@@H] (C[C@H]1N)N)O)O[C @H]1OC[C@H] ([C@@H]1OCCNCCC  c1ccccc1)O[C@@H]1[ | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Aminoglycoside derivative 22 | Target\_lig\_27 1 | Bacterial ribosomal A- site | Target\_3 | 6 |

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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]  (C[C@@H] (O1)CN)O)N)N)O)O |  |  |  |  |  |  |
| 346 | [C@H]1([C@H]  ([C@H]([C@@H]  (O[C@H]1CO)O[C@  @H]1[C@H]([C@@H] ([C@@H] (C[C@H]1N)N)O)O[C @H]1OC[C@@H] ([C@H]1OCCNCCCCc  1ccccc1)O[C@H]1[C@ @H]([C@H](C[C@H]  (O1)CN)O)N)N)O)O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Aminoglycoside derivative 24 | Target\_lig\_27 2 | Bacterial ribosomal A- site | Target\_3 | 6.15490195  998574 |
| 347 | [C@H]1([C@H]  ([C@@H]([C@H]  (O[C@H]1CO)O[C@  @H]1[C@H]([C@H] ([C@@H] (C[C@H]1N)N)O)O[C  @@H]1OC[C@@H] ([C@@H]1OCCNCCc  1ccc(cc1)c1ccccc1)O[C @H]1[C@H]([C@@H] (C[C@@H] (O1)CN)O)N)N)O)O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Aminoglycoside derivative 25 | Target\_lig\_27 3 | Bacterial ribosomal A- site | Target\_3 | 6.04575749  056068 |
| 348 | [C@H]1([C@H]  ([C@@H]([C@H]  (O[C@H]1CO)O[C@H  ]1[C@@H]([C@@H] ([C@H] (C[C@H]1N)N)O)O[C  @@H]1OC[C@@H] ([C@H]1OCCN)O[C@  @H]1[C@H]([C@@H] (C[C@@H] (O1)CN)O)NCCc1cc2c  (cc1)cccc2)N)O)O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Aminoglycoside derivative 33 | Target\_lig\_27 4 | Bacterial ribosomal A- site | Target\_3 | 6.15490195  998574 |
| 349 | [C@@H]1([C@H]  ([C@H]([C@@H]  (O[C@H]1CN(C)C)O[ C@H]1[C@@H] ([C@H]([C@H]  (C[C@H]1N)N)O)O[C  @@H]1O[C@@H] ([C@@H] ([C@@H]1O)O[C@H] 1CO[C@@H] ([C@@H] ([C@H]1O)O)CN)CO) N)O)O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Perazidoparomo mycin derivative 1 | Target\_lig\_27 5 | Bacterial ribosomal A- site | Target\_3 | 6.22184874  961636 |
| 350 | [C@@H]1([C@H]  ([C@H]([C@H] (O[C@@H]1CNCCCN  )O[C@H]1[C@@H]  ([C@H]([C@H]  (C[C@H]1N)N)O)O[C  @@H]1O[C@@H] ([C@H] ([C@@H]1O)O[C@@ H]1CO[C@@H] ([C@@H] ([C@H]1O)O)CN)CO) N)O)O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Perazidoparomo mycin derivative 2 | Target\_lig\_27 6 | Bacterial ribosomal A- site | Target\_3 | 5.79588001  734408 |
| 351 | [C@@H]1([C@@H]  ([C@H]([C@H] (O[C@H]1CCN1CCO CC1)O[C@H]1[C@@ H]([C@H]([C@H]  (C[C@H]1N)N)O)O[C @H]1O[C@@H] | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Perazidoparomo mycin derivative 3 | Target\_lig\_27 7 | Bacterial ribosomal A- site | Target\_3 | 5.44369749  923271 |

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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]1O)O[C@@ H]1CO[C@@H] ([C@@H] ([C@H]1O)O)CN)CO) N)O)O |  |  |  |  |  |  |
| 352 | [C@@H]1([C@H]  ([C@H]([C@H]  (O[C@H]1CNNC(=O) OC(C) (C)C)O[C@H]1[C@@  H]([C@H]([C@H]  (C[C@H]1N)N)O)O[C @H]1O[C@@H] ([C@H] ([C@@H]1O)O[C@@ H]1CO[C@H] ([C@@H] ([C@H]1O)O)CN)CO) N)O)O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Perazidoparomo mycin derivative 4 | Target\_lig\_27 8 | Bacterial ribosomal A- site | Target\_3 | 8 |
| 353 | [C@H]1([C@H]  ([C@H]([C@H]  (O[C@H]1CNC)O[C@  H]1[C@@H]([C@H] ([C@H] (C[C@H]1N)N)O)O[C  @@H]1O[C@@H] ([C@H] ([C@@H]1O)O[C@@ H]1CO[C@@H] ([C@@H] ([C@H]1O)O)CN)CO) N)O)O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Perazidoparomo mycin derivative 5 | Target\_lig\_27 9 | Bacterial ribosomal A- site | Target\_3 | 6.39794000  867204 |
| 354 | [C@@H]1([C@H]  ([C@H]([C@H] (O[C@@H]1CNCCCC N)O[C@H]1[C@@H]  ([C@H]([C@H]  (C[C@H]1N)N)O)O[C @H]1O[C@@H] ([C@H] ([C@@H]1O)O[C@@ H]1CO[C@H] ([C@@H] ([C@H]1O)O)CN)CO) N)O)O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Perazidoparomo mycin derivative 6 | Target\_lig\_28 0 | Bacterial ribosomal A- site | Target\_3 | 5.20065945  054642 |
| 355 | [C@H]1([C@@H]  ([C@H]([C@H]  (O[C@@H]1CNCC(C)  C)O[C@H]1[C@@H]  ([C@H]([C@H]  (C[C@H]1N)N)O)O[C @H]1O[C@@H] ([C@H] ([C@@H]1O)O[C@@ H]1CO[C@H] ([C@@H] ([C@H]1O)O)CN)CO) N)O)O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Perazidoparomo mycin derivative 8 | Target\_lig\_28 1 | Bacterial ribosomal A- site | Target\_3 | 5.92081875  395238 |
| 356 | [C@@H]1([C@@H]  ([C@H]([C@H]  (O[C@H]1CNN)O[C@  H]1[C@@H]([C@H] ([C@H] (C[C@H]1N)N)O)O[C @H]1O[C@@H] ([C@H] ([C@@H]1O)O[C@@ H]1CO[C@@H] ([C@@H] ([C@H]1O)O)CN)CO) N)O)O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Perazidoparomo mycin derivative 9 | Target\_lig\_28 2 | Bacterial ribosomal A- site | Target\_3 | 6.22184874  961636 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
| 357 | [C@H]1([C@H]  ([C@H]([C@H] (O[C@@H]1CNCCc1c  cccc1)O[C@H]1[C@@ H]([C@H]([C@H]  (C[C@H]1N)N)O)O[C @H]1O[C@@H] ([C@@H] ([C@@H]1O)O[C@H] 1CO[C@@H] ([C@@H] ([C@H]1O)O)CN)CO) N)O)O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Perazidoparomo mycin derivative 10 | Target\_lig\_28 3 | Bacterial ribosomal A- site | Target\_3 | 6.30102999  566398 |
| 358 | [C@@H]1([C@@H]  ([C@H]([C@H] (O[C@H]1CN(CCc1cc ccc1)C)O[C@H]1[C@ @H]([C@H]([C@H]  (C[C@H]1N)N)O)O[C  @@H]1O[C@@H] ([C@@H] ([C@H]1O)O[C@H]1C  O[C@@H]([C@@H]  ([C@H]1O)O)CN)CO) N)O)O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Perazidoparomo mycin derivative 11 | Target\_lig\_28 4 | Bacterial ribosomal A- site | Target\_3 | 5.65757731  917779 |
| 359 | [C@@H]1([C@H]  ([C@@H]([C@H] (O[C@@H]1CNCCCc  1ccccc1)O[C@H]1[C@ @H]([C@H]([C@H]  (C[C@H]1N)N)O)O[C @H]1O[C@@H] ([C@H] ([C@@H]1O)O[C@@ H]1CO[C@@H] ([C@@H] ([C@H]1O)O)CN)CO) N)O)O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Perazidoparomo mycin derivative 12 | Target\_lig\_28 5 | Bacterial ribosomal A- site | Target\_3 | 5.85387196  432176 |
| 360 | [C@H]1([C@H]  ([C@H]([C@H] (O[C@@H]1CNCCc1c cc(cc1)C1CCCCC1)O[ C@H]1[C@@H] ([C@H]([C@H]  (C[C@H]1N)N)O)O[C @H]1O[C@@H] ([C@@H] ([C@@H]1O)O[C@H] 1CO[C@@H] ([C@@H] ([C@H]1O)O)CN)CO) N)O)O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Perazidoparomo mycin derivative 13 | Target\_lig\_28 6 | Bacterial ribosomal A- site | Target\_3 | 5.31875876  262441 |
| 361 | [C@@H]1([C@@H]  ([C@H]([C@H] (O[C@H]1CNCCc1c(c ccc1)OC)O[C@H]1[C @@H]([C@H]([C@H]  (C[C@H]1N)N)O)O[C @H]1O[C@@H] ([C@H] ([C@@H]1O)O[C@@ H]1CO[C@@H] ([C@@H] ([C@H]1O)O)CN)CO) N)O)O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Perazidoparomo mycin derivative 14 | Target\_lig\_28 7 | Bacterial ribosomal A- site | Target\_3 | 5.09691001  300806 |
| 362 | [C@H]1([C@H]  ([C@H]([C@H] (O[C@H]1CNCCc1ccc (cc1)F)O[C@H]1[C@  @H]([C@H]([C@H]  (C[C@H]1N)N)O)O[C  @@H]1O[C@@H] | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Perazidoparomo mycin derivative 15 | Target\_lig\_28 8 | Bacterial ribosomal A- site | Target\_3 | 2.85387196  432176 |

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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]1O)O[C@H] 1CO[C@@H] ([C@@H] ([C@H]1O)O)CN)CO) N)O)O |  |  |  |  |  |  |
| 363 | [C@H]1([C@H]  ([C@H]([C@H] (O[C@@H]1CN[C@@ H]  (Cc1ccccc1)C)O[C@H] 1[C@@H]([C@H] ([C@H] (C[C@H]1N)N)O)O[C @H]1O[C@@H] ([C@H] ([C@@H]1O)O[C@@ H]1CO[C@@H] ([C@@H] ([C@H]1O)O)CN)CO) N)O)O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Perazidoparomo mycin derivative 16 | Target\_lig\_28 9 | Bacterial ribosomal A- site | Target\_3 | 2.63827216  398241 |
| 364 | [C@H]1([C@H]  ([C@H]([C@H] (O[C@@H]1CNCCc1c  cc(cc1)C(F) (F)F)O[C@H]1[C@@  H]([C@H]([C@H]  (C[C@H]1N)N)O)O[C  @@H]1O[C@@H] ([C@@H] ([C@@H]1O)O[C@H] 1CO[C@@H] ([C@@H] ([C@H]1O)O)CN)CO) N)O)O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Perazidoparomo mycin derivative 17 | Target\_lig\_29 0 | Bacterial ribosomal A- site | Target\_3 | 2.53760200  210104 |
| 365 | [C@@H]1([C@H]  ([C@H]([C@H] (O[C@@H]1CNCCc1c cc(cc1)OC)O[C@H]1[ C@@H]([C@H]  ([C@H] (C[C@H]1N)N)O)O[C  @@H]1O[C@@H] ([C@H] ([C@@H]1O)O[C@@ H]1CO[C@@H] ([C@@H] ([C@H]1O)O)CN)CO) N)O)O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Perazidoparomo mycin derivative 18 | Target\_lig\_29 1 | Bacterial ribosomal A- site | Target\_3 | 2.20760831  050175 |
| 366 | [C@H]1([C@H]  ([C@H]([C@H] (O[C@@H]1CN1C[C @H]2[C@H] (C1)CCCC2)O[C@H]1 [C@@H]([C@H] ([C@H] (C[C@H]1N)N)O)O[C @H]1O[C@@H] ([C@@H] ([C@@H]1O)O[C@H] 1CO[C@@H] ([C@@H] ([C@H]1O)O)CN)CO) N)O)O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Perazidoparomo mycin derivative 19 | Target\_lig\_29 2 | Bacterial ribosomal A- site | Target\_3 | 1.88941028  970075 |
| 367 | [C@@H]1([C@@H]  ([C@H]([C@H] (O[C@H]1CN[C@@H  ]([C@@H]  (c1ccccc1)O)C)O[C@ H]1[C@@H]([C@H] ([C@H] (C[C@H]1N)N)O)O[C | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Perazidoparomo mycin derivative 20 | Target\_lig\_29 3 | Bacterial ribosomal A- site | Target\_3 | 1.78781239  559604 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  | @H]1O[C@@H] ([C@H] ([C@@H]1O)O[C@@ H]1CO[C@@H] ([C@@H] ([C@H]1O)O)CN)CO) N)O)O |  |  |  |  |  |  |
| 368 | [C@H]1([C@H]  ([C@H]([C@H] (O[C@H]1CNCCc1cc(  ccc1)C(F) (F)F)O[C@H]1[C@@  H]([C@H]([C@H]  (C[C@H]1N)N)O)O[C  @@H]1O[C@@H] ([C@@H] ([C@@H]1O)O[C@H]  1CO[C@@H]([C@H]  ([C@H]1O)O)CN)CO) N)O)O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Perazidoparomo mycin derivative 21 | Target\_lig\_29 4 | Bacterial ribosomal A- site | Target\_3 | 1.69464863  055338 |
| 369 | [C@H]1([C@H]  ([C@H]([C@H] (O[C@@H]1CNCCc1c c(ccc1)OC)O[C@H]1[ C@@H]([C@H]  ([C@H] (C[C@H]1N)N)O)O[C @H]1O[C@@H] ([C@@H] ([C@@H]1O)O[C@H] 1CO[C@@H] ([C@@H] ([C@H]1O)O)CN)CO) N)O)O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Perazidoparomo mycin derivative 22 | Target\_lig\_29 5 | Bacterial ribosomal A- site | Target\_3 | 7 |
| 370 | [C@H]1([C@H]  ([C@@H]([C@H] (O[C@@H]1CCN1C[C @@H]2[C@H] (C1)CCCC2)O[C@H]1 [C@@H]([C@H] ([C@H] (C[C@H]1N)N)O)O[C @H]1O[C@@H] ([C@H] ([C@@H]1O)O[C@@ H]1CO[C@@H] ([C@@H] ([C@H]1O)O)CN)CO) N)O)O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Perazidoparomo mycin derivative 23 | Target\_lig\_29 6 | Bacterial ribosomal A- site | Target\_3 | 3 |
| 371 | [C@@H]1([C@H]  ([C@H]([C@H] (O[C@@H]1CNCC[C @H]1CCCNC1)O[C@ H]1[C@@H]([C@H] ([C@H] (C[C@H]1N)N)O)O[C @H]1O[C@@H] ([C@@H] ([C@@H]1O)O[C@H] 1CO[C@@H] ([C@@H] ([C@H]1O)O)CN)CO) N)O)O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Perazidoparomo mycin derivative 26 | Target\_lig\_29 7 | Bacterial ribosomal A- site | Target\_3 | 5.28399665  63652 |
| 372 | [C@@H]1([C@H]  ([C@H]([C@H] (O[C@@H]1CNCC[C @H]1NCCCC1)O[C@ H]1[C@@H]([C@H] ([C@H] (C[C@H]1N)N)O)O[C  @@H]1O[C@@H] ([C@H] | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Perazidoparomo mycin derivative 27 | Target\_lig\_29 8 | Bacterial ribosomal A- site | Target\_3 | 5.44369749  923271 |

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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]1CO[C@@H] ([C@@H] ([C@H]1O)O)CN)CO) N)O)O |  |  |  |  |  |  |
| 373 | [C@H]1([C@H]  ([C@@H]([C@H]  (C[C@@H]1CO)O[C  @@H]1[C@@H] ([C@H]([C@@H]  (C[C@@H]1N)N)O)O[  C@@H]1O[C@@H] ([C@H] ([C@H]1OCCN(CCc1c  cccc1)C(=O)c1ccccc1) O[C@@H]1[C@H] ([C@H]([C@@H] ([C@H] (O1)N)O)O)N)CO)N)O  )O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Benzoyl paromomycin derivative | Target\_lig\_29 9 | Bacterial ribosomal A- site | Target\_3 | 5.40893539  29735 |
| 374 | [C@@H]1([C@@H]  ([C@H]([C@@H]  (C[C@@H]1CO)O[C  @@H]1[C@H]([C@H] ([C@@H] (C[C@@H]1N)N)O)O[ C@H]1O[C@H] ([C@H] ([C@@H]1OCCN(CCc 1ccccc1)C(=O)C)O[C @@H]1[C@H] ([C@@H]([C@H] ([C@H] (O1)N)O)O)N)CO)N)O  )O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Acetyl parmomycin derivative | Target\_lig\_30 0 | Bacterial ribosomal A- site | Target\_3 | 5.82390874  094432 |
| 375 | [C@@H]1([C@@H]  ([C@H]([C@@H]  (C[C@@H]1CO)O[C  @@H]1[C@H]([C@H] ([C@@H] (C[C@@H]1N)N)O)O[ C@H]1O[C@H] ([C@H] ([C@@H]1OCCN(CCc 1ccccc1)C(=O)C)O[C @@H]1[C@H] ([C@@H]([C@H] ([C@H] (O1)N)O)O)N)CO)N)O  )O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Ether paromomycin derivative 1 | Target\_lig\_111 2 | Bacterial ribosomal A- site | Target\_3 | 6.04575749  056068 |
| 376 | [C@@H]1([C@H]  ([C@H]([C@@H]  (C[C@H]1CO)O[C@H  ]1[C@H]([C@H] ([C@@H] (C[C@@H]1N)N)O)O[  C@@H]1O[C@@H] ([C@H] ([C@@H]1OC[C@@H  ]  (O)c1ccccc1)O[C@H]1 [C@H]([C@@H]  ([C@H]([C@H]  (O1)N)O)O)N)CO)N)O  )O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Ether paromomycin derivative 3 | Target\_lig\_30 1 | Bacterial ribosomal A- site | Target\_3 | 5.56863623  584101 |
| 377 | [C@H]1([C@@H]  ([C@H]([C@@H]  (C[C@H]1CO)O[C@  @H]1[C@@H]([C@H] ([C@@H] (C[C@H]1N)N)O)O[C @H]1O[C@@H] | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Ether paromomycin derivative 4 | Target\_lig\_30 2 | Bacterial ribosomal A- site | Target\_3 | 4.72124639  904717 |

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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]1OCCN)O)C O)N)O)O |  |  |  |  |  |  |
| 378 | [C@H]1([C@H]  ([C@H]([C@@H]  (C[C@@H]1CO)O[C @H]1[C@@H] ([C@@H]([C@H]  (C[C@H]1N)N)O)O[C  @@H]1O[C@@H] ([C@H] ([C@H]1OCCNCN)O) CO)N)O)O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Ether paromomycin derivative 5 | Target\_lig\_30 3 | Bacterial ribosomal A- site | Target\_3 | 5.03621217  265444 |
| 379 | [C@H]1([C@@H]  ([C@H]([C@H]  (C[C@@H]1CO)O[C @H]1[C@@H] ([C@@H]([C@H]  (C[C@H]1N)N)O)O[C  @@H]1O[C@@H] ([C@H] ([C@H]1O)O[C@H]1[ C@@H]([C@H] ([C@@H]([C@@H]  (O1)CN)O)O)N)COCN  (C)C)N)O)O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Ethyl paromomycin derivative 2 | Target\_lig\_30 4 | Bacterial ribosomal A- site | Target\_3 | 5.38721614  328026 |
| 380 | [C@H]1([C@H]  ([C@@H]([C@@H]  (C[C@H]1CO)O[C@  @H]1[C@H]([C@H] ([C@@H] (C[C@@H]1N)N)O)O[  C@@H]1O[C@@H] ([C@H] ([C@H]1O)O[C@@H]  1[C@@H]([C@H]  ([C@H]([C@H]  (O1)CN)O)O)N)COF) N)O)O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Deoxy fluoro paromomycin | Target\_lig\_30 5 | Bacterial ribosomal A- site | Target\_3 | 5.95860731  484177 |
| 381 | C1C(C(C(C(C1N)OC2 C(C(C(C(O2)CO)O)N)  O)O)OC3C(C(C(C(O3) CN)O)O)N)N | GAGCGUCACACCUU CGGGUGAAGUCGCU C | KANAMYCIN B | Target\_lig\_8 | A-site for Kanamycin B | Target\_3 | 7.09691001  300806 |
| 382 | CC1C(CC(C(O1)OC2C (C(C(C(C2O)O)O)O)O  )N)N=C(C(=O)O)N | UUGGCUACUAUGCC AGCUGGUGGAUUG CUCGGCUCAGGCGC UGAUGAAGGACGU GCCAAGCUGCGAUA AGCCAUGGGGAGCC GCACGGAGGCGAAG AACCAUGGAUUUCC GAAUGAGAAUCUC UCUAACAAUUGCUU CGCGCAAUGAGGAA CCCCGAGAACUGAA ACAUCUCAGUAUCG GGAGGAACAGAAA ACGCAAUGUGAUG UCGUUAGUAACCGC GAGUGAACGCGAU ACAGCCCAAACCGA AGCCCUCACGGGCA AUGUGGUGUCAGG GCUACCUCUCAUCA GCCGACCGUCUCGA CGAAGUCUCUUGGA ACAGAGCGUGAUAC AGGGUGACAACCCC GUACUCGAGACCAG UACGACGUGCGGUA GUGCCAGAGUAGCG GGGGUUGGAUAUC | Kasugamycin | Target\_lig\_78 | Bacterial 70S ribosome | Target\_99 | 4.82390874  094432 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | CCUCGCGAAUAACG CAGGCAUCGACUGC GAAGGCUAAACACA ACCUGAGACCGAUA GUGAACAAGUAGU GUGAACGAACGCUG CAAAGUACCCUCAG AAGGGAGGCGAAA UAGAGCAUGAAAU CAGUUGGCGAUCGA GCGACAGGGCAUAC AAGGUCCCUCGACG AAUGACCGACGCGC GAGCGUCCAGUAAG ACUCACGGGAAGCC GAUGUUCUGUCGU ACGUUUUGAAAAA CGAGCCAGGGAGUG UGUCUGCAUGGCAA GUCUAACCGGAGUA UCCGGGGAGGCACA GGGAAACCGACAUG GCCGCAGGGCUUUG CCCGAGGGCCGCCG UCUUCAAGGGCGGG GAGCCAUGUGGACA CGACCCGAAUCCGG ACGAUCUACGCAUG GACAAGAUGAAGC GUGCCGAAAGGCAC GUGGAAGUCUGUU AGAGUUGGUGUCC UACAAUACCCUCUC GUGAUCUAUGUGU AGGGGUGAAAGGC CCAUCGAGUCCGGC AACAGCUGGUUCCA AUCGAAACAUGUCG AAGCAUGACCUCCG CCGAGGUAGUCUGU GAGGUAGAGCGACC GAUUGGUGUGUCC GCCUCCGAGAGGAG UCGGCACACCUGUC AAACUCCAAACUUA CAGACGCCGUUUGA CGCGGGGAUUCCGG UGCGCGGGGUAAGC CUGUGUACCAGGAG GGGAACAACCCAGA GAUAGGUUAAGGU CCCCAAGUGUGGAU UAAGUGUAAUCCUC UGAAGGUGGUCUC GAGCCCUAGACAGC CGGGAGGUGAGCU UAGAAGCAGCUACC CUCUAAGAAAAGCG UAACAGCUUACCGG CCGAGGUUUGAGGC GCCCAAAAUGAUCG GGACUCAAAUCCAC CACCGAGACCUGUC CGUACCACUCAUAC UGGUAAUCGAGUA GAUUGGCGCUCUAA UUGGAUGGAAGUA GGGGUGAAAACUCC UAUGGACCGAUUA GUGACGAAAAUCCU GGCCAUAGUAGCAG CGAUAGUCGGGUG AGAACCCCGACGGC CUAAUGGAUAAGG GUUCCUCAGCACUG |  |  |  |  |  |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | CUGAUCAGCUGAGG GUUAGCCGGUCCUA AGUCAUACCGCAAC UCGACUAUGACGAA AUGGGAAACGGGU UAAUAUUCCCGUGC CACUAUGCAGUGAA AGUUGACGCCCUGG GGUCGAUCACGCUG GGCAUUCGCCCAGU CGAACCGUCCAACU CCGUGGAAGCCGUA AUGGCAGGAAGCG GACGAACGGCGGCA UAGGGAAACGUGA UUCAACCUGGGGCC CAUGAAAAGACGA GCAUAGUGUCCGUA CCGAGAACCGACAC AGGUGUCCAUGGCG GCGAAAGCCAAGGC CUGUCGGGAGCAAC CAACGUUAGGGAA UUCGGCAAGUUAG UCCCGUACCUUCGG AAGAAGGGAUGCC UGCUCCGGAACGGA GCAGGUCGCAGUGA CUCGGAAGCUCGGA CUGUCUAGUAACAA CAUAGGUGACCGCA AAUCCGCAAGGACU CGUACGGUCACUGA AUCCUGCCCAGUGC AGGUAUCUGAACAC CUCGUACAAGAGGA CGAAGGACCUGUCA ACGGCGGGGGUAAC UAUGACCCUCUUAA GGUAGCGUAGUACC UUGCCGCAUCAGUA GCGGCUUGCAUGAA UGGAUUAACCAGA GCUUCACUGUCCCA ACGUUGGGCCCGGU GAACUGUACAUUCC AGUGCGGAGUCUG GAGACACCCAGGGG GAAGCGAAGACCCU AUGGAGCUUUACU GCAGGCUGUCGCUG AGACGUGGUCGCCG AUGUGCAGCAUAG GUAGGAGACACUAC ACAGGUACCCGCGC UAGCGGGCCACCGA GUCAACAGUGAAA UACUACCCGUCGGU GACUGCGACUCUCA CUCCGGGAGGAGGA CACCGAUAGCCGGG CAGUUUGACUGGG GCGGUACGCGCUCG AAAAGAUAUCGAG CGCGCCCUAUGGCU AUCUCAGCCGGGAC AGAGACCCGGCGAA GAGUGCAAGAGCA AAAGAUAGCUUGA CAGUGUUCUUCCCA ACGAGGAACGCUGA CGCGAAAGCGUGGU CUAGCGAACCAAUU AGCCUGCUUGAUGC GGGCAAUUGAUGA |  |  |  |  |  |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | CAGAAAAGCUACCC UAGGGAUAACAGA GUCGUCACUCGCAA GAGCACAUAUCGAC CGAGUGGCUUGCUA CCUCGAUGUCGGUU CCCUCCAUCCUGCC CGUGCAGAAGCGGG CAAGGGUGAGGUU GUUCGCCUAUUAAA GGAGGUCGUGAGC UGGGUUUAGACCG UCGUGAGACAGGUC GGCUGCUAUCUACU GGGUGUGUAAUGG UGUCUGACAAGAAC GACCGUAUAGUACG AGAGGAACUACGG UUGGUGGCCACUGG UGUACCGGUUGUUC GAGAGAGCACGUGC CGGGUAGCCACGCC ACACGGGGUAAGA GCUGAACGCAUCUA AGCUCGAAACCCAC UUGGAAAAGAGAC ACCGCCGAGGUCCC GCGUACAAGACGCG GUCGAUAGACUCGG GGUGUGCGCGUCGA GGUAACGAGACGU UAAGCCCACGAGCA CUAACAGACCAAAG CCAUCAU |  |  |  |  |  |
| 383 | CC1=C(C(=O)NC(=O) N1)C=CC(=O)NC(CO) CS(=O)CSC | UUGGCUACUAUGCC AGCUGGUGGAUUG CUCGGCUCAGGCGC UGAUGAAGGACGU GCCAAGCUGCGAUA AGCCAUGGGGAGCC GCACGGAGGCGAAG AACCAUGGAUUUCC GAAUGAGAAUCUC UCUAACAAUUGCUU CGCGCAAUGAGGAA CCCCGAGAACUGAA ACAUCUCAGUAUCG GGAGGAACAGAAA ACGCAAUGUGAUG UCGUUAGUAACCGC GAGUGAACGCGAU ACAGCCCAAACCGA AGCCCUCACGGGCA AUGUGGUGUCAGG GCUACCUCUCAUCA GCCGACCGUCUCGA CGAAGUCUCUUGGA ACAGAGCGUGAUAC AGGGUGACAACCCC GUACUCGAGACCAG UACGACGUGCGGUA GUGCCAGAGUAGCG GGGGUUGGAUAUC CCUCGCGAAUAACG CAGGCAUCGACUGC GAAGGCUAAACACA ACCUGAGACCGAUA GUGAACAAGUAGU GUGAACGAACGCUG CAAAGUACCCUCAG AAGGGAGGCGAAA UAGAGCAUGAAAU CAGUUGGCGAUCGA GCGACAGGGCAUAC AAGGUCCCUCGACG | Sparsomycin | Target\_lig\_30 6 | Bacterial 70S ribosome | Target\_99 | 5.39794000  867204 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | AAUGACCGACGCGC GAGCGUCCAGUAAG ACUCACGGGAAGCC GAUGUUCUGUCGU ACGUUUUGAAAAA CGAGCCAGGGAGUG UGUCUGCAUGGCAA GUCUAACCGGAGUA UCCGGGGAGGCACA GGGAAACCGACAUG GCCGCAGGGCUUUG CCCGAGGGCCGCCG UCUUCAAGGGCGGG GAGCCAUGUGGACA CGACCCGAAUCCGG ACGAUCUACGCAUG GACAAGAUGAAGC GUGCCGAAAGGCAC GUGGAAGUCUGUU AGAGUUGGUGUCC UACAAUACCCUCUC GUGAUCUAUGUGU AGGGGUGAAAGGC CCAUCGAGUCCGGC AACAGCUGGUUCCA AUCGAAACAUGUCG AAGCAUGACCUCCG CCGAGGUAGUCUGU GAGGUAGAGCGACC GAUUGGUGUGUCC GCCUCCGAGAGGAG UCGGCACACCUGUC AAACUCCAAACUUA CAGACGCCGUUUGA CGCGGGGAUUCCGG UGCGCGGGGUAAGC CUGUGUACCAGGAG GGGAACAACCCAGA GAUAGGUUAAGGU CCCCAAGUGUGGAU UAAGUGUAAUCCUC UGAAGGUGGUCUC GAGCCCUAGACAGC CGGGAGGUGAGCU UAGAAGCAGCUACC CUCUAAGAAAAGCG UAACAGCUUACCGG CCGAGGUUUGAGGC GCCCAAAAUGAUCG GGACUCAAAUCCAC CACCGAGACCUGUC CGUACCACUCAUAC UGGUAAUCGAGUA GAUUGGCGCUCUAA UUGGAUGGAAGUA GGGGUGAAAACUCC UAUGGACCGAUUA GUGACGAAAAUCCU GGCCAUAGUAGCAG CGAUAGUCGGGUG AGAACCCCGACGGC CUAAUGGAUAAGG GUUCCUCAGCACUG CUGAUCAGCUGAGG GUUAGCCGGUCCUA AGUCAUACCGCAAC UCGACUAUGACGAA AUGGGAAACGGGU UAAUAUUCCCGUGC CACUAUGCAGUGAA AGUUGACGCCCUGG GGUCGAUCACGCUG GGCAUUCGCCCAGU CGAACCGUCCAACU CCGUGGAAGCCGUA |  |  |  |  |  |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | AUGGCAGGAAGCG GACGAACGGCGGCA UAGGGAAACGUGA UUCAACCUGGGGCC CAUGAAAAGACGA GCAUAGUGUCCGUA CCGAGAACCGACAC AGGUGUCCAUGGCG GCGAAAGCCAAGGC CUGUCGGGAGCAAC CAACGUUAGGGAA UUCGGCAAGUUAG UCCCGUACCUUCGG AAGAAGGGAUGCC UGCUCCGGAACGGA GCAGGUCGCAGUGA CUCGGAAGCUCGGA CUGUCUAGUAACAA CAUAGGUGACCGCA AAUCCGCAAGGACU CGUACGGUCACUGA AUCCUGCCCAGUGC AGGUAUCUGAACAC CUCGUACAAGAGGA CGAAGGACCUGUCA ACGGCGGGGGUAAC UAUGACCCUCUUAA GGUAGCGUAGUACC UUGCCGCAUCAGUA GCGGCUUGCAUGAA UGGAUUAACCAGA GCUUCACUGUCCCA ACGUUGGGCCCGGU GAACUGUACAUUCC AGUGCGGAGUCUG GAGACACCCAGGGG GAAGCGAAGACCCU AUGGAGCUUUACU GCAGGCUGUCGCUG AGACGUGGUCGCCG AUGUGCAGCAUAG GUAGGAGACACUAC ACAGGUACCCGCGC UAGCGGGCCACCGA GUCAACAGUGAAA UACUACCCGUCGGU GACUGCGACUCUCA CUCCGGGAGGAGGA CACCGAUAGCCGGG CAGUUUGACUGGG GCGGUACGCGCUCG AAAAGAUAUCGAG CGCGCCCUAUGGCU AUCUCAGCCGGGAC AGAGACCCGGCGAA GAGUGCAAGAGCA AAAGAUAGCUUGA CAGUGUUCUUCCCA ACGAGGAACGCUGA CGCGAAAGCGUGGU CUAGCGAACCAAUU AGCCUGCUUGAUGC GGGCAAUUGAUGA CAGAAAAGCUACCC UAGGGAUAACAGA GUCGUCACUCGCAA GAGCACAUAUCGAC CGAGUGGCUUGCUA CCUCGAUGUCGGUU CCCUCCAUCCUGCC CGUGCAGAAGCGGG CAAGGGUGAGGUU GUUCGCCUAUUAAA GGAGGUCGUGAGC UGGGUUUAGACCG |  |  |  |  |  |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | UCGUGAGACAGGUC GGCUGCUAUCUACU GGGUGUGUAAUGG UGUCUGACAAGAAC GACCGUAUAGUACG AGAGGAACUACGG UUGGUGGCCACUGG UGUACCGGUUGUUC GAGAGAGCACGUGC CGGGUAGCCACGCC ACACGGGGUAAGA GCUGAACGCAUCUA AGCUCGAAACCCAC UUGGAAAAGAGAC ACCGCCGAGGUCCC GCGUACAAGACGCG GUCGAUAGACUCGG GGUGUGCGCGUCGA GGUAACGAGACGU UAAGCCCACGAGCA CUAACAGACCAAAG CCAUCAU |  |  |  |  |  |
| 384 | CC(=O)NCC1CN(C(= O)O1)C2=CC(=C(C=C 2)N3CCOCC3)F | UUGGCUACUAUGCC AGCUGGUGGAUUG CUCGGCUCAGGCGC UGAUGAAGGACGU GCCAAGCUGCGAUA AGCCAUGGGGAGCC GCACGGAGGCGAAG AACCAUGGAUUUCC GAAUGAGAAUCUC UCUAACAAUUGCUU CGCGCAAUGAGGAA CCCCGAGAACUGAA ACAUCUCAGUAUCG GGAGGAACAGAAA ACGCAAUGUGAUG UCGUUAGUAACCGC GAGUGAACGCGAU ACAGCCCAAACCGA AGCCCUCACGGGCA AUGUGGUGUCAGG GCUACCUCUCAUCA GCCGACCGUCUCGA CGAAGUCUCUUGGA ACAGAGCGUGAUAC AGGGUGACAACCCC GUACUCGAGACCAG UACGACGUGCGGUA GUGCCAGAGUAGCG GGGGUUGGAUAUC CCUCGCGAAUAACG CAGGCAUCGACUGC GAAGGCUAAACACA ACCUGAGACCGAUA GUGAACAAGUAGU GUGAACGAACGCUG CAAAGUACCCUCAG AAGGGAGGCGAAA UAGAGCAUGAAAU CAGUUGGCGAUCGA GCGACAGGGCAUAC AAGGUCCCUCGACG AAUGACCGACGCGC GAGCGUCCAGUAAG ACUCACGGGAAGCC GAUGUUCUGUCGU ACGUUUUGAAAAA CGAGCCAGGGAGUG UGUCUGCAUGGCAA GUCUAACCGGAGUA UCCGGGGAGGCACA GGGAAACCGACAUG GCCGCAGGGCUUUG CCCGAGGGCCGCCG | Linezolid | Target\_lig\_30 7 | Bacterial ribosome | Target\_99 | 4.39794000  867204 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | UCUUCAAGGGCGGG GAGCCAUGUGGACA CGACCCGAAUCCGG ACGAUCUACGCAUG GACAAGAUGAAGC GUGCCGAAAGGCAC GUGGAAGUCUGUU AGAGUUGGUGUCC UACAAUACCCUCUC GUGAUCUAUGUGU AGGGGUGAAAGGC CCAUCGAGUCCGGC AACAGCUGGUUCCA AUCGAAACAUGUCG AAGCAUGACCUCCG CCGAGGUAGUCUGU GAGGUAGAGCGACC GAUUGGUGUGUCC GCCUCCGAGAGGAG UCGGCACACCUGUC AAACUCCAAACUUA CAGACGCCGUUUGA CGCGGGGAUUCCGG UGCGCGGGGUAAGC CUGUGUACCAGGAG GGGAACAACCCAGA GAUAGGUUAAGGU CCCCAAGUGUGGAU UAAGUGUAAUCCUC UGAAGGUGGUCUC GAGCCCUAGACAGC CGGGAGGUGAGCU UAGAAGCAGCUACC CUCUAAGAAAAGCG UAACAGCUUACCGG CCGAGGUUUGAGGC GCCCAAAAUGAUCG GGACUCAAAUCCAC CACCGAGACCUGUC CGUACCACUCAUAC UGGUAAUCGAGUA GAUUGGCGCUCUAA UUGGAUGGAAGUA GGGGUGAAAACUCC UAUGGACCGAUUA GUGACGAAAAUCCU GGCCAUAGUAGCAG CGAUAGUCGGGUG AGAACCCCGACGGC CUAAUGGAUAAGG GUUCCUCAGCACUG CUGAUCAGCUGAGG GUUAGCCGGUCCUA AGUCAUACCGCAAC UCGACUAUGACGAA AUGGGAAACGGGU UAAUAUUCCCGUGC CACUAUGCAGUGAA AGUUGACGCCCUGG GGUCGAUCACGCUG GGCAUUCGCCCAGU CGAACCGUCCAACU CCGUGGAAGCCGUA AUGGCAGGAAGCG GACGAACGGCGGCA UAGGGAAACGUGA UUCAACCUGGGGCC CAUGAAAAGACGA GCAUAGUGUCCGUA CCGAGAACCGACAC AGGUGUCCAUGGCG GCGAAAGCCAAGGC CUGUCGGGAGCAAC CAACGUUAGGGAA UUCGGCAAGUUAG |  |  |  |  |  |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | UCCCGUACCUUCGG AAGAAGGGAUGCC UGCUCCGGAACGGA GCAGGUCGCAGUGA CUCGGAAGCUCGGA CUGUCUAGUAACAA CAUAGGUGACCGCA AAUCCGCAAGGACU CGUACGGUCACUGA AUCCUGCCCAGUGC AGGUAUCUGAACAC CUCGUACAAGAGGA CGAAGGACCUGUCA ACGGCGGGGGUAAC UAUGACCCUCUUAA GGUAGCGUAGUACC UUGCCGCAUCAGUA GCGGCUUGCAUGAA UGGAUUAACCAGA GCUUCACUGUCCCA ACGUUGGGCCCGGU GAACUGUACAUUCC AGUGCGGAGUCUG GAGACACCCAGGGG GAAGCGAAGACCCU AUGGAGCUUUACU GCAGGCUGUCGCUG AGACGUGGUCGCCG AUGUGCAGCAUAG GUAGGAGACACUAC ACAGGUACCCGCGC UAGCGGGCCACCGA GUCAACAGUGAAA UACUACCCGUCGGU GACUGCGACUCUCA CUCCGGGAGGAGGA CACCGAUAGCCGGG CAGUUUGACUGGG GCGGUACGCGCUCG AAAAGAUAUCGAG CGCGCCCUAUGGCU AUCUCAGCCGGGAC AGAGACCCGGCGAA GAGUGCAAGAGCA AAAGAUAGCUUGA CAGUGUUCUUCCCA ACGAGGAACGCUGA CGCGAAAGCGUGGU CUAGCGAACCAAUU AGCCUGCUUGAUGC GGGCAAUUGAUGA CAGAAAAGCUACCC UAGGGAUAACAGA GUCGUCACUCGCAA GAGCACAUAUCGAC CGAGUGGCUUGCUA CCUCGAUGUCGGUU CCCUCCAUCCUGCC CGUGCAGAAGCGGG CAAGGGUGAGGUU GUUCGCCUAUUAAA GGAGGUCGUGAGC UGGGUUUAGACCG UCGUGAGACAGGUC GGCUGCUAUCUACU GGGUGUGUAAUGG UGUCUGACAAGAAC GACCGUAUAGUACG AGAGGAACUACGG UUGGUGGCCACUGG UGUACCGGUUGUUC GAGAGAGCACGUGC CGGGUAGCCACGCC ACACGGGGUAAGA GCUGAACGCAUCUA |  |  |  |  |  |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | AGCUCGAAACCCAC UUGGAAAAGAGAC ACCGCCGAGGUCCC GCGUACAAGACGCG GUCGAUAGACUCGG GGUGUGCGCGUCGA GGUAACGAGACGU UAAGCCCACGAGCA CUAACAGACCAAAG CCAUCAU |  |  |  |  |  |
| 386 | CC=C1C2=NC(=CS2) C(=O)NC(C3=NC(=CS 3)C(=O)NC(C4=NC(= CS4)C5=C(C=CC(=N5  )C6=NC(=CS6)C7=NC (=CS7)C(=O)NC(=CC) C(=O)NCC(C)O)C8=N C(=CS8)C(=O)NC(C(= O)N1)C(C)O)C(C)O)C( C)C | GCUGGGAUGUUGG CUUAGAAGCAGCCA UCAUUUAAAGAGU GCGUAACAGCUCAC CAGC | Micrococcin | Target\_lig\_30 9 | L11 binding BD RNA | Target\_122 | 7.09691001  300806 |
| 387 | CC=C1C2=NC(=CS2) C(=O)NC3CC(C(=O)O CC4=C5C(=C(C(=O)S CC(C6=NC(=CS6)C7= NC(=C(C=C7C8=NC(= CS8)C(=O)NC(C(=O)N  1)C(C)O)O)C9=NC(=C  S9)C(=O)NC(=C)C(=O  )N)NC(=O)C1=CSC3= N1)NC5=CC=C4)C)O | GCUGGGAUGUUGG CUUAGAAGCAGCCA UCAUUUAAAGAGU GCGUAACAGCUCAC CAGC | Nosiheptide | Target\_lig\_31 0 | L11 binding BD RNA | Target\_122 | 5.30102999  566398 |
| 389 | C1C(C(C(C(C1N)OC2 C(C(C(C(O2)CO)O)O) N)O)O)N | UACCUGGUUGAUCC UGCCAGUAGCAUAU GCUUGUCUCAAAGA UUAAGCCAUGCAUG UCUAAGUACGCACG GCCGGUACAGUGAA ACUGCGAAUGGCUC AUUAAAUCAGUUA UGGUUCCUUUGGUC GCUCGCUCCUCUCC CACUUGGAUAACUG UGGUAAUUCUAGA GCUAAUACAUGCCG ACGGGCGCUGACCC CCUUCGCGGGGGGG AUGCGUGCAUUUA UCAGAUCAAAACCA ACCCGGUCAGCCCC UCUCCGGCCCCGGC CGGGGGGCGGGCGC CGGCGGCUUUGGUG ACUCUAGAUAACCU CGGGCCGAUCGCAC GCCCCCCGUGGCGG CGACGACCCAUUCG AACGUCUGCCCUAU CAACUUUCGAUGGU AGUCGCCGUGCCUA CCAUGGUGACCACG GGUGACGGGGAAU CAGGGUUCGAUUCC GGAGAGGGAGCCU GAGAAACGGCUACC ACAUCCAAGGAAGG CAGCAGGCGCGCAA AUUACCCACUCCCG ACCCGGGGAGGUAG UGACGAAAAAUAA CAAUACAGGACUCU UUCGAGGCCCUGUA AUUGGAAUGAGUC CACUUUAAAUCCUU CCGCGAGGAUCCAU | Paromamine | Target\_lig\_311 | Human A-site | Target\_103 | 4 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | UGGAGGGCAAGUC UGGUGCCAGCAGCC GCGGUAAUUCCAGC UCCAAUAGCGUAUA UUAAAGUUGCUGC AGUUAAAAAGCUC GUAGUUGGAUCUU GGGAGCGGGCGGGC GGUCCGCCGCGAGG CGAGCCACCGCCCG UCCCCGCCCCUUGC CUCUCGGCGCCCCC UCGAUGCUCUUAGC UGAGUGUCCCGCGG GGCCCGAAGCAUUU ACUUUGAAAAAAU UAGAGUGUUCAAA GCAGGCCCGAGCCG CCUGGAUACCGCAG CUAGGAAUAAUGG AAUAGGACCGCGGU UCUAUUUUGUUGG UUUUCGGAACUGA GGCCAUGAUUAAG AGGGACGGCCGGGG GCAUUCGUAUUGCG CCGCUAGAGGUGAA AUUCUUGGACCGGC GCAAGACGGACCAG AGCGAAAGCAUUU GCCAAGAAUGUUU UCAUUAAUCAAGA ACGAAAGUCGGAG GUUCGAAGACGAUC AGAUACCGUCGUAG UUCCGACCAUAAAC GAUGCCGACUGGCG AUGCGGCGGCGUUA UUCCCAUGACCCGC CGGGCAGCUUCCGG GAAACCAAAGUCUU UGGGUUCCGGGGG GAGUAUGGUUGCA AAGCUGAAACUUA AAGGAAUUGACGG AAGGGCACCACCAG GAGUGGAGCCUGCG GCUUAAUUUGACUC AACACGGGAAACCU CACCCGGCCCGGAC ACGGACAGGAUUG ACAGAUUGAUAGC UCUUUCUCGAUUCC GUGGGUGGUGGUG CAUGGCCGUUCUUA GUUGGUGGAGCGA UUUGUCUGGUUAA UUCCGAUAACGAAC GAGACUCUGGCAUG CUAACUAGUUACGC GACCCCCGAGCGGU CGGCGUCCCCCAAC UUCUUAGAGGGAC AAGUGGCGUUCAGC CACCCGAGAUUGAG CAAUAACAGGUCUG UGAUGCCCUUAGAU GUCCGGGGCUGCAC GCGCGCUACACUGA CUGGCUCAGCGUGU GCCUACCCUACGCC GGCAGGCGCGGGUA ACCCGUUGAACCCC AUUCGUGAUGGGG AUCGGGGAUUGCA |  |  |  |  |  |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | AUUAUUCCCCAUGA ACGAGGAAUUCCCA GUAAGUGCGGGUC AUAAGCUUGCGUU GAUUAAGUCCCUGC CCUUUGUACACACC GCCCGUCGCUACUA CCGAUUGGAUGGU UUAGUGAGGCCCUC GGAUCGGCCCCGCC GGGGUCGGCCCACG GCCCUGGCGGAGCG CUGAGAAGACGGUC GAACUUGACUAUCU AGAGGAAGUAAAA GUCGUAACAAGGU UUCCGUAGGUGAAC CUGCGGAAGGAUCA UUA |  |  |  |  |  |
| 390 | CN(C)C1=NC=NC2=C 1N=CN2C3C(C(C(O3) CO)NC(=O)C(CC4=C C=C(C=C4)OC)N)O | GGUUAAGCGACUA AGCGUACACGGUGG AUGCCCUGGCAGUC AGAGGCGAUGAAG GACGUGCUAAUCUG CGAUAAGCGUCGGU AAGGUGAUAUGAA CCGUUAUAACCGGC GAUUUCCGAAUGG GGAAACCCAGUGUG UUUCGACACACUAU CAUUAACUGAAUCC AUAGGUUAAUGAG GCGAACCGGGGGAA CUGAAACAUCUAAG UACCCCGAGGAAAA GAAAUCAACCGAGA UUCCCCCAGUAGCG GCGAGCGAACGGGG AGCAGCCCAGAGCC UGAAUCAGUGUGU GUGUUAGUGGAAG CGUCUGGAAAGGCG CGCGAUACAGGGUG ACAGCCCCGUACAC AAAAAUGCACAUGC UGUGAGCUCGAUG AGUAGGGCGGGAC ACGUGGUAUCCUGU CUGAAUAUGGGGG GACCAUCCUCCAAG GCUAAAUACUCCUG ACUGACCGAUAGUG AACCAGUACCGUGA GGGAAAGGCGAAA AGAACCCCGGCGAG GGGAGUGAAAAAG AACCUGAAACCGUG UACGUACAAGCAGU GGGAGCACGCUUAG GCGUGUGACUGCGU ACCUUUUGUAUAA UGGGUCAGCGACUU AUAUUCUGUAGCA AGGUUAACCGAAU AGGGGAGCCGAAG GGAAACCGAGUCUU AACUGGGCGUUAA GUUGCAGGGUAUA GACCCGAAACCCGG UGAUCUAGCCAUGG GCAGGUUGAAGGU UGGGUAACACUAAC UGGAGGACCGAACC GACUAAUGUUGAA AAAUUAGCGGAUG | Puromycin | Target\_lig\_31 2 | 50S A-site for puromycin | Target\_100 | 3.31875876  262441 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | ACUUGUGGCUGGG GGUGAAAGGCCAA UCAAACCGGGAGAU AGCUGGUUCUCCCC GAAAGCUAUUUAG GUAGCGCCUCGUGA AUUCAUCUCCGGGG GUAGAGCACUGUU UCGGCAAGGGGGUC ACUUACCAACCCGA UGCAAACUGCGAAU ACCGGAGAAUGUU AUCACGGGAGACAC ACGGCGGGUGCUAA CGUCCGUCGUGAAG AGGGAAACAACCCA GACCGCCAGCUAAG GUCCCAAAGUCAUG GUUAAGUGGGAAA CGAUGUGGGAAGG CCCAGACAGCCAGG AUGUUGGCUUAGA AGCAGCCAUCAUUU AAAGAAAGCGUAA UAGCUCACUGGUCG AGUCGGCCUGCGCG GAAGAUGUAACGG GGCUAAACCAUGCA CCGAAGCUGCGGCA GCGACGCUUAUGCG UUGUUGGGUAGGG GAGCGUUCUGUAA GCCUGCGAAGGUGU GCUGUGAGGCAUGC UGGAGGUAUCAGA AGUGCGAAUGCUG ACAUAAGUAACGA UAAAGCGGGUGAA AAGCCCGCUCGCCG GAAGACCAAGGGU UCCUGUCCAACGUU AAUCGGGGCAGGG UGAGUCGACCCCUA AGGCGAGGCCGAAA GGCGUAGUCGAUG GGAAACAGGUUAA UAUUCCUGUACUUG GUGUUACUGCGAA GGGGGGACGGAGA AGGCUAUGUUGGCC GGGCGACGGUUGUC CCGGUUUAAGCGUG UAGGCUGGUUUUCC AGGCAAAUCCGGAA AAUCAAGGCUGAG GCGUGAUGACGAG GCACUACGGUGCUG AAGCAACAAAUGCC CUGCUUCCAGGAAA AGCCUCUAAGCAUC AGGUAACAUCAAA UCGUACCCCAAACC GACACAGGUGGUCA GGUAGAGAAUACC AAGGCGCUUGAGA GAACUCGGGUGAA GGAACUAGGCAAA AUGGUGCCGUAACU UCGGGAGAAGGCAC GCUGAUAUGUAGG UGAGGUCCCUCGCG GAUGGAGCUGAAA UCAGUCGAAGAUAC CAGCUGGCUGCAAC UGUUUAUUAAAAA |  |  |  |  |  |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | CACAGCACUGUGCA AACACGAAAGUGG ACGUAUACGGUGU GACGCCUGCCCGGU GCCGGAAGGUUAA UUGAUGGGGUUAG CGCAAGCGAAGCUC UUGAUCGAAGCCCC GGUAAACGGCGGCC GUAACXAUAACGG UCCUAAGGUAGCGA AAUUCCUUGUCGGG UAAGUUCCGACCUG CACGAAUGGCGUAA UGAUGGCCAGGCUG UCUCCACCCGAGAC UCAGUGAAAUUGA ACUCGCUGUGAAGA UGCAGUGUACCCGC GGCAAGACGGAAA GACCCCGUGAACCU UUACUAUAGCUUG ACACUGAACAUUGA GCCUUGAUGUGUA GGAUAGGUGGGAG GCUUUGAAGUGUG GACGCCAGUCUGCA UGGAGCCGACCUUG AAAUACCACCCUUU AAUGUUUGAUGUU CUAACGUUGACCCG UAAUCCGGGUUGCG GACAGUGUCUGGU GGGUAGUUUGACU GGGGCGGUCUCCUC CUAAAGAGUAACG GAGGAGCACGAAG GUUGGCUAAUCCUG GUCGGACAUCAGGA GGUUAGUGCAAUG GCAUAAGCCAGCUU GACUGCGAGCGUGA CGGCGCGAGCAGGU GCGAAAGCAGGUCA UAGUGAUCCGGUG GUUCUGAAUGGAA GGGCCAUCGCUCAA CGGAUAAAAGGUA CUCCGGGGAUAACA GGCUGAUACCGCCC AAGAGUUCAUAUC GACGGCGGUGUUU GGCACCUCGAUGUC GGCUCAUCACAUCC UGGGGCUGAAGUA GGUCCCAAGGGUAU GGCUGUUCGCCAUU UAAAGUGGUACGC GAGCUGGGUUUAG AACGUCGUGAGACA GUUCGGUCCCUAUC UGCCGUGGGCGCUG GAGAACUGAGGGG GGCUGCUCCUAGUA CGAGAGGACCGGAG UGGACGCAUCACUG GUGUUCGGGUUGU CAUGCCAAUGGCAC UGCCCGGUAGCUAA AUGCGGAAGAGAU AAGUGCUGAAAGC AUCUAAGCACGAAA CUUGCCCCGAGAUG AGUUCUCCCUGACC CUUUAAGGGUCCUG |  |  |  |  |  |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | AAGGAACGUUGAA GACGACGACGUUGA UAGGCCGGGUGUG UAAGCGCAGCGAUG CGUUGAGCUAACCG GUACUAAUGAACCG UGAGGCUUAACCU |  |  |  |  |  |
| 391 | CC1CCC23CCC(=O)C 2C1(C(CC(C(C3C)O) (C)C=C)OC(=O)CSC4 CC5CCC(C4)N5C)C | GGUUAAGCGACUA AGCGUACACGGUGG AUGCCCUGGCAGUC AGAGGCGAUGAAG GACGUGCUAAUCUG CGAUAAGCGUCGGU AAGGUGAUAUGAA CCGUUAUAACCGGC GAUUUCCGAAUGG GGAAACCCAGUGUG UUUCGACACACUAU CAUUAACUGAAUCC AUAGGUUAAUGAG GCGAACCGGGGGAA CUGAAACAUCUAAG UACCCCGAGGAAAA GAAAUCAACCGAGA UUCCCCCAGUAGCG GCGAGCGAACGGGG AGCAGCCCAGAGCC UGAAUCAGUGUGU GUGUUAGUGGAAG CGUCUGGAAAGGCG CGCGAUACAGGGUG ACAGCCCCGUACAC AAAAAUGCACAUGC UGUGAGCUCGAUG AGUAGGGCGGGAC ACGUGGUAUCCUGU CUGAAUAUGGGGG GACCAUCCUCCAAG GCUAAAUACUCCUG ACUGACCGAUAGUG AACCAGUACCGUGA GGGAAAGGCGAAA AGAACCCCGGCGAG GGGAGUGAAAAAG AACCUGAAACCGUG UACGUACAAGCAGU GGGAGCACGCUUAG GCGUGUGACUGCGU ACCUUUUGUAUAA UGGGUCAGCGACUU AUAUUCUGUAGCA AGGUUAACCGAAU AGGGGAGCCGAAG GGAAACCGAGUCUU AACUGGGCGUUAA GUUGCAGGGUAUA GACCCGAAACCCGG UGAUCUAGCCAUGG GCAGGUUGAAGGU UGGGUAACACUAAC UGGAGGACCGAACC GACUAAUGUUGAA AAAUUAGCGGAUG ACUUGUGGCUGGG GGUGAAAGGCCAA UCAAACCGGGAGAU AGCUGGUUCUCCCC GAAAGCUAUUUAG GUAGCGCCUCGUGA AUUCAUCUCCGGGG GUAGAGCACUGUU UCGGCAAGGGGGUC ACUUACCAACCCGA UGCAAACUGCGAAU ACCGGAGAAUGUU | Retapamulin | Target\_lig\_31 3 | large ribosomal subunit from Deinococcus radiodurans | Target\_100 | 8.69897000  433602 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | AUCACGGGAGACAC ACGGCGGGUGCUAA CGUCCGUCGUGAAG AGGGAAACAACCCA GACCGCCAGCUAAG GUCCCAAAGUCAUG GUUAAGUGGGAAA CGAUGUGGGAAGG CCCAGACAGCCAGG AUGUUGGCUUAGA AGCAGCCAUCAUUU AAAGAAAGCGUAA UAGCUCACUGGUCG AGUCGGCCUGCGCG GAAGAUGUAACGG GGCUAAACCAUGCA CCGAAGCUGCGGCA GCGACGCUUAUGCG UUGUUGGGUAGGG GAGCGUUCUGUAA GCCUGCGAAGGUGU GCUGUGAGGCAUGC UGGAGGUAUCAGA AGUGCGAAUGCUG ACAUAAGUAACGA UAAAGCGGGUGAA AAGCCCGCUCGCCG GAAGACCAAGGGU UCCUGUCCAACGUU AAUCGGGGCAGGG UGAGUCGACCCCUA AGGCGAGGCCGAAA GGCGUAGUCGAUG GGAAACAGGUUAA UAUUCCUGUACUUG GUGUUACUGCGAA GGGGGGACGGAGA AGGCUAUGUUGGCC GGGCGACGGUUGUC CCGGUUUAAGCGUG UAGGCUGGUUUUCC AGGCAAAUCCGGAA AAUCAAGGCUGAG GCGUGAUGACGAG GCACUACGGUGCUG AAGCAACAAAUGCC CUGCUUCCAGGAAA AGCCUCUAAGCAUC AGGUAACAUCAAA UCGUACCCCAAACC GACACAGGUGGUCA GGUAGAGAAUACC AAGGCGCUUGAGA GAACUCGGGUGAA GGAACUAGGCAAA AUGGUGCCGUAACU UCGGGAGAAGGCAC GCUGAUAUGUAGG UGAGGUCCCUCGCG GAUGGAGCUGAAA UCAGUCGAAGAUAC CAGCUGGCUGCAAC UGUUUAUUAAAAA CACAGCACUGUGCA AACACGAAAGUGG ACGUAUACGGUGU GACGCCUGCCCGGU GCCGGAAGGUUAA UUGAUGGGGUUAG CGCAAGCGAAGCUC UUGAUCGAAGCCCC GGUAAACGGCGGCC GUAACXAUAACGG UCCUAAGGUAGCGA AAUUCCUUGUCGGG |  |  |  |  |  |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | UAAGUUCCGACCUG CACGAAUGGCGUAA UGAUGGCCAGGCUG UCUCCACCCGAGAC UCAGUGAAAUUGA ACUCGCUGUGAAGA UGCAGUGUACCCGC GGCAAGACGGAAA GACCCCGUGAACCU UUACUAUAGCUUG ACACUGAACAUUGA GCCUUGAUGUGUA GGAUAGGUGGGAG GCUUUGAAGUGUG GACGCCAGUCUGCA UGGAGCCGACCUUG AAAUACCACCCUUU AAUGUUUGAUGUU CUAACGUUGACCCG UAAUCCGGGUUGCG GACAGUGUCUGGU GGGUAGUUUGACU GGGGCGGUCUCCUC CUAAAGAGUAACG GAGGAGCACGAAG GUUGGCUAAUCCUG GUCGGACAUCAGGA GGUUAGUGCAAUG GCAUAAGCCAGCUU GACUGCGAGCGUGA CGGCGCGAGCAGGU GCGAAAGCAGGUCA UAGUGAUCCGGUG GUUCUGAAUGGAA GGGCCAUCGCUCAA CGGAUAAAAGGUA CUCCGGGGAUAACA GGCUGAUACCGCCC AAGAGUUCAUAUC GACGGCGGUGUUU GGCACCUCGAUGUC GGCUCAUCACAUCC UGGGGCUGAAGUA GGUCCCAAGGGUAU GGCUGUUCGCCAUU UAAAGUGGUACGC GAGCUGGGUUUAG AACGUCGUGAGACA GUUCGGUCCCUAUC UGCCGUGGGCGCUG GAGAACUGAGGGG GGCUGCUCCUAGUA CGAGAGGACCGGAG UGGACGCAUCACUG GUGUUCGGGUUGU CAUGCCAAUGGCAC UGCCCGGUAGCUAA AUGCGGAAGAGAU AAGUGCUGAAAGC AUCUAAGCACGAAA CUUGCCCCGAGAUG AGUUCUCCCUGACC CUUUAAGGGUCCUG AAGGAACGUUGAA GACGACGACGUUGA UAGGCCGGGUGUG UAAGCGCAGCGAUG CGUUGAGCUAACCG GUACUAAUGAACCG UGAGGCUUAACCU |  |  |  |  |  |
| 394 | CC1CC=CC=CC(C(CC (C(C(C(CC(=O)O1)O)  OC)OC2C(C(C(C(O2)  C)OC3CC(C(C(O3)C) O) | GGUUAAGCGACUA AGCGUACACGGUGG AUGCCCUGGCAGUC AGAGGCGAUGAAG GACGUGCUAAUCUG | Spiramycin A | Target\_lig\_31 5 | 50S exit tunnel for SPIRAMYCI N A | Target\_100 | 5.74472749  489669 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  | (C)O)N(C)C)O)CC=O) C)OC4CCC(C(O4)C)N (C)C | CGAUAAGCGUCGGU AAGGUGAUAUGAA CCGUUAUAACCGGC GAUUUCCGAAUGG GGAAACCCAGUGUG UUUCGACACACUAU CAUUAACUGAAUCC AUAGGUUAAUGAG GCGAACCGGGGGAA CUGAAACAUCUAAG UACCCCGAGGAAAA GAAAUCAACCGAGA UUCCCCCAGUAGCG GCGAGCGAACGGGG AGCAGCCCAGAGCC UGAAUCAGUGUGU GUGUUAGUGGAAG CGUCUGGAAAGGCG CGCGAUACAGGGUG ACAGCCCCGUACAC AAAAAUGCACAUGC UGUGAGCUCGAUG AGUAGGGCGGGAC ACGUGGUAUCCUGU CUGAAUAUGGGGG GACCAUCCUCCAAG GCUAAAUACUCCUG ACUGACCGAUAGUG AACCAGUACCGUGA GGGAAAGGCGAAA AGAACCCCGGCGAG GGGAGUGAAAAAG AACCUGAAACCGUG UACGUACAAGCAGU GGGAGCACGCUUAG GCGUGUGACUGCGU ACCUUUUGUAUAA UGGGUCAGCGACUU AUAUUCUGUAGCA AGGUUAACCGAAU AGGGGAGCCGAAG GGAAACCGAGUCUU AACUGGGCGUUAA GUUGCAGGGUAUA GACCCGAAACCCGG UGAUCUAGCCAUGG GCAGGUUGAAGGU UGGGUAACACUAAC UGGAGGACCGAACC GACUAAUGUUGAA AAAUUAGCGGAUG ACUUGUGGCUGGG GGUGAAAGGCCAA UCAAACCGGGAGAU AGCUGGUUCUCCCC GAAAGCUAUUUAG GUAGCGCCUCGUGA AUUCAUCUCCGGGG GUAGAGCACUGUU UCGGCAAGGGGGUC ACUUACCAACCCGA UGCAAACUGCGAAU ACCGGAGAAUGUU AUCACGGGAGACAC ACGGCGGGUGCUAA CGUCCGUCGUGAAG AGGGAAACAACCCA GACCGCCAGCUAAG GUCCCAAAGUCAUG GUUAAGUGGGAAA CGAUGUGGGAAGG CCCAGACAGCCAGG AUGUUGGCUUAGA AGCAGCCAUCAUUU AAAGAAAGCGUAA |  |  |  |  |  |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | UAGCUCACUGGUCG AGUCGGCCUGCGCG GAAGAUGUAACGG GGCUAAACCAUGCA CCGAAGCUGCGGCA GCGACGCUUAUGCG UUGUUGGGUAGGG GAGCGUUCUGUAA GCCUGCGAAGGUGU GCUGUGAGGCAUGC UGGAGGUAUCAGA AGUGCGAAUGCUG ACAUAAGUAACGA UAAAGCGGGUGAA AAGCCCGCUCGCCG GAAGACCAAGGGU UCCUGUCCAACGUU AAUCGGGGCAGGG UGAGUCGACCCCUA AGGCGAGGCCGAAA GGCGUAGUCGAUG GGAAACAGGUUAA UAUUCCUGUACUUG GUGUUACUGCGAA GGGGGGACGGAGA AGGCUAUGUUGGCC GGGCGACGGUUGUC CCGGUUUAAGCGUG UAGGCUGGUUUUCC AGGCAAAUCCGGAA AAUCAAGGCUGAG GCGUGAUGACGAG GCACUACGGUGCUG AAGCAACAAAUGCC CUGCUUCCAGGAAA AGCCUCUAAGCAUC AGGUAACAUCAAA UCGUACCCCAAACC GACACAGGUGGUCA GGUAGAGAAUACC AAGGCGCUUGAGA GAACUCGGGUGAA GGAACUAGGCAAA AUGGUGCCGUAACU UCGGGAGAAGGCAC GCUGAUAUGUAGG UGAGGUCCCUCGCG GAUGGAGCUGAAA UCAGUCGAAGAUAC CAGCUGGCUGCAAC UGUUUAUUAAAAA CACAGCACUGUGCA AACACGAAAGUGG ACGUAUACGGUGU GACGCCUGCCCGGU GCCGGAAGGUUAA UUGAUGGGGUUAG CGCAAGCGAAGCUC UUGAUCGAAGCCCC GGUAAACGGCGGCC GUAACXAUAACGG UCCUAAGGUAGCGA AAUUCCUUGUCGGG UAAGUUCCGACCUG CACGAAUGGCGUAA UGAUGGCCAGGCUG UCUCCACCCGAGAC UCAGUGAAAUUGA ACUCGCUGUGAAGA UGCAGUGUACCCGC GGCAAGACGGAAA GACCCCGUGAACCU UUACUAUAGCUUG ACACUGAACAUUGA GCCUUGAUGUGUA |  |  |  |  |  |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | GGAUAGGUGGGAG GCUUUGAAGUGUG GACGCCAGUCUGCA UGGAGCCGACCUUG AAAUACCACCCUUU AAUGUUUGAUGUU CUAACGUUGACCCG UAAUCCGGGUUGCG GACAGUGUCUGGU GGGUAGUUUGACU GGGGCGGUCUCCUC CUAAAGAGUAACG GAGGAGCACGAAG GUUGGCUAAUCCUG GUCGGACAUCAGGA GGUUAGUGCAAUG GCAUAAGCCAGCUU GACUGCGAGCGUGA CGGCGCGAGCAGGU GCGAAAGCAGGUCA UAGUGAUCCGGUG GUUCUGAAUGGAA GGGCCAUCGCUCAA CGGAUAAAAGGUA CUCCGGGGAUAACA GGCUGAUACCGCCC AAGAGUUCAUAUC GACGGCGGUGUUU GGCACCUCGAUGUC GGCUCAUCACAUCC UGGGGCUGAAGUA GGUCCCAAGGGUAU GGCUGUUCGCCAUU UAAAGUGGUACGC GAGCUGGGUUUAG AACGUCGUGAGACA GUUCGGUCCCUAUC UGCCGUGGGCGCUG GAGAACUGAGGGG GGCUGCUCCUAGUA CGAGAGGACCGGAG UGGACGCAUCACUG GUGUUCGGGUUGU CAUGCCAAUGGCAC UGCCCGGUAGCUAA AUGCGGAAGAGAU AAGUGCUGAAAGC AUCUAAGCACGAAA CUUGCCCCGAGAUG AGUUCUCCCUGACC CUUUAAGGGUCCUG AAGGAACGUUGAA GACGACGACGUUGA UAGGCCGGGUGUG UAAGCGCAGCGAUG CGUUGAGCUAACCG GUACUAAUGAACCG UGAGGCUUAACCU |  |  |  |  |  |
| 396 | CCC1C2(C(C(C(=O)C(  CC(C(C(C(=O)C(C(=O  )O1)C)C)OC3C(C(CC(  O3)C)N(C)C)O)  (C)OC)C)C)N(C(=O)O 2)CCCCN4C=C(N=C4) C5=CN=CC=C5)C | GGUUAAGCGACUA AGCGUACACGGUGG AUGCCCUGGCAGUC AGAGGCGAUGAAG GACGUGCUAAUCUG CGAUAAGCGUCGGU AAGGUGAUAUGAA CCGUUAUAACCGGC GAUUUCCGAAUGG GGAAACCCAGUGUG UUUCGACACACUAU CAUUAACUGAAUCC AUAGGUUAAUGAG GCGAACCGGGGGAA CUGAAACAUCUAAG UACCCCGAGGAAAA GAAAUCAACCGAGA | Telithromycin | Target\_lig\_31 7 | Large subunit (TELITHRO MYCIN) | Target\_100 | 8.88605664  769316 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | UUCCCCCAGUAGCG GCGAGCGAACGGGG AGCAGCCCAGAGCC UGAAUCAGUGUGU GUGUUAGUGGAAG CGUCUGGAAAGGCG CGCGAUACAGGGUG ACAGCCCCGUACAC AAAAAUGCACAUGC UGUGAGCUCGAUG AGUAGGGCGGGAC ACGUGGUAUCCUGU CUGAAUAUGGGGG GACCAUCCUCCAAG GCUAAAUACUCCUG ACUGACCGAUAGUG AACCAGUACCGUGA GGGAAAGGCGAAA AGAACCCCGGCGAG GGGAGUGAAAAAG AACCUGAAACCGUG UACGUACAAGCAGU GGGAGCACGCUUAG GCGUGUGACUGCGU ACCUUUUGUAUAA UGGGUCAGCGACUU AUAUUCUGUAGCA AGGUUAACCGAAU AGGGGAGCCGAAG GGAAACCGAGUCUU AACUGGGCGUUAA GUUGCAGGGUAUA GACCCGAAACCCGG UGAUCUAGCCAUGG GCAGGUUGAAGGU UGGGUAACACUAAC UGGAGGACCGAACC GACUAAUGUUGAA AAAUUAGCGGAUG ACUUGUGGCUGGG GGUGAAAGGCCAA UCAAACCGGGAGAU AGCUGGUUCUCCCC GAAAGCUAUUUAG GUAGCGCCUCGUGA AUUCAUCUCCGGGG GUAGAGCACUGUU UCGGCAAGGGGGUC ACUUACCAACCCGA UGCAAACUGCGAAU ACCGGAGAAUGUU AUCACGGGAGACAC ACGGCGGGUGCUAA CGUCCGUCGUGAAG AGGGAAACAACCCA GACCGCCAGCUAAG GUCCCAAAGUCAUG GUUAAGUGGGAAA CGAUGUGGGAAGG CCCAGACAGCCAGG AUGUUGGCUUAGA AGCAGCCAUCAUUU AAAGAAAGCGUAA UAGCUCACUGGUCG AGUCGGCCUGCGCG GAAGAUGUAACGG GGCUAAACCAUGCA CCGAAGCUGCGGCA GCGACGCUUAUGCG UUGUUGGGUAGGG GAGCGUUCUGUAA GCCUGCGAAGGUGU GCUGUGAGGCAUGC UGGAGGUAUCAGA AGUGCGAAUGCUG |  |  |  |  |  |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | ACAUAAGUAACGA UAAAGCGGGUGAA AAGCCCGCUCGCCG GAAGACCAAGGGU UCCUGUCCAACGUU AAUCGGGGCAGGG UGAGUCGACCCCUA AGGCGAGGCCGAAA GGCGUAGUCGAUG GGAAACAGGUUAA UAUUCCUGUACUUG GUGUUACUGCGAA GGGGGGACGGAGA AGGCUAUGUUGGCC GGGCGACGGUUGUC CCGGUUUAAGCGUG UAGGCUGGUUUUCC AGGCAAAUCCGGAA AAUCAAGGCUGAG GCGUGAUGACGAG GCACUACGGUGCUG AAGCAACAAAUGCC CUGCUUCCAGGAAA AGCCUCUAAGCAUC AGGUAACAUCAAA UCGUACCCCAAACC GACACAGGUGGUCA GGUAGAGAAUACC AAGGCGCUUGAGA GAACUCGGGUGAA GGAACUAGGCAAA AUGGUGCCGUAACU UCGGGAGAAGGCAC GCUGAUAUGUAGG UGAGGUCCCUCGCG GAUGGAGCUGAAA UCAGUCGAAGAUAC CAGCUGGCUGCAAC UGUUUAUUAAAAA CACAGCACUGUGCA AACACGAAAGUGG ACGUAUACGGUGU GACGCCUGCCCGGU GCCGGAAGGUUAA UUGAUGGGGUUAG CGCAAGCGAAGCUC UUGAUCGAAGCCCC GGUAAACGGCGGCC GUAACXAUAACGG UCCUAAGGUAGCGA AAUUCCUUGUCGGG UAAGUUCCGACCUG CACGAAUGGCGUAA UGAUGGCCAGGCUG UCUCCACCCGAGAC UCAGUGAAAUUGA ACUCGCUGUGAAGA UGCAGUGUACCCGC GGCAAGACGGAAA GACCCCGUGAACCU UUACUAUAGCUUG ACACUGAACAUUGA GCCUUGAUGUGUA GGAUAGGUGGGAG GCUUUGAAGUGUG GACGCCAGUCUGCA UGGAGCCGACCUUG AAAUACCACCCUUU AAUGUUUGAUGUU CUAACGUUGACCCG UAAUCCGGGUUGCG GACAGUGUCUGGU GGGUAGUUUGACU GGGGCGGUCUCCUC CUAAAGAGUAACG |  |  |  |  |  |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | GAGGAGCACGAAG GUUGGCUAAUCCUG GUCGGACAUCAGGA GGUUAGUGCAAUG GCAUAAGCCAGCUU GACUGCGAGCGUGA CGGCGCGAGCAGGU GCGAAAGCAGGUCA UAGUGAUCCGGUG GUUCUGAAUGGAA GGGCCAUCGCUCAA CGGAUAAAAGGUA CUCCGGGGAUAACA GGCUGAUACCGCCC AAGAGUUCAUAUC GACGGCGGUGUUU GGCACCUCGAUGUC GGCUCAUCACAUCC UGGGGCUGAAGUA GGUCCCAAGGGUAU GGCUGUUCGCCAUU UAAAGUGGUACGC GAGCUGGGUUUAG AACGUCGUGAGACA GUUCGGUCCCUAUC UGCCGUGGGCGCUG GAGAACUGAGGGG GGCUGCUCCUAGUA CGAGAGGACCGGAG UGGACGCAUCACUG GUGUUCGGGUUGU CAUGCCAAUGGCAC UGCCCGGUAGCUAA AUGCGGAAGAGAU AAGUGCUGAAAGC AUCUAAGCACGAAA CUUGCCCCGAGAUG AGUUCUCCCUGACC CUUUAAGGGUCCUG AAGGAACGUUGAA GACGACGACGUUGA UAGGCCGGGUGUG UAAGCGCAGCGAUG CGUUGAGCUAACCG GUACUAAUGAACCG UGAGGCUUAACCU |  |  |  |  |  |
| 397 | 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 | AAAUUGAAGAGUU UGAUCAUGGCUCAG AUUGAACGCUGGCG GCAGGCCUAACACA UGCAAGUCGAACGG UAACAGGAAGAAG CUUGCUUCUUUGCU GACGAGUGGCGGAC GGGUGAGUAAUGU CUGGGAAACUGCCU GAUGGAGGGGGAU AACUACUGGAAACG GUAGCUAAUACCGC AUAACGUCGCAAGA CCAAAGAGGGGGAC CUUCGGGCCUCUUG CCAUCGGAUGUGCC CAGAUGGGAUUAG CUAGUAGGUGGGG UAACGGCUCACCUA GGCGACGAUCCCUA GCUGGUCUGAGAG GAUGACCAGCCACA CUGGAACUGAGACA CGGUCCAGACUCCU ACGGGAGGCAGCAG UGGGGAAUAUUGC ACAAUGGGCGCAAG CCUGAUGCAGCCAU | tetracyclin | Target\_lig\_74 | Small subunit tetracycline | Target\_101 | 5.45593195  564972 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | GCCGCGUGUAUGAA GAAGGCCUUCGGGU UGUAAAGUACUUU CAGCGGGGAGGAA GGGAGUAAAGUUA AUACCUUUGCUCAU UGACGUUACCCGCA GAAGAAGCACCGGC UAACUCCGUGCCAG CAGCCGCGGUAAUA CGGAGGGUGCAAGC GUUAAUCGGAAUU ACUGGGCGUAAAGC GCACGCAGGCGGUU UGUUAAGUCAGAU GUGAAAUCCCCGGG CUCAACCUGGGAAC UGCAUCUGAUACUG GCAAGCUUGAGUCU CGUAGAGGGGGGU AGAAUUCCAGGUG UAGCGGUGAAAUG CGUAGAGAUCUGG AGGAAUACCGGUG GCGAAGGCGGCCCC CUGGACGAAGACUG ACGCUCAGGUGCGA AAGCGUGGGGAGC AAACAGGAUUAGA UACCCUGGUAGUCC ACGCCGUAAACGAU GUCGACUUGGAGG UUGUGCCCUUGAGG CGUGGCUUCCGGAG CUAACGCGUUAAGU CGACCGCCUGGGGA GUACGGCCGCAAGG UUAAAACUCAAAU GAAUUGACGGGGG CCCGCACAAGCGGU GGAGCAUGUGGUU UAAUUCGAUGCAAC GCGAAGAACCUUAC CUGGUCUUGACAUC CACGGAAGUUUUCA GAGAUGAGAAUGU GCCUUCGGGAACCG UGAGACAGGUGCU GCAUGGCUGUCGUC AGCUCGUGUUGUG AAAUGUUGGGUUA AGUCCCGCAACGAG CGCAACCCUUAUCC UUUGUUGCCAGCGG UCCGGCCGGGAACU CAAAGGAGACUGCC AGUGAUAAACUGG AGGAAGGUGGGGA UGACGUCAAGUCAU CAUGGCCCUUACGA CCAGGGCUACACAC GUGCUACAAUGGCG CAUACAAAGAGAA GCGACCUCGCGAGA GCAAGCGGACCUCA UAAAGUGCGUCGU AGUCCGGAUUGGA GUCUGCAACUCGAC UCCAUGAAGUCGGA AUCGCUAGUAAUCG UGGAUCAGAAUGCC ACGGUGAAUACGU UCCCGGGCCUUGUA CACACCGCCCGUCA CACCAUGGGAGUGG |  |  |  |  |  |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | GUUGCAAAAGAAG UAGGUAGCUUAACC UUCGGGAGGGCGCU UACCACUUUGUGAU UCAUGACUGGGGU GAAGUCGUAACAA GGUAACCGUAGGG GAACCUGCGGUUGG AUCACCUCCUUA |  |  |  |  |  |
| 399 | CCC(C)C1C(=O)NC(C (=O)NC(=C)C(=O)NC( C(=O)NC23CCC(=NC 2C4=CSC(=N4)C(C(O C(=O)C5=NC6=C(C=C C(C6O)N1)C(=C5)C(C  )O)C)NC(=O)C7=CSC(  =N7)C(NC(=O)C8CSC (=N8)C(=CC)NC(=O)C (NC(=O)C9=CSC3=N9  )C(C)O)C(C)  (C(C)O)O)C1=NC(=CS  1)C(=O)NC(=C)C(=O)  NC(=C)C(=O)N)C)C | GCUGGGAUGUUGG CUUAGAAGCAGCCA UCAUUUAAAGAGU GCGUAACAGCUCAC CAGC | Thiostrepton | Target\_lig\_31 9 | L11 BD RNA | Target\_122 | 5.88605664  769316 |
| 400 | CCC1C(C=C(C=CC(= O)C(CC(C(C(C(CC(=O  )O1)O)C)OC2C(C(C(C  (O2)C)OC3CC(C(C(O3  )C)O) (C)O)N(C)C)O)CC=O)  C)C)COC4C(C(C(C(O 4)C)O)OC)OC | GGUUAAGCGACUA AGCGUACACGGUGG AUGCCCUGGCAGUC AGAGGCGAUGAAG GACGUGCUAAUCUG CGAUAAGCGUCGGU AAGGUGAUAUGAA CCGUUAUAACCGGC GAUUUCCGAAUGG GGAAACCCAGUGUG UUUCGACACACUAU CAUUAACUGAAUCC AUAGGUUAAUGAG GCGAACCGGGGGAA CUGAAACAUCUAAG UACCCCGAGGAAAA GAAAUCAACCGAGA UUCCCCCAGUAGCG GCGAGCGAACGGGG AGCAGCCCAGAGCC UGAAUCAGUGUGU GUGUUAGUGGAAG CGUCUGGAAAGGCG CGCGAUACAGGGUG ACAGCCCCGUACAC AAAAAUGCACAUGC UGUGAGCUCGAUG AGUAGGGCGGGAC ACGUGGUAUCCUGU CUGAAUAUGGGGG GACCAUCCUCCAAG GCUAAAUACUCCUG ACUGACCGAUAGUG AACCAGUACCGUGA GGGAAAGGCGAAA AGAACCCCGGCGAG GGGAGUGAAAAAG AACCUGAAACCGUG UACGUACAAGCAGU GGGAGCACGCUUAG GCGUGUGACUGCGU ACCUUUUGUAUAA UGGGUCAGCGACUU AUAUUCUGUAGCA AGGUUAACCGAAU AGGGGAGCCGAAG GGAAACCGAGUCUU AACUGGGCGUUAA GUUGCAGGGUAUA GACCCGAAACCCGG UGAUCUAGCCAUGG | Tylosin | Target\_lig\_32 0 | Exit tunnel for TYLOSIN | Target\_100 | 8.56066730  616974 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | GCAGGUUGAAGGU UGGGUAACACUAAC UGGAGGACCGAACC GACUAAUGUUGAA AAAUUAGCGGAUG ACUUGUGGCUGGG GGUGAAAGGCCAA UCAAACCGGGAGAU AGCUGGUUCUCCCC GAAAGCUAUUUAG GUAGCGCCUCGUGA AUUCAUCUCCGGGG GUAGAGCACUGUU UCGGCAAGGGGGUC ACUUACCAACCCGA UGCAAACUGCGAAU ACCGGAGAAUGUU AUCACGGGAGACAC ACGGCGGGUGCUAA CGUCCGUCGUGAAG AGGGAAACAACCCA GACCGCCAGCUAAG GUCCCAAAGUCAUG GUUAAGUGGGAAA CGAUGUGGGAAGG CCCAGACAGCCAGG AUGUUGGCUUAGA AGCAGCCAUCAUUU AAAGAAAGCGUAA UAGCUCACUGGUCG AGUCGGCCUGCGCG GAAGAUGUAACGG GGCUAAACCAUGCA CCGAAGCUGCGGCA GCGACGCUUAUGCG UUGUUGGGUAGGG GAGCGUUCUGUAA GCCUGCGAAGGUGU GCUGUGAGGCAUGC UGGAGGUAUCAGA AGUGCGAAUGCUG ACAUAAGUAACGA UAAAGCGGGUGAA AAGCCCGCUCGCCG GAAGACCAAGGGU UCCUGUCCAACGUU AAUCGGGGCAGGG UGAGUCGACCCCUA AGGCGAGGCCGAAA GGCGUAGUCGAUG GGAAACAGGUUAA UAUUCCUGUACUUG GUGUUACUGCGAA GGGGGGACGGAGA AGGCUAUGUUGGCC GGGCGACGGUUGUC CCGGUUUAAGCGUG UAGGCUGGUUUUCC AGGCAAAUCCGGAA AAUCAAGGCUGAG GCGUGAUGACGAG GCACUACGGUGCUG AAGCAACAAAUGCC CUGCUUCCAGGAAA AGCCUCUAAGCAUC AGGUAACAUCAAA UCGUACCCCAAACC GACACAGGUGGUCA GGUAGAGAAUACC AAGGCGCUUGAGA GAACUCGGGUGAA GGAACUAGGCAAA AUGGUGCCGUAACU UCGGGAGAAGGCAC GCUGAUAUGUAGG |  |  |  |  |  |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | UGAGGUCCCUCGCG GAUGGAGCUGAAA UCAGUCGAAGAUAC CAGCUGGCUGCAAC UGUUUAUUAAAAA CACAGCACUGUGCA AACACGAAAGUGG ACGUAUACGGUGU GACGCCUGCCCGGU GCCGGAAGGUUAA UUGAUGGGGUUAG CGCAAGCGAAGCUC UUGAUCGAAGCCCC GGUAAACGGCGGCC GUAACXAUAACGG UCCUAAGGUAGCGA AAUUCCUUGUCGGG UAAGUUCCGACCUG CACGAAUGGCGUAA UGAUGGCCAGGCUG UCUCCACCCGAGAC UCAGUGAAAUUGA ACUCGCUGUGAAGA UGCAGUGUACCCGC GGCAAGACGGAAA GACCCCGUGAACCU UUACUAUAGCUUG ACACUGAACAUUGA GCCUUGAUGUGUA GGAUAGGUGGGAG GCUUUGAAGUGUG GACGCCAGUCUGCA UGGAGCCGACCUUG AAAUACCACCCUUU AAUGUUUGAUGUU CUAACGUUGACCCG UAAUCCGGGUUGCG GACAGUGUCUGGU GGGUAGUUUGACU GGGGCGGUCUCCUC CUAAAGAGUAACG GAGGAGCACGAAG GUUGGCUAAUCCUG GUCGGACAUCAGGA GGUUAGUGCAAUG GCAUAAGCCAGCUU GACUGCGAGCGUGA CGGCGCGAGCAGGU GCGAAAGCAGGUCA UAGUGAUCCGGUG GUUCUGAAUGGAA GGGCCAUCGCUCAA CGGAUAAAAGGUA CUCCGGGGAUAACA GGCUGAUACCGCCC AAGAGUUCAUAUC GACGGCGGUGUUU GGCACCUCGAUGUC GGCUCAUCACAUCC UGGGGCUGAAGUA GGUCCCAAGGGUAU GGCUGUUCGCCAUU UAAAGUGGUACGC GAGCUGGGUUUAG AACGUCGUGAGACA GUUCGGUCCCUAUC UGCCGUGGGCGCUG GAGAACUGAGGGG GGCUGCUCCUAGUA CGAGAGGACCGGAG UGGACGCAUCACUG GUGUUCGGGUUGU CAUGCCAAUGGCAC UGCCCGGUAGCUAA AUGCGGAAGAGAU |  |  |  |  |  |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | AAGUGCUGAAAGC AUCUAAGCACGAAA CUUGCCCCGAGAUG AGUUCUCCCUGACC CUUUAAGGGUCCUG AAGGAACGUUGAA GACGACGACGUUGA UAGGCCGGGUGUG UAAGCGCAGCGAUG CGUUGAGCUAACCG GUACUAAUGAACCG UGAGGCUUAACCU |  |  |  |  |  |
| 401 | CCCC1CC(N(C1)C)C(  =O)NC(C2C(C(C(C(O2  )SC)O)O)O)C(C)Cl | GGUUAAGCGACUA AGCGUACACGGUGG AUGCCCUGGCAGUC AGAGGCGAUGAAG GACGUGCUAAUCUG CGAUAAGCGUCGGU AAGGUGAUAUGAA CCGUUAUAACCGGC GAUUUCCGAAUGG GGAAACCCAGUGUG UUUCGACACACUAU CAUUAACUGAAUCC AUAGGUUAAUGAG GCGAACCGGGGGAA CUGAAACAUCUAAG UACCCCGAGGAAAA GAAAUCAACCGAGA UUCCCCCAGUAGCG GCGAGCGAACGGGG AGCAGCCCAGAGCC UGAAUCAGUGUGU GUGUUAGUGGAAG CGUCUGGAAAGGCG CGCGAUACAGGGUG ACAGCCCCGUACAC AAAAAUGCACAUGC UGUGAGCUCGAUG AGUAGGGCGGGAC ACGUGGUAUCCUGU CUGAAUAUGGGGG GACCAUCCUCCAAG GCUAAAUACUCCUG ACUGACCGAUAGUG AACCAGUACCGUGA GGGAAAGGCGAAA AGAACCCCGGCGAG GGGAGUGAAAAAG AACCUGAAACCGUG UACGUACAAGCAGU GGGAGCACGCUUAG GCGUGUGACUGCGU ACCUUUUGUAUAA UGGGUCAGCGACUU AUAUUCUGUAGCA AGGUUAACCGAAU AGGGGAGCCGAAG GGAAACCGAGUCUU AACUGGGCGUUAA GUUGCAGGGUAUA GACCCGAAACCCGG UGAUCUAGCCAUGG GCAGGUUGAAGGU UGGGUAACACUAAC UGGAGGACCGAACC GACUAAUGUUGAA AAAUUAGCGGAUG ACUUGUGGCUGGG GGUGAAAGGCCAA UCAAACCGGGAGAU AGCUGGUUCUCCCC GAAAGCUAUUUAG GUAGCGCCUCGUGA AUUCAUCUCCGGGG | Clindamycin | Target\_lig\_32 4 | 50S ribosome (CLINDAM YCIN) | Target\_100 | 5.09691001  300806 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | GUAGAGCACUGUU UCGGCAAGGGGGUC ACUUACCAACCCGA UGCAAACUGCGAAU ACCGGAGAAUGUU AUCACGGGAGACAC ACGGCGGGUGCUAA CGUCCGUCGUGAAG AGGGAAACAACCCA GACCGCCAGCUAAG GUCCCAAAGUCAUG GUUAAGUGGGAAA CGAUGUGGGAAGG CCCAGACAGCCAGG AUGUUGGCUUAGA AGCAGCCAUCAUUU AAAGAAAGCGUAA UAGCUCACUGGUCG AGUCGGCCUGCGCG GAAGAUGUAACGG GGCUAAACCAUGCA CCGAAGCUGCGGCA GCGACGCUUAUGCG UUGUUGGGUAGGG GAGCGUUCUGUAA GCCUGCGAAGGUGU GCUGUGAGGCAUGC UGGAGGUAUCAGA AGUGCGAAUGCUG ACAUAAGUAACGA UAAAGCGGGUGAA AAGCCCGCUCGCCG GAAGACCAAGGGU UCCUGUCCAACGUU AAUCGGGGCAGGG UGAGUCGACCCCUA AGGCGAGGCCGAAA GGCGUAGUCGAUG GGAAACAGGUUAA UAUUCCUGUACUUG GUGUUACUGCGAA GGGGGGACGGAGA AGGCUAUGUUGGCC GGGCGACGGUUGUC CCGGUUUAAGCGUG UAGGCUGGUUUUCC AGGCAAAUCCGGAA AAUCAAGGCUGAG GCGUGAUGACGAG GCACUACGGUGCUG AAGCAACAAAUGCC CUGCUUCCAGGAAA AGCCUCUAAGCAUC AGGUAACAUCAAA UCGUACCCCAAACC GACACAGGUGGUCA GGUAGAGAAUACC AAGGCGCUUGAGA GAACUCGGGUGAA GGAACUAGGCAAA AUGGUGCCGUAACU UCGGGAGAAGGCAC GCUGAUAUGUAGG UGAGGUCCCUCGCG GAUGGAGCUGAAA UCAGUCGAAGAUAC CAGCUGGCUGCAAC UGUUUAUUAAAAA CACAGCACUGUGCA AACACGAAAGUGG ACGUAUACGGUGU GACGCCUGCCCGGU GCCGGAAGGUUAA UUGAUGGGGUUAG CGCAAGCGAAGCUC |  |  |  |  |  |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | UUGAUCGAAGCCCC GGUAAACGGCGGCC GUAACXAUAACGG UCCUAAGGUAGCGA AAUUCCUUGUCGGG UAAGUUCCGACCUG CACGAAUGGCGUAA UGAUGGCCAGGCUG UCUCCACCCGAGAC UCAGUGAAAUUGA ACUCGCUGUGAAGA UGCAGUGUACCCGC GGCAAGACGGAAA GACCCCGUGAACCU UUACUAUAGCUUG ACACUGAACAUUGA GCCUUGAUGUGUA GGAUAGGUGGGAG GCUUUGAAGUGUG GACGCCAGUCUGCA UGGAGCCGACCUUG AAAUACCACCCUUU AAUGUUUGAUGUU CUAACGUUGACCCG UAAUCCGGGUUGCG GACAGUGUCUGGU GGGUAGUUUGACU GGGGCGGUCUCCUC CUAAAGAGUAACG GAGGAGCACGAAG GUUGGCUAAUCCUG GUCGGACAUCAGGA GGUUAGUGCAAUG GCAUAAGCCAGCUU GACUGCGAGCGUGA CGGCGCGAGCAGGU GCGAAAGCAGGUCA UAGUGAUCCGGUG GUUCUGAAUGGAA GGGCCAUCGCUCAA CGGAUAAAAGGUA CUCCGGGGAUAACA GGCUGAUACCGCCC AAGAGUUCAUAUC GACGGCGGUGUUU GGCACCUCGAUGUC GGCUCAUCACAUCC UGGGGCUGAAGUA GGUCCCAAGGGUAU GGCUGUUCGCCAUU UAAAGUGGUACGC GAGCUGGGUUUAG AACGUCGUGAGACA GUUCGGUCCCUAUC UGCCGUGGGCGCUG GAGAACUGAGGGG GGCUGCUCCUAGUA CGAGAGGACCGGAG UGGACGCAUCACUG GUGUUCGGGUUGU CAUGCCAAUGGCAC UGCCCGGUAGCUAA AUGCGGAAGAGAU AAGUGCUGAAAGC AUCUAAGCACGAAA CUUGCCCCGAGAUG AGUUCUCCCUGACC CUUUAAGGGUCCUG AAGGAACGUUGAA GACGACGACGUUGA UAGGCCGGGUGUG UAAGCGCAGCGAUG CGUUGAGCUAACCG GUACUAAUGAACCG UGAGGCUUAACCU |  |  |  |  |  |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
| 403 | CC1C=CC(=O)NCC=C C(=CC(CC(=O)CC2=N C(=CO2)C(=O)N3CCC  =C3C(=O)OC1C(C)C) O)C | GGUUAAGCGACUA AGCGUACACGGUGG AUGCCCUGGCAGUC AGAGGCGAUGAAG GACGUGCUAAUCUG CGAUAAGCGUCGGU AAGGUGAUAUGAA CCGUUAUAACCGGC GAUUUCCGAAUGG GGAAACCCAGUGUG UUUCGACACACUAU CAUUAACUGAAUCC AUAGGUUAAUGAG GCGAACCGGGGGAA CUGAAACAUCUAAG UACCCCGAGGAAAA GAAAUCAACCGAGA UUCCCCCAGUAGCG GCGAGCGAACGGGG AGCAGCCCAGAGCC UGAAUCAGUGUGU GUGUUAGUGGAAG CGUCUGGAAAGGCG CGCGAUACAGGGUG ACAGCCCCGUACAC AAAAAUGCACAUGC UGUGAGCUCGAUG AGUAGGGCGGGAC ACGUGGUAUCCUGU CUGAAUAUGGGGG GACCAUCCUCCAAG GCUAAAUACUCCUG ACUGACCGAUAGUG AACCAGUACCGUGA GGGAAAGGCGAAA AGAACCCCGGCGAG GGGAGUGAAAAAG AACCUGAAACCGUG UACGUACAAGCAGU GGGAGCACGCUUAG GCGUGUGACUGCGU ACCUUUUGUAUAA UGGGUCAGCGACUU AUAUUCUGUAGCA AGGUUAACCGAAU AGGGGAGCCGAAG GGAAACCGAGUCUU AACUGGGCGUUAA GUUGCAGGGUAUA GACCCGAAACCCGG UGAUCUAGCCAUGG GCAGGUUGAAGGU UGGGUAACACUAAC UGGAGGACCGAACC GACUAAUGUUGAA AAAUUAGCGGAUG ACUUGUGGCUGGG GGUGAAAGGCCAA UCAAACCGGGAGAU AGCUGGUUCUCCCC GAAAGCUAUUUAG GUAGCGCCUCGUGA AUUCAUCUCCGGGG GUAGAGCACUGUU UCGGCAAGGGGGUC ACUUACCAACCCGA UGCAAACUGCGAAU ACCGGAGAAUGUU AUCACGGGAGACAC ACGGCGGGUGCUAA CGUCCGUCGUGAAG AGGGAAACAACCCA GACCGCCAGCUAAG GUCCCAAAGUCAUG GUUAAGUGGGAAA | Virginiamycin M | Target\_lig\_111 3 | 50S ribosome (Virginiamyci n M) | Target\_100 | 5.09691001  300806 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | CGAUGUGGGAAGG CCCAGACAGCCAGG AUGUUGGCUUAGA AGCAGCCAUCAUUU AAAGAAAGCGUAA UAGCUCACUGGUCG AGUCGGCCUGCGCG GAAGAUGUAACGG GGCUAAACCAUGCA CCGAAGCUGCGGCA GCGACGCUUAUGCG UUGUUGGGUAGGG GAGCGUUCUGUAA GCCUGCGAAGGUGU GCUGUGAGGCAUGC UGGAGGUAUCAGA AGUGCGAAUGCUG ACAUAAGUAACGA UAAAGCGGGUGAA AAGCCCGCUCGCCG GAAGACCAAGGGU UCCUGUCCAACGUU AAUCGGGGCAGGG UGAGUCGACCCCUA AGGCGAGGCCGAAA GGCGUAGUCGAUG GGAAACAGGUUAA UAUUCCUGUACUUG GUGUUACUGCGAA GGGGGGACGGAGA AGGCUAUGUUGGCC GGGCGACGGUUGUC CCGGUUUAAGCGUG UAGGCUGGUUUUCC AGGCAAAUCCGGAA AAUCAAGGCUGAG GCGUGAUGACGAG GCACUACGGUGCUG AAGCAACAAAUGCC CUGCUUCCAGGAAA AGCCUCUAAGCAUC AGGUAACAUCAAA UCGUACCCCAAACC GACACAGGUGGUCA GGUAGAGAAUACC AAGGCGCUUGAGA GAACUCGGGUGAA GGAACUAGGCAAA AUGGUGCCGUAACU UCGGGAGAAGGCAC GCUGAUAUGUAGG UGAGGUCCCUCGCG GAUGGAGCUGAAA UCAGUCGAAGAUAC CAGCUGGCUGCAAC UGUUUAUUAAAAA CACAGCACUGUGCA AACACGAAAGUGG ACGUAUACGGUGU GACGCCUGCCCGGU GCCGGAAGGUUAA UUGAUGGGGUUAG CGCAAGCGAAGCUC UUGAUCGAAGCCCC GGUAAACGGCGGCC GUAACXAUAACGG UCCUAAGGUAGCGA AAUUCCUUGUCGGG UAAGUUCCGACCUG CACGAAUGGCGUAA UGAUGGCCAGGCUG UCUCCACCCGAGAC UCAGUGAAAUUGA ACUCGCUGUGAAGA UGCAGUGUACCCGC |  |  |  |  |  |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | GGCAAGACGGAAA GACCCCGUGAACCU UUACUAUAGCUUG ACACUGAACAUUGA GCCUUGAUGUGUA GGAUAGGUGGGAG GCUUUGAAGUGUG GACGCCAGUCUGCA UGGAGCCGACCUUG AAAUACCACCCUUU AAUGUUUGAUGUU CUAACGUUGACCCG UAAUCCGGGUUGCG GACAGUGUCUGGU GGGUAGUUUGACU GGGGCGGUCUCCUC CUAAAGAGUAACG GAGGAGCACGAAG GUUGGCUAAUCCUG GUCGGACAUCAGGA GGUUAGUGCAAUG GCAUAAGCCAGCUU GACUGCGAGCGUGA CGGCGCGAGCAGGU GCGAAAGCAGGUCA UAGUGAUCCGGUG GUUCUGAAUGGAA GGGCCAUCGCUCAA CGGAUAAAAGGUA CUCCGGGGAUAACA GGCUGAUACCGCCC AAGAGUUCAUAUC GACGGCGGUGUUU GGCACCUCGAUGUC GGCUCAUCACAUCC UGGGGCUGAAGUA GGUCCCAAGGGUAU GGCUGUUCGCCAUU UAAAGUGGUACGC GAGCUGGGUUUAG AACGUCGUGAGACA GUUCGGUCCCUAUC UGCCGUGGGCGCUG GAGAACUGAGGGG GGCUGCUCCUAGUA CGAGAGGACCGGAG UGGACGCAUCACUG GUGUUCGGGUUGU CAUGCCAAUGGCAC UGCCCGGUAGCUAA AUGCGGAAGAGAU AAGUGCUGAAAGC AUCUAAGCACGAAA CUUGCCCCGAGAUG AGUUCUCCCUGACC CUUUAAGGGUCCUG AAGGAACGUUGAA GACGACGACGUUGA UAGGCCGGGUGUG UAAGCGCAGCGAUG CGUUGAGCUAACCG GUACUAAUGAACCG UGAGGCUUAACCU |  |  |  |  |  |
| 404 | CC(=O)NCC1CN(C(= O)O1)C2=CC(=C(C=C 2)N3CCOCC3)F | GGUUAAGCGACUA AGCGUACACGGUGG AUGCCCUGGCAGUC AGAGGCGAUGAAG GACGUGCUAAUCUG CGAUAAGCGUCGGU AAGGUGAUAUGAA CCGUUAUAACCGGC GAUUUCCGAAUGG GGAAACCCAGUGUG UUUCGACACACUAU CAUUAACUGAAUCC | Linezolid | Target\_lig\_30 7 | 23SrRNA | Target\_104 | 6 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | AUAGGUUAAUGAG GCGAACCGGGGGAA CUGAAACAUCUAAG UACCCCGAGGAAAA GAAAUCAACCGAGA UUCCCCCAGUAGCG GCGAGCGAACGGGG AGCAGCCCAGAGCC UGAAUCAGUGUGU GUGUUAGUGGAAG CGUCUGGAAAGGCG CGCGAUACAGGGUG ACAGCCCCGUACAC AAAAAUGCACAUGC UGUGAGCUCGAUG AGUAGGGCGGGAC ACGUGGUAUCCUGU CUGAAUAUGGGGG GACCAUCCUCCAAG GCUAAAUACUCCUG ACUGACCGAUAGUG AACCAGUACCGUGA GGGAAAGGCGAAA AGAACCCCGGCGAG GGGAGUGAAAAAG AACCUGAAACCGUG UACGUACAAGCAGU GGGAGCACGCUUAG GCGUGUGACUGCGU ACCUUUUGUAUAA UGGGUCAGCGACUU AUAUUCUGUAGCA AGGUUAACCGAAU AGGGGAGCCGAAG GGAAACCGAGUCUU AACUGGGCGUUAA GUUGCAGGGUAUA GACCCGAAACCCGG UGAUCUAGCCAUGG GCAGGUUGAAGGU UGGGUAACACUAAC UGGAGGACCGAACC GACUAAUGUUGAA AAAUUAGCGGAUG ACUUGUGGCUGGG GGUGAAAGGCCAA UCAAACCGGGAGAU AGCUGGUUCUCCCC GAAAGCUAUUUAG GUAGCGCCUCGUGA AUUCAUCUCCGGGG GUAGAGCACUGUU UCGGCAAGGGGGUC AUCCCGACUUACCA ACCCGAUGCAAACU GCGAAUACCGGAGA AUGUUAUCACGGG AGACACACGGCGGG UGCUAACGUCCGUC GUGAAGAGGGAAA CAACCCAGACCGCC AGCUAAGGUCCCAA AGUCAUGGUUAAG UGGGAAACGAUGU GGGAAGGCCCAGAC AGCCAGGAUGUUG GCUUAGAAGCAGCC AUCAUUUAAAGAA AGCGUAAUAGCUCA CUGGUCGAGUCGGC CUGCGCGGAAGAUG UAACGGGGCUAAAC CAUGCACCGAAGCU GCGGCAGCGACGCU UAUGCGUUGUUGG |  |  |  |  |  |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | GUAGGGGAGCGUU CUGUAAGCCUGCGA AGGUGUGCUGUGA GGCAUGCUGGAGG UAUCAGAAGUGCG AAUGCUGACAUAA GUAACGAUAAAGC GGGUGAAAAGCCCG CUCGCCGGAAGACC AAGGGUUCCUGUCC AACGUUAAUCGGG GCAGGGUGAGUCG ACCCCUAAGGCGAG GCCGAAAGGCGUAG UCGAUGGGAAACA GGUUAAUAUUCCU GUACUUGGUGUUA CUGCGAAGGGGGG ACGGAGAAGGCUA UGUUGGCCGGGCGA CGGUUGUCCCGGUU UAAGCGUGUAGGC UGGUUUUCCAGGCA AAUCCGGAAAAUCA AGGCUGAGGCGUG AUGACGAGGCACUA CGGUGCUGAAGCAA CAAAUGCCCUGCUU CCAGGAAAAGCCUC UAAGCAUCAGGUA ACAUCAAAUCGUAC CCCAAACCGACACU GGUGGUCAGGUAG AGAAUACCAAGGCG CUUGAGAGAACUCG GGUGAAGGAACUA GGCAAAAUGGUGCC GUAACUUCGGGAG AAGGCACGCUGAUA UGUAGGUGAGGUC CCUCGCGGAUGGAG CUGAAAUCAGUCGA AGAUACCAGCUGGC UGCAACUGUUUAU UAAAAACACAGCAC UGUGCAAACACGAA AGUGGACGUAUAC GGUGUGACGCCUGC CCGGUGCCGGAAGG UUAAUUGAUGGGG UUAGCGCAAGCGAA GCUCUUGAUCGAAG CCCCGGUAAACGGC GGCCGUAACUAUAA CGGUCCUAAGGUAG CGAAAUUCCUUGUC GGGUAAGUUCCGAC CUGCACGAAUGGCG UAAUGAUGGCCAG GCUGUCUCCACCCG AGACUCAGUGAAA UUGAACUCGCUGUG CAGAUGCAGUGUAC CCGCGGCAAGACGG AAAGACCCCGUGAA CCUUUACUAUAGCU UGACACUGAACAUU GAGCCUUGAUGUG UAGGAUAGGUGGG AGGCUUUGAAGUG UGGACGCCAGUCUG CAUGGAGCCGACCU UGAAAUACCACCCU UUAAUGUUUGAUG UUCUAACGUUGACC |  |  |  |  |  |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | CGUAAUCCGGGUUG CGGACAGUGUCUGG UGGGUAGUUUGAC UGGGGCGGUCUCCU CCUAAAGAGUAACG GAGGAGCACGAAG GUUGGCUAAUCCUG GUCGGACAUCAGGA GGUUAGUGCAAUG GCAUAAGCCAGCUU GACUGCGAGCGUGA CGGCGCGAGCAGGU GCGAAAGCAGGUCA UAGUGAUCCGGUG GUUCUGAAUGGAA GGGCCAUCGCUCAA CGGAUAAAAGGUA CUCCGGGGAUAACA GGCUGAUACCGCCC AAGAGUUCAUAUC GACGGCGGUGUUU GGCACCUCGAUGUC GGCUCAUCACAUCC UGGGGCUGAAGUA GGUCCCAAGGGUAU GGCUGUUCGCCAUU UAAAGUGGUACGC GAGCUGGGUUUAG AACGUCGUGAGACA GUUCGGUCCCUAUC UGCCGUGGGCGCUG GAGAACUGAGGGG GGCUGCUCCUAGUA CGAGAGGACCGGAG UGGACGCAUCACUG GUGUUCGGGUUGU CAUGCCAAUGGCAC UGCCCGGUAGCUAA AUGCGGAAGAGAU AAGUGCUGAAAGC AUCUAAGCACGAAA CUUGCCCCGAGAUG AGUUCUCCCUGACC CUUUAAGGGUCCUG AAGGAACGUUGAA GACGACGACGUUGA UAGGCCGGGUGUG UAAGCGCAGCGAUG CGUUGAGCUAACCG GUACUAAUGAACCG UGAGGCUUAACCUU |  |  |  |  |  |
| 405 | CC(=O)NC[C@H]1CN (C(=O)O1)C2=CC(=C( C=C2)N3CCN(CC3)C(  =O)CO)F | GGUUAAGCGACUA AGCGUACACGGUGG AUGCCCUGGCAGUC AGAGGCGAUGAAG GACGUGCUAAUCUG CGAUAAGCGUCGGU AAGGUGAUAUGAA CCGUUAUAACCGGC GAUUUCCGAAUGG GGAAACCCAGUGUG UUUCGACACACUAU CAUUAACUGAAUCC AUAGGUUAAUGAG GCGAACCGGGGGAA CUGAAACAUCUAAG UACCCCGAGGAAAA GAAAUCAACCGAGA UUCCCCCAGUAGCG GCGAGCGAACGGGG AGCAGCCCAGAGCC UGAAUCAGUGUGU GUGUUAGUGGAAG CGUCUGGAAAGGCG CGCGAUACAGGGUG | LINEZOLID\_DE RIVATIVE\_1 | Target\_lig\_32 6 | 23SrRNA | Target\_104 | 3.70996538  863748 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | ACAGCCCCGUACAC AAAAAUGCACAUGC UGUGAGCUCGAUG AGUAGGGCGGGAC ACGUGGUAUCCUGU CUGAAUAUGGGGG GACCAUCCUCCAAG GCUAAAUACUCCUG ACUGACCGAUAGUG AACCAGUACCGUGA GGGAAAGGCGAAA AGAACCCCGGCGAG GGGAGUGAAAAAG AACCUGAAACCGUG UACGUACAAGCAGU GGGAGCACGCUUAG GCGUGUGACUGCGU ACCUUUUGUAUAA UGGGUCAGCGACUU AUAUUCUGUAGCA AGGUUAACCGAAU AGGGGAGCCGAAG GGAAACCGAGUCUU AACUGGGCGUUAA GUUGCAGGGUAUA GACCCGAAACCCGG UGAUCUAGCCAUGG GCAGGUUGAAGGU UGGGUAACACUAAC UGGAGGACCGAACC GACUAAUGUUGAA AAAUUAGCGGAUG ACUUGUGGCUGGG GGUGAAAGGCCAA UCAAACCGGGAGAU AGCUGGUUCUCCCC GAAAGCUAUUUAG GUAGCGCCUCGUGA AUUCAUCUCCGGGG GUAGAGCACUGUU UCGGCAAGGGGGUC AUCCCGACUUACCA ACCCGAUGCAAACU GCGAAUACCGGAGA AUGUUAUCACGGG AGACACACGGCGGG UGCUAACGUCCGUC GUGAAGAGGGAAA CAACCCAGACCGCC AGCUAAGGUCCCAA AGUCAUGGUUAAG UGGGAAACGAUGU GGGAAGGCCCAGAC AGCCAGGAUGUUG GCUUAGAAGCAGCC AUCAUUUAAAGAA AGCGUAAUAGCUCA CUGGUCGAGUCGGC CUGCGCGGAAGAUG UAACGGGGCUAAAC CAUGCACCGAAGCU GCGGCAGCGACGCU UAUGCGUUGUUGG GUAGGGGAGCGUU CUGUAAGCCUGCGA AGGUGUGCUGUGA GGCAUGCUGGAGG UAUCAGAAGUGCG AAUGCUGACAUAA GUAACGAUAAAGC GGGUGAAAAGCCCG CUCGCCGGAAGACC AAGGGUUCCUGUCC AACGUUAAUCGGG GCAGGGUGAGUCG |  |  |  |  |  |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | ACCCCUAAGGCGAG GCCGAAAGGCGUAG UCGAUGGGAAACA GGUUAAUAUUCCU GUACUUGGUGUUA CUGCGAAGGGGGG ACGGAGAAGGCUA UGUUGGCCGGGCGA CGGUUGUCCCGGUU UAAGCGUGUAGGC UGGUUUUCCAGGCA AAUCCGGAAAAUCA AGGCUGAGGCGUG AUGACGAGGCACUA CGGUGCUGAAGCAA CAAAUGCCCUGCUU CCAGGAAAAGCCUC UAAGCAUCAGGUA ACAUCAAAUCGUAC CCCAAACCGACACU GGUGGUCAGGUAG AGAAUACCAAGGCG CUUGAGAGAACUCG GGUGAAGGAACUA GGCAAAAUGGUGCC GUAACUUCGGGAG AAGGCACGCUGAUA UGUAGGUGAGGUC CCUCGCGGAUGGAG CUGAAAUCAGUCGA AGAUACCAGCUGGC UGCAACUGUUUAU UAAAAACACAGCAC UGUGCAAACACGAA AGUGGACGUAUAC GGUGUGACGCCUGC CCGGUGCCGGAAGG UUAAUUGAUGGGG UUAGCGCAAGCGAA GCUCUUGAUCGAAG CCCCGGUAAACGGC GGCCGUAACUAUAA CGGUCCUAAGGUAG CGAAAUUCCUUGUC GGGUAAGUUCCGAC CUGCACGAAUGGCG UAAUGAUGGCCAG GCUGUCUCCACCCG AGACUCAGUGAAA UUGAACUCGCUGUG CAGAUGCAGUGUAC CCGCGGCAAGACGG AAAGACCCCGUGAA CCUUUACUAUAGCU UGACACUGAACAUU GAGCCUUGAUGUG UAGGAUAGGUGGG AGGCUUUGAAGUG UGGACGCCAGUCUG CAUGGAGCCGACCU UGAAAUACCACCCU UUAAUGUUUGAUG UUCUAACGUUGACC CGUAAUCCGGGUUG CGGACAGUGUCUGG UGGGUAGUUUGAC UGGGGCGGUCUCCU CCUAAAGAGUAACG GAGGAGCACGAAG GUUGGCUAAUCCUG GUCGGACAUCAGGA GGUUAGUGCAAUG GCAUAAGCCAGCUU GACUGCGAGCGUGA CGGCGCGAGCAGGU |  |  |  |  |  |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | GCGAAAGCAGGUCA UAGUGAUCCGGUG GUUCUGAAUGGAA GGGCCAUCGCUCAA CGGAUAAAAGGUA CUCCGGGGAUAACA GGCUGAUACCGCCC AAGAGUUCAUAUC GACGGCGGUGUUU GGCACCUCGAUGUC GGCUCAUCACAUCC UGGGGCUGAAGUA GGUCCCAAGGGUAU GGCUGUUCGCCAUU UAAAGUGGUACGC GAGCUGGGUUUAG AACGUCGUGAGACA GUUCGGUCCCUAUC UGCCGUGGGCGCUG GAGAACUGAGGGG GGCUGCUCCUAGUA CGAGAGGACCGGAG UGGACGCAUCACUG GUGUUCGGGUUGU CAUGCCAAUGGCAC UGCCCGGUAGCUAA AUGCGGAAGAGAU AAGUGCUGAAAGC AUCUAAGCACGAAA CUUGCCCCGAGAUG AGUUCUCCCUGACC CUUUAAGGGUCCUG AAGGAACGUUGAA GACGACGACGUUGA UAGGCCGGGUGUG UAAGCGCAGCGAUG CGUUGAGCUAACCG GUACUAAUGAACCG UGAGGCUUAACCUU |  |  |  |  |  |
| 406 | CC(=O)NC[C@@H]1C N(C(=O)O1)C2=CC(= C(C=C2)N3CCN(CC3) C(=O)CO)F | GGUUAAGCGACUA AGCGUACACGGUGG AUGCCCUGGCAGUC AGAGGCGAUGAAG GACGUGCUAAUCUG CGAUAAGCGUCGGU AAGGUGAUAUGAA CCGUUAUAACCGGC GAUUUCCGAAUGG GGAAACCCAGUGUG UUUCGACACACUAU CAUUAACUGAAUCC AUAGGUUAAUGAG GCGAACCGGGGGAA CUGAAACAUCUAAG UACCCCGAGGAAAA GAAAUCAACCGAGA UUCCCCCAGUAGCG GCGAGCGAACGGGG AGCAGCCCAGAGCC UGAAUCAGUGUGU GUGUUAGUGGAAG CGUCUGGAAAGGCG CGCGAUACAGGGUG ACAGCCCCGUACAC AAAAAUGCACAUGC UGUGAGCUCGAUG AGUAGGGCGGGAC ACGUGGUAUCCUGU CUGAAUAUGGGGG GACCAUCCUCCAAG GCUAAAUACUCCUG ACUGACCGAUAGUG AACCAGUACCGUGA GGGAAAGGCGAAA AGAACCCCGGCGAG | LINEZOLID\_DE RIVATIVE\_2 | Target\_lig\_32 7 | 23SrRNA | Target\_104 | 3.11861534  322943 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | GGGAGUGAAAAAG AACCUGAAACCGUG UACGUACAAGCAGU GGGAGCACGCUUAG GCGUGUGACUGCGU ACCUUUUGUAUAA UGGGUCAGCGACUU AUAUUCUGUAGCA AGGUUAACCGAAU AGGGGAGCCGAAG GGAAACCGAGUCUU AACUGGGCGUUAA GUUGCAGGGUAUA GACCCGAAACCCGG UGAUCUAGCCAUGG GCAGGUUGAAGGU UGGGUAACACUAAC UGGAGGACCGAACC GACUAAUGUUGAA AAAUUAGCGGAUG ACUUGUGGCUGGG GGUGAAAGGCCAA UCAAACCGGGAGAU AGCUGGUUCUCCCC GAAAGCUAUUUAG GUAGCGCCUCGUGA AUUCAUCUCCGGGG GUAGAGCACUGUU UCGGCAAGGGGGUC AUCCCGACUUACCA ACCCGAUGCAAACU GCGAAUACCGGAGA AUGUUAUCACGGG AGACACACGGCGGG UGCUAACGUCCGUC GUGAAGAGGGAAA CAACCCAGACCGCC AGCUAAGGUCCCAA AGUCAUGGUUAAG UGGGAAACGAUGU GGGAAGGCCCAGAC AGCCAGGAUGUUG GCUUAGAAGCAGCC AUCAUUUAAAGAA AGCGUAAUAGCUCA CUGGUCGAGUCGGC CUGCGCGGAAGAUG UAACGGGGCUAAAC CAUGCACCGAAGCU GCGGCAGCGACGCU UAUGCGUUGUUGG GUAGGGGAGCGUU CUGUAAGCCUGCGA AGGUGUGCUGUGA GGCAUGCUGGAGG UAUCAGAAGUGCG AAUGCUGACAUAA GUAACGAUAAAGC GGGUGAAAAGCCCG CUCGCCGGAAGACC AAGGGUUCCUGUCC AACGUUAAUCGGG GCAGGGUGAGUCG ACCCCUAAGGCGAG GCCGAAAGGCGUAG UCGAUGGGAAACA GGUUAAUAUUCCU GUACUUGGUGUUA CUGCGAAGGGGGG ACGGAGAAGGCUA UGUUGGCCGGGCGA CGGUUGUCCCGGUU UAAGCGUGUAGGC UGGUUUUCCAGGCA AAUCCGGAAAAUCA |  |  |  |  |  |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | AGGCUGAGGCGUG AUGACGAGGCACUA CGGUGCUGAAGCAA CAAAUGCCCUGCUU CCAGGAAAAGCCUC UAAGCAUCAGGUA ACAUCAAAUCGUAC CCCAAACCGACACU GGUGGUCAGGUAG AGAAUACCAAGGCG CUUGAGAGAACUCG GGUGAAGGAACUA GGCAAAAUGGUGCC GUAACUUCGGGAG AAGGCACGCUGAUA UGUAGGUGAGGUC CCUCGCGGAUGGAG CUGAAAUCAGUCGA AGAUACCAGCUGGC UGCAACUGUUUAU UAAAAACACAGCAC UGUGCAAACACGAA AGUGGACGUAUAC GGUGUGACGCCUGC CCGGUGCCGGAAGG UUAAUUGAUGGGG UUAGCGCAAGCGAA GCUCUUGAUCGAAG CCCCGGUAAACGGC GGCCGUAACUAUAA CGGUCCUAAGGUAG CGAAAUUCCUUGUC GGGUAAGUUCCGAC CUGCACGAAUGGCG UAAUGAUGGCCAG GCUGUCUCCACCCG AGACUCAGUGAAA UUGAACUCGCUGUG CAGAUGCAGUGUAC CCGCGGCAAGACGG AAAGACCCCGUGAA CCUUUACUAUAGCU UGACACUGAACAUU GAGCCUUGAUGUG UAGGAUAGGUGGG AGGCUUUGAAGUG UGGACGCCAGUCUG CAUGGAGCCGACCU UGAAAUACCACCCU UUAAUGUUUGAUG UUCUAACGUUGACC CGUAAUCCGGGUUG CGGACAGUGUCUGG UGGGUAGUUUGAC UGGGGCGGUCUCCU CCUAAAGAGUAACG GAGGAGCACGAAG GUUGGCUAAUCCUG GUCGGACAUCAGGA GGUUAGUGCAAUG GCAUAAGCCAGCUU GACUGCGAGCGUGA CGGCGCGAGCAGGU GCGAAAGCAGGUCA UAGUGAUCCGGUG GUUCUGAAUGGAA GGGCCAUCGCUCAA CGGAUAAAAGGUA CUCCGGGGAUAACA GGCUGAUACCGCCC AAGAGUUCAUAUC GACGGCGGUGUUU GGCACCUCGAUGUC GGCUCAUCACAUCC UGGGGCUGAAGUA |  |  |  |  |  |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | GGUCCCAAGGGUAU GGCUGUUCGCCAUU UAAAGUGGUACGC GAGCUGGGUUUAG AACGUCGUGAGACA GUUCGGUCCCUAUC UGCCGUGGGCGCUG GAGAACUGAGGGG GGCUGCUCCUAGUA CGAGAGGACCGGAG UGGACGCAUCACUG GUGUUCGGGUUGU CAUGCCAAUGGCAC UGCCCGGUAGCUAA AUGCGGAAGAGAU AAGUGCUGAAAGC AUCUAAGCACGAAA CUUGCCCCGAGAUG AGUUCUCCCUGACC CUUUAAGGGUCCUG AAGGAACGUUGAA GACGACGACGUUGA UAGGCCGGGUGUG UAAGCGCAGCGAUG CGUUGAGCUAACCG GUACUAAUGAACCG UGAGGCUUAACCUU |  |  |  |  |  |
| 407 | CC(=S)NC[C@@H]1C N(C(=O)O1)C2=CC(= C(C=C2)N3CCS(=O)C C3)F | GGUUAAGCGACUA AGCGUACACGGUGG AUGCCCUGGCAGUC AGAGGCGAUGAAG GACGUGCUAAUCUG CGAUAAGCGUCGGU AAGGUGAUAUGAA CCGUUAUAACCGGC GAUUUCCGAAUGG GGAAACCCAGUGUG UUUCGACACACUAU CAUUAACUGAAUCC AUAGGUUAAUGAG GCGAACCGGGGGAA CUGAAACAUCUAAG UACCCCGAGGAAAA GAAAUCAACCGAGA UUCCCCCAGUAGCG GCGAGCGAACGGGG AGCAGCCCAGAGCC UGAAUCAGUGUGU GUGUUAGUGGAAG CGUCUGGAAAGGCG CGCGAUACAGGGUG ACAGCCCCGUACAC AAAAAUGCACAUGC UGUGAGCUCGAUG AGUAGGGCGGGAC ACGUGGUAUCCUGU CUGAAUAUGGGGG GACCAUCCUCCAAG GCUAAAUACUCCUG ACUGACCGAUAGUG AACCAGUACCGUGA GGGAAAGGCGAAA AGAACCCCGGCGAG GGGAGUGAAAAAG AACCUGAAACCGUG UACGUACAAGCAGU GGGAGCACGCUUAG GCGUGUGACUGCGU ACCUUUUGUAUAA UGGGUCAGCGACUU AUAUUCUGUAGCA AGGUUAACCGAAU AGGGGAGCCGAAG GGAAACCGAGUCUU AACUGGGCGUUAA | LINEZOLID\_DE RIVATIVE\_3 | Target\_lig\_32 8 | 23SrRNA | Target\_104 | 4.02687214  64003 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | GUUGCAGGGUAUA GACCCGAAACCCGG UGAUCUAGCCAUGG GCAGGUUGAAGGU UGGGUAACACUAAC UGGAGGACCGAACC GACUAAUGUUGAA AAAUUAGCGGAUG ACUUGUGGCUGGG GGUGAAAGGCCAA UCAAACCGGGAGAU AGCUGGUUCUCCCC GAAAGCUAUUUAG GUAGCGCCUCGUGA AUUCAUCUCCGGGG GUAGAGCACUGUU UCGGCAAGGGGGUC AUCCCGACUUACCA ACCCGAUGCAAACU GCGAAUACCGGAGA AUGUUAUCACGGG AGACACACGGCGGG UGCUAACGUCCGUC GUGAAGAGGGAAA CAACCCAGACCGCC AGCUAAGGUCCCAA AGUCAUGGUUAAG UGGGAAACGAUGU GGGAAGGCCCAGAC AGCCAGGAUGUUG GCUUAGAAGCAGCC AUCAUUUAAAGAA AGCGUAAUAGCUCA CUGGUCGAGUCGGC CUGCGCGGAAGAUG UAACGGGGCUAAAC CAUGCACCGAAGCU GCGGCAGCGACGCU UAUGCGUUGUUGG GUAGGGGAGCGUU CUGUAAGCCUGCGA AGGUGUGCUGUGA GGCAUGCUGGAGG UAUCAGAAGUGCG AAUGCUGACAUAA GUAACGAUAAAGC GGGUGAAAAGCCCG CUCGCCGGAAGACC AAGGGUUCCUGUCC AACGUUAAUCGGG GCAGGGUGAGUCG ACCCCUAAGGCGAG GCCGAAAGGCGUAG UCGAUGGGAAACA GGUUAAUAUUCCU GUACUUGGUGUUA CUGCGAAGGGGGG ACGGAGAAGGCUA UGUUGGCCGGGCGA CGGUUGUCCCGGUU UAAGCGUGUAGGC UGGUUUUCCAGGCA AAUCCGGAAAAUCA AGGCUGAGGCGUG AUGACGAGGCACUA CGGUGCUGAAGCAA CAAAUGCCCUGCUU CCAGGAAAAGCCUC UAAGCAUCAGGUA ACAUCAAAUCGUAC CCCAAACCGACACU GGUGGUCAGGUAG AGAAUACCAAGGCG CUUGAGAGAACUCG GGUGAAGGAACUA |  |  |  |  |  |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | GGCAAAAUGGUGCC GUAACUUCGGGAG AAGGCACGCUGAUA UGUAGGUGAGGUC CCUCGCGGAUGGAG CUGAAAUCAGUCGA AGAUACCAGCUGGC UGCAACUGUUUAU UAAAAACACAGCAC UGUGCAAACACGAA AGUGGACGUAUAC GGUGUGACGCCUGC CCGGUGCCGGAAGG UUAAUUGAUGGGG UUAGCGCAAGCGAA GCUCUUGAUCGAAG CCCCGGUAAACGGC GGCCGUAACUAUAA CGGUCCUAAGGUAG CGAAAUUCCUUGUC GGGUAAGUUCCGAC CUGCACGAAUGGCG UAAUGAUGGCCAG GCUGUCUCCACCCG AGACUCAGUGAAA UUGAACUCGCUGUG CAGAUGCAGUGUAC CCGCGGCAAGACGG AAAGACCCCGUGAA CCUUUACUAUAGCU UGACACUGAACAUU GAGCCUUGAUGUG UAGGAUAGGUGGG AGGCUUUGAAGUG UGGACGCCAGUCUG CAUGGAGCCGACCU UGAAAUACCACCCU UUAAUGUUUGAUG UUCUAACGUUGACC CGUAAUCCGGGUUG CGGACAGUGUCUGG UGGGUAGUUUGAC UGGGGCGGUCUCCU CCUAAAGAGUAACG GAGGAGCACGAAG GUUGGCUAAUCCUG GUCGGACAUCAGGA GGUUAGUGCAAUG GCAUAAGCCAGCUU GACUGCGAGCGUGA CGGCGCGAGCAGGU GCGAAAGCAGGUCA UAGUGAUCCGGUG GUUCUGAAUGGAA GGGCCAUCGCUCAA CGGAUAAAAGGUA CUCCGGGGAUAACA GGCUGAUACCGCCC AAGAGUUCAUAUC GACGGCGGUGUUU GGCACCUCGAUGUC GGCUCAUCACAUCC UGGGGCUGAAGUA GGUCCCAAGGGUAU GGCUGUUCGCCAUU UAAAGUGGUACGC GAGCUGGGUUUAG AACGUCGUGAGACA GUUCGGUCCCUAUC UGCCGUGGGCGCUG GAGAACUGAGGGG GGCUGCUCCUAGUA CGAGAGGACCGGAG UGGACGCAUCACUG GUGUUCGGGUUGU |  |  |  |  |  |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | CAUGCCAAUGGCAC UGCCCGGUAGCUAA AUGCGGAAGAGAU AAGUGCUGAAAGC AUCUAAGCACGAAA CUUGCCCCGAGAUG AGUUCUCCCUGACC CUUUAAGGGUCCUG AAGGAACGUUGAA GACGACGACGUUGA UAGGCCGGGUGUG UAAGCGCAGCGAUG CGUUGAGCUAACCG GUACUAAUGAACCG UGAGGCUUAACCUU |  |  |  |  |  |
| 408 | CC(=S)NC[C@@H]1C N(C(=O)O1)C2=CC(= C(C=C2)N3CCS(=O)C C3)F | GGUUAAGCGACUA AGCGUACACGGUGG AUGCCCUGGCAGUC AGAGGCGAUGAAG GACGUGCUAAUCUG CGAUAAGCGUCGGU AAGGUGAUAUGAA CCGUUAUAACCGGC GAUUUCCGAAUGG GGAAACCCAGUGUG UUUCGACACACUAU CAUUAACUGAAUCC AUAGGUUAAUGAG GCGAACCGGGGGAA CUGAAACAUCUAAG UACCCCGAGGAAAA GAAAUCAACCGAGA UUCCCCCAGUAGCG GCGAGCGAACGGGG AGCAGCCCAGAGCC UGAAUCAGUGUGU GUGUUAGUGGAAG CGUCUGGAAAGGCG CGCGAUACAGGGUG ACAGCCCCGUACAC AAAAAUGCACAUGC UGUGAGCUCGAUG AGUAGGGCGGGAC ACGUGGUAUCCUGU CUGAAUAUGGGGG GACCAUCCUCCAAG GCUAAAUACUCCUG ACUGACCGAUAGUG AACCAGUACCGUGA GGGAAAGGCGAAA AGAACCCCGGCGAG GGGAGUGAAAAAG AACCUGAAACCGUG UACGUACAAGCAGU GGGAGCACGCUUAG GCGUGUGACUGCGU ACCUUUUGUAUAA UGGGUCAGCGACUU AUAUUCUGUAGCA AGGUUAACCGAAU AGGGGAGCCGAAG GGAAACCGAGUCUU AACUGGGCGUUAA GUUGCAGGGUAUA GACCCGAAACCCGG UGAUCUAGCCAUGG GCAGGUUGAAGGU UGGGUAACACUAAC UGGAGGACCGAACC GACUAAUGUUGAA AAAUUAGCGGAUG ACUUGUGGCUGGG GGUGAAAGGCCAA UCAAACCGGGAGAU AGCUGGUUCUCCCC | LINEZOLID\_DE RIVATIVE\_4 | Target\_lig\_32 9 | 23SrRNA | Target\_104 | 3.32422165  832591 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | GAAAGCUAUUUAG GUAGCGCCUCGUGA AUUCAUCUCCGGGG GUAGAGCACUGUU UCGGCAAGGGGGUC AUCCCGACUUACCA ACCCGAUGCAAACU GCGAAUACCGGAGA AUGUUAUCACGGG AGACACACGGCGGG UGCUAACGUCCGUC GUGAAGAGGGAAA CAACCCAGACCGCC AGCUAAGGUCCCAA AGUCAUGGUUAAG UGGGAAACGAUGU GGGAAGGCCCAGAC AGCCAGGAUGUUG GCUUAGAAGCAGCC AUCAUUUAAAGAA AGCGUAAUAGCUCA CUGGUCGAGUCGGC CUGCGCGGAAGAUG UAACGGGGCUAAAC CAUGCACCGAAGCU GCGGCAGCGACGCU UAUGCGUUGUUGG GUAGGGGAGCGUU CUGUAAGCCUGCGA AGGUGUGCUGUGA GGCAUGCUGGAGG UAUCAGAAGUGCG AAUGCUGACAUAA GUAACGAUAAAGC GGGUGAAAAGCCCG CUCGCCGGAAGACC AAGGGUUCCUGUCC AACGUUAAUCGGG GCAGGGUGAGUCG ACCCCUAAGGCGAG GCCGAAAGGCGUAG UCGAUGGGAAACA GGUUAAUAUUCCU GUACUUGGUGUUA CUGCGAAGGGGGG ACGGAGAAGGCUA UGUUGGCCGGGCGA CGGUUGUCCCGGUU UAAGCGUGUAGGC UGGUUUUCCAGGCA AAUCCGGAAAAUCA AGGCUGAGGCGUG AUGACGAGGCACUA CGGUGCUGAAGCAA CAAAUGCCCUGCUU CCAGGAAAAGCCUC UAAGCAUCAGGUA ACAUCAAAUCGUAC CCCAAACCGACACU GGUGGUCAGGUAG AGAAUACCAAGGCG CUUGAGAGAACUCG GGUGAAGGAACUA GGCAAAAUGGUGCC GUAACUUCGGGAG AAGGCACGCUGAUA UGUAGGUGAGGUC CCUCGCGGAUGGAG CUGAAAUCAGUCGA AGAUACCAGCUGGC UGCAACUGUUUAU UAAAAACACAGCAC UGUGCAAACACGAA AGUGGACGUAUAC GGUGUGACGCCUGC |  |  |  |  |  |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | CCGGUGCCGGAAGG UUAAUUGAUGGGG UUAGCGCAAGCGAA GCUCUUGAUCGAAG CCCCGGUAAACGGC GGCCGUAACUAUAA CGGUCCUAAGGUAG CGAAAUUCCUUGUC GGGUAAGUUCCGAC CUGCACGAAUGGCG UAAUGAUGGCCAG GCUGUCUCCACCCG AGACUCAGUGAAA UUGAACUCGCUGUG CAGAUGCAGUGUAC CCGCGGCAAGACGG AAAGACCCCGUGAA CCUUUACUAUAGCU UGACACUGAACAUU GAGCCUUGAUGUG UAGGAUAGGUGGG AGGCUUUGAAGUG UGGACGCCAGUCUG CAUGGAGCCGACCU UGAAAUACCACCCU UUAAUGUUUGAUG UUCUAACGUUGACC CGUAAUCCGGGUUG CGGACAGUGUCUGG UGGGUAGUUUGAC UGGGGCGGUCUCCU CCUAAAGAGUAACG GAGGAGCACGAAG GUUGGCUAAUCCUG GUCGGACAUCAGGA GGUUAGUGCAAUG GCAUAAGCCAGCUU GACUGCGAGCGUGA CGGCGCGAGCAGGU GCGAAAGCAGGUCA UAGUGAUCCGGUG GUUCUGAAUGGAA GGGCCAUCGCUCAA CGGAUAAAAGGUA CUCCGGGGAUAACA GGCUGAUACCGCCC AAGAGUUCAUAUC GACGGCGGUGUUU GGCACCUCGAUGUC GGCUCAUCACAUCC UGGGGCUGAAGUA GGUCCCAAGGGUAU GGCUGUUCGCCAUU UAAAGUGGUACGC GAGCUGGGUUUAG AACGUCGUGAGACA GUUCGGUCCCUAUC UGCCGUGGGCGCUG GAGAACUGAGGGG GGCUGCUCCUAGUA CGAGAGGACCGGAG UGGACGCAUCACUG GUGUUCGGGUUGU CAUGCCAAUGGCAC UGCCCGGUAGCUAA AUGCGGAAGAGAU AAGUGCUGAAAGC AUCUAAGCACGAAA CUUGCCCCGAGAUG AGUUCUCCCUGACC CUUUAAGGGUCCUG AAGGAACGUUGAA GACGACGACGUUGA UAGGCCGGGUGUG UAAGCGCAGCGAUG |  |  |  |  |  |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | CGUUGAGCUAACCG GUACUAAUGAACCG UGAGGCUUAACCUU |  |  |  |  |  |
| 419 | CC1CCC23CCC(=O)C 2C1(C(CC(C(C3C)O) (C)C=C)OC(=O)CSC4 CCNCC4)C | GGUUAAGCGACUA AGCGUACACGGUGG AUGCCCUGGCAGUC AGAGGCGAUGAAG GACGUGCUAAUCUG CGAUAAGCGUCGGU AAGGUGAUAUGAA CCGUUAUAACCGGC GAUUUCCGAAUGG GGAAACCCAGUGUG UUUCGACACACUAU CAUUAACUGAAUCC AUAGGUUAAUGAG GCGAACCGGGGGAA CUGAAACAUCUAAG UACCCCGAGGAAAA GAAAUCAACCGAGA UUCCCCCAGUAGCG GCGAGCGAACGGGG AGCAGCCCAGAGCC UGAAUCAGUGUGU GUGUUAGUGGAAG CGUCUGGAAAGGCG CGCGAUACAGGGUG ACAGCCCCGUACAC AAAAAUGCACAUGC UGUGAGCUCGAUG AGUAGGGCGGGAC ACGUGGUAUCCUGU CUGAAUAUGGGGG GACCAUCCUCCAAG GCUAAAUACUCCUG ACUGACCGAUAGUG AACCAGUACCGUGA GGGAAAGGCGAAA AGAACCCCGGCGAG GGGAGUGAAAAAG AACCUGAAACCGUG UACGUACAAGCAGU GGGAGCACGCUUAG GCGUGUGACUGCGU ACCUUUUGUAUAA UGGGUCAGCGACUU AUAUUCUGUAGCA AGGUUAACCGAAU AGGGGAGCCGAAG GGAAACCGAGUCUU AACUGGGCGUUAA GUUGCAGGGUAUA GACCCGAAACCCGG UGAUCUAGCCAUGG GCAGGUUGAAGGU UGGGUAACACUAAC UGGAGGACCGAACC GACUAAUGUUGAA AAAUUAGCGGAUG ACUUGUGGCUGGG GGUGAAAGGCCAA UCAAACCGGGAGAU AGCUGGUUCUCCCC GAAAGCUAUUUAG GUAGCGCCUCGUGA AUUCAUCUCCGGGG GUAGAGCACUGUU UCGGCAAGGGGGUC ACUUACCAACCCGA UGCAAACUGCGAAU ACCGGAGAAUGUU AUCACGGGAGACAC ACGGCGGGUGCUAA CGUCCGUCGUGAAG AGGGAAACAACCCA | SB-280080 | Target\_lig\_33 4 | 50S SB  280080 | Target\_100 | 8.12493873  66083 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | GACCGCCAGCUAAG GUCCCAAAGUCAUG GUUAAGUGGGAAA CGAUGUGGGAAGG CCCAGACAGCCAGG AUGUUGGCUUAGA AGCAGCCAUCAUUU AAAGAAAGCGUAA UAGCUCACUGGUCG AGUCGGCCUGCGCG GAAGAUGUAACGG GGCUAAACCAUGCA CCGAAGCUGCGGCA GCGACGCUUAUGCG UUGUUGGGUAGGG GAGCGUUCUGUAA GCCUGCGAAGGUGU GCUGUGAGGCAUGC UGGAGGUAUCAGA AGUGCGAAUGCUG ACAUAAGUAACGA UAAAGCGGGUGAA AAGCCCGCUCGCCG GAAGACCAAGGGU UCCUGUCCAACGUU AAUCGGGGCAGGG UGAGUCGACCCCUA AGGCGAGGCCGAAA GGCGUAGUCGAUG GGAAACAGGUUAA UAUUCCUGUACUUG GUGUUACUGCGAA GGGGGGACGGAGA AGGCUAUGUUGGCC GGGCGACGGUUGUC CCGGUUUAAGCGUG UAGGCUGGUUUUCC AGGCAAAUCCGGAA AAUCAAGGCUGAG GCGUGAUGACGAG GCACUACGGUGCUG AAGCAACAAAUGCC CUGCUUCCAGGAAA AGCCUCUAAGCAUC AGGUAACAUCAAA UCGUACCCCAAACC GACACAGGUGGUCA GGUAGAGAAUACC AAGGCGCUUGAGA GAACUCGGGUGAA GGAACUAGGCAAA AUGGUGCCGUAACU UCGGGAGAAGGCAC GCUGAUAUGUAGG UGAGGUCCCUCGCG GAUGGAGCUGAAA UCAGUCGAAGAUAC CAGCUGGCUGCAAC UGUUUAUUAAAAA CACAGCACUGUGCA AACACGAAAGUGG ACGUAUACGGUGU GACGCCUGCCCGGU GCCGGAAGGUUAA UUGAUGGGGUUAG CGCAAGCGAAGCUC UUGAUCGAAGCCCC GGUAAACGGCGGCC GUAACXAUAACGG UCCUAAGGUAGCGA AAUUCCUUGUCGGG UAAGUUCCGACCUG CACGAAUGGCGUAA UGAUGGCCAGGCUG UCUCCACCCGAGAC |  |  |  |  |  |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | UCAGUGAAAUUGA ACUCGCUGUGAAGA UGCAGUGUACCCGC GGCAAGACGGAAA GACCCCGUGAACCU UUACUAUAGCUUG ACACUGAACAUUGA GCCUUGAUGUGUA GGAUAGGUGGGAG GCUUUGAAGUGUG GACGCCAGUCUGCA UGGAGCCGACCUUG AAAUACCACCCUUU AAUGUUUGAUGUU CUAACGUUGACCCG UAAUCCGGGUUGCG GACAGUGUCUGGU GGGUAGUUUGACU GGGGCGGUCUCCUC CUAAAGAGUAACG GAGGAGCACGAAG GUUGGCUAAUCCUG GUCGGACAUCAGGA GGUUAGUGCAAUG GCAUAAGCCAGCUU GACUGCGAGCGUGA CGGCGCGAGCAGGU GCGAAAGCAGGUCA UAGUGAUCCGGUG GUUCUGAAUGGAA GGGCCAUCGCUCAA CGGAUAAAAGGUA CUCCGGGGAUAACA GGCUGAUACCGCCC AAGAGUUCAUAUC GACGGCGGUGUUU GGCACCUCGAUGUC GGCUCAUCACAUCC UGGGGCUGAAGUA GGUCCCAAGGGUAU GGCUGUUCGCCAUU UAAAGUGGUACGC GAGCUGGGUUUAG AACGUCGUGAGACA GUUCGGUCCCUAUC UGCCGUGGGCGCUG GAGAACUGAGGGG GGCUGCUCCUAGUA CGAGAGGACCGGAG UGGACGCAUCACUG GUGUUCGGGUUGU CAUGCCAAUGGCAC UGCCCGGUAGCUAA AUGCGGAAGAGAU AAGUGCUGAAAGC AUCUAAGCACGAAA CUUGCCCCGAGAUG AGUUCUCCCUGACC CUUUAAGGGUCCUG AAGGAACGUUGAA GACGACGACGUUGA UAGGCCGGGUGUG UAAGCGCAGCGAUG CGUUGAGCUAACCG GUACUAAUGAACCG UGAGGCUUAACCU |  |  |  |  |  |
| 420 | [C@@H]1(C[C@]  ([C@@H]([C@@H]  ([C@]23[C@@H]  ([C@]1([C@@H]  (CC3)C)C)C(=O)  [C@H](C2)O)C)O)  (C)C=C)OC(=O)NC(=  O)c1ccc(nn1)N | GGUUAAGCGACUA AGCGUACACGGUGG AUGCCCUGGCAGUC AGAGGCGAUGAAG GACGUGCUAAUCUG CGAUAAGCGUCGGU AAGGUGAUAUGAA CCGUUAUAACCGGC GAUUUCCGAAUGG | SB-571519 | Target\_lig\_33 5 | 50S SB571519 | Target\_100 | 7.95467702  121334 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | GGAAACCCAGUGUG UUUCGACACACUAU CAUUAACUGAAUCC AUAGGUUAAUGAG GCGAACCGGGGGAA CUGAAACAUCUAAG UACCCCGAGGAAAA GAAAUCAACCGAGA UUCCCCCAGUAGCG GCGAGCGAACGGGG AGCAGCCCAGAGCC UGAAUCAGUGUGU GUGUUAGUGGAAG CGUCUGGAAAGGCG CGCGAUACAGGGUG ACAGCCCCGUACAC AAAAAUGCACAUGC UGUGAGCUCGAUG AGUAGGGCGGGAC ACGUGGUAUCCUGU CUGAAUAUGGGGG GACCAUCCUCCAAG GCUAAAUACUCCUG ACUGACCGAUAGUG AACCAGUACCGUGA GGGAAAGGCGAAA AGAACCCCGGCGAG GGGAGUGAAAAAG AACCUGAAACCGUG UACGUACAAGCAGU GGGAGCACGCUUAG GCGUGUGACUGCGU ACCUUUUGUAUAA UGGGUCAGCGACUU AUAUUCUGUAGCA AGGUUAACCGAAU AGGGGAGCCGAAG GGAAACCGAGUCUU AACUGGGCGUUAA GUUGCAGGGUAUA GACCCGAAACCCGG UGAUCUAGCCAUGG GCAGGUUGAAGGU UGGGUAACACUAAC UGGAGGACCGAACC GACUAAUGUUGAA AAAUUAGCGGAUG ACUUGUGGCUGGG GGUGAAAGGCCAA UCAAACCGGGAGAU AGCUGGUUCUCCCC GAAAGCUAUUUAG GUAGCGCCUCGUGA AUUCAUCUCCGGGG GUAGAGCACUGUU UCGGCAAGGGGGUC ACUUACCAACCCGA UGCAAACUGCGAAU ACCGGAGAAUGUU AUCACGGGAGACAC ACGGCGGGUGCUAA CGUCCGUCGUGAAG AGGGAAACAACCCA GACCGCCAGCUAAG GUCCCAAAGUCAUG GUUAAGUGGGAAA CGAUGUGGGAAGG CCCAGACAGCCAGG AUGUUGGCUUAGA AGCAGCCAUCAUUU AAAGAAAGCGUAA UAGCUCACUGGUCG AGUCGGCCUGCGCG GAAGAUGUAACGG GGCUAAACCAUGCA |  |  |  |  |  |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | CCGAAGCUGCGGCA GCGACGCUUAUGCG UUGUUGGGUAGGG GAGCGUUCUGUAA GCCUGCGAAGGUGU GCUGUGAGGCAUGC UGGAGGUAUCAGA AGUGCGAAUGCUG ACAUAAGUAACGA UAAAGCGGGUGAA AAGCCCGCUCGCCG GAAGACCAAGGGU UCCUGUCCAACGUU AAUCGGGGCAGGG UGAGUCGACCCCUA AGGCGAGGCCGAAA GGCGUAGUCGAUG GGAAACAGGUUAA UAUUCCUGUACUUG GUGUUACUGCGAA GGGGGGACGGAGA AGGCUAUGUUGGCC GGGCGACGGUUGUC CCGGUUUAAGCGUG UAGGCUGGUUUUCC AGGCAAAUCCGGAA AAUCAAGGCUGAG GCGUGAUGACGAG GCACUACGGUGCUG AAGCAACAAAUGCC CUGCUUCCAGGAAA AGCCUCUAAGCAUC AGGUAACAUCAAA UCGUACCCCAAACC GACACAGGUGGUCA GGUAGAGAAUACC AAGGCGCUUGAGA GAACUCGGGUGAA GGAACUAGGCAAA AUGGUGCCGUAACU UCGGGAGAAGGCAC GCUGAUAUGUAGG UGAGGUCCCUCGCG GAUGGAGCUGAAA UCAGUCGAAGAUAC CAGCUGGCUGCAAC UGUUUAUUAAAAA CACAGCACUGUGCA AACACGAAAGUGG ACGUAUACGGUGU GACGCCUGCCCGGU GCCGGAAGGUUAA UUGAUGGGGUUAG CGCAAGCGAAGCUC UUGAUCGAAGCCCC GGUAAACGGCGGCC GUAACXAUAACGG UCCUAAGGUAGCGA AAUUCCUUGUCGGG UAAGUUCCGACCUG CACGAAUGGCGUAA UGAUGGCCAGGCUG UCUCCACCCGAGAC UCAGUGAAAUUGA ACUCGCUGUGAAGA UGCAGUGUACCCGC GGCAAGACGGAAA GACCCCGUGAACCU UUACUAUAGCUUG ACACUGAACAUUGA GCCUUGAUGUGUA GGAUAGGUGGGAG GCUUUGAAGUGUG GACGCCAGUCUGCA UGGAGCCGACCUUG |  |  |  |  |  |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | AAAUACCACCCUUU AAUGUUUGAUGUU CUAACGUUGACCCG UAAUCCGGGUUGCG GACAGUGUCUGGU GGGUAGUUUGACU GGGGCGGUCUCCUC CUAAAGAGUAACG GAGGAGCACGAAG GUUGGCUAAUCCUG GUCGGACAUCAGGA GGUUAGUGCAAUG GCAUAAGCCAGCUU GACUGCGAGCGUGA CGGCGCGAGCAGGU GCGAAAGCAGGUCA UAGUGAUCCGGUG GUUCUGAAUGGAA GGGCCAUCGCUCAA CGGAUAAAAGGUA CUCCGGGGAUAACA GGCUGAUACCGCCC AAGAGUUCAUAUC GACGGCGGUGUUU GGCACCUCGAUGUC GGCUCAUCACAUCC UGGGGCUGAAGUA GGUCCCAAGGGUAU GGCUGUUCGCCAUU UAAAGUGGUACGC GAGCUGGGUUUAG AACGUCGUGAGACA GUUCGGUCCCUAUC UGCCGUGGGCGCUG GAGAACUGAGGGG GGCUGCUCCUAGUA CGAGAGGACCGGAG UGGACGCAUCACUG GUGUUCGGGUUGU CAUGCCAAUGGCAC UGCCCGGUAGCUAA AUGCGGAAGAGAU AAGUGCUGAAAGC AUCUAAGCACGAAA CUUGCCCCGAGAUG AGUUCUCCCUGACC CUUUAAGGGUCCUG AAGGAACGUUGAA GACGACGACGUUGA UAGGCCGGGUGUG UAAGCGCAGCGAUG CGUUGAGCUAACCG GUACUAAUGAACCG UGAGGCUUAACCU |  |  |  |  |  |
| 596 | C1C(C(C(C(C1N)OC2 C(C(C(C(O2)CO)O)O)   1. OC3C(C(C(O3)CO)   OC4C(C(C(C(O4)CN)   1. O)N)O)O)N | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Paromomycin\_m ol\_mol | Target\_lig\_111 6 | 16s\_rRNA A SITE | Target\_3 | 6.88605664  769316 |
| 600 | C1C(C(C(C(C1N)OC2 C(C(C(C(O2)CN)O)O)   1. OC3C(C(C(O3)CO)   OC4C(C(C(C(O4)CN)   1. O)N)O)O)N | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Neomycin B | Target\_lig\_12 51 | 16s\_rRNA A SITE | Target\_3 | 5.82390874  094432 |
| 607 | [C@H]1([C@@H]  ([C@@H]([C@@H]  (O[C@@H]1CN)O[C  @@H]1[C@@H] ([C@@H]([C@@H]  (C[C@@H]1N)N)O)O CC(=O)NCCCCCNC(= O)CO[C@@H]1[C@@ H]([C@H](C[C@@H] | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Bifunctional\_ami noglycoside\_deri vative\_1 | Target\_lig\_35 3 | 16s\_rRNA A SITE | Target\_3 | 6.09691001  300806 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  | ([C@H]1O)N)N)O[C@  H]1[C@H]([C@H]  ([C@H]([C@@H]  (O1)CN)O)O)N)N)O)O |  |  |  |  |  |  |
| 608 | [C@H]1([C@@H]  ([C@@H]([C@@H]  (O[C@H]1CN)O[C@H  ]1[C@H]([C@H] ([C@H] (C[C@@H]1N)N)O)O C[C@@H] (CN(CCCCN(C[C@@ H] (CO[C@H]1[C@@H]  ([C@H](C[C@H]  ([C@@H]1O)N)N)O[C  @H]1[C@H]([C@@H]  ([C@@H]([C@@H]  (O1)CN)O)O)N)O)C)C  )O)N)O)O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Bifunctional\_ami noglycoside\_deri vative\_2 | Target\_lig\_35 4 | 16s\_rRNA A SITE | Target\_3 | 7.39794000  867204 |
| 609 | [C@@H]1([C@H]  ([C@H]([C@@H]  (O[C@@H]1CN)OC[C  @@H] (CN(CCCCCCN(C)C[ C@H] (CO[C@@H]1O[C@H  ]([C@@H]([C@@H]  ([C@H]1N)O)O)CN)O  )C)O)N)O)O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Bifunctional\_ami noglycoside\_deri vative\_3 | Target\_lig\_35 5 | 16s\_rRNA A SITE | Target\_3 | 4.95860731  484177 |
| 610 | [C@@H]1([C@H]  ([C@H]([C@@H] ([C@@H] (C1)N)OC[C@@H]  (CN(CCCCCCN(C)C[  C@@H] (CO[C@@H]1[C@@H  ](C[C@H]([C@@H]  ([C@H]1O)O)N)N)O) C)O)O)O)N | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Bifunctional\_ami noglycoside\_deri vative\_4 | Target\_lig\_35 6 | 16s\_rRNA A SITE | Target\_3 | 4.67778070  526608 |
| 611 | [C@H]1([C@H]  ([C@@H]([C@H]  (O[C@H]1CO)OC[C@  @H] (CN(CCCCCCN(C)C[ C@H] (CO[C@@H]1O[C@H  ]([C@@H]([C@@H]  ([C@H]1N)O)O)CO)O  )C)O)N)O)O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Bifunctional\_ami noglycoside\_deri vative\_5 | Target\_lig\_35 7 | 16s\_rRNA A SITE | Target\_3 | 4.28399665  63652 |
| 612 | [C@H]1([C@H]  ([C@@H]([C@H] ([C@@H] (C1)N)OC[C@@H]  (CN(CCCCCCN(C)C[ C@H] (CO[C@@H]1O[C@@ H]([C@H]([C@H]  ([C@H]1N)O)O)CO)O  )C)O)O)O)N | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Bifunctional\_ami noglycoside\_deri vative\_6 | Target\_lig\_35 8 | 16s\_rRNA A SITE | Target\_3 | 4.40893539  29735 |
| 613 | [C@H]1([C@H]  ([C@@H]([C@H] ([C@@H] (C1)N)OC[C@@H]  (CN(CCCCCCN(C)C[ C@H] (CO[C@@H]1O[C@H  ]([C@@H]([C@@H]  ([C@H]1N)O)O)CN)O  )C)O)O)O)N | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Bifunctional\_ami noglycoside\_deri vative\_7 | Target\_lig\_35 9 | 16s\_rRNA A SITE | Target\_3 | 4.49485002  168009 |
| 614 | [C@H]1([C@H] | GAGCGUCACACCUU | Neamine | Target\_lig\_36 | 16s\_rRNA A | Target\_3 | 2.92081875 |

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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]  (O[C@@H]1CN)O[C  @@H]1[C@@H] ([C@H]([C@@H]  (C[C@@H]1N)NC(=O  )[C@@H] (CCN)O)OCCNCCN)O  )N)O)O | CGGGUGAAGUCGCU C | derivative\_1 | 0 | SITE |  | 395238 |
| 615 | C1[C@@H]([C@H]  ([C@@H]([C@H]  ([C@@H]1NC(=O) [C@H] (CCN)O)OCCNCCCN) O)O[C@@H]2[C@@H  ]([C@H]([C@@H] ([C@H] (O2)CN)O)O)N)N | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Neamine derivative\_2 | Target\_lig\_36 1 | 16s\_rRNA A SITE | Target\_3 | 5.22914798  835786 |
| 616 | [C@H]1([C@H]  ([C@@H]([C@@H]  (O[C@@H]1CN)O[C  @H]1[C@H]([C@@H] ([C@H] (C[C@H]1N)NC(=O)  [C@@H] (CCN)O)OCCNCCCC N)O)N)O)O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Neamine derivative\_3 | Target\_lig\_36 2 | 16s\_rRNA A SITE | Target\_3 | 5.40893539  29735 |
| 617 | [C@@H]1([C@@H]  ([C@H]([C@H]  (O[C@H]1CN)O[C@  @H]1[C@@H]([C@H] ([C@@H] (C[C@H]1N)N)OCCN  CCCN)O)N)O)O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Neamine derivative\_4 | Target\_lig\_36 3 | 16s\_rRNA A SITE | Target\_3 | 5.79588001  734408 |
| 618 | [C@H]1([C@@H]  ([C@H]([C@H]  (O[C@@H]1CN)O[C  @@H]1[C@@H] ([C@@H]([C@H]  (C[C@H]1N)NC(=O) [C@H] (CCN)O)OCCN(CCCN  )C(=O)[C@H]  (CCN)O)O)N)O)O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Neamine derivative\_5 | Target\_lig\_36 4 | 16s\_rRNA A SITE | Target\_3 | 4.95860731  484177 |
| 619 | [C@H]1([C@H]  ([C@@H]([C@@H]  (O[C@H]1CN)O[C@  @H]1[C@@H]([C@H] ([C@@H] (C[C@@H]1N)NC(=O  )Cc1ccc(cc1)N)OCCN CCCCN)O)N)O)O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Neamine derivative\_6 | Target\_lig\_36 5 | 16s\_rRNA A SITE | Target\_3 | 4.61978875  828839 |
| 620 | [C@H]1([C@H]  ([C@@H]([C@@H]  (O[C@@H]1CN)O[C  @H]1[C@H]([C@H] ([C@@H] (C[C@H]1N)NC(=O)C  c1cccc(c1)N)OCCNCC CCN)O)N)O)O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Neamine derivative\_7 | Target\_lig\_36 6 | 16s\_rRNA A SITE | Target\_3 | 4.61978875  828839 |
| 621 | [C@H]1([C@H]  ([C@@H]([C@H]  (O[C@H]1CO)O[C@H  ]1[C@@H]([C@H] (O[C@H] ([C@@H]1N)OC)CN) O)N)O)O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Neamine mimic\_1 | Target\_lig\_36 7 | 16s\_rRNA A SITE | Target\_3 | 4.30980391  997149 |
| 622 | [C@@H]1([C@@H]  ([C@H]([C@H]  (O[C@@H]1CN)O[C @@H]1[C@H] | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Neamine mimic\_2 | Target\_lig\_36 8 | 16s\_rRNA A SITE | Target\_3 | 4.43179827  593301 |

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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]1N)OC)CN)O) N)O)O |  |  |  |  |  |  |
| 623 | [C@@H]1([C@H]  ([C@H]([C@H]  (O[C@@H]1CN)O[C  @H]1[C@H]([C@@H] ([C@H] (O[C@H]1CO)OC)N) O)N)O)O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Neamine mimic\_3 | Target\_lig\_36 9 | 16s\_rRNA A SITE | Target\_3 | 4.39794000  867204 |
| 624 | [C@@H]1([C@@H]  ([C@@H]([C@H]  (O[C@@H]1CO)O[C  @H]1[C@H]([C@@H] ([C@H] (O[C@@H]1CN)OC)N  )O)N)O)O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Neamine mimic\_4 | Target\_lig\_37 0 | 16s\_rRNA A SITE | Target\_3 | 4.58502665  202918 |
| 625 | [C@@H]1([C@H]  ([C@H]([C@@H]  (O[C@@H]1CN)O[C  @@H]1[C@@H] ([C@H]([C@@H]  (O[C@H]1CN)OC)N) O)N)O)O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Neamine mimic\_5 | Target\_lig\_37 1 | 16s\_rRNA A SITE | Target\_3 | 4.95860731  484177 |
| 626 | [C@H]1([C@H]  ([C@@H]([C@H]  (O[C@H]1CN)O[C@  @H]1[C@H]([C@@H] ([C@H] (O[C@H]1CN)OC)N) O)N)O)O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Neamine mimic\_6 | Target\_lig\_37 2 | 16s\_rRNA A SITE | Target\_3 | 4.40893539  29735 |
| 627 | [C@H]1([C@H]  ([C@@H]([C@@H]  (O[C@@H]1CN)O[C  @@H]1[C@@H] ([C@H](O[C@H]  ([C@@H]1N)OC)CN) O[C@H]1[C@@H] ([C@H]([C@H] ([C@H] (O1)C)N)O)O)N)O)O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Neamine mimic\_7 | Target\_lig\_37 3 | 16s\_rRNA A SITE | Target\_3 | 3.55129368  009492 |
| 628 | [C@H]1([C@@H]  ([C@@H]([C@H]  (O[C@H]1CN)O[C@ @H]1[C@@H] ([C@@H]([C@H]  (O[C@@H]1CN)OC)N  )O[C@H]1[C@H]  ([C@H]([C@@H]  (O1)CO)O)O)N)O)O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Neamine mimic\_8 | Target\_lig\_37 4 | 16s\_rRNA A SITE | Target\_3 | 4.36653154  442041 |
| 629 | [C@H]1([C@H]  ([C@@H]([C@@H]  (O[C@@H]1CN)O[C @@H]1[C@H] ([C@@H]([C@H]  (O[C@H]1CN)OC)N) O[C@@H]1[C@H] ([C@H]([C@H] ([C@H] (O1)C)N)O)O)N)O)O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Neamine mimic\_9 | Target\_lig\_37 5 | 16s\_rRNA A SITE | Target\_3 | 5.69897000  433602 |
| 630 | C1[C@@H]([C@@H]  ([C@H]([C@@H]  ([C@@H]1N)O[C@H]  1O[C@H]([C@@H] ([C@H] ([C@@H]1N)O)O)CO) O[C@@H]1[C@H] ([C@H]([C@H]  (O1)CO)O[C@H]1O[C  @@H]([C@@H] | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Paromomycin\_m ol derivative 1 16S A-site RNA | Target\_lig\_37 6 | 16s\_rRNA A SITE | Target\_3 | 6.63827216  398241 |

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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]1N)O)O)CN) OCCN)O)N |  |  |  |  |  |  |
| 631 | C1[C@@H]([C@@H]  ([C@H]([C@H]  ([C@@H]1N)O[C@@  H]1O[C@H]([C@@H] ([C@@H] ([C@@H]1N)O)O)CO) O[C@@H]1[C@H] ([C@H]([C@H]  (O1)CO)O[C@H]1O[C  @H]([C@@H]([C@H]  ([C@@H]1N)O)O)CN) OCCCN)O)N | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Paromomycin\_m ol derivative 2 16S A-site RNA | Target\_lig\_37 7 | 16s\_rRNA A SITE | Target\_3 | 7 |
| 632 | C1[C@@H]([C@@H]  ([C@@H]([C@H]  ([C@@H]1N)O[C@@  H]1O[C@H]([C@@H] ([C@H] ([C@@H]1N)O)O)CO) O[C@@H]1[C@H] ([C@@H]([C@H]  (O1)CO)O[C@H]1O[C  @H]([C@@H]([C@H]  ([C@@H]1N)O)O)CN)  OCc1cccnc1)O)N | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Paromomycin\_m ol derivative 3 16S A-site RNA | Target\_lig\_37 8 | 16s\_rRNA A SITE | Target\_3 | 6.88605664  769316 |
| 633 | C1[C@@H]([C@H]  ([C@@H]([C@H] ([C@@H]1N)OCN2C= NC3=C2N=CNC3=O) O)O)N | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Heterocyclic paromomycin derivative 1 | Target\_lig\_37 9 | 16s\_rRNA A SITE | Target\_3 | 4 |
| 634 | C1[C@@H]([C@H]  ([C@@H]([C@H] ([C@@H]1N)OCN2C= CN=C2)O)O)N | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Heterocyclic paromomycin derivative 2 | Target\_lig\_38 0 | 16s\_rRNA A SITE | Target\_3 | 3.56066730  616974 |
| 635 | C1[C@@H]([C@H]  ([C@@H]([C@H] ([C@@H]1N)OCN2C= CN=N2)O)O)N | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Heterocyclic paromomycin derivative 3 | Target\_lig\_38 1 | 16s\_rRNA A SITE | Target\_3 | 3.44977164  694491 |
| 636 | C1[C@@H]([C@H]  ([C@@H]([C@H] ([C@@H]1N)OCN2C= NC=N2)O)O)N | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Heterocyclic paromomycin derivative 4 | Target\_lig\_38 2 | 16s\_rRNA A SITE | Target\_3 | 3.42250820  016277 |
| 637 | C1[C@@H](N) [C@@H](O)[C@H] ([C@@H]  ([C@H]1N)OCSc1ccnc 2c1ccc(c2)C(F)(F)F)O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Quinolinyl\_DOS  \_der | Target\_lig\_38 3 | 16s\_rRNA A SITE | Target\_3 | 4.16749108  729376 |
| 638 | C1[C@@H](N)[C@H]  (O)[C@H]([C@@H]  ([C@H]1N)OCSc1ccnc 2c1ccc(c2)C(F) (F)F)O[C@@H]1O[C @@H]([C@H] ([C@H]1O)O[C@H]1[ C@@H]([C@H] ([C@@H]([C@@H]  (O1)CN)O)O)N)CO | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Quinolinyl\_DOS  \_paromomycin\_d er\_1 | Target\_lig\_38 4 | 16s\_rRNA A SITE | Target\_3 | 6 |
| 639 | C1[C@H](N)[C@@H] (OCCNCCCN)[C@H] ([C@H] ([C@@H]1N)OCSc1cc  nc2c1ccc(c2)C(F) (F)F)O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Quinolinyl\_DOS  \_paromomycin\_d er\_2 | Target\_lig\_38 5 | 16s\_rRNA A SITE | Target\_3 | 5.82390874  094432 |
| 640 | C1[C@H]([C@@H]  ([C@H]([C@@H] ([C@H]1N)OCSC2=C3 C=CC(=CC3=NC=C2) | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Quinolinyl\_DOS  \_paromomycin\_d er\_3 | Target\_lig\_38 6 | 16s\_rRNA A SITE | Target\_3 | 5.69897000  433602 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  | C(F) (F)F)OCCNCCCN)O)N |  |  |  |  |  |  |
| 641 | c1cccc(c1)c1ccc(cc1)C O[C@H] (CO[C@@H]1O[C@@ H]([C@H](O)[C@@H]  (O)[C@H]1N)CN)CN | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Acyclic DOS mimic 1\_biphenyl substituent | Target\_lig\_38 7 | 16s\_rRNA A SITE | Target\_3 | 5.63827216  398241 |
| 642 | C(O[C@@H] (CO[C@@H]1O[C@H  ]([C@@H](O)[C@H] (O) [C@H]1N)CN)CN)c1c  c2ccccc2cc1 | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Acyclic DOS mimic 2\_naphthyl substituent | Target\_lig\_38 8 | 16s\_rRNA A SITE | Target\_3 | 5.55284196  865778 |
| 643 | C(O[C@@H] (CO[C@@H]1O[C@H  ]([C@H](O)[C@@H] (O) [C@H]1N)CN)CN)c1c  cccc1 | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Acyclic DOS mimic 3\_benzyl substituent | Target\_lig\_38 9 | 16s\_rRNA A SITE | Target\_3 | 3 |
| 649 | O1[C@H] (O[C@@H]2C[C@@H  ](NCC[C@H]2N)CO)  [C@H]([C@@H] ([C@H] ([C@@H]1CN)O)O)N | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Azepane aminoglycoside mimic 1 | Target\_lig\_39 5 | 16s\_rRNA A SITE | Target\_3 | 4.95860731  484177 |
| 650 | O1[C@H] (O[C@@H]2C[C@@H  ](NCC[C@H]2N)CO)  [C@H]([C@@H] ([C@H] ([C@@H]1CN)O)O)N | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Azepane aminoglycoside mimic 2 | Target\_lig\_111 4 | 16s\_rRNA A SITE | Target\_3 | 4.92081875  395238 |
| 651 | O1[C@H] (O[C@@H]2C[C@H]  (NCC[C@H]2N)CO)  [C@H]([C@@H] ([C@H] ([C@@H]1CN)O)O)N | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Azepane aminoglycoside mimic 3 | Target\_lig\_39 6 | 16s\_rRNA A SITE | Target\_3 | 4.09691001  300806 |
| 653 | C1[C@H] (CN(C[C@H]1N)c1nc( nc(N2C[C@H] (C[C@@H]  (C2)N)N)n1)Nc1ccc(cc 1)NC(=O)c1c(cc2c(c1) cccc2)O)N | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Diamino\_piperidi nyl\_triazine\_2 | Target\_lig\_39 8 | 16s\_rRNA A SITE | Target\_3 | 8.69897000  433602 |
| 655 | C1CNCCC1C2=NC3= C(N2)C=C(C=C3)N | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Benzimidazole 16S A-site RNA | Target\_lig\_41 7 | 16s\_rRNA A SITE | Target\_3 | 3.30102999  566398 |
| 656 | C1CNCCC1C2=NC3= C(N2)C=C(C=C3)[N+]  (=O)[O-] | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Nitro substituted benzimidazole 16S A-site RNA | Target\_lig\_41 8 | 16s\_rRNA A SITE | Target\_3 | 3.51144928  349956 |
| 657 | C1CNCCC1C2=NC3= CC(=C(C=C3N2)Cl)Cl | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Halogen substituted benzimidazole | Target\_lig\_41 9 | 16s\_rRNA A SITE | Target\_3 | 3.75945075  17174 |
| 658 | C1C[C@@H] (C[C@@H]1C2=NC3= C(N2)C=C(C=C3)[N+]  (=O)[O-])N | GAGCGUCACACCUU CGGGUGAAGUCGCU C | benzimidazole\_a nalog\_rRNA\_1 | Target\_lig\_42 0 | 16s\_rRNA A SITE | Target\_3 | 3.30102999  566398 |
| 660 | COC(=O)C1=CC=C(C  =C1)CN2C3=CC(=C(C  =C3N=C2C4CCNCC4)  Cl)Cl | GAGCGUCACACCUU CGGGUGAAGUCGCU C | benzimidazole\_a nalog\_rRNA\_3 | Target\_lig\_44 6 | 16s\_rRNA A SITE | Target\_3 | 3 |
| 661 | C1CCC(CC1)C2=NC3  =C(N2)C=C(C=C3) [N+](=O)[O-] | GAGCGUCACACCUU CGGGUGAAGUCGCU C | benzimidazole\_a nalog\_rRNA\_4 | Target\_lig\_42 1 | 16s\_rRNA A SITE | Target\_3 | 3 |
| 662 | C1=CC2=C(C=C1[N+] (=O) | GAGCGUCACACCUU CGGGUGAAGUCGCU | benzimidazole\_a nalog\_rRNA\_5 | Target\_lig\_42 2 | 16s\_rRNA A SITE | Target\_3 | 3 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  | [O-])NC(=N2)C3=CC= NC=C3 | C |  |  |  |  |  |
| 663 | C1=CC(=CN=C1)C2= NC3=C(N2)C=C(C=C3  )[N+](=O)[O-] | GAGCGUCACACCUU CGGGUGAAGUCGCU C | benzimidazole\_a nalog\_rRNA\_6 | Target\_lig\_42 3 | 16s\_rRNA A SITE | Target\_3 | 3 |
| 664 | C1=CC(=CC=C1C2=N C3=C(N2)C=C(C=C3) [N+](=O)[O-])N | GAGCGUCACACCUU CGGGUGAAGUCGCU C | benzimidazole\_a nalog\_rRNA\_7 | Target\_lig\_42 4 | 16s\_rRNA A SITE | Target\_3 | 3 |
| 665 | C1=CC(=CC(=C1)N)C 2=NC3=C(N2)C=C(C= C3)[N+](=O)[O-] | GAGCGUCACACCUU CGGGUGAAGUCGCU C | benzimidazole\_a nalog\_rRNA\_8 | Target\_lig\_42 5 | 16s\_rRNA A SITE | Target\_3 | 3.91009488  85606 |
| 666 | C1CC(CCC1C2=NC3= C(N2)C=C(C=C3)[N+]  (=O)[O-])N | GAGCGUCACACCUU CGGGUGAAGUCGCU C | benzimidazole\_a nalog\_rRNA\_9 | Target\_lig\_42 6 | 16s\_rRNA A SITE | Target\_3 | 3.97881070  093006 |
| 667 | c1c(cc2c(c1)[nH]c(n2) [C@H]1C[C@H]  (CCC1)N)N(=O)O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | benzimidazole\_a nalog\_rRNA\_10 | Target\_lig\_42 7 | 16s\_rRNA A SITE | Target\_3 | 3.65560772  631489 |
| 668 | CC(=O)N1CCC(CC1)C 2=NC3=C(N2)C=C(C= C3)[N+](=O)[O-] | GAGCGUCACACCUU CGGGUGAAGUCGCU C | benzimidazole\_a nalog\_rRNA\_11 | Target\_lig\_42 8 | 16s\_rRNA A SITE | Target\_3 | 3 |
| 669 | CN1CCC(CC1)C2=NC 3=C(N2)C=C(C=C3) [N+](=O)[O-] | GAGCGUCACACCUU CGGGUGAAGUCGCU C | benzimidazole\_a nalog\_rRNA\_12 | Target\_lig\_42 9 | 16s\_rRNA A SITE | Target\_3 | 3 |
| 670 | COC1=CC2=C(C=C1) N=C(N2)C3CCNCC3 | GAGCGUCACACCUU CGGGUGAAGUCGCU C | benzimidazole\_a nalog\_rRNA\_13 | Target\_lig\_43 0 | 16s\_rRNA A SITE | Target\_3 | 3.23062267  392386 |
| 671 | CC1=CC2=C(C=C1)N  =C(N2)C3CCNCC3 | GAGCGUCACACCUU CGGGUGAAGUCGCU C | benzimidazole\_a nalog\_rRNA\_14 | Target\_lig\_43 1 | 16s\_rRNA A SITE | Target\_3 | 3.35753547  975788 |
| 672 | C1CNCCC1C2=NC3= C(N2)C=C(C=C3)Br | GAGCGUCACACCUU CGGGUGAAGUCGCU C | benzimidazole\_a nalog\_rRNA\_15 | Target\_lig\_43 2 | 16s\_rRNA A SITE | Target\_3 | 3.44249279  809434 |
| 673 | C1CNCCC1C2=NC3= C(N2)C=C(C=C3)Cl | GAGCGUCACACCUU CGGGUGAAGUCGCU C | benzimidazole\_a nalog\_rRNA\_16 | Target\_lig\_43 3 | 16s\_rRNA A SITE | Target\_3 | 3.29413628  771608 |
| 674 | C1CNCCC1C2=NC3= C(N2)C=C(C=C3)C(F) (F)F | GAGCGUCACACCUU CGGGUGAAGUCGCU C | benzimidazole\_a nalog\_rRNA\_17 | Target\_lig\_43 4 | 16s\_rRNA A SITE | Target\_3 | 3.55129368  009492 |
| 675 | CC1=CC2=C(C=C1Cl) N=C(N2)C3CCNCC3 | GAGCGUCACACCUU CGGGUGAAGUCGCU C | benzimidazole\_a nalog\_rRNA\_18 | Target\_lig\_43 5 | 16s\_rRNA A SITE | Target\_3 | 3.42021640  338319 |
| 676 | c1(c(cc2c(c1) [nH]c(n2)C1CCNCC1)  Cl)Cl | GAGCGUCACACCUU CGGGUGAAGUCGCU C | benzimidazole\_a nalog\_rRNA\_19 | Target\_lig\_111 5 | 16s\_rRNA A SITE | Target\_3 | 3.75945075  17174 |
| 677 | C1CNCCC1C2=NC3= CC=CC=C3N2 | GAGCGUCACACCUU CGGGUGAAGUCGCU C | benzimidazole\_a nalog\_rRNA\_20 | Target\_lig\_43 6 | 16s\_rRNA A SITE | Target\_3 | 3.74472749  489669 |
| 678 | C1CNCCC1C2=NC3= C(N2)C=NC=C3 | GAGCGUCACACCUU CGGGUGAAGUCGCU C | benzimidazole\_a nalog\_rRNA\_21 | Target\_lig\_43 7 | 16s\_rRNA A SITE | Target\_3 | 3.95860731  484177 |
| 679 | C1CNCCC1C2=NC3= C(N2)C=CC=N3 | GAGCGUCACACCUU CGGGUGAAGUCGCU C | benzimidazole\_a nalog\_rRNA\_22 | Target\_lig\_43 8 | 16s\_rRNA A SITE | Target\_3 | 3.27164621  797877 |
| 680 | C1CNCCC1C2=NC3= NC=NC=C3N2 | GAGCGUCACACCUU CGGGUGAAGUCGCU C | benzimidazole\_a nalog\_rRNA\_23 | Target\_lig\_43 9 | 16s\_rRNA A SITE | Target\_3 | 3.03905380  426617 |
| 681 | C1CNCCC1C2=NC3= CC=CC=C3S2 | GAGCGUCACACCUU CGGGUGAAGUCGCU C | benzimidazole\_a nalog\_rRNA\_24 | Target\_lig\_44 0 | 16s\_rRNA A SITE | Target\_3 | 3 |
| 682 | C1CNCCC1C2=NC3= CC(=C(C=C3N2CC4= CC=C(C=C4)C(F) | GAGCGUCACACCUU CGGGUGAAGUCGCU C | benzimidazole\_a nalog\_rRNA\_25 | Target\_lig\_44 1 | 16s\_rRNA A SITE | Target\_3 | 3.66958622  665081 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  | (F)F)Cl)Cl |  |  |  |  |  |  |
| 683 | C1CNCCC1C2=NC3= CC(=C(C=C3N2CC4= C(C=C(C=C4)C(F) (F)F)C(F)(F)F)Cl)Cl | GAGCGUCACACCUU CGGGUGAAGUCGCU C | benzimidazole\_a nalog\_rRNA\_26 | Target\_lig\_44 2 | 16s\_rRNA A SITE | Target\_3 | 3.79860287  567955 |
| 684 | C1CNCCC1C2=NC3= CC(=C(C=C3N2CC4= C(C(=C(C(=C4F)F)F)F  )F)Cl)Cl | GAGCGUCACACCUU CGGGUGAAGUCGCU C | benzimidazole\_a nalog\_rRNA\_27 | Target\_lig\_44 3 | 16s\_rRNA A SITE | Target\_3 | 3.62525165  39899 |
| 685 | C1CNCCC1C2=NC3= CC(=C(C=C3N2CC4= C(C(=C(C(=C4F)F)C(F  )(F)F)F)F)Cl)Cl | GAGCGUCACACCUU CGGGUGAAGUCGCU C | benzimidazole\_a nalog\_rRNA\_28 | Target\_lig\_44 4 | 16s\_rRNA A SITE | Target\_3 | 3.93181413  825384 |
| 686 | C1CNCCC1C2=NC3= CC(=C(C=C3N2CC4= CC=C(C=C4)[N+](=O)  [O-])Cl)Cl | GAGCGUCACACCUU CGGGUGAAGUCGCU C | benzimidazole\_a nalog\_rRNA\_29 | Target\_lig\_44 5 | 16s\_rRNA A SITE | Target\_3 | 3.61798295  742513 |
| 687 | COC(=O)C1=CC=C(C  =C1)CN2C3=CC(=C(C  =C3N=C2C4CCNCC4)  Cl)Cl | GAGCGUCACACCUU CGGGUGAAGUCGCU C | benzimidazole\_a nalog\_rRNA\_30 | Target\_lig\_44 6 | 16s\_rRNA A SITE | Target\_3 | 3.64975198  166584 |
| 688 | C1CNCCC1C2=NC3= CC(=C(C=C3N2CC4= CC=C(C=C4)I)Cl)Cl | GAGCGUCACACCUU CGGGUGAAGUCGCU C | benzimidazole\_a nalog\_rRNA\_31 | Target\_lig\_44 7 | 16s\_rRNA A SITE | Target\_3 | 3.70333480  973847 |
| 689 | C1CNCCC1C2=NC3= CC(=C(C=C3N2CC4= CC(=CC=C4)I)Cl)Cl | GAGCGUCACACCUU CGGGUGAAGUCGCU C | benzimidazole\_a nalog\_rRNA\_32 | Target\_lig\_44 8 | 16s\_rRNA A SITE | Target\_3 | 3.39254497  678533 |
| 690 | C1CNCCC1C2=NC3= CC(=C(C=C3N2CC4= CC=C(C=C4)Br)Cl)Cl | GAGCGUCACACCUU CGGGUGAAGUCGCU C | benzimidazole\_a nalog\_rRNA\_33 | Target\_lig\_44 9 | 16s\_rRNA A SITE | Target\_3 | 3.36251027  048749 |
| 691 | CC(C) (C)C1=CC=C(C=C1)C N2C3=CC(=C(C=C3N  =C2C4CCNCC4)Cl)Cl | GAGCGUCACACCUU CGGGUGAAGUCGCU C | benzimidazole\_a nalog\_rRNA\_34 | Target\_lig\_45 0 | 16s\_rRNA A SITE | Target\_3 | 3.24033215  531037 |
| 692 | C1CNCCC1C2=NC3= CC(=C(C=C3N2CC4= CC=NC=C4)Cl)Cl | GAGCGUCACACCUU CGGGUGAAGUCGCU C | benzimidazole\_a nalog\_rRNA\_35 | Target\_lig\_45 1 | 16s\_rRNA A SITE | Target\_3 | 4.22184874  961636 |
| 693 | C1CNCCC1C2=NC3= CC(=C(C=C3N2CC4= CN=CC=C4)Cl)Cl | GAGCGUCACACCUU CGGGUGAAGUCGCU C | benzimidazole\_a nalog\_rRNA\_36 | Target\_lig\_45 2 | 16s\_rRNA A SITE | Target\_3 | 4.17392519  729917 |
| 694 | CCCCN1C2=CC(=C(C  =C2N=C1C3CCNCC3)  Cl)Cl | GAGCGUCACACCUU CGGGUGAAGUCGCU C | benzimidazole\_a nalog\_rRNA\_37 | Target\_lig\_45 3 | 16s\_rRNA A SITE | Target\_3 | 3.55595520  408192 |
| 695 | CN1C2=CC(=C(C=C2 N=C1C3CCNCC3)Cl)  Cl | GAGCGUCACACCUU CGGGUGAAGUCGCU C | benzimidazole\_a nalog\_rRNA\_38 | Target\_lig\_45 4 | 16s\_rRNA A SITE | Target\_3 | 3.62160209  905186 |
| 696 | COC(=O)CN1C2=CC(  =C(C=C2N=C1C3CCN CC3)Cl)Cl | GAGCGUCACACCUU CGGGUGAAGUCGCU C | benzimidazole\_a nalog\_rRNA\_39 | Target\_lig\_45 5 | 16s\_rRNA A SITE | Target\_3 | 3.52143350  440616 |
| 697 | C1CNCCC1C2=NC3= CC(=C(C=C3N2CC4= CC=CC=C4Br)Cl)Cl | GAGCGUCACACCUU CGGGUGAAGUCGCU C | benzimidazole\_a nalog\_rRNA\_40 | Target\_lig\_45 6 | 16s\_rRNA A SITE | Target\_3 | 3.22694530  663574 |
| 698 | C1CNCCC1C2=NC3= CC(=C(C=C3N2CC4= CSC5=C4C=C(C=C5)  Cl)Cl)Cl | GAGCGUCACACCUU CGGGUGAAGUCGCU C | benzimidazole\_a nalog\_rRNA\_41 | Target\_lig\_45 7 | 16s\_rRNA A SITE | Target\_3 | 3 |
| 699 | c1(c(cc2c(c1)nc(n2Cc1 ccc(cc1N(=O)O)C(F) (F)F)C1CCNCC1)Cl)Cl | GAGCGUCACACCUU CGGGUGAAGUCGCU C | benzimidazole\_a nalog\_rRNA\_42 | Target\_lig\_45 8 | 16s\_rRNA A SITE | Target\_3 | 3.91364016  932525 |
| 700 | c1(c(cc2c(c1)nc(n2Cc1 ccc(cc1N(=O)O)N(=O) O)C1CCNCC1)Cl)Cl | GAGCGUCACACCUU CGGGUGAAGUCGCU C | benzimidazole\_a nalog\_rRNA\_43 | Target\_lig\_45 9 | 16s\_rRNA A SITE | Target\_3 | 3.61439372  640169 |
| 701 | c1(c(cc2c(c1)nc(n2Cc1 | GAGCGUCACACCUU | benzimidazole\_a | Target\_lig\_46 | 16s\_rRNA A | Target\_3 | 3.17263072 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  | ncccn1)C1CCNCC1)Cl  )Cl | CGGGUGAAGUCGCU C | nalog\_rRNA\_44 | 0 | SITE |  | 694617 |
| 702 | c1(c(cc2c(c1)nc(n2CS(  =O)  (=O)c1ccc(cc1)C)C1C CNCC1)Cl)Cl | GAGCGUCACACCUU CGGGUGAAGUCGCU C | benzimidazole\_a nalog\_rRNA\_45 | Target\_lig\_46 1 | 16s\_rRNA A SITE | Target\_3 | 3 |
| 703 | c1(c(cc2c(c1)nc(n2CC(  =O)Oc1ccc(cc1)C)C1C CNCC1)Cl)Cl | GAGCGUCACACCUU CGGGUGAAGUCGCU C | benzimidazole\_a nalog\_rRNA\_46 | Target\_lig\_46 2 | 16s\_rRNA A SITE | Target\_3 | 3 |
| 875 | c12c(c(c3c(n1)cccc3)N c1ccc(cc1)CN)cccc2C(  =O)N[C@@H] (C(=O)N[C@H]  (C(=O)N[C@H] (C(=O)O)CCCCN)CCC CN)CN | AAAUUGAAGAGUU UGAUCAUGGCUCAG AUUGAACGCUGGCG GCAGGCCUAACACA UGCAAGUCGAACGG UAACAGGAAGAAG CUUGCUUCUUUGCU GACGAGUGGCGGAC GGGUGAGUAAUGU CUGGGAAACUGCCU GAUGGAGGGGGAU AACUACUGGAAACG GUAGCUAAUACCGC AUAACGUCGCAAGA CCAAAGAGGGGGAC CUUCGGGCCUCUUG CCAUCGGAUGUGCC CAGAUGGGAUUAG CUAGUAGGUGGGG UAACGGCUCACCUA GGCGACGAUCCCUA GCUGGUCUGAGAG GAUGACCAGCCACA CUGGAACUGAGACA CGGUCCAGACUCCU ACGGGAGGCAGCAG UGGGGAAUAUUGC ACAAUGGGCGCAAG CCUGAUGCAGCCAU GCCGCGUGUAUGAA GAAGGCCUUCGGGU UGUAAAGUACUUU CAGCGGGGAGGAA GGGAGUAAAGUUA AUACCUUUGCUCAU UGACGUUACCCGCA GAAGAAGCACCGGC UAACUCCGUGCCAG CAGCCGCGGUAAUA CGGAGGGUGCAAGC GUUAAUCGGAAUU ACUGGGCGUAAAGC GCACGCAGGCGGUU UGUUAAGUCAGAU GUGAAAUCCCCGGG CUCAACCUGGGAAC UGCAUCUGAUACUG GCAAGCUUGAGUCU CGUAGAGGGGGGU AGAAUUCCAGGUG UAGCGGUGAAAUG CGUAGAGAUCUGG AGGAAUACCGGUG GCGAAGGCGGCCCC CUGGACGAAGACUG ACGCUCAGGUGCGA AAGCGUGGGGAGC AAACAGGAUUAGA UACCCUGGUAGUCC ACGCCGUAAACGAU GUCGACUUGGAGG UUGUGCCCUUGAGG CGUGGCUUCCGGAG CUAACGCGUUAAGU | HTP 21 | Target\_lig\_52 8 | Helix 22 of E.coli 16s RNA | Target\_98 | 4.79588001  734408 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | CGACCGCCUGGGGA GUACGGCCGCAAGG UUAAAACUCAAAU GAAUUGACGGGGG CCCGCACAAGCGGU GGAGCAUGUGGUU UAAUUCGAUGCAAC GCGAAGAACCUUAC CUGGUCUUGACAUC CACGGAAGUUUUCA GAGAUGAGAAUGU GCCUUCGGGAACCG UGAGACAGGUGCU GCAUGGCUGUCGUC AGCUCGUGUUGUG AAAUGUUGGGUUA AGUCCCGCAACGAG CGCAACCCUUAUCC UUUGUUGCCAGCGG UCCGGCCGGGAACU CAAAGGAGACUGCC AGUGAUAAACUGG AGGAAGGUGGGGA UGACGUCAAGUCAU CAUGGCCCUUACGA CCAGGGCUACACAC GUGCUACAAUGGCG CAUACAAAGAGAA GCGACCUCGCGAGA GCAAGCGGACCUCA UAAAGUGCGUCGU AGUCCGGAUUGGA GUCUGCAACUCGAC UCCAUGAAGUCGGA AUCGCUAGUAAUCG UGGAUCAGAAUGCC ACGGUGAAUACGU UCCCGGGCCUUGUA CACACCGCCCGUCA CACCAUGGGAGUGG GUUGCAAAAGAAG UAGGUAGCUUAACC UUCGGGAGGGCGCU UACCACUUUGUGAU UCAUGACUGGGGU GAAGUCGUAACAA GGUAACCGUAGGG GAACCUGCGGUUGG AUCACCUCCUUA |  |  |  |  |  |
| 898 | CC(=O)C1=CC2=C(C= C1)SC3=CC=CC=C3N 2CCCN(C)C | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Acetylpromazine | Target\_lig\_17 6 | A-site bindings | Target\_3 | 3.44369749  923271 |
| 946 | c12cc(ccc1c(c1c(n2)ccc (c1)OC)NCCCCc1c(nc( nc1N)N)N)Cl | GAGCGUCACACCUU CGGGUGAAGUCGCU C | MBNL CCUG  ligand 3 | Target\_lig\_56 3 | RNA A | Target\_3 | 3.52287874  528034 |
| 1802 | CC1=C(C2=C(N=C1C) N=C(C=C2)NCCN)C | GAGCGUCACACCUU CGGGUGAAGUCGCU C | ATMND-C2- NH2 | Target\_lig\_10 12 | Bacterial rRNA A-site | Target\_3 | 6.35654732  351381 |
| 1804 | CC1=C(C2=C(N=C1C) N=C(C=C2)NCCCN)C | GAGCGUCACACCUU CGGGUGAAGUCGCU C | ATMND-C3- NH2 | Target\_lig\_10 14 | Bacterial rRNA A-site | Target\_3 | 6 |
| 1805 | NCCCCNc1ccc2c(n1)n c(c(c2C)C)C | GAGCGUCACACCUU CGGGUGAAGUCGCU C | ATMND-C4- NH2 | Target\_lig\_10 15 | Bacterial rRNA A-site | Target\_3 | 5.79588001  734408 |
| 1806 | NCCNc1ccc2c(n1)nccc 2 | GAGCGUCACACCUU CGGGUGAAGUCGCU C | AMND-C2-NH2 | Target\_lig\_10 16 | Bacterial rRNA A-site | Target\_3 | 4.58502665  202918 |
| 1807 | NCCNc1ccc2c(n1)nc(c c2C)C | GAGCGUCACACCUU CGGGUGAAGUCGCU C | ADMND-C2- NH2 | Target\_lig\_10 17 | Bacterial rRNA A-site | Target\_3 | 5.63827216  398241 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
| 1808 | Cc1cc(NCCN)ncc1 | GAGCGUCACACCUU CGGGUGAAGUCGCU C | MPED | Target\_lig\_12 77 | Bacterial rRNA A-site | Target\_3 | 4.92081875  395238 |
| 2101 | CCC1C(C(C(N(CC(CC (C(C(C(C(C(=O)O1)C) OC2CC(C(C(O2)C)O)  (C)OC)C)OC3C(C(CC(  O3)C)N(C)C)O) (C)O)C)C)C)O)(C)O | GGUUAAGCGACUA AGCGUACACGGUGG AUGCCCUGGCAGUC AGAGGCGAUGAAG GACGUGCUAAUCUG CGAUAAGCGUCGGU AAGGUGAUAUGAA CCGUUAUAACCGGC GAUUUCCGAAUGG GGAAACCCAGUGUG UUUCGACACACUAU CAUUAACUGAAUCC AUAGGUUAAUGAG GCGAACCGGGGGAA CUGAAACAUCUAAG UACCCCGAGGAAAA GAAAUCAACCGAGA UUCCCCCAGUAGCG GCGAGCGAACGGGG AGCAGCCCAGAGCC UGAAUCAGUGUGU GUGUUAGUGGAAG CGUCUGGAAAGGCG CGCGAUACAGGGUG ACAGCCCCGUACAC AAAAAUGCACAUGC UGUGAGCUCGAUG AGUAGGGCGGGAC ACGUGGUAUCCUGU CUGAAUAUGGGGG GACCAUCCUCCAAG GCUAAAUACUCCUG ACUGACCGAUAGUG AACCAGUACCGUGA GGGAAAGGCGAAA AGAACCCCGGCGAG GGGAGUGAAAAAG AACCUGAAACCGUG UACGUACAAGCAGU GGGAGCACGCUUAG GCGUGUGACUGCGU ACCUUUUGUAUAA UGGGUCAGCGACUU AUAUUCUGUAGCA AGGUUAACCGAAU AGGGGAGCCGAAG GGAAACCGAGUCUU AACUGGGCGUUAA GUUGCAGGGUAUA GACCCGAAACCCGG UGAUCUAGCCAUGG GCAGGUUGAAGGU UGGGUAACACUAAC UGGAGGACCGAACC GACUAAUGUUGAA AAAUUAGCGGAUG ACUUGUGGCUGGG GGUGAAAGGCCAA UCAAACCGGGAGAU AGCUGGUUCUCCCC GAAAGCUAUUUAG GUAGCGCCUCGUGA AUUCAUCUCCGGGG GUAGAGCACUGUU UCGGCAAGGGGGUC ACUUACCAACCCGA UGCAAACUGCGAAU ACCGGAGAAUGUU AUCACGGGAGACAC ACGGCGGGUGCUAA CGUCCGUCGUGAAG AGGGAAACAACCCA | Azithromycin | Target\_lig\_22 3 | 50S subunit | Target\_100 | 8.42021640  338319 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | GACCGCCAGCUAAG GUCCCAAAGUCAUG GUUAAGUGGGAAA CGAUGUGGGAAGG CCCAGACAGCCAGG AUGUUGGCUUAGA AGCAGCCAUCAUUU AAAGAAAGCGUAA UAGCUCACUGGUCG AGUCGGCCUGCGCG GAAGAUGUAACGG GGCUAAACCAUGCA CCGAAGCUGCGGCA GCGACGCUUAUGCG UUGUUGGGUAGGG GAGCGUUCUGUAA GCCUGCGAAGGUGU GCUGUGAGGCAUGC UGGAGGUAUCAGA AGUGCGAAUGCUG ACAUAAGUAACGA UAAAGCGGGUGAA AAGCCCGCUCGCCG GAAGACCAAGGGU UCCUGUCCAACGUU AAUCGGGGCAGGG UGAGUCGACCCCUA AGGCGAGGCCGAAA GGCGUAGUCGAUG GGAAACAGGUUAA UAUUCCUGUACUUG GUGUUACUGCGAA GGGGGGACGGAGA AGGCUAUGUUGGCC GGGCGACGGUUGUC CCGGUUUAAGCGUG UAGGCUGGUUUUCC AGGCAAAUCCGGAA AAUCAAGGCUGAG GCGUGAUGACGAG GCACUACGGUGCUG AAGCAACAAAUGCC CUGCUUCCAGGAAA AGCCUCUAAGCAUC AGGUAACAUCAAA UCGUACCCCAAACC GACACAGGUGGUCA GGUAGAGAAUACC AAGGCGCUUGAGA GAACUCGGGUGAA GGAACUAGGCAAA AUGGUGCCGUAACU UCGGGAGAAGGCAC GCUGAUAUGUAGG UGAGGUCCCUCGCG GAUGGAGCUGAAA UCAGUCGAAGAUAC CAGCUGGCUGCAAC UGUUUAUUAAAAA CACAGCACUGUGCA AACACGAAAGUGG ACGUAUACGGUGU GACGCCUGCCCGGU GCCGGAAGGUUAA UUGAUGGGGUUAG CGCAAGCGAAGCUC UUGAUCGAAGCCCC GGUAAACGGCGGCC GUAACXAUAACGG UCCUAAGGUAGCGA AAUUCCUUGUCGGG UAAGUUCCGACCUG CACGAAUGGCGUAA UGAUGGCCAGGCUG UCUCCACCCGAGAC |  |  |  |  |  |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | UCAGUGAAAUUGA ACUCGCUGUGAAGA UGCAGUGUACCCGC GGCAAGACGGAAA GACCCCGUGAACCU UUACUAUAGCUUG ACACUGAACAUUGA GCCUUGAUGUGUA GGAUAGGUGGGAG GCUUUGAAGUGUG GACGCCAGUCUGCA UGGAGCCGACCUUG AAAUACCACCCUUU AAUGUUUGAUGUU CUAACGUUGACCCG UAAUCCGGGUUGCG GACAGUGUCUGGU GGGUAGUUUGACU GGGGCGGUCUCCUC CUAAAGAGUAACG GAGGAGCACGAAG GUUGGCUAAUCCUG GUCGGACAUCAGGA GGUUAGUGCAAUG GCAUAAGCCAGCUU GACUGCGAGCGUGA CGGCGCGAGCAGGU GCGAAAGCAGGUCA UAGUGAUCCGGUG GUUCUGAAUGGAA GGGCCAUCGCUCAA CGGAUAAAAGGUA CUCCGGGGAUAACA GGCUGAUACCGCCC AAGAGUUCAUAUC GACGGCGGUGUUU GGCACCUCGAUGUC GGCUCAUCACAUCC UGGGGCUGAAGUA GGUCCCAAGGGUAU GGCUGUUCGCCAUU UAAAGUGGUACGC GAGCUGGGUUUAG AACGUCGUGAGACA GUUCGGUCCCUAUC UGCCGUGGGCGCUG GAGAACUGAGGGG GGCUGCUCCUAGUA CGAGAGGACCGGAG UGGACGCAUCACUG GUGUUCGGGUUGU CAUGCCAAUGGCAC UGCCCGGUAGCUAA AUGCGGAAGAGAU AAGUGCUGAAAGC AUCUAAGCACGAAA CUUGCCCCGAGAUG AGUUCUCCCUGACC CUUUAAGGGUCCUG AAGGAACGUUGAA GACGACGACGUUGA UAGGCCGGGUGUG UAAGCGCAGCGAUG CGUUGAGCUAACCG GUACUAAUGAACCG UGAGGCUUAACCU |  |  |  |  |  |
| 2104 | CC1CC=CC=CC(C(CC (C(C(C(CC(=O)O1)O)  OC)OC2C(C(C(C(O2)  C)OC3CC(C(C(O3)C) O) (C)C)N(C)C)O)CC=O) C)O | GGUUAAGCGACUA AGCGUACACGGUGG AUGCCCUGGCAGUC AGAGGCGAUGAAG GACGUGCUAAUCUG CGAUAAGCGUCGGU AAGGUGAUAUGAA CCGUUAUAACCGGC GAUUUCCGAAUGG | Kitasamycin | Target\_lig\_114 4 | 50S subunit | Target\_100 | 8.17069622  716898 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | GGAAACCCAGUGUG UUUCGACACACUAU CAUUAACUGAAUCC AUAGGUUAAUGAG GCGAACCGGGGGAA CUGAAACAUCUAAG UACCCCGAGGAAAA GAAAUCAACCGAGA UUCCCCCAGUAGCG GCGAGCGAACGGGG AGCAGCCCAGAGCC UGAAUCAGUGUGU GUGUUAGUGGAAG CGUCUGGAAAGGCG CGCGAUACAGGGUG ACAGCCCCGUACAC AAAAAUGCACAUGC UGUGAGCUCGAUG AGUAGGGCGGGAC ACGUGGUAUCCUGU CUGAAUAUGGGGG GACCAUCCUCCAAG GCUAAAUACUCCUG ACUGACCGAUAGUG AACCAGUACCGUGA GGGAAAGGCGAAA AGAACCCCGGCGAG GGGAGUGAAAAAG AACCUGAAACCGUG UACGUACAAGCAGU GGGAGCACGCUUAG GCGUGUGACUGCGU ACCUUUUGUAUAA UGGGUCAGCGACUU AUAUUCUGUAGCA AGGUUAACCGAAU AGGGGAGCCGAAG GGAAACCGAGUCUU AACUGGGCGUUAA GUUGCAGGGUAUA GACCCGAAACCCGG UGAUCUAGCCAUGG GCAGGUUGAAGGU UGGGUAACACUAAC UGGAGGACCGAACC GACUAAUGUUGAA AAAUUAGCGGAUG ACUUGUGGCUGGG GGUGAAAGGCCAA UCAAACCGGGAGAU AGCUGGUUCUCCCC GAAAGCUAUUUAG GUAGCGCCUCGUGA AUUCAUCUCCGGGG GUAGAGCACUGUU UCGGCAAGGGGGUC ACUUACCAACCCGA UGCAAACUGCGAAU ACCGGAGAAUGUU AUCACGGGAGACAC ACGGCGGGUGCUAA CGUCCGUCGUGAAG AGGGAAACAACCCA GACCGCCAGCUAAG GUCCCAAAGUCAUG GUUAAGUGGGAAA CGAUGUGGGAAGG CCCAGACAGCCAGG AUGUUGGCUUAGA AGCAGCCAUCAUUU AAAGAAAGCGUAA UAGCUCACUGGUCG AGUCGGCCUGCGCG GAAGAUGUAACGG GGCUAAACCAUGCA |  |  |  |  |  |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | CCGAAGCUGCGGCA GCGACGCUUAUGCG UUGUUGGGUAGGG GAGCGUUCUGUAA GCCUGCGAAGGUGU GCUGUGAGGCAUGC UGGAGGUAUCAGA AGUGCGAAUGCUG ACAUAAGUAACGA UAAAGCGGGUGAA AAGCCCGCUCGCCG GAAGACCAAGGGU UCCUGUCCAACGUU AAUCGGGGCAGGG UGAGUCGACCCCUA AGGCGAGGCCGAAA GGCGUAGUCGAUG GGAAACAGGUUAA UAUUCCUGUACUUG GUGUUACUGCGAA GGGGGGACGGAGA AGGCUAUGUUGGCC GGGCGACGGUUGUC CCGGUUUAAGCGUG UAGGCUGGUUUUCC AGGCAAAUCCGGAA AAUCAAGGCUGAG GCGUGAUGACGAG GCACUACGGUGCUG AAGCAACAAAUGCC CUGCUUCCAGGAAA AGCCUCUAAGCAUC AGGUAACAUCAAA UCGUACCCCAAACC GACACAGGUGGUCA GGUAGAGAAUACC AAGGCGCUUGAGA GAACUCGGGUGAA GGAACUAGGCAAA AUGGUGCCGUAACU UCGGGAGAAGGCAC GCUGAUAUGUAGG UGAGGUCCCUCGCG GAUGGAGCUGAAA UCAGUCGAAGAUAC CAGCUGGCUGCAAC UGUUUAUUAAAAA CACAGCACUGUGCA AACACGAAAGUGG ACGUAUACGGUGU GACGCCUGCCCGGU GCCGGAAGGUUAA UUGAUGGGGUUAG CGCAAGCGAAGCUC UUGAUCGAAGCCCC GGUAAACGGCGGCC GUAACXAUAACGG UCCUAAGGUAGCGA AAUUCCUUGUCGGG UAAGUUCCGACCUG CACGAAUGGCGUAA UGAUGGCCAGGCUG UCUCCACCCGAGAC UCAGUGAAAUUGA ACUCGCUGUGAAGA UGCAGUGUACCCGC GGCAAGACGGAAA GACCCCGUGAACCU UUACUAUAGCUUG ACACUGAACAUUGA GCCUUGAUGUGUA GGAUAGGUGGGAG GCUUUGAAGUGUG GACGCCAGUCUGCA UGGAGCCGACCUUG |  |  |  |  |  |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | AAAUACCACCCUUU AAUGUUUGAUGUU CUAACGUUGACCCG UAAUCCGGGUUGCG GACAGUGUCUGGU GGGUAGUUUGACU GGGGCGGUCUCCUC CUAAAGAGUAACG GAGGAGCACGAAG GUUGGCUAAUCCUG GUCGGACAUCAGGA GGUUAGUGCAAUG GCAUAAGCCAGCUU GACUGCGAGCGUGA CGGCGCGAGCAGGU GCGAAAGCAGGUCA UAGUGAUCCGGUG GUUCUGAAUGGAA GGGCCAUCGCUCAA CGGAUAAAAGGUA CUCCGGGGAUAACA GGCUGAUACCGCCC AAGAGUUCAUAUC GACGGCGGUGUUU GGCACCUCGAUGUC GGCUCAUCACAUCC UGGGGCUGAAGUA GGUCCCAAGGGUAU GGCUGUUCGCCAUU UAAAGUGGUACGC GAGCUGGGUUUAG AACGUCGUGAGACA GUUCGGUCCCUAUC UGCCGUGGGCGCUG GAGAACUGAGGGG GGCUGCUCCUAGUA CGAGAGGACCGGAG UGGACGCAUCACUG GUGUUCGGGUUGU CAUGCCAAUGGCAC UGCCCGGUAGCUAA AUGCGGAAGAGAU AAGUGCUGAAAGC AUCUAAGCACGAAA CUUGCCCCGAGAUG AGUUCUCCCUGACC CUUUAAGGGUCCUG AAGGAACGUUGAA GACGACGACGUUGA UAGGCCGGGUGUG UAAGCGCAGCGAUG CGUUGAGCUAACCG GUACUAAUGAACCG UGAGGCUUAACCU |  |  |  |  |  |
| 2105 | CC1CC=CC=CC(C(CC (C(C(C(CC(=O)O1)OC  (=O)C)OC)OC2C(C(C(  C(O2)C)OC3CC(C(C(  O3)C)OC(=O)CC(C)C)  (C)O)N(C)C)O)CC=O) C)O | GGUUAAGCGACUA AGCGUACACGGUGG AUGCCCUGGCAGUC AGAGGCGAUGAAG GACGUGCUAAUCUG CGAUAAGCGUCGGU AAGGUGAUAUGAA CCGUUAUAACCGGC GAUUUCCGAAUGG GGAAACCCAGUGUG UUUCGACACACUAU CAUUAACUGAAUCC AUAGGUUAAUGAG GCGAACCGGGGGAA CUGAAACAUCUAAG UACCCCGAGGAAAA GAAAUCAACCGAGA UUCCCCCAGUAGCG GCGAGCGAACGGGG AGCAGCCCAGAGCC UGAAUCAGUGUGU | Josamycin | Target\_lig\_114 5 | 50S subunit | Target\_100 | 8.08884239  126002 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | GUGUUAGUGGAAG CGUCUGGAAAGGCG CGCGAUACAGGGUG ACAGCCCCGUACAC AAAAAUGCACAUGC UGUGAGCUCGAUG AGUAGGGCGGGAC ACGUGGUAUCCUGU CUGAAUAUGGGGG GACCAUCCUCCAAG GCUAAAUACUCCUG ACUGACCGAUAGUG AACCAGUACCGUGA GGGAAAGGCGAAA AGAACCCCGGCGAG GGGAGUGAAAAAG AACCUGAAACCGUG UACGUACAAGCAGU GGGAGCACGCUUAG GCGUGUGACUGCGU ACCUUUUGUAUAA UGGGUCAGCGACUU AUAUUCUGUAGCA AGGUUAACCGAAU AGGGGAGCCGAAG GGAAACCGAGUCUU AACUGGGCGUUAA GUUGCAGGGUAUA GACCCGAAACCCGG UGAUCUAGCCAUGG GCAGGUUGAAGGU UGGGUAACACUAAC UGGAGGACCGAACC GACUAAUGUUGAA AAAUUAGCGGAUG ACUUGUGGCUGGG GGUGAAAGGCCAA UCAAACCGGGAGAU AGCUGGUUCUCCCC GAAAGCUAUUUAG GUAGCGCCUCGUGA AUUCAUCUCCGGGG GUAGAGCACUGUU UCGGCAAGGGGGUC ACUUACCAACCCGA UGCAAACUGCGAAU ACCGGAGAAUGUU AUCACGGGAGACAC ACGGCGGGUGCUAA CGUCCGUCGUGAAG AGGGAAACAACCCA GACCGCCAGCUAAG GUCCCAAAGUCAUG GUUAAGUGGGAAA CGAUGUGGGAAGG CCCAGACAGCCAGG AUGUUGGCUUAGA AGCAGCCAUCAUUU AAAGAAAGCGUAA UAGCUCACUGGUCG AGUCGGCCUGCGCG GAAGAUGUAACGG GGCUAAACCAUGCA CCGAAGCUGCGGCA GCGACGCUUAUGCG UUGUUGGGUAGGG GAGCGUUCUGUAA GCCUGCGAAGGUGU GCUGUGAGGCAUGC UGGAGGUAUCAGA AGUGCGAAUGCUG ACAUAAGUAACGA UAAAGCGGGUGAA AAGCCCGCUCGCCG GAAGACCAAGGGU |  |  |  |  |  |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | UCCUGUCCAACGUU AAUCGGGGCAGGG UGAGUCGACCCCUA AGGCGAGGCCGAAA GGCGUAGUCGAUG GGAAACAGGUUAA UAUUCCUGUACUUG GUGUUACUGCGAA GGGGGGACGGAGA AGGCUAUGUUGGCC GGGCGACGGUUGUC CCGGUUUAAGCGUG UAGGCUGGUUUUCC AGGCAAAUCCGGAA AAUCAAGGCUGAG GCGUGAUGACGAG GCACUACGGUGCUG AAGCAACAAAUGCC CUGCUUCCAGGAAA AGCCUCUAAGCAUC AGGUAACAUCAAA UCGUACCCCAAACC GACACAGGUGGUCA GGUAGAGAAUACC AAGGCGCUUGAGA GAACUCGGGUGAA GGAACUAGGCAAA AUGGUGCCGUAACU UCGGGAGAAGGCAC GCUGAUAUGUAGG UGAGGUCCCUCGCG GAUGGAGCUGAAA UCAGUCGAAGAUAC CAGCUGGCUGCAAC UGUUUAUUAAAAA CACAGCACUGUGCA AACACGAAAGUGG ACGUAUACGGUGU GACGCCUGCCCGGU GCCGGAAGGUUAA UUGAUGGGGUUAG CGCAAGCGAAGCUC UUGAUCGAAGCCCC GGUAAACGGCGGCC GUAACXAUAACGG UCCUAAGGUAGCGA AAUUCCUUGUCGGG UAAGUUCCGACCUG CACGAAUGGCGUAA UGAUGGCCAGGCUG UCUCCACCCGAGAC UCAGUGAAAUUGA ACUCGCUGUGAAGA UGCAGUGUACCCGC GGCAAGACGGAAA GACCCCGUGAACCU UUACUAUAGCUUG ACACUGAACAUUGA GCCUUGAUGUGUA GGAUAGGUGGGAG GCUUUGAAGUGUG GACGCCAGUCUGCA UGGAGCCGACCUUG AAAUACCACCCUUU AAUGUUUGAUGUU CUAACGUUGACCCG UAAUCCGGGUUGCG GACAGUGUCUGGU GGGUAGUUUGACU GGGGCGGUCUCCUC CUAAAGAGUAACG GAGGAGCACGAAG GUUGGCUAAUCCUG GUCGGACAUCAGGA GGUUAGUGCAAUG |  |  |  |  |  |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | GCAUAAGCCAGCUU GACUGCGAGCGUGA CGGCGCGAGCAGGU GCGAAAGCAGGUCA UAGUGAUCCGGUG GUUCUGAAUGGAA GGGCCAUCGCUCAA CGGAUAAAAGGUA CUCCGGGGAUAACA GGCUGAUACCGCCC AAGAGUUCAUAUC GACGGCGGUGUUU GGCACCUCGAUGUC GGCUCAUCACAUCC UGGGGCUGAAGUA GGUCCCAAGGGUAU GGCUGUUCGCCAUU UAAAGUGGUACGC GAGCUGGGUUUAG AACGUCGUGAGACA GUUCGGUCCCUAUC UGCCGUGGGCGCUG GAGAACUGAGGGG GGCUGCUCCUAGUA CGAGAGGACCGGAG UGGACGCAUCACUG GUGUUCGGGUUGU CAUGCCAAUGGCAC UGCCCGGUAGCUAA AUGCGGAAGAGAU AAGUGCUGAAAGC AUCUAAGCACGAAA CUUGCCCCGAGAUG AGUUCUCCCUGACC CUUUAAGGGUCCUG AAGGAACGUUGAA GACGACGACGUUGA UAGGCCGGGUGUG UAAGCGCAGCGAUG CGUUGAGCUAACCG GUACUAAUGAACCG UGAGGCUUAACCU |  |  |  |  |  |
| 2106 | CCCC(=O)OC1C(OC( CC1(C)OC(=O)CC)OC 2C(OC(C(C2N(C)C)O) OC3C(CC(C(C=CC=C CC(OC(=O)CC(C3OC) O)C)O)C)CC=O)C)C | GGUUAAGCGACUA AGCGUACACGGUGG AUGCCCUGGCAGUC AGAGGCGAUGAAG GACGUGCUAAUCUG CGAUAAGCGUCGGU AAGGUGAUAUGAA CCGUUAUAACCGGC GAUUUCCGAAUGG GGAAACCCAGUGUG UUUCGACACACUAU CAUUAACUGAAUCC AUAGGUUAAUGAG GCGAACCGGGGGAA CUGAAACAUCUAAG UACCCCGAGGAAAA GAAAUCAACCGAGA UUCCCCCAGUAGCG GCGAGCGAACGGGG AGCAGCCCAGAGCC UGAAUCAGUGUGU GUGUUAGUGGAAG CGUCUGGAAAGGCG CGCGAUACAGGGUG ACAGCCCCGUACAC AAAAAUGCACAUGC UGUGAGCUCGAUG AGUAGGGCGGGAC ACGUGGUAUCCUGU CUGAAUAUGGGGG GACCAUCCUCCAAG GCUAAAUACUCCUG ACUGACCGAUAGUG | Rokitamycin | Target\_lig\_114 6 | 50S subunit | Target\_100 | 7.71331903  064507 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | AACCAGUACCGUGA GGGAAAGGCGAAA AGAACCCCGGCGAG GGGAGUGAAAAAG AACCUGAAACCGUG UACGUACAAGCAGU GGGAGCACGCUUAG GCGUGUGACUGCGU ACCUUUUGUAUAA UGGGUCAGCGACUU AUAUUCUGUAGCA AGGUUAACCGAAU AGGGGAGCCGAAG GGAAACCGAGUCUU AACUGGGCGUUAA GUUGCAGGGUAUA GACCCGAAACCCGG UGAUCUAGCCAUGG GCAGGUUGAAGGU UGGGUAACACUAAC UGGAGGACCGAACC GACUAAUGUUGAA AAAUUAGCGGAUG ACUUGUGGCUGGG GGUGAAAGGCCAA UCAAACCGGGAGAU AGCUGGUUCUCCCC GAAAGCUAUUUAG GUAGCGCCUCGUGA AUUCAUCUCCGGGG GUAGAGCACUGUU UCGGCAAGGGGGUC ACUUACCAACCCGA UGCAAACUGCGAAU ACCGGAGAAUGUU AUCACGGGAGACAC ACGGCGGGUGCUAA CGUCCGUCGUGAAG AGGGAAACAACCCA GACCGCCAGCUAAG GUCCCAAAGUCAUG GUUAAGUGGGAAA CGAUGUGGGAAGG CCCAGACAGCCAGG AUGUUGGCUUAGA AGCAGCCAUCAUUU AAAGAAAGCGUAA UAGCUCACUGGUCG AGUCGGCCUGCGCG GAAGAUGUAACGG GGCUAAACCAUGCA CCGAAGCUGCGGCA GCGACGCUUAUGCG UUGUUGGGUAGGG GAGCGUUCUGUAA GCCUGCGAAGGUGU GCUGUGAGGCAUGC UGGAGGUAUCAGA AGUGCGAAUGCUG ACAUAAGUAACGA UAAAGCGGGUGAA AAGCCCGCUCGCCG GAAGACCAAGGGU UCCUGUCCAACGUU AAUCGGGGCAGGG UGAGUCGACCCCUA AGGCGAGGCCGAAA GGCGUAGUCGAUG GGAAACAGGUUAA UAUUCCUGUACUUG GUGUUACUGCGAA GGGGGGACGGAGA AGGCUAUGUUGGCC GGGCGACGGUUGUC CCGGUUUAAGCGUG |  |  |  |  |  |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | UAGGCUGGUUUUCC AGGCAAAUCCGGAA AAUCAAGGCUGAG GCGUGAUGACGAG GCACUACGGUGCUG AAGCAACAAAUGCC CUGCUUCCAGGAAA AGCCUCUAAGCAUC AGGUAACAUCAAA UCGUACCCCAAACC GACACAGGUGGUCA GGUAGAGAAUACC AAGGCGCUUGAGA GAACUCGGGUGAA GGAACUAGGCAAA AUGGUGCCGUAACU UCGGGAGAAGGCAC GCUGAUAUGUAGG UGAGGUCCCUCGCG GAUGGAGCUGAAA UCAGUCGAAGAUAC CAGCUGGCUGCAAC UGUUUAUUAAAAA CACAGCACUGUGCA AACACGAAAGUGG ACGUAUACGGUGU GACGCCUGCCCGGU GCCGGAAGGUUAA UUGAUGGGGUUAG CGCAAGCGAAGCUC UUGAUCGAAGCCCC GGUAAACGGCGGCC GUAACXAUAACGG UCCUAAGGUAGCGA AAUUCCUUGUCGGG UAAGUUCCGACCUG CACGAAUGGCGUAA UGAUGGCCAGGCUG UCUCCACCCGAGAC UCAGUGAAAUUGA ACUCGCUGUGAAGA UGCAGUGUACCCGC GGCAAGACGGAAA GACCCCGUGAACCU UUACUAUAGCUUG ACACUGAACAUUGA GCCUUGAUGUGUA GGAUAGGUGGGAG GCUUUGAAGUGUG GACGCCAGUCUGCA UGGAGCCGACCUUG AAAUACCACCCUUU AAUGUUUGAUGUU CUAACGUUGACCCG UAAUCCGGGUUGCG GACAGUGUCUGGU GGGUAGUUUGACU GGGGCGGUCUCCUC CUAAAGAGUAACG GAGGAGCACGAAG GUUGGCUAAUCCUG GUCGGACAUCAGGA GGUUAGUGCAAUG GCAUAAGCCAGCUU GACUGCGAGCGUGA CGGCGCGAGCAGGU GCGAAAGCAGGUCA UAGUGAUCCGGUG GUUCUGAAUGGAA GGGCCAUCGCUCAA CGGAUAAAAGGUA CUCCGGGGAUAACA GGCUGAUACCGCCC AAGAGUUCAUAUC GACGGCGGUGUUU |  |  |  |  |  |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | GGCACCUCGAUGUC GGCUCAUCACAUCC UGGGGCUGAAGUA GGUCCCAAGGGUAU GGCUGUUCGCCAUU UAAAGUGGUACGC GAGCUGGGUUUAG AACGUCGUGAGACA GUUCGGUCCCUAUC UGCCGUGGGCGCUG GAGAACUGAGGGG GGCUGCUCCUAGUA CGAGAGGACCGGAG UGGACGCAUCACUG GUGUUCGGGUUGU CAUGCCAAUGGCAC UGCCCGGUAGCUAA AUGCGGAAGAGAU AAGUGCUGAAAGC AUCUAAGCACGAAA CUUGCCCCGAGAUG AGUUCUCCCUGACC CUUUAAGGGUCCUG AAGGAACGUUGAA GACGACGACGUUGA UAGGCCGGGUGUG UAAGCGCAGCGAUG CGUUGAGCUAACCG GUACUAAUGAACCG UGAGGCUUAACCU |  |  |  |  |  |
| 2107 | CCC1C(C(C(C(=O)C(  CC(C(C(C(C(C(=O)O1  )C)OC2CC(C(C(O2)C) O) (C)OC)C)OC3C(C(CC(  O3)C)N(C)C)O)  (C)O)C)C)O)(C)O | GGUUAAGCGACUA AGCGUACACGGUGG AUGCCCUGGCAGUC AGAGGCGAUGAAG GACGUGCUAAUCUG CGAUAAGCGUCGGU AAGGUGAUAUGAA CCGUUAUAACCGGC GAUUUCCGAAUGG GGAAACCCAGUGUG UUUCGACACACUAU CAUUAACUGAAUCC AUAGGUUAAUGAG GCGAACCGGGGGAA CUGAAACAUCUAAG UACCCCGAGGAAAA GAAAUCAACCGAGA UUCCCCCAGUAGCG GCGAGCGAACGGGG AGCAGCCCAGAGCC UGAAUCAGUGUGU GUGUUAGUGGAAG CGUCUGGAAAGGCG CGCGAUACAGGGUG ACAGCCCCGUACAC AAAAAUGCACAUGC UGUGAGCUCGAUG AGUAGGGCGGGAC ACGUGGUAUCCUGU CUGAAUAUGGGGG GACCAUCCUCCAAG GCUAAAUACUCCUG ACUGACCGAUAGUG AACCAGUACCGUGA GGGAAAGGCGAAA AGAACCCCGGCGAG GGGAGUGAAAAAG AACCUGAAACCGUG UACGUACAAGCAGU GGGAGCACGCUUAG GCGUGUGACUGCGU ACCUUUUGUAUAA UGGGUCAGCGACUU AUAUUCUGUAGCA AGGUUAACCGAAU | Eryrthromycin | Target\_lig\_23 3 | 50S subunit | Target\_100 | 8.11350927  482752 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | AGGGGAGCCGAAG GGAAACCGAGUCUU AACUGGGCGUUAA GUUGCAGGGUAUA GACCCGAAACCCGG UGAUCUAGCCAUGG GCAGGUUGAAGGU UGGGUAACACUAAC UGGAGGACCGAACC GACUAAUGUUGAA AAAUUAGCGGAUG ACUUGUGGCUGGG GGUGAAAGGCCAA UCAAACCGGGAGAU AGCUGGUUCUCCCC GAAAGCUAUUUAG GUAGCGCCUCGUGA AUUCAUCUCCGGGG GUAGAGCACUGUU UCGGCAAGGGGGUC ACUUACCAACCCGA UGCAAACUGCGAAU ACCGGAGAAUGUU AUCACGGGAGACAC ACGGCGGGUGCUAA CGUCCGUCGUGAAG AGGGAAACAACCCA GACCGCCAGCUAAG GUCCCAAAGUCAUG GUUAAGUGGGAAA CGAUGUGGGAAGG CCCAGACAGCCAGG AUGUUGGCUUAGA AGCAGCCAUCAUUU AAAGAAAGCGUAA UAGCUCACUGGUCG AGUCGGCCUGCGCG GAAGAUGUAACGG GGCUAAACCAUGCA CCGAAGCUGCGGCA GCGACGCUUAUGCG UUGUUGGGUAGGG GAGCGUUCUGUAA GCCUGCGAAGGUGU GCUGUGAGGCAUGC UGGAGGUAUCAGA AGUGCGAAUGCUG ACAUAAGUAACGA UAAAGCGGGUGAA AAGCCCGCUCGCCG GAAGACCAAGGGU UCCUGUCCAACGUU AAUCGGGGCAGGG UGAGUCGACCCCUA AGGCGAGGCCGAAA GGCGUAGUCGAUG GGAAACAGGUUAA UAUUCCUGUACUUG GUGUUACUGCGAA GGGGGGACGGAGA AGGCUAUGUUGGCC GGGCGACGGUUGUC CCGGUUUAAGCGUG UAGGCUGGUUUUCC AGGCAAAUCCGGAA AAUCAAGGCUGAG GCGUGAUGACGAG GCACUACGGUGCUG AAGCAACAAAUGCC CUGCUUCCAGGAAA AGCCUCUAAGCAUC AGGUAACAUCAAA UCGUACCCCAAACC GACACAGGUGGUCA GGUAGAGAAUACC |  |  |  |  |  |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | AAGGCGCUUGAGA GAACUCGGGUGAA GGAACUAGGCAAA AUGGUGCCGUAACU UCGGGAGAAGGCAC GCUGAUAUGUAGG UGAGGUCCCUCGCG GAUGGAGCUGAAA UCAGUCGAAGAUAC CAGCUGGCUGCAAC UGUUUAUUAAAAA CACAGCACUGUGCA AACACGAAAGUGG ACGUAUACGGUGU GACGCCUGCCCGGU GCCGGAAGGUUAA UUGAUGGGGUUAG CGCAAGCGAAGCUC UUGAUCGAAGCCCC GGUAAACGGCGGCC GUAACXAUAACGG UCCUAAGGUAGCGA AAUUCCUUGUCGGG UAAGUUCCGACCUG CACGAAUGGCGUAA UGAUGGCCAGGCUG UCUCCACCCGAGAC UCAGUGAAAUUGA ACUCGCUGUGAAGA UGCAGUGUACCCGC GGCAAGACGGAAA GACCCCGUGAACCU UUACUAUAGCUUG ACACUGAACAUUGA GCCUUGAUGUGUA GGAUAGGUGGGAG GCUUUGAAGUGUG GACGCCAGUCUGCA UGGAGCCGACCUUG AAAUACCACCCUUU AAUGUUUGAUGUU CUAACGUUGACCCG UAAUCCGGGUUGCG GACAGUGUCUGGU GGGUAGUUUGACU GGGGCGGUCUCCUC CUAAAGAGUAACG GAGGAGCACGAAG GUUGGCUAAUCCUG GUCGGACAUCAGGA GGUUAGUGCAAUG GCAUAAGCCAGCUU GACUGCGAGCGUGA CGGCGCGAGCAGGU GCGAAAGCAGGUCA UAGUGAUCCGGUG GUUCUGAAUGGAA GGGCCAUCGCUCAA CGGAUAAAAGGUA CUCCGGGGAUAACA GGCUGAUACCGCCC AAGAGUUCAUAUC GACGGCGGUGUUU GGCACCUCGAUGUC GGCUCAUCACAUCC UGGGGCUGAAGUA GGUCCCAAGGGUAU GGCUGUUCGCCAUU UAAAGUGGUACGC GAGCUGGGUUUAG AACGUCGUGAGACA GUUCGGUCCCUAUC UGCCGUGGGCGCUG GAGAACUGAGGGG GGCUGCUCCUAGUA |  |  |  |  |  |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | CGAGAGGACCGGAG UGGACGCAUCACUG GUGUUCGGGUUGU CAUGCCAAUGGCAC UGCCCGGUAGCUAA AUGCGGAAGAGAU AAGUGCUGAAAGC AUCUAAGCACGAAA CUUGCCCCGAGAUG AGUUCUCCCUGACC CUUUAAGGGUCCUG AAGGAACGUUGAA GACGACGACGUUGA UAGGCCGGGUGUG UAAGCGCAGCGAUG CGUUGAGCUAACCG GUACUAAUGAACCG UGAGGCUUAACCU |  |  |  |  |  |
| 2286 | CCC1C(C=C(C=CC(= O)C(CC(C(C(C(CC(=O  )O1)O)C)OC2C(C(C(C  (O2)C)OC3CC(C(C(O3  )C)O) (C)O)N(C)C)O)CC=O)  C)C)COC4C(C(C(C(O 4)C)O)OC)OC | UUGGCUACUAUGCC AGCUGGUGGAUUG CUCGGCUCAGGCGC UGAUGAAGGACGU GCCAAGCUGCGAUA AGCCAUGGGGAGCC GCACGGAGGCGAAG AACCAUGGAUUUCC GAAUGAGAAUCUC UCUAACAAUUGCUU CGCGCAAUGAGGAA CCCCGAGAACUGAA ACAUCUCAGUAUCG GGAGGAACAGAAA ACGCAAUGUGAUG UCGUUAGUAACCGC GAGUGAACGCGAU ACAGCCCAAACCGA AGCCCUCACGGGCA AUGUGGUGUCAGG GCUACCUCUCAUCA GCCGACCGUCUCGA CGAAGUCUCUUGGA ACAGAGCGUGAUAC AGGGUGACAACCCC GUACUCGAGACCAG UACGACGUGCGGUA GUGCCAGAGUAGCG GGGGUUGGAUAUC CCUCGCGAAUAACG CAGGCAUCGACUGC GAAGGCUAAACACA ACCUGAGACCGAUA GUGAACAAGUAGU GUGAACGAACGCUG CAAAGUACCCUCAG AAGGGAGGCGAAA UAGAGCAUGAAAU CAGUUGGCGAUCGA GCGACAGGGCAUAC AAGGUCCCUCGACG AAUGACCGACGCGC GAGCGUCCAGUAAG ACUCACGGGAAGCC GAUGUUCUGUCGU ACGUUUUGAAAAA CGAGCCAGGGAGUG UGUCUGCAUGGCAA GUCUAACCGGAGUA UCCGGGGAGGCACA GGGAAACCGACAUG GCCGCAGGGCUUUG CCCGAGGGCCGCCG UCUUCAAGGGCGGG GAGCCAUGUGGACA CGACCCGAAUCCGG ACGAUCUACGCAUG | Tylosin | Target\_lig\_32 0 | U2609\_Ecoli  \_ribosome | Target\_99 | 7.12027350  336042 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | GACAAGAUGAAGC GUGCCGAAAGGCAC GUGGAAGUCUGUU AGAGUUGGUGUCC UACAAUACCCUCUC GUGAUCUAUGUGU AGGGGUGAAAGGC CCAUCGAGUCCGGC AACAGCUGGUUCCA AUCGAAACAUGUCG AAGCAUGACCUCCG CCGAGGUAGUCUGU GAGGUAGAGCGACC GAUUGGUGUGUCC GCCUCCGAGAGGAG UCGGCACACCUGUC AAACUCCAAACUUA CAGACGCCGUUUGA CGCGGGGAUUCCGG UGCGCGGGGUAAGC CUGUGUACCAGGAG GGGAACAACCCAGA GAUAGGUUAAGGU CCCCAAGUGUGGAU UAAGUGUAAUCCUC UGAAGGUGGUCUC GAGCCCUAGACAGC CGGGAGGUGAGCU UAGAAGCAGCUACC CUCUAAGAAAAGCG UAACAGCUUACCGG CCGAGGUUUGAGGC GCCCAAAAUGAUCG GGACUCAAAUCCAC CACCGAGACCUGUC CGUACCACUCAUAC UGGUAAUCGAGUA GAUUGGCGCUCUAA UUGGAUGGAAGUA GGGGUGAAAACUCC UAUGGACCGAUUA GUGACGAAAAUCCU GGCCAUAGUAGCAG CGAUAGUCGGGUG AGAACCCCGACGGC CUAAUGGAUAAGG GUUCCUCAGCACUG CUGAUCAGCUGAGG GUUAGCCGGUCCUA AGUCAUACCGCAAC UCGACUAUGACGAA AUGGGAAACGGGU UAAUAUUCCCGUGC CACUAUGCAGUGAA AGUUGACGCCCUGG GGUCGAUCACGCUG GGCAUUCGCCCAGU CGAACCGUCCAACU CCGUGGAAGCCGUA AUGGCAGGAAGCG GACGAACGGCGGCA UAGGGAAACGUGA UUCAACCUGGGGCC CAUGAAAAGACGA GCAUAGUGUCCGUA CCGAGAACCGACAC AGGUGUCCAUGGCG GCGAAAGCCAAGGC CUGUCGGGAGCAAC CAACGUUAGGGAA UUCGGCAAGUUAG UCCCGUACCUUCGG AAGAAGGGAUGCC UGCUCCGGAACGGA GCAGGUCGCAGUGA |  |  |  |  |  |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | CUCGGAAGCUCGGA CUGUCUAGUAACAA CAUAGGUGACCGCA AAUCCGCAAGGACU CGUACGGUCACUGA AUCCUGCCCAGUGC AGGUAUCUGAACAC CUCGUACAAGAGGA CGAAGGACCUGUCA ACGGCGGGGGUAAC UAUGACCCUCUUAA GGUAGCGUAGUACC UUGCCGCAUCAGUA GCGGCUUGCAUGAA UGGAUUAACCAGA GCUUCACUGUCCCA ACGUUGGGCCCGGU GAACUGUACAUUCC AGUGCGGAGUCUG GAGACACCCAGGGG GAAGCGAAGACCCU AUGGAGCUUUACU GCAGGCUGUCGCUG AGACGUGGUCGCCG AUGUGCAGCAUAG GUAGGAGACACUAC ACAGGUACCCGCGC UAGCGGGCCACCGA GUCAACAGUGAAA UACUACCCGUCGGU GACUGCGACUCUCA CUCCGGGAGGAGGA CACCGAUAGCCGGG CAGUUUGACUGGG GCGGUACGCGCUCG AAAAGAUAUCGAG CGCGCCCUAUGGCU AUCUCAGCCGGGAC AGAGACCCGGCGAA GAGUGCAAGAGCA AAAGAUAGCUUGA CAGUGUUCUUCCCA ACGAGGAACGCUGA CGCGAAAGCGUGGU CUAGCGAACCAAUU AGCCUGCUUGAUGC GGGCAAUUGAUGA CAGAAAAGCUACCC UAGGGAUAACAGA GUCGUCACUCGCAA GAGCACAUAUCGAC CGAGUGGCUUGCUA CCUCGAUGUCGGUU CCCUCCAUCCUGCC CGUGCAGAAGCGGG CAAGGGUGAGGUU GUUCGCCUAUUAAA GGAGGUCGUGAGC UGGGUUUAGACCG UCGUGAGACAGGUC GGCUGCUAUCUACU GGGUGUGUAAUGG UGUCUGACAAGAAC GACCGUAUAGUACG AGAGGAACUACGG UUGGUGGCCACUGG UGUACCGGUUGUUC GAGAGAGCACGUGC CGGGUAGCCACGCC ACACGGGGUAAGA GCUGAACGCAUCUA AGCUCGAAACCCAC UUGGAAAAGAGAC ACCGCCGAGGUCCC GCGUACAAGACGCG |  |  |  |  |  |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | GUCGAUAGACUCGG GGUGUGCGCGUCGA GGUAACGAGACGU UAAGCCCACGAGCA CUAACAGACCAAAG CCAUCAU |  |  |  |  |  |
| 2288 | CCCC1CC(N(C1)C)C(  =O)NC(C2C(C(C(C(O2  )SC)O)O)O)C(C)O | GGUUAAGCGACUA AGCGUACACGGUGG AUGCCCUGGCAGUC AGAGGCGAUGAAG GACGUGCUAAUCUG CGAUAAGCGUCGGU AAGGUGAUAUGAA CCGUUAUAACCGGC GAUUUCCGAAUGG GGAAACCCAGUGUG UUUCGACACACUAU CAUUAACUGAAUCC AUAGGUUAAUGAG GCGAACCGGGGGAA CUGAAACAUCUAAG UACCCCGAGGAAAA GAAAUCAACCGAGA UUCCCCCAGUAGCG GCGAGCGAACGGGG AGCAGCCCAGAGCC UGAAUCAGUGUGU GUGUUAGUGGAAG CGUCUGGAAAGGCG CGCGAUACAGGGUG ACAGCCCCGUACAC AAAAAUGCACAUGC UGUGAGCUCGAUG AGUAGGGCGGGAC ACGUGGUAUCCUGU CUGAAUAUGGGGG GACCAUCCUCCAAG GCUAAAUACUCCUG ACUGACCGAUAGUG AACCAGUACCGUGA GGGAAAGGCGAAA AGAACCCCGGCGAG GGGAGUGAAAAAG AACCUGAAACCGUG UACGUACAAGCAGU GGGAGCACGCUUAG GCGUGUGACUGCGU ACCUUUUGUAUAA UGGGUCAGCGACUU AUAUUCUGUAGCA AGGUUAACCGAAU AGGGGAGCCGAAG GGAAACCGAGUCUU AACUGGGCGUUAA GUUGCAGGGUAUA GACCCGAAACCCGG UGAUCUAGCCAUGG GCAGGUUGAAGGU UGGGUAACACUAAC UGGAGGACCGAACC GACUAAUGUUGAA AAAUUAGCGGAUG ACUUGUGGCUGGG GGUGAAAGGCCAA UCAAACCGGGAGAU AGCUGGUUCUCCCC GAAAGCUAUUUAG GUAGCGCCUCGUGA AUUCAUCUCCGGGG GUAGAGCACUGUU UCGGCAAGGGGGUC ACUUACCAACCCGA UGCAAACUGCGAAU ACCGGAGAAUGUU AUCACGGGAGACAC | Lincomycin | Target\_lig\_117 5 | 50S ribosome (CLINDAM YCIN) | Target\_100 | 5.30102999  566398 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | ACGGCGGGUGCUAA CGUCCGUCGUGAAG AGGGAAACAACCCA GACCGCCAGCUAAG GUCCCAAAGUCAUG GUUAAGUGGGAAA CGAUGUGGGAAGG CCCAGACAGCCAGG AUGUUGGCUUAGA AGCAGCCAUCAUUU AAAGAAAGCGUAA UAGCUCACUGGUCG AGUCGGCCUGCGCG GAAGAUGUAACGG GGCUAAACCAUGCA CCGAAGCUGCGGCA GCGACGCUUAUGCG UUGUUGGGUAGGG GAGCGUUCUGUAA GCCUGCGAAGGUGU GCUGUGAGGCAUGC UGGAGGUAUCAGA AGUGCGAAUGCUG ACAUAAGUAACGA UAAAGCGGGUGAA AAGCCCGCUCGCCG GAAGACCAAGGGU UCCUGUCCAACGUU AAUCGGGGCAGGG UGAGUCGACCCCUA AGGCGAGGCCGAAA GGCGUAGUCGAUG GGAAACAGGUUAA UAUUCCUGUACUUG GUGUUACUGCGAA GGGGGGACGGAGA AGGCUAUGUUGGCC GGGCGACGGUUGUC CCGGUUUAAGCGUG UAGGCUGGUUUUCC AGGCAAAUCCGGAA AAUCAAGGCUGAG GCGUGAUGACGAG GCACUACGGUGCUG AAGCAACAAAUGCC CUGCUUCCAGGAAA AGCCUCUAAGCAUC AGGUAACAUCAAA UCGUACCCCAAACC GACACAGGUGGUCA GGUAGAGAAUACC AAGGCGCUUGAGA GAACUCGGGUGAA GGAACUAGGCAAA AUGGUGCCGUAACU UCGGGAGAAGGCAC GCUGAUAUGUAGG UGAGGUCCCUCGCG GAUGGAGCUGAAA UCAGUCGAAGAUAC CAGCUGGCUGCAAC UGUUUAUUAAAAA CACAGCACUGUGCA AACACGAAAGUGG ACGUAUACGGUGU GACGCCUGCCCGGU GCCGGAAGGUUAA UUGAUGGGGUUAG CGCAAGCGAAGCUC UUGAUCGAAGCCCC GGUAAACGGCGGCC GUAACXAUAACGG UCCUAAGGUAGCGA AAUUCCUUGUCGGG UAAGUUCCGACCUG |  |  |  |  |  |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | CACGAAUGGCGUAA UGAUGGCCAGGCUG UCUCCACCCGAGAC UCAGUGAAAUUGA ACUCGCUGUGAAGA UGCAGUGUACCCGC GGCAAGACGGAAA GACCCCGUGAACCU UUACUAUAGCUUG ACACUGAACAUUGA GCCUUGAUGUGUA GGAUAGGUGGGAG GCUUUGAAGUGUG GACGCCAGUCUGCA UGGAGCCGACCUUG AAAUACCACCCUUU AAUGUUUGAUGUU CUAACGUUGACCCG UAAUCCGGGUUGCG GACAGUGUCUGGU GGGUAGUUUGACU GGGGCGGUCUCCUC CUAAAGAGUAACG GAGGAGCACGAAG GUUGGCUAAUCCUG GUCGGACAUCAGGA GGUUAGUGCAAUG GCAUAAGCCAGCUU GACUGCGAGCGUGA CGGCGCGAGCAGGU GCGAAAGCAGGUCA UAGUGAUCCGGUG GUUCUGAAUGGAA GGGCCAUCGCUCAA CGGAUAAAAGGUA CUCCGGGGAUAACA GGCUGAUACCGCCC AAGAGUUCAUAUC GACGGCGGUGUUU GGCACCUCGAUGUC GGCUCAUCACAUCC UGGGGCUGAAGUA GGUCCCAAGGGUAU GGCUGUUCGCCAUU UAAAGUGGUACGC GAGCUGGGUUUAG AACGUCGUGAGACA GUUCGGUCCCUAUC UGCCGUGGGCGCUG GAGAACUGAGGGG GGCUGCUCCUAGUA CGAGAGGACCGGAG UGGACGCAUCACUG GUGUUCGGGUUGU CAUGCCAAUGGCAC UGCCCGGUAGCUAA AUGCGGAAGAGAU AAGUGCUGAAAGC AUCUAAGCACGAAA CUUGCCCCGAGAUG AGUUCUCCCUGACC CUUUAAGGGUCCUG AAGGAACGUUGAA GACGACGACGUUGA UAGGCCGGGUGUG UAAGCGCAGCGAUG CGUUGAGCUAACCG GUACUAAUGAACCG UGAGGCUUAACCU |  |  |  |  |  |
| 2292 | CCC1C(=O)N2CCCC2 C(=O)N(C(C(=O)N3C CC(=O)CC3C(=O)NC( C(=O)OC(C(C(=O)N1) NC(=O)C4=C(C=CC= N4)O)C)C5=CC=CC= | GGUUAAGCGACUA AGCGUACACGGUGG AUGCCCUGGCAGUC AGAGGCGAUGAAG GACGUGCUAAUCUG CGAUAAGCGUCGGU | Virginiamycin S | Target\_lig\_117 6 | 50S ribosome (Virginiamyci n M) | Target\_100 | 6.39794000  867204 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  | C5)CC6=CC=CC=C6) C | AAGGUGAUAUGAA CCGUUAUAACCGGC GAUUUCCGAAUGG GGAAACCCAGUGUG UUUCGACACACUAU CAUUAACUGAAUCC AUAGGUUAAUGAG GCGAACCGGGGGAA CUGAAACAUCUAAG UACCCCGAGGAAAA GAAAUCAACCGAGA UUCCCCCAGUAGCG GCGAGCGAACGGGG AGCAGCCCAGAGCC UGAAUCAGUGUGU GUGUUAGUGGAAG CGUCUGGAAAGGCG CGCGAUACAGGGUG ACAGCCCCGUACAC AAAAAUGCACAUGC UGUGAGCUCGAUG AGUAGGGCGGGAC ACGUGGUAUCCUGU CUGAAUAUGGGGG GACCAUCCUCCAAG GCUAAAUACUCCUG ACUGACCGAUAGUG AACCAGUACCGUGA GGGAAAGGCGAAA AGAACCCCGGCGAG GGGAGUGAAAAAG AACCUGAAACCGUG UACGUACAAGCAGU GGGAGCACGCUUAG GCGUGUGACUGCGU ACCUUUUGUAUAA UGGGUCAGCGACUU AUAUUCUGUAGCA AGGUUAACCGAAU AGGGGAGCCGAAG GGAAACCGAGUCUU AACUGGGCGUUAA GUUGCAGGGUAUA GACCCGAAACCCGG UGAUCUAGCCAUGG GCAGGUUGAAGGU UGGGUAACACUAAC UGGAGGACCGAACC GACUAAUGUUGAA AAAUUAGCGGAUG ACUUGUGGCUGGG GGUGAAAGGCCAA UCAAACCGGGAGAU AGCUGGUUCUCCCC GAAAGCUAUUUAG GUAGCGCCUCGUGA AUUCAUCUCCGGGG GUAGAGCACUGUU UCGGCAAGGGGGUC ACUUACCAACCCGA UGCAAACUGCGAAU ACCGGAGAAUGUU AUCACGGGAGACAC ACGGCGGGUGCUAA CGUCCGUCGUGAAG AGGGAAACAACCCA GACCGCCAGCUAAG GUCCCAAAGUCAUG GUUAAGUGGGAAA CGAUGUGGGAAGG CCCAGACAGCCAGG AUGUUGGCUUAGA AGCAGCCAUCAUUU AAAGAAAGCGUAA UAGCUCACUGGUCG |  |  |  |  |  |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | AGUCGGCCUGCGCG GAAGAUGUAACGG GGCUAAACCAUGCA CCGAAGCUGCGGCA GCGACGCUUAUGCG UUGUUGGGUAGGG GAGCGUUCUGUAA GCCUGCGAAGGUGU GCUGUGAGGCAUGC UGGAGGUAUCAGA AGUGCGAAUGCUG ACAUAAGUAACGA UAAAGCGGGUGAA AAGCCCGCUCGCCG GAAGACCAAGGGU UCCUGUCCAACGUU AAUCGGGGCAGGG UGAGUCGACCCCUA AGGCGAGGCCGAAA GGCGUAGUCGAUG GGAAACAGGUUAA UAUUCCUGUACUUG GUGUUACUGCGAA GGGGGGACGGAGA AGGCUAUGUUGGCC GGGCGACGGUUGUC CCGGUUUAAGCGUG UAGGCUGGUUUUCC AGGCAAAUCCGGAA AAUCAAGGCUGAG GCGUGAUGACGAG GCACUACGGUGCUG AAGCAACAAAUGCC CUGCUUCCAGGAAA AGCCUCUAAGCAUC AGGUAACAUCAAA UCGUACCCCAAACC GACACAGGUGGUCA GGUAGAGAAUACC AAGGCGCUUGAGA GAACUCGGGUGAA GGAACUAGGCAAA AUGGUGCCGUAACU UCGGGAGAAGGCAC GCUGAUAUGUAGG UGAGGUCCCUCGCG GAUGGAGCUGAAA UCAGUCGAAGAUAC CAGCUGGCUGCAAC UGUUUAUUAAAAA CACAGCACUGUGCA AACACGAAAGUGG ACGUAUACGGUGU GACGCCUGCCCGGU GCCGGAAGGUUAA UUGAUGGGGUUAG CGCAAGCGAAGCUC UUGAUCGAAGCCCC GGUAAACGGCGGCC GUAACXAUAACGG UCCUAAGGUAGCGA AAUUCCUUGUCGGG UAAGUUCCGACCUG CACGAAUGGCGUAA UGAUGGCCAGGCUG UCUCCACCCGAGAC UCAGUGAAAUUGA ACUCGCUGUGAAGA UGCAGUGUACCCGC GGCAAGACGGAAA GACCCCGUGAACCU UUACUAUAGCUUG ACACUGAACAUUGA GCCUUGAUGUGUA GGAUAGGUGGGAG |  |  |  |  |  |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA**  **\_name** | **Target\_RNA\_ ID** | **pKd** |
|  |  | GCUUUGAAGUGUG GACGCCAGUCUGCA UGGAGCCGACCUUG AAAUACCACCCUUU AAUGUUUGAUGUU CUAACGUUGACCCG UAAUCCGGGUUGCG GACAGUGUCUGGU GGGUAGUUUGACU GGGGCGGUCUCCUC CUAAAGAGUAACG GAGGAGCACGAAG GUUGGCUAAUCCUG GUCGGACAUCAGGA GGUUAGUGCAAUG GCAUAAGCCAGCUU GACUGCGAGCGUGA CGGCGCGAGCAGGU GCGAAAGCAGGUCA UAGUGAUCCGGUG GUUCUGAAUGGAA GGGCCAUCGCUCAA CGGAUAAAAGGUA CUCCGGGGAUAACA GGCUGAUACCGCCC AAGAGUUCAUAUC GACGGCGGUGUUU GGCACCUCGAUGUC GGCUCAUCACAUCC UGGGGCUGAAGUA GGUCCCAAGGGUAU GGCUGUUCGCCAUU UAAAGUGGUACGC GAGCUGGGUUUAG AACGUCGUGAGACA GUUCGGUCCCUAUC UGCCGUGGGCGCUG GAGAACUGAGGGG GGCUGCUCCUAGUA CGAGAGGACCGGAG UGGACGCAUCACUG GUGUUCGGGUUGU CAUGCCAAUGGCAC UGCCCGGUAGCUAA AUGCGGAAGAGAU AAGUGCUGAAAGC AUCUAAGCACGAAA CUUGCCCCGAGAUG AGUUCUCCCUGACC CUUUAAGGGUCCUG AAGGAACGUUGAA GACGACGACGUUGA UAGGCCGGGUGUG UAAGCGCAGCGAUG CGUUGAGCUAACCG GUACUAAUGAACCG UGAGGCUUAACCU |  |  |  |  |  |
| 2348 | [C@H]1([C@H]  ([C@@H]([C@H]  (O[C@H]1CO)O[C@H  ]1[C@@H]([C@H] (O[C@H] ([C@@H]1N)OC)CN) O)N)O)O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Neamine mimic\_10 | Target\_lig\_12 85 | 16s\_rRNA A SITE | Target\_3 | 4.16115090  926274 |
| 2349 | N[C@@H]1C[C@H] (N)[C@H]([C@@H]  ([C@H]1OCn1cnc2c1c ccc2)O)O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Neamine\_derivat ive\_14 | Target\_lig\_12 01 | 16s\_rRNA A SITE | Target\_3 | 3.17587416  608345 |
| 2350 | N[C@@H]1C[C@H] (N)[C@H]([C@@H]  ([C@H]1OCn1c2ccccc 2nc1C(F)(F)F)O)O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Neamine\_derivat ive\_15 | Target\_lig\_12 02 | 16s\_rRNA A SITE | Target\_3 | 3.35753547  975788 |
| 2351 | N[C@@H]1C[C@H] | GAGCGUCACACCUU | Neamine\_derivat | Target\_lig\_12 | 16s\_rRNA A | Target\_3 | 3.16621562 |

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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@@H]  ([C@H]1OCn1ccc(n1)I  )O)O | CGGGUGAAGUCGCU C | ive\_18 | 03 | SITE |  | 534352 |
| 2352 | N[C@@H]1C[C@H] (N)[C@H]([C@@H]  ([C@H]1OSc1cncnc1) O)O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Neamine\_derivat ive\_19 | Target\_lig\_12 04 | 16s\_rRNA A SITE | Target\_3 | 3.31158017  799729 |
| 2353 | N[C@@H]1C[C@H] (N)[C@H]([C@@H]  ([C@H]1OSc1cnc(nc1) C(F)(F)F)O)O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Neamine\_derivat ive\_20 | Target\_lig\_12 05 | 16s\_rRNA A SITE | Target\_3 | 2.96697855  531709 |
| 2354 | N[C@@H]1C[C@H] (N)[C@H]([C@@H] ([C@H]1OC[N+]1N=N  c2c1nccc2)O)O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Neamine\_derivat ive\_26 | Target\_lig\_12 06 | 16s\_rRNA A SITE | Target\_3 | 3.25649023  527157 |
| 2355 | N[C@@H]1C[C@H] (N)[C@H]([C@@H] ([C@H]1OC[N+]1N=N  c2c1cccn2)O)O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Neamine\_derivat ive\_27 | Target\_lig\_12 07 | 16s\_rRNA A SITE | Target\_3 | 3.25649023  527157 |
| 2356 | N[C@@H]1C[C@H] (N)[C@H]([C@@H]  ([C@H]1OCn1nc2c(n1  )cccn2)O)O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Neamine\_derivat ive\_28 | Target\_lig\_12 08 | 16s\_rRNA A SITE | Target\_3 | 3.25649023  527157 |
| 2357 | N[C@@H]1C[C@H] (N)[C@H]([C@@H]  ([C@H]1OCn1ccc(n1) C(F)(F)F)O)O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Neamine\_derivat ive\_29 | Target\_lig\_12 09 | 16s\_rRNA A SITE | Target\_3 | 3.35556141  053216 |
| 2358 | N[C@@H]1C[C@H] (N)[C@H]([C@@H]  ([C@H]1OCn1nccc1C( F)(F)F)O)O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Neamine\_derivat ive\_30 | Target\_lig\_12 10 | 16s\_rRNA A SITE | Target\_3 | 3.35556141  053216 |
| 2359 | N[C@@H]1C[C@H] (N)[C@H]([C@@H]  ([C@H]1OCn1cnc2c1n c[nH]c2=O)O)O | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Neamine\_derivat ive\_33 | Target\_lig\_12 11 | 16s\_rRNA A SITE | Target\_3 | 4 |
| 2361 | CNC1C(OC2OC(Cn3n  nc(c3)CCC(=O)Nc3ccc c(c3)c3csc(n3)NC(=O) C)C(C(C2O)O)N)OC2  C(C1O)OC(C(C2)N)O  C1C(N)CC(C(C1O)O) N | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Apramycin | Target\_lig\_77 2 | 16s\_rRNA A SITE | Target\_3 | 5.69897000  433602 |
| 2362 | C1C(C(C(C(C1N)OC2 C(C(C(C(O2)CO)O)N)  O)O)OC3C(C(C(C(O3) CN)O)O)N)N | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Bekanamycin | Target\_lig\_12 86 | 16s\_rRNA A SITE | Target\_3 | 5.69897000  433602 |
| 2364 | C1C(C(C(C(C1N)OC2 C(C(C(C(O2)CO)O)O)   1. OC3C(C(C(O3)CO)   OC4C(C(C(C(O4)CN)   1. O)N)O)O)N | GAGCGUCACACCUU CGGGUGAAGUCGCU C | Paromomycin | Target\_lig\_5 | 16s\_rRNA A SITE | Target\_3 | 6.95860731  484177 |