Training dataset curated from [R-SIM](https://web.iitm.ac.in/bioinfo2/R_SIM/) database for the “miRNA” 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** |
| 1060 | CCCN(CC(=O)N(CC C)CC(=O)N(CC(N)= O)CC1=CN(CCCNC(  =O)CCCOC2=C(C=C (C=C2C(C) (C)C)C2=NC3=CC(= CC=C3N2)N2CC[NH  +](C)CC2)C(C)  (C)C)N=N1)C(=O)CC COC1=CC=CC(=C1) C1=NC2=CC(=CC=C 2N1)C1=NC2=CC(=C C=C2N1)N1CC[NH+] (C)CC1 | GGGAGAGGGUUUA AUUACGAAAGUAA UUGGAUCCGCAAG G | Targaprimir-96 | Target\_lig\_62 7 | Pri-miR-96 RNAC (UU  loop mutant to AU basepair) | Target\_159 | 5.3979400086  7204 |
| 1061 | CCCN(CC(=O)N(CC C)CC(=O)N(CC(N)= O)CC1=CN(CCCNC(  =O)CCCOC2=C(C=C (C=C2C(C) (C)C)C2=NC3=CC(= CC=C3N2)N2CC[NH  +](C)CC2)C(C)  (C)C)N=N1)C(=O)CC COC1=CC=CC(=C1) C1=NC2=CC(=CC=C 2N1)C1=NC2=CC(=C C=C2N1)N1CC[NH+] (C)CC1 | GGGAGAGGGUUUA UUUACGAAAGUAU AUGGAUCCGCAAG G | Targaprimir-96 | Target\_lig\_62 7 | Pri-miR-96 RNA1 (Drosha processing site only) | Target\_160 | 5.9208187539  5238 |
| 1062 | CCCN(CC(=O)N(CC C)CC(=O)N(CC(N)= O)CC1=CN(CCCNC(  =O)CCCOC2=C(C=C (C=C2C(C) (C)C)C2=NC3=CC(= CC=C3N2)N2CC[NH  +](C)CC2)C(C)  (C)C)N=N1)C(=O)CC COC1=CC=CC(=C1) C1=NC2=CC(=CC=C 2N1)C1=NC2=CC(=C C=C2N1)N1CC[NH+] (C)CC1 | GGGAGAGGGUUUA CGAACGAAAGUUG GUGGAUCCGCAAG G | Targaprimir-96 | Target\_lig\_62 7 | Pri-miR-96 RNA2 (desired GG loop only) | Target\_161 | 6.0457574905  6068 |
| 1063 | CCCN(CC(=O)N(CC C)CC(=O)N(CC(N)= O)CC1=CN(CCCNC(  =O)CCCOC2=C(C=C (C=C2C(C) (C)C)C2=NC3=CC(= CC=C3N2)N2CC[NH  +](C)CC2)C(C)  (C)C)N=N1)C(=O)CC COC1=CC=CC(=C1) C1=NC2=CC(=CC=C 2N1)C1=NC2=CC(=C C=C2N1)N1CC[NH+] (C)CC1 | GGGAGAGGGUUUA CGAUUUACGAAAG UAUAUGGUGGAUC CGCAAGG | Targaprimir-96 | Target\_lig\_62 7 | Pri-miR-96 RNA3 (both the Drosha target site and adjacent target site) | Target\_162 | 4.6989700043  3602 |
| 1064 | CCCN(CC(=O)N(CC C)CC(=O)N(CC(N)= O)CC1=CN(CCCNC(  =O)CCCOC2=C(C=C (C=C2C(C) (C)C)C2=NC3=CC(= CC=C3N2)N2CC[NH  +](C)CC2)C(C)  (C)C)N=N1)C(=O)CC COC1=CC=CC(=C1) C1=NC2=CC(=CC=C 2N1)C1=NC2=CC(=C C=C2N1)N1CC[NH+] (C)CC1 | GGGAGAGGGUUUA CGAUUUACGAAAG UAUAUCGUGGAUC CGCAAGG | Targaprimir-96 | Target\_lig\_62 7 | Pri-miR-96 RNA4 (GG to  GC loop mutation) | Target\_163 | 5.9208187539  5238 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA\_ ID** | **pKd** |
| 1065 | CCCN(CC(=O)N(CC C)CC(=O)N(CC(N)= O)CC1=CN(CCCNC(  =O)CCCOC2=C(C=C (C=C2C(C) (C)C)C2=NC3=CC(= CC=C3N2)N2CC[NH  +](C)CC2)C(C)  (C)C)N=N1)C(=O)CC COC1=CC=CC(=C1) C1=NC2=CC(=CC=C 2N1)C1=NC2=CC(=C C=C2N1)N1CC[NH+] (C)CC1 | GGGAGAGGGUUUA CGAUUUACGAAAG UAAAUGGUGGAUC CGCAAGG | Targaprimir-96 | Target\_lig\_62 7 | Pri-miR-96 RNA5 (UU  loop mutant to UA loop) | Target\_164 | 5.8239087409  4432 |
| 1066 | CCCN(CC(=O)N(CC C)CC(=O)N(CC(N)= O)CC1=CN(CCCNC(  =O)CCCOC2=C(C=C (C=C2C(C) (C)C)C2=NC3=CC(= CC=C3N2)N2CC[NH  +](C)CC2)C(C)  (C)C)N=N1)C(=O)CC COC1=CC=CC(=C1) C1=NC2=CC(=CC=C 2N1)C1=NC2=CC(=C C=C2N1)N1CC[NH+] (C)CC1 | CGCGAATTCGCGTT TTCGCGAATTCGCG | Targaprimir-96 | Target\_lig\_62 7 | Pri-miR-96 AT- rich DNA hairpin | Target\_165 | 4.3010299956  6398 |
| 1190 | CC(C) (C)C1=CC(=CC(=C1 OCCCC(=O)NCCCN  =[N+]=[N-])C(C) (C)C)C2=NC3=C(N2) C=C(C=C3)N4CCN(C C4)C | UGGCCGAUUUUGG CACUAGCACAUUU UUGCUUGUGUCUC UCCGCUCUGAGCAA UCAUGUGCAGUGC CAAUAUGGGAAA | Benzimidazole 1  (2014) | Target\_lig\_67 8 | 5'UUU/3'AUA,  miR-96 Precursor Processing Site | Target\_202 | 5.8860566476  9316 |
| 1191 | CC(C) (C)C1=CC(=CC(=C1 OCCCC(=O)NCCCN  =[N+]=[N-])C(C) (C)C)C2=NC3=C(N2) C=C(C=C3)N4CCN(C C4)C | UGGCCGAUUUUGG CACUAGCACAUUU UUGCUUGUGUCUC UCCGCUCUGAGCAA UCAUGUGCAGUGC CAAUAUGGGAAA | Benzimidazole 1  (2014) | Target\_lig\_67 8 | 5'CGAUUU/  3'GGUAUA,  Expanded miR- 96 Precursor Processing Site | Target\_203 | 5.4685210829  5774 |
| 1271 | CN1CCN(CC1)C2=C C3=C(C=C2)N=C(N3  )C4=CC5=C(C=C4)N  =C(N5)C6=CC(=CC= C6)OCCCC(=O)NCC CN=[N+]=[N-] | AGCCCCUGCCCACC GCACACUGCGCUGC CCCAGACCCACUGU GCGUGUGACAGCG GCUGA | Targaprimir-210 | Target\_lig\_70 9 | Pre-miR-210 | Target\_227 | 6.1791420105  603 |
| 1331 | COC1=CC=C(C=C1) NCC(CN2C3=C(C=C( C=C3)Br)C4=C2C=C C(=C4)Br)O | GGGUUGACUGUUG AAUCUCAUGGCAA CCC | Aniline\_analog\_ 2 | Target\_lig\_72 6 | miR-21 hairpin | Target\_265 | 6.1549019599  8574 |
| 1332 | COC1=CC(=C(C=C1) NCC(CN2C3=C(C=C( C=C3)Br)C4=C2C=C C(=C4)Br)O)OC | GGGUUGACUGUUG AAUCUCAUGGCAA CCC | Aniline\_analog\_ 3 | Target\_lig\_72 7 | miR-21 hairpin | Target\_265 | 5.5228787452  8034 |
| 1333 | COC1=C(C=C(C=C1) NCC(CN2C3=C(C=C( C=C3)Br)C4=C2C=C C(=C4)Br)O)OC | GGGUUGACUGUUG AAUCUCAUGGCAA CCC | Aniline\_analog\_ 4 | Target\_lig\_72 8 | miR-21 hairpin | Target\_265 | 5.8538719643  2176 |
| 1334 | CCOc1ccc(cn1)NCC( Cn1c2ccc(cc2c2c1ccc( c2)Br)Br)O | GGGUUGACUGUUG AAUCUCAUGGCAA CCC | Aniline\_analog\_ 5 | Target\_lig\_72 9 | miR-21 hairpin | Target\_265 | 5.3187587626  2441 |
| 1335 | CCCOc1ccc(cc1)NCC (Cn1c2ccc(cc2c2c1ccc (c2)Br)Br)O | GGGUUGACUGUUG AAUCUCAUGGCAA CCC | Aniline\_analog\_ 6 | Target\_lig\_73 0 | miR-21 hairpin | Target\_265 | 5.6575773191  7779 |
| 1336 | OC(Cn1c2ccc(cc2c2c1 ccc(c2)Br)Br)CNc1ccc (cc1)N1CCOCC1 | GGGUUGACUGUUG AAUCUCAUGGCAA CCC | Aniline\_analog\_ 7 | Target\_lig\_73 1 | miR-21 hairpin | Target\_265 | 5.6777807052  6608 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA\_ ID** | **pKd** |
| 1338 | CCOc1ccc(cc1Cl)NC C(Cn1c2ccc(cc2c2c1c cc(c2)Br)Br)O | GGGUUGACUGUUG AAUCUCAUGGCAA CCC | Aniline\_analog\_ 9 | Target\_lig\_73 3 | miR-21 hairpin | Target\_265 | 5.5376020021  0104 |
| 1339 | C1=CC=C(C=C1)NC C(CN2C3=C(C=C(C= C3)Br)C4=C2C=CC(= C4)Br)O | GGGUUGACUGUUG AAUCUCAUGGCAA CCC | Aniline\_analog\_ 10 | Target\_lig\_73 4 | miR-21 hairpin | Target\_265 | 5.6777807052  6608 |
| 1342 | CCOC1=CC=C(C=C1  )NCC(CN2C3=C(C=C (C=C3)Br)C4=C2C=C C(=C4)Br)O | GGGUUGACUGUUG AAUCUCAUGGCAA CCC | Aniline\_analog\_ 13 | Target\_lig\_73 7 | miR-21 hairpin | Target\_265 | 5.9208187539  5238 |
| 1350 | CCOC1=CC=C(C=C1  )NCC(CN2C3=C(C=C (C=C3)Cl)C4=C2C=C C(=C4)Cl)O | GGGUUGACUGUUG AAUCUCAUGGCAA CCC | Carbazole\_analo g\_23 | Target\_lig\_74 5 | miR-21 hairpin | Target\_265 | 5.4948500216  8009 |
| 1351 | CCOc1ccc(cc1)NCC( Cn1c2ccc(cc2c(c1C)C  )Br)O | GGGUUGACUGUUG AAUCUCAUGGCAA CCC | Carbazole\_analo g\_24 | Target\_lig\_74 6 | miR-21 hairpin | Target\_265 | 5 |
| 1352 | CCOc1ccc(cc1)NCC( CN(c1ccc(cc1)Br)c1cc c(cc1)Br)O | GGGUUGACUGUUG AAUCUCAUGGCAA CCC | Carbazole\_analo g\_25 | Target\_lig\_74 7 | miR-21 hairpin | Target\_265 | 5.6382721639  8241 |
| 1355 | CC1=CC=CC=C1NC C(CN2C3=C(C=C(C= C3)Br)C4=C2C=CC(= C4)Br)O | GGGUUGACUGUUG AAUCUCAUGGCAA CCC | Aniline\_analog\_ 1 | Target\_lig\_72 5 | miR-21 hairpin | Target\_265 | 5.6382721639  8241 |
| 1362 | CC1=C(C=CC=C1Cl) NCC(CN2C3=C(C=C( C=C3)Br)C4=C2C=C C(=C4)Br)O | GGGUUGACUGUUG AAUCUCAUGGCAA CCC | Aniline\_analog\_ 8 | Target\_lig\_73 2 | miR-21 hairpin | Target\_265 | 5.4948500216  8009 |
| 1365 | C1=CC(=CC(=C1)Cl) NCC(CN2C3=C(C=C( C=C3)Br)C4=C2C=C C(=C4)Br)O | GGGUUGACUGUUG AAUCUCAUGGCAA CCC | Aniline\_analog\_ 11 | Target\_lig\_73 5 | miR-21 hairpin | Target\_265 | 5.9208187539  5238 |
| 1366 | OC(Cn1c2ccc(cc2c2c1 ccc(c2)Br)Br)CNc1ccc 2c(c1)cccc2 | GGGUUGACUGUUG AAUCUCAUGGCAA CCC | Aniline\_analog\_ 12 | Target\_lig\_73 6 | miR-21 hairpin | Target\_265 | 6.0969100130  0806 |
| 1368 | CC1=CC(=C(C=C1)N CC(CN2C3=C(C=C(C  =C3)Br)C4=C2C=CC(  =C4)Br)O)C | GGGUUGACUGUUG AAUCUCAUGGCAA CCC | Aniline\_analog\_ 14 | Target\_lig\_73 8 | miR-21 hairpin | Target\_265 | 5.2924298239  0206 |
| 1369 | C1=CC=C(C=C1)NC C(CN2C3=CC=CC=C 3C4=CC=CC=C42)O | GGGUUGACUGUUG AAUCUCAUGGCAA CCC | Carbazole\_analo g\_17 | Target\_lig\_73 9 | miR-21 hairpin | Target\_265 | 5.0809219076  2393 |
| 1370 | CCOC1=CC=C(C=C1  )NCC(CN2C3=C(C=C (C=C3)Br)C4=CC=C C=C42)O | GGGUUGACUGUUG AAUCUCAUGGCAA CCC | Carbazole\_analo g\_18 | Target\_lig\_74 0 | miR-21 hairpin | Target\_265 | 5.6989700043  3602 |
| 1371 | OC(Cn1c2ccc(cc2c2c1 cccc2)Br)CNc1ccc(cc 1)N1CCOCC1 | GGGUUGACUGUUG AAUCUCAUGGCAA CCC | Carbazole\_analo g\_19 | Target\_lig\_74 1 | miR-21 hairpin | Target\_265 | 5.4948500216  8009 |
| 1372 | CCOc1ccc(cc1)NCC( Cn1c2cc(Br)ccc2c2c1 cc(Br)cc2)O | GGGUUGACUGUUG AAUCUCAUGGCAA CCC | Carbazole\_analo g\_20 | Target\_lig\_74 2 | miR-21 hairpin | Target\_265 | 6 |
| 1373 | OC(Cn1c2cc(Br)ccc2c 2c1cc(Br)cc2)CNc1cc c(cc1)N1CCOCC1 | GGGUUGACUGUUG AAUCUCAUGGCAA CCC | Carbazole\_analo g\_21 | Target\_lig\_74 3 | miR-21 hairpin | Target\_265 | 5.6777807052  6608 |
| 1374 | OC(Cn1c2cc(Br)ccc2c 2c1cc(Br)cc2)CNc1cc ccc1C | GGGUUGACUGUUG AAUCUCAUGGCAA CCC | Carbazole\_analo g\_22 | Target\_lig\_74 4 | miR-21 hairpin | Target\_265 | 5.5686362358  4101 |
| 1378 | OC(CN(c1ccc(cc1)Br) c1ccc(cc1)Br)CNc1cc c(cc1)N1CCOCC1 | GGGUUGACUGUUG AAUCUCAUGGCAA CCC | Carbazole\_analo g\_26 | Target\_lig\_74 8 | miR-21 hairpin | Target\_265 | 5.4436974992  3271 |
| 1379 | OC(CN(c1ccc(cc1)Br) c1ccc(cc1)Br)CNc1cc | GGGUUGACUGUUG AAUCUCAUGGCAA | Carbazole\_analo g\_27 | Target\_lig\_74 9 | miR-21 hairpin | Target\_265 | 5.3565473235  1381 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA\_ ID** | **pKd** |
|  | ccc1C | CCC |  |  |  |  |  |
| 1380 | CNC(=O)C1=NC=CC (=C1)OC2=CC(=C(C  =C2)NC(=O)NC3=CC (=C(C=C3)Cl)C(F) (F)F)F | GGGUUGACUGUUG AAUCUCAUGGCAA CCC | Regorafenib | Target\_lig\_75 0 | miR-21 hairpin | Target\_265 | 6.1366771398  7954 |
| 1381 | C1C(C(C(C(C1N)OC2 C(C(C(C(O2)CN)O)O  )N)OC3C(C(C(O3)CO  )OC4C(C(C(C(O4)CN  )O)O)N)O)O)N | GUGGGCCUCAAAU GUGGAGCACUAUU CUGAUGUCCAAGU GGAAAGUGCUGCG ACAUUUGAGCGUC AC | Neomycin | Target\_lig\_4 | Pre-miR-372 | Target\_266 | 2.1307682802  6902 |
| 1382 | NCC1OC(OC2C(Cn3  nnc(c3)Cn3cnc4c3ncn c4N)OC(C2O)OC2C( O)C(N)CC(C2OC2OC (CN)C(C(C2N)O)O)N  )C(C(C1O)O)N | GUGGGCCUCAAAU GUGGAGCACUAUU CUGAUGUCCAAGU GGAAAGUGCUGCG ACAUUUGAGCGUC AC | Neomycin\_nucl eobase\_3a | Target\_lig\_75 1 | Pre-miR-372 | Target\_266 | 3.3142582613  9774 |
| 1383 | NCC1OC(OC2C(Cn3  nnc(c3)Cn3ccc(=O) [nH]c3=O)OC(C2O)O C2C(O)C(N)CC(C2O  C2OC(CN)C(C(C2N)  O)O)N)C(C(C1O)O)N | GUGGGCCUCAAAU GUGGAGCACUAUU CUGAUGUCCAAGU GGAAAGUGCUGCG ACAUUUGAGCGUC AC | Neomycin\_nucl eobase\_3b | Target\_lig\_75 2 | Pre-miR-372 | Target\_266 | 2.9788107009  3006 |
| 1384 | NCC1OC(OC2C(Cn3  nnc(c3)Cn3ccc(nc3=O  )N)OC(C2O)OC2C(O) C(N)CC(C2OC2OC(C N)C(C(C2N)O)O)N)C (C(C1O)O)N | GUGGGCCUCAAAU GUGGAGCACUAUU CUGAUGUCCAAGU GGAAAGUGCUGCG ACAUUUGAGCGUC AC | Neomycin\_nucl eobase\_3c | Target\_lig\_75 3 | Pre-miR-372 | Target\_266 | 3.2240256688  7063 |
| 1385 | NCC1OC(OC2C(Cn3  nnc(c3)Cn3cnc4c3[nH  ]c(N)nc4=O)OC(C2O)  OC2C(O)C(N)CC(C2 OC2OC(CN)C(C(C2N  )O)O)N)C(C(C1O)O) N | GUGGGCCUCAAAU GUGGAGCACUAUU CUGAUGUCCAAGU GGAAAGUGCUGCG ACAUUUGAGCGUC AC | Neomycin\_nucl eobase\_3d | Target\_lig\_75 4 | Pre-miR-372 | Target\_266 | 3.8386319977  6503 |
| 1386 | NCC1OC(OC2C(Cn3 nnc(c3)CCCC(=O)Nc  3cccc(c3)c3ncc(s3)NC (=O)C)OC(C2O)OC2  C(O)C(N)CC(C2OC2  OC(CN)C(C(C2N)O)  O)N)C(C(C1O)O)N | GUGGGCCUCAAAU GUGGAGCACUAUU CUGAUGUCCAAGU GGAAAGUGCUGCG ACAUUUGAGCGUC AC | Neomycin\_nucl eobase\_3e | Target\_lig\_75 5 | Pre-miR-372 | Target\_266 | 4.7958800173  4408 |
| 1387 | NCC1OC(OC2C(Cn3  nnc(c3)Cc3nc4c(o3)cc c(c4)NC(=O)Nc3ccccc 3)OC(C2O)OC2C(O) C(N)CC(C2OC2OC(C N)C(C(C2N)O)O)N)C (C(C1O)O)N | GUGGGCCUCAAAU GUGGAGCACUAUU CUGAUGUCCAAGU GGAAAGUGCUGCG ACAUUUGAGCGUC AC | Neomycin\_nucl eobase\_3f | Target\_lig\_75 6 | Pre-miR-372 | Target\_266 | 4.8569851997  4591 |
| 1388 | CCCCNC(=O)Nc1ccc  2c(c1)nc(o2)Cc1nnn(c 1)CC1OC(C(C1OC1O C(CN)C(C(C1N)O)O)  O)OC1C(O)C(N)CC( C1OC1OC(CN)C(C(C 1N)O)O)N | GUGGGCCUCAAAU GUGGAGCACUAUU CUGAUGUCCAAGU GGAAAGUGCUGCG ACAUUUGAGCGUC AC | Neomycin\_nucl eobase\_3g | Target\_lig\_75 7 | Pre-miR-372 | Target\_266 | 4.7055337738  3841 |
| 1389 | NCC1OC(OC2C(Cn3  nnc(c3)Cn3cnc(c3)c3c ccc(c3)NC(=O)c3cccc c3)OC(C2O)OC2C(O) C(N)CC(C2OC2OC(C N)C(C(C2N)O)O)N)C (C(C1O)O)N | GUGGGCCUCAAAU GUGGAGCACUAUU CUGAUGUCCAAGU GGAAAGUGCUGCG ACAUUUGAGCGUC AC | Neomycin\_nucl eobase\_3h | Target\_lig\_75 8 | Pre-miR-372 | Target\_266 | 4.7235381958  2676 |
| 1390 | CCCCNC(=O)Nc1ccc  c(c1)c1ncn(c1)Cc1nnn (c1)CC1OC(C(C1OC1 | GUGGGCCUCAAAU GUGGAGCACUAUU CUGAUGUCCAAGU | Neomycin\_nucl eobase\_3i | Target\_lig\_75 9 | Pre-miR-372 | Target\_266 | 4.3362990746  1035 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA\_ ID** | **pKd** |
|  | OC(CN)C(C(C1N)O)  O)O)OC1C(O)C(N)C C(C1OC1OC(CN)C(C (C1N)O)O)N | GGAAAGUGCUGCG ACAUUUGAGCGUC AC |  |  |  |  |  |
| 1391 | NCC1OC(OC2C(Cn3 nnc(c3)CCC(=O)NCC  (=O)Nc3nc4c([nH]3)c ccc4)OC(C2O)OC2C( O)C(N)CC(C2OC2OC (CN)C(C(C2N)O)O)N  )C(C(C1O)O)N | GUGGGCCUCAAAU GUGGAGCACUAUU CUGAUGUCCAAGU GGAAAGUGCUGCG ACAUUUGAGCGUC AC | Neomycin\_nucl eobase\_3j | Target\_lig\_76 0 | Pre-miR-372 | Target\_266 | 4.8297382846  0504 |
| 1392 | NCC1OC(OC2C(Cn3  nnc(c3)CCC(=O)Nc3c ccc(c3)c3csc(n3)NC(= O)C)OC(C2O)OC2C( O)C(N)CC(C2OC2OC (CN)C(C(C2N)O)O)N  )C(C(C1O)O)N | GUGGGCCUCAAAU GUGGAGCACUAUU CUGAUGUCCAAGU GGAAAGUGCUGCG ACAUUUGAGCGUC AC | Neomycin-S | Target\_lig\_76 1 | Pre-miR-372 | Target\_266 | 4.7958800173  4408 |
| 1393 | NCC1OC(OC2C(Cn3  nnc(c3)CCC(=O)Nc3c ccc(c3)c3csc(n3)NC(= O)c3ccc(cc3)C)OC(C2 O)OC2C(O)C(N)CC( C2OC2OC(CN)C(C(C 2N)O)O)N)C(C(C1O) O)N | GUGGGCCUCAAAU GUGGAGCACUAUU CUGAUGUCCAAGU GGAAAGUGCUGCG ACAUUUGAGCGUC AC | Neomycin-3a | Target\_lig\_76 2 | Pre-miR-372 | Target\_266 | 4.2798406965  9404 |
| 1394 | NCC1OC(OC2C(Cn3  nnc(c3)CCC(=O)Nc3c ccc(c3)c3csc(n3)NC(= O)c3ccc(cc3)Cl)OC(C 2O)OC2C(O)C(N)CC( C2OC2OC(CN)C(C(C 2N)O)O)N)C(C(C1O) O)N | GUGGGCCUCAAAU GUGGAGCACUAUU CUGAUGUCCAAGU GGAAAGUGCUGCG ACAUUUGAGCGUC AC | Neomycin-3b | Target\_lig\_76 3 | Pre-miR-372 | Target\_266 | 4.3001622741  3275 |
| 1395 | NCC1OC(OC2C(Cn3  nnc(c3)CCC(=O)Nc3c ccc(c3)c3csc(n3)NC(= O)c3ccc(cc3)F)OC(C2 O)OC2C(O)C(N)CC( C2OC2OC(CN)C(C(C 2N)O)O)N)C(C(C1O) O)N | GUGGGCCUCAAAU GUGGAGCACUAUU CUGAUGUCCAAGU GGAAAGUGCUGCG ACAUUUGAGCGUC AC | Neomycin-3c | Target\_lig\_76 4 | Pre-miR-372 | Target\_266 | 4.6478174818  8864 |
| 1396 | NCC1OC(OC2C(Cn3  nnc(c3)CCC(=O)Nc3c ccc(c3)c3csc(n3)NC(= O)c3ccc(cc3)N)OC(C 2O)OC2C(O)C(N)CC( C2OC2OC(CN)C(C(C 2N)O)O)N)C(C(C1O) O)N | GUGGGCCUCAAAU GUGGAGCACUAUU CUGAUGUCCAAGU GGAAAGUGCUGCG ACAUUUGAGCGUC AC | Neomycin-3d | Target\_lig\_76 5 | Pre-miR-372 | Target\_266 | 4.5686362358  4101 |
| 1397 | NCC1OC(OC2C(Cn3 nnc(c3)CCCCC(=O)N  c3cccc(c3)c3csc(n3)N C(=O)C)OC(C2O)OC  2C(O)C(N)CC(C2OC  2OC(CN)C(C(C2N)O)  O)N)C(C(C1O)O)N | GUGGGCCUCAAAU GUGGAGCACUAUU CUGAUGUCCAAGU GGAAAGUGCUGCG ACAUUUGAGCGUC AC | Neomycin-4a | Target\_lig\_76 6 | Pre-miR-372 | Target\_266 | 4.5606673061  6974 |
| 1398 | NCC1OC(OC2C(Cn3 nnc(c3)CCCCCC(=O)  Nc3cccc(c3)c3csc(n3) NC(=O)C)OC(C2O)O  C2C(O)C(N)CC(C2O  C2OC(CN)C(C(C2N)  O)O)N)C(C(C1O)O)N | GUGGGCCUCAAAU GUGGAGCACUAUU CUGAUGUCCAAGU GGAAAGUGCUGCG ACAUUUGAGCGUC AC | Neomycin-4b | Target\_lig\_76 7 | Pre-miR-372 | Target\_266 | 4.5867002359  1875 |
| 1399 | NCC1OC(OC2C(Cn3  nnc(c3)c3ccc(cc3)C(= O)Nc3cccc(c3)c3csc(n 3)NC(=O)C)OC(C2O)  OC2C(O)C(N)CC(C2 | GUGGGCCUCAAAU GUGGAGCACUAUU CUGAUGUCCAAGU GGAAAGUGCUGCG ACAUUUGAGCGUC | Neomycin-4c | Target\_lig\_76 8 | Pre-miR-372 | Target\_266 | 4.4710832997  2235 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA\_ ID** | **pKd** |
|  | OC2OC(CN)C(C(C2N  )O)O)N)C(C(C1O)O) N | AC |  |  |  |  |  |
| 1400 | NCC1OC(OC2C(Cn3  nnc(c3)c3cccc(c3)C(= O)Nc3cccc(c3)c3csc(n 3)NC(=O)C)OC(C2O)  OC2C(O)C(N)CC(C2 OC2OC(CN)C(C(C2N  )O)O)N)C(C(C1O)O) N | GUGGGCCUCAAAU GUGGAGCACUAUU CUGAUGUCCAAGU GGAAAGUGCUGCG ACAUUUGAGCGUC AC | Neomycin-4d | Target\_lig\_76 9 | Pre-miR-372 | Target\_266 | 4.3925449767  8533 |
| 1401 | NCC1OC(OC2C(Cn3  nnc(c3)Oc3ccc(cc3)C(  =O)Nc3cccc(c3)c3csc( n3)NC(=O)C)OC(C2  O)OC2C(O)C(N)CC( C2OC2OC(CN)C(C(C 2N)O)O)N)C(C(C1O) O)N | GUGGGCCUCAAAU GUGGAGCACUAUU CUGAUGUCCAAGU GGAAAGUGCUGCG ACAUUUGAGCGUC AC | Neomycin-4e | Target\_lig\_77 0 | Pre-miR-372 | Target\_266 | 4.4907974776  689 |
| 1402 | NCC1OC(OC2C(Cn3  nnc(c3)Oc3cccc(c3)C(  =O)Nc3cccc(c3)c3csc( n3)NC(=O)C)OC(C2  O)OC2C(O)C(N)CC( C2OC2OC(CN)C(C(C 2N)O)O)N)C(C(C1O) O)N | GUGGGCCUCAAAU GUGGAGCACUAUU CUGAUGUCCAAGU GGAAAGUGCUGCG ACAUUUGAGCGUC AC | Neomycin-4f | Target\_lig\_77 1 | Pre-miR-372 | Target\_266 | 4.6307841425  8986 |
| 1403 | CNC1C(OC2OC(Cn3  nnc(c3)CCC(=O)Nc3c ccc(c3)c3csc(n3)NC(= O)C)C(C(C2O)O)N)O  C2C(C1O)OC(C(C2)  N)OC1C(N)CC(C(C1 O)O)N | GUGGGCCUCAAAU GUGGAGCACUAUU CUGAUGUCCAAGU GGAAAGUGCUGCG ACAUUUGAGCGUC AC | Apramycin-6a | Target\_lig\_77 2 | Pre-miR-372 | Target\_266 | 3.6819366650  3724 |
| 1404 | NCC1OC(OC2C(N)C C(C(C2O)O)N)C(C(C 1OCn1nnc(c1)CC(=O)  Nc1cccc(c1)c1csc(n1) NC(=O)C)O)N | GUGGGCCUCAAAU GUGGAGCACUAUU CUGAUGUCCAAGU GGAAAGUGCUGCG ACAUUUGAGCGUC AC | Neamine-6b | Target\_lig\_77 3 | Pre-miR-372 | Target\_266 | 3.4948500216  8009 |
| 1405 | O=C(Cc1nnn(c1)COC 1C(N)CC(C(C1O)O)N  )Nc1cccc(c1)c1csc(n1) NC(=O)C | GUGGGCCUCAAAU GUGGAGCACUAUU CUGAUGUCCAAGU GGAAAGUGCUGCG ACAUUUGAGCGUC AC | 2-DOS-6c | Target\_lig\_77 4 | Pre-miR-372 | Target\_266 | 3.1687703061  3294 |
| 1406 | NCC1OC(OC2C(Cn3  nnc(c3)CCC(=O)Nc3c ccc(c3)c3csc(n3)NC(= O)C)OC(C2O)OC2C( O)C(N)CC(C2OC2OC (CN)C(C(C2N)O)O)N  )C(C(C1O)O)N | GGGAUACUCAAAA UGGGGGCGCUUUC CUUUUUGUCUGUA CUGGGAAGUGCUU CGAUUUUGGGGUG UCCC | Neomycin-S | Target\_lig\_76 1 | Pre-miR-373 | Target\_267 | 4.9507819773  2982 |
| 1407 | NCC1OC(OC2C(Cn3  nnc(c3)CCC(=O)Nc3c ccc(c3)c3csc(n3)NC(= O)c3ccc(cc3)C)OC(C2 O)OC2C(O)C(N)CC( C2OC2OC(CN)C(C(C 2N)O)O)N)C(C(C1O) O)N | GGGAUACUCAAAA UGGGGGCGCUUUC CUUUUUGUCUGUA CUGGGAAGUGCUU CGAUUUUGGGGUG UCCC | Neomycin-3a | Target\_lig\_76 2 | Pre-miR-373 | Target\_267 | 4.3665315444  2041 |
| 1408 | NCC1OC(OC2C(Cn3  nnc(c3)CCC(=O)Nc3c ccc(c3)c3csc(n3)NC(= O)c3ccc(cc3)Cl)OC(C 2O)OC2C(O)C(N)CC( C2OC2OC(CN)C(C(C 2N)O)O)N)C(C(C1O) O)N | GGGAUACUCAAAA UGGGGGCGCUUUC CUUUUUGUCUGUA CUGGGAAGUGCUU CGAUUUUGGGGUG UCCC | Neomycin-3b | Target\_lig\_76 3 | Pre-miR-373 | Target\_267 | 4.4596705252  0913 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA\_ ID** | **pKd** |
| 1409 | NCC1OC(OC2C(Cn3  nnc(c3)CCC(=O)Nc3c ccc(c3)c3csc(n3)NC(= O)c3ccc(cc3)F)OC(C2 O)OC2C(O)C(N)CC( C2OC2OC(CN)C(C(C 2N)O)O)N)C(C(C1O) O)N | GGGAUACUCAAAA UGGGGGCGCUUUC CUUUUUGUCUGUA CUGGGAAGUGCUU CGAUUUUGGGGUG UCCC | Neomycin-3c | Target\_lig\_76 4 | Pre-miR-373 | Target\_267 | 4.4723700991  2866 |
| 1410 | NCC1OC(OC2C(Cn3  nnc(c3)CCC(=O)Nc3c ccc(c3)c3csc(n3)NC(= O)c3ccc(cc3)N)OC(C 2O)OC2C(O)C(N)CC( C2OC2OC(CN)C(C(C 2N)O)O)N)C(C(C1O) O)N | GGGAUACUCAAAA UGGGGGCGCUUUC CUUUUUGUCUGUA CUGGGAAGUGCUU CGAUUUUGGGGUG UCCC | Neomycin-3d | Target\_lig\_76 5 | Pre-miR-373 | Target\_267 | 4.3233063903  7513 |
| 1411 | NCC1OC(OC2C(Cn3 nnc(c3)CCCCC(=O)N  c3cccc(c3)c3csc(n3)N C(=O)C)OC(C2O)OC  2C(O)C(N)CC(C2OC  2OC(CN)C(C(C2N)O)  O)N)C(C(C1O)O)N | GGGAUACUCAAAA UGGGGGCGCUUUC CUUUUUGUCUGUA CUGGGAAGUGCUU CGAUUUUGGGGUG UCCC | Neomycin-4a | Target\_lig\_76 6 | Pre-miR-373 | Target\_267 | 4.6363880201  0786 |
| 1412 | NCC1OC(OC2C(Cn3 nnc(c3)CCCCCC(=O)  Nc3cccc(c3)c3csc(n3) NC(=O)C)OC(C2O)O  C2C(O)C(N)CC(C2O  C2OC(CN)C(C(C2N)  O)O)N)C(C(C1O)O)N | GGGAUACUCAAAA UGGGGGCGCUUUC CUUUUUGUCUGUA CUGGGAAGUGCUU CGAUUUUGGGGUG UCCC | Neomycin-4b | Target\_lig\_76 7 | Pre-miR-373 | Target\_267 | 4.3746875490  3833 |
| 1413 | NCC1OC(OC2C(Cn3  nnc(c3)c3ccc(cc3)C(= O)Nc3cccc(c3)c3csc(n 3)NC(=O)C)OC(C2O)  OC2C(O)C(N)CC(C2 OC2OC(CN)C(C(C2N  )O)O)N)C(C(C1O)O) N | GGGAUACUCAAAA UGGGGGCGCUUUC CUUUUUGUCUGUA CUGGGAAGUGCUU CGAUUUUGGGGUG UCCC | Neomycin-4c | Target\_lig\_76 8 | Pre-miR-373 | Target\_267 | 4.4762535331  8844 |
| 1414 | NCC1OC(OC2C(Cn3  nnc(c3)c3cccc(c3)C(= O)Nc3cccc(c3)c3csc(n 3)NC(=O)C)OC(C2O)  OC2C(O)C(N)CC(C2 OC2OC(CN)C(C(C2N  )O)O)N)C(C(C1O)O) N | GGGAUACUCAAAA UGGGGGCGCUUUC CUUUUUGUCUGUA CUGGGAAGUGCUU CGAUUUUGGGGUG UCCC | Neomycin-4d | Target\_lig\_76 9 | Pre-miR-373 | Target\_267 | 4.4634415574  2847 |
| 1415 | NCC1OC(OC2C(Cn3  nnc(c3)Oc3ccc(cc3)C(  =O)Nc3cccc(c3)c3csc( n3)NC(=O)C)OC(C2  O)OC2C(O)C(N)CC( C2OC2OC(CN)C(C(C 2N)O)O)N)C(C(C1O) O)N | GGGAUACUCAAAA UGGGGGCGCUUUC CUUUUUGUCUGUA CUGGGAAGUGCUU CGAUUUUGGGGUG UCCC | Neomycin-4e | Target\_lig\_77 0 | Pre-miR-373 | Target\_267 | 4.4248121550  7234 |
| 1416 | NCC1OC(OC2C(Cn3  nnc(c3)Oc3cccc(c3)C(  =O)Nc3cccc(c3)c3csc( n3)NC(=O)C)OC(C2  O)OC2C(O)C(N)CC( C2OC2OC(CN)C(C(C 2N)O)O)N)C(C(C1O) O)N | GGGAUACUCAAAA UGGGGGCGCUUUC CUUUUUGUCUGUA CUGGGAAGUGCUU CGAUUUUGGGGUG UCCC | Neomycin-4f | Target\_lig\_77 1 | Pre-miR-373 | Target\_267 | 4.4736607226  1016 |
| 1417 | CNC1C(OC2OC(Cn3  nnc(c3)CCC(=O)Nc3c ccc(c3)c3csc(n3)NC(= O)C)C(C(C2O)O)N)O  C2C(C1O)OC(C(C2)  N)OC1C(N)CC(C(C1 O)O)N | GGGAUACUCAAAA UGGGGGCGCUUUC CUUUUUGUCUGUA CUGGGAAGUGCUU CGAUUUUGGGGUG UCCC | Apramycin-6a | Target\_lig\_77 2 | Pre-miR-373 | Target\_267 | 3.9956786262  1736 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA\_ ID** | **pKd** |
| 1418 | NCC1OC(OC2C(N)C C(C(C2O)O)N)C(C(C 1OCn1nnc(c1)CC(=O)  Nc1cccc(c1)c1csc(n1) NC(=O)C)O)N | GGGAUACUCAAAA UGGGGGCGCUUUC CUUUUUGUCUGUA CUGGGAAGUGCUU CGAUUUUGGGGUG UCCC | Neamine-6b | Target\_lig\_77 3 | Pre-miR-373 | Target\_267 | 3.9746941347  3523 |
| 1419 | O=C(Cc1nnn(c1)COC 1C(N)CC(C(C1O)O)N  )Nc1cccc(c1)c1csc(n1) NC(=O)C | GGGAUACUCAAAA UGGGGGCGCUUUC CUUUUUGUCUGUA CUGGGAAGUGCUU CGAUUUUGGGGUG UCCC | 2-DOS-6c | Target\_lig\_77 4 | Pre-miR-373 | Target\_267 | 2.5030703519  2679 |
| 1420 | CC1(C(C2=CC=CC= C2NC1=NCCCNCCC CNCCCN)N(C)C3=C C=CC=C3)C | GUGGGCCUCAAAU GUGGAGCACUAUU CUGAUGUCCAAGU GGAAAGUGCUGCG ACAUUUGAGCGUC AC | PA-1 | Target\_lig\_77 5 | Pre-miR-372 | Target\_266 | 6.8239087409  4432 |
| 1421 | C(CCNCCCCNCCCC N)CN | GUGGGCCUCAAAU GUGGAGCACUAUU CUGAUGUCCAAGU GGAAAGUGCUGCG ACAUUUGAGCGUC AC | PA-2 | Target\_lig\_77 6 | Pre-miR-372 | Target\_266 | 6.2757241303  9921 |
| 1422 | NCCCCN/C(=C/1\ C(=O)C=C2C(C1=O) (C)c1c(O)c(C)c(c(c1O 2)C(=O)C)O)/C | GUGGGCCUCAAAU GUGGAGCACUAUU CUGAUGUCCAAGU GGAAAGUGCUGCG ACAUUUGAGCGUC AC | PA-3 | Target\_lig\_77 7 | Pre-miR-372 | Target\_266 | 5.9393021596  4639 |
| 1423 | CN1CCN(CC1)C2=C C3=C(C=C2)N=C(N3  )C4=CC5=C(C=C4)N  =C(N5)C6=CC(=CC= C6)OCCCC(=O)NCC CN=[N+]=[N-] | AGCCCCUGCCCACC GCACACUGCGCUGC CCCAGACCCACUGU GCGUGUGACAGCG GCUGA | Targapremir-210 | Target\_lig\_12 62 | Pre-miR-210 | Target\_227 | 6.7958800173  4408 |
| 1424 | CN1CCN(CC1)C2=C C3=C(C=C2)N=C(N3  )C4=CC5=C(C=C4)N  =C(N5)C6=CC(=CC= C6)OCCCC(=O)NCC CN=[N+]=[N-] | AGCCCCUGCCCACC GCACACUGCGCUGC CCCAGACCCACUGU GCGUGUGACAGCG GCUGA | Targapremir- 210-RL | Target\_lig\_12 63 | Pre-miR-210 | Target\_227 | 6.7212463990  4717 |
| 1425 | N=[N+]=NCCCNC(=  O)CCCOc1c(cc(cc1C( C)  (C)C)c1nc2c([nH]1)cc  c(c2)c1nc2c([nH]1)cc( cc2)N1CCN(CC1)C)C (C)(C)C | GGGAGAGGGUUUA AUUCUUACGAAAG UAAUAAUUGGAUC CGCAAGG | Targapremir- 515/885 | Target\_lig\_77 8 | Pri-miR-515 drosha site (RNA 1) | Target\_268 | 5.0457574905  6068 |
| 1426 | N=[N+]=NCCCNC(=  O)CCCOc1c(cc(cc1C( C)  (C)C)c1nc2c([nH]1)cc  c(c2)c1nc2c([nH]1)cc( cc2)N1CCN(CC1)C)C (C)(C)C | GGGAGAGGGUUUA AUUUCUACGAAAG UAGCGAUUGGAUC CGCAAGG | Targapremir- 515/885 | Target\_lig\_77 8 | Pri-miR-885 drosha site (RNA 2) | Target\_269 | 4.9208187539  5238 |
| 1427 | N=[N+]=NCCCNC(=  O)CCCOc1c(cc(cc1C( C)  (C)C)c1nc2c([nH]1)cc  c(c2)c1nc2c([nH]1)cc( cc2)N1CCN(CC1)C)C (C)(C)C | GGGAGAGGGUUUA AUUCAUACGAAAG UAUUAAUUGGAUC CGCAAGG | Targapremir- 515/885 | Target\_lig\_77 8 | Pri-miR-515 (RNA 3) | Target\_270 | 5.1249387366  083 |
| 1432 | N=[N+]=NCCCNC(=  O)CCCOc1c(cc(cc1C( C)  (C)C)c1nc2c([nH]1)cc  c(c2)c1nc2c([nH]1)cc( cc2)N1CCN(CC1)C)C | GGGAGAGGGUUUA AUUCAUUCUACGA AAGUAGCGUUAAU UGGAUCCGCAAGG | Targapremir-515 | Target\_lig\_77 8 | Pri-miR-515 and the adjacent RNA motif (RNA 4) | Target\_271 | 7.2218487496  1636 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA\_ ID** | **pKd** |
|  | (C)(C)C |  |  |  |  |  |  |
| 1433 | CCCN(C(=O)CN(C(= O)CNCc1nnn(c1)N=[ N+]=N)CCC)CC(=O)  N(CC(=O)N(CC(=O)  N(CC(=O)N)CCC)CC C)CCC | GGGAGAGGGUUUA AUUCAUUCUACGA AAGUAGCGUUAAU UGGAUCCGCAAGG | Compound 1a | Target\_lig\_78 0 | Pri-miR-515 and the adjacent RNA motif (RNA 4) | Target\_271 | 4.7447274948  9669 |
| 1434 | CCCN(C(=O)CNCc1n  nn(c1)N=[N+]=Nn1nn c(c1)CO)CC(=O)N(C  C(=O)N(CC(=O)N(C  C(=O)N(CC(=O)N)C CC)CCC)CCC)CCC | GGGAGAGGGUUUA AUUCAUUCUACGA AAGUAGCGUUAAU UGGAUCCGCAAGG | Compound 1b | Target\_lig\_78 1 | Pri-miR-515 and the adjacent RNA motif (RNA 4) | Target\_271 | 4.6989700043  3602 |
| 1576 | C1C(C(C(C(C1N)OC2 C(C(C(C(O2)CN)O)O  )N)OC3C(C(C(O3)CO  )OC4C(C(C(C(O4)CN  )O)O)N)O)O)N | CCGACUGAUGUUG ACUGUUGAAUCUC AUGGCAACACCAG UCGG | Neomycin | Target\_lig\_4 | Oligonucleotide 3 | Target\_282 | 5.3979400086  7204 |
| 1577 | CC1(COC(C(C1NC)O  )OC2C(CC(C(C2O)O C3C(CC=C(O3)CN)N  )N)N)O | CCGACUGAUGUUG ACUGUUGAAUCUC AUGGCAACACCAG UCGG | Sisomycin | Target\_lig\_12 69 | Oligonucleotide 3 | Target\_282 | 5.3979400086  7204 |
| 1578 | [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)CNc1c2ccccc2nc 2c1cccc2)O)N)O | CCGACUGAUGUUG ACUGUUGAAUCUC AUGGCAACACCAG UCGG | Tobramycin | Target\_lig\_54 0 | Oligonucleotide 3 | Target\_282 | 5.0969100130  0806 |
| 1579 | C1C(C(C(C(C1NC(=  O)C(CCN)O)OC2C(C (C(C(O2)CO)O)N)O)  O)OC3C(C(C(C(O3)C N)O)O)O)N | CCGACUGAUGUUG ACUGUUGAAUCUC AUGGCAACACCAG UCGG | Amikacin | Target\_lig\_17 5 | Oligonucleotide 3 | Target\_282 | 4.8239087409  4432 |
| 1580 | CC(C1CCC(C(O1)OC 2C(CC(C(C2O)OC3C( C(C(CO3) (C)O)NC)O)N)N)N)N C | CCGACUGAUGUUG ACUGUUGAAUCUC AUGGCAACACCAG UCGG | Gentamycin | Target\_lig\_12 70 | Oligonucleotide 3 | Target\_282 | 4.7958800173  4408 |
| 1581 | CNC1C(OC2OC(Cn3  nnc(c3)CCC(=O)Nc3c ccc(c3)c3csc(n3)NC(= O)C)C(C(C2O)O)N)O  C2C(C1O)OC(C(C2)  N)OC1C(N)CC(C(C1 O)O)N | CCGACUGAUGUUG ACUGUUGAAUCUC AUGGCAACACCAG UCGG | Apramycin | Target\_lig\_77 2 | Oligonucleotide 3 | Target\_282 | 4.6575773191  7779 |
| 1582 | CCNC1CC(C(C(C1O C2C(C(C(CO2) (C)O)NC)O)O)OC3C( CC=C(O3)CN)N)N | CCGACUGAUGUUG ACUGUUGAAUCUC AUGGCAACACCAG UCGG | Netilmicin | Target\_lig\_12 71 | Oligonucleotide 3 | Target\_282 | 4.4559319556  4972 |
| 1583 | C1C(C(C(C(C1N)OC2 C(C(C(C(O2)CN)O)O  )O)O)OC3C(C(C(C(O  3)CO)O)N)O)N | CCGACUGAUGUUG ACUGUUGAAUCUC AUGGCAACACCAG UCGG | Kanamycin-A | Target\_lig\_12 72 | Oligonucleotide 3 | Target\_282 | 4.3565473235  1381 |
| 1584 | C1C(C(C(C(C1N)OC2 C(C(C(C(O2)CN)O)O  )N)OC3C(C(C(O3)CO  )O)O)O)N | CCGACUGAUGUUG ACUGUUGAAUCUC AUGGCAACACCAG UCGG | Ribostamycin | Target\_lig\_12 73 | Oligonucleotide 3 | Target\_282 | 4.0457574905  6068 |
| 1585 | CC(C1C(C(C(C(O1)O C2C(CC(C(C2O)OC3 C(C(C(CO3) (C)O)NC)O)N)N)N)O  )O)O | CCGACUGAUGUUG ACUGUUGAAUCUC AUGGCAACACCAG UCGG | Geneticin | Target\_lig\_14 0 | Oligonucleotide 3 | Target\_282 | 3.9956786262  1736 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA\_ ID** | **pKd** |
| 1586 | CC1C(C(C(O1)OC2C( C(C(C(C2O)O)N=C(  N)N)O)N=C(N)N)OC  3C(C(C(C(O3)CO)O) O)NC)(C=O)O | CCGACUGAUGUUG ACUGUUGAAUCUC AUGGCAACACCAG UCGG | Streptomycin | Target\_lig\_63 | Oligonucleotide 3 | Target\_282 | 3.8728952016  3519 |
| 1587 | CNC1CC(C(C(C1O)O C2C3C(C(C(O2)CO)  O)OC4(O3)C(C(C(C(  O4)C(CO)N)O)O)O)O  )N | CCGACUGAUGUUG ACUGUUGAAUCUC AUGGCAACACCAG UCGG | Hygromycin | Target\_lig\_3 | Oligonucleotide 3 | Target\_282 | 3.5833594926  6172 |
| 1588 | C1C(C(C(C(C1N)OC2 C(C(C(C(O2)CN)O)O  )N)OC3C(C(C(O3)CO  )OC4C(C(C(C(O4)CN  )O)O)N)O)O)N | CCGACUGAUGUUG AXUGUUGAAUYUC AUGGCAACACCAG UCGG | Neomycin | Target\_lig\_4 | Oligonucleotide 4 | Target\_283 | 5.5228787452  8034 |
| 1589 | CC1(COC(C(C1NC)O  )OC2C(CC(C(C2O)O C3C(CC=C(O3)CN)N  )N)N)O | CCGACUGAUGUUG AXUGUUGAAUYUC AUGGCAACACCAG UCGG | Sisomycin | Target\_lig\_12 69 | Oligonucleotide 4 | Target\_283 | 5.3979400086  7204 |
| 1590 | [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)CNc1c2ccccc2nc 2c1cccc2)O)N)O | CCGACUGAUGUUG AXUGUUGAAUYUC AUGGCAACACCAG UCGG | Tobramycin | Target\_lig\_54 0 | Oligonucleotide 4 | Target\_283 | 5.0969100130  0806 |
| 1591 | C1C(C(C(C(C1NC(=  O)C(CCN)O)OC2C(C (C(C(O2)CO)O)N)O)  O)OC3C(C(C(C(O3)C N)O)O)O)N | CCGACUGAUGUUG AXUGUUGAAUYUC AUGGCAACACCAG UCGG | Amikacin | Target\_lig\_17 5 | Oligonucleotide 4 | Target\_283 | 4.8538719643  2176 |
| 1592 | CC(C1CCC(C(O1)OC 2C(CC(C(C2O)OC3C( C(C(CO3) (C)O)NC)O)N)N)N)N C | CCGACUGAUGUUG AXUGUUGAAUYUC AUGGCAACACCAG UCGG | Gentamycin | Target\_lig\_12 70 | Oligonucleotide 4 | Target\_283 | 4.8860566476  9316 |
| 1593 | CNC1C(OC2OC(Cn3  nnc(c3)CCC(=O)Nc3c ccc(c3)c3csc(n3)NC(= O)C)C(C(C2O)O)N)O  C2C(C1O)OC(C(C2)  N)OC1C(N)CC(C(C1 O)O)N | CCGACUGAUGUUG AXUGUUGAAUYUC AUGGCAACACCAG UCGG | Apramycin | Target\_lig\_77 2 | Oligonucleotide 4 | Target\_283 | 4.6382721639  8241 |
| 1594 | CCNC1CC(C(C(C1O C2C(C(C(CO2) (C)O)NC)O)O)OC3C( CC=C(O3)CN)N)N | CCGACUGAUGUUG AXUGUUGAAUYUC AUGGCAACACCAG UCGG | Netilmicin | Target\_lig\_12 71 | Oligonucleotide 4 | Target\_283 | 4.4685210829  5774 |
| 1595 | C1C(C(C(C(C1N)OC2 C(C(C(C(O2)CN)O)O  )O)O)OC3C(C(C(C(O  3)CO)O)N)O)N | CCGACUGAUGUUG AXUGUUGAAUYUC AUGGCAACACCAG UCGG | Kanamycin-A | Target\_lig\_12 72 | Oligonucleotide 4 | Target\_283 | 4.3467874862  2466 |
| 1596 | C1C(C(C(C(C1N)OC2 C(C(C(C(O2)CN)O)O  )N)OC3C(C(C(O3)CO  )O)O)O)N | CCGACUGAUGUUG AXUGUUGAAUYUC AUGGCAACACCAG UCGG | Ribostamycin | Target\_lig\_12 73 | Oligonucleotide 4 | Target\_283 | 4.1079053973  0952 |
| 1597 | CC(C1C(C(C(C(O1)O C2C(CC(C(C2O)OC3 C(C(C(CO3) (C)O)NC)O)N)N)N)O  )O)O | CCGACUGAUGUUG AXUGUUGAAUYUC AUGGCAACACCAG UCGG | Geneticin | Target\_lig\_14 0 | Oligonucleotide 4 | Target\_283 | 4.0268721464  003 |
| 1598 | CC1C(C(C(O1)OC2C( C(C(C(C2O)O)N=C(  N)N)O)N=C(N)N)OC  3C(C(C(C(O3)CO)O) | CCGACUGAUGUUG AXUGUUGAAUYUC AUGGCAACACCAG UCGG | Streptomycin | Target\_lig\_63 | Oligonucleotide 4 | Target\_283 | 3.9393021596  4639 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA\_ ID** | **pKd** |
|  | O)NC)(C=O)O |  |  |  |  |  |  |
| 1599 | CNC1CC(C(C(C1O)O C2C3C(C(C(O2)CO)  O)OC4(O3)C(C(C(C(  O4)C(CO)N)O)O)O)O  )N | CCGACUGAUGUUG AXUGUUGAAUYUC AUGGCAACACCAG UCGG | Hygromycin | Target\_lig\_3 | Oligonucleotide 4 | Target\_283 | 3.5361070110  1409 |
| 1729 | N=[N+]=NCCCNC(=  O)CCCOc1ccc(cc1)c1 nc2c([nH]1)cc(cc2)c1c cc(cc1)N1CCN(CC1) C | AGCCCCUGCCCACC GCACACUGCGCUGC CCCAGACCCACUGU GCGUGUGACAGCG GCUGA | Compound1 | Target\_lig\_96 5 | Pre-miR-21 | Target\_227 | 4.7447274948  9669 |
| 1730 | CN1CCN(CC1)c1ccc(  cc1)c1ccc2c(c1) [nH]c(n2)c1ccc(cc1)O CCCC(=O)N1CCN(C  C1)c1nncc2c1ccs2 | AGCCCCUGCCCACC GCACACUGCGCUGC CCCAGACCCACUGU GCGUGUGACAGCG GCUGA | Compound9 | Target\_lig\_96 6 | Pre-miR-21 | Target\_227 | 6 |
| 1731 | CN1CCN(CC1)c1ccc(  cc1)c1ccc2c(c1) [nH]c(n2)c1ccc(cc1)O CCCC(=O)N(Cc1ccnc  c1)CCNC(=O)c1ccc(c (c1)C)F | AGCCCCUGCCCACC GCACACUGCGCUGC CCCAGACCCACUGU GCGUGUGACAGCG GCUGA | Compound7 | Target\_lig\_96 7 | Pre-miR-21 | Target\_227 | 6.8927900303  5213 |
| 1732 | Coc1ccc(cc1OCC1=N C2N(C1)C=CC=C2)N  C(=O)CCCOc1ccc(cc 1)c1[nH]c2c(n1)ccc(c 2)c1ccc(cc1)N1CCN( CC1)C | AGCCCCUGCCCACC GCACACUGCGCUGC CCCAGACCCACUGU GCGUGUGACAGCG GCUGA | Compound8 | Target\_lig\_96 8 | Pre-miR-21 | Target\_227 | 6.5702477199  9759 |
| 1733 | CN1CCN(CC1)c1ccc(  cc1)c1ccc2c(c1) [nH]c(n2)c1ccc(cc1)O CCCC(=O)N1CCN(C  C1)c1nncc2c1ccs2 | GUUGACUGUUGAA UCUCAUGGCAAC | Compound9 | Target\_lig\_96 6 | miR-21 WT | Target\_301 | 6.4736607226  1016 |
| 1734 | CN1CCN(CC1)c1ccc(  cc1)c1ccc2c(c1) [nH]c(n2)c1ccc(cc1)O CCCC(=O)N1CCN(C  C1)c1nncc2c1ccs2 | GUUGACUGUUGAA UCUCAAUGGUCAA C | Compound9 | Target\_lig\_96 6 | miR-21 BP | Target\_302 | 5 |
| 1735 | CN1CCN(CC1)c1ccc(  cc1)c1ccc2c(c1) [nH]c(n2)c1ccc(cc1)O CCCC(=O)N1CCN(C  C1)c1nncc2c1ccs2 | GUUGACUGUUGAA UCUCAAUGGUCAA C | Compound9 | Target\_lig\_96 6 | miR-21 A bulge | Target\_303 | 6.6382721639  8241 |
| 1736 | CN1CCN(CC1)c1ccc(  cc1)c1ccc2c(c1) [nH]c(n2)c1ccc(cc1)O CCCC(=O)N1CCN(C  C1)c1nncc2c1ccs2 | GUUGACUGUUGAA UCUCAUGGUCAAC | Compound9 | Target\_lig\_96 6 | miR-21 U  bulge | Target\_304 | 5 |
| 1737 | CN1CCN(CC1)c1ccc(  cc1)c1ccc2c(c1) [nH]c(n2)c1ccc(cc1)O CCCC(=O)N1CCN(C  C1)c1nncc2c1ccs2 | GUUGACUGUUGAA UCUCAUAGCAAC | Compound9 | Target\_lig\_96 6 | miR-21 G-A | Target\_305 | 5.4814860601  2211 |
| 1775 | C1=CC(=CC(=C1)C2  =NC3=C(N2)C=C(C= C3)N)C4=NC5=C(N4  )C=C(C=C5)N | GCAGAGGUUGCCC UUGGUGAAUUCGC UUUAUUUAUGUUG AAUCACACAAAGG CAACUUUUGU | Compound C1 | Target\_lig\_99 4 | Pre-miR-377 dicer processing site | Target\_312 | 4.5376020021  0104 |
| 1776 | CN1CCN(CC1)c1cc(  Nc2nccc(c2)Nc2ccc3c (n2)cccc3)nc(n1)C | GCAGAGGUUGCCC UUGGUGAAUUCGC UUUAUUUAUGUUG AAUCACACAAAGG CAACUUUUGU | Compound C2 | Target\_lig\_99 5 | Pre-miR-377 5′-G\_G/3′-CAC  bulge | Target\_313 | 5.5228787452  8034 |
| 1777 | CCOC(=O)CCCOC1= CC(=CC(=C1)C2=NC 3=C(N2)C=C(C=C3) N)C4=NC5=C(N4)C= | GCAGAGGUUGCCC UUGGUGAAUUCGC UUUAUUUAUGUUG AAUCACACAAAGG | Compound C1- COOEt | Target\_lig\_99 6 | Pre-miR-377 dicer processing site | Target\_312 | 6.0969100130  0806 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA\_ ID** | **pKd** |
|  | C(C=C5)N | CAACUUUUGU |  |  |  |  |  |
| 1778 | C#CCc1nc(Nc2nccc(c 2)Nc2ccc3c(n2)cccc3) cc(n1)N1CCN(CC1)C | GCAGAGGUUGCCC UUGGUGAAUUCGC UUUAUUUAUGUUG AAUCACACAAAGG CAACUUUUGU | Compound C2- Ak | Target\_lig\_99 7 | Pre-miR-377 5′-G\_G/3′-CAC  bulge | Target\_313 | 5.7958800173  4408 |
| 1779 | CCCN(C(=O)CN(C(=  O)CN(C(=O)CN(C(=  O)CCCOc1cc(cc(c1)c 1[nH]c2c(n1)cc(cc2)N  )c1[nH]c2c(n1)ccc(c2) N)CCC)CCC)CCC)C C(=O)N(CC(=O)N)C CCn1cnc(c1)CN1CCN  (CC1)c1nc(CC)nc(c1) Nc1nccc(c1)Nc1ccc2c (n1)cccc2 | GCAGAGGUUGCCC UUGGUGAAUUCGC UUUAUUUAUGUUG AAUCACACAAAGG CAACUUUUGU | Targapremir-377 | Target\_lig\_99 8 | Pre-miR-377 | Target\_312 | 6.7212463990  4717 |
| 1794 | N=[N+]=NCCCNC(=  O)CCCOc1ccc(cc1)c1 nc2c([nH]1)ccc(c2)c1c cc(cc1)N1CCN(CC1) C | AGCCCCUGCCCACC GCACACUGCGCUGC CCCAGACCCACUGU GCGUGUGACAGCG GCUGA | miR-21 binder compound 1 | Target\_lig\_10 08 | miR-21 | Target\_227 | 4.6989700043  3602 |
| 1795 | CCCN(C(=O)CN(C(= O)NCc1nnn(c1)CCCN  C(=O)CCCOc1ccc(cc 1)c1nc2c([nH]1)ccc(c 2)c1ccc(cc1)N1CCN( CC1)C)CCC)CC(=O) N(CC(=O)N(Cc1nnn( c1)CCCNC(=O)CCC  Oc1ccc(cc1)c1nc2c([n H]1)ccc(c2)c1ccc(cc1) N1CCN(CC1)C)CC(= O)N)CCC | AGCCCCUGCCCACC GCACACUGCGCUGC CCCAGACCCACUGU GCGUGUGACAGCG GCUGA | miR-21 binder compound 2 | Target\_lig\_10 09 | miR-21 | Target\_227 | 6.0087739243  0751 |
| 1797 | NC(=[NH2+])C1=CC  =C(NC2=CC=C(C=C 2)C2=CC3=CC=C(C= C3N2)C(N)=[NH2+]) C=C1 | GUGCAGGUAGUGA UAUGUGCAUCUAC UGCAC | Compound 2 | Target\_lig\_67 6 | miR-17 Dicer site | Target\_316 | 6.9208187539  5238 |
| 1798 | NC(=[NH2+])C1=CC  =C(NC2=CC=C(C=C 2)C2=CC3=CC=C(C= C3N2)C(N)=[NH2+]) C=C1 | GUGCAGGUAGUGA UAUGUGCAUCUAC UGCAC | Compound 2 | Target\_lig\_67 6 | miR-17 G-  bulge | Target\_317 | 4.8239087409  4432 |
| 1799 | NC(=[NH2+])C1=CC  =C(NC2=CC=C(C=C 2)C2=CC3=CC=C(C= C3N2)C(N)=[NH2+]) C=C1 | GUGCAGGUAGUGA UAUGUGCAUCUAC CUGCAC | Compound 2 | Target\_lig\_67 6 | miR-17 U-  bulge | Target\_318 | 4.7212463990  4717 |
| 1800 | NC(=[NH2+])C1=CC  =C(NC2=CC=C(C=C 2)C2=CC3=CC=C(C= C3N2)C(N)=[NH2+]) C=C1 | GUGCAGGUAGAUG AUAUGUGCAUCUA CCUGCAC | Compound 2 | Target\_lig\_67 6 | miR-17 Base pairing control | Target\_319 | 4 |
| 1801 | NC(=[NH2+])C1=CC  =C(NC2=CC=C(C=C 2)C2=CC3=CC=C(C= C3N2)C(N)=[NH2+]) C=C1 | UGCAGAUAGUGAA GUAGAUAGGCAUC UACUGCA | Compound 2 | Target\_lig\_67 6 | miR-18a Dicer site | Target\_320 | 6.9065783148  3777 |
| 1809 | NCCCC(=O)NCCCN  1Cc2ccc3c(n2)nc(cc3) NC(=O)OCC/C=C/ CCOC(=O)Nc2nc3nc(  C1)ccc3cc2 | GCUGAUUUCUUUU GGUGUUCAGAGGG GUCGGUGGUGGUG GUGGUGGUGGUUC UAGCACCAUCUGA AAUCGGUUA | CMBL-3aL | Target\_lig\_10 18 | R-Seq1 | Target\_321 | 6.6615435063  954 |
| 1810 | NCCCC(=O)NCCCN  1Cc2ccc3c(n2)nc(cc3) NC(=O)OCC/C=C/ | GCUGAUUUCUUUU GGUGUUCAGAGUG GUCGGUGGUUGGU | CMBL-3aL | Target\_lig\_10 18 | R-Seq2 | Target\_322 | 5.8827287043  4424 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA\_ ID** | **pKd** |
|  | CCOC(=O)Nc2nc3nc(  C1)ccc3cc2 | GGUGGGUGGUGGU UCUAGCACCAUCUG AAAUCGGUUA |  |  |  |  |  |
| 1811 | NCCCC(=O)NCCCN  1Cc2ccc3c(n2)nc(cc3) NC(=O)OCC/C=C/ CCOC(=O)Nc2nc3nc(  C1)ccc3cc2 | GCUGAUUUCUUUU GGUGUUCAGAGAG GUCGGUGGUUGGU GGUGGGUGGUGGU UCUAGCACCAUCUG AAAUCGGUUA | CMBL-3aL | Target\_lig\_10 18 | R-Seq3 | Target\_323 | 6.1662156253  4352 |
| 1812 | NCCCC(=O)NCCCN  1Cc2ccc3c(n2)nc(cc3) NC(=O)OCC/C=C/ CCOC(=O)Nc2nc3nc(  C1)ccc3cc2 | GCUGAUUUCUUUU GGUGUUCAGAGUG GGGUGAGCUUUCU AGCACCAUCUGAA AUCGGUUA | CMBL-3aL | Target\_lig\_10 18 | R-Seq4 | Target\_324 | 6.8696662315  0499 |
| 1813 | NCCCC(=O)NCCCN  1Cc2ccc3c(n2)nc(cc3) NC(=O)OCC/C=C/ CCOC(=O)Nc2nc3nc(  C1)ccc3cc2 | GUGCAUUGUAGUU GCAUUGCAUGUUC UGGUGGUACCCAU CGAAUGUUUCCAC AGUGCAUCAC | CMBL-3aL | Target\_lig\_10 18 | Pre-miR-33a | Target\_325 | 8.8601209135  9876 |
| 1814 | NCCCC(=O)NCCCN  1Cc2ccc3c(n2)nc(cc3) NC(=O)OCC/C=C/ CCOC(=O)Nc2nc3nc(  C1)ccc3cc2 | GUGCAUUGUAGUU GCAUUGCAUGUUC UGGUAGUACCCAU CGAAUGUUUCCAC AGUGCAUCAC | CMBL-3aL | Target\_lig\_10 18 | Pre-miR-33a- G31A | Target\_326 | 8.6497519816  6584 |
| 1815 | NCCCC(=O)NCCCN  1Cc2ccc3c(n2)nc(cc3) NC(=O)OCC/C=C/ CCOC(=O)Nc2nc3nc(  C1)ccc3cc2 | GUGCAUUGUAGUU GCAUUGCAUGUUC UGGUGAUACCCAU CGAAUGUUUCCAC AGUGCAUCAC | CMBL-3aL | Target\_lig\_10 18 | Pre-miR-33a- G32A | Target\_327 | 8.5934598195  6604 |
| 1816 | NCCCC(=O)NCCCN  1Cc2ccc3c(n2)nc(cc3) NC(=O)OCC/C=C/ CCOC(=O)Nc2nc3nc(  C1)ccc3cc2 | UGCCUACUGAGCU GAAACACAGUUGG UUUGUGUACACUG GCUCAGUUCAGCA GGAACAG | CMBL-3aL | Target\_lig\_10 18 | Pre-miR-24-2 | Target\_328 | 8.6903698325  741 |
| 1820 | N=[N+]=NCCCNC(=  O)CCCOc1cccc(c1)c1 nc2c([nH]1)ccc(c2)c1 nc2c([nH]1)cc(cc2)N1 CCN(CC1)C | AGCCCCUGCCCACC GCACACUGCGCUGC CCCAGACCCACUGU GCGUGUGACAGCG GCUGA | SMB1 | Target\_lig\_12 78 | Pre-miR-210 | Target\_227 | 6.7958800173  4408 |
| 1821 | CCCN(C(=O)NCc1nn n(c1)CCCCC(=O)CC  COc1c(cc(cc1C(C) (C)C)c1[nH]c2c(n1)cc (cc2)N1CCN(CC1)C) C(C) (C)C)CC(=O)N(C(=O  )CCCOc1ccc(cc1)c1[n H]c2c(n1)cc(cc2)N1C CN(CC1)C)CCC | GGGAGAGGGUUUA AUUACGAAAGUAA UUGGAUCCGCAAG G | SMB2 | Target\_lig\_10 22 | Pri-miR-96 | Target\_159 | 7.6989700043  3602 |
| 1822 | CCCN(C(=O)CN(C(= O)NCc1nnn(c1)CCCC  C(=O)CCCOc1ccc(cc 1)c1nc2c([nH]1)ccc(c 2)c1ccc(cc1)N1CCN( CC1)C)CCC)CC(=O) N(CC(=O)N(Cc1nnn( c1)CCCCC(=O)CCC  Oc1ccc(cc1)c1nc2c([n H]1)ccc(c2)c1ccc(cc1) N1CCN(CC1)C)CC(= O)N)CCC | AGCCCCUGCCCACC GCACACUGCGCUGC CCCAGACCCACUGU GCGUGUGACAGCG GCUGA | SMB3 | Target\_lig\_10 23 | Pre-miR-21 | Target\_227 | 6.0087739243  0751 |
| 1823 | CCCN(C(=O)CN(C(= O)NCc1nnn(c1)CCCC  C(=O)CCCOc1c(cc(cc 1C(C)  (C)C)c1nc2c([nH]1)cc c(c2)c1ccc(cc1)N1CC N(CC1)C)C(C)  (C)C)CCC)CC(=O)N( | UAGCUUAUCAGAC UGAUGUUGACUGU UGAAUCUCAUGGC AACACCAGUCGAU GGGCUGU | SMB4 | Target\_lig\_12 79 | Pre-miR- 17/18a/20a | Target\_331 | 6.9208187539  5238 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA\_ ID** | **pKd** |
|  | CC(=O)N(Cc1nnn(c1) CCCCC(=O)CCCOc1  c(cc(cc1C(C) (C)C)c1nc2c([nH]1)cc c(c2)c1ccc(cc1)N1CC N(CC1)C)C(C)  (C)C)CC(=O)N)CCC |  |  |  |  |  |  |
| 1824 | OC(COP(=O) (OC1C(O)C(OC1n1cn  c2c1ncnc2N)COP(=O) (OC1C(O)C(OC1n1cn  c2c1ncnc2N)COP(=O) (OC1C(O)C(OC1n1cn  c2c1ncnc2N)COP(=O) (OC1C(O)C(OC1n1cn  c2c1ncnc2N)COP(=O) (O)O)O)O)O)O)COC CCNC(=O)CCCOc1cc  cc(c1)c1nc2c([nH]1)cc c(c2)c1nc2c([nH]1)cc( cc2)N1CCN(CC1)C | AGCCCCUGCCCACC GCACACUGCGCUGC CCCAGACCCACUGU GCGUGUGACAGCG GCUGA | SMC1 | Target\_lig\_10 24 | Pre-miR-210 | Target\_227 | 6.7212463990  4717 |
| 1825 | CCCN(C(=O)N(Cc1n nn(c1)CCCCC(=O)CC  COc1c(cc(cc1C(C) (C)C)c1nc2c([nH]1)cc c(c2)N1CCN(CC1)C) C(C) (C)C)CCOCCOCCOP (=O) (OC1C(O)C(OC1n1cn  c2c1ncnc2N)COP(=O) (OC1C(O)C(OC1n1cn  c2c1ncnc2N)COP(=O) (OC1C(O)C(OC1n1cn  c2c1ncnc2N)COP(=O) (OC1C(O)C(OC1n1cn  c2c1ncnc2N)COP(=O) (O)O)O)O)O)O)CC(= O)N(C(=O)CCCOc1c  cc(cc1)c1nc2c([nH]1)c cc(c2)N1CCN(CC1)C) CCC | GGGAGAGGGUUUA AUUACGAAAGUAA UUGGAUCCGCAAG G | SMC2 | Target\_lig\_10 25 | Pri-miR-96 | Target\_159 | 7.0757207139  3812 |
| 1826 | CCCN(C(=O)N(Cc1n nn(c1)CCCCC(=O)CC  COc1c(cc(cc1C(C) (C)C)c1nc2c([nH]1)cc c(c2)N1CCN(CC1)C) C(C) (C)C)CC(=O)NCCCC NCCCNC(=O)c1csc(n 1)c1csc(n1)CCNC(=O  )C(C(O)C)NC(=O)C(  C(C(NC(=O)C(C(c1cn c[nH]1)OC1OC(CO)C (C(C1OC1OC(CO)C(  C(C1O)OC(=O)N)O)  O)O)NC(=O)c1nc(nc(  c1C)N)C(CC(=O)N)N  CC(C(=O)N)N)C)O)C  )CC(=O)N(C(=O)CC  COc1ccc(cc1)c1nc2c([ nH]1)ccc(c2)N1CCN( CC1)C)CCC | GGGAGAGGGUUUA AUUACGAAAGUAA UUGGAUCCGCAAG G | SMC2-2 | Target\_lig\_10 26 | Pri-miR-96 | Target\_159 | 7.1938200260  1611 |