Training dataset curated from [R-SIM](https://web.iitm.ac.in/bioinfo2/R_SIM/) database for the “Viral RNA (Old)” 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** |
| 204 | CC1C(C(C(C(O1)OC2 C3CC#CC4C(O4) (C#CC3=CC2OC(=O)C 5=C(C=CC6=C5C=C( C=C6C)OC)O)C7COC(  =O)O7)NC)O)O | GGCCAGAUUGAGCC UGGGAGCUCUCUGG CC | neocarzinostatin | Target\_lig\_148 | RNA\_Str\_HIV- 2 TAR | Target\_20 | 4.85387  1964321  76 |
| 205 | c12c(cc(cc1C)OC) [C@@]1(C(=O)C=C2)  C(=O)O[C@@H]2[C@ H]1c1c([C@@H]2O[C @H]2[C@@H] ([C@@H]([C@H] ([C@H] (O2)C)O)O)NC)cc2c(c  1)[C@](C=C2)  ([C@H]1OC(=O)OC1) O | GGCCAGAUUGAGCC UGGGAGCUCUCUGG CC | Neocarzinostatin\_ chromophore\_deri vative\_1 | Target\_lig\_149 | RNA\_Str\_HIV- 2 TAR | Target\_20 | 4.85387  1964321  76 |
| 206 | c12c(cccc1) [C@]1(C(=O)C=C2)  [C@@H] (O[C@@H]2[C@@H]  1c1c(C2=O)cc2c(c1)cc cc2)O[C@@H]1[C@H  ]([C@@H]([C@H] ([C@H] (O1)CO)O)O)N | GGCCAGAUUGAGCC UGGGAGCUCUCUGG CC | Neocarzinostatin\_ chromophore\_deri vative\_2 | Target\_lig\_150 | RNA\_Str\_HIV- 2 TAR | Target\_20 | 4.85387  1964321  76 |
| 207 | c12c(cccc1) [C@]1([C@@H]  (C=C2)O[C@H]2[C@  @H]([C@H]([C@@H] ([C@@H] (O2)CO)O)O)N)C(=O) O[C@H]2[C@@H]1c1  c(C2=O)cc2c(c1)cccc2 | GGCCAGAUUGAGCC UGGGAGCUCUCUGG CC | Neocarzinostatin\_ chromophore\_deri vative\_3 | Target\_lig\_151 | RNA\_Str\_HIV- 2 TAR | Target\_20 | 4.88605  6647693  16 |
| 208 | c12c(cc(cc1)OC) [C@@]1(C(=O)C=C2) C=C[C@@H]2[C@@ H]1c1c([C@H]2O[C@ @H]2[C@H]([C@@H]  ([C@@H]([C@@H]  (O2)C)O)O)NC)cc2c(c  1)cccc2 | GGCCAGAUUGAGCC UGGGAGCUCUCUGG CC | Neocarzinostatin\_ chromophore\_deri vative\_5 | Target\_lig\_152 | RNA\_Str\_HIV- 2 TAR | Target\_20 | 5.09691  0013008  06 |
| 209 | c12c(cc(cc1)OC) [C@@]1(C(=O)C=C2) C=C[C@H]2[C@H]1c  1c([C@@H]2O[C@@ H]2[C@H]([C@@H]  ([C@@H]([C@@H]  (O2)C)O)O)NC)cc2c(c  1)cccc2 | GGCCAGAUUGAGCC UGGGAGCUCUCUGG CC | Neocarzinostatin\_ chromophore\_deri vative\_6 | Target\_lig\_153 | RNA\_Str\_HIV- 2 TAR | Target\_20 | 5.04575  7490560  68 |
| 233 | CC1(COC(C(C1NC)O) OC2C(CC(C(C2O)OC3 C(CC=C(O3)CN)N)N) N)O | GGCAGAUCUGAGCC UGGGAGCUCUCUGC C | sisomicin | Target\_lig\_10 | HIV-1 TAR RNA | Target\_19 | 6.13667  7139879  54 |
| 234 | 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 | GGCAGAUCUGAGCC UGGGAGCUCUCUGC C | Amikacin | Target\_lig\_175 | HIV-1 TAR RNA | Target\_19 | 5.81247  9279163  54 |
| 235 | CC(=O)C1=CC2=C(C= C1)SC3=CC=CC=C3N 2CCCN(C)C | GGCAGAUCUGAGCC UGGGAGCUCUCUGC C | Acetylpromazine | Target\_lig\_176 | HIV-1 TAR RNA | Target\_19 | 3.56863  6235841  01 |
| 238 | CN1CCN(CC1)C2=CC 3=C(C=C2)N=C(N3)C  4=CC5=C(C=C4)N=C( N5)C6=CC(=C(C(=C6) | GGCAGAUCUGAGCC UGGGAGCUCUCUGC C | CMC3\_Hoechst3 3258 | Target\_lig\_179 | HIV-1 TAR RNA | Target\_19 | 5 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA**  **\_ID** | **pKd** |
|  | O)O)O |  |  |  |  |  |  |
| 239 | CN1CCN(CC1)C1=C= C=c2c(=C1) [nH]c(n2)C1=C=C=c2c (=C1)nc([nH]2)C1=C= C=C(C=C1)O | GGCAGAUCUGAGCC UGGGAGCUCUCUGC C | CMC3-  2\_Hoechst33258 | Target\_lig\_180 | HIV-1 TAR RNA | Target\_19 | 5 |
| 240 | C1=CC=C2C(=C1)C(= O)C3=CC4=C(C=C3N 2)C(=O)C5=CC=CC=C  5N4 | GGCAGAUCUGAGCC UGGGAGCUCUCUGC C | Quinacridone | Target\_lig\_181 | HIV-1 TAR RNA | Target\_19 | 6 |
| 241 | C1=CC(=C2C(=C1NC CNCCO)C(=O)C3=C( C=CC(=C3C2=O)O)O) NCCNCCO | GGCAGAUCUGAGCC UGGGAGCUCUCUGC C | Mitoxantrone | Target\_lig\_182 | HIV-1 TAR RNA | Target\_19 | 7.25963  7310505  76 |
| 242 | COC1=CC(=C(C=C1) OCCN=C(N)N)CNCC CCN=C(N)N | GGCAGAUCUGAGCC UGGGAGCUCUCUGC C | Rbt203 | Target\_lig\_183 | HIV-1 TAR RNA | Target\_19 | 5.69897  0004336  02 |
| 243 | C1=CC=C2C(=C1)C= C(S2)C3=CC(=C(C=C3  )OCCN=C(N)N)CNCC CCN=C(N)N | GGCAGAUCUGAGCC UGGGAGCUCUCUGC C | Rbt417 | Target\_lig\_184 | HIV-1 TAR RNA | Target\_19 | 6.82973  8284605  04 |
| 244 | C1=CC=C2C(=C1)C= C(O2)C3=CC(=C(C=C 3)OCCN=C(N)N)CNC CCCN=C(N)N | GGCAGAUCUGAGCC UGGGAGCUCUCUGC C | Rbt418 | Target\_lig\_185 | HIV-1 TAR RNA | Target\_19 | 6.79317  4123968  15 |
| 245 | C1=CC=C2C(=C1)C= C(S2)C3=CC(=C(C=C3  )OCCCN)CNCCCCN= C(N)N | GGCAGAUCUGAGCC UGGGAGCUCUCUGC C | Rbt428 | Target\_lig\_186 | HIV-1 TAR RNA | Target\_19 | 6.90308  9986991  94 |
| 246 | C1CN(CCN1)CCNCC2  =C(C=CC(=C2)C3=CC 4=C(C=C3)NC=C4)OC CCN | GGCAGAUCUGAGCC UGGGAGCUCUCUGC C | Rbt550 | Target\_lig\_187 | HIV-1 TAR RNA | Target\_19 | 7.30102  9995663  98 |
| 247 | CCSC1=CC2=C(C=C1) SC3=CC=CC=C3N2C CCN4CCN(CC4)C | GGCAGAUCUGAGCC UGGGAGCUCUCUGC C | Thiethylperazine | Target\_lig\_188 | HIV-1 TAR RNA | Target\_19 | 3.56863  6235841  01 |
| 248 | CN1CCN(CC1)CCCN2 C3=CC=CC=C3SC4=C 2C=C(C=C4)C(F)(F)F | GGCAGAUCUGAGCC UGGGAGCUCUCUGC C | Trifluoperazine | Target\_lig\_189 | HIV-1 TAR RNA | Target\_19 | 3.56863  6235841  01 |
| 249 | CC1=C(C(=C2C(=C1O  )C3(C(=CC(=O)C(C3=  O)C(=O)C)O2)C)C(=O  )C)O | GGCAGAUCUGAGCC UGGGAGCUCUCUGC C | Usnic acid | Target\_lig\_190 | HIV-1 TAR RNA | Target\_19 | 6 |
| 250 | CN1C=C(C(=O)C2=C C(=C(C=C21)N3CCN( CC3)C4=CC=CC=N4) N)C(=O)O | GGCAGAUCUGAGCC UGGGAGCUCUCUGC C | Wm5 | Target\_lig\_191 | HIV-1 TAR RNA | Target\_19 | 7.72124  6399047  17 |
| 251 | CN1C2=C(C(=O)N(C1  =O)C)N(C=N2)CC(CN (C)CCO)O | GGCAGAUCUGAGCC UGGGAGCUCUCUGC C | Xanthinol | Target\_lig\_192 | HIV-1 TAR RNA | Target\_19 | 6 |
| 252 | COC(=O)C1C(CCC2C 1CC3C4=C(CCN3C2) C5=CC=CC=C5N4)O | GGCAGAUCUGAGCC UGGGAGCUCUCUGC C | Yohimbine | Target\_lig\_193 | HIV-1 TAR RNA | Target\_19 | 6 |
| 253 | CCNC1CC(C(C(C1OC 2C(C(C(CO2) (C)O)NC)O)O)OC3C( CC=C(O3)CN)N)N | GGCAGAUCUGAGCC UGGGAGCUCUCUGC C | netilmicin | Target\_lig\_194 | HIV-1 TAR RNA | Target\_19 | 5.86966  6231504  99 |
| 254 | c1c(ccc2Sc3ccccc3N(c 12)CCCN1CCC[C@H] (C1)CO)C(=O)C | GGCAGAUCUGAGCC UGGGAGCUCUCUGC C | hydroxymethyl\_pi peridinyl\_propyl\_ phenothiazinyl\_et hanone | Target\_lig\_195 | HIV-1 TAR RNA | Target\_19 | 3.74472  7494896  69 |
| 255 | CO[C@H]1CCCN(C1)  CCCCN1c2cc(ccc2Sc2 c1cccc2)C(=O)C | GGCAGAUCUGAGCC UGGGAGCUCUCUGC C | methoxypiperidin  \_butyl\_der | Target\_lig\_196 | HIV-1 TAR RNA | Target\_19 | 3.85387  1964321  76 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA**  **\_ID** | **pKd** |
| 256 | CC(=O)C1=CC2=C(C= C1)SC3=CC=CC=C3N 2CCCN(C)C | GGCAGAUCUGAGCC UGGGAGCUCUCUGC C | dimethylamino\_pr opyl\_phenothiazin yl\_ethanone | Target\_lig\_197 | HIV-1 TAR RNA | Target\_19 | 3.56863  6235841  01 |
| 257 | CN(C)CCCN1C2=CC= CC=C2SC3=C1C=C(C  =C3)OC | GGCAGAUCUGAGCC UGGGAGCUCUCUGC C | 3-(2-methoxy- 10H-  phenothiazin-10- yl)-N,N-  dimethylpropan- 1-amine | Target\_lig\_198 | HIV-1 TAR RNA | Target\_19 | 2.52287  8745280  34 |
| 258 | CN(C)CCCN1C2=CC= CC=C2SC3=C1C=C(C  =C3)Cl | GGCAGAUCUGAGCC UGGGAGCUCUCUGC C | 3-(2-chloro-10H- phenothiazin-10- yl)-N,N-  dimethylpropan- 1-amine | Target\_lig\_199 | HIV-1 TAR RNA | Target\_19 | 3.25963  7310505  76 |
| 259 | CC=1C=CC=2N(C3=C C=C(C=C3SC2C1)C)C CCN(C)C | GGCAGAUCUGAGCC UGGGAGCUCUCUGC C | 3-(3,7-dimethyl- 10H-  phenothiazin-10- yl)-N,N-  dimethylpropan- 1-amine | Target\_lig\_200 | HIV-1 TAR RNA | Target\_19 | 2.30102  9995663  98 |
| 260 | COC1=CC=CC=2N(C3  =CC=CC=C3SC12)CC CN(C)C | GGCAGAUCUGAGCC UGGGAGCUCUCUGC C | 3-(4-methoxy- 10H-  phenothiazin-10- yl)-N,N-  dimethylpropan- 1-amine | Target\_lig\_201 | HIV-1 TAR RNA | Target\_19 | 2.52287  8745280  34 |
| 261 | CN(C)CCCN1C2=CC= CC=C2SC3=C1C=C(C  =C3)O | GGCAGAUCUGAGCC UGGGAGCUCUCUGC C | dimethylamino\_pr opyl\_phenothiazin  \_der\_2 | Target\_lig\_202 | HIV-1 TAR RNA | Target\_19 | 2.52287  8745280  34 |
| 262 | CN(CCCN1C2=CC=C C=C2SC=2C(=CC=CC 12)O)C | GGCAGAUCUGAGCC UGGGAGCUCUCUGC C | 10-(3-  (dimethylamino)p ropyl)-10H- phenothiazin-4-ol | Target\_lig\_203 | HIV-1 TAR RNA | Target\_19 | 2.52287  8745280  34 |
| 263 | CN(C)CCCN1C2=CC= CC=C2SC3=C1C=C(C  =C3)C(F)(F)F | GGCAGAUCUGAGCC UGGGAGCUCUCUGC C | N,N-dimethyl-3- (2-  (trifluoromethyl)- 10H-  phenothiazin-10- yl)propan-1- amine | Target\_lig\_204 | HIV-1 TAR RNA | Target\_19 | 3.25963  7310505  76 |
| 264 | CN(CCCN1C2=CC=C C=C2SC=2C=C(C=CC 12)C)C | GGCAGAUCUGAGCC UGGGAGCUCUCUGC C | N,N-dimethyl-3- (3-methyl-10H- phenothiazin-10- yl)propan-1- amine | Target\_lig\_205 | HIV-1 TAR RNA | Target\_19 | 2.52287  8745280  34 |
| 265 | CN(C)CCCN1C2=CC= CC=C2SC3=CC=CC= C31 | GGCAGAUCUGAGCC UGGGAGCUCUCUGC C | N,N-dimethyl-3- (10H-  phenothiazin-10- yl)propan-1- amine | Target\_lig\_206 | HIV-1 TAR RNA | Target\_19 | 2.30102  9995663  98 |
| 266 | CN(C)CCCN1C2=CC= CC=C2SC3=C1C=C(C  =C3)Cl | GGCAGAUCUGAGCC UGGGAGCUCUCUGC C | [3-(2-chloro-10H- phenothiazin-10 | Target\_lig\_207 | HIV-1 TAR RNA | Target\_19 | 3.25963  7310505  76 |
| 268 | c1c(ccc2Sc3ccccc3N(c 12)CCCCN1CCC[C@ H](C1)CO)C(=O)C | GGCAGAUCUGAGCC UGGGAGCUCUCUGC C | hydroxymethyl\_pi peridinyl\_butyl | Target\_lig\_208 | HIV-1 TAR RNA | Target\_19 | 3.25963  7310505  76 |
| 269 | c1c(ccc2Sc3ccccc3N(c 12)CCCCCN1CCC[C @H](C1)CO)C(=O)C | GGCAGAUCUGAGCC UGGGAGCUCUCUGC C | hydroxymethyl\_pi peridinyl\_pentyl | Target\_lig\_209 | HIV-1 TAR RNA | Target\_19 | 2.52287  8745280  34 |
| 270 | c1c(ccc2Sc3ccccc3N(c 12)CCCNCN(CO)CO) C(=O)C | GGCAGAUCUGAGCC UGGGAGCUCUCUGC C | 3\_phenothiazine\_ analog\_1 | Target\_lig\_210 | HIV-1 TAR RNA | Target\_19 | 2.52287  8745280  34 |
| 271 | c1c(ccc2Sc3ccccc3N(c 12)CCCN[C@H] (CCSC)O)C(=O)C | GGCAGAUCUGAGCC UGGGAGCUCUCUGC C | 3\_phenothiazine\_ analog\_2 | Target\_lig\_211 | HIV-1 TAR RNA | Target\_19 | 2.30102  9995663  98 |
| 272 | C1=CC=C2C(=C1)N(C | GGCAGAUCUGAGCC | 3\_phenothiazine\_ | Target\_lig\_212 | HIV-1 TAR | Target\_19 | 3.25963 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA**  **\_ID** | **pKd** |
|  | 3=C(S2)C=CC(=C3)Cl) CCCNCCO | UGGGAGCUCUCUGC C | analog\_3 |  | RNA |  | 7310505  76 |
| 273 | c1cccc2Sc3ccc(cc3N(c 12)CCCNCCCCC)Cl | GGCAGAUCUGAGCC UGGGAGCUCUCUGC C | 2-chloro-10- pyrrolidin\_phenot hiazine\_der | Target\_lig\_213 | HIV-1 TAR RNA | Target\_19 | 3.25963  7310505  76 |
| 274 | c1cccc2Sc3ccc(cc3N(c 12)CCN1CCCC1)Cl | GGCAGAUCUGAGCC UGGGAGCUCUCUGC C | 2-chloro-10- methylpyrrolidin\_ phenothiazine\_der | Target\_lig\_214 | HIV-1 TAR RNA | Target\_19 | 2.30102  9995663  98 |
| 275 | c1cccc2Sc3ccc(cc3N(c 12)CCN1CCC[C@@H  ]1C)Cl | GGCAGAUCUGAGCC UGGGAGCUCUCUGC C | 2-chloro-10-[2-(2- methylpyrrolidin- 1-  yl)ethyl]\_phenothi azine\_der | Target\_lig\_215 | HIV-1 TAR RNA | Target\_19 | 2.30102  9995663  98 |
| 276 | C1CCN(CC1)CCCN2C 3=CC=CC=C3SC4=C2 C=C(C=C4)Cl | GGCAGAUCUGAGCC UGGGAGCUCUCUGC C | chloro\_piperidine  \_propyl\_der | Target\_lig\_216 | HIV-1 TAR RNA | Target\_19 | 3.25963  7310505  76 |
| 277 | CN1CCN(CC1)CCCN2 C3=CC=CC=C3SC4=C 2C=C(C=C4)Cl | GGCAGAUCUGAGCC UGGGAGCUCUCUGC C | chloro\_methylpip erazinyl\_propyl\_p henothiazine\_der | Target\_lig\_217 | HIV-1 TAR RNA | Target\_19 | 2.52287  8745280  34 |
| 278 | c1cccc2Sc3ccc(cc3N(c 12)CCn1cncc1)Cl | GGCAGAUCUGAGCC UGGGAGCUCUCUGC C | choro\_imidazole\_ phenothiazine\_der | Target\_lig\_218 | HIV-1 TAR RNA | Target\_19 | 2.30102  9995663  98 |
| 279 | C1=CC=C(C=C1)CNC CN2C3=CC=CC=C3S C4=C2C=C(C=C4)Cl | GGCAGAUCUGAGCC UGGGAGCUCUCUGC C | benzyl\_phenothia zin\_der | Target\_lig\_219 | HIV-1 TAR RNA | Target\_19 | 2.30102  9995663  98 |
| 280 | C1C(C(C(C(C1NC(=O)  C(CCN)O)O)OC2C(C(  C(O2)CO)O)O)OC3C(  C(C(C(O3)CN)O)O)N) N | GGCAGAUCUGAGCC UGGGAGCUCUCUGC C | Butirosin | Target\_lig\_220 | HIV-1 TAR RNA | Target\_19 | 5.32057  2103387  88 |
| 281 | CN(C)C1=NC(=C(N=C 1Cl)C(=O)N=C(N)N)N | GGCAGAUCUGAGCC UGGGAGCUCUCUGC C | N\_N\_dimethyl\_a miloride | Target\_lig\_221 | HIV-1 TAR RNA | Target\_19 | 3.91417  4466479  26 |
| 286 | c1c2OC[C@@H] (Cc2c2c(c1)N=C1[C@ H]2C[C@@H] (CN1)CN(C)C)CN(C)C | GGCCGAGUAGUGU UGGGUCGCGAAAG GCC | Benzimidazole13i bis | Target\_lig\_225 | HCV IRES  Domain II | Target\_66 | 6.14266  7503568  73 |
| 287 | CN(C)CCCN1C2=C(C  =CC(=C2)OCCCN(C)C  )N=C1N | GGCCGAGUAGUGU UGGGUCGCGAAAG GCC | Benzimidazole3ib is | Target\_lig\_226 | HCV IRES  Domain II | Target\_66 | 4.76955  1078621  73 |
| 305 | CC(C)N=C(C1=CC=C C(=C1)C2=CC=C(O2) C3=CC(=CC=C3)C(=N C(C)C)N)N | GCACUAUGGGCGCC AGCGUCAAUGACGC UGACGGUACAGCCA GACAAUUAUUGUC UGGUAUAGUGC | CMC6\_diphenylf uran | Target\_lig\_243 | HIV-1 RRE | Target\_80 | 5.30102  9995663  98 |
| 306 | CN(C)CCN=C(C1=CC  =CC(=C1)C2=CC=C(O 2)C3=CC(=CC=C3)C(  =NCCN(C)C)N)N | GCACUAUGGGCGCC AGCGUCAAUGACGC UGACGGUACAGCCA GACAAUUAUUGUC UGGUAUAGUGC | CMC7\_diphenylf uran | Target\_lig\_244 | HIV-1 RRE | Target\_80 | 7 |
| 307 | CN(C)CCCN=C(C1=C C=CC(=C1)C2=CC=C( O2)C3=CC(=CC=C3)C (=NCCCN(C)C)N)N | GCACUAUGGGCGCC AGCGUCAAUGACGC UGACGGUACAGCCA GACAAUUAUUGUC UGGUAUAGUGC | CMC8\_diphenylf uran | Target\_lig\_245 | HIV-1 RRE | Target\_80 | 5.79588  0017344  08 |
| 393 | CC1(COC(C(C1NC)O) OC2C(CC(C(C2O)OC3 C(CC=C(O3)CN)N)N) N)O | GGCCGAGUAGUGU UGGGUCGCGAAAG GCC | sisomicin | Target\_lig\_10 | HCV IRES  Domain IIId | Target\_66 | 6.58502  6652029  18 |
| 710 | C1(=O)N(C(=O)c2c([C  @H]1C)ncn2C[C@H] (O)N(C)C)C | GGCAGAUCUGAGCC UGGGAGCUCUCUGC C | Phenothiazine 1 | Target\_lig\_474 | RNA\_Str\_HIV- 1 TAR | Target\_19 | 5.84466  3962534  94 |
| 711 | CN1CCN(CC1)CCCN2 C3=CC=CC=C3SC4=C | GGCAGAUCUGAGCC UGGGAGCUCUCUGC | Phenothiazine 2 | Target\_lig\_475 | RNA\_Str\_HIV- 1 TAR | Target\_19 | 4.92445  3038607 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA**  **\_ID** | **pKd** |
|  | 2C=C(C=C4)Cl | C |  |  |  |  | 47 |
| 712 | C1=CC2=C(C=C1N=C  =S)C(=O)OC23C4=C( C=C(C=C4)O)OC5=C3 C=CC(=C5)O | GGCAGAUCUGAGCC UGGGAGCUCUCUGC C | Phenothiazine 3 | Target\_lig\_476 | RNA\_Str\_HIV- 1 TAR | Target\_19 | 4.92445  3038607  47 |
| 713 | C1=CC=C2C(=C1)C(= O)OC2(C3=CC=C(C= C3)O)C4=CC=C(C=C4  )O | GGCAGAUCUGAGCC UGGGAGCUCUCUGC C | Phenothiazine 4 | Target\_lig\_477 | RNA\_Str\_HIV- 1 TAR | Target\_19 | 4.59345  9819566  04 |
| 714 | CC(=O)C1=CC2=C(C= C1)SC3=CC=CC=C3N 2CCCN(C)C | GGCAGAUCUGAGCC UGGGAGCUCUCUGC C | Phenothiazine 6 | Target\_lig\_478 | RNA\_Str\_HIV- 1 TAR | Target\_19 | 3.79860  2875679  55 |
| 715 | C1=CC=C2C(=C1)C(= O)C3=CC4=C(C=C3N 2)C(=O)C5=CC=CC=C  5N4 | GGCAGAUCUGAGCC UGGGAGCUCUCUGC C | Phenothiazine 7 | Target\_lig\_479 | RNA\_Str\_HIV- 1 TAR | Target\_19 | 3.43770  7135543  53 |
| 716 | [C@H]12[C@@H]  (C[C@@H]3[N@@] (C1)  (CCc1c3[nH]c3c1cccc3  )C)[C@H]([C@H]  (CC2)O)C(=O)OC | GGCAGAUCUGAGCC UGGGAGCUCUCUGC C | Phenothiazine 8 | Target\_lig\_480 | RNA\_Str\_HIV- 1 TAR | Target\_19 | 3.04720  7556955  91 |
| 717 | [C@@H]1(C[C@H]  ([C@H]2[C@@H]  ([C@@H]1C(=O)C)O[  C@H]1[C@@]2(C(=O  )[C@@H] (C(=O)C1)C(=O)C)C) O)O | GGCAGAUCUGAGCC UGGGAGCUCUCUGC C | Phenothiazine 9 | Target\_lig\_481 | RNA\_Str\_HIV- 1 TAR | Target\_19 | 2.40671  3932979  54 |
| 718 | CN(C)CCCN1C2=CC= CC=C2SC3=C1C=C(C  =C3)Cl | GGCAGAUCUGAGCC UGGGAGCUCUCUGC C | Phenothiazine 10 | Target\_lig\_482 | RNA\_Str\_HIV- 1 TAR | Target\_19 | 2.00921  7308196  86 |
| 731 | [C@@H]1([C@H]  ([C@H]([C@H]  (O[C@@H]1CNC(=N) N)O[C@@H]1[C@@H  ]([C@@H]([C@H]  (C[C@H]1NC(=N)N)N  C(=N)N)O)O[C@H]1[ C@@H]([C@H]  ([C@@H] (O1)CO)O[C@H]1O[C  @H]([C@H]([C@@H]  ([C@@H]1NC(=N)N)  O)O)CNC(=N)N)O)NC (=N)N)O)O | UUUUUUAGGGAAG AUCUGGCCUUCCCA CAAGGGAAGGCCAG GGAAUUUUCUU | guanidinoneomyci n\_B | Target\_lig\_495 | HIV- 1FRAMESHIF T STEM LOOP STRUCTURE | Target\_109 | 8 |
| 732 | C[C@H]1[C@H] ([C@H](C[C@@H]  (O1)O[C@H]2C[C@@  ] (CC3=C2C(=C4C(=C3  O)C(=O)C5=C(C4=O) C(=CC=C5)OC)O) (C(=O)CO)O)N)O | UUUUUUAGGGAAG AUCUGGCCUUCCCA CAAGGGAAGGCCAG GGAAUUUUCUU | doxorubicin | Target\_lig\_496 | HIV- 1FRAMESHIF T STEM LOOP STRUCTURE | Target\_109 | 5.55284  1968657  78 |
| 733 | c1cc(ccc1)C[C@H] (NC(=O) [C@@H]1CCCN1C(= O)[C@@H]  (NC(=O)c1cc2ccccc2nc 1CC)CSSC[C@H] (C(=O)N1CCC[C@H]1 C(=O)N[C@H] (C(=O)NCCCN)Cc1ccc  cc1)NC(=O)c1c(nc2c(c 1)cccc2)CC)C(=O)NC CCN | UUUUUUAGGGAAG AUCUGGCCUUCCCA CAAGGGAAGGCCAG GGAAUUUUCUU | ethylquinoline\_ca rboxamide derivative | Target\_lig\_497 | HIV- 1FRAMESHIF T STEM LOOP STRUCTURE | Target\_109 | 6.45593  1955649  72 |
| 734 | CC1=NC2=NC(=NN2C (=C1)N3CCN(CC3)C) | AGGACUCGGCUUGC UGAAGCGCGCGACG | methylpiperazine derivative | Target\_lig\_498 | SL-3 of HIV- 1\_SITE | Target\_146 | 4.95860  7314841 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA**  **\_ID** | **pKd** |
|  | C4=CC=C(C=C4)Cl | GCAAGAGGCGAGG GGCGGCGACUGGUG AGUACGCCAAAAAU UUUGACUAGCGGA GGCUAGAAGGAGA GAGAUGGGUGCGA GAGCGUCGGU |  |  |  |  | 77 |
| 735 | CC1=C(C(=O)C2=C(C 1=O)N3C[C@H]4[C@  @H] (C3=C2COC(=O)N)N4 C)OC | AGGACUCGGCUUGC UGAAGCGCGCGACG GCAAGAGGCGAGG GGCGGCGACUGGUG AGUACGCCAAAAAU UUUGACUAGCGGA GGCUAGAAGGAGA GAGAUGGGUGCGA GAGCGUCGGU | methyl\_carbamate derivative | Target\_lig\_499 | SL-3 of HIV- 1\_SITE | Target\_146 | 4.00877  3924307  51 |
| 798 | CC1C(C(C(O1)OC2C( C(C(C(C2O)O)N=C(N)  N)O)N=C(N)N)OC3C(  C(C(C(O3)CO)O)O)N C)(C=O)O | GGCAGAUCUGAGCC UGGGAGCUCUCUGC C | Streptomycin | Target\_lig\_63 | Argininamide- TAR complex | Target\_19 | 5.61978  8758288  39 |
| 799 | 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 | GGCAGAUCUGAGCC UGGGAGCUCUCUGC C | Neomycin\_B | Target\_lig\_124 6 | Argininamide- TAR complex | Target\_19 | 6.15490  1959985  74 |
| 800 | CC1(COC(C(C1NC)O) OC2C(CC(C(C2O)OC3 C(CCC(O3)CN)N)N)N  )O | GGCAGAUCUGAGCC UGGGAGCUCUCUGC C | gentamicin\_mol | Target\_lig\_76 | Argininamide- TAR complex | Target\_19 | 5.36653  1544420  41 |
| 847 | CC1C(C(C(O1)OC2C( C(C(C(C2O)O)N=C(N)  N)O)N=C(N)N)OC3C(  C(C(C(O3)CO)O)O)N C)(C=O)O | GCACUAUGGGCGCC AGCGUCAAUGACGC UGACGGUACAGCCA GACAAUUAUUGUC UGGUAUAGUGC | Streptomycin | Target\_lig\_63 | RRE-RNA | Target\_80 | 6 |
| 849 | [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 | GCACUAUGGGCGCC AGCGUCAAUGACGC UGACGGUACAGCCA GACAAUUAUUGUC UGGUAUAGUGC | Tobramycin | Target\_lig\_540 | RRE-RNA | Target\_80 | 5.52287  8745280  34 |
| 850 | 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 | GCACUAUGGGCGCC AGCGUCAAUGACGC UGACGGUACAGCCA GACAAUUAUUGUC UGGUAUAGUGC | Kanamycin A | Target\_lig\_7 | RRE-RNA | Target\_80 | 3.12493  8736608  3 |
| 851 | 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 | GCACUAUGGGCGCC AGCGUCAAUGACGC UGACGGUACAGCCA GACAAUUAUUGUC UGGUAUAGUGC | KANAMYCIN B | Target\_lig\_8 | RRE-RNA | Target\_80 | 4.04575  7490560  68 |
| 852 | 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 | GCACUAUGGGCGCC AGCGUCAAUGACGC UGACGGUACAGCCA GACAAUUAUUGUC UGGUAUAGUGC | Neomycin\_B | Target\_lig\_124 6 | RRE-RNA | Target\_80 | 6.82390  8740944  32 |
| 853 | 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 | GGUGGGCGCAGCUU CGGCUGCGGUACAC C | Neomycin | Target\_lig\_4 | RRE1 | Target\_81 | 6.79588  0017344  08 |
| 854 | C1C(C(C(C(C1N)OC2 C(C(C(C(O2)CN)O)O) | GGUGUCGCAGCUUC GCCUCGCACACC | Neomycin | Target\_lig\_4 | RRE2 | Target\_82 | 5.12262  8654130 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA**  **\_ID** | **pKd** |
|  | 1. OC3C(C(C(O3)CO)   OC4C(C(C(C(O4)CN)   1. O)N)O)O)N |  |  |  |  |  | 23 |
| 855 | 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 | GGUGGGCGCAGCUU CGGCUGCGCCCACC | Neomycin | Target\_lig\_4 | RRE3 | Target\_83 | 5.19382  0026016  11 |
| 856 | 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 | GGUGGGCGCAGCUU CGGCUGCGGACACC | Neomycin | Target\_lig\_4 | RRE4 | Target\_84 | 6.31875  8762624  41 |
| 857 | 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 | GGUGGGCGCAGCUU CGGCUGCGCACACC | Neomycin | Target\_lig\_4 | RRE5 | Target\_85 | 5.92811  7992693  88 |
| 858 | 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 | GGUGGCCGCAGCUU CGGCUGCGGACACC | Neomycin | Target\_lig\_4 | RRE6 | Target\_86 | 5.53313  2379645  89 |
| 859 | 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 | GGUGGGCGCAGCUU CGGCUGCGGCCACC | Neomycin | Target\_lig\_4 | RRE7 | Target\_87 | 5.75696  1951313  71 |
| 860 | 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 | GGUGUGCCGCAGCU UCGGCUGCGGACAC C | Neomycin | Target\_lig\_4 | RRE8 | Target\_88 | 5.56224  9437179  61 |
| 861 | 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 | GGUGGAGCGCAGCU UCGGCUGCGCCCAC C | Neomycin | Target\_lig\_4 | RRE9 | Target\_89 | 5.90308  9986991  94 |
| 862 | 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 | GGUGGGCGCAGCUU CGGCUGCGCACCAC C | Neomycin | Target\_lig\_4 | RRE10 | Target\_90 | 6.18708  6643357  14 |
| 863 | 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 | GGUGGGCGCAGCUU CGGCUGCGCAACCA CC | Neomycin | Target\_lig\_4 | RRE11 | Target\_91 | 6.26760  6240177  03 |
| 864 | 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 | GGUGGGCGCAGCUU CGGCUGCGCAAACC ACC | Neomycin | Target\_lig\_4 | RRE12 | Target\_92 | 6.18708  6643357  14 |
| 865 | 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 | GGUGGGCGCAGCUU CGGCUGCGCAAAAC CACC | Neomycin | Target\_lig\_4 | RRE13 | Target\_93 | 6.21467  0164989  23 |
| 866 | 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 | GGUGGGCGCAGCUU CGGCUGCGCGGCCA CC | Neomycin | Target\_lig\_4 | RRE14 | Target\_94 | 6.35654  7323513  81 |
| 867 | 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) | GGUGGGCGCAGCUU CGGCUGCGCUUCCA CC | Neomycin | Target\_lig\_4 | RRE15 | Target\_95 | 6.28399  6656365  2 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA**  **\_ID** | **pKd** |
|  | O)O)N)O)O)N |  |  |  |  |  |  |
| 897 | c1ccc2c(c1)Sc1c(N2CC CN(C)C)cc(cc1)C(=O) C | GGCAGAUCUGAGCC UGGGAGCUCUCUGC C | Phenothiazine 5 | Target\_lig\_125 3 | Acetylpromazi ne TAR RNA | Target\_19 | 4.129011  1862394  3 |
| 899 | CC(=O)C1=CC2=C(C= C1)SC3=CC=CC=C3N 2CCCN(C)C | GGGCUAGCACUCUG GUAUCACGGUACCU UUGUGCGCCC | Acetylpromazine | Target\_lig\_176 | Coxsackie virus B3 RNA | Target\_130 | 3.48148  6060122  11 |
| 900 | CC(=O)C1=CC2=C(C= C1)SC3=CC=CC=C3N 2CCCN(C)C | GGGGUUGUACCCAC CCC | Acetylpromazine | Target\_lig\_176 | Polio virus loop B construct | Target\_131 | 2.74472  7494896  69 |
| 949 | N([C@@H] (C(=O)N1[C@@H]  (CCC1)C(=O)N[C@@ H]  (Cc1ccccc1)C(=O)NCC CCCCN)CSSC[C@@H  ]  (NC(=O)c1c(nc2c(cccc 2)c1)CC)C(=O)N1[C@  @H] (CCC1)C(=O)N[C@@ H]  (Cc1ccccc1)C(=O)NCC CCCCN)C(=O)c1c2c(n  c(c1)CC)cccc2 | GGCCUUCCCACAAG GGAAGGCC | disulfide\_der\_0 | Target\_lig\_564 | HIV-1 FSS | Target\_188 | 6.45593  1955649  72 |
| 950 | N([C@@H] (C(=O)N1[C@@H]  (CCC1)C(=O)N[C@@ H]  (Cc1ccccc1)C(=O)NCC CN)CSSC[C@@H]  (NC(=O)c1c(nc2c(cccc 2)c1)CC)C(=O)N1[C@  @H] (CCC1)C(=O)N[C@@ H]  (Cc1ccccc1)C(=O)NCC CN)C(=O)c1c2c(nc(c1) CC)cccc2 | GGCCUUCCCACAAG GGAAGGCC | disulfide\_der\_1 | Target\_lig\_565 | HIV-1 FSS | Target\_188 | 6.45593  1955649  72 |
| 951 | N([C@H] (C(=O)N1[C@H]  (CCC1)C(=O)N[C@H]  (Cc1ccccc1)C(=O)NCC CN)CSSC[C@@H]  (NC(=O)c1c(nc2c(cccc 2)c1)C)C(=O)N1[C@  @H] (CCC1)C(=O)N[C@@ H]  (Cc1ccccc1)C(=O)NCC CN)C(=O)c1c2c(nc(c1) C)cccc2 | GGCCUUCCCACAAG GGAAGGCC | disulfide\_der\_2 | Target\_lig\_566 | HIV-1 FSS | Target\_188 | 6.36653  1544420  41 |
| 952 | N([C@@H] (C(=O)N1[C@@H]  (CCC1)C(=O)N[C@H]  (Cc1ccccc1)C(=O)NCC CN)CSSC[C@@H]  (NC(=O)c1cnc2c(cccc2  )c1)C(=O)N1[C@@H]  (CCC1)C(=O)N[C@@ H]  (Cc1ccccc1)C(=O)NCC CN)C(=O)c1c2c(ncc1)c ccc2 | GGCCUUCCCACAAG GGAAGGCC | disulfide\_der\_3 | Target\_lig\_567 | HIV-1 FSS | Target\_188 | 6.18708  6643357  14 |
| 953 | N([C@@H] (C(=O)N1[C@H]  (CCC1)C(=O)N[C@@ H]  (Cc1ccccc1)C(=O)NCC CN)CSSC[C@@H] | GGCCUUCCCACAAG GGAAGGCC | disulfide\_der\_6 | Target\_lig\_568 | HIV-1 FSS | Target\_188 | 5.84771  1655616  94 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA**  **\_ID** | **pKd** |
|  | (NC(=O)c1c(nc2c(cc3c (c2)OCO3)c1)CC)C(= O)N1[C@@H] (CCC1)C(=O)N[C@@ H]  (Cc1ccccc1)C(=O)NCC CN)C(=O)c1c2c(nc(c1) CC)cc1c(c2)OCO1 |  |  |  |  |  |  |
| 954 | N([C@H] (C(=O)N1[C@@H]  (CCC1)C(=O)N[C@@ H]  (Cc1ccccc1)C(=O)NCC CN)CSSC[C@H] (NC(=O)c1c(nc2c(c1)C (=O)  [C@@H]1[C@@H] (C2=O)C=CC=C1)CC) C(=O)N1[C@@H]  (CCC1)C(=O)N[C@@ H]  (Cc1ccccc1)C(=O)NCC CN)C(=O)c1c2c(nc(c1) CC)C(=O)  [C@@H]1[C@H] (C2=O)C=CC=C1 | GGCCUUCCCACAAG GGAAGGCC | disulfide\_der\_7 | Target\_lig\_569 | HIV-1 FSS | Target\_188 | 6.63827  2163982  41 |
| 955 | N([C@H] (C(=O)N1[C@H]  (CCC1)C(=O)N[C@H]  (Cc1ccccc1)C(=O)NCC CN)CC=C)C(=O)c1c2c  (nc(c1)CC)cccc2 | AGGACUCGGCUUGC UGAAGCGCGCGACG GCAAGAGGCGAGG GGCGGCGACUGGUG AGUACGCCAAAAAU UUUGACUAGCGGA GGCUAGAAGGAGA GAGAUGGGUGCGA GAGCGUCGGU | carba\_der | Target\_lig\_570 | HIV-1 genomic SL3 rna | Target\_146 | 6.32790  2142064  28 |
| 956 | N([C@H] (C(=O)N1[C@H]  (CCC1)C(=O)N[C@@ H]  (Cc1ccccc1)C(=O)NCC CN)C/C=C/C[C@H]  (NC(=O)c1c(nc2c(c1)c ccc2)CC)C(=O)N1[C@  @H] (CCC1)C(=O)N[C@@ H]  (Cc1ccccc1)C(=O)NCC CN)C(=O)c1c2c(nc(c1) CC)cccc2 | AGGACUCGGCUUGC UGAAGCGCGCGACG GCAAGAGGCGAGG GGCGGCGACUGGUG AGUACGCCAAAAAU UUUGACUAGCGGA GGCUAGAAGGAGA GAGAUGGGUGCGA GAGCGUCGGU | dicarba\_analog\_1 | Target\_lig\_571 | HIV-1 genomic SL3 rna | Target\_146 | 6.48148  6060122  11 |
| 957 | N([C@H] (C(=O)N1[C@H]  (CCC1)C(=O)N[C@H]  (Cc1ccccc1)C(=O)NCC CN)CCCC[C@H]  (NC(=O)c1c(nc2c(c1)c ccc2)CC)C(=O)N1[C@  @H] (CCC1)C(=O)N[C@@ H]  (Cc1ccccc1)C(=O)NCC CN)C(=O)c1c2c(nc(c1) CC)cccc2 | AGGACUCGGCUUGC UGAAGCGCGCGACG GCAAGAGGCGAGG GGCGGCGACUGGUG AGUACGCCAAAAAU UUUGACUAGCGGA GGCUAGAAGGAGA GAGAUGGGUGCGA GAGCGUCGGU | dicarba\_analog\_2 | Target\_lig\_572 | HIV-1 genomic SL3 rna | Target\_146 | 5.89619  6279044  04 |
| 958 | CN(C)CCNC1=CC(=N C2=CC=CC=C21)C3= CC=CC=C3 | AGGACUCGGCUUGC UGAAGCGCGCGACG GCAAGAGGCGAGG GGCGGCGACUGGUG AGUACGCCAAAAAU UUUGACUAGCGGA GGCUAGAAGGAGA GAGAUGGGUGCGA GAGCGUCGGU | quinoline\_der | Target\_lig\_24 | HIV-1 genomic SL3 rna | Target\_146 | 6.53760  2002101  04 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA**  **\_ID** | **pKd** |
| 959 | C1=C(N(C(=C=1)c1c(c c(cc1C)C)C)[Ru]  (=Cc1ccccc1)(Cl) (Cl)P(C1CCCCC1) (C1CCCCC1)C1CCCC  C1)c1c(cc(cc1C)C)C | AGGACUCGGCUUGC UGAAGCGCGCGACG GCAAGAGGCGAGG GGCGGCGACUGGUG AGUACGCCAAAAAU UUUGACUAGCGGA GGCUAGAAGGAGA GAGAUGGGUGCGA GAGCGUCGGU | Ruthenium\_der | Target\_lig\_574 | HIV-1 genomic SL3 rna | Target\_146 | 6.45593  1955649  72 |
| 960 | CN(C)C1=NC=NC2=C 1N=CN2CCN3C=NC4  =C3N=CN=C4N(C)C | AGGACUCGGCUUGC UGAAGCGCGCGACG GCAAGAGGCGAGG GGCGGCGACUGGUG AGUACGCCAAAAAU UUUGACUAGCGGA GGCUAGAAGGAGA GAGAUGGGUGCGA GAGCGUCGGU | NSC54101 | Target\_lig\_575 | HIV-1 genomic SL3 rna | Target\_146 | 4.49485  0021680  09 |
| 961 | C[N+]1(CCCC2=CC=C C=C21)NCC[N+](C)  (C)C.[I-] | AGGACUCGGCUUGC UGAAGCGCGCGACG GCAAGAGGCGAGG GGCGGCGACUGGUG AGUACGCCAAAAAU UUUGACUAGCGGA GGCUAGAAGGAGA GAGAUGGGUGCGA GAGCGUCGGU | NSC18613 | Target\_lig\_576 | HIV-1 genomic SL3 rna | Target\_146 | 5.82390  8740944  32 |
| 962 | CC1=NC2=NC(=NN2C (=C1)N3CCN(CC3)C) C4=CC=C(C=C4)Cl | AGGACUCGGCUUGC UGAAGCGCGCGACG GCAAGAGGCGAGG GGCGGCGACUGGUG AGUACGCCAAAAAU UUUGACUAGCGGA GGCUAGAAGGAGA GAGAUGGGUGCGA GAGCGUCGGU | NSC252359 | Target\_lig\_577 | HIV-1 genomic SL3 rna | Target\_146 | 4.95860  7314841  77 |
| 963 | CN1C2=C(N=C1OCC N(C)C)N(C(=O)N(C2= O)C)C | AGGACUCGGCUUGC UGAAGCGCGCGACG GCAAGAGGCGAGG GGCGGCGACUGGUG AGUACGCCAAAAAU UUUGACUAGCGGA GGCUAGAAGGAGA GAGAUGGGUGCGA GAGCGUCGGU | NSC11936 | Target\_lig\_578 | HIV-1 genomic SL3 rna | Target\_146 | 5.85387  1964321  76 |
| 964 | CC1=C(C(=O)C2=C(C 1=O)N3C[C@H]4[C@  @H] (C3=C2COC(=O)N)N4 C)OC | AGGACUCGGCUUGC UGAAGCGCGCGACG GCAAGAGGCGAGG GGCGGCGACUGGUG AGUACGCCAAAAAU UUUGACUAGCGGA GGCUAGAAGGAGA GAGAUGGGUGCGA GAGCGUCGGU | NSC123111 | Target\_lig\_579 | HIV-1 genomic SL3 rna | Target\_146 | 4.00877  3924307  51 |
| 965 | CN1C2=NC=NC3=C2 C(=CN3C4C(C(C(O4) CO)O)O)C(=N1)N | AGGACUCGGCUUGC UGAAGCGCGCGACG GCAAGAGGCGAGG GGCGGCGACUGGUG AGUACGCCAAAAAU UUUGACUAGCGGA GGCUAGAAGGAGA GAGAUGGGUGCGA GAGCGUCGGU | NSC154020 | Target\_lig\_580 | HIV-1 genomic SL3 rna | Target\_146 | 3.92811  7992693  87 |
| 966 | C[N+]1(CCC2=CC(=C( C=C2C1CC3=CC(=C( C=C3)O)O)O)O)C.  [Br-] | AGGACUCGGCUUGC UGAAGCGCGCGACG GCAAGAGGCGAGG GGCGGCGACUGGUG AGUACGCCAAAAAU UUUGACUAGCGGA GGCUAGAAGGAGA GAGAUGGGUGCGA | NSC121848 | Target\_lig\_581 | HIV-1 genomic SL3 rna | Target\_146 | 3.86966  6231504  99 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA**  **\_ID** | **pKd** |
|  |  | GAGCGUCGGU |  |  |  |  |  |
| 967 | C1=CC=C(C(=C1)/  C=C\2/ C(=O)N(C(=O)N2)/  C=C\3/ C(=O)C4=CC=CC=C4 OC3=O)O | AGGACUCGGCUUGC UGAAGCGCGCGACG GCAAGAGGCGAGG GGCGGCGACUGGUG AGUACGCCAAAAAU UUUGACUAGCGGA GGCUAGAAGGAGA GAGAUGGGUGCGA GAGCGUCGGU | NSC657704 | Target\_lig\_582 | HIV-1 genomic SL3 rna | Target\_146 | 3.78781  2395596  04 |
| 968 | C[N+]1(C2CC(CC1C3 C2O3)OC(=O)C(CO)C 4=CC=CC=C4)C | AGGACUCGGCUUGC UGAAGCGCGCGACG GCAAGAGGCGAGG GGCGGCGACUGGUG AGUACGCCAAAAAU UUUGACUAGCGGA GGCUAGAAGGAGA GAGAUGGGUGCGA GAGCGUCGGU | NSC61809 | Target\_lig\_583 | HIV-1 genomic SL3 rna | Target\_146 | 3.80410  0347590  77 |
| 969 | c1c(cc2c(c1)c(c1c(n2)c c(c(c1)OC)C)Nc1ccc(c( c1)CN1CCN(CC1)C)O  )Cl | AGGACUCGGCUUGC UGAAGCGCGCGACG GCAAGAGGCGAGG GGCGGCGACUGGUG AGUACGCCAAAAAU UUUGACUAGCGGA GGCUAGAAGGAGA GAGAUGGGUGCGA GAGCGUCGGU | acridine\_new\_der v | Target\_lig\_584 | HIV-1 genomic SL3 rna | Target\_146 | 6.17392  5197299  17 |
| 990 | CC1=CC=CN2C1=NC 3=C(C2=O)C=C(C(=N) N3CCOCCO)C(=O)N[  C@@H] (C)C4=CC=CC=C4 | AGGACUCGGCUUGC UGAAGCGCGCGACG GCAAGAGGCGAGG GGCGGCGACUGGUG AGUACGCCAAAAAU UUUGACUAGCGGA GGCUAGAAGGAGA GAGAUGGGUGCGA GAGCGUCGGU | SL3  RNA\_ligand1 | Target\_lig\_605 | SL3 RNA | Target\_146 | 3.78781  2395596  04 |
| 991 | C1=CC=C2C=C(C=CC 2=C1)/C=C/3\ C(=O)N=C(S3)N | AGGACUCGGCUUGC UGAAGCGCGCGACG GCAAGAGGCGAGG GGCGGCGACUGGUG AGUACGCCAAAAAU UUUGACUAGCGGA GGCUAGAAGGAGA GAGAUGGGUGCGA GAGCGUCGGU | SL3  RNA\_ligand3 | Target\_lig\_606 | SL3 RNA | Target\_146 | 4.95860  7314841  77 |
| 992 | COC1=C(C=C(C=C1) NCC2=CC=C(S2)[N+] (=O)[O-])OC | AGGACUCGGCUUGC UGAAGCGCGCGACG GCAAGAGGCGAGG GGCGGCGACUGGUG AGUACGCCAAAAAU UUUGACUAGCGGA GGCUAGAAGGAGA GAGAUGGGUGCGA GAGCGUCGGU | SL3  RNA\_ligand4 | Target\_lig\_607 | SL3 RNA | Target\_146 | 5.95860  7314841  77 |
| 993 | C1=CC=C2C=C(C=CC 2=C1)/C=C/3\ C(=O)NC(=S)N3 | AGGACUCGGCUUGC UGAAGCGCGCGACG GCAAGAGGCGAGG GGCGGCGACUGGUG AGUACGCCAAAAAU UUUGACUAGCGGA GGCUAGAAGGAGA GAGAUGGGUGCGA GAGCGUCGGU | SL3  RNA\_ligand5 | Target\_lig\_608 | SL3 RNA | Target\_146 | 5.45593  1955649  72 |
| 994 | C1=CC=C(C=C1)C[N+  ]2=CC=C(C=C2)C(=O)  N/N=C\ C3=CC=C(C=C3)Br | AGGACUCGGCUUGC UGAAGCGCGCGACG GCAAGAGGCGAGG GGCGGCGACUGGUG AGUACGCCAAAAAU UUUGACUAGCGGA | SL3  RNA\_ligand6 | Target\_lig\_609 | SL3 RNA | Target\_146 | 5.30102  9995663  98 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA**  **\_ID** | **pKd** |
|  |  | GGCUAGAAGGAGA GAGAUGGGUGCGA GAGCGUCGGU |  |  |  |  |  |
| 995 | CC1CCN(CC1)C2=CC  =C(C=C2)N | AGGACUCGGCUUGC UGAAGCGCGCGACG GCAAGAGGCGAGG GGCGGCGACUGGUG AGUACGCCAAAAAU UUUGACUAGCGGA GGCUAGAAGGAGA GAGAUGGGUGCGA GAGCGUCGGU | SL3  RNA\_ligand7 | Target\_lig\_610 | SL3 RNA | Target\_146 | 5 |
| 996 | C1=CC=C(C=C1)OCC NC2=CC=CC=C2N | AGGACUCGGCUUGC UGAAGCGCGCGACG GCAAGAGGCGAGG GGCGGCGACUGGUG AGUACGCCAAAAAU UUUGACUAGCGGA GGCUAGAAGGAGA GAGAUGGGUGCGA GAGCGUCGGU | SL3  RNA\_ligand8 | Target\_lig\_611 | SL3 RNA | Target\_146 | 4.16749  1087293  76 |
| 997 | C1=CC2=C(C=CC(=C 2N=C1)SCCO)[N+] (=O)[O-] | AGGACUCGGCUUGC UGAAGCGCGCGACG GCAAGAGGCGAGG GGCGGCGACUGGUG AGUACGCCAAAAAU UUUGACUAGCGGA GGCUAGAAGGAGA GAGAUGGGUGCGA GAGCGUCGGU | SL3  RNA\_ligand9 | Target\_lig\_612 | SL3 RNA | Target\_146 | 5.76955  1078621  73 |
| 998 | C1=CC=C(C(=C1)/  C=C\2/ C(=O)N(C(=O)N2)/  C=C/3\ C(=O)C4=CC=CC=C4 OC3=O)O | AGGACUCGGCUUGC UGAAGCGCGCGACG GCAAGAGGCGAGG GGCGGCGACUGGUG AGUACGCCAAAAAU UUUGACUAGCGGA GGCUAGAAGGAGA GAGAUGGGUGCGA GAGCGUCGGU | SL3  RNA\_ligand10 | Target\_lig\_613 | SL3 RNA | Target\_146 | 5.34678  7486224  66 |
| 999 | C1=CC=C2C(=C1)C(= O)C3=C(C2=O)C(=C( C=C3NC4=CC=C(C=C 4)S(=O)(=O)N)S(=O) (=O)O)N | AGGACUCGGCUUGC UGAAGCGCGCGACG GCAAGAGGCGAGG GGCGGCGACUGGUG AGUACGCCAAAAAU UUUGACUAGCGGA GGCUAGAAGGAGA GAGAUGGGUGCGA GAGCGUCGGU | SL3  RNA\_ligand11 | Target\_lig\_614 | SL3 RNA | Target\_146 | 4.95860  7314841  77 |
| 1000 | c12ccccc1C(=O) [C@H]1[C@H] (C2=O)C(=CC=C1NC CO)NCCO | AGGACUCGGCUUGC UGAAGCGCGCGACG GCAAGAGGCGAGG GGCGGCGACUGGUG AGUACGCCAAAAAU UUUGACUAGCGGA GGCUAGAAGGAGA GAGAUGGGUGCGA GAGCGUCGGU | SL3  RNA\_ligand12 | Target\_lig\_615 | SL3 RNA | Target\_146 | 4.95467  7021213  34 |
| 1001 | CC1=CC=CN2C1=NC 3=C(C2=O)C=C(C(=N) N3CCCO)C(=O)NC | AGGACUCGGCUUGC UGAAGCGCGCGACG GCAAGAGGCGAGG GGCGGCGACUGGUG AGUACGCCAAAAAU UUUGACUAGCGGA GGCUAGAAGGAGA GAGAUGGGUGCGA GAGCGUCGGU | SL3  RNA\_ligand13 | Target\_lig\_616 | SL3 RNA | Target\_146 | 4.87942  6068794  15 |
| 1002 | CC1=CC=CN2C1=NC 3=C(C2=O)C=C(C(=N) N3CC4=CN=CC=C4)C (=O)NCCN5CCOCC5 | AGGACUCGGCUUGC UGAAGCGCGCGACG GCAAGAGGCGAGG GGCGGCGACUGGUG | SL3  RNA\_ligand14 | Target\_lig\_617 | SL3 RNA | Target\_146 | 4.48148  6060122  11 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA**  **\_ID** | **pKd** |
|  |  | AGUACGCCAAAAAU UUUGACUAGCGGA GGCUAGAAGGAGA GAGAUGGGUGCGA GAGCGUCGGU |  |  |  |  |  |
| 1003 | CC1=CC=CN2C1=NC 3=C(C2=O)C=C(C(=N) N3C[C@H]4CCCO4)C (=O)N5CCN(CC5)C | AGGACUCGGCUUGC UGAAGCGCGCGACG GCAAGAGGCGAGG GGCGGCGACUGGUG AGUACGCCAAAAAU UUUGACUAGCGGA GGCUAGAAGGAGA GAGAUGGGUGCGA GAGCGUCGGU | SL3  RNA\_ligand15 | Target\_lig\_618 | SL3 RNA | Target\_146 | 4.35654  7323513  81 |
| 1004 | C1=CC=C(C=C1)N2C  =C(C(=N2)C3=CC4=C (C=CC5=CC=CC=C54  )OC3=O)C=C6C(=O)N C(=S)NC6=O | AGGACUCGGCUUGC UGAAGCGCGCGACG GCAAGAGGCGAGG GGCGGCGACUGGUG AGUACGCCAAAAAU UUUGACUAGCGGA GGCUAGAAGGAGA GAGAUGGGUGCGA GAGCGUCGGU | SL3  RNA\_ligand16 | Target\_lig\_619 | SL3 RNA | Target\_146 | 4.29242  9823902  06 |
| 1005 | CN1CCN(CC1)CCCN2 C3=CC=CC=C3SC4=C 2C=C(C=C4)C(F)(F)F | AGGACUCGGCUUGC UGAAGCGCGCGACG GCAAGAGGCGAGG GGCGGCGACUGGUG AGUACGCCAAAAAU UUUGACUAGCGGA GGCUAGAAGGAGA GAGAUGGGUGCGA GAGCGUCGGU | SL3  RNA\_ligand17 | Target\_lig\_620 | SL3 RNA | Target\_146 | 4.04575  7490560  68 |
| 1107 | NC1=NC(N)=[NH+]C( NCCCCNC(=[NH2+]) C2=CC=C(C=C2)C(=[ NH2+])NCCCCNC2=[ NH+]C(N)=NC(N)=N2  )=N1 | UUUUUUAGGGAAG AUCUGGCCUUCCCA CAAGGGAAGGCCAG GGAAUUUUCUU | Bisamidinium 2 | Target\_lig\_649 | HIV-1 FSS RNA | Target\_109 | 3.69897  0004336  02 |
| 1126 | CCC1=C(C=C2C=C3C  =CC=CC3=CC2=N1)C (=O)N1CCC[C@H]1C(  =O)N[C@@H](CCC\ C=C\CCC[C@H] (NC(=O) [C@@H]1CCCN1C(= O)C1=C(CC)N=C2C= C3C=CC=CC3=CC2= C1)C(=O)N[C@@H]  (CCCC[NH3+])C(=O) NCCC[NH3+])C(=O)N  [C@@H] (CCCC[NH3+])C(=O) NCCC[NH3+] | UUUUUUAGGGAAG AUCUGGCCUUCCCA CAAGGGAAGGCCAG GGAAUUUUCUU | DCC 11 (2012) | Target\_lig\_653 | HIV-1 FSS RNA | Target\_109 | 5.69897  0004336  02 |
| 1129 | CCC1=C(C=C2C=C3C  =CC=CC3=CC2=N1)C (=O)N(C)[C@@H](C\ C=C\C[C@H] (N(C)C(=O)C1=C(CC) N=C2C=C3C=CC=CC 3=CC2=C1)C(=O)N1C CC[C@H]1C(=O)N(C)  [C@@H] (CC1=CC=CC=C1)C(= O)NCCC[NH3+])C(=O  )N1CCC[C@H]1C(=O) N(C)[C@@H] (CC1=CC=CC=C1)C(= O)NCCC[NH3+] | UUUUUUAGGGAAG AUCUGGCCUUCCCA CAAGGGAAGGCCAG GGAAUUUUCUU | Compound 4E | Target\_lig\_654 | HIV-1 FSS RNA | Target\_109 | 8.30102  9995663  98 |
| 1130 | CCC1=C(C=C2C=C3C  =CC=CC3=CC2=N1)C (=O)N(C)[C@@H](C\ | GGCCUUCCCACAAG GGAAGGCC | Compound 4E | Target\_lig\_654 | HIV-1 FSS DNA | Target\_188 | 7.46852  1082957  74 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA**  **\_ID** | **pKd** |
|  | C=C\C[C@H] (N(C)C(=O)C1=C(CC) N=C2C=C3C=CC=CC 3=CC2=C1)C(=O)N1C CC[C@H]1C(=O)N(C)  [C@@H] (CC1=CC=CC=C1)C(= O)NCCC[NH3+])C(=O  )N1CCC[C@H]1C(=O) N(C)[C@@H] (CC1=CC=CC=C1)C(= O)NCCC[NH3+] |  |  |  |  |  |  |
| 1134 | CCC1=C(C=C2C=C3C  =CC=CC3=CC2=N1)C (=O)N1CCC[C@H]1C(  =O)N[C@@H](C\C=C/ C[C@H](NC(=O) [C@@H]1CCCN1C(= O)C1=C(CC)N=C2C= C3C=CC=CC3=CC2= C1)C(=O)N[C@@H]  (CCCC[NH3+])C(=O) NCCC[NH3+])C(=O)N  [C@@H] (CCCC[NH3+])C(=O) NCCC[NH3+] | GGCCUUCCCACAAG GGAAGGCC | DCC 4 (2012) | Target\_lig\_652 | HIV-1 FSS DNA | Target\_188 | 7.14874  1651280  92 |
| 1135 | CCC1=C(C=C2C=C3C  =CC=CC3=CC2=N1)C (=O)N1CCC[C@H]1C(  =O)N[C@@H](C\C=C/ C[C@H](NC(=O) [C@@H]1CCCN1C(= O)C1=C(CC)N=C2C= C3C=CC=CC3=CC2= C1)C(=O)N[C@@H]  (CCCC[NH3+])C(=O) NCCC[NH3+])C(=O)N  [C@@H] (CCCC[NH3+])C(=O) NCCC[NH3+] | UUUUUUAGGGAAG AUCUGGCCUUCCCA CAAGGGAAGGCCAG GGAAUUUUCUU | DCC 4 (2012) | Target\_lig\_652 | HIV-1 FSS RNA | Target\_109 | 7.18045  6064458  13 |
| 1138 | CCC1=C(C=C2C=C3C  =CC=CC3=CC2=N1)C (=O)N[C@@H](C\ C=C\C[C@H] (NC(=O)C1=C(CC)N= C2C=C3C=CC=CC3= CC2=C1)C(=O)N1CCC [C@H]1C(=O)N[C@@ H] (CC1=CC=CC=C1)C(= O)NCCC[NH3+])C(=O  )N1CCC[C@H]1C(=O) N[C@@H] (CC1=CC=CC=C1)C(= O)NCCC[NH3+] | UUUUUUAGGGAAG AUCUGGCCUUCCCA CAAGGGAAGGCCAG GGAAUUUUCUU | DCC 5 (2012) | Target\_lig\_655 | HIV-1 FSS RNA | Target\_109 | 7.05060  9993355  09 |
| 1139 | CCC1=C(C=C2C=C3C  =CC=CC3=CC2=N1)C (=O)N[C@@H](C\ C=C\C[C@H] (NC(=O)C1=C(CC)N= C2C=C3C=CC=CC3= CC2=C1)C(=O)N1CCC [C@H]1C(=O)N[C@@ H] (CC1=CC=CC=C1)C(= O)NCCC[NH3+])C(=O  )N1CCC[C@H]1C(=O) N[C@@H] (CC1=CC=CC=C1)C(= O)NCCC[NH3+] | GGCCUUCCCACAAG GGAAGGCC | DCC 5 (2012) | Target\_lig\_655 | HIV-1 FSS DNA | Target\_188 | 7.01772  8766960  43 |
| 1143 | CC(=O)NC1=NC(=CS1  )C1=CC(NC(=O)C(CN | GGCAGAUCUGAGCC UGGGAGCUCUCUGC | S-Amino acid conjugate 13b | Target\_lig\_656 | HIV-1 TAR RNA | Target\_19 | 6.61978  8758288 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA**  **\_ID** | **pKd** |
|  | C(=O)[C@@H] ([NH3+])CCCC[NH3+]  )NC(=O)[C@@H]  ([NH3+])CCCC[NH3+]  )=CC=C1 | C |  |  |  |  | 39 |
| 1146 | CC(=O)NC1=NC(=CS1  )C1=CC(NC(=O)C(CN C(=O)[C@@H] ([NH3+])CCCNC(N)=[ NH2+])NC(=O)  [C@@H] ([NH3+])CCCNC(N)=[ NH2+])=CC=C1 | GGCAGAUCUGAGCC UGGGAGCUCUCUGC C | S-Amino acid conjugate 14b | Target\_lig\_657 | HIV-1 TAR RNA | Target\_19 | 6.95860  7314841  77 |
| 1150 | CCC1=C(C=C2C=C3C  =CC=CC3=CC2=N1)C (=O)N[C@@H] (CCN1C=C(C[C@H] (NC(=O)C2=C(CC)N= C3C=C4C=CC=CC4= CC3=C2)C(=O)N2CCC [C@H]2C(=O)N[C@@ H] (CC2=CC=CC=C2)C(= O)NCCC[NH3+])N=N 1)C(=O)N1CCC[C@H]  1C(=O)N[C@@H] (CC1=CC=CC=C1)C(= O)NCCC[NH3+] | UUUUUUAGGGAAG AUCUGGCCUUCCCA CAAGGGAAGGCCAG GGAAUUUUCUU | DCC 3 (2017) | Target\_lig\_658 | HIV-1 FSS  RNA; 5-fold excess tRNA | Target\_109 | 7.49485  0021680  09 |
| 1152 | CCC1=C(C=C2C=C3C  =CC=CC3=CC2=N1)C (=O)N[C@@H] (CC1=CN(CC[C@H] (N(C)C(=O)C2=C(CC) N=C3C=C4C=CC=CC 4=CC3=C2)C(=O)N2C CC[C@H]2C(=O)N(C)  [C@@H] (CC2=CC=CC=C2)C(= O)NCCC[NH3+])N=N 1)C(=O)N1CCC[C@H]  1C(=O)N[C@@H] (CC1=CC=CC=C1)C(= O)NCCC[NH3+] | UUUUUUAGGGAAG AUCUGGCCUUCCCA CAAGGGAAGGCCAG GGAAUUUUCUU | DCC 4 (2017) | Target\_lig\_659 | HIV-1 FSS  RNA; 5-fold excess tRNA | Target\_109 | 7.20760  8310501  75 |
| 1154 | CCC1=C(C=C2C=C3C  =CC=CC3=CC2=N1)C (=O)N[C@@H] (CC1=CN(CC[C@H] (N(C)C(=O)C2=C(CC) N=C3C=C4C=CC=CC 4=CC3=C2)C(=O)N2C CC[C@H]2C(=O)N[C  @@H] (CC2=CC=CC=C2)C(= O)NCCC[NH3+])N=N 1)C(=O)N1CCC[C@H]  1C(=O)N(C)[C@@H] (CC1=CC=CC=C1)C(= O)NCCC[NH3+] | UUUUUUAGGGAAG AUCUGGCCUUCCCA CAAGGGAAGGCCAG GGAAUUUUCUU | DCC 5 (2017) | Target\_lig\_660 | HIV-1 FSS  RNA; 5-fold excess tRNA | Target\_109 | 7.50863  8306165  73 |
| 1155 | CCC1=C(C=C2C=C3C  =CC=CC3=CC2=N1)C (=O)N(C)[C@@H] (CCN1C=C(C[C@H] (N(C)C(=O)C2=C(CC) N=C3C=C4C=CC=CC 4=CC3=C2)C(=O)N2C CC[C@H]2C(=O)N(C)  [C@@H] (CC2=CC=CC=C2)C(= O)NCCC[NH3+])N=N 1)C(=O)N1CCC[C@H]  1C(=O)N(C)[C@@H] (CC1=CC=CC=C1)C(= | UUUUUUAGGGAAG AUCUGGCCUUCCCA CAAGGGAAGGCCAG GGAAUUUUCUU | DCC 7 (2017) | Target\_lig\_661 | HIV-1 FSS RNA | Target\_109 | 7.79588  0017344  08 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA**  **\_ID** | **pKd** |
|  | O)NCCC[NH3+] |  |  |  |  |  |  |
| 1226 | C[NH+] (C)CCCOC1=CC=C2[ NH+]=C(N)N(CCC[N  H+](C)C)C2=C1 | CUCCCCUGUGAGGA ACUACUGUCUUCAC GCAGAAAGCGUCUA GCCAUGGCGUUAGU AUGAGUGUCGUGC AGCCUCCAGG | Benzimidazole 3 | Target\_lig\_125 6 | HCV IRES IIa  40-mer | Target\_67 | 4.76955  1078621  73 |
| 1227 | C[NH+] (C)CCCOC1=CC=C2N  =C3NCC(C[NH+] (C)C)CN3C2=C1 | CUCCCCUGUGAGGA ACUACUGUCUUCAC GCAGAAAGCGUCUA GCCAUGGCGUUAGU AUGAGUGUCGUGC AGCCUCCAGG | Benzimidazole 10 | Target\_lig\_689 | HCV IRES IIa  40-mer | Target\_67 | 5.45593  1955649  72 |
| 1228 | C[NH+] (C)CCCN1C(N)=[NH+  ]C2=CC=C3OC(CC[N H+](C)C)CC3=C12 | CUCCCCUGUGAGGA ACUACUGUCUUCAC GCAGAAAGCGUCUA GCCAUGGCGUUAGU AUGAGUGUCGUGC AGCCUCCAGG | Benzimidazole 11 / Isis-11 | Target\_lig\_690 | HCV IRES IIa  40-mer | Target\_67 | 5.76955  1078621  73 |
| 1230 | C[NH+] (C)CCCN1C(N)=[NH+  ]C2=CC=C3OCC(C[N H+](C)C)CC3=C12 | CUCCCCUGUGAGGA ACUACUGUCUUCAC GCAGAAAGCGUCUA GCCAUGGCGUUAGU AUGAGUGUCGUGC AGCCUCCAGG | Benzimidazole 12 | Target\_lig\_691 | HCV IRES IIa  40-mer | Target\_67 | 6.06048  0747381  38 |
| 1231 | C[NH+] (C)CC1CNC2=[NH+]C 3=CC=C4OCC(C[NH+  ](C)C)CC4=C3N2C1 | CUCCCCUGUGAGGA ACUACUGUCUUCAC GCAGAAAGCGUCUA GCCAUGGCGUUAGU AUGAGUGUCGUGC AGCCUCCAGG | Benzimidazole 13  / Isis-13 | Target\_lig\_125 7 | HCV IRES IIa  40-mer | Target\_67 | 6.14266  7503568  73 |
| 1233 | C[NH+] (C)CC1CC2=C3N4CC( C[NH+] (C)C)CNC4=[NH+]C3  =CC=C2O1 | GAGGAACUACUGG AGACGUGCAGCCUC | Isis-22 | Target\_lig\_692 | HCV IRES RNA | Target\_68 | 5.65757  7319177  79 |
| 1234 | C[NH+] (C)CCC[NH+]=C(C1= CC=C(C=C1)C(=[NH+  ]CCC[NH+](C)C)N)N | UUUUUUAGGGAAG AUCUGGCCUUCCCA CAAGGGAAGGCCAG GGAAUUUUCUU | DB213 | Target\_lig\_693 | HIV-1 FSS RNA | Target\_109 | 3.44369  7499232  71 |
| 1236 | CC[NH+] (CC)CCOC1=CC=C(C  =C1)/C(=C(\ C2=CC=CC=C2)/Cl)/ C3=CC=CC=C3 | GCACUAUGGGCGCC AGCGUCAAUGACGC UGACGGUACAGCCA GACAAUUAUUGUC UGGUAUAGUGC | Clomiphene | Target\_lig\_694 | HIV-1 RRE  IIB, 100-fold Excess tRNA | Target\_80 | 5.22184  8749616  36 |
| 1240 | C[NH+]1CCC(=C2C3= CC=CC=C3C=CC4=C C=CC=C42)CC1 | GCACUAUGGGCGCC AGCGUCAAUGACGC UGACGGUACAGCCA GACAAUUAUUGUC UGGUAUAGUGC | Cyproheptadine | Target\_lig\_695 | HIV-1 RRE IIB | Target\_80 | 5.74472  7494896  69 |
| 1245 | CN1C=C(C([O-])=O)C (=O)C2=CC(N)=C(C= C12)N1CCN(CC1)C1= CC=CC=N1 | GGCAGAUCUGAGCC UGGGAGCUCUCUGC C | WM5 | Target\_lig\_125 8 | HIV-1 TAR | Target\_19 | 7.72124  6399047  17 |
| 1251 | CC(=O)NC1=NC(=CS1  )C1=CC(NC(=O)  [C@@H] ([NH3+])CCCC[NH3+]  )=CC=C1 | GGCAGAUCUGAGCC UGGGAGCUCUCUGC C | S-Amino acid conjugate 1b | Target\_lig\_698 | HIV-1 TAR | Target\_19 | 5.12493  8736608  3 |
| 1252 | CC(=O)NC1=NC(=CS1  )C1=CC(NC(=O)  [C@@H] ([NH3+])CC2=CNC=N 2)=CC=C1 | GGCAGAUCUGAGCC UGGGAGCUCUCUGC C | S-Amino acid conjugate 3b | Target\_lig\_699 | HIV-1 TAR | Target\_19 | 4.75696  1951313  71 |
| 1253 | CC1=NC2=C(C=C1)C(  =C(S2)C(=O)NC3=CC  =CC(=C3)C(F)(F)F)N | GGCAGAUCUGAGCC UGGGAGCUCUCUGC C | ST4133609 | Target\_lig\_700 | HIV-1 TAR | Target\_19 | 5.61978  8758288  39 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA**  **\_ID** | **pKd** |
| 1255 | COC1=C(C=C2C(=C1) C(=NC(=N2)N3CC[NH 2+]CC3)N)OC | GAGUAGAAACAAG GCUUCGGCCUGCUU UUGCU | DPQ | Target\_lig\_701 | Influenza RNA promoter | Target\_217 | 4.29670  8621881  34 |
| 1256 | CCC(=O)N1CCN(CC1) C1=NC(N)=C2C=C(O C)C(OC)=CC2=[NH+] 1 | GAGUAGAAACAAG GCUUCGGCCUGCUU UUGCU | DPQ6 | Target\_lig\_702 | Influenza RNA promoter | Target\_217 | 3.94233  3896090  17 |
| 1257 | COC1=CC2=[NH+]C(  =NC(N)=C2C=C1OC) N1CCN(CC1)C(=O)C( C)C | GAGUAGAAACAAG GCUUCGGCCUGCUU UUGCU | DPQ7 | Target\_lig\_703 | Influenza RNA promoter | Target\_217 | 3.79997  0733446  23 |
| 1258 | CCCC(=O)N1CCN(CC 1)C1=NC(N)=C2C=C( OC)C(OC)=CC2=[NH+  ]1 | GAGUAGAAACAAG GCUUCGGCCUGCUU UUGCU | DPQ8 | Target\_lig\_704 | Influenza RNA promoter | Target\_217 | 4.35310  6375832  25 |
| 1259 | COC1=CC2=[NH+]C(  =NC(N)=C2C=C1OC) N1CCN(CC1)C(=O)C1 CC1 | GAGUAGAAACAAG GCUUCGGCCUGCUU UUGCU | DPQ10 | Target\_lig\_705 | Influenza RNA promoter | Target\_217 | 3.89551  2888687  6 |
| 1260 | CCOC(=O)C1=CC=CC  =C1NC(=O)N2CCCN( CC2)CC3=CSC(=N3)C | CGGUGUAAGUGCA GCCCGUCUUACACC GUGCGGCACAGCGG AAACGCUGAUGUCG UAUACAGGGCU | Compound 43 (MTDB) | Target\_lig\_706 | SARS-  Pseudoknot Construct | Target\_218 | 3.67778  0705266  08 |
| 1261 | CCN(CC)CCOC1=CC= C(C=C1)NC2=NC(=N C3=CC=CC=C32)C4= CC=CC=C4NC(=O)CC N5CCN(CC5)C | GGAGGAGGGGGAG GAGGA | Compound 1  (2017) | Target\_lig\_707 | HCV IRES-A | Target\_219 | 6.03245  2023781  14 |
| 1262 | CCN(CC)CCOC1=CC= C(C=C1)NC2=NC(=N C3=CC=CC=C32)C4= CC=CC=C4NC(=O)CC N5CCN(CC5)C | UGAUGAGUGUGAG GAGGA | Compound 1  (2017) | Target\_lig\_707 | HCV IRES-A 1  Mutant | Target\_220 | 5.43062  6090384  95 |
| 1266 | CCN(CC)CCOC1=CC= C(C=C1)NC2=NC(=N C3=CC=CC=C32)C4= CC=CC=C4NC(=O)CC N5CCN(CC5)C | CCUGACUAGUCUUU CAGG | Compound 1  (2017) | Target\_lig\_707 | HCV IRES-A DNA | Target\_222 | 4.83863  1997765  03 |
| 1275 | COC1=CC(CC[NH3+])  =C(C(CC[NH3+])=C1) C1=CC(C)=C(C(C)=C1  )C1=CC(CC[NH3+])= C(O)C(CC[NH3+])=C1 | GCACUAUGGGCGCC AGCGUCAAUGACGC UGACGGUACAGCCA GACAAUUAUUGUC UGGUAUAGUGC | p-Terphenyl 6b | Target\_lig\_711 | HIV-1 RRE IIB | Target\_80 | 6.22184  8749616  36 |
| 1322 | C(CN1C=C(CNC2=C3 C=CC=CC3=[NH+]C3  =C2OC2=C3C=CC=C2  )N=N1)C[NH+]1CCCC C1 | GGAGGAGGGGGAG GAGGA | Quindoline CK1- 14 | Target\_lig\_723 | IRES RNA G-  quadruplex | Target\_257 | 5.86012  0913598  76 |
| 1710 | COC1=C(C=C2C(=C1) C(=NC(=N2)N3CC[NH 2+]CC3)N)OC | GGCAGAUCUGAGCC UGGGAGCUCUCUGC C | DPQ | Target\_lig\_701 | HIV-1 TAR RNA | Target\_19 | 4.36653  1544420  41 |
| 1713 | C1=CC(=CC=C1C(=N) N)OCCCCCOC2=CC= C(C=C2)C(=N)N | GGCAGAUCUGAGCC UGGGAGCUCUCUGC C | Pentamidine | Target\_lig\_953 | HIV-1 TAR RNA | Target\_19 | 3.47886  1916295  96 |
| 1780 | 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 | GGCAGAUCUGAGCC UGGGAGCUCUCUGC C | Neomycin | Target\_lig\_4 | HIV-1 TAR RNA | Target\_19 | 4.67778  0705266  08 |
| 1781 | NCCCCC(C(=O)OCO C[C@H]1O[C@H] (C[C@@H]1O)C(=O)  Nc1cccc(c1)c1csc(n1)N C(=O)C)N | GGCAGAUCUGAGCC UGGGAGCUCUCUGC C | Compound 3ab | Target\_lig\_999 | HIV-1 TAR RNA | Target\_19 | 4.52287  8745280  34 |
| 1782 | NCCCCC(C(=O)OCO[ | GGCAGAUCUGAGCC | Compound 3bb | Target\_lig\_100 | HIV-1 TAR | Target\_19 | 5.09691 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA**  **\_ID** | **pKd** |
|  | C@H]1C[C@@H] (O[C@@H]1COCOC(  =O)C(CCCCN)N)C(=O  )Nc1cccc(c1)c1csc(n1) NC(=O)C)N | UGGGAGCUCUCUGC C |  | 0 | RNA |  | 0013008  06 |
| 1783 | CC(=O)Nc1scc(n1)c1cc cc(c1)NC(=O)  [C@H]1C[C@@H]  ([C@H] (O1)COCOC(=O)C(CC CN=C(N)N)N)O | GGCAGAUCUGAGCC UGGGAGCUCUCUGC C | Compound 3cb | Target\_lig\_100 1 | HIV-1 TAR RNA | Target\_19 | 4.88605  6647693  16 |
| 1784 | CC(=O)Nc1scc(n1)c1cc cc(c1)NC(=O)  [C@H]1C[C@@H]  ([C@H] (O1)COCOC(=O)C(CC CN=C(N)N)N)OCOC(  =O)C(CCCN=C(N)N)N | GGCAGAUCUGAGCC UGGGAGCUCUCUGC C | Compound 3db | Target\_lig\_100 2 | HIV-1 TAR RNA | Target\_19 | 5 |
| 1785 | NCCCCC(C(=O)OCO C[C@H]1OC(C[C@@  H]1O)C(=O)Nc1cccc(c 1)c1csc(n1)NC(=O)C) N | GGCAGAUCUGAGCC UGGGAGCUCUCUGC C | Compound 3aa | Target\_lig\_100 3 | HIV-1 TAR RNA | Target\_19 | 4.85387  1964321  76 |
| 1786 | NCCCCC(C(=O)OCO[ C@H]1CC(O[C@@H] 1COCOC(=O)C(CCCC  N)N)C(=O)Nc1cccc(c1  )c1csc(n1)NC(=O)C)N | GGCAGAUCUGAGCC UGGGAGCUCUCUGC C | Compound 3ba | Target\_lig\_100 4 | HIV-1 TAR RNA | Target\_19 | 4.88605  6647693  16 |
| 1787 | 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 | GGCAGAUCUGAGCC UGGGAGCUCUCUGC C | Neomycin | Target\_lig\_4 | HIV-1 TAR ab | Target\_19 | 4.50863  8306165  73 |
| 1817 | CN(C)C1=C(N=C(C(= N1)N)C(=O) [NH+]=C(N)N)C#CC2  =CC=CC=C2 | GGAUCAAUAGCAG GUGUGGCACACCAG UCAUACCUUGAUCC | DMA-135 | Target\_lig\_101 9 | EV71 SLII RNA | Target\_329 | 6.28399  6656365  2 |
| 1818 | O=C(c1nc(Cl)c(nc1N) N(C)C)NC(=[NH2+])N | GGAUCAAUAGCAG GUGUGGCACACCAG UCAUACCUUGAUCC | DMA-001 | Target\_lig\_102 0 | EV71 SLII RNA | Target\_329 | 6.23657  2006437  06 |
| 1819 | CN(c1nc(N)c(nc1c1ccc (cc1)c1ccccc1)C(=O)N C(=[NH2+])N)C | GGAUCAAUAGCAG GUGUGGCACACCAG UCAUACCUUGAUCC | DMA-155 | Target\_lig\_102 1 | EV71 SLII RNA | Target\_329 | 6.25181  1972993  8 |
| 2047 | CC(=O)C1=CC2=C(C= C1)SC3=CC=CC=C3N 2CCCN(C)C | GGGCUAGCACUCUG GUAUCACGGUACCU UUGUGCGCCC | Acetylpromazine | Target\_lig\_176 | CVB loop D RNA | Target\_373 | 3.48148  6060122  11 |
| 2048 | CC(=O)C1=CC2=C(C= C1)SC3=CC=CC=C3N 2CCCN(C)C | GGGGUUGUACCCAC CCCAC | Acetylpromazine | Target\_lig\_176 | Polio virus loop B RNA | Target\_374 | 2.74472  7494896  69 |
| 2049 | NCCCOc1ccc(cc1CNC CCCNC(=N)N)c1cscc1 | GGCAGAUCUGAGCC UGGGAGCUCUCUGC C | Rbt427 | Target\_lig\_112 4 | HIV-1 TAR RNA | Target\_19 | 6.06550  1548756  43 |
| 2050 | NCCCOc1ccc(cc1CNC CCCNC(=N)N)c1cc2c(  o1)cccc2 | GGCAGAUCUGAGCC UGGGAGCUCUCUGC C | Rbt429 | Target\_lig\_112 5 | HIV-1 TAR RNA | Target\_19 | 6.72124  6399047  17 |
| 2051 | NCCCOc1ccc(cc1CNC Cc1ccc(cc1)CNC(=N)N  )c1cc2c(s1)cccc2 | GGCAGAUCUGAGCC UGGGAGCUCUCUGC C | Rbt446 | Target\_lig\_112 6 | HIV-1 TAR RNA | Target\_19 | 6.65955  5885159  88 |
| 2052 | NCCCOc1ccc(cc1CNC CCCN(C)C)c1cc2c(s1)  cccc2 | GGCAGAUCUGAGCC UGGGAGCUCUCUGC C | Rbt489 | Target\_lig\_112 7 | HIV-1 TAR RNA | Target\_19 | 6.22914  7988357  86 |
| 2053 | NCCCOc1ccc(cc1CNC CC1CCNCC1)c1cc2c(s  1)cccc2 | GGCAGAUCUGAGCC UGGGAGCUCUCUGC C | Rbt537 | Target\_lig\_112 8 | HIV-1 TAR RNA | Target\_19 | 6.32239  3047279  51 |
| 2054 | NCCCOc1ccc(cc1CNC | GGCAGAUCUGAGCC | Rbt549 | Target\_lig\_112 | HIV-1 TAR | Target\_19 | 6.82102 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA**  **\_ID** | **pKd** |
|  | CC1CCNCC1)c1ccc2c(  c1)[nH]cc2 | UGGGAGCUCUCUGC C |  | 9 | RNA |  | 3052706  83 |
| 2055 | NCCCOc1ccc(cc1CNC CC1CCNCC1)c1ccc2c( c1)oc(c2)C(=O)NC | GGCAGAUCUGAGCC UGGGAGCUCUCUGC C | Rbt551 | Target\_lig\_113 0 | HIV-1 TAR RNA | Target\_19 | 5.47366  0722610  16 |
| 2056 | NCCCOc1ccc(cc1CNC CC1CCNCC1)c1ccccn 1 | GGCAGAUCUGAGCC UGGGAGCUCUCUGC C | Rbt552 | Target\_lig\_113 1 | HIV-1 TAR RNA | Target\_19 | 6.36855  6230986  83 |
| 2057 | NCCCOc1ccc(cc1CNC CC1CCNCC1)c1ccc2c(  c1)c(=O)cco2 | GGCAGAUCUGAGCC UGGGAGCUCUCUGC C | Rbt555 | Target\_lig\_113 2 | HIV-1 TAR RNA | Target\_19 | 5.51712  6416391  25 |
| 2058 | NCCCOc1ccc(cc1CNC CC1CCNCC1)c1ccc2c(  n1)cccc2 | GGCAGAUCUGAGCC UGGGAGCUCUCUGC C | Rbt556 | Target\_lig\_113 3 | HIV-1 TAR RNA | Target\_19 | 6.35066  5141287  86 |
| 2059 | NCCCOc1ccc(cc1CNC CC1CCNCC1)c1ccccc1 | GGCAGAUCUGAGCC UGGGAGCUCUCUGC C | Rbt567 | Target\_lig\_113 4 | HIV-1 TAR RNA | Target\_19 | 5.92445  3038607  47 |
| 2060 | N1CCN(CC1)CCCNCc  1cc(ccc1OCc1cc2c(s1)c ccc2)c1cc2c(s1)cccc2 | GGCAGAUCUGAGCC UGGGAGCUCUCUGC C | Rbt603 | Target\_lig\_113 5 | HIV-1 TAR RNA | Target\_19 | 5.53910  2157243  45 |
| 2061 | CN(CCCCOc1ccc(cc1 CNCCCN1CCNCC1)c  1cc2c(s1)cccc2)C | GGCAGAUCUGAGCC UGGGAGCUCUCUGC C | Rbt605 | Target\_lig\_113 6 | HIV-1 TAR RNA | Target\_19 | 5.94692  1556516  58 |
| 2098 | CN(CCCOc1ccc2c(c1) n1CC(CNc1n2)CN(C)C  )C | GGCCGAGUAGUGU UGGGUCGCGAAAG GCC | Benzimidazole10 | Target\_lig\_114 1 | HCV IRES  Domain II | Target\_66 | 5.45593  1955649  72 |
| 2099 | CN(CCCn1c(N)nc2c1c 1CC(Oc1cc2)CN(C)C) C | GGCCGAGUAGUGU UGGGUCGCGAAAG GCC | Benzimidazole11 | Target\_lig\_114 2 | HCV IRES  Domain II | Target\_66 | 5.76955  1078621  73 |
| 2100 | CN(CCCn1c(N)nc2c1c 1CC(COc1cc2)CN(C)C  )C | GGCCGAGUAGUGU UGGGUCGCGAAAG GCC | Benzimidazole12 | Target\_lig\_114 3 | HCV IRES  Domain II | Target\_66 | 6.06550  1548756  43 |
| 2142 | [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 | GGCCGAGUAGUGU UGGGUCGCGAAAG GCC | Tobramycin | Target\_lig\_540 | HCV IRES  Domain IIId | Target\_66 | 5.65757  7319177  79 |
| 2143 | 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 | GGCCGAGUAGUGU UGGGUCGCGAAAG GCC | Neomycin B | Target\_lig\_125 1 | HCV IRES  Domain IIId | Target\_66 | 5.53760  2002101  04 |
| 2144 | NCC1OC(OC2C(N)CC (C(C2O)OC2OC(CN)C (C(C2O)O)N)N)C(CC1 O)N | GGCCGAGUAGUGU UGGGUCGCGAAAG GCC | Compd 32 | Target\_lig\_115 5 | HCV IRES  Domain IIId | Target\_66 | 5.16749  1087293  76 |
| 2145 | NCC1OC(OC2C(N)CC (C(C2O)OC2OC(CN)C (CC2N)O)N)C(C(C1O C1OC(CO)C(C(C1O)O  )N)N)O | GGCCGAGUAGUGU UGGGUCGCGAAAG GCC | Compd 33 | Target\_lig\_115 6 | HCV IRES  Domain IIId | Target\_66 | 6.15490  1959985  74 |
| 2146 | NCC1OC(OC2C(N)CC (C(C2O)OC2OC(CN)C (CC2N)O)N)C(C(C1O C1OC(CO)C(C(C1O)N  )O)O)N | GGCCGAGUAGUGU UGGGUCGCGAAAG GCC | Compd 34 | Target\_lig\_115 7 | HCV IRES  Domain IIId | Target\_66 | 6.60205  9991327  96 |
| 2147 | NCC1OC(OC2C(N)CC (C(C2O)OC2OC(CN)C (C(C2O)N)O)N)C(CC1 | GGCCGAGUAGUGU UGGGUCGCGAAAG GCC | Compd 35 | Target\_lig\_115 8 | HCV IRES  Domain IIId | Target\_66 | 5.56863  6235841  01 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA**  **\_ID** | **pKd** |
|  | O)N |  |  |  |  |  |  |
| 2148 | NCC1OC(OC2C(N)CC (C(C2O)OC2OC(CN)C (CC2N)O)N)C(C(C1O) OC1OC(CO)C(C(C1O) O)N)O | GGCCGAGUAGUGU UGGGUCGCGAAAG GCC | Compd 37 | Target\_lig\_115 9 | HCV IRES  Domain IIId | Target\_66 | 5.63827  2163982  41 |
| 2149 | NCC1OC(OC2C(N)CC (C(C2O)OC2OC(CN)C (CC2N)O)N)C(C(C1O C1OC(CO)C(C(C1N)O  )O)N)O | GGCCGAGUAGUGU UGGGUCGCGAAAG GCC | Compd 38 | Target\_lig\_116 0 | HCV IRES  Domain IIId | Target\_66 | 5.63827  2163982  41 |
| 2150 | NCC1OC(OC2C(N)CC (C(C2O)OC2OC(COC3 OC(CN)C(C(C3O)O)O  )C(C(C2N)O)N)N)C(C C1O)N | GGCCGAGUAGUGU UGGGUCGCGAAAG GCC | Compd 39 | Target\_lig\_116 1 | HCV IRES  Domain IIId | Target\_66 | 5.39794  0008672  04 |
| 2151 | NCC1OC(OC2C(N)CC (C(C2O)OC2OC(COC3 OC(CN)C(C(C3O)O)O  )C(C(C2N)O)N)N)C(C C1O)N | GGCCGAGUAGUGU UGGGUCGCGAAAG GCC | Compd 40 | Target\_lig\_128 1 | HCV IRES  Domain IIId | Target\_66 | 5.48148  6060122  11 |
| 2152 | NCC1OC(OC2C(N)CC (C(C2O)OC2OC(CN)C (CC2N)O)N)C(C(C1O) OC1OC(CO)C(C(C1N) O)O)N | GGCCGAGUAGUGU UGGGUCGCGAAAG GCC | Compd 41 | Target\_lig\_116 2 | HCV IRES  Domain IIId | Target\_66 | 6.27572  4130399  21 |
| 2153 | NCC1OC(OC2C(N)CC (C(C2O)OC2OC(CN)C (CC2N)O)N)C(C(C1O) OC1OC(CO)C(C(C1N) O)O)N | GGCCGAGUAGUGU UGGGUCGCGAAAG GCC | Compd 42 | Target\_lig\_128 2 | HCV IRES  Domain IIId | Target\_66 | 5.69897  0004336  02 |
| 2154 | NCC1OC(OC2C(N)CC (C(C2O)OC2OC(CN)C (CC2N)O)N)C(C(C1O C1OC(CO)C(C(C1N)O  )O)N)O | GGCCGAGUAGUGU UGGGUCGCGAAAG GCC | Compd 43 | Target\_lig\_128 3 | HCV IRES  Domain IIId | Target\_66 | 6 |
| 2185 | CC1(COC(C(C1NC)O) OC2C(CC(C(C2O)OC3 C(CC=C(O3)CN)N)N) N)O | CUGUCUUCACGCAG AAAGCGUCUAGCCA UGGCGUUAGUAUG AGUGUCG | sisomicin | Target\_lig\_10 | HCV IRES  Domain Iib | Target\_408 | 5.36653  1544420  41 |
| 2186 | [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 | CUGUCUUCACGCAG AAAGCGUCUAGCCA UGGCGUUAGUAUG AGUGUCG | Tobramycin | Target\_lig\_540 | HCV IRES  Domain Iib | Target\_408 | 5.56863  6235841  01 |
| 2187 | 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 | CUGUCUUCACGCAG AAAGCGUCUAGCCA UGGCGUUAGUAUG AGUGUCG | Neomycin B | Target\_lig\_125 1 | HCV IRES  Domain Iib | Target\_408 | 5.53760  2002101  04 |
| 2188 | NCC1OC(OC2C(N)CC (C(C2O)OC2OC(CN)C (C(C2O)O)N)N)C(CC1 O)N | CUGUCUUCACGCAG AAAGCGUCUAGCCA UGGCGUUAGUAUG AGUGUCG | Compd 32 | Target\_lig\_115 5 | HCV IRES  Domain Iib | Target\_408 | 4.92081  8753952  38 |
| 2189 | NCC1OC(OC2C(N)CC (C(C2O)OC2OC(CN)C (CC2N)O)N)C(C(C1O C1OC(CO)C(C(C1O)O  )N)N)O | CUGUCUUCACGCAG AAAGCGUCUAGCCA UGGCGUUAGUAUG AGUGUCG | Compd 33 | Target\_lig\_115 6 | HCV IRES  Domain Iib | Target\_408 | 5.52287  8745280  34 |
| 2190 | NCC1OC(OC2C(N)CC (C(C2O)OC2OC(CN)C | CUGUCUUCACGCAG AAAGCGUCUAGCCA | Compd 34 | Target\_lig\_115 7 | HCV IRES  Domain Iib | Target\_408 | 6.37675  0709602 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA**  **\_ID** | **pKd** |
|  | (CC2N)O)N)C(C(C1O C1OC(CO)C(C(C1O)N  )O)O)N | UGGCGUUAGUAUG AGUGUCG |  |  |  |  | 1 |
| 2191 | NCC1OC(OC2C(N)CC (C(C2O)OC2OC(CN)C (C(C2O)N)O)N)C(CC1 O)N | CUGUCUUCACGCAG AAAGCGUCUAGCCA UGGCGUUAGUAUG AGUGUCG | Compd 35 | Target\_lig\_115 8 | HCV IRES  Domain Iib | Target\_408 | 5.74472  7494896  69 |
| 2192 | NCC1OC(OC2C(N)CC (C(C2O)OC2OC(COC3 OC(CO)C(C(C3N)O)O  )C(C(C2N)O)O)N)C(C C1O)N | CUGUCUUCACGCAG AAAGCGUCUAGCCA UGGCGUUAGUAUG AGUGUCG | Compd 36 | Target\_lig\_116 3 | HCV IRES  Domain Iib | Target\_408 | 5.02687  2146400  3 |
| 2193 | NCC1OC(OC2C(N)CC (C(C2O)OC2OC(CN)C (CC2N)O)N)C(C(C1O) OC1OC(CO)C(C(C1O) O)N)O | CUGUCUUCACGCAG AAAGCGUCUAGCCA UGGCGUUAGUAUG AGUGUCG | Compd 37 | Target\_lig\_115 9 | HCV IRES  Domain Iib | Target\_408 | 6.55284  1968657  78 |
| 2194 | NCC1OC(OC2C(N)CC (C(C2O)OC2OC(CN)C (CC2N)O)N)C(C(C1O C1OC(CO)C(C(C1N)O  )O)N)O | CUGUCUUCACGCAG AAAGCGUCUAGCCA UGGCGUUAGUAUG AGUGUCG | Compd 38 | Target\_lig\_116 0 | HCV IRES  Domain Iib | Target\_408 | 4.92081  8753952  38 |
| 2195 | NCC1OC(OC2C(N)CC (C(C2O)OC2OC(COC3 OC(CN)C(C(C3O)O)O  )C(C(C2N)O)N)N)C(C C1O)N | CUGUCUUCACGCAG AAAGCGUCUAGCCA UGGCGUUAGUAUG AGUGUCG | Compd 39 | Target\_lig\_116 1 | HCV IRES  Domain Iib | Target\_408 | 5.58502  6652029  18 |
| 2196 | NCC1OC(OC2C(N)CC (C(C2O)OC2OC(COC3 OC(CN)C(C(C3O)O)O  )C(C(C2N)O)N)N)C(C C1O)N | CUGUCUUCACGCAG AAAGCGUCUAGCCA UGGCGUUAGUAUG AGUGUCG | Compd 40 | Target\_lig\_128 1 | HCV IRES  Domain Iib | Target\_408 | 5.42021  6403383  19 |
| 2197 | NCC1OC(OC2C(N)CC (C(C2O)OC2OC(CN)C (CC2N)O)N)C(C(C1O) OC1OC(CO)C(C(C1N) O)O)N | CUGUCUUCACGCAG AAAGCGUCUAGCCA UGGCGUUAGUAUG AGUGUCG | Compd 41 | Target\_lig\_116 2 | HCV IRES  Domain Iib | Target\_408 | 5.45593  1955649  72 |
| 2198 | NCC1OC(OC2C(N)CC (C(C2O)OC2OC(CN)C (CC2N)O)N)C(C(C1O) OC1OC(CO)C(C(C1N) O)O)N | CUGUCUUCACGCAG AAAGCGUCUAGCCA UGGCGUUAGUAUG AGUGUCG | Compd 42 | Target\_lig\_128 2 | HCV IRES  Domain Iib | Target\_408 | 5.50863  8306165  73 |
| 2199 | NCC1OC(OC2C(N)CC (C(C2O)OC2OC(CN)C (CC2N)O)N)C(C(C1O C1OC(CO)C(C(C1N)O  )O)N)O | CUGUCUUCACGCAG AAAGCGUCUAGCCA UGGCGUUAGUAUG AGUGUCG | Compd 43 | Target\_lig\_128 3 | HCV IRES  Domain Iib | Target\_408 | 5.02227  6394711  15 |
| 2215 | CC1(COC(C(C1NC)O) OC2C(CC(C(C2O)OC3 C(CC=C(O3)CN)N)N) N)O | GGCUGACCAUCAAU AAGGAAGAAGCCCU UCAGCGGCCAGUA | sisomicin | Target\_lig\_10 | HIV protease active site (PAS) mRNA | Target\_409 | 4.82390  8740944  32 |
| 2216 | [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 | GGCUGACCAUCAAU AAGGAAGAAGCCCU UCAGCGGCCAGUA | Tobramycin | Target\_lig\_540 | HIV protease active site (PAS) mRNA | Target\_409 | 4.85387  1964321  76 |
| 2217 | 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 | GGCUGACCAUCAAU AAGGAAGAAGCCCU UCAGCGGCCAGUA | Neomycin B | Target\_lig\_125 1 | HIV protease active site (PAS) mRNA | Target\_409 | 5.69897  0004336  02 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA**  **\_ID** | **pKd** |
| 2218 | NCC1OC(OC2C(N)CC (C(C2O)OC2OC(CN)C (C(C2O)O)N)N)C(CC1 O)N | GGCUGACCAUCAAU AAGGAAGAAGCCCU UCAGCGGCCAGUA | Compd 32 | Target\_lig\_115 5 | HIV protease active site (PAS) mRNA | Target\_409 | 4.72124  6399047  17 |
| 2219 | NCC1OC(OC2C(N)CC (C(C2O)OC2OC(CN)C (CC2N)O)N)C(C(C1O C1OC(CO)C(C(C1O)O  )N)N)O | GGCUGACCAUCAAU AAGGAAGAAGCCCU UCAGCGGCCAGUA | Compd 33 | Target\_lig\_115 6 | HIV protease active site (PAS) mRNA | Target\_409 | 5.95860  7314841  77 |
| 2220 | NCC1OC(OC2C(N)CC (C(C2O)OC2OC(CN)C (CC2N)O)N)C(C(C1O C1OC(CO)C(C(C1O)N  )O)O)N | GGCUGACCAUCAAU AAGGAAGAAGCCCU UCAGCGGCCAGUA | Compd 34 | Target\_lig\_115 7 | HIV protease active site (PAS) mRNA | Target\_409 | 6.08092  1907623  93 |
| 2221 | NCC1OC(OC2C(N)CC (C(C2O)OC2OC(CN)C (C(C2O)N)O)N)C(CC1 O)N | GGCUGACCAUCAAU AAGGAAGAAGCCCU UCAGCGGCCAGUA | Compd 35 | Target\_lig\_115 8 | HIV protease active site (PAS) mRNA | Target\_409 | 5.16749  1087293  76 |
| 2222 | NCC1OC(OC2C(N)CC (C(C2O)OC2OC(COC3 OC(CO)C(C(C3N)O)O  )C(C(C2N)O)O)N)C(C C1O)N | GGCUGACCAUCAAU AAGGAAGAAGCCCU UCAGCGGCCAGUA | Compd 36 | Target\_lig\_116 3 | HIV protease active site (PAS) mRNA | Target\_409 | 5.29242  9823902  06 |
| 2223 | NCC1OC(OC2C(N)CC (C(C2O)OC2OC(CN)C (CC2N)O)N)C(C(C1O) OC1OC(CO)C(C(C1O) O)N)O | GGCUGACCAUCAAU AAGGAAGAAGCCCU UCAGCGGCCAGUA | Compd 37 | Target\_lig\_115 9 | HIV protease active site (PAS) mRNA | Target\_409 | 5.52287  8745280  34 |
| 2224 | NCC1OC(OC2C(N)CC (C(C2O)OC2OC(CN)C (CC2N)O)N)C(C(C1O C1OC(CO)C(C(C1N)O  )O)N)O | GGCUGACCAUCAAU AAGGAAGAAGCCCU UCAGCGGCCAGUA | Compd 38 | Target\_lig\_116 0 | HIV protease active site (PAS) mRNA | Target\_409 | 5.30102  9995663  98 |
| 2225 | NCC1OC(OC2C(N)CC (C(C2O)OC2OC(COC3 OC(CN)C(C(C3O)O)O  )C(C(C2N)O)N)N)C(C C1O)N | GGCUGACCAUCAAU AAGGAAGAAGCCCU UCAGCGGCCAGUA | Compd 39 | Target\_lig\_116 1 | HIV protease active site (PAS) mRNA | Target\_409 | 5.39794  0008672  04 |
| 2226 | NCC1OC(OC2C(N)CC (C(C2O)OC2OC(COC3 OC(CN)C(C(C3O)O)O  )C(C(C2N)O)N)N)C(C C1O)N | GGCUGACCAUCAAU AAGGAAGAAGCCCU UCAGCGGCCAGUA | Compd 40 | Target\_lig\_128 1 | HIV protease active site (PAS) mRNA | Target\_409 | 4.85387  1964321  76 |
| 2227 | NCC1OC(OC2C(N)CC (C(C2O)OC2OC(CN)C (CC2N)O)N)C(C(C1O) OC1OC(CO)C(C(C1N) O)O)N | GGCUGACCAUCAAU AAGGAAGAAGCCCU UCAGCGGCCAGUA | Compd 41 | Target\_lig\_116 2 | HIV protease active site (PAS) mRNA | Target\_409 | 5.92081  8753952  38 |
| 2228 | NCC1OC(OC2C(N)CC (C(C2O)OC2OC(CN)C (CC2N)O)N)C(C(C1O) OC1OC(CO)C(C(C1N) O)O)N | GGCUGACCAUCAAU AAGGAAGAAGCCCU UCAGCGGCCAGUA | Compd 42 | Target\_lig\_128 2 | HIV protease active site (PAS) mRNA | Target\_409 | 5.15490  1959985  74 |
| 2229 | NCC1OC(OC2C(N)CC (C(C2O)OC2OC(CN)C (CC2N)O)N)C(C(C1O C1OC(CO)C(C(C1N)O  )O)N)O | GGCUGACCAUCAAU AAGGAAGAAGCCCU UCAGCGGCCAGUA | Compd 43 | Target\_lig\_128 3 | HIV protease active site (PAS) mRNA | Target\_409 | 5.22184  8749616  36 |
| 2375 | C=CC1CN2CCC1CC2 C(C3=CC=NC4=CC=C C=C34)O | UUUUUUAGGGAAG AUCUGGCCUUCCCA CAAGGGAAGGCCAG GGAAUUUUCUU | Cinchonidine | Target\_lig\_122 1 | HIV- 1FRAMESHIF T STEM LOOP STRUCTURE | Target\_109 | 3.71399  2877920  53 |
| 2376 | CCCCOC(=O)C1=CC= C(C=C1)N | UUUUUUAGGGAAG AUCUGGCCUUCCCA CAAGGGAAGGCCAG GGAAUUUUCUU | Butamben | Target\_lig\_122 2 | HIV- 1FRAMESHIF T STEM LOOP STRUCTURE | Target\_109 | 4.40450  3778174  43 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA**  **\_ID** | **pKd** |
| 2377 | CC1C(C(CC(O1)OC2C C(CC3=C2C(=C4C(=C 3O)C(=O)C5=CC=CC= C5C4=O)O) (C(=O)C)O)N)O | UUUUUUAGGGAAG AUCUGGCCUUCCCA CAAGGGAAGGCCAG GGAAUUUUCUU | Idarubicin | Target\_lig\_122 3 | HIV- 1FRAMESHIF T STEM LOOP STRUCTURE | Target\_109 | 5.04095  8607678  91 |
| 2378 | c1cc(ccc1)C[C@H] (NC(=O) [C@@H]1CCCN1C(= O)[C@@H]  (NC(=O)c1cc2ccccc2nc 1CC)CSSC[C@H] (C(=O)N1CCC[C@H]1 C(=O)N[C@H] (C(=O)NCCCN)Cc1ccc  cc1)NC(=O)c1c(nc2c(c 1)cccc2)CC)C(=O)NC CCN | GGCCUUCCUACAAG GGAAGGCC | ethylquinoline\_ca rboxamide derivative | Target\_lig\_497 | FSS\_mutant\_1 | Target\_431 | 6.34678  7486224  66 |
| 2379 | c1cc(ccc1)C[C@H] (NC(=O) [C@@H]1CCCN1C(= O)[C@@H]  (NC(=O)c1cc2ccccc2nc 1CC)CSSC[C@H] (C(=O)N1CCC[C@H]1 C(=O)N[C@H] (C(=O)NCCCN)Cc1ccc  cc1)NC(=O)c1c(nc2c(c 1)cccc2)CC)C(=O)NC CCN | CCGGAAGGGACAAC CCUUCCGG | ethylquinoline\_ca rboxamide derivative | Target\_lig\_497 | FSS\_mutant\_2 | Target\_432 | 6.48148  6060122  11 |
| 2380 | c1cc(ccc1)C[C@H] (NC(=O) [C@@H]1CCCN1C(= O)[C@@H]  (NC(=O)c1cc2ccccc2nc 1CC)CSSC[C@H] (C(=O)N1CCC[C@H]1 C(=O)N[C@H] (C(=O)NCCCN)Cc1ccc  cc1)NC(=O)c1c(nc2c(c 1)cccc2)CC)C(=O)NC CCN | GGCCUUCCCGCAAG GGAAGGCC | ethylquinoline\_ca rboxamide derivative | Target\_lig\_497 | FSS\_mutant\_3 | Target\_433 | 6.11918  6407719  21 |
| 2381 | c1cc(ccc1)C[C@H] (NC(=O) [C@@H]1CCCN1C(= O)[C@@H]  (NC(=O)c1cc2ccccc2nc 1CC)CSSC[C@H] (C(=O)N1CCC[C@H]1 C(=O)N[C@H] (C(=O)NCCCN)Cc1ccc  cc1)NC(=O)c1c(nc2c(c 1)cccc2)CC)C(=O)NC CCN | GGCCUUCCCCACCG GGAAGGCC | ethylquinoline\_ca rboxamide derivative | Target\_lig\_497 | FSS\_mutant\_4 | Target\_434 | 5.95860  7314841  77 |
| 2382 | c1cc(ccc1)C[C@H] (NC(=O) [C@@H]1CCCN1C(= O)[C@@H]  (NC(=O)c1cc2ccccc2nc 1CC)CSSC[C@H] (C(=O)N1CCC[C@H]1 C(=O)N[C@H] (C(=O)NCCCN)Cc1ccc  cc1)NC(=O)c1c(nc2c(c 1)cccc2)CC)C(=O)NC CCN | CCGCUGCUGCUGCU GCUGCUGCUGCUGC UGCUGCGG | ethylquinoline\_ca rboxamide derivative | Target\_lig\_497 | FSS\_mutant\_5 | Target\_435 | 4.39794  0008672  04 |
| 2383 | NCCCNC(=O)[C@H]  (Cc1ccccc1)NC(=O) [C@@H]1CCCN1C(= O)[C@H]  (NC(=O)c1cc2ccccc2nc 1C)CSSC[C@@H] | UUUUUUAGGGAAG AUCUGGCCUUCCCA CAAGGGAAGGCCAG GGAAUUUUCUU | ethylquinoline\_ca rboxamide derivative 2 | Target\_lig\_122 4 | HIV- 1FRAMESHIF T STEM LOOP STRUCTURE | Target\_109 | 6.36653  1544420  41 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA**  **\_ID** | **pKd** |
|  | (C(=O)N1CCC[C@H]1 C(=O)N[C@H] (C(=O)NCCCN)Cc1ccc  cc1)NC(=O)c1cc2ccccc 2nc1C |  |  |  |  |  |  |
| 2384 | NCCCNC(=O)[C@H]  (Cc1ccccc1)NC(=O) [C@@H]1CCCN1C(= O)[C@H]  (NC(=O)c1cnc2c(c1)cc cc2)CSSC[C@@H] (C(=O)N1CCC[C@H]1 C(=O)N[C@H] (C(=O)NCCCN)Cc1ccc  cc1)NC(=O)c1cnc2c(c1  )cccc2 | UUUUUUAGGGAAG AUCUGGCCUUCCCA CAAGGGAAGGCCAG GGAAUUUUCUU | ethylquinoline\_ca rboxamide derivative 3 | Target\_lig\_122 5 | HIV- 1FRAMESHIF T STEM LOOP STRUCTURE | Target\_109 | 6.18708  6643357  14 |
| 2385 | NCCCNC(=O)[C@H]  (Cc1ccccc1)NC(=O) [C@@H]1CCCN1C(= O)[C@H] (NC(=O)c1cc2cc3OCO c3cc2nc1CC)CSSC[C  @@H] (C(=O)N1CCC[C@H]1 C(=O)N[C@H] (C(=O)NCCCN)Cc1ccc  cc1)NC(=O)c1cc2cc3O COc3cc2nc1CC | UUUUUUAGGGAAG AUCUGGCCUUCCCA CAAGGGAAGGCCAG GGAAUUUUCUU | ethylquinoline\_ca rboxamide derivative 4 | Target\_lig\_122 6 | HIV- 1FRAMESHIF T STEM LOOP STRUCTURE | Target\_109 | 5.84771  1655616  94 |
| 2386 | NCCCNC(=O)[C@H]  (Cc1ccccc1)NC(=O) [C@@H]1CCCN1C(= O)[C@H]  (Nc1ccc2c(c1)C(=O)c1 c(C2=O)cccc1)CSSC[C  @@H] (C(=O)N1CCC[C@H]1 C(=O)N[C@H] (C(=O)NCCCN)Cc1ccc  cc1)Nc1ccc2c(c1)C(=O  )c1c(C2=O)cccc1 | UUUUUUAGGGAAG AUCUGGCCUUCCCA CAAGGGAAGGCCAG GGAAUUUUCUU | ethylquinoline\_ca rboxamide derivative 5 | Target\_lig\_122 7 | HIV- 1FRAMESHIF T STEM LOOP STRUCTURE | Target\_109 | 6.63827  2163982  41 |
| 2387 | Ccc1nc2ccccc2cc1C(= O)O | UUUUUUAGGGAAG AUCUGGCCUUCCCA CAAGGGAAGGCCAG GGAAUUUUCUU | 2-ethylquinoline- 3-carboxylic acid | Target\_lig\_122 8 | HIV- 1FRAMESHIF T STEM LOOP STRUCTURE | Target\_109 | 6.53760  2002101  04 |
| 2388 | C=CC[C@@H] (C(=O)N1CCCC1C(=O  )NC(C(=O)NCCCN)Cc  1ccccc1)NC(=O)c1cc2c cccc2nc1CC | UUUUUUAGGGAAG AUCUGGCCUUCCCA CAAGGGAAGGCCAG GGAAUUUUCUU | Dicarba\_derivativ e\_8 | Target\_lig\_122 9 | HIV- 1FRAMESHIF T STEM LOOP STRUCTURE | Target\_109 | 6.32790  2142064  28 |
| 2389 | NCCCNC(=O)C(Cc1cc ccc1)NC(=O)C1CCCN 1C(=O)C(NC(=O)c1cc  2ccccc2nc1CC)C/C=C/ C[C@@H] (C(=O)N1CCCC1C(=O  )NC(C(=O)NCCCN)Cc  1ccccc1)NC(=O)c1cc2c cccc2nc1CC | UUUUUUAGGGAAG AUCUGGCCUUCCCA CAAGGGAAGGCCAG GGAAUUUUCUU | Dicarba\_derivativ e\_9 | Target\_lig\_123 0 | HIV- 1FRAMESHIF T STEM LOOP STRUCTURE | Target\_109 | 6.48148  6060122  11 |
| 2390 | Coc1ccc2c(c1)c(Nc1cc c(c(c1)CN1CCN(CC1)  C)O)c1c(n2)cc(cc1)Cl | AGGACUCGGCUUGC UGAAGCGCGCGACG GCAAGAGGCGAGG GGCGGCGACUGGUG AGUACGCCAAAAAU UUUGACUAGCGGA GGCUAGAAGGAGA GAGAUGGGUGCGA GAGCGUCGGU | Acridine\_derivati ve\_2 (AD2) | Target\_lig\_123 1 | SL-3 of HIV- 1\_SITE | Target\_146 | 6.17392  5197299  17 |
| 2391 | CCOC(=O)C1=C2C=C C=CN2C3=C1C(=O)C 4=CC=CC=C4C3=O | AGGACUCGGCUUGC UGAAGCGCGCGACG GCAAGAGGCGAGG | NSC119236 | Target\_lig\_123 2 | SL-3 of HIV- 1\_SITE | Target\_146 | 5.85387  1964321  76 |

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| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA**  **\_ID** | **pKd** |
|  |  | GGCGGCGACUGGUG AGUACGCCAAAAAU UUUGACUAGCGGA GGCUAGAAGGAGA GAGAUGGGUGCGA GAGCGUCGGU |  |  |  |  |  |
| 2392 | C[N+] (CCN[N+]1(C)CCCc2c  1cccc2)(C)C | AGGACUCGGCUUGC UGAAGCGCGCGACG GCAAGAGGCGAGG GGCGGCGACUGGUG AGUACGCCAAAAAU UUUGACUAGCGGA GGCUAGAAGGAGA GAGAUGGGUGCGA GAGCGUCGGU | SL3\_compound\_6 | Target\_lig\_123 3 | SL-3 of HIV- 1\_SITE | Target\_146 | 5.82390  8740944  32 |
| 2393 | CN(c1ncnc2c1n(CCn1c nc3c1ncnc3N(C)C)cn2) C | AGGACUCGGCUUGC UGAAGCGCGCGACG GCAAGAGGCGAGG GGCGGCGACUGGUG AGUACGCCAAAAAU UUUGACUAGCGGA GGCUAGAAGGAGA GAGAUGGGUGCGA GAGCGUCGGU | SL3\_compound\_2 | Target\_lig\_123 4 | SL-3 of HIV- 1\_SITE | Target\_146 | 4.49485  0021680  09 |
| 2472 | 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 | GGUCGGCGCAGCUU CGGCUGCGGUAGAC C | Neomycin | Target\_lig\_4 | RRE16 | Target\_447 | 6.24412  5144327  51 |
| 2473 | 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 | GGUGUGCGCAGCUU CGGCUGCGGUACAC C | Neomycin | Target\_lig\_4 | RRE17 | Target\_448 | 6.20065  9450546  42 |
| 2474 | 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 | GGUGCGCGCAGCUU CGGCUGCGGUACAC C | Neomycin | Target\_lig\_4 | RRE18 | Target\_449 | 6.29242  9823902  06 |
| 2475 | 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 | GGUGGACGCAGCUU CGGCUGACUGUACA CC | Neomycin | Target\_lig\_4 | RRE19 | Target\_450 | 6.07572  0713938  12 |
| 2476 | 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 | GGUGGCCGCAGCUU CGGCUGACGGUACA CC | Neomycin | Target\_lig\_4 | RRE20 | Target\_451 | 5.46852  1082957  74 |
| 2477 | 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 | GGUGGGAGCAGCU UCGGCUGAUGGUAC ACC | Neomycin | Target\_lig\_4 | RRE21 | Target\_452 | 6.22184  8749616  36 |
| 2478 | 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 | GGUGGGCUCAGCUU CGGCUGACGGUACA CC | Neomycin | Target\_lig\_4 | RRE22 | Target\_453 | 6.30980  3919971  49 |
| 2479 | 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 | GCACUAUGGGCGCC AGCGUCAAUGACGC UGACGGUACAGCCA GACAAUUAUUGUC UGGUAUAGUGC | Paromomycin | Target\_lig\_5 | RRE-RNA | Target\_80 | 5.08092  1907623  93 |
| 2480 | 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 | GCACUAUGGGCGCC AGCGUCAAUGACGC UGACGGUACAGCCA GACAAUUAUUGUC | Kanamycin B | Target\_lig\_128 7 | RRE-RNA | Target\_80 | 5.25181  1972993  8 |

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| --- | --- | --- | --- | --- | --- | --- | --- |
| **Entry\_ID** | **SMILES** | **Target\_RNA\_sequence** | **Molecule\_name** | **Molecule\_ID** | **Target\_RNA\_ name** | **Target\_RNA**  **\_ID** | **pKd** |
|  |  | UGGUAUAGUGC |  |  |  |  |  |
| 2481 | 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 | GGUGGGCGCAGCUU CGGCUGCGCCCACC | Paromomycin | Target\_lig\_5 | RRE3 | Target\_83 | 4.60205  9991327  96 |
| 2482 | 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 | GGUGGGCGCAGCUU CGGCUGCGGACACC | Paromomycin | Target\_lig\_5 | RRE4 | Target\_84 | 4.80966  8301829  71 |
| 2483 | 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 | GGUGGGCGCAGCUU CGGCUGCGCAACCA CC | Paromomycin | Target\_lig\_5 | RRE11 | Target\_91 | 4.72815  8393463  5 |
| 2484 | 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 | GGUGGGCGCAGCUU CGGCUGCGCCCACC | Kanamycin B | Target\_lig\_128 7 | RRE3 | Target\_83 | 4.90308  9986991  94 |
| 2485 | 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 | GGUGGGCGCAGCUU CGGCUGCGGACACC | Kanamycin B | Target\_lig\_128 7 | RRE4 | Target\_84 | 5.20065  9450546  42 |
| 2486 | 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 | GGUGGGCGCAGCUU CGGCUGCGCAACCA CC | Kanamycin B | Target\_lig\_128 7 | RRE11 | Target\_91 | 4.87614  8359032  91 |