

Training dataset curated from [R-SIM](#) database for the “Viral RNA (Old)” model in [RSAPred](#)

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
204	<chem>CC1C(C(C(C(O1)OC2C3CC#CC4C(O4)(C#CC3=CC2OC(=O)C5=C(C=CC6=C5C=C(C=C6C)OC)O)C7COC(=O)O7)NC)O)O</chem>	GGCCAGAUUGAGCC UGGGAGCUCUCUGG CC	neocarzinostatin	Target_lig_148	RNA_Str_HIV- 2 TAR	Target_20	4.85387 1964321 76
205	<chem>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(c1)[C@](C=C2)([C@H]1OC(=O)OC1)O</chem>	GGCCAGAUUGAGCC UGGGAGCUCUCUGG CC	Neocarzinostatin_ chromophore_deriva tive_1	Target_lig_149	RNA_Str_HIV- 2 TAR	Target_20	4.85387 1964321 76
206	<chem>c12c(cccc1)[C@@]1(C(=O)C=C2)[C@@H](O[C@@H]2[C@@H]1c1c(C2=O)cc2c(c1)cc2)O[C@@H]1[C@H]([C@@H]([C@H]([C@H](O1)CO)O)O)N</chem>	GGCCAGAUUGAGCC UGGGAGCUCUCUGG CC	Neocarzinostatin_ chromophore_deriva tive_2	Target_lig_150	RNA_Str_HIV- 2 TAR	Target_20	4.85387 1964321 76
207	<chem>c12c(cccc1)[C@@]1([C@@H](C=C2)O[C@H]2[C@@H]([C@H]([C@@H]([C@@H](O2)CO)O)O)N)C(=O)O[C@@H]2[C@@H]1c1c(C2=O)cc2c(c1)cccc2</chem>	GGCCAGAUUGAGCC UGGGAGCUCUCUGG CC	Neocarzinostatin_ chromophore_deriva tive_3	Target_lig_151	RNA_Str_HIV- 2 TAR	Target_20	4.88605 6647693 16
208	<chem>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](O2)C)O)O)NC)cc2c(c1)cccc2</chem>	GGCCAGAUUGAGCC UGGGAGCUCUCUGG CC	Neocarzinostatin_ chromophore_deriva tive_5	Target_lig_152	RNA_Str_HIV- 2 TAR	Target_20	5.09691 0013008 06
209	<chem>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](O2)C)O)O)NC)cc2c(c1)cccc2</chem>	GGCCAGAUUGAGCC UGGGAGCUCUCUGG CC	Neocarzinostatin_ chromophore_deriva tive_6	Target_lig_153	RNA_Str_HIV- 2 TAR	Target_20	5.04575 7490560 68
233	<chem>CC1(COC(C(C1NC)O)OC2C(CC(C(C2O)OC3C(CC=C(O3)CN)N)N)O</chem>	GGCAGAUCUGAGCC UGGGAGCUCUCUGC C	sisomicin	Target_lig_10	HIV-1 TAR RNA	Target_19	6.13667 7139879 54
234	<chem>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</chem>	GGCAGAUCUGAGCC UGGGAGCUCUCUGC C	Amikacin	Target_lig_175	HIV-1 TAR RNA	Target_19	5.81247 9279163 54
235	<chem>CC(=O)C1=CC2=C(C=C1)SC3=CC=CC=C3N2CCCN(C)C</chem>	GGCAGAUCUGAGCC UGGGAGCUCUCUGC C	Acetylpromazine	Target_lig_176	HIV-1 TAR RNA	Target_19	3.56863 6235841 01
238	<chem>CN1CCN(CC1)C2=CC3=C(C=C2)N=C(N3)C4=CC5=C(C=C4)N=C(N5)C6=CC=C(C(C=C6)</chem>	GGCAGAUCUGAGCC UGGGAGCUCUCUGC C	CMC3_Hoechst3 3258	Target_lig_179	HIV-1 TAR RNA	Target_19	5

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=C3N2)C(=O)C5=CC=CC=C5N4	GGCAGAUCUGAGCC UGGGAGCUCUCUGC C	Quinacridone	Target_lig_181	HIV-1 TAR RNA	Target_19	6
241	C1=CC(=C2C(=C1NCNCCO)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)CNCCCN=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)CNCCCN=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=C3)OCCN=C(N)N)CNCNCCN=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)CNCCCN=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=CC4=C(C=C3)NC=C4)OCCN	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=C3N2CCN4CCN(CC4)C	GGCAGAUCUGAGCC UGGGAGCUCUCUGC C	Thiethylperazine	Target_lig_188	HIV-1 TAR RNA	Target_19	3.56863 6235841 01
248	CN1CCN(CC1)CCCN2C3=CC=CC=C3SC4=C2C=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(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(CCC2C1CC3C4=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(C1OC2C(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(c12)CCCN1CCC[C@H](C1)CO)C(=O)C	GGCAGAUCUGAGCC UGGGAGCUCUCUGC C	hydroxymethyl_pi peridinyI_propyl phenothiazinyI_et hanone	Target_lig_195	HIV-1 TAR RNA	Target_19	3.74472 7494896 69
255	CO[C@H]1CCCN(C1)CCCN1c2cc(ccc2Sc2c1ccccc2)C(=O)C	GGCAGAUCUGAGCC UGGGAGCUCUCUGC C	methoxypiperidin _butyl_der	Target_lig_196	HIV-1 TAR RNA	Target_19	3.85387 1964321 76

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
256	<chem>CC(=O)C1=CC2=C(C=C1)SC3=CC=CC=C3N2CCCN(C)C</chem>	GGCAGAU CUGAGCC UGGGAGCUCUCUGC C	dimethylamino_p ropyl_phenothiazin yl_ethanone	Target_lig_197	HIV-1 TAR RNA	Target_19	3.56863 6235841 01
257	<chem>CN(C)CCCN1C2=CC=CC=C2SC3=C1C=C(C=C3)OC</chem>	GGCAGAU CUGAGCC 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	<chem>CN(C)CCCN1C2=CC=CC=C2SC3=C1C=C(C=C3)Cl</chem>	GGCAGAU CUGAGCC 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	<chem>CC=1C=CC=2N(C3=C(C=C(C3SC2C1)C)CCN(C)C</chem>	GGCAGAU CUGAGCC 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	<chem>COC1=CC=CC=2N(C3=CC=CC=C3SC12)CCN(C)C</chem>	GGCAGAU CUGAGCC 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	<chem>CN(C)CCCN1C2=CC=CC=C2SC3=C1C=C(C=C3)O</chem>	GGCAGAU CUGAGCC UGGGAGCUCUCUGC C	dimethylamino_p ropyl_phenothiazin _der_2	Target_lig_202	HIV-1 TAR RNA	Target_19	2.52287 8745280 34
262	<chem>CN(CCCN1C2=CC=C(C=C2SC=2C(=CC=CC12)O)C</chem>	GGCAGAU CUGAGCC UGGGAGCUCUCUGC C	10-(3-(dimethylamino)propyl)-10H-phenothiazin-4-ol	Target_lig_203	HIV-1 TAR RNA	Target_19	2.52287 8745280 34
263	<chem>CN(C)CCCN1C2=CC=CC=C2SC3=C1C=C(C=C3)C(F)(F)F</chem>	GGCAGAU CUGAGCC 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	<chem>CN(CCCN1C2=CC=C(C=C2SC=2C(C=CC12)C)C</chem>	GGCAGAU CUGAGCC 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	<chem>CN(C)CCCN1C2=CC=CC=C2SC3=CC=CC=C31</chem>	GGCAGAU CUGAGCC 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	<chem>CN(C)CCCN1C2=CC=CC=C2SC3=C1C=C(C=C3)Cl</chem>	GGCAGAU CUGAGCC UGGGAGCUCUCUGC C	[3-(2-chloro-10H-phenothiazin-10	Target_lig_207	HIV-1 TAR RNA	Target_19	3.25963 7310505 76
268	<chem>c1c(ccc2Sc3ccccc3N(c12)CCCCN1CCC[C@H](C1)CO)C(=O)C</chem>	GGCAGAU CUGAGCC UGGGAGCUCUCUGC C	hydroxymethyl_pi peridiny1_butyl	Target_lig_208	HIV-1 TAR RNA	Target_19	3.25963 7310505 76
269	<chem>c1c(ccc2Sc3ccccc3N(c12)CCCCCN1CCC[C@H](C1)CO)C(=O)C</chem>	GGCAGAU CUGAGCC UGGGAGCUCUCUGC C	hydroxymethyl_pi peridiny1_penty1	Target_lig_209	HIV-1 TAR RNA	Target_19	2.52287 8745280 34
270	<chem>c1c(ccc2Sc3ccccc3N(c12)CCCN(CN(CO)CO)C(=O)C</chem>	GGCAGAU CUGAGCC UGGGAGCUCUCUGC C	3_phenothiazine_ analog_1	Target_lig_210	HIV-1 TAR RNA	Target_19	2.52287 8745280 34
271	<chem>c1c(ccc2Sc3ccccc3N(c12)CCCN[C@H](CCSC)O)C(=O)C</chem>	GGCAGAU CUGAGCC UGGGAGCUCUCUGC C	3_phenothiazine_ analog_2	Target_lig_211	HIV-1 TAR RNA	Target_19	2.30102 9995663 98
272	<chem>C1=CC=C2C(=C1)N(C</chem>	GGCAGAU CUGAGCC	3_phenothiazine_	Target_lig_212	HIV-1 TAR	Target_19	3.25963

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	<chem>3=C(S2)C=CC(=C3)Cl</chem> <chem>CCCNCCO</chem>	UGGGAGCUCUCUGC C	analog_3		RNA		7310505 76
273	<chem>c1cccc2Sc3ccc(cc3N(c12)CCCNCCCCC)Cl</chem>	GGCAGAUCUGAGCC UGGGAGCUCUCUGC C	2-chloro-10-pyrrolidin_phenothiazine_der	Target_lig_213	HIV-1 TAR RNA	Target_19	3.25963 7310505 76
274	<chem>c1cccc2Sc3ccc(cc3N(c12)CCN1CCCC1)Cl</chem>	GGCAGAUCUGAGCC UGGGAGCUCUCUGC C	2-chloro-10-methylpyrrolidin_phenothiazine_der	Target_lig_214	HIV-1 TAR RNA	Target_19	2.30102 9995663 98
275	<chem>c1cccc2Sc3ccc(cc3N(c12)CCN1CCC[C@@H]1C)Cl</chem>	GGCAGAUCUGAGCC UGGGAGCUCUCUGC C	2-chloro-10-[2-(2-methylpyrrolidin-1-yl)ethyl]_phenothiazine_der	Target_lig_215	HIV-1 TAR RNA	Target_19	2.30102 9995663 98
276	<chem>C1CCN(CC1)CCCN2C3=CC=CC=C3SC4=C2C=C(C=C4)Cl</chem>	GGCAGAUCUGAGCC UGGGAGCUCUCUGC C	chloro_piperidine_propyl_der	Target_lig_216	HIV-1 TAR RNA	Target_19	3.25963 7310505 76
277	<chem>CN1CCN(CC1)CCCN2C3=CC=CC=C3SC4=C2C=C(C=C4)Cl</chem>	GGCAGAUCUGAGCC UGGGAGCUCUCUGC C	chloro_methylpiperazinyl_propyl_phenothiazine_der	Target_lig_217	HIV-1 TAR RNA	Target_19	2.52287 8745280 34
278	<chem>c1cccc2Sc3ccc(cc3N(c12)CCn1cccc1)Cl</chem>	GGCAGAUCUGAGCC UGGGAGCUCUCUGC C	choro_imidazole_phenothiazine_der	Target_lig_218	HIV-1 TAR RNA	Target_19	2.30102 9995663 98
279	<chem>C1=CC=C(C=C1)CNCN2C3=CC=CC=C3SC4=C2C=C(C=C4)Cl</chem>	GGCAGAUCUGAGCC UGGGAGCUCUCUGC C	benzyl_phenothiazine_der	Target_lig_219	HIV-1 TAR RNA	Target_19	2.30102 9995663 98
280	<chem>C1C(C(C(C1NC(=O)C(CCN)O)O)OC2C(C(C(O2)CO)O)O)OC3C(C(C(C(O3)CN)O)O)N</chem>	GGCAGAUCUGAGCC UGGGAGCUCUCUGC C	Butirosin	Target_lig_220	HIV-1 TAR RNA	Target_19	5.32057 2103387 88
281	<chem>CN(C)C1=NC(=C(N=C1Cl)C(=O)N=C(N)N)N</chem>	GGCAGAUCUGAGCC UGGGAGCUCUCUGC C	N_N_dimethyl_amiloride	Target_lig_221	HIV-1 TAR RNA	Target_19	3.91417 4466479 26
286	<chem>c1c2OC[C@@H](Cc2c(c1)N=C1[C@H]2C[C@@H](CN1)CN(C)C)CN(C)C</chem>	GGCCGAGUAGUGU UGGGUCGCGAAAG GCC	Benzimidazole13ibis	Target_lig_225	HCV IRES Domain II	Target_66	6.14266 7503568 73
287	<chem>CN(C)CCCN1C2=C(C=CC(=C2)OCCCN(C)C)N=C1N</chem>	GGCCGAGUAGUGU UGGGUCGCGAAAG GCC	Benzimidazole3ibis	Target_lig_226	HCV IRES Domain II	Target_66	4.76955 1078621 73
305	<chem>CC(C)N=C(C1=CC=C(C=C1)C2=CC=C(O2)C3=CC(=CC=C3)C(=N(C(C)C)N)N</chem>	GCACUAUGGGCGCC AGCGUCAAUGACGC UGACGGUACAGCCA GACAAUUAUUGUC UGGUAUAGUGC	CMC6_diphenylfuran	Target_lig_243	HIV-1 RRE	Target_80	5.30102 9995663 98
306	<chem>CN(C)CCN=C(C1=CC=CC(=C1)C2=CC=C(O2)C3=CC(=CC=C3)C(=NCCN(C)C)N)N</chem>	GCACUAUGGGCGCC AGCGUCAAUGACGC UGACGGUACAGCCA GACAAUUAUUGUC UGGUAUAGUGC	CMC7_diphenylfuran	Target_lig_244	HIV-1 RRE	Target_80	7
307	<chem>CN(C)CCCN=C(C1=C(C=CC(=C1)C2=CC=C(O2)C3=CC(=CC=C3)C(=NCCCN(C)C)N)N</chem>	GCACUAUGGGCGCC AGCGUCAAUGACGC UGACGGUACAGCCA GACAAUUAUUGUC UGGUAUAGUGC	CMC8_diphenylfuran	Target_lig_245	HIV-1 RRE	Target_80	5.79588 0017344 08
393	<chem>CC1(COC(C(C1NC)O)OC2C(CC(C(C2O)OC3C(CC=C(O3)CN)N)N)N)O</chem>	GGCCGAGUAGUGU UGGGUCGCGAAAG GCC	sisomicin	Target_lig_10	HCV IRES Domain IIIId	Target_66	6.58502 6652029 18
710	<chem>C1(=O)N(C(=O)c2c([C@H]1C)ncn2[C@H](O)N(C)C)C</chem>	GGCAGAUCUGAGCC UGGGAGCUCUCUGC C	Phenothiazine 1	Target_lig_474	RNA_Str_HIV-1 TAR	Target_19	5.84466 3962534 94
711	<chem>CN1CCN(CC1)CCCN2C3=CC=CC=C3SC4=C</chem>	GGCAGAUCUGAGCC UGGGAGCUCUCUGC	Phenothiazine 2	Target_lig_475	RNA_Str_HIV-1 TAR	Target_19	4.92445 3038607

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	<chem>2C=C(C=C4)C1</chem>	C					47
712	<chem>C1=CC2=C(C=C1N=C=S)C(=O)OC23C4=C(C=C(C=C4)O)OC5=C3C=CC(=C5)O</chem>	GGCAGAUCUGAGCC UGGGAGCUCUCUGC C	Phenothiazine 3	Target_lig_476	RNA_Str_HIV-1 TAR	Target_19	4.92445 3038607 47
713	<chem>C1=CC=C2C(=C1)C(=O)OC2(C3=CC=C(C=C3)O)C4=CC=C(C=C4)O</chem>	GGCAGAUCUGAGCC UGGGAGCUCUCUGC C	Phenothiazine 4	Target_lig_477	RNA_Str_HIV-1 TAR	Target_19	4.59345 9819566 04
714	<chem>CC(=O)C1=CC2=C(C=C1)SC3=CC=CC=C3N2CCCN(C)C</chem>	GGCAGAUCUGAGCC UGGGAGCUCUCUGC C	Phenothiazine 6	Target_lig_478	RNA_Str_HIV-1 TAR	Target_19	3.79860 2875679 55
715	<chem>C1=CC=C2C(=C1)C(=O)C3=CC4=C(C=C3N2)C(=O)C5=CC=CC=C5N4</chem>	GGCAGAUCUGAGCC UGGGAGCUCUCUGC C	Phenothiazine 7	Target_lig_479	RNA_Str_HIV-1 TAR	Target_19	3.43770 7135543 53
716	<chem>[C@H]12[C@@H](C[C@@H]3[N@](C1)(CCc1c3[nH]c3c1cccc3)C)[C@H]([C@H](CC2)O)C(=O)OC</chem>	GGCAGAUCUGAGCC UGGGAGCUCUCUGC C	Phenothiazine 8	Target_lig_480	RNA_Str_HIV-1 TAR	Target_19	3.04720 7556955 91
717	<chem>[C@@H]1([C@H]([C@H]2[C@@H]([C@H]1C(=O)C)O[C@H]1[C@@H]2C(=O)[C@@H](C(=O)C1)C(=O)C)CO</chem>	GGCAGAUCUGAGCC UGGGAGCUCUCUGC C	Phenothiazine 9	Target_lig_481	RNA_Str_HIV-1 TAR	Target_19	2.40671 3932979 54
718	<chem>CN(C)CCCN1C2=CC=CC=C2SC3=C1C=C(C=C3)C1</chem>	GGCAGAUCUGAGCC UGGGAGCUCUCUGC C	Phenothiazine 10	Target_lig_482	RNA_Str_HIV-1 TAR	Target_19	2.00921 7308196 86
731	<chem>[C@@H]1([C@H]([C@H]([C@H]1O[C@H]1CNC(=N)N)O[C@H]1[C@@H]([C@H]([C@H]([C@H]1C[C@H]1NC(=N)N)N)C(=N)N)O)O[C@H]1[C@@H]([C@H]([C@H]([C@H]1O)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</chem>	UUUUUUAGGGAAG AUCUGGCCUCCCCA CAAGGGAAGGCCAG GGAAUUUUUCUU	guanidinoneomycin_B	Target_lig_495	HIV-1FRAMESHIFT STEM LOOP STRUCTURE	Target_109	8
732	<chem>C[C@H]1[C@H]([C@H]([C@H]1O)O[C@H]2C[C@@H](CC3=C2C(=C4C(=C3O)C(=O)C5=C(C4=O)C(=CC=C5)OC)O)C(=O)CO)N)O</chem>	UUUUUUAGGGAAG AUCUGGCCUCCCCA CAAGGGAAGGCCAG GGAAUUUUUCUU	doxorubicin	Target_lig_496	HIV-1FRAMESHIFT STEM LOOP STRUCTURE	Target_109	5.55284 1968657 78
733	<chem>c1cc(ccc1)C[C@H](NC(=O)[C@@H]1CCCN1C(=O)[C@H]1NC(=O)c1cc2cccc2nc1CC)CSSC[C@H](C(=O)N1CCC[C@H]1C(=O)N[C@H](C(=O)NCCCN)Cc1ccc(cc1)NC(=O)c1c(nc2c(c1)cccc2)CC)C(=O)NCCCN</chem>	UUUUUUAGGGAAG AUCUGGCCUCCCCA CAAGGGAAGGCCAG GGAAUUUUUCUU	ethylquinoline_carboxamide derivative	Target_lig_497	HIV-1FRAMESHIFT STEM LOOP STRUCTURE	Target_109	6.45593 1955649 72
734	<chem>CC1=NC2=NC(=NN2C(=C1)N3CCN(CC3)C)</chem>	AGGACUCGGCUUGC UGAAGCGCGCGACG	methylpiperazine derivative	Target_lig_498	SL-3 of HIV-1_SITE	Target_146	4.95860 7314841

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	<chem>C4=CC=C(C=C4)Cl</chem>	GCAAGAGGCGAGG GGCGGCGACUGGUG AGUACGCCAAAAAU UUUGACUAGCGGA GGCUAGAAGGAGA GAGAUUGGUGCGA GAGCGUCGGU					77
735	<chem>CC1=C(C(=O)C2=C(C1=O)N3C[C@H]4[C@@H](C3=C2COC(=O)N)N4C)OC</chem>	AGGACUCGGCUUGC UGAAGCGCGCGACG GCAAGAGGCGAGG GGCGGCGACUGGUG AGUACGCCAAAAAU UUUGACUAGCGGA GGCUAGAAGGAGA GAGAUUGGUGCGA GAGCGUCGGU	methyl_carbamate derivative	Target_lig_499	SL-3 of HIV- 1_SITE	Target_146	4.00877 3924307 51
798	<chem>CC1C(C(C(O1)OC2C(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</chem>	GGCAGAUCUGAGCC UGGGAGCUCUCUGC C	Streptomycin	Target_lig_63	Argininamide- TAR complex	Target_19	5.61978 8758288 39
799	<chem>C1C(C(C(C1N)OC2C(C(C(C2)CN)O)O)N)OC3C(C(C(O3)CO)OC4C(C(C(C(O4)CN)O)O)N)O)O)N</chem>	GGCAGAUCUGAGCC UGGGAGCUCUCUGC C	Neomycin_B	Target_lig_124 6	Argininamide- TAR complex	Target_19	6.15490 1959985 74
800	<chem>CC1(COC(C(C1NC)O)OC2C(CC(C(C2O)OC3C(CCC(O3)CN)N)N)O)O</chem>	GGCAGAUCUGAGCC UGGGAGCUCUCUGC C	gentamicin_mol	Target_lig_76	Argininamide- TAR complex	Target_19	5.36653 1544420 41
847	<chem>CC1C(C(C(O1)OC2C(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</chem>	GCACUAUGGGCGCC AGCGUCAAUGACGC UGACGGUACAGCCA GACAAUUAUUGUC UGGUAUAGUGC	Streptomycin	Target_lig_63	RRE-RNA	Target_80	6
849	<chem>[C@H]1([C@H](C[C@H]([C@H]([C@H]1O)O)[C@H]1[C@@H](C[C@H]([C@@H]([C@@H](O1)CN)O)N)N)O)[C@@H]1[C@H]([C@@H]([C@@H](O1)CNe1c2ccccc2nc2c1cccc2)O)N)O</chem>	GCACUAUGGGCGCC AGCGUCAAUGACGC UGACGGUACAGCCA GACAAUUAUUGUC UGGUAUAGUGC	Tobramycin	Target_lig_540	RRE-RNA	Target_80	5.52287 8745280 34
850	<chem>C1C(C(C(C(C1N)OC2C(C(C(C2)CN)O)O)O)OC3C(C(C(C(O3)CO)O)N)O)N</chem>	GCACUAUGGGCGCC AGCGUCAAUGACGC UGACGGUACAGCCA GACAAUUAUUGUC UGGUAUAGUGC	Kanamycin A	Target_lig_7	RRE-RNA	Target_80	3.12493 8736608 3
851	<chem>C1C(C(C(C(C1N)OC2C(C(C(C2)CO)O)N)O)OC3C(C(C(C(O3)CN)O)O)N)N</chem>	GCACUAUGGGCGCC AGCGUCAAUGACGC UGACGGUACAGCCA GACAAUUAUUGUC UGGUAUAGUGC	KANAMYCIN B	Target_lig_8	RRE-RNA	Target_80	4.04575 7490560 68
852	<chem>C1C(C(C(C(C1N)OC2C(C(C(C2)CN)O)O)N)OC3C(C(C(O3)CO)OC4C(C(C(C(O4)CN)O)O)N)O)N</chem>	GCACUAUGGGCGCC AGCGUCAAUGACGC UGACGGUACAGCCA GACAAUUAUUGUC UGGUAUAGUGC	Neomycin_B	Target_lig_124 6	RRE-RNA	Target_80	6.82390 8740944 32
853	<chem>C1C(C(C(C(C1N)OC2C(C(C(C2)CN)O)O)N)OC3C(C(C(O3)CO)OC4C(C(C(C(O4)CN)O)O)N)O)O)N</chem>	GGUGGGCGCAGCUU CGGCUGCGGUACAC C	Neomycin	Target_lig_4	RRE1	Target_81	6.79588 0017344 08
854	<chem>C1C(C(C(C(C1N)OC2C(C(C(C2)CN)O)O)O)O)O</chem>	GGUGUCGCAGCUUC GCCUCGCACACC	Neomycin	Target_lig_4	RRE2	Target_82	5.12262 8654130

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	N)OC3C(C(C(O3)CO)OC4C(C(C(C(O4)CN)O)O)N)O)O)N						23
855	C1C(C(C(C(C1N)OC2C(C(C(C(O2)CN)O)O)N)OC3C(C(C(O3)CO)OC4C(C(C(C(O4)CN)O)O)N)O)O)N	GGUGGGCGCAGCUUCGGCUGCGCCCACC	Neomycin	Target_lig_4	RRE3	Target_83	5.19382002601611
856	C1C(C(C(C(C1N)OC2C(C(C(C(O2)CN)O)O)N)OC3C(C(C(O3)CO)OC4C(C(C(C(O4)CN)O)O)N)O)O)N	GGUGGGCGCAGCUUCGGCUGCGGACACC	Neomycin	Target_lig_4	RRE4	Target_84	6.31875876262441
857	C1C(C(C(C(C1N)OC2C(C(C(C(O2)CN)O)O)N)OC3C(C(C(O3)CO)OC4C(C(C(C(O4)CN)O)O)N)O)O)N	GGUGGGCGCAGCUUCGGCUGCGCACACC	Neomycin	Target_lig_4	RRE5	Target_85	5.92811799269388
858	C1C(C(C(C(C1N)OC2C(C(C(C(O2)CN)O)O)N)OC3C(C(C(O3)CO)OC4C(C(C(C(O4)CN)O)O)N)O)O)N	GGUGGCCGCGAGCUUCGGCUGCGGACACC	Neomycin	Target_lig_4	RRE6	Target_86	5.53313237964589
859	C1C(C(C(C(C1N)OC2C(C(C(C(O2)CN)O)O)N)OC3C(C(C(O3)CO)OC4C(C(C(C(O4)CN)O)O)N)O)O)N	GGUGGGCGCAGCUUCGGCUGCGGCCACC	Neomycin	Target_lig_4	RRE7	Target_87	5.75696195131371
860	C1C(C(C(C(C1N)OC2C(C(C(C(O2)CN)O)O)N)OC3C(C(C(O3)CO)OC4C(C(C(C(O4)CN)O)O)N)O)O)N	GGUGUGCCGCGAGCUUCGGCUGCGGACACC	Neomycin	Target_lig_4	RRE8	Target_88	5.56224943717961
861	C1C(C(C(C(C1N)OC2C(C(C(C(O2)CN)O)O)N)OC3C(C(C(O3)CO)OC4C(C(C(C(O4)CN)O)O)N)O)O)N	GGUGGAGCGCAGCUUCGGCUGCGCCCACC	Neomycin	Target_lig_4	RRE9	Target_89	5.90308998699194
862	C1C(C(C(C(C1N)OC2C(C(C(C(O2)CN)O)O)N)OC3C(C(C(O3)CO)OC4C(C(C(C(O4)CN)O)O)N)O)O)N	GGUGGGCGCAGCUUCGGCUGCGCACCACC	Neomycin	Target_lig_4	RRE10	Target_90	6.18708664335714
863	C1C(C(C(C(C1N)OC2C(C(C(C(O2)CN)O)O)N)OC3C(C(C(O3)CO)OC4C(C(C(C(O4)CN)O)O)N)O)O)N	GGUGGGCGCAGCUUCGGCUGCGCAACCAACC	Neomycin	Target_lig_4	RRE11	Target_91	6.26760624017703
864	C1C(C(C(C(C1N)OC2C(C(C(C(O2)CN)O)O)N)OC3C(C(C(O3)CO)OC4C(C(C(C(O4)CN)O)O)N)O)O)N	GGUGGGCGCAGCUUCGGCUGCGCAAACCAACC	Neomycin	Target_lig_4	RRE12	Target_92	6.18708664335714
865	C1C(C(C(C(C1N)OC2C(C(C(C(O2)CN)O)O)N)OC3C(C(C(O3)CO)OC4C(C(C(C(O4)CN)O)O)N)O)O)N	GGUGGGCGCAGCUUCGGCUGCGCAAAACCAACC	Neomycin	Target_lig_4	RRE13	Target_93	6.21467016498923
866	C1C(C(C(C(C1N)OC2C(C(C(C(O2)CN)O)O)N)OC3C(C(C(O3)CO)OC4C(C(C(C(O4)CN)O)O)N)O)O)N	GGUGGGCGCAGCUUCGGCUGCGCGGCCAACCC	Neomycin	Target_lig_4	RRE14	Target_94	6.35654732351381
867	C1C(C(C(C(C1N)OC2C(C(C(C(O2)CN)O)O)N)OC3C(C(C(O3)CO)OC4C(C(C(C(O4)CN)O)O)N)O)O)N	GGUGGGCGCAGCUUCGGCUGCGCUUCCCAACC	Neomycin	Target_lig_4	RRE15	Target_95	6.2839966563652

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	O)O)N)O)O)N						
897	<chem>c1ccc2c(c1)Sc1c(N2CCCN(C)C)cc(cc1)C(=O)C</chem>	GGCAGAUCUGAGCC UGGGAGCUCUCUGC C	Phenothiazine 5	Target_lig_1253	Acetylpromazine TAR RNA	Target_19	4.129011 18623943
899	<chem>CC(=O)C1=CC2=C(C=C1)SC3=CC=CC=C3N2CCCN(C)C</chem>	GGGCUAGCACUCUG GUAUCACGGUACCU UUGUGCGCCC	Acetylpromazine	Target_lig_176	Coxsackie virus B3 RNA	Target_130	3.48148 606012211
900	<chem>CC(=O)C1=CC2=C(C=C1)SC3=CC=CC=C3N2CCCN(C)C</chem>	GGGGUUGUACCCAC CCC	Acetylpromazine	Target_lig_176	Polio virus loop B construct	Target_131	2.74472 749489669
949	<chem>N([C@@H](C(=O)N1[C@@H](CCC1)C(=O)N[C@@H](Cc1ccccc1)C(=O)NCCC(CCCN)CSSC[C@@H]1)(NC(=O)c1c(nc2c(cccc2)c1)CC)C(=O)N1[C@@H](CCC1)C(=O)N[C@@H](Cc1ccccc1)C(=O)NCCC(CCCN)C(=O)c1c2c(nc(c1)CC)cccc2</chem>	GGCCUUCCCAAG GGAAGGCC	disulfide_der_0	Target_lig_564	HIV-1 FSS	Target_188	6.45593 195564972
950	<chem>N([C@@H](C(=O)N1[C@@H](CCC1)C(=O)N[C@@H](Cc1ccccc1)C(=O)NCC(CN)CSSC[C@@H]1)(NC(=O)c1c(nc2c(cccc2)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</chem>	GGCCUUCCCAAG GGAAGGCC	disulfide_der_1	Target_lig_565	HIV-1 FSS	Target_188	6.45593 195564972
951	<chem>N([C@H](C(=O)N1[C@@H](CCC1)C(=O)N[C@@H](Cc1ccccc1)C(=O)NCC(CN)CSSC[C@@H]1)(NC(=O)c1c(nc2c(cccc2)c1)C(=O)N1[C@@H](CCC1)C(=O)N[C@@H](Cc1ccccc1)C(=O)NCC(CN)C(=O)c1c2c(nc(c1)C)cccc2</chem>	GGCCUUCCCAAG GGAAGGCC	disulfide_der_2	Target_lig_566	HIV-1 FSS	Target_188	6.36653 154442041
952	<chem>N([C@@H](C(=O)N1[C@@H](CCC1)C(=O)N[C@@H](Cc1ccccc1)C(=O)NCC(CN)CSSC[C@@H]1)(NC(=O)c1cnc2c(cccc2)c1)C(=O)N1[C@@H](CCC1)C(=O)N[C@@H](Cc1ccccc1)C(=O)NCC(CN)C(=O)c1c2c(nc(c1)c2)cccc2</chem>	GGCCUUCCCAAG GGAAGGCC	disulfide_der_3	Target_lig_567	HIV-1 FSS	Target_188	6.18708 664335714
953	<chem>N([C@@H](C(=O)N1[C@@H](CCC1)C(=O)N[C@@H](Cc1ccccc1)C(=O)NCC(CN)CSSC[C@@H]1</chem>	GGCCUUCCCAAG GGAAGGCC	disulfide_der_6	Target_lig_568	HIV-1 FSS	Target_188	5.84771 165561694

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	<chem>(NC(=O)c1c(nc2c(cc3c(c2)OCO3)c1)CC)C(=O)N1[C@@H](CCC1)C(=O)N[C@@H](Cc1ccccc1)C(=O)NCCCN)C(=O)c1c2c(nc(c1)CC)cc1c(c2)OCO1</chem>						
954	<chem>N([C@H](C(=O)N1[C@@H](CCC1)C(=O)N[C@@H](Cc1ccccc1)C(=O)NCCCN)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)NCCCN)C(=O)c1c2c(nc(c1)CC)C(=O)[C@@H]1[C@H](C2=O)C=CC=C1</chem>	GGCCUCCCCACAAG GGAAGGCC	disulfide_der_7	Target_lig_569	HIV-1 FSS	Target_188	6.63827 2163982 41
955	<chem>N([C@H](C(=O)N1[C@@H](CCC1)C(=O)N[C@@H](Cc1ccccc1)C(=O)NCCCN)CC=C)C(=O)c1c2c(nc(c1)CC)cccc2</chem>	AGGACUCGGCUUGC UGAAGCGCGCGACG GCAAGAGGCGAGG GGCGGCGACUGGUG AGUACGCCAAAAAU UUUGACUAGCGGA GGCUAGAAGGAGA GAGAUUGGUGCGA GAGCGUCGGU	carba_der	Target_lig_570	HIV-1 genomic SL3 ma	Target_146	6.32790 2142064 28
956	<chem>N([C@H](C(=O)N1[C@@H](CCC1)C(=O)N[C@@H](Cc1ccccc1)C(=O)NCCCN)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)NCCCN)C(=O)c1c2c(nc(c1)CC)cccc2</chem>	AGGACUCGGCUUGC UGAAGCGCGCGACG GCAAGAGGCGAGG GGCGGCGACUGGUG AGUACGCCAAAAAU UUUGACUAGCGGA GGCUAGAAGGAGA GAGAUUGGUGCGA GAGCGUCGGU	dicarba_analog_1	Target_lig_571	HIV-1 genomic SL3 ma	Target_146	6.48148 6060122 11
957	<chem>N([C@H](C(=O)N1[C@@H](CCC1)C(=O)N[C@@H](Cc1ccccc1)C(=O)NCCCN)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)NCCCN)C(=O)c1c2c(nc(c1)CC)cccc2</chem>	AGGACUCGGCUUGC UGAAGCGCGCGACG GCAAGAGGCGAGG GGCGGCGACUGGUG AGUACGCCAAAAAU UUUGACUAGCGGA GGCUAGAAGGAGA GAGAUUGGUGCGA GAGCGUCGGU	dicarba_analog_2	Target_lig_572	HIV-1 genomic SL3 ma	Target_146	5.89619 6279044 04
958	<chem>CN(C)CCNC1=CC(=NC2=CC=CC=C21)C3=CC=CC=C3</chem>	AGGACUCGGCUUGC UGAAGCGCGCGACG GCAAGAGGCGAGG GGCGGCGACUGGUG AGUACGCCAAAAAU UUUGACUAGCGGA GGCUAGAAGGAGA GAGAUUGGUGCGA GAGCGUCGGU	quinoline_der	Target_lig_24	HIV-1 genomic SL3 ma	Target_146	6.53760 2002101 04

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
959	<chem>C1=C(N(C(=C=1)c1c(c(c(cc1C)C)C)[Ru](=Cc1cccc1)(Cl)(Cl)P(C1CCCC1)(C1CCCC1)C1CCCC1)c1c(cc(cc1C)C)C</chem>	AGGACUCGGCUUGC UGAAGCGCGCGACG GCAAGAGGCGAGG GGCGGCGACUGGUG AGUACGCCAAAAAU UUUGACUAGCGGA GGCUAGAAGGAGA GAGAUGGGUGCGA GAGCGUCGGU	Ruthenium_der	Target_lig_574	HIV-1 genomic SL3 ma	Target_146	6.45593 1955649 72
960	<chem>CN(C)C1=NC=NC2=C1N=CN2CCN3C=NC4=C3N=CN=C4N(C)C</chem>	AGGACUCGGCUUGC UGAAGCGCGCGACG GCAAGAGGCGAGG GGCGGCGACUGGUG AGUACGCCAAAAAU UUUGACUAGCGGA GGCUAGAAGGAGA GAGAUGGGUGCGA GAGCGUCGGU	NSC54101	Target_lig_575	HIV-1 genomic SL3 ma	Target_146	4.49485 0021680 09
961	<chem>C[N+](CCCC2=CC=C(C=C2)NCC[N+](C)(C)C.[I-]</chem>	AGGACUCGGCUUGC UGAAGCGCGCGACG GCAAGAGGCGAGG GGCGGCGACUGGUG AGUACGCCAAAAAU UUUGACUAGCGGA GGCUAGAAGGAGA GAGAUGGGUGCGA GAGCGUCGGU	NSC18613	Target_lig_576	HIV-1 genomic SL3 ma	Target_146	5.82390 8740944 32
962	<chem>CC1=NC2=NC(=NN2C(=C1)N3CCN(CC3)C)C4=CC=C(C(=C4)C1</chem>	AGGACUCGGCUUGC UGAAGCGCGCGACG GCAAGAGGCGAGG GGCGGCGACUGGUG AGUACGCCAAAAAU UUUGACUAGCGGA GGCUAGAAGGAGA GAGAUGGGUGCGA GAGCGUCGGU	NSC252359	Target_lig_577	HIV-1 genomic SL3 ma	Target_146	4.95860 7314841 77
963	<chem>CN1C2=C(N(=C1OCCN(C)C)N(C(=O)N(C2=O)C)C</chem>	AGGACUCGGCUUGC UGAAGCGCGCGACG GCAAGAGGCGAGG GGCGGCGACUGGUG AGUACGCCAAAAAU UUUGACUAGCGGA GGCUAGAAGGAGA GAGAUGGGUGCGA GAGCGUCGGU	NSC11936	Target_lig_578	HIV-1 genomic SL3 ma	Target_146	5.85387 1964321 76
964	<chem>CC1=C(C(=O)C2=C(C1=O)N3C[C@H]4[C@@H](C3=C2COC(=O)N)N4C)OC</chem>	AGGACUCGGCUUGC UGAAGCGCGCGACG GCAAGAGGCGAGG GGCGGCGACUGGUG AGUACGCCAAAAAU UUUGACUAGCGGA GGCUAGAAGGAGA GAGAUGGGUGCGA GAGCGUCGGU	NSC123111	Target_lig_579	HIV-1 genomic SL3 ma	Target_146	4.00877 3924307 51
965	<chem>CN1C2=NC=NC3=C2C(=CN3C4C(C(C(O4)CO)O)O)C(=N1)N</chem>	AGGACUCGGCUUGC UGAAGCGCGCGACG GCAAGAGGCGAGG GGCGGCGACUGGUG AGUACGCCAAAAAU UUUGACUAGCGGA GGCUAGAAGGAGA GAGAUGGGUGCGA GAGCGUCGGU	NSC154020	Target_lig_580	HIV-1 genomic SL3 ma	Target_146	3.92811 7992693 87
966	<chem>C[N+](CCCC2=CC(=C(C=C2C1CC3=CC(=C(C=C3)O)O)O)O)C.[Br-]</chem>	AGGACUCGGCUUGC UGAAGCGCGCGACG GCAAGAGGCGAGG GGCGGCGACUGGUG AGUACGCCAAAAAU UUUGACUAGCGGA GGCUAGAAGGAGA GAGAUGGGUGCGA GAGCGUCGGU	NSC121848	Target_lig_581	HIV-1 genomic SL3 ma	Target_146	3.86966 6231504 99

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		GAGCGUCGGU					
967	<chem>C1=CC=C(C(=C1)/C=C\2/C(=O)N(C(=O)N2)/C=C\3/C(=O)C4=CC=CC=C4OC3=O)O</chem>	AGGACUCGGCUUGC UGAAGCGCGCGACG GCAAGAGGCGAGG GGCGGCGACUGGUG AGUACGCCAAAAAU UUUGACUAGCGGA GGCUAGAAGGAGA GAGAUUGGUGCGA GAGCGUCGGU	NSC657704	Target_lig_582	HIV-1 genomic SL3 ma	Target_146	3.78781 2395596 04
968	<chem>C[N+]1(C2CC(CC1C3C2O3)OC(=O)C(CO)C4=CC=CC=C4)C</chem>	AGGACUCGGCUUGC UGAAGCGCGCGACG GCAAGAGGCGAGG GGCGGCGACUGGUG AGUACGCCAAAAAU UUUGACUAGCGGA GGCUAGAAGGAGA GAGAUUGGUGCGA GAGCGUCGGU	NSC61809	Target_lig_583	HIV-1 genomic SL3 ma	Target_146	3.80410 0347590 77
969	<chem>c1c(cc2c(c1)c(c1c(n2)c(c(c1)OC)C)Nc1ccc(c(c1)CN1CCN(CC1)C)O)Cl</chem>	AGGACUCGGCUUGC UGAAGCGCGCGACG GCAAGAGGCGAGG GGCGGCGACUGGUG AGUACGCCAAAAAU UUUGACUAGCGGA GGCUAGAAGGAGA GAGAUUGGUGCGA GAGCGUCGGU	acridine_new_der v	Target_lig_584	HIV-1 genomic SL3 ma	Target_146	6.17392 5197299 17
990	<chem>CC1=CC=CN2C1=NC3=C(C2=O)C=C(C(=N)N3CCOCCO)C(=O)N[C@@H](C)C4=CC=CC=C4</chem>	AGGACUCGGCUUGC UGAAGCGCGCGACG GCAAGAGGCGAGG GGCGGCGACUGGUG AGUACGCCAAAAAU UUUGACUAGCGGA GGCUAGAAGGAGA GAGAUUGGUGCGA GAGCGUCGGU	SL3 RNA_ligand1	Target_lig_605	SL3 RNA	Target_146	3.78781 2395596 04
991	<chem>C1=CC=C2C=C(C(=CC2=C1)/C=C/3\C(=O)N=C(S3)N</chem>	AGGACUCGGCUUGC UGAAGCGCGCGACG GCAAGAGGCGAGG GGCGGCGACUGGUG AGUACGCCAAAAAU UUUGACUAGCGGA GGCUAGAAGGAGA GAGAUUGGUGCGA GAGCGUCGGU	SL3 RNA_ligand3	Target_lig_606	SL3 RNA	Target_146	4.95860 7314841 77
992	<chem>COC1=C(C(=C(C=C1)NCC2=CC=C(S2)[N-](=O)[O-])OC</chem>	AGGACUCGGCUUGC UGAAGCGCGCGACG GCAAGAGGCGAGG GGCGGCGACUGGUG AGUACGCCAAAAAU UUUGACUAGCGGA GGCUAGAAGGAGA GAGAUUGGUGCGA GAGCGUCGGU	SL3 RNA_ligand4	Target_lig_607	SL3 RNA	Target_146	5.95860 7314841 77
993	<chem>C1=CC=C2C=C(C(=CC2=C1)/C=C/3\C(=O)NC(=S)N3</chem>	AGGACUCGGCUUGC UGAAGCGCGCGACG GCAAGAGGCGAGG GGCGGCGACUGGUG AGUACGCCAAAAAU UUUGACUAGCGGA GGCUAGAAGGAGA GAGAUUGGUGCGA GAGCGUCGGU	SL3 RNA_ligand5	Target_lig_608	SL3 RNA	Target_146	5.45593 1955649 72
994	<chem>C1=CC=C(C(=C1)C[N+]2=CC=C(C(=C2)C(=O)N/N=C\C3=CC=C(C(=C3)Br</chem>	AGGACUCGGCUUGC UGAAGCGCGCGACG GCAAGAGGCGAGG GGCGGCGACUGGUG AGUACGCCAAAAAU UUUGACUAGCGGA	SL3 RNA_ligand6	Target_lig_609	SL3 RNA	Target_146	5.30102 9995663 98

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=C2/ 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=C3 NC4=CC=C(C=C4)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	c12cccc1C(=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

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		AGUACGCCAAAAAU UUUGACUAGCGGA GGCUAGAAGGAGA GAGAUUGGUGCGA GAGCGUCGGU					
1003	<chem>CC1=CC=CN2C1=NC3=C(C2=O)C=C(C(=N)N3C[C@H]4CCCCO4)C(=O)N5CCN(CC5)C</chem>	AGGACUCGGCUUGC UGAAGCGCGCGACG GCAAGAGGCGAGG GGCGGCGACUGGUG AGUACGCCAAAAAU UUUGACUAGCGGA GGCUAGAAGGAGA GAGAUUGGUGCGA GAGCGUCGGU	SL3 RNA_ligand15	Target_lig_618	SL3 RNA	Target_146	4.35654 7323513 81
1004	<chem>C1=CC=C(C(C=C1)N2C=C(C(=N2)C3=CC4=C(C=CC5=CC=CC=C54)OC3=O)C=C6C(=O)NC(=S)NC6=O</chem>	AGGACUCGGCUUGC UGAAGCGCGCGACG GCAAGAGGCGAGG GGCGGCGACUGGUG AGUACGCCAAAAAU UUUGACUAGCGGA GGCUAGAAGGAGA GAGAUUGGUGCGA GAGCGUCGGU	SL3 RNA_ligand16	Target_lig_619	SL3 RNA	Target_146	4.29242 9823902 06
1005	<chem>CN1CCN(CC1)CCCN2C3=CC=CC=C3SC4=C2C=C(C=C4)C(F)(F)F</chem>	AGGACUCGGCUUGC UGAAGCGCGCGACG GCAAGAGGCGAGG GGCGGCGACUGGUG AGUACGCCAAAAAU UUUGACUAGCGGA GGCUAGAAGGAGA GAGAUUGGUGCGA GAGCGUCGGU	SL3 RNA_ligand17	Target_lig_620	SL3 RNA	Target_146	4.04575 7490560 68
1107	<chem>NC1=NC(N)=[NH+]C(NCCCCNC(=[NH2+])C2=CC=C(C=C2)C(=[NH2+])NCCCCNC2=[NH+]C(N)=NC(N)=N2)=N1</chem>	UUUUUUAGGGAAG AUCUGGCCUUCCCA CAAGGGAAGGCCAG GGAAUUUUUCUU	Bisamidinium 2	Target_lig_649	HIV-1 FSS RNA	Target_109	3.69897 0004336 02
1126	<chem>CCC1=C(C=C2C=C3C=CC=CC3=CC2=N1)C(=O)N1CCC[C@H]1C(=O)N[C@@H](CCC\C=C\C[C@H]1CCCN1C(=O)C1=C(CC)N=C2C=C3C=CC=CC2=C1)C(=O)N[C@@H](CCCC[NH3+])C(=O)NCCCC[NH3+]C(=O)N[C@@H](CCCC[NH3+])C(=O)NCCCC[NH3+]</chem>	UUUUUUAGGGAAG AUCUGGCCUUCCCA CAAGGGAAGGCCAG GGAAUUUUUCUU	DCC 11 (2012)	Target_lig_653	HIV-1 FSS RNA	Target_109	5.69897 0004336 02
1129	<chem>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=CC2=C1)C(=O)N1C CC[C@H]1C(=O)N(C)[C@@H](CC1=CC=CC=C1)C(=O)NCCCC[NH3+])C(=O)N1CCC[C@H]1C(=O)N(C)[C@@H](CC1=CC=CC=C1)C(=O)NCCCC[NH3+]</chem>	UUUUUUAGGGAAG AUCUGGCCUUCCCA CAAGGGAAGGCCAG GGAAUUUUUCUU	Compound 4E	Target_lig_654	HIV-1 FSS RNA	Target_109	8.30102 9995663 98
1130	<chem>CCC1=C(C=C2C=C3C=CC=CC3=CC2=N1)C(=O)N(C)[C@@H](C\C</chem>	GGCCUUCACAAAG GGAAGGCC	Compound 4E	Target_lig_654	HIV-1 FSS DNA	Target_188	7.46852 1082957 74

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	<chem>C=C\C[C@H](N(C)C(=O)C1=C(CC)N=C2C=C3C=CC=CC3=CC2=C1)C(=O)N1CC[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+]</chem>						
1134	<chem>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+]</chem>	GGCCUUCCACAAAG GGAAGGCC	DCC 4 (2012)	Target_lig_652	HIV-1 FSS DNA	Target_188	7.14874 1651280 92
1135	<chem>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+]</chem>	UUUUUUAGGGAAG AUCUGGCCUCCCA CAAGGGAAGGCCAG GGAAUUUUUCUU	DCC 4 (2012)	Target_lig_652	HIV-1 FSS RNA	Target_109	7.18045 6064458 13
1138	<chem>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]N[C@@H](CC1=CC=CC=C1)C(=O)NCCC[NH3+]</chem>	UUUUUUAGGGAAG AUCUGGCCUCCCA CAAGGGAAGGCCAG GGAAUUUUUCUU	DCC 5 (2012)	Target_lig_655	HIV-1 FSS RNA	Target_109	7.05060 9993355 09
1139	<chem>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]N[C@@H](CC1=CC=CC=C1)C(=O)NCCC[NH3+]</chem>	GGCCUUCCACAAAG GGAAGGCC	DCC 5 (2012)	Target_lig_655	HIV-1 FSS DNA	Target_188	7.01772 8766960 43
1143	<chem>CC(=O)NC1=NC(=CS1)C1=CC(NC(=O)C(CN</chem>	GGCAGAUCUGAGCC UGGGAGCUCUCUGC	S-Amino acid conjugate 13b	Target_lig_656	HIV-1 TAR RNA	Target_19	6.61978 8758288

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	<chem>C(=O)[C@@H]([NH3+])CCCC[NH3+]NC(=O)[C@@H]([NH3+])CCCC[NH3+])=CC=C1</chem>	C					39
1146	<chem>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</chem>	GGCAGAUCUGAGCC UGGGAGCUCUCUGC C	S-Amino acid conjugate 14b	Target_lig_657	HIV-1 TAR RNA	Target_19	6.95860 7314841 77
1150	<chem>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=N1)C(=O)N1CCC[C@H]1C(=O)N[C@@H](CC1=CC=CC=C1)C(=O)NCCC[NH3+]</chem>	UUUUUUAGGGAAG AUCUGGCCUCCCA CAAGGGAAGGCCAG GGAAUUUUUCUU	DCC 3 (2017)	Target_lig_658	HIV-1 FSS RNA; 5-fold excess tRNA	Target_109	7.49485 0021680 09
1152	<chem>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=CC4=CC3=C2)C(=O)N2CC[C@H]2C(=O)N(C)[C@@H](CC2=CC=CC=C2)C(=O)NCCC[NH3+])N=N1)C(=O)N1CCC[C@H]1C(=O)N[C@@H](CC1=CC=CC=C1)C(=O)NCCC[NH3+]</chem>	UUUUUUAGGGAAG AUCUGGCCUCCCA CAAGGGAAGGCCAG GGAAUUUUUCUU	DCC 4 (2017)	Target_lig_659	HIV-1 FSS RNA; 5-fold excess tRNA	Target_109	7.20760 8310501 75
1154	<chem>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=CC4=CC3=C2)C(=O)N2CC[C@H]2C(=O)N[C@@H](CC2=CC=CC=C2)C(=O)NCCC[NH3+])N=N1)C(=O)N1CCC[C@H]1C(=O)N(C)[C@@H](CC1=CC=CC=C1)C(=O)NCCC[NH3+]</chem>	UUUUUUAGGGAAG AUCUGGCCUCCCA CAAGGGAAGGCCAG GGAAUUUUUCUU	DCC 5 (2017)	Target_lig_660	HIV-1 FSS RNA; 5-fold excess tRNA	Target_109	7.50863 8306165 73
1155	<chem>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=CC4=CC3=C2)C(=O)N2CC[C@H]2C(=O)N(C)[C@@H](CC2=CC=CC=C2)C(=O)NCCC[NH3+])N=N1)C(=O)N1CCC[C@H]1C(=O)N(C)[C@@H](CC1=CC=CC=C1)C(=O)NCCC[NH3+]</chem>	UUUUUUAGGGAAG AUCUGGCCUCCCA CAAGGGAAGGCCAG GGAAUUUUUCUU	DCC 7 (2017)	Target_lig_661	HIV-1 FSS RNA	Target_109	7.79588 0017344 08

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[NH+])(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)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[NH+])(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[NH+])(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+]C3=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	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)/C1/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=N2)=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

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
1255	<chem>COC1=C(C=C2C(=C1)C(=NC(=N2)N3CC[NH2+]CC3)N)OC</chem>	GAGUAGAAACAAG GCUUCGGCCUGCUU UUGCU	DPQ	Target_lig_701	Influenza RNA promoter	Target_217	4.29670 8621881 34
1256	<chem>CCC(=O)N1CCN(CC1)C1=NC(N)=C2C=C(C(OC)C(OC)=CC2=[NH+]1</chem>	GAGUAGAAACAAG GCUUCGGCCUGCUU UUGCU	DPQ6	Target_lig_702	Influenza RNA promoter	Target_217	3.94233 3896090 17
1257	<chem>COC1=CC2=[NH+]C(=NC(N)=C2C=C1OC)N1CCN(CC1)C(=O)C(C)C</chem>	GAGUAGAAACAAG GCUUCGGCCUGCUU UUGCU	DPQ7	Target_lig_703	Influenza RNA promoter	Target_217	3.79997 0733446 23
1258	<chem>CCCC(=O)N1CCN(CC1)C1=NC(N)=C2C=C(OC)C(OC)=CC2=[NH+]1</chem>	GAGUAGAAACAAG GCUUCGGCCUGCUU UUGCU	DPQ8	Target_lig_704	Influenza RNA promoter	Target_217	4.35310 6375832 25
1259	<chem>COC1=CC2=[NH+]C(=NC(N)=C2C=C1OC)N1CCN(CC1)C(=O)C1CC1</chem>	GAGUAGAAACAAG GCUUCGGCCUGCUU UUGCU	DPQ10	Target_lig_705	Influenza RNA promoter	Target_217	3.89551 2888687 6
1260	<chem>CCOC(=O)C1=CC=CC=C1NC(=O)N2CCCN(CC2)CC3=CSC(=N3)C</chem>	CGGUGUAAGUGCA GCCCCGUCUUACACC GUGCGGCACAGCGG AAACGCUGAUGUCG UAUACAGGGCU	Compound 43 (MTDB)	Target_lig_706	SARS- Pseudoknot Construct	Target_218	3.67778 0705266 08
1261	<chem>CCN(CC)CCOC1=CC=C(C=C1)NC2=NC(=NC3=CC=CC=C32)C4=CC=CC=C4NC(=O)CCN5CCN(CC5)C</chem>	GGAGGAGGGGGAG GAGGA	Compound 1 (2017)	Target_lig_707	HCV IRES-A	Target_219	6.03245 2023781 14
1262	<chem>CCN(CC)CCOC1=CC=C(C=C1)NC2=NC(=NC3=CC=CC=C32)C4=CC=CC=C4NC(=O)CCN5CCN(CC5)C</chem>	UGAUGAGUGUGAG GAGGA	Compound 1 (2017)	Target_lig_707	HCV IRES-A 1 Mutant	Target_220	5.43062 6090384 95
1266	<chem>CCN(CC)CCOC1=CC=C(C=C1)NC2=NC(=NC3=CC=CC=C32)C4=CC=CC=C4NC(=O)CCN5CCN(CC5)C</chem>	CCUGACUAGUCUUU CAGG	Compound 1 (2017)	Target_lig_707	HCV IRES-A DNA	Target_222	4.83863 1997765 03
1275	<chem>COC1=CC(CC[NH3+])=C(C(C[NH3+])=C1)C1=CC(C)=C(C(C)=C1)C1=CC(CC[NH3+])=C(O)C(CC[NH3+])=C1</chem>	GCACUAUGGGCGCC AGCGUCAUAGACGC UGACGGUACAGCCA GACAAUUAUUGUC UGGUAUAGUGC	p-Terphenyl 6b	Target_lig_711	HIV-1 RRE IIB	Target_80	6.22184 8749616 36
1322	<chem>C(CN1C=C(CNC2=C3C=CC=CC3=[NH+]C3=C2OC2=C3C=CC=C2)N=N1)C[NH+]1CCCCC1</chem>	GGAGGAGGGGGAG GAGGA	Quindoline CK1- 14	Target_lig_723	IRES RNA G- quadruplex	Target_257	5.86012 0913598 76
1710	<chem>COC1=C(C=C2C(=C1)C(=NC(=N2)N3CC[NH2+]CC3)N)OC</chem>	GGCAGAUCUGAGCC UGGGAGCUCUCUGC C	DPQ	Target_lig_701	HIV-1 TAR RNA	Target_19	4.36653 1544420 41
1713	<chem>C1=CC(=CC=C1C(=N)N)OCCCCOC2=CC=C(C=C2)C(=N)N</chem>	GGCAGAUCUGAGCC UGGGAGCUCUCUGC C	Pentamidine	Target_lig_953	HIV-1 TAR RNA	Target_19	3.47886 1916295 96
1780	<chem>C1C(C(C(C(C1N)OC2C(C(C(C(O2)CN)O)O)N)OC3C(C(C(O3)CO)OC4C(C(C(C(O4)CN)O)O)N)O)O)N</chem>	GGCAGAUCUGAGCC UGGGAGCUCUCUGC C	Neomycin	Target_lig_4	HIV-1 TAR RNA	Target_19	4.67778 0705266 08
1781	<chem>NCCCCC(C(=O)OCO[C@H]1O[C@H](C[C@H]1O)C(=O)Nc1cccc(c1)c1sc(c(n1)N(C(=O)C)N</chem>	GGCAGAUCUGAGCC UGGGAGCUCUCUGC C	Compound 3ab	Target_lig_999	HIV-1 TAR RNA	Target_19	4.52287 8745280 34
1782	<chem>NCCCCC(C(=O)OCO[</chem>	GGCAGAUCUGAGCC	Compound 3bb	Target_lig_100	HIV-1 TAR	Target_19	5.09691

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	<chem>C@H]1C[C@@H](O[C@@H]1COCOC(=O)C(CCCCN)N)C(=O)Nc1cccc(c1)c1csc(n1)NC(=O)C)N</chem>	UGGGAGCUCUCUGC C		0	RNA		0013008 06
1783	<chem>CC(=O)Nc1ccc(n1)c1ccc(c1)NC(=O)[C@H]1C[C@@H]([C@H](O1)COCOC(=O)C(CCN=C(N)N)N)O</chem>	GGCAGAUCUGAGCC UGGGAGCUCUCUGC C	Compound 3cb	Target_lig_100 1	HIV-1 TAR RNA	Target_19	4.88605 6647693 16
1784	<chem>CC(=O)Nc1ccc(n1)c1ccc(c1)NC(=O)[C@H]1C[C@@H]([C@H](O1)COCOC(=O)C(CCN=C(N)N)N)OCOC(=O)C(CCCN=C(N)N)N</chem>	GGCAGAUCUGAGCC UGGGAGCUCUCUGC C	Compound 3db	Target_lig_100 2	HIV-1 TAR RNA	Target_19	5
1785	<chem>NCCCCC(C(=O)OCO[C@H]1OC(C[C@@H]1O)C(=O)Nc1cccc(c1)c1csc(n1)NC(=O)C)N</chem>	GGCAGAUCUGAGCC UGGGAGCUCUCUGC C	Compound 3aa	Target_lig_100 3	HIV-1 TAR RNA	Target_19	4.85387 1964321 76
1786	<chem>NCCCCC(C(=O)OCO[C@H]1CC(O[C@@H]1COCOC(=O)C(CCCCN)N)C(=O)Nc1cccc(c1)c1csc(n1)NC(=O)C)N</chem>	GGCAGAUCUGAGCC UGGGAGCUCUCUGC C	Compound 3ba	Target_lig_100 4	HIV-1 TAR RNA	Target_19	4.88605 6647693 16
1787	<chem>C1C(C(C(C1N)OC2C(C(C(C(O2)CN)O)O)N)OC3C(C(C(O3)CO)OC4C(C(C(C(O4)CN)O)O)N)O)O)N</chem>	GGCAGAUCUGAGCC UGGGAGCUCUCUGC C	Neomycin	Target_lig_4	HIV-1 TAR ab	Target_19	4.50863 8306165 73
1817	<chem>CN(C)C1=C(N=C(C(=N1)N)C(=O)[NH+]=C(N)N)C#CC2=CC=CC=C2</chem>	GGAUCAAUAGCAG GUGUGGCACACCAG UCAUACCUUGAUCC	DMA-135	Target_lig_101 9	EV71 SLII RNA	Target_329	6.28399 6656365 2
1818	<chem>O=C(c1nc(Cl)c(nc1N)N(C)C)NC(=[NH2+])N</chem>	GGAUCAAUAGCAG GUGUGGCACACCAG UCAUACCUUGAUCC	DMA-001	Target_lig_102 0	EV71 SLII RNA	Target_329	6.23657 2006437 06
1819	<chem>CN(c1nc(N)c(nc1c1ccc(cc1)c1cccc1)C(=O)N)C(=[NH2+])N)C</chem>	GGAUCAAUAGCAG GUGUGGCACACCAG UCAUACCUUGAUCC	DMA-155	Target_lig_102 1	EV71 SLII RNA	Target_329	6.25181 1972993 8
2047	<chem>CC(=O)C1=CC2=C(C=C1)SC3=CC=CC=C3N2CCCN(C)C</chem>	GGGCUAGCACUCUG GUAUCACGGUACCU UUGUGCGCCC	Acetylpromazine	Target_lig_176	CVB loop D RNA	Target_373	3.48148 6060122 11
2048	<chem>CC(=O)C1=CC2=C(C=C1)SC3=CC=CC=C3N2CCCN(C)C</chem>	GGGGUUGUACCCAC CCCAC	Acetylpromazine	Target_lig_176	Polio virus loop B RNA	Target_374	2.74472 7494896 69
2049	<chem>NCCCOc1ccc(cc1CNC)CCCNC(=N)N)c1csc1</chem>	GGCAGAUCUGAGCC UGGGAGCUCUCUGC C	Rbt427	Target_lig_112 4	HIV-1 TAR RNA	Target_19	6.06550 1548756 43
2050	<chem>NCCCOc1ccc(cc1CNC)CCCNC(=N)N)c1cc2c(o1)cccc2</chem>	GGCAGAUCUGAGCC UGGGAGCUCUCUGC C	Rbt429	Target_lig_112 5	HIV-1 TAR RNA	Target_19	6.72124 6399047 17
2051	<chem>NCCCOc1ccc(cc1CNC)Cc1ccc(cc1CNC(=N)N)c1cc2c(s1)cccc2</chem>	GGCAGAUCUGAGCC UGGGAGCUCUCUGC C	Rbt446	Target_lig_112 6	HIV-1 TAR RNA	Target_19	6.65955 5885159 88
2052	<chem>NCCCOc1ccc(cc1CNC)CCCN(C)C)c1cc2c(s1)cccc2</chem>	GGCAGAUCUGAGCC UGGGAGCUCUCUGC C	Rbt489	Target_lig_112 7	HIV-1 TAR RNA	Target_19	6.22914 7988357 86
2053	<chem>NCCCOc1ccc(cc1CNC)CC1CCNCC1)c1cc2c(s1)cccc2</chem>	GGCAGAUCUGAGCC UGGGAGCUCUCUGC C	Rbt537	Target_lig_112 8	HIV-1 TAR RNA	Target_19	6.32239 3047279 51
2054	<chem>NCCCOc1ccc(cc1CNC)</chem>	GGCAGAUCUGAGCC	Rbt549	Target_lig_112	HIV-1 TAR	Target_19	6.82102

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)c1cccn1	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)c1cccc1	GGCAGAUcUGAGCC UGGGAGCUCUCUGC C	Rbt567	Target_lig_113 4	HIV-1 TAR RNA	Target_19	5.92445 3038607 47
2060	N1CCN(CC1)CCCNCc1cc(cce1OCc1cc2c(s1)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 CNCCCNC1CCNCC1)c1cc2c(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)O[C@@H]1[C@H] ([C@@H]([C@H] ([C@@H] (O1)CNc1c2cccc2nc2 c1cccc2)O)N)O	GGCCGAGUAGUGU UGGGUCGCGAAAG GCC	Tobramycin	Target_lig_540	HCV IRES Domain IIIId	Target_66	5.65757 7319177 79
2143	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)N)O)O)N	GGCCGAGUAGUGU UGGGUCGCGAAAG GCC	Neomycin B	Target_lig_125 1	HCV IRES Domain IIIId	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 IIIId	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 IIIId	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)N)N	GGCCGAGUAGUGU UGGGUCGCGAAAG GCC	Compd 34	Target_lig_115 7	HCV IRES Domain IIIId	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 IIIId	Target_66	5.56863 6235841 01

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 IIIId	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 IIIId	Target_66	5.63827 2163982 41
2150	NCC1OC(OC2C(N)CC(C(C2O)OC2OC(COC3OC(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 IIIId	Target_66	5.39794 0008672 04
2151	NCC1OC(OC2C(N)CC(C(C2O)OC2OC(COC3OC(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 IIIId	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 IIIId	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 IIIId	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 IIIId	Target_66	6
2185	CC1(COC(C(C1NC)O)OC2C(CC(C(C2O)OC3C(CC=C(O3)CN)N)N)N)O	CUGUCUUCACGCAG AAAGCGUCUAGCCA UGGCGUUAGUAUG AGUGUCG	sisomicin	Target_lig_10	HCV IRES Domain lib	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@H]([C@@H](O1)CN)O)N)N)O[C@@H]1[C@H]([C@@H]([C@H]([C@@H](O1)CN)c1c2ccccc2nc2c1cccc2)O)N)O	CUGUCUUCACGCAG AAAGCGUCUAGCCA UGGCGUUAGUAUG AGUGUCG	Tobramycin	Target_lig_540	HCV IRES Domain lib	Target_408	5.56863 6235841 01
2187	C1C(C(C(C(C1N)OC2C(C(C(C(O2)CN)O)O)N)OC3C(C(C(O3)CO)OC4C(C(C(C(O4)CN)O)O)N)O)O)N	CUGUCUUCACGCAG AAAGCGUCUAGCCA UGGCGUUAGUAUG AGUGUCG	Neomycin B	Target_lig_125 1	HCV IRES Domain lib	Target_408	5.53760 2002101 04
2188	NCC1OC(OC2C(N)CC(C(C2O)OC2OC(CN)C(C(C2O)O)N)N)C(CC1O)N	CUGUCUUCACGCAG AAAGCGUCUAGCCA UGGCGUUAGUAUG AGUGUCG	Compd 32	Target_lig_115 5	HCV IRES Domain lib	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 lib	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 lib	Target_408	6.37675 0709602

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	<chem>(CC2N)O)N)C(C(C1OC(CO)C(C(C1O)N)O)O)N</chem>	UGGCGUUAGUAUG AGUGUCG					1
2191	<chem>NCC1OC(OC2C(N)CC(C(C2O)OC2OC(CN)C(C(C2O)N)O)N)C(C(C1O)N</chem>	CUGUCUUCACGCAG AAAGCGUCUAGCCA UGGCGUUAGUAUG AGUGUCG	Compd 35	Target_lig_115 8	HCV IRES Domain Lib	Target_408	5.74472 7494896 69
2192	<chem>NCC1OC(OC2C(N)CC(C(C2O)OC2OC(COC3OC(CO)C(C(C3N)O)O)C(C(C2N)O)O)N)C(C(C1O)N</chem>	CUGUCUUCACGCAG AAAGCGUCUAGCCA UGGCGUUAGUAUG AGUGUCG	Compd 36	Target_lig_116 3	HCV IRES Domain Lib	Target_408	5.02687 2146400 3
2193	<chem>NCC1OC(OC2C(N)CC(C(C2O)OC2OC(CN)C(C(C2N)O)N)C(C(C1O)OC1OC(CO)C(C(C1O)O)N)O</chem>	CUGUCUUCACGCAG AAAGCGUCUAGCCA UGGCGUUAGUAUG AGUGUCG	Compd 37	Target_lig_115 9	HCV IRES Domain Lib	Target_408	6.55284 1968657 78
2194	<chem>NCC1OC(OC2C(N)CC(C(C2O)OC2OC(CN)C(C(C2N)O)N)C(C(C1OC1OC(CO)C(C(C1N)O)O)N)O</chem>	CUGUCUUCACGCAG AAAGCGUCUAGCCA UGGCGUUAGUAUG AGUGUCG	Compd 38	Target_lig_116 0	HCV IRES Domain Lib	Target_408	4.92081 8753952 38
2195	<chem>NCC1OC(OC2C(N)CC(C(C2O)OC2OC(COC3OC(CN)C(C(C3O)O)O)C(C(C2N)O)N)N)C(C(C1O)N</chem>	CUGUCUUCACGCAG AAAGCGUCUAGCCA UGGCGUUAGUAUG AGUGUCG	Compd 39	Target_lig_116 1	HCV IRES Domain Lib	Target_408	5.58502 6652029 18
2196	<chem>NCC1OC(OC2C(N)CC(C(C2O)OC2OC(COC3OC(CN)C(C(C3O)O)O)C(C(C2N)O)N)N)C(C(C1O)N</chem>	CUGUCUUCACGCAG AAAGCGUCUAGCCA UGGCGUUAGUAUG AGUGUCG	Compd 40	Target_lig_128 1	HCV IRES Domain Lib	Target_408	5.42021 6403383 19
2197	<chem>NCC1OC(OC2C(N)CC(C(C2O)OC2OC(CN)C(C(C2N)O)N)C(C(C1O)OC1OC(CO)C(C(C1N)O)O)N</chem>	CUGUCUUCACGCAG AAAGCGUCUAGCCA UGGCGUUAGUAUG AGUGUCG	Compd 41	Target_lig_116 2	HCV IRES Domain Lib	Target_408	5.45593 1955649 72
2198	<chem>NCC1OC(OC2C(N)CC(C(C2O)OC2OC(CN)C(C(C2N)O)N)C(C(C1O)OC1OC(CO)C(C(C1N)O)O)N</chem>	CUGUCUUCACGCAG AAAGCGUCUAGCCA UGGCGUUAGUAUG AGUGUCG	Compd 42	Target_lig_128 2	HCV IRES Domain Lib	Target_408	5.50863 8306165 73
2199	<chem>NCC1OC(OC2C(N)CC(C(C2O)OC2OC(CN)C(C(C2N)O)N)C(C(C1OC1OC(CO)C(C(C1N)O)O)N)O</chem>	CUGUCUUCACGCAG AAAGCGUCUAGCCA UGGCGUUAGUAUG AGUGUCG	Compd 43	Target_lig_128 3	HCV IRES Domain Lib	Target_408	5.02227 6394711 15
2215	<chem>CC1(COC(C(C1NC)O)OC2C(CC(C(C2O)OC3C(CC=C(O3)CN)N)N)N)O</chem>	GGCUGACCAUCAAU AAGGAAGAAGCCCU UCAGCGGCCAGUA	sisomicin	Target_lig_10	HIV protease active site (PAS) mRNA	Target_409	4.82390 8740944 32
2216	<chem>[C@H]1([C@H](C[C@H]1([C@H]([C@H]1O)O)[C@@H]1[C@@H]([C@H]([C@@H]([C@H]1O1)CN)O)N)N)O[C@@H]1[C@H]([C@@H]([C@H]([C@@H]([C@H]1O1)CN)C1c2ccccc2nc2c1ccccc2)O)N)O</chem>	GGCUGACCAUCAAU AAGGAAGAAGCCCU UCAGCGGCCAGUA	Tobramycin	Target_lig_540	HIV protease active site (PAS) mRNA	Target_409	4.85387 1964321 76
2217	<chem>C1C(C(C(C(C1N)OC2C(C(C(C(O2)CN)O)O)N)OC3C(C(C(O3)CO)OC4C(C(C(C(O4)CN)O)O)N)O)O)N</chem>	GGCUGACCAUCAAU AAGGAAGAAGCCCU UCAGCGGCCAGUA	Neomycin B	Target_lig_125 1	HIV protease active site (PAS) mRNA	Target_409	5.69897 0004336 02

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
2218	<chem>NCC1OC(OC2C(N)CC(C(C2O)OC2OC(CN)C(CC2N)O)N)C(C(C1O)C(C2O)O)N</chem>	GGCUGACCAUCAAU AAGGAAGAAGCCCU UCAGCGGCCAGUA	Compd 32	Target_lig_115 5	HIV protease active site (PAS) mRNA	Target_409	4.72124 6399047 17
2219	<chem>NCC1OC(OC2C(N)CC(C(C2O)OC2OC(CN)C(CC2N)O)N)C(C(C1O)C1OC(CO)C(C(C1O)O)N)N)O</chem>	GGCUGACCAUCAAU AAGGAAGAAGCCCU UCAGCGGCCAGUA	Compd 33	Target_lig_115 6	HIV protease active site (PAS) mRNA	Target_409	5.95860 7314841 77
2220	<chem>NCC1OC(OC2C(N)CC(C(C2O)OC2OC(CN)C(CC2N)O)N)C(C(C1O)C1OC(CO)C(C(C1O)N)O)O)N</chem>	GGCUGACCAUCAAU AAGGAAGAAGCCCU UCAGCGGCCAGUA	Compd 34	Target_lig_115 7	HIV protease active site (PAS) mRNA	Target_409	6.08092 1907623 93
2221	<chem>NCC1OC(OC2C(N)CC(C(C2O)OC2OC(CN)C(C(C2O)N)O)N)C(C(C1O)C(C2O)O)N</chem>	GGCUGACCAUCAAU AAGGAAGAAGCCCU UCAGCGGCCAGUA	Compd 35	Target_lig_115 8	HIV protease active site (PAS) mRNA	Target_409	5.16749 1087293 76
2222	<chem>NCC1OC(OC2C(N)CC(C(C2O)OC2OC(COC3OC(CO)C(C(C3N)O)O)C(C(C2N)O)O)N)C(C(C1O)N</chem>	GGCUGACCAUCAAU AAGGAAGAAGCCCU UCAGCGGCCAGUA	Compd 36	Target_lig_116 3	HIV protease active site (PAS) mRNA	Target_409	5.29242 9823902 06
2223	<chem>NCC1OC(OC2C(N)CC(C(C2O)OC2OC(CN)C(CC2N)O)N)C(C(C1O)OC1OC(CO)C(C(C1O)O)N)O</chem>	GGCUGACCAUCAAU AAGGAAGAAGCCCU UCAGCGGCCAGUA	Compd 37	Target_lig_115 9	HIV protease active site (PAS) mRNA	Target_409	5.52287 8745280 34
2224	<chem>NCC1OC(OC2C(N)CC(C(C2O)OC2OC(CN)C(CC2N)O)N)C(C(C1O)C1OC(CO)C(C(C1N)O)O)N)O</chem>	GGCUGACCAUCAAU AAGGAAGAAGCCCU UCAGCGGCCAGUA	Compd 38	Target_lig_116 0	HIV protease active site (PAS) mRNA	Target_409	5.30102 9995663 98
2225	<chem>NCC1OC(OC2C(N)CC(C(C2O)OC2OC(COC3OC(CN)C(C(C3O)O)O)C(C(C2N)O)N)N)C(C(C1O)N</chem>	GGCUGACCAUCAAU AAGGAAGAAGCCCU UCAGCGGCCAGUA	Compd 39	Target_lig_116 1	HIV protease active site (PAS) mRNA	Target_409	5.39794 0008672 04
2226	<chem>NCC1OC(OC2C(N)CC(C(C2O)OC2OC(COC3OC(CN)C(C(C3O)O)O)C(C(C2N)O)N)N)C(C(C1O)N</chem>	GGCUGACCAUCAAU AAGGAAGAAGCCCU UCAGCGGCCAGUA	Compd 40	Target_lig_128 1	HIV protease active site (PAS) mRNA	Target_409	4.85387 1964321 76
2227	<chem>NCC1OC(OC2C(N)CC(C(C2O)OC2OC(CN)C(CC2N)O)N)C(C(C1O)OC1OC(CO)C(C(C1N)O)O)N</chem>	GGCUGACCAUCAAU AAGGAAGAAGCCCU UCAGCGGCCAGUA	Compd 41	Target_lig_116 2	HIV protease active site (PAS) mRNA	Target_409	5.92081 8753952 38
2228	<chem>NCC1OC(OC2C(N)CC(C(C2O)OC2OC(CN)C(CC2N)O)N)C(C(C1O)OC1OC(CO)C(C(C1N)O)O)N</chem>	GGCUGACCAUCAAU AAGGAAGAAGCCCU UCAGCGGCCAGUA	Compd 42	Target_lig_128 2	HIV protease active site (PAS) mRNA	Target_409	5.15490 1959985 74
2229	<chem>NCC1OC(OC2C(N)CC(C(C2O)OC2OC(CN)C(CC2N)O)N)C(C(C1O)C1OC(CO)C(C(C1N)O)O)N)O</chem>	GGCUGACCAUCAAU AAGGAAGAAGCCCU UCAGCGGCCAGUA	Compd 43	Target_lig_128 3	HIV protease active site (PAS) mRNA	Target_409	5.22184 8749616 36
2375	<chem>C=CC1CN2CCC1CC2C(C3=CC=NC4=CC=C(C=C34)O</chem>	UUUUUUAGGGAAG AUCUGGCCUUCCCA CAAGGGAAGGCCAG GGAAUUUUUCUU	Cinchonidine	Target_lig_122 1	HIV- 1FRAMESHIF T STEM LOOP STRUCTURE	Target_109	3.71399 2877920 53
2376	<chem>CCCCOC(=O)C1=CC=C(C=C1)N</chem>	UUUUUUAGGGAAG AUCUGGCCUUCCCA CAAGGGAAGGCCAG GGAAUUUUUCUU	Butamben	Target_lig_122 2	HIV- 1FRAMESHIF T STEM LOOP STRUCTURE	Target_109	4.40450 3778174 43

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
2377	<chem>CC1C(C(CC(O)OC2C(C(C3=C2C(=C4C(=C3O)C(=O)C5=CC=CC=C5C4=O)O)(C(=O)C)O)N)O</chem>	UUUUUUAGGGAAG AUCUGGCCUCCCCA CAAGGGAAGGCCAG GGAAUUUUUCUU	Idarubicin	Target_lig_122 3	HIV- 1FRAMESHIF T STEM LOOP STRUCTURE	Target_109	5.04095 8607678 91
2378	<chem>c1cc(ccc1)C[C@H](NC(=O)[C@@H]1CCCN1C(=O)[C@@H](NC(=O)c1cc2ccccc2nc1CC)CSSC[C@H](C(=O)N1CCC[C@H]1C(=O)N[C@H](C(=O)NCCCN)Cc1cccc1)NC(=O)c1c(nc2c(c1)cccc2)CC)C(=O)NCCN</chem>	GGCCUCCUACAAG GGAAGGCC	ethylquinoline_ca rboxamide derivative	Target_lig_497	FSS_mutant_1	Target_431	6.34678 7486224 66
2379	<chem>c1cc(ccc1)C[C@H](NC(=O)[C@@H]1CCCN1C(=O)[C@@H](NC(=O)c1cc2ccccc2nc1CC)CSSC[C@H](C(=O)N1CCC[C@H]1C(=O)N[C@H](C(=O)NCCCN)Cc1cccc1)NC(=O)c1c(nc2c(c1)cccc2)CC)C(=O)NCCN</chem>	CCGGAAGGGACAAC CCUCCGG	ethylquinoline_ca rboxamide derivative	Target_lig_497	FSS_mutant_2	Target_432	6.48148 6060122 11
2380	<chem>c1cc(ccc1)C[C@H](NC(=O)[C@@H]1CCCN1C(=O)[C@@H](NC(=O)c1cc2ccccc2nc1CC)CSSC[C@H](C(=O)N1CCC[C@H]1C(=O)N[C@H](C(=O)NCCCN)Cc1cccc1)NC(=O)c1c(nc2c(c1)cccc2)CC)C(=O)NCCN</chem>	GGCCUCCCCGCAAG GGAAGGCC	ethylquinoline_ca rboxamide derivative	Target_lig_497	FSS_mutant_3	Target_433	6.11918 6407719 21
2381	<chem>c1cc(ccc1)C[C@H](NC(=O)[C@@H]1CCCN1C(=O)[C@@H](NC(=O)c1cc2ccccc2nc1CC)CSSC[C@H](C(=O)N1CCC[C@H]1C(=O)N[C@H](C(=O)NCCCN)Cc1cccc1)NC(=O)c1c(nc2c(c1)cccc2)CC)C(=O)NCCN</chem>	GGCCUCCCCACCG GGAAGGCC	ethylquinoline_ca rboxamide derivative	Target_lig_497	FSS_mutant_4	Target_434	5.95860 7314841 77
2382	<chem>c1cc(ccc1)C[C@H](NC(=O)[C@@H]1CCCN1C(=O)[C@@H](NC(=O)c1cc2ccccc2nc1CC)CSSC[C@H](C(=O)N1CCC[C@H]1C(=O)N[C@H](C(=O)NCCCN)Cc1cccc1)NC(=O)c1c(nc2c(c1)cccc2)CC)C(=O)NCCN</chem>	CCGUGCUGCUGCU GCUGCUGCUGCUGC UGCUGCGG	ethylquinoline_ca rboxamide derivative	Target_lig_497	FSS_mutant_5	Target_435	4.39794 0008672 04
2383	<chem>NCCCNC(=O)[C@H](Cc1ccccc1)NC(=O)[C@@H]1CCCN1C(=O)[C@@H](NC(=O)c1cc2ccccc2nc1C)CSSC[C@@H]</chem>	UUUUUUAGGGAAG AUCUGGCCUCCCCA CAAGGGAAGGCCAG GGAAUUUUUCUU	ethylquinoline_ca rboxamide derivative 2	Target_lig_122 4	HIV- 1FRAMESHIF T STEM LOOP STRUCTURE	Target_109	6.36653 1544420 41

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
	<chem>(C(=O)N1CCC[C@H]1C(=O)N[C@H](C(=O)NCCCN)Cc1ccc(cc1)NC(=O)c1cc2ccccc2nc1C</chem>						
2384	<chem>NCCCN(C(=O)[C@H](Cc1ccccc1)NC(=O)[C@@H]1CCCN1C(=O)[C@H](NC(=O)c1cnc2c(c1)ccc2)CSSC[C@H](C(=O)N1CCC[C@H]1C(=O)N[C@H](C(=O)NCCCN)Cc1ccc(cc1)NC(=O)c1cnc2c(c1)ccc2</chem>	UUUUUUAGGGAAG AUCUGGCCUCCCA CAAGGGAAGGCCAG GGAAUUUUCUU	ethylquinoline_carboxamide derivative 3	Target_lig_122_5	HIV-1FRAMESHIFT STEM LOOP STRUCTURE	Target_109	6.18708 6643357 14
2385	<chem>NCCCN(C(=O)[C@H](Cc1ccccc1)NC(=O)[C@@H]1CCCN1C(=O)[C@H](NC(=O)c1cc2cc3OCOC3cc2nc1CC)CSSC[C@H](C(=O)N1CCC[C@H]1C(=O)N[C@H](C(=O)NCCCN)Cc1ccc(cc1)NC(=O)c1cc2cc3OCOC3cc2nc1CC</chem>	UUUUUUAGGGAAG AUCUGGCCUCCCA CAAGGGAAGGCCAG GGAAUUUUCUU	ethylquinoline_carboxamide derivative 4	Target_lig_122_6	HIV-1FRAMESHIFT STEM LOOP STRUCTURE	Target_109	5.84771 1655616 94
2386	<chem>NCCCN(C(=O)[C@H](Cc1ccccc1)NC(=O)[C@@H]1CCCN1C(=O)[C@H](Nc1ccc2c(c1)C(=O)c(C2=O)cccc1)CSSC[C@H](C(=O)N1CCC[C@H]1C(=O)N[C@H](C(=O)NCCCN)Cc1ccc(cc1)Nc1ccc2c(c1)C(=O)c1c(C2=O)cccc1</chem>	UUUUUUAGGGAAG AUCUGGCCUCCCA CAAGGGAAGGCCAG GGAAUUUUCUU	ethylquinoline_carboxamide derivative 5	Target_lig_122_7	HIV-1FRAMESHIFT STEM LOOP STRUCTURE	Target_109	6.63827 2163982 41
2387	<chem>Ccc1nc2ccccc2cc1C(=O)O</chem>	UUUUUUAGGGAAG AUCUGGCCUCCCA CAAGGGAAGGCCAG GGAAUUUUCUU	2-ethylquinoline-3-carboxylic acid	Target_lig_122_8	HIV-1FRAMESHIFT STEM LOOP STRUCTURE	Target_109	6.53760 2002101 04
2388	<chem>C=CC[C@@H](C(=O)N1CCCC1C(=O)NC(C(=O)NCCCN)Cc1ccc(cc1)NC(=O)c1cc2ccccc2nc1CC</chem>	UUUUUUAGGGAAG AUCUGGCCUCCCA CAAGGGAAGGCCAG GGAAUUUUCUU	Dicarbaldehyde_8	Target_lig_122_9	HIV-1FRAMESHIFT STEM LOOP STRUCTURE	Target_109	6.32790 2142064 28
2389	<chem>NCCCN(C(=O)C(Cc1ccc(cc1)NC(=O)C1CCCN1C(=O)C(NC(=O)c1cc2ccccc2nc1CC)/C=C/C[C@H](C(=O)N1CCCC1C(=O)NC(C(=O)NCCCN)Cc1ccc(cc1)NC(=O)c1cc2ccccc2nc1CC</chem>	UUUUUUAGGGAAG AUCUGGCCUCCCA CAAGGGAAGGCCAG GGAAUUUUCUU	Dicarbaldehyde_9	Target_lig_123_0	HIV-1FRAMESHIFT STEM LOOP STRUCTURE	Target_109	6.48148 6060122 11
2390	<chem>Coc1ccc2c(c1)c(Nc1ccc(c(c1)CN1CCN(CC1)C)O)c1c(n2)cc(cc1)Cl</chem>	AGGACUCGGCUUGC UGAAGCGCGGACG GCAAGAGGCGAGG GGCGGCGACUGGUG AGUACGCCAAAAAU UUUGACUAGCGGA GAGUAGGAGGAGA GAGAUGGGUGCGA GAGCGUCGGU	Acridine_derivative_2 (AD2)	Target_lig_123_1	SL-3 of HIV-1_SITE	Target_146	6.17392 5197299 17
2391	<chem>CCOC(=O)C1=C2C=C(C=CN2C3=C1C(=O)C4=CC=CC=C4C3=O</chem>	AGGACUCGGCUUGC UGAAGCGCGGACG GCAAGAGGCGAGG	NSC119236	Target_lig_123_2	SL-3 of HIV-1_SITE	Target_146	5.85387 1964321 76

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		GGCGGCGACUGGUG AGUACGCCAAAAAU UUUGACUAGCGGA GGCUAGAAGGAGA GAGAUGGGUGCGA GAGCGUCGGU					
2392	<chem>C[N+](CCN[N+](C)CCCc2c1cccc2)(C)C</chem>	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	<chem>CN(c1ncnc2c1n(Cc1cnc3c1ncnc3N(C)C)cn2)C</chem>	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	<chem>C1C(C(C(C(C1N)OC2C(C(C(C(O2)CN)O)O)N)OC3C(C(C(O3)CO)OC4C(C(C(C(O4)CN)O)O)N)O)O)N</chem>	GGUCGGCGCAGCUU CGGCUGCGGUACAC C	Neomycin	Target_lig_4	RRE16	Target_447	6.24412 5144327 51
2473	<chem>C1C(C(C(C(C1N)OC2C(C(C(C(O2)CN)O)O)N)OC3C(C(C(O3)CO)OC4C(C(C(C(O4)CN)O)O)N)O)O)N</chem>	GGUGUGCGCAGCUU CGGCUGCGGUACAC C	Neomycin	Target_lig_4	RRE17	Target_448	6.20065 9450546 42
2474	<chem>C1C(C(C(C(C1N)OC2C(C(C(C(O2)CN)O)O)N)OC3C(C(C(O3)CO)OC4C(C(C(C(O4)CN)O)O)N)O)O)N</chem>	GGUGCGCGCAGCUU CGGCUGCGGUACAC C	Neomycin	Target_lig_4	RRE18	Target_449	6.29242 9823902 06
2475	<chem>C1C(C(C(C(C1N)OC2C(C(C(C(O2)CN)O)O)N)OC3C(C(C(O3)CO)OC4C(C(C(C(O4)CN)O)O)N)O)O)N</chem>	GGUGGACGCAGCUU CGGCUGACUGUACA CC	Neomycin	Target_lig_4	RRE19	Target_450	6.07572 0713938 12
2476	<chem>C1C(C(C(C(C1N)OC2C(C(C(C(O2)CN)O)O)N)OC3C(C(C(O3)CO)OC4C(C(C(C(O4)CN)O)O)N)O)O)N</chem>	GGUGGCCGCAGCUU CGGCUGACGGUACA CC	Neomycin	Target_lig_4	RRE20	Target_451	5.46852 1082957 74
2477	<chem>C1C(C(C(C(C1N)OC2C(C(C(C(O2)CN)O)O)N)OC3C(C(C(O3)CO)OC4C(C(C(C(O4)CN)O)O)N)O)O)N</chem>	GGUGGGAGCAGCU UCGGCUGAUGGUAC ACC	Neomycin	Target_lig_4	RRE21	Target_452	6.22184 8749616 36
2478	<chem>C1C(C(C(C(C1N)OC2C(C(C(C(O2)CN)O)O)N)OC3C(C(C(O3)CO)OC4C(C(C(C(O4)CN)O)O)N)O)O)N</chem>	GGUGGGCUCAGCUU CGGCUGACGGUACA CC	Neomycin	Target_lig_4	RRE22	Target_453	6.30980 3919971 49
2479	<chem>C1C(C(C(C(C1N)OC2C(C(C(C(O2)CO)O)O)N)OC3C(C(C(O3)CO)OC4C(C(C(C(O4)CN)O)O)N)O)O)N</chem>	GCACUAUGGGCGCC AGCGUCAAUGACGC UGACGGUACAGCCA GACAAUUAUUGUC UGGUAUAGUGC	Paromomycin	Target_lig_5	RRE-RNA	Target_80	5.08092 1907623 93
2480	<chem>C1C(C(C(C(C1N)OC2C(C(C(C(O2)CO)O)O)N)OC3C(C(C(C(O3)CN)O)O)N)O)O)N</chem>	GCACUAUGGGCGCC AGCGUCAAUGACGC UGACGGUACAGCCA GACAAUUAUUGUC	Kanamycin B	Target_lig_128_7	RRE-RNA	Target_80	5.25181 1972993 8

Entry_ID	SMILES	Target_RNA_sequence	Molecule_name	Molecule_ID	Target_RNA_name	Target_RNA_ID	pKd
		UGGUAUAGUGC					
2481	<chem>C1C(C(C(C(C1N)OC2C(C(C(C(O2)CO)O)O)N)OC3C(C(C(O3)CO)OC4C(C(C(O4)CN)O)O)N)O)O)N</chem>	GGUGGGCGCAGCUUCGGCUGCGCCACC	Paromomycin	Target_lig_5	RRE3	Target_83	4.60205 9991327 96
2482	<chem>C1C(C(C(C(C1N)OC2C(C(C(C(O2)CO)O)O)N)OC3C(C(C(O3)CO)OC4C(C(C(O4)CN)O)O)N)O)O)N</chem>	GGUGGGCGCAGCUUCGGCUGCGGACACC	Paromomycin	Target_lig_5	RRE4	Target_84	4.80966 8301829 71
2483	<chem>C1C(C(C(C(C1N)OC2C(C(C(C(O2)CO)O)O)N)OC3C(C(C(O3)CO)OC4C(C(C(O4)CN)O)O)N)O)O)N</chem>	GGUGGGCGCAGCUUCGGCUGCGCAACCA CC	Paromomycin	Target_lig_5	RRE11	Target_91	4.72815 8393463 5
2484	<chem>C1C(C(C(C(C1N)OC2C(C(C(C(O2)CO)O)O)N)OC3C(C(C(O3)CO)OC4C(C(C(O4)CN)O)O)N)O)O)N</chem>	GGUGGGCGCAGCUUCGGCUGCGCCACC	Kanamycin B	Target_lig_128 7	RRE3	Target_83	4.90308 9986991 94
2485	<chem>C1C(C(C(C(C1N)OC2C(C(C(C(O2)CO)O)O)N)OC3C(C(C(O3)CO)OC4C(C(C(O4)CN)O)O)N)O)O)N</chem>	GGUGGGCGCAGCUUCGGCUGCGGACACC	Kanamycin B	Target_lig_128 7	RRE4	Target_84	5.20065 9450546 42
2486	<chem>C1C(C(C(C(C1N)OC2C(C(C(C(O2)CO)O)O)N)OC3C(C(C(O3)CO)OC4C(C(C(O4)CN)O)O)N)O)O)N</chem>	GGUGGGCGCAGCUUCGGCUGCGCAACCA CC	Kanamycin B	Target_lig_128 7	RRE11	Target_91	4.87614 8359032 91