HIV-1 TAR RNA QSAR test dataset (taken from Cai et al., 2022)

HIV_QSAR_SMILES	Mol_ID	pKd
NC[C@@H]1O[C@H](O[C@@H]2[C@@H](CO)O[C@@H](O[C@@H]3[C@@H](O)[C@H](N)C[C@H](N)[C@H]3O[C@H]3O[C@H](CO)[C@@H](O)[C@H](O)[C@H]3N)[C@@H]2O)[C@H](N)[C@@H](O)[C@@H]1O	HIV_QSAR_1	5.43651891460559
CN[C@H]1[C@H](O)[C@@H](O)[C@H](CO)O[C@H]1O[C@H]1[C@H](O[C@H]2[C@H](O)[C@@H](O)[C@H](NC(N)=N)[C@@H](O)[C@@H]2NC(N)=N)O[C@@H](C)[C@]1(O)C=O	HIV_QSAR_2	4.95860731484177
NC[C@H]1O[C@H](O[C@@H]2[C@@H](N)C[C@@H](N)[C@H](O[C@H]3O[C@H](CO)[C@@H](O)[C@H](N)[C@H]3O)[C@H]2O)[C@H](N)C[C@@H]1O	HIV_QSAR_3	5.44977164694491
CNC(C)C1CCC(N)C(OC2C(N)CC(N)C(OC3OCC(C)(O)C(NC)C3O)C2O)O1	HIV_QSAR_4	5.42021640338319
NC[C@H]1O[C@H](O[C@@H]2[C@@H](N)C[C@@H](N)[C@H](O)[C@H]2O)[C@H](N)[C@@H](O)[C@@H]1O	HIV_QSAR_5	5.58737147945562
NC[C@H]1O[C@H](O[C@@H]2[C@@H](N)C[C@@H](N)[C@H](O[C@H]3O[C@H](CO)[C@@H](O)[C@H](N)[C@H]3O)[C@H]2O)[C@H](O)[C@@H](O)[C@@H]1O	HIV_QSAR_6	4.91904899562052
CN(C)C1=C(Cl)N=C(C(=O)NC(N)=[NH2+])C(N)=N1	HIV_QSAR_7	3.48469985672782
NCCNC1=C(Cl)N=C(C(=O)NC(N)=[NH2+])C(N)=N1	HIV_QSAR_8	5.24511677174783
CN(C)C1=C(N=C(C(=O)NC(N)=[NH2+])C(N)=N1)C1=CC=C(C=C1)C#N	HIV_QSAR_9	3.04667530361081
CN1CCN(CCNC2=C(Cl)N=C(C(=O)NC(N)=[NH2+])C(N)=N2)CC1	HIV_QSAR_10	4.43203309317685
NC(=[NH2+])NC(=O)C1=NC(C2=CC=CC=C2)=C(NCCC2=NC3=C(N2)C=CC=C3)N=C1N	HIV_QSAR_11	3.62598525970809
NC(=[NH2+])NC(=O)C1=NC(C2=CN=CN=C2)=C(N=C1N)N1CCCC1	HIV_QSAR_12	2.70524000796455
CN1CCN(CCNC2=C(N=C(C(=O)NC(N)=[NH2+])C(N)=N2)C2=CC=CC=C2)CC1	HIV_QSAR_13	4.63469925136201
NC(=[NH2+])NC(=O)C1=NC(=C(NCCC2=CNC3=C2C=CC=C3)N=C1N)C1=CC=NC=C1	HIV_QSAR_14	4.48818345869691
NC(=[NH2+])NC(=O)C1=NC(=C(NCCC2=CNC3=C2C=CC=C3)N=C1N)C1=CN=CN=C1	HIV_QSAR_15	4.48858459279123
NC(=[NH2+])NC(=O)C1=NC(=C(NCCC2=CNC3=C2C=CC=C3)N=C1N)C1=CN=C(NCCCN2C=CN=C2)N=C1	HIV_QSAR_16	4.57438427542307
NC(=[NH2+])NC(=O)C1=NC(=C(NCCC2=CNC3=C2C=CC=C3)N=C1N)C1=CN=C(N=C1)N1CCCC1	HIV_QSAR_17	4.90187566170576
[I-].[I-].C[N+]1=C(SC2=C1C=CC=C2)\C=C1/C=CN(CCC[N+](C)(C)C)C2=C1C=CC=C2	HIV_QSAR_18	6.17848647159523
CN(C)CCCNC(=N)C1=CC(=CC=C1)C1=CC=C(O1)C1=CC(=CC=C1)C(=N)NCCCN(C)C	HIV_QSAR_19	6.94692155651658
CN(C)CCCNC(=N)C1=CC=C(C=C1)C1=CC=C(O1)C1=CC=C(C=C1)C(=N)NCCCN(C)C	HIV_QSAR_20	7.10127481841051
NC(=N)C1=CC=C(C=C1)C1=CC=C(O1)C1=CC=C(C=C1)C(N)=N	HIV_QSAR_21	5.59911678445164
[Br-].CC[N+]1=C(C2C=C(N)C=CC2C2=CC=C(N)C=C12)C1=CC=CC=C1	HIV_QSAR_22	5.95860731484177
[H][N+]1=C(NC2=C1C=C(C=C2)N1CC[N+]([H])(C)CC1)C1=CC2=C(NC(=[N+]2[H])C2=CC=C(O)C=C2)C=C1	HIV_QSAR_23	5.141102042768
CN(C)C1=NC(N)=C(N=C1C1=CC=C(CNC2=CC=C3N=CC=NC3=C2)C=C1)C(=O)NC(N)=[NH2+]	HIV_QSAR_24	4.34345143906787
CN(C)C1=NC(N)=C(N=C1C1=CC=C(CNC2=CC=C(C=C2)N2C=CN=C2)C=C1)C(=O)NC(N)=[NH2+]	HIV_QSAR_25	4.05827991762937
CN(C)C1=NC(N)=C(N=C1C1=CC=C(CNC2=CC3=C(NC=N3)C=C2)C=C1)C(=O)NC(N)=[NH2+]	HIV_QSAR_26	3.77408364750598
CN(C)C1=NC(N)=C(N=C1C1=CC=C(CNC2=CC=C(C=C2)N2CCOCC2)C=C1)C(=O)NC(N)=[NH2+]	HIV_QSAR_27	4.48731560378284
CN(C)C1=NC(N)=C(N=C1C1=CC=C(CNC2=CC=NN2)C=C1)C(=O)NC(N)=[NH2+]	HIV_QSAR_28	3.125309492778
CN(C)C1=NC(N)=C(N=C1C1=CC=C(CNC2=CC=CC=C2)C=C1)C(=O)NC(N)=[NH2+]	HIV_QSAR_29	3.2134792693533
CC1=CC=C(C=C1)S([O-])(=O)=O.CN1\C(SC2=CC=CC=C12)=C\C1=CC=[N+](C)C2=CC=CC=C12	HIV_QSAR_30	5.06348625752111
N=C(NCCC1=CC=CN=C1)C2=CC(C3=CC=C(C4=CC(C(NCCC5=CC=CN=C5)=N)=CC=C4)O3)=CC=C2	HIV_QSAR_31	5.41987367458842
N=C(NCCN1CCNCC1)C2=CC(C3=CC=C(C4=CC(C(NCCN5CCNCC5)=N)=CC=C4)O3)	HIV_QSAR_32	5.93930215964639

HIV_QSAR_SMILES	Mol_ID	pKd
=CC=C2		
N=C(NCCN1CCN(C)CC1)C2=CC(C3=CC=C(C4=CC(C(NCCN5CCN(C)CC5)=N)=CC=C4)O3)=CC=C2	HIV_QSAR_33	6.24488773360493
N=C(NCC1=CC=CC=C1Cl)C(C=C2)=CC=C2C3=CC=C(C4=CC=C(C(NCC5=CC=CC=C5Cl)=N)C=C4)O3	HIV_QSAR_34	4.24123945609002
[NH2+]=C(N[C@H]1CCC[NH+](CC2=CC=CC=C2)C1)C1=CC=C(C=C1)C1=CC=C(O1)C1=CC=C(C=C1)C(=[NH2+])N[C@H]1CCC[NH+](CC2=CC=CC=C2)C1	HIV_QSAR_35	5.95467702121334
CN(C)C1=CC2=NC3=C(C=CC(=C3)N(C)C)C=C2C=C1	HIV_QSAR_36	5.24641694110709
N=C(NCCC1=CC=CC=C1)C2=CC(C3=CC=C(C4=CC(C(NCCC5=CC=CC=C5)=N)=CC=C4)O3)=CC=C2	HIV_QSAR_37	5.42021640338319
N=C(NCCC1=CC=CC=C1)C(C=C2)=CC=C2C3=CC=C(C4=CC=C(C(NCCC5=CC=CC=C5)=N)C=C4)O3	HIV_QSAR_38	5.41680122603138
N=C(NCC1=CC=C(Cl)C=C1)C(C=C2)=CC=C2C3=CC=C(C4=CC=C(C(NCC5=CC=C(Cl)C=C5)=N)C=C4)O3	HIV_QSAR_39	5.36451625318509
N=C(NC1CCN(CC2=CC=CC=C2)CC1)C(C=C3)=CC=C3C4=CC=C(C5=CC=C(C(NC6CCN(CC7=CC=CC=C7)CC6)=N)C=C5)O4	HIV_QSAR_40	6.20830935097988
[NH2+]=C(NCCC1CC[NH+](CC2=CC=CC=C2)CC1)C1=CC=C(C=C1)C1=CC=C(O1)C1=CC=C(C=C1)C(=[NH2+])NCCC1CC[NH+](CC2=CC=CC=C2)CC1	HIV_QSAR_41	6.1681302257195
N=C(NCCC1=CC=CN=C1)C1=CC(=CC=C1)N=NNC1=CC(=CC=C1)C(=N)NCCC1=CC=CN=C1	HIV_QSAR_42	5.65757731917779
N=C(NC1CCN(CC2=CC=CC=C2)CC1)C1=CC=C(N\\N=N\C2=CC=C(C=C2)C(=N)NC2CCN(CC3=CC=CC=C3)CC2)C=C1	HIV_QSAR_43	6.08354605145007
N=C(NCCC1CCN(CC2=CC=CC=C2)CC1)C1=CC=C(N\\N=N\C2=CC=C(C=C2)C(=N)NCCC2CCN(CC3=CC=CC=C3)CC2)C=C1	HIV_QSAR_44	6.09528445472132