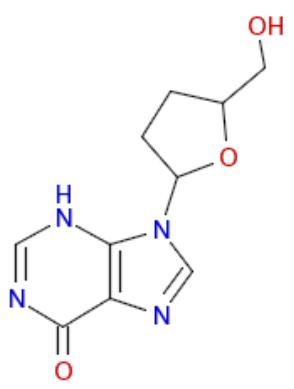


Figure S2. HIV drugs grouped by molecular structure similarity

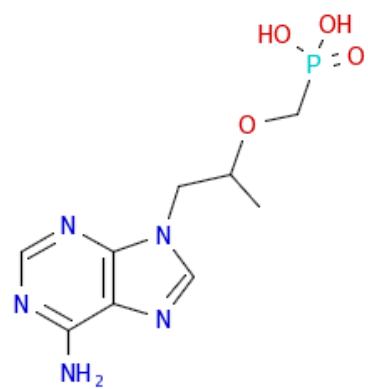
SimilarityGroup: 1



Abacavir

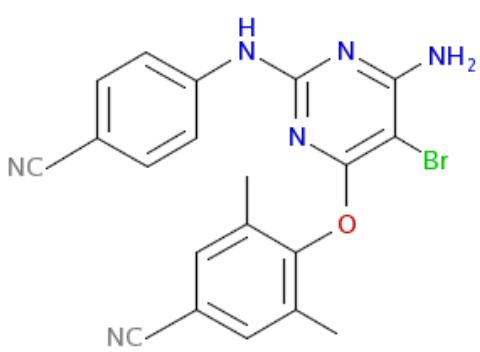


Didanosine

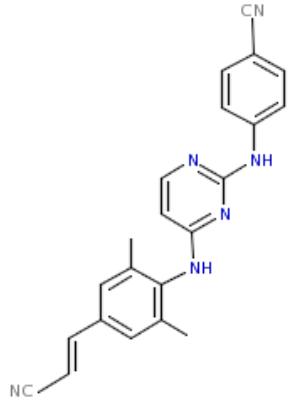


Tenofovir

SimilarityGroup: 2

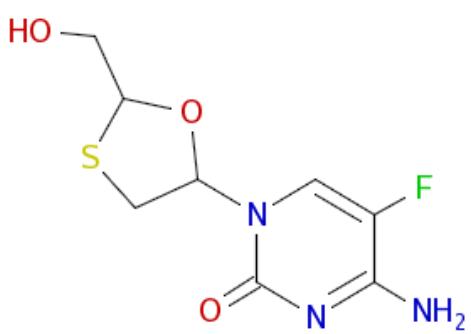


Etravirine

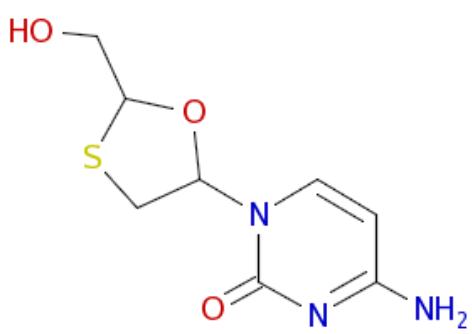


Rilpivirine

SimilarityGroup: 3

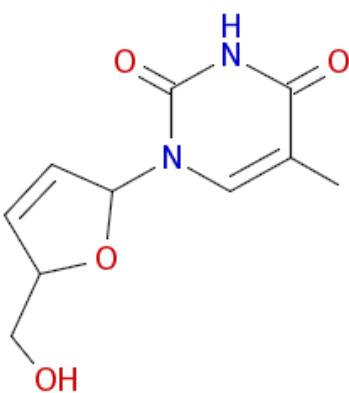


Emtricitabine

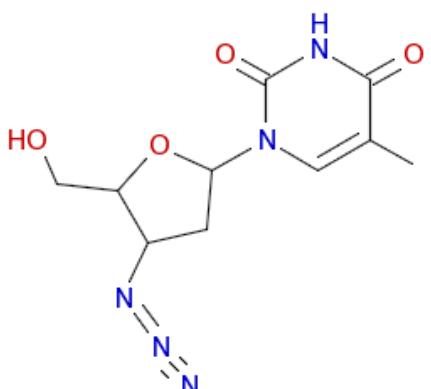


Lamivudine

SimilarityGroup: 4

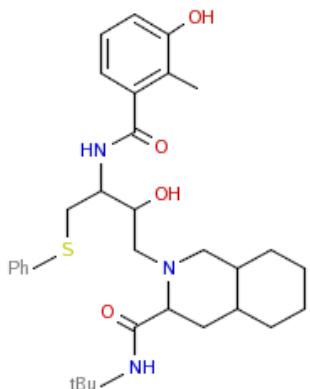


Stavudine

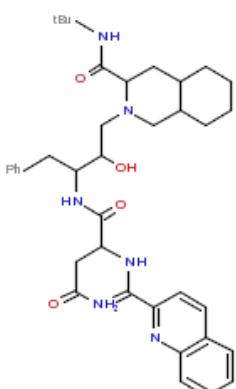


Zidovudine

SimilarityGroup: 5

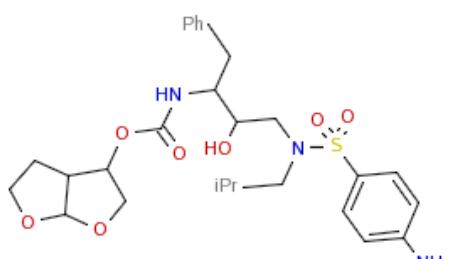


Nelfinavir

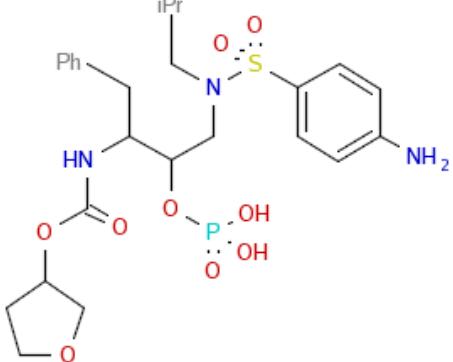


Saquinavir

SimilarityGroup: 6

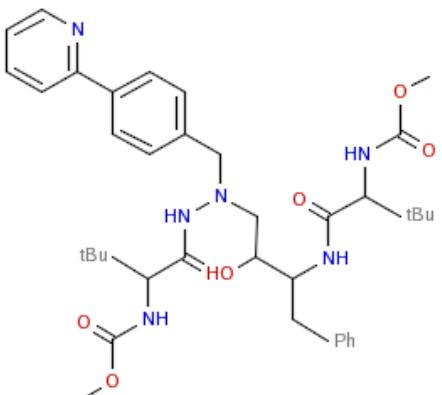


Darunavir

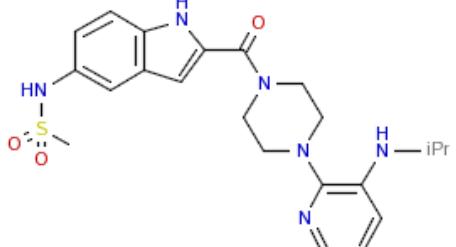


Fosamprenavir

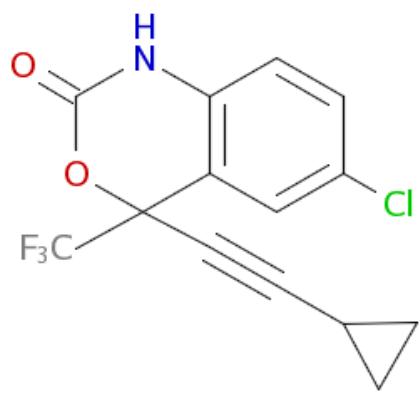
SimilarityGroup: Singletons



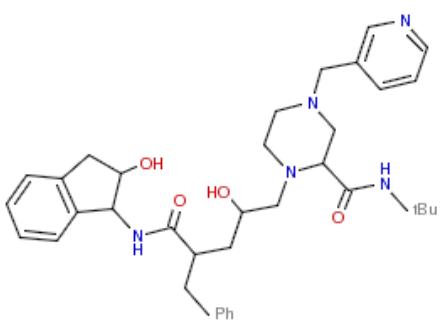
Atazanavir



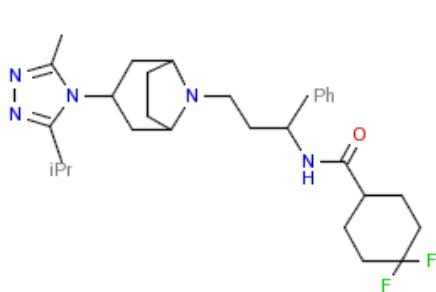
Delavirdine



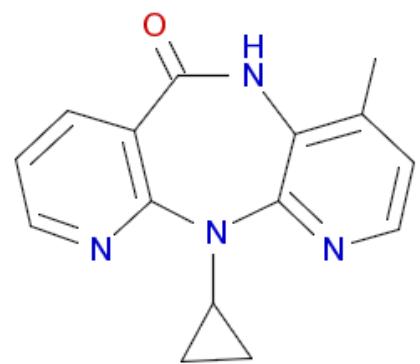
Efavirenz



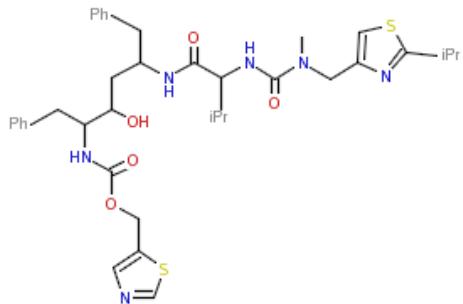
Indinavir



Maraviroc



Nevirapine



Ritonavir