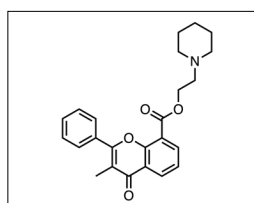


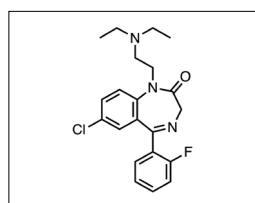
Examples of fully-synthetic molecules from 1970 and 2021

1970



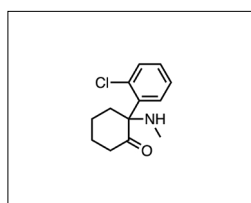
flavoxate

MW = 392
LogP = 4.3
HBA = 5
HBD = 0
Fsp³ = 0.33



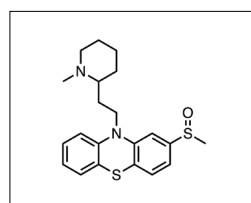
flurazepam

MW = 388
LogP = 3.0
HBA = 4
HBD = 0
Fsp³ = 0.33



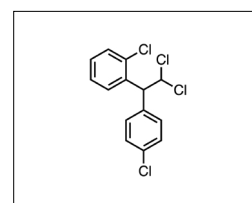
ketamine

MW = 238
LogP = 2.2
HBA = 2
HBD = 1
Fsp³ = 0.46



mesoridazine

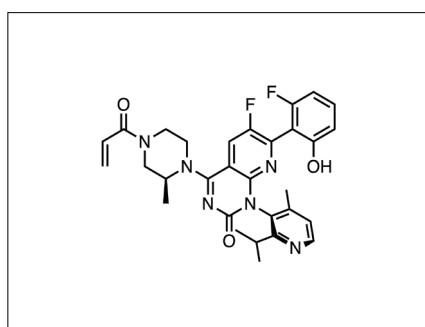
MW = 387
LogP = 4.5
HBA = 5
HBD = 0
Fsp³ = 0.43



mitotane

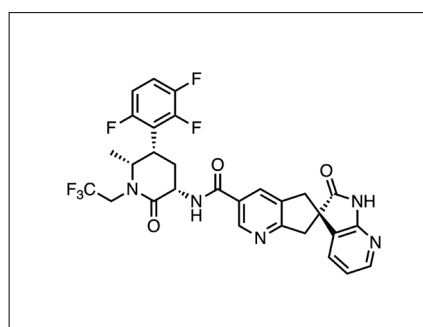
MW = 320
LogP = 6.2
HBA = 0
HBD = 0
Fsp³ = 0.14

2021



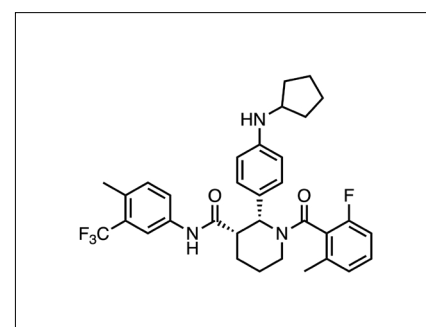
sotorasib

MW = 561
LogP = 4.0
HBA = 7
HBD = 1
Fsp³ = 0.30



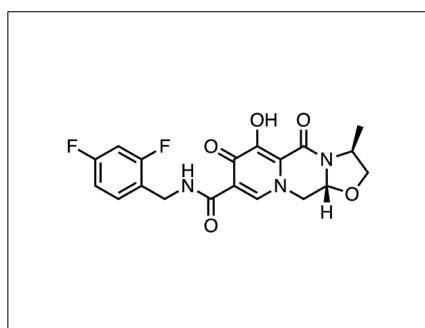
atogepant

MW = 604
LogP = 3.4
HBA = 11
HBD = 2
Fsp³ = 0.34



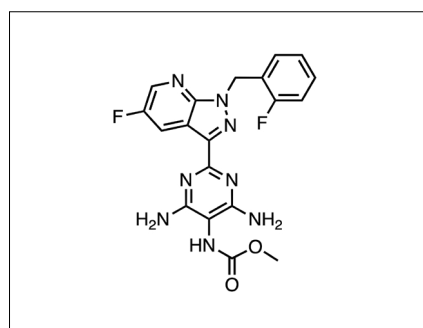
avacopan

MW = 582
LogP = 7.2
HBA = 7
HBD = 2
Fsp³ = 0.39



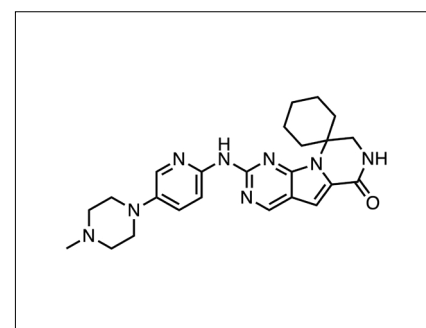
cabotegravir

MW = 405
LogP = 2.1
HBA = 8
HBD = 2
Fsp³ = 0.32



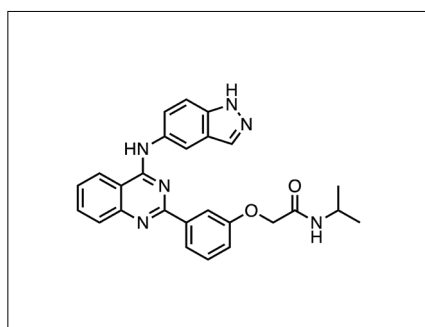
vericiguat

MW = 426
LogP = 1.5
HBA = 10
HBD = 3
Fsp³ = 0.10



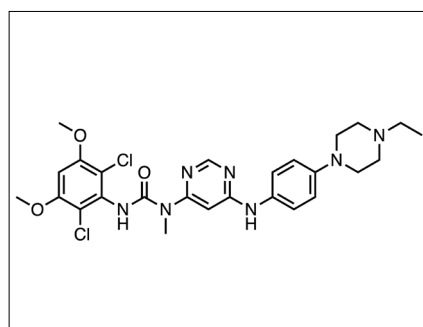
trilaciclib

MW = 447
LogP = 2.6
HBA = 7
HBD = 2
Fsp³ = 0.50



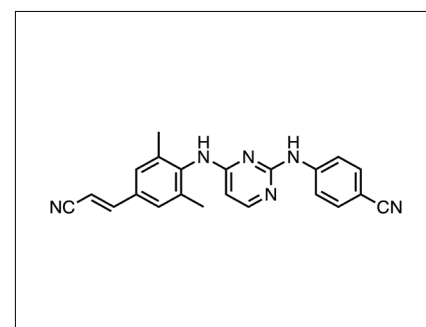
belumosudil

MW = 453
LogP = 4.8
HBA = 6
HBD = 3
Fsp³ = 0.15



infigratinib

MW = 561
LogP = 4.7
HBA = 8
HBD = 2
Fsp³ = 0.35



rilpivirine

MW = 366
LogP = 4.5
HBA = 6
HBD = 2
Fsp³ = 0.09