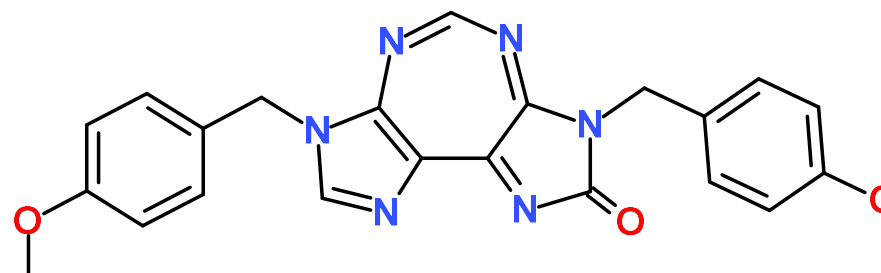


O=C(OC(C)(C)C)N/C1=C/C=CN(C1=O)[C@@]([H])(C[C@@]2([H])CC2)C(=O)N[C@@]([H])(C[C@]3([H])CCNC3=O)[C@](O)([H])C(=O)NCc4ccccc4 6Y2F

IUPAC NAME: tert-butyl N-[1-[(1S)-2-[[[(1S,2R)-3-(benzylamino)-2-hydroxy-3-oxo-1-[[[(3S)-2-oxopyrrolidin-3-yl]methyl]propyl]amino]-1-(cyclopropylmethyl)-2-oxo-ethyl]-2-oxo-3-pyridyl]carbamate

Reference (ref) compound for Mpro



COc1ccc(CN2C(=O)N=C3C2=NC=Nc4c3ncn4Cc5ccc(OC)cc5)cc1 RK-33

IUPAC NAME: 5,11-bis[(4-methoxyphenyl)methyl]-3,5,7,9,11,13-hexazatricyclo[8.3.0.0<sup>2,6</sup>]trideca-1(10),2,6,8,12-pentaen-4-one

Reference (ref) compound for DDX3

Supplementary Figure S1. 2D structures for ref compounds.