MOLNOVA
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Datasheet (Version 1.0)

Product Name	:	Darunavir
Synonyms	:	TMC-114;UIC-94017
Cat No.	:	M13207
CAS Number	:	206361-99-1
Molecular Formula	:	C27H37N3O7S
Formula Weight	:	547.66
Chemical Name	:	Carbamic acid, N-[(1S,2R)-3-[[(4-aminophenyl)sulfonyl](2-methylpropyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-, (3R,3aS,6aR)-hexahydrofuro[2,3-b]furan-3-yl ester
Description	:	A potent, selective HIV-1 protease inhibitor that is extremely potent against laboratory HIV-1 strains and primary clinical isolates with IC50 of 3 nM, IC90 of 9 nM; blockes the infectivity and replication of HIV-1(NL4-3) variants with IC50 of 3-29 nM, also potent against multi-PI-resistant clinical HIV-1 variants isolated from patients; used to treat and prevent HIV/AIDS.HIV Infection Approved
Pathway	:	Microbiology/Virology
Target	:	HIV
Receptor	:	HIVProtease
Solubility	:	10 mM in DMSO
SMILES	:	CC(C)CN(C[C@H]([C@H](CC1=CC=CC=C1)NC(=O)O[C@H]2CO[C@@H]3[C@H]2CCO3)O)S(=O)(=O)C4=CC=C(C=C4)N
Storage	:	(-20℃)
Stability	:	≥ 2 years
Reference	:	

1. Surleraux DL, et al. J Med Chem. 2005 Mar 24;48(6):1813-22.| 2. Koh Y, et al. Antimicrob Agents Chemother. 2003 Oct;47(10):3123-9.| 3. King NM, et al. J Virol. 2004 Nov;78(21):12012-21.