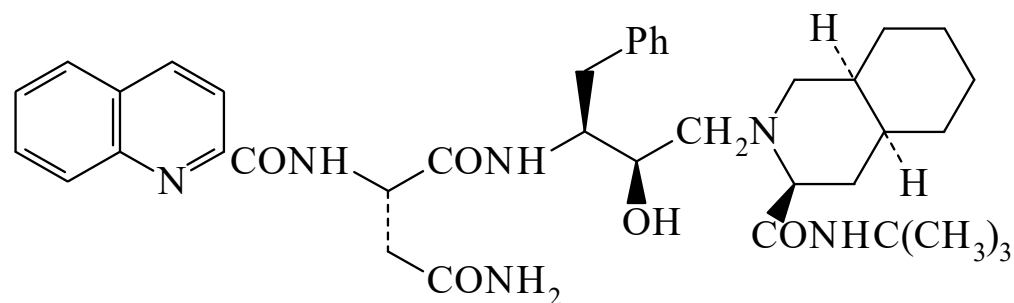




>>Entry Name: Saquinavir, BAN, INN, USAN

Synonym(s): *N'*-[3-[3-[[[(1*H*)-isoquinolinyl]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]butanediamide, 9Cl. Fortovase. Invirase. Ro 31-8959



CAS Registry Number: 127779-20-8

Related CAS Registry Numbers(s): 128053-46-3 137622-85-6 147922-51-8 147922-52-9

Molecular Formula: C₃₈H₅₀N₆O₅

Molecular Weight: 670.85

Accurate Mass: 670.384269

Percentage Composition: C 68.04%; H 7.51%; N 12.53%; O 11.92%

Use/Importance: Potent and selective inhibitor of HIV proteinase. Antiviral agent

Physical Description: Foam

Development Status: Launched 1995 (US)

Optical Rotation: $[\alpha]_D^{20} -55.9$ (c, 0.5 in MeOH)

Calculated Log P Data: Log P 4.22 (calc)

>>Derivative: Methanesulfonate

Synonym(s): Saquinavir mesylate, USAN

CAS Registry Number: 149845-06-7

References:

- Eur. Pat.*, 1989, *Hoffmann-La Roche*, 346 847; *CA*, **113**, 41332e, (*synth, pharmacol*)
Craig, J.C. *et al.*, *Antiviral Res.*, 1991, **16**, 295, (*pharmacol*)
Martin, J.A. *et al.*, *Biochem. Biophys. Res. Commun.*, 1991, **176**, 180, (*pharmacol*)
Krohn, A. *et al.*, *J. Med. Chem.*, 1991, **34**, 3340, (*activity, bibl*)
Craig, J.C. *et al.*, *Antiviral Chem. Chemother.*, 1993, **4**, 335; 1994, **5**, 43, (*pharmacol*)
Thompson, W.J. *et al.*, *J.A.C.S.*, 1993, **115**, 801, (*activity, bibl*)
Parkes, K.E.B. *et al.*, *J.O.C.*, 1994, **59**, 3656, (*synth, bibl*)
Noble, S. *et al.*, *Drugs*, 1996, **52**, 93, (*rev, pharmacol*)
Perry, C.M. *et al.*, *Drugs*, 1998, **55**, 461-486, (*rev*)
Tawa, G.J. *et al.*, *J.A.C.S.*, 1998, **120**, 8856-8863, (*drug-enzyme binding*)
Figgitt, D.P. *et al.*, *Drugs*, 2000, **60**, 481-516, (*rev*)