

Product Data Sheet

Product Name: Indinavir
Cat. No.: GC36309

Chemical Properties

Cas. No. 150378-17-9

SMILES O=C([C@@H](C[C@H](O)CN(CCN(CC1=CN=CC=C1)C2)[C@@H]2C(NC(C)(C)C)=O)CC3=CC=CC=C3)N[C@H]4C(C=CC=C5)=C5C[C@H]4O

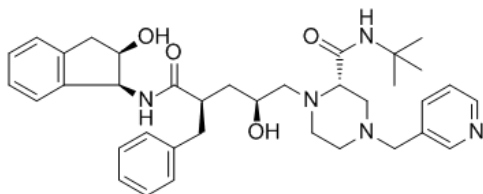
Formula $C_{36}H_{47}N_5O_4$ M.Wt 613.79

Solubility Soluble in DMSO Storage Store at -20°C

General tips For obtaining a higher solubility, please warm the tube at 37 °C and shake it in the ultrasonic bath for a while. Stock solution can be stored below -20°C for several months.

Shipping Condition Evaluation sample solution: ship with blue ice. All other available size: ship with RT, or blue ice upon request.

Structure



Background

Indinavir (MK-639; L735524) is a potent and specific HIV protease inhibitor that appears to have good oral bioavailability. Target: HIV Protease. Indinavir (MK-639) is a protease inhibitor used as a component of highly active antiretroviral therapy (HAART) to treat HIV infection and AIDS. MK-639 appears to have significant dose-related antiviral activity and is well tolerated [1]. Inhibition constants (K_i) of the antiviral drug indinavir for the reaction catalyzed by the mutant enzymes were about threefold and 50-fold higher for PR(L24I) and PR(I50V), respectively, relative to PR and PR(G73S).

Caution: Product has not been fully validated for medical applications. For research use only.

Tel: (909) 407-4943 Fax: (626) 353-8530 E-mail: tech@glpbio.com

Address: 10292 Central Ave. #205, Montclair, CA, USA

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The dimer dissociation constant ($K(d)$) was estimated to be approximately 20 nM for both PR(L24I) and PR(I50V), and below 5 nM for PR(G73S) and PR. Crystal structures of the mutants PR(L24I), PR(I50V) and PR(G73S) were determined in complexes with indinavir, or the p2/NC substrate analog at resolutions of 1.10-1.50 Angstrom [2].

[1]. Stein, D.S., et al., A 24-week open-label phase I/II evaluation of the HIV protease inhibitor MK-639 (indinavir). AIDS, 1996. 10(5): p. 485-92. [2]. Liu, F., et al., Kinetic, stability, and structural changes in high-resolution crystal structures of HIV-1 protease with drug-resistant mutations L24I, I50V, and G73S. J Mol Biol, 2005. 354(4): p. 789-800.

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