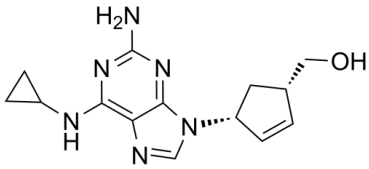
Data Sheet

Product Name:	Abacavir
Cat. No.:	CS-1354
CAS No.:	136470-78-5
Molecular Formula:	C14H18N6O
Molecular Weight:	286.33
Target:	Apoptosis; HIV; Reverse Transcriptase
Pathway:	Anti-infection; Apoptosis
Solubility:	DMSO : 100 mg/mL (349.25 mM; Need ultrasonic); H2O : 2 mg/mL (6.98 mM; Need ultrasonic)



BIOLOGICAL ACTIVITY:

Abacavir is a powerful nucleoside analog reverse transcriptase inhibitor (NRTI) used to treat HIV and AIDS. IC50 value: Target: NRTI; reverse transcriptase inhibitor Abacavir is a nucleoside reverse transcriptase inhibitor marketed since 1999 for the treatment of infection with the human immunodeficiency virus type 1 (HIV). Despite its clinical efficacy, abacavir administration has been associated with serious and sometimes fatal toxic events. Abacavir has been reported to undergo bioactivation in vitro, yielding reactive species that bind covalently to human serum albumin, but the haptenation mechanism and its significance to the toxic events induced by this anti-HIV drug have yet to be elucidated. The mechanism underlying abacavir hypersensitivity syndrome is related to the change in the HLA-B*5701 protein product. Abacavir binds with high specificity to the HLA-B*5701 protein, changing the shape and chemistry of the antigen-binding cleft. This results in a change in immunological tolerance and the subsequent activation of abacavir-specific cytotoxic T cells, which produce a systemic reaction known as abacavir hypersensitivity syndrome.

References:

[1]. Charneira C, et al. Reactive aldehyde metabolites from the anti-HIV drug abacavir: amino acid adducts as possible factors in abacavir toxicity. Chem Res Toxicol. 2011 Dec 19;24(12):2129-41.

[2]. Hervey PS, et al. Abacavir: a review of its clinical potential in patients with HIV infection. Drugs. 2000 Aug;60(2):447-79.

CAIndexNames:

2-Cyclopentene-1-methanol, 4-[2-amino-6-(cyclopropylamino)-9H-purin-9-yl]-, (1S,4R)-

SMILES:

NC1=NC(NC2CC2)=C3N=CN([C@H]4C=C[C@@H](CO)C4)C3=N1

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

Tel: 732-484-9848 Fax: 888-484-5008 E-mail: sales@ChemScene.com

Address: 1 Deer Park Dr, Suite Q, Monmouth Junction, NJ 08852, USA