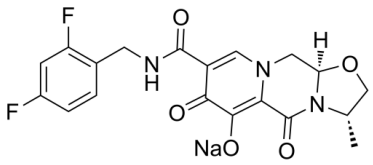
Data Sheet

Product Name:	Cabotegravir (sodium)
Cat. No.:	CS-0007799
CAS No.:	1051375-13-3
Molecular Formula:	$C_{19}H_{16}F_2N_3NaO_5$
Molecular Weight:	427.33
Target:	HIV; HIV Integrase
Pathway:	Anti-infection; Metabolic Enzyme/Protease
Solubility:	DMSO : 6.9 mg/mL (ultrasonic;warming;heat to 60°C)



BIOLOGICAL ACTIVITY:

Cabotegravir (GSK-1265744) sodium is a orally active and long-acting **HIV integrase** strand transfer inhibitor and organic anion transporter 1/3 (**OAT1**/**OAT3**) inhibitor with **IC_{50}** values of 2.5 nM, 0.41 μM and 0.81 μM for HIV_{ADA}, OAT3 and OAT1, respectively. Cabotegravir sodium is primarily metabolized by uridine diphosphate glucuronosyltransferase (UGT) 1A1, with low potential to interact with other antiretroviral drugs (ARVs). Cabotegravir sodium can be used to research AIDS[1][2]. IC50 & Target:IC_{50}: 2.5 nM (HIV_{ADA})[1]

IC_{50}: 0.41 μM (OAT3), 0.81 μM (OAT1)[2] ***In Vitro:*** Cabotegravir (GSK-1265744) inhibits the HIV-1 integrase catalyzed strand transfer reaction with an IC_{50} of 3.0 nM in vitro. The antiviral EC_{50} against HIV-1 Ba-L is 0.22 nM and that against NL432 is 0.34 nM in PBMCs, 0.57 nM using CellTiter-Glo and 1.3 nM using MTT in MT-4, and 0.5 nM in the PHIV assay, which uses a pseudotyped self-inactivating virus[3]. ***In Vivo:*** The half-life of Cabotegravir is up to 54 days in mice[1].

Cabotegravir (25 or 50 mg/kg; i.v.; single dose or twice) protects Macaques against intravenous challenge with SIVmac251[4].

References:

[1]. Zhou T, et al. Creation of a nanoformulated cabotegravir prodrug with improved antiretroviral profiles. Biomaterials. 2018 Jan;151:53-65.

[2]. Reese MJ, et al. Drug interaction profile of the HIV integrase inhibitor cabotegravir: assessment from in vitro studies and a clinical investigation with midazolam. Xenobiotica. 2016;46(5):445-56.

[3]. Yoshinaga T, et al. Antiviral characteristics of GSK1265744, an HIV integrase inhibitor dosed orally or by long-acting injection. Antimicrob Agents Chemother. 2015 Jan;59(1):397-406.

[4]. Andrews CD, et al. Cabotegravir long acting injection protects macaques against intravenous challenge with SIVmac251. AIDS. 2017 Feb 20;31(4):461-467.

CAIndexNames:

Oxazolo[3,2-a]pyrido[1,2-d]pyrazine-8-carboxamide, N-[(2,4-difluorophenyl)methyl]-2,3,5,7,11,11a-hexahydro-6-hydroxy-3-methyl-5,7-dioxo-, sodium salt (1:1), (3S,11aR)-

SMILES:

FC1=C(CNC(C2=CN3C(C(N([C@@H](C)CO4)[C@@]4([H])C3)=O)=C(O[Na])C2=O)=O)C=CC(F)=C1

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

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