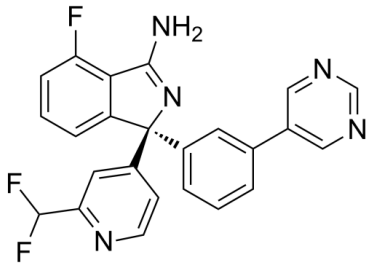
Data Sheet

Product Name:	AZD3839 (free base)
Cat. No.:	CS-5933
CAS No.:	1227163-84-9
Molecular Formula:	$C_{24}H_{16}F_3N_5$
Molecular Weight:	431.41
Target:	Beta-secretase
Pathway:	Neuronal Signaling
Solubility:	DMSO : 125 mg/mL (ultrasonic)



BIOLOGICAL ACTIVITY:

AZD3839 free base is a potent and selective orally active, brain-permeable **BACE1** inhibitor ($\mathbf{K_i}$=26 nM). AZD3839 free base shows 14 and >1000-fold selectivity against BACE2 and cathepsin D, respectively. AZD3839 free base exhibits dose- and time-dependent lowering of plasma, brain, and cerebrospinal fluid Aβ levels in mouse, guinea pig, and non-human primate. AZD3839 free base can be used for the research of Alzheimer's disease[1][2].

PROTOCOL (Extracted from published papers and Only for reference)

cell assay [1] Effects on hERG-encoded potassium channel–expressing Chinese hamster ovary cells were recorded at room temperature in the whole-cell configuration of the patch-clamp technique. AZD3839 was investigated in five cells, into each of which was added vehicle solution (0.1% dimethylsulfoxide) and AZD3839 at six ascending nominal concentrations (0.3–100 μM). Following application of the highest test concentration, vehicle solution was reapplied to test the reversibility of the effect. The positive control (3 μM cisapride) was then applied. For each cell recorded, data obtained in the presence of the test compound were expressed as a percentage of the first application of vehicle solution. The IC50 value is based on test concentrations measured using a high-pressure liquid chromatography–tandem mass spectroscopy method.

References:

[1]. Sparve E et al. Prediction and modeling of effects on the QTc interval for clinical safety margin assessment, based on single-ascending-dose study data with AZD3839. J Pharmacol Exp Ther. 2014 Aug;350(2):469-78.

[2]. Jeppsson F et al. Discovery of AZD3839, a potent and selective BACE1 inhibitor clinical candidate for the treatment of Alzheimer disease. J Biol Chem. 2012 Nov 30;287(49):41245-57.

CAIndexNames:

1H-Isoindol-3-amine, 1-[2-(difluoromethyl)-4-pyridinyl]-4-fluoro-1-[3-(5-pyrimidinyl)phenyl]-, (1S)-

SMILES:

FC1=C2C([C@](C3=CC=CC(C4=CN=CN=C4)=C3)(C5=CC(C(F)F)=NC=C5)N=C2N)=CC=C1

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

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