AZ13705339 hemihydrate

Cat. No.: HY-120940A

Molecular Formula: $C_{33}H_{36}FN_7O_3S.{}_1/_2H_2O$

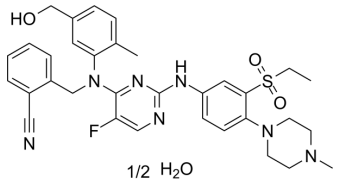
Molecular Weight: 638.77

Target: PAK

Pathway: Cell Cycle/DNA Damage; Cytoskeleton

Storage:

Powder	-20°C	3 years
In solvent	-80°C	6 months
	-20°C	1 month



SOLVENT & SOLUBILITY

In Vitro

DMSO : 100 mg/mL (156.55 mM; Need ultrasonic)

Preparing Stock Solutions	Mass / Solvent / Concentration	1 mg	5 mg	10 mg
	1 mM	1.5655 mL	7.8275 mL	15.6551 mL
	5 mM	0.3131 mL	1.5655 mL	3.1310 mL
	10 mM	0.1566 mL	0.7828 mL	1.5655 mL

Please refer to the solubility information to select the appropriate solvent.

BIOLOGICAL ACTIVITY

Description

AZ13705339 hemihydrate is a highly potent and selective PAK1 inhibitor with IC_{50}s of 0.33 nM and 59 nM for PAK1 and pPAK1, respectively. AZ13705339 hemihydrate has binding affinities to PAK1 and PAK2, with K_ds of 0.28 nM and 0.32 nM, respectively. AZ13705339 hemihydrate can be used in the research of cancers[1].

IC_{50} & Target				
	PAK2 0.32 nM (Kd)	PAK1 0.28 nM (Kd)	PAK1 0.33 nM (IC_{50})	pPAK1 59 nM (IC_{50})

In Vitro

AZ13705339 (1 μM) hemihydrate inhibits αIgM-controlled adhesion and not PMA-induced adhesion in Namalwa cells[2].
AZ13705339 (300 nM, 30 min) prevents Siglec-8 engagement-induced eosinophil death[3].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

In Vivo

AZ13705339 hemihydrate (100 mg/kg, P.O.) has moderate clearance and oral C_{max} of 7.7 μM in rats[1].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. McCoull W, et al. Optimization of Highly Kinase Selective Bis-anilino Pyrimidine PAK1 Inhibitors. ACS Med Chem Lett. 2016;7(12):1118-1123. Published 2016 Sep 14.

[2]. Martin F M de Rooij, et al. A loss-of-adhesion CRISPR-Cas9 screening platform to identify cell adhesion-regulatory proteins and signaling pathways. Nat Commun. 2022 Apr 19;13(1):2136.

[3]. Daniela J Carroll, et al. Siglec-8 Signals Through a Non-Canonical Pathway to Cause Human Eosinophil Death In Vitro. Front Immunol. 2021 Oct 11;12:737988.

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