Tagtociclib hydrate

Cat. No.: HY-137894A

CAS No.: 2733575-91-0

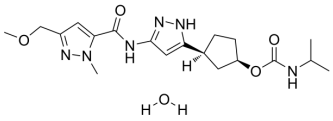
Molecular Formula: $C_{19}H_{30}N_6O_5$

Molecular Weight: 422.48

Target: CDK; GSK-3

Pathway: Cell Cycle/DNA Damage; PI3K/Akt/mTOR; Stem Cell/Wnt

Storage: 4°C, sealed storage, away from moisture and light
* In solvent : -80°C, 6 months; -20°C, 1 month (sealed storage, away from moisture and light)



SOLVENT & SOLUBILITY

In Vitro

DMSO : 200 mg/mL (473.40 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.3670 mL	11.8349 mL	23.6698 mL
	5 mM	0.4734 mL	2.3670 mL	4.7340 mL
	10 mM	0.2367 mL	1.1835 mL	2.3670 mL

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

In Vivo

1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: ≥ 5 mg/mL (11.83 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 5 mg/mL (11.83 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 5 mg/mL (11.83 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

PF-07104091 hydrate is a potent and selective CDK2/cyclin E_1 and GSK3β inhibitor, with K_is of 1.16 and 537.81 nM, respectively. PF-07104091 hydrate has anti-tumor activity for cyclin E_1-amplified cancers. (patent WO2020157652A2).

IC_{50} & Target

CDK2/cyclin E1	GSK3β
1.16 nM (Ki)	537.81 nM (Ki)

In Vitro

PF-07104091 hydrate (Example 13) inhibits CDK1/cyclin A_2, CDK4/cyclin D_1, CDK6/cyclin D_3 and CDK9, with K_is of 110, 238, 465 and 117 nM, respectively[1].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. Douglas Carl BEHENNA, et al. Cdk2 inhibitors. WO2020157652A2.

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

Tel: 609-228-6898 Fax: 609-228-5909 E-mail: tech@MedChemExpress.com
Address: 1 Deer Park Dr, Suite Q, Monmouth Junction, NJ 08852, USA