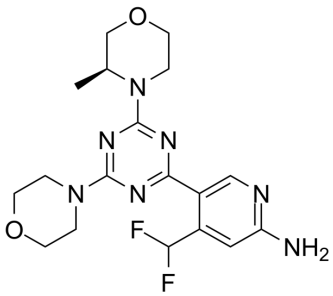
PQR530

Cat. No.:	HY-107365
CAS No.:	1927857-61-1
Molecular Formula:	$C_{18}H_{23}F_2N_7O_2$
Molecular Weight:	407.42
Target:	PI3K; mTOR
Pathway:	PI3K/Akt/mTOR
Storage:	Powder -20°C 3 years 4°C 2 years In solvent -80°C 6 months -20°C 1 month



SOLVENT & SOLUBILITY

In Vitro

DMSO : 33.33 mg/mL (81.81 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.4545 mL	12.2723 mL	24.5447 mL
	5 mM	0.4909 mL	2.4545 mL	4.9089 mL
	10 mM	0.2454 mL	1.2272 mL	2.4545 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: 2.5 mg/mL (6.14 mM); Suspended solution; Need ultrasonic
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.5 mg/mL (6.14 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (6.14 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

PQR530 is a potent, ATP-competitive, orally bioavailable and brain-penetrant dual pan-PI3K/mTORC1/2 inhibitor, with a subnanomolar K_d toward PI3Kα and mTOR (0.84 and 0.33 nM, respectively). Antitumor activity[1][2].

IC_{50} & Target

mTOR 0.33 nM (Kd)	PI3Kα 0.84 nM (Kd)	PI3Kβ 6.1 nM (Kd)	PI3Kγ 10 nM (Kd)
PI3Kδ 11 nM (Kd)	PI3KC2β 100 nM (Kd)		

In Vitro	PQR-530 is a potent, oral and brain-penetrant dual pan-PI3K/mTORC1/2 inhibitor, exhibiting antitumor activity. PQR-530 inhibits all PI3K isoforms and mTOR complexes C1/2 potently and selectively. PQR-530 inhibits protein kinase B (PKB, pSer473) and ribosomal protein S6 (pS6, pSer235/236) phosphorylation with IC_{50} values of 0.07 μM in A2058 melanoma cells. PQR-530 shows inhibitory activity against the growth of 44 cancer cell lines with mean GI_{50} of 426 nM[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. Denise Rageot, et al. Abstract 140: Discovery and biological evaluation of PQR530, a highly potent dual pan-PI3K/mTORC1/2 inhibitor. Cancer Res 2017;77(13 Suppl).

[2]. Rageot D, et al. (S)-4-(Difluoromethyl)-5-(4-(3-methylmorpholino)-6-morpholino-1,3,5-triazin-2-yl)pyridin-2-amine (PQR530), a Potent, Orally Bioavailable, and Brain-Penetrable Dual Inhibitor of Class I PI3K and mTOR Kinase. J Med Chem. 2019;62(13):6241-6261.

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