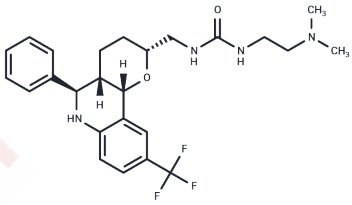
Data Sheet (Cat.No.TQ0314)

TargetMol

EMD534085

Chemical Properties



CAS No. : 858668-07-2

Formula: C25H31F3N4O2

Molecular Weight: 476.53

Storage: Powder: -20°C for 3 years | In solvent: -80°C for 1 year
Actual storage temperature shall be subject to the COA.

Biological Description

Description	EMD534085 is an effective and selective mitotic kinesin-5 inhibitor (IC50: 8 nM).
Targets(IC50)	Kinesin
In vitro	EMD 534085 does not inhibit other tested kinesins at 1 μM or 10 μM concentrations, showing selectivity for kinesin-5. EMD 534085 binds to the allosteric pocket of kinesin-5 [1]. It induces rapid cell death in HL60 cells during mitotic arrest, activating caspase-8, -9, -3, -7; cleaving Parp1; and degrading Mcl1 and XIAP. Additionally, EMD 534085-treated HL60 cells exhibit a significantly increased phospho-histone H3 level starting 6 hours post thymidine release [2].
In vivo	In a pharmacokinetic study of EMD 534085 conducted at a low dose in mice, average clearance was observed at 1.8 L/h/kg, with a volume of distribution of 7.4 L/kg and a half-life approximately 2.5 hours. High dose experiments (>10 mg/kg) consistently demonstrated a bioavailability exceeding 50% in mice. Intraperitoneal administration of EMD 534085 resulted in significant systemic exposure, contributing to a notable reduction in tumor growth without inducing toxic side effects [1].
Cell Research	Epithelial cell lines HeLa and MCF7 are synchronized in G2-phase using RO-3306. Cells are treated with 10 μM RO-3306 for 16 hrs, and then are ished and released to either warm growth medium or medium supplemented with 500 nM EMD534085 [2].

Solubility Information

Solubility	DMSO: 25 mg/mL (52.46 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.0985 mL	10.4925 mL	20.985 mL
5 mM	0.4197 mL	2.0985 mL	4.197 mL
10 mM	0.2099 mL	1.0493 mL	2.0985 mL
50 mM	0.042 mL	0.2099 mL	0.4197 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. Please use it as soon as possible.

Note: The dilution table applies only to solid products. For liquid products, please calculate the stock solution based on the stated concentration and/or density.

Reference

Schiemann K, et al. The discovery and optimization of hexahydro-2H-pyrano[3,2-c]quinolines (HHPQs) as potent and selective inhibitors of the mitotic kinesin-5. Bioorg Med Chem Lett. 2010 Mar 1;20(5):1491-5.
Tang Y, et al. Rapid induction of apoptosis during Kinesin-5 inhibitor-induced mitotic arrest in HL60 cells. Cancer Lett. 2011 Nov 1;310(1):15-24.