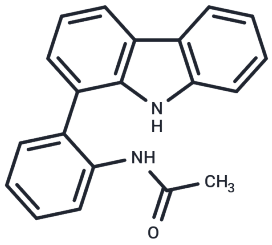
Data Sheet (Cat.No.T5399)

TargetMol

GeA-69

Chemical Properties



CAS No. : 2143475-98-1

Formula: C20H16N2O

Molecular Weight: 300.35

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	GeA-69 (GeA69) is a selective and allosteric PARP14 macrodomain 2 (MD2) inhibitor (Kd: 0.86 μM in ITC assays).
Targets(IC50)	PARP
In vitro	The macrodomain recruitment was significantly decreased in cells pre-treated with 50 μM GeA-69 and completely prevented in cells exposed to 250 μM GeA-69.
Kinase Assay	Binding experiments were carried out on a VP-ITC microcalorimeter. All experiments were performed in 50 mM HEPES (pH 7.4), 300 mM NaCl, 5 % glycerol, 0.5 mM TCEP at 12 °C, a reference power of 12 μCal/sec and a stirring speed of 307 rpm. The titrations were conducted using an initial injection of 2 μL followed by 28 identical injections of 10 μL with duration of 4 sec (per injection) and a spacing of 240 sec between injections. Competition experiments were performed on an iTC200 instrument at 20 °C, a reference power of 12 μCal/sec and a stirring speed of 1000 rpm. Following an initial injection of 0.2 μL, 20 identical injections of 2 μL were run with a duration of 4 sec (per injection) and a spacing of 150 sec between injections. Data analysis was carried out using Origin software with the MicroCal plugin. Thermodynamic parameters were calculated using ΔG = ΔH ? TΔS = ?RTlnKB, where ΔG, ΔH, and ΔS are the changes in free energy, enthalpy, and entropy of binding, respectively. In all cases, a single binding site model was employed.

Solubility Information

Solubility	DMSO: 120 mg/mL (399.53 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
In vivo Formulation	10% DMSO+40% PEG300+5% Tween 80+45% Saline: 4 mg/mL (13.32 mM),Sonication is recommended. *Please add the solvents sequentially, clarifying the solution as much as possible before adding the next one. Dissolve by heating and/or sonication if necessary. Working solution is recommended to be prepared and used immediately. The formulation provided above is for reference purposes only. In vivo formulations may vary and should be modified based on specific experimental conditions.*

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	3.3294 mL	16.6472 mL	33.2945 mL
5 mM	0.6659 mL	3.3294 mL	6.6589 mL
10 mM	0.3329 mL	1.6647 mL	3.3294 mL
50 mM	0.0666 mL	0.3329 mL	0.6659 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

Schuller M, et al. Discovery of a Selective Allosteric Inhibitor Targeting Macrodomain 2 of Polyadenosine-Diphosphate-Ribose Polymerase 14. ACS Chem Biol. 2017 Nov 17;12(11):2866-2874.