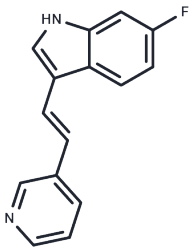
Data Sheet (Cat.No.T22251)

TargetMol

680C91

Chemical Properties



CAS No. : 163239-22-3

Formula: C15H11FN2

Molecular Weight: 238.26

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	680C91 is a potent and selective inhibitor of TDO, and its Ki is 51 nM.
Targets(IC50)	Others
In vitro	68OC91, a potent (Ki = 51 nM) and selective TDO inhibitor, has no inhibitory activity against monoamine oxidase A and B, indoleamine 2,3-dioxygenase (EC 1.13.11.17), 5-HT uptake and 5-HT1A,5-HT1D,5-HT2A and 5-HT2c receptors at a concentration of 10 μM. 68OC91 has no effect on the binding of tryptophan to albumin in plasma and inhibited TDO competitively with respect to its substrate tryptophan. 68OC91 inhibits the catabolism of tryptophan by rat liver cells and rat liver perfused in situ.[1]
In vivo	Prior administration of 68OC91 inhibits the catabolism of L-[ring-2-14C]-tryptophan and a load dose of tryptophan (100 mg/kg) in vivo. Administration of 68OC91 alone significantly increases brain tryptophan, 5-HIAA and 5-HT. A load dose of tryptophan (100 mg/kg), producing increases in brain tryptophan 4-fold greater than that seen with 68OC91, does not increase brain 5-HIAA and 5-HT to levels greater than those seen with 68OC91 and produces a shorter-lasting increase in these parameters.[1]
Cell Research	Cell lines: rat liver cells. Concentrations: 0.1 μM, 0.5 μM, 2 μM. Incubation Time: 0 min - 120 min. Method: The combined concentration of non-labelled L-tryptophan and the L-[ring-2-14C]-tryptophan used in the assays is 20 μM and is added either with or without 68OC91 at time zero.
Animal Research	Animal Models: Male Wistar rats. Dosages: 15 mg/kg. Administration: Oral gavage

Solubility Information

Solubility	DMSO: 125 mg/mL (524.64 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: 5 mg/mL (20.99 mM) *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	4.1971 mL	20.9855 mL	41.971 mL
5 mM	0.8394 mL	4.1971 mL	8.3942 mL
10 mM	0.4197 mL	2.0985 mL	4.1971 mL
50 mM	0.0839 mL	0.4197 mL	0.8394 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

M Salter, et al. Biochem Pharmacol. 1995 May 17;49(10):1435-42.
Sophie Imbeault, et al. Acta Neuropsychiatr. 2020 Feb;32(1):43-53.