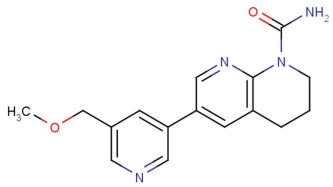
Data Sheet (Cat.No.T14664)

TargetMol
A DRUG SCREENING EXPERT

BI 689648

Chemical Properties



CAS No.:	1633009-87-6
Formula:	C16H18N4O2
Molecular Weight:	298.34
Appearance:	N/A
Storage:	0-4℃ for short term (days to weeks), or -20℃ for long term (months).

Biological Description

Description	BI 689648 is a highly selective inhibitor of aldosterone synthase(CYP11B1 and CYP11B2 with IC50s of 310 and 2.1 nM, respectively).
Targets(IC_{50})	CYP11B1: 310 nM CYP11B2: 2.1 nM
In vitro	Compare with the FADs and LCI699, BI 689648 is highly selective in vitro, providing an IC50 for CYP11B2 of 2.1 nM and a selectivity factor of 149 over CYP11B1. FAD286, by comparison, shows a similar IC50 for CYP11B2 (2.5 nM). However, its greater potency against CYP11B1 (94 nM) results in a comparatively modest selectivity factor of 38, approximately 4-fold less than BI 689648[1].
In vivo	After oral administration in cyno monkeys, BI 689648 (5 mg/kg) exhibits a peak plasma concentration of ~500 nM. BI 689648 exhibits minimal impact on 11-DC and only at very high plasma concentrations (~10 μM)[1]. For BI 689648 (aldosterone EC50=2 nM), appreciable changes in 11-DOC are only noted at plasma concentrations >2000 nM or >1000-fold its aldosterone EC50 while FAD286 shows a window of ~100-fold.

Solubility Information

Solubility	DMSO: 30 mg/mL (100.56 mM) (< 1 mg/ml refers to the product slightly soluble or insoluble)

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	3.352 mL	16.759 mL	33.519 mL
5 mM	0.67 mL	3.352 mL	6.704 mL
10 mM	0.335 mL	1.676 mL	3.352 mL
50 mM	0.067 mL	0.335 mL	0.67 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. The storage conditions and period of the stock solution: - 80 ℃ for 6 months; - 20 ℃ for 1 month. Please use it as soon as possible.

Reference

1. Weldon SM, et al. Selectivity of BI 689648, a Novel, Highly Selective Aldosterone Synthase Inhibitor: Comparison with FAD286 and LCI699 in Nonhuman Primates. J Pharmacol Exp Ther. 2016 Oct;359(1):142-50.

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