

产品名称 : Autotaxin inhibitor compound 1

同义词 : Autotaxin-IN-1

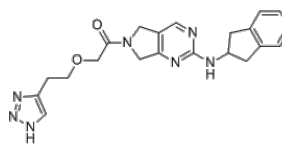
产品货号 : M12375

CAS Number : 1619971-30-0

分子式 : C₂₁H₂₃N₇O₂

分子量 : 405.462

化学全名 : 2-(2-(1H-1,2,3-triazol-4-yl)ethoxy)-1-((2,3-dihydro-1H-inden-2-yl)amino)-5,7-dihydro-6H-pyrrolo[3,4-d]pyrimidin-6-yl)ethan-1-one



产品描述 : Autotaxin inhibitor compound 1 (Autotaxin-IN-1) is a potent, selective, orally bioavailable inhibitor of autotaxin with IC₅₀ of 2.2 nM in ex vivo human whole blood assay, does not inhibit related proteins ENPP1 and ENPP7; demonstrates significant anti-inflammatory and analgesic effects in the carrageenan-induced paw inflammation and acetic acid-induced visceral pain tests, respectively; also significantly inhibits disease activity score in the dextran sodium sulfate-induced model of inflammatory bowel disease (IBD) and in autoimmune encephalomyelitis model of multiple sclerosis (MS).

通路 : Wnt/Notch/Hedgehog

靶点 : Autotaxin

受体 : Autotaxin

溶解度 : ——

SMILES : O=C(N1CC2=NC(NC3CC4=C(C=CC=C4)C3)=NC=C2C1)COC(=O)C5=CN=CN5

存储条件 : (-20℃)

稳定性 : ≥ 2 years

参考文献 :

1. Thirunavukkarasu K, et al. J Pharmacol Exp Ther. 2016 Oct;359(1):207-14. 2. Jones SB, et al. ACS Med Chem Lett. 2016 Aug 2;7(9):857-61.