Product Datasheet

NIK SMI1

Catalog No. **BP-02148** · CAS **1660114-31-7** · Form **free base** · Physical state **other** · Color **off-white to pink** · Version **1.0** · Revision **2026-09-03**

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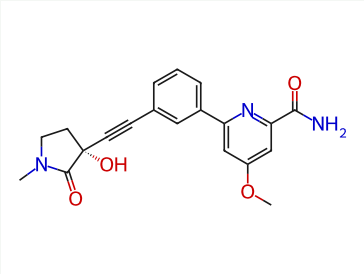
Target	Research area
NF-κB	**Inflammation/Immunology**

Molecular formula	$C_{20}H_{19}N_3O_4$
Molecular weight	**365.3826**

STRUCTURE



DESCRIPTION

NIK SMI1 is a highly potent and selective NF-κB-inducing kinase (NIK) inhibitor with Ki of 0.23 nM for NIK-catalyzed hydrolysis of ATP to ADP.

BIOLOGICAL ACTIVITY

In Vitro

NIK SMI1 (Compound 4f) inhibits NIK-catalyzed hydrolysis of ATP to ADP (fluorescence polarization, FP) with an IC50 of 0.23±0.17 nM. NIK SMI1 inhibits the expression of NIK SMI1 response elementregulated firefly luciferase reporter gene in HEK293 cells with an IC50 of 34±6 nM. Consistent with expectations for a NIK inhibitor, NIK SMI1 is shown to inhibit nuclear translocation of p52 (RelB) (IC50=70 nM). NIK SMI1 inhibits BAFF-induced B cell (mouse) survival in vitro with an IC50 of 373±64 nM.

n Vivo

C57BL/6 mice are treated twice daily for 7 days with orally administered NIK SMI1 or with three injections of recombinant BAFF receptor fusion protein (Br3- mIgG2a) over the course of the 7-day experiment as a positive control. The nonlinearity of exposure relative to dose between 100 and 200 mg/kg is a result of saturation of clearance mechanisms. The pharmacology of NIK SMI1 is examined in SD rat, CD-1 mouse, beagle, and cynomologous monkey with 20, 32, 18, and 7.8 mL/kg per min, respectively. Volume of distribution (Vd, L/kg) is 1.35, 1.58, 0.778, and 1.39, respectively.

SOLUBILITY

Soluble in DMSO

REFERENCES

[1]. Blaquiere N, et al. Scaffold-Hopping Approach To Discover Potent, Selective, and Efficacious Inhibitors of NF-κB Inducing Kinase. J Med Chem. 2018 Aug 9;61(15):6801-6813.

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