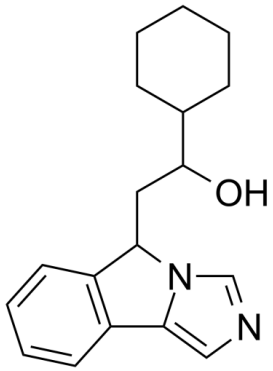
Data Sheet

Product Name:	IDO-IN-7
Cat. No.:	CS-3512
CAS No.:	1402836-58-1
Molecular Formula:	C18H22N2O
Molecular Weight:	282.38
Target:	Indoleamine 2,3-Dioxygenase (IDO)
Pathway:	Metabolic Enzyme/Protease
Solubility:	DMSO : 15 mg/mL (53.12 mM; Need warming); Ethanol : 25 mg/mL (88.53 mM; Need ultrasonic)



BIOLOGICAL ACTIVITY:

IDO-IN-7 (NLG-919 analogue) is a a potent **IDO1** inhibitor with an **IC_{50}** of 38 nM. IC50 & Target: IC50: 38 nM (IDO1)[1] **In Vitro:** IDO-IN-7 (NLG-919 analogue) is a potent IDO1 inhibitor (IC_{50}=38 nM). The binding mode of IDO-IN-7 to IDO1 is experimentally available and shows a direct coordinative interaction to the sixth coordination site of ferric heme. IDO-IN-7 has been used as reference compound in other studies to validate high-throughput screening assay for IDO1 inhibition and develop immunostimulatory nanomicellar carrier[1].

PROTOCOL (Extracted from published papers and Only for reference)

Cell Assay: IDO-IN-7 (NLG-919 analogue) and the selected fragments 8, 15, and 18 are tested in cellular assay for their ability to cross cell membrane and inhibit IDO1 catalytic activity. The cell line of murine mastocytoma P1.HTR stably transfected with murine IDO1 (P1.IDO1) is cultured for 16 hrs in the presence of each compound at the concentration of 30 mM. The ability of P1.IDO1 cells to convert LTrp contained in the culture medium at the concentration of 78.4 μM into L-Kyn is then assessed after 16 hrs of incubation[1].

References:

[1]. Coletti A, et al. Fragment-based approach to identify IDO1 inhibitor building blocks. Eur J Med Chem. 2017 Dec 1;141:169-177.

CAIndexNames:

5H-Imidazo[5,1-a]isoindole-5-ethanol, α-cyclohexyl-

SMILES:

OC(C1CCCCC1)CC(C2=C3C=CC=C2)N4C3=CN=C4

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