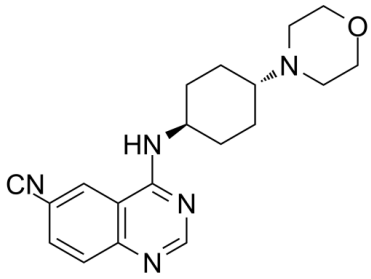
Data Sheet

Product Name:	IRAK4-IN-1
Cat. No.:	CS-7925
CAS No.:	1820787-94-7
Molecular Formula:	C19H23N5O
Molecular Weight:	337.42
Target:	IRAK
Pathway:	Immunology/Inflammation; Protein Tyrosine Kinase/RTK
Solubility:	H2O : < 0.1 mg/mL (insoluble); DMSO : 14.29 mg/mL (42.35 mM; Need ultrasonic)



BIOLOGICAL ACTIVITY:

IRAK4-IN-1 is an interleukin-1 receptor associated kinase 4 (**IRAK4**) inhibitor with an **IC_{50}** of 7 nM. IC50 & Target: IC50: 7 nM (IRAK4)[1]
In Vitro: The in vitro metabolic stability profiles of IRAK4-IN-1 (Compound 23) is measured, with EC_{50} of 2300 nM for the rat whole blood (RWB) [1]. **In Vivo:** Oral pharmacokinetic studies of IRAK4-IN-1 (Compound 23) show it to have high bioavailability of 73% and low plasma clearance (Clp=22 mL/min/kg) leading to a reasonable half-life of 1.3 h[1].

PROTOCOL (Extracted from published papers and Only for reference)

Animal Administration: [1]Rat[1]
In the TLR driven in vivo model, female Lewis rats are dosed with either vehicle or IRAK4-IN-1 (Compound 23; 3, 10, 30, and 100 mg/kg; p.o.) dosed at 1 h prior to stimulation with Resiquimod, R848 (5 mg/kg, IP). At 1.5 h post R848 stimulation, blood samples are obtained from the animals and cytokine levels are measured.

References:

[1]. Smith GF, et al. Identification of quinazoline based inhibitors of IRAK4 for the treatment of inflammation. Bioorg Med Chem Lett. 2017 Jun 15;27(12):2721-2726.

CAIndexNames:

6-Quinazolinecarbonitrile, 4-[[trans-4-(4-morpholinyl)cyclohexyl]amino]-

SMILES:

N#CC1=CC2=C(N=CN=C2N[C@@H]3CC[C@@H](N4CCOCC4)CC3)C=C1

Caution: Product has not been fully validated for medical applications. For research use only.

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