THS-044

Cat. No.: HY-19621

CAS No.: 62054-67-5

Molecular Formula: $C_{11}H_{12}F_3N_3O_3$

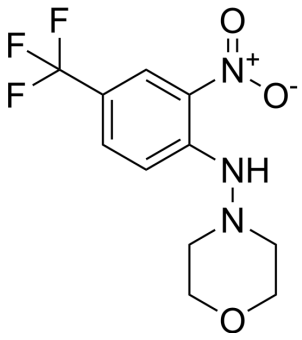
Molecular Weight: 291.23

Target: HIF/HIF Prolyl-Hydroxylase

Pathway: Metabolic Enzyme/Protease

Storage:

Powder	-20°C	3 years
	4°C	2 years
In solvent	-80°C	2 years
	-20°C	1 year



SOLVENT & SOLUBILITY

In Vitro

DMSO : 125 mg/mL (429.21 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	3.4337 mL	17.1686 mL	34.3371 mL
	5 mM	0.6867 mL	3.4337 mL	6.8674 mL
	10 mM	0.3434 mL	1.7169 mL	3.4337 mL

Please refer to the solubility information to select the appropriate solvent.

BIOLOGICAL ACTIVITY

Description

THS-044 binding stabilizes the HIF2α PAS-B folded state, for regulating HIF2 activity in endogenous and clinical settings.Target: HIF2αLimited trypsin proteolysis reveals that both apo and THS-044-bound protein are efficiently cut at R330 in the extended HI loop. In the THS-044 bound state, there appears no additional proteolysis at the remaining candidate trypsin sites. In contrast, these THS-044-protected sites are protease accessible in the unliganded protein, leading its complete degradation. In parallel, NMR-based deuterium exchange measurements revealed a dramatic stabilization of the THS-044-bound protein β-sheet, with some sites experiencing 100-fold enhanced protection factors relative to the ligand-free protein.

REFERENCES

[1]. Motto I, et al. New aryl hydrocarbon receptor homology model targeted to improve docking reliability. J Chem Inf Model. 2011 Nov 28;51(11):2868-2881.

[2]. Scheuermann TH, et al. Artificial ligand binding within the HIF2alpha PAS-B domain of the HIF2 transcription factor. Proc Natl Acad Sci U S A. 2009 Jan 13;106(2):450-

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