Product Data Sheet

Product Name: THS-044
Cat. No.: GC32945

Chemical Properties

Cas. No.	62054-67-5		
SMILES	FC(C1=CC=C(NN2CCOCC2)C([N+]([O-])=O)=C1)(F)F		
Formula	$C_{11}H_{12}F_3N_3O_3$	M.Wt	291.23
Solubility	Soluble in DMSO	Storage	Store at -20°C
General tips	For obtaining a higher solubility , please warm the tube at 37 ℃ and shake it in the ultrasonic bath for a while.Stock solution can be stored below -20℃ for several months.		
Shipping Condition	Evaluation sample solution : ship with blue ice All other available size: ship with RT , or blue ice upon request.		
Structure	THS-044		

Background

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.

[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):450-455.

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