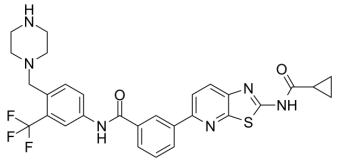
HG-12-6

Cat. No.:	HY-123956
CAS No.:	2222354-57-4
Molecular Formula:	$C_{29}H_{27}F_3N_6O_2S$
Molecular Weight:	580.62
Target:	IRAK
Pathway:	Immunology/Inflammation
Storage:	Please store the product under the recommended conditions in the Certificate of Analysis.



BIOLOGICAL ACTIVITY

Description	HG-12-6 is a type II inhibitor of IRAK4. HG-12-6 shows preferential binding to unphosphorylated inactive IRAK4 with an IC_{50} of 165 nM. HG-12-6 can modulate IRAK4 activity in autoimmunity and inflammation[1].	
IC_{50} & Target	IRAK4 165 nM (IC_{50}, Unphosphorylated inactive IRAK4)	IRAK4 2876 nM (IC_{50}, Phosphorylated active IRAK4)
In Vitro	The in-house compound HG-12-6 has a similar chemical scaffold as Ponatinib. The most differentiating components are the head of the inhibitor and the lack of a methyl substituent on ring A. Without the methyl substituent on ring A, the entire HG-12-6 molecule shifts inward to the ATP pocket in comparison with the binding mode of Ponatinib[1]. HG-12-6 has a better binding affinity for the unphosphorylated inactive IRAK4 kinase domain (IC_{50} of 165 nM) than the phosphorylated active IRAK4 kinase domain (IC_{50} of 2876 nM)[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.	

REFERENCES

[1]. Wang L, et al. Conformational flexibility and inhibitor binding to unphosphorylated interleukin-1 receptor-associated kinase 4 (IRAK4). J Biol Chem. 2019 Mar 22;294(12):4511-4519.

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