Product Name	:	TH1020
Synonyms	:	——
Cat No.	:	M22635
CAS Number	:	1841460-82-9
Molecular Formula	:	C23H15N7S2
Formula Weight	:	453.54
Chemical Name	:	——
Description	:	TH1020 is a novel Inhibitor of Toll-Like Receptor 5 (TLR5)/Flagellin Complex with promising activity (IC50 =0.85±0.12?μm) and specificity.TH1020 was repress the expression of downstream TNF-α signaling pathways mediated by the TLR5/flagellin complex formation.?Based on molecular docking simulation, TH1020 is suggested to compete with flagellin and disrupt its association with TLR5.?TH1020 provides a much-needed molecular probe for studying this important protein-protein interaction and a lead compound for identifying novel therapeutics targeting TLR5.
Pathway	:	GPCR/G Protein
Target	:	Antibacterial
Receptor	:	TLR5;Bacterial
Solubility	:	DMSO:2 mg/mL (4.41 mM; ultrasonic and warming and adjust pH to 2 with 1M HCl and heat to 80°C)
SMILES	:	C(c1ccccc1)n1c(Sc2ncnc3c4cccnc4sc23)nnc1-c1ccncc1
Storage	:	(-20℃)
Stability	:	≥ 2 years
Reference	:	

1.Lei Yan, et al. Pyrimidine Triazole Thioether Derivatives as Toll-Like Receptor 5 (TLR5)/Flagellin Complex Inhibitors. ChemMedChem. 2016 Apr 19;11(8):822-6.