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## Product Data Sheet

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Product Name: ITK inhibitor  
 Cat. No.: GC12167

### Chemical Properties

Cas. No. 439574-61-5

Chemical Name N-[5-[5-(4-acetyl piperazine-1-carbonyl)-4-methoxy-2-methylphenyl]sulfanyl-1,3-thiazol-2-yl]-4-[(3-methylbutan-2-ylamino)methyl]benzamide

SMILES CC1=C(C=C(C(=C1)OC)C(=O)N2CCN(CC2)C(=O)C)SC3=CN=C(S3)NC(=O)C4=CC=C(C=C4)CNC(C)C(C)C

Formula C<sub>31</sub>H<sub>39</sub>N<sub>5</sub>O<sub>4</sub>S<sub>2</sub>

M.Wt

609.82

Solubility Soluble in DMSO

Storage

Store at -20°C

General tips For obtaining a higher solubility, please warm the tube at 37 °C and shake it in the ultrasonic bath for a while. Stock solution can be stored below -20°C 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

### Background

Interleukin-2-inducible T cell kinase (ITK) is a non-receptor tyrosine kinase expressed in T cells, NKT cells and mast cells which plays a crucial role in regulating the T cell receptor (TCR), CD28, CD2, chemokine receptor CXCR4, and FcεpsilonR-mediated signaling pathways. ITK inhibitors can be used for the treatment of inflammation and immune-mediated disorders. ITK inhibitor (N-[5-[[3-[(4-Acetylpiperazin-1-yl)carbonyl]-4-methyl-6-methoxyphenyl]thio]thiazol-2-yl]-4-(N-1,2-dimethylpropylaminomethyl)benzamide) is the analogue of BMS-509744, which can potently and selectively inhibit Itk kinase activity.

In vitro: BMS-509744 could reduce TCR-induced functions including PLCγ1 tyrosine phosphorylation, calcium mobilization, IL-2 secretion, and T-cell proliferation in vitro in both human and mouse cells [1].

In vivo: BMS-509744 suppressed the production of IL-2 induced by anti-TCR antibody administered to mice. BMS-509744 also significantly diminishes lung inflammation in a mouse model of ovalbumin-induced allergy/asthma [1].

Clinical trial: Up to now, both BMS-509744 and ITK inhibitor is still in the preclinical development stage.

### Reference:

[1] Lin TA, McIntyre KW, Das J, Liu C, O'Day KD, Penhallow B, Hung CY, Whitney GS, Shuster DJ, Yang X, Townsend R, Postelnek J, Spergel SH, Lin J, Moquin RV, Furch JA, Kamath AV, Zhang H, Marathe PH, Perez-Villar JJ, Doweiko A, Killar L, Dodd JH, Barrish JC, Wityak J, Kanner SB. Selective Itk inhibitors block T-cell activation and murine lung inflammation. *Biochemistry*. 2004 Aug 31;43(34):11056-62.

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

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