

**Product Name:** TH 1020

**Catalog No.:** 6191

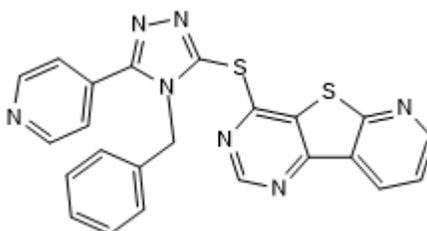
**Batch No.:** 1

CAS Number: 1841460-82-9

IUPAC Name: 4-[[4-(Phenylmethyl)-5-(4-pyridinyl)-4H-1,2,4-triazol-3-yl]thio]-pyrido[3',2':4,5]thieno[3,2-d]pyrimidine

## 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:**  $C_{23}H_{15}N_7S_2 \cdot \frac{1}{2}H_2O$   
**Batch Molecular Weight:** 462.55  
**Physical Appearance:** Off White solid  
**Solubility:** DMSO to 5 mM with gentle warming  
**Storage:** Store at +4°C  
**Batch Molecular Structure:**



## 2. ANALYTICAL DATA

**TLC:**  $R_f = 0.43$  (Dichloromethane:Methanol [95:5])  
**HPLC:** Shows 99.5% purity  
**<sup>1</sup>H NMR:** Consistent with structure  
**Mass Spectrum:** Consistent with structure  
**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	59.72	3.49	21.2
Found	59.74	3.22	21.14

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**Description:**

Toll-like receptor (TLR) 5/Flagellin complex antagonist (IC<sub>50</sub> = 0.85 μM). Competes with flagellin for TLR5 binding to inhibit the TLR5:flagellin interaction and subsequent downstream TNF-α secretion.

**Physical and Chemical Properties:**

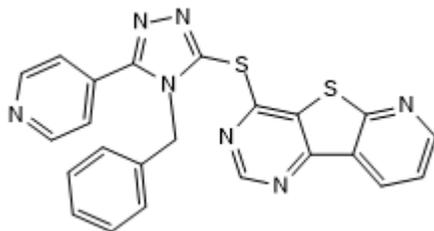
Batch Molecular Formula: C<sub>23</sub>H<sub>15</sub>N<sub>7</sub>S<sub>2</sub>·½H<sub>2</sub>O

Batch Molecular Weight: 462.55

Physical Appearance: Off White solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**



**Storage:** Store at +4°C

**Solubility & Usage Info:**

DMSO to 5 mM with gentle warming

**Stability and Solubility Advice:**

Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a 45-60°C water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. Our standard recommendations are:

**SOLIDS:** Provided storage is as stated on the product label and the vial is kept tightly sealed, the product can be stored for up to 6 months from date of receipt.

**SOLUTIONS:** We recommend that stock solutions, once prepared, are stored aliquoted in tightly sealed vials at -20°C or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

**References:**

Yan *et al* (2016) Pyrimidine triazole thioether derivatives as toll-like receptor 5 (TLR5)/flagellin complex inhibitors. *Chem.Med.Chem.* **11** 822. PMID: 26634412.

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