

**Product Name:** IKK 16

**Catalog No.:** 2539

**Batch No.:** 2

**CAS Number:** 1186195-62-9

**IUPAC Name:** *N*-(4-Pyrrolidin-1-yl-piperidin-1-yl)-[4-(4-benzo[*b*]thiophen-2-yl-pyrimidin-2-ylamino)phenyl]carboxamide hydrochloride

## 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>28</sub>H<sub>29</sub>N<sub>5</sub>OS.HCl.¼H<sub>2</sub>O

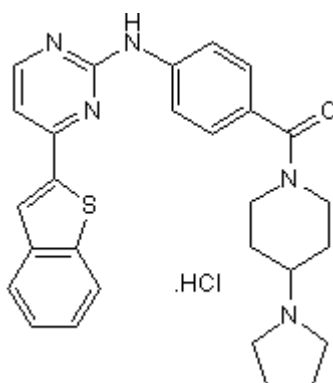
**Batch Molecular Weight:** 524.59

**Physical Appearance:** Beige solid

**Solubility:** water to 50 mM  
DMSO to 50 mM

**Storage:** Desiccate at -20°C

**Batch Molecular Structure:**



## 2. ANALYTICAL DATA

**TLC:** R<sub>f</sub> = 0.44 (Dichloromethane:Methanol:Ammonia soln. [90:9:1])

**HPLC:** Shows >98.7% purity

**<sup>1</sup>H NMR:** Consistent with structure

**Mass Spectrum:** Consistent with structure

**UV Spectrum:** 14-0735

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	64.11	5.86	13.35
Found	63.88	5.82	13.04

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**Description:**

Selective inhibitor of IκB kinase (IKK) (IC<sub>50</sub> values are 40, 70 and 200 nM for IKKβ, IKK complex and IKKα respectively). Inhibits TNF-α-stimulated IκB degradation and expression of adhesion molecules E-selectin, ICAM and VCAM (IC<sub>50</sub> values are 1.0, 0.5, 0.3 and 0.3 μM respectively). Inhibits LPS-induced TNF-α release in vivo and neutrophil extravasion in thioglycollate-induced peritonitis.

**Physical and Chemical Properties:**

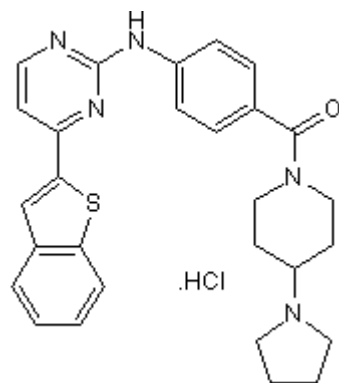
Batch Molecular Formula: C<sub>28</sub>H<sub>29</sub>N<sub>5</sub>OS.HCl.¼H<sub>2</sub>O

Batch Molecular Weight: 524.59

Physical Appearance: Beige solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**



**Storage:** Desiccate at -20°C

**Solubility & Usage Info:**

water to 50 mM  
DMSO to 50 mM

**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:**

Waelchli *et al* (2006) Design and preparation of 2-benzoamido-pyrimidines as inhibitors of IKK. *Bioorg.Med.Chem.Lett.* **16** 108. PMID: 16236504.

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