

Product Name: IKK 16

Catalog No.: 2539

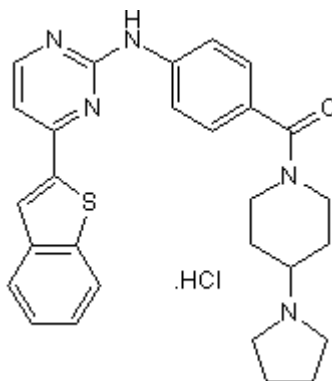
Batch No.: 2

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: C₂₈H₂₉N₅OS.HCl.¼H₂O
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_f = 0.44 (Dichloromethane:Methanol:Ammonia soln. [90:9:1])
HPLC: Shows >98.7% purity
¹H 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) (IC₅₀ 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 (IC₅₀ 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:

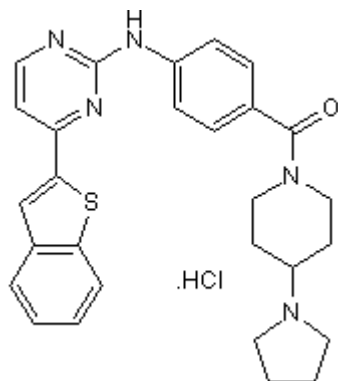
Batch Molecular Formula: C₂₈H₂₉N₅OS.HCl.¼H₂O

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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bio-techne.com

info@bio-techne.com

techsupport@bio-techne.com

North America

Tel: (800) 343 7475

China

info.cn@bio-techne.com

Tel: +86 (21) 52380373

Europe Middle East Africa

Tel: +44 (0)1235 529449

Rest of World

www.tocris.com/distributors

Tel: +1 612 379 2956