

Product Name: HJC 0416 hydrochloride

Catalog No.: 6110

Batch No.: 1

IUPAC Name: 2-(3-Aminopropoxy)-5-chloro-N-(1,1-dioxidobenzo[*b*]thien-6-yl)benzamide hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₈H₁₇ClN₂O₄S.HCl.1½H₂O

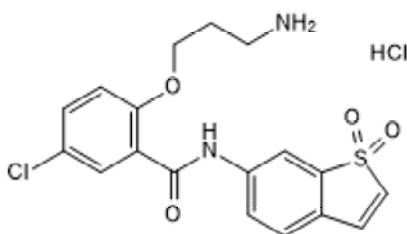
Batch Molecular Weight: 456.34

Physical Appearance: Off White solid

Solubility: DMSO to 100 mM
water to 20 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 97.5% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	47.38	4.64	6.14
Found	47.04	4.53	5.99

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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Description:

STAT3 inhibitor. Downregulates phosphorylation of STAT3 and increases the expression of cleaved caspase-3. Inhibits cell-cycle progression and proliferation in breast and pancreatic cancer cells in vitro (IC₅₀ values are in the range 0.04 - 1.97 μM). Also inhibits growth of ER-negative breast cancer xenografts in mice. Orally bioavailable.

Physical and Chemical Properties:

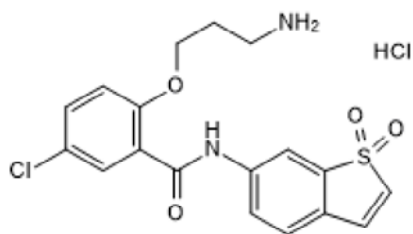
Batch Molecular Formula: C₁₈H₁₇ClN₂O₄S.HCl.1½H₂O

Batch Molecular Weight: 456.34

Physical Appearance: Off White solid

Minimum Purity: ≥97%

Batch Molecular Structure:



References:

Chen et al (2014) Discovery of potent anticancer agent HJC0416, an orally bioavailable small molecule inhibitor of signal transducer and activator of transcription 3 (STAT3). *Eur.J.Med.Chem.* **82** 195. PMID: 24904966.

Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM

water to 20 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.

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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