

Product Name: BI 605906

Catalog No.: 5300

Batch No.: 1

CAS Number: 960293-88-3

IUPAC Name: 3-Amino-4-(1,1-difluoropropyl)-6-[4-(methylsulfonyl)-1-piperidinyl]thieno[2,3-b]pyridine-2-carboxamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₇H₂₂F₂N₄O₃S₂

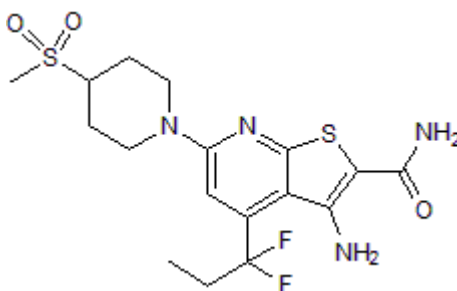
Batch Molecular Weight: 432.51

Physical Appearance: Yellow solid

Solubility: DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.5 (Dichloromethane:Methanol [9:1])

HPLC: Shows 98.3% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	47.21	5.13	12.95
Found	47.06	5.04	12.84

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Description:

Selective IKK β inhibitor (IC₅₀ = 380 nM). Displays no effect on a panel of 100 kinases, except at IGF1 (IC₅₀ = 7.6 μ M).

Physical and Chemical Properties:

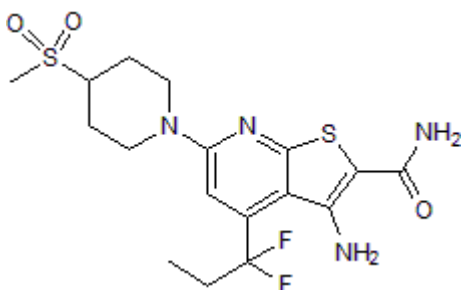
Batch Molecular Formula: C₁₇H₂₂F₂N₄O₃S₂

Batch Molecular Weight: 432.51

Physical Appearance: Yellow solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 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:

Zhang *et al* (2014) An unexpected twist to the activation of IKK β : TAK1 primes IKK β for activation by autophosphorylation. *Biochem.J.* **461** 531. PMID: 24911653.

Clark *et al* (2011) Novel cross-talk within the IKK family controls innate immunity. *Biochem.J.* **434** 93. PMID: 21138416.

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