

Product Name: ACHP

Catalog No.: 4547

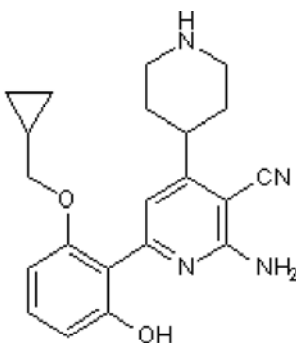
Batch No.: 4

CAS Number: 406208-42-2

IUPAC Name: 2-Amino-6-[2-(cyclopropylmethoxy)-6-hydroxyphenyl]-4-(4-piperidinyl)-3-pyridinecarbonitrile

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₁H₂₄N₄O₂
Batch Molecular Weight: 364.44
Physical Appearance: Yellow solid
Solubility: DMSO to 20 mM
Storage: Store at -20°C
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.48 (Dichloromethane:Methanol:Ammonia soln. [9:1:0.3])
HPLC: Shows 98.0% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	69.21	6.64	15.37
Found	69.18	6.69	15.03

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

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Description:

IκB kinase inhibitor (IC₅₀ values are 8.5 and 250 nM for IKKβ and IKKα respectively). Selective for IKKα and IKKβ over IKK3, Syk and MAPKKK4 (IC₅₀ values are > 20 μM). Inhibits DNA binding activity of NF-κB. Blocks NF-κB pathway in multiple myeloma cell lines; induces cell growth arrest and apoptosis. Also inhibits STAT3 signaling in NSCLC in vitro.

Physical and Chemical Properties:

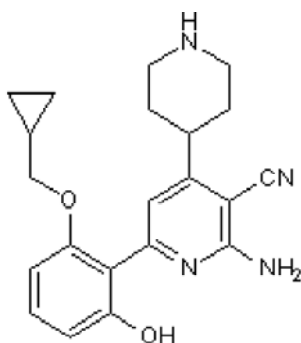
Batch Molecular Formula: C₂₁H₂₄N₄O₂

Batch Molecular Weight: 364.44

Physical Appearance: Yellow solid

Minimum Purity: ≥97%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO 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.

References:

Lee et al (2019) The IκB kinase inhibitor ACHP targets the STAT3 signaling pathway in human non-small cell lung carcinoma cells. *Biomolecules* **9** 875. PMID: 31847229.

Sanda et al (2005) Growth inhibition of multiple myeloma cells by a novel IκB kinase inhibitor. *Clin.Cancer Res.* **11** 1974. PMID: 15756023.

Murata et al (2004) Synthesis and structure-activity relationships of novel IKK-β inhibitors. Part 3: Orally active anti-inflammatory agents. *Bioorg.Med.Chem.Lett.* **14** 4019. PMID: 15225718 .

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