

Certificate of Analysis

Product Name: AZ 12080282 dihydrochloride

Catalog No.: 4838

Batch No.: 1

IUPAC Name: *N*-[5-(1*H*-Imidazol-2-yl)-2-methylphenyl]-4-(2-pyridinylmethoxy)benzamide dihydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₃H₂₀N₄O₂·2HCl·2H₂O

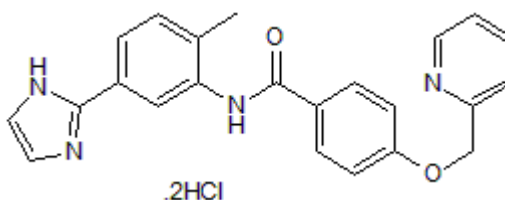
Batch Molecular Weight: 493.38

Physical Appearance: Yellow solid

Solubility: water to 100 mM
DMSO to 100 mM

Storage: Desiccate at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.53 (Dichloromethane:Methanol [9:1])

HPLC: Shows 99.9% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	55.99	5.31	11.36
Found	55.67	5.1	11.38

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

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Description:

Inhibitor of Hedgehog (Hh) signaling (IC₅₀ <0.012 μM in a firefly reporter assay against the Hh pathway). Shown to displace cyclopamine in HeLa cells expressing Smoothened. Exhibits selectivity against p38α. Orally bioavailable.

Physical and Chemical Properties:

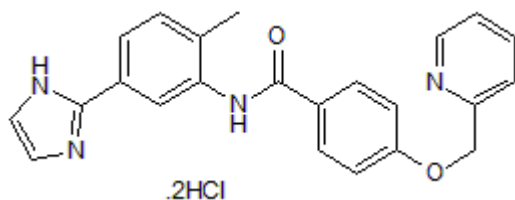
Batch Molecular Formula: C₂₃H₂₀N₄O₂·2HCl·2H₂O

Batch Molecular Weight: 493.38

Physical Appearance: Yellow solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Desiccate at RT

Solubility & Usage Info:

water to 100 mM
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:

Yang *et al* (2012) Discovery of novel hedgehog antagonists from cell-based screening: isoteric modification of p38 bisamides as potent inhibitors of SMO. *Bioorg.Med.Chem.Lett.* **22** 4907. PMID: 22704236.

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