

Product Name: CC 401 dihydrochloride

Catalog No.: 6258

Batch No.: 1

CAS Number: 2250025-96-6

IUPAC Name: 3-[3-[2-(1-Piperidinyl)ethoxy]phenyl]-5-(1*H*-1,2,4-triazol-5-yl)-1*H*-indazole dihydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₂H₂₄N₆O.2HCl.¾H₂O

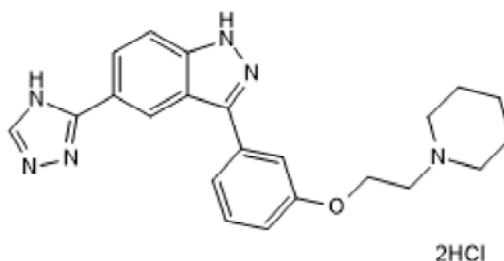
Batch Molecular Weight: 474.9

Physical Appearance: Off White solid

Solubility: water to 100 mM
DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 98.7% purity

¹H NMR: consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	55.64	5.84	17.7
Found	55.52	5.98	17.94

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

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Description:

CC 401 dihydrochloride is a high affinity JNK inhibitor (K_i values are 25-50 nM). Inhibits JNK via competitive binding of the ATP-binding site of active, phosphorylated JNK. Exhibits > 40-fold selectivity for JNK over p38, ERK, IKK2, protein kinase C, Lck and ZAP70. Hepatoprotective. Also inhibits HCMV replication.

Physical and Chemical Properties:

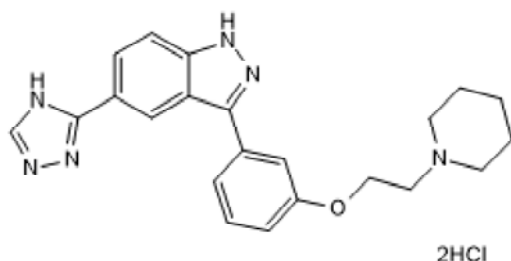
Batch Molecular Formula: $C_{22}H_{24}N_6O \cdot 2HCl \cdot \frac{3}{4}H_2O$

Batch Molecular Weight: 474.9

Physical Appearance: Off White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



References:

Vasilevskaya et al (2015) Inhibition of JNK sensitizes hypoxic colon cancer cells to DNA-damaging agents. *Clin.Cancer.Res.* **21** 4143. PMID: 26023085.

Zhang et al (2015) The c-Jun N-terminal kinase inhibitor SP600125 inhibits human cytomegalovirus replication. *J.Med.Virol.* **87** 2135. PMID: 26058558 .

Ma et al (2009) Blockade of the c-Jun amino terminal kinase prevents crescent formation and halts established anti-GBM glomerulonephritis in the rat. *Lab.Invest.* **89** 470. PMID: 19188913 .

Storage: Store at -20°C

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.

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