

Solubility:

Certificate of Analysis

Print Date: Nov 20th 2024

Batch No.: 1

www.tocris.com

Catalog No.: 5964

Product Name: SI-2 hydrochloride

CAS Number: 1992052-49-9

IUPAC Name: 1-(2-Pyridinyl)ethanone 2-(1-methyl-1*H*-benzimidazol-2-yl)hydrazone hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₅H₁₅N₅.HCl.½H₂O

Batch Molecular Weight: 306.28

Physical Appearance: Orange solid

water to 50 mM DMSO to 20 mM

Storage: Store at +4°C

Batch Molecular Structure:

2. ANALYTICAL DATA

TLC: $R_f = 0.22 (10\% \text{ MeOH in DCM } 0.05\% \text{ 7N NH3 in MeOH})$

HPLC: Shows 99.3% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen Chlorine

Theoretical 58.82 5.43 22.87 11.58 Found 58.83 5.21 23 11.7

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



Product Information

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Description:

SI-2 hydrochloride is a potent steroid receptor coactivator 3 (SRC-3) inhibitor. Reduces SRC1, SRC2 and SRC3 levels in breast cancer cell lines. Inhibits cell growth (IC $_{50}$ = 3.4 nM), induces apoptosis and attenuates migration of MDA-MB48 breast cancer cells in vitro. Inhibits tumor growth in a MDA-MB48 cell breast cancer mouse model. Orally available.

Physical and Chemical Properties:

Batch Molecular Formula: C₁₅H₁₅N₅.HCl.½H₂O

Batch Molecular Weight: 306.28 Physical Appearance: Orange solid

Minimum Purity: ≥98%

Batch Molecular Structure:

Storage: Store at +4°C

Solubility & Usage Info:

water to 50 mM 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).

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Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. *Unless contradicted by product-specific protocols or instructions, our standard recommendations apply:

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:

Song *et al* (2016) Development of potent small-molecule inhibitors to drug the undruggable steroid receptor coactivator-3. Proc.Natl.Acad.Sci.U.S.A. *113* 4970. PMID: 27084884 .

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