

Certificate of Analysis

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Product Name: SI-2 hydrochloride

Catalog No.: 5964

Batch No.: 1

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

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₅H₁₅N₅·HCl·¼H₂O

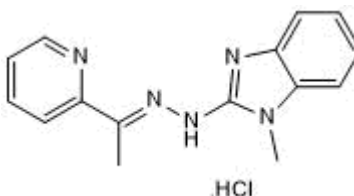
Batch Molecular Weight: 306.28

Physical Appearance: Orange solid

Solubility: 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% MeOH in DCM 0.05% 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

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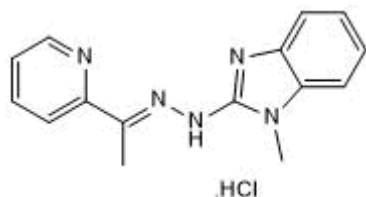
Description:

Potent steroid receptor coactivator 3 (SRC-3) inhibitor. Reduces SRC1, SRC2 and SRC3 levels in breast cancer cell lines. Inhibits cell growth (IC₅₀ = 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·¼H₂O

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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).

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:

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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