

Certificate of Analysis

Product Name: SID 7969543

Catalog No.: 3440

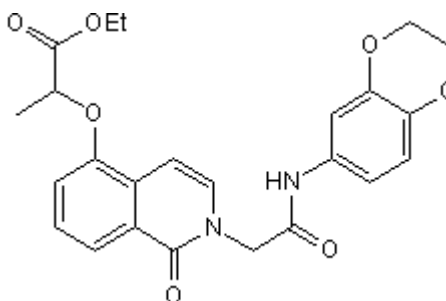
Batch No.: 1

CAS Number: 868224-64-0

IUPAC Name: Ethyl 2-[[2-[2-[(2,3-Dihydro-1,4-benzodioxin-6-yl)amino]-2-oxoethyl]-1,2-dihydro-1-oxo-5-isoquinolinyloxy]propanoate

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula:	$C_{24}H_{24}N_2O_7 \cdot \frac{1}{4}H_2O$
Batch Molecular Weight:	456.96
Physical Appearance:	White solid
Solubility:	DMSO to 100 mM
Storage:	Store at +4°C
Batch Molecular Structure:	



2. ANALYTICAL DATA

HPLC:	Shows 98% purity
¹H NMR:	Consistent with structure
Mass Spectrum:	Consistent with structure
Microanalysis:	

	Carbon	Hydrogen	Nitrogen
Theoretical	63.08	5.4	6.13
Found	63.2	5.3	6.24

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

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Description:

Selective steroidogenic factor-1 (SF-1, NR5A1) inhibitor (IC₅₀ values are 0.76, >33 and >33 μM at SF-1, RORα and VP16 respectively). Inhibits SF-1-dependent luciferase expression in HEK 293T cells in vitro (IC₅₀ = 30 nM).

Physical and Chemical Properties:

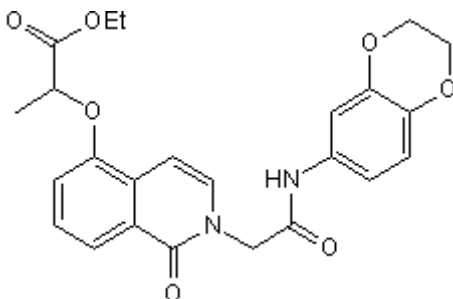
Batch Molecular Formula: C₂₄H₂₄N₂O₇ · ¼H₂O

Batch Molecular Weight: 456.96

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

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:

Roth et al (2008) Synthesis of small molecule inhibitors of the orphan nuclear receptor steroidogenic factor-1 (NR5A1) based on isoquinolinone scaffolds. *Bioorg.med.Chem.Lett.* **18** 2628. PMID: 18374567.

Madoux et al (2008) Potent, selective and cell penetrant inhibitors of SF-1 by functional ultra-high-throughput screening. *Mol.Pharmacol.* **73** 1776. PMID: 18334597.

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