

Certificate of Analysis

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Product Name: 5J 4

Catalog No.: 5490

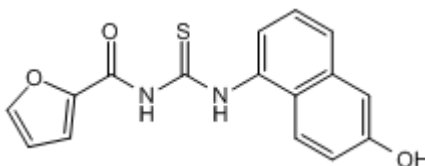
Batch No.: 1

CAS Number: 827001-82-1

IUPAC Name: *N*-[[[(6-Hydroxy-1-naphthalenyl)amino]thioxomethyl]-2-furancarboxamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₆H₁₂N₂O₃S
Batch Molecular Weight: 312.34
Physical Appearance: Yellow solid
Solubility: DMSO to 100 mM
 ethanol to 10 mM
Storage: Store at -20°C
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.5 (Ethyl acetate:Petroleum ether [1:2])
HPLC: Shows 99.7% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

| | Carbon | Hydrogen | Nitrogen |
|-------------|--------|----------|----------|
| Theoretical | 61.53 | 3.87 | 8.97 |
| Found | 61.87 | 3.8 | 9 |

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

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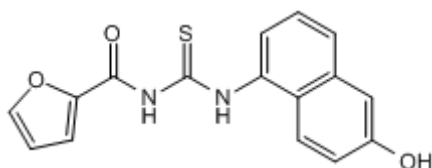
IUPAC Name: *N*-[[[(6-Hydroxy-1-naphthalenyl)amino]thioxomethyl]-2-furancarboxamide**Description:**

Calcium release-activated calcium (CRAC) channel blocker. Blocks store-operated calcium entry (SOCE) in HeLa-O+S cells and Th17 cells in vitro. Ameliorates symptoms and reduces CNS infiltration by mononuclear cells in a mouse model of experimental autoimmune encephalomyelitis (EAE) in vivo.

Physical and Chemical Properties:Batch Molecular Formula: C₁₆H₁₂N₂O₃S

Batch Molecular Weight: 312.34

Physical Appearance: Yellow solid

Minimum Purity: >98%**Batch Molecular Structure:****Storage:** Store at -20°C

CAUTION - This product is light sensitive and we recommend that the solid material and any solutions obtained are protected from exposure to light.

Solubility & Usage Info:

DMSO to 100 mM

ethanol to 10 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:

Kim *et al* (2014) Calcium signaling via Orai1 is essential for induction of the nuclear orphan receptor pathway to drive Th17 differentiation. *J.Immunol.* **192** 110. PMID: 24307733 .

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