

Certificate of Analysis

Print Date: May 10th 2024

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Product Name: NDT 30805 Catalog No.: 7808 Batch No.: 1

IUPAC Name: 2-((1,2,3,5,6,7-Hexahydro-s-indacen-4-yl)amino)-5-(pyridin-2-ylmethyl)-[1,2,4]triazolo[1,5-a]pyrimidine-7(4H)-thione

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{23}H_{22}N_6S$ Batch Molecular Weight: 414.53

Physical Appearance: Off White solid
Solubility: DMSO to 100 mM
Storage: Store at -20°C

Batch Molecular Structure:

2. ANALYTICAL DATA

HPLC: Shows 96.9% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

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Product Information

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Description:

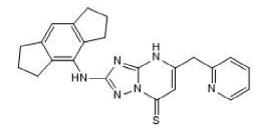
NDT 30805 is a potent NLRP3 inflammasome inhibitor. Inhibits IL-1 β release in peripheral blood mononuclear cell assay, ASC speck assay and in whole blood (IC $_{50}$ values are 13 nM, 34 nM and 1500 nM). Inhibits nigericin (Cat.No. 4312) and ATP-induced IL-1 β release. Soluble and uncharged at physiological pH.

Physical and Chemical Properties:

Batch Molecular Formula: C₂₃H₂₂N₆S Batch Molecular Weight: 414.53 Physical Appearance: Off White solid

Minimum Purity: ≥95%

Batch Molecular Structure:



Storage: Store at -20°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. *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:

Harrison et al (2022) Discovery and optimization of triazolopyrimidinone derivatives as selective NLRP3 inflammasome inhibitors. ACS Med.Chem.Lett. 13 1321. PMID: 35978696.

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