Certificate of Analysis

Product Name: **NMS 873** **Catalog No.: 6180** **Batch No.: 1**

CAS Number: 1418013-75-8

IUPAC Name: 3-[3-(Cyclopentylthio)-5-[[[2-methyl-4'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]oxy]methyl]-4*H*-1,2,4-triazol-4-yl]pyridine

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{27}H_{28}N_4O_3S_2$

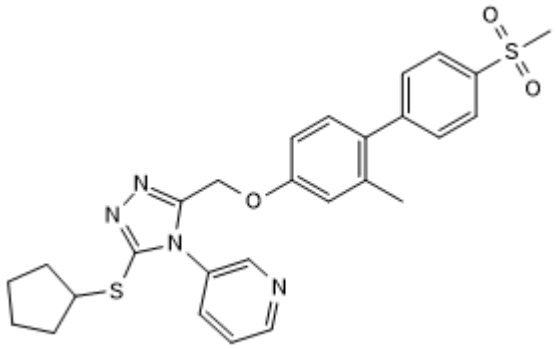
Batch Molecular Weight: 520.67

Physical Appearance: White solid

Solubility: DMSO to 100 mM
ethanol to 10 mM with gentle warming

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.6% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	62.28	5.42	10.76
Found	62.32	5.45	10.62

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Product Information

Product Name: **NMS 873** **Catalog No.: 6180** **Batch No.: 1**

CAS Number: 1418013-75-8

IUPAC Name: 3-[3-(Cyclopentylthio)-5-[[[2-methyl-4'-(methylsulfonyl)[1,1'-biphenyl]-4-yl]oxy]methyl]-4*H*-1,2,4-triazol-4-yl]pyridine

Description:

Potent p97 ATPase (VCP) allosteric inhibitor (IC_{50} = 30 nM). Selective over all other AAA ATPases, HSP90 and kinases tested (IC_{50} >10 nM). Activates the unfolded protein response (UPR) and modulates autophagosome maturation. Exhibits antiproliferative activity in cancer cells in vitro (IC_{50} values are 400 and 700 nM for HCT116 and HeLa cells respectively). Reduces p97-sensitization to trypsin digestion.

Physical and Chemical Properties:

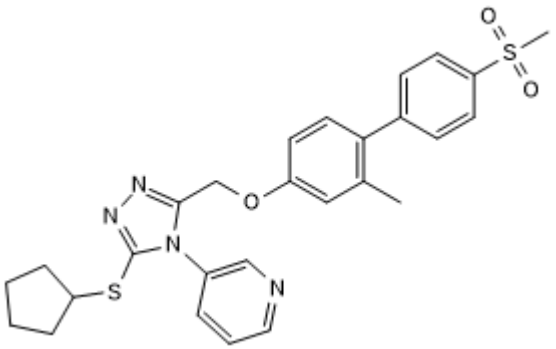
Batch Molecular Formula: $C_{27}H_{28}N_4O_3S_2$

Batch Molecular Weight: 520.67

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 100 mM
ethanol to 10 mM with gentle warming

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:

Anderson *et al* (2015) Targeting the AAA ATPase p97 as an approach to treat cancer through disruption of protein homeostasis. Cancer Cell ***28*** 653. PMID: 26555175.

Magnaghi *et al* (2013) Covalent and allosteric inhibitors of the ATPase VCP/p97 induce cancer cell death. Nat.Chem.Biol. ***9*** 548. PMID: 23892893.

Polucci *et al* (2013) Alkylsulfanyl-1,2,4-triazoles, a new class of allosteric valosine containing protein inhibitors. Synthesis and structure-activity relationships. J.Med.Chem. ***56*** 437. PMID: 23245311.

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