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Certificate of Analysis

www.tocris.com

Product Name: CST 530

Catalog No.: 8065 Batch No.: 1

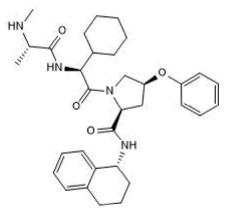
CAS Number: 847137-53-5

IUPAC Name:

(2S,4S)-1-((S)-2-Cyclohexyl-2-((S)-2-(methylamino)propanamido)acetyl)-4-phenoxy-N-((R)-1,2,3,4-tetrahydronaphthalen-1-yl)pyrrolidine-2-carboxamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: Batch Molecular Weight: Physical Appearance: Solubility: Storage: Batch Molecular Structure: $C_{33}H_{44}N_4O_4.1^3/_4H_2O$ 592.26 White solid DMSO to 100 mM Store at -20°C



2. ANALYTICAL DATA

HPLC: ¹H NMR: Mass Spectrum: Microanalysis:

Shows 97.7% purity						
Consistent with structure						
Consistent with structure						
Carbon Hydrogen Nitrogen						
Theoretical	66.92	8.08	9.46			

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

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Catalog No.: 8065 E

Batch No.: 1

CAS Number: 847137-53-5

IUPAC Name:

(2S,4S)-1-((S)-2-Cyclohexyl-2-((S)-2-(methylamino)propanamido)acetyl)-4-phenoxy-N-((R)-1,2,3,4-tetrahydronaphthalen-1-yl)pyrrolidine-2-carboxamide

Description:

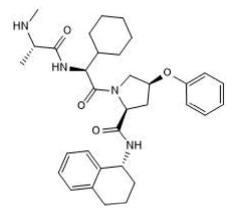
CST 530 is a monovalent IAP antagonist. Induces cIAP1 and cIAP2 autodegradation in MM.1S cells (degrades cIAP1 at 0.1 μ M and cIAP2 at 1 μ M, after 16h). CST 530 reduces cell viability in a variety of cancer cell lines including SUDHL6, MOLM13 and HEL (IC₅₀ values are 170 nM, 420 nM and 450 nM respectively).

Physical and Chemical Properties:

Batch Molecular Formula: $C_{33}H_{44}N_4O_4$.1³/₄H₂O Batch Molecular Weight: 592.26 Physical Appearance: White solid

Minimum Purity: ≥97%

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 $45-60^{\circ}C$ 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:

Ng et al (2023) Heterobifunctional ligase recruiters enable pan-degradation of inhibitor of apoptosis proteins. J.Med.Chem. 66 4703. PMID: 36996313.

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