

Product Name: UNC 3866

Catalog No.: 6096

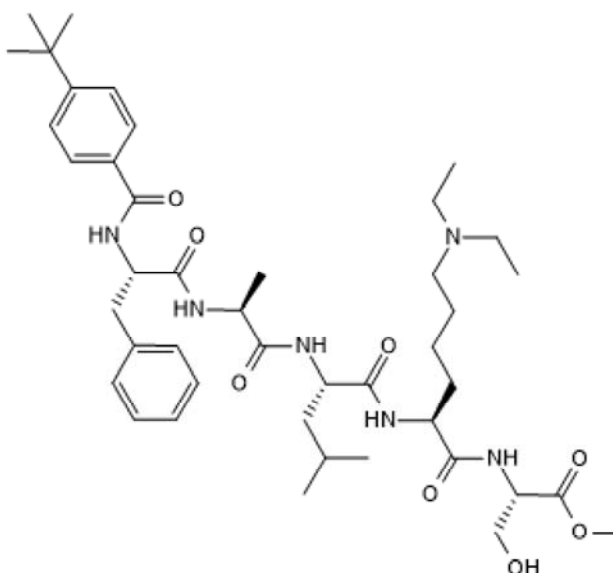
Batch No.: 1

CAS Number: 1872382-47-2

IUPAC Name: *N*-[4-(1,1-Dimethylethyl)benzoyl]-L-phenylalanyl-L-alanyl-L-leucyl-*N,N*-diethyl-L-lysyl-L-serine methyl ester

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₄₃H₆₆N₆O₈ · 1.67H₂O
Batch Molecular Weight: 825.06
Physical Appearance: White solid
Solubility: DMSO to 100 mM
 ethanol to 20 mM with gentle warming
Storage: Store at -20°C
Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 93.5% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	62.61	8.47	10.19
Found	62.34	8.12	10.58

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

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Description:

High affinity CBX4 and CBX7 inhibitor (K_i values are 94 and 97 nM, respectively). Exhibits >6-fold selectivity for CBX4/7 over other CBX and CDY family members. Inhibits proliferation of PC3 cells in vitro.

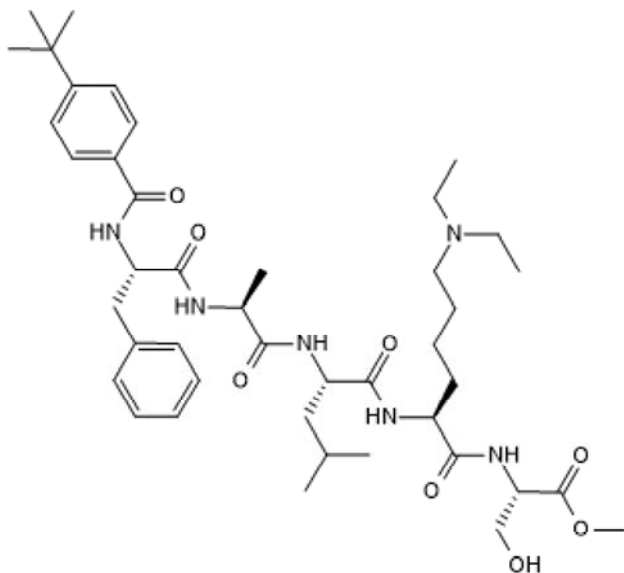
Physical and Chemical Properties:

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Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM

ethanol to 20 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:

Barnash et al (2016) Chromodomain ligand optimization via target-class directed combinatorial repurposing. *ACS Chem.Biol.* **11** 2475. PMID: 27356154.

Stuckey et al (2016) Structure-activity relationships and kinetic studies of peptidic antagonists of CBX chromodomains. *J.Med.Chem.* **59** 8913. PMID: 27571219.

Stuckey et al (2016) A cellular chemical probe targeting the chromodomains of Polycomb repressive complex 1. *Nat.Chem.Biol.* **12** 180. PMID: 26807715.

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