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: C_{43}H_{66}N_{6}O_{8}.1.67H_{2}O

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:

![Chemical Structure](image)

2. ANALYTICAL DATA

HPLC: Shows 93.5% purity

^1^H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

<table>
<thead>
<tr>
<th></th>
<th>Carbon</th>
<th>Hydrogen</th>
<th>Nitrogen</th>
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<td>Theoretical</td>
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<td>8.47</td>
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<td>8.12</td>
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</table>

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use
Description:
High affinity CBX4 and CBX7 inhibitor (K 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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Batch Molecular Weight: 825.06
Physical Appearance: White solid

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: