Certificate of Analysis

Product Name: **CU CPT 4a** **Catalog No.: 4883** **Batch No.: 2**

CAS Number: 1279713-77-7

IUPAC Name: *N*-[(3-Chloro-6-fluorobenzo[*b*]thien-2-yl)carbonyl]-D-phenylalanine

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{18}H_{13}ClFNO_3S$

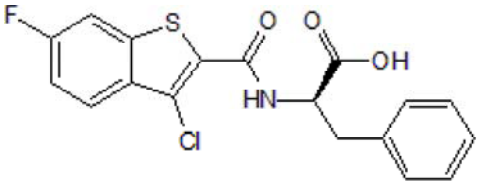
Batch Molecular Weight: 377.82

Physical Appearance: White solid

Solubility: DMSO to 100 mM

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.5 (Chloroform:Methanol [9:1])

HPLC: Shows 100% purity

Chiral HPLC: Shows 100% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: $[\alpha]_D$ = -20.8 (Concentration = .37, Solvent = Chloroform)

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	57.22	3.47	3.71
Found	57.19	3.55	3.6

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Description:

Selective TLR3 inhibitor (IC_{50} = 3.44 µM in RAW 264.7 cells); suppresses downstream signaling pathways mediated by the TLR3/dsRNA complex, inhibiting TNF-α and IL-1β production in whole cells. Reduces death of crypt cells and improves gastrointestinal syndrome in mice.

Physical and Chemical Properties:

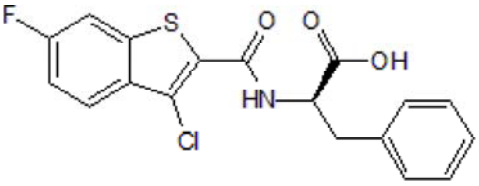
Batch Molecular Formula: $C_{18}H_{13}ClFNO_3S$

Batch Molecular Weight: 377.82

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at +4°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. 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.

Licensing Information:

Sold under license from the University of Colorado

References:

Takemura *et al* (2014) Blockade of TLR3 protects mice from lethal radiation-induced gastrointestinal syndrome. Nat.Commun. ***18***. PMID: 24637670 .

Cheng *et al* (2011) Small-molecule inhibitors of the TLR3/dsRNA complex. J.Am.Chem.Soc. ***133*** 3764. PMID: 21355588.