

Certificate of Analysis

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Product Name: Santacruzamate A

Catalog No.: 7191

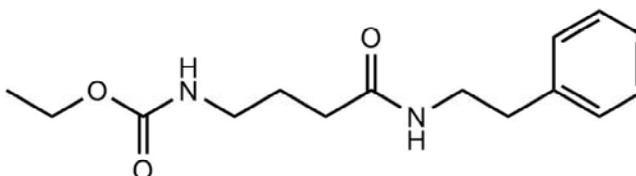
Batch No.: 1

CAS Number: 1477949-42-0

IUPAC Name: Ethyl N-[4-oxo-4-[(2-phenylethyl)amino]butyl]carbamate

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₅H₂₂N₂O₃
Batch Molecular Weight: 278.35
Physical Appearance: White solid
Solubility: DMSO to 100 mM
Storage: Store at -20°C
Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.7% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	64.73	7.97	10.06
Found	64.44	8.09	10.1

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

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Batch No.: 1

CAS Number: 1477949-42-0

IUPAC Name: Ethyl N-[4-oxo-4-[(2-phenylethyl)amino]butyl]carbamate

Description:

Highly potent and selective histone deacetylase 2 (HDAC2) inhibitor (IC₅₀ = 112 - 119 pM). Also inhibits HDAC6 in nanomolar range (IC₅₀ = 433 nM). Displays >3500 fold selectivity for HDAC2 over HDAC6, and >8500-fold selectivity over HDAC4 (IC₅₀ >1 μM for HDAC4). Inhibits growth of HuT-78 cutaneous T-cell lymphoma cell line. Identified as targeting human host proteins that interact with SARS-CoV-2.

Physical and Chemical Properties:

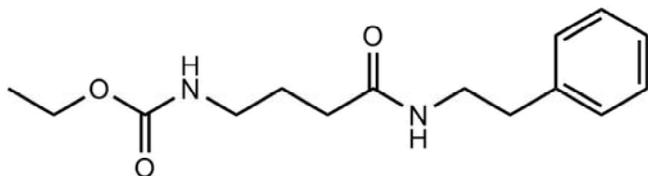
Batch Molecular Formula: C₁₅H₂₂N₂O₃

Batch Molecular Weight: 278.35

Physical Appearance: White solid

Minimum Purity: ≥98%

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°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:

Gordon et al (2020) A SARS-CoV-2 protein interaction map reveals targets for drug repurposing. *Nature*. **583** 459. PMID: 32353859.

Pavlik et al (2013) Santacruzamate A, a potent and selective histone deacetylase inhibitor from the Panamanian marine cyanobacterium cf. *Symploca* sp. *J.Nat.Prod.* **76** 2026. PMID: 24164245.

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