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### **Certificate of Analysis**

### www.tocris.com

Print Date: Mar 22nd 2023

#### Product Name: Ac-Cys-NHMe

CAS Number: 10061-65-1 IUPAC Name: (2R)-2-(Acetylamino)-3-mercapto-N-methylpropanamide

### 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula: Batch Molecular Weight: Physical Appearance:** Solubility:

 $C_6H_{12}N_2O_2S$ 176.23 White solid DMSO to 100 mM water to 100 mM Store at -20°C

Storage: **Batch Molecular Structure:** 

41.07

6.9

15.79

#### 2. ANALYTICAL DATA

<sup>1</sup>H NMR: Consistent with structure Mass Spectrum: Consistent with structure  $[\alpha]_D = -19.7$  (Concentration = 1, Solvent = Water) **Optical Rotation: Microanalysis:** Carbon Hydrogen Nitrogen Theoretical 40.89 6.86 15.9

Found

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

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Catalog No.: 7936 Batch No.: 2

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#### Product Name: Ac-Cys-NHMe

CAS Number: 10061-65-1

IUPAC Name: (2R)-2-(Acetylamino)-3-mercapto-N-methylpropanamide

#### **Description:**

Ac-Cys-NHMe is a non-canonical amino acid that is an essential building block for lysine acylation using conjugating enzymes (LACE) technique. LACE is a chemoenzymatic approach that uses an E2 small ubiquitin-like modifier (SUMO)-conjugating enzyme, Ubc9, to conjugate peptide thioesters containing a C-terminal ubiquitin-derived sequence (LRLRGG) to a lysine residue located in a recognition sequence (IKQE) on a protein via an isopeptide bond. Ac-Cys-NHMe can be reacted with a peptide hydrazide to form a reactive peptide thioester, which is the substrate for Ubc9. LACE enables the site-specific modification of proteins at lysine residues to all... Please see product specific page on www.tocris.com for full description.

#### **Physical and Chemical Properties:**

Batch Molecular Formula: C<sub>6</sub>H<sub>12</sub>N<sub>2</sub>O<sub>2</sub>S Batch Molecular Weight: 176.23 Physical Appearance: White solid

#### **Batch Molecular Structure:**

### **Storage:** Store at -20°C. This product is packaged under an inert atmosphere.

Catalog No.: 7936

#### Solubility & Usage Info:

DMSO to 100 mM water 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:**

Levasseur *et al* (2022) Post-assembly modification of protein cages by Ubc9-mediated lysine acylation. Chembiochem **23** e202200332. PMID: 35951442.

**Hofmann** *et al* (2020) Lysine acylation using conjugating enzymes for site-specific modification and ubiquitination of recombinant proteins. Nat.Chem. **12** 1008. PMID: 32929246.

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