Print Date: May 23rd 2022

Certificate of Analysis

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Product Name: **EDA-DA** **Catalog No.: 7714** **Batch No.: 1**

CAS Number: 87156-01-2

IUPAC Name: *N*-(4,4,5,5-Tetradehydro-D-norvalyl)-D-alanine trifluoroacetate

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_8H_{12}N_2O_3.CF_3CO_2H.$

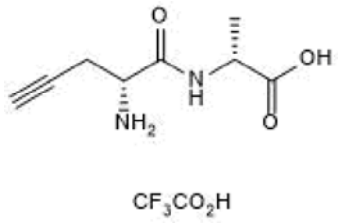
Batch Molecular Weight: 298.22

Physical Appearance: White solid

Solubility: DMSO to 100 mM
water to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.4% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	40.28	4.39	9.39
Found	40.51	4.41	9.33

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Description:

EDA-DA is an unnatural dipeptide building block (an ethynyl-D-alanine and a D-alanine). It incorporates a biorthogonal alkyne group into peptidoglycan (PG) through MurF in the cytoplasmic pathway, which enables selective labeling via a click-chemistry reaction. EDA-DA allows labeling of PG in Gram-positive (B. subtilis), Gram-negative (E. coli and C. trachomatis), Mycobacterium (M. smegmatis) and moss plastids (P. patens) with azide modified fluorescent dyes such as Alexa Fluor 488.

Physical and Chemical Properties:

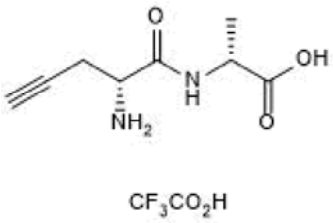
Batch Molecular Formula: $C_8H_{12}N_2O_3.CF_3CO_2H$.

Batch Molecular Weight: 298.22

Physical Appearance: White solid

Minimum Purity: ≥95%

Batch Molecular Structure:



Storage: Store at -20°C

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:

Banahene *et al* (2022) Chemical reporters for bacterial glycans: development and applications. Chem.Rev. ***122*** (3) 3336. PMID: 34905344.

Kuru *et al* (2019) Mechanisms of incorporation for D-amino acid probes that target peptidoglycan biosynthesis. ACS Chem.Biol. ***14*** (12) 2745. PMID: 31743648.

Hirano *et al* (2016) Moss chloroplasts are surrounded by a peptidoglycan wall containing D-amino acids. Plant Cell ***28*** (7) 1521. PMID: 27325639.