biotechne[®] TOCRIS

IUPAC Name:

Batch No.: 2

Certificate of Analysis

www.tocris.com

Catalog No.: 7860

Product Name: sBADA

CAS Number: 2376838-11-6

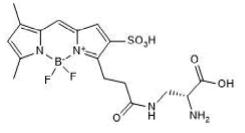
(*R*)-2-Amino-3-(3-(5,5-difluoro-7,9-dimethyl-2-sulfo-5*H*-4λ⁴,5λ⁴-dipyrrolo[1,2-c:2',1'-f][1,3,2]diazaborinin-3-yl) propanamido)propanoic acid

1. PHYSICAL AND CHEMICAL PROPERTIES

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

Batch Molecular Structure:

 $C_{17}H_{21}BF_2N_4O_6S$ 458.24 Brown solid DMSO to 10 mM Store at -20°C



2. ANALYTICAL DATA

HPLC: ¹H NMR: Mass Spectrum: UV Spectrum: λ_{max} : λ_{ex} : λ_{em} : Shows 94.9% purity at 491 nm Consistent with structure Consistent with structure Consistent with structure 490 nm (pbs) 490 nm (pbs) 505 nm (pbs)

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

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Print Date: Mar 3rd 2025

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Product Name: sBADA

CAS Number: 2376838-11-6

(*R*)-2-Amino-3-(3-(5,5-difluoro-7,9-dimethyl-2-sulfo-5*H*- $4\lambda^4$, $5\lambda^4$ -dipyrrolo[1,2-*c*:2',1'-*f*][1,3,2]diazaborinin-3-yl) propanamido)propanoic acid

Description:

IUPAC Name:

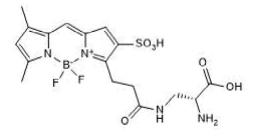
sBADA is a green sulfonated BODIPY-FL 3-amino-D-alanine (sBADA) or fluorescent D-amino acid (FFDA). Labels peptidoglycans in live bacteria. Sulfonated form of BADA with increased hydrophilicity and thermostability. Excitation/emission $\lambda \sim$ 490/510 nm.

Physical and Chemical Properties:

Batch Molecular Formula: C₁₇H₂₁BF₂N₄O₆S Batch Molecular Weight: 458.24 Physical Appearance: Brown solid

Minimum Purity: ≥95%

Batch Molecular Structure:



Storage: Store at -20°C

CAUTION - This product is light sensitive and we recommend that the solid material and any solutions obtained are protected from exposure to light.

Catalog No.: 7860

Solubility & Usage Info:

DMSO to 10 mM

This product is supplied in lyophilized form. It may appear as a solid, gel or film and be very hard to visualize. Solutions should be made by adding solvent directly to the vial. The vial should then be vortexed vigorously to ensure the product has completely dissolved.

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. *Unless contradicted by product-specific protocols or instructions, our standard recommendations apply:

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:

Hsu et al (2017) Full color palette of fluorescent d-amino acids for in situ labeling of bacterial cell walls. Chem.Sci. 8 6313. PMID: 28989665.

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