Certificate of Analysis

www.tocris.com

Print Date: Feb 13th 2023

Product Name: HADA

a biotechne

Catalog No.: 6647 Batch

Batch No.: 2

CAS Number: IUPAC Name: 2253733-10-5

3-[[(7-Hydroxy-2-oxo-2H-1-benzopyran-3-yl)carbonyl]amino]-D-alanine hydrocholoride

1. PHYSICAL AND CHEMICAL PROPERTIES

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

Batch Molecular Structure:

 $C_{13}H_{12}N_2O_6.HCI.H_2O$ 346.73 White solid DMSO to 100 mM Store at -20°C



2. ANALYTICAL DATA

HPLC:	Shows 99.9% purity at 405 nm			
¹ H NMR:	Consistent with structure			
Mass Spectrum:	Consistent with structure			
UV Spectrum:	Consistent with structure			
λ _{max} :	405 nm (PBS)			
λ _{ex} :	405 nm (PBS)			
λ _{em} :	448 nm (PBS)			
Optical Rotation:	$[\alpha]_D$ = -1.7 (Concentration = 2, Solvent = DMSO)			
Microanalysis:	Carbon Hydrogen Nitrogen			
	Theoretical 45.03 4.36 8.08			
	Found 44.41 4.11 7.8			

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

bio-techne.com	North America	China	Europe Middle East Africa	Rest of World
info@bio-techne.com techsupport@bio-techne.com	Tel: (800) 343 7475	info.cn@bio-techne.com Tel: +86 (21) 52380373	Tel: +44 (0)1235 529449	www.tocris.com/distributors Tel:+1 612 379 2956

TOCRIS a biotechne brand

Product Information

Print Date: Feb 13th 2023

2

Product Name: HADA

CAS Number: 2253733-10-5

3-[[(7-Hydroxy-2-oxo-2H-1-benzopyran-3-yl)carbonyl]amino]-D-alanine hydrocholoride

Description:

IUPAC Name:

HADA is a fluorescent D-amino acid. Suitable for labeling peptidoglycans in live bacteria. Results in strong peripheral and septal labeling of diverse bacterial cell populations without affecting growth rates. Displays mitochondrial outer membrane permeability. Excitation/emission $\lambda \sim 405/450$ nm.

Physical and Chemical Properties:

Batch Molecular Formula: C₁₃H₁₂N₂O₆.HCl.H₂O Batch Molecular Weight: 346.73 Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



References:

Botella *et al* (2017) Distinct spatiotemporal dynamics of peptidoglycan synthesis between *Mycobacterium smegmatis* and *Mycobacterium tuberculosis*. Mbio. *8* e01183. PMID: 28900018.

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.

Kuru et al (2012) In Situ probing of newly synthesized peptidoglycan in live bacteria with fluorescent D-amino acids. Angew.Chem.Int.Ed. 51 12519. PMID: 23055266.

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

bio-techne.com	North America	China	Europe Middle East Africa	Rest of World
info@bio-techne.com techsupport@bio-techne.com	Tel: (800) 343 7475	info.cn@bio-techne.com Tel: +86 (21) 52380373	Tel: +44 (0)1235 529449	www.tocris.com/distributors Tel:+1 612 379 2956

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.: 6647

Solubility & Usage Info:

DMSO to 100 mM Solutions in DMSO may appear hazy.

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.