bio-techne
TOCRIS

Print Date: Jun 12th 2024

Certificate of Analysis

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Product Name: **BTD S-sulfenic acid probe** **Catalog No.: 8059** **Batch No.: 1**

CAS Number: 2095485-22-4

IUPAC Name: 1-(4-Pentyn-1-yl)-1*H*-2,1-benzothiazin-4(3*H*)-one 2,2-dioxide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{13}H_{13}NO_3S$.

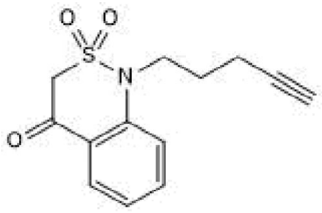
Batch Molecular Weight: 263.31

Physical Appearance: Off White solid

Solubility: DMSO to 100 mM
ethanol to 20 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 98.9% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	59.3	4.98	5.32
Found	59.2	4.96	5.26

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Description:

BTD S-sulfenic acid probe is a nucleophilic fragment that can selectively modify sulfenic acid residues in proteins, and can be used as a tool to identify ligandable S-sulfenation sites. Covalently modifies oxidized cysteines on proteins. Quantitatively labels hyper-reactive sulfenic acids at low BTD concentrations, less reactive sites exhibit concentration-dependent increases in probe labeling. Incorporates an alkyne handle for click chemistry and chemoproteomic profiling.

Physical and Chemical Properties:

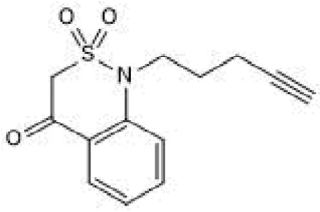
Batch Molecular Formula: $C_{13}H_{13}NO_3S$.

Batch Molecular Weight: 263.31

Physical Appearance: Off White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM
ethanol to 20 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. *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:

Fu *et al* (2023) Nucleophilic covalent ligand discovery for the cysteine redoxome. Nat.Chem.Biol. ***19*** 1309. PMID: 37248412.

Gupta *et al* (2017) Diverse redoxome reactivity profiles of carbon nucleophiles. J.Am.Chem.Soc. ***139*** 5588. PMID: 28355876.