



# **Certificate of Analysis**

www.tocris.com

Product Name: BromoTag® AGB1 Catalog No.: 7686 Batch No.: 1

CAS Number: 2776190-62-4

IUPAC Name: (S)-13-((2S,4R)-4-Hydroxy-2-((4-(4-methylthiazol-5-yl)benzyl)carbamoyl)pyrrolidine-1-carbonyl)-14,14-dimethyl-11-

oxo-3,6,9-trioxa-12-azapentadecyl (R)-2-((S)-4-(4-chlorophenyl)-2,3,9-trimethyl-6H-thieno[3,2-f][1,2,4]triazolo[4,3-a]

[1,4]diazepin-6-yl)butanoate

## 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:**  $C_{51}H_{63}CIN_8O_9S_2.H_2O$ 

Batch Molecular Weight: 1049.7

Physical Appearance: Off White solid

Solubility: DMSO to 100 mM

Storage: Store at -20°C

**Batch Molecular Structure:** 

#### 2. ANALYTICAL DATA

**HPLC:** Shows 99.5% purity

<sup>1</sup>H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 58.36 6.24 10.68 Found 58.05 6.26 10.6

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

# **Product Information**

Print Date: Nov 14th 2022

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oxo-3,6,9-trioxa-12-azapentadecyl (R)-2-((S)-4-(4-chlorophenyl)-2,3,9-trimethyl-6H-thieno[3,2-f][1,2,4]triazolo[4,3-a]

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#### **Description:**

BromoTag® AGB1 is a highly selective and potent "Bump & Hole" TAG Degrader (DC $_{50,6h}$  < 15 nM,  $t_{1/2}$  for protein degradation = 40 min). BromoTag AGB1 comprises a VHL E3 ligase ligand joined by a linker to a (+)-JQ1 (Cat. No. 4499) derivative (the "bump" bearer) that selectively binds the Brd4BD2 L387A variant (the "hole"). In cell lines expressing a fusion of the target protein with the tag, Brd4BD2 L387A, BromoTag AGB1 drives formation of a ternary complex between VHL and the "BromoTagged" protein, leading to ubiquitination of the protein and its subsequent proteasomal degradation. BromoTag... Please see product specific page on www.tocris.com for full description.

## **Physical and Chemical Properties:**

Batch Molecular Formula: C<sub>51</sub>H<sub>63</sub>CIN<sub>8</sub>O<sub>9</sub>S<sub>2</sub>.H<sub>2</sub>O

Batch Molecular Weight: 1049.7 Physical Appearance: Off White solid

**Minimum Purity:** ≥98%

# **Batch Molecular Structure:**

Storage: Store at -20°C

## Solubility & Usage Info:

DMSO 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.

#### **Licensing Information:**

Sold under exclusive licence from the University of Dundee

References:

**Bond** *et al* (2021) Development of BromoTag: a 'Bump-and-Hole'-PROTAC system to induce potent, rapid, and selective degradation of tagged target proteins. J.Med.Chem. *64* 15477. PMID: 34652918.

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