

**Product Name:** BromoTag® AGB3

**Catalog No.:** 7688

**Batch No.:** 1

CAS Number: 2776191-07-0

IUPAC Name: (2*S*,4*R*)-1-((2*S*,17*R*)-2-(*tert*-Butyl)-17-((*S*)-4-(4-chlorophenyl)-2,3,9-trimethyl-6*H*-thieno[3,2-*f*][1,2,4]triazolo[4,3-*a*][1,4]diazepin-6-yl)-4,16-dioxo-6,9,12-trioxa-3,15-diazanonadecanoyl)-4-hydroxy-*N*-(4-(4-methylthiazol-5-yl)benzyl)pyrrolidine-2-carboxamide

## 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>51</sub>H<sub>64</sub>ClN<sub>9</sub>O<sub>8</sub>S<sub>2</sub>·2H<sub>2</sub>O

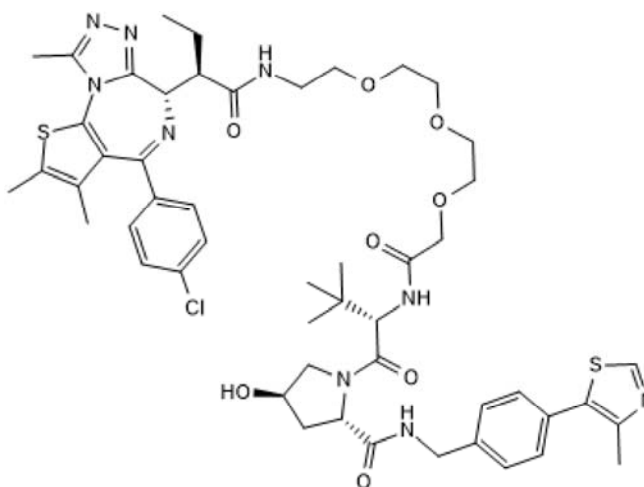
**Batch Molecular Weight:** 1066.73

**Physical Appearance:** White solid

**Solubility:** DMSO to 100 mM

**Storage:** Store at -20°C

**Batch Molecular Structure:**



## 2. ANALYTICAL DATA

**HPLC:** Shows 98.4% purity

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

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	57.42	6.43	11.82
Found	57.1	6.31	11.47

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**1**

CAS Number: 2776191-07-0

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**Description:**

BromoTag® AGB3 is a selective "Bump & Hole" TAG Degrader (DC<sub>50</sub> 210 - 290 nM, protein degradation t<sub>1/2</sub> = 113 min, D<sub>max</sub> = 92%). BromoTag AGB3 comprises a VHL E3 ligase ligand joined by a linker to a (+)-JQ1 (Cat. No. 4499) derivative (the "bump" bearer) that selectively binds the Brd4<sup>BD2 L387A</sup> variant (the "hole"). In cell lines expressing a fusion of the target protein with the tag, Brd4<sup>BD2 L387A</sup>, BromoTag AGB3 drives formation of a ternary complex between VHL and the "BromoTagged" protein, leading to ubiquitination of the protein and its subsequent proteasomal degradation. BromoTag® is a reg... Please see product specific page on www.tocris.com for full description.

**Physical and Chemical Properties:**

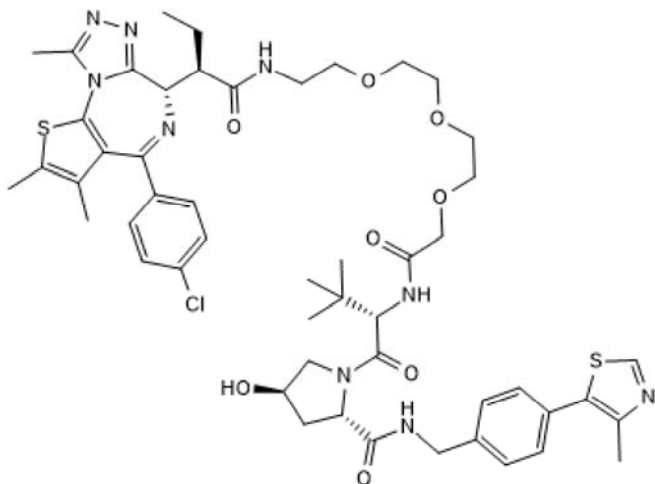
Batch Molecular Formula: C<sub>51</sub>H<sub>64</sub>ClN<sub>9</sub>O<sub>8</sub>S<sub>2</sub>·2H<sub>2</sub>O

Batch Molecular Weight: 1066.73

Physical Appearance: White solid

**Minimum Purity:** ≥98%

**Batch Molecular Structure:**



**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.

**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

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