

**Product Name:** BAY 299

**Catalog No.:** 5970

**Batch No.:** 3

CAS Number: 2080306-23-4

IUPAC Name: 6-(3-Hydroxypropyl)-2-(1,3,6-trimethyl-2-oxo-2,3-dihydro-1*H*-benzimidazol-5-yl)-1*H*-benzo[*de*]isoquinoline-1,3(2*H*)-dione

## 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>25</sub>H<sub>23</sub>N<sub>3</sub>O<sub>4</sub>·½H<sub>2</sub>O

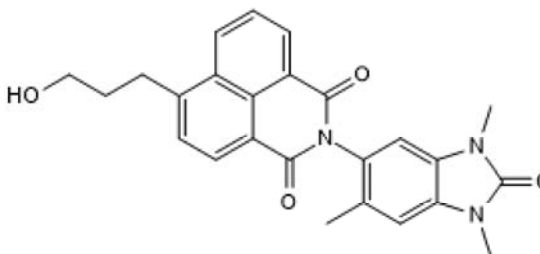
**Batch Molecular Weight:** 438.48

**Physical Appearance:** Pale yellow solid

**Solubility:** DMSO to 100 mM

**Storage:** Store at -20°C

**Batch Molecular Structure:**



## 2. ANALYTICAL DATA

**HPLC:** Shows 98.8% purity

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

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	68.48	5.52	9.58
Found	68.17	5.28	9.59

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**bio-techne.com**

info@bio-techne.com

techsupport@bio-techne.com

**North America**

Tel: (800) 343 7475

**China**

info.cn@bio-techne.com

Tel: +86 (21) 52380373

**Europe Middle East Africa**

Tel: +44 (0)1235 529449

**Rest of World**

www.tocris.com/distributors

Tel: +1 612 379 2956

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**3**

CAS Number: 2080306-23-4

IUPAC Name: 6-(3-Hydroxypropyl)-2-(1,3,6-trimethyl-2-oxo-2,3-dihydro-1H-benzimidazol-5-yl)-1H-benzo[de]isoquinoline-1,3(2H)-dione

**Description:**

BAY 299 is a potent and selective BRD1 and TAF1 inhibitor (IC<sub>50</sub> values are 6-67 and 8-13 nM, respectively). Displays selectivity over other bromodomains (>30-fold over other members of the BRPF family; BRD9 and ATAD2; >300-fold over BRD4). Displays BRD1 and TAF1 inhibition in a NanoBRET cell assay. Inhibits binding of BRD1 and TAF1 to histone H4 (IC<sub>50</sub> values are 575 nM and 0.9 μM, respectively) and histone H3.3 (IC<sub>50</sub> values are 825 nM and 1.4 μM, respectively).

**Physical and Chemical Properties:**

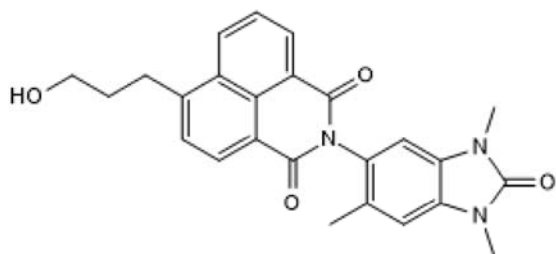
Batch Molecular Formula: C<sub>25</sub>H<sub>23</sub>N<sub>3</sub>O<sub>4</sub>·½H<sub>2</sub>O

Batch Molecular Weight: 438.48

Physical Appearance: Pale yellow solid

**Minimum Purity:** ≥98%

**Batch Molecular Structure:**



**References:**

**Bouche et al** (2017) Benzoisoquinolinediones as potent and selective inhibitors of BRPF2 and TAF1/TAF1L bromodomains. *J.Med.Chem.* **60** 4002. PMID: 28402630.

**Klein et al** (2014) Crosstalk between epigenetic readers regulates the MOZ/MORF HAT complexes. *Epigenetics* **9** 186. PMID: 24169304.

**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:**

This probe is supplied in conjunction with the Structural Genomics Consortium. For further characterization details, please visit the BAY 299 probe summary on the SGC website.

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