Print Date: Feb 26th 2020

Certificate of Analysis

www.tocris.com

Product Name: **BAY 299** **Catalog No.: 5970** **Batch No.: 2**

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: $C_{25}H_{23}N_3O_4.¼H_2O$

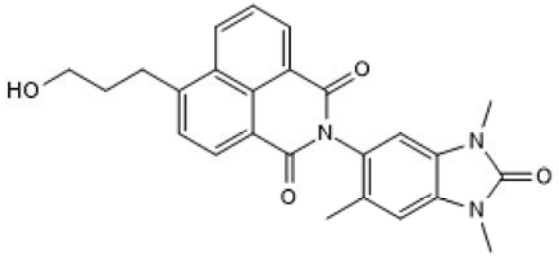
Batch Molecular Weight: 433.97

Physical Appearance: Pale yellow solid

Solubility: DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.4% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	69.19	5.46	9.68
Found	69.27	5.44	9.77

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Description:

Potent and selective BRD1 and TAF1 inhibitor (IC_{50} 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_{50} values are 575 nM and 0.9 µM, respectively) and histone H3.3 (IC_{50} values are 825 nM and 1.4 µM, respectively).

Physical and Chemical Properties:

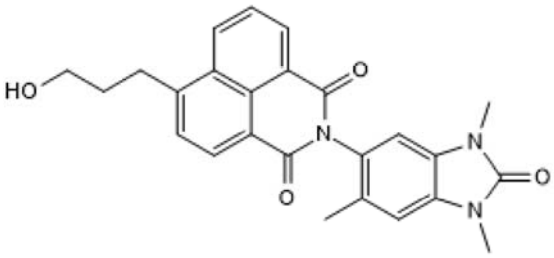
Batch Molecular Formula: $C_{25}H_{23}N_3O_4.¼H_2O$

Batch Molecular Weight: 433.97

Physical Appearance: Pale yellow 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:

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.

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.