TOCRIS
a bio-techne brand

Print Date: Oct 12th 2022

Certificate of Analysis

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Product Name: **BAY 1816032** **Catalog No.: 7549** **Batch No.: 1**

CAS Number: 1891087-61-8

IUPAC Name: 2-[3,5-Difluoro-4-[[3-[5-methoxy-4-[(3-methoxy-4-pyridinyl)amino]-2-pyrimidinyl]-1*H*-indazol-1-yl]methyl]phenoxy] ethanol

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{27}H_{24}F_2N_6O_4.¼H_2O$

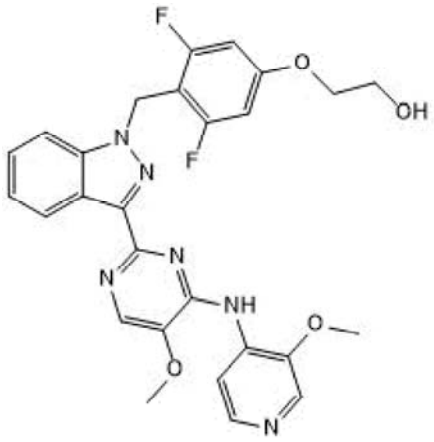
Batch Molecular Weight: 539.02

Physical Appearance: Off White solid

Solubility: DMSO to 50 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 100.0% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	60.16	4.58	15.59
Found	60.09	4.68	15.35

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Description:

BAY 1816032 is a potent and selective inhibitor of BUB1 kinase, a mitotic checkpoint serine/threonine kinase (IC_{50} = 6.1 nM). BAY 1816032 shows 17-fold selectivity over a panel of 403 other human kinases. In vivo, BAY 1816032 decreases tumor size in tumor xenograft models. BAY 181603 is orally bioavailable.

Physical and Chemical Properties:

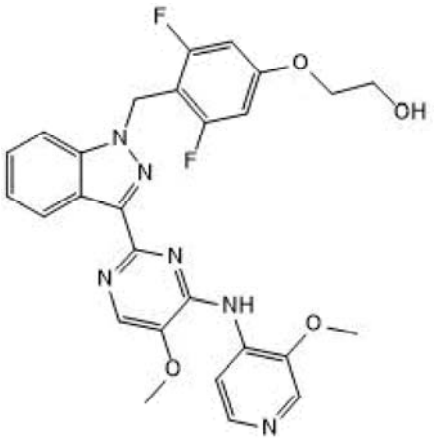
Batch Molecular Formula: $C_{27}H_{24}F_2N_6O_4.¼H_2O$

Batch Molecular Weight: 539.02

Physical Appearance: Off White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 50 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.

References:

Siemeister *et al* (2019) Inhibition of BUB1 kinase by BAY 1816032 sensitizes tumor cells toward taxanes, ATR, and PARP inhibitors *in vitro* and *in vivo*. Clin.Cancer Res. ***25*** 1404. PMID: 30429199.