

Product Name: AZ 3451

Catalog No.: 6806

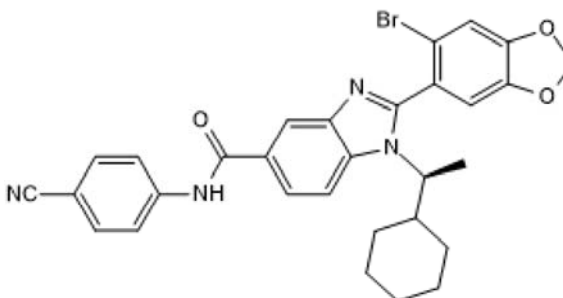
Batch No.: 1

CAS Number: 2100284-59-9

IUPAC Name: 2-(6-Bromo-1,3-benzodioxol-5-yl)-N-(4-cyanophenyl)-1-[(1S)-1-cyclohexylethyl]-1H-benzimidazole-5-carboxamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₃₀H₂₇BrN₄O₃
Batch Molecular Weight: 571.46
Physical Appearance: Brown solid
Solubility: DMSO to 100 mM
 ethanol to 100 mM
Storage: Store at -20°C
Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 98.3% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	63.05	4.76	9.8
Found	62.66	4.86	9.63

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

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Description:

Potent negative allosteric modulator of PAR₂ (IC₅₀ = 23 nM); binds to a remote allosteric site outside the helical bundle. Inhibits ERK phosphorylation in 1321N1 cells overexpressing wild-type human PAR₂. Highly lipophilic.

Physical and Chemical Properties:

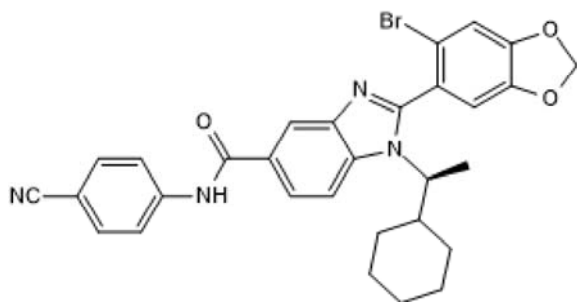
Batch Molecular Formula: C₃₀H₂₇BrN₄O₃

Batch Molecular Weight: 571.46

Physical Appearance: Brown solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM
ethanol 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.

References:

Cheng *et al* (2017) Structural insight into allosteric modulation of protease-activated receptor 2. *Nature* **545** 112. PMID: 28445455.

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