

Product Name: C3

Catalog No.: 5957

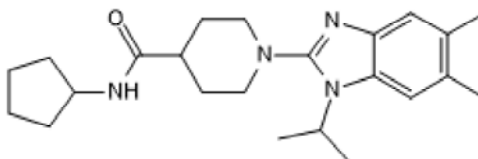
Batch No.: 1

CAS Number: 1268709-57-4

IUPAC Name: *N*-Cyclopentyl-1-[5,6-dimethyl-1-(1-methylethyl)-1*H*-benzimidazol-2-yl]-4-piperidinecarboxamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₃H₃₄N₄O
Batch Molecular Weight: 382.54
Physical Appearance: White solid
Solubility: DMSO to 50 mM
ethanol to 100 mM
Storage: Store at -20°C
Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.4% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	72.21	8.96	14.65
Found	72.05	9	14.58

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

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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IUPAC Name: *N*-Cyclopentyl-1-[5,6-dimethyl-1-(1-methylethyl)-1*H*-benzimidazol-2-yl]-4-piperidinecarboxamide

Description:

Selective microsomal prostaglandin E synthase 1 (mPGES-1) inhibitor (IC₅₀ values are 90 and 900 nM for rat and human mPGES-1, respectively). Displays selectivity for mPGES-1 over COX-1, COX-2, PGIS, hPGDS and iPGDS (% inhibition values are 15, 18, 0, 0 and 60 % inhibition at 50 μM, respectively). Reduces PGE₂ production in vitro and in a localized inflammation animal model. Elevates CD80 expression by tumor associated phagocytes in vitro. Also decreases vascular contractility, in ex vivo human vessels.

Physical and Chemical Properties:

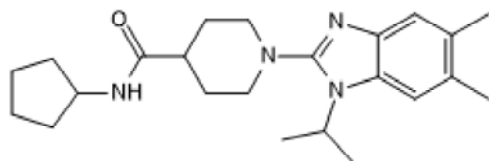
Batch Molecular Formula: C₂₃H₃₄N₄O

Batch Molecular Weight: 382.54

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 50 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:

Ozen et al (2017) Inhibition of microsomal PGE synthase-1 reduces human vascular tone by increasing PGI₂: a safer alternative to COX-2 inhibition. *Br.J.Pharmacol* **174** 4087. PMID: 28675448.

Olesch et al (2015) MPGES-1-derived PGE₂ suppresses CD80 expression on tumor-associated phagocytes to inhibit anti-tumor immune responses in breast cancer. *Oncotarget* **6** 10284. PMID: 25871398.

Leclerc et al (2013) Characterization of a human and murine mPGES-1 inhibitor and comparison to mPGES-1 genetic deletion in mouse models of inflammation. *Prostaglandins Other Lipid Mediat.* **107** 26. PMID: 24045148.

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