

Product Name: BMS 265246

Catalog No.: 5654

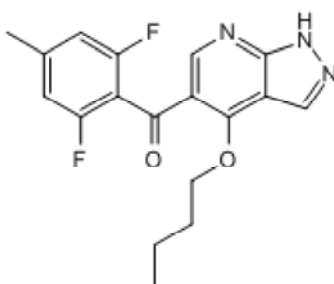
Batch No.: 1

CAS Number: 582315-72-8

IUPAC Name: (4-Butoxy-1*H*-pyrazolo[3,4-*b*]pyridin-5-yl) (2,6-difluoro-4-methylphenyl)methanone

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₈H₁₇F₂N₃O₂
Batch Molecular Weight: 345.34
Physical Appearance: White solid
Solubility: DMSO to 50 mM
Storage: Store at -20°C
Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 97.4% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	62.6	4.96	12.17
Found	62.51	5.06	11.8

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

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Description:

Potent cyclin-dependent kinase 1 (cdk1) and cdk 2 inhibitor (IC₅₀ values are 5.6 - 71 and 6 - 14 nM, respectively). Also inhibits cdk4 and cdk5 in the sub micromolar range and cdk7 and cdk9 in the low micromolar range. Inhibits proliferation of HCT-116 colon cancer cells in vitro.

Physical and Chemical Properties:

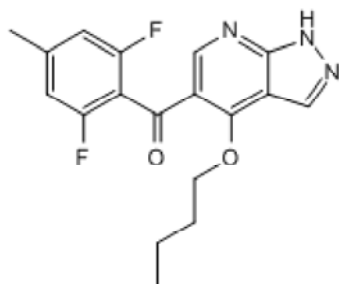
Batch Molecular Formula: C₁₈H₁₇F₂N₃O₂

Batch Molecular Weight: 345.34

Physical Appearance: White solid

Minimum Purity: >97%

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:

Jorda et al (2018) How selective are pharmacological inhibitors of cell-cycle-regulating cyclin-dependent kinases? *J.Med.Chem.* **61** 9105. PMID: 30234987.

Misra et al (2003) 1H-Pyrazolo[3,4-b]pyridine inhibitors of cyclin-dependent kinases: highly potent 2,6-Difluorophenacyl analogues. *Bioorg.Med.Chem.Lett.* **13** 2405. PMID: 12824044.

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