

Product Name: R 547

Catalog No.: 5494

Batch No.: 1

CAS Number: 741713-40-6

IUPAC Name: [4-Amino-2-[[1-(methylsulfonyl)-4-piperidiny]amino]-5-pyrimidinyl](2,3-difluoro-6-methoxyphenyl)methanone

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₈H₂₁F₂N₅O₄S

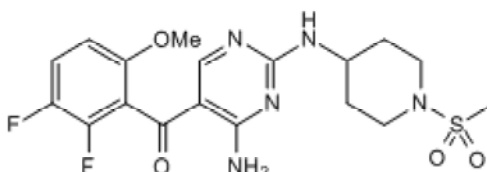
Batch Molecular Weight: 441.45

Physical Appearance: Off White solid

Solubility: DMSO to 100 mM

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.5 (Dichloromethane:Methanol [9:1])

HPLC: Shows 98.4% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	48.97	4.79	15.86
Found	49.15	4.82	15.62

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Description:

Potent and selective inhibitor of CDKs (K_i values are 1, 2, 3, 46, 171 and 260 nM for CDK4/cyclin D1, CDK1/cyclin B, CDK2/cyclin E, GSK3 α , CDK7/cyclin H and GSK3 β). Exhibits no effect against a panel of >120 other kinases ($K_i > 5,000$ nM). Inhibits the proliferation of tumor cell lines independent of multidrug resistant status, or p53 status. Suppresses retinoblastoma protein in tumor cells and xenografts, also inhibits tumor growth in the HCT116 human colorectal tumor xenograft model in nude mice. Orally bioavailable.

Physical and Chemical Properties:

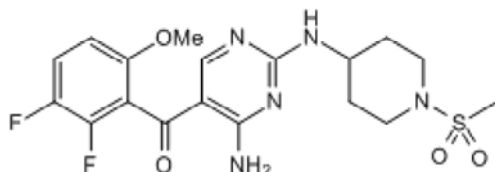
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Minimum Purity: >98%

Batch Molecular Structure:



References:

Chu et al (2006) Discovery of [4-Amino-2-(1-methanesulfonylpiperidin-4-ylamino)pyrimidin-5-yl](2,3-difluoro-6-methoxyphenyl)methanone (R547), a potent and selective cyclin-dependent kinase inhibitor with significant *in vivo* antitumor activity. *J. Med. Chem.* **49** 6549. PMID: 17064073.

DePinto et al (2006) *In vitro* and *in vivo* activity of R547: a potent and selective cyclin-dependent kinase inhibitor currently in phase I clinical trials. *Mol. Cancer Ther.* **5** 2644. PMID: 17121911.

Storage: Store at +4°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.

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