

Product Name: PF 477736

Catalog No.: 4277

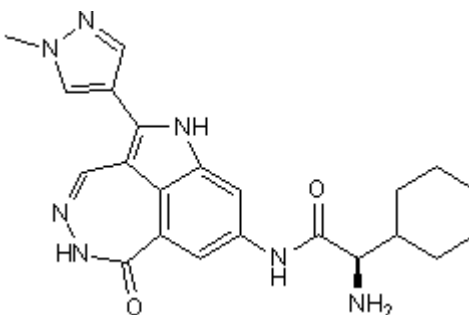
Batch No.: 1

CAS Number: 952021-60-2

IUPAC Name: (*R*)- α -Amino-*N*-[5,6-dihydro-2-(1-methyl-1*H*-pyrazol-4-yl)-6-oxo-1*H*-pyrrolo[4,3,2-*ef*][2,3]benzodiazepin-8-yl]-cyclohexaneacetamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₂H₂₅N₇O₂
Batch Molecular Weight: 419.48
Physical Appearance: Yellow solid
Solubility: DMSO to 75 mM
Storage: Store at +4°C
Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.8% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	62.99	6.01	23.37
Found	62.72	6.03	23.35

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

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Description:

Selective checkpoint kinase 1 (Chk1) inhibitor (K_i values are 0.49 and 47 nM for Chk1 and Chk2 respectively). Abrogates cell cycle arrest at S and G₂-M checkpoints; sensitizes cells to DNA damage. Enhances docetaxel (Cat. No. 4056) efficacy in tumor cells and xenografts.

Physical and Chemical Properties:

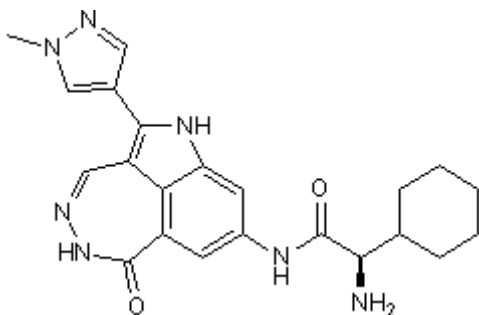
Batch Molecular Formula: C₂₂H₂₅N₇O₂

Batch Molecular Weight: 419.48

Physical Appearance: Yellow solid

Minimum Purity: >99%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 75 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:

Ashwell and Zabludoff (2008) DNA damage detection and repair pathways - recent advances with inhibitors of checkpoint kinases in cancer therapy. *Clin.Cancer Res.* **14** 4032. PMID: 18593978.

Blasina et al (2008) Breaching the DNA damage checkpoint via PF-00477736, a novel small-molecule inhibitor of checkpoint kinase 1. *Mol.Cancer Ther.* **7** 2394. PMID: 18723486.

Zhang et al (2009) PF-00477736 mediates checkpoint kinase 1 signaling pathways and potentiates docetaxel-induced efficacy in xenografts. *Clin.Cancer Res.* **15** 4630. PMID: 19584159.

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