

Product Name: NVS PAK1 C

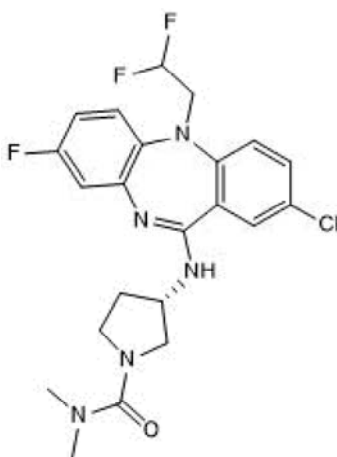
Catalog No.: 6133

Batch No.: 1

IUPAC Name: (3*S*)-3-(2-Chloro-5-(2,2-difluoroethyl)-8-fluoro-5*H*-dibenzo[*b,e*][1,4]diazepin-11-ylamino)-*N,N*-dimethylpyrrolidine-1-carboxamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₂H₂₃ClF₃N₅O
Batch Molecular Weight: 465.91
Physical Appearance: White solid
Solubility: DMSO to 100 mM
ethanol to 20 mM
Storage: Store at -20°C
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.25 (Ethyl acetate:Petroleum ether [1:1])
HPLC: Shows 99.3% purity
Chiral HPLC: Shows >99.9% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	56.72	4.98	15.03
Found	56.64	4.98	14.79

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

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Description:

Negative control of NVS PAK1 1 (Cat. No. 6132), a potent and selective PAK1 inhibitor.

Physical and Chemical Properties:

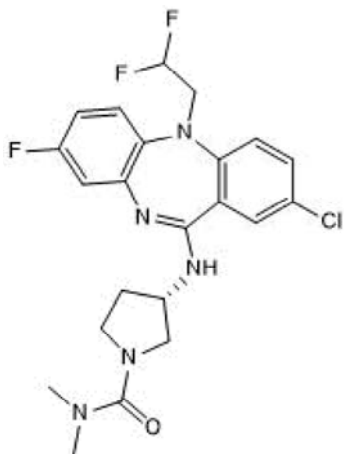
Batch Molecular Formula: C₂₂H₂₃ClF₃N₅O

Batch Molecular Weight: 465.91

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM

ethanol to 20 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.

Licensing Information:

This probe is supplied in conjunction with the Structural Genomics Consortium. For further characterization details, please visit the NVS PAK1 1 probe summary on the SGC website.

References:

Karpov et al (2015) Optimization of a dibenzodiazepine hit to a potent and selective allosteric PAK1 inhibitor. *ACS Med.Chem.Lett* **6** 776. PMID: 26191365.

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