

Product Name: NVS PAK1 1

Catalog No.: 6132

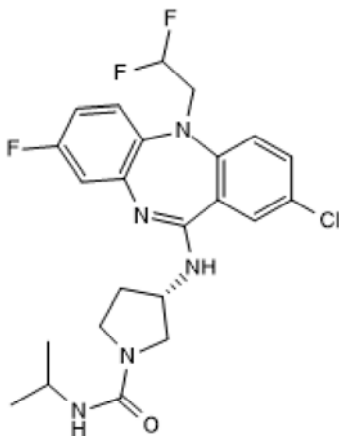
Batch No.: 1

CAS Number: 1783816-74-9

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

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula:	C ₂₃ H ₂₅ ClF ₃ N ₅ O
Batch Molecular Weight:	479.93
Physical Appearance:	Yellow solid
Solubility:	DMSO to 100 mM 1eq. HCl to 100 mM ethanol to 100 mM
Storage:	Store at -20°C
Batch Molecular Structure:	



2. ANALYTICAL DATA

TLC:	R _f = 0.2 (Ethyl acetate:Petroleum ether [1:1])
HPLC:	Shows 99.6% purity
Chiral HPLC:	Shows 99.77% purity
¹H NMR:	Consistent with structure
Mass Spectrum:	Consistent with structure
Microanalysis:	

	Carbon	Hydrogen	Nitrogen
Theoretical	57.56	5.25	14.59
Found	57.43	5.29	14.4

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

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Description:

NVS PAK1 1 is a potent and selective PAK1 inhibitor ($IC_{50} = 5$ nM) that displays selective for PAK1 over PAK2 and a panel of 442 kinases. NVS PAK1 1 inhibits autophosphorylation of PAK1 in KRAS-mutated pancreatic cancer cell lines. A negative control for NVS PAK1 1 is also available; NVS PAK1 C.

Physical and Chemical Properties:

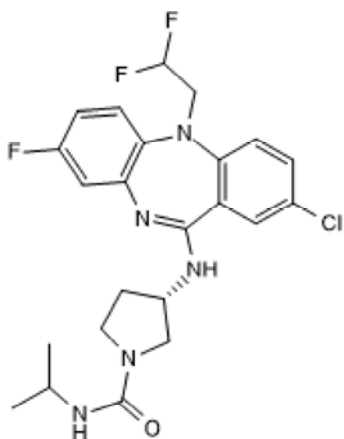
Batch Molecular Formula: $C_{23}H_{25}ClF_3N_5O$

Batch Molecular Weight: 479.93

Physical Appearance: Yellow solid

Minimum Purity: $\geq 98\%$

Batch Molecular Structure:



Storage: Store at $-20^{\circ}C$

Solubility & Usage Info:

DMSO to 100 mM
1eq. HCl to 100 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 $45-60^{\circ}C$ 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 $-20^{\circ}C$ 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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