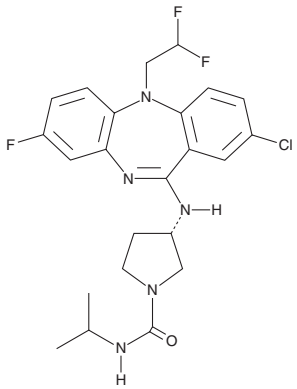
PRODUCT INFORMATION

NVS-PAK1-1

Item No. 19964



CAS Registry No.:	1783816-74-9
Formal Name:	(3S)-3-[[2-chloro-5-(2,2-difluoroethyl)-8-fluoro-5H-dibenzo[b,e][1,4]diazepin-11-yl]amino]-N-(1-methylethyl)-1-pyrrolidinecarboxamide
MF:	$C_{23}H_{25}ClF_3N_5O$
FW:	479.9
Purity:	≥98%
UV/Vis.:	λ_{max}: 264 nm
Supplied as:	A crystalline solid
Storage:	-20°C
Stability:	≥4 years

Information represents the product specifications. Batch specific analytical results are provided on each certificate of analysis.

Laboratory Procedures

NVS-PAK1-1 is supplied as a crystalline solid. A stock solution may be made by dissolving the NVS-PAK1-1 in the solvent of choice, which should be purged with an inert gas. NVS-PAK1-1 is soluble in organic solvents such as ethanol, DMSO, and dimethyl formamide (DMF). The solubility of NVS-PAK1-1 in ethanol is approximately 20 mg/ml and approximately 50 mg/ml in DMSO and DMF.

NVS-PAK1-1 is sparingly soluble in aqueous buffers. For maximum solubility in aqueous buffers, NVS-PAK1-1 should first be dissolved in DMF and then diluted with the aqueous buffer of choice. NVS-PAK1-1 has a solubility of approximately 0.5 mg/ml in a 1:1 solution of DMF:PBS (pH 7.2) using this method. We do not recommend storing the aqueous solution for more than one day.

Description

NVS-PAK1-1 is an allosteric inhibitor of p21-activated kinase 1 (PAK1), a non-receptor serine/threonine kinase involved in tumorigenesis (K_d = 7 nM).[1] It has an IC_{50} value of 5.2 nM in a PAK1 dephosphorylation assay. NVS-PAK1-1 is selective for PAK1 over PAK2 (K_d = 400 nM) and over a panel of 442 kinases, where it did not inhibit any other kinases by greater than 80%.[1,2] It inhibits phosphorylation of MEK Ser289 when used at concentrations ranging from 6 to 20 µM but does not inhibit proliferation of Su86.86 cells at concentrations lower than 2 µM.[1] See the Structural Genomics Consortium (SGC) website for more information.

References

1. Karpov, A.S., Amiri, P., Bellamacina, C., *et al.* Optimization of a dibenzodiazepine hit to a potent and selective allosteric PAK1 inhibitor. *ACS Med. Chem. Lett.* **6(7)**, 776-781 (2015).
2. Semenova, G. and Chernoff, J. Targeting PAK1. *Biochem. Soc. Trans.* **45(1)**, 79-88 (2017).

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