

**Product Name:** NVP 2

**Catalog No.:** 6535

**Batch No.:** 1

CAS Number: 1263373-43-8

IUPAC Name: 4-[[[5'-Chloro-2'-[[*trans*-4-[[*(1R)*-2-methoxy-1-methylethyl]amino]cyclohexyl]amino][2,4'-bipyridin]-6-yl]amino]methyl]tetrahydro-2*H*-pyran-4-carbonitrile

**1. PHYSICAL AND CHEMICAL PROPERTIES**

**Batch Molecular Formula:** C<sub>27</sub>H<sub>37</sub>ClN<sub>6</sub>O<sub>2</sub>·½H<sub>2</sub>O

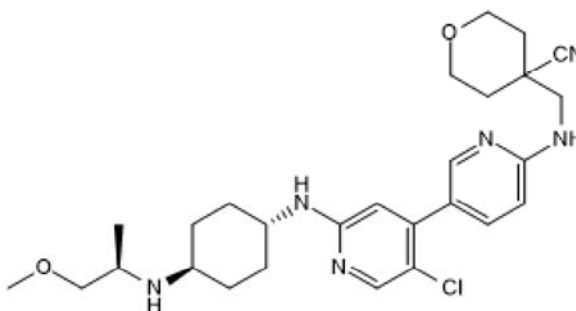
**Batch Molecular Weight:** 522.08

**Physical Appearance:** Cream solid

**Solubility:** DMSO to 100 mM  
ethanol to 100 mM

**Storage:** Store at -20°C

**Batch Molecular Structure:**



**2. ANALYTICAL DATA**

**TLC:** R<sub>f</sub> = 0.4 (Dichloromethane:Methanol [9:1])

**HPLC:** Shows 97.4% purity

**Chiral HPLC:** Shows 99.3% purity

**<sup>1</sup>H NMR:** Consistent with structure

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	62.12	7.34	16.1
Found	61.94	7.33	15.7

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**Description:**

Potent and selective ATP-competitive CDK9 inhibitor ( $IC_{50} = 0.5$  nM). Exhibits selectivity for CDK9 over a panel of 468 kinases, but inhibits DYRK1B ( $IC_{50} = 350$  nM), displays <90% binding to CDK7 ( $IC_{50} >10$   $\mu$ M) and CDK13. Inhibits proliferation of MOLT4 cells in vitro. Induces apoptosis.

**Physical and Chemical Properties:**

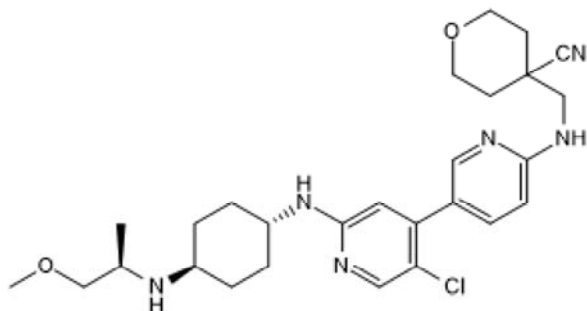
Batch Molecular Formula:  $C_{27}H_{37}ClN_6O_2 \cdot \frac{1}{2}H_2O$

Batch Molecular Weight: 522.08

Physical Appearance: Cream solid

**Minimum Purity:** >97%

**Batch Molecular Structure:**



**Storage:** Store at -20°C

**Solubility & Usage Info:**

DMSO 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°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:**

**Olson *et al*** (2018) Pharmacological perturbation of CDK9 using selective CDK9 inhibition or degradation. *Nat.Chem.Biol.* **14** 163. PMID: 29251720.

**Winter *et al*** (2017) BET bromodomain proteins function as master transcription elongation factors independent of CDK9 recruitment. *Mol.Cell* **67** 5. PMID: 28673542 .

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