

## Certificate of Analysis

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**Product Name:** NVP CXCR2 20

**Catalog No.:** 5660

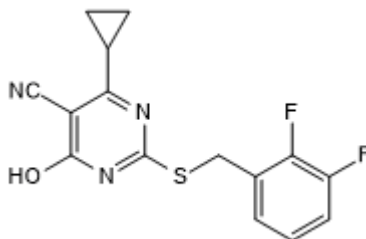
**Batch No.:** 1

**CAS Number:** 1029521-30-9

**IUPAC Name:** 4-Cyclopropyl-2-[[[(2,3-difluorophenyl)methyl]thio]-1,6-dihydro-6-oxo5-pyrimidinecarbonitrile

### 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>15</sub>H<sub>11</sub>F<sub>2</sub>N<sub>3</sub>OS  
**Batch Molecular Weight:** 319.33  
**Physical Appearance:** White solid  
**Solubility:** DMSO to 50 mM  
 1eq. NaOH to 10 mM with sonication  
**Storage:** Store at +4°C  
**Batch Molecular Structure:**



### 2. ANALYTICAL DATA

**TLC:** R<sub>f</sub> = 0.55 (Dichloromethane:Methanol [9:1])  
**HPLC:** Shows >99.8% purity  
<sup>1</sup>H NMR: Consistent with structure  
 Mass Spectrum: Consistent with structure  
 Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	56.42	3.47	13.16
Found	56.59	3.43	13.17

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

## Product Information

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### Description:

Potent and selective CXCR2 antagonist ( $IC_{50} = 40$  nM). Exhibits selectivity for CXCR2 over a panel of 49 other GPCRs. Orally bioavailable.

### Physical and Chemical Properties:

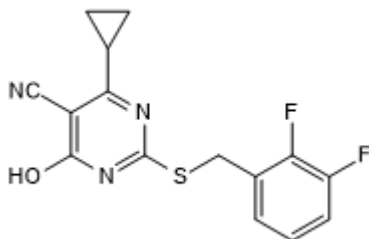
Batch Molecular Formula:  $C_{15}H_{11}F_2N_3OS$

Batch Molecular Weight: 319.33

Physical Appearance: White solid

**Minimum Purity:** >98%

### Batch Molecular Structure:



**Storage:** Store at +4°C

### Solubility & Usage Info:

DMSO to 50 mM

1eq. NaOH to 10 mM with sonication

### 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:

**Porter *et al*** (2014) The discovery of potent, orally bioavailable pyrimidine-5-carbonitrile-6-alkyl CXCR2 receptor antagonists. *Bioorg.Med.Chem.Lett.* **24** 3285. PMID: 24974342.

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