

Product Name: XL 413 hydrochloride

Catalog No.: 5493

Batch No.: 1

CAS Number: 1169562-71-3

IUPAC Name: 8-Chloro-2-(2S)-2-pyrrolidinylbenzofuro[3,2-d]pyrimidin-4(3H)-one hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₄H₁₂ClN₃O₂.HCl.¾H₂O

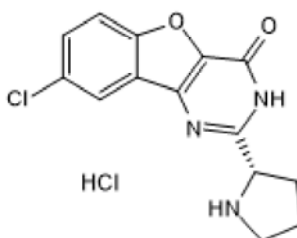
Batch Molecular Weight: 339.69

Physical Appearance: White solid

Solubility: water to 20 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.3% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	49.5	4.3	12.37
Found	49.55	4.23	12.33

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

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Description:

Potent and selective Cdc7 inhibitor (IC₅₀ = 3.4 nM). Exhibits >12-fold selectivity for Cdc7 over PIM-1 kinase and >30-fold selectivity over pMCM and CK2. Inhibits proliferation of Colo 205 cells in vitro and attenuates tumor growth of Colo 205 xenografts in mice.

Physical and Chemical Properties:

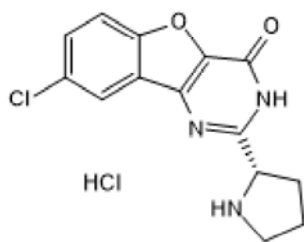
Batch Molecular Formula: C₁₄H₁₂ClN₃O₂.HCl.¾H₂O

Batch Molecular Weight: 339.69

Physical Appearance: White solid

Minimum Purity: ≥99%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

water 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.

References:

Sasi et al (2014) The potent Cdc7-Dbf4 (DDK) kinase inhibitor XL413 has limited activity in many cancer cell lines and discovery of potential new DDK inhibitor scaffolds. *PLoS ONE* **9** e113300. PMID: 25412417.

Koltun et al (2012) Discovery of XL413, a potent and selective CDC7 inhibitor. *Bioorg.Med.Chem.Lett.* **22** 3727. PMID: 22560567.

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