Print Date: Apr 14th 2022

Certificate of Analysis

www.tocris.com

Product Name: **XL 413 hydrochloride** **Catalog No.: 5493** **Batch No.: 1**

CAS Number: 1169562-71-3

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

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{14}H_{12}ClN_3O_2.HCl.¾H_2O$

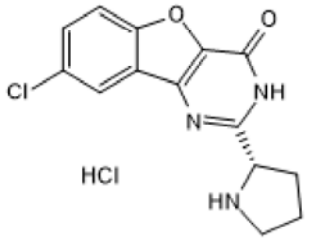
Batch Molecular Weight: 339.69

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

^{1}H 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

bio-techne.com
info@bio-techne.com
techsupport@bio-techne.com

North America
Tel: (800) 343 7475

China
info.cn@bio-techne.com
Tel: +86 (21) 52380373

Europe Middle East Africa
Tel: +44 (0)1235 529449

Rest of World
www.tocris.com/distributors
Tel:+1 612 379 2956

Product Name: **XL 413 hydrochloride** **Catalog No.: 5493** **Batch No.: 1**

CAS Number: 1169562-71-3

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

Description:

XL 413 hydrochloride is a potent and selective Cdc7 inhibitor (IC_{50} = 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. XL 413 also improves homology-directed repair (HDR) editing in hematopoietic stem cells (HSC).

Physical and Chemical Properties:

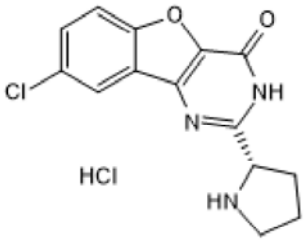
Batch Molecular Formula: $C_{14}H_{12}ClN_3O_2.HCl.¾H_2O$

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:

Azhagiri *et al* (2021) Homology-directed gene-editing approaches for hematopoietic stem and progenitor cell gene therapy. Stem Cell Res.Ther. ***12*** 500. PMID: 34503562.

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.