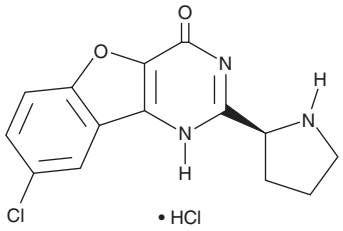
PRODUCT INFORMATION

XL413 (hydrochloride)

Item No. 24906

CAS Registry No.:	2062200-97-7
Formal Name:	8-chloro-2-(2S)-2-pyrrolidinyl-benzofuro[3,2-d]pyrimidin-4(3H)-one, monohydrochloride
MF:	$C_{14}H_{12}ClN_3O_2 \bullet HCl$
FW:	326.2
Purity:	≥98%
UV/Vis.:	λ_{max}: 232, 289 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

XL413 (hydrochloride) is supplied as a crystalline solid. A stock solution may be made by dissolving the XL413 (hydrochloride) in the solvent of choice. XL413 (hydrochloride) is soluble in the organic solvent DMSO, which should be purged with an inert gas, at a concentration of approximately 0.2 mg/ml.

Further dilutions of the stock solution into aqueous buffers or isotonic saline should be made prior to performing biological experiments. Ensure that the residual amount of organic solvent is insignificant, since organic solvents may have physiological effects at low concentrations. Organic solvent-free aqueous solutions of XL413 (hydrochloride) can be prepared by directly dissolving the crystalline solid in aqueous buffers. The solubility of XL413 (hydrochloride) in PBS, pH 7.2, is approximately 10 mg/ml. We do not recommend storing the aqueous solution for more than one day.

Description

XL413 is a potent inhibitor of Cdc7 (IC_{50} = 3.4 nM).[1] It is >60, >10, and >300-fold selective for Cdc7 over CK2, PIM1, and a panel of over 100 protein kinases, respectively. XL413 inhibits the growth of MDA-MB-231T and COLO 205 cells (IC_{50}s = 118 and 140 nM, respectively). It inhibits Cdc7-specific phosphorylation of mini-chromosome maintenance protein (MCM2) and induces cell cycle accumulation in the S and G_2 phases in MDA-MB-231T and COLO 205 cells that overexpress Cdc7. *In vivo*, XL413 inhibits MCM2 phosphorylation (ED_{50} = <3 mg/kg) and reduces tumor growth in a COLO 205 mouse xenograft model when administered orally at doses of 10, 30, and 100 mg/kg.

Reference

1. Koltun, E.S., Tsuhako, A.L., Brown, D.S., *et al.* Discovery of XL413, a potent and selective CDC7 inhibitor. *Bioorg. Med. Chem. Lett.* **22(11)**, 3727-3731 (2012).

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