

**Product Name:** WS 383

**Catalog No.:** 7055

**Batch No.:** 1

CAS Number: 2247544-02-9

IUPAC Name: 5-[[2-[(4-Chlorophenyl)methyl]thio]-5-methyl[1,2,4]triazolo[1,5-a]pyrimidin-7-yl]thio]-*N,N*-dimethyl-1*H*-tetrazole-1-ethanamine hydrochloride

## 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>18</sub>H<sub>20</sub>ClN<sub>9</sub>S<sub>2</sub>.HCl.½H<sub>2</sub>O

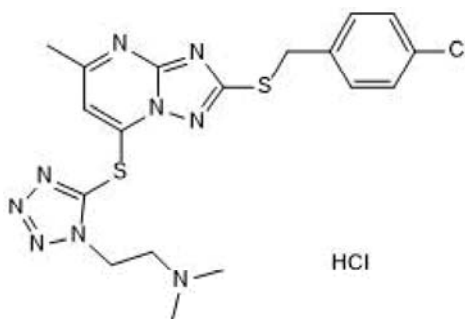
**Batch Molecular Weight:** 507.46

**Physical Appearance:** White solid

**Solubility:** DMSO to 100 mM

**Storage:** Store at -20°C

**Batch Molecular Structure:**



## 2. ANALYTICAL DATA

**HPLC:** Shows 99.4% purity

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

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen	Chlorine
Theoretical	42.6	4.37	24.84	13.97
Found	42.72	4.27	24.7	13.54

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

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**Description:**

WS 383 is a potent and reversible DCN1-UBC12 interaction inhibitor (IC<sub>50</sub> = 11 nM). The compound displays selectivity for DCN1-UBC12 over inhibition of a panel of kinases, including Bruton's tyrosine kinase (BTK), cyclin-dependent kinases (CDKs) and epidermal growth factor receptor (EGFR). In vitro, WS 383 selectively inhibits cullin-3 neddylation over other cullins, and induces accumulation of p21, p27 and NRF2.

**Physical and Chemical Properties:**

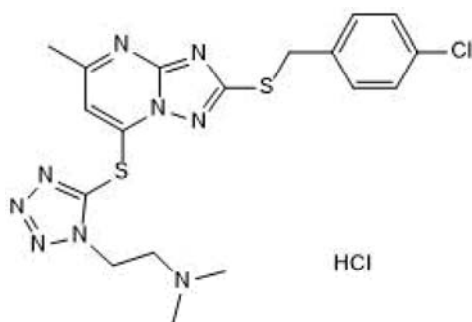
Batch Molecular Formula: C<sub>18</sub>H<sub>20</sub>ClN<sub>9</sub>S<sub>2</sub>.HCl.½H<sub>2</sub>O

Batch Molecular Weight: 507.46

Physical Appearance: White solid

**Minimum Purity:** ≥98%

**Batch Molecular Structure:**



**Storage:** Store at -20°C

**Solubility & Usage Info:**

DMSO 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:**

**Wang et al** (2019) Development of highly potent, selective, and cellular active triazolo[1,5- a]pyrimidine-based inhibitors targeting the DCN1-UBC12 protein-protein interaction. *J.Med.Chem.* **62** 2772. PMID: 30803229.

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