

**Product Name:** Mps1-IN-1 dihydrochloride

**Catalog No.:** 5142

**Batch No.:** 1

CAS Number: 1883548-93-3

IUPAC Name: 1-[3-Methoxy-4-[[4-[[2-[(1-methylethyl)sulfonyl]phenyl]amino]-1*H*-pyrrolo[2,3-*b*]pyridin-6-yl]amino]phenyl]-4-piperidinol dihydrochloride

## 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>28</sub>H<sub>33</sub>N<sub>5</sub>O<sub>4</sub>S.2HCl.2H<sub>2</sub>O

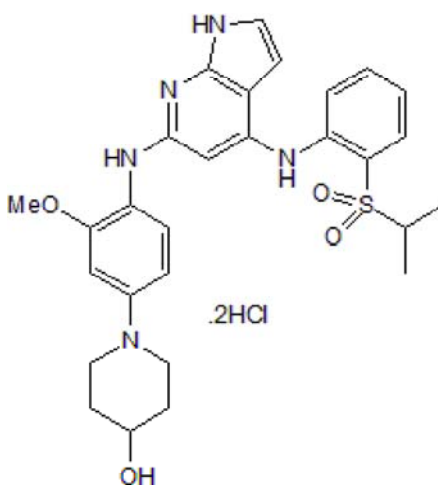
**Batch Molecular Weight:** 644.61

**Physical Appearance:** Beige solid

**Solubility:** water to 100 mM  
DMSO to 100 mM

**Storage:** Desiccate at RT

**Batch Molecular Structure:**



## 2. ANALYTICAL DATA

**TLC:** R<sub>f</sub> = 0.26 (Chloroform:Methanol:Ammonia soln. [94:5:1])

**HPLC:** Shows 99.1% purity

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

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	52.17	6.1	10.86
Found	52.12	6.12	10.77

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**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

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**Description:**

Selective monopolar spindle 1 (Mps1) kinase inhibitor (IC<sub>50</sub> = 367 nM); exhibits >1000 fold-selectivity against a panel of 352 kinases with the exceptions of ALK and Ltk. Disrupts the recruitment of Mad2 to kinetochores. Increases frequency of multipolar mitosis in U2OS cells.

**Physical and Chemical Properties:**

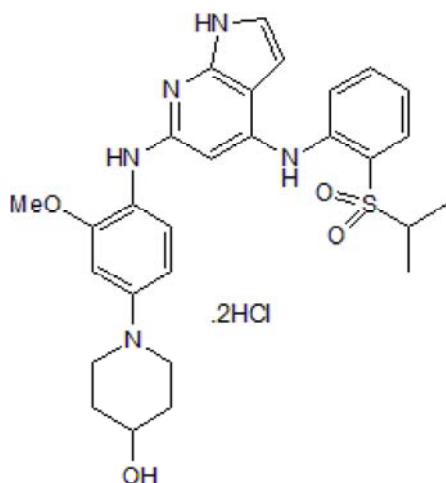
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Batch Molecular Weight: 644.61

Physical Appearance: Beige solid

**Minimum Purity:** ≥98%

**Batch Molecular Structure:**



**Storage:** Desiccate at RT

**Solubility & Usage Info:**

water to 100 mM

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:**

**Miduturu et al** (2011) High-throughput kinase profiling: a more efficient approach toward the discovery of new kinase inhibitors. *Chem.Biol.* **18** 868. PMID: 21802008.

**Kwiatkowski et al** (2010) Small-molecule kinase inhibitors provide insight into Mps1 cell cycle function. *Nat.Chem.Biol.* **6** 359. PMID: 20383151.

**Lan and Cleveland** (2010) A chemical tool box defines mitotic and interphase roles for Mps1 kinase. *J.Cell Biol.* **190** 21. PMID: 20624898.

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