

## Certificate of Analysis

**Product Name:** VX 680

**Catalog No.:** 5907

**Batch No.:** 1

CAS Number: 639089-54-6

IUPAC Name: *N*-[4-[[4-(4-Methyl-1-piperazinyl)-6-[(5-methyl-1*H*-pyrazol-3-yl)amino]-2-pyrimidinyl]thio]phenyl]cyclopropanecarboxamide

### 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>23</sub>H<sub>28</sub>N<sub>8</sub>OS.H<sub>2</sub>O

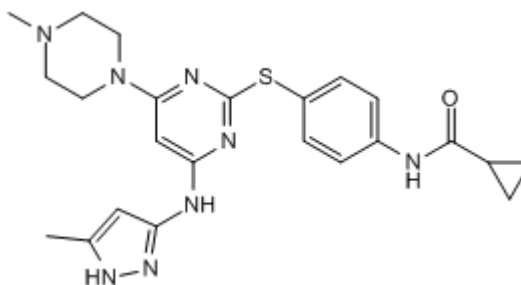
**Batch Molecular Weight:** 482.61

**Physical Appearance:** White solid

**Solubility:** DMSO to 100 mM

**Storage:** Store at -20°C

**Batch Molecular Structure:**



### 2. ANALYTICAL DATA

**HPLC:** Shows 99.9% purity

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

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

Carbon Hydrogen Nitrogen

Theoretical 57.24 6.27 23.22

Found 57.31 6.26 23.17

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

**Product Name:** VX 680

**Catalog No.:** 5907

**Batch No.:** 1

CAS Number: 639089-54-6

IUPAC Name: *N*-[4-[[4-(4-Methyl-1-piperazinyl)-6-[(5-methyl-1*H*-pyrazol-3-yl)amino]-2-pyrimidinyl]thio]phenyl]cyclopropanecarboxamide

**Description:**

High affinity and selective Aurora kinase inhibitor ( $K_i$  values are 0.6, 5 and 18 nM for Aurora A, Aurora C and Aurora B, respectively). Also exhibits affinity for FLT-3 and Abl. Exhibits selectivity for Aurora kinase over 190 other protein kinases. Inhibits proliferation and induces apoptosis in a number of cancer cell lines *in vitro*. Reduces tumor size in leukemia and colon cancer cell xenografts in mice.

**Physical and Chemical Properties:**

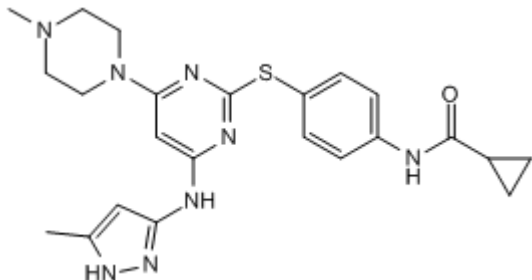
Batch Molecular Formula:  $C_{23}H_{28}N_8OS \cdot H_2O$

Batch Molecular Weight: 482.61

Physical Appearance: White solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**



**References:**

**Bebbington et al** (2009) The discovery of the potent aurora inhibitor MK-0457 (VX-680). *Bioorg.Med.Chem.Lett.* **19** 3586. PMID: 19447622.

**Harrington et al** (2004) VX-680, a potent and selective small-molecule inhibitor of the Aurora kinases, suppresses tumor growth *in vivo*. *Nat.Med.* **10** 262. PMID: 14981513.

**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.

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

**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