

# Certificate of Analysis

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**Product Name:** SB 743921 hydrochloride

**Catalog No.:** 5109

**Batch No.:** 2

**CAS Number:** 940929-33-9

**IUPAC Name:** *N*-(3-Aminopropyl)-*N*-[(1*R*)-1-[7-chloro-4-oxo-3-(phenylmethyl)-4*H*-1-benzopyran-2-yl]-2-methylpropyl]-4-methylbenzamide hydrochloride

## 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>31</sub>H<sub>33</sub>ClN<sub>2</sub>O<sub>3</sub>.HCl.½H<sub>2</sub>O

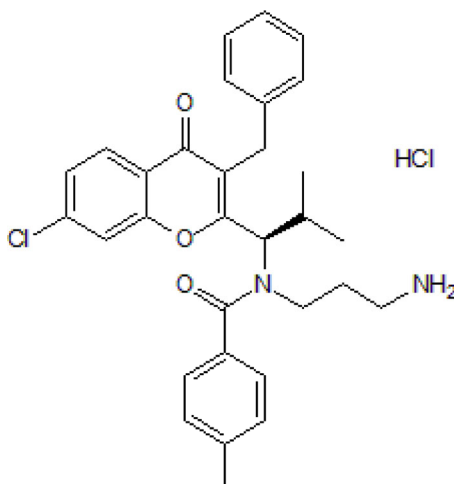
**Batch Molecular Weight:** 558.02

**Physical Appearance:** Off White solid

**Solubility:** DMSO to 100 mM

**Storage:** Store at -20°C

**Batch Molecular Structure:**



## 2. ANALYTICAL DATA

**HPLC:** Shows 98.6% purity

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

**Mass Spectrum:** Consistent with structure

**Optical Rotation:** [α]<sub>D</sub> = +174 (Concentration = 1, Solvent = Methanol)

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen	Chlorine
Theoretical	66.72	6.23	5.02	12.71
Found	65.66	6.12	4.87	12.75

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](http://www.tocris.com/distributors)

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**Description:**

SB 743921 hydrochloride is a potent kinesin spindle protein (KSP) inhibitor ( $K_i = 0.1$  nM). Induces cell mitotic arrest and apoptosis in vitro. Inhibits the growth of a range of tumor cells in vitro, including colon (HCT 116), prostate (PC-3) and leukemia (K-562) cancer cell lines. Causes tumor regression in human tumor xenograft models in vivo, including colon (Colo205), lung (H69) and breast (MCF7) cancer cell xenografts.

**Physical and Chemical Properties:**

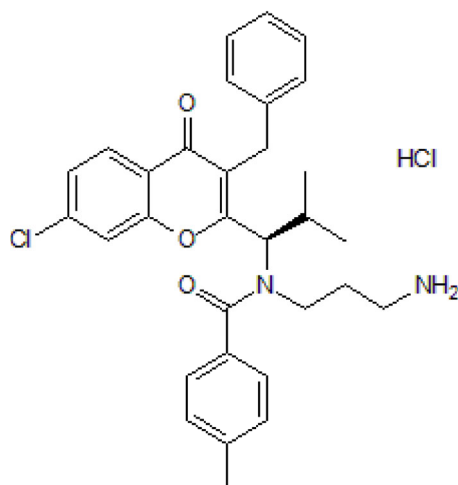
Batch Molecular Formula:  $C_{31}H_{33}ClN_2O_3 \cdot HCl \cdot \frac{1}{4}H_2O$

Batch Molecular Weight: 558.02

Physical Appearance: Off 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. \*Unless contradicted by product-specific protocols or instructions, our standard recommendations apply:

**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.

**Licensing Information:**

Sold with the permission of GlaxoSmithKline.

**References:**

**Good et al** (2013) Optimized S-trityl-L-cysteine-based inhibitors of kinesin spindle protein with potent in vivo antitumor activity in lung cancer xenograft models. *J.Med.Chem.* **56** 1878. PMID: 23394180.

**Talapatra et al** (2013) Mitotic kinesin Eg5 overcomes inhibition to the phase I/II clinical candidate SB743921 by an allosteric resistance mechanism. *J.Med.Chem.* **56** 6317. PMID: 23875972.

**Jackson et al** (2006) A second generation KSP inhibitor, SB-743921, is a highly potent and active therapeutic in preclinical models of cancer. First AACR International Conference on Molecular and Diagnostics in Cancer Therapeutic Development. Abstract (B11).

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