

**Product Name:** SKI II

**Catalog No.:** 2097

**Batch No.:** 3

CAS Number: 312636-16-1

IUPAC Name: 4-[[4-(4-Chlorophenyl)-2-thiazolyl]amino]phenol

**1. PHYSICAL AND CHEMICAL PROPERTIES**

**Batch Molecular Formula:** C<sub>15</sub>H<sub>11</sub>ClN<sub>2</sub>OS·¼H<sub>2</sub>O

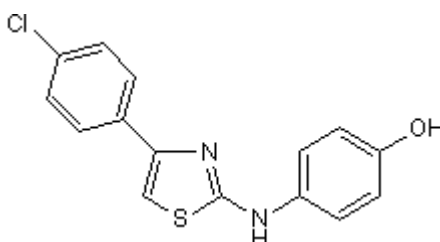
**Batch Molecular Weight:** 307.28

**Physical Appearance:** White solid

**Solubility:** DMSO to 100 mM

**Storage:** Store at -20°C

**Batch Molecular Structure:**



**2. ANALYTICAL DATA**

**TLC:** R<sub>f</sub> = 0.37 (Ethyl acetate:Petroleum ether [3:7])

**HPLC:** Shows 100% purity

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

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	58.63	3.77	9.12
Found	58.6	3.8	9.17

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**Description:**

Selective non-lipid inhibitor of sphingosine kinase ( $IC_{50} = 0.5 \mu M$ ); does not act at ATP-binding site. Displays no inhibition of ERK2, PI 3-kinase, or PKC $\alpha$  at concentrations up to 60  $\mu M$ . Reduces levels of sphingosine-1-phosphate in MDA-MB-231 breast cancer cells. Induces apoptosis and inhibits proliferation in several other tumor cell lines in vitro ( $IC_{50} = 0.9 - 4.6 \mu M$ ).

**Physical and Chemical Properties:**

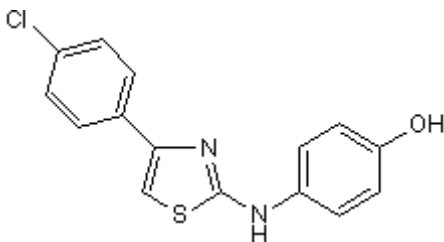
Batch Molecular Formula:  $C_{15}H_{11}ClN_2OS \cdot \frac{1}{4}H_2O$

Batch Molecular Weight: 307.28

Physical Appearance: White solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**



**References:**

**French et al** (2003) Discovery and evaluation of inhibitors of human sphingosine kinase. *Cancer Res.* **63** 5862.

**French et al** (2006) Antitumor activity of sphingosine kinase inhibitors. *J.Pharmacol.Exp.Ther.* **318** 596. PMID: 16632640.

**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.

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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