

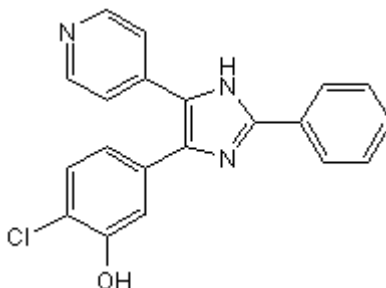
## Certificate of Analysis

**Product Name:** L-779,450  
**CAS Number:** 303727-31-3  
**IUPAC Name:** 2-Chloro-5-[2-Phenyl-5-(4-pyridinyl)-1H-imidazol-4-yl]phenol

**Catalog No.:** 3185 **Batch No.:** 1

### 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:**  $C_{20}H_{14}ClN_3O \cdot \frac{1}{2}H_2O$   
**Batch Molecular Weight:** 356.81  
**Physical Appearance:** Beige solid  
**Solubility:** DMSO to 100 mM  
 ethanol to 100 mM  
**Storage:** Store at +4°C  
**Batch Molecular Structure:**



### 2. ANALYTICAL DATA

**TLC:**  $R_f = 0.36$  (Dichloromethane:Methanol [9:1])  
**HPLC:** Shows 99.7% purity  
**<sup>1</sup>H NMR:** Consistent with structure  
**Mass Spectrum:** Consistent with structure  
**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	67.32	4.24	11.78
Found	67.56	4.43	11.77

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**Description:**

Potent, ATP-competitive Raf kinase inhibitor ( $IC_{50} = 10$  nM) that displays > 7, > 30 and > 70-fold selectivity over p38 $\alpha$ , GSK3 $\beta$  and Lck respectively. Suppresses DNA synthesis and induces apoptosis in cells that proliferate in response to Raf-1 and A-Raf but not B-Raf.

**Physical and Chemical Properties:**

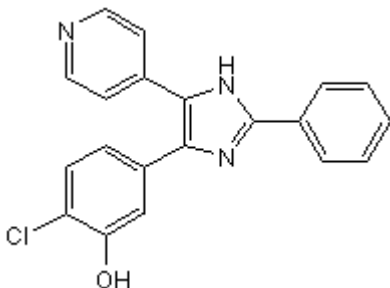
Batch Molecular Formula: C<sub>20</sub>H<sub>14</sub>ClN<sub>3</sub>O · ½H<sub>2</sub>O

Batch Molecular Weight: 356.81

Physical Appearance: Beige solid

**Minimum Purity:** >99%

**Batch Molecular Structure:**



**Storage:** Store at +4°C

**Solubility & Usage Info:**

DMSO to 100 mM  
ethanol 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:**

**White** (2003) Small-molecule inhibitors of signal transduction pathways in leukemia therapeutics: how to assess selectivity for malignant signals. *Leukemia* **17** 1759. PMID: 12970775.

**Shelton et al** (2003) Differential effects of kinase cascade inhibitors on neoplastic and cytokine-mediated cell proliferation. *Leukemia* **17** 1765. PMID: 12970777.

**Take et al** (2006) Identification of potent and selective imidazole-based inhibitors of B-Raf kinase. *Bioorg.Med.Chem.Letts.* **16** 378.

**Röring et al** (2012) Distinct requirement for an intact dimer interface in wild-type, V600E and kinase-dead B-Raf signalling. *EMBO J.* **31** 2629. PMID: 22510884.

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