

## Certificate of Analysis

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

**Product Name:** SB 218795

**Catalog No.:** 1376

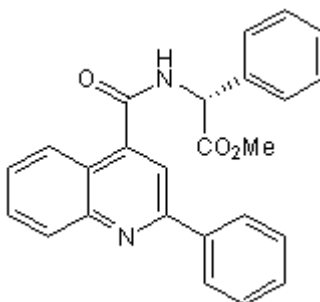
**Batch No.:** 1

**CAS Number:** 174635-53-1

**IUPAC Name:** (R)-[[2-Phenyl-4-quinoliny]carbonyl]amino]-methyl ester benzenecetic acid

### 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>25</sub>H<sub>20</sub>N<sub>2</sub>O<sub>3</sub>  
**Batch Molecular Weight:** 396.44  
**Physical Appearance:** White solid  
**Solubility:** DMSO to 100 mM  
 ethanol to 5 mM  
**Storage:** Store at RT  
**Batch Molecular Structure:**



### 2. ANALYTICAL DATA

**TLC:** R<sub>f</sub> = 0.58 (Ethyl acetate:Petroleum ether [1:1])  
**Melting Point:** At 180°C  
**HPLC:** Shows >99.3% purity  
<sup>1</sup>H NMR: Consistent with structure  
**Optical Rotation:** [α]<sub>D</sub> = -41.6 (Concentration = 0.5, Solvent = Methanol)

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	75.74	5.08	7.07
Found	75.63	5.09	6.88

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

## Product Information

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### Description:

Potent, selective and competitive non-peptide NK<sub>3</sub> receptor antagonist (K<sub>i</sub> = 13 nM at hNK<sub>3</sub>). Displays 90-fold and 7000-fold selectivity over hNK<sub>2</sub> and hNK<sub>1</sub> receptors respectively. Active in vivo, inhibiting agonist-induced pupillary constriction.

### Physical and Chemical Properties:

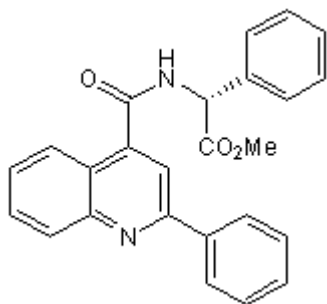
Batch Molecular Formula: C<sub>25</sub>H<sub>20</sub>N<sub>2</sub>O<sub>3</sub>

Batch Molecular Weight: 396.44

Physical Appearance: White solid

**Minimum Purity:** >99%

### Batch Molecular Structure:



**Storage:** Store at RT

### Solubility & Usage Info:

DMSO to 100 mM

ethanol to 5 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:

**Giardina et al** (1997) Discovery of a novel class of selective non-peptide antagonists for the human neurokinin-3 receptor. 1. Identification of the 4-quinolinecarboxamide framework. *J.Med.Chem.* **40** 1794. PMID: 9191956.

**Medhurst et al** (1997) *In vitro* and *in vivo* characterization of NK<sub>3</sub> receptors in the rabbit eye by use of selective non-peptide NK<sub>3</sub> receptor antagonists. *Br.J.Pharmacol.* **122** 469. PMID: 9351503.

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