

## Certificate of Analysis

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**Product Name:** CGS 35066

**Catalog No.:** 2512

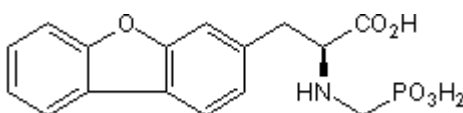
**Batch No.:** 3

CAS Number: 261619-50-5

IUPAC Name:  $\alpha$ -[(S)-(Phosphonomethyl)amino]-3-dibenzofuranpropanoic acid

### 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>16</sub>H<sub>16</sub>NO<sub>6</sub>P·½H<sub>2</sub>O  
**Batch Molecular Weight:** 353.78  
**Physical Appearance:** White solid  
**Solubility:** 1eq. NaOH to 100 mM  
**Storage:** Desiccate at RT  
**Batch Molecular Structure:**



### 2. ANALYTICAL DATA

**TLC:** R<sub>f</sub> = 0.43 (Pyridine:Acetic acid:Water:Butanol [3:8:11:33])  
**HPLC:** Shows 99.8% purity  
**<sup>1</sup>H NMR:** Consistent with structure  
**<sup>13</sup>C NMR:** Consistent with structure  
**Mass Spectrum:** Consistent with structure  
**Optical Rotation:** [α]<sub>D</sub> = +44 (Concentration = 0.235, Solvent = NaOH aq)  
**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	54.32	4.7	3.96
Found	54.4	4.57	3.66

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

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**Description:**

Potent endothelin-converting enzyme (ECE) inhibitor that displays > 100-fold selectivity over neutral endopeptidase 24.11 (IC<sub>50</sub> values are 22 and 2300 nM respectively). Blocks the hypertensive effects induced by big ET-1 in vitro and reduces the magnitude of cerebral vasospasm following subarachnoid hemorrhage (SAH).

**Physical and Chemical Properties:**

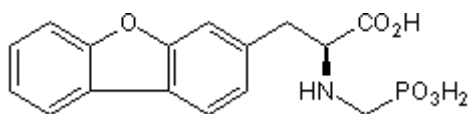
Batch Molecular Formula: C<sub>16</sub>H<sub>16</sub>NO<sub>6</sub>P·¼H<sub>2</sub>O

Batch Molecular Weight: 353.78

Physical Appearance: White solid

**Minimum Purity:** >99%

**Batch Molecular Structure:**



**References:**

**De Lombaert et al** (2000) Potent and selective non-peptidic inhibitors of endothelin-converting enzyme-1 with sustained duration of action. *J.Med.Chem.* **43** 488. PMID: 10669576.

**Trapani et al** (2000) Pharmacological properties of CGS 35066, a potent and selective endothelin-converting enzyme inhibitor, in conscious rats. *J.Cardiovasc.Pharmacol.* **36** (5 Suppl. 1) S40. PMID: 11078331.

**Kwan et al** (2002) Attenuation of SAH-induced cerebral vasospasm by a selective ECE inhibitor. *Neuropharmacol.Neurotoxicol.* **13** 197.

**Storage:** Desiccate at RT

**Solubility & Usage Info:**

1eq. NaOH 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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