

Product Name: CGS 35066

Catalog No.: 2512

Batch No.: 3

CAS Number: 261619-50-5

IUPAC Name: α -[(S)-(Phosphonomethyl)amino]-3-dibenzofuranpropanoic acid

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₆H₁₆NO₆P · ¼H₂O

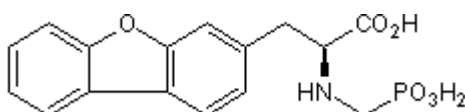
Batch Molecular Weight: 353.78

Physical Appearance: White solid

Solubility: 1eq. NaOH to 100 mM

Storage: Desiccate at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.43 (Pyridine:Acetic acid:Water:Butanol [3:8:11:33])

HPLC: Shows 99.8% purity

¹H NMR: Consistent with structure

¹³C NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: [α]_D = +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

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Description:

Potent endothelin-converting enzyme (ECE) inhibitor that displays > 100-fold selectivity over neutral endopeptidase 24.11 (IC₅₀ 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:

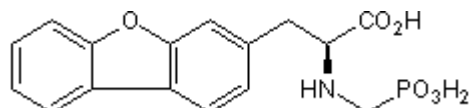
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Physical Appearance: White solid

Minimum Purity: >99%

Batch Molecular Structure:



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.

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.