

**Product Name:** TR 14035

**Catalog No.:** 6908

**Batch No.:** 1

CAS Number: 232271-19-1

IUPAC Name: (αS)-α-[(2,6-Dichlorobenzoyl)amino]-2',6'-dimethoxy[1,1'-biphenyl]-4-propanoic acid

## 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>24</sub>H<sub>21</sub>Cl<sub>2</sub>NO<sub>5</sub>·¼H<sub>2</sub>O

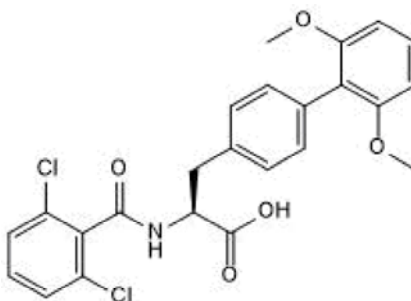
**Batch Molecular Weight:** 478.83

**Physical Appearance:** Off White solid

**Solubility:** DMSO to 100 mM  
ethanol to 20 mM

**Storage:** Store at -20°C

**Batch Molecular Structure:**



## 2. ANALYTICAL DATA

**HPLC:** Shows 97.7% purity

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

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	60.2	4.53	2.93
Found	60.08	4.34	3.04

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

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**Description:**

Potent integrin  $\alpha_4\beta_7$  and  $\alpha_4\beta_1$  antagonist (IC<sub>50</sub> values are 7 and 87 nM, respectively). Inhibits binding of HEK 293 cells to osteopontin forms. Orally bioavailable.

**Physical and Chemical Properties:**

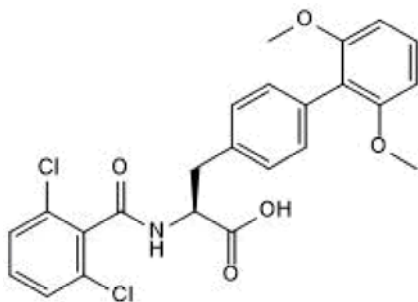
Batch Molecular Formula: C<sub>24</sub>H<sub>21</sub>Cl<sub>2</sub>NO<sub>5</sub>·¼H<sub>2</sub>O

Batch Molecular Weight: 478.83

Physical Appearance: Off White solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**



**References:**

**Jürets *et al*** (2019) Inhibition of cellular adhesion by immunological targeting of osteopontin neopeptides generated through matrix metalloproteinase and thrombin cleavage. *PLoS One* **11** e0148333. PMID: 26840958.

**Sircar *et al*** (2002) Synthesis and SAR of *N*-benzoyl-L-biphenylalanine derivatives: discovery of TR-14035, a dual  $\alpha_4\beta_7/\alpha_4\beta_1$  integrin antagonist. *Bioorg.Med.Chem.* **6** 20151. PMID: 11937364.

**Storage:** Store at -20°C

**Solubility & Usage Info:**

DMSO to 100 mM

ethanol to 20 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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