

Certificate of Analysis

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Product Name: H2L5186303

Catalog No.: 4878

Batch No.: 1

CAS Number: 139262-76-3

IUPAC Name: (Z,Z)-4,4'-[1,3-Phenylenebis(oxy-4,1-phenyleneimino)]bis[4-oxo-2-butenoic acid

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{26}H_{20}N_2O_8 \cdot \frac{3}{4}H_2O$

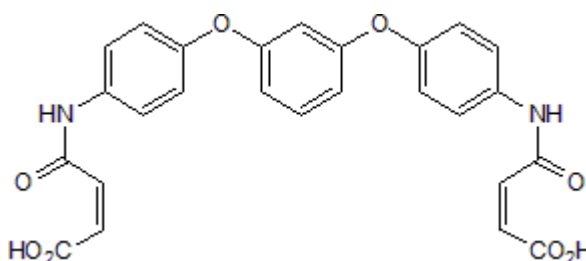
Batch Molecular Weight: 501.96

Physical Appearance: Yellow solid

Solubility: DMSO to 100 mM

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 98.4% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

Carbon Hydrogen Nitrogen

| | Carbon | Hydrogen | Nitrogen |
|-------------|--------|----------|----------|
| Theoretical | 62.21 | 4.32 | 5.58 |
| Found | 62.33 | 4.03 | 5.54 |

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

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Description:

Potent and selective lysophosphatidic acid 2 (LPA₂) receptor antagonist (IC₅₀ values are 8.9, 1230 and 27354 nM for LPA₂, LPA₃ and LPA₁ receptors respectively, in a LPA-elicited calcium mobilization assay).

Physical and Chemical Properties:

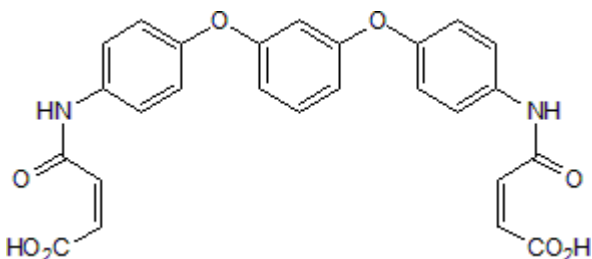
Batch Molecular Formula: C₂₆H₂₀N₂O₈·³/₄H₂O

Batch Molecular Weight: 501.96

Physical Appearance: Yellow solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at +4°C

CAUTION - This product is light sensitive and we recommend that the solid material and any solutions obtained are protected from exposure to light.

Solubility & Usage Info:

DMSO 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:

Fells et al (2008) Identification of non-lipid LPA₃ antagonists by virtual screening. *Bioorg.Med.Chem.* **16** 6207. PMID: 18467108.

Fells et al (2009) Structure-based drug design identifies novel LPA₃ antagonists. *Bioorg.Med.Chem.* **17** 7457. PMID: 19800804.

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