TOCRIS a biotechne brand

Print Date: May 10th 2021

Certificate of Analysis

www.tocris.com

Batch No.: 6

Catalog No.: 3022

Product Name: Edelfosine

CAS Number: 77286-66-9

IUPAC Name:

(7R) - 4 - Hydroxy - 7 - methoxy - N, N, N - trimethyl - 3, 5, 9 - trioxa - 4 - phosphaheptacosan - 1 - aminium - 4 - oxide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: Batch Molecular Weight: Physical Appearance: Solubility: Storage: Batch Molecular Structure: $C_{27}H_{58}NO_6P.2H_2O$ 559.76 White solid water to 5 mM with gentle warming Store at -20°C



2. ANALYTICAL DATA

TLC: ¹H NMR:

Mass Spectrum:

Optical Rotation:

Microanalysis:

R _f = 0.51 (Chloroform:Methanol:Water [65:35:8])							
Consistent with structure							
Consistent with structure							
$[\alpha]_D$ = -2.9 (Concentration = 1, Solvent = Chloroform/Methanol (1:1))							
Carbon Hydrogen Nitrogen							
Theoretical	57.93	11.16	2.5				
Found	57.6	11.26	2.49				

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

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IUPAC Name:

(7R)-4-Hydroxy-7-methoxy-N,N,N-trimethyl-3,5,9-trioxa-4-phosphaheptacosan-1-aminium-4-oxide

Description:

Synthetic lysophospholipid analog that selectively inhibits phosphatidylinositol phospholipase C (IC_{50} = 9.6 µM in fibroblasts and adenocarcinoma cells). Also acts as an agonist at platelet-activating factor (PAF) receptors. Antitumor lipid; selectively induces apoptosis in tumor cells, sparing normal cells.

Physical and Chemical Properties:

Batch Molecular Formula: C₂₇H₅₈NO₆P.2H₂O Batch Molecular Weight: 559.76 Physical Appearance: White solid

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

water to 5 mM with gentle warming

CAUTION - This product is hygroscopic and we recommend that it is desiccated upon arrival. Standard retail vials are prepared by lyophilisation. The product may appear as a solid, a gel or a film. Solutions should be made by adding solvent directly to the vial. The vial should then be vortexed vigorously to ensure the product has completely dissolved

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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:

Shimizu *et al* (2007) Roles of brain phosphatidylinositol-specific phospholipase C and diacylglycerol lipase in centrally administered histamine-induced adrenomedullary outflow in rats. Eur.J.Pharmacol. **571** 138. PMID: 17628524.

Wong et al (2007) Phospholipase C and myosin light chain kinase inhibition define a common step in actin regulation during cytokinesis. BMC Cell Biol. 8 15. PMID: 17509155.

Aoki *et al* (1995) A radioreceptor binding assay for platelet-activating factor (PAF) using membranes from CHO cells expressing human PAF receptor. J.Immunol.Methods **186** 225. PMID: 7594622.

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