

Certificate of Analysis

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Product Name: S 32826

Catalog No.: 3404

Batch No.: 1

CAS Number: 1103672-43-0

IUPAC Name: [4-(Tetradecanoylamino)benzyl]phosphonic acid disodium salt

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{21}H_{34}NO_4PNa_2 \cdot 2\frac{1}{2}H_2O$

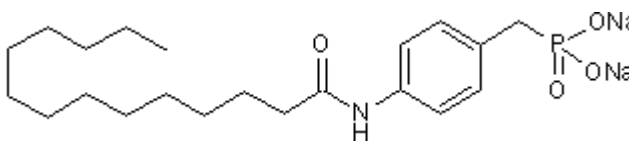
Batch Molecular Weight: 486.49

Physical Appearance: White solid

Solubility: 1eq. NaOH to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: $R_f = 0.5$ (Chloroform:Methanol [4:1])

HPLC: Shows 99.7% purity

1H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	51.85	8.08	2.88
Found	51.86	8.02	2.74

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

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Description:

Inhibitor of autotaxin (IC₅₀ = 9 nM). Displays similar inhibitory effects at all three autotaxin isoforms (α, β and γ). Exhibits no affinity for lysophosphatidic acid receptor 1 (LPA1) at concentrations up to 10 μM. Inhibits LPA release from adipocytes (IC₅₀ = 90 nM).

Physical and Chemical Properties:

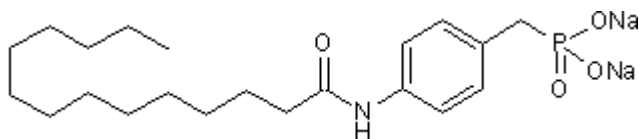
Batch Molecular Formula: C₂₁H₃₄NO₄PNa₂·2½H₂O

Batch Molecular Weight: 486.49

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at -20°C

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:

Ferry et al (2008) S32826, a nanomolar inhibitor of autotaxin: discovery, synthesis and applications as a pharmacological tool. *J.Pharmacol.Exp.Ther.* **327** 809. PMID: 18755937.

Gaetano et al (2009) Inhibition of autotaxin production or activity blocks lysophosphatidylcholine-induced migration of human breast cancer and melanoma cells. *Mol.Carcinogenesis* **48** 801.

Li et al (2011) Autotaxin is induced by TSA through HDAC3 and HDAC7 inhibition and antagonizes the TSA-induced cell apoptosis. *Mol.Cancer* **10** 18. PMID: 21314984.

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