

Certificate of Analysis

Print Date: Jul 13th 2020

www.tocris.com

Product Name: ASB 14780 Catalog No.: 6316 Batch No.: 1

CAS Number: 1069046-00-9

IUPAC Name: 3-(3-Phenethyl-1-(4-phenoxyphenyl)-1*H*-indol-5-yl)propanoic acid tris salt

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{31}H_{27}NO_3.C_4H_{11}NO_3$

Batch Molecular Weight: 582.7

Physical Appearance: Pale orange solid
Solubility: DMSO to 100 mM
Storage: Store at -20°C

Batch Molecular Structure:

2. ANALYTICAL DATA

HPLC: Shows 98.2% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Carbon Hydrogen Nitrogen

Theoretical 72.14 6.57 4.81 Found 72.13 6.61 4.92

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

www.tocris.com/distributors Tel:+1 612 379 2956



Product Information

Print Date: Jul 13th 2020

www.tocris.com

Product Name: ASB 14780 Catalog No.: 6316 Batch No.: 1

CAS Number: 1069046-00-9

IUPAC Name: 3-(3-Phenethyl-1-(4-phenoxyphenyl)-1*H*-indol-5-yl)propanoic acid tris salt

Description:

Potent and selective cytosolic phospholipase A_2 alpha (cPLA₂ α) inhibitor (IC₅₀ = 20 nM). Selective for cPLA₂ α over secreted PLA₂ α (sPLA₂ α ; exhibits no inhibition at 10 μ M). Inhibits cPLA₂ α -dependent inflammatory responses in vitro in guinea pig and human whole-blood assays. Improves diet-induced liver injury and CCl4-induced hepatic fibrosis in vivo. Orally bioavailable.

Physical and Chemical Properties:

Batch Molecular Formula: C₃₁H₂₇NO₃.C₄H₁₁NO₃

Batch Molecular Weight: 582.7

Physical Appearance: Pale orange solid

Minimum Purity: ≥98%

Batch Molecular Structure:

Storage: Store at -20°C

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:

Kanai *et al* (2016) ASB14780, an orally active inhibitor of group IVA phospholipase A₂, Is a pharmacotherapeutic condidate for nonalcoholic fatty liver disease. J.Pharmacol.Exp.Ther. **356** 604. PMID: 26699145.

Tomoo *et al* (2014) Design, synthesis, and biological evaluation of 3-(1-aryl-1H-indol-5-yl)propanoic acids as new indole-based cytosolic phospholipase $A_2\alpha$. J.Med.Chem. *57* 7244. PMID: 25102418.

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