

Certificate of Analysis

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Product Name: H2L 5765834 Catalog No.: 4870 Batch No.: 1

CAS Number: 420841-84-5

IUPAC Name: 2,3-Dihydro-2-[3-(4-nitrophenoxy)phenyl]-1,3-dioxo-1*H*-isoindole-5-carboxylic acid

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{21}H_{12}N_2O_7.4H_2O$

Batch Molecular Weight: 408.83

Physical Appearance: Pale yellow solid

Solubility: DMSO to 100 mM

Storage: Store at +4°C

Batch Molecular Structure:

2. ANALYTICAL DATA

HPLC: Shows 99.3% purity

1H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 61.7 3.08 6.85 Found 61.69 3.03 6.96





Product Information

Print Date: May 23rd 2013

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IUPAC Name: 2,3-Dihydro-2-[3-(4-nitrophenoxy)phenyl]-1,3-dioxo-1*H*-isoindole-5-carboxylic acid

Description:

Antagonist of the lysophosphatidic acid receptors LPA $_1$, LPA $_5$ and LPA $_3$ (IC $_{50}$ values are 94, 463 and 752 nM respectively). Exhibits no effect at LPA $_2$ or LPA $_4$ receptors.

Physical and Chemical Properties:

Batch Molecular Formula: C₂₁H₁₂N₂O₇. ¼H₂O

Batch Molecular Weight: 408.83 Physical Appearance: Pale yellow solid

Minimum Purity: >99%

Batch Molecular Structure:

Storage: Store at +4°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:

Williams et al (2009) Unique ligand selectivity of the GPR92/LPA₅ lysophosphatidate receptor indicates role in human platelet activation. J.Biol.Chem. 284 17304. PMID: 19366702.

Fells et al (2010) 2D binary QSAR modeling of LPA₃ receptor antagonism. J.Mol.Graph Model. 28 828. PMID: 20356772.

Tigyi (2010) Aiming drug discovery at lysophosphatidic acid targets. Br.J.Pharmacol. 161 241. PMID: 20735414.

