



Certificate of Analysis

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Product Name: XEN 445 Catalog No.: 5839 Batch No.: 1

CAS Number: 1515856-92-4

IUPAC Name: 2-[(3S)-3-(2-Pyridinylmethoxy)-1-pyrrolidinyl]-5-(trifluoromethyl)benzoic acid

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{18}H_{17}F_3N_2O_3$

Batch Molecular Weight: 366.33

Physical Appearance: Off White solid

Solubility: DMSO to 100 mM ethanol to 100 mM

Storage: Store at +4°C

Batch Molecular Structure:

2. ANALYTICAL DATA

HPLC: Shows 98.6% purity

¹H NMR: Consistent with structure Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 59.02 4.68 7.65 Found 59.11 4.72 7.5



Product Information

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IUPAC Name: 2-[(3S)-3-(2-Pyridinylmethoxy)-1-pyrrolidinyl]-5-(trifluoromethyl)benzoic acid

Description:

Selective endothelial lipase (EL) inhibitor ($IC_{50} = 237$ nM for human EL). Exhibits >20-fold selectivity for EL over lipoprotein lipase (LPL) and hepatic lipase (HL). Increases high density lipoprotein cholesterol (HDLc) plasma levels in mice. Orally bioavailable.

Physical and Chemical Properties:

Batch Molecular Formula: C₁₈H₁₇F₃N₂O₃ Batch Molecular Weight: 366.33 Physical Appearance: Off White solid

Minimum Purity: >98%

Batch Molecular Structure:

Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 100 mM ethanol 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:

Sun et al (2013) Discovery of XEN445: a potent and selective endothelial lipase inhibitor raises plasma HDL-cholesterol concentration in mice. Bioorg.Med.Chem. 21 7724. PMID: 24211162.

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