

Certificate of Analysis

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Print Date: Jan 15th 2016

Product Name: AC 261066 Catalog No.: 4046 Batch No.: 1

CAS Number: 870773-76-5

IUPAC Name: 4-[4-(2-Butoxyethoxy-)-5-methyl-2-thiazolyl]-2-fluorobenzoic acid

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{17}H_{20}FNO_4S$

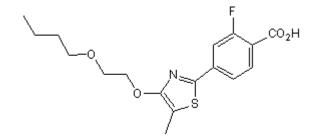
Batch Molecular Weight: 353.41
Physical Appearance: Yellow solid

Solubility: DMSO to 100 mM

ethanol to 100 mM

Storage: Store at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: $R_f = 0.03$ (Dichloromethane:Methanol [95:5])

HPLC: Shows 98.1% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 57.78 5.7 3.96 Found 57.94 5.72 3.9



Product Information

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Description:

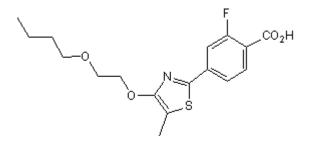
Potent RAR β 2 agonist (pEC $_{50}$ = 8.1). Selective over RAR β 1, RAR α and RAR γ (pEC $_{50}$ values are 6.4, 6.2 and 6.3 respectively). More potent and orally available than AC 55649 (Cat. No. 2436).

Physical and Chemical Properties:

Batch Molecular Formula: C₁₇H₂₀FNO₄S Batch Molecular Weight: 353.41 Physical Appearance: Yellow solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at RT

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:

Lund *et al* (2005) Discovery of a potent, orally available, and isoform-selective retinoic acid β2 receptor agonist. J.Med.Chem. *48* 7517. PMID: 16302793.

Lund *et al* (2009) Design, synthesis, and structure-activity analysis of isoform-selective retinoic acid receptor β ligands. J.Med.Chem. *52* 1540. PMID: 19239230.