1. PHYSICAL AND CHEMICAL PROPERTIES

   Batch Molecular Formula: \( C_{15}H_{11}NS \)
   Batch Molecular Weight: 237.32
   Physical Appearance: Beige solid
   Solubility: DMSO to 100 mM, ethanol to 50 mM
   Storage: Store at +4°C
   Batch Molecular Structure:

2. ANALYTICAL DATA

   Melting Point: At 160°C
   HPLC: Shows 98.2% purity
   \(^1\)H NMR: Consistent with structure
   Mass Spectrum: Consistent with structure
   Microanalysis:

      | Carbon | Hydrogen | Nitrogen |
      |-------|---------|---------|
      | Theoretical | 75.92 | 4.68 | 5.9 |
      | Found | 75.61 | 4.57 | 6.1 |

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use
Product Name: PD 146176

CAS Number: 4079-26-9

IUPAC Name: 6,11-Dihydro[1]benzothiopyrano[4,3-b]indole

Description:
Specific, non-competitive 15-lipoxygenase (15-LOX) inhibitor (K_i = 197nM) that has no demonstrable effect on 5-LOX, 12-LOX, COX-1 or COX-2 (IC_50 = 0.54 μM for 15-LOX in rabbit reticulocytes). Lacks non-specific antioxidant properties and prevents atherogenesis via regulation of monocyte-macrophage enrichment in vivo.

Physical and Chemical Properties:
Batch Molecular Formula: C_{10}H_{14}N_S
Batch Molecular Weight: 237.32
Physical Appearance: Beige solid
Minimum Purity: >98%

Batch Molecular Structure:

Storage: Store at +4°C

Solubility & Usage Info:
DMSO to 100 mM
ethanol to 50 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: