Product Name: PD 146176
CAS Number: 4079-26-9
IUPAC Name: 6,11-Dihydro[1]benzothiopyrano[4,3-b]indole

1. PHYSICAL AND CHEMICAL PROPERTIES

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

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:

<table>
<thead>
<tr>
<th></th>
<th>Theoretical</th>
<th>Found</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carbon</td>
<td>75.92</td>
<td>75.61</td>
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<tr>
<td>Hydrogen</td>
<td>4.68</td>
<td>4.57</td>
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<tr>
<td>Nitrogen</td>
<td>5.90</td>
<td>6.10</td>
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</tbody>
</table>
Product Name: PD 146176
Catalog No.: 2850  Batch No.: 1

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 \( (K_i = 197 \text{nM}) \) that has no demonstrable effect on 5-LOX, 12-LOX, COX-1 or COX-2 \( (IC_{50} = 0.54 \, \mu\text{M} \text{ for 15-LOX in rabbit reticulocytes}) \). Lacks non-specific antioxidant properties and prevents atherogenesis via regulation of monocyte-macrophage enrichment in vivo.

Physical and Chemical Properties:
Batch Molecular Formula: \( \text{C}_{15}\text{H}_{11}\text{NS} \)
Batch Molecular Weight: 237.32
Physical Appearance: Beige solid
Minimum Purity: >98%

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).

References: