Product Name: FR 122047 hydrochloride
Catalog No.: 1507
Batch No.: 3
CAS Number: 130717-51-0
IUPAC Name: 1-[[4,5-bis(4-Methoxyphenyl)-2-thiazolyl]carbonyl]-4-methylpiperazine hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

   Batch Molecular Formula: \( \text{C}_{23}\text{H}_{25}\text{N}_{3}\text{O}_{3}\text{S}\cdot\text{HCl}\cdot\text{H}_{2}\text{O} \)
   
   Batch Molecular Weight: 478.01
   
   Physical Appearance: Pale yellow solid
   
   Solubility:
   - Water to 10 mM
   - 1eq. HCl to 5 mM
   - DMSO to 100 mM
   - Ethanol to 25 mM
   
   Storage: Desiccate at +4°C
   
   Batch Molecular Structure:

2. ANALYTICAL DATA

   TLC: \( R_f = 0.6 \) (Dichloromethane:Methanol:Ammonia soln. [9:1:0.1])
   
   Melting Point: Greater than 250°C(dec)
   
   HPLC: Shows 100% purity
   
   \(^1\text{H NMR:}\) Consistent with structure
   
   Microanalysis:

<table>
<thead>
<tr>
<th></th>
<th>Carbon</th>
<th>Hydrogen</th>
<th>Nitrogen</th>
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<td>Found</td>
<td>57.93</td>
<td>5.89</td>
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</table>
Product Name: FR 122047 hydrochloride
CAS Number: 130717-51-0
IUPAC Name: 1-[[4,5-bis(4-Methoxyphenyl)-2-thiazolyl]carbonyl]-4-methylpiperazine hydrochloride

Description:
Selective cyclooxygenase-1 (COX-1) inhibitor (IC\textsubscript{50} values are 0.028 and 65 μM for COX-1 and COX-2 respectively). Antiplatelet, analgesic and anti-inflammatory following oral administration in vivo.

Physical and Chemical Properties:
Batch Molecular Formula: C\textsubscript{23}H\textsubscript{22}N\textsubscript{2}O\textsubscript{3}S.HCl.H\textsubscript{2}O
Batch Molecular Weight: 478.01
Physical Appearance: Pale yellow solid
Minimum Purity: >98%

Storage: Desiccate at +4°C

Solubility & Usage Info:
water to 10 mM
1eq. HCl to 5 mM
DMSO to 100 mM
ethanol to 25 mM
CAUTION - Avoid heating, this product appears to polymerise at 100°C when in solid form and at lower temperatures in solution.

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: