

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: C₂₃H₂₅N₃O₃S.HCl.H₂O

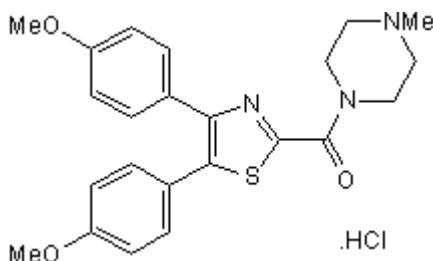
Batch Molecular Weight: 478.01

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

¹H NMR: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	57.79	5.9	8.79
Found	57.93	5.89	8.9

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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Description:

Selective cyclooxygenase-1 (COX-1) inhibitor (IC₅₀ 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:

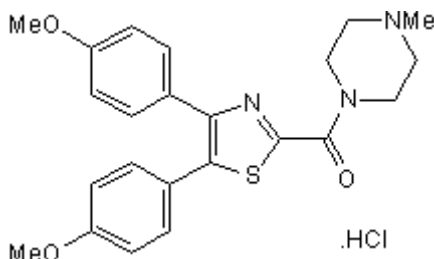
Batch Molecular Formula: C₂₃H₂₅N₃O₃S.HCl.H₂O

Batch Molecular Weight: 478.01

Physical Appearance: Pale yellow solid

Minimum Purity: >98%

Batch Molecular Structure:



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:

Dohi et al (1993) The anti-platelet actions of FR122047, a novel cyclooxygenase inhibitor. *Eur.J.Pharmacol.* **243** 179. PMID: 8276067.

Tanaka et al (1994) Antiplatelet agents based on cyclooxygenase inhibition without ulcerogenesis. Evaluation and synthesis of 4,5-bis(4-methoxyphenyl)-2-substituted-thiazoles. *J.Med.Chem.* **37** 1189. PMID: 8164261.

Ochi et al (2000) The analgesic effect profile of FR122047, a selective cyclo-oxygenase-1 inhibitor, in chemical nociceptive models. *Eur.J.Pharmacol.* **391** 49. PMID: 10720634.

Ochi and Goto (2002) Differential effect of FR122047, a selective cyclo-oxygenase-1 inhibitor, in rat chronic models of arthritis. *Br.J.Pharmacol.* **135** 782. PMID: 11834626.

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