

## Certificate of Analysis

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**Product Name:** DuP 697

**Catalog No.:** 1430

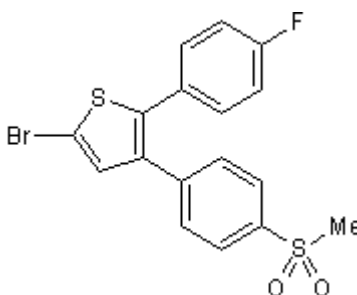
**Batch No.:** 1

CAS Number: 88149-94-4

IUPAC Name: 5-Bromo-2-(4-fluorophenyl)-3-[4-(methylsulfonyl)phenyl]-thiophene

### 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>17</sub>H<sub>12</sub>BrFO<sub>2</sub>S<sub>2</sub>  
**Batch Molecular Weight:** 411.3  
**Physical Appearance:** White solid  
**Solubility:** DMSO to 100 mM  
**Storage:** Store at +4°C  
**Batch Molecular Structure:**



### 2. ANALYTICAL DATA

**TLC:** R<sub>f</sub> = 0.27 (Ethyl acetate:Petroleum ether [1:3])  
**Melting Point:** At 135°C  
**HPLC:** Shows >99.3% purity  
**<sup>1</sup>H NMR:** Consistent with structure  
**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	49.64	2.94	
Found	49.48	2.89	

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

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**Description:**

Potent and selective inhibitor of cyclooxygenase-2 (IC<sub>50</sub> values are 10 and 800 nM for COX-2 and COX-1 respectively). Inhibits prostaglandin synthesis and is anti-inflammatory in vivo. Orally active.

**Physical and Chemical Properties:**

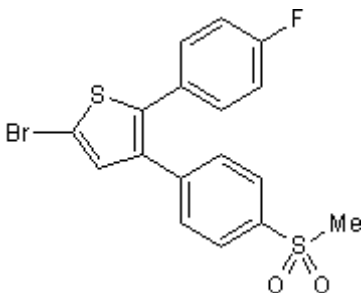
Batch Molecular Formula: C<sub>17</sub>H<sub>12</sub>BrFO<sub>2</sub>S<sub>2</sub>

Batch Molecular Weight: 411.3

Physical Appearance: White solid

**Minimum Purity:** >99%

**Batch Molecular Structure:**



**Storage:** Store at +4°C

**Solubility & Usage Info:**

DMSO 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:**

**Gans *et al*** (1990) Anti-inflammatory and safety profile of DuP 697, a novel orally effective prostaglandin synthesis inhibitor. *J.Pharmacol.Exp.Ther.* **254** 180. PMID: 2366180.

**Gierse *et al*** (1995) Expression and selective inhibition of the constitutive and inducible forms of human cyclo-oxygenase. *Biochem.J.* **305** 479. PMID: 7832763.

**Rossoni *et al*** (2002) Inhibition of cyclo-oxygenase-2 exacerbates ischaemia-induced acute myocardial dysfunction in the rabbit. *Br.J.Pharmacol.* **135** 1540. PMID: 11906968.

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