

# **Certificate of Analysis**

Print Date: Aug 18th 2017

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Product Name: DG 041 Catalog No.: 6240 Batch No.: 1

CAS Number: 861238-35-9

IUPAC Name: (2E)-3-[1-[(2,4-Dichlorophenyl)methyl]-5-fluoro-3-methyl-1H-indol-7-yl]-N-[(4,5-dichloro-2-thienyl)sulfonyl]-2-

propenamide

## 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>23</sub>H<sub>15</sub>Cl<sub>4</sub>FN<sub>2</sub>O<sub>3</sub>S<sub>2</sub>

Batch Molecular Weight: 592.32

Physical Appearance: Yellow solid

Solubility: DMSO to 100 mM Storage: Store at +4°C

**Batch Molecular Structure:** 

## 2. ANALYTICAL DATA

**TLC:**  $R_f = 0.55$  (Dichloromethane:Methanol [9:1])

**HPLC:** Shows 99.3% purity

<sup>1</sup>H NMR: Consistent with structure Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 46.64 2.55 4.73 Found 46.73 2.51 4.52

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## **Product Information**

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propenamide

#### **Description:**

Potent and selective  $EP_3$  antagonist ( $IC_{50}$  = 4.6 nM). Inhibits  $PGE_2$  facilitation of platelet aggregation in vitro and ex vivo. Displays good plasma and metabolic stability. Does not affect bleeding time in rats. Antiplatelet and antithrombotic.

## **Physical and Chemical Properties:**

Batch Molecular Formula: C<sub>23</sub>H<sub>15</sub>Cl<sub>4</sub>FN<sub>2</sub>O<sub>3</sub>S<sub>2</sub>

Batch Molecular Weight: 592.32 Physical Appearance: Yellow solid

Minimum Purity: >98%

#### **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:

**Markovič** *et al* (2017) Structural features of subtype-selective EP receptor modulators. Drug Discov.Today. **22** 57. PMID: 27506873. **Singh** *et al* (2009) Antagonists of the EP<sub>3</sub> receptor for prostaglandin E<sub>2</sub> are novel antiplatelet agents that do not prolong bleeding. ACS Chem. Biol. **4** 115. PMID: 19193156.

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