

# **Certificate of Analysis**

Print Date: Mar 19th 2020

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Product Name: ASP 7663 Catalog No.: 5178 Batch No.: 3

CAS Number: 1190217-35-6

IUPAC Name: (2E)-2-[7-Fluoro-1,2-dihydro-1-(2-methylpropyl)-2-oxo-3H-indol-3-ylidene]acetic acid

### 1. PHYSICAL AND CHEMICAL PROPERTIES

 $\textbf{Batch Molecular Formula:} \qquad \qquad C_{14}H_{14}FNO_3$ 

Batch Molecular Weight: 263.26

Physical Appearance: Orange solid

Solubility: DMSO to 100 mM

ethanol to 100 mM

Storage: Store at +4°C

**Batch Molecular Structure:** 

#### 2. ANALYTICAL DATA

**HPLC:** Shows 99.2% purity

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

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 63.87 5.36 5.32 Found 63.63 5.38 5.3

www.tocris.com/distributors Tel:+1 612 379 2956



## **Product Information**

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IUPAC Name: (2E)-2-[7-Fluoro-1,2-dihydro-1-(2-methylpropyl)-2-oxo-3H-indol-3-ylidene]acetic acid

#### **Description:**

Selective TRPA1 activator (EC $_{50}$  values are ~0.5  $\mu$ M in human, mouse and rat). Displays little or no affinity at more than 60 other related receptors, channels and enzymes. Stimulates 5-HT release from QGP-1 cells. Exhibits an abdominal analgesic effect in vivo. Orally bioavailable.

#### **Physical and Chemical Properties:**

Batch Molecular Formula: C<sub>14</sub>H<sub>14</sub>FNO<sub>3</sub> Batch Molecular Weight: 263.26 Physical Appearance: Orange solid

Minimum Purity: ≥98%

#### **Batch Molecular Structure:**

Storage: Store at +4°C

CAUTION - This product is light sensitive and we recommend that the solid material and any solutions obtained are protected from exposure to light.

#### Solubility & Usage Info:

DMSO to 100 mM ethanol 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:

**Kojima** *et al* (2014) Effects of novel TRPA1 receptor agonist ASP7663 in models of drug-induced constipation and visceral pain. Eur.J.Pharmacol. **723** 288. PMID: 24291101.