

Certificate of Analysis

Print Date: May 20th 2021

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Product Name: LM 10 Catalog No.: 5794 Batch No.: 1

CAS Number: 1316695-35-8

IUPAC Name: 6-Fluoro-3-[(1E)-2-(2H-tetrazol-5-yl)ethenyl]-1H-indole

1. PHYSICAL AND CHEMICAL PROPERTIES

 $C_{11}H_8FN_5$ **Batch Molecular Formula: Batch Molecular Weight:** 229.21

Off White solid **Physical Appearance:** Solubility: DMSO to 100 mM

ethanol to 20 mM with gentle warming

Storage: Store at -20°C

Batch Molecular Structure:

2. ANALYTICAL DATA

HPLC: Shows 99.7% purity

¹H NMR: Consistent with structure Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

> Theoretical 57.64 3.52 30.55 Found 57.78 3.78 30.55



Product Information

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CAS Number: 1316695-35-8

IUPAC Name: 6-Fluoro-3-[(1*E*)-2-(2*H*-tetrazol-5-yl)ethenyl]-1*H*-indole

Description:

Selective tryptophan 2,3-dioxygenase (TDO) inhibitor (IC_{50} values are 0.62 and 2 μ M for human and mouse TDO, respectively). Exhibits selectivity for TDO over IDO, MAO-A, MAO-B, and a panel of receptors and transporters. Reduces growth of TDO-expressing P815 mastocytoma tumors in mice. Orally bioavailable.

Physical and Chemical Properties:

Batch Molecular Formula: C₁₁H₈FN₅ Batch Molecular Weight: 229.21 Physical Appearance: Off White solid

Minimum Purity: ≥98%

Batch Molecular Structure:

Storage: Store at -20°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 20 mM with gentle warming

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:

Pilotte et al (2012) Reversal of tumoral immune resistance by inhibition of tryptophan 2,3-dioxygenase. Proc.Natl.Acad.Sci.U.S.A. 109 2497. PMID: 22308364.

Dolusić *et al* (2011) Tryptophan 2,3-dioxygenase (TDO) inhibitors. 3-(2-(pyridyl)ethenyl)indoles as potential anticancer immunomodulators. J.Med.Chem. *54* 5320. PMID: 21726069 .

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