

Certificate of Analysis

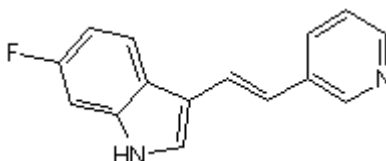
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Product Name: 680C91
CAS Number: 163239-22-3
IUPAC Name: 6-Fluoro-3-[(1*E*)-2-(3-pyridinyl)ethenyl]-1*H*-indole

Catalog No.: 4392 **Batch No.:** 2

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₅H₁₁FN₂
Batch Molecular Weight: 238.26
Physical Appearance: Brown solid
Solubility: DMSO to 100 mM
 ethanol to 50 mM
Storage: Store at +4°C
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.3 (Ethyl acetate:Petroleum ether [1:3])
HPLC: Shows >99.6% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	75.62	4.65	11.75
Found	75.38	4.53	11.88

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

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

Description:

Potent and selective inhibitor of tryptophan 2,3-dioxygenase (TDO) ($K_i = 51$ nM). Exhibits no activity against indoleamine 2,3-dioxygenase, monoamine oxidase A and B, 5-HT uptake or 5-HT_{1A}, 1D, 2A and 2C receptors. Produces large increases in brain tryptophan and serotonin in vitro and in vivo in the rat.

Physical and Chemical Properties:

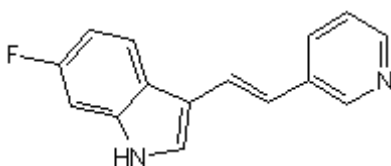
Batch Molecular Formula: C₁₅H₁₁FN₂

Batch Molecular Weight: 238.26

Physical Appearance: Brown solid

Minimum Purity: >98%

Batch Molecular Structure:



References:

Opitz et al (2011) An endogenous tumour-promoting ligand of the human aryl hydrocarbon receptor. *Nature* **478** 197. PMID: 21976023.

Salter et al (1995) The effects of a novel and selective inhibitor of tryptophan 2,3-dioxygenase on tryptophan and serotonin metabolism in the rat. *Biochem.Pharmacol.* **17** 1435. PMID: 7539265.

Salter et al (1995) The effects of an inhibitor of tryptophan 2,3-dioxygenase and a combined inhibitor of tryptophan 2,3-dioxygenase and 5-HT reuptake in the rat. *Neuropharmacology* **34** 217. PMID: 7617147.

Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 100 mM

ethanol to 50 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.

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