# TOCRIS a biotechne brand

## **Certificate of Analysis**

## www.tocris.com

Print Date: Mar 24th 2016

#### Product Name: ML 354

Catalog No.: 5387 Batch No.: 1

CAS Number: 89159-60-4 **IUPAC Name:** 1-Methyl-5-nitro-3-phenyl-1H-indole-2-methanol

### 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula: Batch Molecular Weight: Physical Appearance:** Solubility:

**Batch Molecular Structure:** 

C<sub>16</sub>H<sub>14</sub>N<sub>2</sub>O<sub>3</sub>.¼H<sub>2</sub>O 286.79 Yellow solid DMSO to 100 mM ethanol to 10 mM with gentle warming Store at -20°C



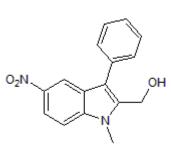
HPLC: <sup>1</sup>H NMR: Mass Spectrum: **Microanalysis:** 

Shows 98.3% purity Consistent with structure Consistent with structure

	Carbon H	ydrogen I	Nitrogen
Theoretical	67.01	5.1	9.77
Found	67.33	4.88	9.82

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

bio-techne.com	North America	China	Europe Middle East Africa	Rest of World
info@bio-techne.com techsupport@bio-techne.com	Tel: (800) 343 7475	info.cn@bio-techne.com Tel: +86 (21) 52380373	Tel: +44 (0)1235 529449	www.tocris.com/distributors Tel:+1 612 379 2956



Storage:

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Catalog No.: 5387 B

Batch No.: 1

CAS Number: 89159-60-4 IUPAC Name: 1-Methyl-5-nitro-3-phenyl-1*H*-indole-2-methanol

#### **Description:**

Selective PAR<sub>4</sub> antagonist (IC<sub>50</sub> = 140 nM). Exhibits 70-fold selectivity for PAR<sub>4</sub> over PAR<sub>1</sub>.

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

Batch Molecular Formula:  $C_{16}H_{14}N_2O_3$ . <sup>1</sup>/<sub>4</sub> $H_2O$ Batch Molecular Weight: 286.79 Physical Appearance: Yellow solid

Minimum Purity: >98%

**Batch Molecular Structure:** 

# O<sub>2</sub>N OH

#### 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 10 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:**

Wen et al (2014) Substituted indoles as selective protease activated receptor 4 (PAR<sub>4</sub>) antagonists: Discovery and SAR of ML354. Bioorg.Med.Chem.Lett. **24** 4708. PMID: 25176330.

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info@bio-techne.com techsupport@bio-techne.com	Tel: (800) 343 7475	info.cn@bio-techne.com Tel: +86 (21) 52380373	Tel: +44 (0)1235 529449	www.tocris.com/distributors Tel:+1 612 379 2956