



# **Certificate of Analysis**

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Product Name: L-732,138 Catalog No.: 0868 Batch No.: 3

CAS Number: 148451-96-1

IUPAC Name: N-Acetyl-L-tryptophan 3,5-bis(trifluoromethyl)benzyl ester

## 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:**  $C_{22}H_{18}F_6N_2O_3$ 

**Batch Molecular Weight:** 472.39 **Physical Appearance:** White solid

**Solubility:** ethanol to 100 mM

DMSO to 100 mM

Storage: Store at RT

**Batch Molecular Structure:** 

## 2. ANALYTICAL DATA

**TLC:**  $R_f = 0.73$  (Ethyl acetate:Petroleum ether [4:1])

HPLC: Shows >99.9% purity

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

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 55.94 3.84 5.93 Found 56.09 3.88 6.07

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



## **Product Information**

Print Date: Jun 17th 2019

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CAS Number: 148451-96-1

IUPAC Name: N-Acetyl-L-tryptophan 3,5-bis(trifluoromethyl)benzyl ester

## **Description:**

Potent and highly selective competitive tachykinin  $NK_1$  receptor antagonist ( $IC_{50} = 2.3 \text{ nM}$ ).

## **Physical and Chemical Properties:**

Batch Molecular Formula: C<sub>22</sub>H<sub>18</sub>F<sub>6</sub>N<sub>2</sub>O<sub>3</sub>

Batch Molecular Weight: 472.39 Physical Appearance: White solid

**Minimum Purity: >98%** 

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

Storage: Store at RT

## Solubility & Usage Info:

ethanol to 100 mM 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.

#### **Licensing Information:**

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### References:

**Kuo** et al (1998) Lipopolysaccharide enhances neurogenic plasma exudation in guinea-pig airways. Br.J.Pharmacol. **125** 711. PMID: 9831906.

**Cascieri** *et al* (1994) Characterization of the interaction of *N-acyl-*L-tryptophan benzyl ester neurokinin antagonists with the human neurokinin-1 receptor. J.Biol.Chem. **269** 6587. PMID: 7509807.

**MacLeod** *et al* (1994) Identification of L-tryptophan derivatives with potent and selective antagonist activity at the NK<sub>1</sub> receptor. J.Med.Chem. **37** 1269. PMID: 7513763.

MacLeod et al (1993) N-Acyl-L-tryptophan benzyl esters: potent substance P receptor antagonists. J.Med.Chem. 36 2044. PMID: 8393115.

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