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Certificate of Analysis

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Product Name: Gavestinel

Catalog No.: 2348 Batch No.: 1

CAS Number: IUPAC Name: 153436-38-5

4,6-Dichloro-3-[(1E)-3-oxo-3-(phenylamino)-1-propenyl]-1H-indole-2-carboxylic acid sodium salt

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: Batch Molecular Weight: Physical Appearance: Solubility: Storage: Batch Molecular Structure: C₁₈H₁₁Cl₂N₂O₃Na.1³/₄H₂O 428.71 Yellow solid DMSO to 40 mM Desiccate at RT



2. ANALYTICAL DATA

TLC:	R _f = 0.5 (Dichloromethane:Methanol [9:1])		
Melting Point:	Greater than 320°C		
HPLC:	Shows >99% purity		
¹ H NMR:	Consistent with structure		
Mass Spectrum:	Consistent with structure		
Microanalysis:	Carbon Hydrogen Nitrogen		

Iheoretical	50.43	3.41	6.53
Found	50.42	3.23	6.45

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

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Print Date: Jan 15th 2016

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4,6-Dichloro-3-[(1E)-3-oxo-3-(phenylamino)-1-propenyl]-1H-indole-2-carboxylic acid sodium salt

Description:

Highly potent and selective non-competitive antagonist acting at the strychnine-insensitive glycine binding site of the NMDA receptor-channel complex ($K_d = 0.8$ nM). Displays > 1000-fold selectivity over NMDA, AMPA and kainate binding sites. Orally bioavailable and active in vivo.

Physical and Chemical Properties:

Batch Molecular Formula: C₁₈H₁₁Cl₂N₂O₃Na.1¾H₂O Batch Molecular Weight: 428.71 Physical Appearance: Yellow solid

153436-38-5

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Desiccate at RT

Solubility & Usage Info: DMSO to 40 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).

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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:

Di Fabio *et al* (1997) Substituted indole-2-carboxylates as *in vivo* potent antagonists acting at the strychnine-insensitive glycine binding site. J.Med.Chem. **40** 841. PMID: 9083472.

Mugnaini *et al* (2000) Receptor binding characteristics of the novel NMDA receptor glycine site antagonist [³H]GV150526A in rat cerebral cortical membranes. Eur.J.Pharmacol. **391** 233. PMID: 10729363.

Kajbaf et al (2003) Pharmacokinetics, metabolism and excretion of the glycine antagonist GV150526A in rat and dog. Xenobiotica. 33 415. PMID: 12745876.

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