

Certificate of Analysis

Print Date: Jan 15th 2016

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Product Name: TCS 1205 Catalog No.: 3941 Batch No.: 1

CAS Number: 355022-97-8

IUPAC Name: 5-Nitro- α -oxo-N-(1R)-phenylethyl]-1H-indole-3-acetamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{18}H_{15}N_3O_4$ Batch Molecular Weight:337.33Physical Appearance:Yellow solid

Solubility: DMSO to 100 mM

Storage: Store at RT

Batch Molecular Structure:

2. ANALYTICAL DATA

TLC: $R_f = 0.6$ (Dichloromethane:Methanol [9:1])

HPLC: Shows 99.6% purity
Chiral HPLC: Shows >99.5% purity

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

Optical Rotation: $[\alpha]_D = -45.7$ (Concentration = 1.2, Solvent = DMF)

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 64.09 4.48 12.46 Found 63.97 4.54 12.41



Product Information

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Description:

 GABA_A $\alpha 2$ agonist and GABA_A $\alpha 1$ partial agonist in vitro (K_i values are 14 and 121 nM respectively). Exhibits non-sedative anxiolytic activity in vivo.

Physical and Chemical Properties:

Batch Molecular Formula: C₁₈H₁₅N₃O₄ Batch Molecular Weight: 337.33 Physical Appearance: Yellow solid

Minimum Purity: >99%

Batch Molecular Structure:

Storage: Store at RT

Solubility & Usage Info:

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.

References:

Primofiore *et al* (2001) Novel *N*-(arylalkyl)indol-3-ylglyoxylamides targeted as ligands of the benzodiazepine receptor: synthesis, biological evaluation, and molecular modeling analysis of the structure-activity relationships. J.Med.Chem. *44* 2286. PMID: 11428922.

Taliani *et al* (2009) Identification of anxiolytic/nonsedative agents among indol-3-ylglyoxylamides acting as functionally selective agonists at the γ-aminobutyric acid-A (GABA_A) κ_2 benzodiazepine receptor. J.Med.Chem. **52** 3723. PMID: 19469479.