

Certificate of Analysis

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Product Name: TCN 213

Catalog No.: 4163

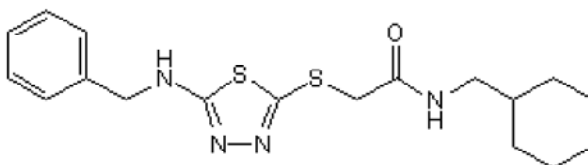
Batch No.: 1

CAS Number: 556803-08-8

IUPAC Name: N-(Cyclohexylmethyl)-2-[(5-[(phenylmethyl)amino]-1,3,4-thiadiazol-2-yl)thio]acetamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₈H₂₄N₄OS₂
Batch Molecular Weight: 376.54
Physical Appearance: Pale yellow solid
Solubility: DMSO to 75 mM
 ethanol to 10 mM
Storage: Store at +4°C
Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.2% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon Hydrogen Nitrogen		
Theoretical	57.42	6.42	14.88
Found	57.46	6.39	14.93

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

bio-techne.com

info@bio-techne.com

techsupport@bio-techne.com

North America

Tel: (800) 343 7475

China

info.cn@bio-techne.com

Tel: +86 (21) 52380373

Europe Middle East Africa

Tel: +44 (0)1235 529449

Rest of World

www.tocris.com/distributors

Tel: +1 612 379 2956

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CAS Number: 556803-08-8

IUPAC Name: N-(Cyclohexylmethyl)-2-[(5-[(phenylmethyl)amino]-1,3,4-thiadiazol-2-yl)thio]acetamide

Description:

NMDA receptor antagonist, selective for GluN1/GluN2A (formally NR1/NR2A) (pIC_{50} = 5.4) over GluN1/GluN2B (formally NR1/NR2B) containing receptors. Please refer to IUPHAR Guide to Pharmacology for the most recent naming conventions.

Physical and Chemical Properties:

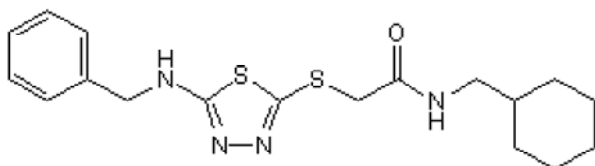
Batch Molecular Formula: C₁₈H₂₄N₄OS₂

Batch Molecular Weight: 376.54

Physical Appearance: Pale yellow solid

Minimum Purity: >99%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 75 mM

ethanol to 10 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:

McKay *et al* (2012) Direct pharmacological monitoring of the developmental switch in NMDAR subunit composition using TCN 213, a GluN2A-selective, glycine-dependent antagonist. *Br.J.Pharmacol.* **166** 924. PMID: 22022974.

Bettini *et al* (2010) Identification and characterization of novel NMDA receptor antagonists selective for NR2A- over NR2B-containing receptors. *J.Pharmacol.Exp.Ther.* **335** 644. PMID: 20810618.

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North America

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