

Certificate of Analysis

Print Date: Feb 24th 2020

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Product Name: SU 3327 Catalog No.: 3607 Batch No.: 1

CAS Number: 40045-50-9

IUPAC Name: 5-[(5-Nitro-2-thiazolyl)thio]-1,3,4thiadiazol-2-amine

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_5H_3N_5O_2S_3$

Batch Molecular Weight: 261.3

Physical Appearance: Yellow solid

Solubility: DMSO to 100 mM

ethanol to 10 mM

Storage: Store at RT

Batch Molecular Structure:

 O_2N S S N N N N

2. ANALYTICAL DATA

TLC: $R_f = 0.32$ (Ethyl acetate:Hexane [9:1])

HPLC: Shows 99.5% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 22.98 1.16 26.8 Found 23.05 1.17 26.72

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Product Information

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IUPAC Name: 5-[(5-Nitro-2-thiazolyl)thio]-1,3,4thiadiazol-2-amine

Description:

Selective inhibitor of c-Jun N-terminal kinase (JNK) ($IC_{50} = 0.7 \mu M$). Inhibits the protein-protein interaction between JNK and JIP ($IC_{50} = 239 \mu M$). Displays selectivity over p38 MAPK and Akt. Restores insulin sensitivity in a mouse model of type-2 diabetes. Displays antibiotic activity against a range of bacteria including S.aureus, A.baumanni, C.difficile and M.tuberculosis.

Physical and Chemical Properties:

Batch Molecular Formula: C₅H₃N₅O₂S₃

Batch Molecular Weight: 261.3 Physical Appearance: Yellow solid

Minimum Purity: ≥99%

Batch Molecular Structure:

Storage: Store at RT

Solubility & Usage Info:

DMSO to 100 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:

De *et al* (2009) Design, synthesis and structure-activity relationship of substrate competitive, selective, and in vivo active triazole and thiadiazole inhibitors of the c-jun N-terminal kinase. J.Med.Chem. *52* 1943. PMID: 19271755.