

Certificate of Analysis

Print Date: Aug 8th 2018

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Product Name: SR 9009 Catalog No.: 5855 Batch No.: 1

CAS Number: 1379686-30-2

IUPAC Name: Ethyl 3-[[[(4-chlorophenyl)methyl][(5-nitro-2-thienyl)methyl]amino]methyl]-1-pyrrolidinecarboxylate

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₀H₂₄ClN₃O₄S

Batch Molecular Weight: 437.94

Physical Appearance: Off White solid

Solubility: DMSO to 100 mM

ethanol to 100 mM

Storage: Store at +4°C

Batch Molecular Structure:

2. ANALYTICAL DATA

HPLC: Shows 99.8% purity

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

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 54.85 5.52 9.6 Found 55.22 5.49 9.62

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Product Information

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IUPAC Name: Ethyl 3-[[(4-chlorophenyl)methyl][(5-nitro-2-thienyl)methyl]amino]methyl]-1-pyrrolidinecarboxylate

Description:

Rev-Erb α/β agonist (EC $_{50}$ = 710 nM; K $_{d}$ = 800 nM). Alters circadian locomotor activity and core clock hypothalamic gene expression in mice. Induces weight loss in diet-induced obese mice. Brain penetrant.

Physical and Chemical Properties:

Batch Molecular Formula: C₂₀H₂₄ClN₃O₄S

Batch Molecular Weight: 437.94 Physical Appearance: Off White solid

Minimum Purity: >98%

Batch Molecular Structure:

Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 100 mM ethanol 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:

Shin et al (2012) Small molecule tertiary amines as agonists of the nuclear hormone receptor Rev-erbα. Bioorg.Med.Chem.Lett. 22 4413. PMID: 22633688.

Solt et al (2012) Regulation of circadian behaviour and metabolism by synthetic REV-ERB agonists. Nature 485 62. PMID: 22460951.

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