

# Certificate of Analysis

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**Product Name:** GSK 4112

**Catalog No.:** 3663

**Batch No.:** 1

CAS Number: 1216744-19-2

IUPAC Name: 1,1-Dimethylethyl-*N*-[(4-chlorophenyl)methyl]-*N*-[(5-nitro-2-thienyl)methyl]glycinate

## 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>18</sub>H<sub>21</sub>ClN<sub>2</sub>O<sub>4</sub>S

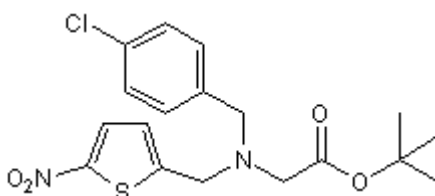
**Batch Molecular Weight:** 396.89

**Physical Appearance:** Off-white solid

**Solubility:** DMSO to 25 mM

**Storage:** Store at +4°C

**Batch Molecular Structure:**



## 2. ANALYTICAL DATA

**TLC:** R<sub>f</sub> = 0.61 (Ethyl acetate:Petroleum ether [1:1])

**HPLC:** Shows 98.9% purity

**<sup>1</sup>H NMR:** Consistent with structure

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	54.47	5.33	7.06
Found	54.47	5.34	7.13

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**Description:**

Selective Rev-Erb $\alpha$  agonist (EC<sub>50</sub> = 250 nM). Enhances recruitment of nuclear receptor co-repressor (NCoR) peptide to Rev-Erb $\alpha$ ; causes acute suppression of Bmal1 gene transcription. Induces phase shifts in the circadian clock.

**Physical and Chemical Properties:**

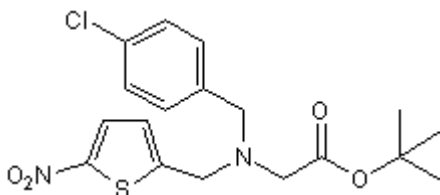
Batch Molecular Formula: C<sub>18</sub>H<sub>21</sub>ClN<sub>2</sub>O<sub>4</sub>S

Batch Molecular Weight: 396.89

Physical Appearance: Off-white solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**



**Storage:** Store at +4°C

**Solubility & Usage Info:**

DMSO to 25 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:**

**Meng *et al*** (2008) Ligand modulation of REV-ERB $\alpha$  function resets the peripheral circadian clock in a phasic manner. *J.Cell Science* **121** 3629.

**Kojetin *et al*** (2011) Identification of SR8278, a synthetic antagonist of the nuclear heme receptor REV-ERB. *ACS Chem.Biol.* **6** 131. PMID: 21043485.

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