TOCRIS
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Print Date: Oct 7th 2021

Certificate of Analysis

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Product Name: **GPR52 Comp-43** **Catalog No.: 7445** **Batch No.: 1**

CAS Number: 1239987-91-7

IUPAC Name: (2*E*)-5-Phenyl-1-(2-thienyl)-2-penten-1-one

1. PHYSICAL AND CHEMICAL PROPERTIES

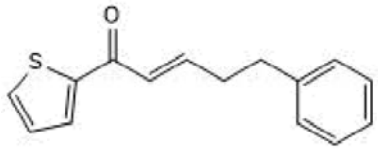
Batch Molecular Formula: $C_{15}H_{14}OS$.

Batch Molecular Weight: 242.34

Physical Appearance: White solid

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.9% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	74.35	5.82	
Found	74.35	5.84	

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Product Information

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CAS Number: 1239987-91-7

IUPAC Name: (2*E*)-5-Phenyl-1-(2-thienyl)-2-penten-1-one

Description:

GPR52 Comp-43 is a GPR52 receptor antagonist (IC_{50} = 0.63 µM). The use of GPR52 Comp-43 in animal models of Huntington's Disease leads to degradation and reduction of soluble and aggregated mutant huntingtin protein in the striatum. It also reduces neuronal loss, promotes neuronal survival and improves motor functions in vivo. GPR52 Comp-43 is active in vitro and brain penetrant.

Physical and Chemical Properties:

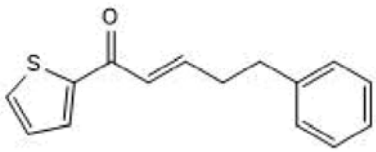
Batch Molecular Formula: $C_{15}H_{14}OS$.

Batch Molecular Weight: 242.34

Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°C

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:

Komatsu (2021) Discovery of the first druggable GPR52 antagonist to treat Huntington's disease. J.Med.Chem. ***64*** 938. PMID: 33443413.

Wang *et al* (2021) GPR52 antagonist reduces huntingtin levels and ameliorates Huntington's disease-related phenotypes. J.Med.Chem. ***64*** 941. PMID: 33185430.

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