

Product Name: GPR52 Comp-43

Catalog No.: 7445

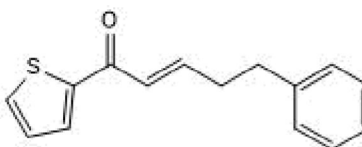
Batch No.: 1

CAS Number: 1239987-91-7

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

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₅H₁₄OS.
Batch Molecular Weight: 242.34
Physical Appearance: White solid
Solubility: DMSO to 100 mM
 ethanol to 100 mM
Storage: Store at -20°C
Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.9% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	74.35	5.82	
Found	74.35	5.84	

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

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

Description:

GPR52 Comp-43 is a GPR52 receptor antagonist ($IC_{50} = 0.63 \mu M$). 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:

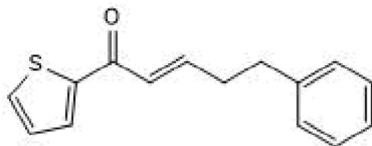
Batch Molecular Formula: $C_{15}H_{14}OS$.

Batch Molecular Weight: 242.34

Physical Appearance: White solid

Minimum Purity: $\geq 98\%$

Batch Molecular Structure:



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.

Storage: Store at $-20^{\circ}C$

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 $45-60^{\circ}C$ water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. *Unless contradicted by product-specific protocols or instructions, our standard recommendations apply:

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 $-20^{\circ}C$ or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

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