

Certificate of Analysis

Product Name: S 07662

Catalog No.: 5188

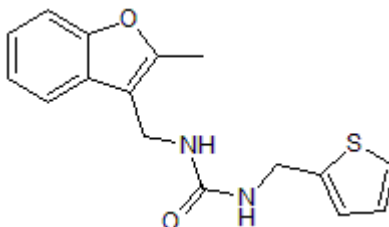
Batch No.: 1

CAS Number: 883226-64-0

IUPAC Name: *N*-[(2-Methyl-3-benzofuranyl)methyl]-*N*-(2-thienylmethyl)urea

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₆H₁₆N₂O₂S
Batch Molecular Weight: 300.38
Physical Appearance: White solid
Solubility: DMSO to 100 mM
ethanol to 50 mM
Storage: Store at +4°C
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.46 (Ethyl acetate:Petroleum ether [2:3])
HPLC: Shows 98.3% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	63.98	5.37	9.33
Found	64.03	5.42	9.3

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

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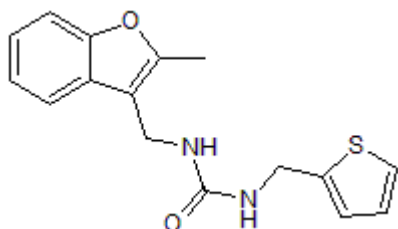
IUPAC Name: *N*-[(2-Methyl-3-benzofuranyl)methyl]-*N*-(2-thienylmethyl)urea**Description:**

Inverse agonist of the constitutive androstane receptor (CAR). Inhibits CAR activity via recruitment of nuclear receptor co-repressor (NCoR). Suppresses CITCO-induced CYP2B6 gene expression in human primary hepatocytes.

Physical and Chemical Properties:Batch Molecular Formula: C₁₆H₁₆N₂O₂S

Batch Molecular Weight: 300.38

Physical Appearance: White solid

Minimum Purity: >98%**Batch Molecular Structure:****References:**

Küblbeck *et al* (2011) New in vitro tools to study human constitutive androstane receptor (CAR) biology: discovery and comparison of human CAR inverse agonists. *Mol.Pharm.* **8** 2424. PMID: 22044162.

Storage: Store at +4°C**Solubility & Usage Info:**

DMSO to 100 mM

ethanol to 50 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.

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