

# Certificate of Analysis

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**Product Name:** SHA 68

**Catalog No.:** 4510

**Batch No.:** 1

CAS Number: 847553-89-3

IUPAC Name: *N*-[(4-Fluorophenyl)methyl]tetrahydro-3-oxo-1,1-diphenyl-3*H*-oxazolo[3,4-*a*]pyrazine-7(1*H*)-carboxamide

## 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>26</sub>H<sub>24</sub>FN<sub>3</sub>O<sub>3</sub>·¼H<sub>2</sub>O

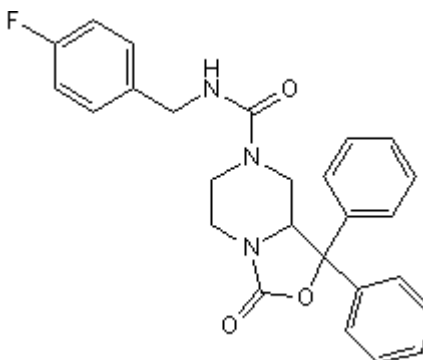
**Batch Molecular Weight:** 449.99

**Physical Appearance:** 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

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

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	69.4	5.49	9.34
Found	69.33	5.38	9.33

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

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**Description:**

Selective neuropeptide S receptor (NPSR) antagonist (IC<sub>50</sub> values are 22.0 and 23.8 nM for human NPSR Asn107 and Ile107 variants respectively). Displays no activity against a range of 14 GPCRs, including vasopressin and oxytocin receptors.

**Physical and Chemical Properties:**

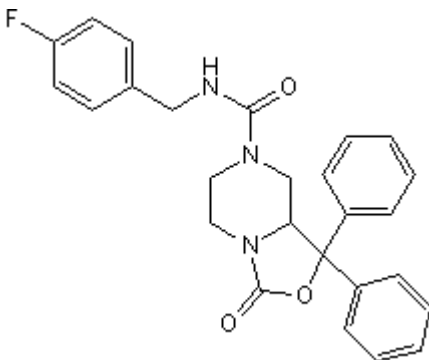
Batch Molecular Formula: C<sub>26</sub>H<sub>24</sub>FN<sub>3</sub>O<sub>3</sub>·¼H<sub>2</sub>O

Batch Molecular Weight: 449.99

Physical Appearance: 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:**

**Okamura et al (2008)** Synthesis and pharmacological in vitro and in vivo profile of 3-oxo-1,1-diphenyl-tetrahydro-oxazolo[3,4-*a*]pyrazine-7-carboxylic acid 4-fluoro-benzylamide (SHA 68), a selective antagonist of the neuropeptide S receptor. *J.Pharmacol.Exp.Ther.* **325** 893. PMID: 18337476.

**Okamura et al (2011)** Neuropeptide S enhances memory during the consolidation phase and interacts with noradrenergic systems in the brain. *Neuropsychopharmacology* **36** 744. PMID: 21150909.

**Trapella et al (2011)** Synthesis and separation of the enantiomers of the neuropeptide S receptor antagonist (9*R/S*)-3-oxo-1,1-diphenyl-tetrahydro-oxazolo[3,4*a*]pyrazine-7-carboxylic acid 4-fluoro-benzylamide (SHA 68). *J.Med.Chem.* **54** 2738. PMID: 21466221.

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