

## Certificate of Analysis

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**Product Name:** WQ 1

**Catalog No.:** 7156

**Batch No.:** 1

CAS Number: 1204401-49-9

IUPAC Name: 2,3-Dihydro-2-[1-(phenylmethyl)-4-piperidinyl]-4H-1-benzothiopyran-4-one

### 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>21</sub>H<sub>23</sub>NOS  
**Batch Molecular Weight:** 337.48  
**Physical Appearance:** Beige solid  
**Solubility:** DMSO to 50 mM  
 ethanol to 10 mM  
**Storage:** Store at -20°C

### 2. ANALYTICAL DATA

**HPLC:** Shows 99.7% purity  
**<sup>1</sup>H NMR:** Consistent with structure  
**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	74.74	6.87	4.15
Found	74.55	6.99	4.22

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

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## Product Information

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### Description:

High affinity and selective  $\sigma_1$  receptor antagonist ( $pK_i$  values are 10.28-10.85, 5.81-6.53 and 5.80 at  $\sigma_1$ ,  $\sigma_2$  and DAT). Displays  $\sigma_1/\sigma_2$  selectivity ratio of 29512. Selectively blocks binge eating without a general inhibition of food intake in rats.

### Physical and Chemical Properties:

Batch Molecular Formula:  $C_{21}H_{23}NOS$

Batch Molecular Weight: 337.48

Physical Appearance: Beige solid

**Minimum Purity:**  $\geq 98\%$

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

### Solubility & Usage Info:

DMSO to 50 mM

ethanol to 10 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  $45-60^\circ\text{C}$  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  $-20^\circ\text{C}$  or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

### References:

**Bello *et al*** (2019) Investigation of the role of chirality in the interaction with  $\sigma$  receptors and effect on binge eating episode of a potent  $\sigma_1$  antagonist analogue of spipethiane. *ACS Chem.Neurosci.* **10** 3391. PMID: 31298830.

**Piergentili *et al*** (2010) Novel highly potent and selective sigma 1 receptor antagonists related to spipethiane. *J.Med.Chem.* **53** 1261. PMID: 20067271.

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