

Certificate of Analysis

Print Date: May 1st 2018

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Product Name: NS 6740 Catalog No.: 6139 Batch No.: 1

CAS Number: 753499-14-8

IUPAC Name: 1,4-Diazabicyclo[3.2.2]non-4-yl[5-[3-(trifluoromethyl)phenyl]-2-furanyl]methanone hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{19}H_{19}F_3N_2O_2 \ HCl.\frac{1}{4}H_2O$

Batch Molecular Weight: 405.32 **Physical Appearance:** White solid

Solubility: water to 100 mM

DMSO to 50 mM

Storage: Store at RT

Batch Molecular Structure:

2. ANALYTICAL DATA

TLC: $R_f = 0.4 (10\% \text{ MeOH/DCM w. 5 drops NH4OH (FB)})$

HPLC: Shows 99.1% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 56.3 5.1 6.91 Found 56.07 5.17 6.89

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Product Information

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IUPAC Name: 1,4-Diazabicyclo[3.2.2]non-4-yl[5-[3-(trifluoromethyl)phenyl]-2-furanyl]methanone hydrochloride

Description:

High affinity $\alpha 7$ nAChR partial agonist (K_i = 1.1 nM in rat; E_{max} < 10% of the response to ACh in rat and human). Inhibits ACh (IC₅₀ = 2.7 nM) at $\alpha 7$ nAChR. Reduces LPS-induced TNF- α release from microglia enriched cultures. Anti-inflammatory.

Physical and Chemical Properties:

Batch Molecular Formula: C₁₉H₁₉F₃N₂O₂ HCI.½H₂O

Batch Molecular Weight: 405.32 Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:

Storage: Store at RT

Solubility & Usage Info:

water to 100 mM DMSO 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.

References:

Papke et al (2015) The analgesic-like properties of the alpha7 nAChR silent agonist NS6740 is associated with non-conducting conformations of the receptor. Neuropharmacology 91 34. PMID: 25497451.

Thomsen et al (2012) The $\alpha 7$ nicotinic acetylcholine receptor ligands methyllycaconitine, NS6740 and GTS-21 reduce lipopolysaccharide-induced TNF- α release from microglia. J.Neuroimmunol. **251** 65. PMID: 22884467 .

Briggs et al (2009) Role of channel activation in cognitive enhancement mediated by α 7 nicotinic acetylcholine receptors. Br.J.Pharmacol. **158** 1486. PMID: 19845675.

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