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Certificate of Analysis

www.tocris.com

Catalog No.: 2737

Print Date: Apr 5th 2023

Batch No.: 2

Product Name: TC 2559 difumarate

CAS Number: 2454492-41-0 IUPAC Name: 4-(5-ethoxy-3-r

4-(5-ethoxy-3-pyridinyl)-N-methyl-(3E)-3-buten-1-amine difumarate

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: Batch Molecular Weight: Physical Appearance: Solubility: Storage: Batch Molecular Structure: $\begin{array}{c} \mathbf{S} \\ C_{12}H_{18}N_{2}O. \ 2C_{4}H_{4}O_{4} \\ 438.43 \\ \text{White solid} \\ \text{water to 100 mM} \\ \text{Desiccate at RT} \\ \\ \hline MeHN \\ \hline .2C_{4}H_{4}O_{4} \\ OEt \\ \end{array}$

2. ANALYTICAL DATA

HPLC: ¹H NMR: Mass Spectrum: Microanalysis:

Shows 98.4% purity					
Consistent with structure					
Consistent with structure					
Carbon Hydrogen Nitrogen					
Theoretical 54.79	5.98	6.39			

54.45

6.29

6.33

Found

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

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Product Information

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CAS Number: 2454492-41-0

IUPAC Name: 4-(5-ethoxy-3-pyridinyl)-*N*-methyl-(3*E*)-3-buten-1-amine difumarate

Description:

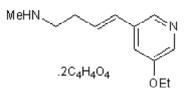
TC 2559 difumarate is a subtype-selective partial agonist for $\alpha4\beta2$ nicotinic acetylcholine receptors (EC₅₀ values are 0.18, 12.5, 14.0, > 30, > 100 and > 100 μ M for $\alpha4\beta2$, $\alpha4\beta4$, $\alpha2\beta4$, $\alpha3\beta4$, $\alpha3\beta2$ and $\alpha7$ receptor subtypes respectively). Displays selectivity for ($\alpha4$)₂($\beta2$)₃ receptor stoichiometry and enhanced CNS-PNS selectivity ratio. Attenuates scopolamine-induced cognitive deficits in a step-through passive avoidance task.

Physical and Chemical Properties:

Batch Molecular Formula: $C_{12}H_{18}N_2O$. $2C_4H_4O_4$ Batch Molecular Weight: 438.43 Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Desiccate at RT

Solubility & Usage Info: water 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:

Zwart *et al* (2006) 5-I A-85380 and TC-2559 differentially activate heterologously expressed α4β2 nicotinic receptors. Eur.J.Pharmacol. **539** 10. PMID: 16674940.

Chen *et al* (2003) The nicotinic α4β2 receptor selective agonist, TC-2559, increases DA neuronal activity in the ventral tegmental area of rat midbrain slices. Neuropharmacology **45** 334. PMID: 12871651.

Bencherif *et al* (2000) TC-2559: a novel orally active ligand selective at neuronal acetylcholine receptors. Eur.J.Pharmacol. **409** 45. PMID: 11099699.

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