

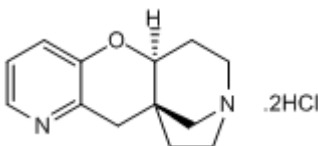
Certificate of Analysis

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Product Name: Dianicline **Catalog No.:** 5557 **Batch No.:** 1
CAS Number: 292634-27-6
IUPAC Name: (5a*S*,8*S*,10a*R*)-5a,6,9,10-Tetrahydro-7*H*,11*H*-8,10a-methanopyrido[2',3':5,6]pyrano[2,3-*d*]azepine

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₃H₁₆N₂O.2HCl.½H₂O
Batch Molecular Weight: 298.21
Physical Appearance: White solid
Solubility: water to 100 mM
DMSO to 20 mM
Storage: Store at -20°C
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.2 (Chloroform:Methanol [4:1])
HPLC: Shows >99.4% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Optical Rotation: [α]_D = -90.4 (Concentration = 1, Solvent = Methanol)
Microanalysis:

	Carbon	Hydrogen	Nitrogen	Chlorine
Theoretical	52.36	6.42	9.39	23.78
Found	52.13	6.43	9.25	23.42

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Description:

Selective $\alpha 4\beta 2$ nAChR partial agonist ($IC_{50} = 105$ nM). Exhibits >20-fold selectivity for $\alpha 4\beta 2$ over other nAChR subtypes. Increases dopamine turnover in rat nucleus accumbens in vivo. Orally bioavailable.

Physical and Chemical Properties:

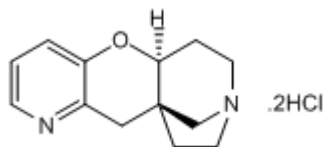
Batch Molecular Formula: $C_{13}H_{16}N_2O \cdot 2HCl \cdot \frac{1}{2}H_2O$

Batch Molecular Weight: 298.21

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

water to 100 mM

DMSO to 20 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:

Rollema et al (2010) Pre-clinical properties of the $\alpha 4\beta 2$ nicotinic acetylcholine receptor partial agonists varenicline, cytisine and dianicline translate to clinical efficacy for nicotine dependence. *Br.J.Pharmacol.* **160** 334. PMID: 20331614 .

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