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Print Date: Jun 8th 2016

Certificate of Analysis

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Product Name: **CC4** **Catalog No.: 5236** **Batch No.: 1**

CAS Number: 492-02-4

IUPAC Name: (1*R*,5*S*)-1,2,3,4,5,6-Hexahydro-3-[2-[(1*R*,5*S*)-1,5,6,8-tetrahydro-8-oxo-1,5-methano-2*H*-pyrido[1,2-*a*][1,5]diazocin-3(4*H*)-yl]ethyl]-1,5-methano-8*H*-pyrido[1,2-*a*][1,5]diazocin-8-one

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{24}H_{30}N_4O_2.¼H_2O$

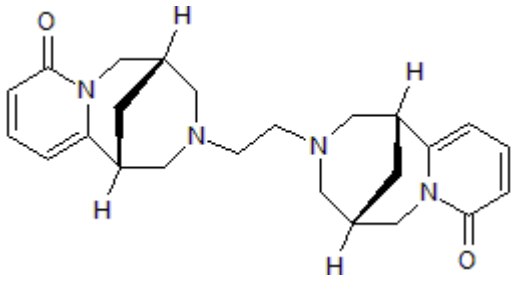
Batch Molecular Weight: 411.02

Physical Appearance:

Solubility: water to 20 mM
DMSO to 100 mM

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.62 (Chloroform:Methanol:Ammonia soln. [90:8:2])

HPLC: Shows 98.8% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: $[\alpha]_D$ = -246.2 (Concentration = 1, Solvent = Chloroform)

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	70.13	7.48	13.63
Found	69.95	7.53	13.47

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CAS Number: 492-02-4

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Description:

High affinity and subtype selective α6β2 and α4β2 partial agonist (K_i values are 12 and 26nM for rat α6β2 and α4β2 receptors respectively). Has low affinity for α3β4 and α7 receptors (K_i values are 4.8 and 13 μM for human α3β4 and rat α7 receptors respectively). Stimulates dopamine release from striatal slices in vitro. Attenuates nicotine-induced self-administration and conditional place preference in rats.

Physical and Chemical Properties:

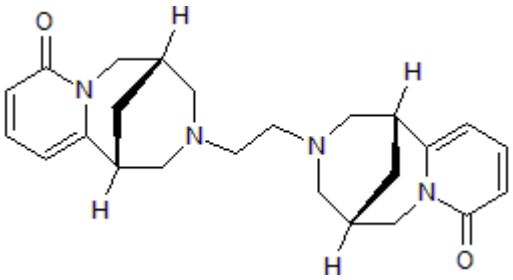
Batch Molecular Formula: $C_{24}H_{30}N_4O_2.¼H_2O$

Batch Molecular Weight: 411.02

Physical Appearance:

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

water to 20 mM
DMSO 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:

Sala *et al* (2013) CC4, a dimer of cytisine, is a selective partial agonist at α4β2/α6β2 nAChR with improved selectivity for tobacco smoking cessation. Br.J.Pharmacol. ***168*** 835. PMID: 22957729.

Riganti *et al* (2005) Long-term exposure to the new nicotinic antagonist 1,2-bisN-cytisinylethane upregulates nicotinic receptor subtypes of SH-SY5Y human neuroblastoma cells. Br.J.Pharmacol. ***146*** 1096. PMID: 16273122.

Carbonnelle *et al* (2003) Nitrogen substitution modifies the activity of cytisine on neuronal nicotinic receptor subtypes. Eur.J.Pharmacol. ***471*** 85. PMID: 12818695.

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