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

CAS Number: 492-02-4
IUPAC Name: (1R,5S)-1,2,3,4,5,6-Hexahydro-3-[2-[(1R,5S)-1,5,6,8-tetrahydro-8-oxo-1,5-methano-2H-pyrido[1,2-a][1,5]diazocin-3(4H)-yl]ethyl]-1,5-methano-8H-pyrido[1,2-a][1,5]diazocin-8-one

1. PHYSICAL AND CHEMICAL PROPERTIES

   Batch Molecular Formula: \( C_{24}H_{30}N_4O_2 \cdot \frac{1}{4}H_2O \)
   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 (Kᵢ values are 12 and 26nM for rat α6β2 and α4β2 receptors respectively). Has low affinity for α3β4 and α7 receptors (Kᵢ 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: C₇₄H₅₀N₄O₁₂.¾H₂O
Batch Molecular Weight: 411.02
Physical Appearance:
Minimum Purity: >98%

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: