

Product Name: TCS 46b

Catalog No.: 2782

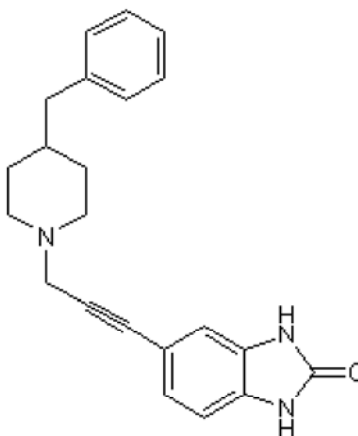
Batch No.: 2

CAS Number: 302799-86-6

IUPAC Name: 1,3-Dihydro-5-[3-[4-(phenylmethyl)-1-2H-benzimidazol-2-one

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₂H₂₃N₃O
Batch Molecular Weight: 345.44
Physical Appearance: White solid
Solubility: DMSO to 100 mM
 ethanol to 100 mM
Storage: Store at RT
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.17 (Ethyl acetate)
HPLC: Shows >99% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	76.49	6.71	12.16
Found	76.48	6.72	11.99

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

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Description:

Orally active, subtype-selective GluN1A/GluN2B (formally NR1A/NR2B) NMDA receptor antagonist (IC₅₀ values are 5.3, 35000 and > 100000 nM for GluN1A/2B (NR1A/2B), GluN1A/2B (NR1A/2B) and GluN1A/2C (NR1A/2C) receptor subtypes respectively). Potentiates the effect of L-DOPA in 6-OHDA-lesioned rats following oral administration. Please refer to IUPHAR Guide to Pharmacology for the most recent naming conventions.

Physical and Chemical Properties:

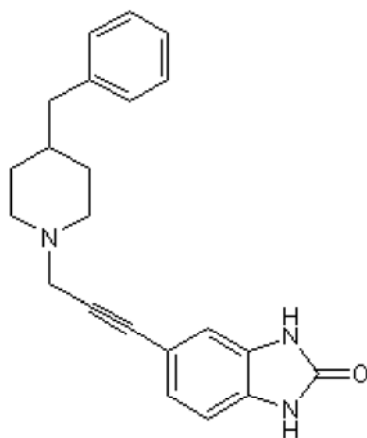
Batch Molecular Formula: C₂₂H₂₃N₃O

Batch Molecular Weight: 345.44

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



References:

Roger et al (2003) Synthesis, radiosynthesis and in vivo evaluation of 5-[3-(4-benzylpiperidin-1-yl)prop-1-ynyl]-1,3-dihydrobenzimidazol-2-[¹¹C]one, as a potent NR_{1A/2B} subtype selective NMDA PET radiotracer. *Bioorg.Med.Chem.* **11** 5401. PMID: 14642584.

Wright et al (2000) Subtype-selective N-methyl-D-aspartate receptor antagonists: synthesis and biological evaluation of 1-(heteroarylalkynyl)-4-benzylpiperidines. *J.Med.Chem.* **43** 3408. PMID: 10978188.

Storage: Store at RT

Solubility & Usage Info:

DMSO to 100 mM
ethanol 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.

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