

Product Name: DR 4485 hydrochloride

Catalog No.: 5005

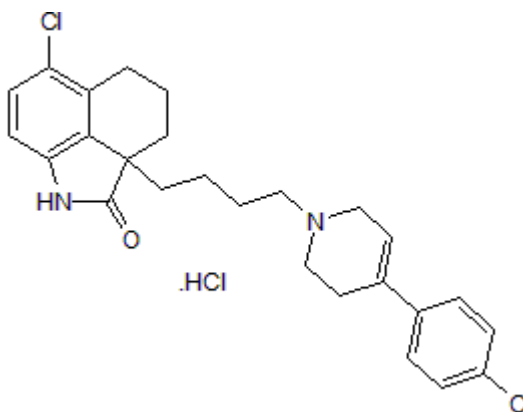
Batch No.: 1

CAS Number: 402942-53-4

IUPAC Name: 6-Chloro-2a-[4-[4-(4-chlorophenyl)-3,6-dihydro-1(2*H*)-pyridinyl]butyl]-2a,3,4,5-tetrahydrobenz[*cd*]indol-2(1*H*)-one hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₆H₂₈Cl₂N₂O.HCl.H₂O
Batch Molecular Weight: 509.9
Physical Appearance: Off-white solid
Solubility: DMSO to 100 mM
Storage: Desiccate at RT
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.12 (Chloroform:Methanol [95:5])
HPLC: Shows >99.5% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	61.24	6.13	5.49
Found	61.22	6.01	5.46

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

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Description:

High affinity and selective 5-HT₇ antagonist (pK_i = 8.14). Exhibits selectivity for 5-HT₇ over other 5-HT receptors. Inhibits 5-HT-induced cAMP accumulation in HEK-293 cells expressing the 5-HT₇ receptor. Orally bioavailable.

Physical and Chemical Properties:

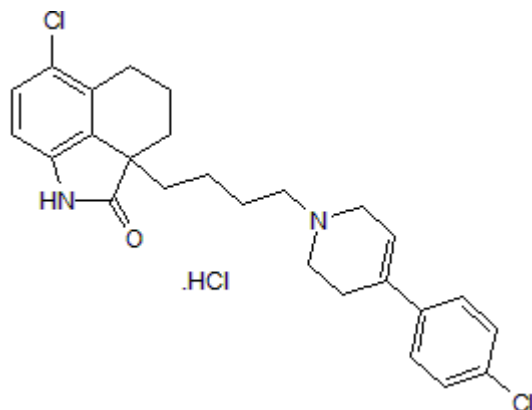
Batch Molecular Formula: C₂₆H₂₈Cl₂N₂O.HCl.H₂O

Batch Molecular Weight: 509.9

Physical Appearance: Off-white solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Desiccate at RT

Solubility & Usage Info:

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:

Kikuchi *et al* (2003) New tetrahydrobenzindoles as potent and selective 5-HT(7) antagonists with increased In vitro metabolic stability. *Bioorg.Med.Chem.Lett.* **13** 61. PMID: 12467617.

Medina *et al* (2009) Synthesis of new serotonin 5-HT7 receptor ligands. Determinants of 5-HT7/5-HT1A receptor selectivity. *J.Med.Chem.* **52** 2384. PMID: 19326916.

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