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Print Date: Jan 13th 2016

Certificate of Analysis

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Product Name: **PD 135158** **Catalog No.: 2608** **Batch No.: 2**

CAS Number: 130285-87-9

IUPAC Name: 4-[[(1*R*)-2-[[(2*R*)-3-(1*H*-Indol-3-yl)-2-methyl-1-oxo-2-[[[[(1*S*,2*R*,4*S*)-1,7,7-trimethylbicyclo[2.2.1]hept-2-yl]oxy] carbonyl]amino]propyl]amino]-1-phenylethyl]amino]-4-oxobutanoic acid

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{35}H_{44}N_4O_6 \cdot \frac{1}{2}H_2O$

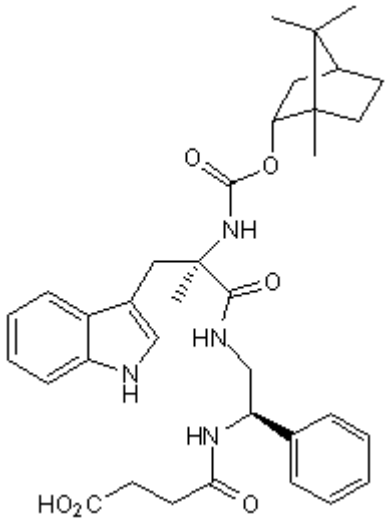
Batch Molecular Weight: 625.77

Physical Appearance: White solid

Solubility: DMSO to 100 mM

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.31 (Dichloromethane:Methanol [90:10])

HPLC: Shows >98.5% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: $[\alpha]_D$ = -23.6 (Concentration = 1, Solvent = Acetone)

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	67.18	7.25	8.95
Found	67.16	7.25	9.09

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Description:

Potent and selective, nonpeptide CCK_2 receptor antagonist (IC_{50} values are 2.8 and 1232 nM for CCK_2 and CCK_1 respectively) that displays negligible affinity at $GABA_A$, benzodiazepine, substance P, neurotensin, opioid, bradykinin and $5\text{-}HT_3$ receptors (IC_{50} > 10 µM). Exhibits anxiolytic activity in elevated plus maze and social interaction tests and increases food intake in rats.

Physical and Chemical Properties:

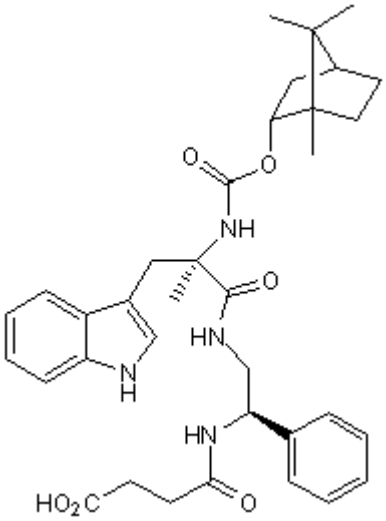
Batch Molecular Formula: $C_{35}H_{44}N_4O_6.½H_2O$

Batch Molecular Weight: 625.77

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at +4°C

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:

Hughes *et al* (1990) Development of a class of selective cholecystokinin type B receptor antagonists having potent anxiolytic activity. Proc.Natl.Acad.Sci.USA ***87*** 6728.

Dorre and Smith (1998) $Cholecystokinin_B$ receptor antagonist increases food intake in rats. Physiol.Behav. ***65*** 11. PMID: 9811359.

Tsutsumi *et al* (1999) Suppression of conditioned fear by administration of CCKB receptor antagonist PD135158. Neuropeptides ***33*** 483. PMID: 10657528.

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