TOCRIS
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Print Date: Jan 13th 2016

Certificate of Analysis

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Product Name: **RP 67580** **Catalog No.: 1635** **Batch No.: 3**

CAS Number: 135911-02-3

IUPAC Name: (3a*R*,7a*R*)-Octahydro-2-[1-imino-2-(2-methoxyphenyl)ethyl]-7,7-diphenyl-4*H*-isoindol

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{29}H_{30}N_2O_2 .¼H_2O$

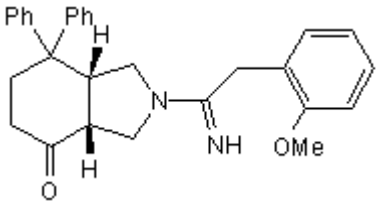
Batch Molecular Weight: 443.07

Physical Appearance: Pale yellow solid

Solubility: ethanol to 100 mM
DMSO to 50 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.17 (Dichloromethane:Methanol [98:2])

Melting Point: Between 176 - 177°C

HPLC: Shows 97.4% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: $[\alpha]_D$ = -262 (Concentration = 1, Solvent = Methanol)

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	78.61	6.94	6.32
Found	78.73	7.08	6.26

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Description:

Potent and selective tachykinin NK_1 receptor antagonist (K_i values are 2.9 nM and > 10 µM for rat NK_1, and rat NK_2 and NK_3 receptors respectively). Displays higher affinity at rat and mouse than human receptors. Antinociceptive in vivo, possibly partly via inhibition of calcium channels.

Physical and Chemical Properties:

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Batch Molecular Weight: 443.07

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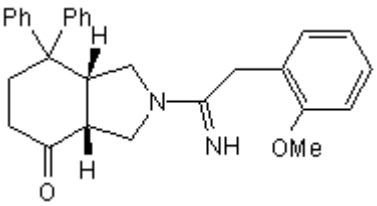
Minimum Purity: >97%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

ethanol to 100 mM
DMSO to 50 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:

Garret *et al* (1991) Pharmacological properties of a potent and selective nonpeptide substance P antagonist. Proc.Natl.Acad.Sci.U.S.A. ***88*** 10208. PMID: 1719549.

Fong *et al* (1992) Molecular basis for the species selectivity of the neurokinin-1 receptor antagonists CP-96,345 and RP67580. J.Biol.Chem. ***267*** 25668. PMID: 1281470.

Beaujouan *et al* (1993) Higher potency of RP 67580, in the mouse and the rat compared with other nonpeptide and peptide tachykinin NK_1 antagonists. Br.J.Pharmacol. ***108*** 793. PMID: 7682138.

Rupniak *et al* (1993) Antinociceptive activity of NK_1 receptor antagonists: non-specific effects of racemic RP67580. Br.J.Pharmacol. ***110*** 1607. PMID: 8306108.