TOCRIS
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Print Date: Jan 13th 2016

Certificate of Analysis

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Product Name: **J 104129 fumarate** **Catalog No.: 2507** **Batch No.: 3**

CAS Number: 257603-40-0

IUPAC Name: (α*R*)-α-Cyclopentyl-α-hydroxy-*N*-[1-(4-methyl-3-pentenyl)-4-piperidinyl]benzeneacetamide fumarate

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{24}H_{36}N_2O_2.C_4H_4O_4$

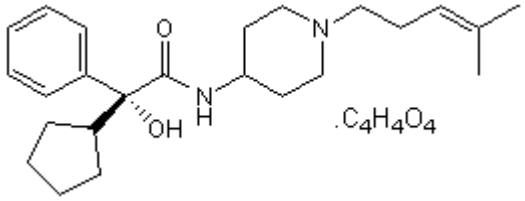
Batch Molecular Weight: 500.63

Physical Appearance: White solid

Solubility: DMSO to 100 mM
ethanol to 50 mM

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.52 (Dichloromethane:Methanol:Ammonia soln. [9:1:0.05])

HPLC: Shows 99.4% purity

Chiral HPLC: Shows 100% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: $[\alpha]_D$ = -7.9 (Concentration = 1, Solvent = Methanol)

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	67.18	8.05	5.6
Found	67.41	7.97	5.74

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Description:

Potent M_3 muscarinic receptor antagonist that displays ~ 120-fold selectivity over M_2 receptors (K_i values are 4.2, 19 and 490 nM for human M_3, M_1 and M_2 receptors respectively). Exhibits > 250-fold bronchial selectivity; inhibits ACh-induced bronchoconstriction but not ACh-induced bradycardia (K_B values are 3.3 and 170 nM for rat trachea M_3 and rat right atria M_2 receptors respectively).

Physical and Chemical Properties:

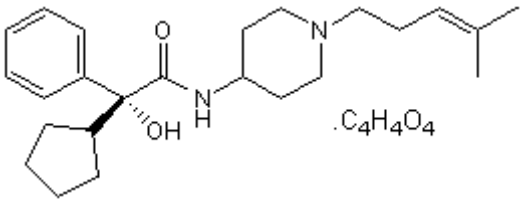
Batch Molecular Formula: $C_{24}H_{36}N_2O_2.C_4H_4O_4$

Batch Molecular Weight: 500.63

Physical Appearance: White solid

Minimum Purity: >99%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 100 mM
ethanol 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:

Mitsuya *et al* (1999) J-104129, a novel muscarinic M_3 receptor antagonist with high selectivity for M_3 over M_2 receptors. Bioorg.Med.Chem. ***7*** 2555. PMID: 10632066.

Mitsuya *et al* (1999) Stereoselective synthesis of a new muscarinic M_3 receptor antagonist, J-104129. Bioorrg.Med.Chem.Lett. ***9*** 2037.

Mitsuya *et al* (2000) Discovery of a muscarinic M_3 receptor antagonist with high selectivity for M_3 over M_2 receptors among 2-[(1*S*,3*S*)-3-sulfonylaminocyclopentyl]phenylacetamide derivatives. Bioorg.Med.Chem. ***8*** 825. PMID: 10819171.