

Certificate of Analysis

Print Date: Jan 11th 2016

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Product Name: Xamoterol hemifumarate Catalog No.: 0950 Batch No.: 4

CAS Number: 73210-73-8 EC Number: 277-319-9 IUPAC Name: 1-(4-Hydroxyphenoxy)-3-[2-(4-morpholinocarboxamido)ethylamino]-2-propanol hemifumarate

1. PHYSICAL AND CHEMICAL PROPERTIES

 $\textbf{Batch Molecular Formula:} \qquad \qquad \textbf{C}_{16}\textbf{H}_{25}\textbf{N}_{3}\textbf{O}_{5}.0.5\textbf{C}_{4}\textbf{H}_{4}\textbf{O}_{4}.^{1/4}\textbf{H}_{2}\textbf{O}$

Batch Molecular Weight: 401.93

Physical Appearance: White solid

Solubility: water to 50 mM

DMSO to 100 mM

Storage: Store at RT

2. ANALYTICAL DATA

Batch Molecular Structure:

TLC: $R_f = 0.11$ (Ethyl acetate:Methanol:Triethylamine [4:1:0.6])

HPLC: Shows 100% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 53.79 6.9 10.45 Found 53.74 6.82 10.52



Product Information

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Description:

 β_1 -adrenoceptor-selective partial agonist (pA₂ values are 7.4 - 7.8 and 5.2 - 6.2 at β_1 - and β_2 -adrenoceptors respectively).

Physical and Chemical Properties:

Batch Molecular Formula: $C_{16}H_{25}N_3O_5.0.5C_4H_4O_4.$ $^{1}4H_2O$

Batch Molecular Weight: 401.93 Physical Appearance: White solid

Minimum Purity: >97%

Batch Molecular Structure:

Storage: Store at RT

Solubility & Usage Info:

water to 50 mM 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:

Barlow *et al* (1981) β-Adrenoceptor stimulant properties of aminoalkylamino-substituted 1-aryl-2-ethanols and 1-(aryloxy)-2-propanols. J.Med.Chem. **24** 315. PMID: 6115058.

Nuttall and Snow (1982) The cardiovascular effects of ICI 118,587: a β_1 -adrenoceptor partial agonist. Br.J.Pharmacol. **77** 381. PMID: 6128041.

Malta et al (1985) The in vitro pharmacology of xamoterol (ICI 118,587). Br.J.Pharmacol. 85 179. PMID: 2862938.