

Certificate of Analysis

Print Date: Jan 15th 2016

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Product Name: Cyclofenil Catalog No.: 3999 Batch No.: 1

CAS Number: 2624-43-3 EC Number: 220-089-1

IUPAC Name: 4,4'-(Cyclohexylidenemethylene)bisphenol 1,1'-diacetate

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{23}H_{24}O_4$ Batch Molecular Weight: 364.43

Physical Appearance:White crystalline solidSolubility:DMSO to 10 mM

ethanol to 5 mM with gentle warming

Storage: Store at +4°C

Batch Molecular Structure:

i. Chi

2. ANALYTICAL DATA

Microanalysis:

HPLC: Shows 99.6% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Carbon Hydrogen Nitrogen

Theoretical 75.8 6.64 Found 75.38 6.6



Product Information

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CAS Number: 2624-43-3 EC Number: 220-089-1

IUPAC Name: 4,4'-(Cyclohexylidenemethylene)bisphenol 1,1'-diacetate

Description:

Non-steroidal selective estrogen receptor modulator (SERM). Displays higher affinity for estrogen receptor β (ER β) than for ERα.

Physical and Chemical Properties:

Batch Molecular Formula: C23H24O4 Batch Molecular Weight: 364.43

Physical Appearance: White crystalline solid

Minimum Purity: >99%

Batch Molecular Structure:

Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 10 mM

ethanol to 5 mM with gentle warming

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:

Seo et al (2006) Fluorine-substituted cyclofenil derivatives as estrogen receptor ligands: synthesis and structure-affinity relationship study of potential PET agents for imaging estrogen receptors in breast cancer. J.Med.Chem. 49 2496. PMID: 16610793.

Kieser et al (2010) Characterization of the pharmacore properties of novel selective estrogen receptor downregulators (SERDs). J.Med.Chem. 53 3320. PMID: 20334372.

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