



Certificate of Analysis

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Product Name: Y 134 Catalog No.: 2676 Batch No.: 1

CAS Number: 849662-80-2

IUPAC Name: [6-Hydroxy-2-(4-hydroxyphenyl)benzo[b]thien-3-yl]-[4-[4-(1-methylethyl)-1-piperazinyl]phenyl]methanone

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₈H₂₈N₂O₃S.H₂O

Batch Molecular Weight: 490.62 **Physical Appearance:** Yellow solid

Solubility: DMSO to 100 mM

ethanol to 100 mM

Storage: Desiccate at RT

Batch Molecular Structure:

2. ANALYTICAL DATA

TLC: $R_f = 0.58$ (Ethyl acetate:Methanol [9:1])

HPLC: Shows >98.1% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 68.55 6.16 5.71 Found 68.72 5.73 5.67



Product Information

Print Date: Apr 26th 2018

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IUPAC Name: [6-Hydroxy-2-(4-hydroxyphenyl)benzo[b]thien-3-yl]-[4-[4-(1-methylethyl)-1-piperazinyl]phenyl]methanone

Description:

Selective estrogen receptor modulator (SERM) that displays selectivity for ER α over ER β (K_i values are 0.09 and 11.31 nM respectively) and no cross-reactivity with mineralocorticoid, glucocorticoid, androgen and progesterone receptors. Acts as an agonist in the bone and antagonist in reproductive tissue. Suppresses estrogen-stimulated proliferation of ER-positive human breast cancer MCF-7 and T47D cells.

Physical and Chemical Properties:

Batch Molecular Formula: C28H28N2O3S.H2O

Batch Molecular Weight: 490.62 Physical Appearance: Yellow solid

Minimum Purity: >98%

Batch Molecular Structure:

N N OH

Storage: Desiccate at RT

Solubility & Usage Info:

DMSO to 100 mM ethanol 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:

Ning *et al* (2007) Biological activities of a novel selective oestrogen receptor modulator derived from raloxifene (Y134). Br.J.Pharmacol. *150* 19. PMID: 17115070.

Yang et al (2005) Benzothiophenes containing a piperazine side chain as selective ligands for the estrogen receptor α and their bioactivities in vivo. Bioorg.Med.Chem.Lett. **15** 1505. PMID: 15713417.

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use