

Certificate of Analysis

Print Date: Jan 15th 2016

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Product Name: GSK 4716 Catalog No.: 3075 Batch No.: 1

CAS Number: 101574-65-6

IUPAC Name: 4-Hydroxy-2-[(1*E*)-[4-(1-methylethyl)phenyl]methylene]hydrazide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{17}H_{18}N_2O_2.H_2O$

Batch Molecular Weight: 300.36 **Physical Appearance:** White solid

Solubility: DMSO to 100 mM ethanol to 100 mM

Ctore of 14°C

Storage: Store at +4°C

Batch Molecular Structure:

2. ANALYTICAL DATA

Melting Point: At 195°C

HPLC: Shows >99.9% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 67.98 6.71 9.33 Found 67.83 6.7 9.36



Product Information

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IUPAC Name: 4-Hydroxy-2-[(1*E*)-[4-(1-methylethyl)phenyl]methylene]hydrazide

Description:

Selective agonist at estrogen-related receptors ERR β and ERR γ . Displays selectivity over ERR α and the classical estrogen receptors.

Physical and Chemical Properties:

Batch Molecular Formula: $C_{17}H_{18}N_2O_2.H_2O$

Batch Molecular Weight: 300.36 Physical Appearance: White solid

Minimum Purity: >99%

Batch Molecular Structure:

Storage: Store at +4°C

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:

Zuercher *et al* (2005) Identification and structure-activity relationship of phenolic acyl hydrazones as selective agonists for the estrogen-related orphan nuclear receptors ERRβ and ERRγ. J.Med.Chem. *48* 3107. PMID: 15857113.

Ariazi and Jordan (2006) Estrogen-related receptors as emerging targets in cancer and metabolic disorders. Curr.Top.Med.Chem. 6 203. PMID: 16515477.

Wang et al (2006) X-ray crystal structures of the estrogen-related receptor-gamma ligand binding domain in three functional states reveal the molecular basis of small molecule regulation. J.Biol.Chem. 281 37773. PMID: 16990259.