

**Product Name:** ZK 164015

**Catalog No.:** 2183

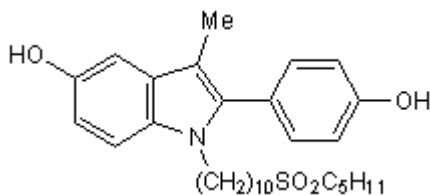
**Batch No.:** 1

CAS Number: 177583-70-9

IUPAC Name: 2-(4-Hydroxyphenyl)-3-methyl-1-[10-(pentylsulfonyl)decyl]-1*H*-indol-5-ol

**1. PHYSICAL AND CHEMICAL PROPERTIES**

**Batch Molecular Formula:** C<sub>30</sub>H<sub>43</sub>NO<sub>4</sub>S  
**Batch Molecular Weight:** 513.73  
**Physical Appearance:** Pale yellow solid  
**Solubility:** ethanol to 25 mM  
DMSO to 100 mM  
**Storage:** Store at RT  
**Batch Molecular Structure:**



**2. ANALYTICAL DATA**

**TLC:** R<sub>f</sub> = 0.53 (Dichloromethane:Ethyl acetate [7:1])  
**Melting Point:** At 119°C  
**HPLC:** Shows >99.4% purity  
**<sup>1</sup>H NMR:** Consistent with structure  
**<sup>13</sup>C NMR:** Consistent with structure  
**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	70.14	8.44	2.73
Found	70.03	8.55	2.7

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

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**Description:**

Potent estrogen receptor silent antagonist. Inhibits 17β-estradiol stimulation of luciferase activity (IC<sub>50</sub> = 0.025 μM); potently inhibits the growth of estrogen-sensitive human MCF-7 breast cancer cells in vitro (IC<sub>50</sub> ~ 1 nM).

**Physical and Chemical Properties:**

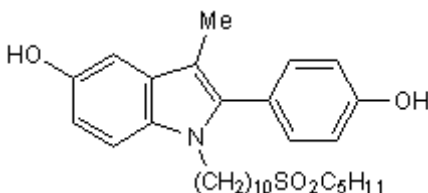
Batch Molecular Formula: C<sub>30</sub>H<sub>43</sub>NO<sub>4</sub>S

Batch Molecular Weight: 513.73

Physical Appearance: Pale yellow solid

**Minimum Purity:** >99%

**Batch Molecular Structure:**



**Storage:** Store at RT

**Solubility & Usage Info:**

ethanol to 25 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:**

**Biberger and von Angerer** (1996) 2-Phenylindoles with sulfur containing side chains. Estrogen receptor affinity, antiestrogenic potency, and antitumour activity. *J.Steroid Biochem.Molec.Biol.* **58** 31.

**Liu et al** (1999) The anti-estrogen hydroxytamoxifen is a potent antagonist in a novel yeast system. *Biol.Chem.* **380** 1341. PMID: 10614829.

**Walter et al** (2004) Synthesis and biological evaluation of stilbene-based pure estrogen antagonists. *Bioorg.Med.Chem.Lett.* **14** 4659. PMID: 15324884.

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