

Certificate of Analysis

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Product Name: (S)-Equol

Catalog No.: 6158

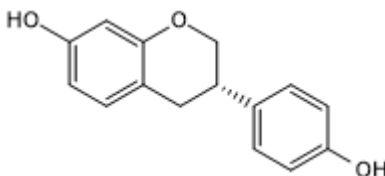
Batch No.: 1

CAS Number: 531-95-3

IUPAC Name: (3S)-3,4-Dihydro-3-(4-hydroxyphenyl)-2H-1-benzopyran-7-ol

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₅H₁₄O₃
Batch Molecular Weight: 242.27
Physical Appearance: White solid
Solubility: DMSO to 100 mM
 ethanol to 100 mM
Storage: Store at -20°C
Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 98.5% purity
Chiral HPLC: Shows 99.1% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Optical Rotation: [α]_D = -21.4 (Concentration = 0.14, Solvent = Methanol)
Microanalysis:

| | Carbon | Hydrogen | Nitrogen |
|-------------|--------|----------|----------|
| Theoretical | 74.36 | 5.82 | |
| Found | 74.35 | 5.85 | |

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

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Description:

Potent estrogen receptor β (ER β) agonist (EC₅₀ = 65 nM). Exhibits 13-fold selectivity for ER β over ER α . Atheroprotective. Protects against t-BHP induced apoptosis and attenuates ER stress in HUVECs. Activates Nrf2 signaling in vitro and in vivo. Inhibits tumor growth. Also dihydrotestosterone antagonist in vivo.

Physical and Chemical Properties:

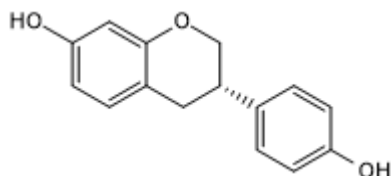
Batch Molecular Formula: C₁₅H₁₄O₃

Batch Molecular Weight: 242.27

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at -20°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:

Yuan et al (2016) Tyrosine phosphorylation regulates ER β ubiquitination, protein turnover, and inhibition of breast cancer. *Oncotarget*. **7** 42585. PMID: 27323858.

Zhang et al (2016) Equol attenuates atherosclerosis in apolipoprotein e-deficient mice by inhibiting endoplasmic reticulum stress via activation of Nrf2 in endothelial cells. *PLoS One*. **11**. PMID: 27907038 .

Setchell et al (2005) S-equol, a potent ligand for estrogen receptor beta, is the exclusive enantiomeric form of the soy isoflavone metabolite produced by human intestinal bacterial flora. *Am.J.Clin.Nutr.* **81** 1079. PMID: 15883431.

Muthyala et al (2004) Equol, a natural estrogenic metabolite from soy isoflavones: convenient preparation and resolution of R- and S-equols and their differing binding and biological activity through estrogen receptors alpha and beta. *Bioorg.Med.Chem.* **12** 1559. PMID: 15018930.

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bio-techne.com

info@bio-techne.com

techsupport@bio-techne.com

North America

Tel: (800) 343 7475

China

info.cn@bio-techne.com

Tel: +86 (21) 52380373

Europe Middle East Africa

Tel: +44 (0)1235 529449

Rest of World

www.tocris.com/distributors

Tel: +1 612 379 2956