

Certificate of Analysis

Print Date: Mar 6th 2018

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Product Name: ERB 041 Catalog No.: 4276 Batch No.: 3

CAS Number: 524684-52-4

IUPAC Name: 7-Ethenyl-2-(3-fluoro-4-hydroxyphenyl)-5-benzoxazolol

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₅H₁₀FNO₃.0.2H₂O

Batch Molecular Weight: 274.84 **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 98.7% purity

¹H NMR: Consistent with structure Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

> Theoretical 65.55 3.81 5.1 Found 65.85 5.08 3.69

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Product Information

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IUPAC Name: 7-Ethenyl-2-(3-fluoro-4-hydroxyphenyl)-5-benzoxazolol

Description:

Potent ER β agonist; displays >200-fold selectivity for ER β over ER α (IC $_{50}$ values are 5 and 1216 nM for human ER β and ER α ; 3.1 and 620 nM for rat ER β and ER α ; and 3.7 and 750 nM for mouse ER β and ER α respectively).

Physical and Chemical Properties:

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Batch Molecular Weight: 274.84 Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:

Storage: Store at -20°C

CAUTION - This product is light sensitive and we recommend that the solid material and any solutions obtained are protected from exposure to light.

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.

Licensing Information:

Sold for research purposes under agreement from Pfizer Inc.

References:

Cvoro *et al* (2008) Selective estrogen receptor-γ agonists repress transcription of proinflammatory genes. J.Immunol. *180* 630. PMID: 18097065.

Malamas *et al* (2004) Design and synthesis of aryl diphenolic azoles as potent and selective estrogen receptor-β ligands. J.Med.Chem. **47** 5021. PMID: 15456246.

Harris *et al* (2003) Evaluaton of an estrogen receptor-β agonist in animal models of human disease. Endocrinology *144* 4241. PMID: 14500559.