

## Certificate of Analysis

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**Product Name:** Fluorobexarotene

**Catalog No.:** 4064

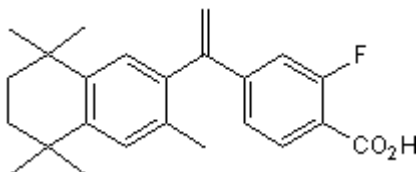
**Batch No.:** 2

**CAS Number:** 1190848-23-7

**IUPAC Name:** 2-Fluoro-4-[1-(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)ethenyl]benzoic acid

### 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>24</sub>H<sub>27</sub>FO<sub>2</sub>  
**Batch Molecular Weight:** 366.47  
**Physical Appearance:** White solid  
**Solubility:** DMSO to 100 mM  
 ethanol to 25 mM  
**Storage:** Store at +4°C  
**Batch Molecular Structure:**



### 2. ANALYTICAL DATA

**HPLC:** Shows 97.5% purity  
**<sup>1</sup>H NMR:** Consistent with structure  
**Mass Spectrum:** Consistent with structure  
**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	78.66	7.43	
Found	78.29	7.14	

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

## Product Information

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### Description:

RXR agonist ( $K_i$  = 12 nM;  $EC_{50}$  = 43 nM at RXR $\alpha$  receptors). Displays similar RAR agonist activity to bexarotene; exhibits an apparent RXR binding affinity 75% greater than bexarotene.

### Physical and Chemical Properties:

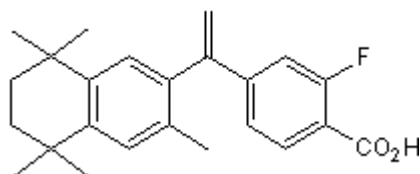
Batch Molecular Formula:  $C_{24}H_{27}FO_2$

Batch Molecular Weight: 366.47

Physical Appearance: White solid

**Minimum Purity:** >97%

### Batch Molecular Structure:



**Storage:** Store at +4°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 25 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:

Manufactured and sold under license from Arizona State University - Patent Pending

### References:

**Wagner *et al*** (2009) Modeling, synthesis and biological evaluation of potential retinoid X receptor (RXR) selective agonists: novel analogues of 4-[1-(3,5,5,8,8-Pentamethyl-5,6,7,8-tetrahydro-2-naphthyl)ethynyl]benzoic acid (bexarotene). *J.Med.Chem.* **52** 5950. PMID: 19791803.

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