

## Certificate of Analysis

**Product Name:** BMS 453

**Catalog No.:** 3409

**Batch No.:** 3

CAS Number: 166977-43-1

IUPAC Name: 4-[(1E)-2-(5,6-Dihydro-5,5-dimethyl-8-phenyl-2-naphthalenyl)ethenyl]-benzoic acid

### 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:**  $C_{27}H_{24}O_2 \cdot \frac{1}{2}H_2O$

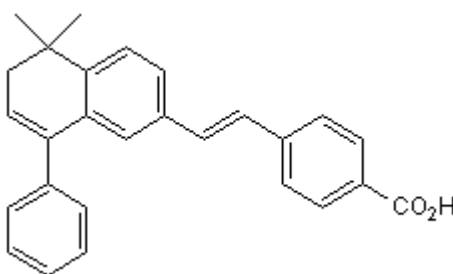
**Batch Molecular Weight:** 389.49

**Physical Appearance:** Off-white solid

**Solubility:** DMSO to 100 mM

**Storage:** Store at -20°C

**Batch Molecular Structure:**



### 2. ANALYTICAL DATA

**TLC:**  $R_f = 0.1$  (Ethyl acetate:Petroleum ether [9:1])

**HPLC:** Shows 98% purity

**<sup>1</sup>H NMR:** Consistent with structure

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

Carbon Hydrogen Nitrogen

Theoretical 83.26 6.47

Found 83.55 6.29

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**Description:**

Synthetic retinoid. Retinoic acid receptor  $\beta$  (RAR $\beta$ ) agonist in vivo; RAR $\alpha$  and RAR $\gamma$  antagonist in vitro. Inhibits breast cell proliferation by inducing active transforming growth factor  $\beta$  (TGF $\beta$ ) and causes G<sub>1</sub> arrest.

**Physical and Chemical Properties:**

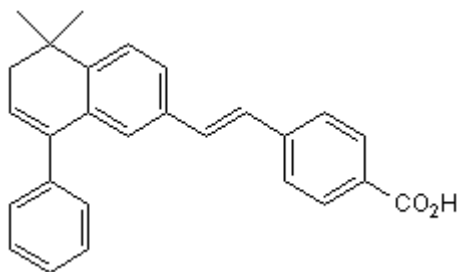
Batch Molecular Formula: C<sub>27</sub>H<sub>24</sub>O<sub>2</sub>·½H<sub>2</sub>O

Batch Molecular Weight: 389.49

Physical Appearance: Off-white solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**



**Storage:** Store at -20°C

**Solubility & Usage Info:**

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:**

**Chen *et al*** (1995) RAR-specific agonist/antagonists which dissociate transactivation and AP1 transrepression inhibit anchorage-independent cell proliferation. *EMBO J.* **14** 1187. PMID: 7720709.

**Yang *et al*** (2001) The retinoic acid receptor antagonist, BMS543, inhibits normal breast cell growth by inducing active TGFB and causing cell cycle arrest. *Oncogene* **20** 8025. PMID: 11753686.

**Monteiro *et al*** (2009) Commitment of mouse embryonic stem cells to the adipocyte lineage requires retinoic acid receptor beta and active GSK3. *Stem Cells Dev.* **18** 457. PMID: 18690793.

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