

**Product Name:** BMS 195614

**Catalog No.:** 3660

**Batch No.:** 2

CAS Number: 182135-66-6

IUPAC Name: 4-[[[5,6-Dihydro-5,5-dimethyl-8-(3-quinolinyl)-2-naphthalenyl]carbonyl]amino]benzoic acid

**1. PHYSICAL AND CHEMICAL PROPERTIES**

**Batch Molecular Formula:** C<sub>29</sub>H<sub>24</sub>N<sub>2</sub>O<sub>3</sub>·½H<sub>2</sub>O

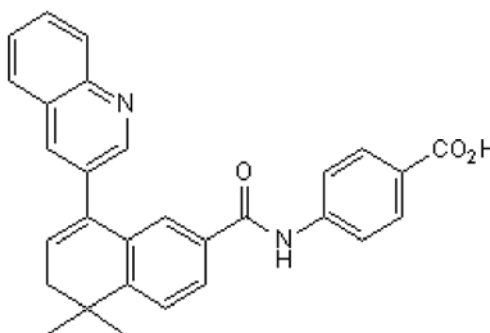
**Batch Molecular Weight:** 457.52

**Physical Appearance:** Off-white solid

**Solubility:** DMSO to 25 mM

**Storage:** Store at -20°C

**Batch Molecular Structure:**



**2. ANALYTICAL DATA**

**TLC:** R<sub>f</sub> = 0.87 (Pyridine:Acetic acid:Water:Butanol [3:8:11:198])

**HPLC:** Shows 98.5% purity

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

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	76.13	5.51	6.12
Found	76.2	5.45	6.22

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**Description:**

Neutral retinoic acid receptor (RAR)  $\alpha$ -selective antagonist ( $K_i$  = 2.5 nM). Displays no significant effect on nuclear receptor corepressor (NCoR) binding; moderately decreases SMRT binding to RAR. Antagonizes agonist-induced coactivator (CoA) recruitment.

**Physical and Chemical Properties:**

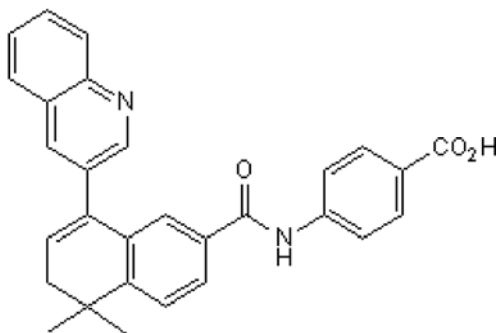
Batch Molecular Formula: C<sub>29</sub>H<sub>24</sub>N<sub>2</sub>O<sub>3</sub>·½H<sub>2</sub>O

Batch Molecular Weight: 457.52

Physical Appearance: Off-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 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.

**References:**

**Germain *et al*** (2009) Differential action on coregulator interaction defines retinoid agonists and neutral antagonists. *Chem.Biol.* **16** 479. PMID: 19477412.

**Gehin *et al*** (1999) Structural basis for engineering of retinoic acid receptor isotype-selective agonists and antagonists. *Chem.Biol.* **6** 519. PMID: 10421757.

**Schoenemark *et al*** (1999) Retinoid-mediated suppression of tumor invasion and matrix metalloproteinase synthesis. *Ann.N.Y.Acad.Sci.* **30** 878.

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