

Certificate of Analysis

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Product Name: BMS 961

Catalog No.: 3410

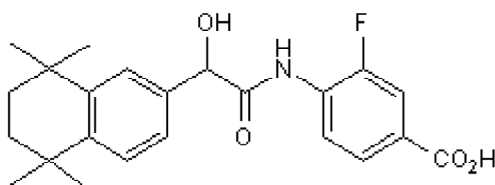
Batch No.: 1

CAS Number: 185629-22-5

IUPAC Name: 3-Fluoro-4-[[2-hydroxy-2-(5,5,8,8-tetramethyl-5,6,7,8,-tetrahydro-2-naphthalenyl)acetyl]amino]-benzoic acid

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₃H₂₆FNO₄
Batch Molecular Weight: 399.46
Physical Appearance: Off-white solid
Solubility: DMSO to 100 mM
Storage: Store at +4°C
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.2 (Dichloromethane:Methanol [9:1])
HPLC: Shows 96.8% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	69.16	6.56	3.51
Found	69.19	6.54	3.68

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

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Description:

BMS 961 is a selective RAR γ agonist (EC₅₀ values are 30 and 1000 nM at RAR γ and RAR β respectively). Displays no activity at RAR α receptors.

Physical and Chemical Properties:

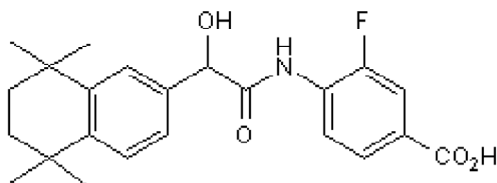
Batch Molecular Formula: C₂₃H₂₆FNO₄

Batch Molecular Weight: 399.46

Physical Appearance: Off-white solid

Minimum Purity: ≥95%

Batch Molecular Structure:



Storage: Store at +4°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. *Unless contradicted by product-specific protocols or instructions, our standard recommendations apply:

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:

Klaholz *et al* (2000) Enantiomer discrimination illustrated by high-resolution crystal structures of the human nuclear receptor hRAR γ . *Proc.Natl.Acad.Sci.* **97** 6322.

Abu-Abed *et al* (1998) Mouse *P450RAI* (CYP26) expression and retinoic acid-inducible retinoic acid metabolism in F9 cells are regulated by retinoic acid receptor γ and retinoid X receptor α . *J.Biol.Chem.* **273** 2409. PMID: 9442090.

Taneja *et al* (1996) Cell-type and promoter-context dependent retinoic acid receptor (RAR) redundancies for *RAR β 2* and *Hoxa-1* activation in F9 and P19 cells can be artefactually generated by gene knockouts. *Proc.Natl.Acad.Sci.USA* **93** 6197.

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