

Certificate of Analysis

Print Date: Jan 15th 2016

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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: $C_{23}H_{26}FNO_4$

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 97.8% 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



Product Information

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Description:

Selective RAR γ agonist (EC $_{50}$ values are 30 and 1000 nM at RAR γ and RAR β respectively). Displays no activity at RAR α receptors.

receptors.

Physical and Chemical Properties:

Batch Molecular Formula: C₂₃H₂₆FNO₄ Batch Molecular Weight: 399.46 Physical Appearance: Off-white solid

Minimum Purity: >97%

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. 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:

Taneja et al (1996) Cell-type and promoter-context dependent retinoic acid receptor (RAR) redundancies for RARβ2 and Hoxa-1 activation in F9 and P19 cells can be artefactually generated by gene knockouts. Proc.Natl.Acad.Sci.USA 93 6197.

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.

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