

# Certificate of Analysis

**Product Name:** Fexaramine

**Catalog No.:** 2563

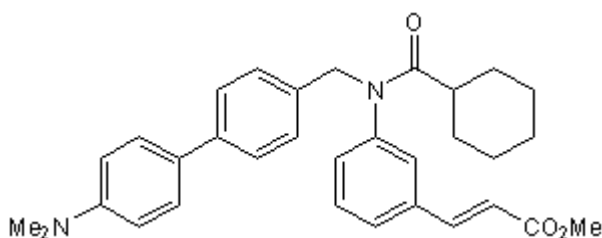
**Batch No.:** 2

CAS Number: 574013-66-4

IUPAC Name: 3-[3-[(Cyclohexylcarbonyl)-[[4'-(dimethylamino)-[1,1'-biphenyl]-4-yl]methyl]amino]phenyl]-2-propenoic acid methyl ester

## 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>32</sub>H<sub>36</sub>N<sub>2</sub>O<sub>3</sub>  
**Batch Molecular Weight:** 496.64  
**Physical Appearance:** Yellow solid  
**Solubility:** DMSO to 100 mM  
**Storage:** Desiccate at +4°C  
**Batch Molecular Structure:**



## 2. ANALYTICAL DATA

**TLC:** R<sub>f</sub> = 0.18 (Ethyl acetate:Petroleum ether [3:7])  
**HPLC:** Shows 97.9% purity  
**<sup>1</sup>H NMR:** Consistent with structure  
**Mass Spectrum:** Consistent with structure  
**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	77.39	7.31	5.64
Found	77.53	7.34	5.7

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**Description:**

Potent, selective farnesoid X receptor agonist ( $EC_{50} = 25$  nM). Displays no activity at hRXR $\alpha$ , hPPAR $\alpha$ , hPPAR $\gamma$ , hPPAR $\delta$ , mPXR, hPXR, hLXR $\alpha$ , hTR $\beta$ , hRAR $\beta$ , mCAR, mERR $\gamma$  and hVDR receptors.

**Physical and Chemical Properties:**

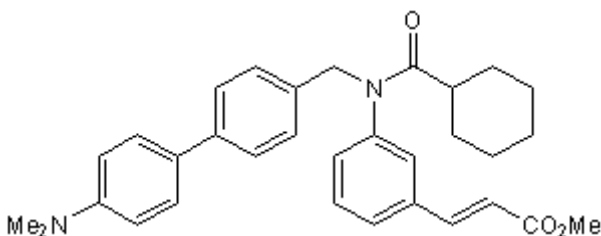
Batch Molecular Formula: C<sub>32</sub>H<sub>36</sub>N<sub>2</sub>O<sub>3</sub>

Batch Molecular Weight: 496.64

Physical Appearance: Yellow solid

**Minimum Purity:** >97%

**Batch Molecular Structure:**



**Storage:** Desiccate 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:**

**Nicolaou et al** (2003) Discovery and optimization of non-steroidal FXR agonists from natural product-like libraries. *Org.Biomol.Chem.* **1** 908. PMID: 12929628.

**Downes et al** (2003) A chemical, genetic, and structural analysis of the nuclear bile acid receptor FXR. *Mol.Cell* **11** 1079. PMID: 12718892.

**Pellicciari et al** (2006) Back door modulation of the farnesoid X receptor: design, synthesis, and biological evaluation of a series of side chain modified chenodeoxycholic acid derivatives. *J.Med.Chem.* **49** 4208. PMID: 16821780.

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