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: $\text{C}_{32}\text{H}_{36}\text{N}_{2}\text{O}_{3}$

Batch Molecular Weight: 496.64

Physical Appearance: Yellow solid

Solubility: DMSO to 100 mM

Storage: Desiccate at +4°C

Batch Molecular Structure:

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2. ANALYTICAL DATA

TLC: $R_f = 0.18$ (Ethyl acetate:Petroleum ether [3:7])

HPLC: Shows 97.9% purity

$^1\text{H}$ NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

<table>
<thead>
<tr>
<th></th>
<th>Theoretical</th>
<th>Found</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carbon</td>
<td>77.39</td>
<td>77.53</td>
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<tr>
<td>Hydrogen</td>
<td>7.31</td>
<td>7.34</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>5.64</td>
<td>5.7</td>
</tr>
</tbody>
</table>

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

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Description:
Potent, selective farnesoid X receptor agonist (EC<sub>50</sub> = 25 nM). Displays no activity at hRXR<sub>α</sub>, hPPAR<sub>α</sub>, hPPAR<sub>γ</sub>, hPPAR<sub>δ</sub>, mPXR, hPXR, hLXR<sub>α</sub>, hTR<sub>β</sub>, hRAR<sub>β</sub>, mCAR, mERR<sub>γ</sub> and hVDR receptors.

Physical and Chemical Properties:
Batch Molecular Formula: C<sub>32</sub>H<sub>35</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: