Product Name: Atorvastatin hemicalcium salt
Catalog No.: 3776 Batch No.: 2
CAS Number: 134523-03-8
IUPAC Name: \((R,R)-2-(4-\text{Fluorophenyl})-\beta,\delta\text{-dihydroxy}-5\{(1\text{-methylethyl})-3\text{-phenyl}-4-\{(\text{phenylamino})\text{carbonyl}\}-1\text{H-pyrrole-1-heptanoic acid hemicalcium salt}\)

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: \(C_{33}H_{34}FN_2O_5\cdot\frac{1}{2}\text{Ca.H}_2\text{O}\)
Batch Molecular Weight: 595.69
Physical Appearance: White solid
Solubility: DMSO to 100 mM
Storage: Store at +4°C

2. ANALYTICAL DATA

HPLC: Shows 99.6% purity
\(^1\)H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Optical Rotation: \([\alpha]_D = -12\) (Concentration = 1, Solvent = DMSO)
Microanalysis:

<table>
<thead>
<tr>
<th></th>
<th>Carbon</th>
<th>Hydrogen</th>
<th>Nitrogen</th>
</tr>
</thead>
<tbody>
<tr>
<td>Theoretical</td>
<td>66.54</td>
<td>6.09</td>
<td>4.7</td>
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<tr>
<td>Found</td>
<td>66.48</td>
<td>6.19</td>
<td>4.67</td>
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</tbody>
</table>

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use
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CAS Number: 134523-03-8
IUPAC Name: \((R,R)\)-2-(4-Fluorophenyl)-β,δ-dihydroxy-5-(1-methylethyl)-3-phenyl-4-[[phenylamino]carbonyl]-1H-pyrrole-1-heptanoic acid hemicalcium salt

Description:
Potent HMG-CoA reductase inhibitor (IC\textsubscript{50} = 8 nM). Reduces circulating LDL-C by inhibiting cholesterol biosynthesis and inducing expression of LDL receptors. Inhibits smooth muscle cell proliferation in vitro and exhibits antinociceptive effects in the inflammatory hypernociception model.

Physical and Chemical Properties:
Batch Molecular Formula: C\textsubscript{33}H\textsubscript{32}FN\textsubscript{2}O\textsubscript{5}·½Ca·H\textsubscript{2}O
Batch Molecular Weight: 595.69
Physical Appearance: White solid
Minimum Purity: >99%

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.

Licensing Information:
Sold for research purposes under agreement from Pfizer Inc.

References: