1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C_{23}H_{22}F_{2}N_{4}O_{4}

**Batch Molecular Weight:** 456.44

**Physical Appearance:** White solid

**Solubility:** DMSO to 100 mM
1eq. NaOH to 10 mM with gentle warming

**Storage:** Store at +4°C

**Batch Molecular Structure:**

![Molecular Structure Diagram]

(and enantiomer)

2. ANALYTICAL DATA

**TLC:** R_f = 0.57 (Dichloromethane:Methanol [95:5])

**HPLC:** Shows 98.9% purity

**^1H 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>60.52</td>
<td>60.52</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>4.86</td>
<td>4.85</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>12.27</td>
<td>12.29</td>
</tr>
</tbody>
</table>

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use
Product Name: AZD 3988
Catalog No.: 4837
Batch No.: 1

CAS Number: 892489-52-0
IUPAC Name: trans-4-[[[5-(3,4-Difluorophenyl)amino]-1,3,4-oxadiazol-2-yl]carbonyl]amino]phenyl)cyclohexaneacetic acid

Description:
Potent and selective diacylglycerol acyltransferase (DGAT-1) inhibitor (IC₅₀ = 0.6 nM). Exhibits selectivity for DGAT-1 over DGAT-2, Kᵦ₁₁.1 (hERG) and cytochrome P450 enzymes. Suppresses triacylglyceride (TAG) plasma excursion and adipose tissue TAG synthesis in rats. Reduces body weight of diet-induced obese rats. Cell permeable and orally bioavailable.

Physical and Chemical Properties:
Batch Molecular Formula: C₂₉H₂₅F₂N₄O₄
Batch Molecular Weight: 456.44
Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:

Storage: Store at +4°C

Solubility & Usage Info:
DMSO to 100 mM
1eq. NaOH to 10 mM with gentle warming

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: