

Product Name: AZD 3988

Catalog No.: 4837

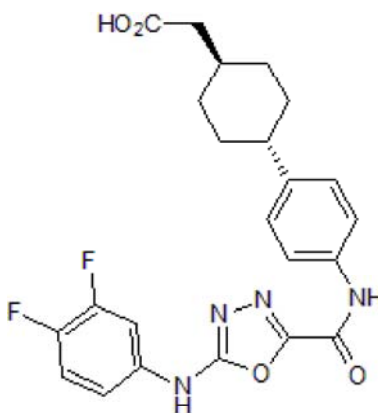
Batch No.: 1

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

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₃H₂₂F₂N₄O₄
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:



(and enantiomer)

2. ANALYTICAL DATA

TLC: R_f = 0.57 (Dichloromethane:Methanol [95:5])
HPLC: Shows 98.7% purity
¹H NMR: Consistent with structure
 Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	60.52	4.86	12.27
Found	60.52	4.85	12.29

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Description:

Potent and selective diacylglycerol acyltransferase (DGAT-1) inhibitor (IC_{50} = 0.6 nM). Exhibits selectivity for DGAT-1 over DGAT-2, K_v 11.1 (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:

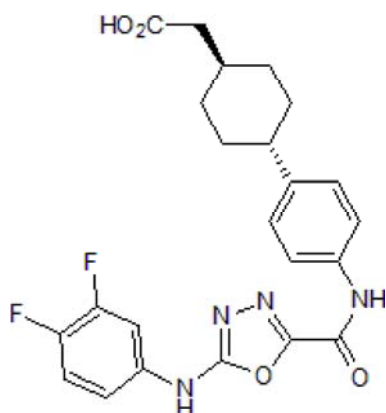
Batch Molecular Formula: $C_{23}H_{22}F_2N_4O_4$

Batch Molecular Weight: 456.44

Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



(and enantiomer)

References:

McCoull *et al* (2012) Identification, optimisation and *in vivo* evaluation of oxadiazole DGAT-1 inhibitors for the treatment of obesity and diabetes. *Bioorg.Med.Chem.Lett.* **22** 3873. PMID: 22608962.

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.

Licensing Information:

Sold with the permission of AstraZeneca UK Ltd.

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