

Product Name: PF 8380

Catalog No.: 4078

Batch No.: 1

CAS Number: 1144035-53-9

IUPAC Name: 3,5-Dichlorobenzyl-[4-[3-oxo-3-(2-oxo-2,3-dihydrobenzoxazol-6-yl)propyl]]piperazine-1-carboxylate

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₂H₂₁Cl₂N₃O₅·¼H₂O

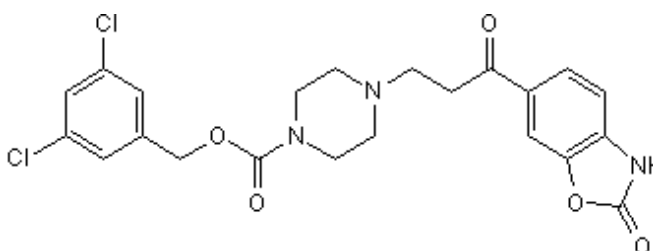
Batch Molecular Weight: 482.83

Physical Appearance: Yellow solid

Solubility: DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.3 (Dichloromethane:Methanol [95:5])

HPLC: Shows 97.7% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	54.73	4.49	8.7
Found	54.62	4.41	8.61

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

Product Name: PF 8380

Catalog No.: 4078

Batch No.: 1

CAS Number: 1144035-53-9

IUPAC Name: 3,5-Dichlorobenzyl-[4-[3-oxo-3-(2-oxo-2,3-dihydrobenzoxazol-6-yl)propyl]]piperazine-1-carboxylate

Description:

Potent autotaxin inhibitor (IC₅₀ = 2.8 nM in isolated enzyme assay; 101 nM in human whole blood). Modulates lysophosphatidic acid (LPA) levels in vivo and in vitro by directly inhibiting autotaxin; reduces LPA levels both in plasma and at site of inflammation. Orally available.

Physical and Chemical Properties:

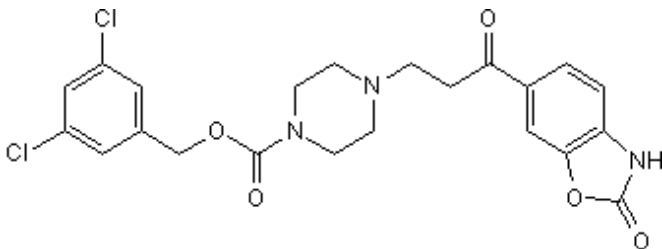
Batch Molecular Formula: C₂₂H₂₁Cl₂N₃O₅ · ¼H₂O

Batch Molecular Weight: 482.83

Physical Appearance: Yellow solid

Minimum Purity: >97%

Batch Molecular Structure:



References:

Gierse *et al* (2010) A novel autotaxin inhibitor reduces lysophosphatidic acid levels in plasma and the site of inflammation. *J.Pharmacol.Exp.Ther.* **334** 310. PMID: 20392816.

Jankowski (2011) Autotaxin: its role in biology of melanoma cells and as a pharmacological target. *Enzyme Res.* 194857. PMID: 21423677.

Storage: Store at -20°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.

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

bio-techne.com

info@bio-techne.com

techsupport@bio-techne.com

North America

Tel: (800) 343 7475

China

info.cn@bio-techne.com

Tel: +86 (21) 52380373

Europe Middle East Africa

Tel: +44 (0)1235 529449

Rest of World

www.tocris.com/distributors

Tel:+1 612 379 2956