

Product Name: HA 130

Catalog No.: 4196

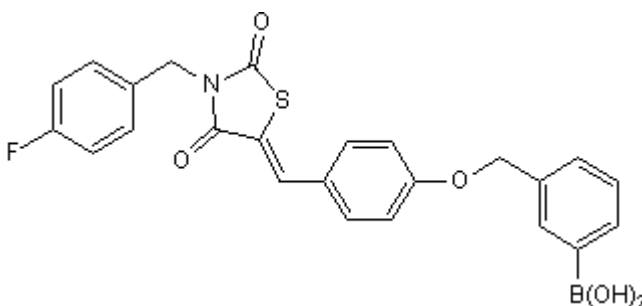
Batch No.: 1

CAS Number: 1229652-21-4

IUPAC Name: *B*-[3-[[4-[[3-[(4-Fluorophenyl)methyl]-2,4-dioxo-5-thiazolidinylidene)methyl]phenoxy]methyl]phenyl]-boronic acid

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₄H₁₉BFNO₅S
Batch Molecular Weight: 463.29
Physical Appearance: White solid
Solubility: DMSO to 100 mM
Storage: Store at -20°C
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.6 (Ethyl acetate:Petroleum ether [2:1])
HPLC: Shows 99.3% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	62.22	4.13	3.02
Found	62.2	4.06	3.01

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

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Description:

Potent and selective autotaxin inhibitor ($IC_{50} = 28$ nM). Binds and inhibits autotaxin reversibly. Displays no activity against the proteasome, recombinant NPP1 or alkaline phosphatase. Inhibits ATX-mediated cell migration in an A2058 melanoma cell assay.

Physical and Chemical Properties:

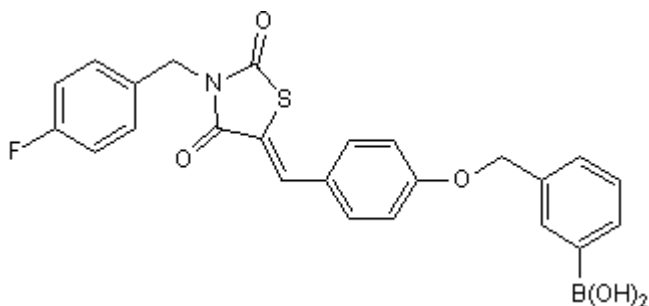
Batch Molecular Formula: $C_{24}H_{19}BFNO_5S$

Batch Molecular Weight: 463.29

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM

Note this product may decompose if dissolved in ethanol or other alcohol solvents.

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:

Albers et al (2010) Discovery and optimization of boronic acid based inhibitors of autotaxin. *J.Med.Chem.* **53** 4958. PMID: 20536182.

Albers et al (2010) Boronic acid-based inhibitor of autotaxin reveals rapid turnover of LPA in the circulation. *Proc.Natl.Acad.Sci.USA* **107** 7257. PMID: 20360563.

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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