

Product Name: 142D6

Catalog No.: 8018

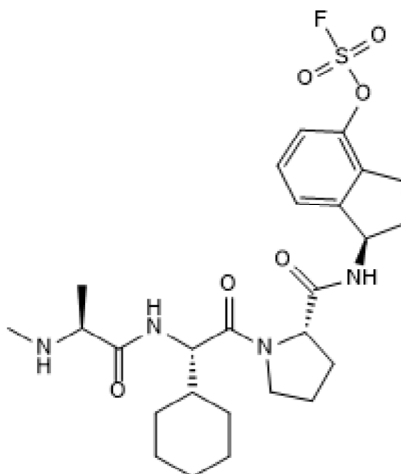
Batch No.: 1

CAS Number: 2410953-19-2

IUPAC Name: (R)-1-((S)-1-((S)-2-Cyclohexyl-2-((S)-2-(methylamino)propanamido)acetyl)pyrrolidine-2-carboxamido)-2,3-dihydro-1H-inden-4-yl sulfurofluoridate

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula:	C ₂₆ H ₃₇ FN ₄ O ₆ S.
Batch Molecular Weight:	552.66
Physical Appearance:	White solid
Solubility:	DMSO to 100 mM
Storage:	Store at -20°C
Batch Molecular Structure:	



2. ANALYTICAL DATA

HPLC:	Shows 95.5% purity
¹H NMR:	Consistent with structure
Mass Spectrum:	Consistent with structure

Microanalysis:	Carbon	Hydrogen	Nitrogen
Theoretical	56.5	6.75	10.14
Found	55.61	6.8	9.81

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

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Description:

142D6 is a potent pan-IAP inhibitor (IC₅₀ values are 21, 21 and 43 nM for cIAP1, cIAP2 and XIAP respectively). 142D6 covalently targets Lys residues in the BIR3 domain of the inhibitor of the apoptosis protein (IAP) family. In vitro, 142D6 reduces viability of cultured breast cancer MDA-MB-231 cells (EC₅₀ values are 44 and 61 nM in cell viability and apoptosis assays, respectively). 142D6 is chemically stable in buffer and plasma and is orally bioavailable.

Physical and Chemical Properties:

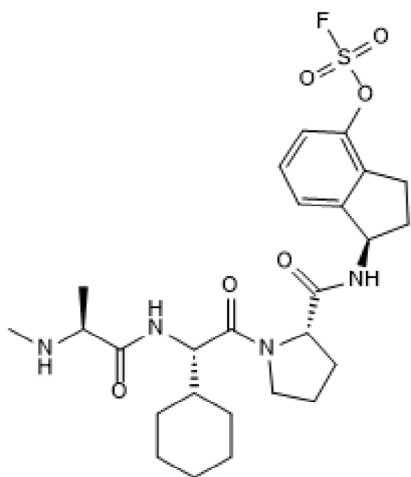
Batch Molecular Formula: C₂₆H₃₇FN₄O₆S.

Batch Molecular Weight: 552.66

Physical Appearance: White solid

Minimum Purity: ≥95%

Batch Molecular Structure:



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. *Unless contradicted by product-specific protocols or instructions, our standard recommendations apply:

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 under patent license from The Regents of the University of California

References:

Udompholkul et al (2023) Characterization of a potent and orally bioavailable Lys-covalent inhibitor of apoptosis protein (IAP) antagonist. *J.Med.Chem.* **66** 8159. PMID: 37262387.

Baggio et al (2019) Aryl-fluorosulfate-based lysine covalent pan-inhibitors of apoptosis protein (IAP) antagonists with cellular efficacy. *J.Med.Chem.* **62** 9188. PMID: 31550155.

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