

Product Name: XL01126

Catalog No.: 8968

Batch No.: 1

CAS Number: 3011029-58-3

IUPAC Name: (2*S*,4*R*)-1-((*R*)-3-((((1*r*,4*R*)-4-((4-(4-((5-Chloro-4-(methyl-λ²-azaneyl)pyrimidin-2-yl)amino)-3-methoxybenzoyl)piperazin-1-yl)methyl)cyclohexyl)methyl)thio)-2-(1-fluorocyclopropane-1-carboxamido)-3-methylbutanoyl)-4-hydroxy-*N*-(4-(4-methylthiazol-5-yl)benzyl)pyrrolidine-2-carboxamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₅₀H₆₄ClFN₁₀O₆S₂·½H₂O

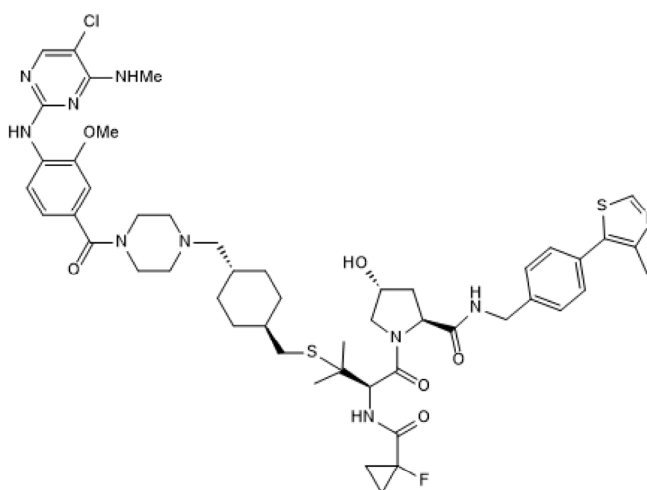
Batch Molecular Weight: 1028.7

Physical Appearance: White solid

Solubility: DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 98.4% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon Hydrogen Nitrogen		
Theoretical	58.38	6.37	13.62
Found	57.46	6.37	13.22

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Description:

XL01126 is a fast and potent degrader of LRRK2 in multiple cell lines (DC₅₀ values within 15-72 nM, Dmax values range from 82-90%). XL01126 exhibits high cell permeability and forms a positively cooperative ternary complex with VHL and LRRK2, which compensates for a substantial loss of binary binding affinities to VHL and LRRK2, underscoring its strong degradation performance in cells. XL01126 is orally bioavailable (F=15%) and can penetrate the blood brain barrier after either oral or parenteral dosing in mice. PROTAC® is a registered trademark of Arvinas Operations, Inc., and is used under license

Physical and Chemical Properties:

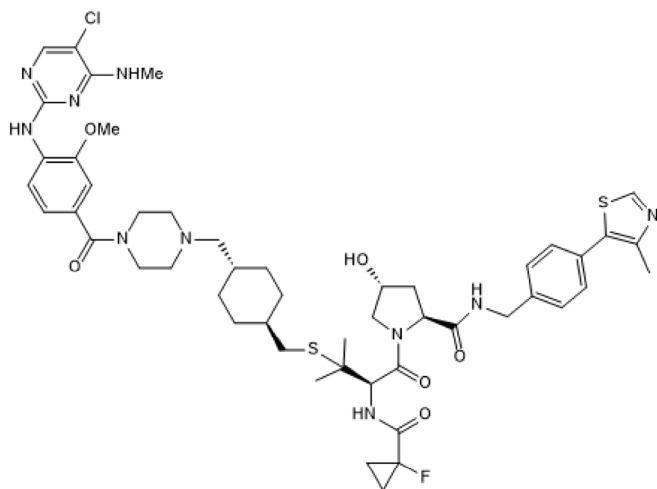
Batch Molecular Formula: C₅₀H₆₄ClF₁₀O₆S₂·½H₂O

Batch Molecular Weight: 1028.7

Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



References:

Liu *et al* (2022) Discovery of XL01126: a potent, fast, cooperative, selective, orally bioavailable, and blood-brain barrier penetrant PROTAC degrader of leucine-rich repeat kinase 2. JACS **144** 16930. PMID: 36007011.

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 licence from the University of Dundee

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