

Product Name: SJF 0628

Catalog No.: 7463

Batch No.: 2

CAS Number: 2413035-41-1

IUPAC Name: (2*S*,4*R*)-1-((*S*)-2-(2-(4-(4-(3-(2,6-Difluoro-3-(propylsulfonamido)benzoyl)-1*H*-pyrrolo[2,3-*b*]pyridin-5-yl)phenyl)piperazin-1-yl)acetamido)-3,3-dimethylbutanoyl)-4-hydroxy-*N*-(4-(4-methylthiazol-5-yl)benzyl)pyrrolidine-2-carboxamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₅₁H₅₇F₂N₉O₇S₂·1¾H₂O

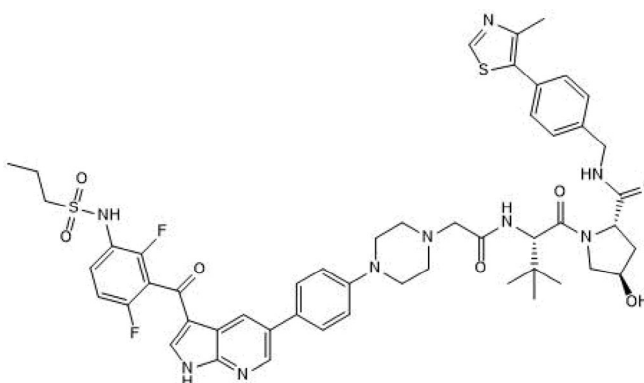
Batch Molecular Weight: 1041.71

Physical Appearance: Yellow solid

Solubility: DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 98.5% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	58.8	5.85	12.1
Found	58	5.59	11.68

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Description:

SJF 0628 is a potent, high affinity and mutant-selective Degradator (PROTAC®) of BRAF, comprising a ligand for the von Hippel Lindau E3 ligase joined by a piperazine linker to the BRAF kinase inhibitor vemurafenib. SJF 0628 induces degradation of all 3 classes of BRAF mutant in BRAF-dependent cancer cells without inducing degradation of the BRAF^{WT} protein. The product degrades mutant BRAF^{V600E} in BRAF-driven cancer cell lines (DC₅₀ = 6.8 nM - 28 nM). SJ 0628 inhibits phosphorylation of MEK and ERK in SK-MEL-28 cells (DC₅₀ = 10 nM) and inhibits cell growth in mutant-BRAF driven cancer cells (EC₅₀ = 37 nM). SJF 0661 negative control (Cat... Please see product specific page on www.tocris.com for full description.

Physical and Chemical Properties:

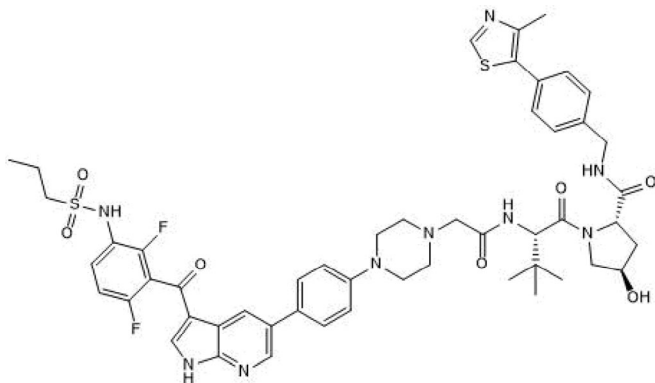
Batch Molecular Formula: C₅₁H₅₇F₂N₉O₇S₂·1¾H₂O

Batch Molecular Weight: 1041.71

Physical Appearance: Yellow solid

Minimum Purity: ≥98%

Batch Molecular Structure:



References:

Alabi *et al* (2021) Mutant-selective degradation by BRAF-targeting PROTACs. *Nat. Commun.* **12**. PMID: 33568647.

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.

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