

Product Name: SJF 0628

Catalog No.: 7463

Batch No.: 1

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 · 1½H₂O

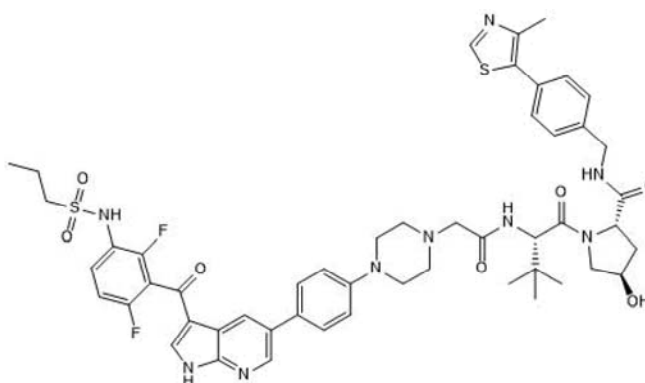
Batch Molecular Weight: 1037.21

Physical Appearance: Pale yellow solid

Solubility: DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 98.6% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	59.06	5.83	12.15
Found	58.68	5.67	12.06

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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:

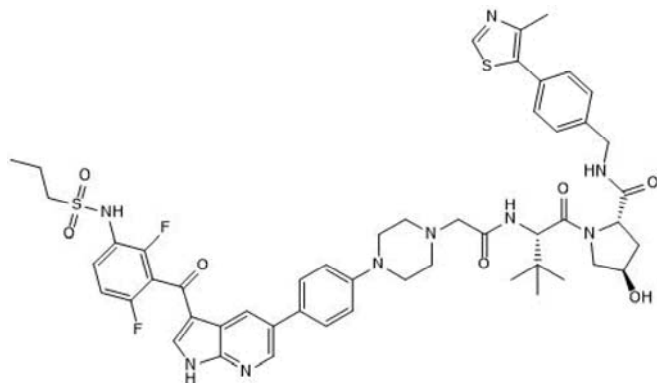
Batch Molecular Formula: C₅₁H₅₇F₂N₉O₇S₂·1½H₂O

Batch Molecular Weight: 1037.21

Physical Appearance: Pale 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.

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