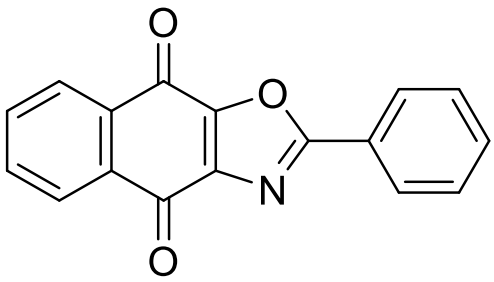
Product data sheet

MedKoo Cat#: 563362 Name: SJB2-043 CAS#: 63388-44-3 Chemical Formula: $C_{17}H_9NO_3$ Exact Mass: 275.0582 Molecular Weight: 275.26	
Product supplied as:	Powder
Purity (by HPLC):	≥ 98%
Shipping conditions	Ambient temperature
Storage conditions:	Powder: -20°C 3 years; 4°C 2 years.
	In solvent: -80°C 3 months; -20°C 2 weeks.

1. Product description:
SJB2-043 is an inhibitor of USP1 target ID1 degradation in leukemic cells.

2. CoA, QC data, SDS, and handling instruction
SDS and handling instruction, CoA with copies of QC data (NMR, HPLC and MS analytical spectra) can be downloaded from the product web page under "QC And Documents" section. Note: copies of analytical spectra may not be available if the product is being supplied by MedKoo partners. Whether the product was made by MedKoo or provided by its partners, the quality is 100% guaranteed.

3. Solubility data

Solvent	Max Conc. mg/mL	Max Conc. mM
DMF	2	
DMSO	1	

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	3.63 mL	18.16 mL	36.33 mL
5 mM	0.73 mL	3.63 mL	7.27 mL
10 mM	0.36 mL	1.82 mL	3.63 mL
50 mM	0.07 mL	0.36 mL	0.73 mL

5. Molarity Calculator, Reconstitution Calculator, Dilution Calculator
Please refer the product web page under section of "Calculator"

6. Recommended literature which reported protocols for in vitro and in vivo study
In vitro study

1. Cho CC, Li SG, Lalonde TJ, Yang KS, Yu G, Qiao Y, Xu S, Ray Liu W. Drug Repurposing for the SARS-CoV-2 Papain-Like Protease. ChemMedChem. 2022 Jan 5;17(1):e202100455. doi: 10.1002/cmdc.202100455. Epub 2021 Oct 12. Erratum in: ChemMedChem. 2022 Mar 4;17(5):e202200053. PMID: 34423563; PMCID: PMC8653067.
2. Mistry H, Hsieh G, Buhrlage SJ, Huang M, Park E, Cuny GD, Galinsky I, Stone RM, Gray NS, D'Andrea AD, Parmar K. Small-molecule inhibitors of USP1 target ID1 degradation in leukemic cells. Mol Cancer Ther. 2013 Dec;12(12):2651-62. doi: 10.1158/1535-7163.MCT-13-0103-T. Epub 2013 Oct 15. PMID: 24130053; PMCID: PMC4089878.

In vivo study

To be determined

7. Bioactivity
Biological target:

SJB2-043 is a dual inhibitor of USP1 and the USP1-UAF1 complex (IC50 = 0.544 μM for deubiquitinase activity) and also targets the SARS-CoV-2 papain-like protease (PLpro). It demonstrates antiproliferative effects in K562 cells (EC50 = 1.07 μM), inducing concentration-dependent apoptosis. Additionally, SJB2-043 effectively inhibits SARS-CoV-2 PLpro, with IC50 values of 0.56 μM and 0.091 μM using the fluorogenic substrates Z-LRGG-AMC and ubiquitin-AMC (Ub-AMC), respectively.

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In vitro activity

SJB2-043 inhibits the DUB activity of native USP1 complexes isolated from human cells. After treating cells with SJB2-043 for 24 hours, the formation of the Ub-USP1 conjugate was suppressed. SJB2-043 also showed specificity by inhibiting the labeling of a limited number of endogenous DUB enzymes. Furthermore, SJB2-043 demonstrated a dose-dependent inhibition of the labeling of USP1 with Ub-VS. In summary, these findings establish SJB2-043 as an inhibitor of the native USP1/UAF1 complex.

Reference: Mol Cancer Ther. 2013 Dec;12(12):2651-62. https://pubmed.ncbi.nlm.nih.gov/24130053/

In vivo activity

To be determined

Note: The information listed here was extracted from literature. MedKoo has not independently retested and confirmed the accuracy of these methods. Customer should use it just for a reference only.