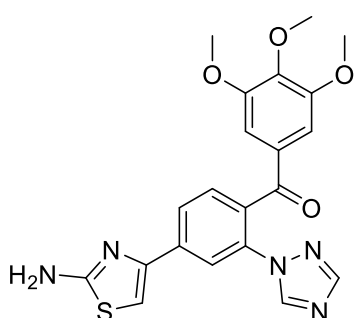


# Product data sheet



MedKoo Cat#: 462379 Name: S516 CAS#: 1016543-77-3 Chemical Formula: C <sub>21</sub> H <sub>19</sub> N <sub>5</sub> O <sub>4</sub> S Exact Mass: 437.1158 Molecular Weight: 437.47	
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:

S516 is an active metabolite of CKD-516 and a potent tubulin polymerization inhibitor.

## 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
DMSO	12.5	28.57

## 4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	2.29 mL	11.43 mL	22.86 mL
5 mM	0.46 mL	2.29 mL	4.57 mL
10 mM	0.23 mL	1.14 mL	2.29 mL
50 mM	0.05 mL	0.23 mL	0.46 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

- Kim SJ, Jegal KH, Im JH, Park G, Kim S, Jeong HG, Cho IJ, Kang KW. Involvement of ER stress and reactive oxygen species generation in anti-cancer effect of CKD-516 for lung cancer. *Cancer Chemother Pharmacol.* 2020 Apr;85(4):685-697. doi: 10.1007/s00280-020-04043-x. Epub 2020 Mar 11. PMID: 32157413.
- Moon CH, Lee SJ, Lee HY, Dung le TK, Cho WJ, Cha H, Park JW, Min YJ. CKD-516 displays vascular disrupting properties and enhances anti-tumor activity in combination with chemotherapy in a murine tumor model. *Invest New Drugs.* 2014 Jun;32(3):400-11. doi: 10.1007/s10637-013-0043-8. Epub 2013 Nov 8. PMID: 24202729.

### In vivo study

- Kim HK, Kang JW, Park YW, Kim JY, Kim M, Kim SJ, Kim SM, Ho Ryu K, Yoon S, Kim Y, Cho JY, Lee KS, Yun T, Kim K, Kwak MH, Kim TS, Chung J, Park JW. Phase I and pharmacokinetic study of the vascular-disrupting agent CKD-516 (NOV120401) in patients with refractory solid tumors. *Pharmacol Res Perspect.* 2020 Apr;8(2):e00568. doi: 10.1002/prp2.568. PMID: 32162844; PMCID: PMC7066534.
- Lee J, Kim SJ, Choi H, Kim YH, Lim IT, Yang HM, Lee CS, Kang HR, Ahn SK, Moon SK, Kim DH, Lee S, Choi NS, Lee KJ. Identification of CKD-516: a potent tubulin polymerization inhibitor with marked antitumor activity against murine and human solid tumors. *J Med Chem.* 2010 Sep 9;53(17):6337-54. doi: 10.1021/jm1002414. PMID: 20690624.

## 7. Bioactivity

Biological target:

# Product data sheet



S516 is a potent tubulin polymerization inhibitor with an IC<sub>50</sub> of 4.29  $\mu$ M. S516 has antitumor activity.

## In vitro activity

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This study evaluated the effects of S516 in HUVECs and three lung cancer cell lines. In lung cancer cells, S516 increased endoplasmic reticulum stress and induced reactive oxygen species generation by mitochondria and the endoplasmic reticulum. S516 targeted the colchicine binding site on  $\beta$ -tubulin.

Reference: Cancer Chemother Pharmacol. 2020 Apr;85(4):685-697. <https://pubmed.ncbi.nlm.nih.gov/32157413/>

## In vivo activity

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S516 showed marked antitumor efficacy against both murine tumors (CT26 and 3LL) and human xenografts (HCT116 and HCT15) in mice.

Reference: J Med Chem. 2010 Sep 9;53(17):6337-54. <https://pubmed.ncbi.nlm.nih.gov/20690624/>

*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.*