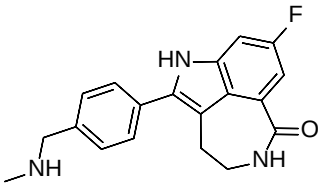
Product data sheet

MedKoo Cat#: 100947 Name: Rucaparib free base CAS#: 283173-50-2 (free base) Chemical Formula: $C_{19}H_{18}FN_3O$ Exact Mass: 323.1434 Molecular Weight: 323.37	
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:
Rucaparib is a tricyclic indole poly(ADP-Ribose) polymerase (PARP1) inhibitor with potential chemosensitizing, radiosensitizing, and antineoplastic activities. Rucaparib selectively binds to PARP1 and inhibits PARP1-mediated DNA repair, thereby enhancing the accumulation of DNA strand breaks and promoting genomic instability and apoptosis.

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	46.67	144.32
Ethanol	16.50	51.03
DMF	30.0	92.77
DMF:PBS (pH 7.2) (1:1)	0.50	1.55

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	3.09 mL	15.46 mL	30.92 mL
5 mM	0.62 mL	3.09 mL	6.18 mL
10 mM	0.31 mL	1.55 mL	3.09 mL
50 mM	0.06 mL	0.31 mL	0.62 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. Liao M, Jaw-Tsai S, Beltman J, Simmons AD, Harding TC, Xiao JJ. Evaluation of in vitro absorption, distribution, metabolism, and excretion and assessment of drug-drug interaction of rucaparib, an orally potent poly(ADP-ribose) polymerase inhibitor. Xenobiotica. 2020 Sep;50(9):1032-1042. doi: 10.1080/00498254.2020.1737759. Epub 2020 Mar 18. PMID: 32129697.

In vivo study

1. Tang M, Liu Q, Zhou L, Chen L, Yang X, Yu J, Wang Y, Qiu H. The poly (ADP-ribose) polymerase inhibitor rucaparib suppresses proliferation and serves as an effective radiosensitizer in cervical cancer. Invest New Drugs. 2019 Feb;37(1):65-75. doi: 10.1007/s10637-018-0616-7. Epub 2018 Jun 6. PMID: 29872938.

7. Bioactivity
Biological target: Rucaparib (AG014699) is an inhibitor of PARP with Ki of 1.4 nM for PARP1 in a cell-free assay.

In vitro activity

Product data sheet

The absorption, distribution, metabolism, elimination, and drug-drug interaction (DDI) potential of the poly(ADP-ribose) polymerase (PARP) inhibitor rucaparib was characterised in vitro. Rucaparib showed moderate cellular permeability, moderate human plasma protein binding (70.2%), and slow metabolism in human liver microsomes (HLMs). In HLMs, cytochrome P450 (CYP) 1A2 and CYP3A contributed to the metabolism of rucaparib to its major metabolite M324 with estimated fractions of metabolism catalysed by CYP (fm,CYP) of 0.27 and 0.64, respectively. Rucaparib reversibly inhibited CYP1A2, CYP2C9, CYP2C19, CYP2D6, and CYP3As (IC50, 3.55, 12.9, 5.42, 41.6, and 17.2-22.9 μM [2 substrates], respectively), but not CYP2B6 or CYP2C8 (>190 μM).

Reference: Xenobiotica. 2020 Sep;50(9):1032-1042.
https://www.tandfonline.com/doi/abs/10.1080/00498254.2020.1737759?journalCode=ixen20

In vivo activity

The effects of rucaparib on the proliferation of cervical cancer cells and sensitivity to radiotherapy were investigated. Animal experiments were performed to evaluate tumor size after treatment with rucaparib. Immunohistochemistry was performed to analyze the expression of Ki-67. Rucaparib suppressed proliferation, induced G2/M phase arrest, and reduced the expression of cyclin D1 and CDK4 in cervical cancer cells. When rucaparib was combined with radiotherapy in cervical cancer cells, clone formation decreased significantly and G2/M phase arrest was accentuated. The expression of the DNA-damage marker γ-H2AX was increased significantly, and rucaparib suppressed tumor growth in vivo. Rucaparib exerts significant anti-proliferative effects and can serve as an effective radiosensitizer in cervical cancer.

Reference: Invest New Drugs. 2019 Feb;37(1):65-75. https://link.springer.com/article/10.1007%2Fs10637-018-0616-7