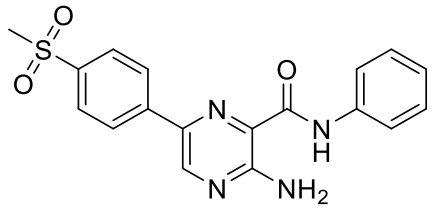
Product data sheet

MedKoo Cat#: 406257 Name: VE-821 CAS#: 1232410-49-9 Chemical Formula: $C_{18}H_{16}N_4O_3S$ Exact Mass: 368.09431 Molecular Weight: 368.40964	
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:
VE-821 is the first highly selective and potent ATR inhibitor. VE-821 inhibited radiation- and gemcitabine-induced phosphorylation of Chk1, confirming inhibition of ATR signaling. Consistently, VE-821 significantly enhanced the sensitivity of PSN-1, MiaPaCa-2 and primary PancM pancreatic cancer cells to radiation and gemcitabine under both normoxic and hypoxic conditions. ATR inhibition by VE-821 led to inhibition of radiation-induced G 2/M arrest in cancer 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
DMSO	50	135.72

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	2.71 mL	13.57 mL	27.14 mL
5 mM	0.54 mL	2.71 mL	5.43 mL
10 mM	0.27 mL	1.36 mL	2.71 mL
50 mM	0.05 mL	0.27 mL	0.54 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. Fujisawa H, Nakajima NI, Sunada S, Lee Y, Hirakawa H, Yajima H, Fujimori A, Uesaka M, Okayasu R. VE-821, an ATR inhibitor, causes radiosensitization in human tumor cells irradiated with high LET radiation. Radiat Oncol. 2015 Aug 19;10:175. doi: 10.1186/s13014-015-0464-y. PMID: 26286029; PMCID: PMC4554350.

2. Prevo R, Fokas E, Reaper PM, Charlton PA, Pollard JR, McKenna WG, Muschel RJ, Brunner TB. The novel ATR inhibitor VE-821 increases sensitivity of pancreatic cancer cells to radiation and chemotherapy. Cancer Biol Ther. 2012 Sep;13(11):1072-81. doi: 10.4161/cbt.21093. Epub 2012 Jul 24. PMID: 22825331; PMCID: PMC3461814.

In vivo study

TBD

7. Bioactivity
Biological target:

VE-821 is a potent ATP-competitive inhibitor of ATR with Ki/IC50 of 13 nM/26 nM.

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In vitro activity

HeLa, U2OS, and 1BR-hTERT (normal) cells were pre-treated with 1 μM VE-821 for 1 hour and irradiated with either high LET carbon ions or X-rays. Cell survival, cell cycle distribution, cell growth, and micronuclei formation were evaluated. VE-821 caused abrogation of G2/M checkpoint and forced irradiated cells to divide into daughter cells. It was also found that carbon ions caused a higher number of multiple micronuclei than X-rays, leading to decreased cell survival in tumor cells when treated with VE-821, while the survival of irradiated normal cells were not significantly affected by this inhibitor.

Reference: Radiat Oncol. 2015 Aug 19;10:175. https://www.ncbi.nlm.nih.gov/pmc/articles/pmid/26286029/

In vivo activity

TBD

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.