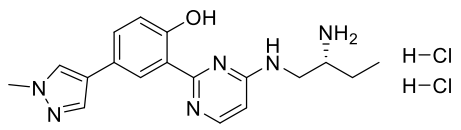
Product data sheet

MedKoo Cat#: 531753 Name: CRT0066101 HCl CAS#: 1883545-60-5 Chemical Formula: $C_{18}H_{24}Cl_2N_6O$ Molecular Weight: 411.33	
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:

CRT 0066101 is a potent inhibitor of protein kinase D (PKD). It inhibits all PKD isoforms (IC50 values are 1, 2 and 2.5 nM for PKD1, PKD3 and PKD2 respectively). CRT 0066101 exhibits selectivity for PKD against a panel of >90 protein kinases, including PKCα, MEK, ERK, c-Raf and c-Src.

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	19.41	47.19
Ethanol	2.0	4.86
Water	57.71	140.30

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	**1 mg**	**5 mg**	**10 mg**
1 mM	2.43 mL	12.16 mL	24.31 mL
5 mM	0.49 mL	2.43 mL	4.86 mL
10 mM	0.24 mL	1.22 mL	2.43 mL
50 mM	0.05 mL	0.24 mL	0.49 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. Liu Y, Wang Y, Yu S, Zhou Y, Ma X, Su Q, An L, Wang F, Shi A, Zhang J, Chen L. The Role and Mechanism of CRT0066101 as an Effective Drug for Treatment of Triple-Negative Breast Cancer. Cell Physiol Biochem. 2019;52(3):382-396. doi: 10.33594/000000027. Epub 2019 Mar 8. PMID: 30845378.
2. Li QQ, Hsu I, Sanford T, Railkar R, Balaji N, Sourbier C, Vocke C, Balaji KC, Agarwal PK. Protein kinase D inhibitor CRT0066101 suppresses bladder cancer growth in vitro and xenografts via blockade of the cell cycle at G2/M. Cell Mol Life Sci. 2018 Mar;75(5):939-963. doi: 10.1007/s00018-017-2681-z. Epub 2017 Oct 25. PMID: 29071385; PMCID: PMC7984729.

In vivo study

1. Li QQ, Hsu I, Sanford T, Railkar R, Balaji N, Sourbier C, Vocke C, Balaji KC, Agarwal PK. Protein kinase D inhibitor CRT0066101 suppresses bladder cancer growth in vitro and xenografts via blockade of the cell cycle at G2/M. Cell Mol Life Sci. 2018 Mar;75(5):939-963. doi: 10.1007/s00018-017-2681-z. Epub 2017 Oct 25. PMID: 29071385; PMCID: PMC7984729.
2. Borges S, Perez EA, Thompson EA, Radisky DC, Geiger XJ, Storz P. Effective Targeting of Estrogen Receptor-Negative Breast Cancers with the Protein Kinase D Inhibitor CRT0066101. Mol Cancer Ther. 2015 Jun;14(6):1306-16. doi: 10.1158/1535-7163.MCT-14-0945. Epub 2015 Apr 7. PMID: 25852060; PMCID: PMC4458391.

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7. Bioactivity

Biological target:

CRT0066101 dihydrochloride is a potent and specific PKD inhibitor with IC50 values of 1, 2.5 and 2 nM for PKD1, 2, and 3 respectively.

In vitro activity

The time-course of CRT0066101 suppression of the proliferation of the four cell lines was characterized in vitro using the MTT assay. All of the four cell lines examined showed a maximal inhibitory effect at day 4 following CRT0066101 treatment (Fig. 2a).

Reference: Cell Mol Life Sci. 2018 Mar; 75(5): 939–963. https://www.ncbi.nlm.nih.gov/pmc/articles/PMC7984729/

In vivo activity

Treatment of mice with CRT0066101 did result in a significant decrease of primary tumor size and weight (Fig. 5A, Supplemental Fig. S9), associated with an approximately 50% decrease in tumor cell proliferation (Fig. 5B), and an increase of apoptosis (Fig. 5C).

Reference: Mol Cancer Ther. 2015 Jun; 14(6): 1306–1316. https://www.ncbi.nlm.nih.gov/pmc/articles/PMC4458391/

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.