

Product Name: Veliparib dihydrochloride

Catalog No.: 7026

Batch No.: 1

CAS Number: 912445-05-7

IUPAC Name: 2-[(2*R*)-2-Methyl-2-pyrrolidinyl]-1*H*-benzimidazole-4-carboxamide dihydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₃H₁₆N₄O.2HCl.¼H₂O

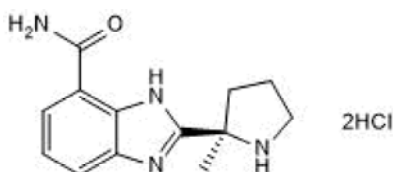
Batch Molecular Weight: 321.71

Physical Appearance: Off-white solid

Solubility: DMSO to 100 mM
water to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 98.6% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: [α]_D = +14.7 (Concentration = 1, Solvent = Methanol)

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	48.53	5.8	17.41
Found	48.57	5.39	17.37

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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Description:

High affinity PARP-2 and PARP-1 inhibitor (K_i values are 2.9 and 5.2 nM, respectively). Inhibits repair of radiation-induced DNA damage and sensitizes lung cancer cells to radiation. Also increases autophagy and apoptosis in lung cancer cells. Enhances radiation-induced tumor growth delay in mice bearing lung tumor xenografts. Also chemosensitizer. Potentiates effects of temozolomide (Cat. No. 2706) in a mouse melanoma model. Orally bioavailable and brain penetrant.

Physical and Chemical Properties:

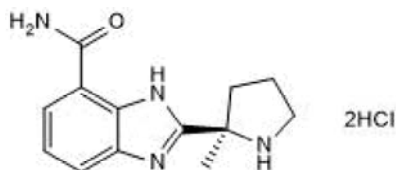
Batch Molecular Formula: $C_{13}H_{16}N_4O \cdot 2HCl \cdot \frac{1}{4}H_2O$

Batch Molecular Weight: 321.71

Physical Appearance: Off-white solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM
water to 100 mM

Stability and Solubility Advice:

Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a 45-60°C water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. Our standard recommendations are:

SOLIDS: Provided storage is as stated on the product label and the vial is kept tightly sealed, the product can be stored for up to 6 months from date of receipt.

SOLUTIONS: We recommend that stock solutions, once prepared, are stored aliquoted in tightly sealed vials at -20°C or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

References:

Albert et al (2007) Inhibition of poly(ADP-ribose) polymerase enhances cell death and improves tumor growth delay in irradiated lung cancer models. *Clin.Cancer Res.* **13** 3033. PMID: 17505006.

Donawho et al (2007) ABT-888, an orally active poly(ADP-ribose) polymerase inhibitor that potentiates DNA-damaging agents in preclinical tumor models. *Clin.Cancer Res.* **13** 2728. PMID: 17473206.

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