

Product data sheet



MedKoo Cat#: 206822 Name: BAY-1895344 HCl CAS#: 1876467-74-1 Chemical Formula: C ₂₀ H ₂₂ ClN ₇ O Molecular Weight: 411.89	
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:

BAY-1895344 HCl, also known as Elimusertib, is a potent and selective ATM inhibitor. BAY 1895344 shows potent anti-tumor efficacy in monotherapy and strong combination potential with the targeted alpha therapy Radium-223 dichloride.

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	54	131.10
Water	50	121.39
Ethanol	82	199.08

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	2.43 mL	12.14 mL	24.28 mL
5 mM	0.49 mL	2.43 mL	4.86 mL
10 mM	0.24 mL	1.21 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. Lücking U, Wortmann L, Wengner AM, Lefranc J, Lienau P, Briem H, Siemeister G, Bömer U, Denner K, Schäfer M, Koppitz M, Eis K, Bartels F, Bader B, Bone W, Moosmayer D, Holton SJ, Eberspächer U, Grudzinska-Goebel J, Schatz C, Deeg G, Mumberg D, von Nussbaum F. Damage Incorporated: Discovery of the Potent, Highly Selective, Orally Available ATR Inhibitor BAY 1895344 with Favorable Pharmacokinetic Properties and Promising Efficacy in Monotherapy and in Combination Treatments in Preclinical Tumor Models. *J Med Chem.* 2020 Jul 9;63(13):7293-7325. doi: 10.1021/acs.jmedchem.0c00369. Epub 2020 Jun 28. PMID: 32502336.

In vivo study

1. Antje Margret Wengner, Gerhard Siemeister, Ulrich Luecking, Julien Lefranc, Philip Lienau, Gesa Deeg, Eleni Lagkadinou, Li Liu, Sven Golfier, Christoph Schatz, Arne Scholz, Franz von Nussbaum, Michael Brands, Dominik Mumberg, Karl Ziegelbauer. ATR inhibitor BAY 1895344 shows potent anti-tumor efficacy in monotherapy and strong combination potential with the targeted alpha therapy Radium-223 dichloride in preclinical tumor models [abstract]. In: Proceedings of the American Association for Cancer Research Annual Meeting 2017; 2017 Apr 1-5; Washington, DC. Philadelphia (PA): AACR; Cancer Res 2017;77(13 Suppl):Abstract nr 836. doi:10.1158/1538-7445.AM2017-836

7. Bioactivity

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Biological target:

Elimusertib (BAY 1895344) hydrochloride is a potent, orally available and selective ATR inhibitor with an IC50 of 7 nM.

In vitro activity

In vitro, BAY 1895344 is shown to be a very potent and highly selective ATR inhibitor (IC50 = 7 nM), which potently inhibits proliferation of a broad spectrum of human tumor cell lines (median IC50 = 78 nM). In cellular mechanistic assays BAY 1895344 potently inhibits hydroxyurea-induced H2AX phosphorylation (IC50 = 36 nM)

Reference: Proceedings of the American Association for Cancer Research Annual Meeting 2017; 2017 Apr 1-5; Washington, DC. Philadelphia (PA): AACR; Cancer Res 2017;77(13 Suppl):Abstract nr 983.
https://cancerres.aacrjournals.org/content/77/13_Supplement/983

In vivo activity

BAY 1895344 is an ATR inhibitor that exhibits strong in vivo anti-tumor efficacy in monotherapy in a variety of xenograft models of different indications that are characterized by DDR deficiencies, inducing stable disease in ovarian and colorectal cancer or even complete tumor remission in mantle cell lymphoma models.

Reference: Proceedings of the American Association for Cancer Research Annual Meeting 2017; 2017 Apr 1-5; Washington, DC. Philadelphia (PA): AACR; Cancer Res 2017;77(13 Suppl):Abstract nr 836.
https://cancerres.aacrjournals.org/content/77/13_Supplement/836

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.