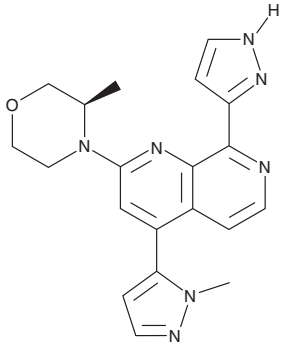
PRODUCT INFORMATION

BAY-1895344

Item No. 33603

CAS Registry No.:	1876467-74-1
Formal Name:	2-[(3R)-3-methyl-4-morpholinyl]-4-(1-methyl-1H-pyrazol-5-yl)-8-(1H-pyrazol-3-yl)-1,7-naphthyridine
Synonym:	Elimusertib
MF:	$C_{20}H_{21}N_7O$
FW:	375.4
Purity:	≥98%
UV/Vis.:	λ_{max}: 221, 282 nm
Supplied as:	A crystalline solid
Storage:	-20°C
Stability:	≥4 years



Information represents the product specifications. Batch specific analytical results are provided on each certificate of analysis.

Laboratory Procedures

BAY-1895344 is supplied as a crystalline solid. A stock solution may be made by dissolving the BAY-1895344 in the solvent of choice, which should be purged with an inert gas. BAY-1895344 is soluble in organic solvents such as ethanol, DMSO, and dimethyl formamide (DMF). The solubility of BAY-1895344 in ethanol is approximately 1 mg/ml and approximately 25 mg/ml in DMSO and DMF.

BAY-1895344 is sparingly soluble in aqueous buffers. For maximum solubility in aqueous buffers, BAY-1895344 should first be dissolved in DMSO and then diluted with the aqueous buffer of choice. BAY-1895344 has a solubility of approximately 0.25 mg/ml in a 1:3 solution of DMSO:PBS (pH 7.2) using this method. We do not recommend storing the aqueous solution for more than one day.

Description

BAY-1895344 is an inhibitor of ataxia-telangiectasia and Rad3-related protein/kinase (ATR; IC_{50} = 0.007 µM).[1,2] It is selective for ATR over DNA protein kinase (DNA-PK), ataxia-telangiectasia mutated kinase (ATM), and PI3Kβ (IC_{50}s = 0.332, 1.42, and 3.27 µM, respectively).[1] BAY-1895344 inhibits proliferation of HT-29 and LoVo colorectal cancer cells and SU-DHL-8 B lymphoma cells with IC_{50} values of 0.16, 0.071, and 0.009 µM, respectively. It reduces tumor growth in a mutant ATM^{K1964E}-containing SU-DHL-8 mouse xenograft model when administered at a dose of 50 mg/kg. BAY-1895344 is synergistic with carboplatin (Item No. 13112), olaparib (Item No. 10621), or radiation in various mouse xenograft models.[1,2]

References

1. Lücking, U., Wortmann, L., Wengner, A.M., *et al.* 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.* **63(13)**, 7293-7325 (2020).
2. Wengner, A.M., Siemeister, G., Lücking, U., *et al.* The novel ATR inhibitor BAY 1895344 is efficacious as monotherapy and combined with DNA damage-inducing or repair-compromising therapies in preclinical cancer models. *Mol. Cancer Ther.* **19(1)**, 26-38 (2020).

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