

PRODUCT INFORMATION

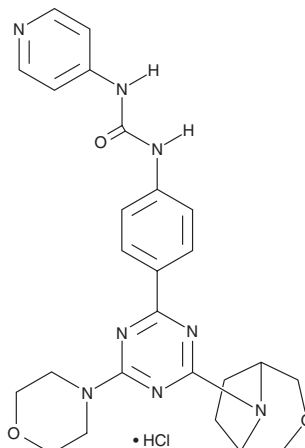


PKI-179 (hydrochloride)

Item No. 21202

CAS Registry No.: 1463510-35-1
Formal Name: N-[4-[4-(4-morpholinyl)-6-(3-oxa-8-azabicyclo[3.2.1]oct-8-yl)-1,3,5-triazin-2-yl]phenyl]-N'-4-pyridinyl-urea, monohydrochloride

MF: C₂₅H₂₈N₈O₃ • HCl
FW: 525.0
Purity: ≥98%
UV/Vis.: λ_{max}: 228, 297 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

PKI-179 (hydrochloride) is supplied as a crystalline solid. A stock solution may be made by dissolving the PKI-179 (hydrochloride) in the solvent of choice, which should be purged with an inert gas. PKI-179 (hydrochloride) is soluble in organic solvents such as DMSO and dimethyl formamide. The solubility of PKI-179 (hydrochloride) in these solvents is approximately 2.5 and 2 mg/ml, respectively. PKI-179 (hydrochloride) is also slightly soluble in ethanol.

PKI-179 (hydrochloride) is sparingly soluble in aqueous buffers. For maximum solubility in aqueous buffers, PKI-179 (hydrochloride) should first be dissolved in DMSO and then diluted with the aqueous buffer of choice. PKI-179 (hydrochloride) 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

PKI-179 is an orally bioavailable dual inhibitor of PI3K and mammalian target of rapamycin (mTOR).¹ In an *in vitro* enzymatic assay, it potently inhibits PI3K (IC₅₀s = 8, 24, 17, and 74 nM for isoforms α, β, δ, and γ, respectively), two common PI3Kα mutants, E545K and H1047R (IC₅₀s = 14 and 11 nM, respectively), and mTOR (IC₅₀ = 0.42 nM). PKI-179 is selective for PI3K and mTOR over a panel of 361 other kinases at IC₅₀ values up to 50 μM, hERG (IC₅₀ > 30 μM), and cytochrome P450 (CYP) isoforms (IC₅₀s > 30 μM), but does have activity for CYP2C8 (IC₅₀ = 3 μM). It inhibits proliferation through the Akt/mTOR signaling pathway in MDA-361 breast and PC3MM2 prostate cancer cell lines *in vitro* (IC₅₀s = 22 and 29 nM, respectively) and inhibits tumor growth in an MDA-361 mouse xenograft model when used at a dose of 50 mg/kg.

Reference

1. Venkatesan, A.M., Chen, Z., dos Santos, O., *et al.* PKI-179: An orally efficacious dual phosphatidylinositol-3-kinase (PI3K)/mammalian target of rapamycin (mTOR) inhibitor. *Bioorg. Med. Chem. Lett.* **20**(19), 5869-5873 (2010).

WARNING

THIS PRODUCT IS FOR RESEARCH ONLY - NOT FOR HUMAN OR VETERINARY DIAGNOSTIC OR THERAPEUTIC USE.

SAFETY DATA

This material should be considered hazardous until further information becomes available. Do not ingest, inhale, get in eyes, on skin, or on clothing. Wash thoroughly after handling. Before use, the user must review the complete Safety Data Sheet, which has been sent via email to your institution.

WARRANTY AND LIMITATION OF REMEDY

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