

Product Name: TAK 960 hydrochloride

Catalog No.: 5403

Batch No.: 1

CAS Number: 2108449-45-0

IUPAC Name: 4-[(9-Cyclopentyl-7,7-difluoro-6,7,8,9-tetrahydro-5-methyl-6-oxo-5H-pyrimido[4,5-b][1,4]diazepin-2-yl)amino]-2-fluoro-5-methoxy-N-(1-methyl-4-piperidiny)benzamide hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₇H₃₄F₃N₇O₃.HCl.2H₂O

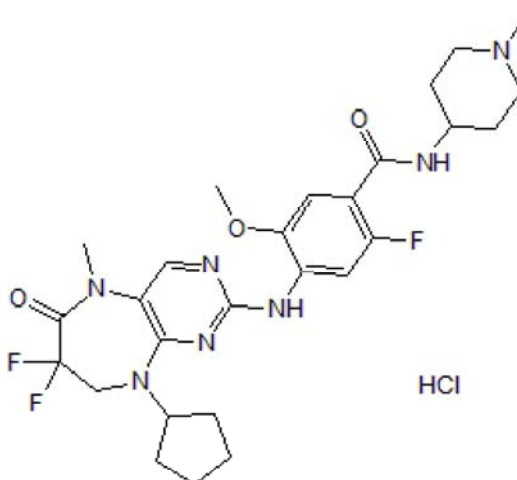
Batch Molecular Weight: 634.09

Physical Appearance: Off-white solid

Solubility: DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 98.5% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	51.14	6.2	15.46
Found	51.35	6.27	15.26

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bio-techne.com

info@bio-techne.com

techsupport@bio-techne.com

North America

Tel: (800) 343 7475

China

info.cn@bio-techne.com

Tel: +86 (21) 52380373

Europe Middle East Africa

Tel: +44 (0)1235 529449

Rest of World

www.tocris.com/distributors

Tel:+1 612 379 2956

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Description:

Potent PLK1 inhibitor (IC₅₀ values are 0.8, 16.9 and 50.2 nM for PLK1, PLK2 and PLK3 respectively). Exhibits >20-fold selectivity for PLK1 over FAK, MLCK and FES, and has minimal activity against a panel of 282 other kinases. Inhibits proliferation of a range of cancer cell lines in vitro and inhibits tumor growth of multiple human cancer cell xenografts in vivo. Orally bioavailable.

Physical and Chemical Properties:

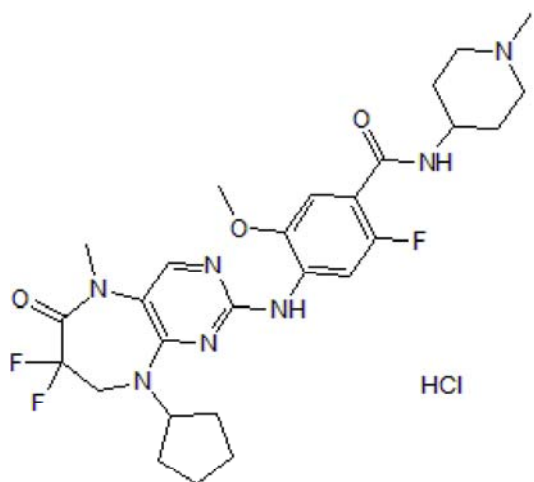
Batch Molecular Formula: C₂₇H₃₄F₃N₇O₃.HCl.2H₂O

Batch Molecular Weight: 634.09

Physical Appearance: Off-white solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO 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:

Nie et al (2013) Discovery of TAK-960: an orally available small molecule inhibitor of polo-like kinase 1 (PLK1). *Bioorg.Med.Chem.Lett.* **23** 3662. PMID: 23664874.

Hikichi et al (2012) TAK-960, a novel, orally available, selective inhibitor of polo-like kinase 1, shows broad-spectrum preclinical antitumor activity in multiple dosing regimens. *Mol.Cancer Ther.* **11** 700. PMID: 22188812.

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