

**Product Name:** TC KHNS 11

**Catalog No.:** 6079

**Batch No.:** 1

CAS Number: 1431540-99-6

IUPAC Name: 5-[4-[3-[(4-Acetyl-1-piperazinyl)carbonyl]phenyl]-6-quinazoliny]-2-methoxy-3-pyridinecarbonitrile

**1. PHYSICAL AND CHEMICAL PROPERTIES**

**Batch Molecular Formula:** C<sub>28</sub>H<sub>24</sub>N<sub>6</sub>O<sub>3</sub>·½H<sub>2</sub>O

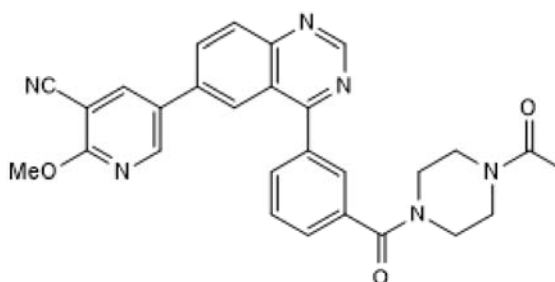
**Batch Molecular Weight:** 501.54

**Physical Appearance:** Yellow solid

**Solubility:** DMSO to 100 mM

**Storage:** Store at -20°C

**Batch Molecular Structure:**



**2. ANALYTICAL DATA**

**TLC:** R<sub>f</sub> = 0.23 (Dichloromethane:Methanol [95:5])

**HPLC:** Shows 98.2% purity

**<sup>1</sup>H NMR:** Consistent with structure

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	67.05	5.02	16.76
Found	66.91	5.06	16.54

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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 and selective PI 3-kinase  $\delta$  inhibitor (biochemical  $IC_{50}$  values are 9, 262, 1650 and 4630 nM for PI 3-K $\delta$ , PI 3-K $\alpha$ , PI 3-K $\beta$  and PI 3-K $\gamma$ , respectively; cellular  $IC_{50}$  values are 49, 3440 and 6530 nM for PI 3-K $\delta$ , PI 3-K $\alpha$  and PI 3-K $\beta$ , respectively). Selective for PI 3-K $\delta$  over a panel of lipid and protein kinases. Inhibits B-cell function. Exhibits moderate oral bioavailability in vivo.

**Physical and Chemical Properties:**

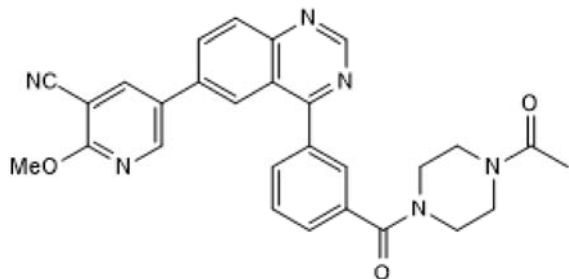
Batch Molecular Formula:  $C_{28}H_{24}N_6O_3 \cdot \frac{1}{2}H_2O$

Batch Molecular Weight: 501.54

Physical Appearance: Yellow 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:**

Hoegenauer *et al* (2016) Discovery and pharmacological characterization of novel quinazoline-based PI3K delta-selective inhibitors. ACS Med.Chem.Lett. 7 762. PMID: 27563400.

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