

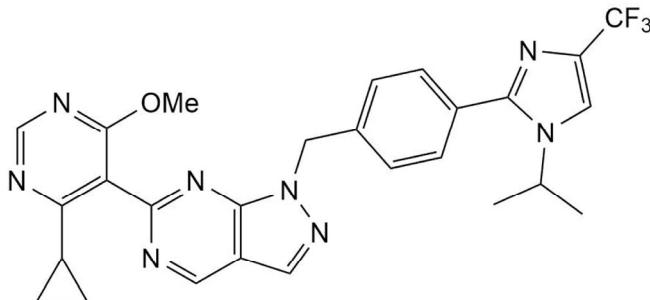
Certificate of Analysis

www.tocris.com**Product Name:** **KSQ 4279****Catalog No.:** **7746****Batch No.:** **1**

CAS Number: 2446480-97-1

IUPAC Name: 6-(4-Cyclopropyl-6-methoxypyrimidin-5-yl)-1-(4-(1-isopropyl-4-(trifluoromethyl)-1*H*-imidazol-2-yl)benzyl)-1*H*-pyrazolo[3,4-*d*]pyrimidine

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₇H₂₅F₃N₈O**Batch Molecular Weight:** 534.54**Physical Appearance:** White solid**Solubility:** DMSO to 100 mM
ethanol to 100 mM**Storage:** Store at -20°C**Batch Molecular Structure:**

2. ANALYTICAL DATA

HPLC: Shows 98.8% purity**¹H NMR:** Consistent with structure**Mass Spectrum:** Consistent with structure**Microanalysis:** Carbon Hydrogen Nitrogen

Theoretical 60.67 4.71 20.96

Found 60.08 4.66 20.56

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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Product Information

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Product Name: **KSQ 4279**

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Description:

KSQ 4279 is a potent and selective allosteric inhibitor of the ubiquitin specific protease 1 (USP1) (IC_{50} = 11 nM; K_i = 1.2 nM), a key regulator of DNA damage repair pathway (distinct from PARP inhibitors). It displays selectivity for USP1 over other USP, UCH and OTU enzymes. KSQ 4279 has strong antiproliferation effects *in vitro*. It induces accumulation of mono-ubiquitinated substrates in MDA-MB-436 cells. *In vivo*, KSQ 4279 induces anti-tumor response in the BRCA1 mutant ovarian PDX model (mouse). It also displays synergistic effects with PARP inhibitor Olaparib (Cat. No. 7579) leading to significant and durable anti-tumor response in mice... Please see product specific page on www.tocris.com for full description.

Physical and Chemical Properties:

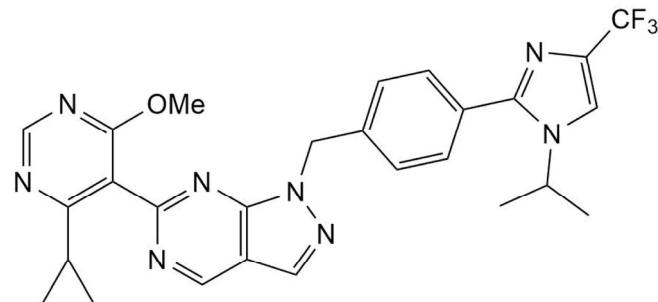
Batch Molecular Formula: C₂₇H₂₅F₃N₈O

Batch Molecular Weight: 534.54

Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



References:

Cadzow *et al* (2024) The USP1 inhibitor KSQ-4279 overcomes PARP inhibitor resistance in homologous recombination-deficient tumors. *Cancer Res.* **84** 3419. PMID: 39402989.

Li *et al* (2024) Design, synthesis, and biological evaluation of pyrido[2,3-*d*]pyrimidin-7(8*H*)-one derivatives as potent USP1 inhibitors. *Eur.J.Med.Chem.* **275** 116568. PMID: 38889606.

Nusawardhana *et al* (2024) USP1-dependent nucleolytic expansion of PRIMPOL-generated nascent DNA strand discontinuities during replication stress. *Nucleic Acids Research* **52** 2340. PMID: 38180818.

Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM
ethanol 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. *Unless contradicted by product-specific protocols or instructions, our standard recommendations apply:

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.

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