

# Certificate of Analysis

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**Product Name:** KSQ 4279

**Catalog No.:** 7746

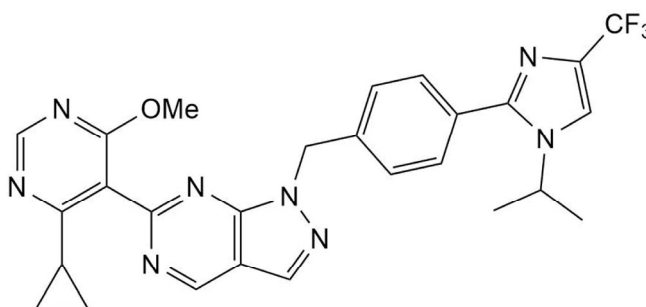
**Batch No.:** 1

**CAS Number:** 2446480-97-1

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

## 1. PHYSICAL AND CHEMICAL PROPERTIES

<b>Batch Molecular Formula:</b>	C <sub>27</sub> H <sub>25</sub> F <sub>3</sub> N <sub>8</sub> O
<b>Batch Molecular Weight:</b>	534.54
<b>Physical Appearance:</b>	White solid
<b>Solubility:</b>	DMSO to 100 mM ethanol to 100 mM
<b>Storage:</b>	Store at -20°C
<b>Batch Molecular Structure:</b>	



## 2. ANALYTICAL DATA

<b>HPLC:</b>	Shows 98.8% purity
<b><sup>1</sup>H NMR:</b>	Consistent with structure
<b>Mass Spectrum:</b>	Consistent with structure
<b>Microanalysis:</b>	

	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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**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](http://www.tocris.com) for full description.

**Physical and Chemical Properties:**

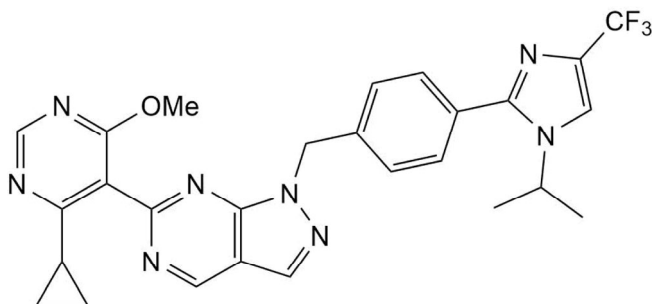
Batch Molecular Formula:  $C_{27}H_{25}F_3N_8O$

Batch Molecular Weight: 534.54

Physical Appearance: White solid

**Minimum Purity:** ≥98%

**Batch Molecular Structure:**



**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.

**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(8H)-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.

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