

**Product Name:** AZD 2461

**Catalog No.:** 6060

**Batch No.:** 1

CAS Number: 1174043-16-3

IUPAC Name: 4-[[4-Fluoro-3-[(4-methoxy-1-piperidiny)carbonyl]phenyl]methyl]-1(2*H*)-phthalazinone

**1. PHYSICAL AND CHEMICAL PROPERTIES**

**Batch Molecular Formula:** C<sub>22</sub>H<sub>22</sub>FN<sub>3</sub>O<sub>3</sub>·¼H<sub>2</sub>O

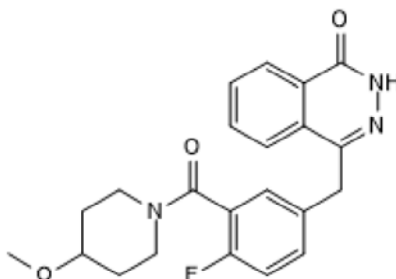
**Batch Molecular Weight:** 399.93

**Physical Appearance:** Light yellow solid

**Solubility:** DMSO to 100 mM  
ethanol to 100 mM

**Storage:** Store at -20°C

**Batch Molecular Structure:**



**2. ANALYTICAL DATA**

**TLC:** R<sub>f</sub> = 0.75 (Dichloromethane:Methanol [85:15])

**HPLC:** Shows >99.2% purity

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

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	66.07	5.67	10.51
Found	66.14	5.63	10.66

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

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**Description:**

AZD 2461 is a potent PARP inhibitor (IC<sub>50</sub> values are 2, 5 and 200 nM for PARP2, PARP1 and PARP3, respectively). Exhibits anticancer effects in BRCA1 mutant, but not wild-type breast cancer cell lines in vitro. Inhibits growth of olaparib-resistant mammary tumors in a mouse model and is a poor substrate for the P-gp transporter. Orally bioavailable.

**Physical and Chemical Properties:**

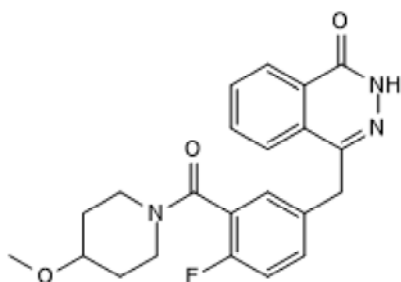
Batch Molecular Formula: C<sub>22</sub>H<sub>22</sub>FN<sub>3</sub>O<sub>3</sub>·1/4H<sub>2</sub>O

Batch Molecular Weight: 399.93

Physical Appearance: Light yellow 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. 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:**

**Oplustil O'Connor et al** (2016) The PARP inhibitor AZD2461 provides insights into the role of PARP3 inhibition for both synthetic lethality and tolerability with chemotherapy in preclinical models. *Cancer Res.* **76** 6084. PMID: 27550455.

**Jaspers et al** (2013) Loss of 53BP1 causes PARP inhibitor resistance in Brca1-mutated mouse mammary tumors. *Cancer Discov.* **3** 68. PMID: 23103855.

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