

Certificate of Analysis

Product Name: AZD 2461

Catalog No.: 6060

Batch No.: 1

CAS Number: 1174043-16-3

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

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₂H₂₂FN₃O₃·¼H₂O

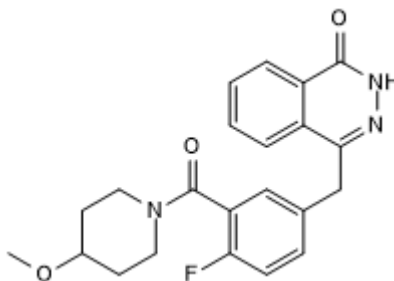
Batch Molecular Weight: 399.93

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_f = 0.75 (Dichloromethane:Methanol [85:15])

HPLC: Shows >99.2% purity

¹H 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

Product Name: AZD 2461

Catalog No.: 6060

Batch No.: 1

CAS Number: 1174043-16-3

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

Description:

Potent PARP inhibitor (IC₅₀ 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:

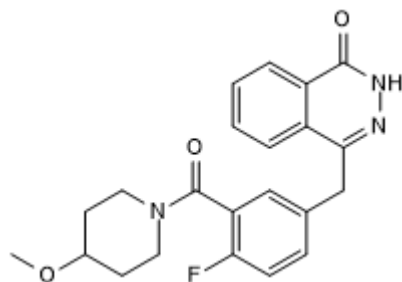
Batch Molecular Formula: C₂₂H₂₂FN₃O₃ · ¼H₂O

Batch Molecular Weight: 399.93

Physical Appearance: Light yellow solid

Minimum Purity: >98%

Batch Molecular Structure:



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.

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.

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

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