# Chemical Properties

**Product Name:** MLN8237 (Alisertib)

**Cas No.:** 1028486-01-2

**M.Wt:** 518.92

**Formula:** C27H20ClFN4O4

**Chemical Name:** 4-[[9-chloro-7-(2-fluoro-6-methoxyphenyl)-5H-pyrimido[5,4-d][2]benzazepin-2-yl]amino]-2-methoxybenzoic acid

**Canonical SMILES:** COC1=C(C(=CC=C1)F)C2=NCC3=CN=C(N=C3C4=C2C=C(C=C4)Cl)NC5=CC(=C(C=C5)C(=O)O)OC

**Solubility:** >25.9mg/mL in DMSO

**Storage:** Store at -20°C

**General tips:** For obtaining a higher solubility, please warm the tube at 37°C and shake it in the ultrasonic bath for a while. Stock solution can be stored below -20°C for several months.

**Shopping Condition:** Evaluation sample solution: ship with blue ice
All other available size: ship with RT, or blue ice upon request

# Biological Activity

**Targets:** Aurora Kinase

**Pathways:** Chromatin/Epigenetics >> Aurora Kinase

**Description:**

The orally bioavailable agent, MLN8237 (also known as alisertib), is a potent small-molecule inhibitor of Aurora A kinase (AAK) which is overexpressed in several types of tumor and associated with oncogenesis and tumor progression. It was developed from its predecessor, MLN8054, in order to minimize the benzodiazepine-like effects seen with MLN8054. The inhibitory effect of MLN8237 is ATP-competitive, reversible and AAK-specific with an inhibition constant (Ki) of 0.43 nmol/L. MLN8237 is being investigated to treat advanced malignancies, due to its both in vitro and in vivo activities against a broad range of tumor types.
Reference:

Protocol

Cell experiment:

Cell lines: TIB-48 and CRL-2396 cells

Preparation method: The solubility of this compound in DMSO is >10 mM. General tips for obtaining a higher concentration: Please warm the tube at 37 °C for 10 minutes and/or shake it in the ultrasonic bath for a while. Stock solution can be stored below -20°C for several months.

Reacting conditions: >100 nM, 48 hours

Applications: TIB-48 and CRL-2396 cells were treated with MLN8237 at 10 nM, 50 nM, 100 nM, 500 nM and 1.0 μM for 48 h. MLN8237 induced apoptosis at concentrations >100 nM, suggesting that induction of apoptosis is dose-dependent. These results were confirmed by demonstrating an increased level of cleaved PARP in treated TIB-48 and CRL-2396 cells. PARP cleavage was observed even at the concentration of MLN8237 as low as 50 nM.

Animal experiment [3]:

Animal models: Female C.B-17 SCID mice injected with OVCAR-5-pWZL-Luc cells

Dosage form: Oral administration, 20 or 30 mg/kg, once daily (QD) or twice daily (BID)

Applications: The mice (n=16/group) were randomly divided into five treatment groups: 1) vehicle, 2) 20 mg/kg alisertib, 3) 30 mg/kg alisertib, 4) 5 mg/kg paclitaxel and 5) 20 mg/kg alisertib + 5 mg/kg paclitaxel. Tumor growth was monitored by weekly BLI and the log-transformed total flux data showed significantly decreased tumor growth rates in mice treated with alisertib (20 or 30 mg/kg) compared to vehicle-treated mice. Treatment with 20 mg/kg and 30 mg/kg alisertib resulted in 51% and 49% TGI, respectively.

Other notes: Please test the solubility of all compounds indoor, and the actual solubility may slightly differ with the theoretical value. This is caused
by an experimental system error and it is normal.

Reference:

Product Validation

Cytotoxicity of MLN8237 against Daoy (Black diamond), IMR-32 (Black square) and MOLT-4 (Black circle) cell lines.

MLN8237 induces G2/M arrest and apoptosis

Caution

FOR RESEARCH PURPOSES ONLY.

NOT FOR HUMAN, VETERINARY DIAGNOSTIC OR THERAPEUTIC USE.

Specific storage and handling information for each product is indicated on the product datasheet. Most ApexBio products are stable under the recommended conditions. Products are sometimes shipped at a temperature that differs from the recommended storage temperature. Shortterm storage of many products are stable in the short-term at temperatures that differ from that required for long-term storage. We ensure that the product is shipped under conditions that will maintain the quality of the reagents. Upon receipt of the product, follow the storage
recommendations on the product data sheet.