**Product Data Sheet**

### Chemical Properties

**Product Name:** ML216  
**Cas No.:** 1430213-30-1  
**M.Wt:** 383.32  
**Formula:** C15H9F4N5OS  

**Chemical Name:** 1-(4-fluoro-3-(trifluoromethyl)phenyl)-3-(5-(pyridin-4-yl)-1,3,4-thiadiazol-2-yl)urea

**Canonical SMILES:** FC(C(\(\text{C}(\text{F})(\text{F})=\text{C}\text{1})=\text{C}\text{CNC(\text{N2}=\text{NNC(\text{C3=CC=NC=NC=NC3}}\text{S2}})=\text{O})

**Solubility:** \(\geq 10.65\text{mg/mL in DMSO with gentle warming}\)

**Storage:** Desiccate 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:** Others  
**Pathways:** Others

**Description:**  
IC50: 3.0 and 0.97 μM for full length BLM and BLM636–1298, respectively

ML216 is a potent inhibitor of the DNA unwinding activity of BLM helicase.

BLM helicase is reported to be a DNA unwinding enzyme critical in DNA repair through the
homologous recombination pathway. BLM gene mutations lead to diminished BLM helicase activity and can cause Bloom’s Syndrome. Similar to other DNA repair enzymes, BLM helicase inhibition shows sensitization of tumor cells to conventional cancer therapies, such as camptothecin.

In vitro: ML216 showed submicromolar potency and selectivity over related helicases including RECQ1, RECQ5, and E. coli UvrD helicases. ML216 also inhibited cell proliferation of BLM-proficient fibroblast cells while had minimal effects on BLM deficient fibroblast cells, indicating on-target activity in a cellular context. Additionally, ML216 increased the frequency of sister chromatid exchanges, which was a diagnostic cellular phenotype consistent with the absence of a functional BLM protein [1].

In vivo: ML216 was a suitable starting point for further mouse tumor xenograft models and for the further development of potential cancer therapeutics [1].

Clinical trial: N/A

Reference:

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.