**Product Data Sheet**

### Chemical Properties

- **Product Name:** MDV3100 (Enzalutamide)
- **Cas No.:** 915087-33-1
- **M.Wt:** 464.4
- **Formula:** C21H16F4N4O2S
- **Synonyms:** Enzalutamide, MDV3100, MDV-3100, MDV 3100
- **Chemical Name:** 4-[3-[4-cyano-3-(trifluoromethyl)phenyl]-5,5-dimethyl-4-oxo-2-sulfanylideneimidazolidin-1-yl]-2-fluoro-N-methylbenzamide
- **Canonical SMILES:** CC1(C(=O)N(C(=S)N1C2=CC(=C(C=C2)C(=O)NC)F)C3=CC(=C(C=C3)C#N)C(F)(F)F)C
- **Solubility:** $\geq 23.22\text{mg/mL}$ in DMSO
- **Storage:** Store at $-20^\circ\text{C}$
- **General tips:** For obtaining a higher solubility, please warm the tube at $37^\circ\text{C}$ and shake it in the ultrasonic bath for a while. Stock solution can be stored below $-20^\circ\text{C}$ 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:** Endocrinology and Hormones
- **Pathways:** Androgen Receptor

**Description:**

MDV3100, known as Enzalutamide, is a second-generation androgen receptor (AR) signaling inhibitor. It has been demonstrated impressive affinity to the AR compared to the first-generation AR inhibitors. It is able to inhibit binding of androgens to the AR, AR nuclear translocation, and the association of the AR with DNA. The AR is a 919-amino acid member of the steroid receptor
transcription factor superfamily with different domains including an N-terminal regulation domain, a central DNA binding domain, and a C-terminal domain, which includes the ligand-binding domain incorporated within its protein structure. MDV3100 was identified by the Sawyers/Jung laboratories by using the nonsteroidal agonist. Testing was showing that it induced apoptosis in VCaP cells, an AR gene amplified human prostate cancer line, while bicalutamide was ineffective.

**Reference:**

**Protocol**

**Cell experiment:**

**Cell lines**
VCaP, LNCaP, 22RV1, DU145 and PC3 prostate cancer cell lines

**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**
10 μM, 12h

**Applications**
Recruitment of AR to target loci was markedly attenuated by MDV3100 and less so by bicalutamide. Interestingly, JQ1 blocked AR recruitment almost as effectively as MDV3100. Limiting our evaluation to AR and BRD4 coincident peaks, we observed that DHT-mediated AR recruitment to these loci was inhibited by MDV3100 and to a lesser extent by JQ1. Corroborating the ChIP seq data, gene expression analysis in VCaP and LNCaP cells showed more efficient repression of DHT-induced AR-target genes by JQ1 than by MDV3100 or bicalutamide.

**Animal experiment [3]:**
Animal models  Four-week-old male SCIDC.B17 mice
Dosage form  10 mg/kg, oral gavage or intraperitoneally, five days a week
Applications  Treatment of VCaP tumour-bearing mice with JQ1 led to a significant reduction in tumour volume/weight, whereas MDV3100 had a less pronounced effect. Recently, several studies described the pro-metastatic effects of MDV3100 in pre-clinical models. To test whether MDV3100 treatment leads to spontaneous metastasis in our VCaP xenograft model, we isolated femur, liver and spleen from MDV3100-treated mice and found evidence of metastases in femur and liver. By contrast, JQ1-treated mice showed no evidence of metastasis. Taken together, these pre-clinical studies suggest that the use of MDV3100 in clinically localized prostate cancer may potentiate the formation of micro-metastases, unlike BET inhibitors.

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 Citations

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. Short-term 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.