Chemical Properties

**Product Name:** Abiraterone acetate  
**Cas No.:** 154229-18-2  
**M.Wt:** 391.55  
**Formula:** C26H33NO2  
**Chemical Name:** \[(3S,8R,9S,10R,13S,14S)-10,13-dimethyl-17-pyridin-3-yl-2,3,4,7,8,9,1,12,14,15-decahydro-1H-cyclopenta[a]phenanthren-3-yl\] acetate  
**Canonical SMILES:** CC(=O)OC1CCC2(C3CCC4(C(C3CC=C2C1)CC=C4C5=CN=CC=C5)C)C  
**Solubility:** ≥15.7mg/mL in Ethanol  
**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:** Metabolism  
**Pathways:** P450  
**Description:**  
Abiraterone acetate is the 3β-acetate form of its active component abiraterone, a potent inhibitor of androgen biosynthesis. Abiraterone, a pregnenolone-derived 3-pyridyl steroidal compound, potently and irreversibly inhibits cytochrome P450 17 alpha-hydroxylase (CYP17), an important enzyme involved in the synthesis of androgen and cortisol, through a covalent binding mechanism with a value of 50% inhibition concentration IC50 of 72 nM, which is 10 to 30 times greater in potency, due to the 3-pyridyl substitution in its chemical structure, than the inhibition by ketoconazole. In order to improve the low solubility of abiraterone, abiraterone acetate has
been developed and used for the treatment of castration-resistant prostate cancer (CRPC).

Reference:
Guru Sonpavde, Gerhardt Attard, Joaquim Bellmunt, Malcolm D. Mason, Bernard Malavaud, Bertrand Tombal and Cora N. Sternberg. The role of abiraterone acetate in the management of prostate cancer: a critical analysis of the literature. EUROPEAN UROLOGY 60 (2011) 270-278

Protocol

Cell experiment:

Cell lines: PC-3 cells
Preparation method: The solubility of this compound in DMSO is limited. 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: Applications

In PC-3 cells co-transfected with ARE3-luciferase and wild type or mutant androgen receptor (AR), Abiraterone Acetate at the dose up to 25 μM did not any obvious increase in luciferase activity. However, Abiraterone Acetate dose-dependently inhibited stimulated wild type and mutant AR activity, with significant inhibition observed at the doses ≤ 10 μM.

Animal experiment [3]:

Animal models: Male NOD/SCID mice bearing LAPC4 cells
Dosage form: 0.5 mmol/kg/d; i.p.; 5 days per week, for 4 weeks

Applications: Abiraterone Acetate at the dose of 0.5 mmol/kg/d resulted in serum concentrations ranging from 0.5 to 1 mmol/L. Compared with the control group, Abiraterone Acetate treatment significantly inhibited "castration-resistant" prostate cancer progression in the robustly growing subset, effectively inhibiting tumor growth over 4 weeks of treatment.

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:

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.

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