
Abiraterone

产品编号: D50727

CAS: 154229-19-3

分子式: C₂₄H₃₁NO

纯度: ≥98%

InChi: InChi=1S/C₂₄H₃₁NO/c1-23-11-9-18(26)14-17(23)5-6-19-21-8-7-20(16-4-3-13-25-15-16)24(21,2)
12-10-22(19)23/h3-5,7,13,15,18-19,21-22,26H,6,8-12,14H2,1-2H3/t18-,19-,21-,22-,23-
,24+/m0/s1

InChi Key: GZOSMCIZMLWJML-VJLLXTKPSA-N

Smiles: C[C@]12CC[C@H]3[C@@H](CC=C4C[C@@H](O)CC[C@@]43C)[C@@H]1CC=C2C1C=NC=CC=1

外观: 固体粉末

作用通路: Cytochrome P450

溶解性: DMSO up to 20mM

保存条件: Store in dry, dark place for one year.

产品介绍: Abiraterone is the first-in-class potent and selective CYP17 (cytochrome P450 17alpha-hydroxylase-17, 20-lyase) inhibitor with IC₅₀ ~4 nM. It was approved by US FDA in 2011 to treat castration-resistant prostate cancer. As prostate cancer cells proliferate in response to androgen steroids, CYP17 inhibition is a new strategy to prevent androgen synthesis and treat lethal metastatic prostate cancer. In recent Nature publication, the structures of cytochrome P450 17A1 with abiraterone was released. A phase I/II clinical trial evaluating abiraterone in advanced breast cancer patients is also underway.