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(54) Title: NOVEL C-17-HETEROARYL STEROIDAL CYP17 INHIBITORS/ANTIANDROGENS: SYNTHESIS, IN VITRO BIOLOGICAL ACTIVITIES, PHARMACOKINETICS AND ANTITUMOR ACTIVITY

(57) Abstract: Described are steroidal C- 17 benzoazoles, pyrimidinoazoles (azabenzoazoles) and diazines. Methods for their synthesis are also described, which include methods having a step of nucleophilic vinylic "addition-elimination" substitution reaction of 3β-acetoxy-17- chloro-16-formylandrosta-5,16-diene or analogs thereof and benzoazole or pyrimidinoazole nucleophiles and methods having a palladium catalyzed cross-coupling reaction of 17- iodoandrosta-5,16-dien-3β-ol or analogs thereof with tributylstannyl diazines. The compounds are potent inhibitors of human CYP 17 enzyme as well as potent antagonists of both wild type and mutant androgen receptors (AR). The compounds are useful for the treatment of human prostate cancer.