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New 17α-picolyl Androstane Derivatives: Synthesis, *In Vitro* Biological Activity and *In Silico* ADME/T Properties

J. Ajduković,[a,*] Đ. Janković,[a] S. Bekić,[a] A. Ćelić[b] and E. Petri[b]

[a] *University of Novi Sad, Faculty of Sciences, Department of Chemistry, Biochemistry and Environmental Protection, Trg Dositeja Obradovića 3, Novi Sad, Serbia*

[b] *University of Novi Sad, Faculty of Sciences, Department of Biology and Ecology, Trg Dositeja Obradovića 2, Novi Sad, Serbia*

*jovana.ajdukovic@dh.uns.ac.rs

Oxyimino ethers are compounds very often used in organic synthesis to obtain various products such as amino alcohols, hydroxylamines and amines, but they have also shown promising anticancer activity.[1] Bearing this in mind, we have efficiently synthesized a new *O*-alkylated oxime derivative in the androstane series, which was then used as a precursor for preparing a 3-hydrazinocarbonylmethyloxyimino derivative.

New androstane derivatives were evaluated for relative binding affinities to the ligand-binding domains of selected steroid receptors (ERα, ERβ, AR and GR) and inhibition potential against recombinant enzymes from aldo-keto reductase 1C subfamily, promising drug targets for cancer treatment. Our results showed the lack of estrogenic or androgenic properties of the tested compounds, suggesting they could be suitable candidates for the development of anticancer agents against hormone-dependent cancers. In addition, *in silico* ADME/T profile and physicochemical properties were determined using the online web tools, where parameters for both compounds were within the optimal range, suggesting them as drug-like molecules.

Keywords: androstane; *O*-alkylated oximes; hormone receptors; AKR1C4

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