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*Abstract*

# Synthesis, Structural Characterization, and *In Silico* ADMET Testing of Novel 17β-Acetoxy-17α-(Pyridin-2-yl) Estrane Derivatives †

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**Abstract:** Steroidal compounds that contain a heterocyclic ring or heteroatom in their structure usually possess good anticancer activity. The main goal of modern medicinal chemistry is to find new potent agonists or antagonists of naturally occurring hormones for the treatment of hormone-dependent cancers, such as the above-mentioned steroid derivatives. Here, we reported on a two-step synthesis of a new 17β-acetoxy-17α-(pyridin-2-yl) derivative of estra-1,3,5(10)-triene. The configuration at the C17 position was determined using the 2D NMR spectra. Furthermore, *in silico* ADME properties were determined for the synthesized compound. The physicochemical properties were calculated with the SwissADME web tool and compared with five different sets of criteria: *Lipinski*, *Veber*, *Egan*, *Ghose*, and *Muegge*. The toxicity of the synthesized compound was predicted and analyzed using a virtual lab ProTox II.

**Keywords:** estrane; heterocycle; SwissADME; 2D NMR



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