

Synthesis, *in vitro* steroid receptor binding and *in silico* testing of novel 17 α -(pyridin-2-yl)estra-1,3,5(10),16-tetraen derivatives

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Steroid compounds incessantly attract attention due to their biological and clinical importance. Considering that many cancers are hormone-dependent, synthetically modified steroid molecules are suitable candidates for the treatment of these malignancies. It has been established that steroid compounds with a heterocyclic ring or heteroatoms in their structure represent potential anticancer agents, and also have other important pharmacological properties. With this in mind, we have synthesized novel 17-(pyridin-2-yl)estra-1,3,5(10),16-tetraen compounds, starting from 17 β -hydroxy-17 α -(pyridin-2-yl)-estra-1,3,5(10)-triene derivatives by dehydration reactions. For all synthesized compounds we analyzed *in silico* ADMET properties using the online SwissADME tool and ProToxII virtual lab. Since these modified compounds are based on steroidal scaffolds, their relative binding affinities for the ligand-binding domains of estrogen receptor α and β and androgen receptor were evaluated using a fluorescent assay in yeast.

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