Molecular Modeling of 17-Picolyl and 17-Picolinylidene Androstane Derivatives with Anticancer Activity

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Abstract : In the present study, the molecular modeling of a series of 24 17-picolyl and 17-picolinylidene androstane derivatives whit significant anticancer activity was carried out. Modelling of studied compounds was performed by CS ChemBioDraw Ultra v12.0 program for drawing 2D molecular structures and CS ChemBio3D Ultra v12.0 for 3D molecular modelling. The obtained 3D structures were subjected to energy minimization using molecular mechanics force field method (MM2). The cutoff for structure optimization was set at a gradient of 0.1 kcal/Åmol. Full geometry optimization was done by the Austin Model 1 (AM1) until the root mean square (RMS) gradient reached a value smaller than 0.0001 kcal/Åmol using Molecular Orbital Package (MOPAC) program. The obtained physicochemical, lipophilicity and topological descriptors were used for analysis of molecular similarities and dissimilarities applying suitable chemometric methods (principal component analysis and cluster analysis). These results are the part of the project No. 114-451-347/2015-02, financially supported by the Provincial Secretariat for Science and Technological Development of Vojvodina and CMST COST Action CM1306.

Keywords : androstane derivatives, anticancer activity, chemometrics, molecular descriptors
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