

Abstract

Application of Both Cluster and Principal Component Analysis for Evaluation of the Lipophilicity Parameters of Selected Antiandrogen Drugs [†]

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Abstract: The aim of this work was the use of both cluster analysis (CA) and Principal Component Analysis (PCA) for the evaluation of the lipophilicity of selected antiandrogen drugs such as abiraterone, bicalutamide, flutamide, nilutamide, leflunomide, teriflunomide and aianthone. Lipophilicity is an important physicochemical parameter that is useful in determining the ADMET properties (absorption, distribution, metabolism, elimination and toxicity) of organic compounds that are being considered as potential drugs or drug candidates. Therefore, there is an urgent need to develop rapid, economical and efficient tools like theoretical methods that include CA and PCA analyses for the evaluation of the lipophilic properties of different bioactive compounds such as antiandrogens. In this study, we used both methods for comparison of the physicochemical properties (including lipophilicity) of seven antiandrogens with different chemical structures. The lipophilicity parameters of the studied compounds were obtained in the form of R_{MW} by using a thin-layer chromatographic method (RP-TLC) under different conditions (i.e., various mobile phases composed of ethanol-water, propan-2-ol-water and acetonitrile-water and chromatographic plates RP2F₂₅₄, RP18F₂₅₄ and RP18WF₂₅₄), as well as logP values predicted using calculation methods (AlogPs, AClogP, AlogP, MlogP, xlogP2 and xlogP3). The CA and PCA analyses allowed the comparison of the examined compounds based on their lipophilicity parameters determined using RP-TLC and calculated logP values. Our study confirms the utility of both statistical methods (i.e., CA and PCA) to evaluate the lipophilicity of bioactive compounds belonging to the class of antiandrogen drugs.

Keywords: cluster analysis; principal component analysis; lipophilicity; antiandrogen drugs



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