Theoretical study in the differentiations of psychoactivity in biological active cannabinoids compounds and their metabolites

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Different cannabinoid metabolites have been investigated from quantum calculations and chemometric methods to establish correlations between chemical structure and psychoactivity. Geometry optimizations and several physical-chemical properties were obtained from calculations semi-empirical (AM1, PM3 e PM5) and theory density functional calculations (DFT). Several molecular descriptors were obtained these properties for multivariate treatment and some chemometric methods were applied including principal component analysis (PCA), hierarchical cluster analysis (HCA), nonhierarchical cluster analysis (K-means), nearest neighbor (KNN) and artificial neural networks (RNAs). Among all the molecular descriptors calculated, the most relevant ones to discriminate according to their psychoactivity were those related to electronic, lipophilic and stereo-geometric properties (lumo, T2 e Log P). Thus, the compounds were classified into psychoactive (A1), moderately psychoactive (A2) and psychoinactive (B) groups. The models obtained were used to study 22 cannabinoids compounds, and our predictions related to the psychoactivity were in good agreement with the experimental evidences.