A THEORETICAL APPROACH TO THE INTERACTION OF BRASSINOLIDE WITH ESSENTIAL AMINOACIDS

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The interaction of the most-active natural brassinosteroid, brassinolide, with the twenty natural amino acids is studied applying the multiple minima hypersurface method to model the molecular interactions explicitly. The resulting thermodynamic data gives useful information about the amino acids with the greatest association for brassinolide and the stabilities of such complexes. B3LYP/6-31G optimizations and single-point energy calculations at the B3LYP/6-311+G(d) level of theory are further carried out to test the performance of the AM1 calculations. The AM1 geometries and stability order of these complexes are in good agreement with the B3LYP results obtained. Polar charged amino acids show the highest affinity for brasinolide forming the most stable complexes. This study could contribute to future investigations of the interaction of brassinosteroids with the receptor protein in plants.