GROMOS53A6 Force Field Parameters for Chalcones and Flavonoids

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INTRODUCTION: Chalcones and flavonoids are polyphenolic compounds extensively distributed in plants, constituting a large family of natural products with a broad spectrum of pharmacological activities. Changes in their structure have been proven useful for the development of new therapeutic agents, thus these biomolecules are being intensively studied and modified. Computational methods such as molecular dynamics (MD) simulations are powerful tools to assess information that is difficult to obtain experimentally. Accurate force fields are essential for describing biological systems in MD simulations, therefore a parameter set associated to a molecule needs to be carefully calibrated to ensure reliable results. **OBJECTIVES:** Considering the relevance of this family of molecules and the lack of validated parameters for the basic structure of chalcones and flavonoids in the GROMOS force field, this work intends to provide a new parameter set for the simulation of these compounds. **MATERIAL AND METHODS:** We employed a protocol combining ab initio calculations, performed using Gaussian03, and MD simulations, using the GROMACS simulation suite with GROMOS53A6 force field. Experimental properties such as density and enthalpy of vaporization were used as comparison to the calculated values in order to validate the parameters. **DISCUSSION AND RESULTS**: A fitting of molecular mechanical to quantum mechanical torsional profiles was performed for each of the dihedrals of interest in the structures, and has generated force field parameters that reproduce well the target data. Additionally, adjustments in charge groups were made in topologies used for the MD simulations and the obtained values of the thermodynamic properties are in good agreement with experimental data. **CONCLUSION:** Once completed, we expect that such parameters will be able to properly describe the conformational distribution of chalcones and flavonoids, a starting point to further studies on the biological role of such molecules at an atomistic level of detail.

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