Molecular Dynamics Modellization and Simulation of Water Diffusion through Plant Cutin

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A theoretical molecular modelling study has been conducted for cutin, the biopolyester that forms the main structural component of the plant cuticle. Molecular dynamics (MD) simulations, extended over several ten picoseconds, suggests that cutin is a moderately flexible netting with motional constraints mainly located at the cross-link sites of functional ester groups. This study also gives structural information essentially in accordance with previously reported experimental data, obtained from X-ray diffraction and nuclear magnetic resonance experiments. MD calculations were also performed to simulate the diffusion of water molecules through the cutin biopolymer. The theoretical analysis gives evidence that water permeation proceedes by a "hopping mechanism". Coefficients for the diffusion of the water molecules in cutin were obtained from their mean-square displacements yielding values in good agreement with experimental data.