ESTIMATING SOLVENT EFFECTS FOR FATTY COMPOUNDS IN SUPERCRITICAL CARBON DIOXIDE FROM LANGEVIN DYNAMIC CALCULATIONS.

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Supercritical carbon dioxide is an attractive solvent for green chemistry and material processing applications based on its low toxicity and cost versus traditional organic solvents. However, carbon dioxide does not display favorable solvent properties for many reactants.

The behavior of a series of fatty acids, fatty alcohols, and esters were calculated in vacuo and in supercritical carbon dioxide. The solvent effects of supercritical carbon dioxide on these compounds were modeled using Langevin dynamics with periodic boundary conditions. These solutions converged more rapidly than similar molecular dynamic calculations using explicitly defined solvent molecules

. This technique permitted the calculation of changes in bond length that lead to chemical reaction of the solute molecule in the presence of the solvent. The results of such calculations can be used to complement transition state searches of the potential energy surface for transition structures and to guide the selection of reaction conditions.