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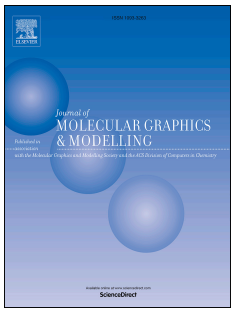

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Computer Simulation for the Study of the Liquid Chromatographic Separation of Explosive Molecules

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Abstract

The application of high performance liquid chromatography (HPLC) to separate explosive chemicals was investigated by molecular dynamics (MD) simulations. The explosive ingredients including NG, RDX, HMX and TNT were assigned as solutes, while methanol (CH_3OH) and acetonitrile (CH_3CN) were assigned as solvents in the solution system. The polymeric-molecular siloxanes (Si-C8) and poly-1,2-methylenedioxy-4-propenyl benzene (PISAF) compounds were treated as stationary phase in the simulation. The simulation results showed that the different species of explosive ingredients were separated successfully in the solutions by each of the constructed stationary phase of Si-C8 and PISAF after a total simulation time of 12.0 ps approximately, which were consistent with the experimental analysis of HPLC spectra. The origin for the separation was found due to the electrostatic interactions between polymer and explosives.

Keyword：molecular simulation, liquid chromatography, explosives.