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Simulation of DBS, DBS-COOH and DBS-CONHNH$_2$ as hydrogelators

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The organic gelator 1,3(R):2,4(S)-dibenzylidene-D-sorbitol (DBS) self-organizes to form a 3-D network at relatively low concentrations in a variety of nonpolar organic solvents and polymer melt. DBS could be transformed into a hydrogelators by introduction of hydrophilic groups, which facilitate its self-assembly in aqueous medium. In this work, we have investigated the hydrogelators DBS-COOH and DBS-CONHNH$_2$ and the organogelator DBS by molecular modeling. We have used quantum mechanics (QM) to elucidate the preferred geometry of one molecule and a dimer of each of the gelators, and molecular dynamics (MD) to simulate the pure gelators and their mixtures with water. The results of the simulation indicate that the interaction between DBS-COOH molecules is the strongest of the three and its water compatibility is the highest. Therefore, DBS-COOH seems to be a better hydrogelator than DBS-CONHNH$_2$ and DBS. Intermolecular H-bonding interactions are formed between DBS, DBS-COOH and DBS-CONHNH$_2$ molecules as pure substances, and they dramatically decrease in the presence of water. In contrast, the intramolecular interactions increase in water. This result indicates that in aqueous environment the molecular structure tend to be more rigid and fixed in the preferred conformation. The most significant intramolecular interaction is formed between O3 acetal and H-O6 groups. Due to the H-bonds, DBS, DBS-COOH and DBS-CONHNH$_2$ molecules form a rigid structure similar to liquid crystal forming molecules, which might explain their tendency to create nano fibrils. It was found that the aromatic rings did not contribute significantly to the inter-and intra-molecular interactions. Their main role is probably to stiffen the molecular structure.

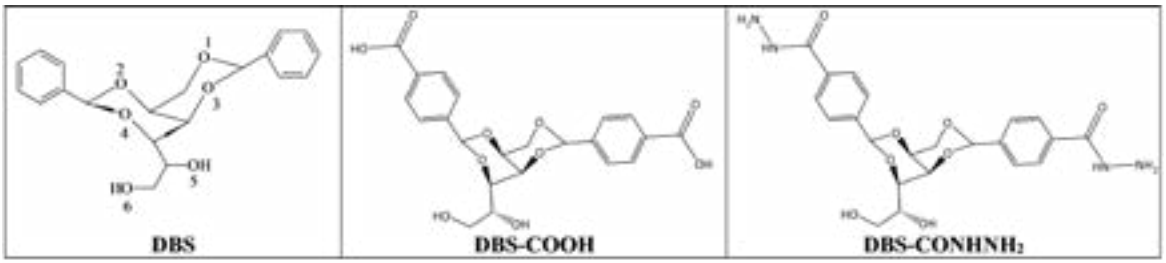

Figure 1: DBS, DBS-COOH and DBS-CONHNH$_2$ molecular structure.

Biography

Dafna Knani is a Senior Lecturer in Department of Biotechnology Engineering, ORT Braude College. She is an Organic Polymer Chemist, graduated from Chemistry Faculty, Technion- Israel Institute of Technology. In the past, she worked for surgical bio-polymeric materials start-up company as a Research Polymer Chemist (developing adhesives for hard tissues) and as a Research Chemist and Project Leader at Israel Chemicals Ltd. (ICL), IMI-Institute for R&D. Her current research focuses on "Molecular modeling of materials and biomaterials". Some of her research topics are simulation of systems used for controlled drug release and tissue engineering and computational design of polymer additives.

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