Mixtures of γ-oryzanol and β-sitosterol can form transparent organogels in edible oils. This process is a nice example of molecular self-assembly, where γ-oryzanol and β-sitosterol molecules form very well-defined supramolecular entities. Small-angle X-ray scattering (SAXS) was used to elucidate the microstructure of the building blocks of these organogels in sunflower oil [3]. The measurements were performed at the high-brilliance ID2 beamline of the European Synchrotron Radiation Facility (ESRF) in Grenoble, France, allowing collection of SAXS data in the range 0.06–q/nm<4.5. Differential Scanning Calorimetry (DSC) was used to study the dissolution, melting and crystallisation behaviour of these systems during a heating-cooling-heating cycle. It was found that the γ-oryzanol + β-sitosterol system forms tubules with a diameter of 7.2±0.1 nm and a wall thickness of 0.8±0.2 nm. Tubules prepared with γ-oryzanol-rich structurant show the least bundle formation, and can be supercooled during formation most easily. The tubes vanish at the melting point of the gel, in agreement with the loss of structuring capacity as observed in earlier experiments. Moreover, a number of alternative sterols (e.g. stigmasterol, cholesterol, cholestanol) can replace β-sitosterol in the tubules. The diameter of the tubules for these systems varies between 7.2 and 8.0 nm, the wall thickness between 0.6 and 1.1 nm. The microstructure of the sterol(esters) in emulsions differs from that in pure oil.


Keywords: organogels, self-assembly, small-angle X-ray scattering

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Structural and systematic studies of a 3x3 isomer grid of nine N-(fluorophenyl)-pyridinecarboxamides

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Nine NxxF isomers (x = 4-, 3- or 2-N/F substitution) were investigated and compared to determine factors underpinning (a) the roles of the F/N atom substituents on molecular conformation and overall supramolecular aggregation, (b) competition between intermolecular amide...amide (in NppF) or intra-/intermolecular amide...pyridine hydrogen bond formation and (c) general structural and physico-chemical properties and trends.

Crystal structure analyses of the nine NxxF isomers reveal different primary interactions as N-H...N or N-H...O=C. NpmF and NpoF are isomorphous and the latter is also disordered. Conformational analysis of the NxxF molecular conformations from DFT calculations differ from the crystal structure results for several isomers and highlighting the cooperative effects of intra-/intermolecular interactions in the solid state.