Characterisation of the properties of polyphenol crystals to aid the design of novel Pickering Emulsion stabilisers

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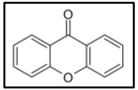
Introduction



- Xanthones are a class of polyphenols found in plants and fungi.
- Sourced from plant waste material they are a sustainable alternative to surfactants.
- Polyphenols can be used as 'clean label' emulsion stabilisers.
- Characterising the properties of each crystal facet can help us elucidate their mechanism of emulsion stabilisation

Methodology

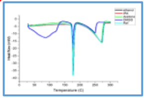
1) Solid-form screening

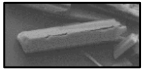
Solution recrystallization
↓
Vary solvent & concentration
↓
XRD, DSC/TGA & SEM analysis

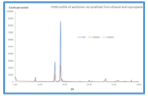
2) Molecular modelling

- Mercury software with VisualHabit to predict morphology
- SystSearch with a probe to identify the intermolecular interactions of each crystal facet

Initial Results

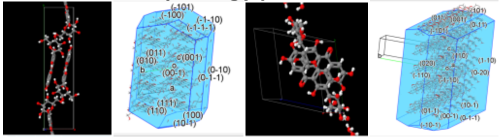






- The xanthone crystals formed at room temperature all had a needle shaped-morphology.
- DSC and XRD analysis confirmed that the crystals formed were consistent with the data obtained for Xanthone Form I (anhydrous). Identical results were obtained irrespective of the solvent used.
- The crystals showed limited surface activity in hand-shaken emulsions and the crystals arranged flat at the at the oil-water interface.

Morphology prediction



Form I (anhydrous) **Form II (hydrate)**

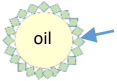
The VisualHabit model in Mercury predicts that Form I is orthorhombic and Form II has a triclinic morphology. The lattice energies were compared and the key intermolecular interactions on the most dominant facets were : VdW > Hydrogen bonding > electrostatic interactions. Probes confirmed the surface interactions of each facet.

Conclusions

- Needles are the dominant morphology at ambient temperature. Higher temperatures may produce different morphologies.
- There is preferential growth of particular facets of the crystals. Not all of the facets predicted in the model were observed.

Future work

- Adaptation of the crystallisation conditions to produce different morphologies.
- Probe the dominant facets with different solvent molecules.
- Evaluate the emulsion stabilising capability of the crystals with different morphologies and dominant facets.



Acknowledgements

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