Neutron- and synchrotron scattering for studying aggregate structures for optimised functionality of green surfactants

THE INDUSTRIAL CHALLENGE

Enza Biotech is developing novel green sugar based surfactants for use in a wide range of products, from pharmaceuticals to cosmetics. The function of any given surfactant system such as foaming, rheology modification and emulsification capacity is directly dependent on the aggregates it forms in solution. In order to optimize the molecular structure of a surfactant to fit a specific application, it is necessary to understand its behaviour in solution, and interactions with other ingredients in a formulation.



WHY USING A LARGE SCALE FACILITY Both neutron scattering (SANS) and synchrotron based small angle Xray scattering (SAXS) can give more detailed information on the structure of associated structures of surfactants, such as micelles, than other techniques such as Dynamic Light Scattering and bench top SAXS. Especially neutron scattering using contrast variation provides considerable additional benefits as it allows different components of a complex formulation to be studied independently.

HOW THE WORK WAS DONE

In order to evaluate if SANS and SAXS can give industrially relevant information concerning the structure of the Enza sugar based surfactants, four different experiments were performed. The Larmor experimental station of ISIS Neutron & Muon Source, England, was used for studying interactions of a surfactants with proteins. We thank Rob Dagleish for help at the beamline. Further, the KWS-2 experimental station of the FRM II neutron facility at MLZ in Germany was used for studies of complex formulations of a surfactants mixed with oligosaccharides using contrast variation SANS. We thank Dr. Christian Lang for help. In addition, two experiments were performed to investigate the dependence of selfaggregation on molecular structure of different sugar surfactants: the experimental stations Sans2 at ISIS and CoSAXS at the MAX IV synchrotron. Dr. Najet Mahmoudi (remote at ISIS) and Dr Ann Terry and Fátima Herranz (MAXIV) are acknowledges for their help.

THE RESULTS AND EXPECTED IMPACT

The four studies showed that SAXS and, in particular, SANS are powerful tools in investigations of the complex structures formed by self-association of different types of sugar-based surfactants. The details of the relationship between the molecular structure of the novel surfactants and the aggregates formed in solution turned out to be completely unexpected and not possible to predict based on textbook knowledge. The increased understanding thus have a direct positive impact on Enza Biotech's ability to design new surfactant structures that are tailored for given applications. In addition, especially the contrast-matched SANS studies allowed us to elucidate how surfactants interact the with other components in a formulation. Again, this type of understanding is extremely valuable in further optimisation of the materials.

"The data obtained by SANS has given us critical insight into the structure-function relationships of our materials" /Stefan Ulvenlund, Enza Biotech AB

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