

Time-of-Flight Secondary Ion Mass Spectrometry (ToF-SIMS) for Imaging Composition and Functional Properties of Surfaces

Kempson, I.¹, Joyce, P.², Denman, J.¹, Cavallaro, A.^{1,3} and Prestidge, C.¹

¹ University of South Australia, Australia, ² Chalmers University of Technology, Sweden, ³ Australian Microscopy and Microanalysis Research Facility, South Australian Node, Australia

Time-of-Flight Secondary Ion Mass Spectrometry (ToF-SIMS) provides compositional analysis of material surfaces to a depth of ~1-2nm providing organic, inorganic and isotopic information. The sensitivity to matrix effects beneficially provides different fragmentation patterns representing physico-chemical properties of the material. This facilitates analysis and imaging of inorganic and organic material with the same composition, but different structure with important ramifications in our understanding of properties such as polymorphs, polyamorphs, crystal orientation, molecular orientation, protein misfolding and denaturation. In our work, this powerful level of characterization has implications with respect to functional and pharmaceutical materials and products.

This presentation provides insight into our research with respect to distributions of peptides and proteins on surfaces and in porous materials for bio-sensing, pharmaceutical products and enzymatic processes. Furthermore, information can be obtained on molecular orientation which can be correlated with material properties and molecular activity. This is shown for examples of: lipase encapsulated within porous silica particles engineered to control the adsorption kinetics and molecular orientation of lipase, which plays critical roles in the digestion kinetics of triglycerides; variations in lipid adsorption kinetics and molecular behavior in porous silica particles as a function of varying hydrophobicities and resulting lipase activity; and semi-quantitative analysis of misfolded proteins in complex mixtures.

1. IM Kempson and C Prestidge. Mass Spectrometry Imaging of Pharmaceuticals: From Tablets to Tissues, *In Analytical Techniques in Delivery Science and Technology, Controlled Release Society, Springer, 2016.*
2. IM Kempson, Y Hwu, CA Prestidge. Probing protein association with nano- and micro-scale structures with ToF-SIMS, *In Proteins at Interfaces III, American Chemical Society, 2012, 1120, pp. 709-729.*

Acknowledgement: This research was supported by the Australian Microscopy and Microanalysis Research Facility (AMMRF), South Australian Node.