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Synthesis of Deuterated Molecules Using Enzyme Catalysis

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Analysis of hydrogen-containing molecules via neutron scattering analyses often benefits from the substitution of hydrogen with deuterium atoms, since hydrogen (protium) and deuterium have different scattering length densities (SLDs). Selective replacement of protium for deuterium in multi-component systems allows the scattering from individual components to be observed in isolation. For this reason, neutron scattering facilities such as the European Spallation Source (ESS) are invested in furthering techniques for producing deuterated molecules.

Current methodologies fall broadly under the categories of 'chemical' – using H/D exchange reactions, or deuterated reagents, to exchange or install deuterons – or 'biological' – growing organisms in D2O, often with a deuterated carbon source, followed by extraction and purification of the molecules of interest. The chemical deuteration laboratory at ESS is aiming to establish a combined chemical-biochemical approach to deuterated molecules exploiting enzyme catalysis. Enzyme catalysis is advantageous because it is safer than and operates under milder conditions than conventional chemical synthesis and because it shows excellent chemo-, regio- and enantioselectivity, greatly increasing efficiency.

We have successfully applied this approach to the synthesis of enantiopure deuterated D- and L-lactic acid-d4; current work focuses on applying this method to tail-deuterated mixed-acyl phospholipids such as 1-palmitoyl-2-oleoyl-sn-glycerol-3-phosphocholine (POPC). Recent results will be presented.

Topic

Chemistry

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