William R. Wiley
EMSL In Brief
Environmental Molecular Sciences Laboratory

Researchers Find Sugars a Sweet Alternative to Oil

EMSL NMR capabilities helped users study mutaroration, an atom-swapping phase that allow metal chloride catalysts to convert natural sugars to HMF.

Nuclear magnetic resonance (NMR) spectrometry capabilities housed at the Environmental Molecular Sciences Laboratory (EMSL) have played a role in helping researchers study direct conversion of natural sugars to an alternative source for plastic, fuels, and other industrial and household chemicals.

Scientists from the Pacific Northwest National Laboratory (PNNL)—who used EMSL NMR capabilities as well as instruments from PNNL's Institute for Interfacial Catalysis to perform the research—converted glucose directly in high yields to a primary building block for fuel and polyesters. This first-ever conversion is reported in *Science* (316:1597-1600).

The building block, hydroxymethylfurfural, or HMF, is a chemical derived from carbohydrates such as glucose and fructose and is a promising surrogate for petroleum-based chemicals. While glucose is an abundant sugar in nature, obtaining a commercially viable yield of HFM from glucose has been challenging and has historically generated many different byproducts.

The scientists experimented with a novel non-acidic catalytic system containing metal chloride catalysts in a solvent capable of dissolving cellulose. The solvent, called ionic liquid, allowed the metal chlorides to convert the sugars to HMF. But while metal chlorides work well for converting fructose, conversion of glucose as initial stock created many impurities. Using a high-throughput reactor to test metals at various temperatures, the scientists discovered that chromium chloride was most effective at converting glucose at low temperature and with few impurities. Upward of 70 percent from glucose and nearly 90 percent from fructose were obtained from the process, while leaving only traces of acid impurities.

EMSL's NMR capabilities were instrumental in verifying that the metal chloride catalysts work during an atom-swapping phase called mutarotation, in which hydrogen and hydroxyl trade places.

The scientists will now continue to evaluate ionic solvents and metal halides combinations to determine if they can increase HMF yield while reducing separation and purification costs. The research is supported by the PNNL Laboratory-Directed Research and Development program.

For more information, contact Mary Ann Showalter (509-376-5751).

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