THE USE OF BIODERIVED MOLECULAR BUILDING BLOCKS FOR THE SIMULTANEOUS PRODUCTION OF FUELS AND CHEMICALS

Andrew D. Sutton, Ty R. Brooks, Rhodri W. Jenkins, William L. Kubic Jr., Cameron M. Moore, Troy A. Semelesberger, Orion Staples.

Los Alamos National Laboratory

PO Box 1663, MS K558

Los Alamos, NM 87544, USA.

adsutton@lanl.gov

Targeting desirable compounds and using retrosynthetic approaches to construct them from small molecules is not a new concept in chemistry. However, its application using readily available bio-building blocks has not extensively explored. By understanding the types of carbon skeleton that can be made and by knowing the optimum amount of defunctionalizion required, our approach is to rationally design molecules and use group contribution methods to identify fuel candidates prior to actual cetane and octane testing. To that end we have been developing strategies to use small bio-derived molecules to construct more complicated molecules and our group's recent work on using two and three carbon units such as acetone, ethanol and glycerol as precursors will be presented. We have been able to construct a variety of carbon skeletons with varying degrees of functionalization and we can convert between the functional groups using simple catalytic approaches to produce molecules with promising gasoline and diesel properties as well as known commodity chemicals. While a large proportion of biomass to chemicals/fuels work concentrates on producing hydrocarbons, there are numerous instances where over-defunctionalizing is not necessary and in fact is detrimental to the final properties and in the process consumes more energy and raw materials.