NREL
NATIONAL RENEWABLE ENERGY LABORATORY

Magnetic Resonance Facility

Liquid and solid-state analysis capability for a variety of biomass, photovoltaic, and materials characterization applications across NREL

This 400 MHz spectrometer is available to all NREL scientists. *Photo by Dennis Schroeder, NREL 19989*

NREL scientists analyze solid and liquid samples on three nuclear magnetic resonance (NMR) spectrometers.

NREL's state-of-the-art Magnetic Resonance Facility provides:

- High-throughput, quantitative liquids analysis using a Bruker Sample Jet
- Cutting-edge analysis of semi-solid samples using an HR MAS probe
- An open-use instrument for NREL scientists to run their own liquid sample analysis
- Solid-state analysis of biomass feedstocks, biomass-related materials, and polymers.

NMR applications include:

- Rapid quantitative analysis of biomass hydrolysates
- Qualitative and quantitative mixture analysis
- Characterization of various catalysts including enzymes
- Protein structure determination
- Lignin composition and nondestructive determination of syringyl and guaiacyl (S/G) ratios
- Fuel composition analysis
- Nanotube characterization
- Temperature-dependent reaction rate determination.

Magnetic Resonance Equipment Specifications

System	Capabilities
600 MHz, 14.7 Tesla Bruker Avance III NMR Spectrometer	Liquid and solid state capabilities Bruker SampleJet for high-throughput analysis High sensitivity liquid-state Bruker CryoProbe High resolution MAS probe for semi-solid samples MAS spinning speeds up to 35 kHz
400 MHz, 9.4 Tesla Bruker Avance III HD NanoBay NMR Spectrometer	Dedicated liquids system Bruker SampleCase autosampler Bruker Prodigy CryoProbe for increased sensitivity Routine ^{1}H, ^{13}C, ^{31}P, and ^{19}F Temperatures studies from -40°C to 80°C
200 MHz, 4.7 Tesla Bruker Avance III HD NMR Spectrometer	Ideal for solid-state ^{13}C NMR studies 10 mm liquids probe for rapid ^{13}C analysis

NREL is a national laboratory of the U.S. Department of Energy, Office of Energy Efficiency and Renewable Energy, operated by the Alliance for Sustainable Energy, LLC.

Applications

High-throughput, quantitative determination of sugars in hydrolysates

- Rapid determination of sugar and degradation product concentrations in hydrolysates.

Solid-state analysis of biomass feedstocks

- Nondestructive, quantitative method to analyze lignin and cellulosic composition of biomass feedstocks
- Multiple cell wall components can be analyzed in a single spectrum.

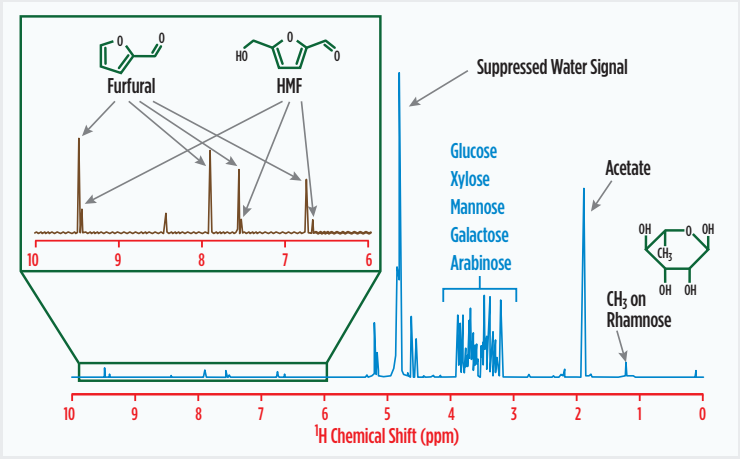
Fundamental structural and chemical compositional analysis

- NREL synthetic chemists can quickly determine both structural and chemical properties of their compounds on the multi-user instrument
- Water suppression techniques allow for high resolution study of biological compounds.

Fundamental studies of the structure and kinetics of catalysts

- 2- and 3-dimensional NMR spectroscopy allows for structural characterization of enzymes
- Determination of exchange rates from variable temperature experiments.

NREL scientist Renee Happs readies samples for high-throughput analysis using the SampleJet on the Bruker 600 MHz spectrometer. *Photo by Dennis Schroeder, NREL 19988*



Sample NMR spectra of a biomass hydrolysate. *Source: National Bioenergy Center. Figure by Ray David, NREL*

Nanotube characterization

- ^{13}C NMR spectroscopy provides valuable information on the metallic and semiconducting properties of single-walled carbon nanotubes (SWNTs)
- 2-dimensional ^{13}C-^{1}H correlation spectra are used to gain insight into nanotube polymer interactions for photovoltaic applications.

Associated publications

Happs, R.M., et al. (2015). "O-Glycosylation Effects on Family 1 Carbohydrate-Binding Module Solution Structures." *FEBS J.* (282:22); pp. 4341–4356.

Mukarakate, C., et al. (2014). "Real-Time Monitoring of the Deactivation of HZSM-5 During Upgrading of Pine Pyrolysis Vapors." *Green Chem.* (16); pp. 1444–1461.

Gjersing, E., et al. (2013). "Rapid Determination of Sugar Content in Biomass Hydrolysates Using Nuclear Magnetic Resonance Spectroscopy." *Biotechnol. Bioeng.* (110:3); pp. 721-728.

Smagala, T.G., et al. (2013). "Hydrocarbon Renewable and Synthetic Diesel Fuel Blendstocks: Composition and Properties." *Energy Fuels* (27:1); pp. 237-246.

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