

G&G Data Depository: Parameters used for NMR spectroscopy, to accompany:
A. Abduriyim et al., “Characterization of “Green Amber” with Infrared and Nuclear Magnetic Resonance Spectroscopy,” Fall 2009 *G&G*, pp. 158–177.

The Bruker spectrometer was operated at 150.9 MHz with a magnetic field strength of 14.1 Tesla, and the ^{13}C chemical shift was calibrated using glycine (176.0 ppm) as an external reference. Approximately 200–300 mg of powder from each sample was enclosed in a 4 mm zirconia sample rotor during the NMR experiments. Sample spinning rate was 6 kHz (6000/s) to ~10 kHz (10000/s), spectrometer pulse power was set at 280 watts for ^{13}C , pulse length was 6 microseconds (RF field strength 60.6 kHz), cross polarization contact time was 1.8 milliseconds, and the number of sampling points was 4096.

The JEOL spectrometer was operated at 125.7 MHz with magnetic field strength of 11.7 Tesla, and the ^{13}C chemical shift was calibrated by hexamethylbenzene (17.7 ppm from tetramethylsilane). Approximately 250–300 mg of powder from each sample was enclosed in a 4 mm zirconia rotor. Sample spinning rate was 15 kHz, spectrometer pulse power was set at 200 watts for ^{13}C , pulse length was 3.5 microseconds (RF field strength 71 kHz), CP contact time was 1.8 milliseconds, and the number of sampling points was 4096. All samples were measured with scanning numbers of 6000–8000 units in both spectrometers. The spectra from different samples and from different instruments were normalized before comparison based on the operating conditions of each instrument.