

## Supplementary Information for

### Operationally Simple Electrochemical Method for the Conversion of Acetone into High-Specification Jet Fuel

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**Materials.** Mesityl oxide was obtained from Acros Organics. Tetrabutylammonium tetrafluoroborate was purchased from TCI America. The Pd/Al<sub>2</sub>O<sub>3</sub> catalyst was purchased from Strem Chemicals Inc. The Pd/C catalyst and n-C<sub>12</sub>H<sub>30</sub> internal standard were purchased from Sigma-Aldrich.

**Fuel Characterization.** All GC-FID spectra were collected on an Agilent 7820A gas chromatograph (Santa Clara, CA). The GC oven method began at 40 °C for 3 min, then ramped to 300 °C at a rate of 10 °C min<sup>-1</sup>, and finally held at 300 °C for 1 min. The gas-phase separation was achieved using an Agilent Technologies DB-5 column, 60 m x 0.620 mm x 0.25 μm. The column was held at 12.6 psi. A manual injection of 1 μL was used for each run. The inlet temperature was held at 250 °C at a pressure of 12.59 psi. Eluted compounds were fed into the flame ionization detector (FID) which was held at the following parameters: 300 °C, a hydrogen gas flow at 40 mL min<sup>-1</sup>, an air flow at 400 mL min<sup>-1</sup>, and a makeup gas flow at 27 mL min<sup>-1</sup>. All GC-MS spectra were collected on a Thermo Scientific Trace™ 1310 Gas Chromatograph / Exactive™ GC Orbitrap mass spectrometer. The GC oven method began at 40 °C for 3 min, then ramped to 300 °C at a rate of 20 °C min<sup>-1</sup>, with a final hold at 300 °C for 30 min. The gas phase separation was achieved using a Thermo Scientific TG-5SILMS column, 30 m x 0.25 mm x 0.25 μm. A split flow mode of injection was used at 25 mL min<sup>-1</sup> with a split ratio of 25.0. The inlet temperature was held at 300 °C. Eluted compounds passed through a heated auxiliary line (300 °C) and were directed toward the ion source region of the mass spectrometer, held at 305 °C, where they were subjected to electron impact ionization (EI). The mass range of the mass spectrometer was set from 50 to 600 amu.

**Kinematic Viscosity and Density Studies.** The kinematic viscosities and densities of the fuels were measured using a Stabinger SVM 3001 viscometer connected to a TC-502 chiller to achieve temperatures down to -40 °C. Each sample was placed in a 5 mL syringe, which was then attached to the viscometer through a Luer lock adapter. Approximately 3 mL of each fuel was then slowly injected to prewet the measurement cells. The sample was allowed to equilibrate at the starting temperature (typically 20 °C). The method was then initiated, and an additional 1 mL of sample was added. Each sample was then cooled to -40 °C (±0.002 °C), and at 5 °C increments, both the kinematic viscosity and density were measured. Reported values were derived from the average of five determinations. After each run, the measuring cells were rinsed three times with hexanes and dried under a stream of nitrogen.

**Heat of Combustion Studies.** The net heats of combustion of fuel samples were measured using the following procedure: A pellet of high purity benzoic acid (~950–1000 mg) was accurately weighed, and ~350–800 mg of fuel was added and allowed to fully saturate the pellet. The pellet was then reweighed and the gross heat of combustion (HOC) was measured in a Parr 6200 Calorimeter. After combustion of the sample, the HOC was corrected by subtracting the contribution due to benzoic acid and combusted wire. The NHOC was then calculated from the corrected HOC by taking into account the hydrogen content (determined by elemental analysis) and the density of the fuel at 15 °C. The NHOC measurements were taken in triplicate and averaged.

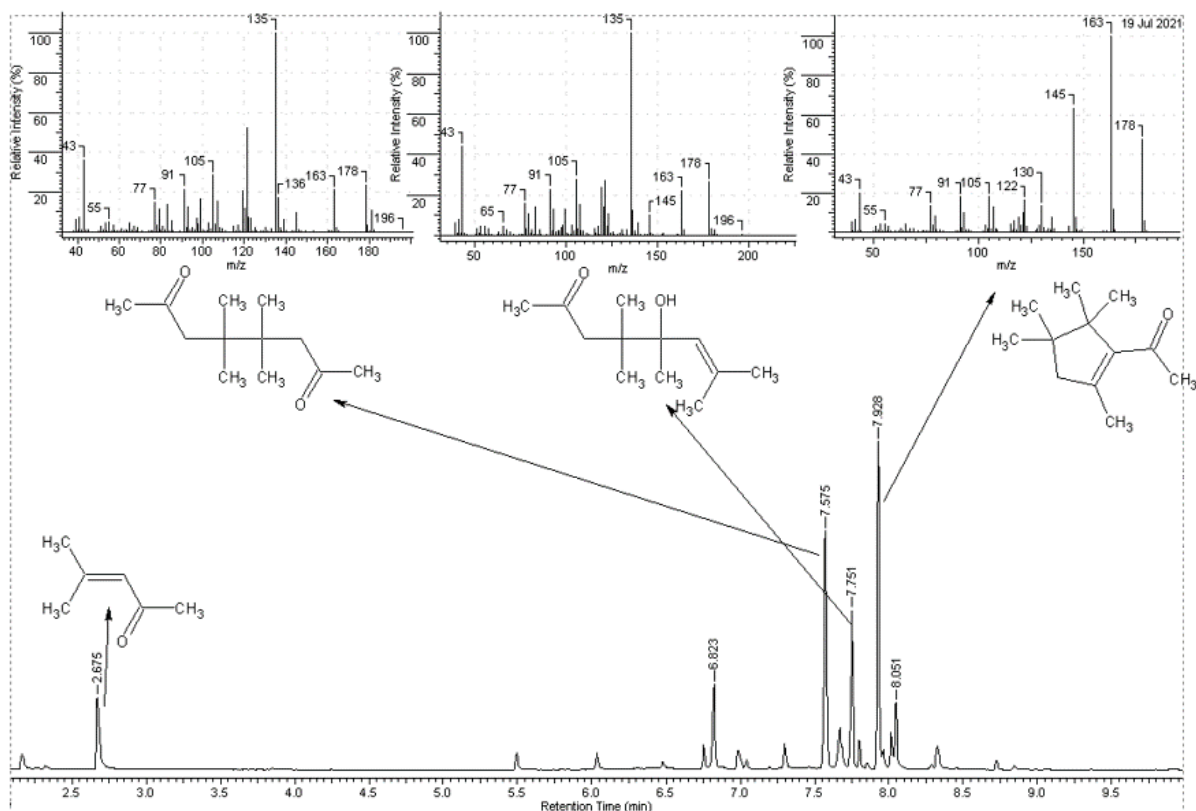
**Flashpoint Measurements.** The flash points of the fuel samples were measured with a Grabner Instruments/Ametek Miniflash FLP Touch according to ASTM D7094. For each measurement, 2 mL of

fuel was transferred via auto pipette to a 7 mL stainless steel sample cup. N-Decane was used as a calibration standard and fuel measurements were conducted in duplicate.

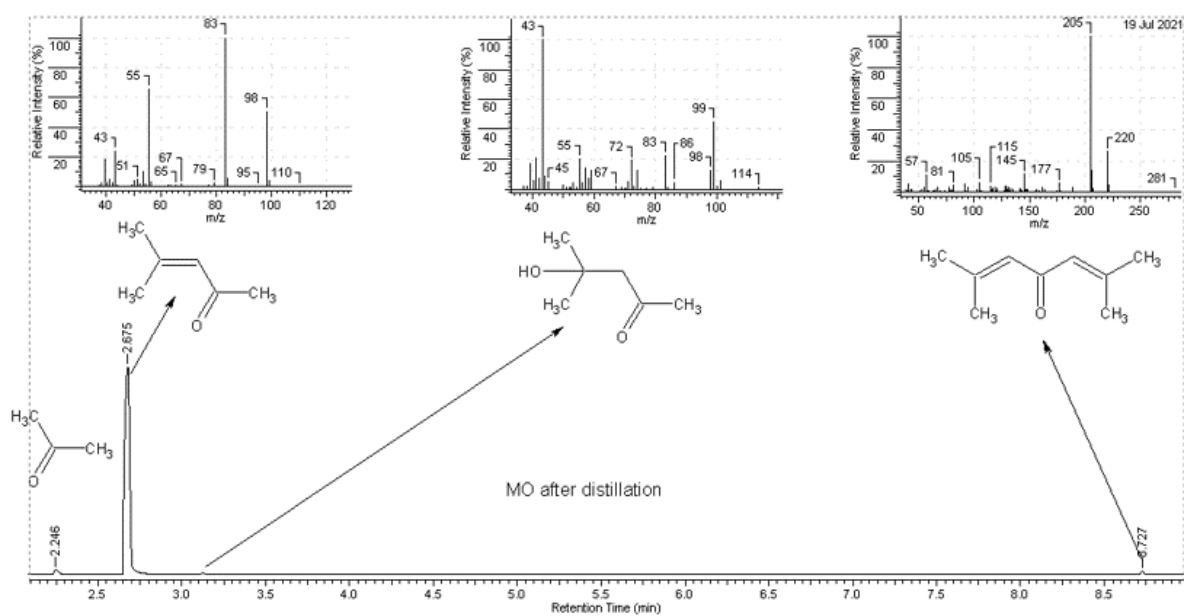
**Commercial DC power supply used in this work**



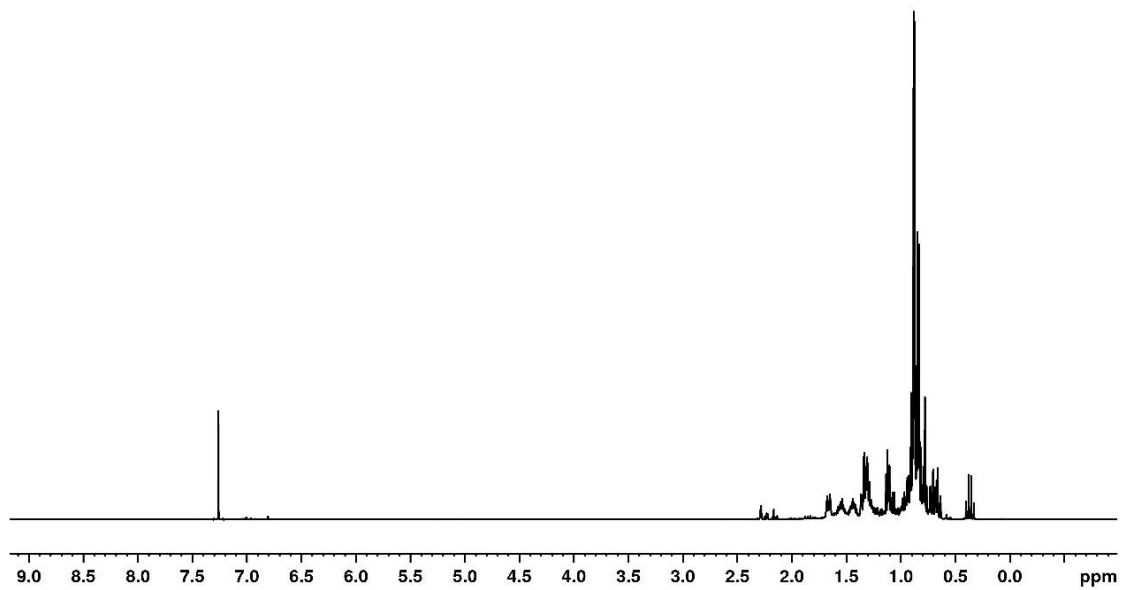
**Figure S1.** Yescom DCP3010D 10 A – 30 V DC power supply.



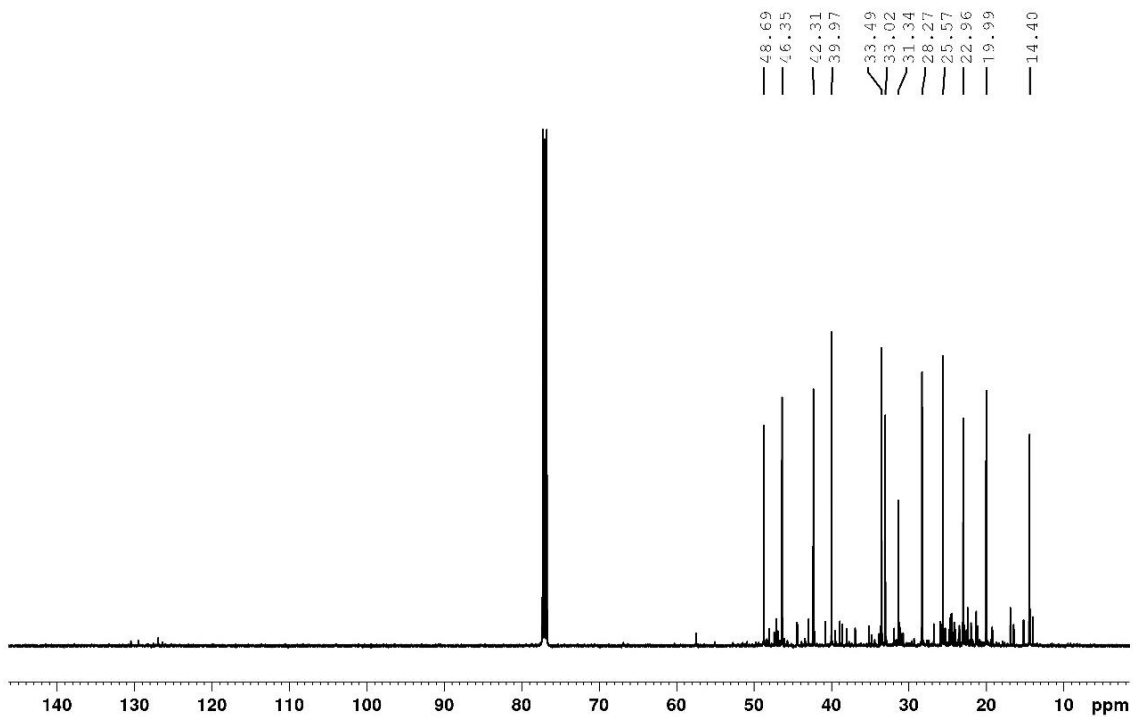
**Figure S2.** GC-MS of the electrolysis product, with structure assignments made based on mass spectral peak matching.



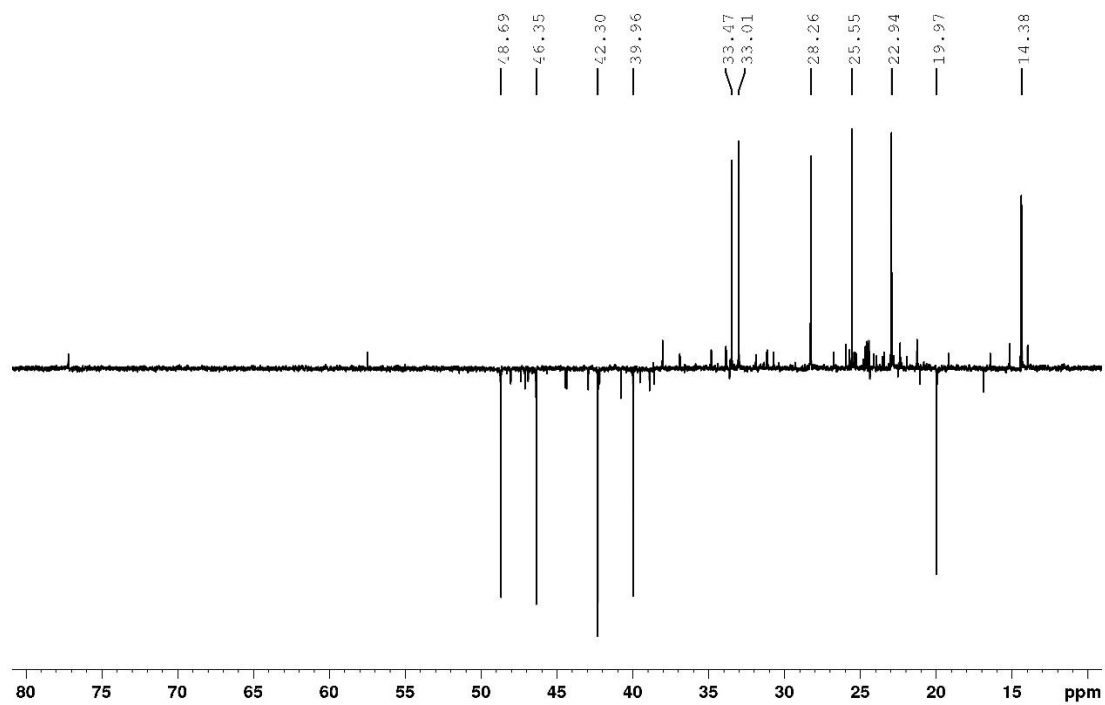
**Figure S3.** GC-MS of blank experiment with no current passed for 12 h, with structure assignments made based on mass spectral peak matching.



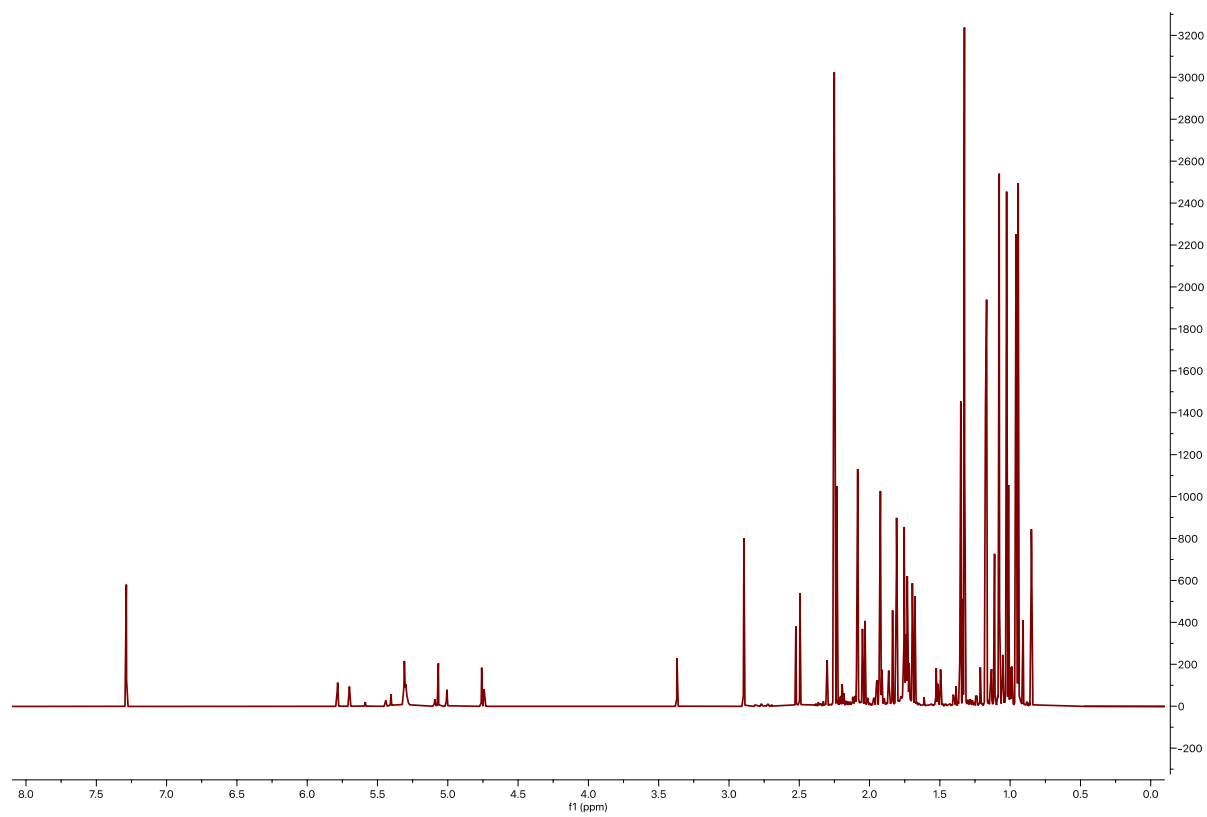
**Figure S4.** 400 MHz  $^1\text{H}$ -NMR of the finished hydrocarbon product ( $\text{CDCl}_3$ ).



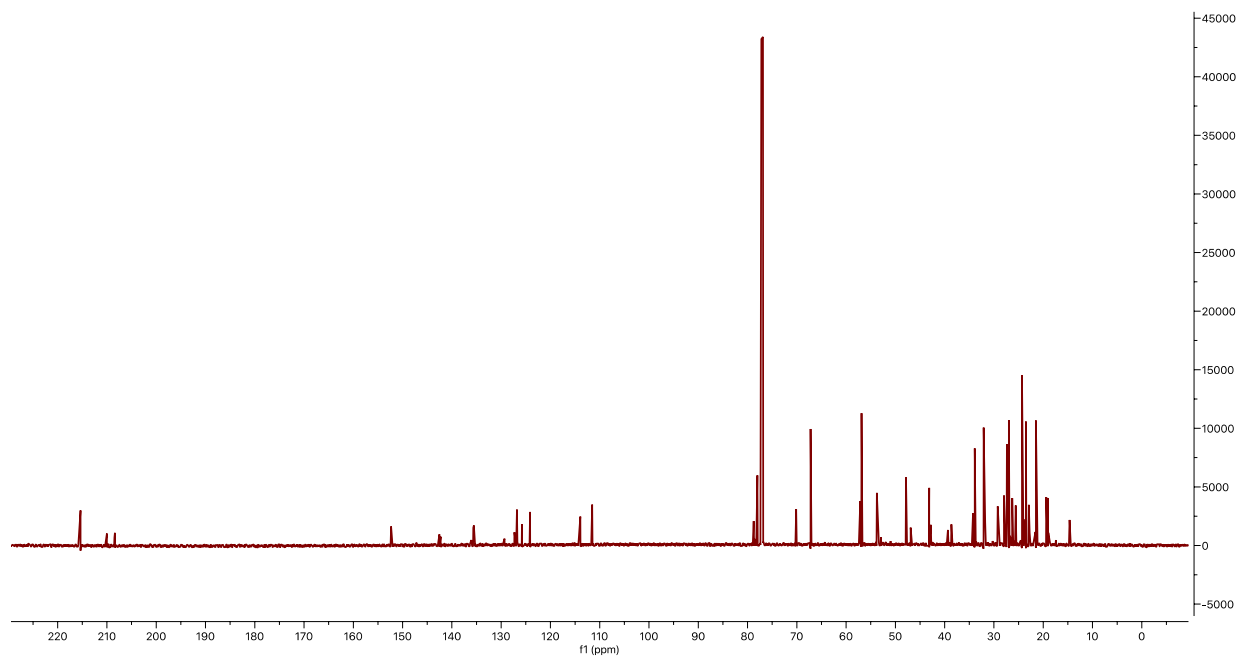
**Figure S5.** 400 MHz  $^{13}\text{C}$ -NMR of the finished hydrocarbon product ( $\text{CDCl}_3$ ).



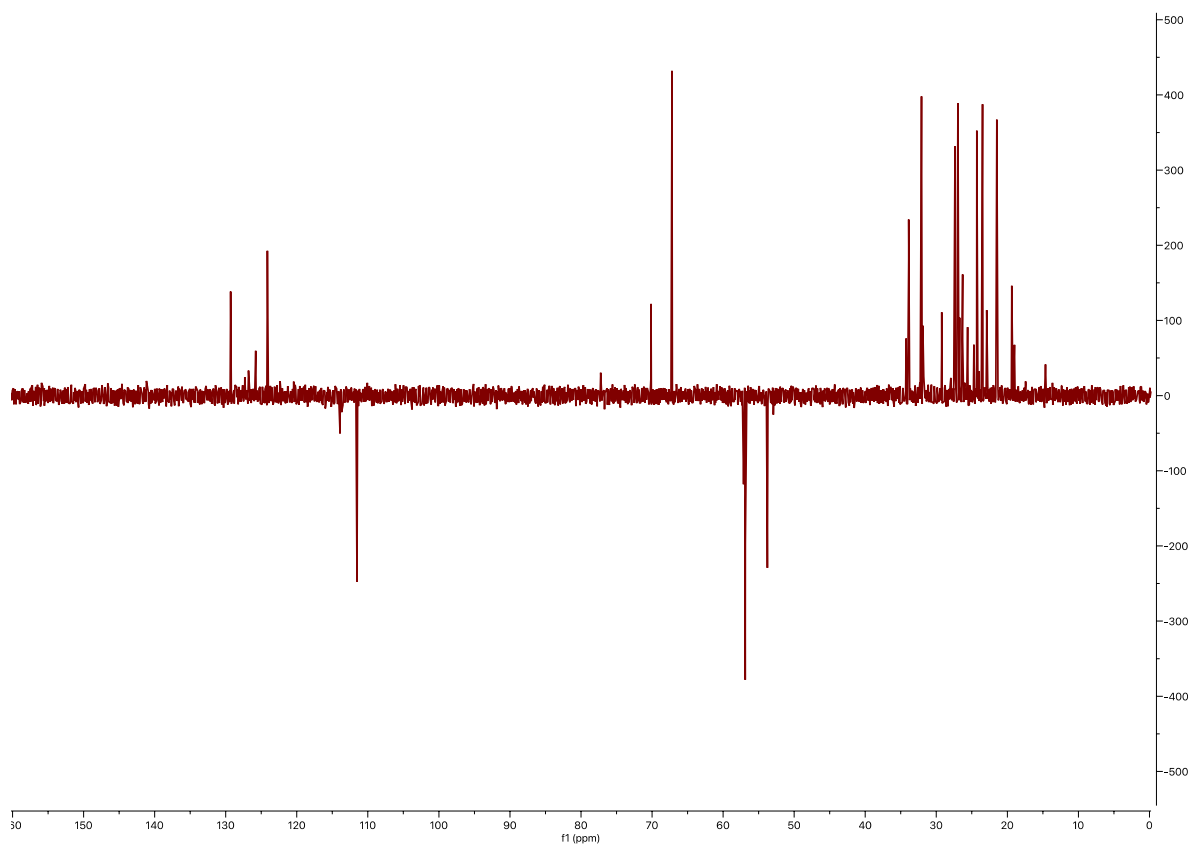
**Figure S6.** 400 MHz DEPT  $^{13}\text{C}$ -NMR of the finished hydrocarbon product ( $\text{CDCl}_3$ ).



**Figure S7.** 800 MHz  $^1\text{H}$ -NMR of the electrolysis product prior to hydrogenation ( $\text{CDCl}_3$ ).



**Figure S8.** 800 MHz <sup>13</sup>C-NMR of the electrolysis product prior to hydrogenation (CDCl<sub>3</sub>).



**Figure S9.** 400 MHz DEPT <sup>13</sup>C-NMR of the electrolysis product prior to hydrogenation (CDCl<sub>3</sub>).