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Supplementary Information

Unsaturated Renewable Oil Transformation into Novel Biofuel Compositions via an Olefin Metathesis-Transesterification-Hydrogenation Sequence

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Calculation of ethenolysis conversion by ^{1}H NMR

The olive oil average molecular weight was calculated according to the literature.[1]

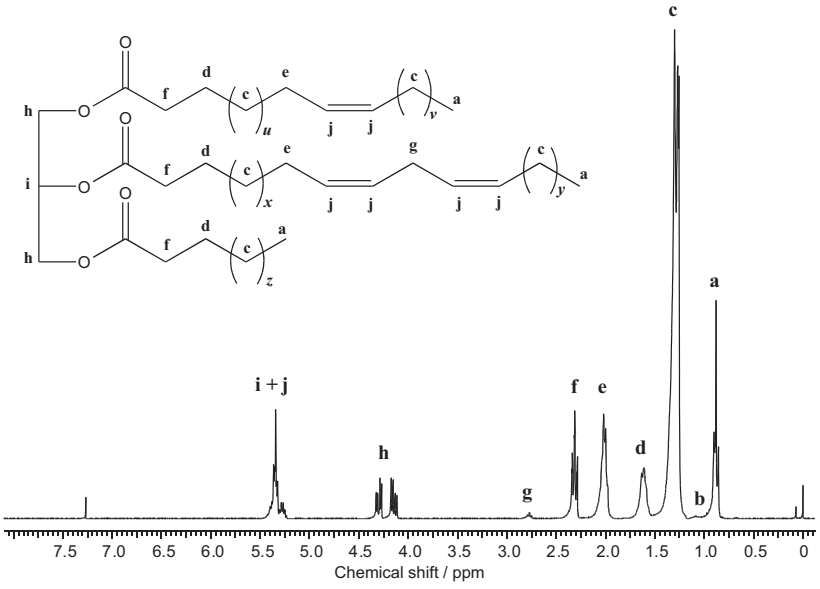

Figure S1. Olive oil ^{1}H NMR (300 MHz, $CDCl_3$) spectrum.

$$MW = 15.03\left(\frac{a}{3\ A_p}\right) + 14.03\left(\frac{b + c + d + e + f + g}{2\ A_p}\right) + 26.02\left(\frac{(i + j) - A_p}{2A_p}\right) + 173.1 \qquad (1)$$

where A_p is the area of one methylene hydrogen of the glycerol moiety and calculated by:

$$A_p = \frac{h}{4} \qquad (2)$$

The ethenolysis conversion can be calculated by ^{1}H NMR, since the olefinic hydrogens of the terminal and internal olefins have different chemical shifts and do not overlap in the spectrum (Figure S2).

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In memoriam of Prof Roberto Fernando de Souza

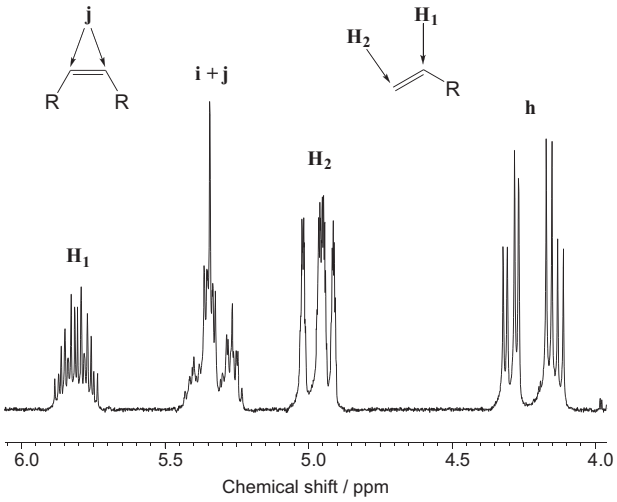

Figure S2. Olefinic hydrogen signals used to calculate the ethenolysis conversion by ^{1}H NMR.

The ethenolysis conversion can be calculated by:

$$\text{conversion (\%)} = \frac{\text{terminal olefin}}{2 \times \text{internal olefin} + \text{terminal olefin}} \times 100 \qquad (3)$$

The molar ratio of the terminal olefins can be obtained from the integral of the signals H_1 and H_2 (Figure S2):

$$\text{terminal olefin} = \frac{(0.5 \times H_2) + H_1}{2} \qquad (4)$$

The molar ratio of the internal olefins can be obtained from the integral of the signal i + j subtracting the area of one hydrogen (A_p):

$$\text{internal olefin} = \frac{(i + j) - A_p}{2} \qquad (5)$$

Replacing equations 4 and 5 into equation 3 results in equation 6:

$$\text{conversion (\%)} = \frac{(0.5 \times H_2) + H_1}{2 \times ((i + j) - A_p) \quad + \quad (0.5 \times H_2) + H_1} \times 100 \qquad (6)$$

References

1. Miyake, Y.; Yokomoto, K.; Matsukaki, N.; *J. Am. Oil Chem. Soc*. **1998**, *75*, 15.