

Ketal-Rich Bio-Petroleum from Lignocellulosic Biomass: A Tunable Feedstock for Green Hydrocarbon Production in Refinery Condition

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Supplementary information material

1. Tubular semi-continuous reactor scheme

The scheme of home-made tubular semi-continuous reactor used for BP production is illustrated in Figure S1.

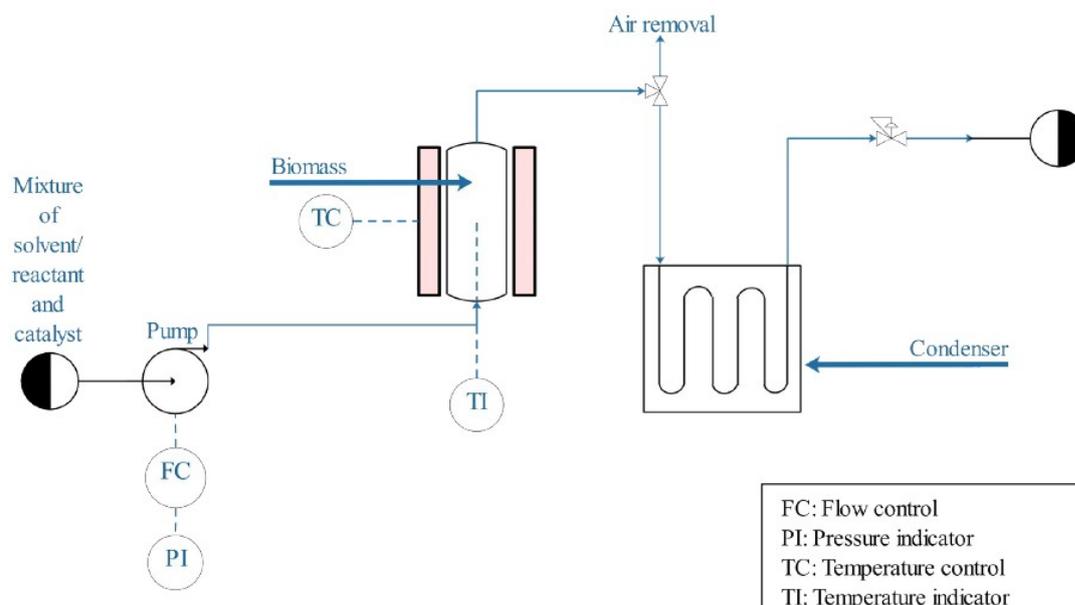


Figure S1 – Semi-continuous tubular reactor scheme (published under permission of Santos et al., 2020)

2. Carbohydrate ketals content in BPs and BP yields

Carbohydrate ketals content (in terms of DG and DX content) in BPs produced from different biomasses and temperatures are displayed in Figure S2.

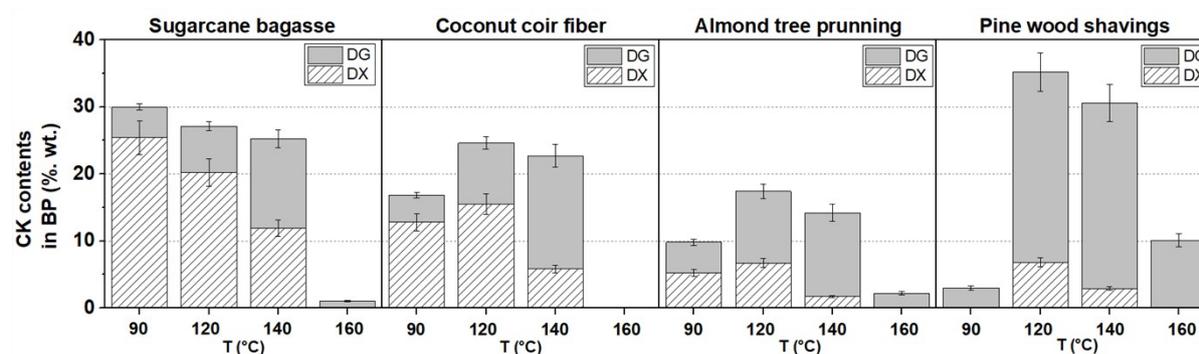


Figure S2 – Carbohydrate ketals (CK) content in BPs produced from different biomasses under different reaction temperatures

Pinus wood shavings and sugarcane bagasse were capable to produce BPs containing more ketals than other biomasses.

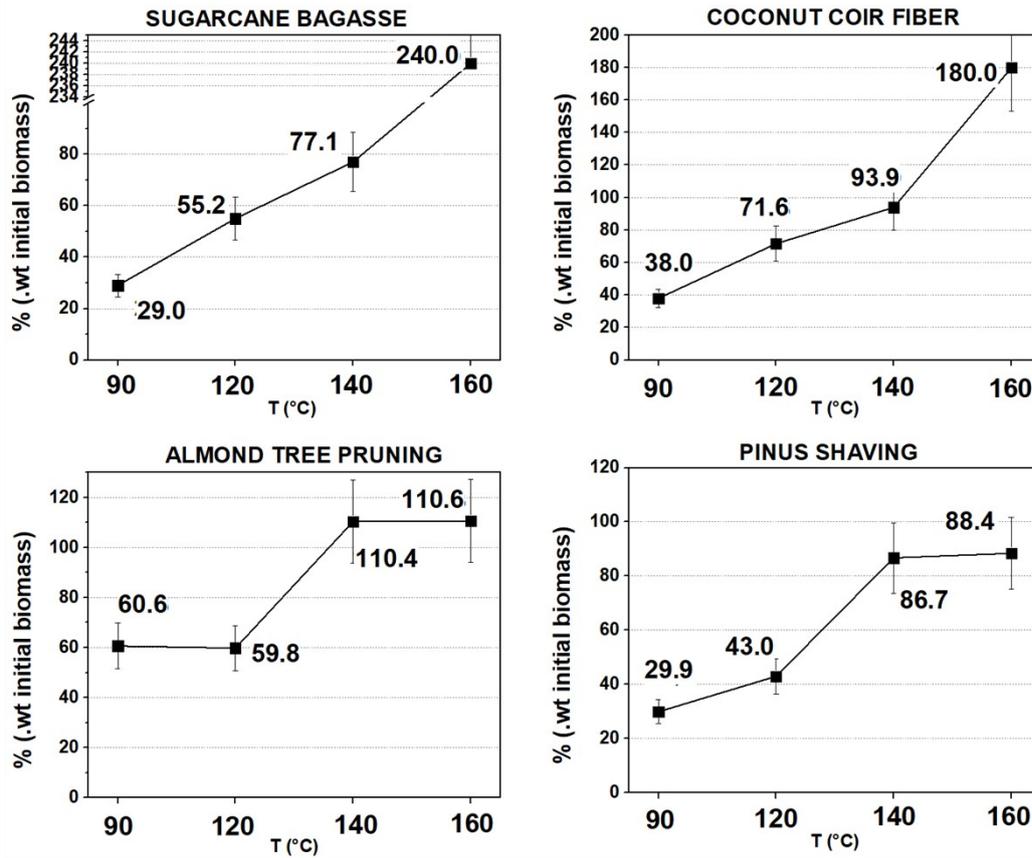


Figure S3 – BP yields from different biomasses and reaction temperatures

BP yields were calculated using Equation S1. BP yields rise abruptly at 160°C due to condensation of acetone. Both CK content in BP and BP yield values for duplicate experiments presented up to 15% of standard deviations which are present as error bars on graphic curves.

Equation S1
$$BP\ yield = \frac{mass\ of\ BP}{mass\ of\ biomass\ fed\ into\ reactor} \times 100$$

3. NMR spectra of different BPs

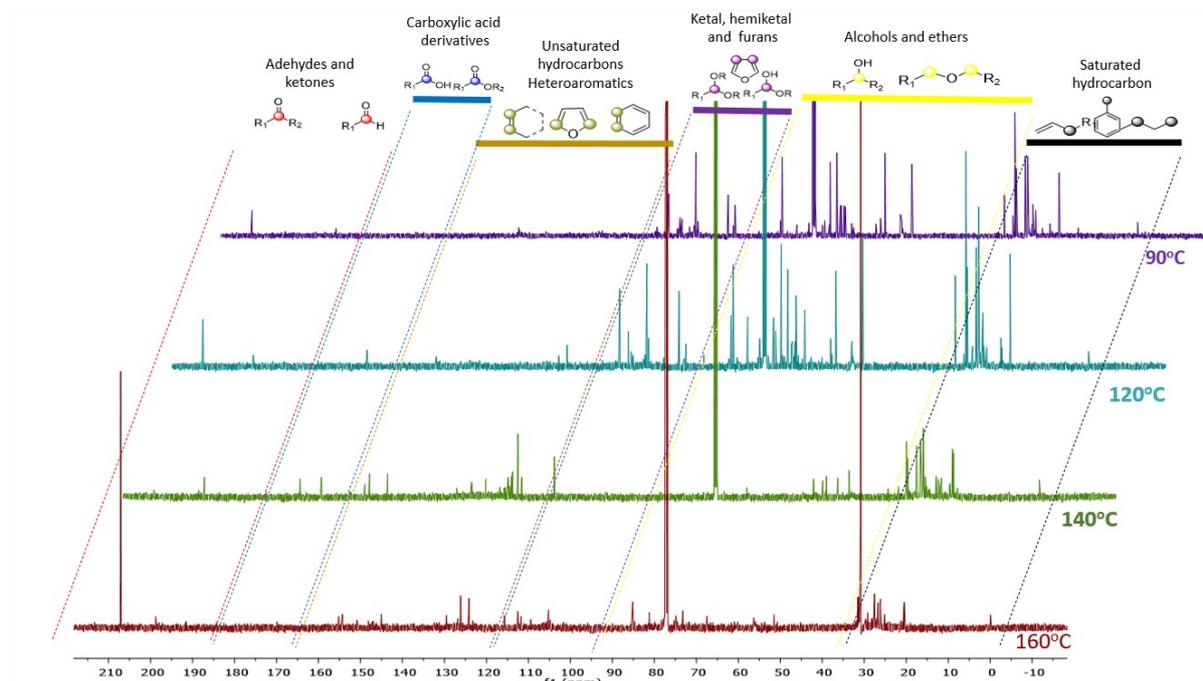


Figure S4 - ^{13}C NMR spectra of BPs produced at different temperatures from almond tree pruning

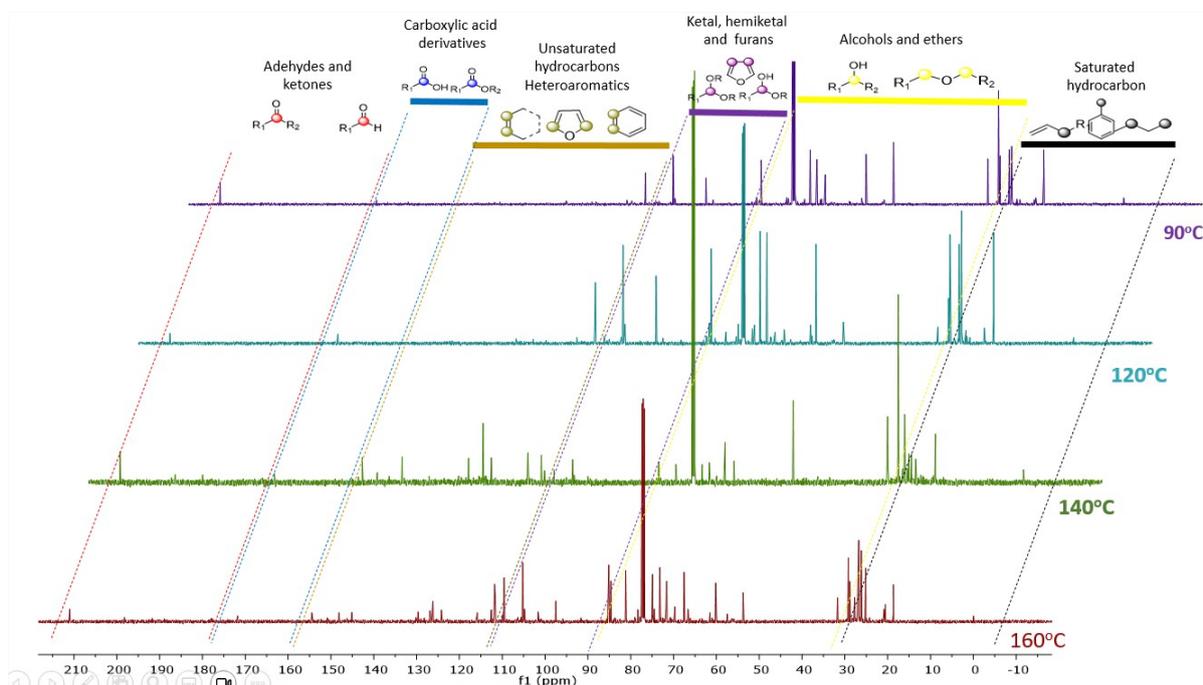


Figure S5 - ^{13}C NMR spectra of BPs produced at different temperatures from sugarcane bagasse

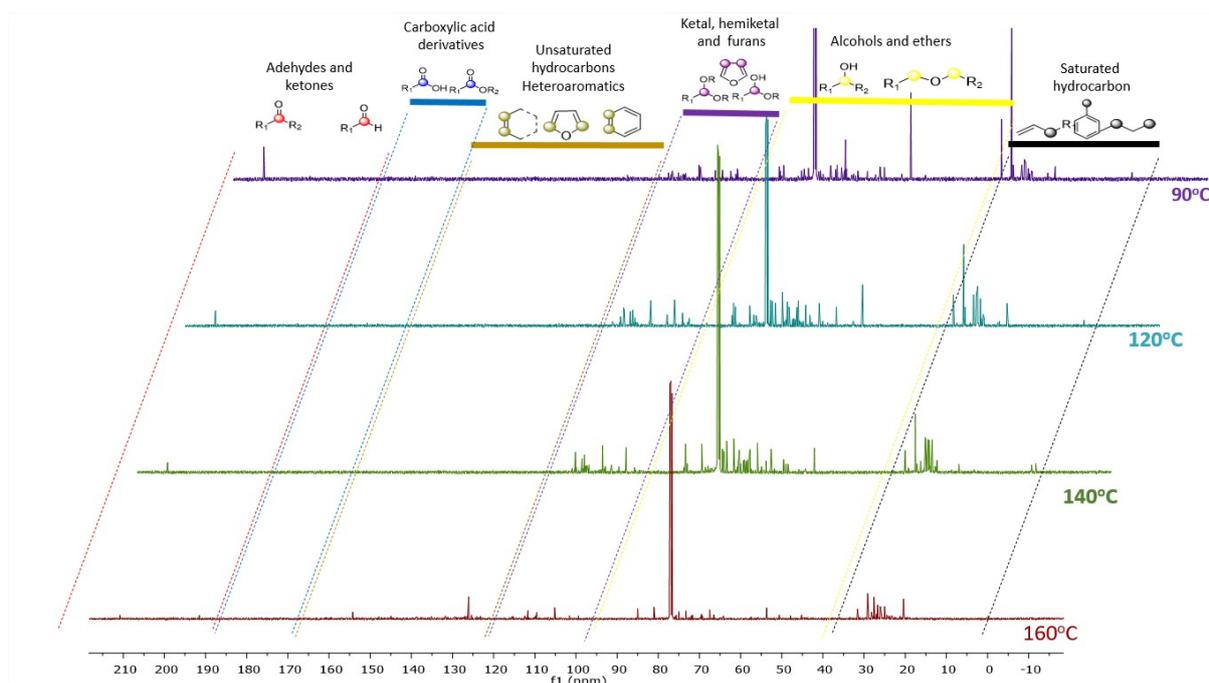


Figure S6 - ^{13}C NMR spectra of BPs produced at different temperatures from pine wood shavings

4. Thermogravimetric curves and mass loss of in natura biomasses and residual biomasses after BP production reactions

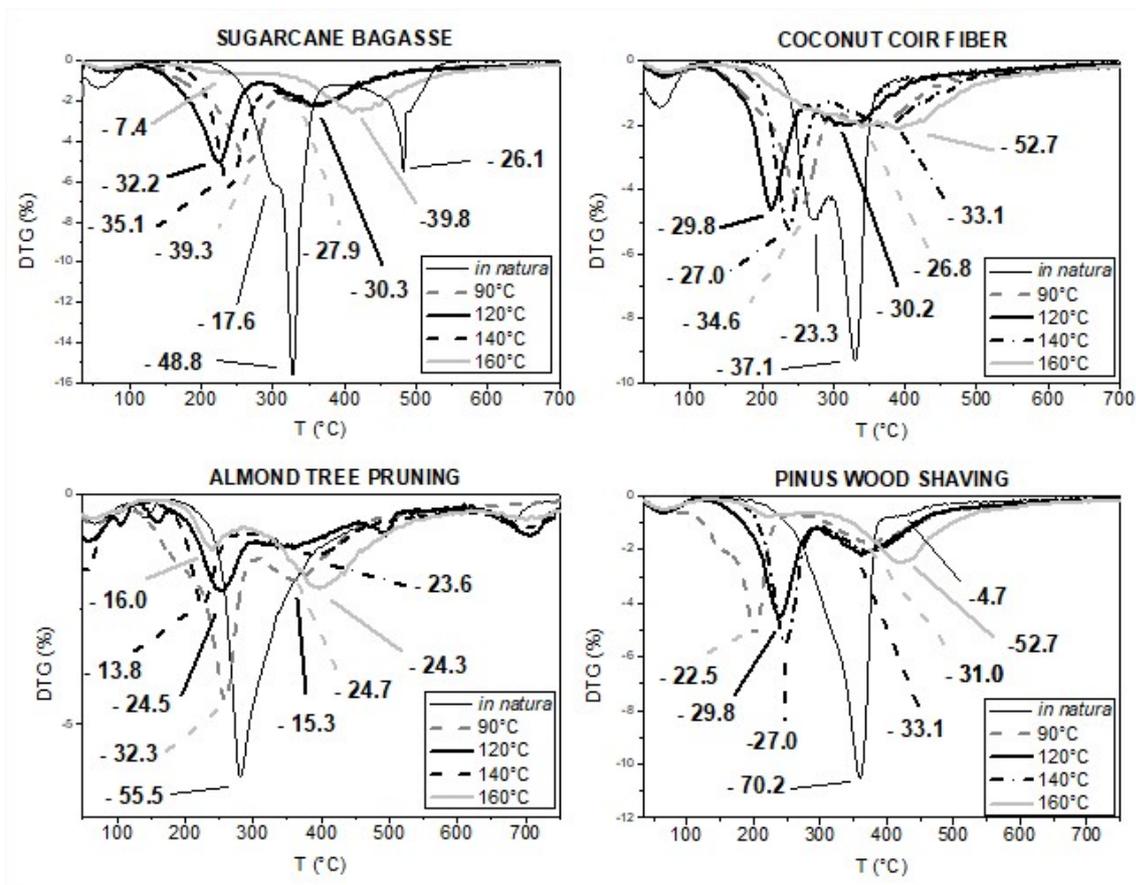


Figure S7 – TGA curves and mass loss of in natura biomasses and residual biomasses from BP reaction

5. Estimative of lignocellulosic composition of biomasses using data from literature

Table S1 summarizes the cellulose, hemicellulose, and lignin contents of the biomasses studied, as reported in the literature. The bold values represent the median content for each fiber and were used as reference values to estimate the relative holocellulose recovery. The effect of temperature on HR is shown in Figure 10.

Table S1 - Cellulose, hemicellulose, and lignin contents in the studied biomass samples, as reported in the literature. (informar nome científico no texto)

Biomass	Sugarcane bagasse	Coconut coir	Almond tree pruning	Pine wood shaving
Lignin (%)	20.57 ²⁷	42.0 ²⁹	31.2 ³¹	12.85 ³²
	23.61 ²⁸	30.46 ³⁰		27.2 ³³
Average content (%)	22.1	44.0	31.2	20.0
Cellulose (%)	37.74 ²⁷	27.41 ²⁹	23.1 ³¹	52.52 ³²

	41.95 ²⁸	32-50 ³⁰		31.4 ³³
Average content (%)	39.8	38.7	23.1	42.0
Hemicellulose	27.23 ²⁷	14.63 ²⁹	31.3 ³¹	16.35 ³²
	21.70 ²⁸	0.15-15 ³⁰		40.2 ³³
Average content (%)	24.5	14.8	31.3	28.3
Holocellulose content (%)	64.3	53.5	54.4	70.3

legend – values in bold were calculated through the average value of the ones associated to a specific fiber

* Median value of a specific fiber obtained from literature (see values on bold in Table 1)