Supplementary Information

Lignin-First Biorefining of Lignocellulose: the Impact of Process Severity on the Uniformity of Lignin Oil Composition

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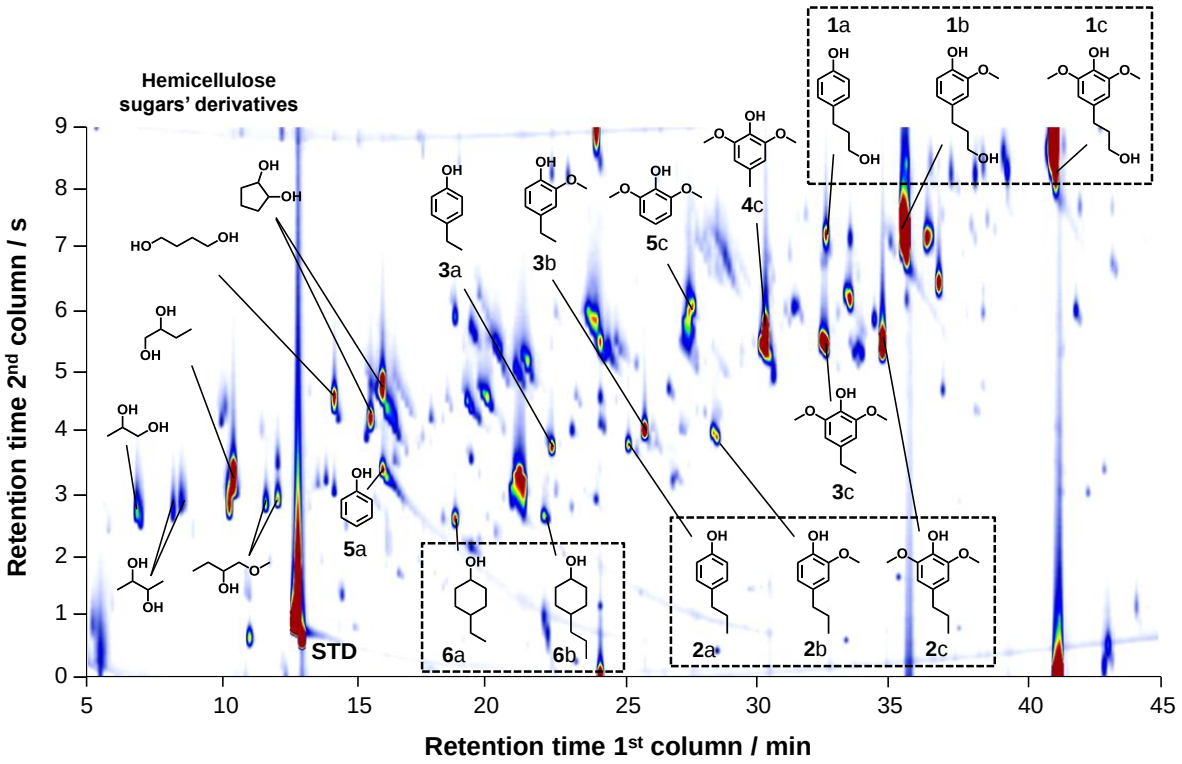

Figure S1. GC × GC trace of the CUB lignin oil obtained in 2-PrOH/H_2O (7:3, v/v) at 160 °C. The EI-mass spectra of species showed a similarity index > 95% either with authentic samples or with MS libraries NIST 08, NIST 08s, and Wiley 9. STD: external standard (di-*n*-butyl ether).

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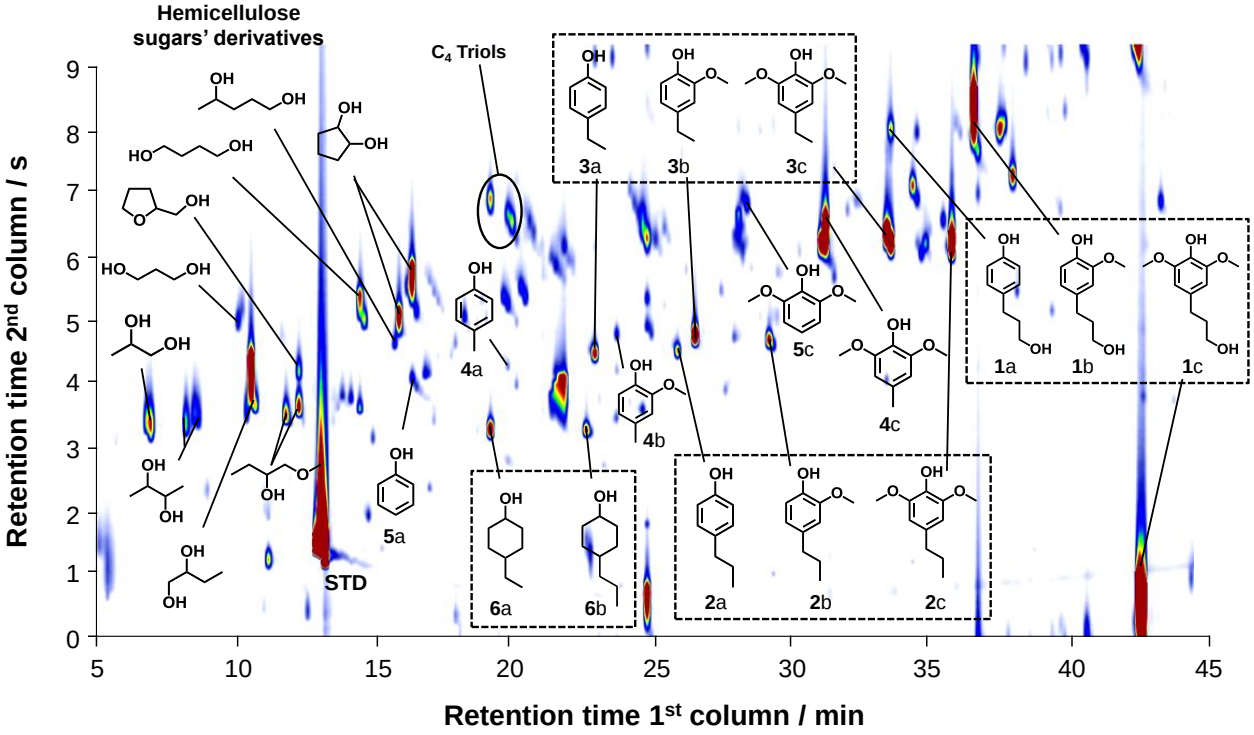

Figure S2. GC × GC trace of the CUB lignin oil obtained in 2-PrOH/H_2O (7:3, v/v) at 180 °C. The EI-mass spectra of species showed a similarity index > 95% either with authentic samples or with MS libraries NIST 08, NIST 08s, and Wiley 9. STD: external standard (di-*n*-butyl ether).

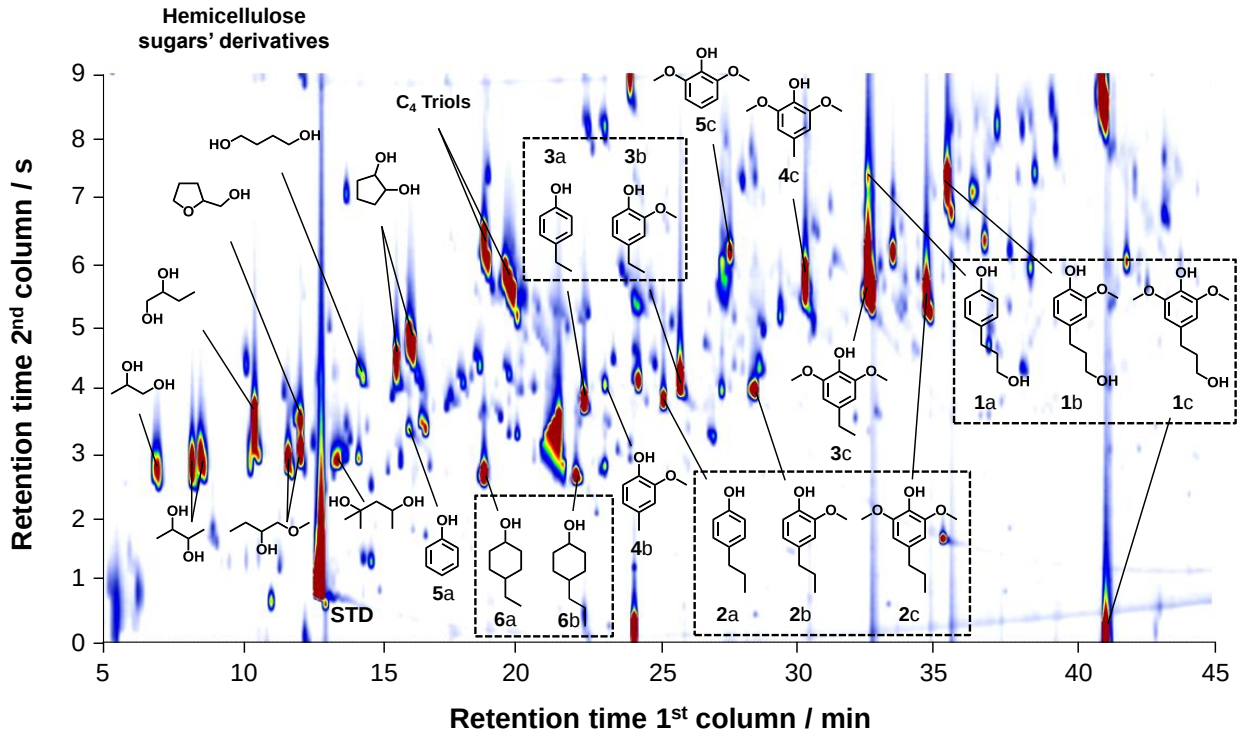

Figure S3. GC × GC trace of the CUB lignin oil obtained in 2-PrOH/H_2O (7:3, v/v) at 200 °C. The EI-mass spectra of species showed a similarity index > 95% either with authentic samples or with MS libraries NIST 08, NIST 08s, and Wiley 9. STD: external standard (di-*n*-butyl ether).

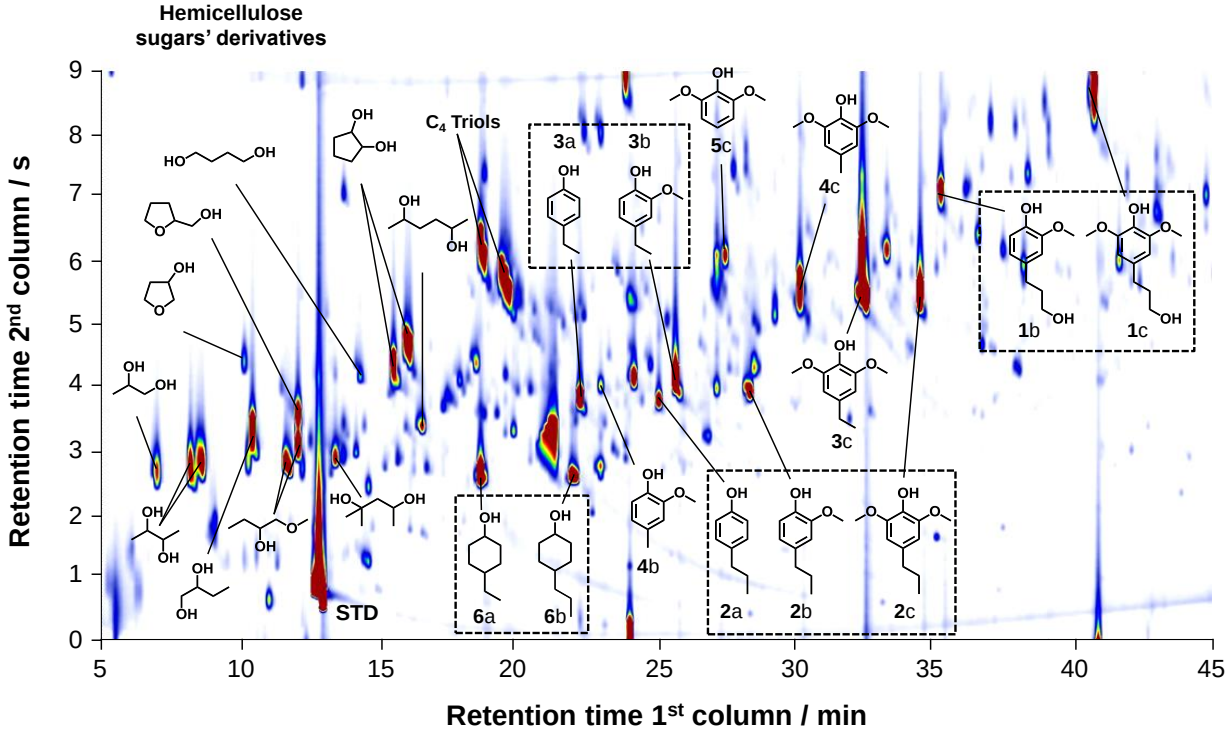

Figure S4. GC × GC trace of the CUB lignin oil obtained in 2-PrOH/H_2O (7:3, v/v) at 220 °C. The EI-mass spectra of species showed a similarity index > 95% either with authentic samples or with MS libraries NIST 08, NIST 08s, and Wiley 9. STD: external standard (di-*n*-butyl ether).

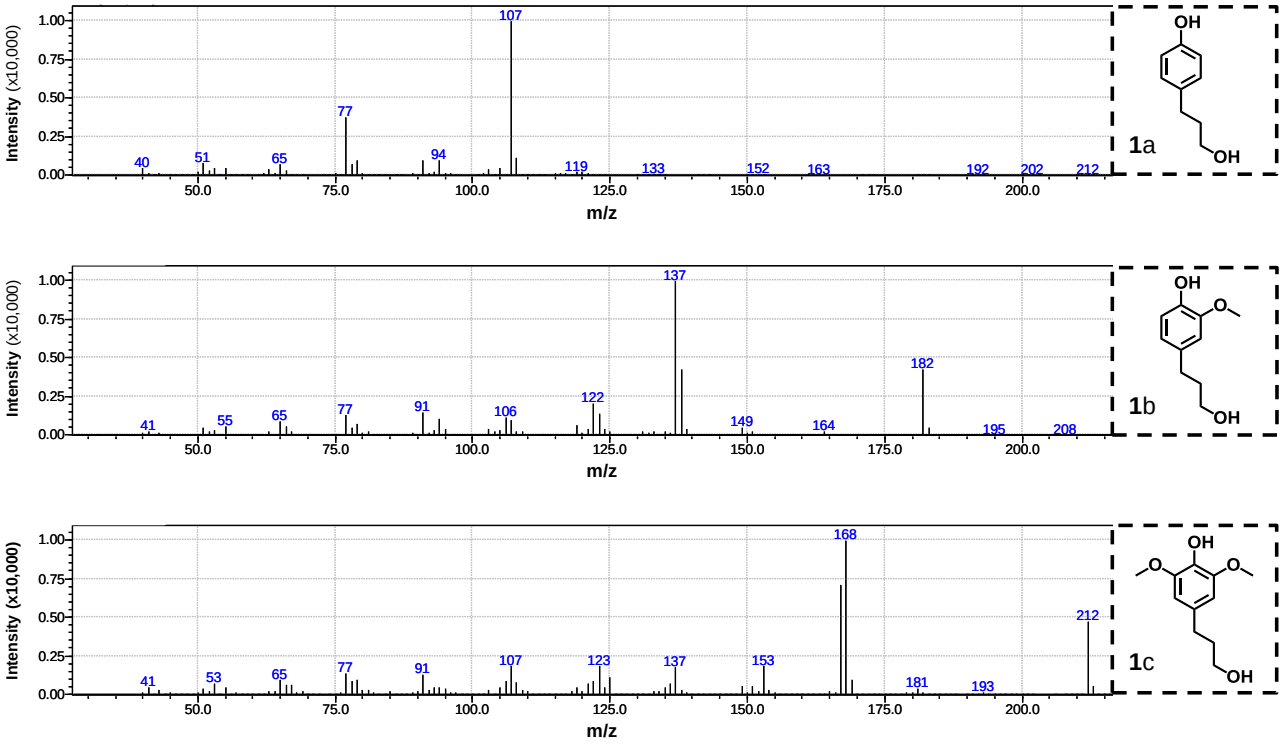

Figure S5. Examples of EI-mass spectra of authentic samples (**1a**, **1b** and **1c**) ran in order to establish similarity indices with compounds identified on GC × GC-MS analysis.

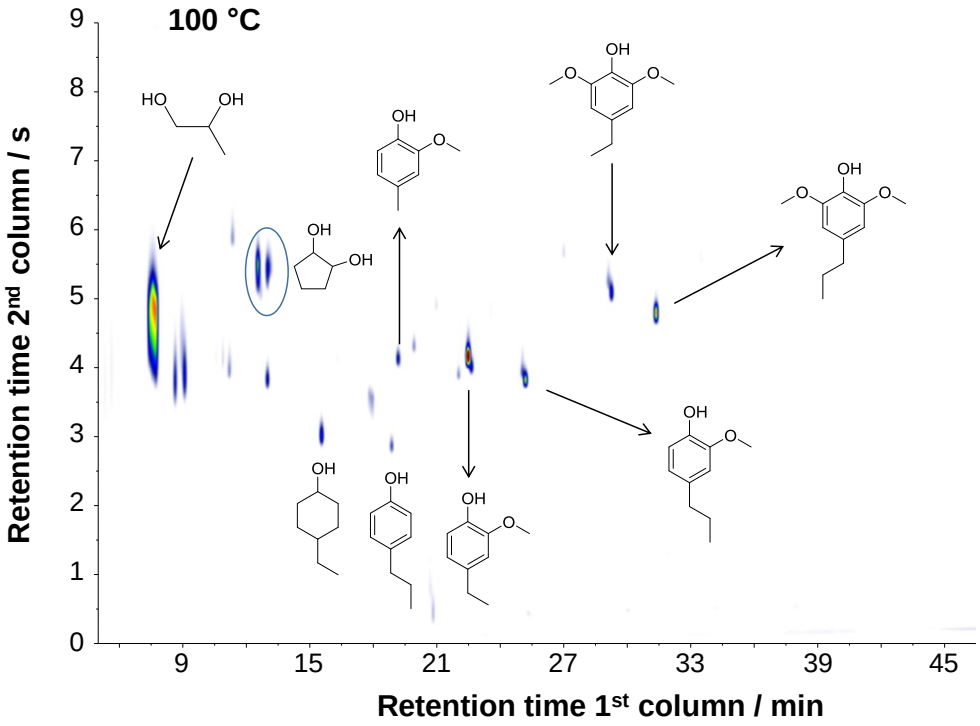

Figure S6. 2D GC × GC image showing the main components of a CUB lignin oil distillation fraction collected at 100 °C. Identification of the peaks was performed using an MS detector and by comparing the spectra with libraries (NIST 08, NIST 08s, and Wiley 9).

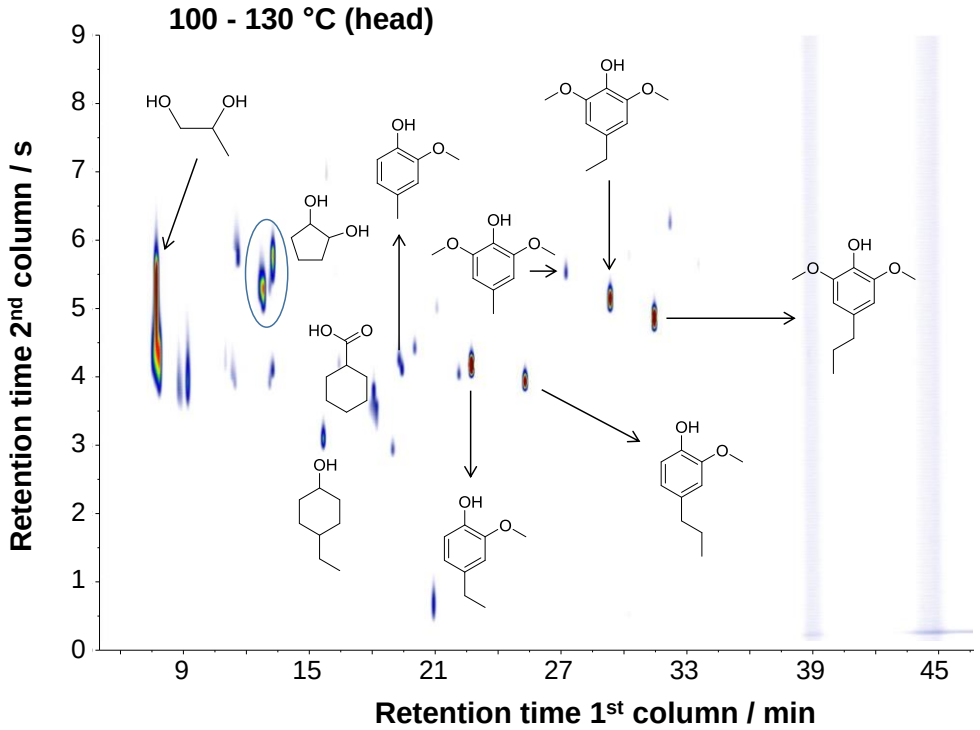

Figure S7. 2D GC × GC image showing the main components of a CUB lignin oil distillation fraction collected at 100-130 °C (head). Identification of the peaks was performed using an MS detector and by comparing the spectra with libraries (NIST 08, NIST 08s, and Wiley 9).

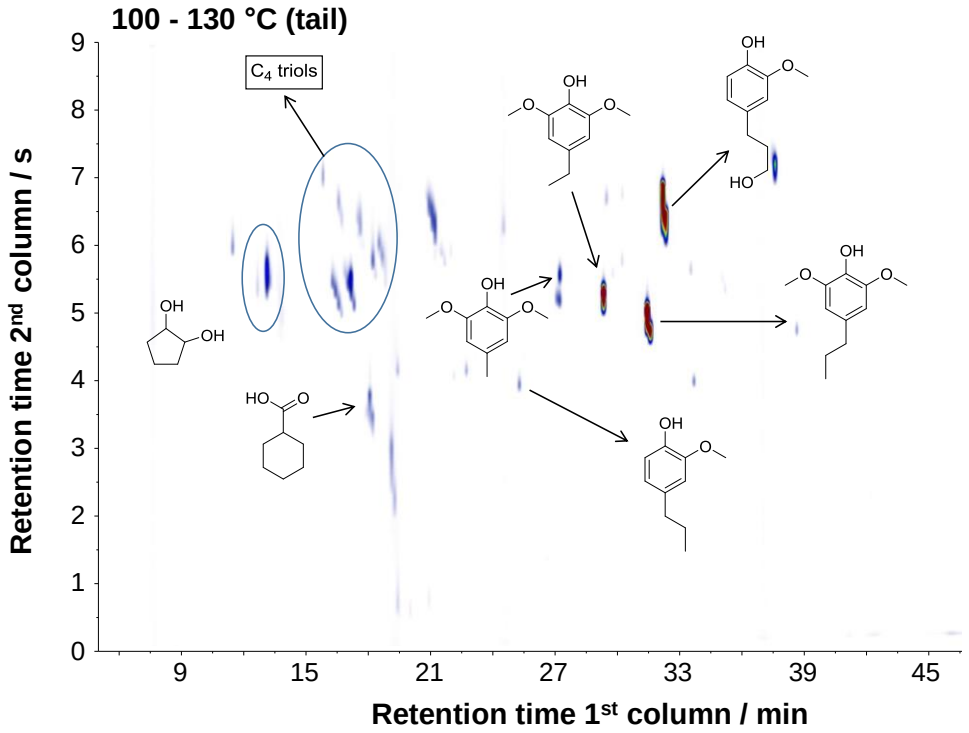

Figure S8. 2D GC × GC image showing the main components of a CUB lignin oil distillation fraction collected at 100-130 °C (tail). Identification of the peaks was performed using an MS detector and by comparing the spectra with libraries (NIST 08, NIST 08s, and Wiley 9).

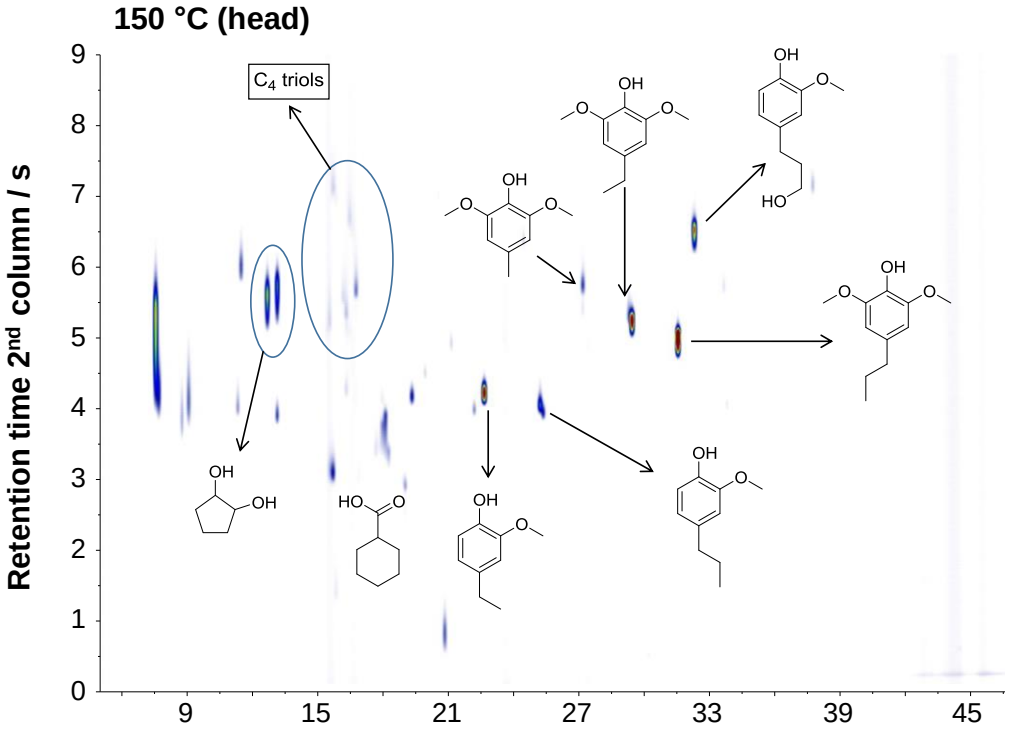

Figure S9. 2D GC × GC image showing the main components of a CUB lignin oil distillation fraction collected at 150 °C (head). Identification of the peaks was performed using an MS detector and by comparing the spectra with libraries (NIST 08, NIST 08s, and Wiley 9).

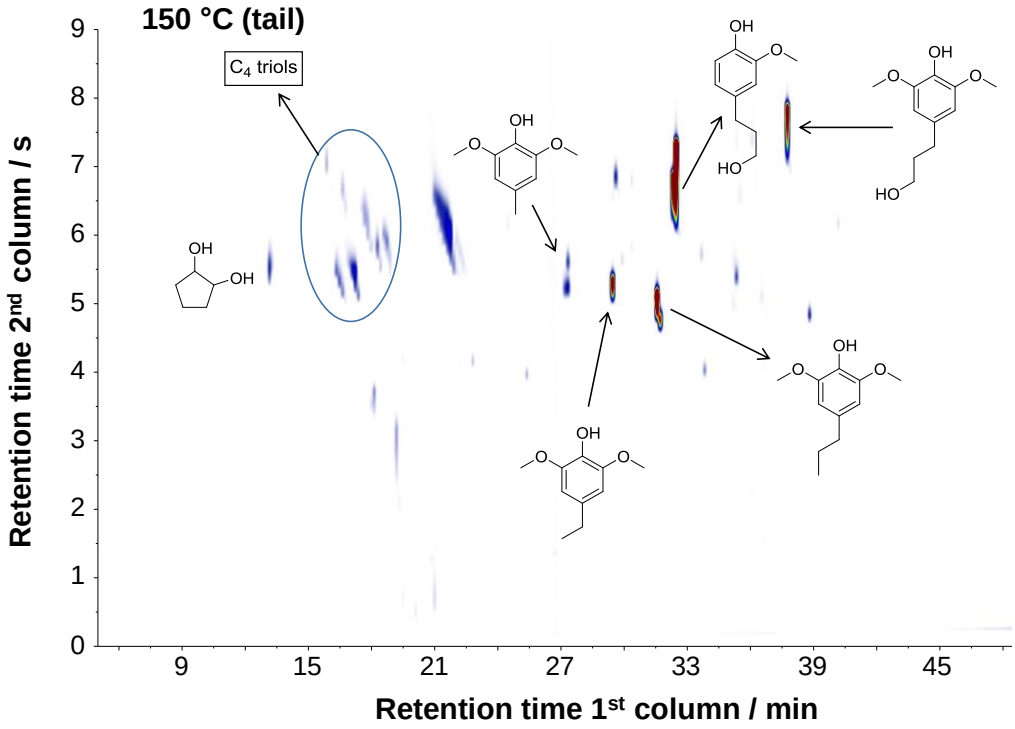

Figure S10. 2D GC × GC image showing the main components of a CUB lignin oil distillation fraction collected at 150 °C (tail). Identification of the peaks was performed using an MS detector and by comparing the spectra with libraries (NIST 08, NIST 08s, and Wiley 9).

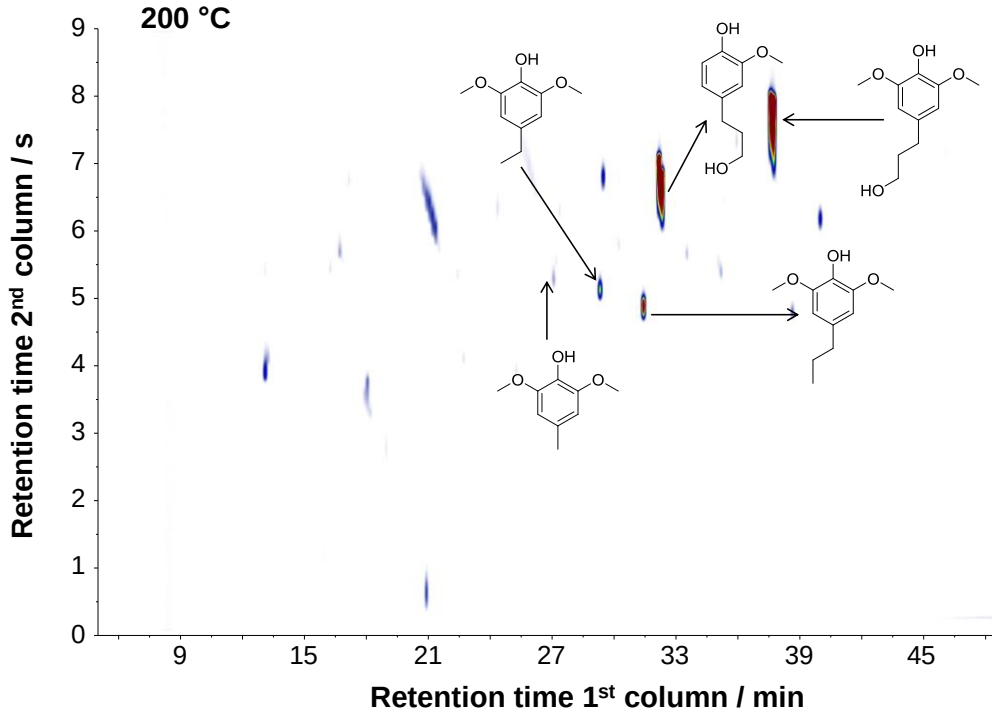

Figure S11. 2D GC × GC image showing the main components of a CUB lignin oil distillation fraction collected at 200 °C. Identification of the peaks was performed using an MS detector and by comparing the spectra with libraries (NIST 08, NIST 08s, and Wiley 9).

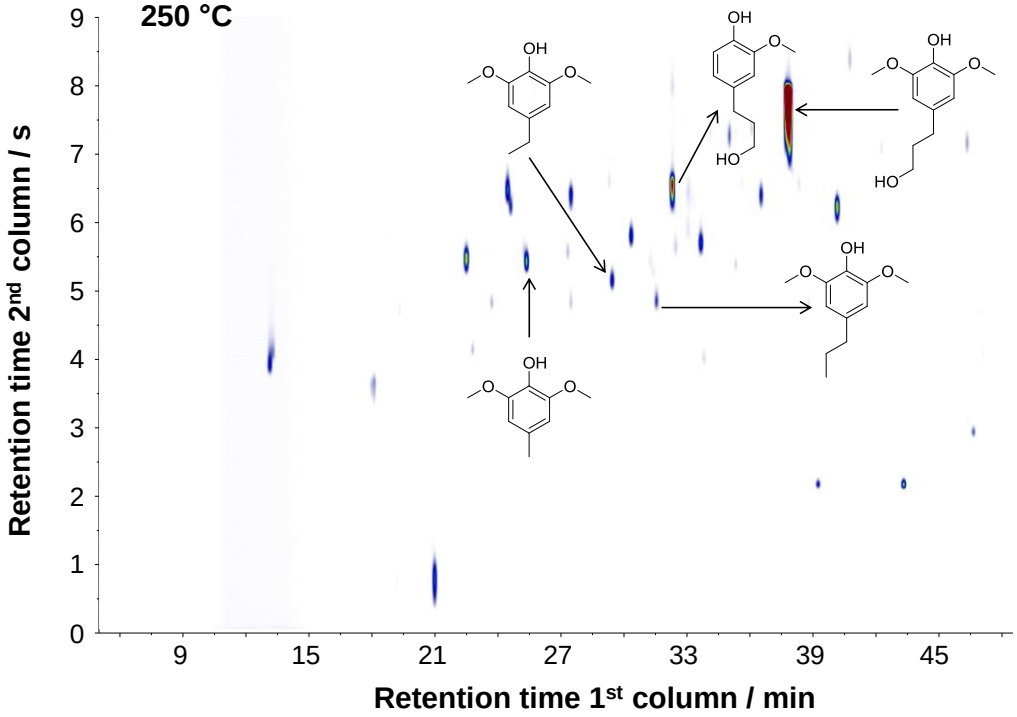

Figure S12. 2D GC × GC image showing the main components of a CUB lignin oil distillation fraction collected at 250 °C. Identification of the peaks was performed using an MS detector and by comparing the spectra with libraries (NIST 08, NIST 08s, and Wiley 9).