

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

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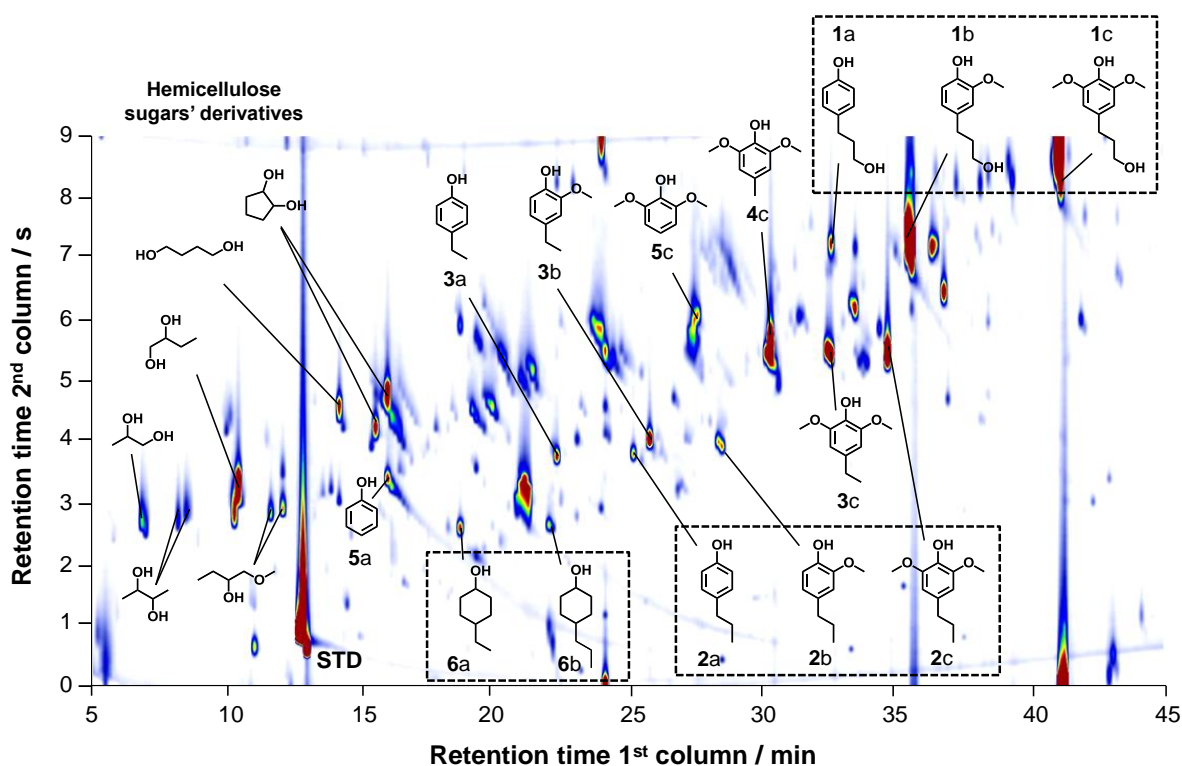


Figure S1. GC × GC trace of the CUB lignin oil obtained in 2-PrOH/H₂O (7:3, v/v) at 160 °C. The EI-mass spectra of species showed a similarity index > 95% either with authentic samples or with MS libraries NIST 08, NIST 08s, and Wiley 9. STD: external standard (di-*n*-butyl ether).

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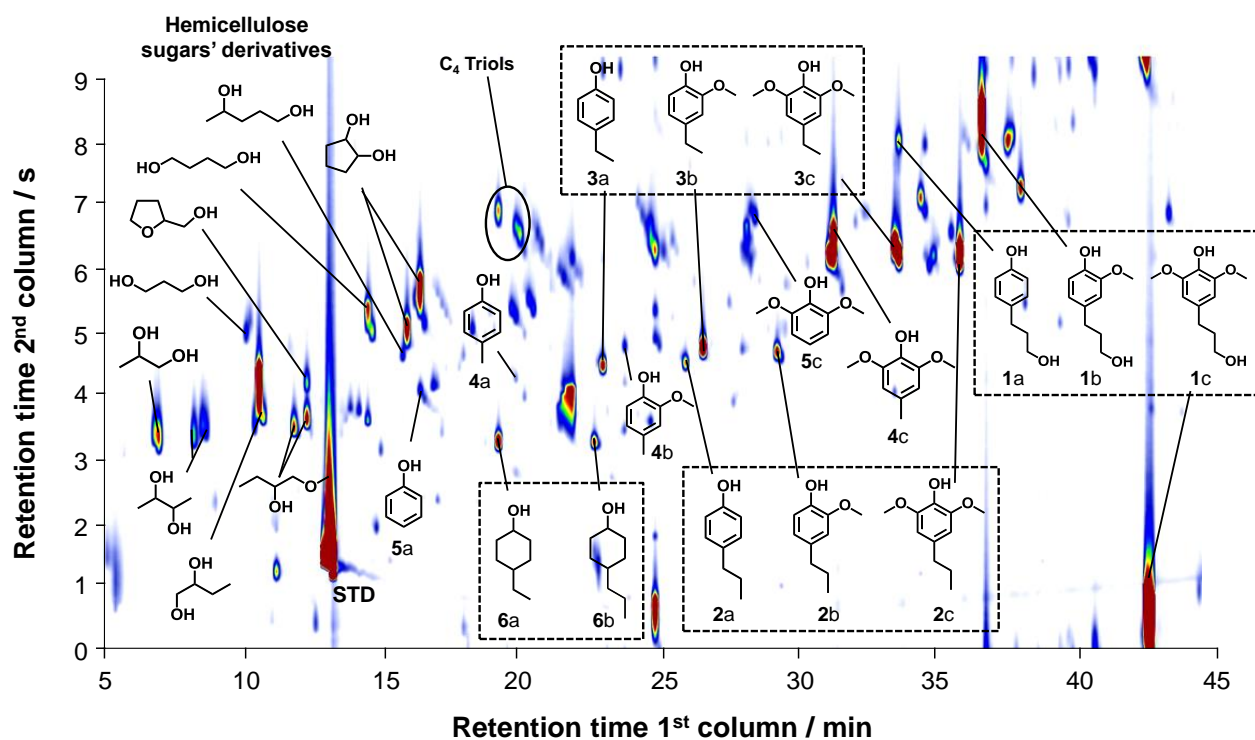


Figure S2. GC \times GC trace of the CUB lignin oil obtained in 2-PrOH/H₂O (7:3, v/v) at 180 °C. The EI-mass spectra of species showed a similarity index > 95% either with authentic samples or with MS libraries NIST 08, NIST 08s, and Wiley 9. STD: external standard (di-*n*-butyl ether).

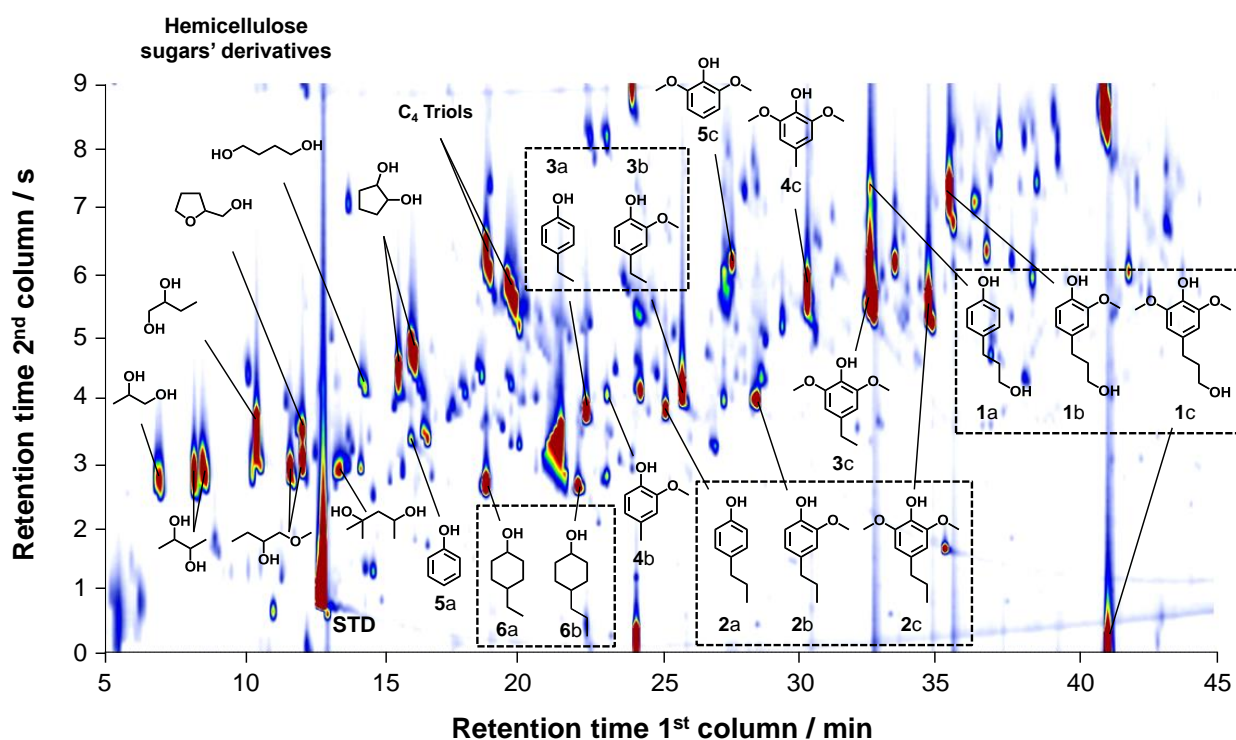


Figure S3. GC \times GC trace of the CUB lignin oil obtained in 2-PrOH/H₂O (7:3, v/v) at 200 °C. The EI-mass spectra of species showed a similarity index > 95% either with authentic samples or with MS libraries NIST 08, NIST 08s, and Wiley 9. STD: external standard (di-*n*-butyl ether).

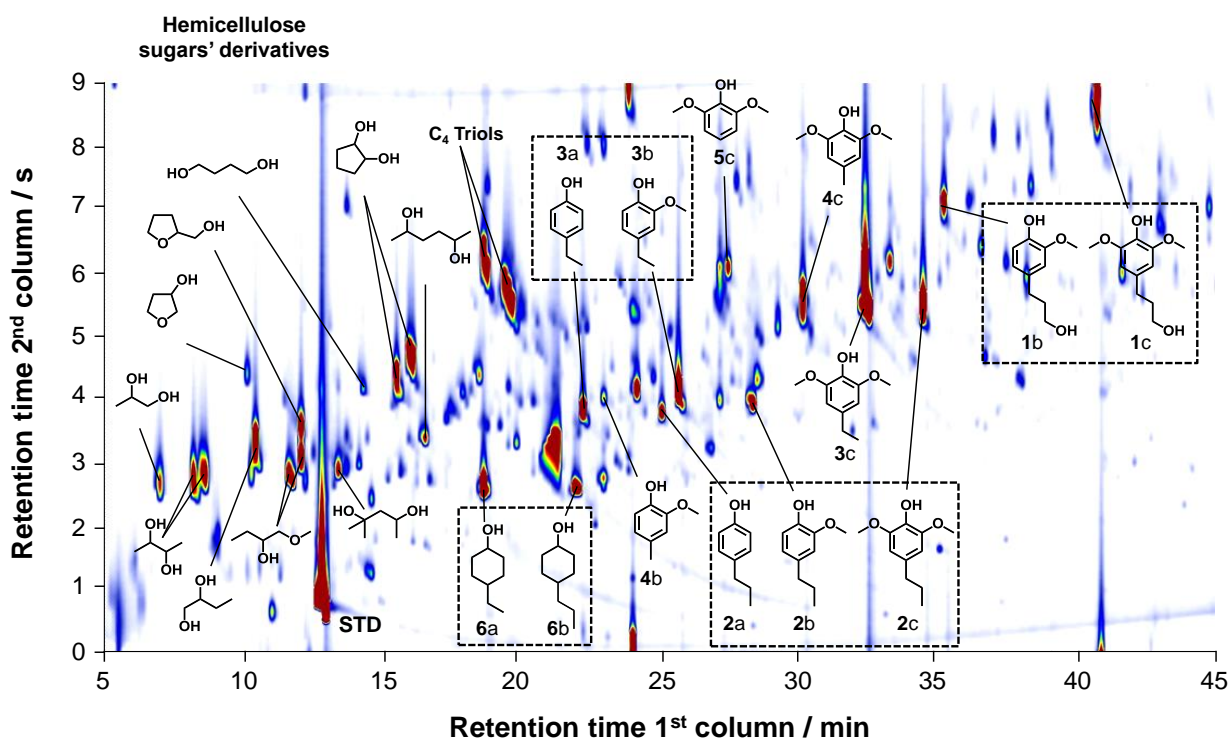


Figure S4. GC × GC trace of the CUB lignin oil obtained in 2-PrOH/H₂O (7:3, v/v) at 220 °C. The EI-mass spectra of species showed a similarity index > 95% either with authentic samples or with MS libraries NIST 08, NIST 08s, and Wiley 9. STD: external standard (di-*n*-butyl ether).

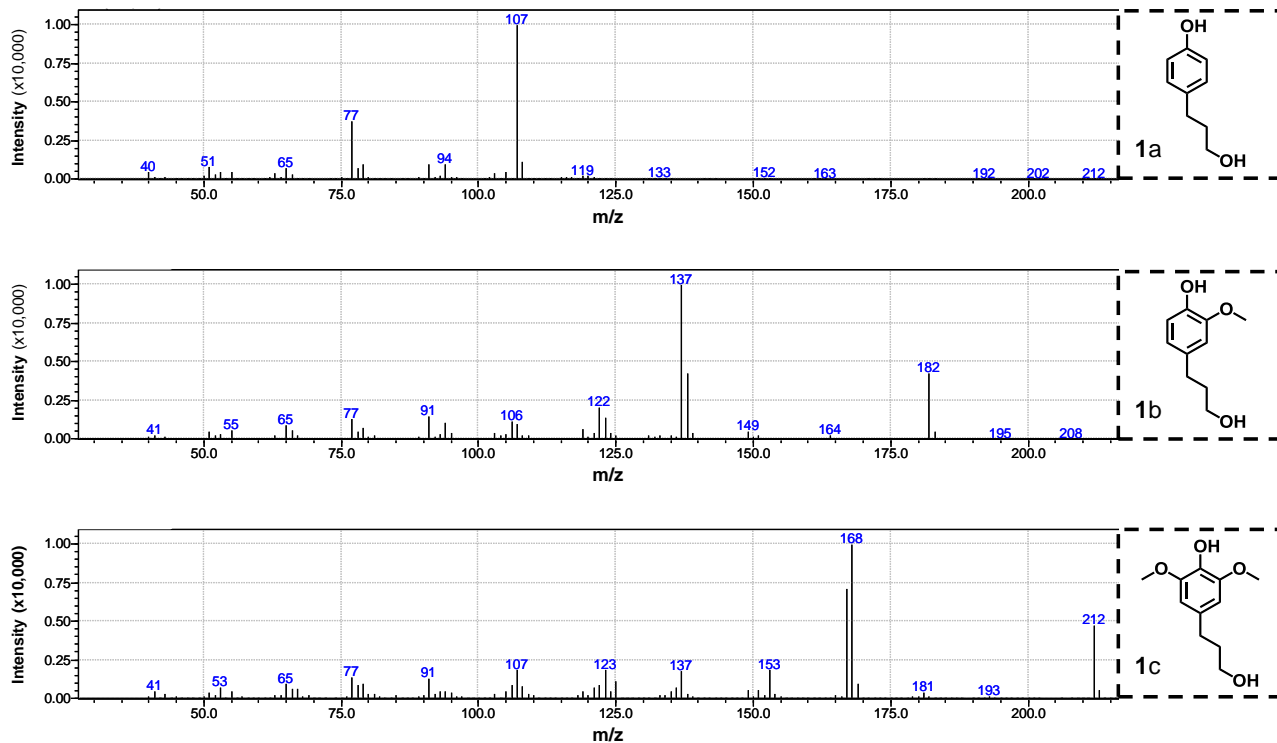


Figure S5. Examples of EI-mass spectra of authentic samples (**1a**, **1b** and **1c**) ran in order to establish similarity indices with compounds identified on GC × GC-MS analysis.

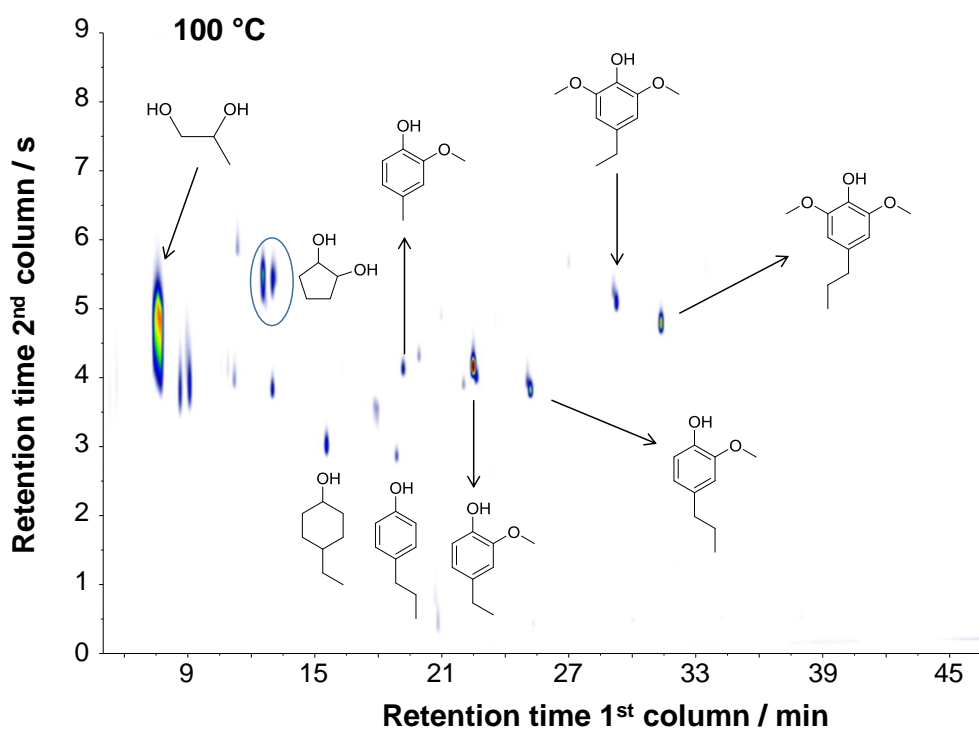


Figure S6. 2D GC \times GC image showing the main components of a CUB lignin oil distillation fraction collected at 100 °C. Identification of the peaks was performed using an MS detector and by comparing the spectra with libraries (NIST 08, NIST 08s, and Wiley 9).

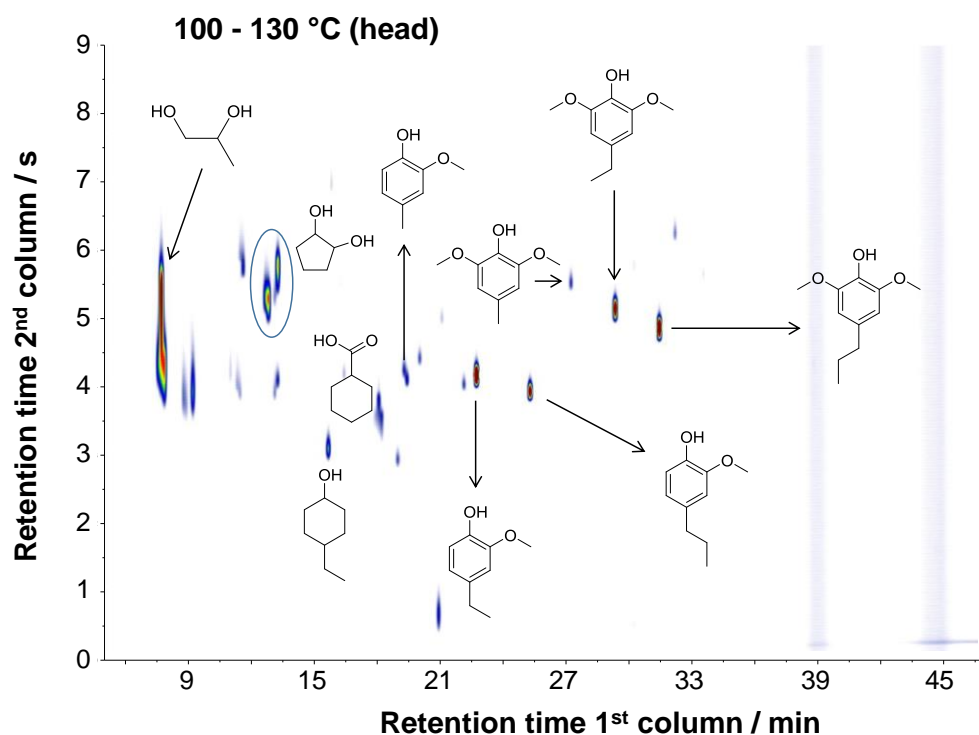


Figure S7. 2D GC \times GC image showing the main components of a CUB lignin oil distillation fraction collected at 100-130 °C (head). Identification of the peaks was performed using an MS detector and by comparing the spectra with libraries (NIST 08, NIST 08s, and Wiley 9).

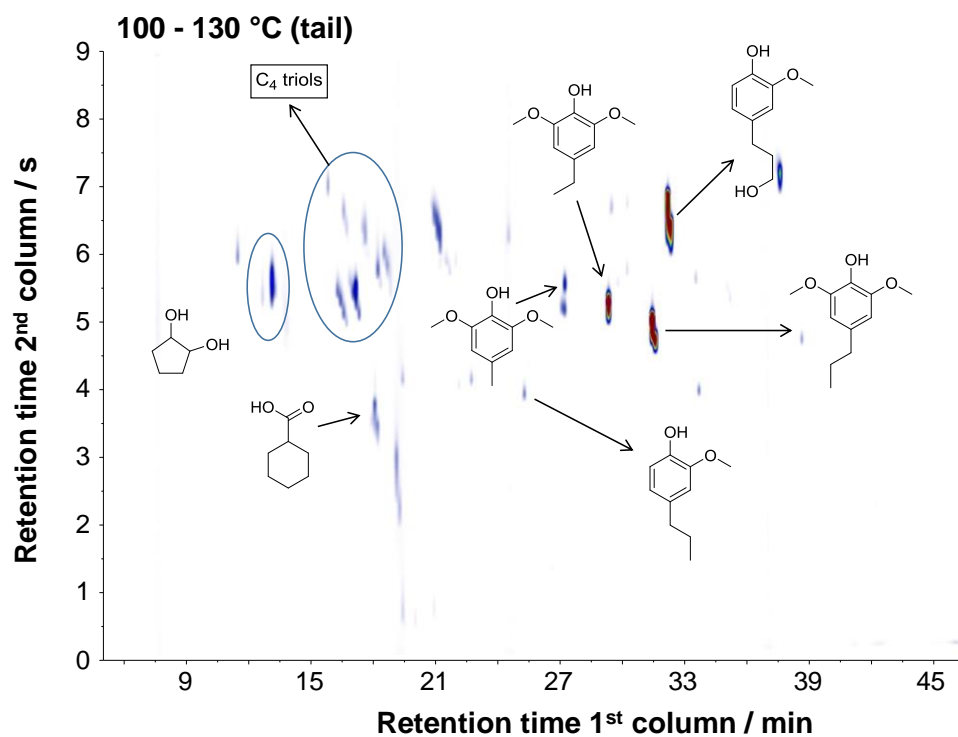


Figure S8. 2D GC \times GC image showing the main components of a CUB lignin oil distillation fraction collected at 100-130 °C (tail). Identification of the peaks was performed using an MS detector and by comparing the spectra with libraries (NIST 08, NIST 08s, and Wiley 9).

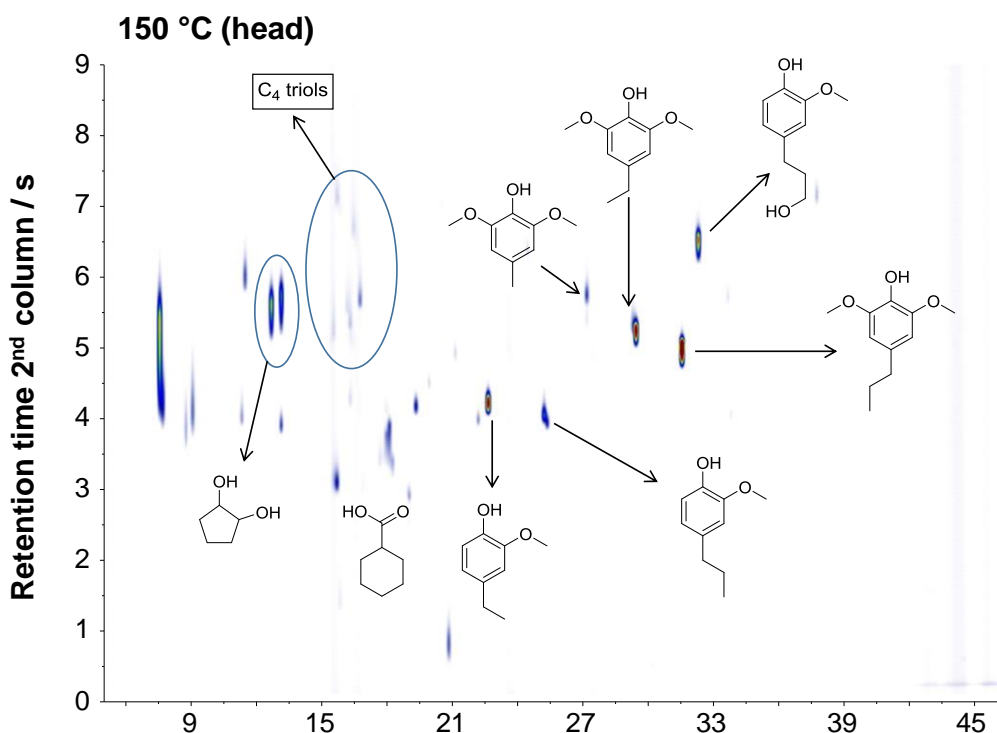


Figure S9. 2D GC \times GC image showing the main components of a CUB lignin oil distillation fraction collected at 150 °C (head). Identification of the peaks was performed using an MS detector and by comparing the spectra with libraries (NIST 08, NIST 08s, and Wiley 9).

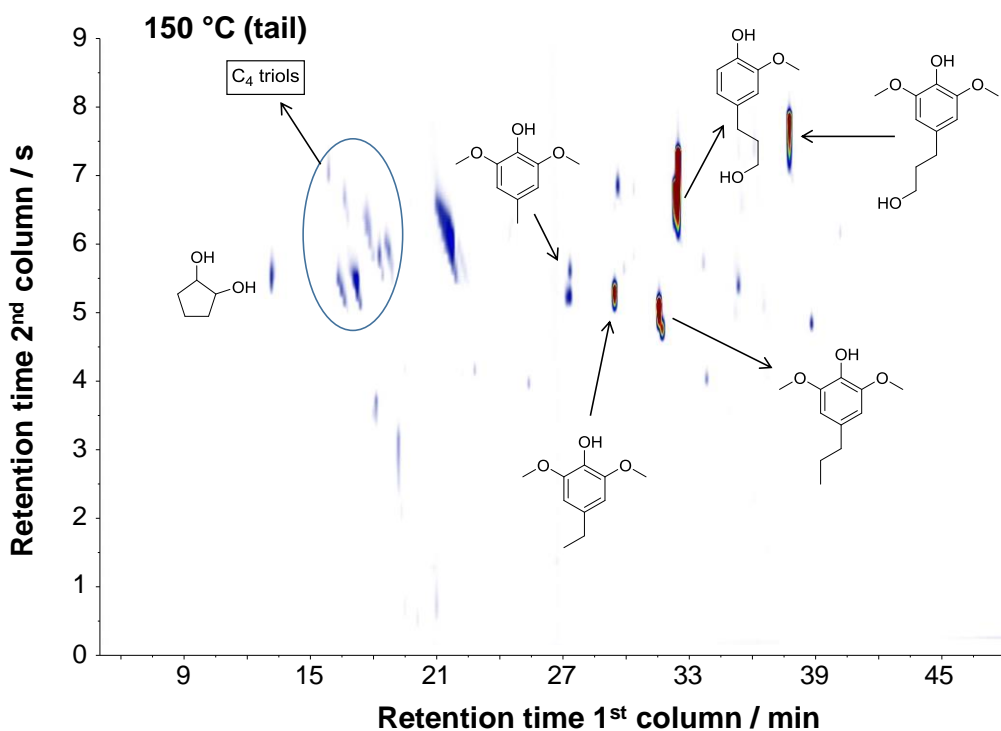


Figure S10. 2D GC \times GC image showing the main components of a CUB lignin oil distillation fraction collected at 150 °C (tail). Identification of the peaks was performed using an MS detector and by comparing the spectra with libraries (NIST 08, NIST 08s, and Wiley 9).

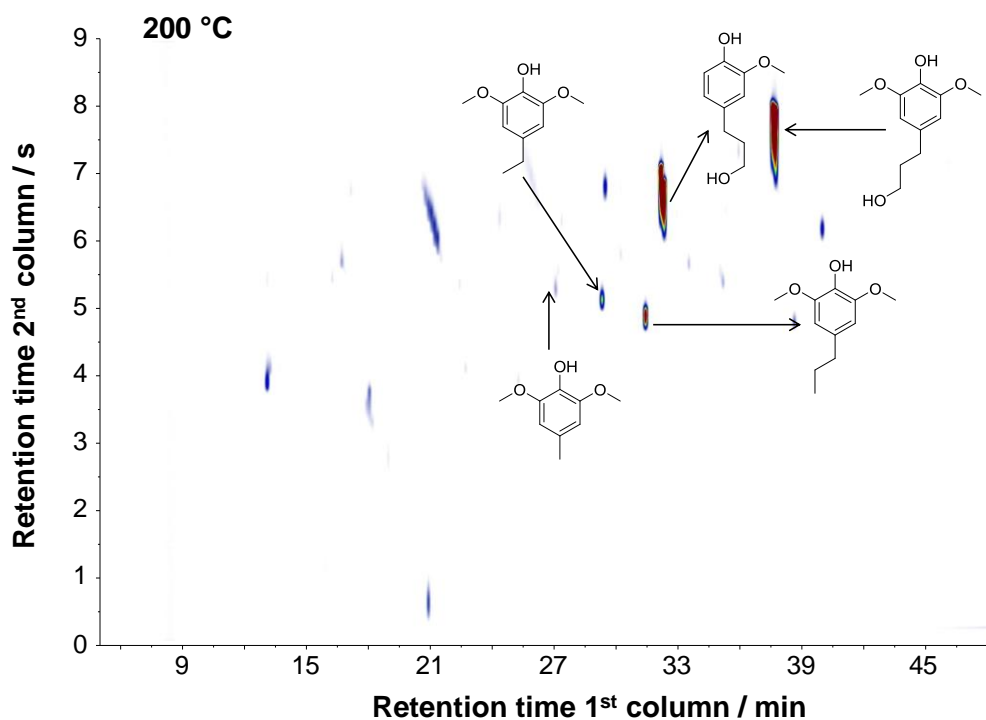


Figure S11. 2D GC \times GC image showing the main components of a CUB lignin oil distillation fraction collected at 200 °C. Identification of the peaks was performed using an MS detector and by comparing the spectra with libraries (NIST 08, NIST 08s, and Wiley 9).

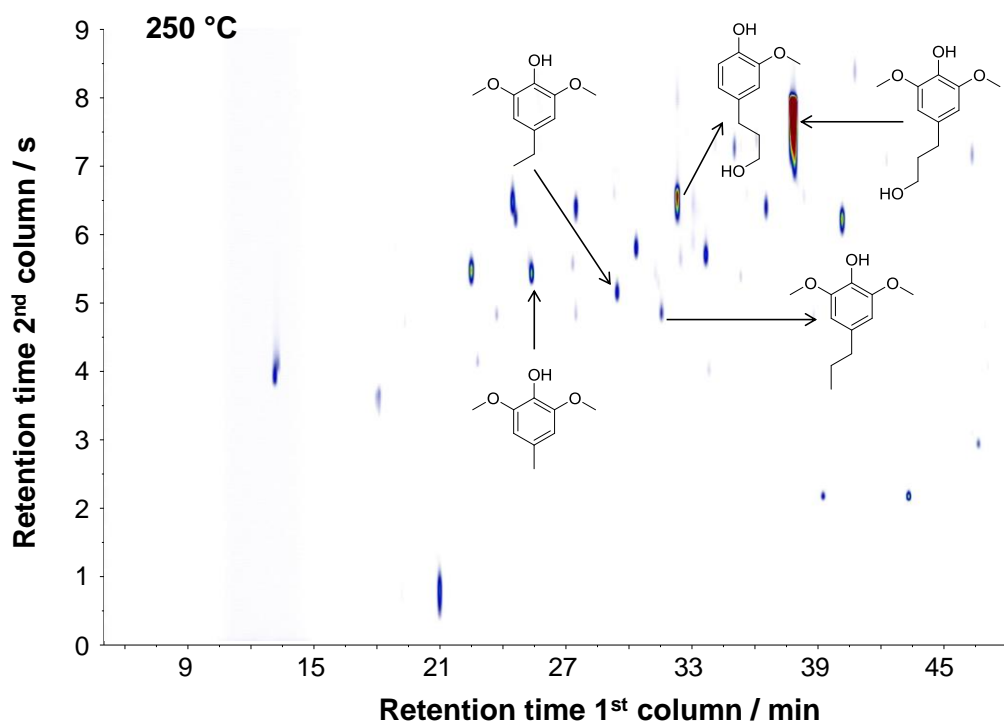


Figure S12. 2D GC × GC image showing the main components of a CUB lignin oil distillation fraction collected at 250 °C. Identification of the peaks was performed using an MS detector and by comparing the spectra with libraries (NIST 08, NIST 08s, and Wiley 9).