Application of Phase Correction to Improve the Characterization of Photooxidation Products of Lignin Using 7 Tesla Fourier-Transform Ion Cyclotron Resonance Mass Spectrometry

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This Supplementary Material contains Figures S1-S6 and Table S1.

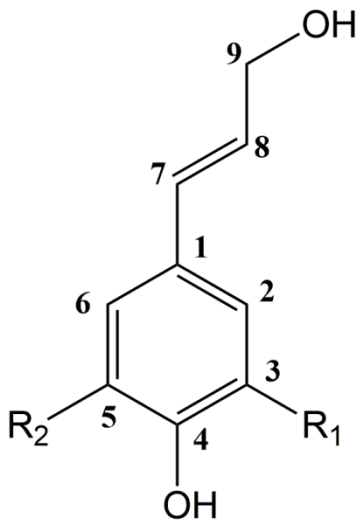

Fig. S1. Structures of the three main lignin monolignols with numbering scheme for the carbon positions: coumaryl alcohol (R1 = R2 = H), coniferyl alcohol (R1 = OCH3, R2 = H), and sinapyl alcohol (R1 = R2 = OCH3).

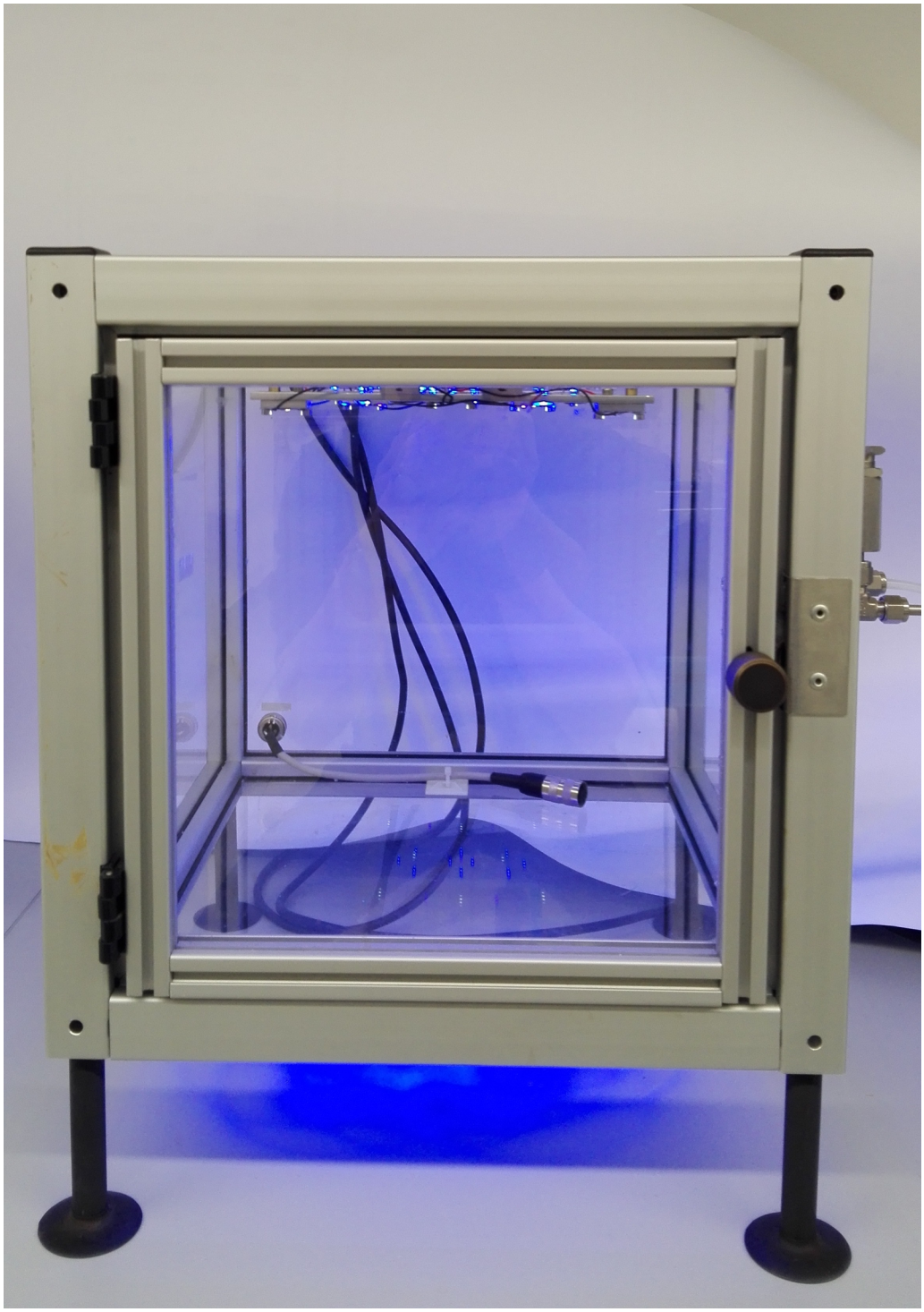

Fig. S2. Custom-built photooxidation chamber for the simulated solar radiation experiments described in this study.

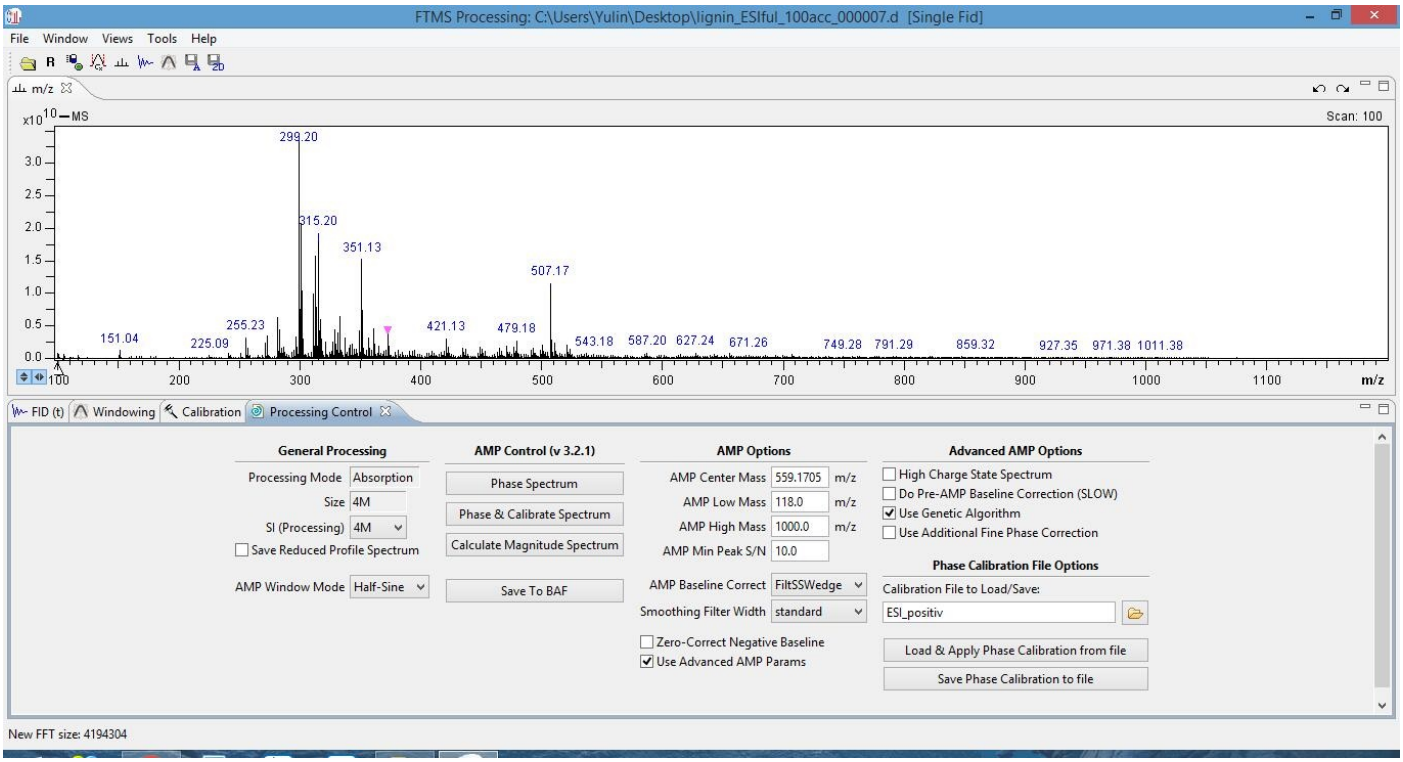

Fig. S3. Screenshot of the Bruker ftms Processing software v2.1.0 interface, to illustrate the essential parameter set required for processing the absorption mode spectra in this paper.

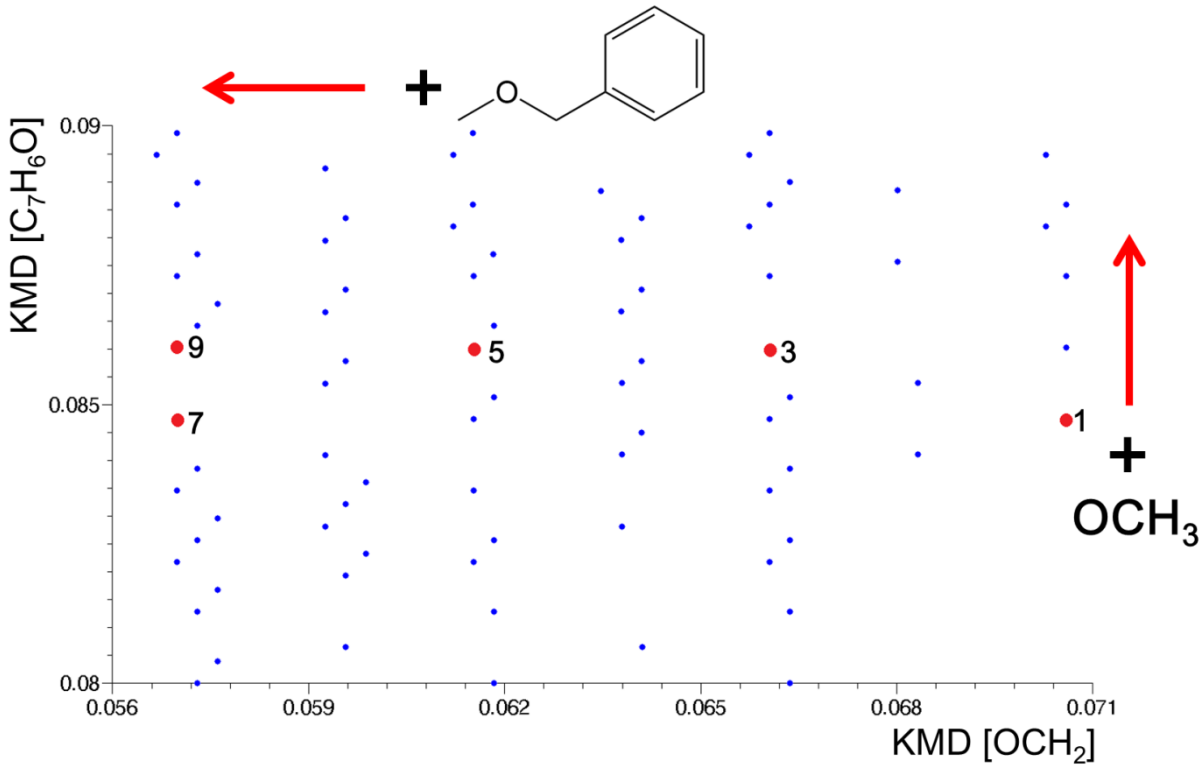

Fig. S4. Two-dimensional mass defect matrix plot, methoxylation (OCH_2) *versus* (C_7H_6O); the lignin compounds selected for Fig. 2 in the main article are highlighted in red.

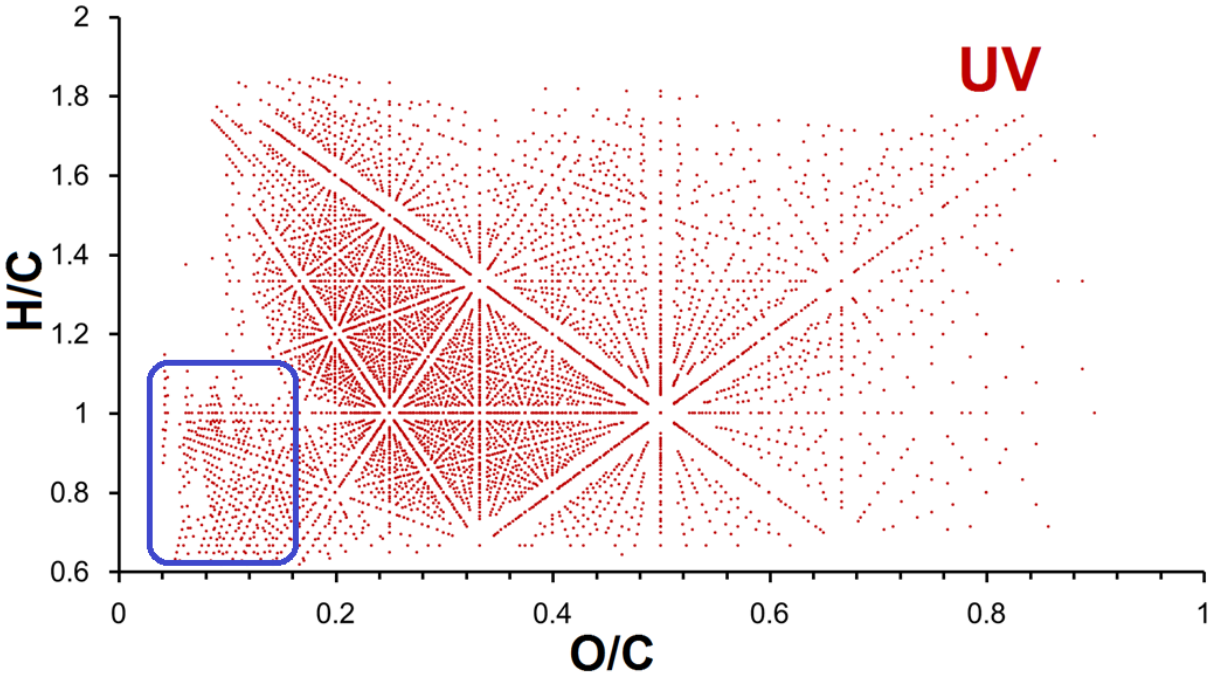

Fig. S5. van Krevelen diagram for species detected in an UV-oxidized lignin samples; the newly-discovered compounds produced by UV fragmentation are in the circled region. Reprinted from (Qi et al. 2016) with permission from Springer.

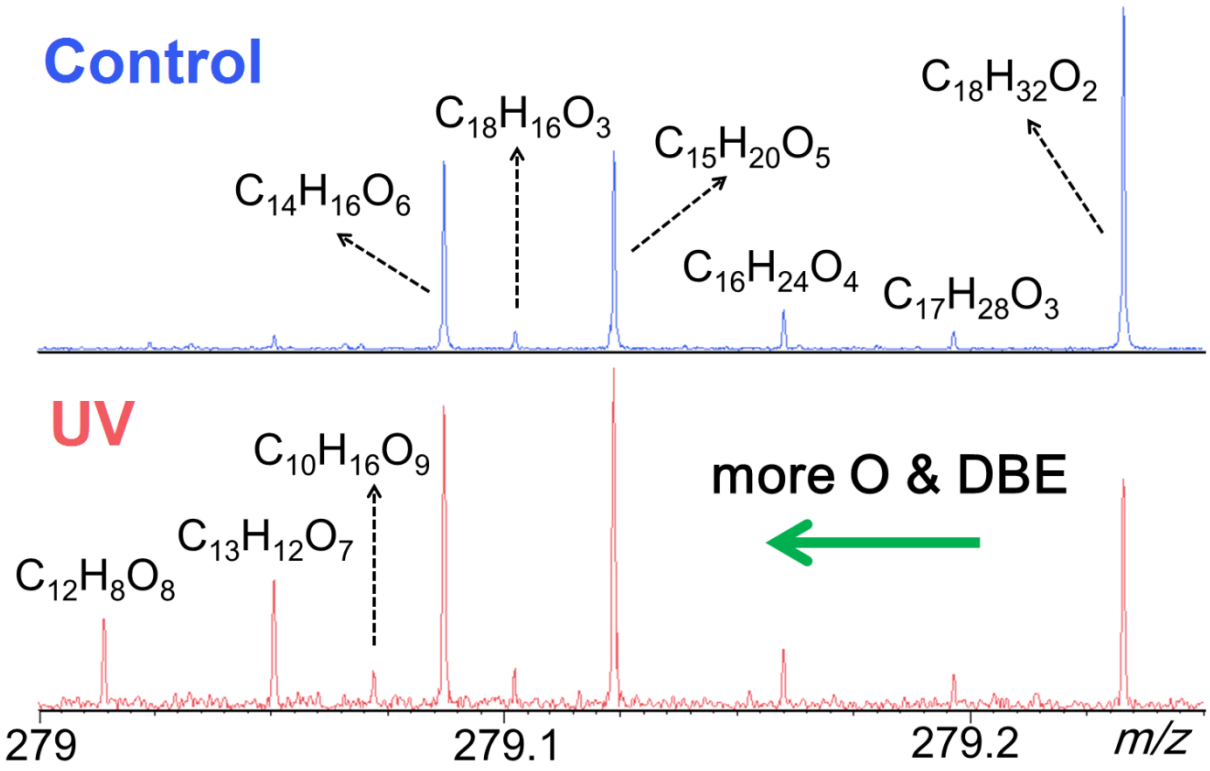

Fig. S6. Mass scale-expanded segments (0.25 u) of the lignin broadband mass spectra. The shift to lower mass defect in the UV-oxidized sample reflects higher oxygen content and DBE value. Reprinted from (Qi et al. 2016) with permission from Springer.

Table S1. Peak assignments for Fig. 6 of the main text.

Compound	Calc. *m/z*	Exp. *m/z*	ppm error
$C_{12}H_8O_8$	279.01464	279.01462	-0.08
$C_{13}H_{12}O_7$	279.05103	279.05100	-0.09
$C_{10}H_{16}O_9$	279.07216	279.07215	-0.04
$C_{14}H_{16}O_6$	279.08741	279.08744	0.10
$C_{18}H_{16}O_3$	279.10267	279.10271	0.15
$C_{15}H_{20}O_5$	279.12380	279.12383	0.12
$C_{16}H_{24}O_4$	279.16018	279.16021	0.10
$C_{17}H_{28}O_3$	279.19657	279.19654	-0.10
$C_{18}H_{32}O_2$	279.23295	279.23297	0.06

References

Qi, Y., Hempelmann, R. & Volmer, D.A., 2016. Shedding light on the structures of lignin compounds: photo-oxidation under artificial UV light and characterization by high resolution mass spectrometry. *Analytical and Bioanalytical Chemistry*, pp.1–8. Available at: http://dx.doi.org/10.1007/s00216-016-9928-7.