

Appendix

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Appendix Data

^1H and ^{13}C spectra from fraction 1.5.3.47 (Appendix Figures S1-S2) were used for structure elucidation. Analysis of spectra and comparison with NMR data of commercial standards (Appendix Figures S3-S5) led to the identification of vaccenic acid.

Appendix Figure S1: ^1H NMR spectrum (600 MHz, CDCl_3)

Appendix Figure S2: ^{13}C NMR spectrum (151 MHz, CDCl_3)

Appendix Figure S3: HSQC NMR spectrum

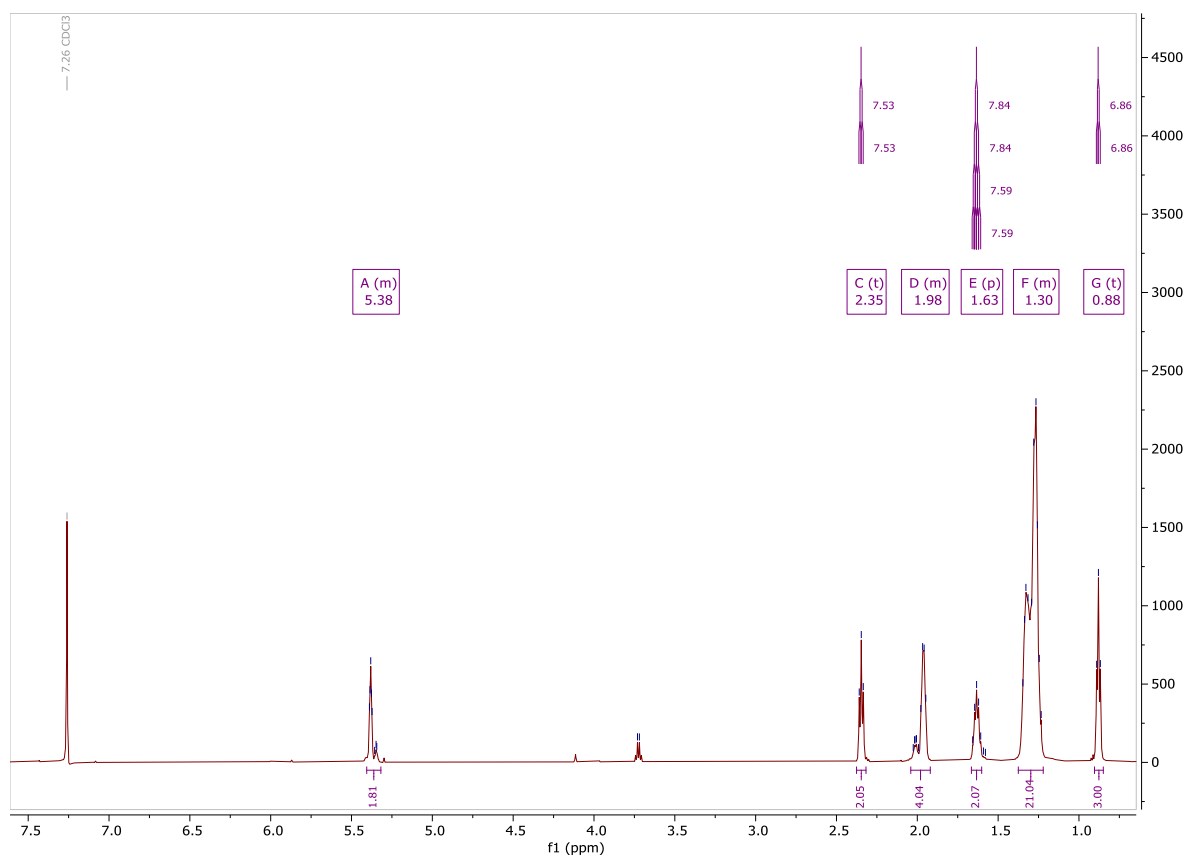
Appendix Figure S4: COSY NMR spectrum

Appendix Figure S5: HMBC NMR spectrum

Appendix Figure S6: EI-MS spectrum

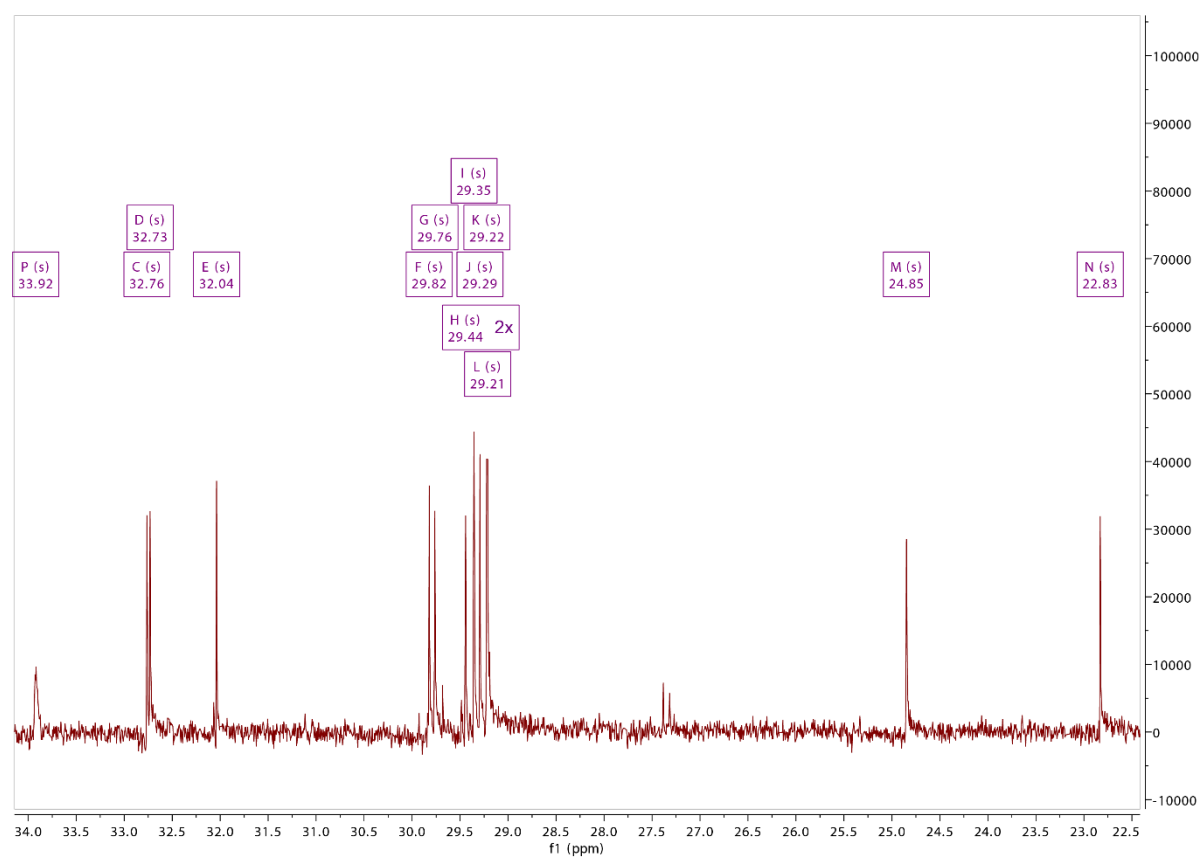
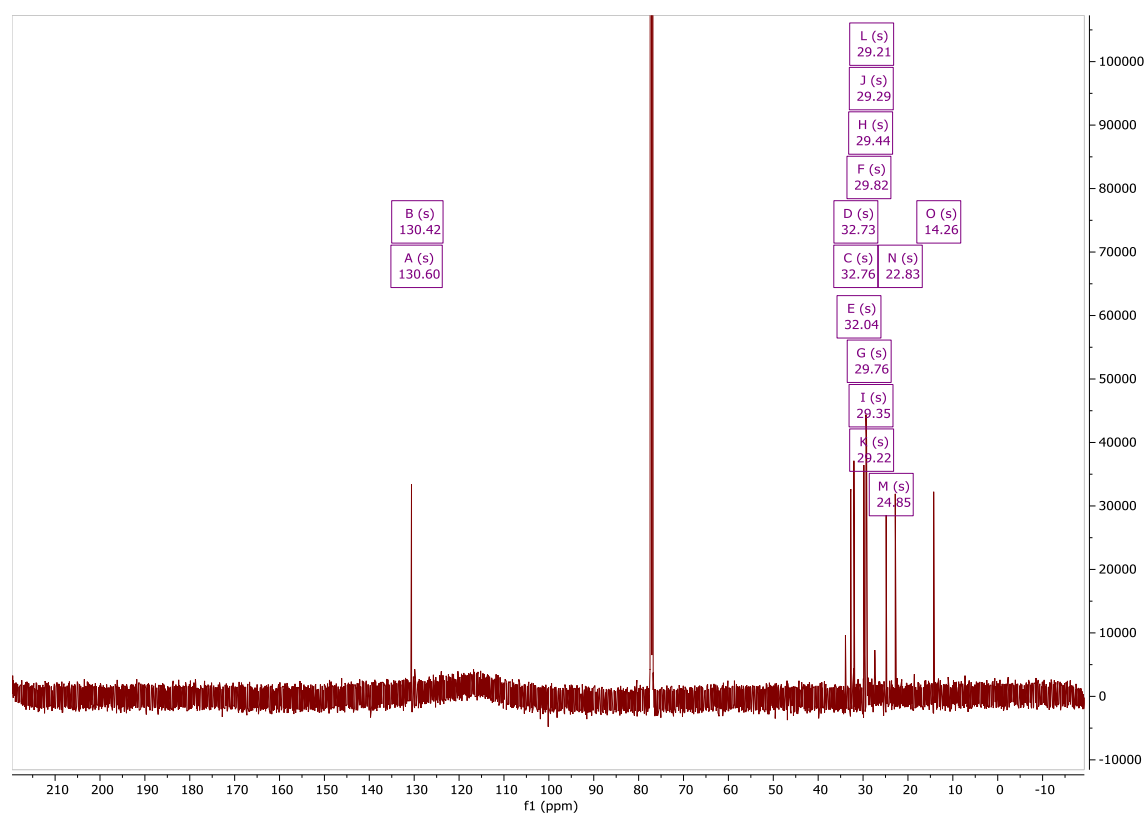
Appendix Figure S7: GC-MS spectrum

Appendix Figure S1: ^1H NMR spectrum (600 MHz, CDCl_3)



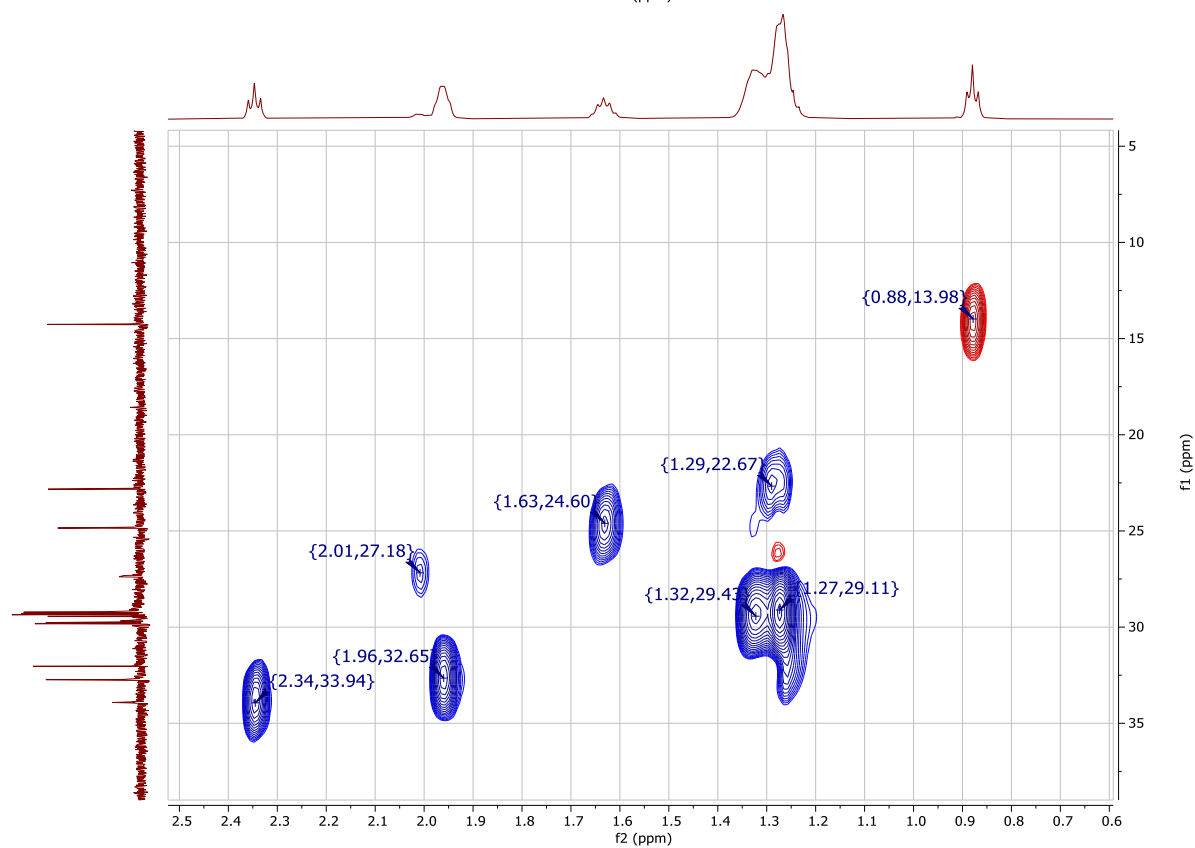
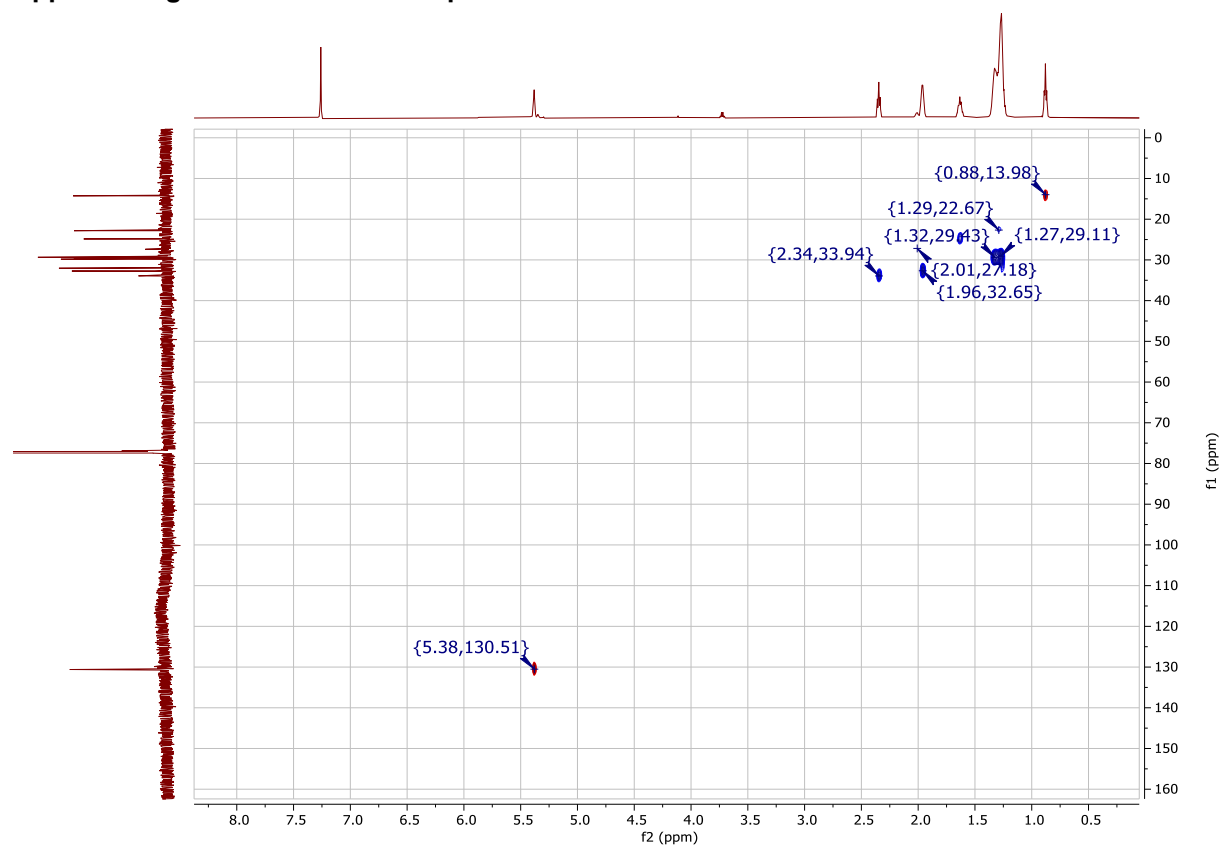
^1H NMR (600 MHz, CDCl_3) δ 5.43 – 5.33 (m, 2H), 2.35 (t, J = 7.5 Hz, 2H), 2.09 – 1.91 (m, 4H), 1.63 (p, J = 7.6 Hz, 2H), 1.34 (d, J = 6.4 Hz, 2H), 1.33 – 1.22 (m, 18H), 0.88 (t, J = 6.9 Hz, 3H).

Appendix Figure S2: ^{13}C NMR spectrum (151 MHz, CDCl_3)

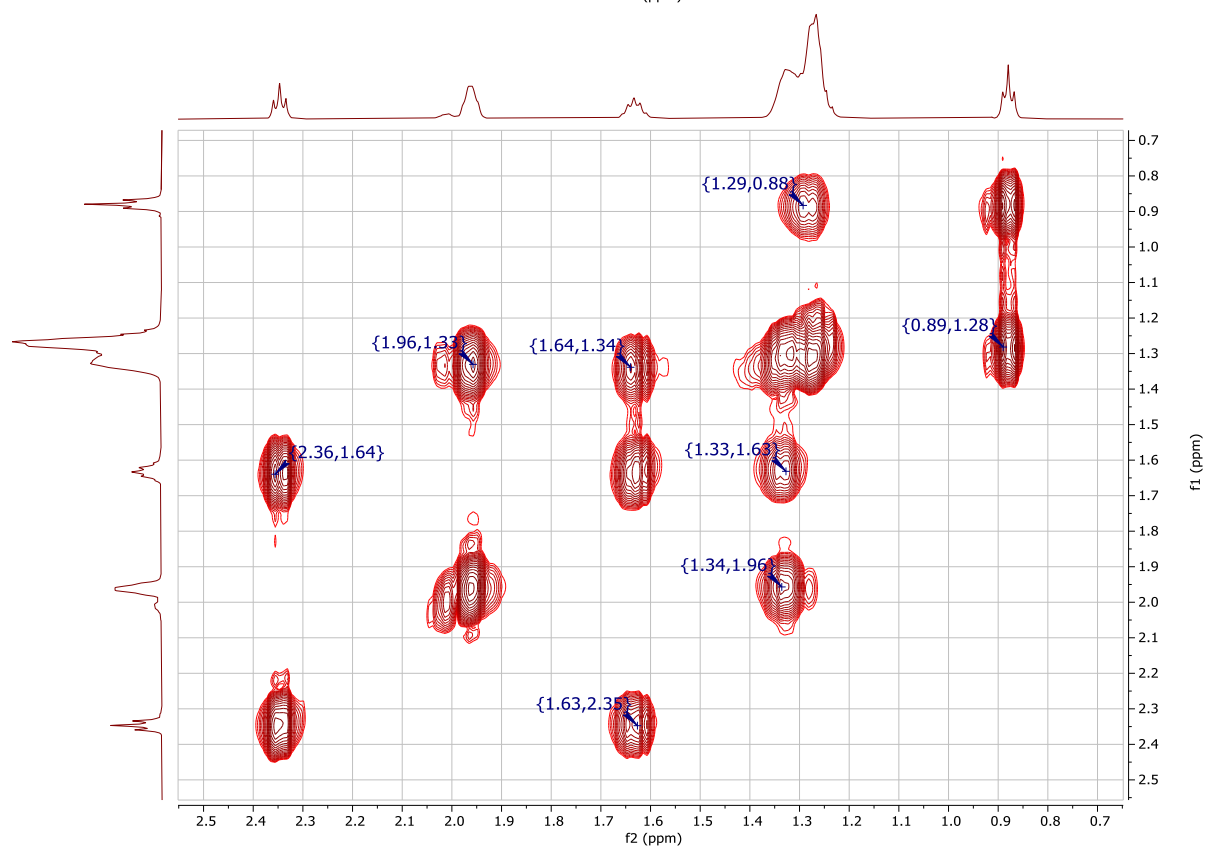
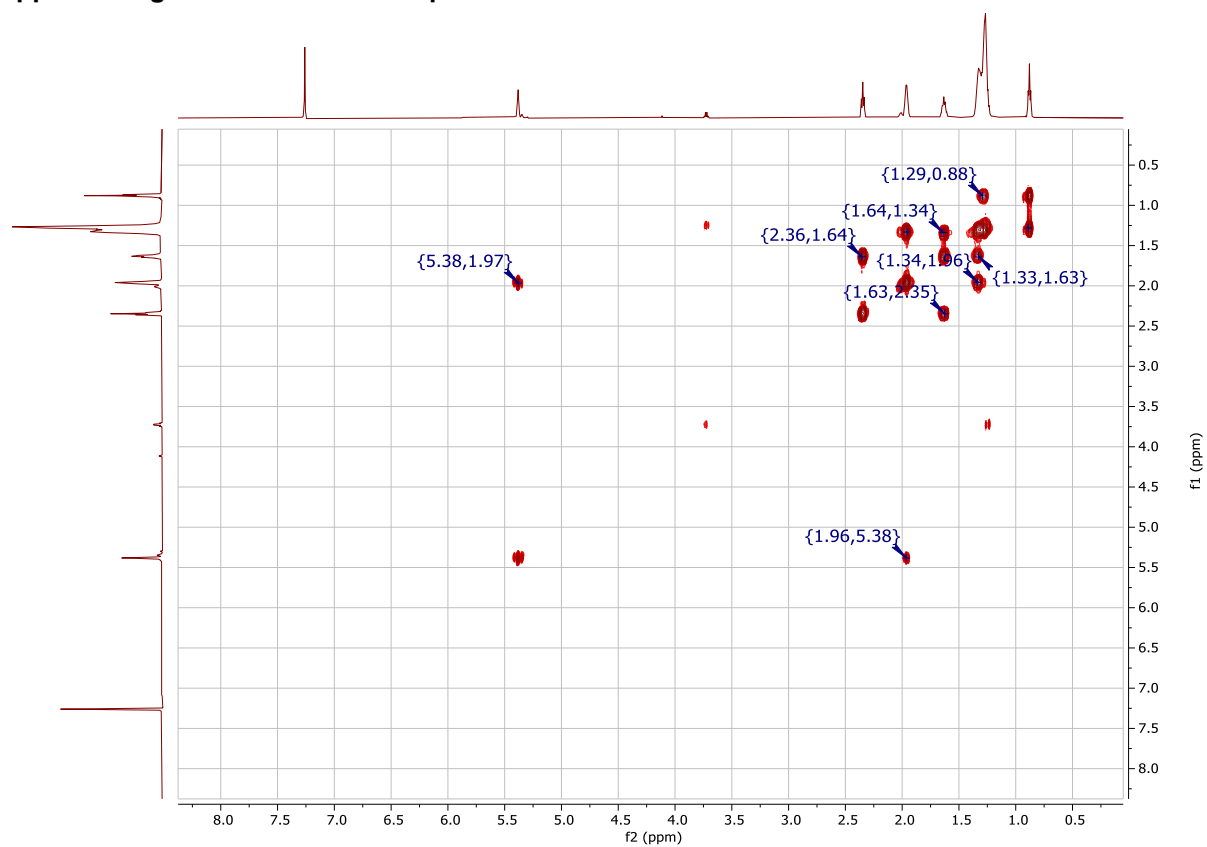


^{13}C NMR (151 MHz, CDCl_3) δ 178.7 (derived from HMBC), 130.6, 130.4, 33.9, 32.8, 32.7, 32.0, 29.8, 29.8, 29.4, 29.4 (2x), 29.3, 29.2, 29.2, 24.8, 22.8, 14.3.

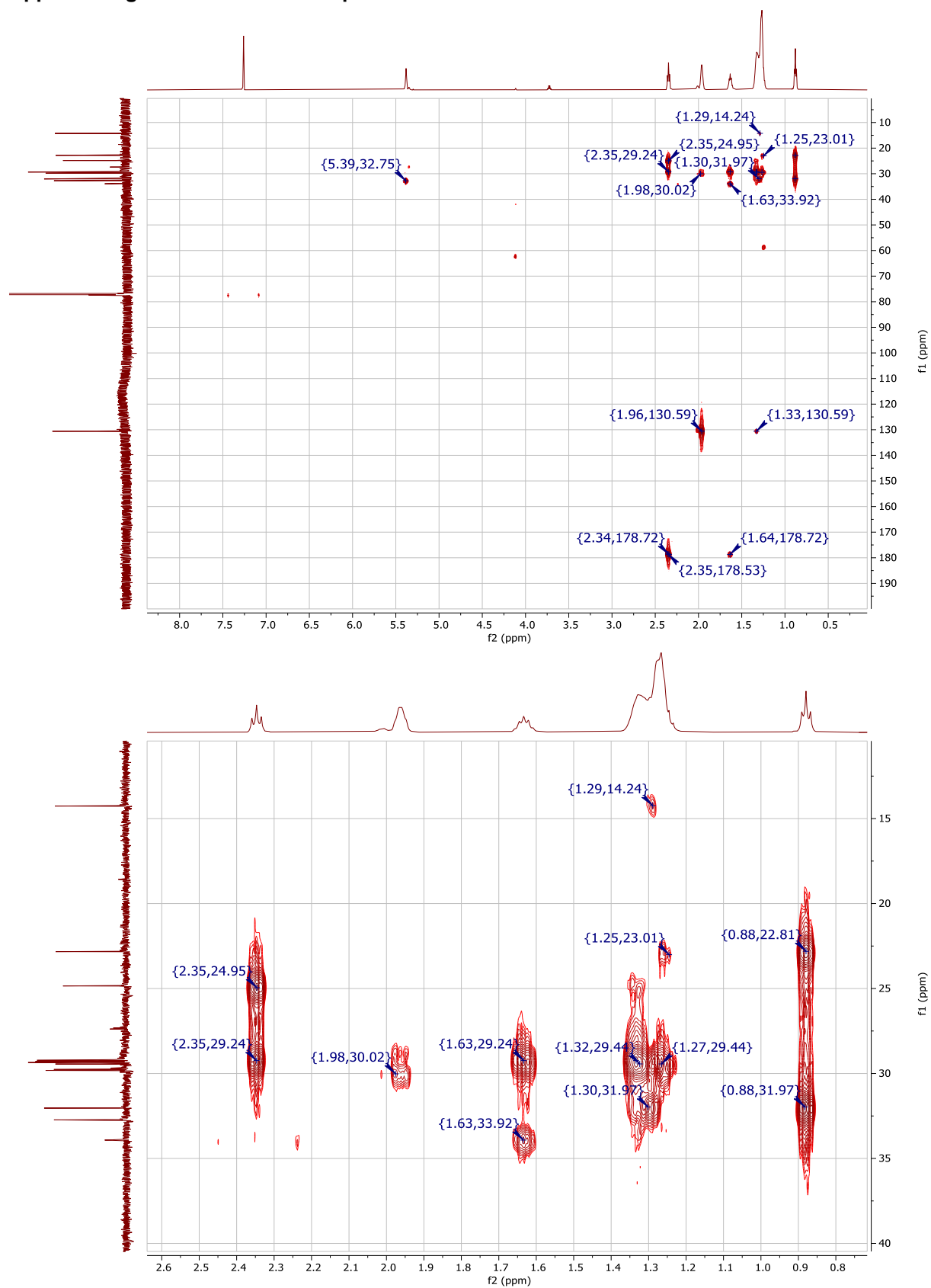
Appendix Figure S3: HSQC NMR spectrum



Appendix Figure S4: COSY NMR spectrum



Appendix Figure S5: HMBC NMR spectrum



Appendix Figure S6: EI-MS spectrum (top panel) and Appendix Figure S7 (bottom panel): GC-MS spectrum

