Electronic Supplementary Material

Developmental mapping of *Clusia minor* L. organs (leaf, flower, fruit and seed) via comparative MS, 1D-, and 2D-NMR metabolomics

Clarice Noleto-Dias[a,b,§], Mohamed A. Farag[c*], Andrea Porzel[b], Josean F. Tavares[a], Ludger A. Wessjohann[b*]

[a] Natural and Synthetic Bioactive Products Graduate Program, Federal University of Paraíba, João Pessoa, PB, 58051-900, Brazil

[b] Department of Bioorganic Chemistry, Leibniz Institute of Plant Biochemistry (IPB), D-06120 Halle (Saale), Germany.

[c] Pharmacognosy Department, College of Pharmacy, Cairo University, Cairo, 11562, Egypt

[§] Present address: Plant Sciences and the Bioeconomy, Rothamsted Research, West Common, Harpenden, Hertfordshire AL5 2JQ, UK.

[*] Corresponding authors email: wessjohann@ipb-halle.de; mohamed.farag@pharma.cu.edu.eg

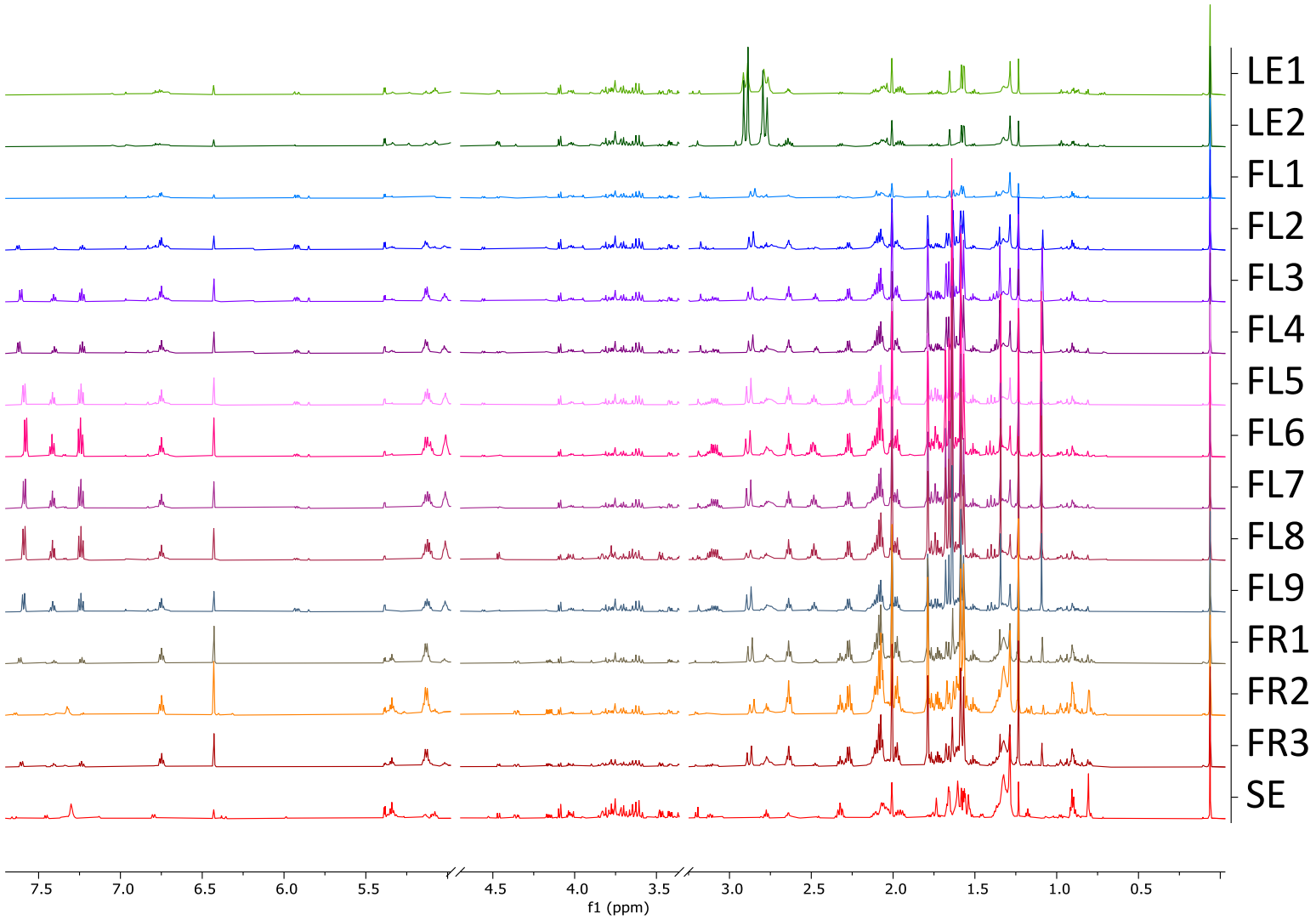

Fig. S1. ^{1}H NMR spectra of different organs and developmental stages of *Clusia minor* L. showing the most relevant peaks in the shift range of δ 0.5 to 8.0 ppm. L1 (expanding leaves), L2 (mature leaves), FL1 (juvenile bud stage), FL2 (second green bud stage), FL3 (third green bud stage), FL4 (fourth green bud stage), FL5 (first pink bud stage), FL6 (fully mature bud), FL7 (preanthesis flower stage), FL8 (fully open flower), FL9 (senescent flower), FR1 (immature fruit), FR2 (mature fruit), FR3 (fully expanded fruit), SE (seeds of expanded fruit).

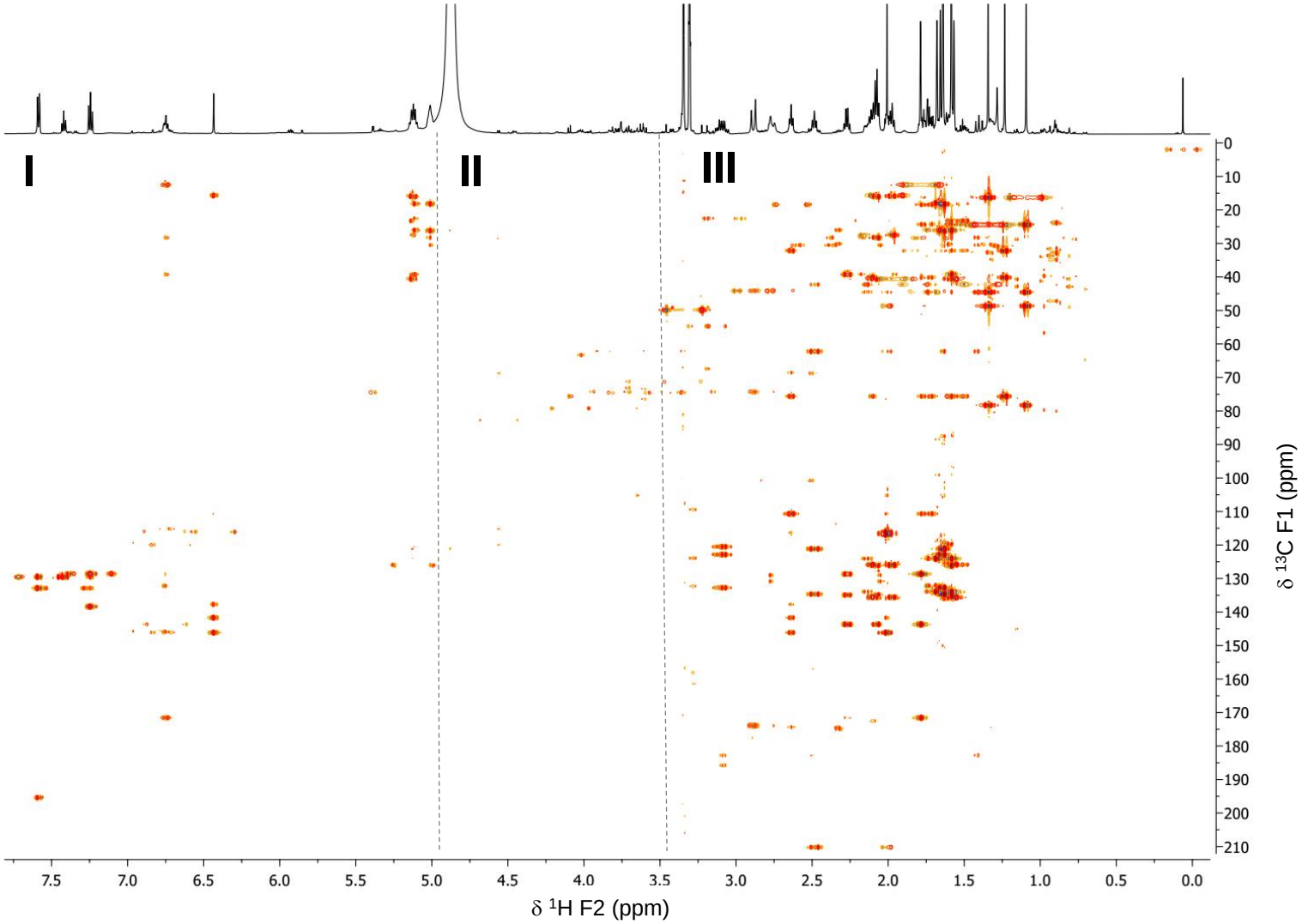

Fig. S2. ^{1}H-^{13}C HMBC NMR spectrum of the methanol extract of *Clusia minor* L. fully mature bud flower **FL6** (CD_3OD, 600 MHz). The spectrum can be visually divided into three main regions along the proton dimension, categorised as: I ($\delta^{1}H$ 5.0 - 8.0 ppm); II ($\delta^{1}H$ 3.5 - 5.0 ppm); and III ($\delta^{1}H$ 0.5 - 3.5 ppm). See text for details.

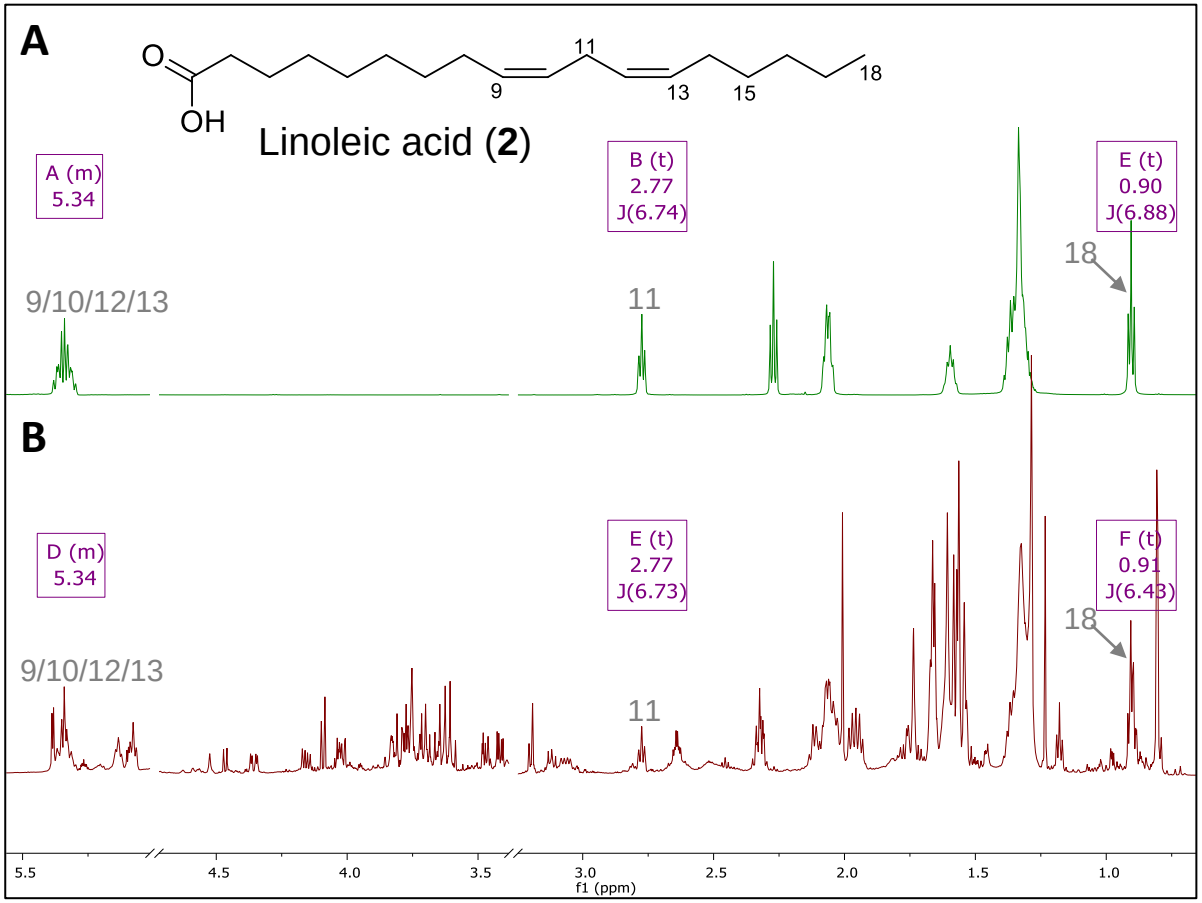

Fig. S3. ^{1}H NMR spectra of the authentic standard of linoleic acid (**A**) and of *Clusia minor* L. seed extract **SE** (**B**) (CD_3OD, 600 MHz).

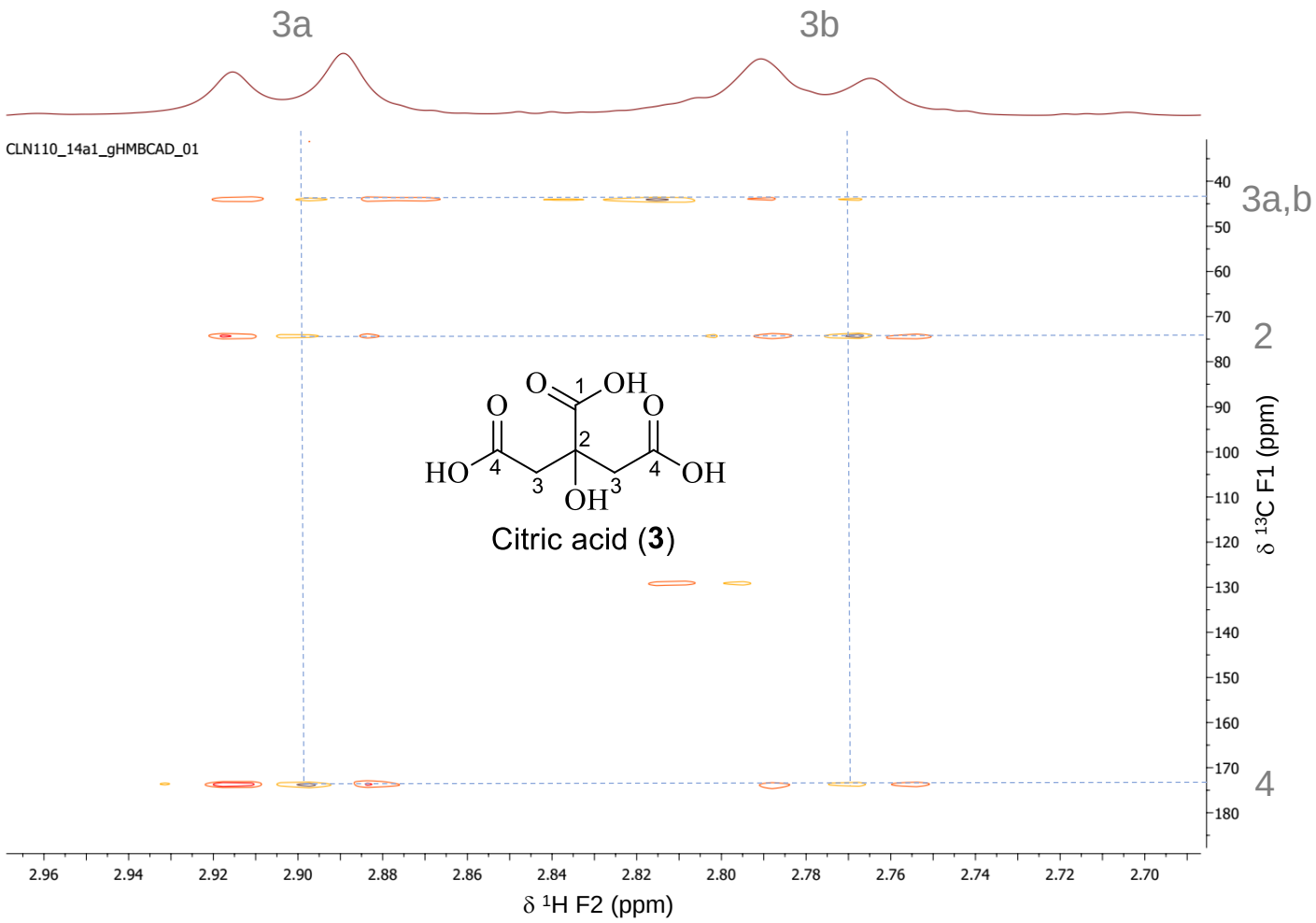

Fig. S4. Extension of the ^{1}H-^{13}C HMBC NMR spectrum of the methanol extract of *Clusia minor* L. leaves **L1** (CD_3OD, 600 MHz), showing the cross peaks of citric acid (**N3**).

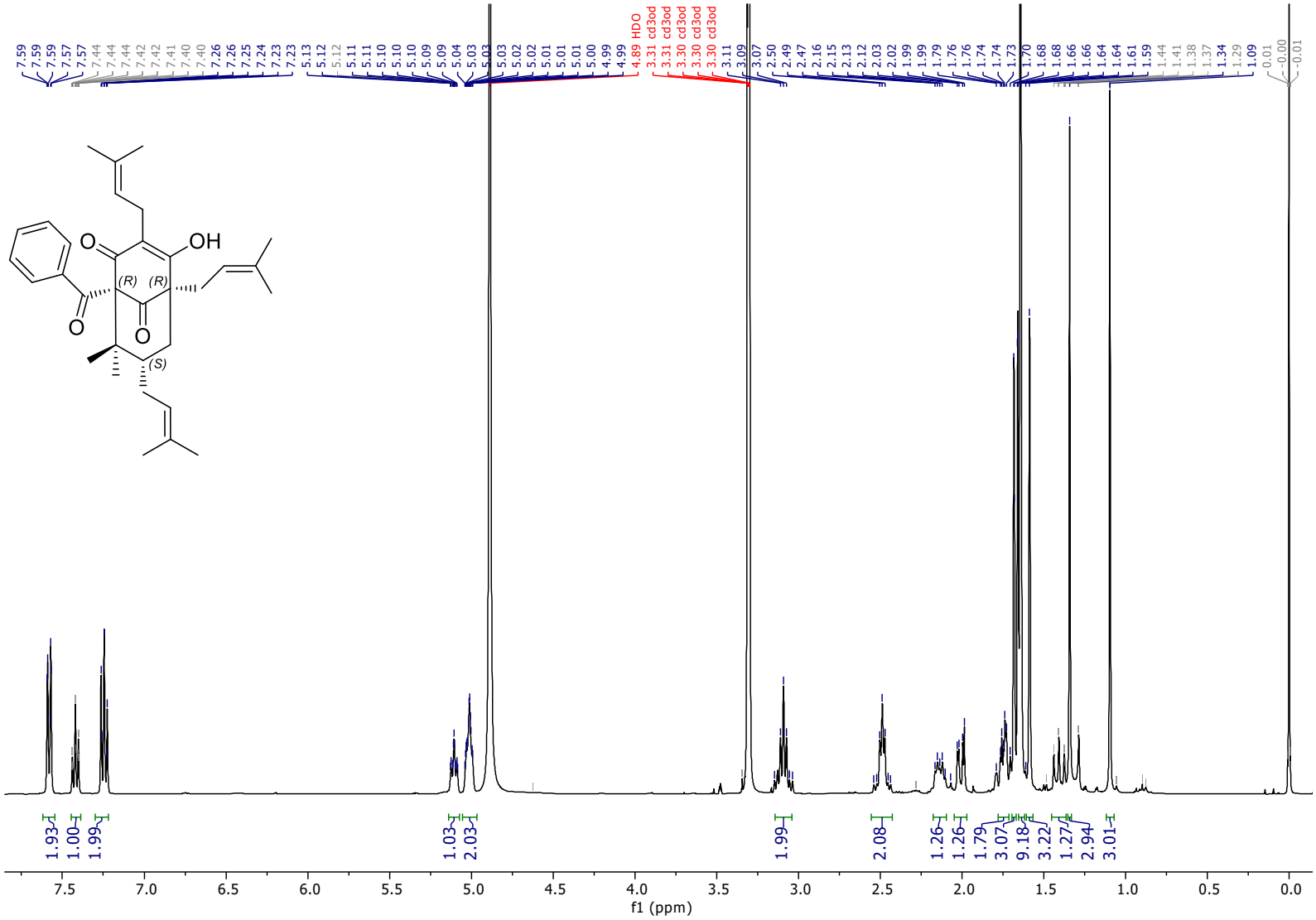

Fig. S5. ^{1}H NMR spectrum of nemorosone (CD_3OD, 600 MHz).

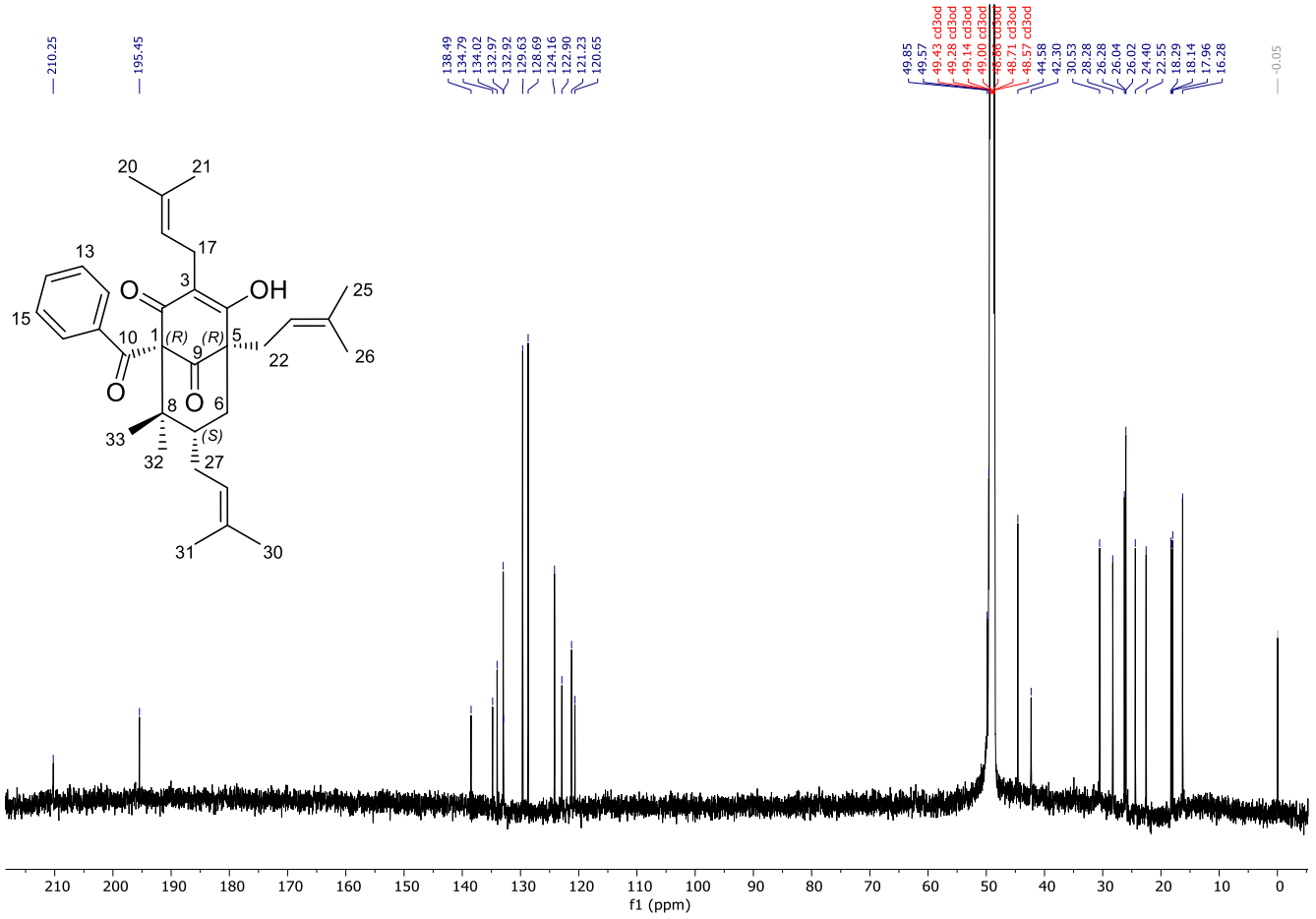

Fig. S6. ^{13}C NMR spectrum of nemorosone (CD_3OD, 600 MHz).

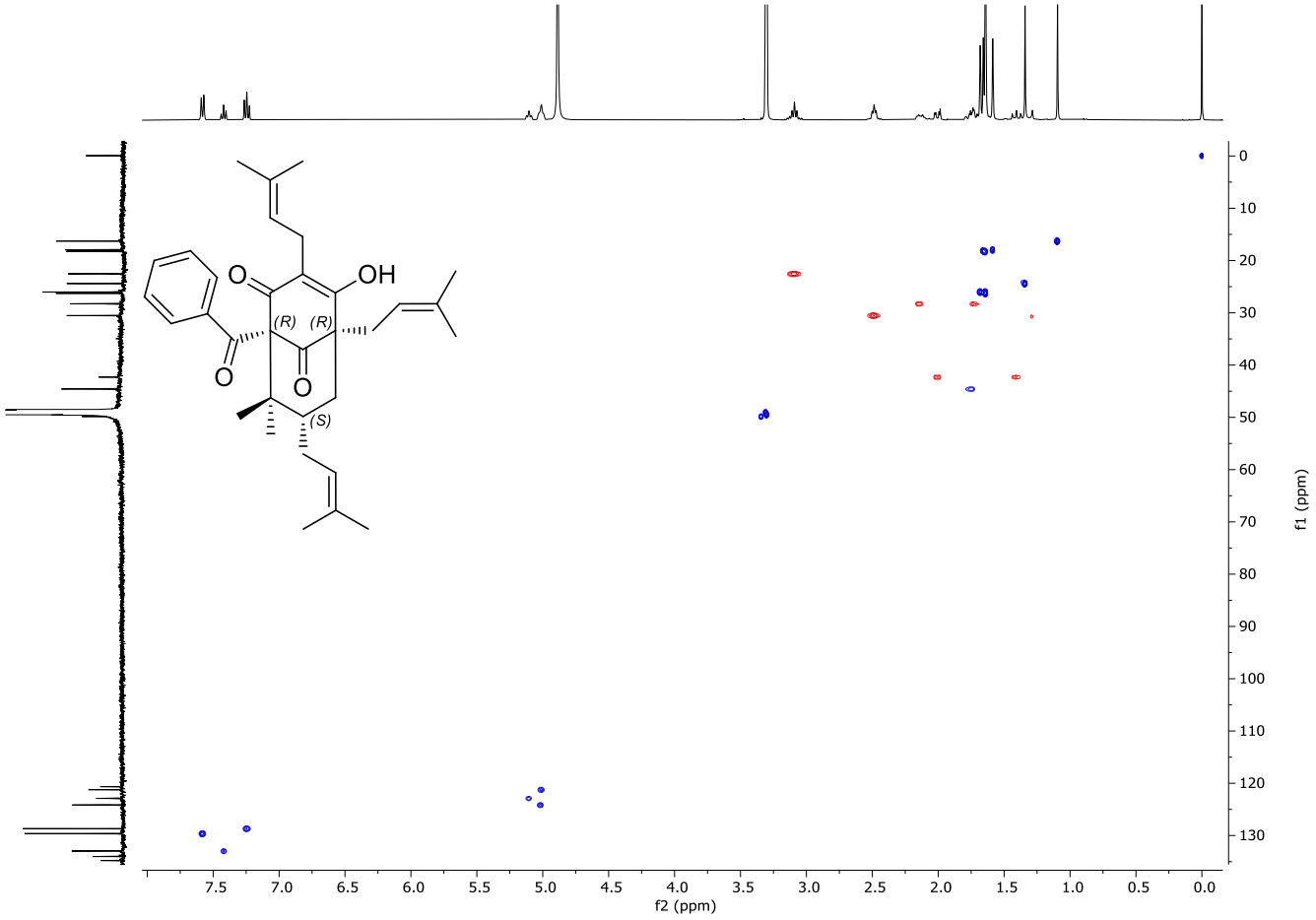

Fig. S7. ^{1}H-^{13}C HSQC NMR spectrum of nemorosone (CD_3OD, 600 MHz).

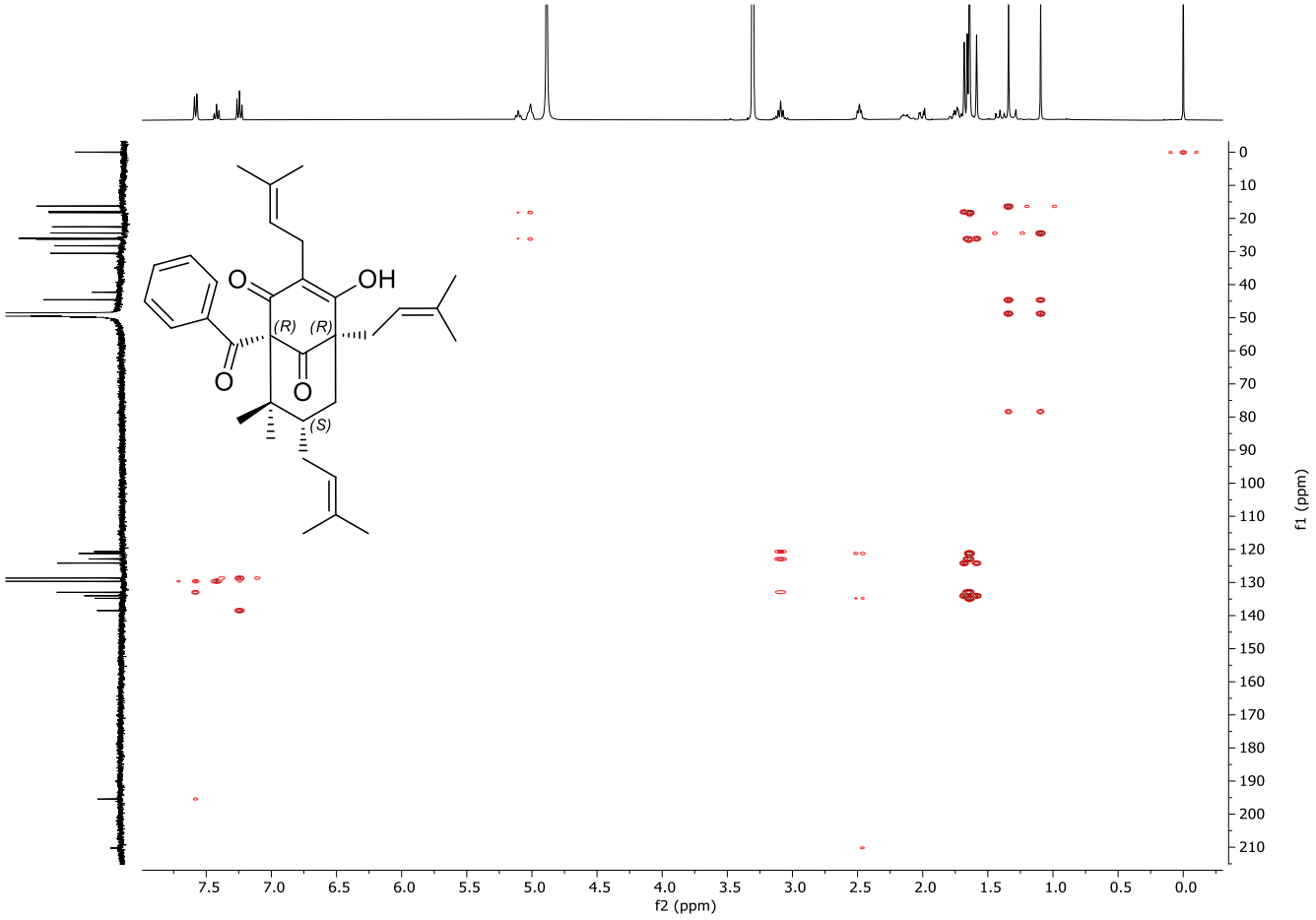

Fig. S8. ^{1}H-^{13}C HMBC NMR spectrum of nemorosone (CD_3OD, 600 MHz).

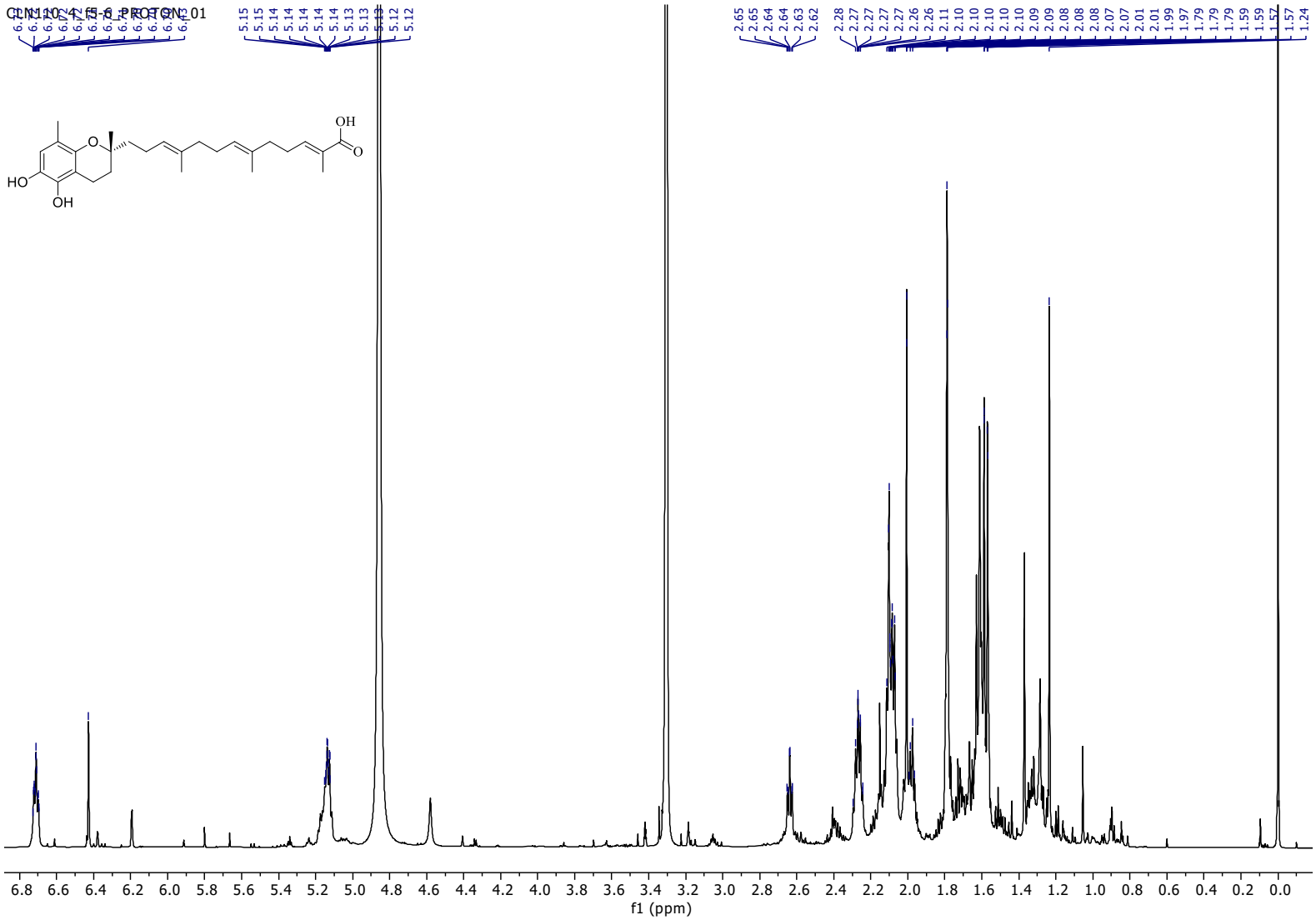

Fig. S9. ^{1}H NMR spectrum of 5-hydroxy tocotrienoloic acid (**N13**) (CD_3OD, 600 MHz).

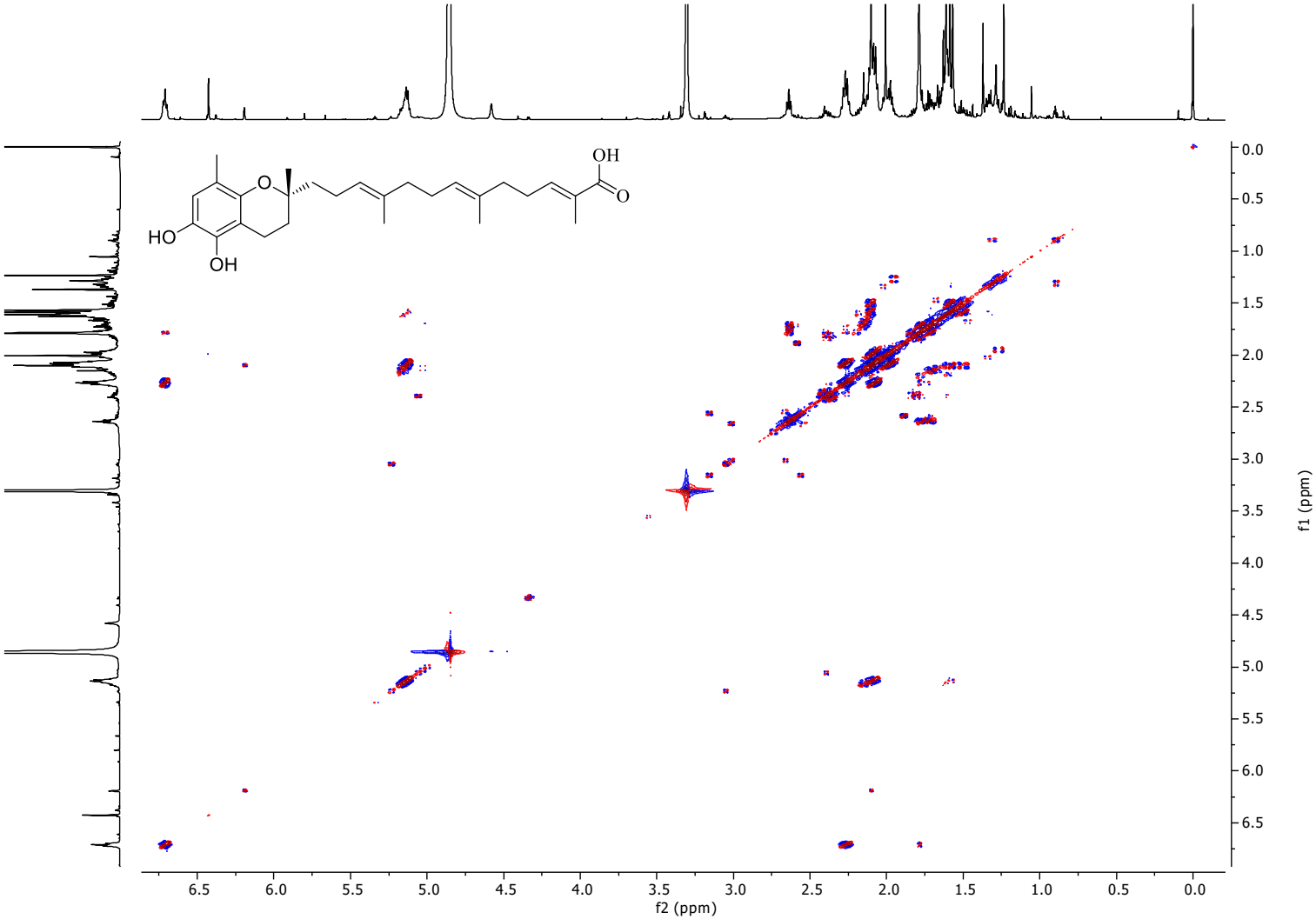

Fig. S10. ^{1}H-^{1}H COSY NMR spectrum of 5-hydroxy tocotrienoloic acid (**N13**) (CD_3OD, 600 MHz).

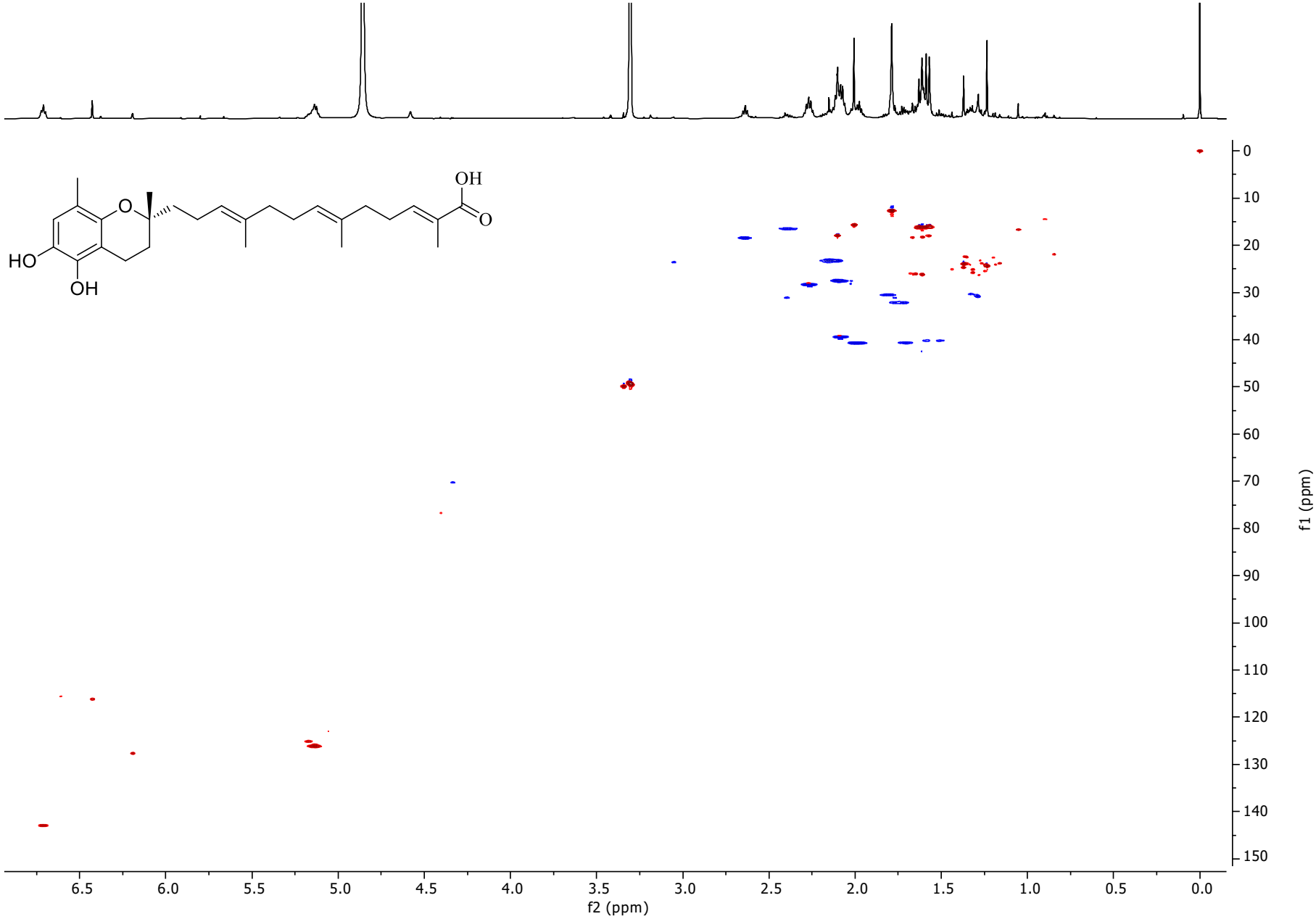

Fig. S11. ^{1}H-^{13}C HSQC NMR spectrum of 5-hydroxy tocotrienoloic acid (**N13**) (CD_3OD, 600 MHz).

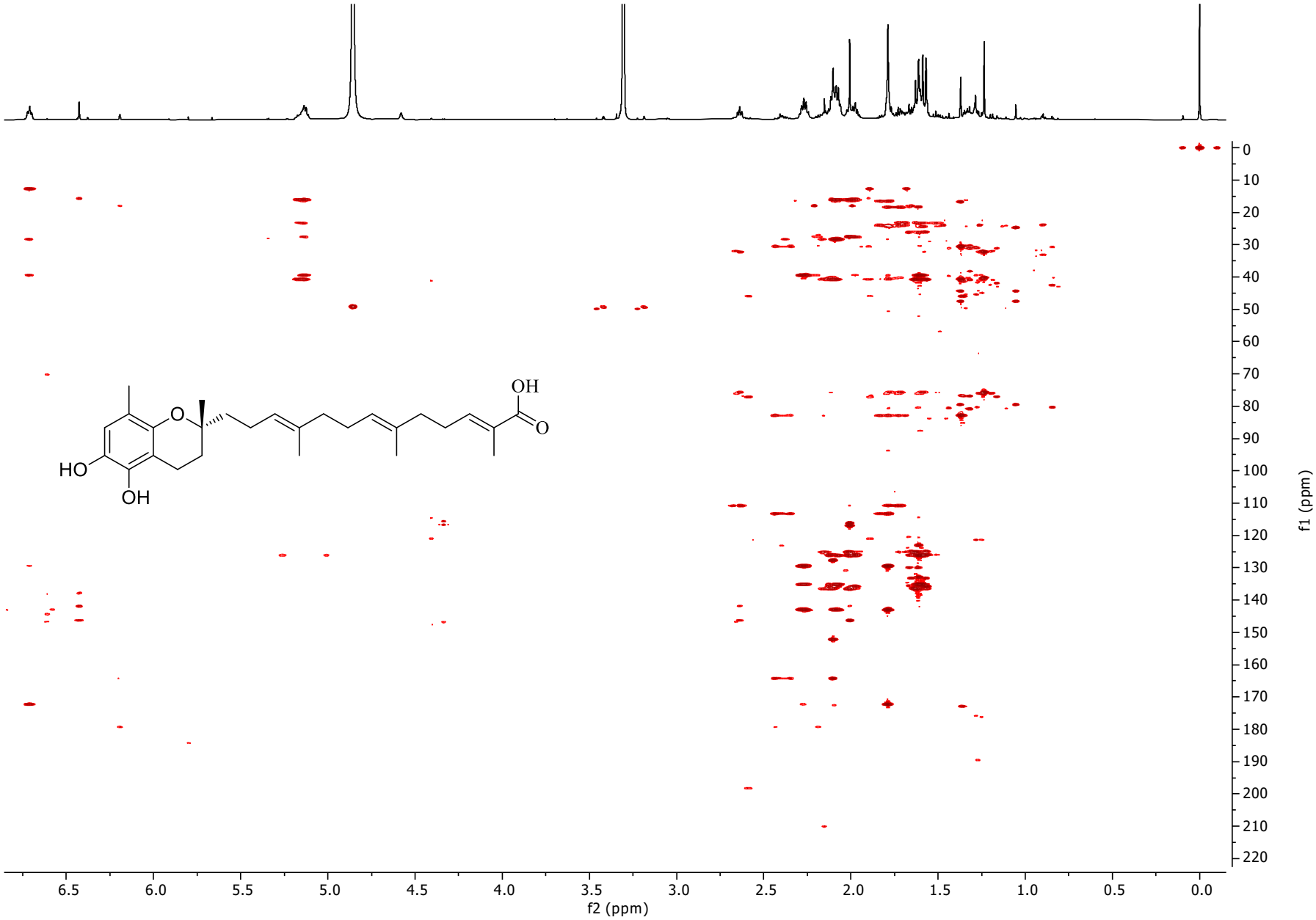

Fig. S12. ^{1}H-^{13}C HMBC NMR spectrum of 5-hydroxy tocotrienoloic acid (**N13**) (CD_3OD, 600 MHz).

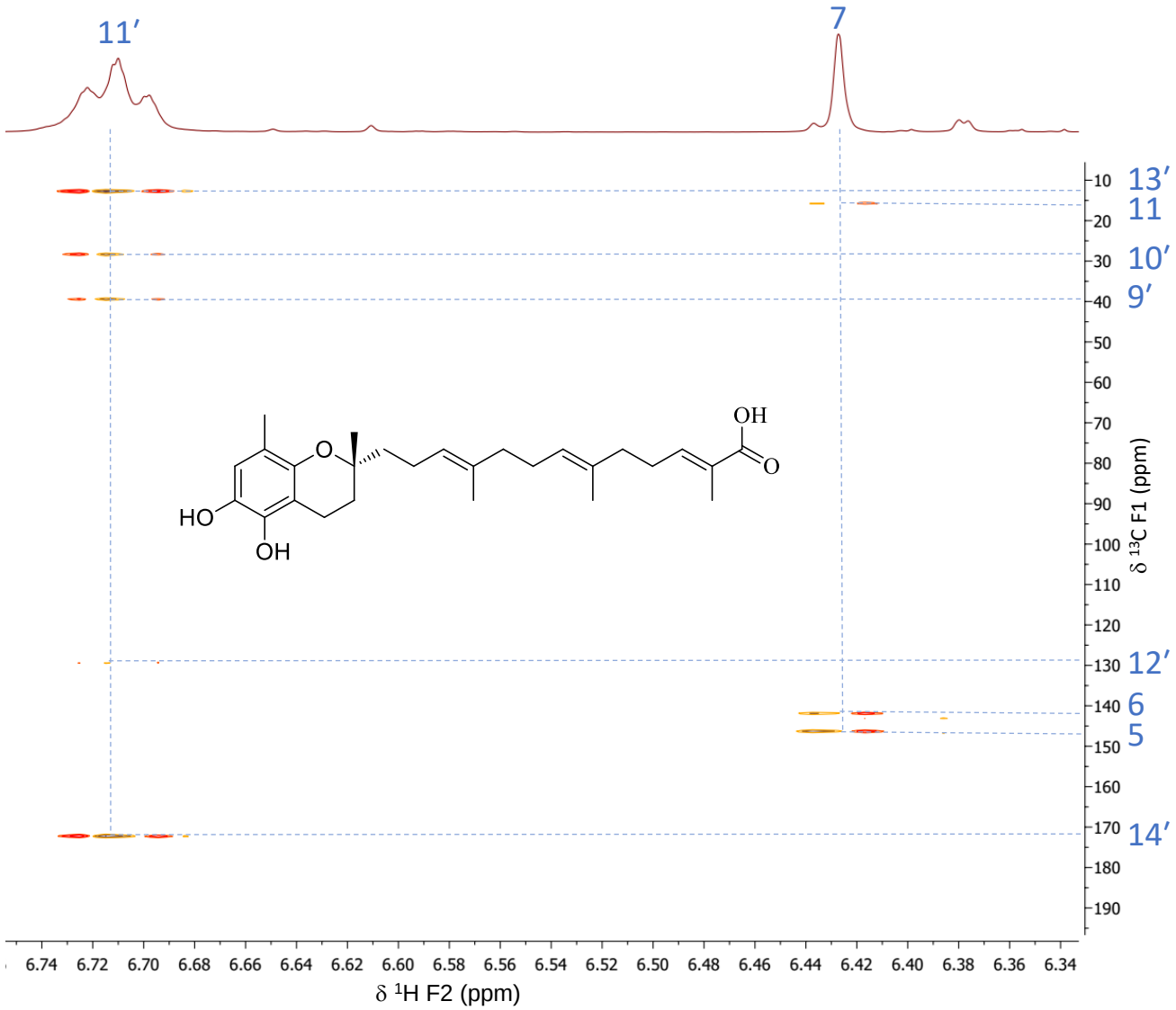

Fig. S13. Extension of the ^{1}H-^{13}C HMBC NMR spectrum of 5-hydroxy tocotrienoloic acid (**N13**), showing cross peaks at δ_H 6.43 (H-7) and 6.75 (H-11') (CD_3OD, 600 MHz).

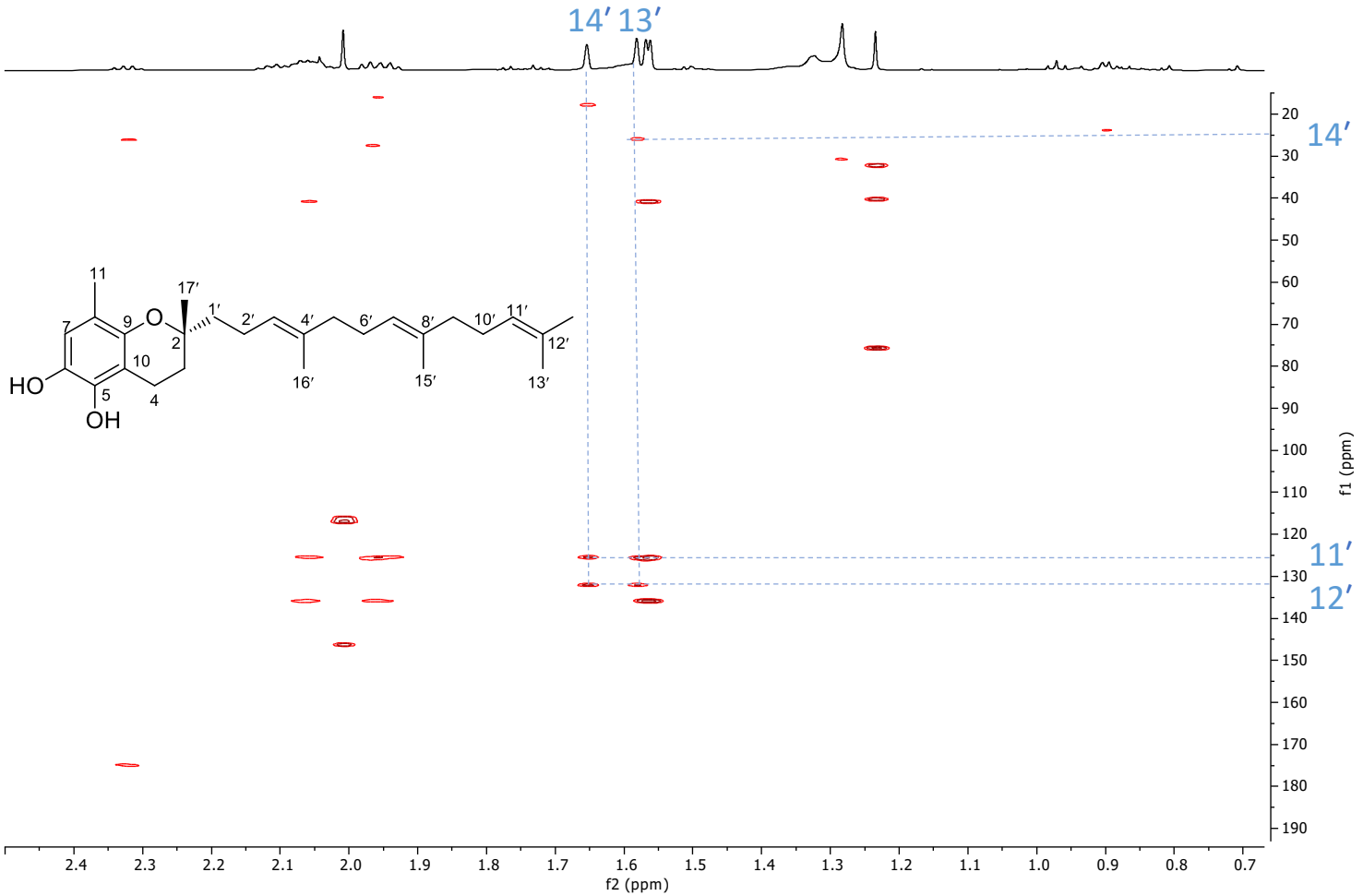

Fig. S14. Extension of the ^{1}H-^{13}C HMBC NMR spectrum of the methanol extract of *Clusia minor* L. leaf **L2**, showing cross peaks of 5-hydroxy-8-methyltocotrienol (**N14**) (CD_3OD, 600 MHz).

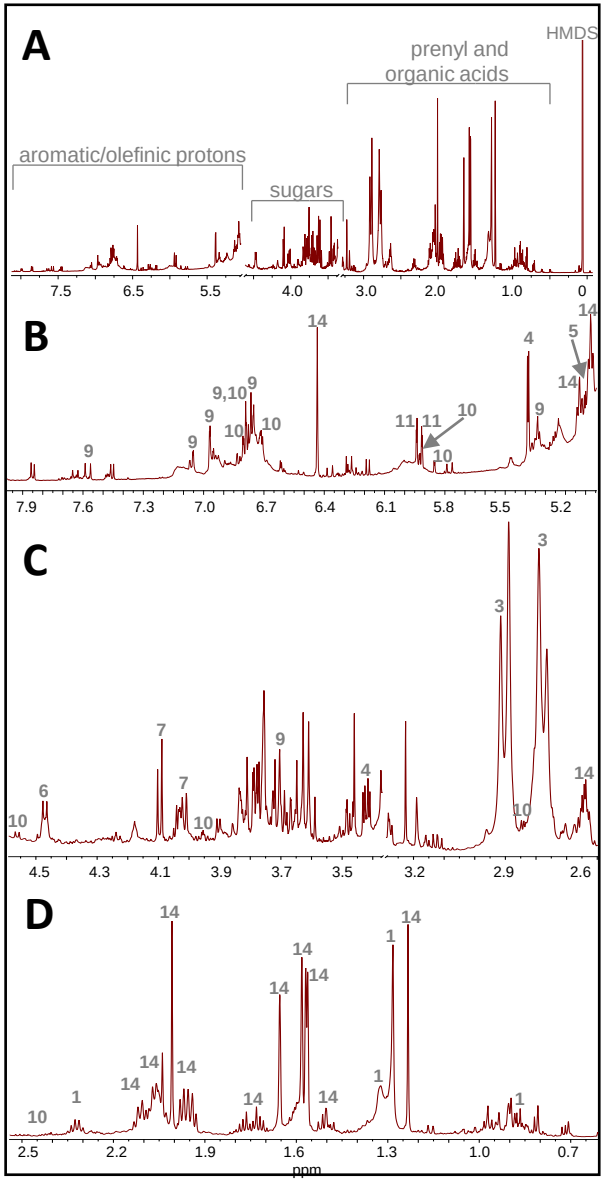

Fig. S15. ^{1}H NMR spectrum of *Clusia minor* L. leaves **L1** (CD_3OD, 600 MHz), showing characteristic signals for metabolites in the most relevant shift range (δ 0.0−8.0 ppm) (A). Expanded spectral region from 5.2–7.9 (B), 2.6–4.7 (C), and 0.5-2.5 (D) ppm with assigned peaks: **N1** (fatty acids), **N3** (citric acid), **N4** (α-sucrose), **N5** (α-glucose), **N6** (β-glucose), **N7** (fructose), **N9** (chlorogenic acid), **N10** (catechin), **N11** (epicatechin) and **N14** (5-hydroxy-8-methyltocotrienol). Signal numbers correspond to those listed in **Table 3** for metabolite identification using ^{1}H-NMR.