

Supplementary Materials

# Characterization of a new trioxilin and a sulfoquinovosyl diacylglycerol with anti-inflammatory properties from the dinoflagellate *Oxyrrhis marina*

Eun Young Yoon, A Reum Yang, Jaeyeon Park, Seung Joo Moon, Eun Ju Jeong and Jung-Rae Rho

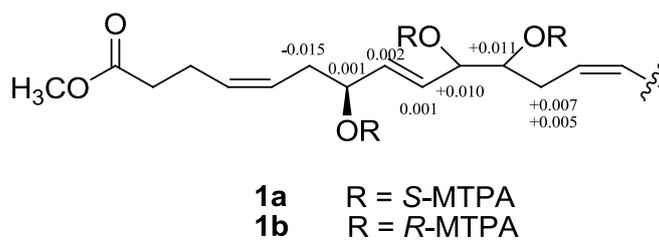
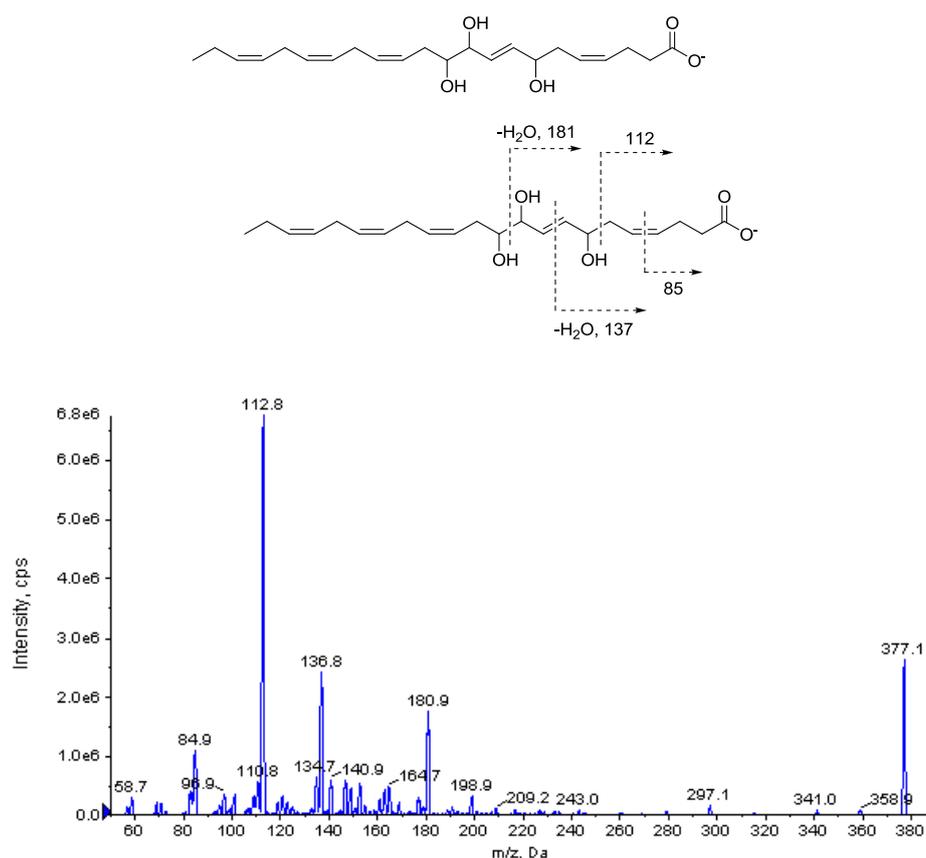


Figure S2. Differences in chemical shifts of key protons of S-MTPA ester (**1a**) and R-MTPA ester (**1b**).

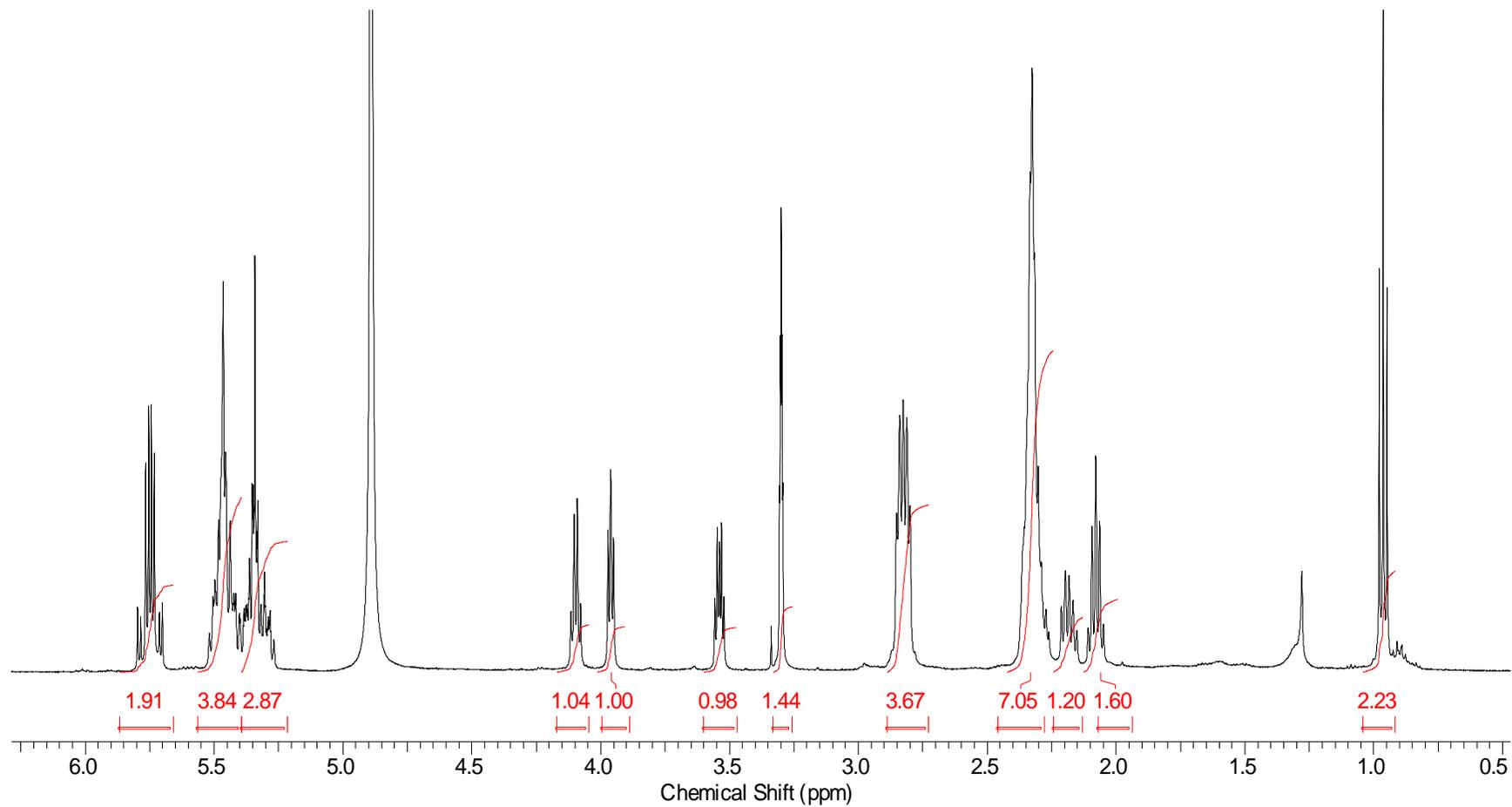
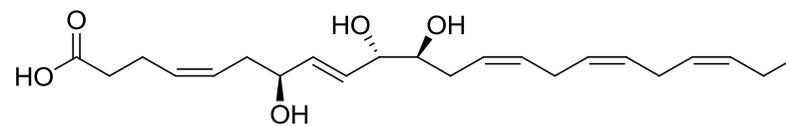


Figure S3. <sup>1</sup>H NMR spectrum of compound 1 at 500 MHz.

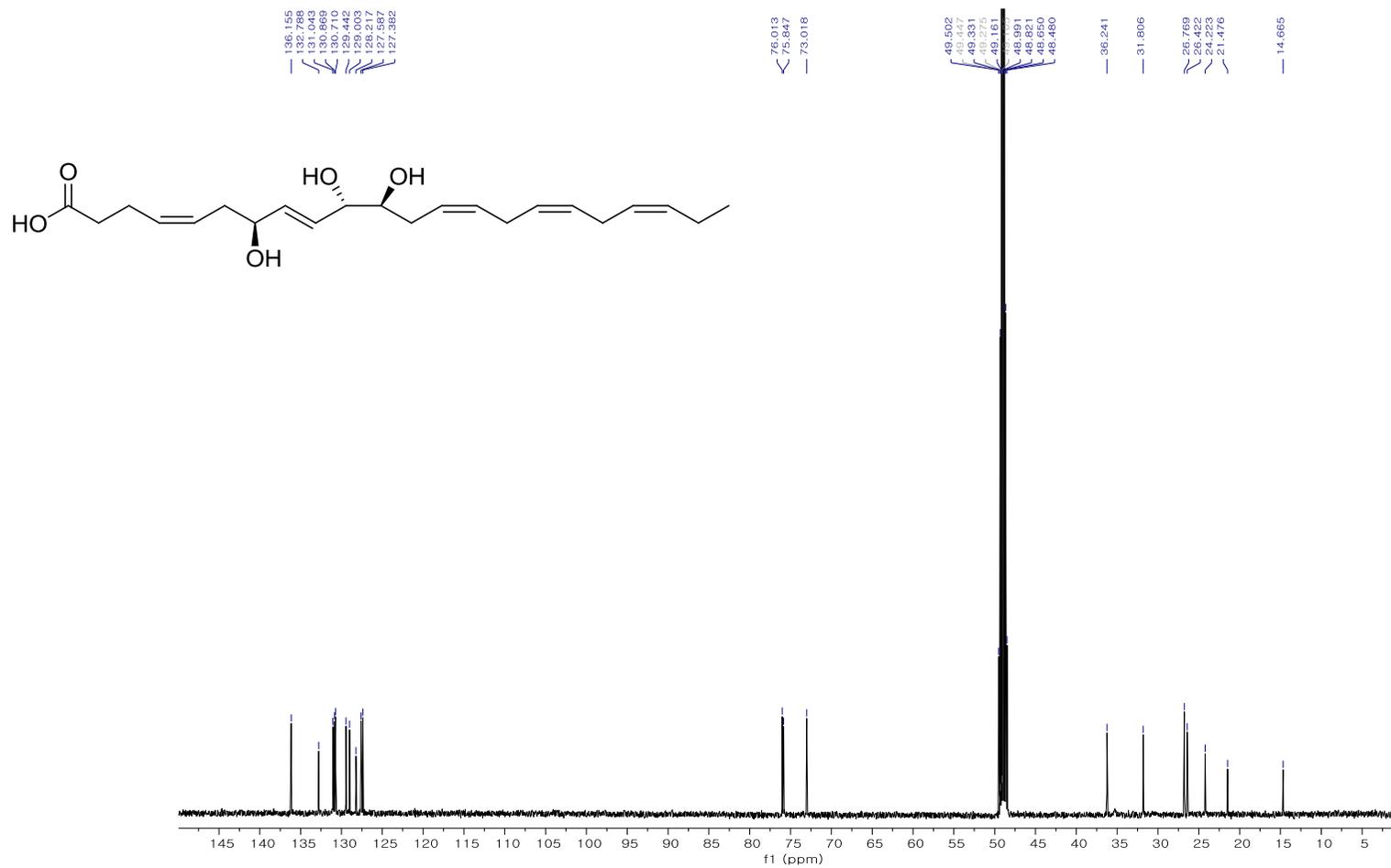


Figure S4. <sup>13</sup>C NMR spectrum of compound 1 at 125 MHz.

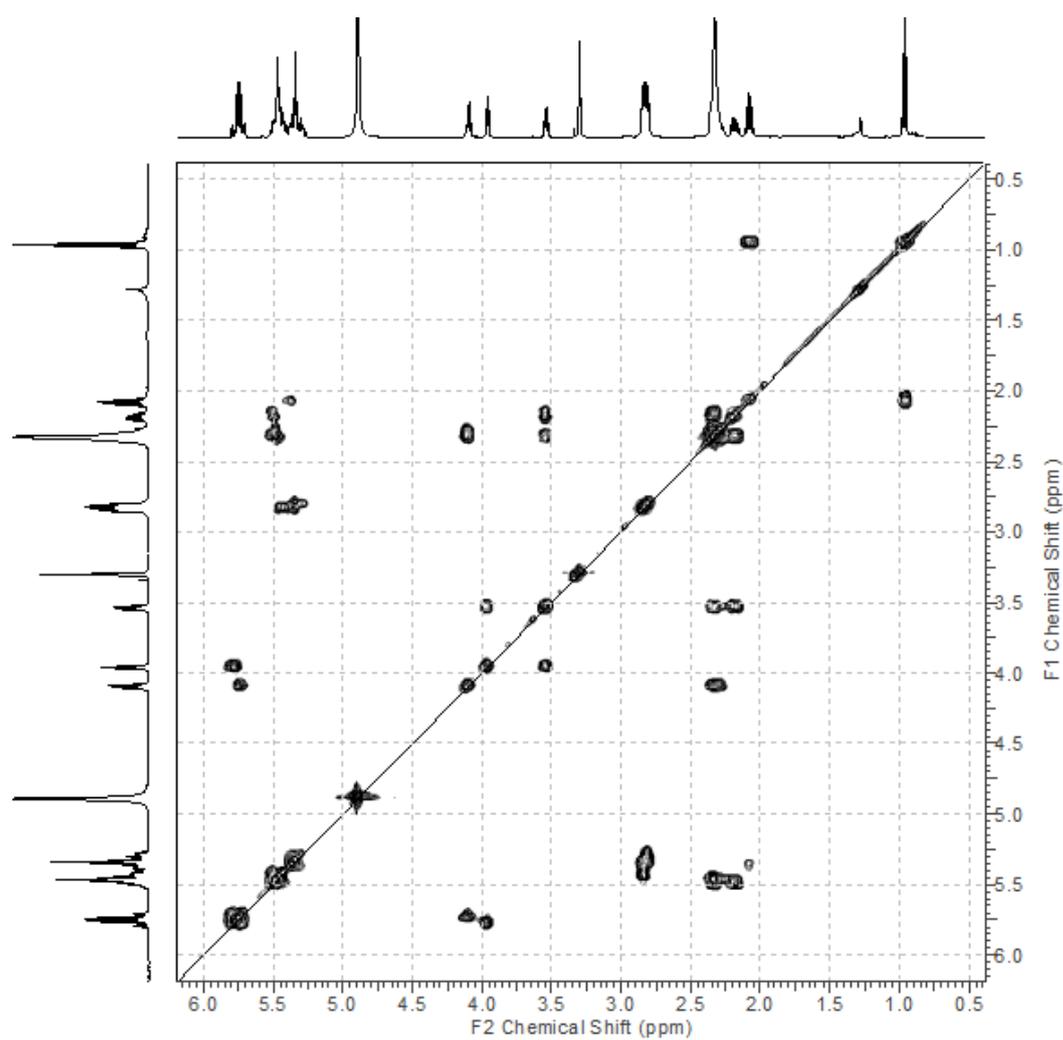
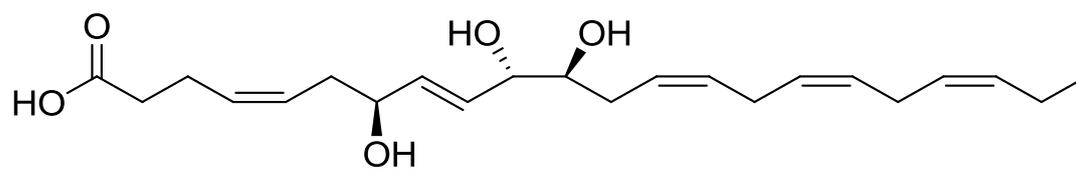


Figure S5. COSY NMR spectrum of compound 1 at 500 MHz.

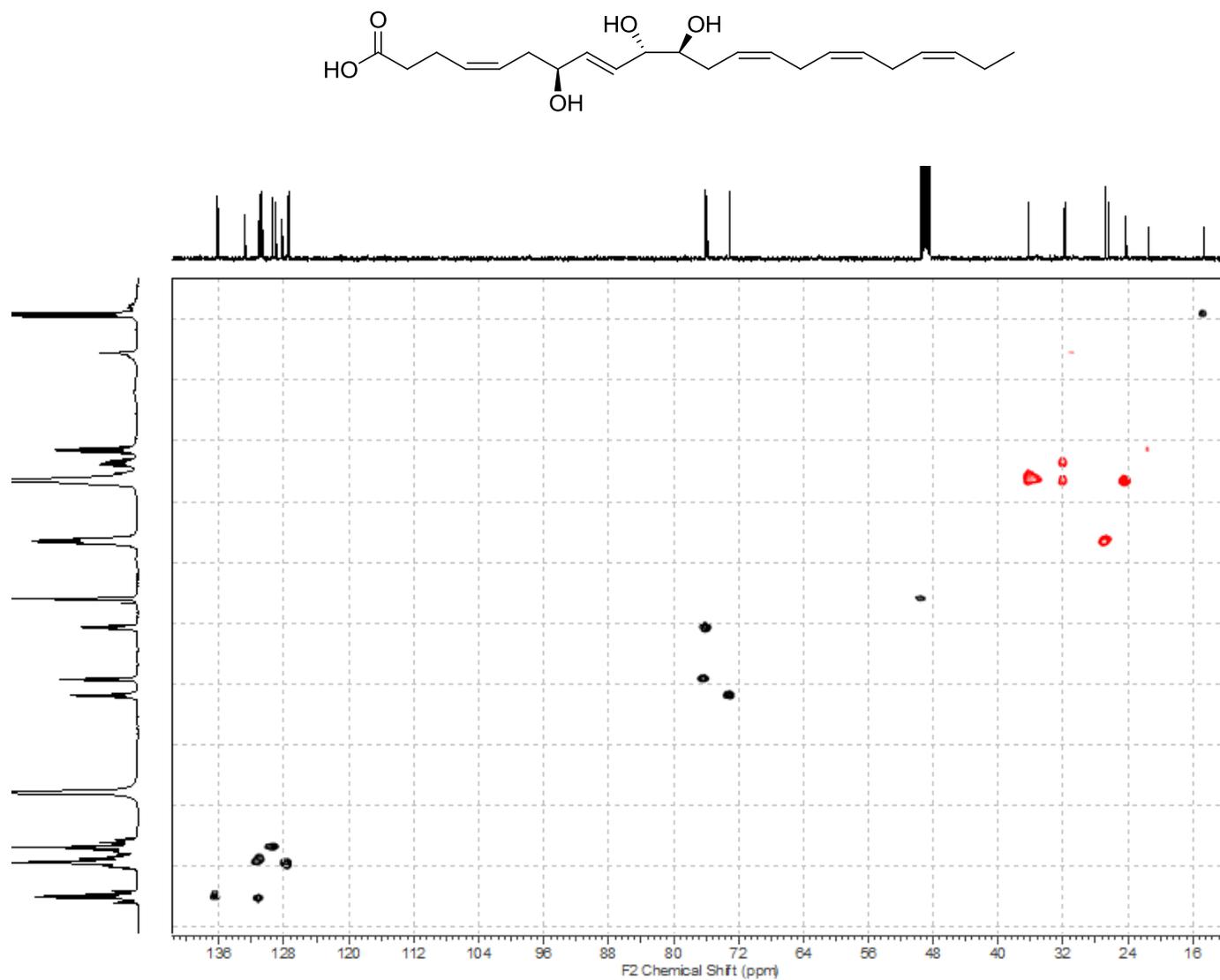


Figure S6. HSQC NMR spectrum of compound 1 at 500 MHz. (Black: CH, CH<sub>3</sub>; Red: CH<sub>2</sub>)

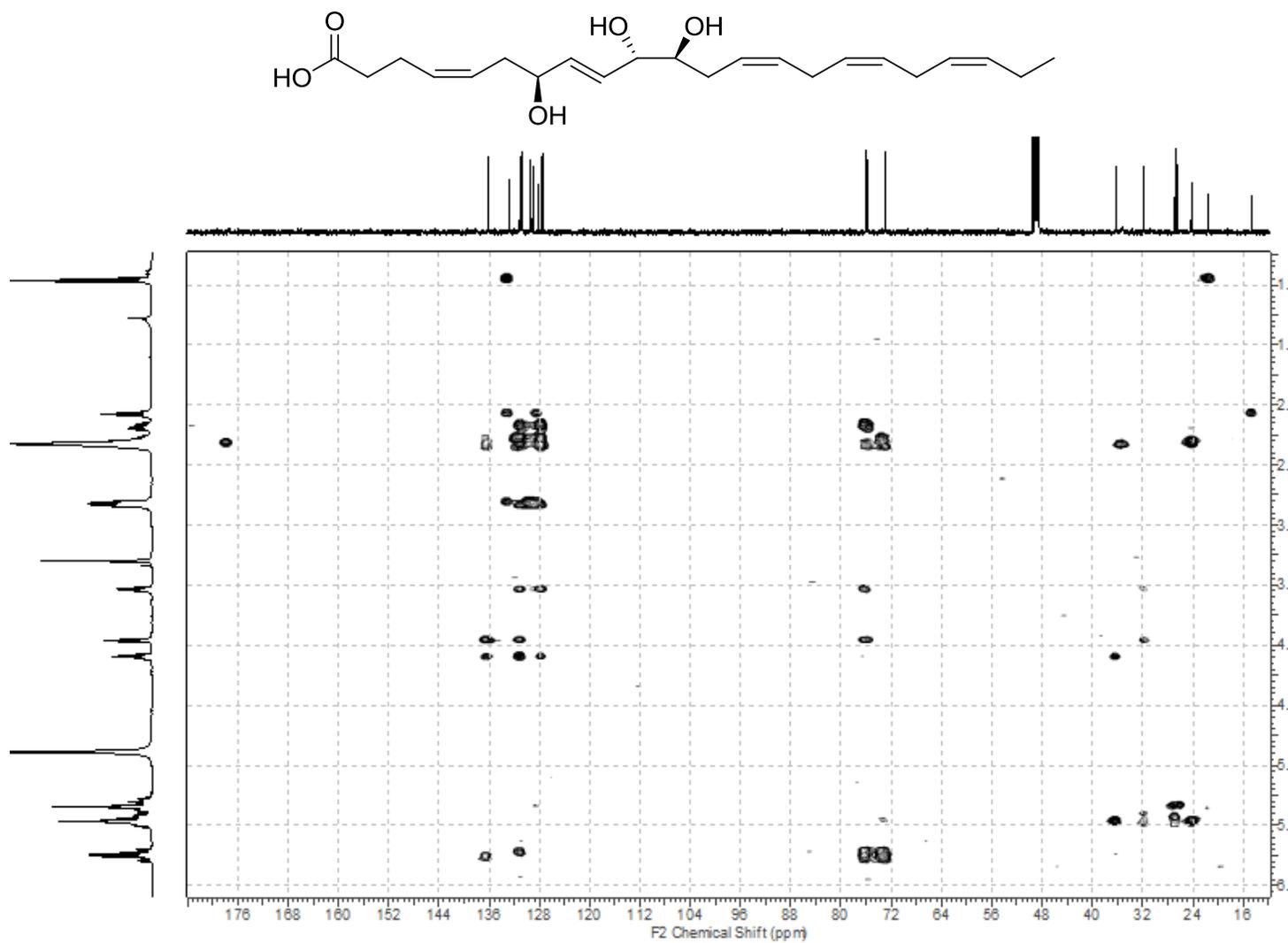
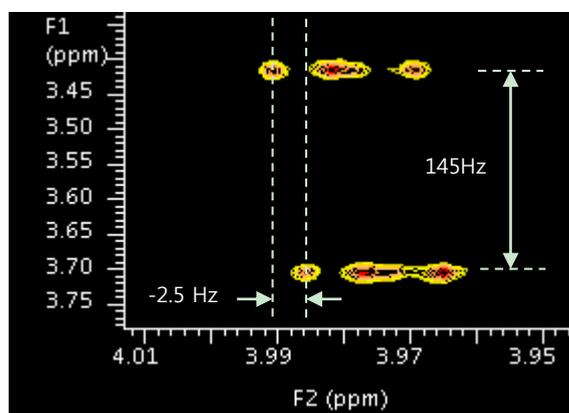
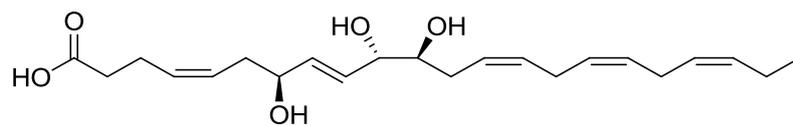
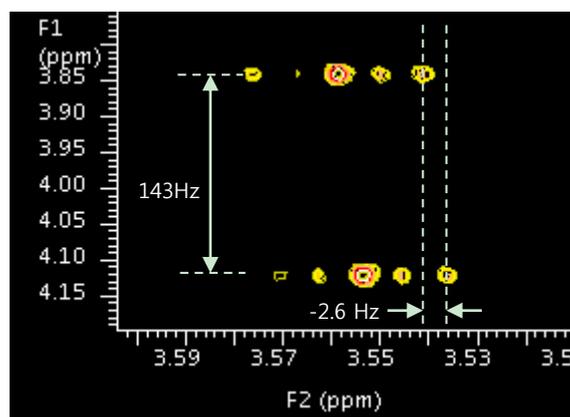


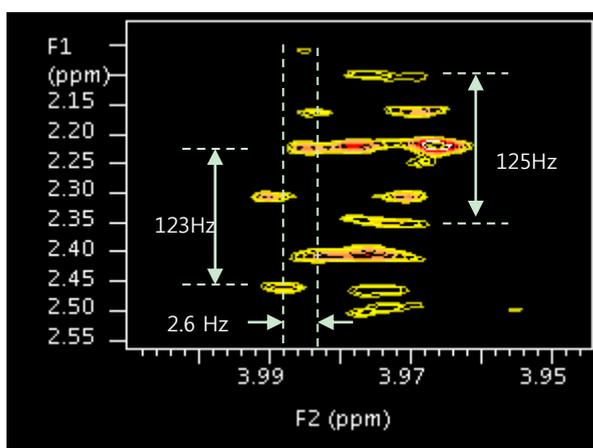
Figure S7. HMBC NMR spectrum of compound 1 at 500 MHz.



$${}^2J_{H_{10}C_{11}} = -2.5 \text{ Hz}$$



$${}^2J_{H_{11}C_{10}} = -2.6 \text{ Hz}$$



$${}^3J_{H_{10}C_{12}} = +2.6 \text{ Hz}$$

Figure S8. Key HETLOC NMR cross peaks of compound 1 at 500 MHz.

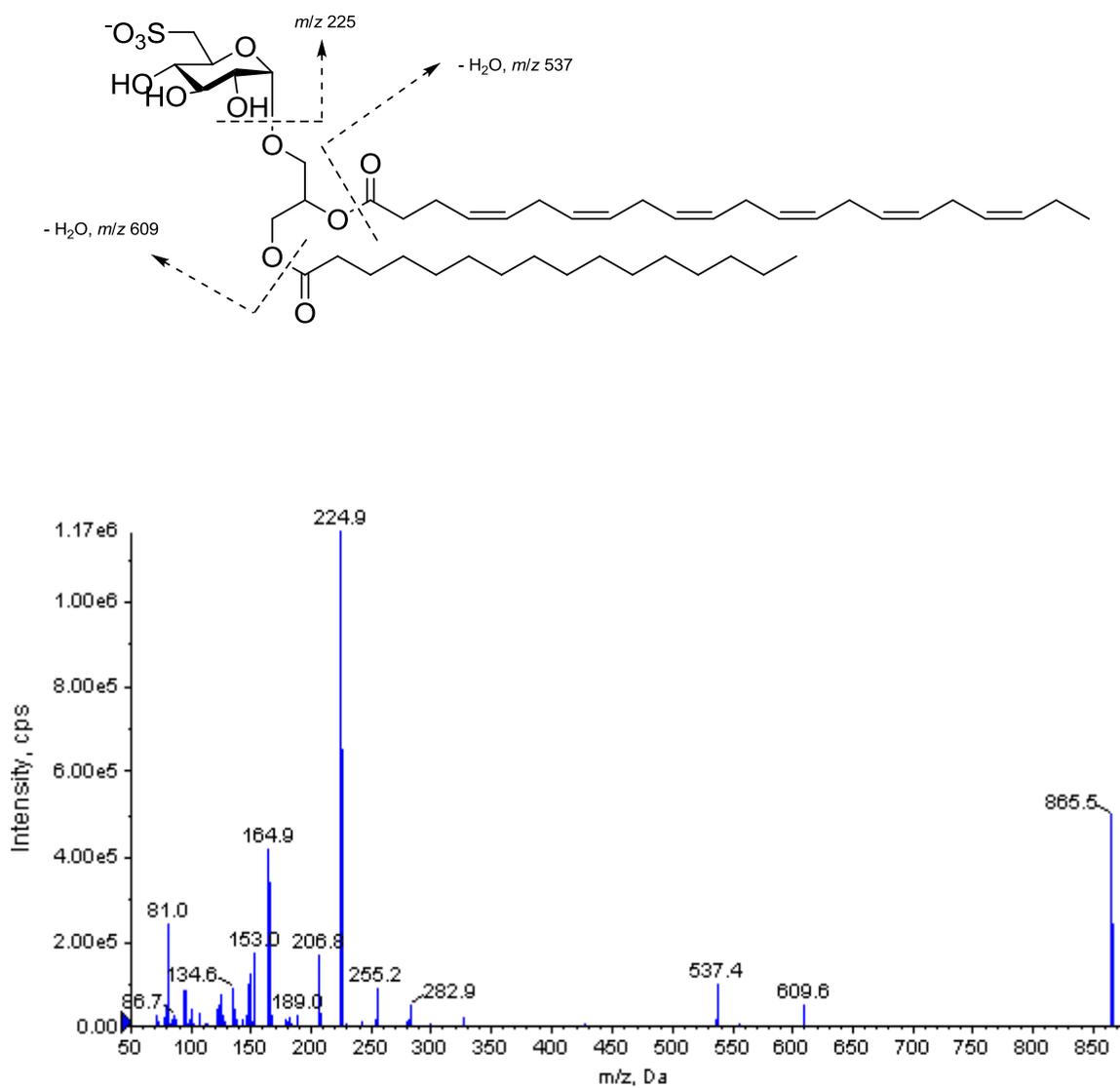


Figure S9. MS/MS fragmentation of compound 2.

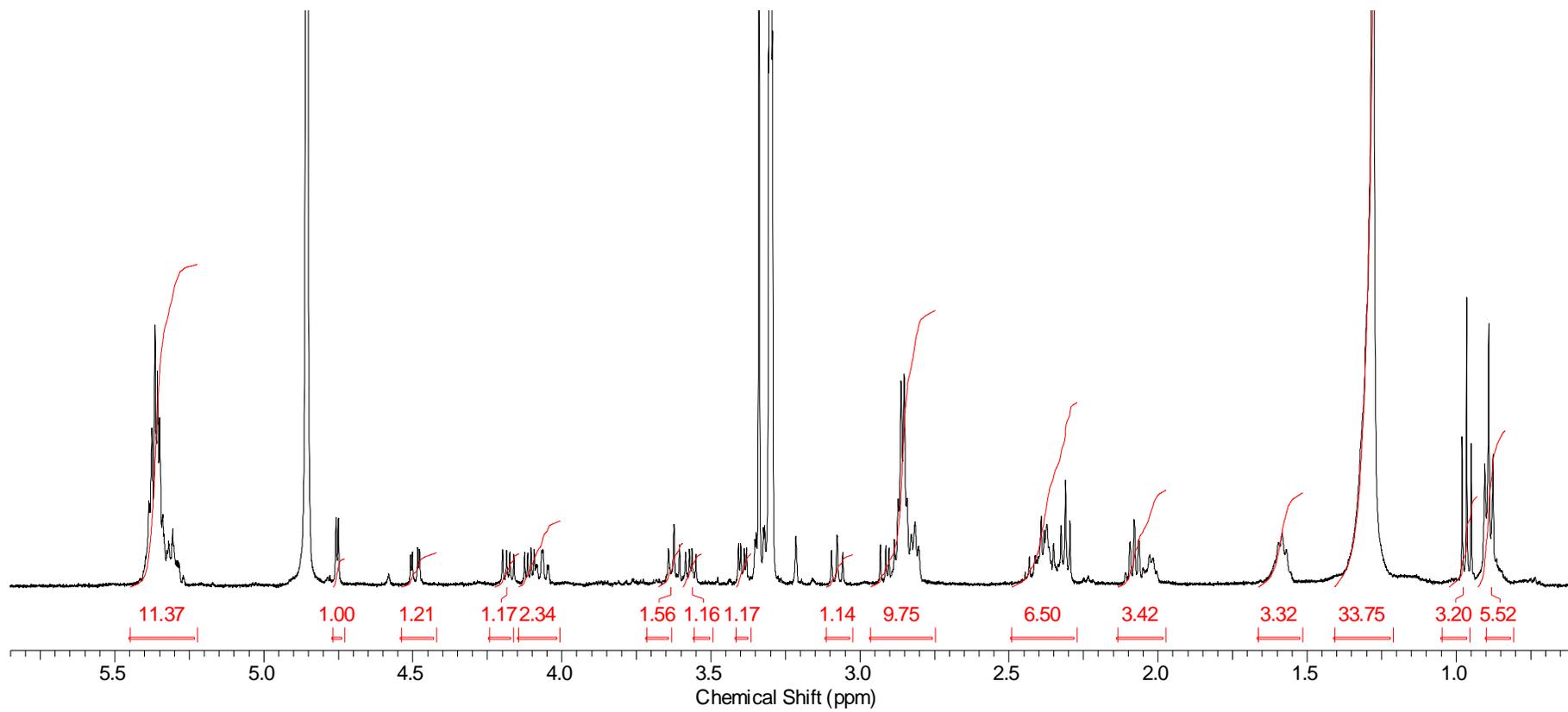
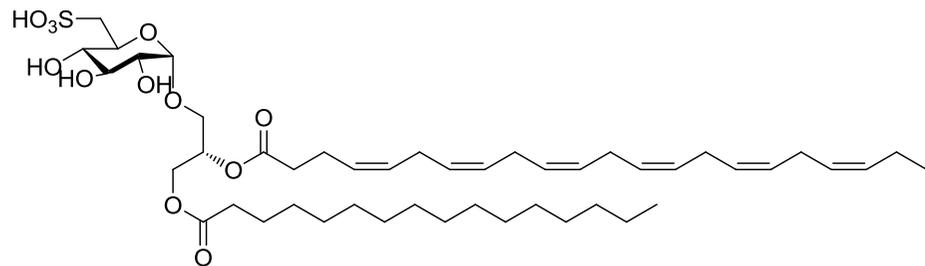


Figure S10.  $^1\text{H}$  NMR spectrum of compound 2 at 500 MHz.

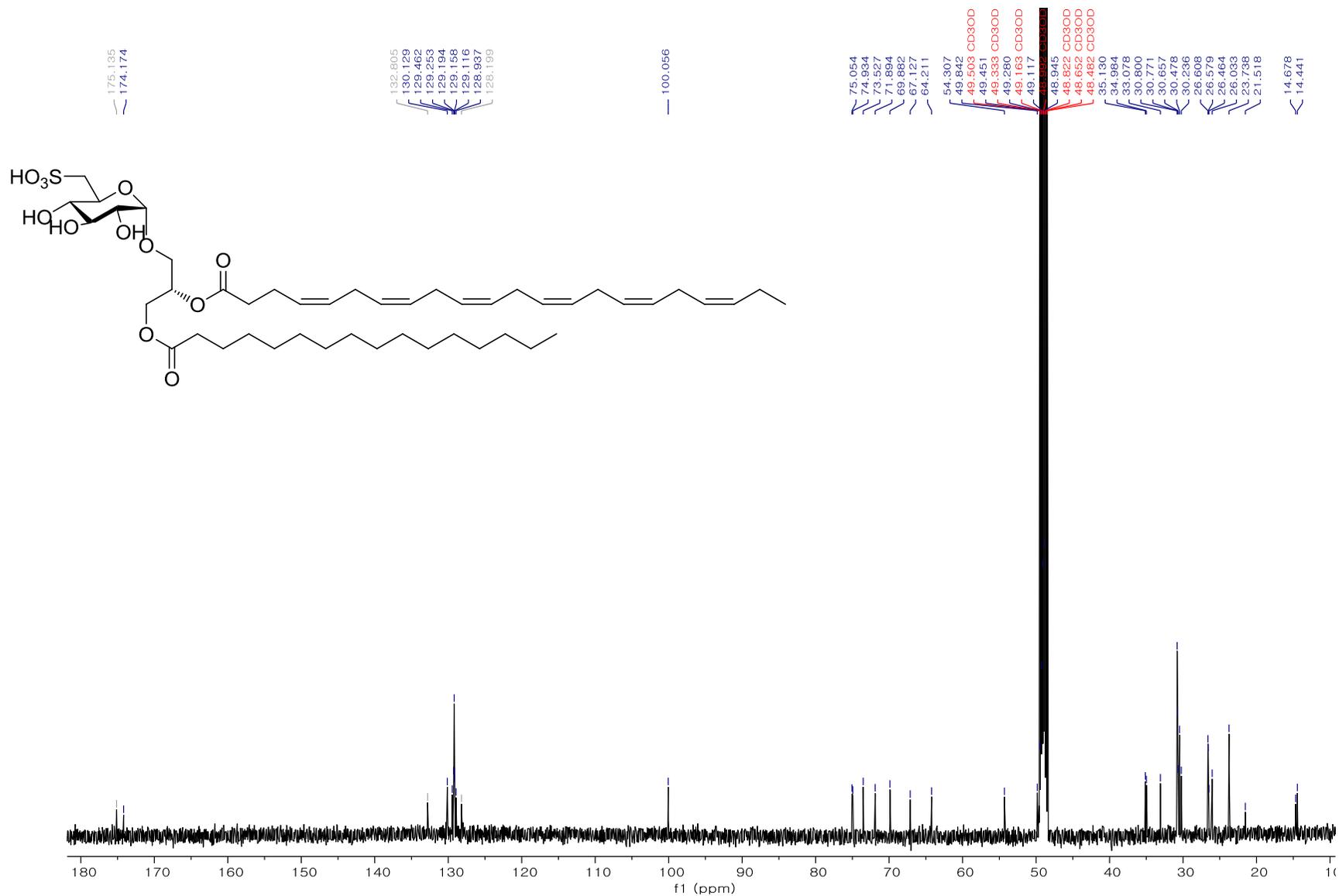


Figure S11. <sup>13</sup>C NMR spectrum of compound 2 at 125 MHz.

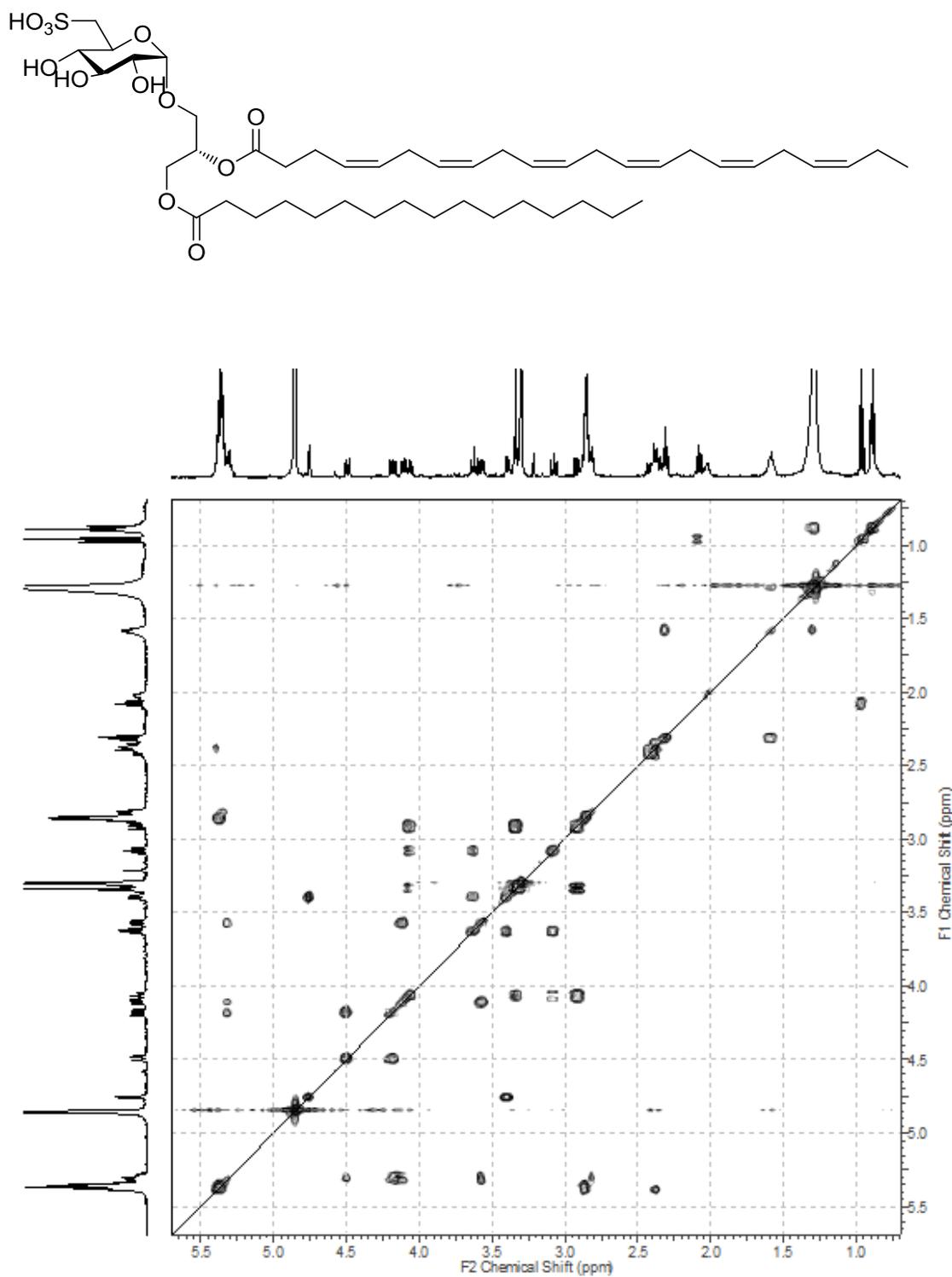


Figure S12. COSY NMR spectrum of compound 2 at 500 MHz.

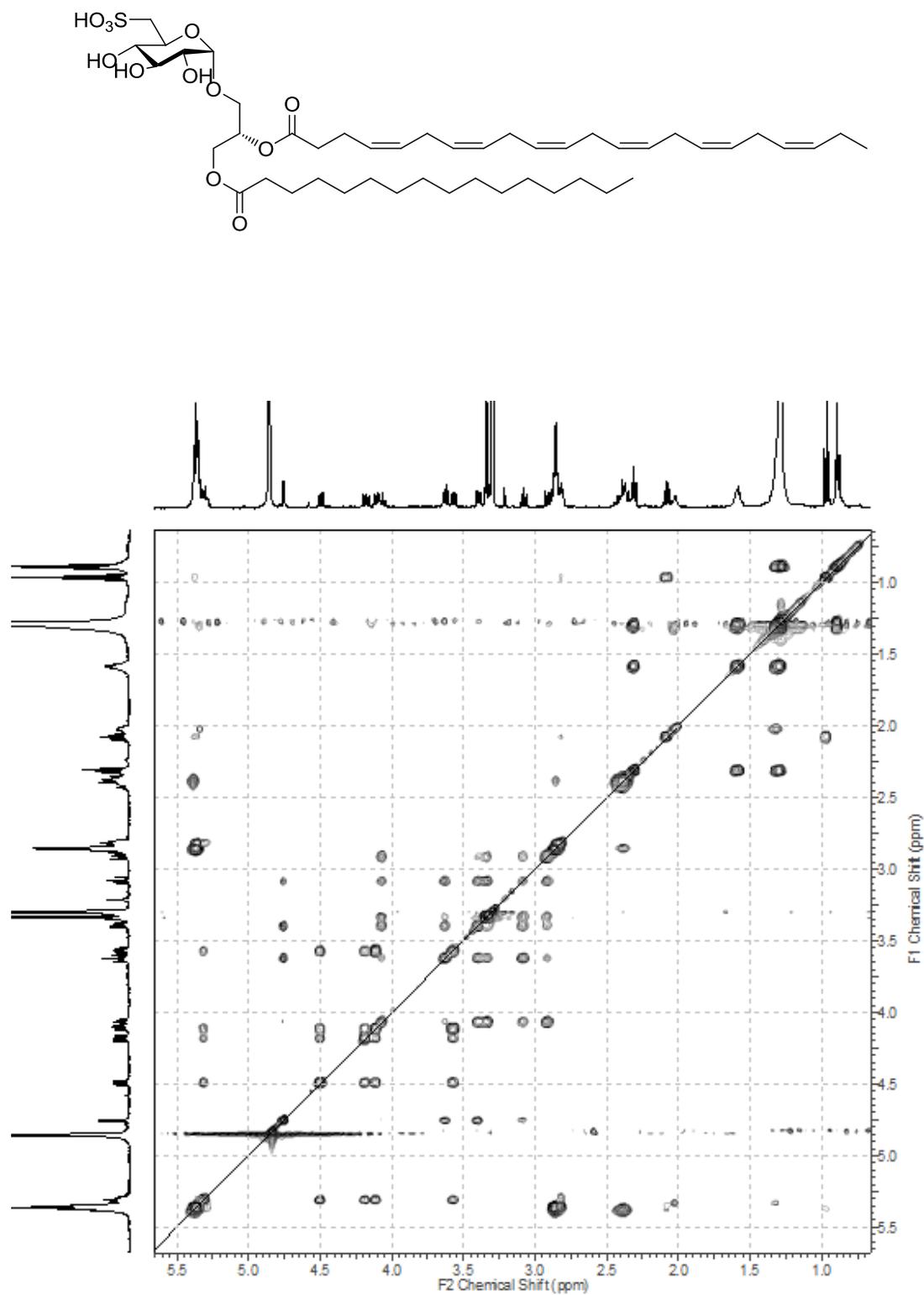


Figure S13. TOCSY NMR spectrum of compound 2 at 500 MHz.

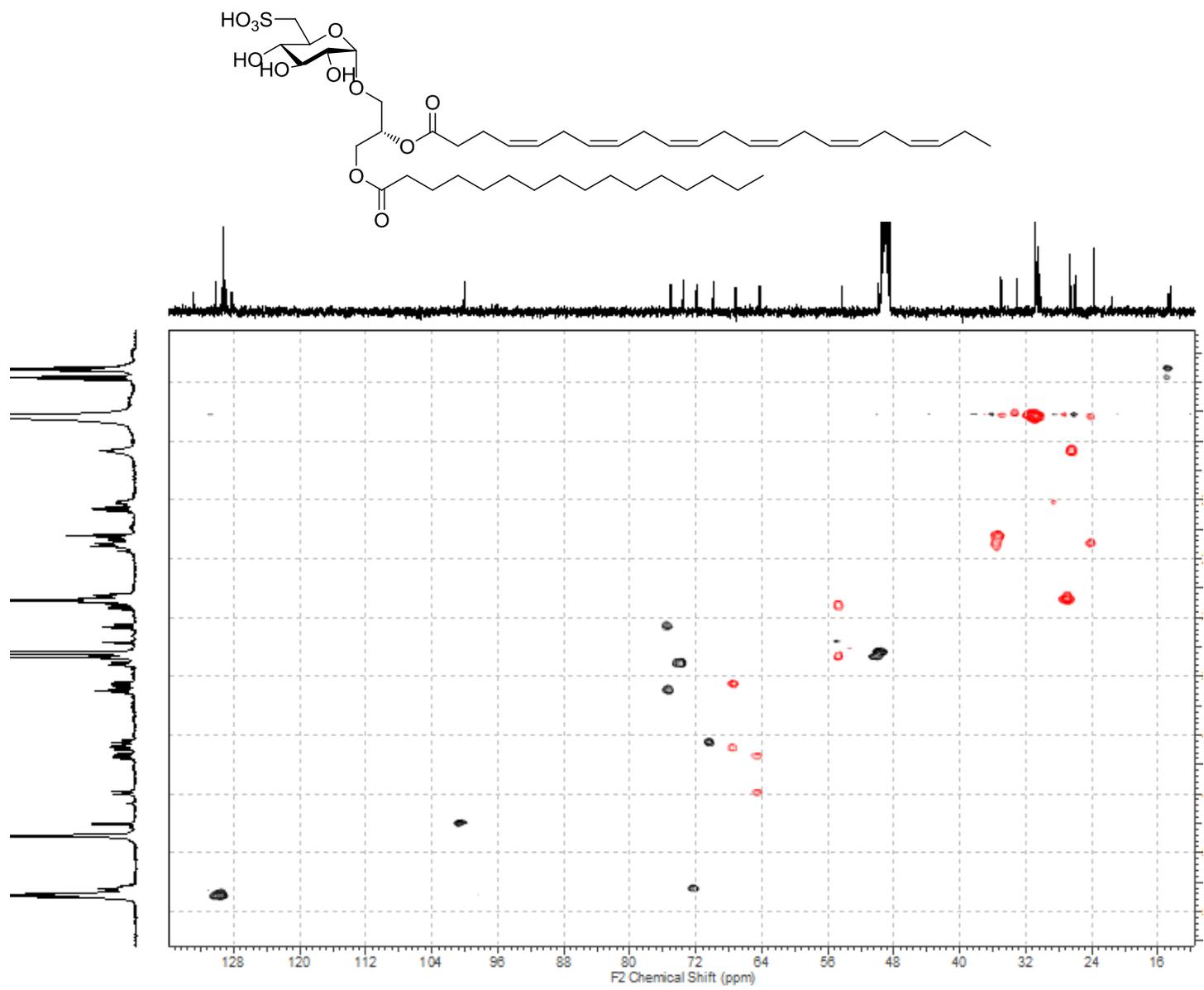


Figure S14. HSQC NMR spectrum of compound 2 at 500 MHz. (Black: CH, CH<sub>3</sub>; Red: CH<sub>2</sub>)

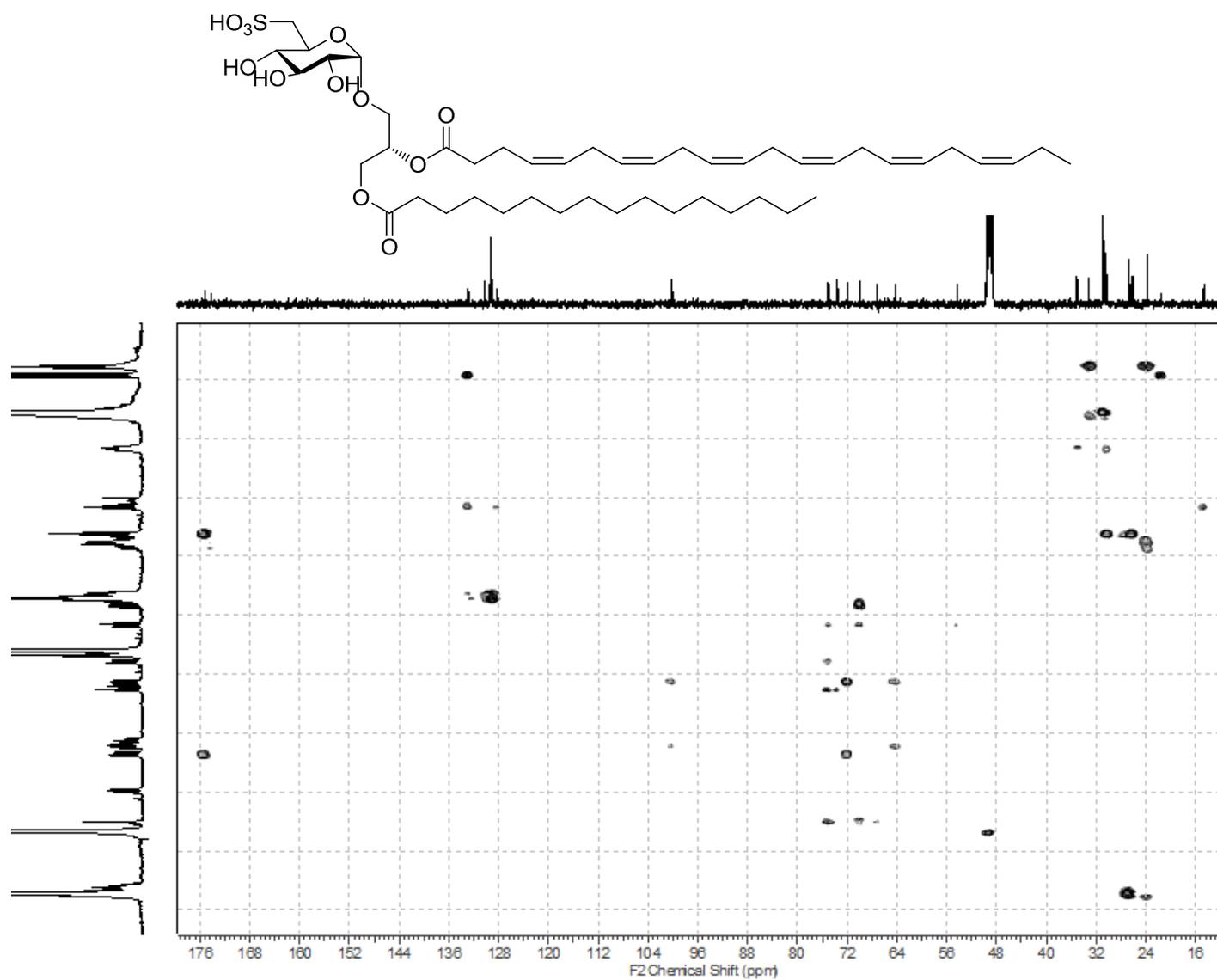


Figure S15. HMBC NMR spectrum of compound 2 at 500 MHz.

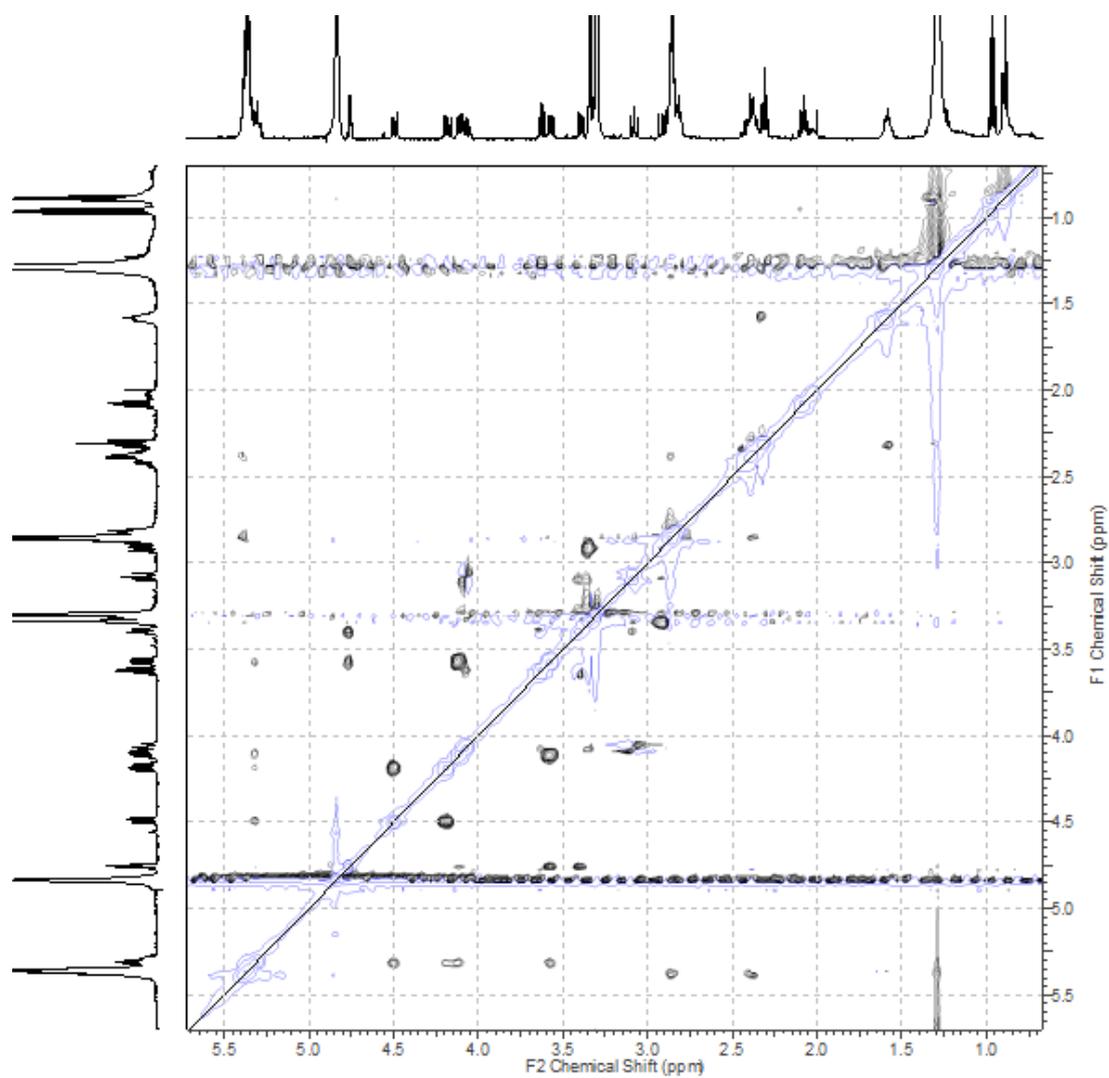
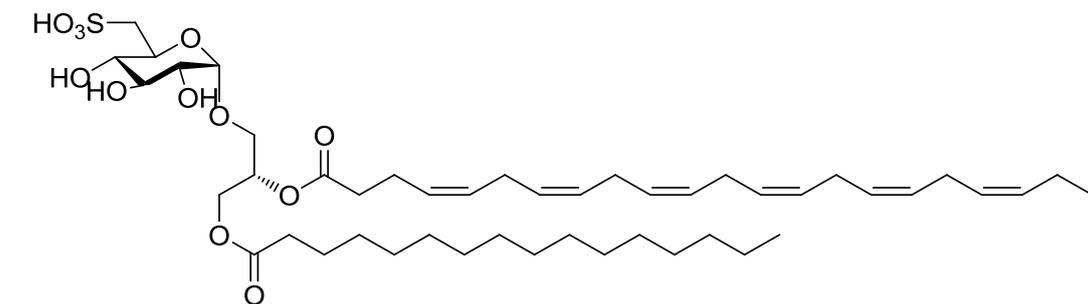


Figure S16. ROESY NMR spectrum of compound 2 at 500 MHz.