

Supporting Information

Determination of the Absolute Configuration of a Monoglyceride Anti-Bolting Compound and Isolation of Related Compounds from Radish Leaves (*Raphanus sativus*)

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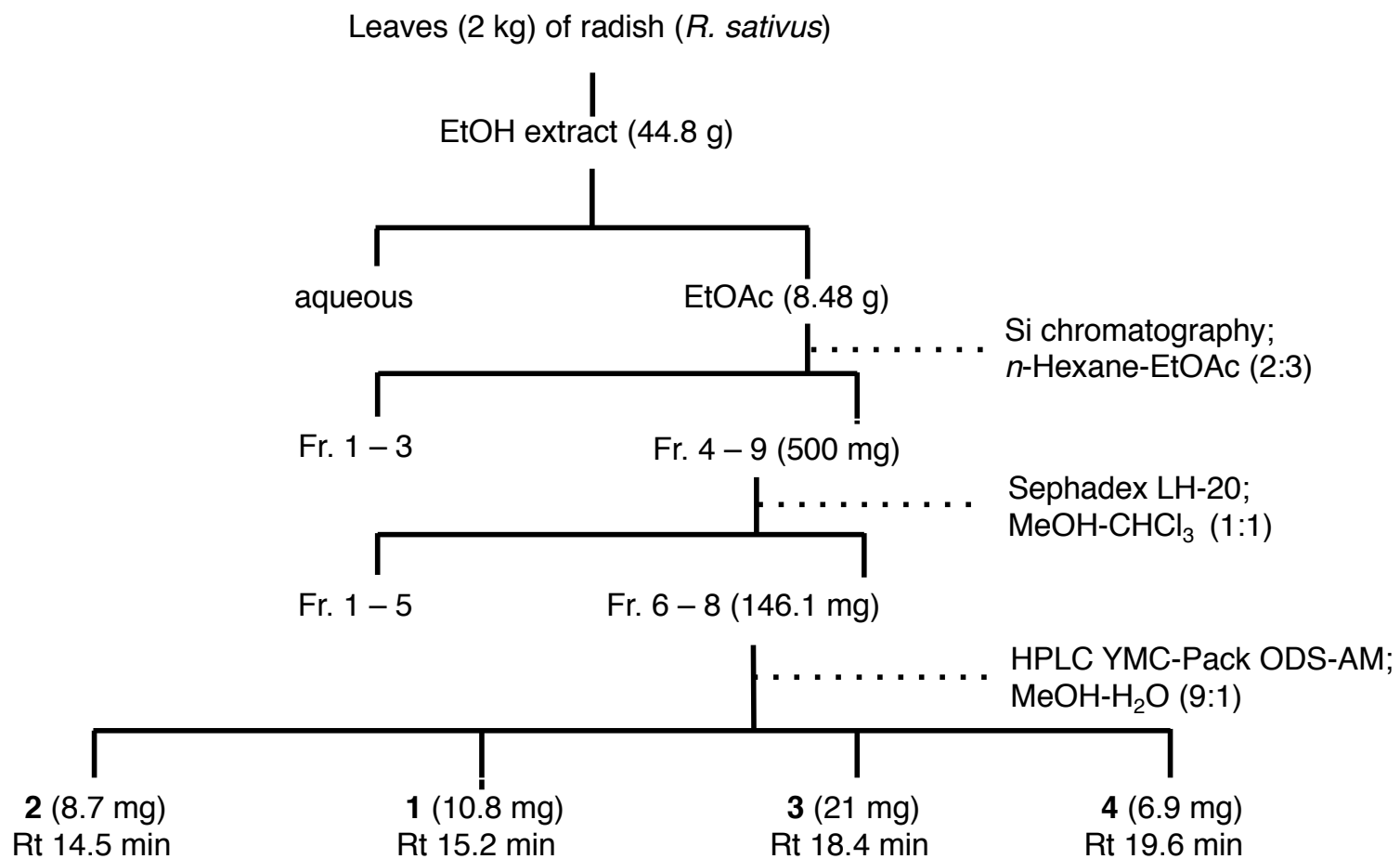


Figure S1. Isolation procedure for 1-4.

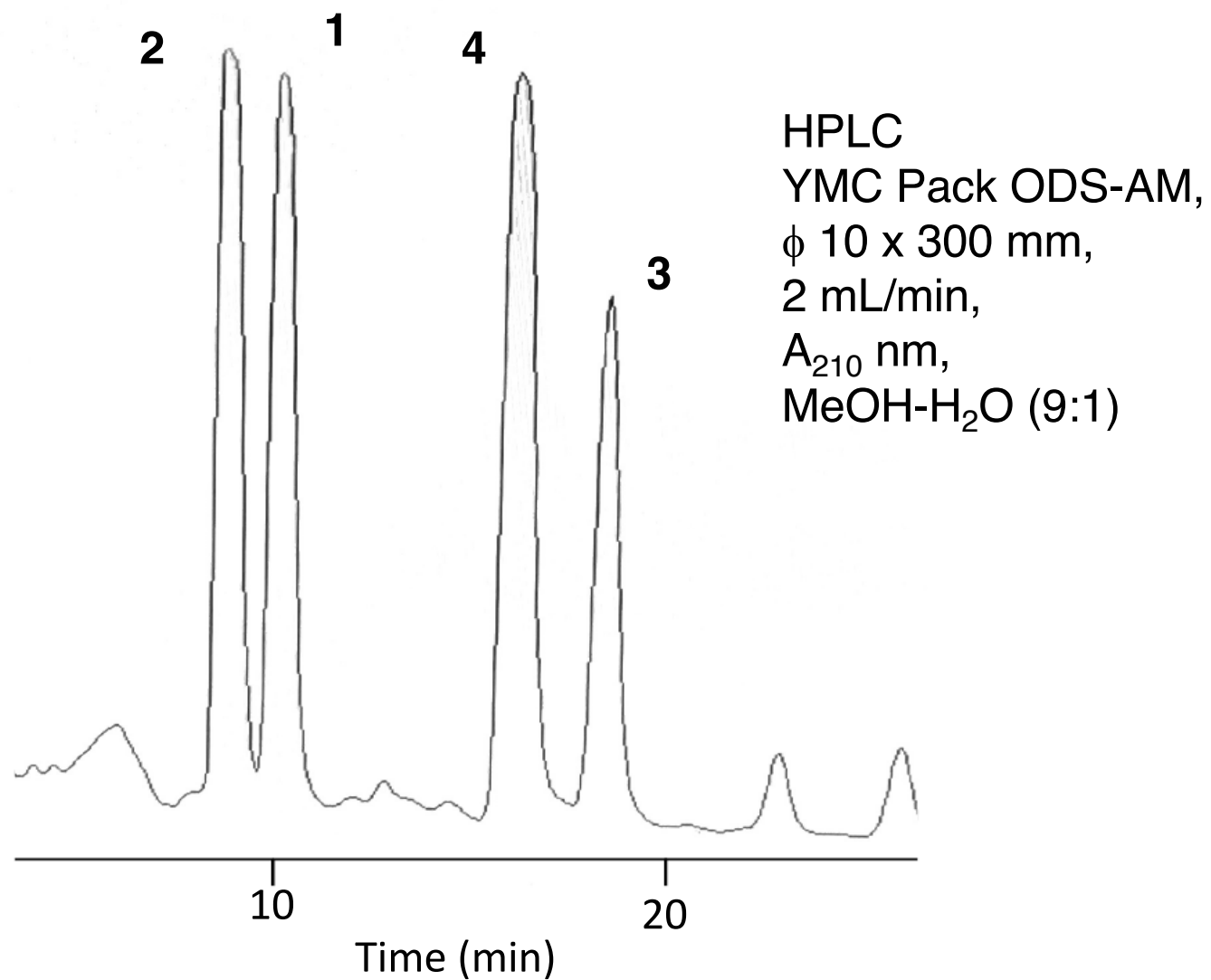


Figure S2. Representative HPLC feature to purify compounds **1-4**.

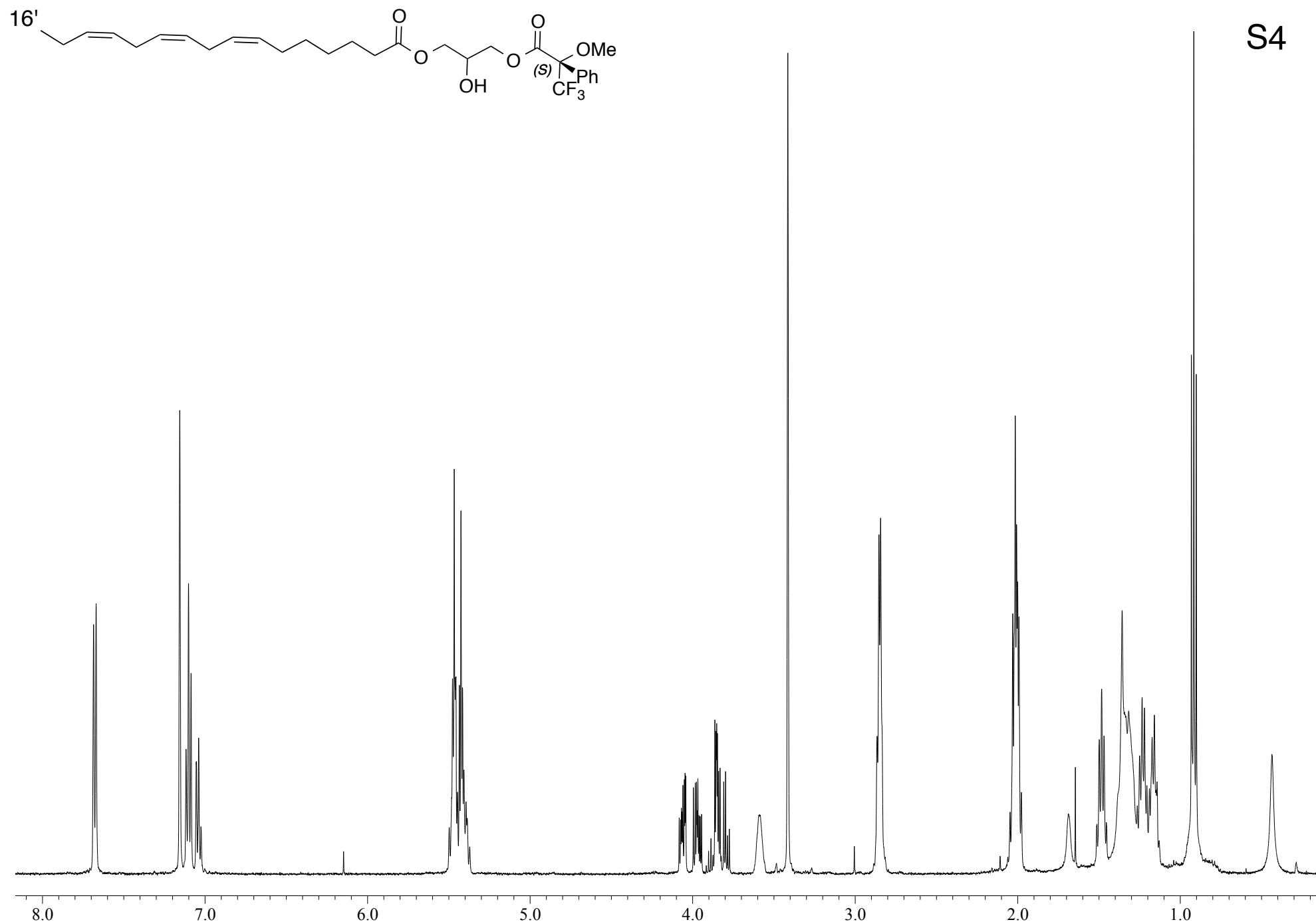


Figure S3. ^1H NMR spectrum of MTPA ester of **1** (500 MHz, benzene-*d*₆)

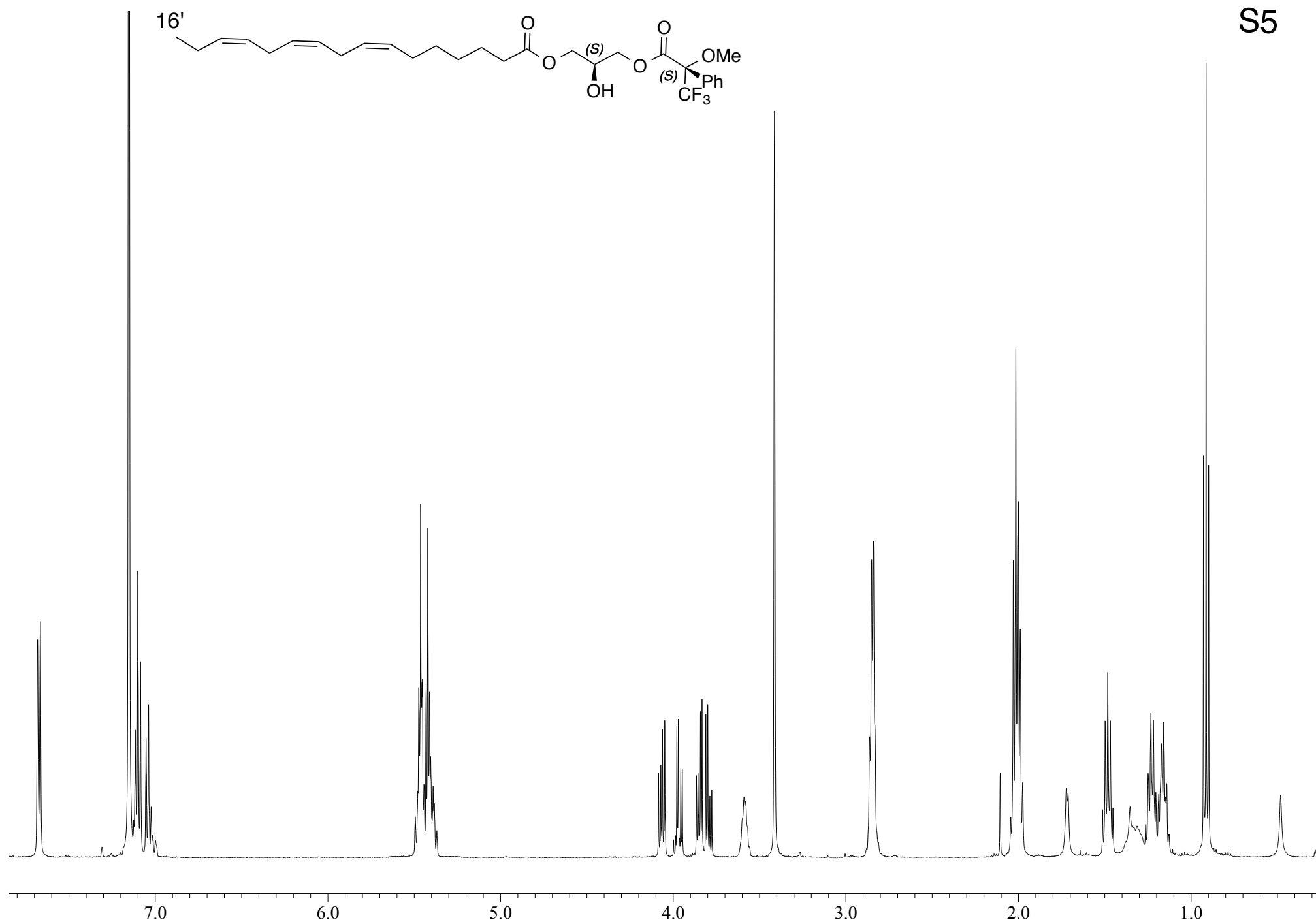
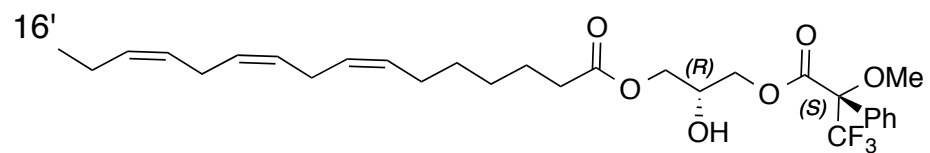


Figure S4. ^1H NMR spectrum of MTPA ester of **1a** (500 MHz, benzene- d_6)



S6

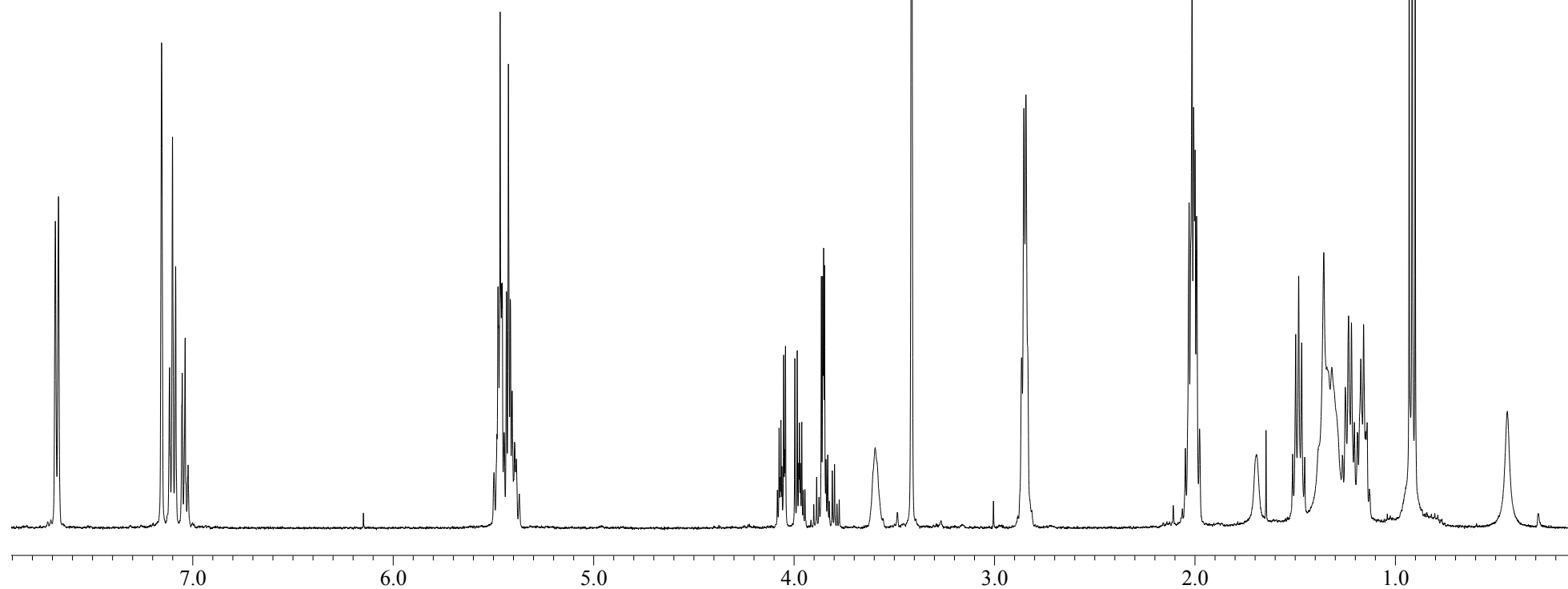


Figure S5. ¹H NMR spectrum of MTPA ester of **1b** (500 MHz, benzene-*d*₆)

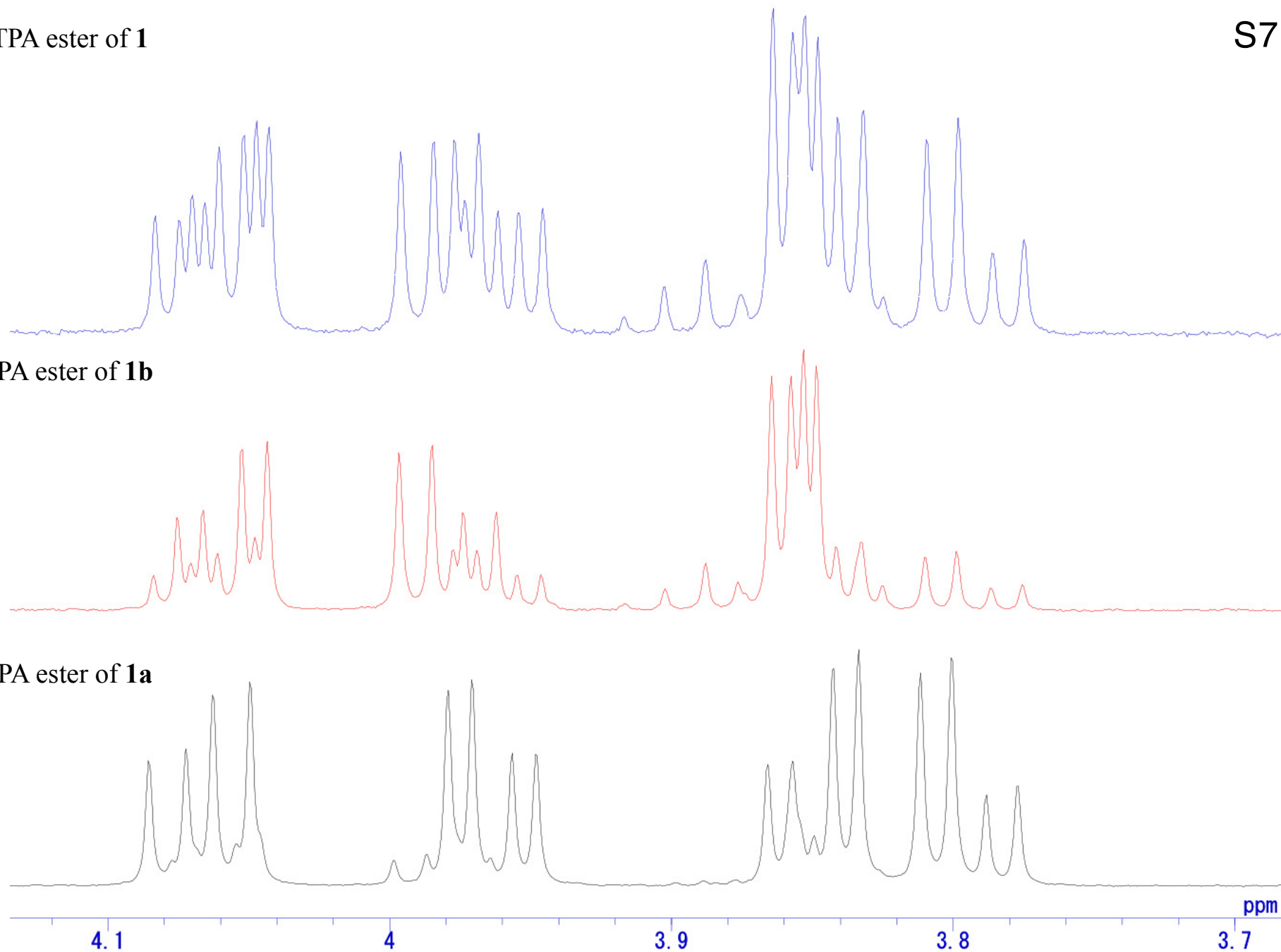
MTPA ester of **1b**MTPA ester of **1a**

Figure S6. Enlarged view of ¹H NMR spectra of MTPA esters of **1**, **1a** and **1b**
(500 MHz, benzene-*d*₆)

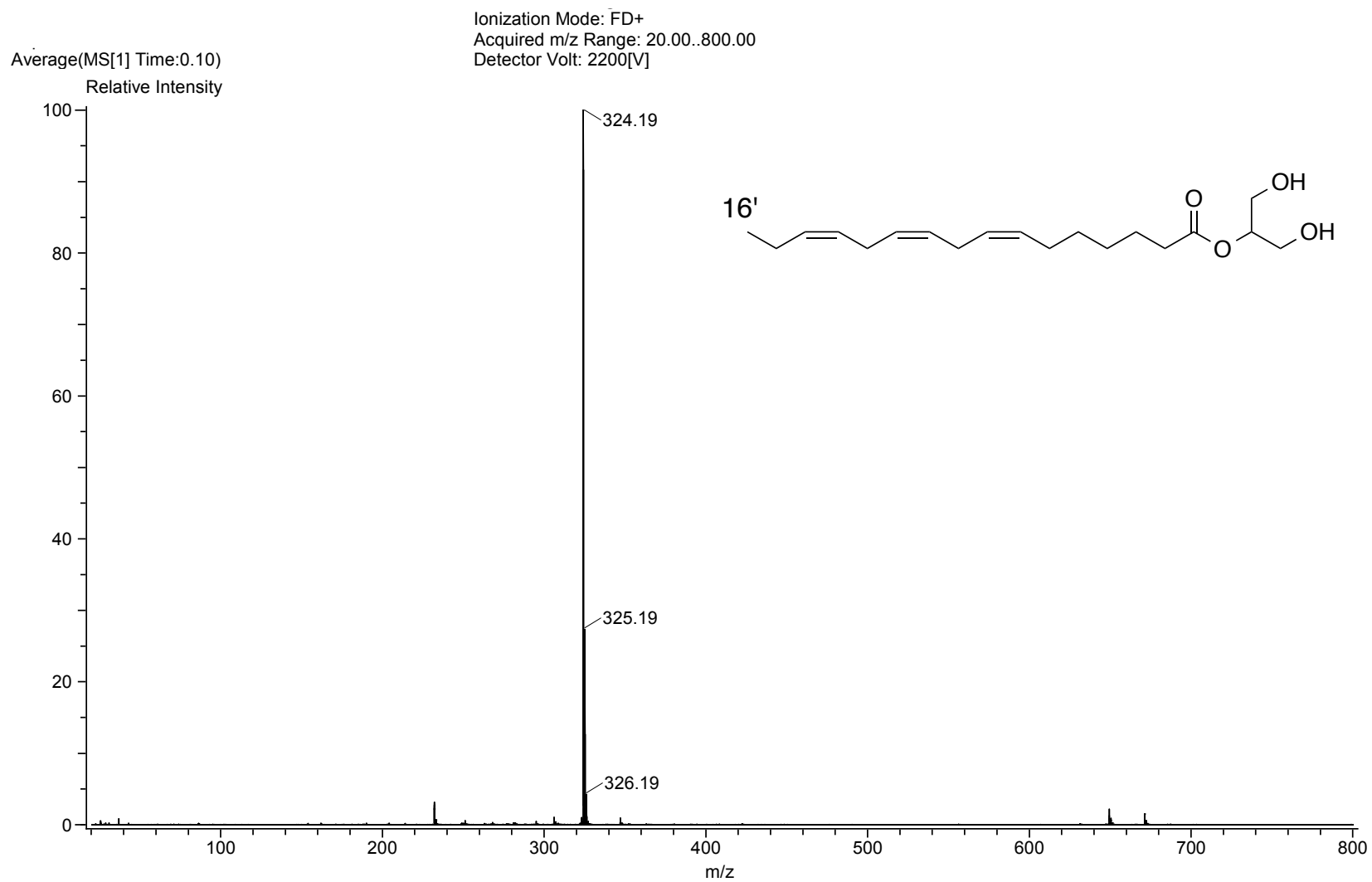


Figure S7. FDMS spectrum of compound **2**

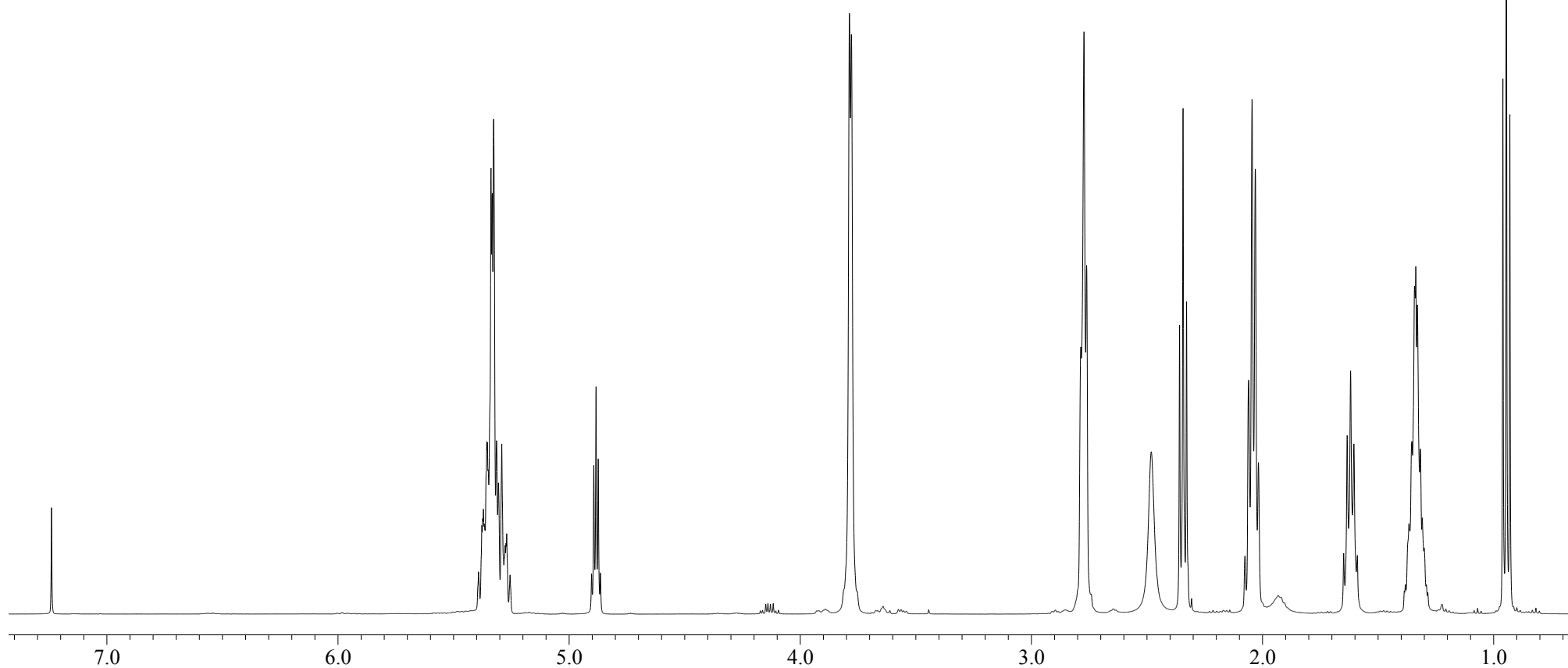
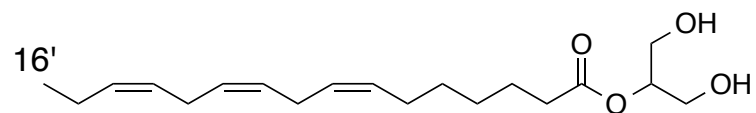


Figure S8. ^1H NMR spectrum of compound **2** (500 MHz, CDCl_3)

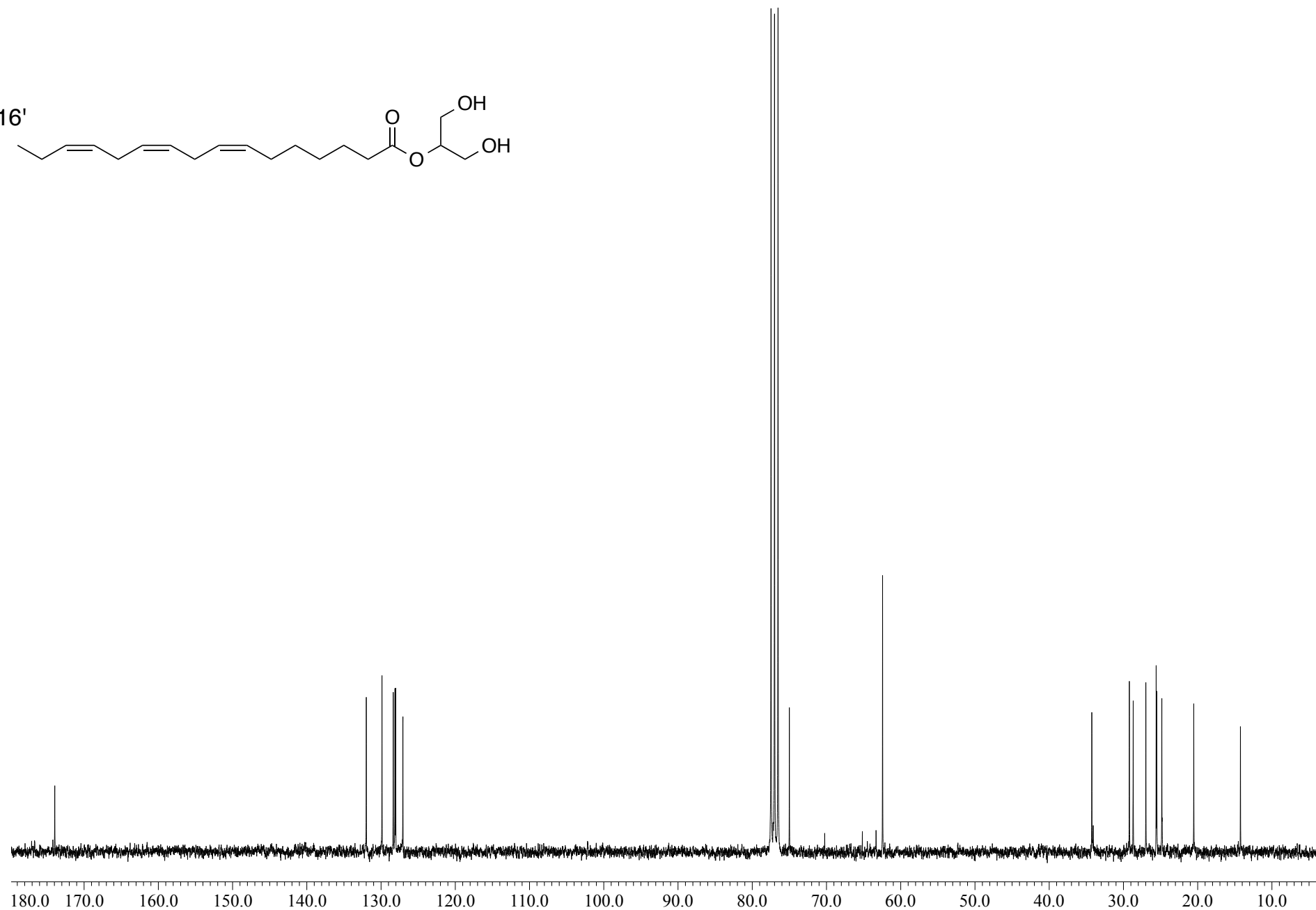
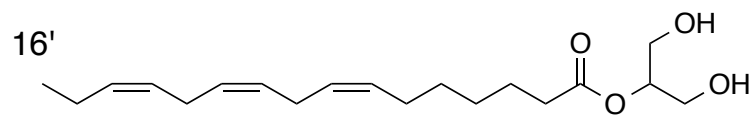
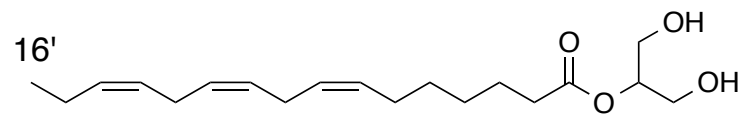


Figure S9. ^{13}C NMR spectra of compound **2** (75 MHz, CDCl_3)



S11

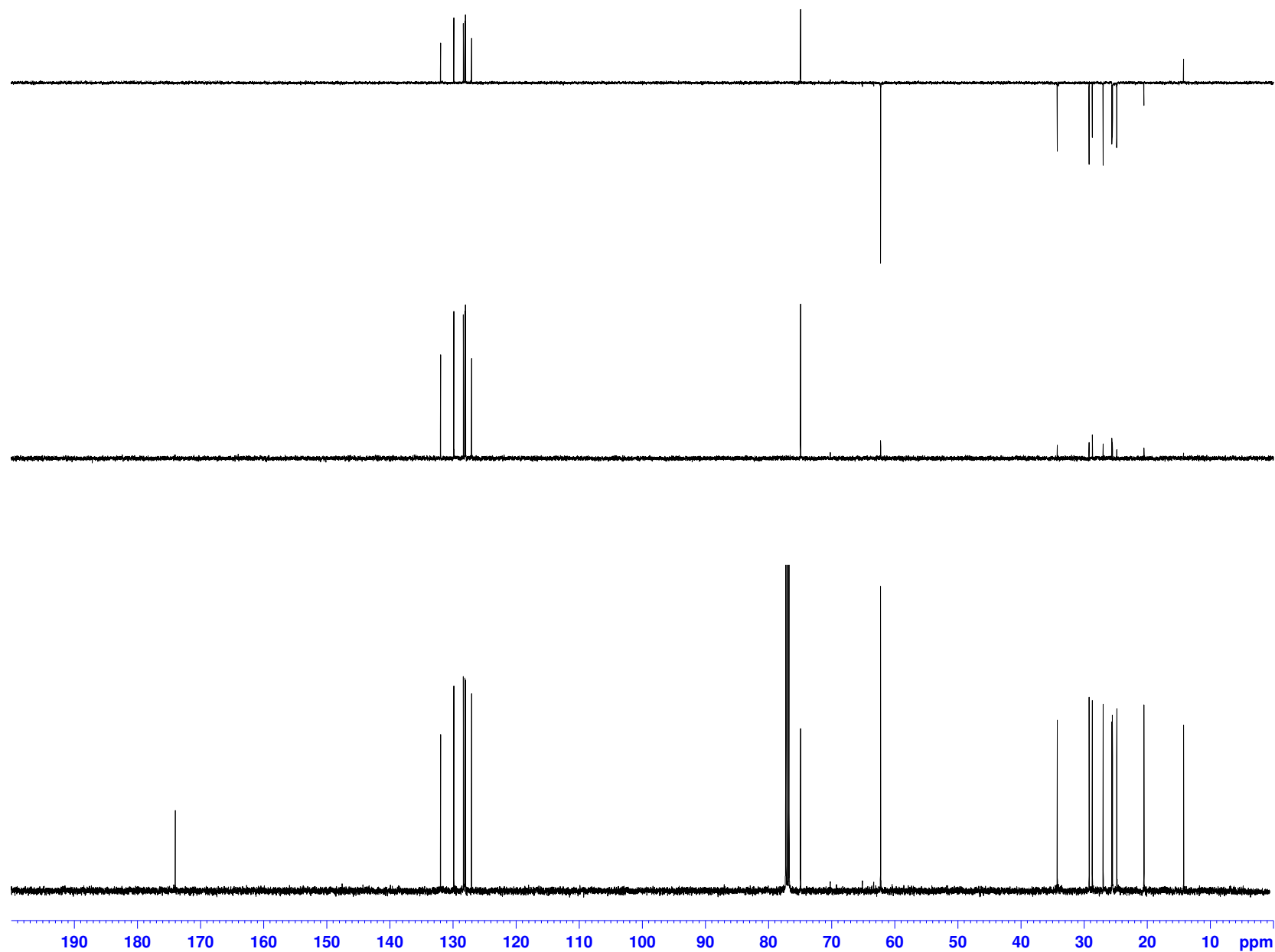
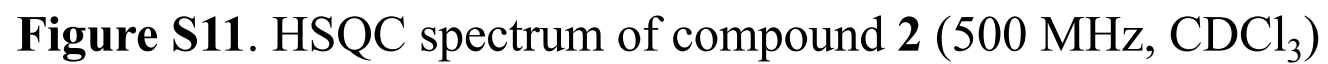
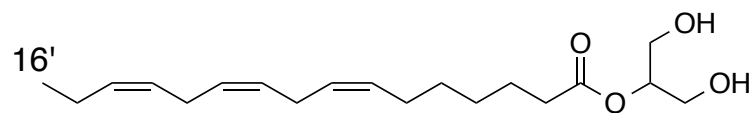


Figure S10. DEPT experiment for compound **2** (126 MHz, CDCl₃)





S13

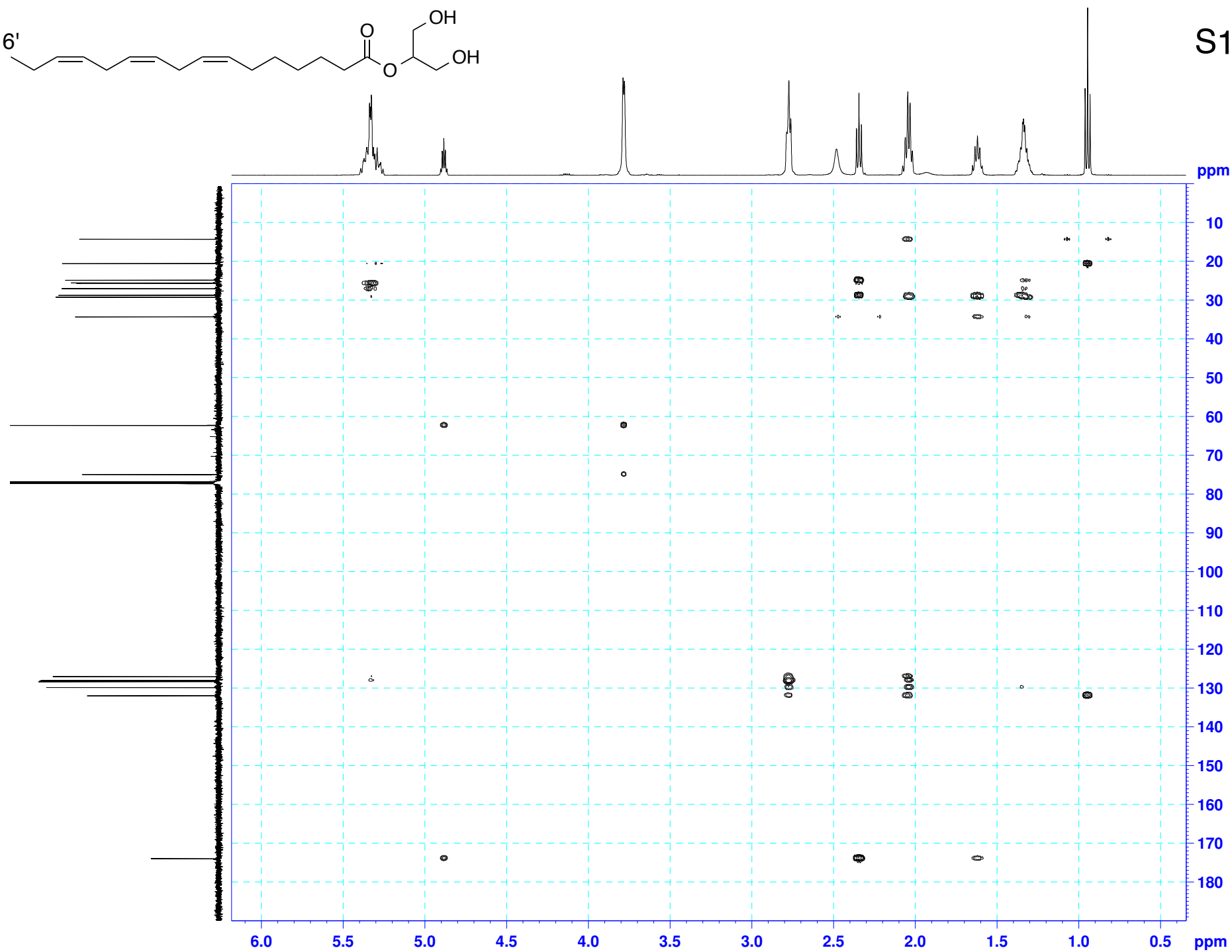
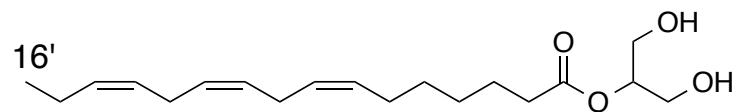


Figure S12. HMBC spectrum of compound **2** (500 MHz, CDCl₃)



S14

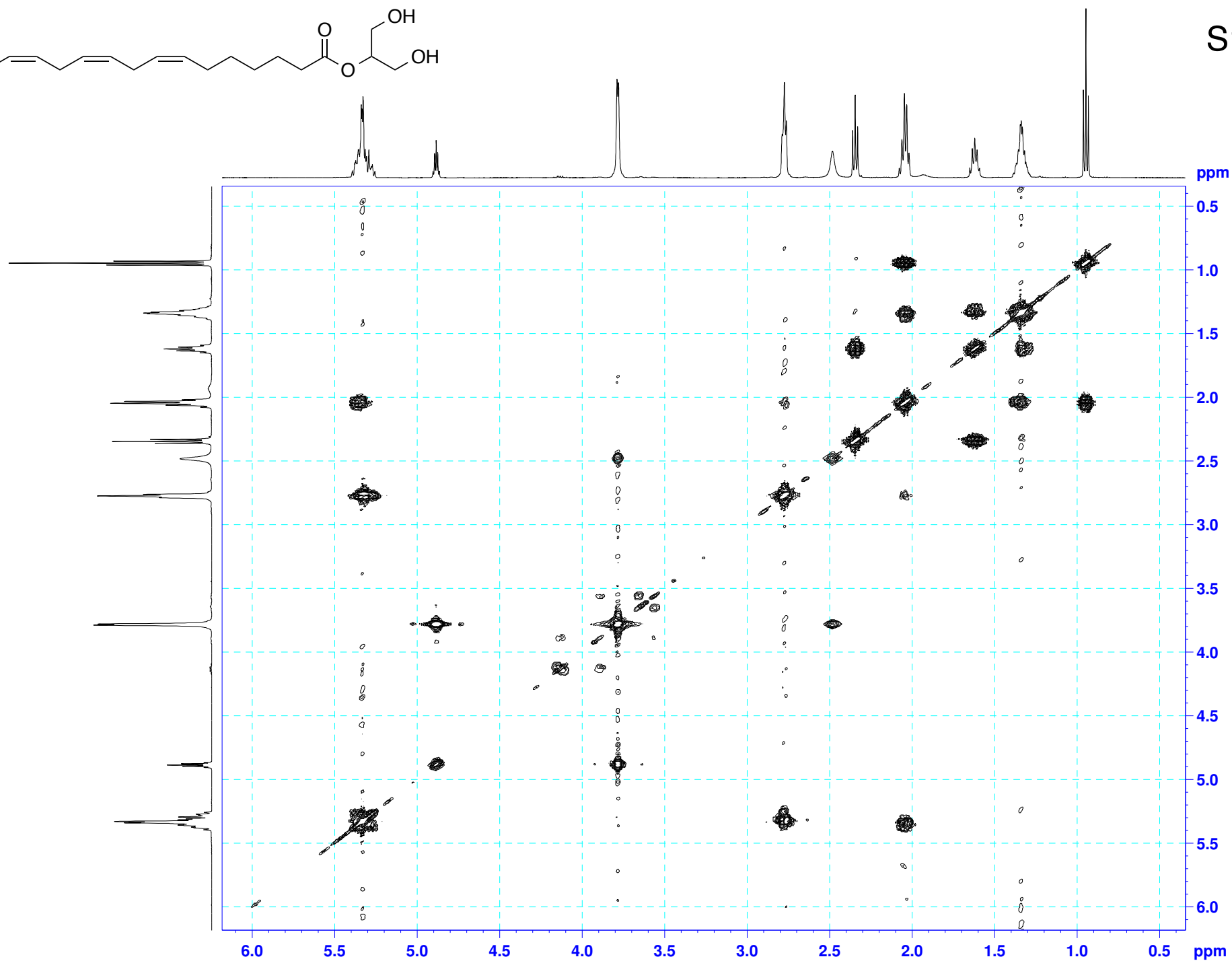


Figure S13. COSY spectrum of compound **2** (270 MHz, CDCl_3)

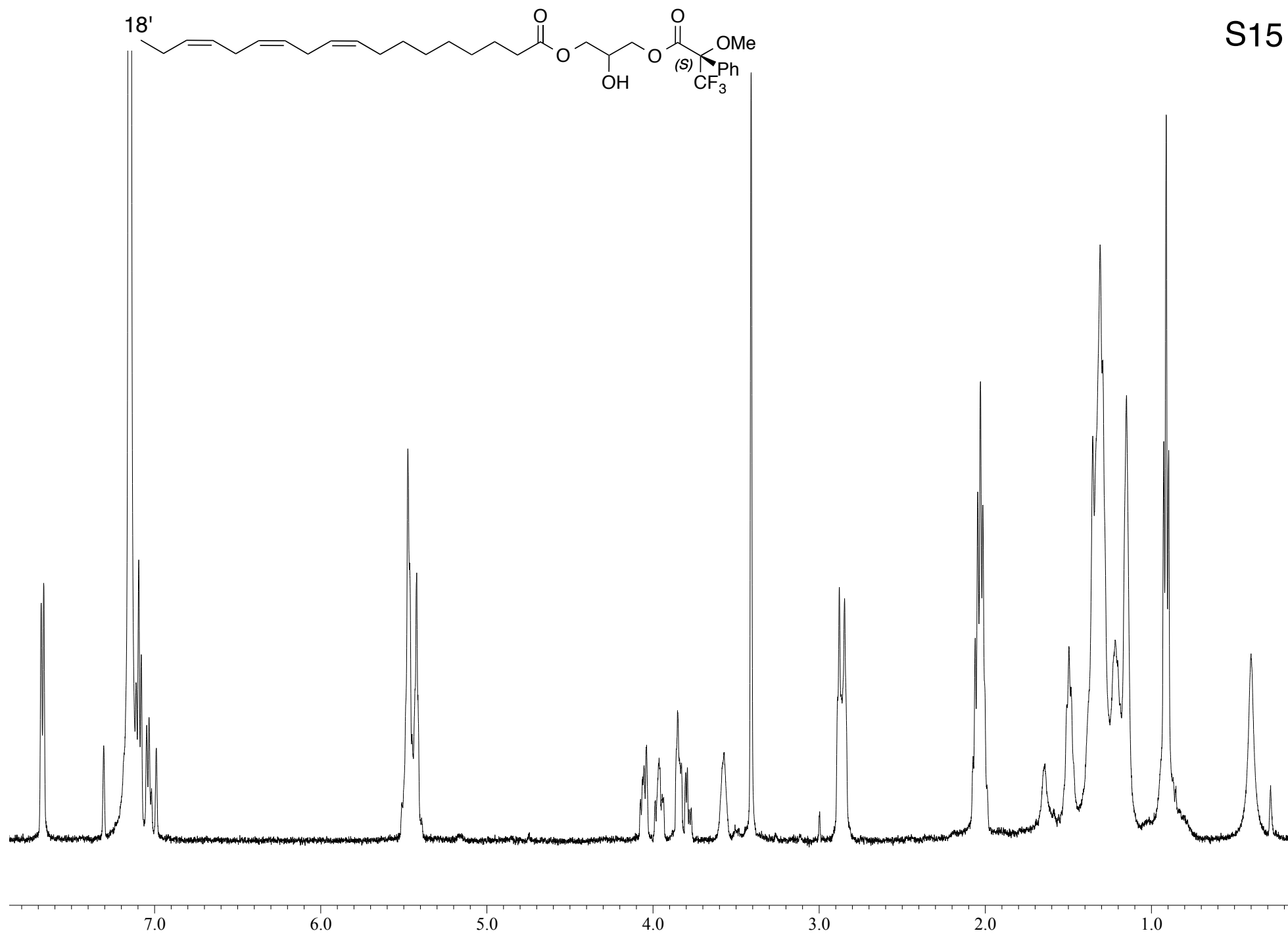


Figure S14. ^1H NMR spectrum of MTPA ester of **3** (500 MHz, benzene- d_6)

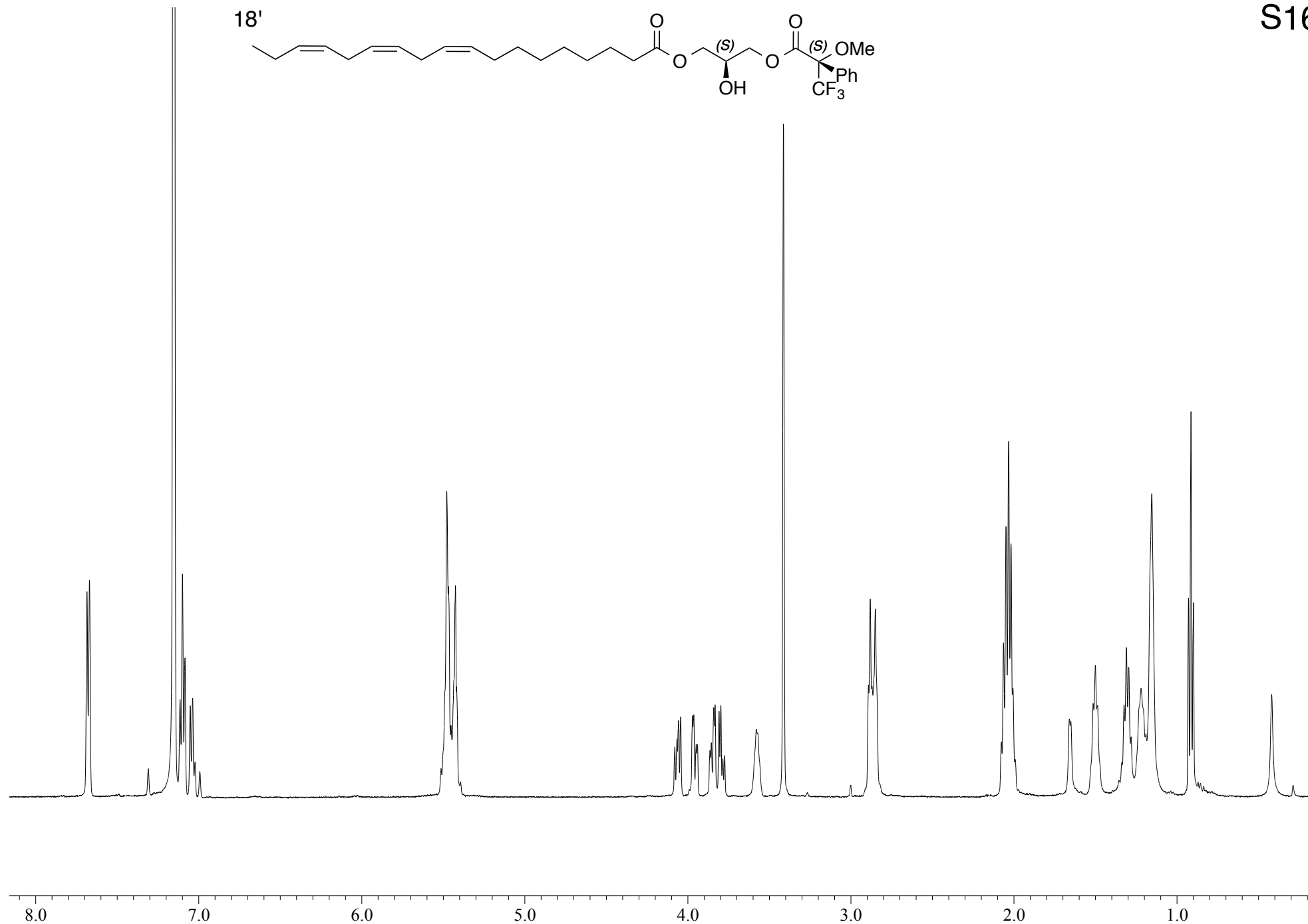


Figure S15. ¹H NMR spectrum of MTPA ester of **3a** (500 MHz, benzene-*d*₆)

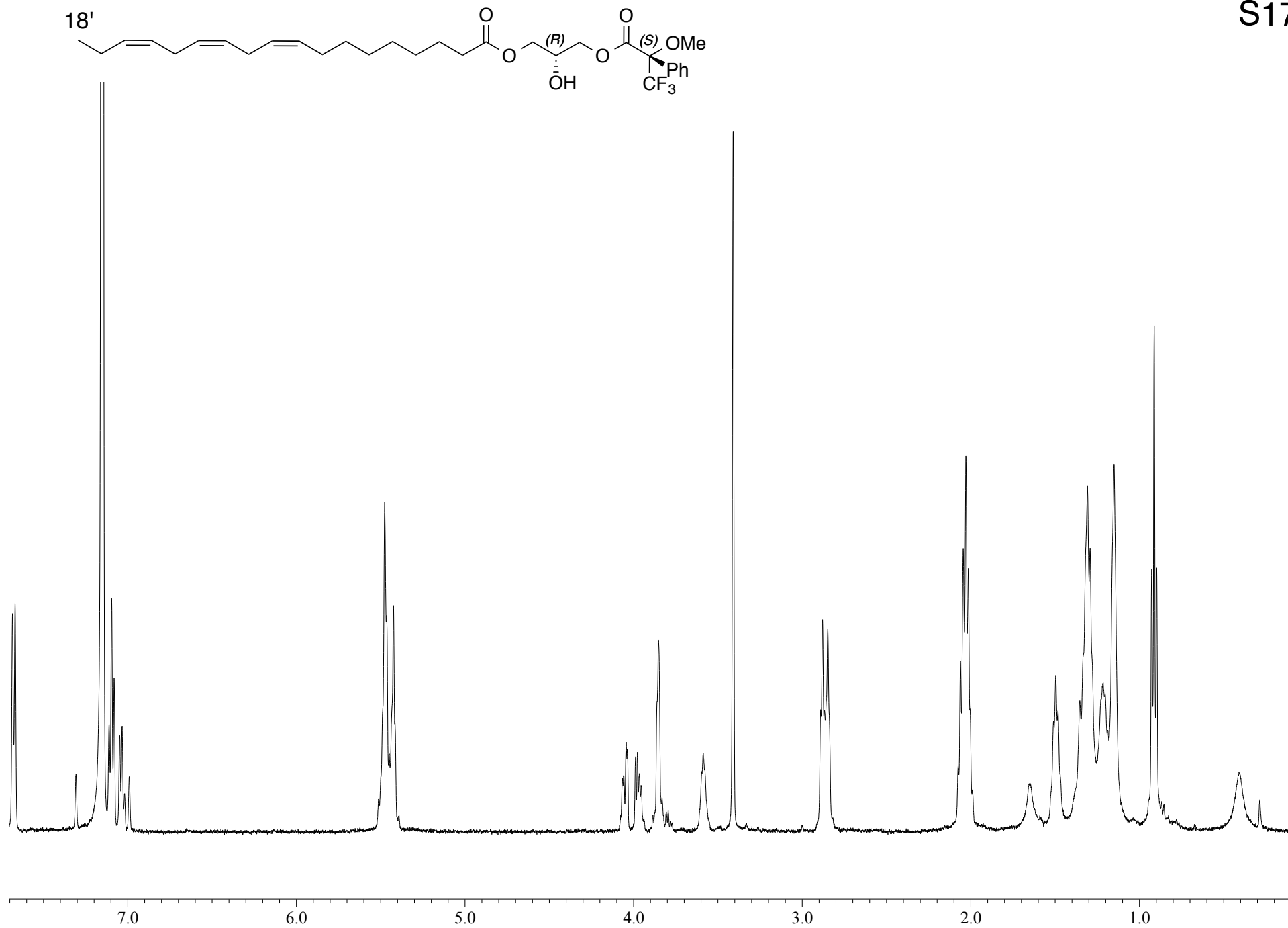


Figure S16. ^1H NMR spectrum of MTPA ester of **3b** (500 MHz, benzene- d_6)

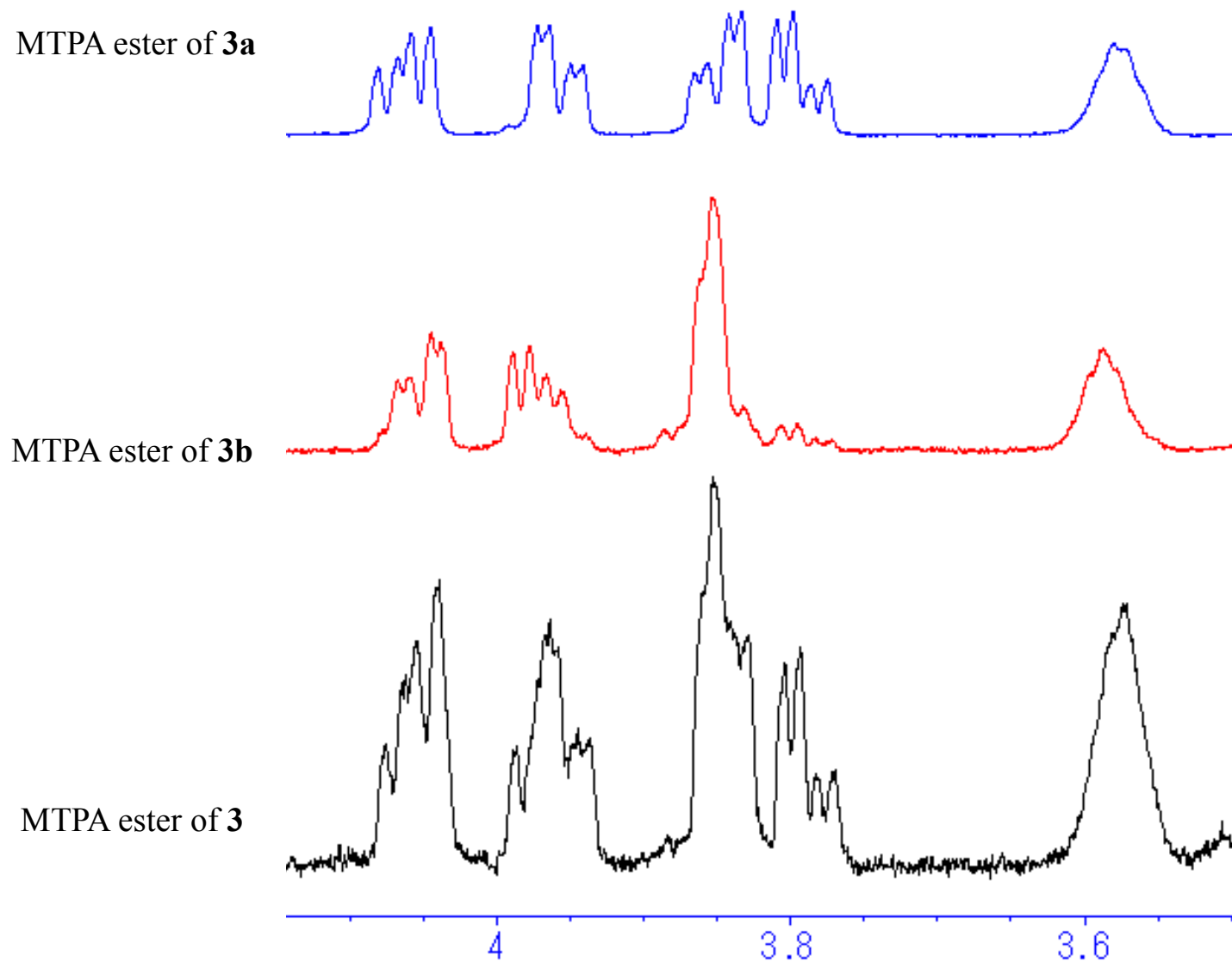
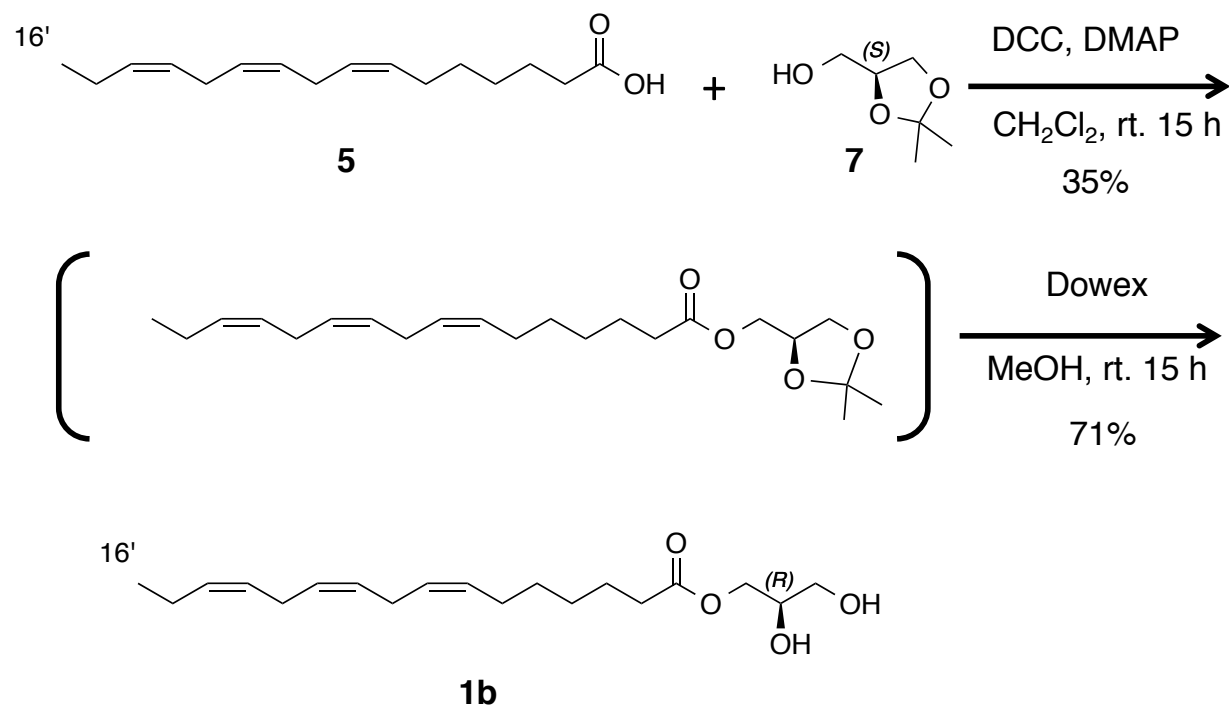
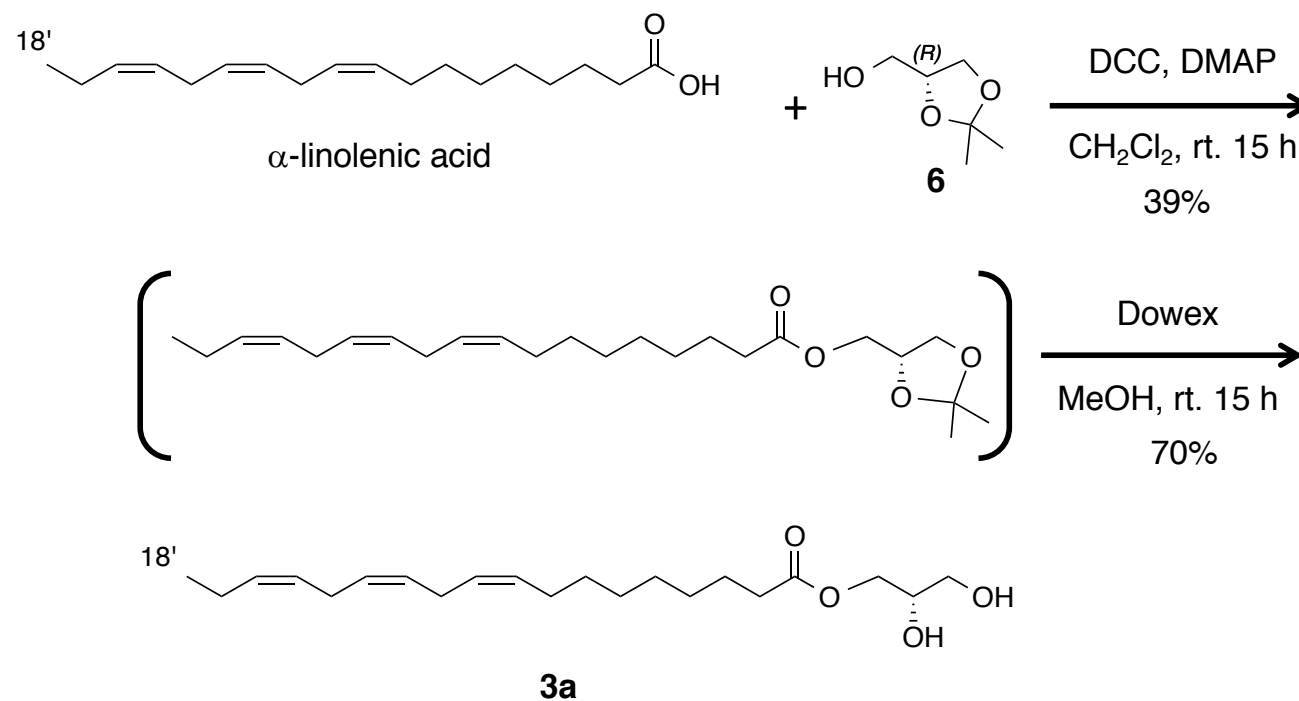


Figure S17. Enlarged view of ¹H NMR spectra of MTPA esters of **3**, **3a** and **3b** (500 MHz, benzene-*d*₆)

Scheme S1. Synthesis (2*R*)- α -(7'*Z*,10'*Z*,13'*Z*)-hexadecatrienoic acid monoglyceride (**1b**)

Scheme S2. Synthesis (2*S*)- α -(7'*Z*,10'*Z*,13'*Z*)-hexadecatrienoic acid monoglyceride (**3a**)

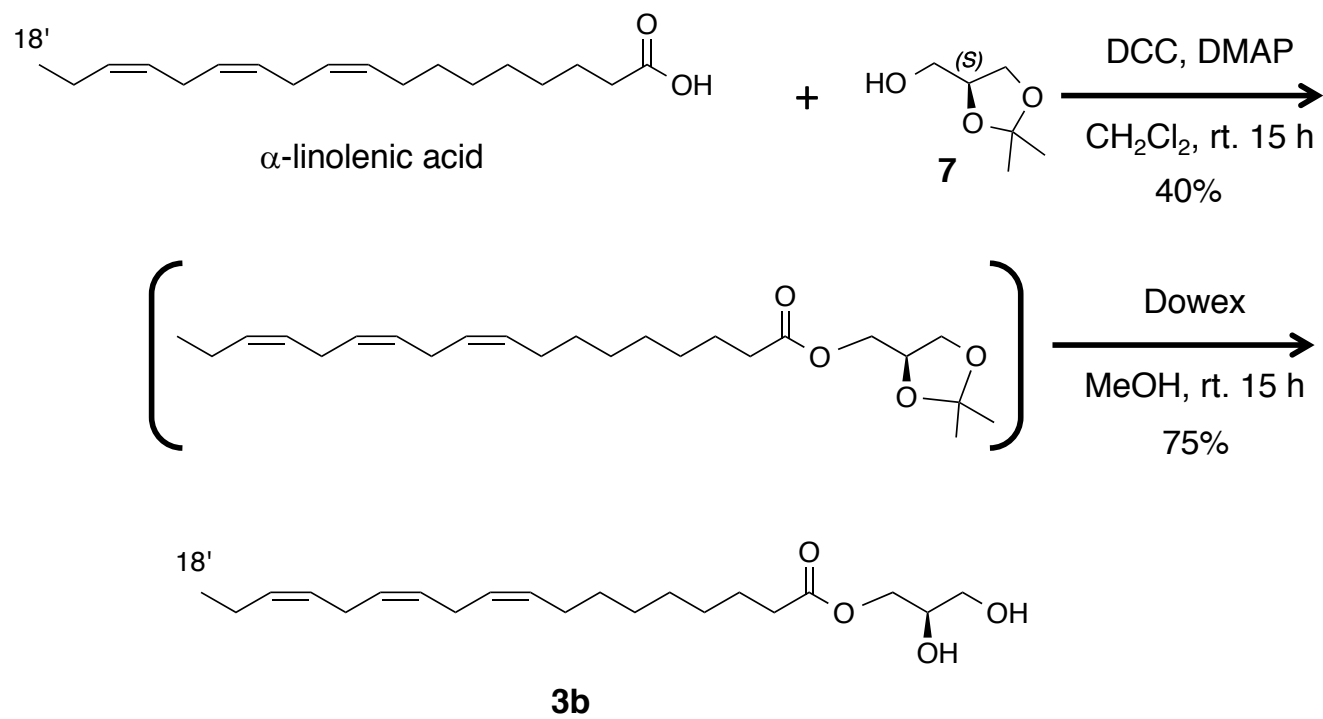
Scheme S3. Synthesis (2*R*)- α -(7'*Z*,10'*Z*,13'*Z*)-hexadecatrienoic acid monoglyceride (**3b**)

Table S1. Conditions of MS Optimization for MRM in Positive Mode

Entry	[M+H] ⁺ (<i>m/z</i>)	Transition ion (<i>m/z</i>)	Cone voltage (V)	Collision energy (eV)
1	325.37	233.14	33	12
8	330.37	233.14	33	12
3	353.37	261.14	33	12
9	358.37	261.14	33	12