

Supporting Information

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Penioctadecatrienoic A: A New Polyketide from Endophytic Fungus *Penicillium pinophilum* J70

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Table of Contents	Page
Figure S1: HR-ESI-MS spectrum of 1 (penioctadecatrienoic A)	2
Figure S2: ¹ H-NMR (600 MHz, CD ₃ OD) spectrum of 1 (penioctadecatrienoic A)	3
Figure S3: ¹³ C-NMR (150 MHz, CD ₃ OD) spectrum of 1 (penioctadecatrienoic A)	4
Figure S4: Enlarged ¹³ C-NMR spectrum of 1 (penioctadecatrienoic A)	4
Figure S5: Enlarged ¹³ C-NMR spectrum of 1 (penioctadecatrienoic A)	5
Figure S6: HSQC spectrum of 1 (penioctadecatrienoic A)	6
Figure S7: ¹ H- ¹ H COSY spectrum of 1 (penioctadecatrienoic A)	7
Figure S8: HMBC spectrum of 1 (penioctadecatrienoic A)	8
Figure S9: Enlarged HMBC correlation of H-3 to C-2 of 1 (penioctadecatrienoic A)	9
Figure S10: NOESY spectrum of 1 (penioctadecatrienoic A)	10
Figure S11: The Scifinder similarity report for new compound 1 (penioctadecatrienoic A)	11
Figure S12: ¹ H-NMR (600 MHz, CDCl ₃) spectrum of 1a (<i>tri</i> -(<i>R</i>)-MPA esters of 1)	12
Figure S13: ¹ H- ¹ H COSY spectrum of 1a (<i>tri</i> -(<i>R</i>)-MPA esters of 1)	13
Figure S14: ¹ H-NMR (600 MHz, CDCl ₃) spectrum of 1b (<i>tri</i> -(<i>S</i>)-MPA esters of 1)	14
Figure S15: ¹ H- ¹ H COSY spectrum of 1b (<i>tri</i> -(<i>S</i>)-MPA esters of 1)	15
Table S1. Comparison of ¹ H and ¹³ C NMR data of 1 with the similar known compound	16

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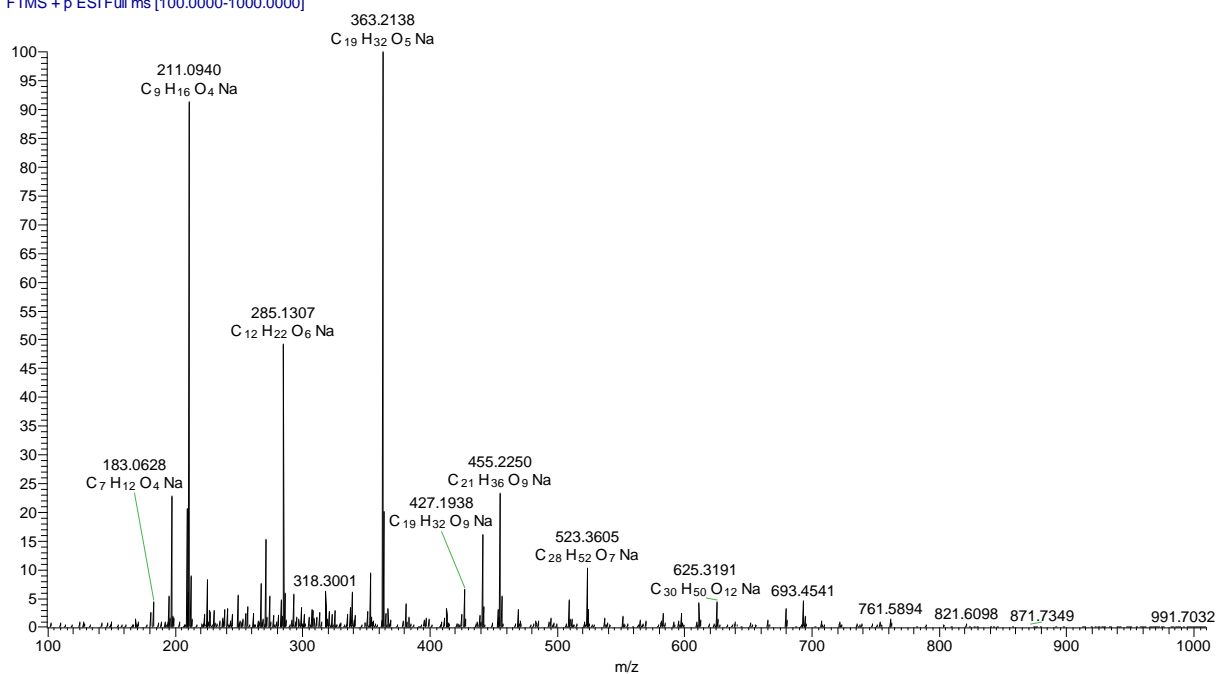
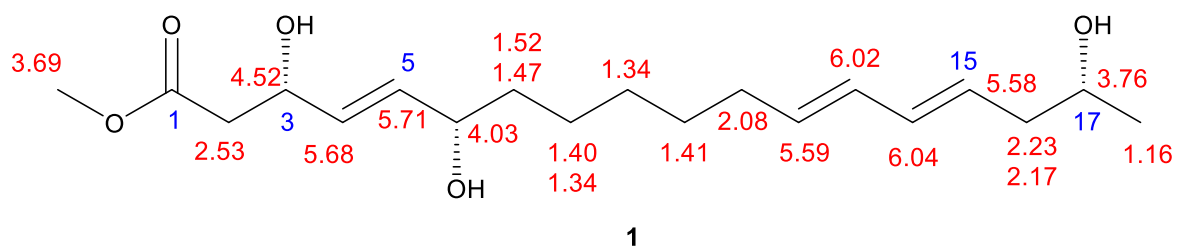


Figure S1: HR-ESI-MS spectrum of **1** (penioctadecatrienoic A)



¹H NMR spectrum of **1** measured in CD₃OD at 600 MHz

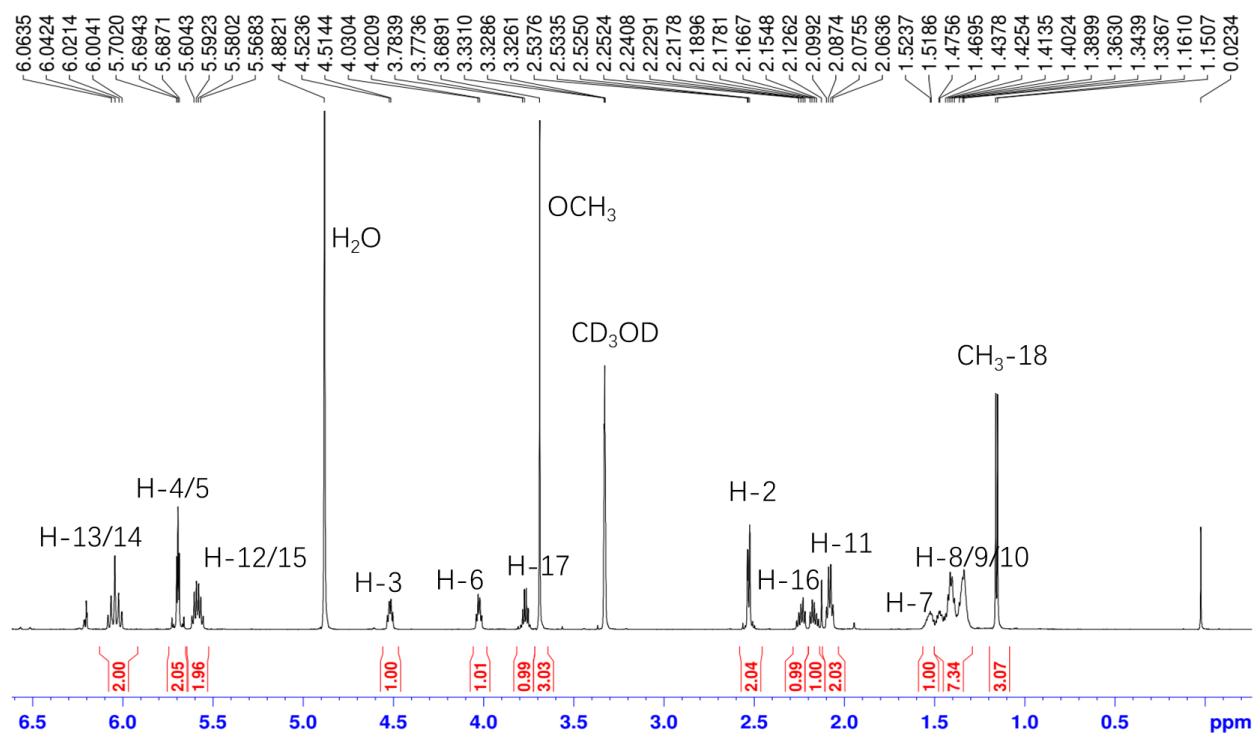


Figure S2: ¹H-NMR (600 MHz, CD₃OD) spectrum of **1** (penioctadecatrienoic A)

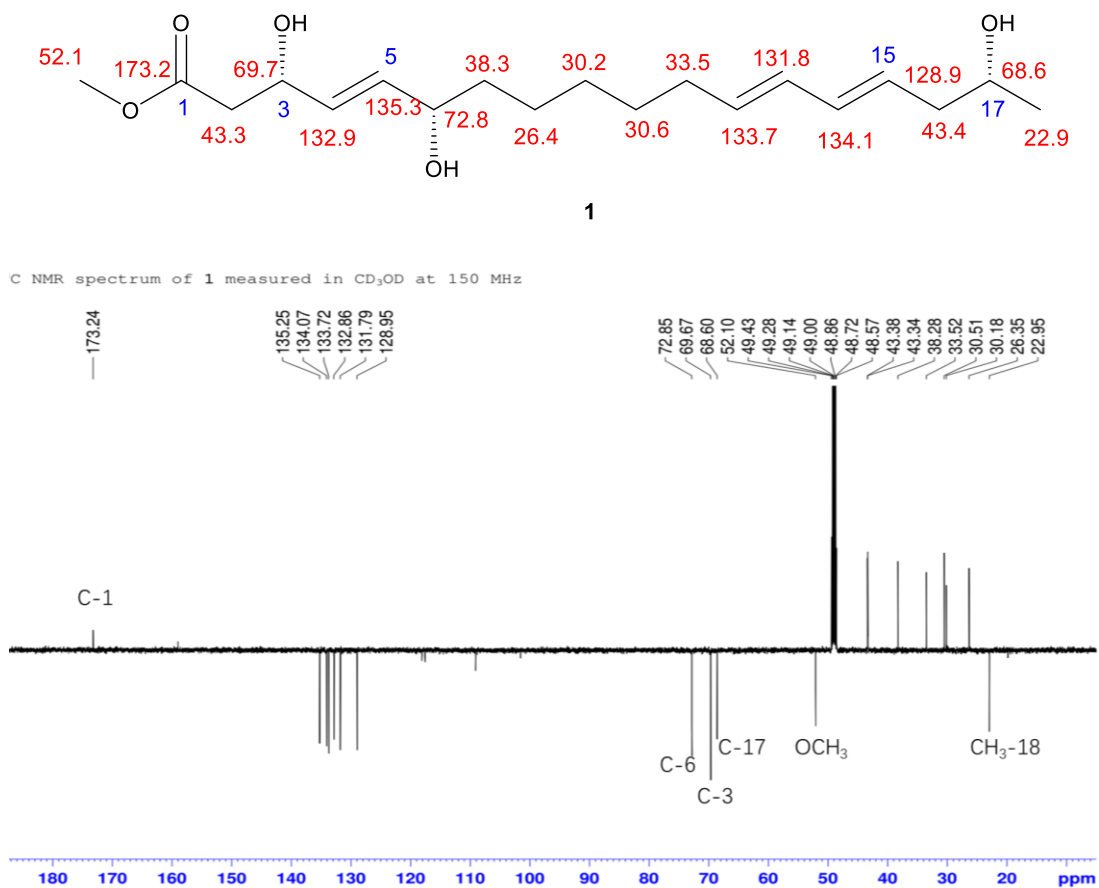


Figure S3: ¹³C-NMR (150 MHz, CD₃OD) spectrum of **1** (penioctadecatrienoic A)

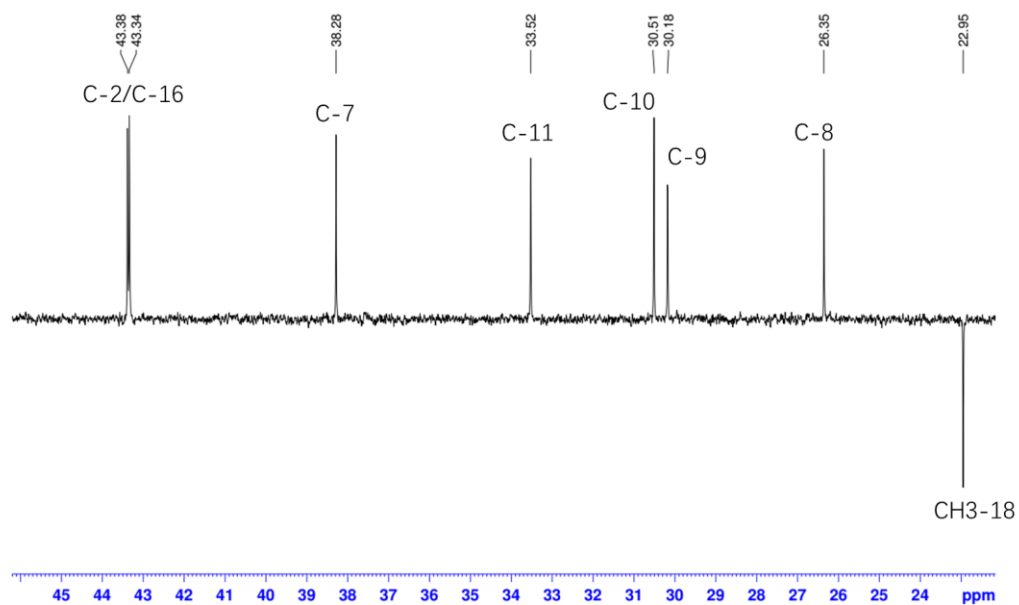


Figure S4: Enlarged ¹³C-NMR spectrum of **1** (penioctadecatrienoic A)

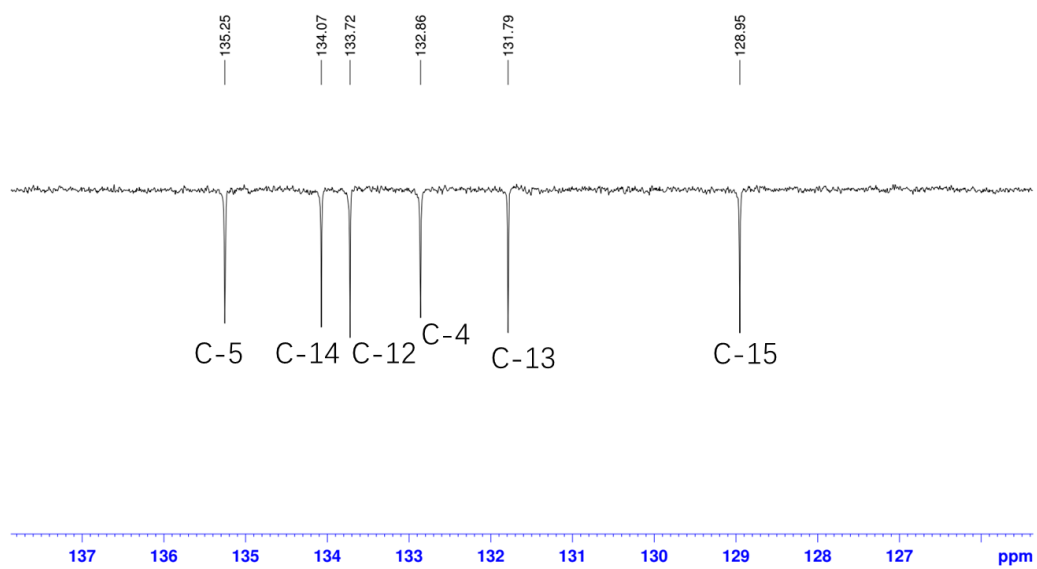


Figure S5: Enlarged ^{13}C -NMR spectrum of **1** (penioctadecatrienoic A)

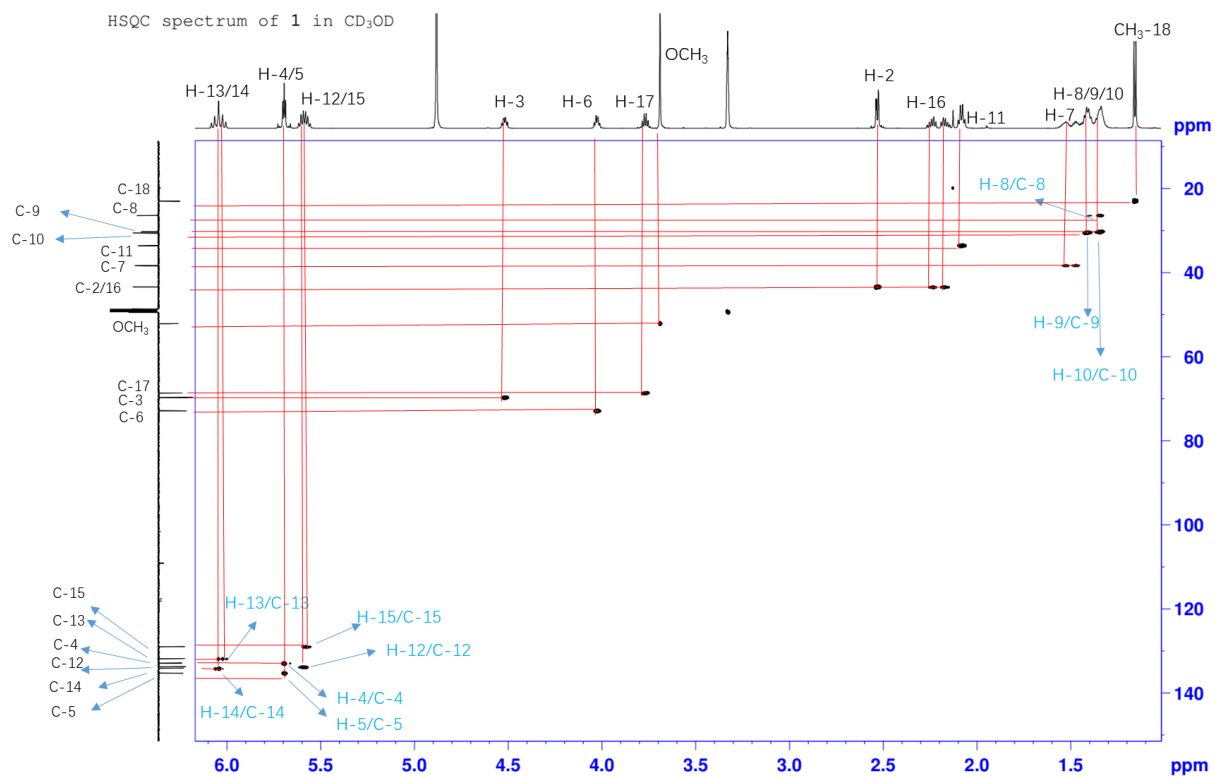
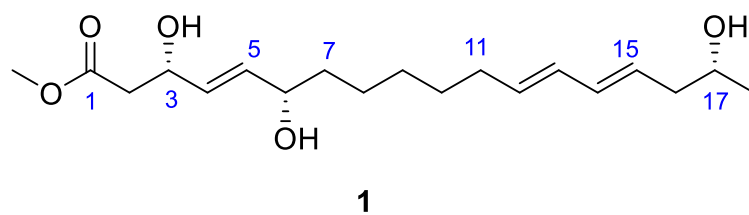
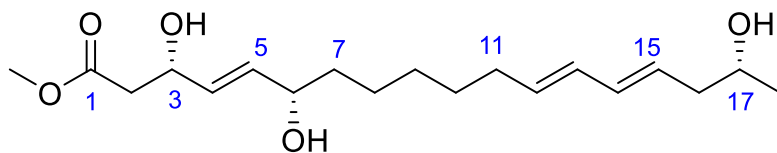


Figure S6: HSQC spectrum of **1** (penioctadecatrienoic A)



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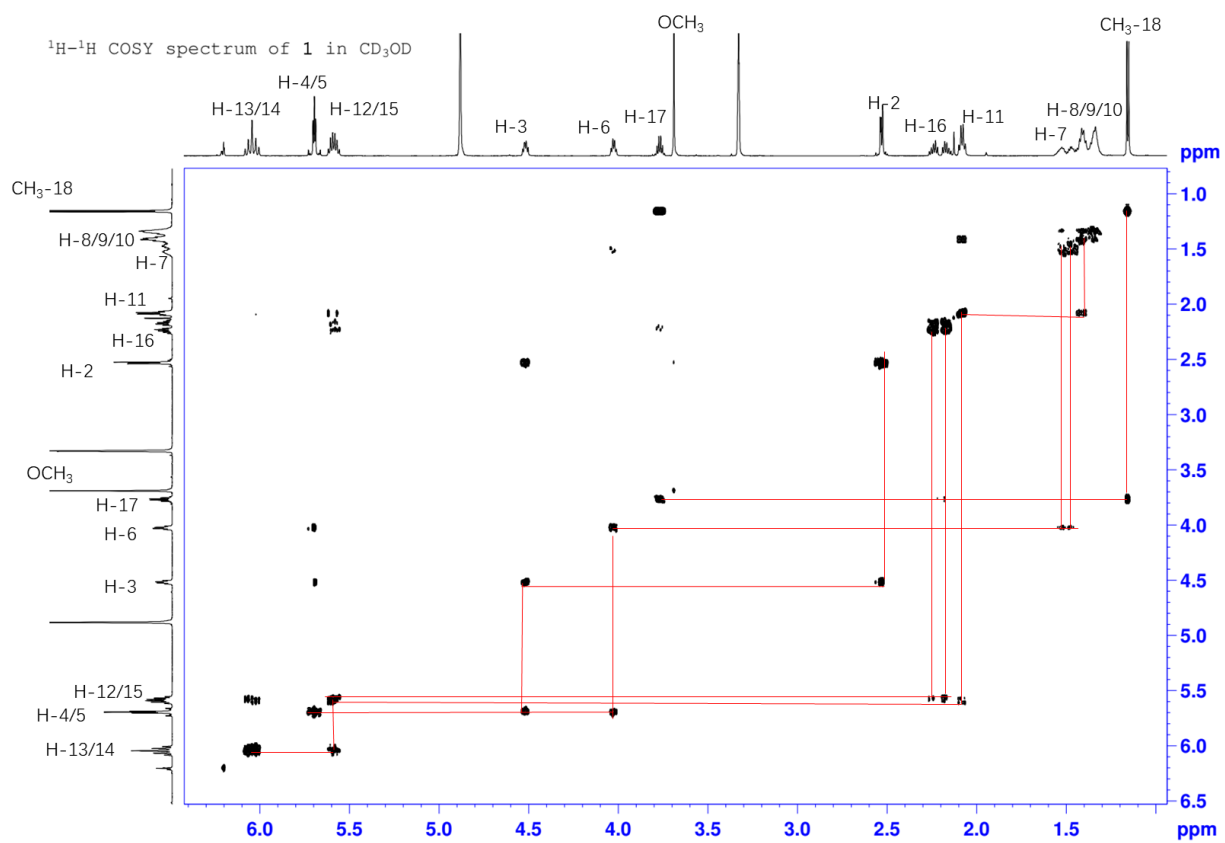
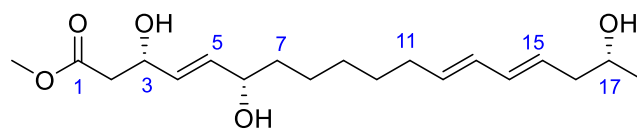


Figure S7: ¹H-¹H COSY spectrum of 1 (penioctadecatrienoic A)



1

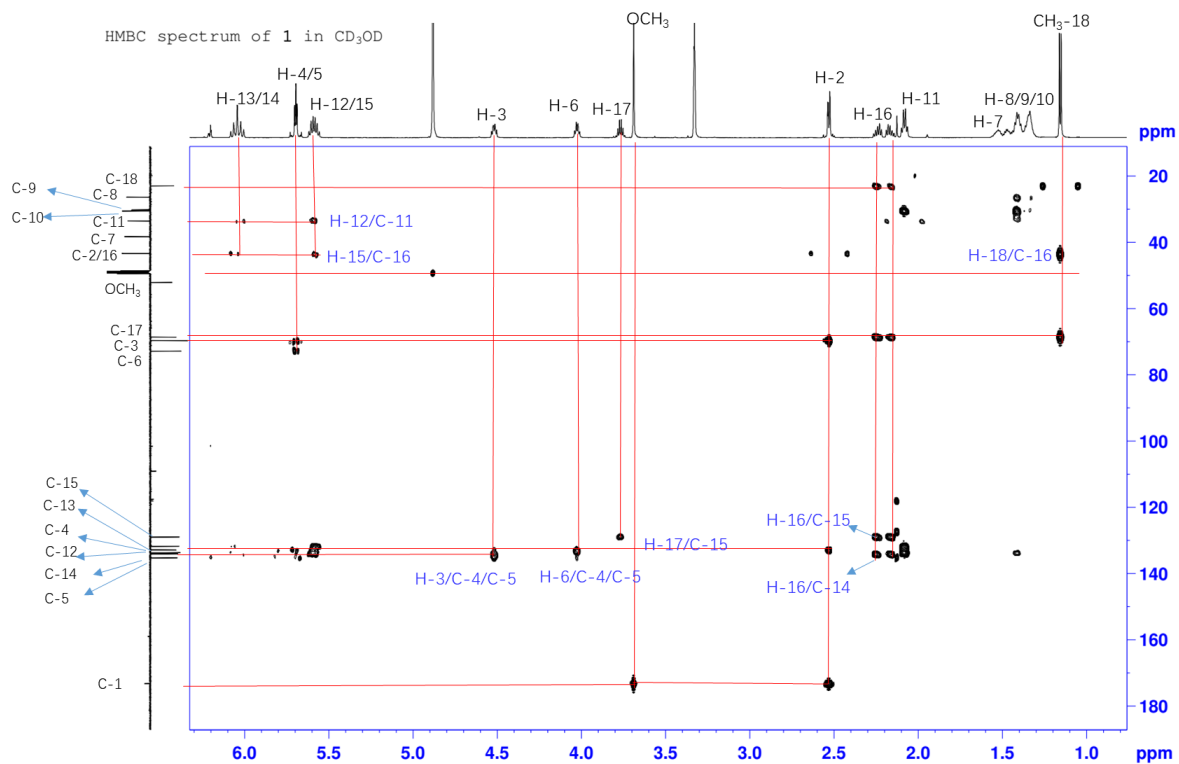


Figure S8: HMBC spectrum of 1 (penioctadecatrienoic A)

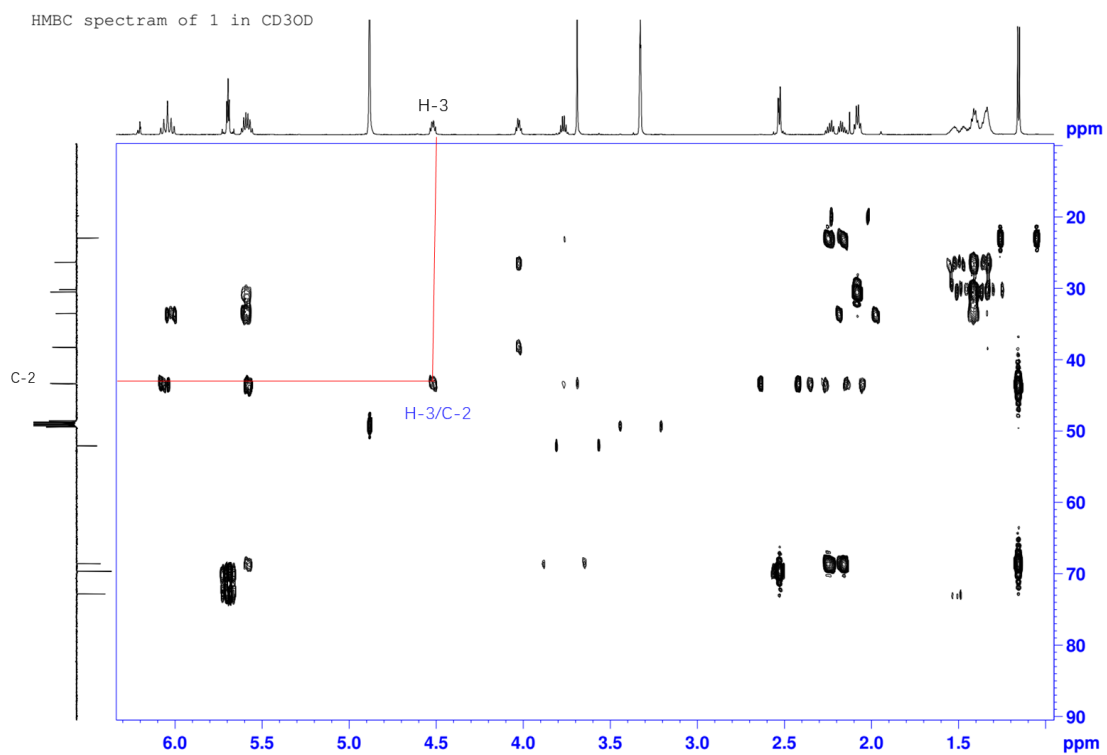
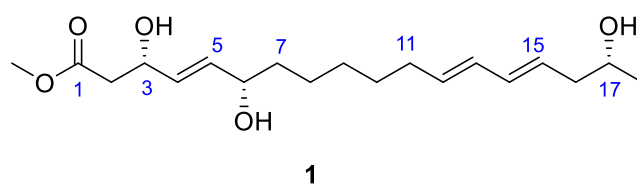
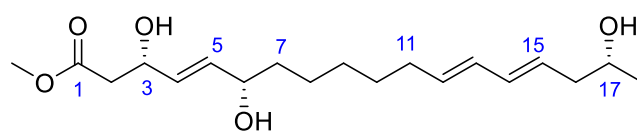


Figure S9: Enlarged HMBC correlation of H-3 to C-2 of **1** (penioctadecatrienoic A)



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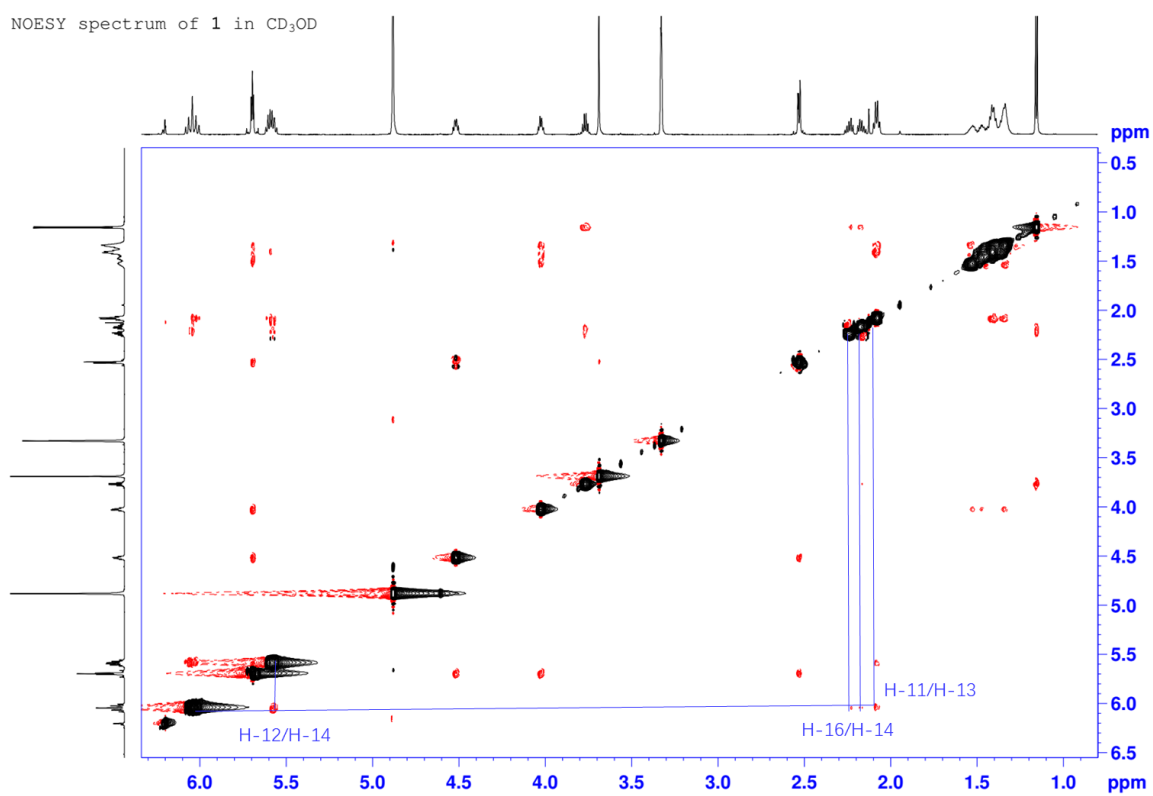
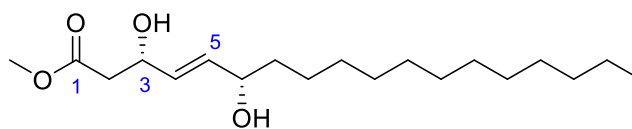


Figure S10: NOESY spectrum of 1 (penioctadecatrienoic A)

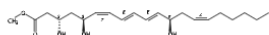


1

Score: 96

1. [157394-88-2](#) 🔍

~2



Double bond geometry as shown.,Absolute stereochemistry.

C₂₁ H₃₄ O₅

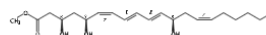
6,8,10,14-Eicosatetraenoic acid, 3,5,12-trihydroxy-, methyl ester, [3*S*-(3*R**,5*R**,6*Z*,8*E*,10*E*,12*S**,14*Z*)]-(9CI)

▶ [Key Physical Properties](#)

Score: 96

2. [157478-55-2](#) 🔍

~2



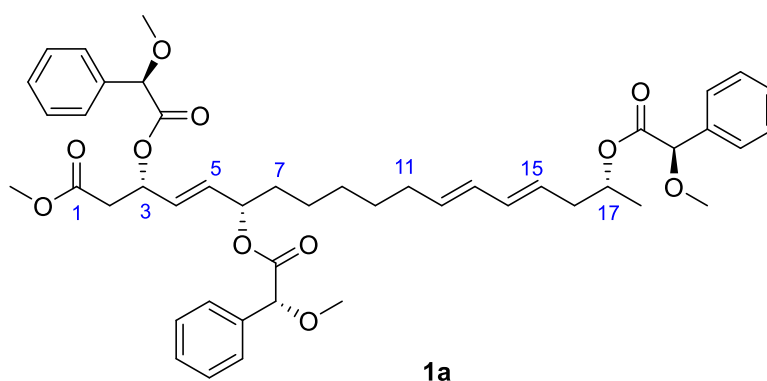
Double bond geometry as shown.,Absolute stereochemistry.

C₂₁ H₃₄ O₅

6,8,10,14-Eicosatetraenoic acid, 3,5,12-trihydroxy-, methyl ester, [3*R*-(3*R**,5*S**,6*Z*,8*E*,10*E*,12*R**,14*Z*)]-(9CI)

▶ [Key Physical Properties](#)

Figure S11: The Scifinder similarity report for new compound **1** (penioctadecatrienoic A)



¹H NMR spectrum of 1a measured in CDCl₃ at 600 MHz

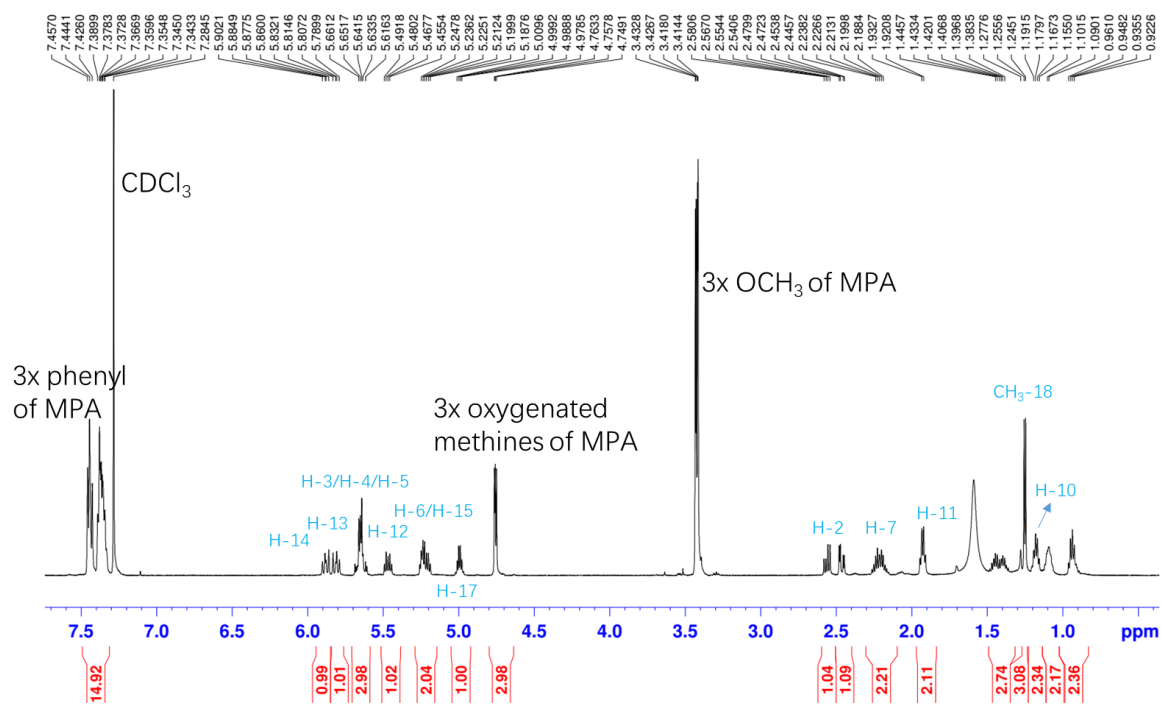
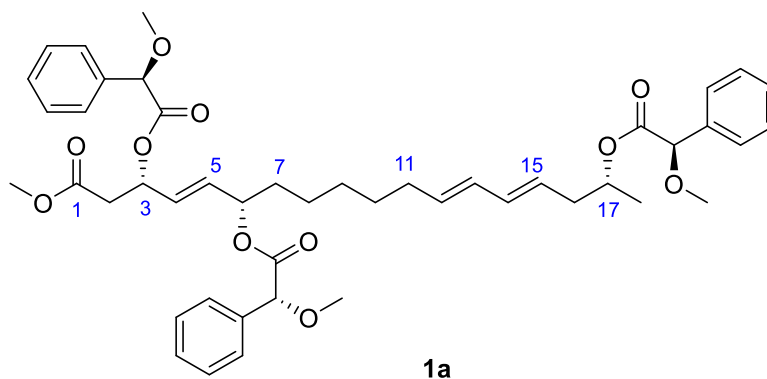


Figure S12: ¹H-NMR (600 MHz, CDCl₃) spectrum of **1a** (*tri-(R)*-MPA esters of **1**)



^1H - ^1H COSY spectrum of **1a** measured in CDCl_3

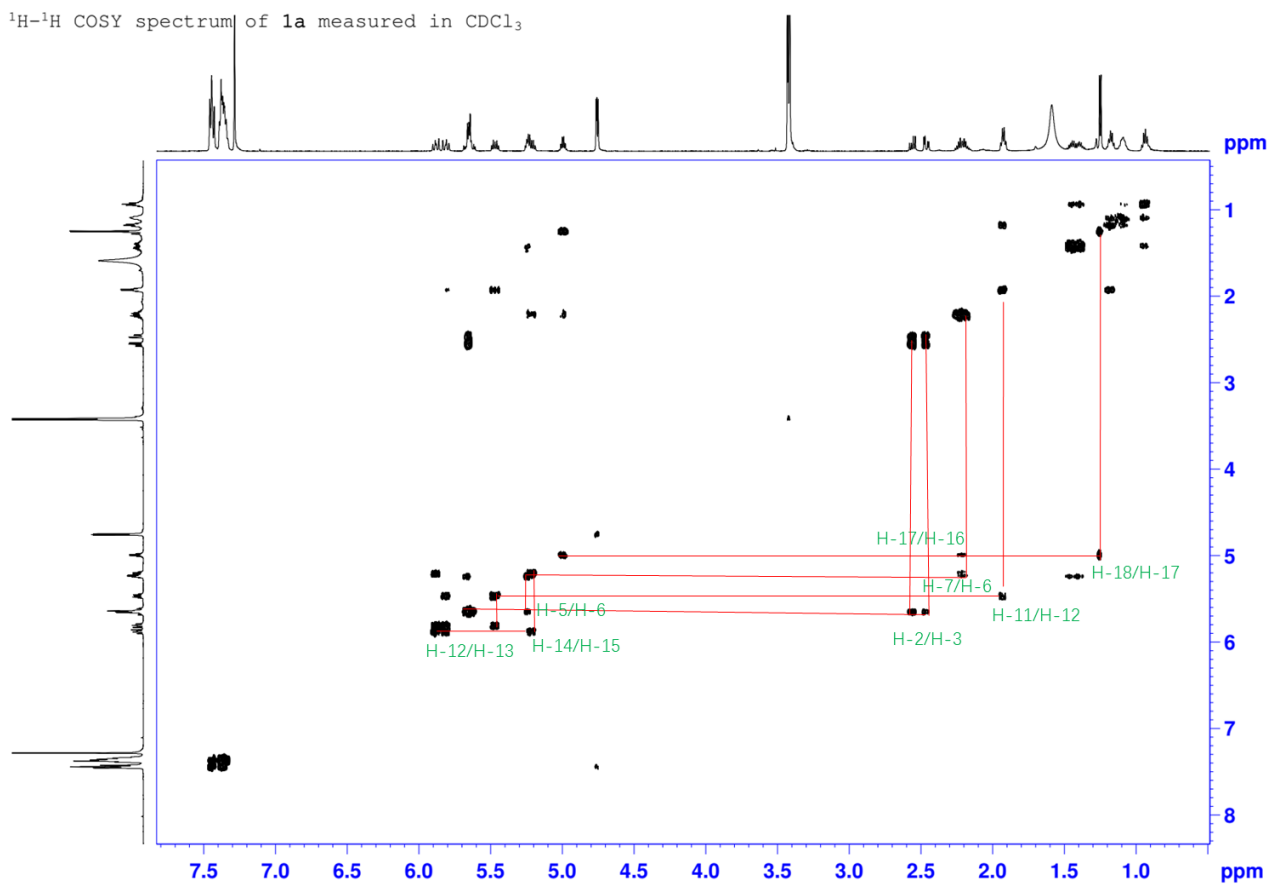
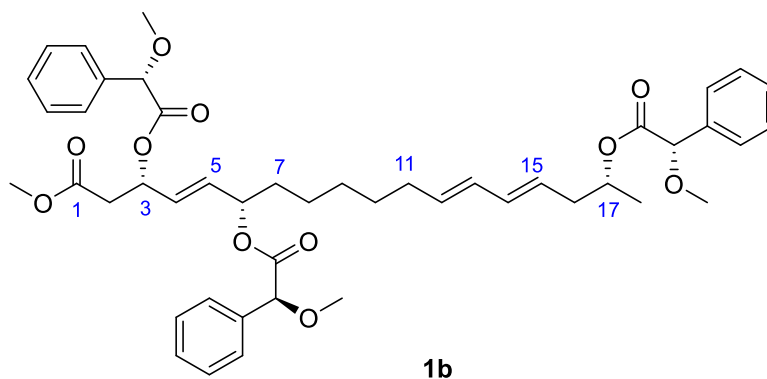


Figure S13: ^1H - ^1H COSY spectrum of **1a** (*tri*-(*R*)-MPA esters of **1**)



¹H NMR spectrum of **1b** measured in CDCl₃ at 600 MHz

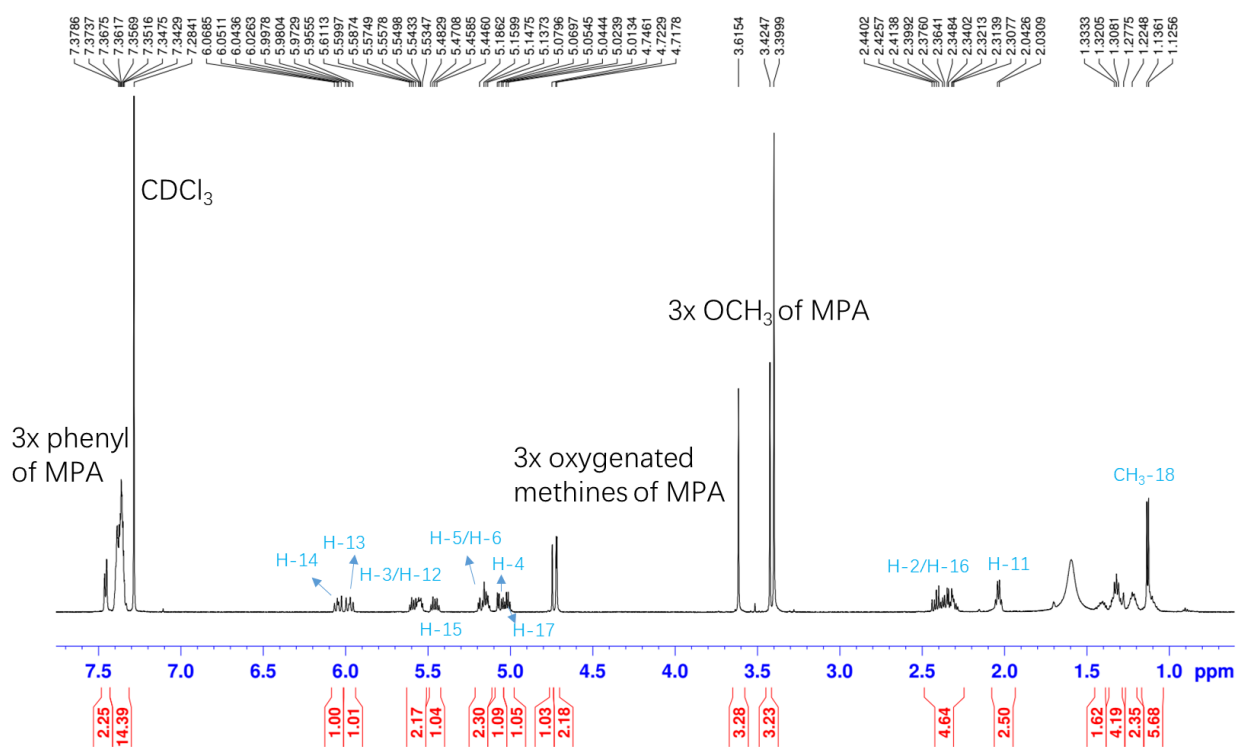


Figure S14: ¹H-NMR (600 MHz, CDCl₃) spectrum of **1b** (*tri*-(*S*)-MPA esters of **1**)

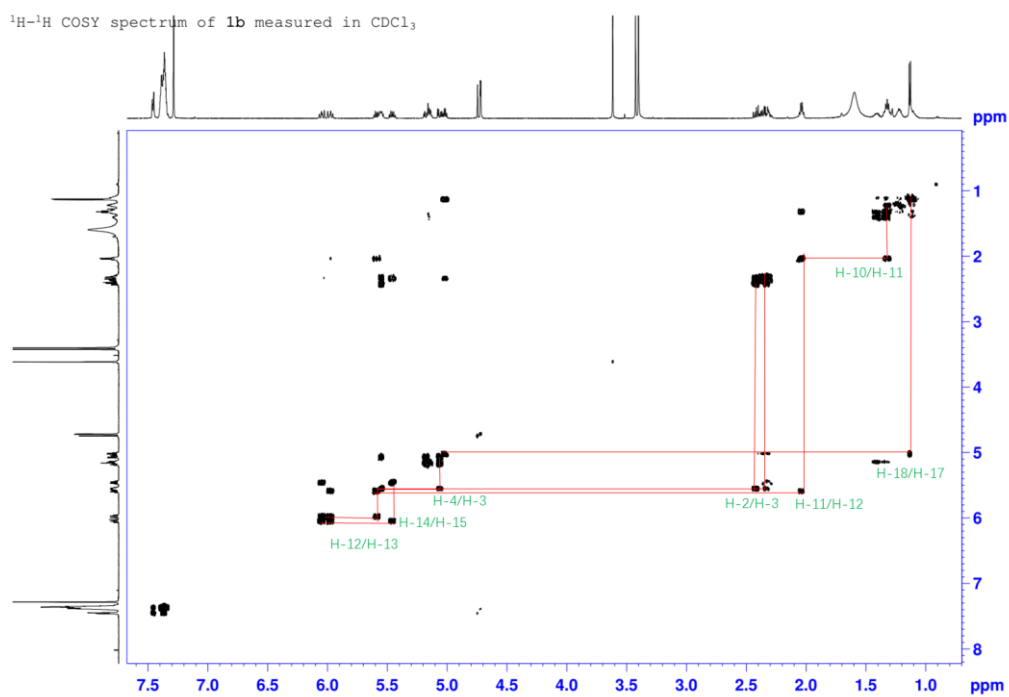
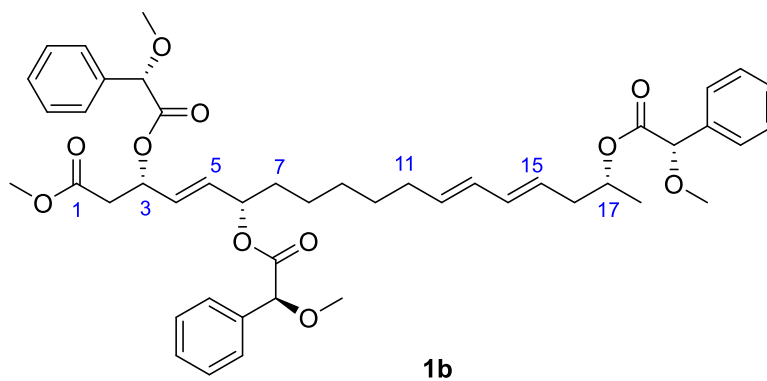


Figure S15: ¹H-¹H COSY spectrum of **1b** (*tri-(S)*-MPA esters of **1**)

Table S1. Comparison of ^1H and ^{13}C NMR data of **1** with the similar known compound [1]

1		Methyl (+)-(3 <i>R</i> ,4 <i>E</i> ,6 <i>Z</i> ,15 <i>E</i>)-3-methoxyoctadecatrienoate		
no.	δ_{C}	δ_{H}	δ_{H}	δ_{C}
1	173.2, C			174.1, C
2	43.3, CH ₂	2.53, m	2.29, m; 2.20, m	34.1, CH ₂
3	69.7, CH	4.52, m	3.64 dt (8.0, 7.0)	82.5, CH
4	132.9, CH	5.68, dd (15.5, 5.0)	5.50, dd (15.5, 8.0)	134.5, CH
5	135.3, CH	5.71, dd (15.5, 5.2)	6.53, dd (15.5, 11.0)	128.5, CH
6	72.8, CH	4.03, m	6.00, dd (11.0, 10.5)	128.9, CH
7	38.3, CH ₂	1.52, m	5.43, dt (10.5, 7.0)	133.0, CH
		1.47, m		
8	26.4, CH ₂	1.40, m	2.20, m	29.3, CH ₂
		1.34, m		
9	30.2, CH ₂	1.34, m	1.39, m	30.0, CH ₂
10	30.6, CH ₂	1.41, m	1.29, m	30.0, CH ₂
11	33.5, CH ₂	2.08, m	1.29, m	30.0, CH ₂
12	133.7, CH	5.59, m	1.29, m	30.0, CH ₂
13	131.8, CH	6.02, m	1.57, m	25.6, CH ₂
14	134.1, CH	6.04, m	2.30, m	34.3, CH ₂
			2.20, m	
15	128.9, CH	5.58, m	5.33, dt (15.5, 7.0)	125.5, CH
16	43.4, CH ₂	2.23, m	5.39, dt (15.0, 7.0)	133.7, CH
		2.17, m		
17	68.6, CH	3.76, m	2.04, m	21.2, CH ₂
18	22.9, CH ₃	1.16, d (6.3)	0.92, t (7.0)	14.4, CH ₃
1-OCH ₃	52.1, CH ₃	3.69, s	3.59, s	51.4, CH ₃
3-OCH ₃			3.20, s	56.2, CH ₃

References

- [1] S. Lin, Y.-L. Zhang, M.-T. Liu, J.-C. Zi, M.-L. Gan, W.-X. Song, X.-N. Fan, S.-J. Wang, Y.-C. Yang and J.-G. Shi (2012). Methoxylated fatty acids from the bark of *Fraxinus sieboldiana*, *J. Asian Nat. Prod. Ees.* **14**, 235-243.