

Supporting information for Stereoselective Synthesis, Pro-resolution and Anti-inflammatory Bioactions of RvD5_{n-3} DPA

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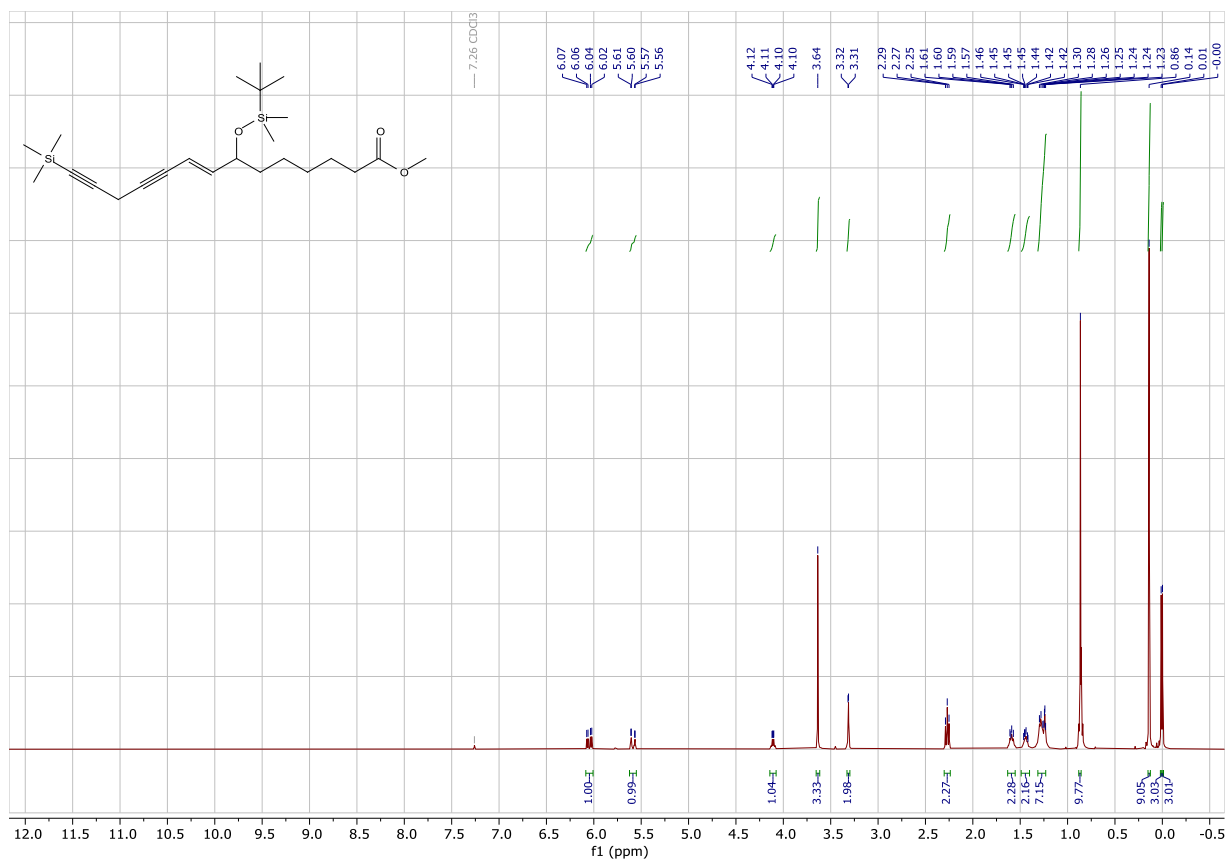


Figure S-1. ^1H NMR spectrum of compound **8**, CDCl_3 , 400 MHz.

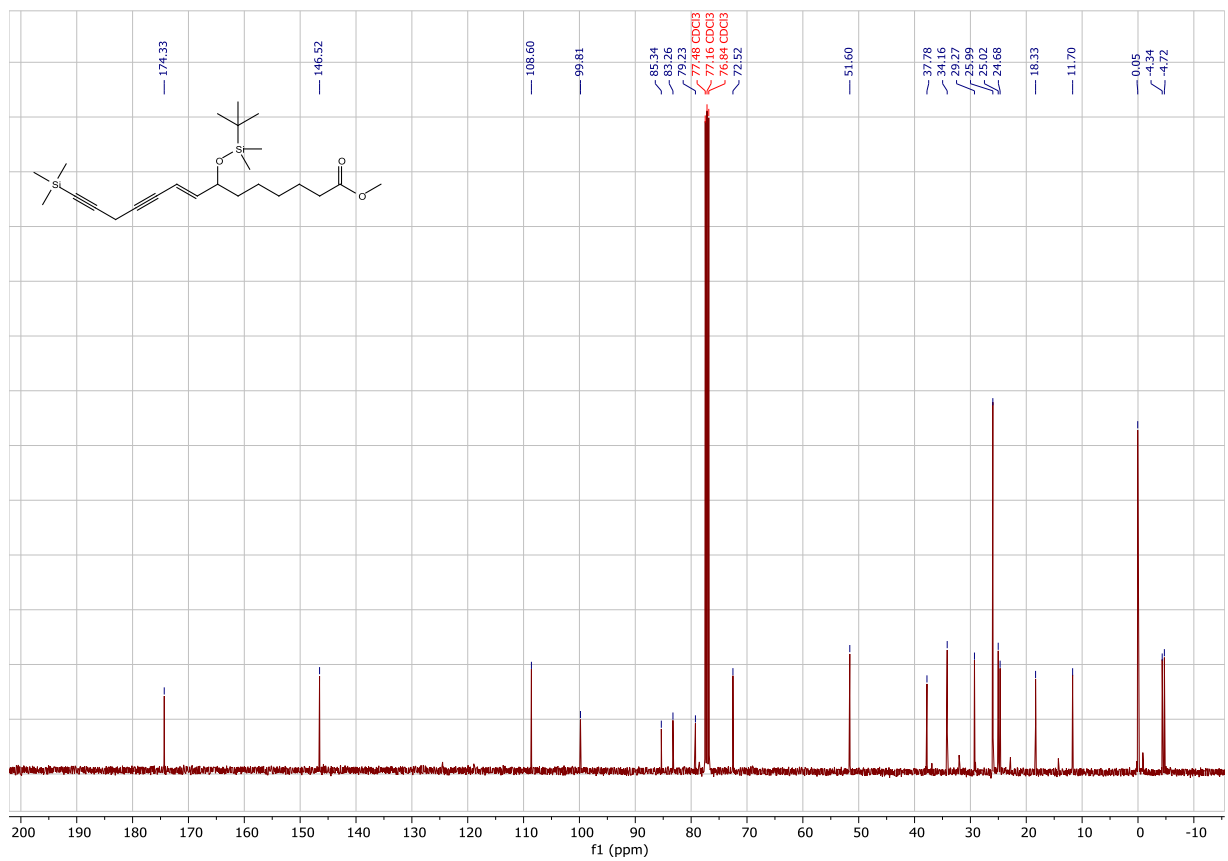


Figure S-2. ^{13}C NMR spectrum of compound **8**, CDCl_3 , 100 MHz.

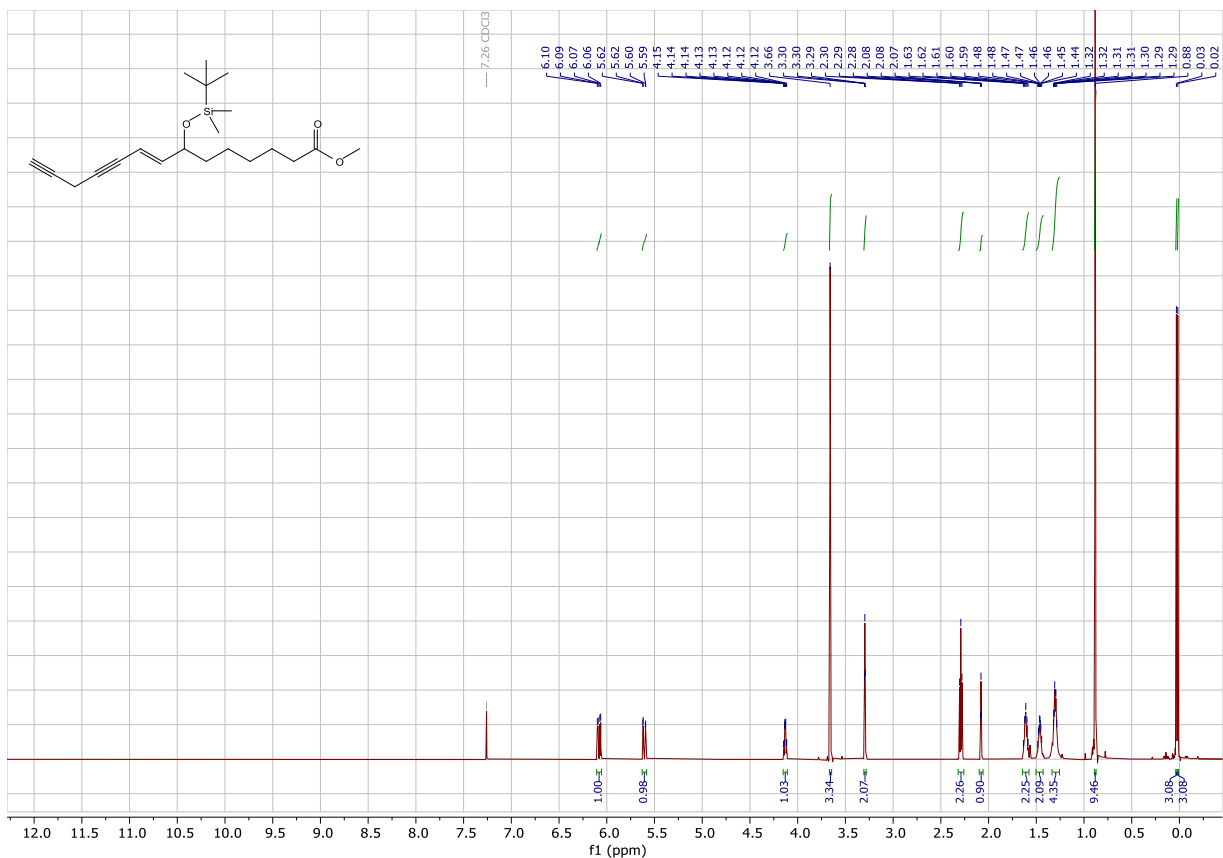


Figure S-3. ^1H NMR spectrum of compound **9**, CDCl_3 , 400 MHz.

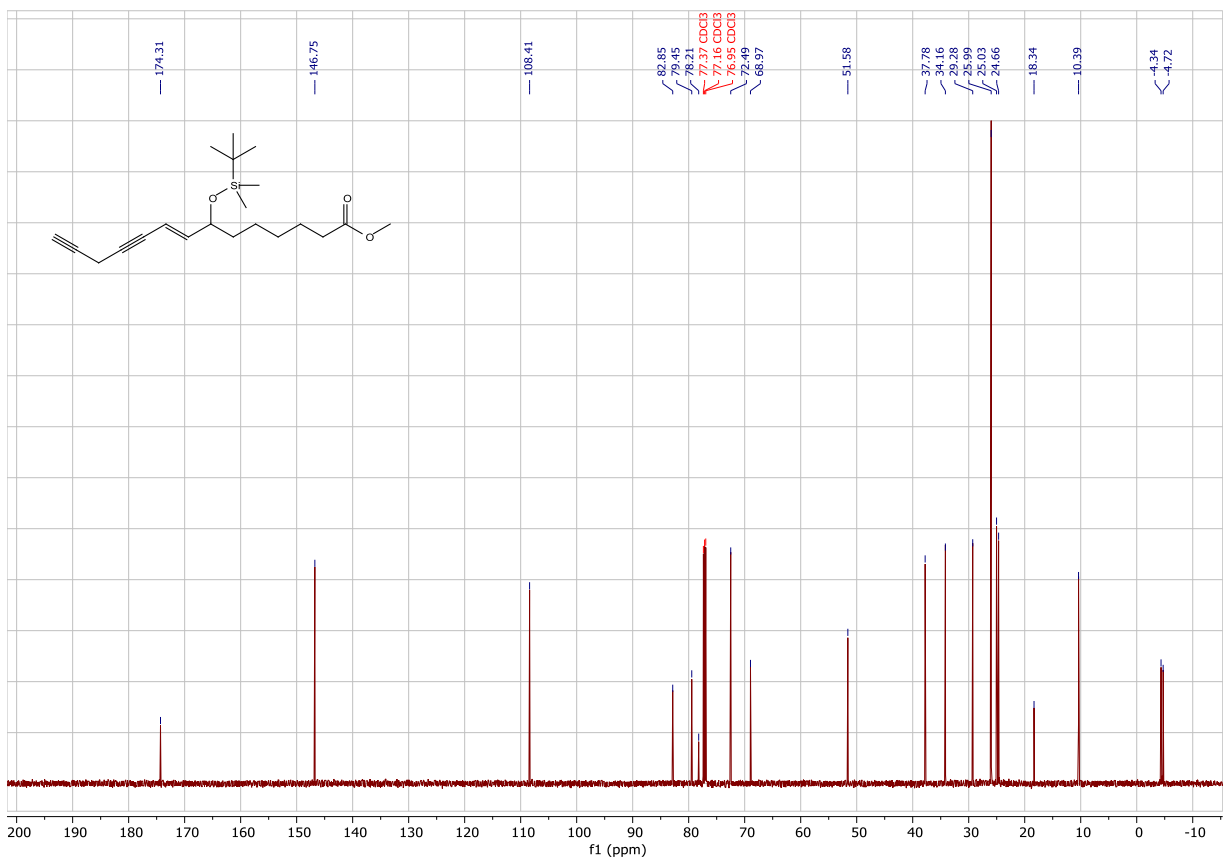


Figure S-4. ^{13}C NMR spectrum of compound **9**, CDCl_3 , 100 MHz.

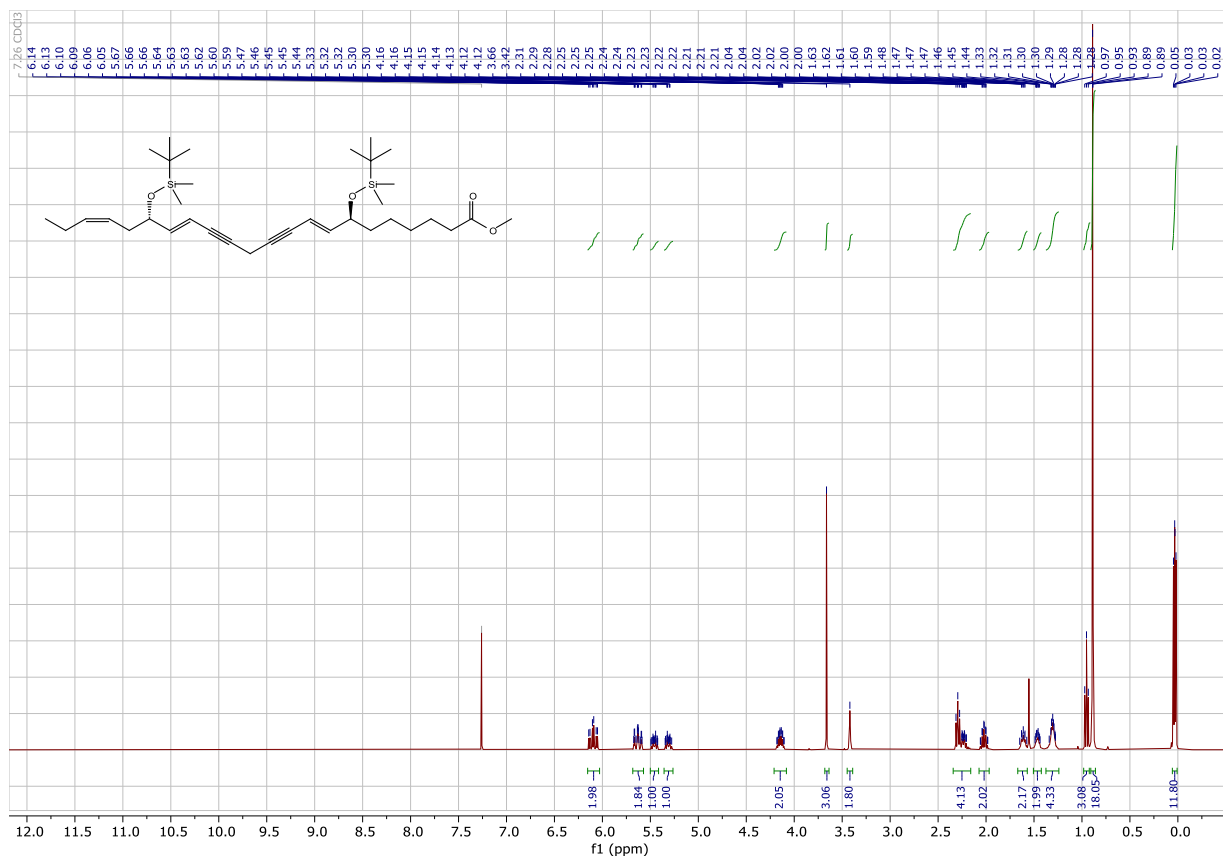


Figure S-5. ¹H NMR spectrum of compound **10**, CDCl₃, 400 MHz.

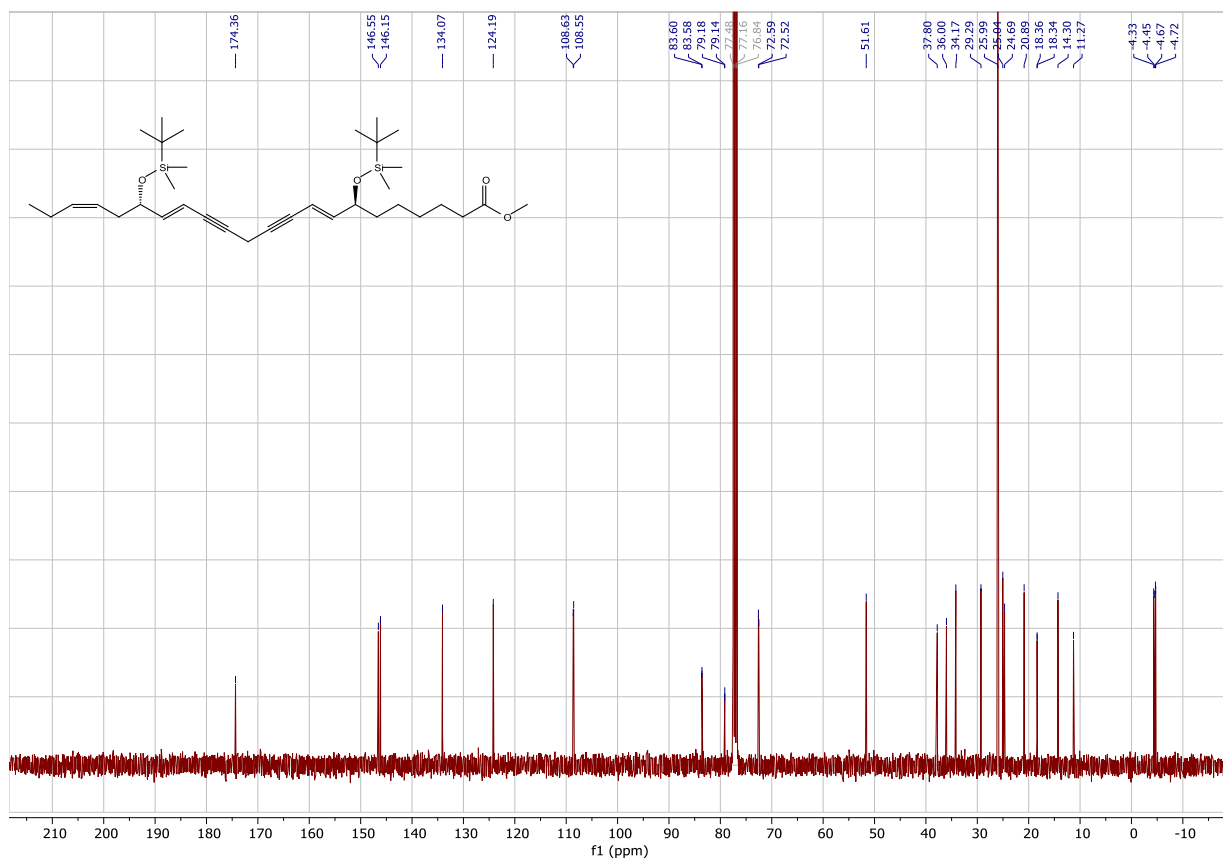


Figure S-6. ¹³C NMR spectrum of compound **10**, CDCl₃, 100 MHz.

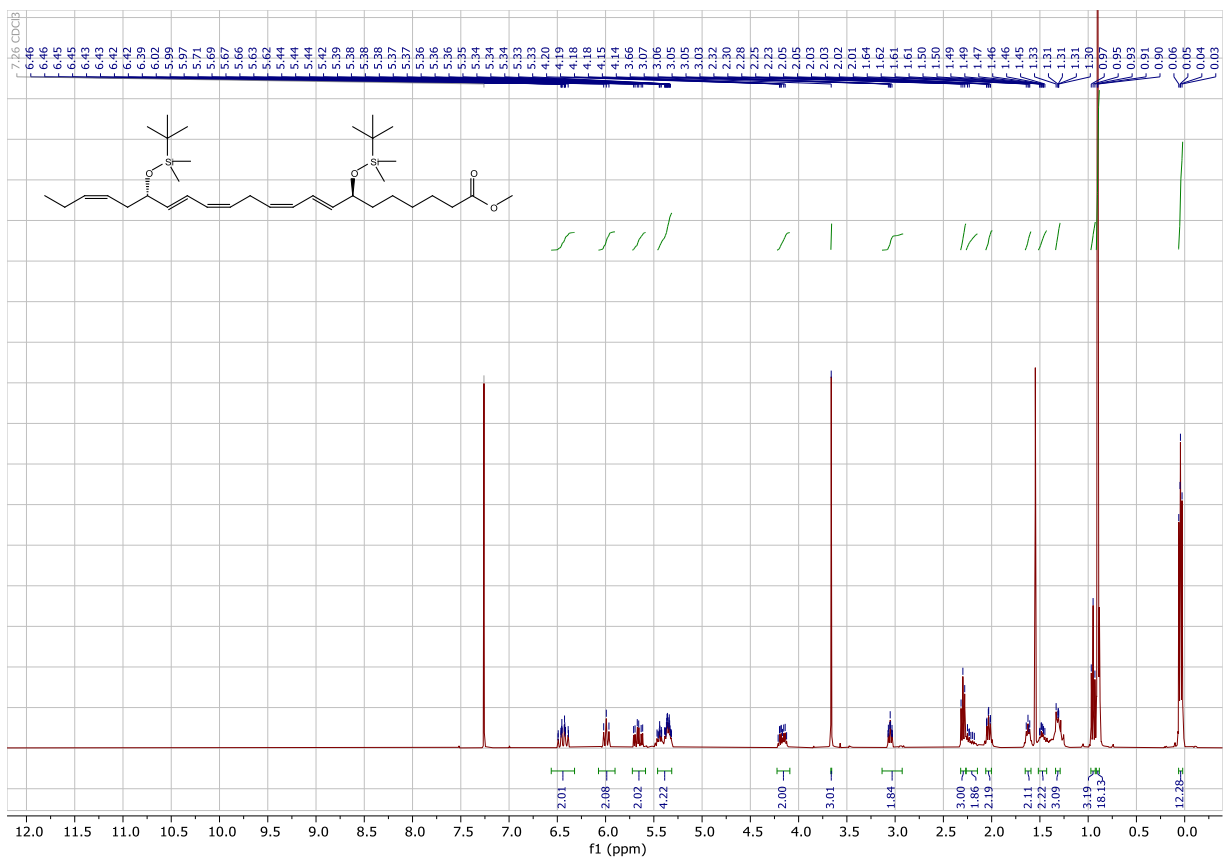


Figure S-7. ¹H NMR spectrum of compound 11, CDCl₃, 400 MHz.

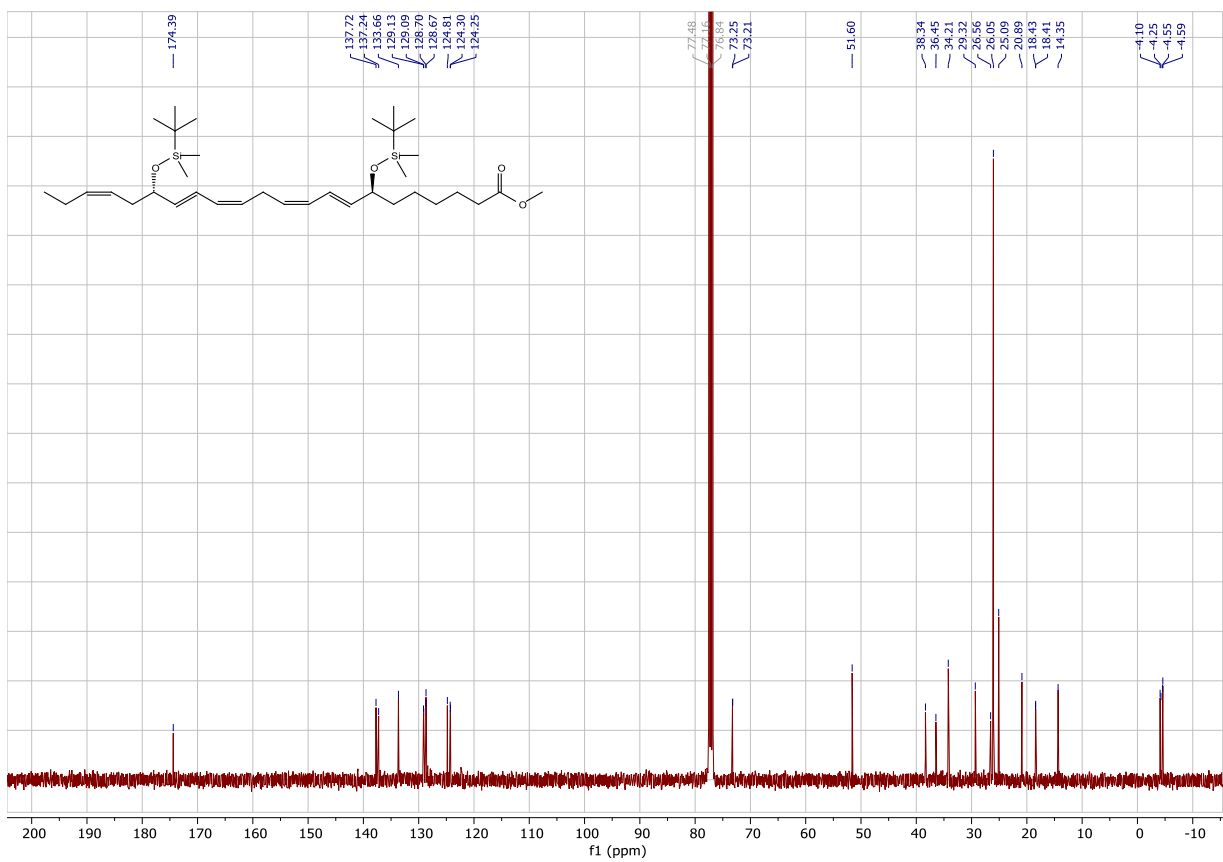


Figure S-8. ¹³C NMR spectrum of compound 11, CDCl₃, 100 MHz.

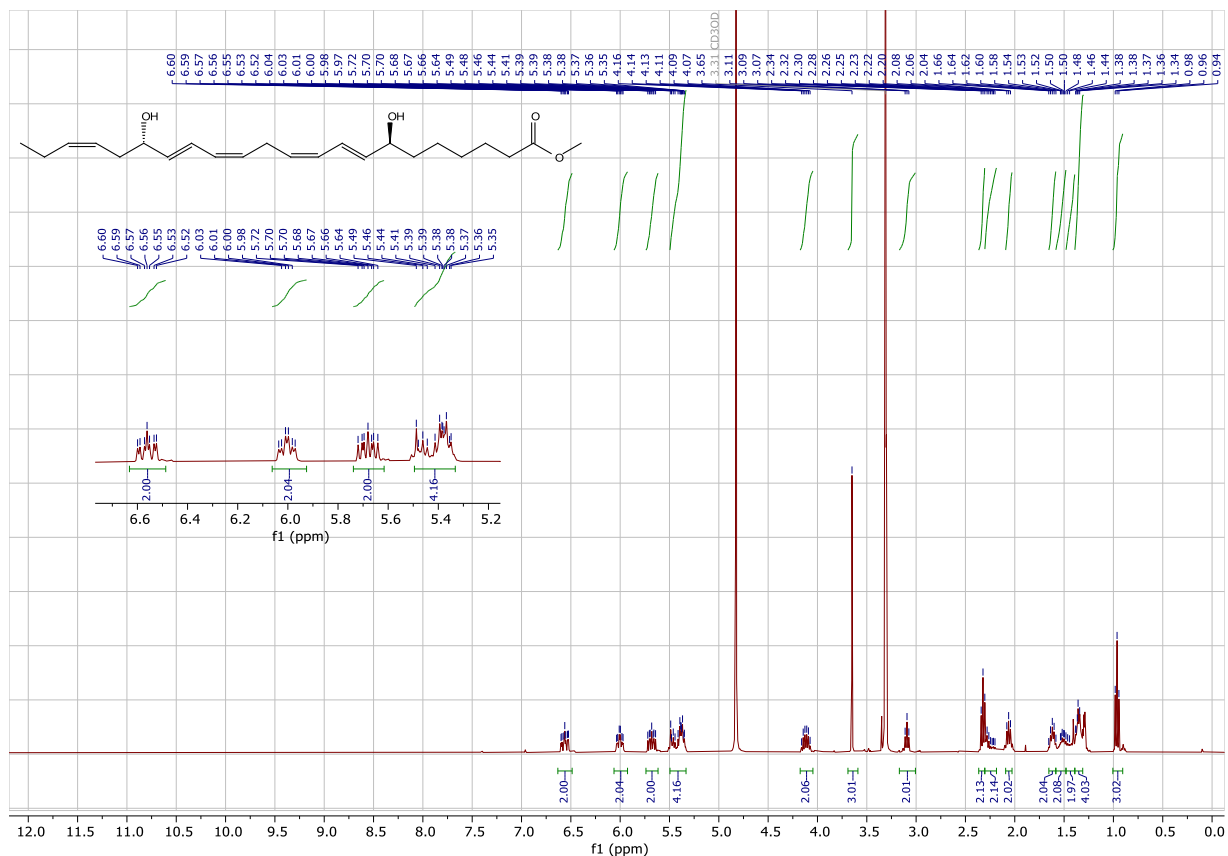


Figure S-9. ¹H NMR spectrum of compound RvD5_{n-3} DPA methyl ester **2**, CD₃OD, 400 MHz.

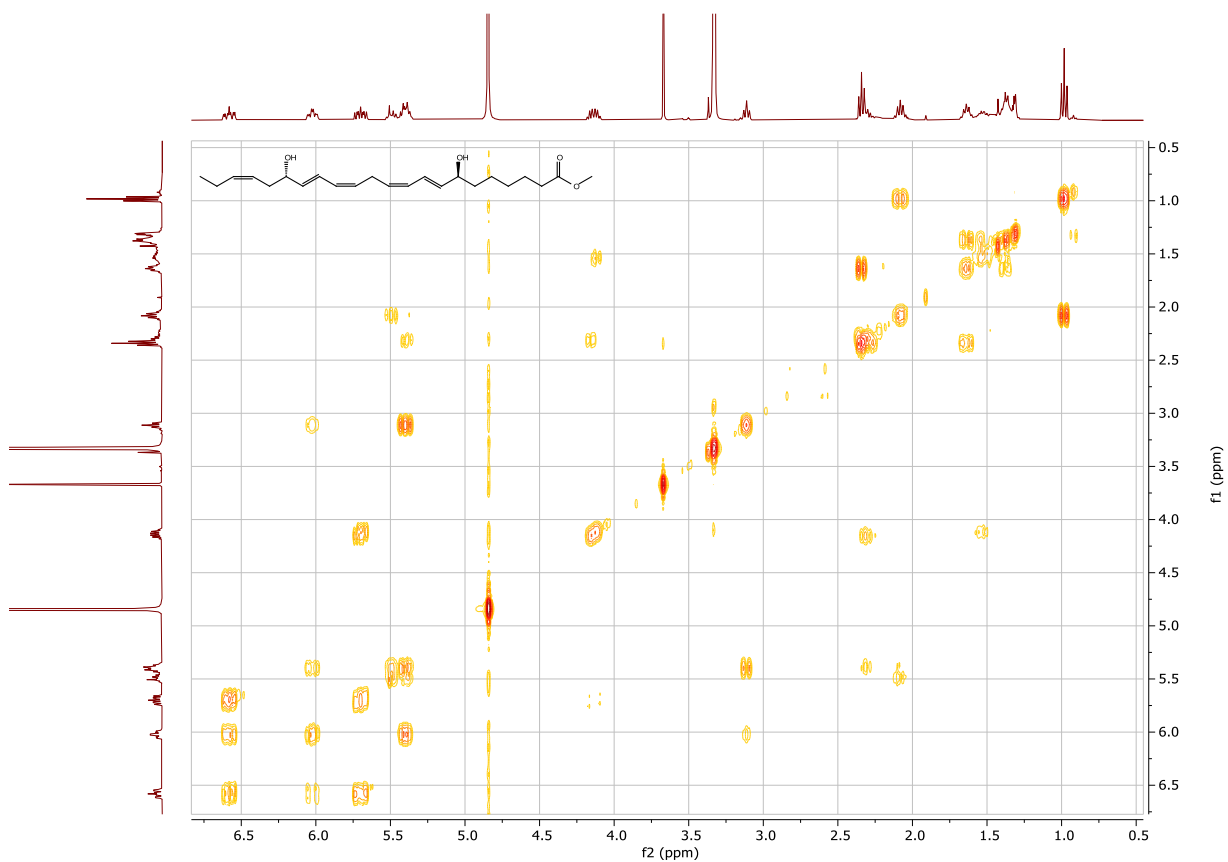


Figure S-10. COSY-spectrum of RvD5_{n-3} DPA methyl ester **2**, CD₃OD, 400 MHz.

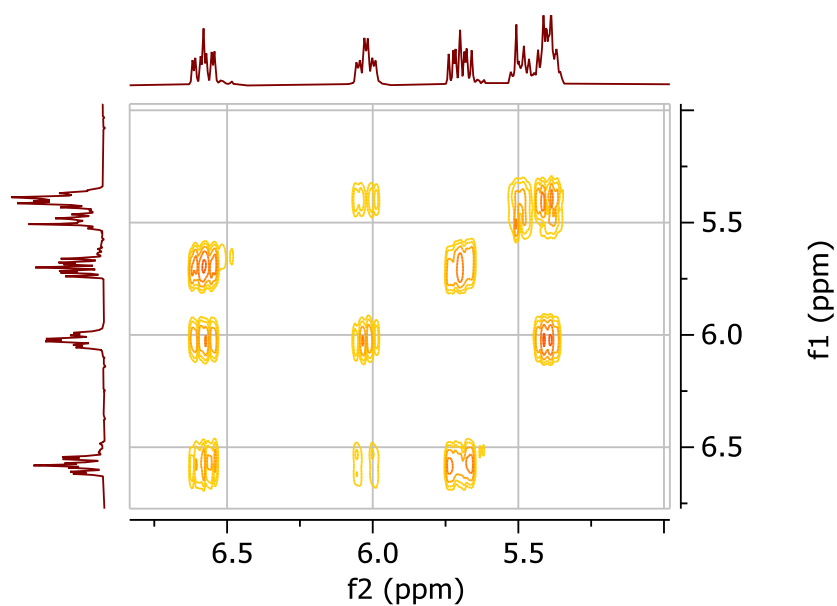


Figure S-11. Expansion of the olefinic area in the COSY NMR spectrum of RvD5_{n-3} DPA methyl ester **2**.

Position	δ (mult, J/Hz)
H ₉ , H ₁₅	6.56 (ddd, $J = 15.0, 11.1, 3.9$ Hz, 2H)
H ₁₀ , H ₁₄	6.00 (td, $J = 10.8, 4.6$ Hz, 2H)
H ₈ , H ₁₆	5.68 (ddd, $J = 15.7, 9.8, 6.6$ Hz, 2H)
H ₁₁ , H ₁₃ , H ₁₉ , H ₂₀	5.49 – 5.35 (m, 4H)

Table S-1. Interpretation of the double bond geometry in RvD5_{n-3} DPA methyl ester (**2**).

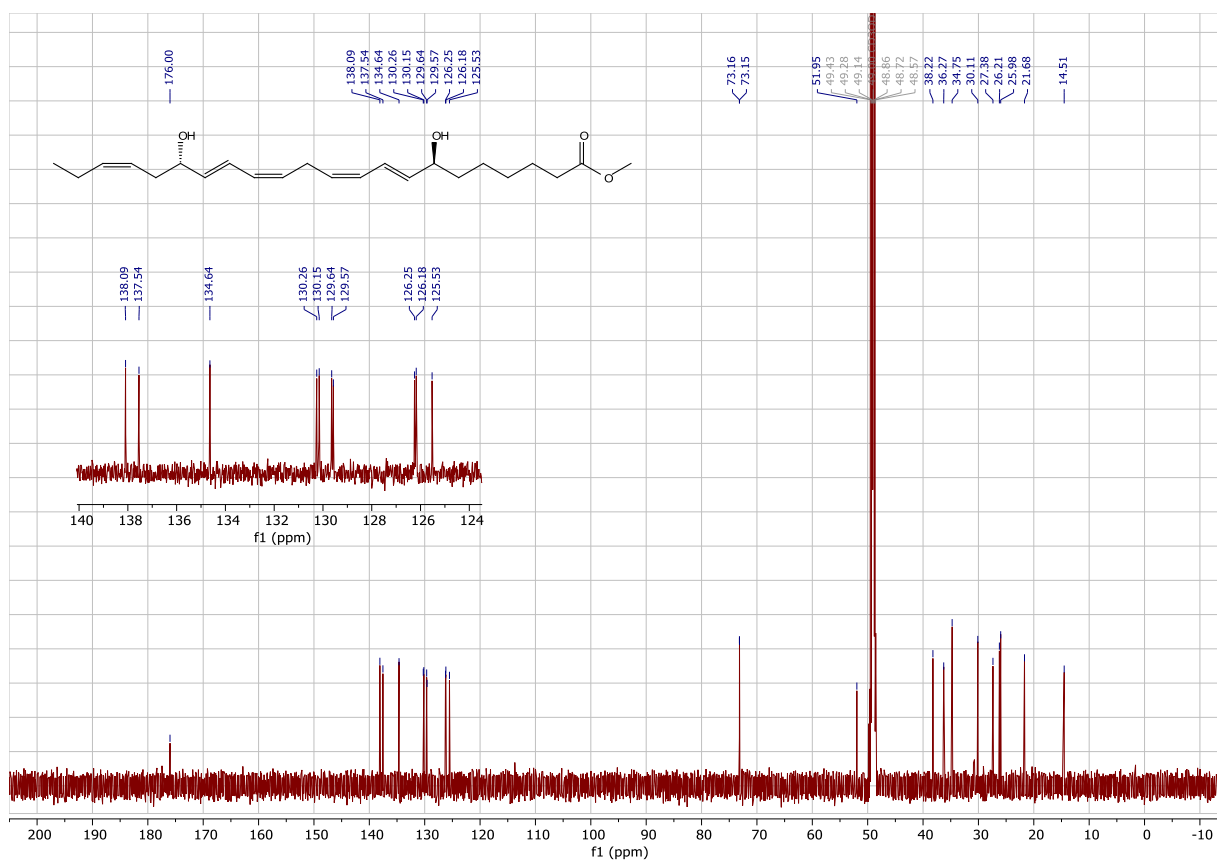


Figure S-12. ^{13}C NMR spectrum of RvD5_{n-3} DPA methyl ester **2**, CD_3OD , 150 MHz.

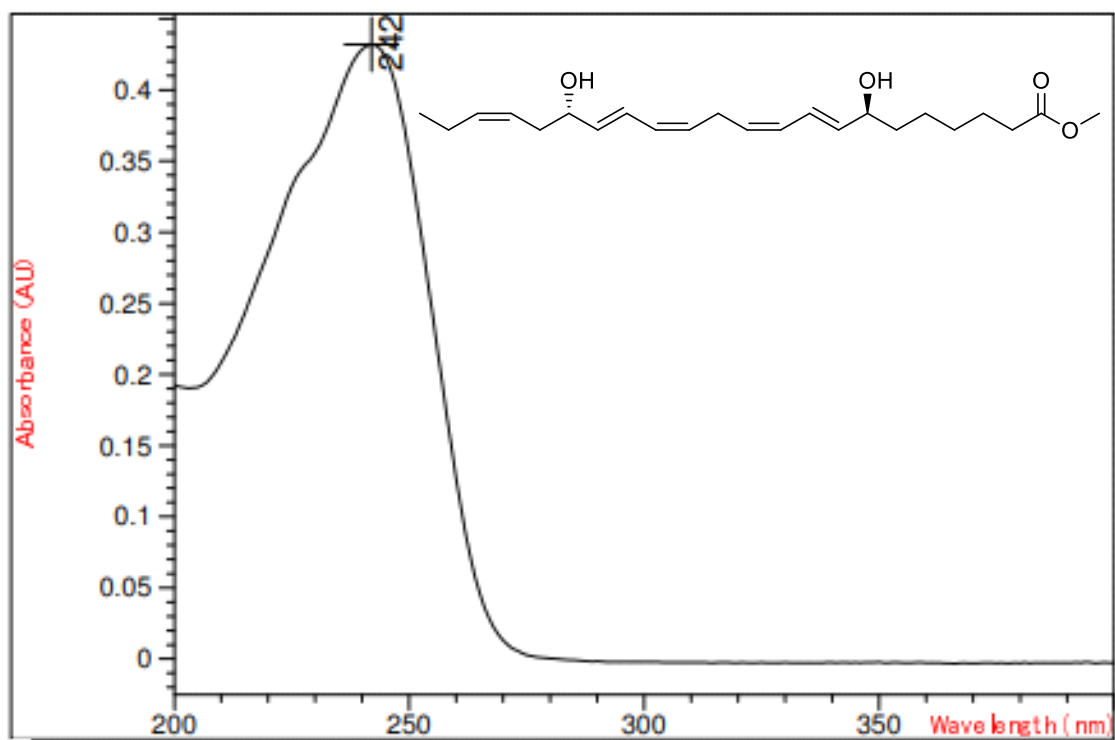


Figure S-13. UV-Vis of RvD5_{n-3} DPA methyl ester **2** in MeOH.

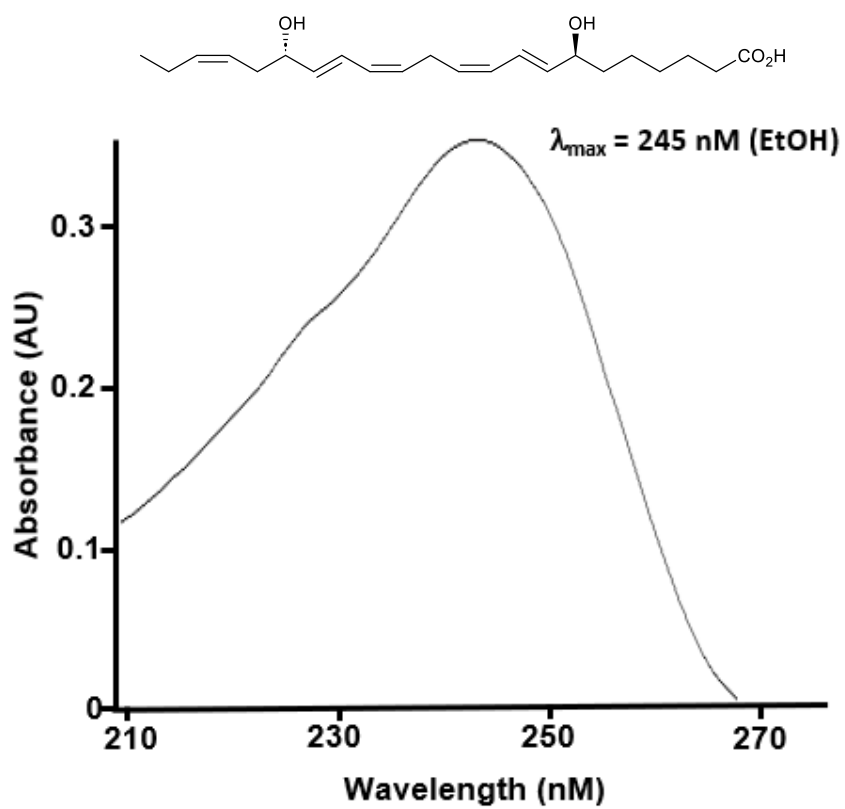
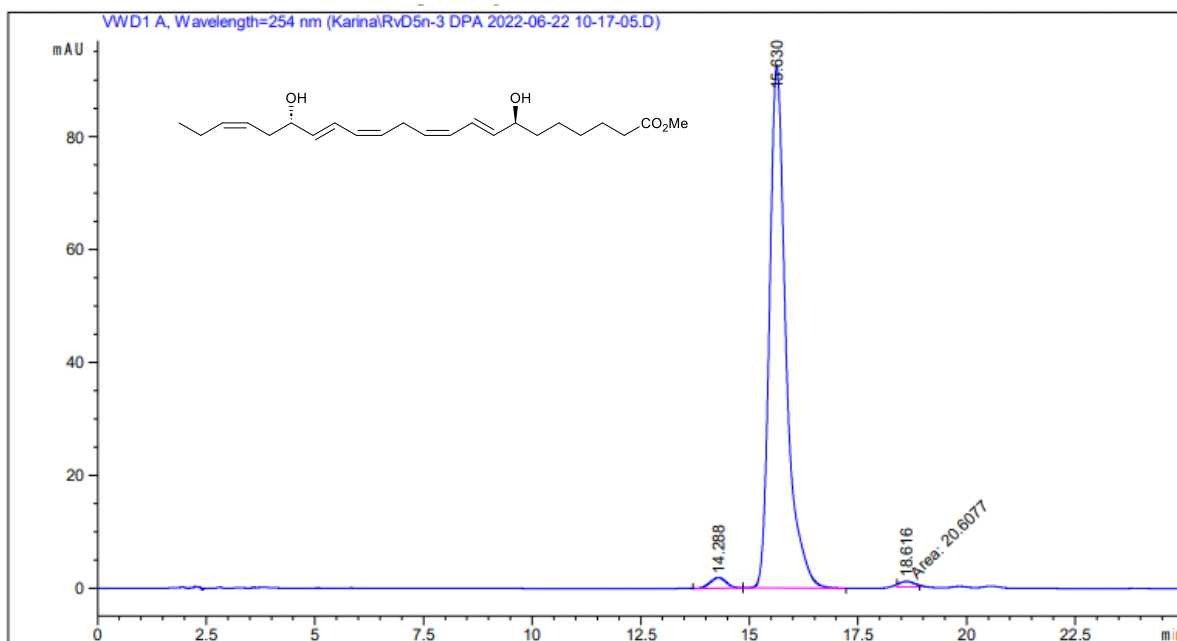


Figure S-14. UV-Vis of RvD5_{n-3} DPA 1.



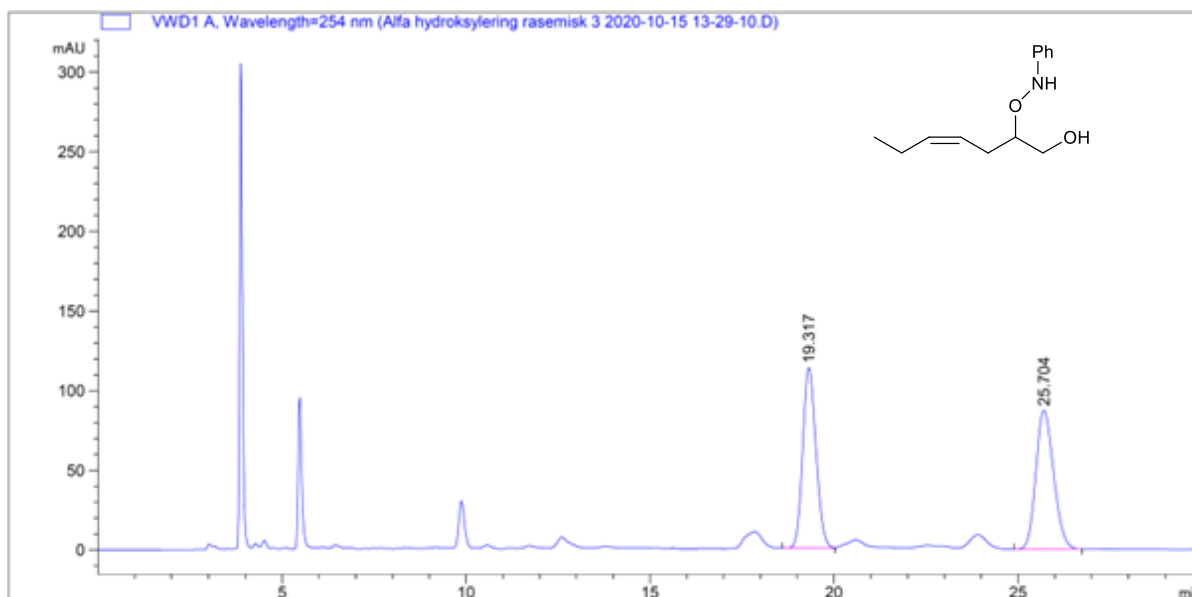
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 Area Percent Report
 =====

Sorted By : Signal
 Multiplier : 1.0000
 Dilution : 1.0000
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.288	BB	0.3929	48.07434	1.87654	1.9158
2	15.630	BB	0.3974	2440.66089	92.33601	97.2629
3	18.616	MM	0.3787	20.60766	9.06916e-1	0.8212

Figure S-15. HPLC chromatogram of RvD5_{n-3} DPA methyl ester 2.



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 Area Percent Report
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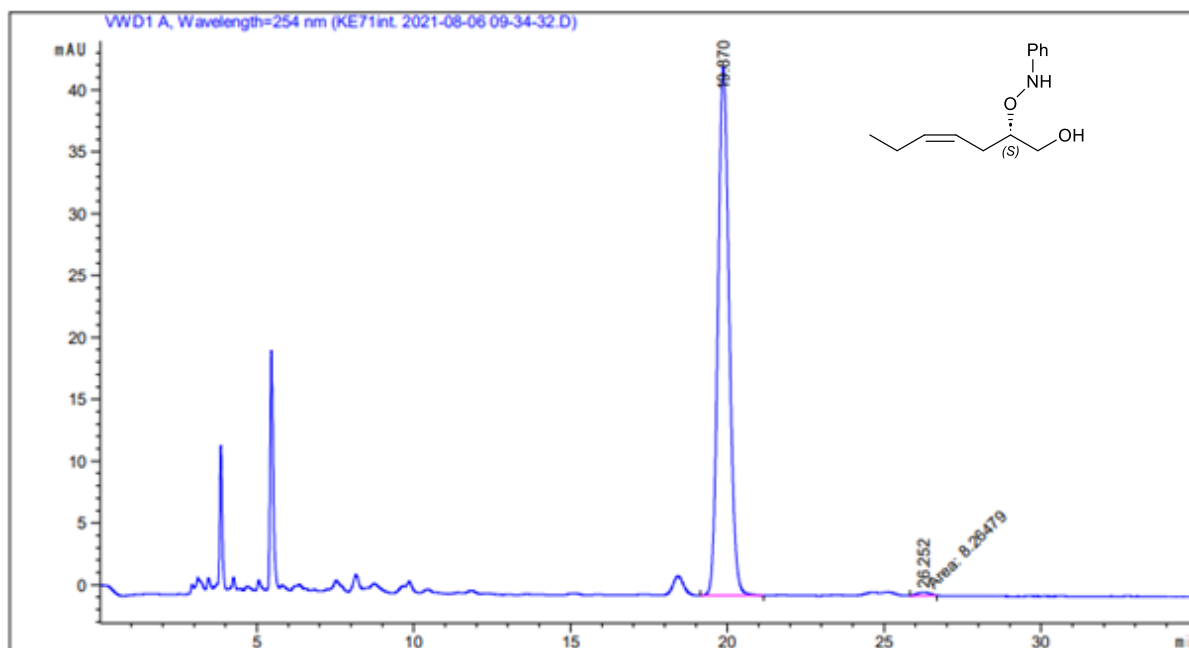
Sorted By : Signal
 Multiplier : 1.0000
 Dilution : 1.0000
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	19.317	BV	0.3891	2837.64722	113.32843	49.2803
2	25.704	BB	0.5210	2920.53052	87.13389	50.7197

Totals : 5758.17773 200.46232

Figure S-16. HPLC chromatogram of racemic α -aminoxylated alcohol intermediate of compound 7.



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 Area Percent Report
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Sorted By : Signal
 Multiplier : 1.0000
 Dilution : 1.0000
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	19.870	BB	0.3840	1057.72974	42.69299	99.2247
2	26.252	MM	0.4983	8.26479	2.76407e-1	0.7753

Figure S-17. HPLC chromatogram of optical α -aminoxylated alcohol intermediate of compound **7**.

Elemental Analysis Report

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Sample Name	KE79	Analysis Name	D:\Data\maxis2021\18137.d
Method	ESI_pos_50_1500_os.m		

Acquisition Parameter

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Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C

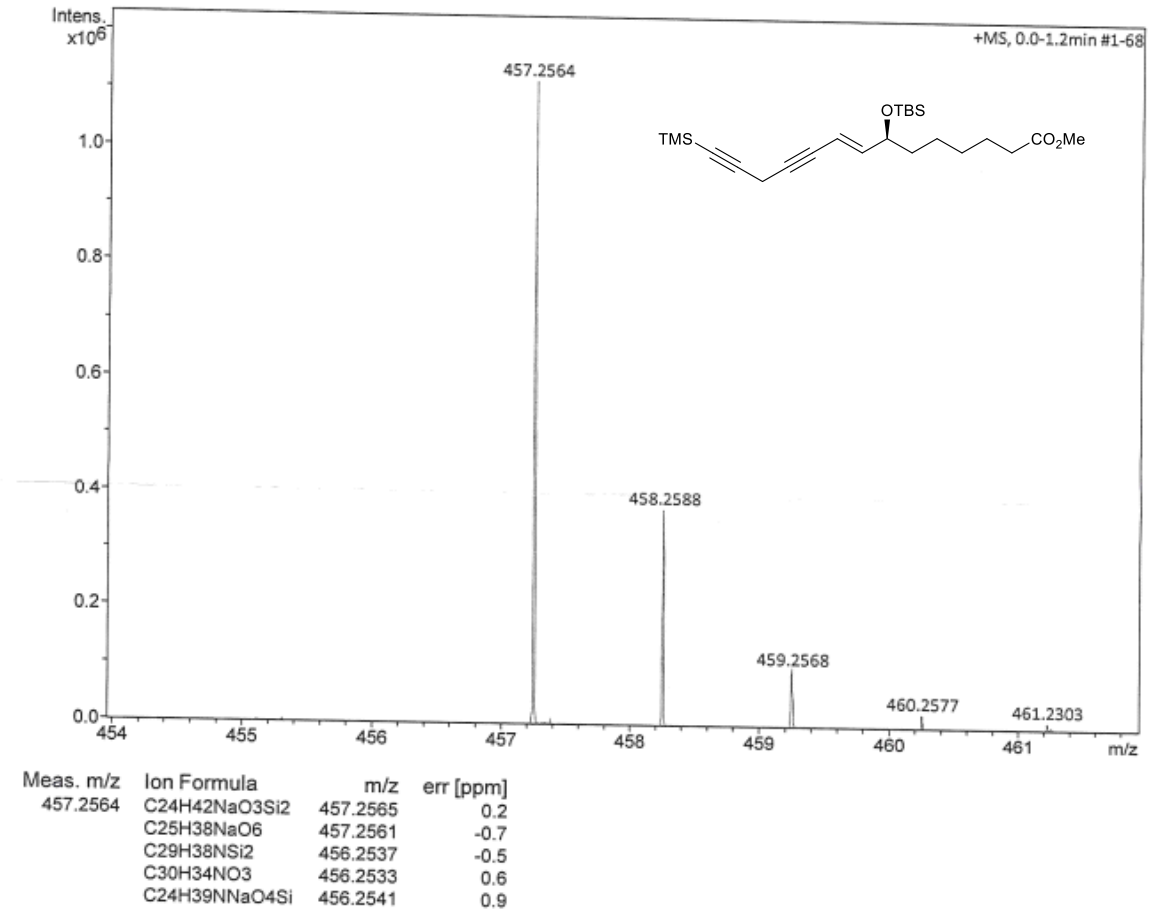


Figure S-18. HRMS spectrum of compound 8.

Elemental Analysis Report

Analysis Info

Sample Name KE80
 Method ESI_pos_50_1500_os.m

Acquisition Date 05-Jan-22 3:48:15 PM
 Analysis Name D:\Data\maxis2022\18362.d

Acquisition Parameter

Source Type	ESI	Set Capillary	3500 V	Set Nebulizer	0.3 Bar
Focus	Not active	Set End Plate Offset	-500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Charging Voltage	2000 V	Set Dry Gas	4.0 l/min
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				Set APCI Heater	0 °C

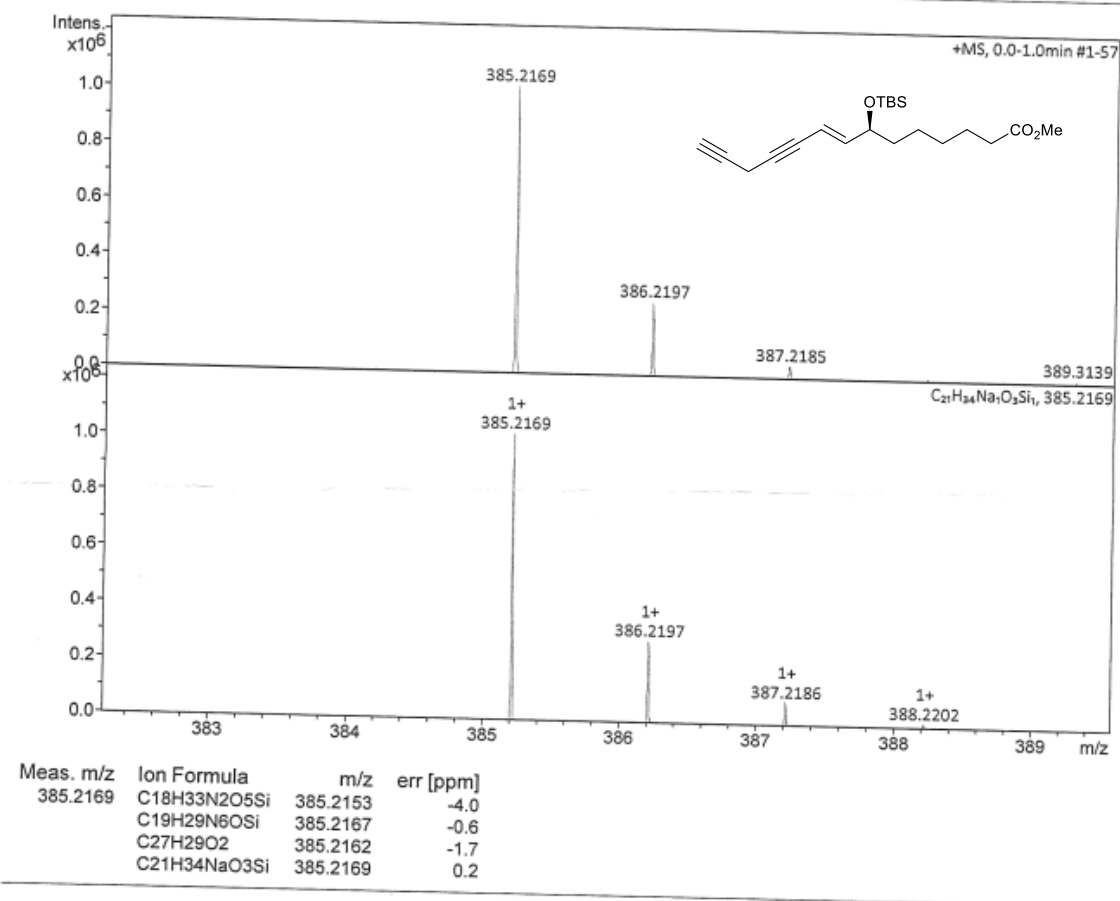


Figure S-19. HRMS spectrum of compound 9.

Elemental Analysis Report

Analysis Info

Sample Name KE81

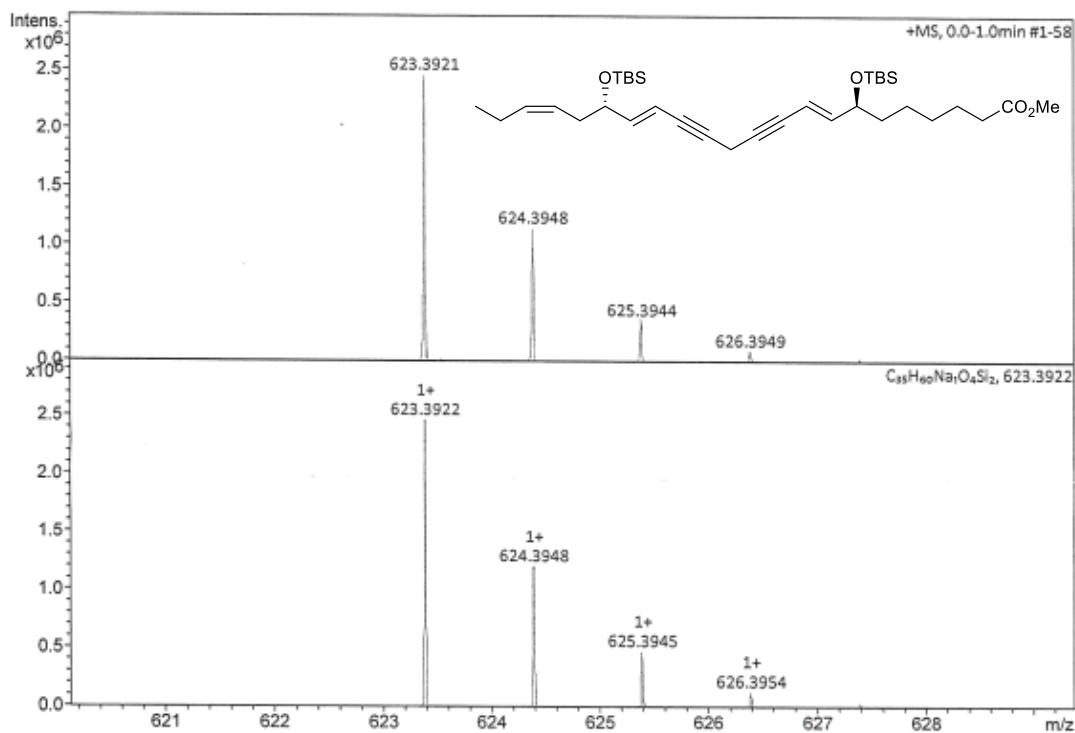
Method ESI_pos_50_1500_os.m

Acquisition Date 07-Jan-22 9:54:56 AM

Analysis Name D:\Data\maxis2022\18371.d

Acquisition Parameter

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Focus	Not active	Set End Plate Offset	-500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Charging Voltage	2000 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Corona	0 nA	Set Divert Valve	Waste
				Set APCI Heater	0 °C



Meas. m/z	Ion Formula	m/z	err [ppm]
623.3921	C36H54N3O4Si	620.3878	0.8
	C41H55O3Si	623.3915	-1.0
	C34H51N6O5	623.3915	-1.0
	C40H56NOSi2	622.3895	-0.0
	C41H52NO4	622.3891	0.5
	C36H57N2O3Si2	621.3902	0.6
	C35H60NaO4Si2	623.3922	0.1
	C36H56NaO7	623.3918	-0.5
	C35H57NNaO5Si	622.3898	1.0
	C38H51N3NaO3	620.3823	-0.9

Figure S-20. HRMS spectrum of compound 10.

Elemental Analysis Report

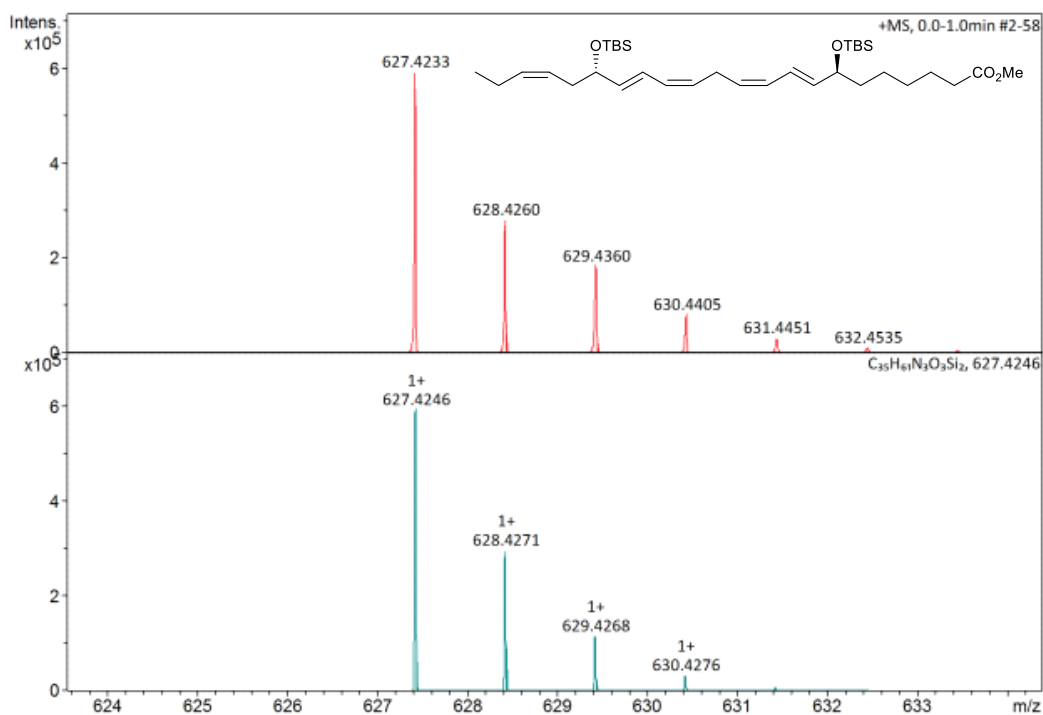
Analysis Info

Sample Name KE107.1
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Acquisition Date 10-Jun-22 1:33:06 PM
 Analysis Name D:\Data\maxis2022\18912.d

Acquisition Parameter

Source Type	ESI	Set Capillary	3500 V	Set Nebulizer	0.5 Bar
Focus	Not active	Set End Plate Offset	-500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Charging Voltage	2000 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Corona	0 nA	Set Divert Valve	Waste
				Set APCI Heater	0 °C



Meas. m/z	Ion Formula	m/z	err [ppm]
627.4233	C ₃₃ H ₅₉ N ₆ O ₂ Si ₂	627.4233	-0.1
	C ₃₅ H ₆₄ NaO ₄ Si ₂	627.4235	0.3

Figure S-21. HRMS spectrum of compound **11**.

Elemental Analysis Report

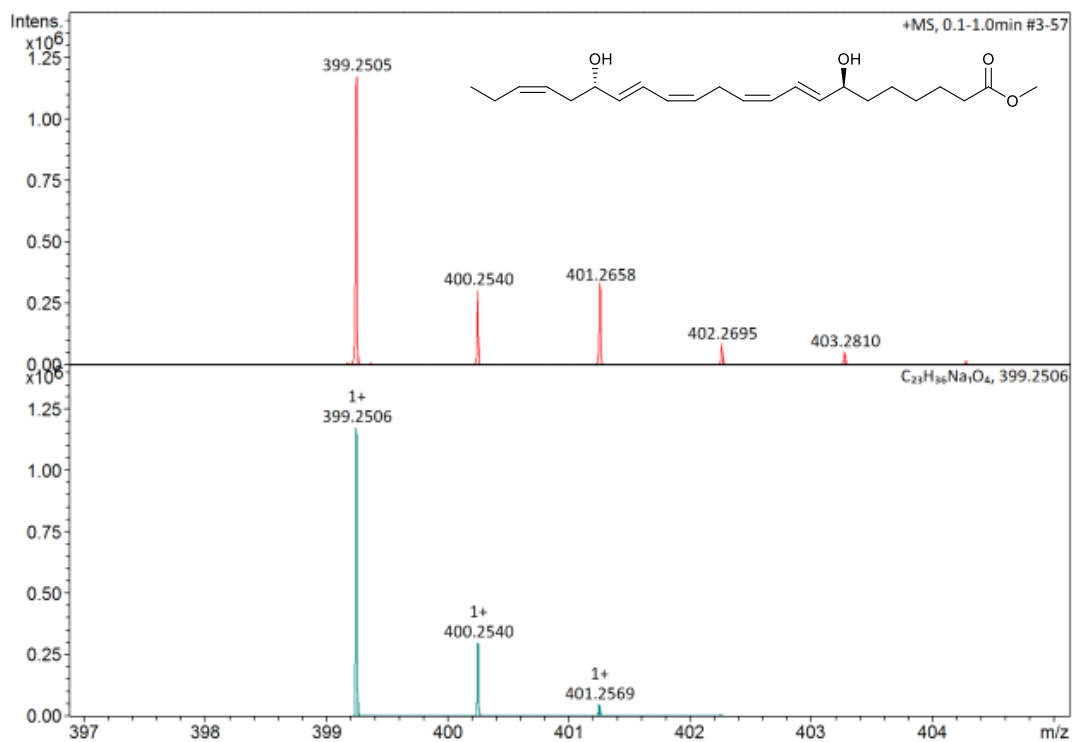
Analysis Info

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 Method ESI_pos_50_1500_os.m

Acquisition Date 21-Jun-22 1:02:18 PM
 Analysis Name D:\Data\maxis2022\18949.d

Acquisition Parameter

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Scan Begin	50 m/z	Set Charging Voltage	2000 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Corona	0 nA	Set Divert Valve	Waste
				Set APCI Heater	0 °C



Meas. m/z	Ion Formula	m/z	err [ppm]
399.2505	C ₂₁ H ₃₁ N ₆ O ₂	399.2503	-0.5
	C ₂₃ H ₃₆ NaO ₄	399.2506	0.2
401.2658	C ₂₁ H ₃₃ N ₆ O ₂	401.2660	0.5
	C ₂₃ H ₃₈ NaO ₄	401.2662	1.2

Figure S-22. HRMS spectrum of RvD5_{n-3}-DPA methyl ester **2**.