

# Supporting Information

## **Glycolipids and a Polyunsaturated Fatty Acid Methyl Ester Isolated from the Marine Dinoflagellate *Karenia mikimotoi***

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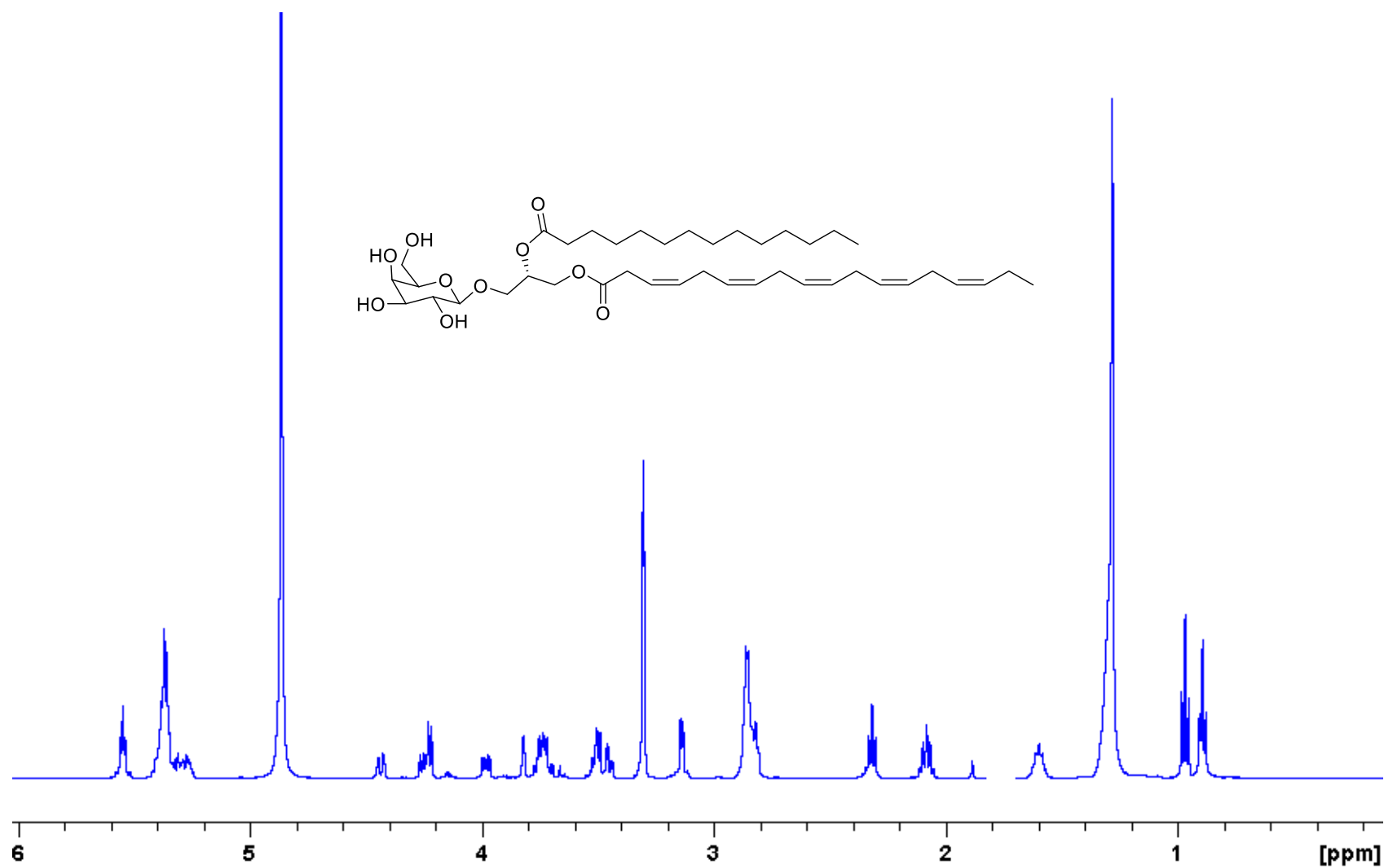
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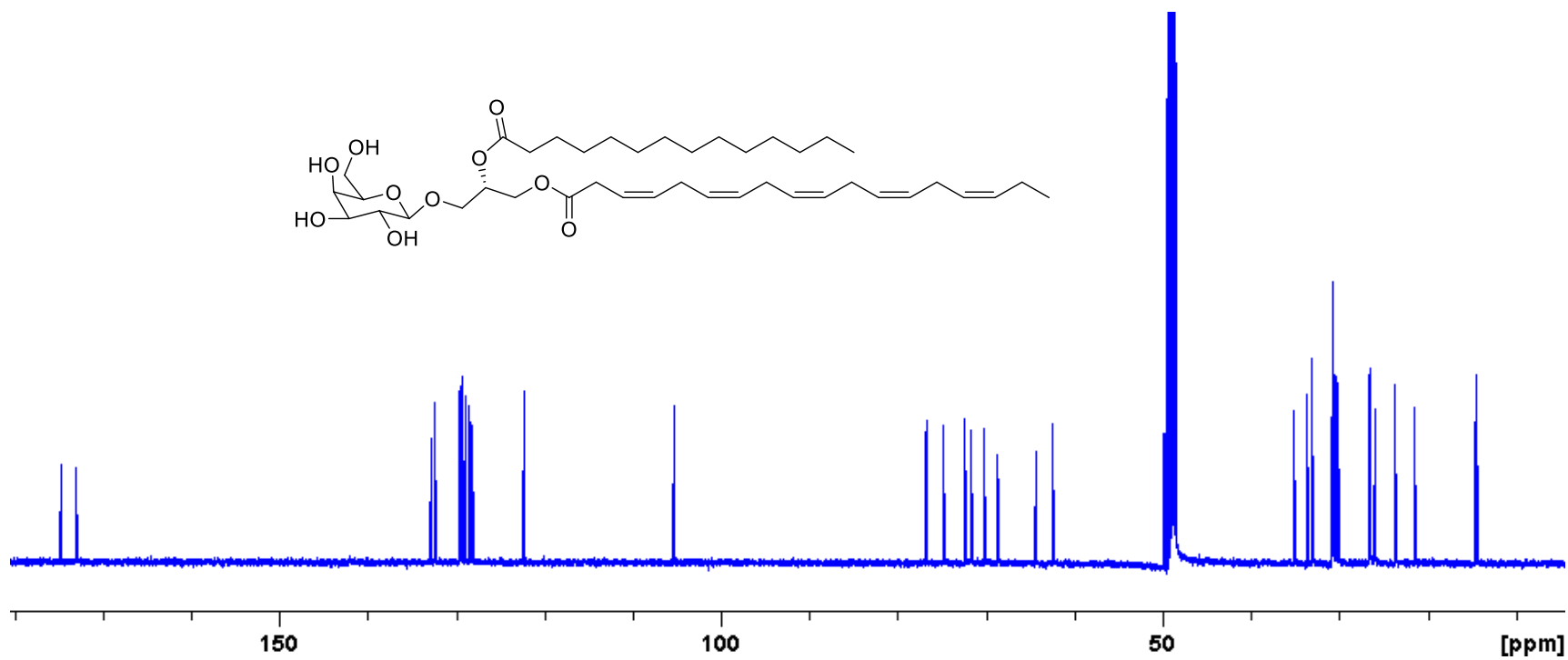
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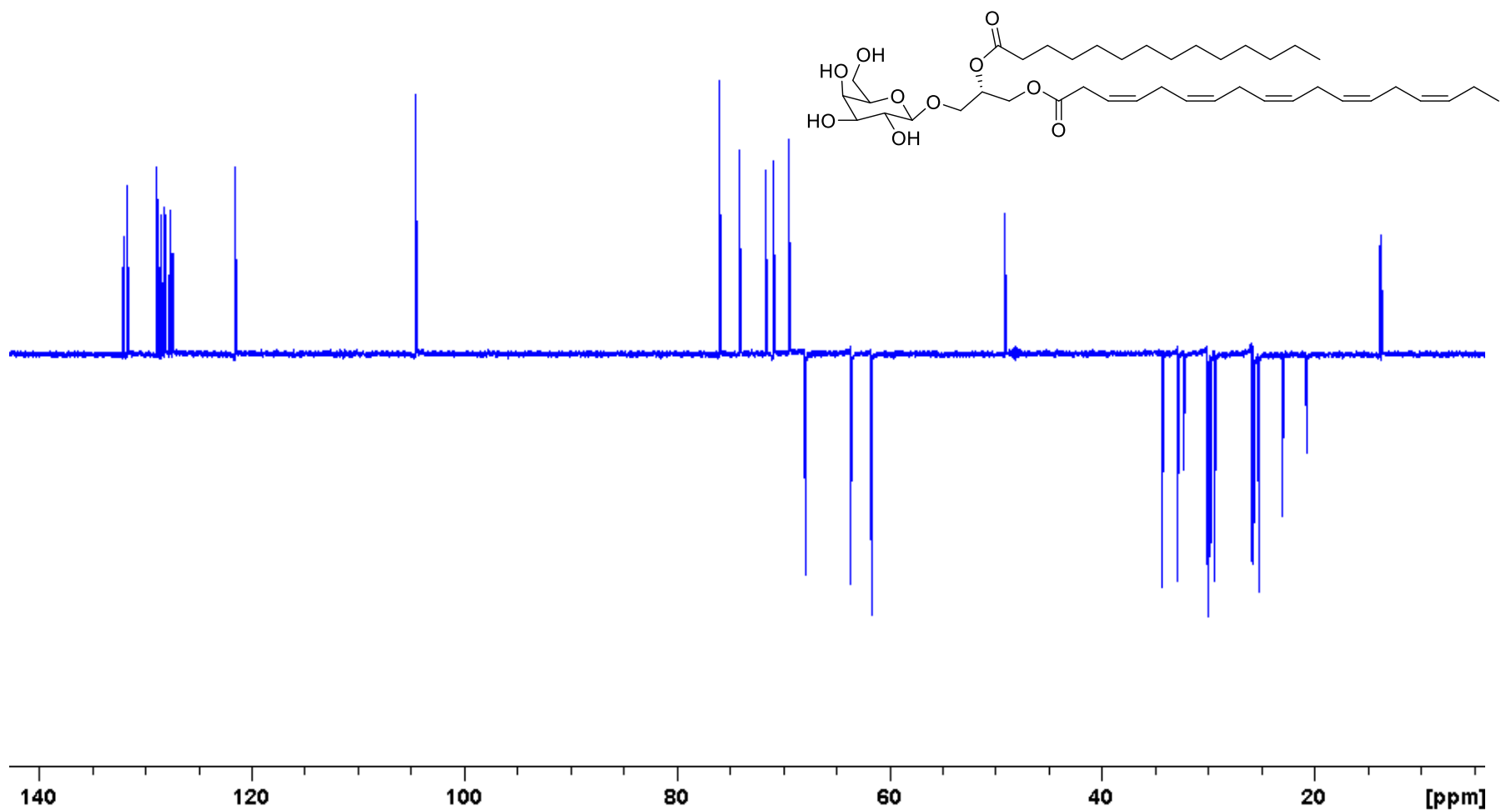
**Figure S1.**  $^1\text{H}$  NMR Spectrum (500 MHz) of Monogalactosyldiacylglycerol (**1**) in  $\text{CD}_3\text{OD}$



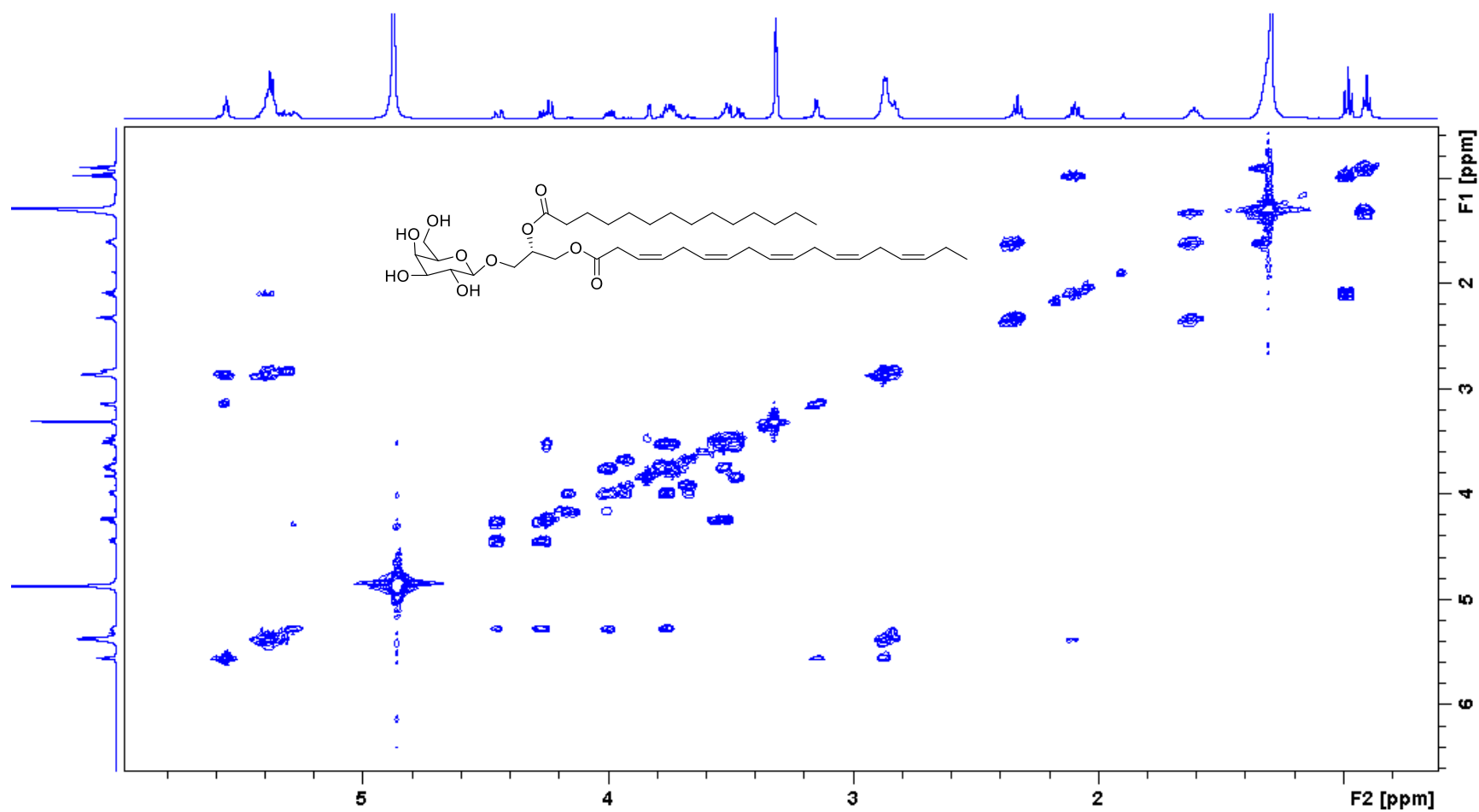
**Figure S2.**  $^{13}\text{C}$  NMR Spectrum (125 MHz) of Monogalactosyldiacylglycerol (**1**) in  $\text{CD}_3\text{OD}$



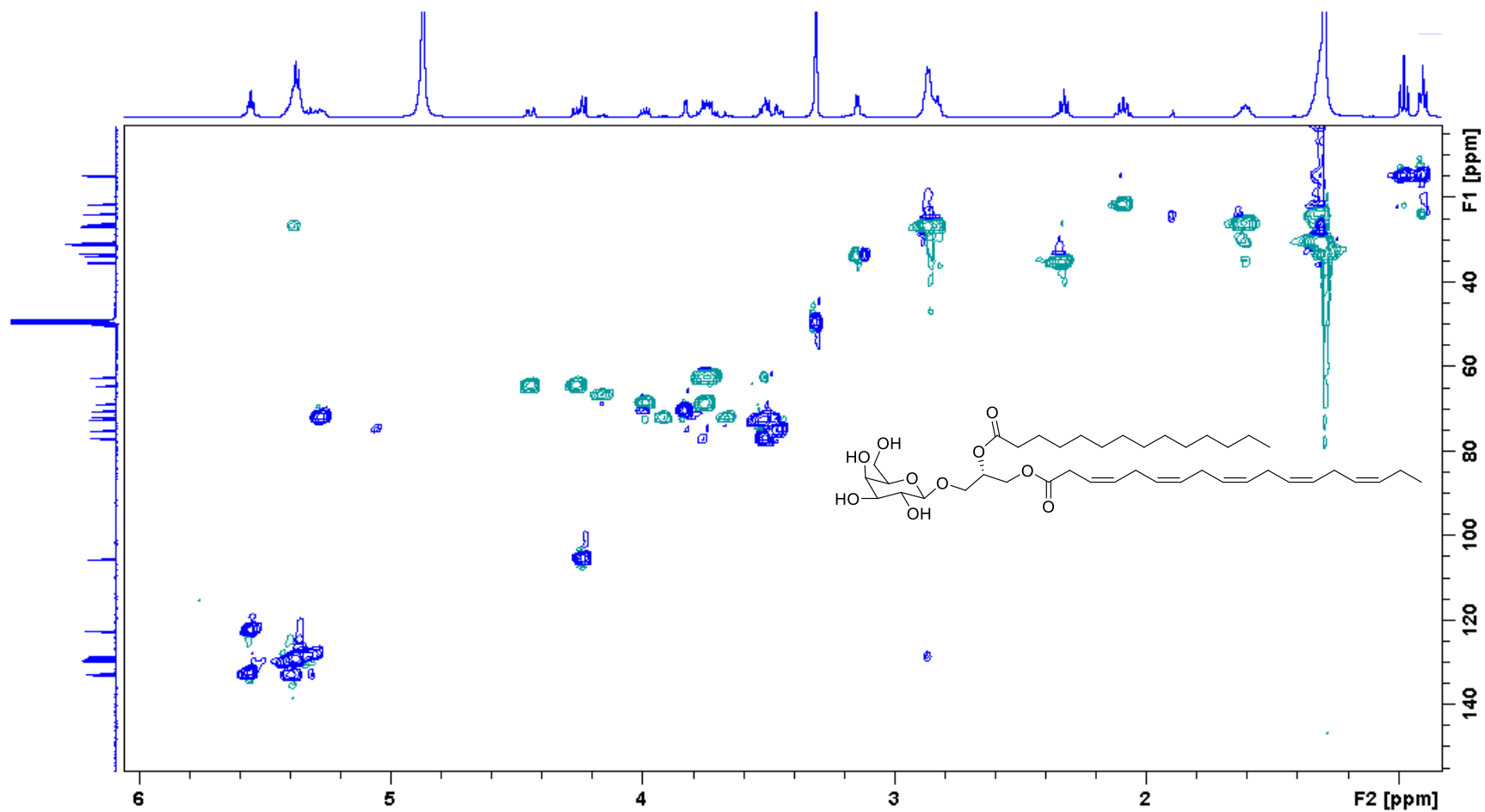
**Figure S3.** DEPT-135 (125 MHz) of Monogalactosyldiacylglycerol (**1**) in CD<sub>3</sub>OD



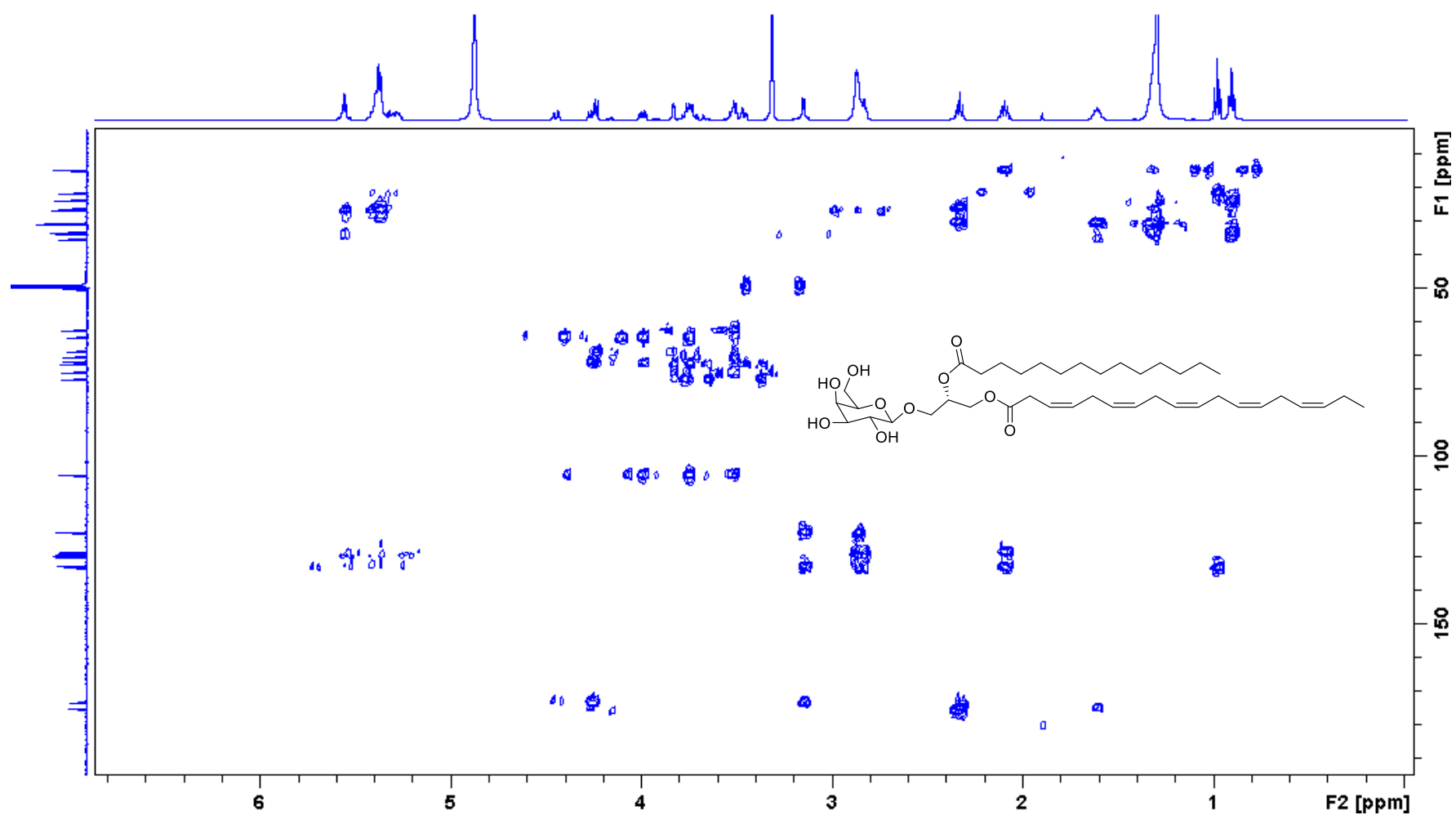
**Figure S4.** COSY Spectra (500 MHz) of Monogalactosyldiacylglycerol (**1**) in CD<sub>3</sub>OD



**Figure S5.** HSQC Spectra (500 MHz) of of Monogalactosyldiacylglycerol (**1**) in CD<sub>3</sub>OD



**Figure S6.** HMBC Spectra (500 MHz) of of Monogalactosyldiacylglycerol (**1**) in CD<sub>3</sub>OD





**Figure S7. HRMS/ESITOF of Monogalactosyldiacylglycerol (1)**

**Single Mass Analysis**

Tolerance = 4.0 PPM / DBE: min = 0.0, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

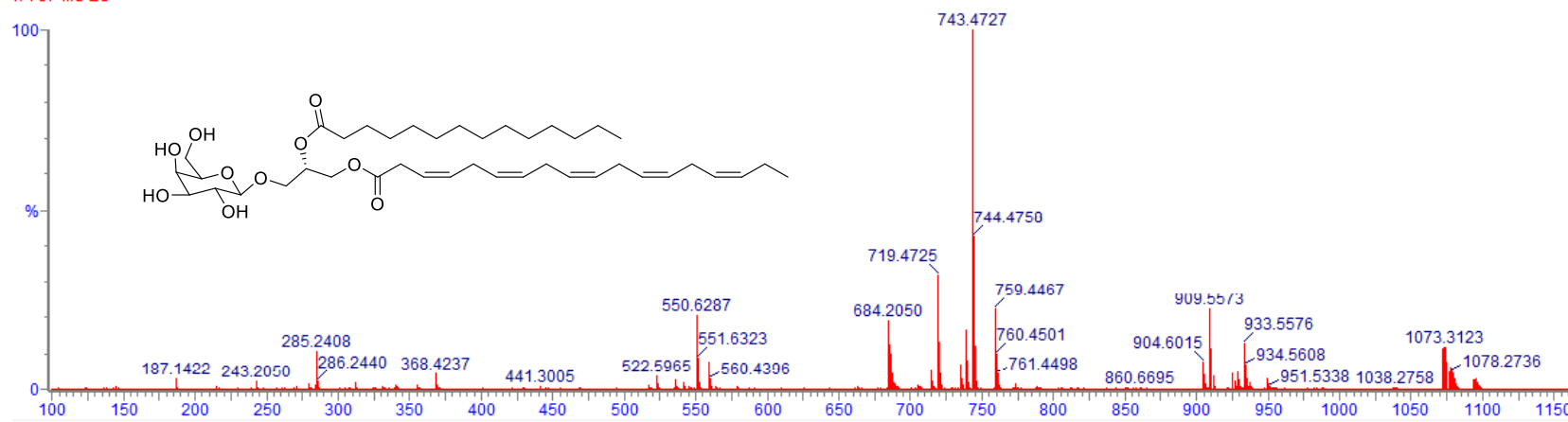
315 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)

Elements Used:

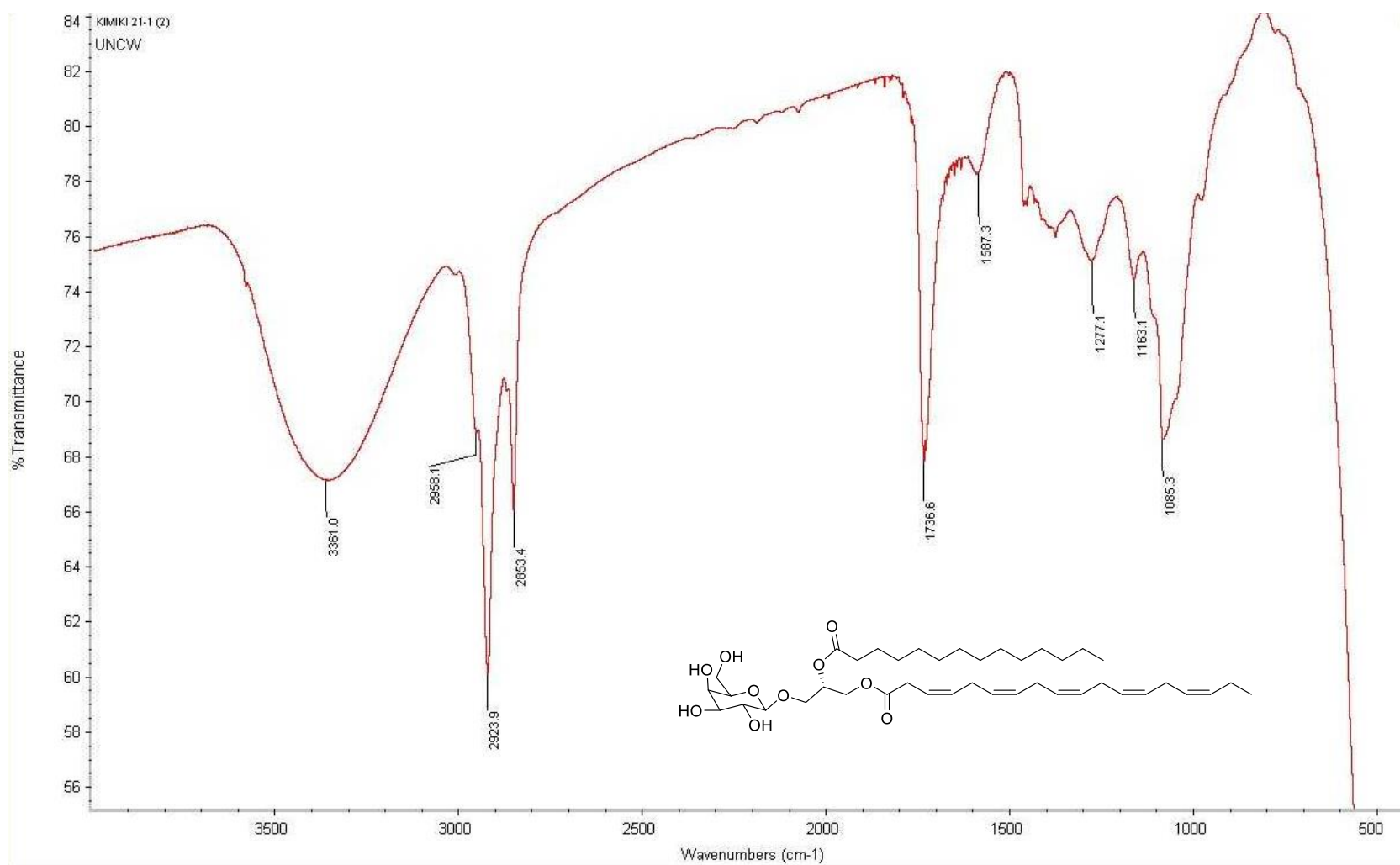
Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	O	Na
743.4727	743.4734	-0.7	-0.9	10.5	C43 H67 O10	444.9	1.606	20.07	43	67	10	
	743.4710	1.7	2.3	7.5	C41 H68 O10 Na	443.5	0.224	79.93	41	68	10	1

<miki 3rd extract meoh 10 2 2844 (5.514)AM2 (Ar,30000.0,556.28,0.00,LS 10); ABS

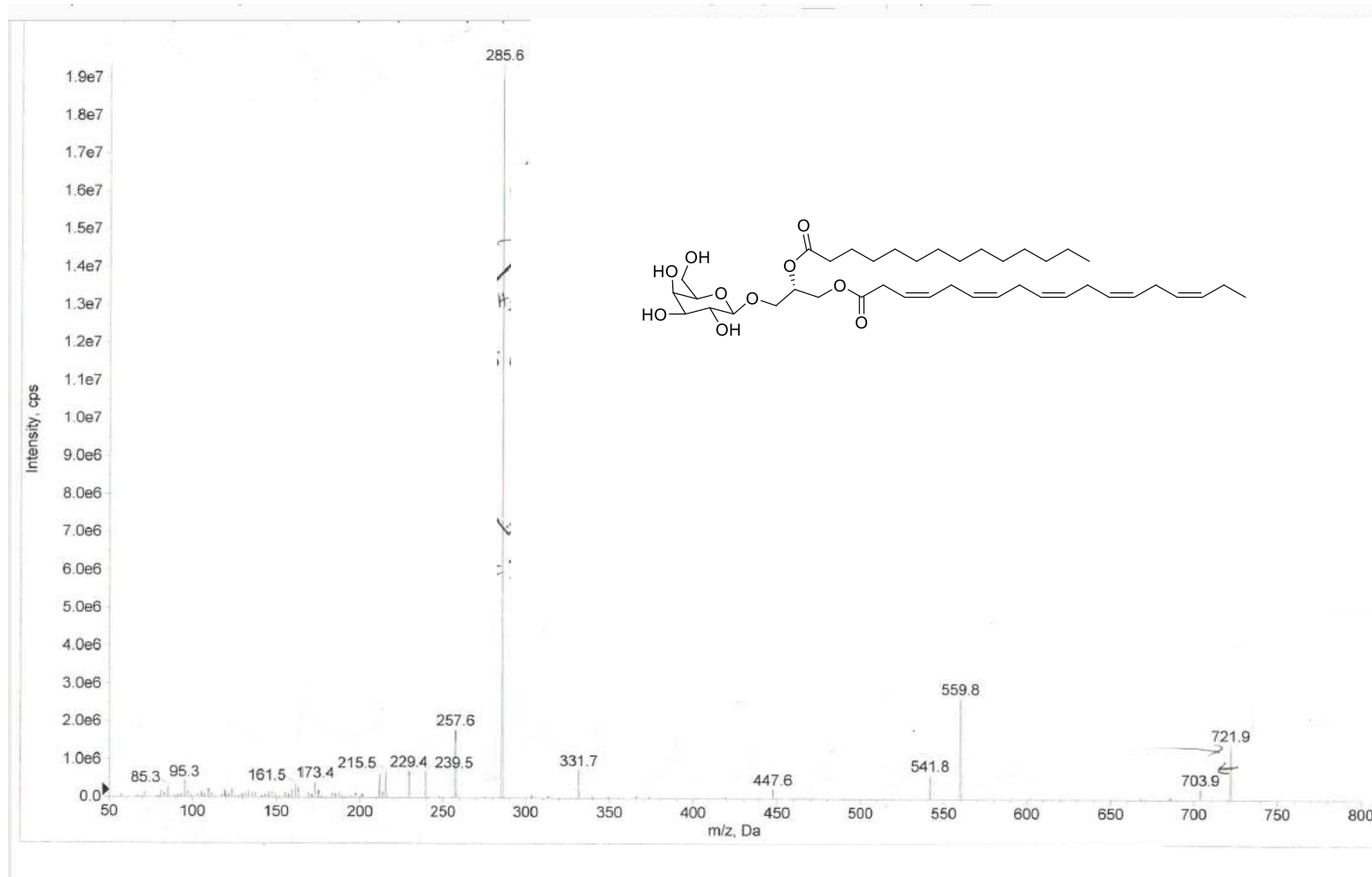
1: TOF MS ES+



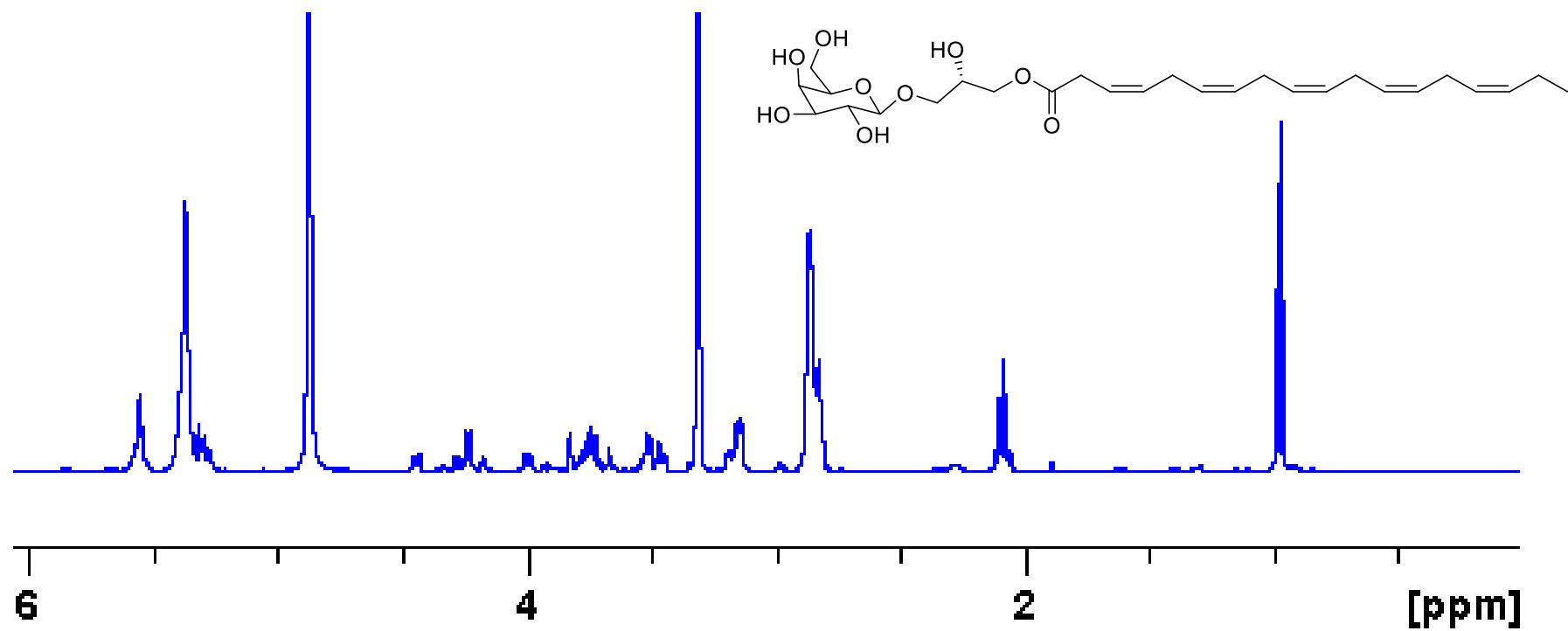
**Figure S8.** IR Spectra of Monogalactosyldiacylglycerol (**1**)



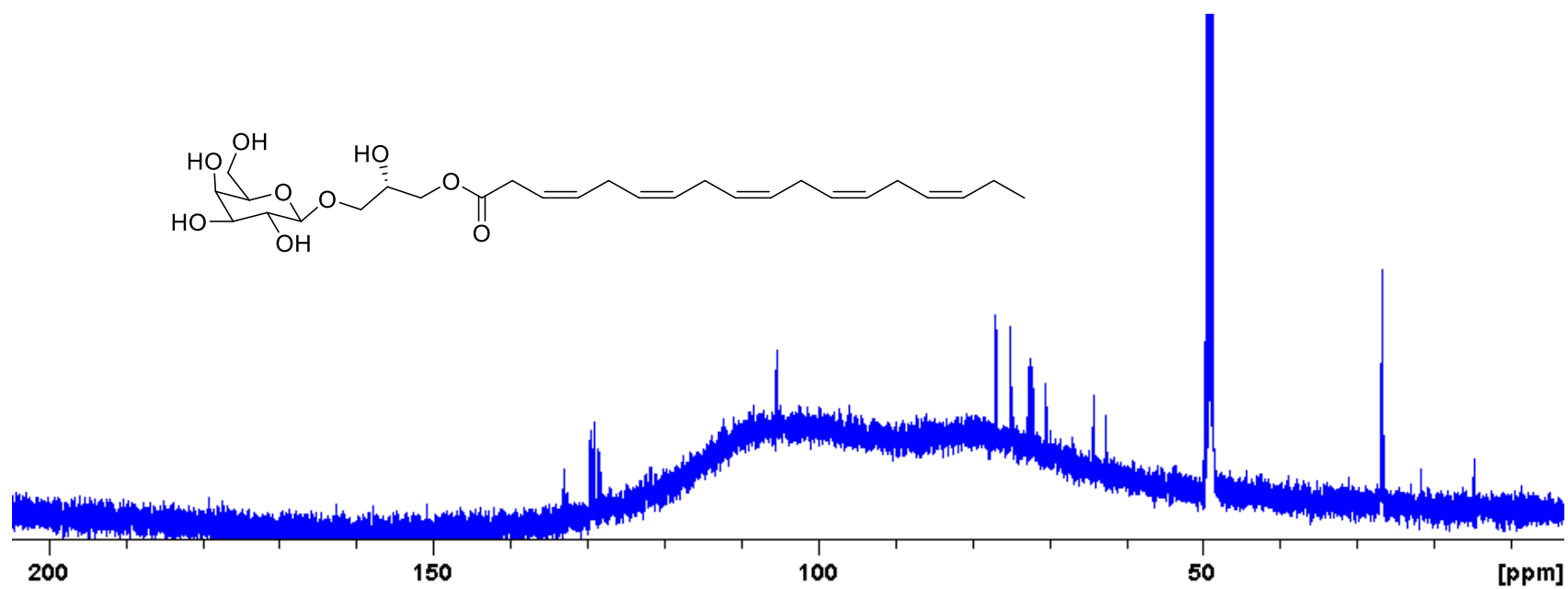
**Figure S9.** Fragmentation ESI-MS of the monogalactosyldiacylglycerol (**1**)



**Figure S10.**  $^1\text{H}$  NMR Spectrum (500 MHz) of Monogalactosylmonoacylglycerol (**2**) in  $\text{CD}_3\text{OD}$



**Figure S11.**  $^{13}\text{C}$  NMR Spectrum (125 MHz) of Monogalactosylmonoacylglycerol (**2**) in  $\text{CD}_3\text{OD}$



**Figure S12.** HRMS/ESI-TOF of Monogalactosylmonoacylglycerol (**2**)

**Single Mass Analysis**

Tolerance = 4.0 PPM / DBE: min = 0.0, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions

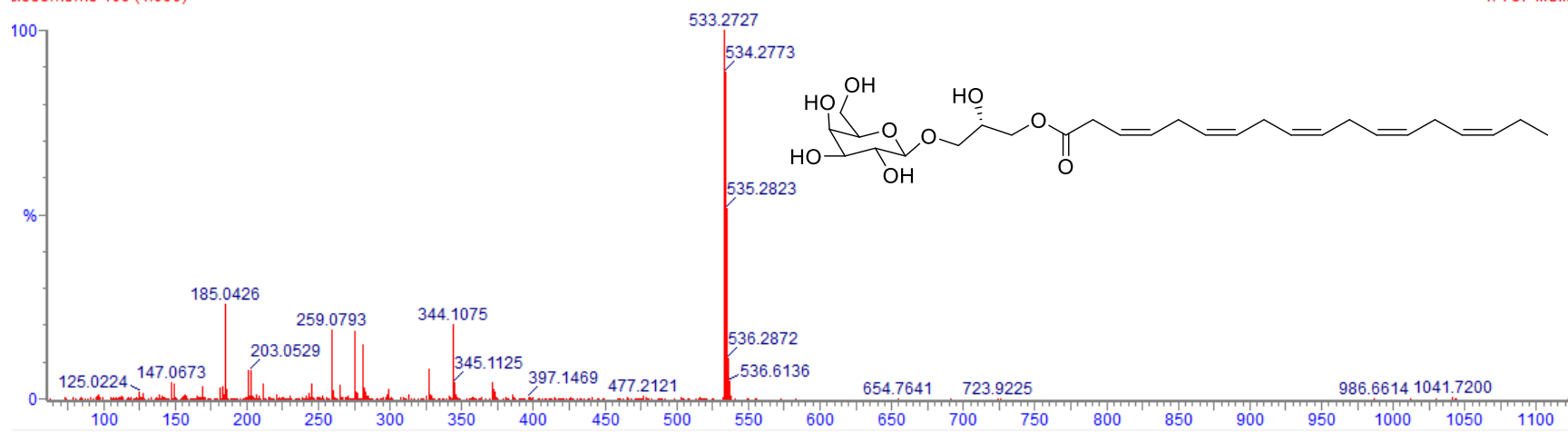
208 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

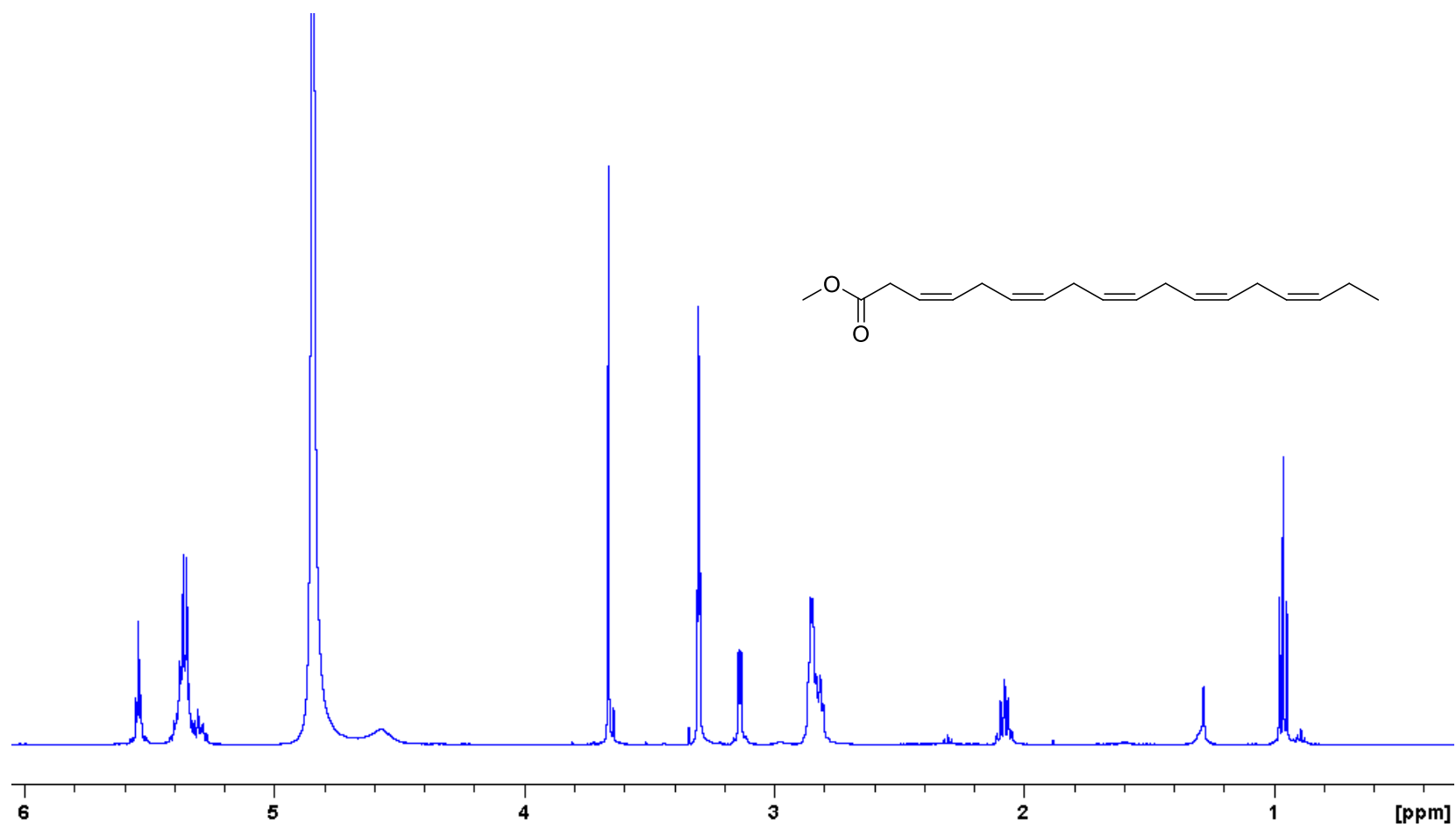
Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	O	Na
533.2727	533.2727	0.0	0.0	6.5	C <sub>27</sub> H <sub>42</sub> O <sub>9</sub> Na	276.3	n/a	n/a	27	42	9	1

msms 533 pos ce40  
1533msms 109 (1.090)

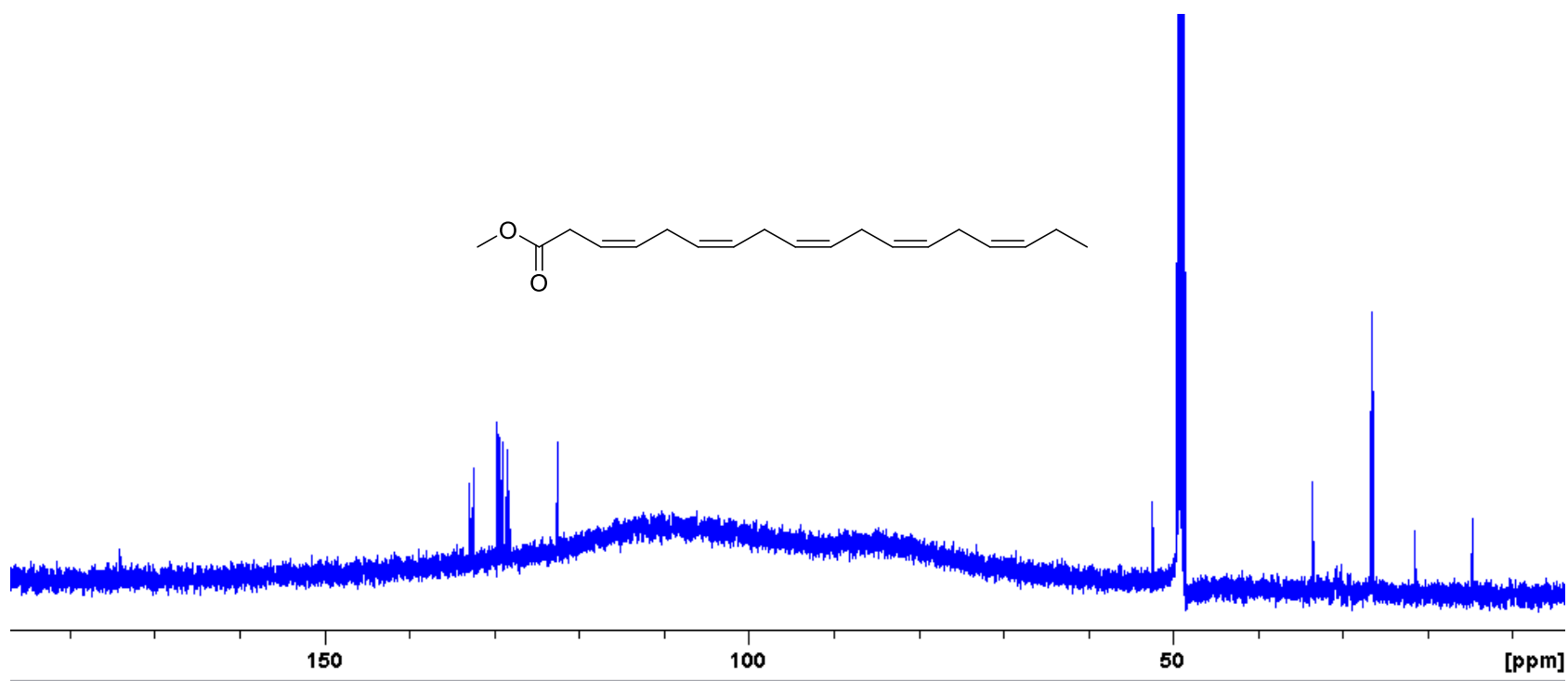
1: TOF MSMS!



**Figure S13.**  $^1\text{H}$  NMR Spectrum (500 MHz) of Polyunsaturated fatty acid methyl ester (**3**) in  $\text{CD}_3\text{OD}$



**Figure S14.**  $^{13}\text{C}$  NMR Spectrum (125 MHz) of Polyunsaturated fatty acid methyl ester (**3**) in  $\text{CD}_3\text{OD}$





**Figure S15.** HRMSEITOF of Polyunsaturated fatty acid methyl ester (**3**)

**Single Mass Analysis**

Tolerance = 4.0 PPM / DBE: min = 0.0, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

84 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	O	Na
289.2169	289.2168	0.1	0.3	5.5	C19 H29 O2	815.8	n/a	n/a	19	29	2	

kmiki 3rd extract meoh 9 1 1983 (3.852) AM2 (Ar,30000.0,556.28,0.00,LS 10); ABS

1: TOF MS ES+

