

# The Antitumoral Effect In Ovo of a New Inclusion Complex from Dimethoxycurcumin with Magnesium and Beta-Cyclodextrin

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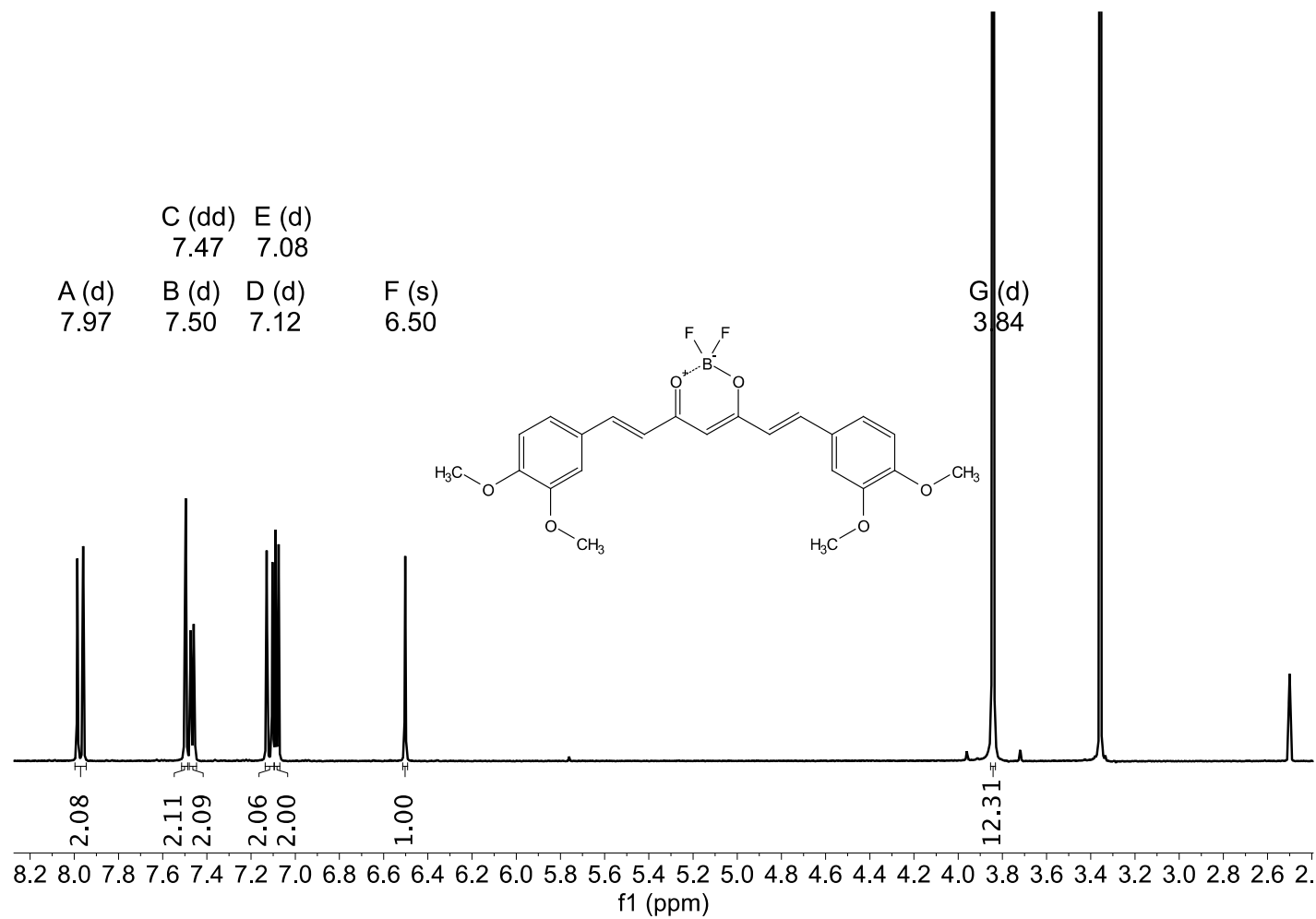
<sup>3</sup> Departamento de Biología de la Reproducción “Dr. Carlos Gual Castro”, Instituto Nacional de Ciencias Médicas y Nutrición Salvador Zubirán, México, Mexico City 14080, Mexico; barrera1912@gmail.com (D.B.-H.); mariol\_48@ciencias.unam.mx (M.G.-O.)

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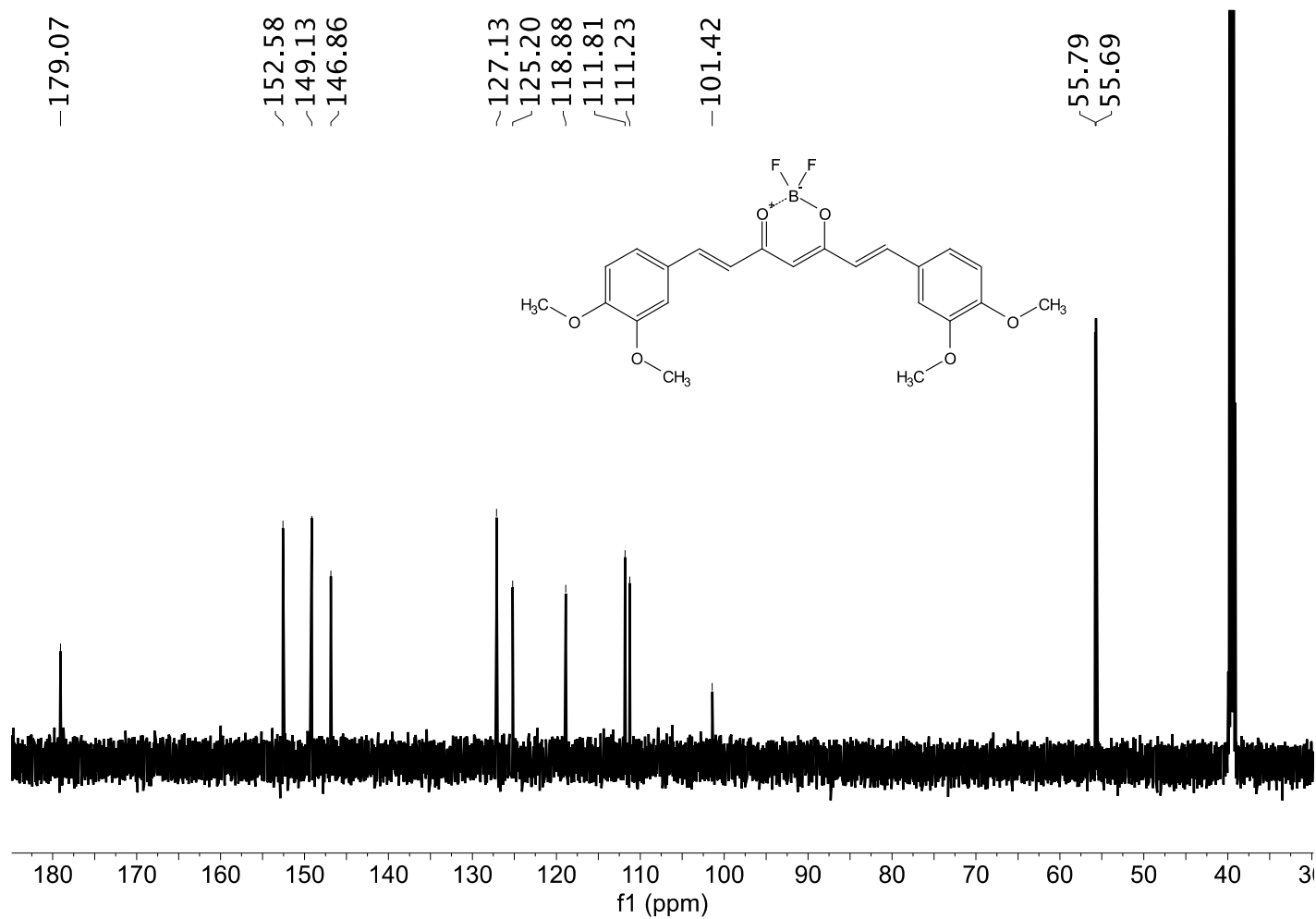
† These authors contributed equally to this work.

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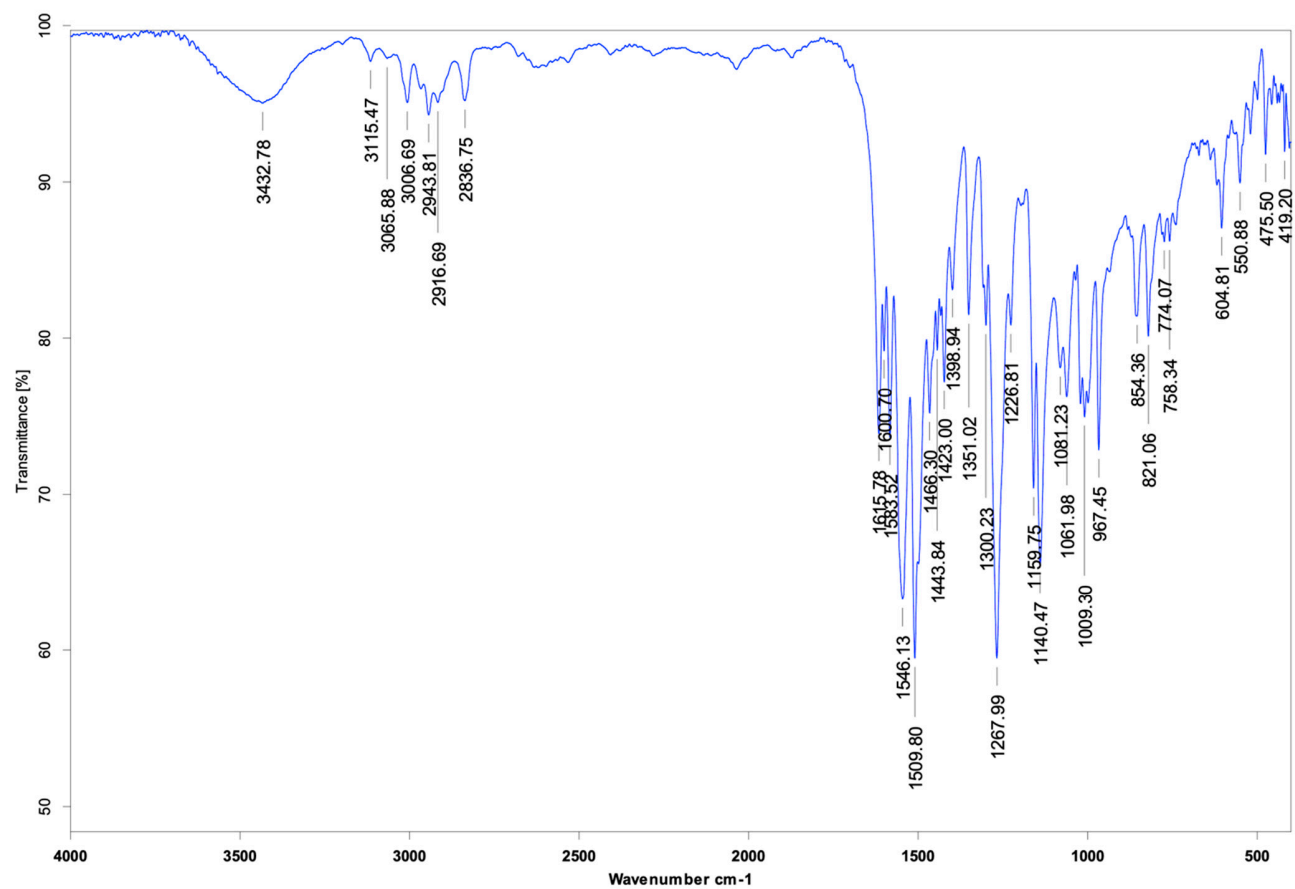
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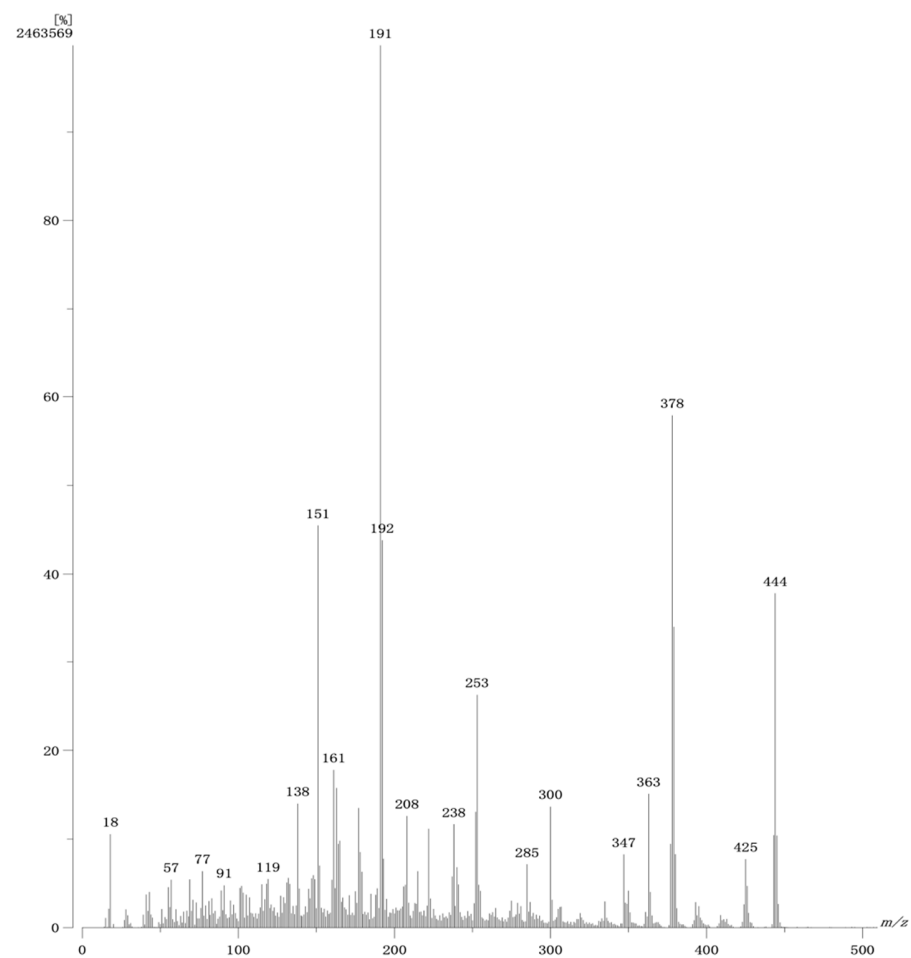
**Fig S1.** <sup>1</sup>H NMR spectrum of Dimethoxycurcumin-BF<sub>2</sub> ( DiMeOC-BF<sub>2</sub>, 400 MHz, DMSO-*d*<sub>6</sub>).



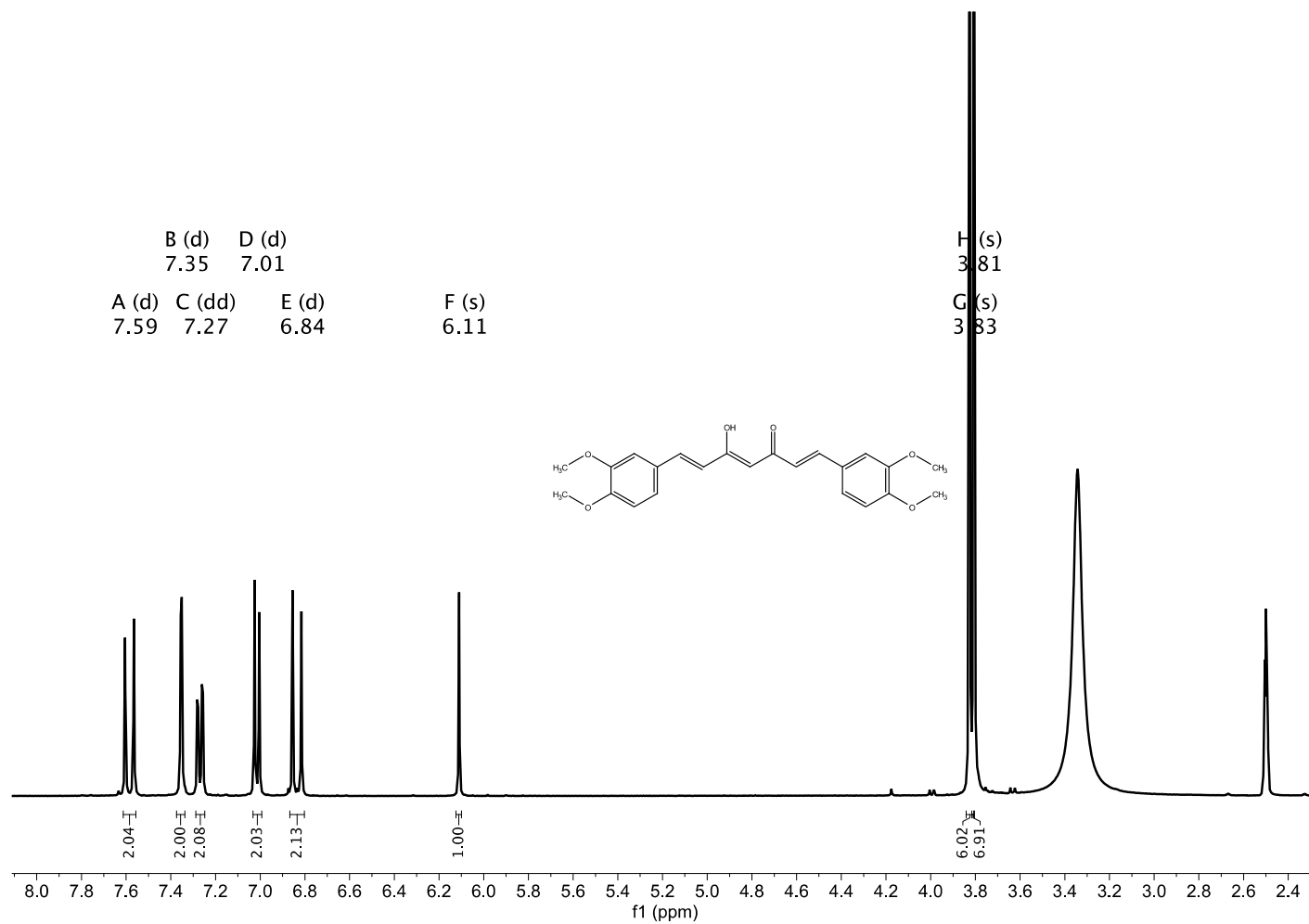
**Fig S2.**  $^{13}\text{C}$  NMR spectrum of Dimethoxycurcumin- $\text{BF}_2$  ( DiMeOC- $\text{BF}_2$ , 100 MHz,  $\text{DMSO-}d_6$ ).



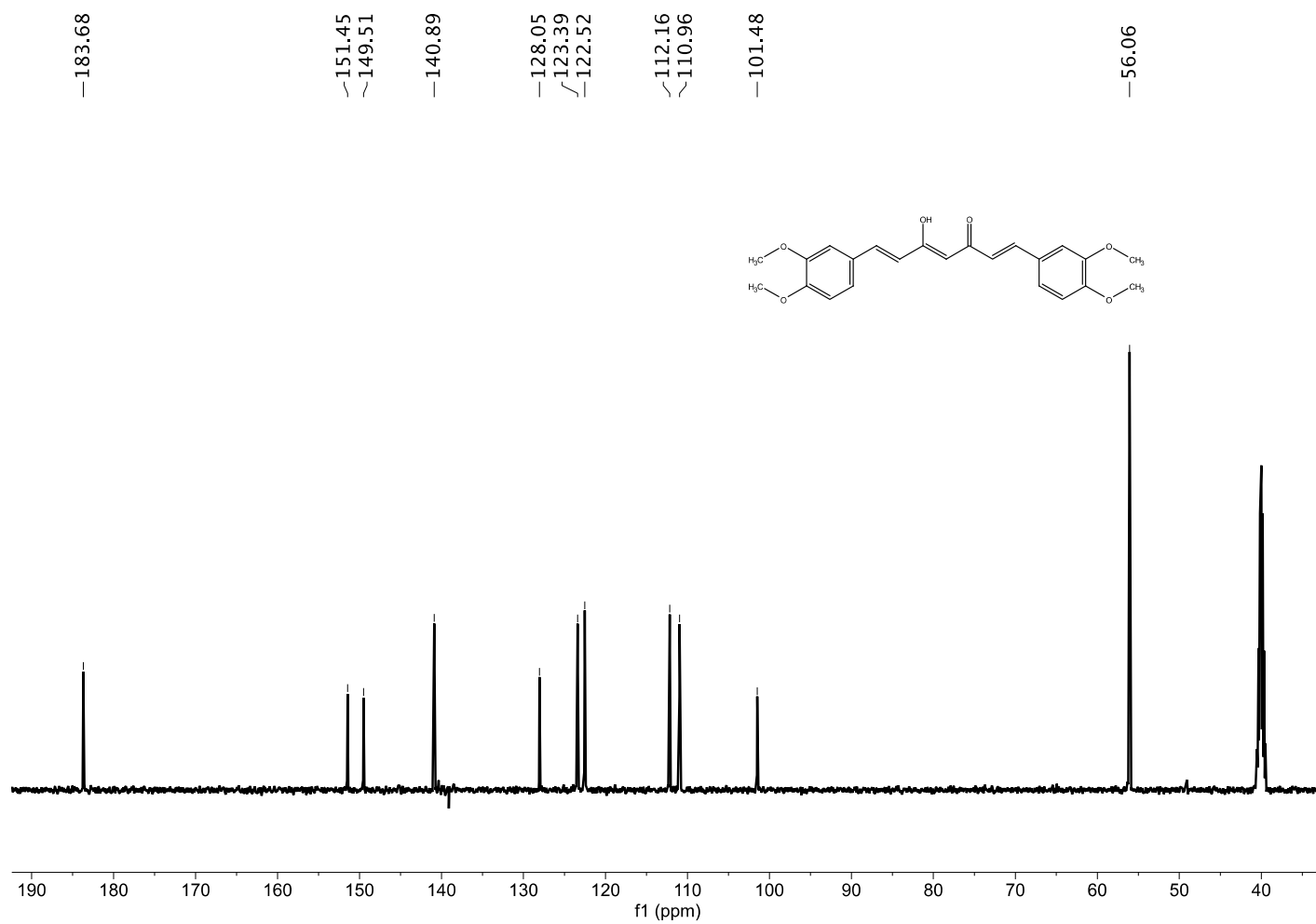
**Fig S3.** IR Spectrum of DiMeOC-BF<sub>2</sub>.



**Fig S4.** Mass Spectrum of DiMeOC-BF<sub>2</sub> (IE<sup>+</sup>).



**Fig S5.** <sup>1</sup>H NMR spectrum of DiMeOC (400 MHz, DMSO- $d_6$ ).



**Fig S6.** <sup>13</sup>C NMR spectrum of DiMeOC (100 MHz, DMSO-*d*<sub>6</sub>).

\*\*\* PEAK-PICK \*\*\*

-- PEAK --		-- VALLEY --	
$\lambda$	ABS	$\lambda$	ABS
417.0	0.975	641.0	-0.002
262.0	0.215	288.0	0.098
220.0	0.271	246.0	0.173

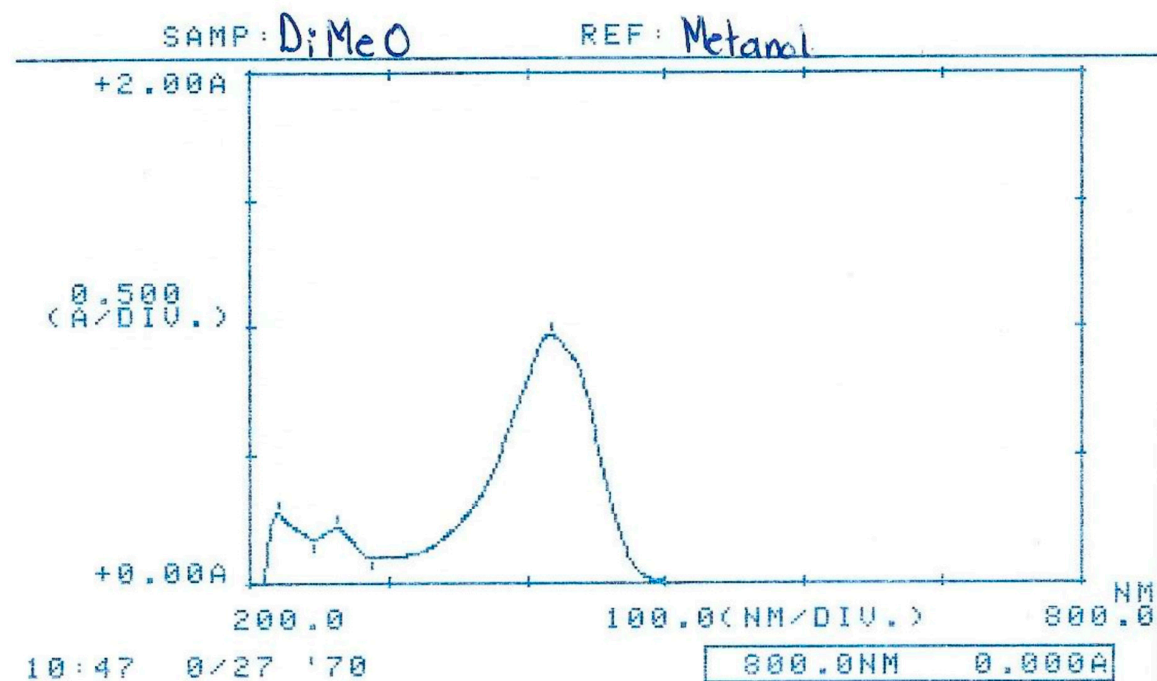
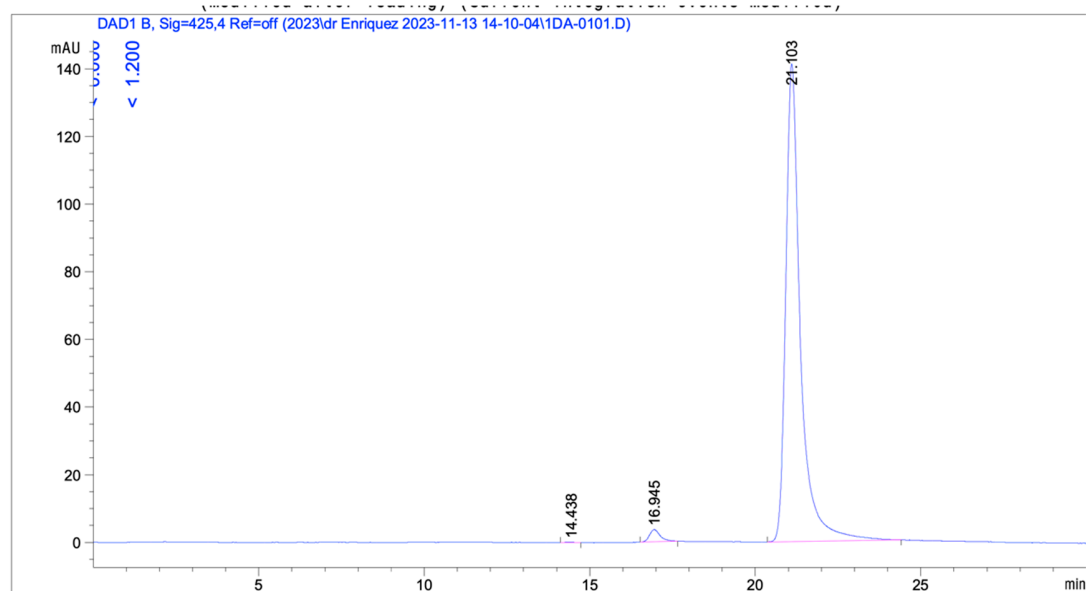


Fig S7. UV-VIS spectrum in methanol of DiMeOC.

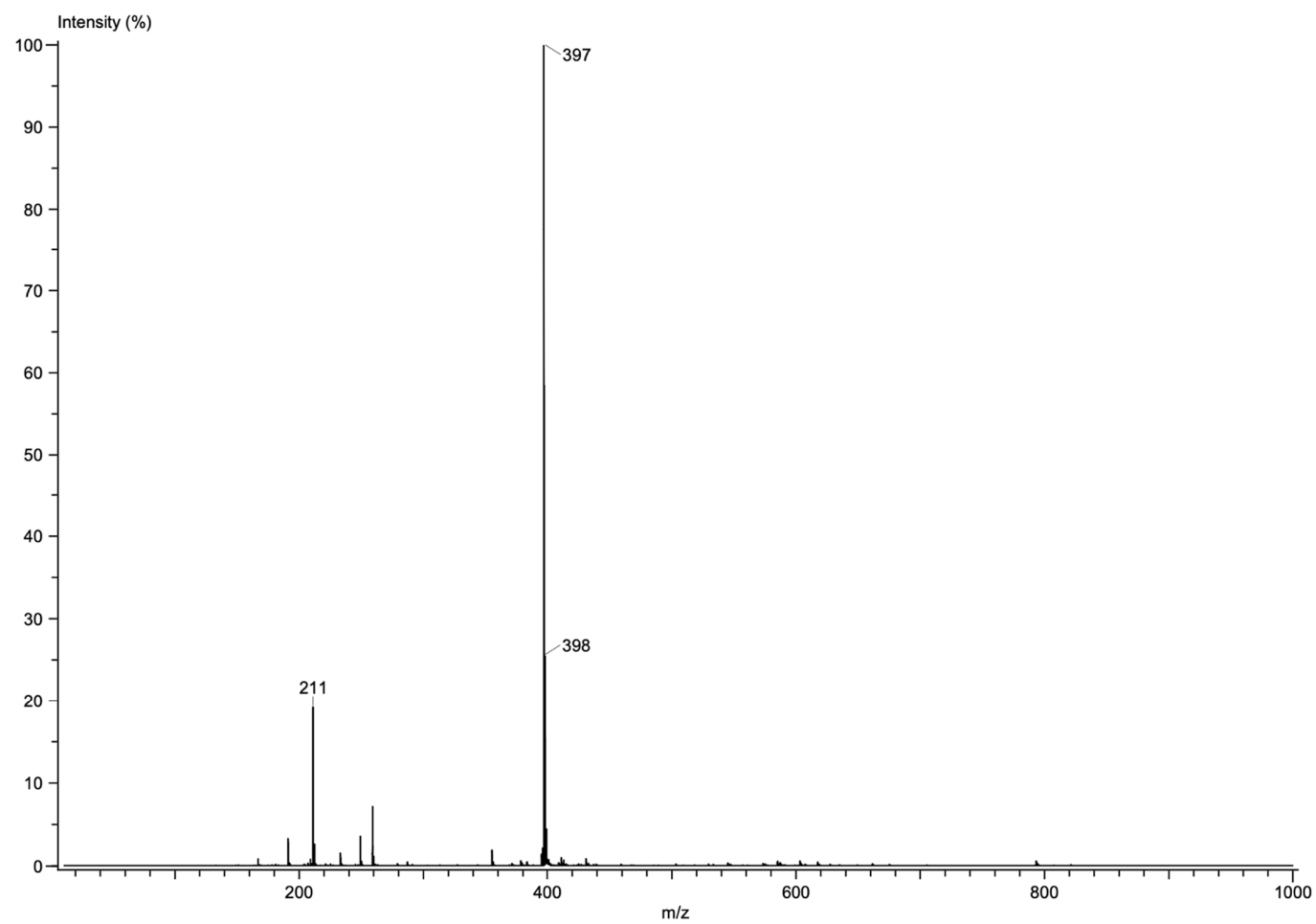


Signal 1: DAD1 B, Sig=425,4 Ref=off

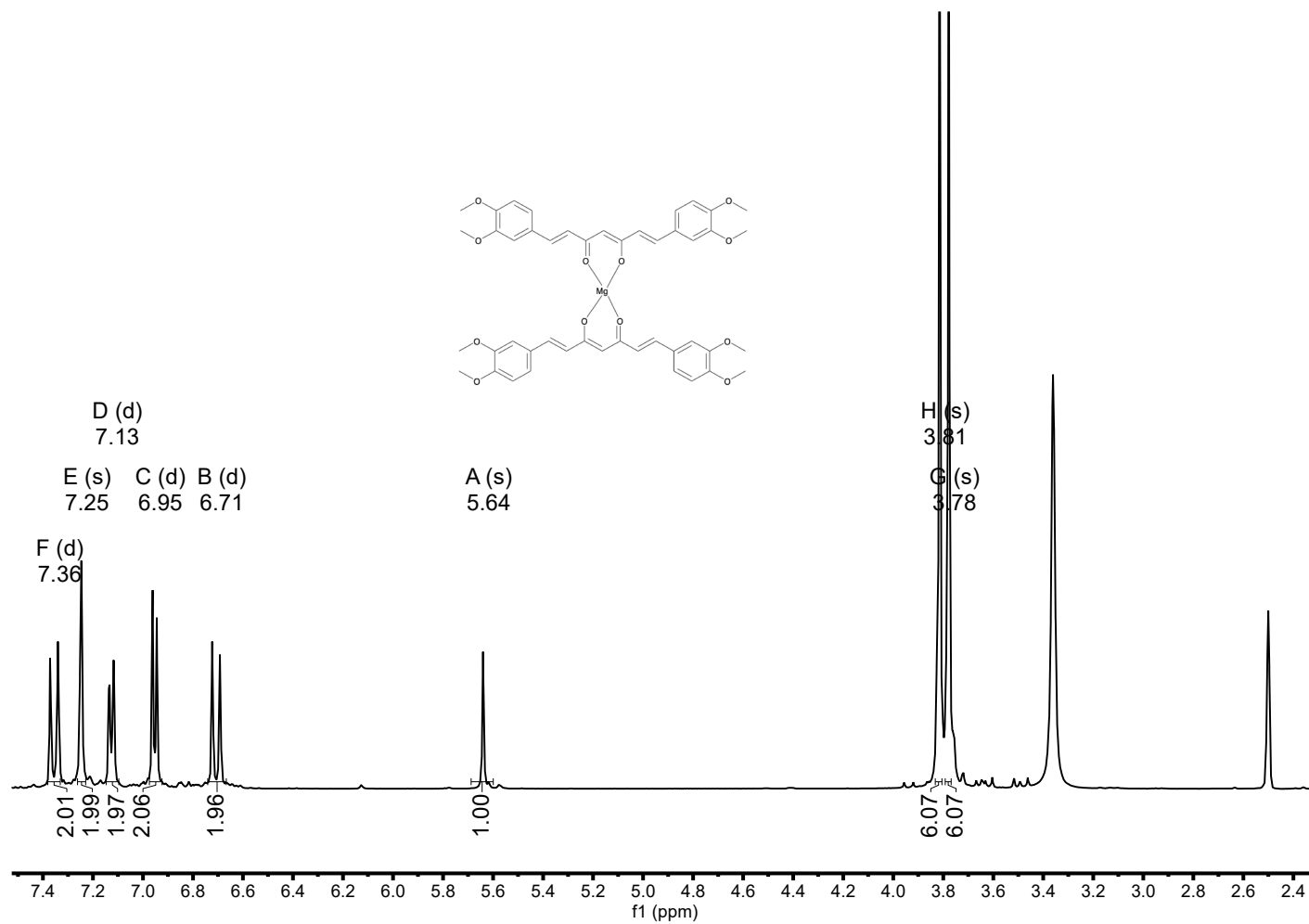
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.438	BB	0.2067	3.60961	2.16300e-1	0.0812
2	16.945	BB	0.3063	82.44865	3.63930	1.8543
3	21.103	BB	0.4564	4360.39209	141.14056	98.0646

Totals : 4446.45035 144.99616

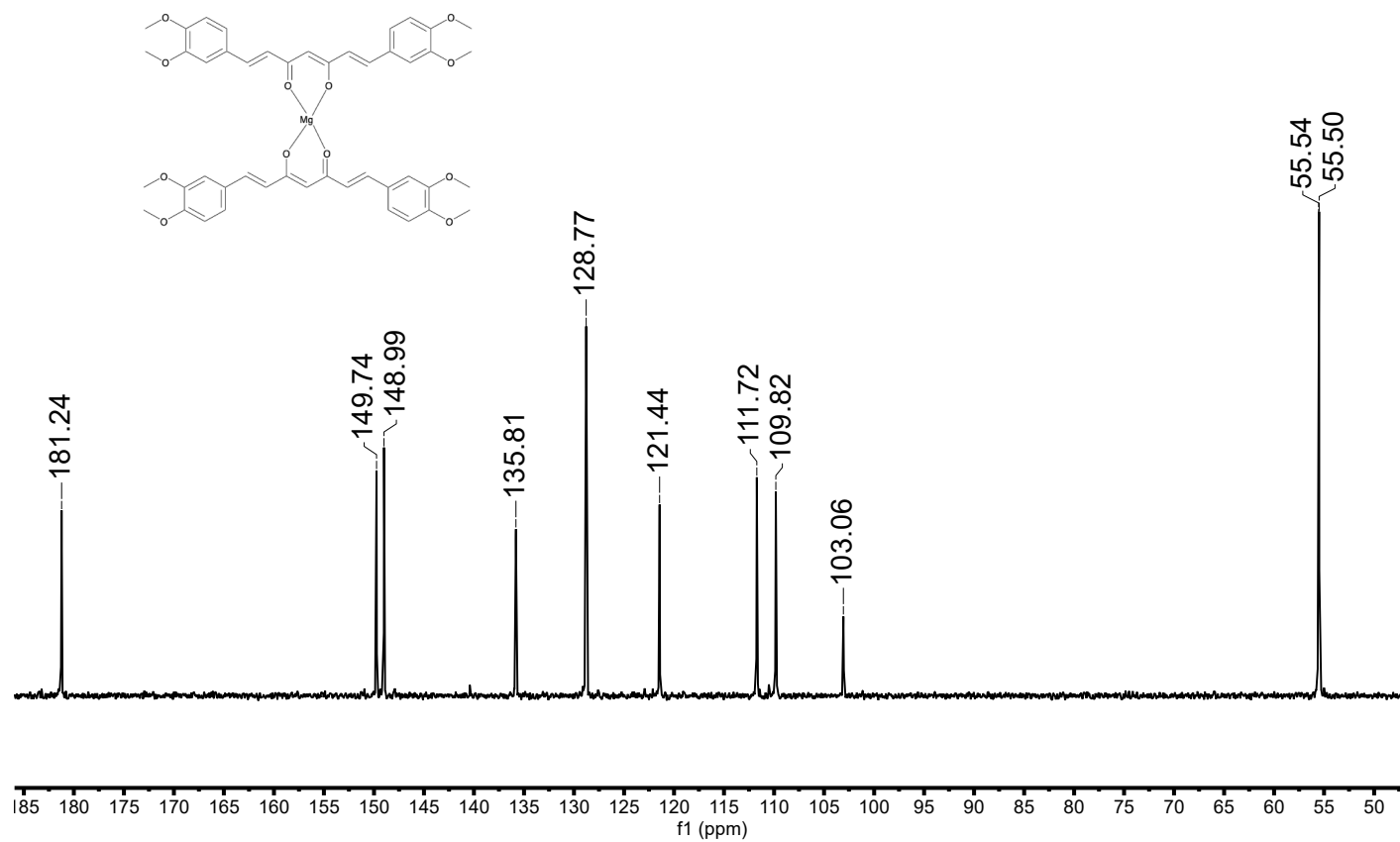
**Fig S8.** HPLC spectrum of DiMeOC (417nm, CH<sub>3</sub>CN/H<sub>2</sub>O (0.02% formic acid) 55:45)



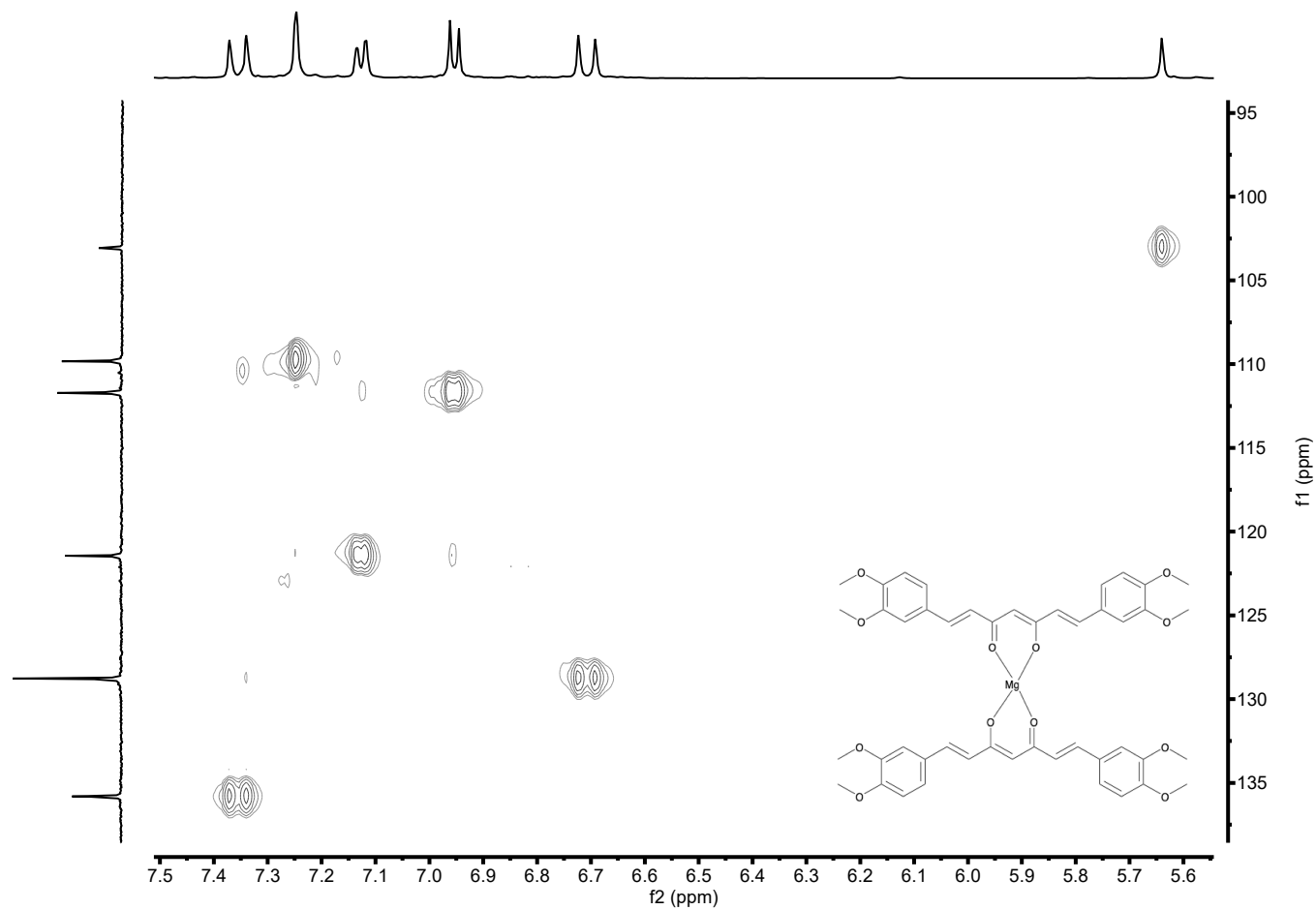
**Fig S9.** Mass Spectrum of DiMeOC (DART<sup>+</sup>).



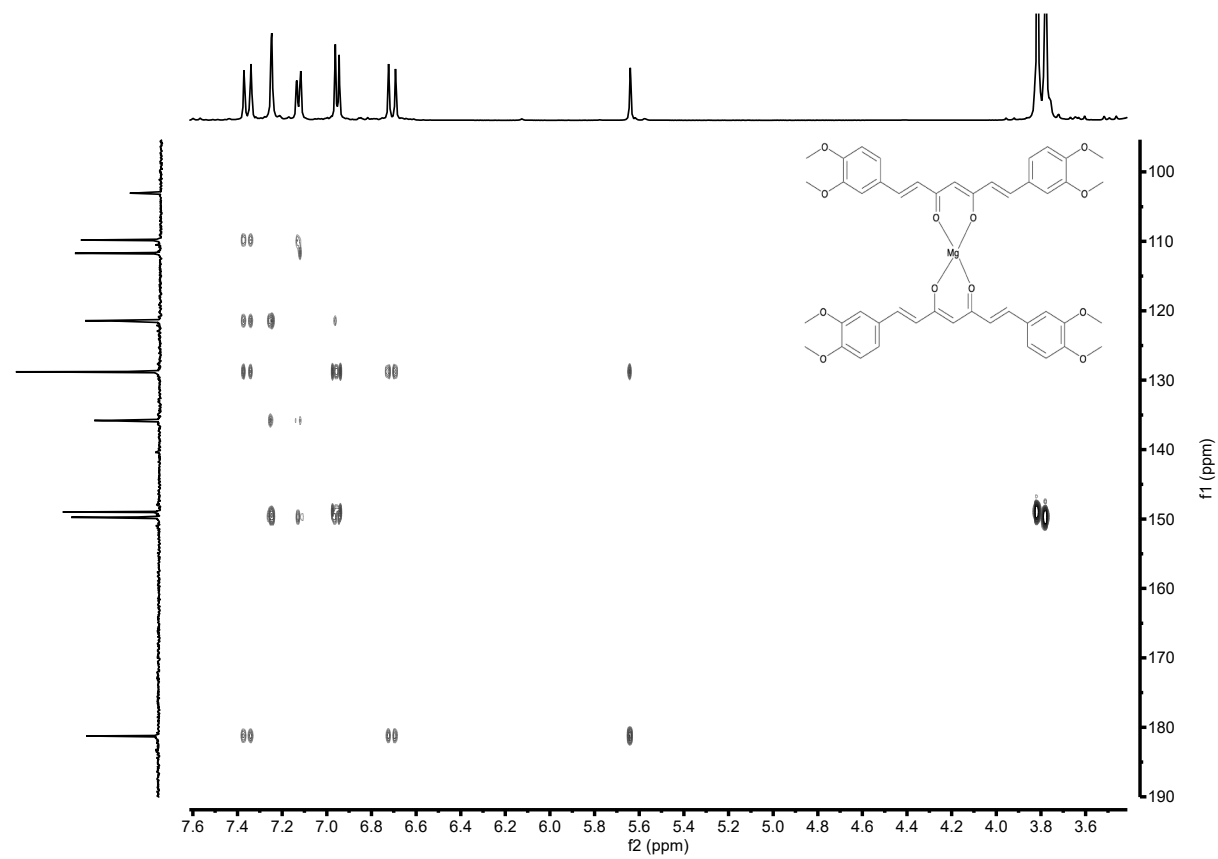
**Fig S10.**  $^1\text{H}$  NMR spectrum of DiMeOC-Mg (400 MHz,  $\text{DMSO}-d_6$ )



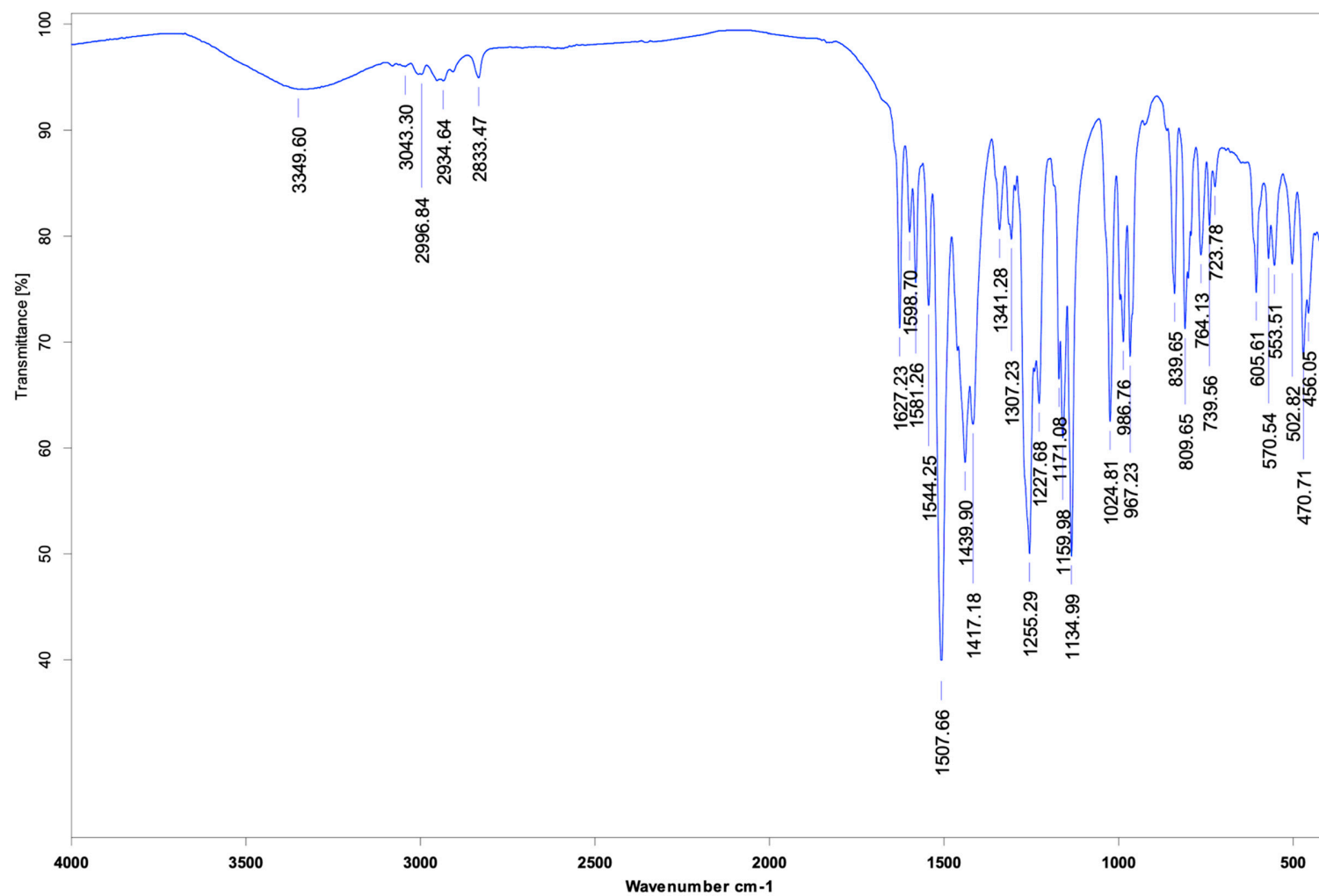
**Fig S11.**  $^{13}\text{C}$  NMR spectrum of DiMeOC-Mg (100 MHz,  $\text{DMSO-}d_6$ ).



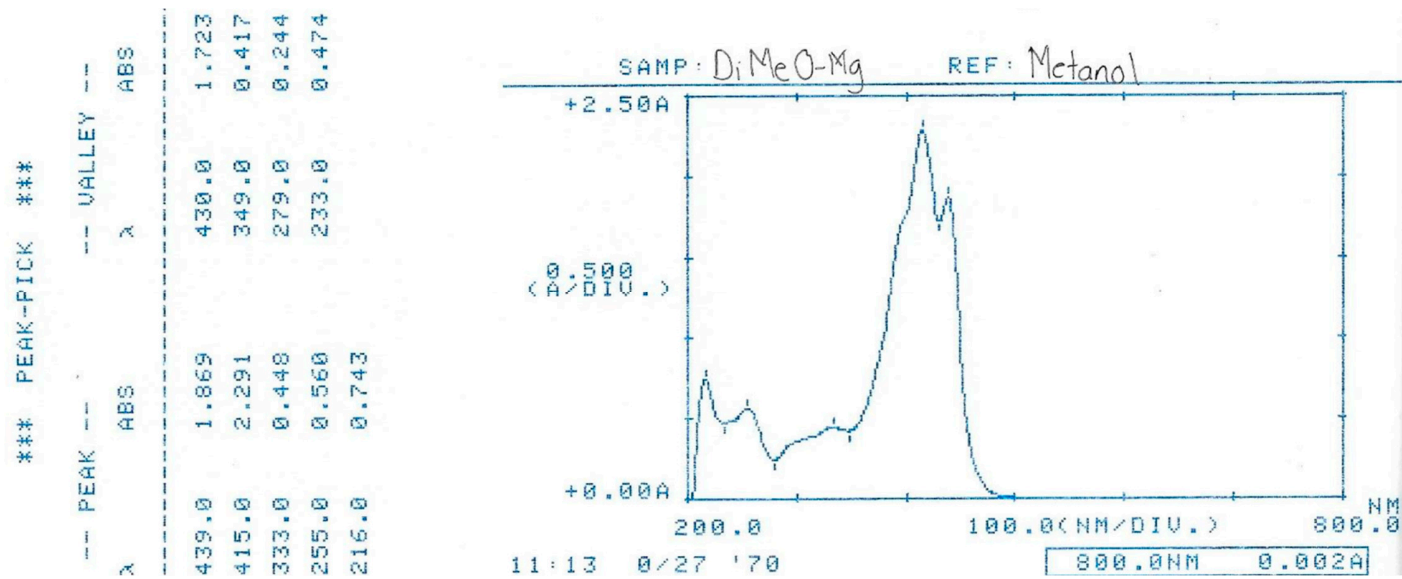
**Fig S12.** HSQC NMR spectrum of DiMeOC-Mg (400 MHz, DMSO- $d_6$ ).



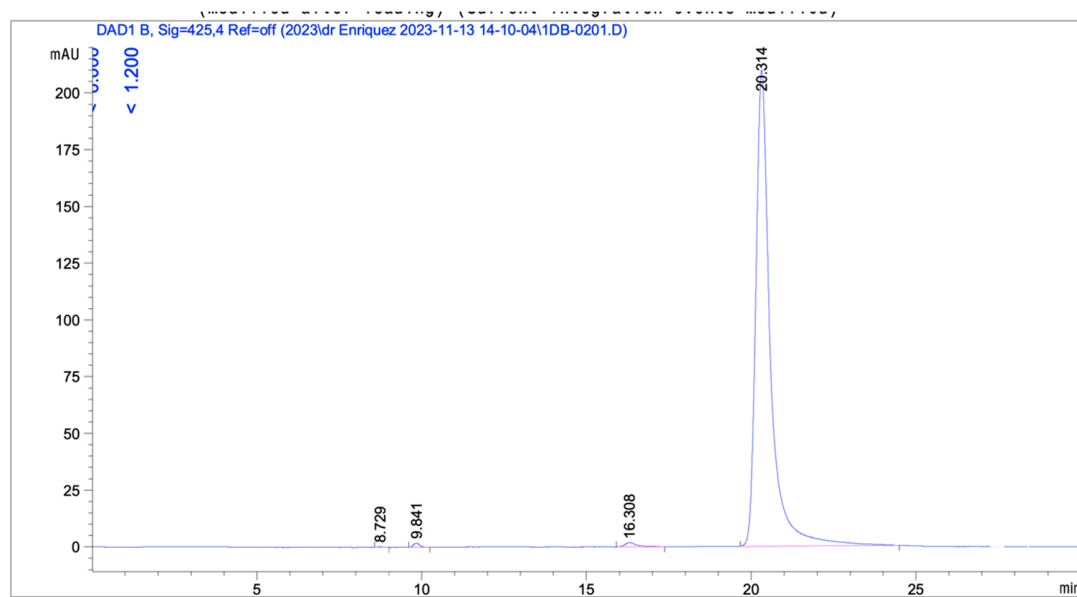
**Fig S13.** HMBC NMR spectrum of DiMeOC-Mg (400 MHz, DMSO-*d*<sub>6</sub>).



**Fig S14.** IR Spectrum of DiMeOC-Mg.



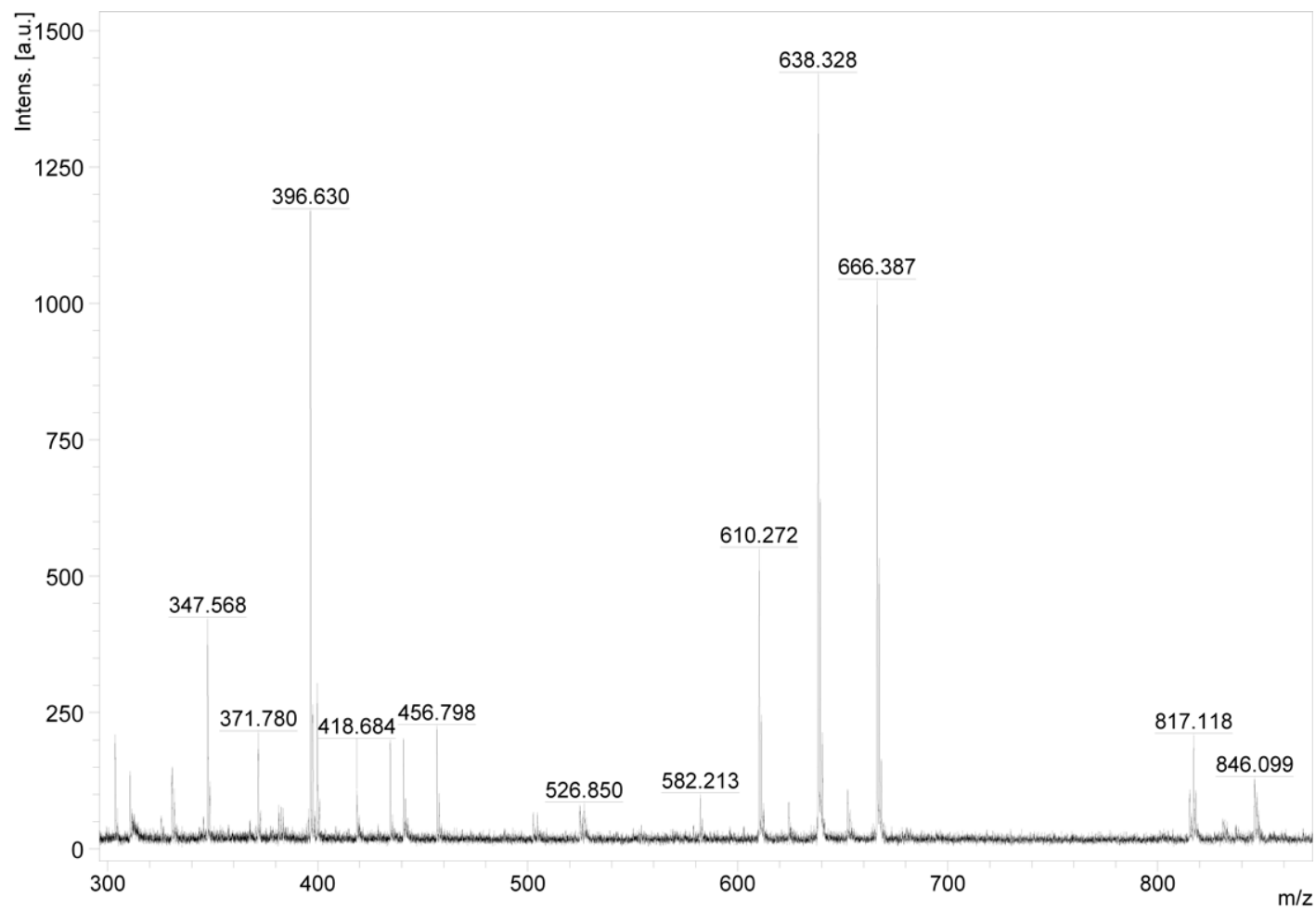
**Fig S15.** UV-VIS spectrum in methanol of DiMeOC-Mg .



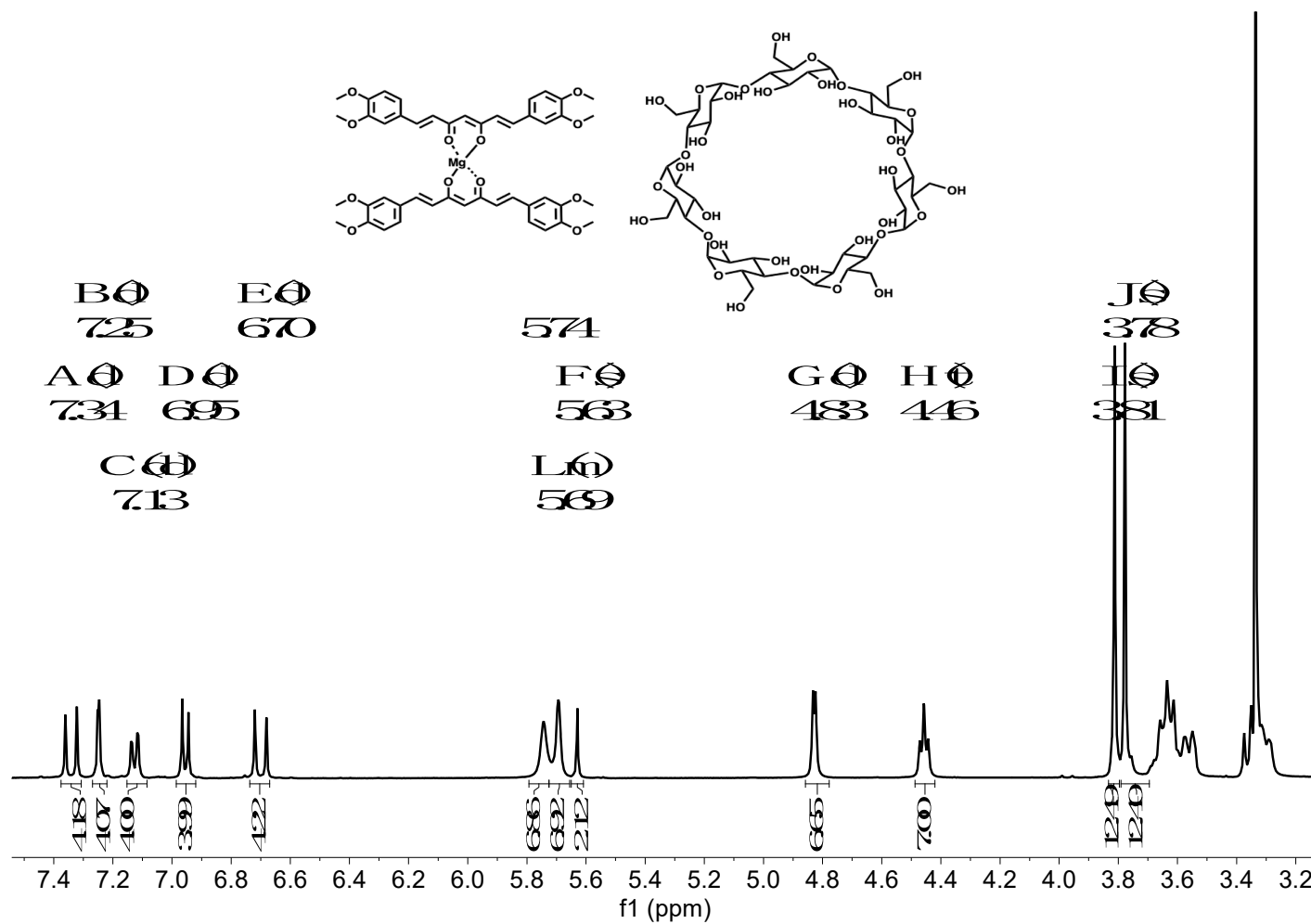
**Fig S16.** HPLC spectrum of DiMeOC-Mg (417 nm, CH<sub>3</sub>CN/H<sub>2</sub>O (0.02% formic acid) 55:45).

Signal 1: DAD1 B, Sig=425,4 Ref=off

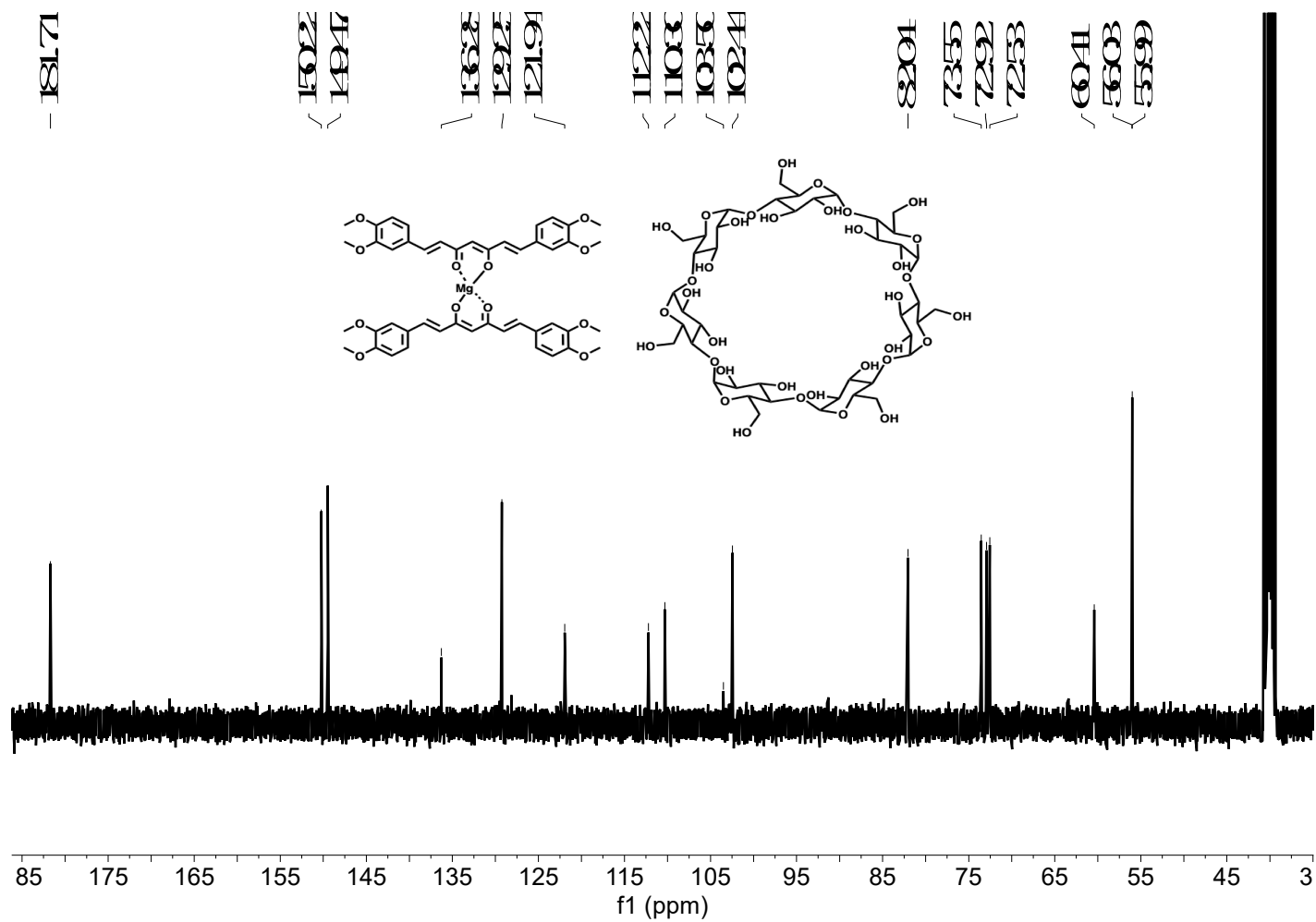
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.729	BB	0.1436	3.30270	3.01962e-1	0.0507
2	9.841	BB	0.1913	23.72007	1.90404	0.3642
3	16.308	BV R	0.3436	50.56177	1.91799	0.7763
4	20.314	BB	0.4502	6435.36230	209.61371	98.8088



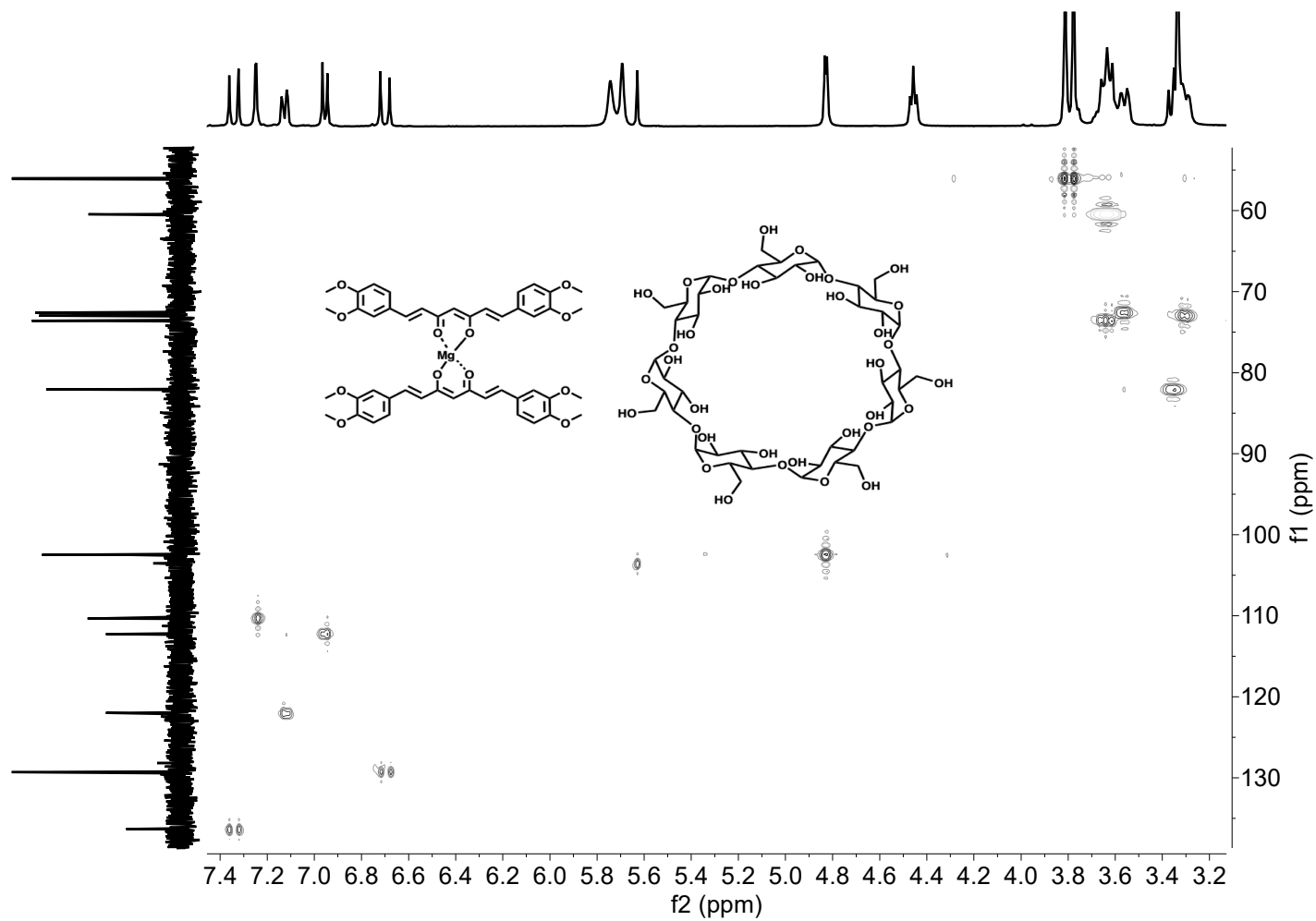
**Fig S17.** Mass Spectrum of DiMeOC-Mg (MALDI-TOF).



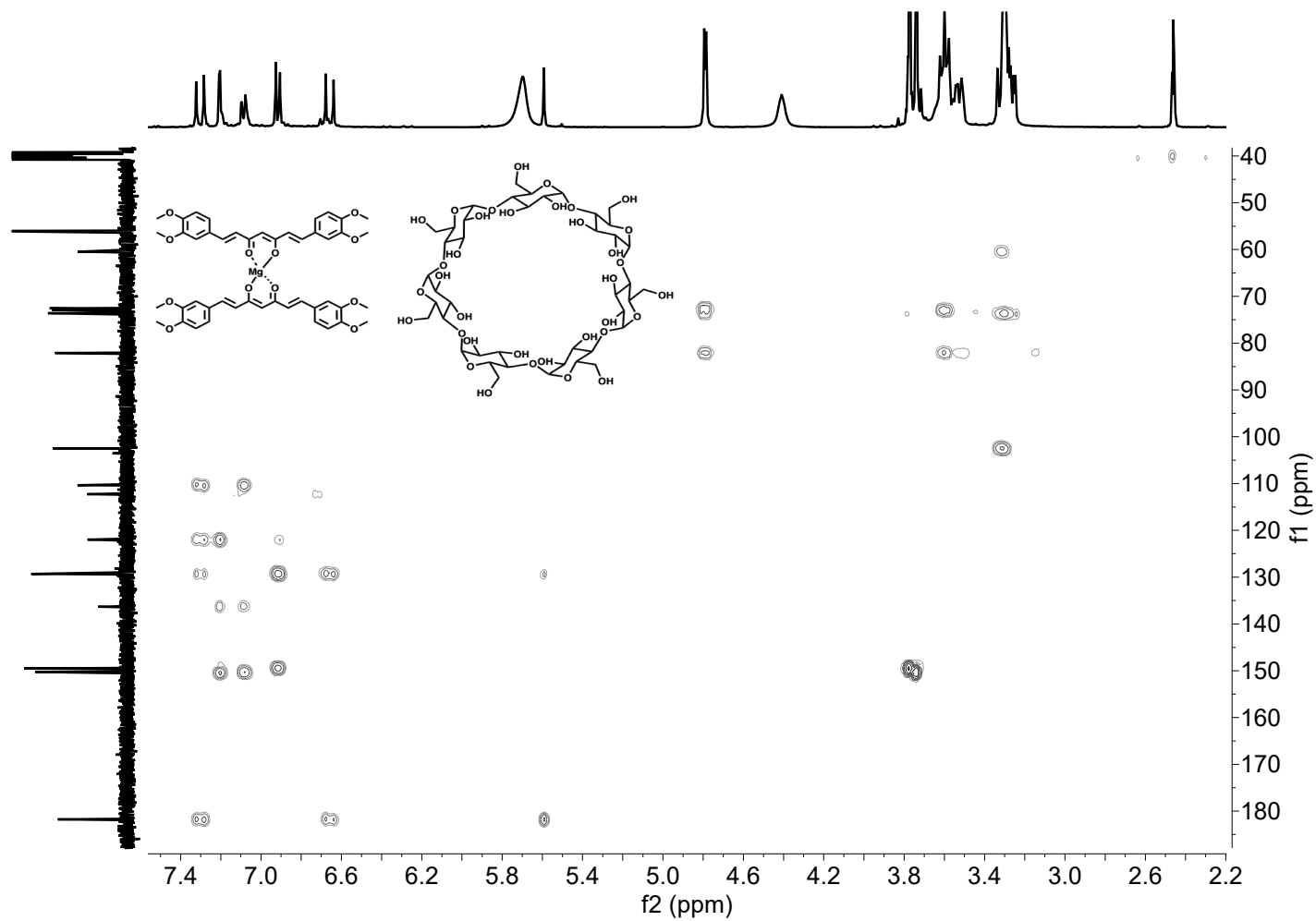
**Fig S18.**  $^1\text{H}$  NMR spectrum of DiMeOC-Mg-BCD (400 MHz,  $\text{DMSO-}d_6$ ).



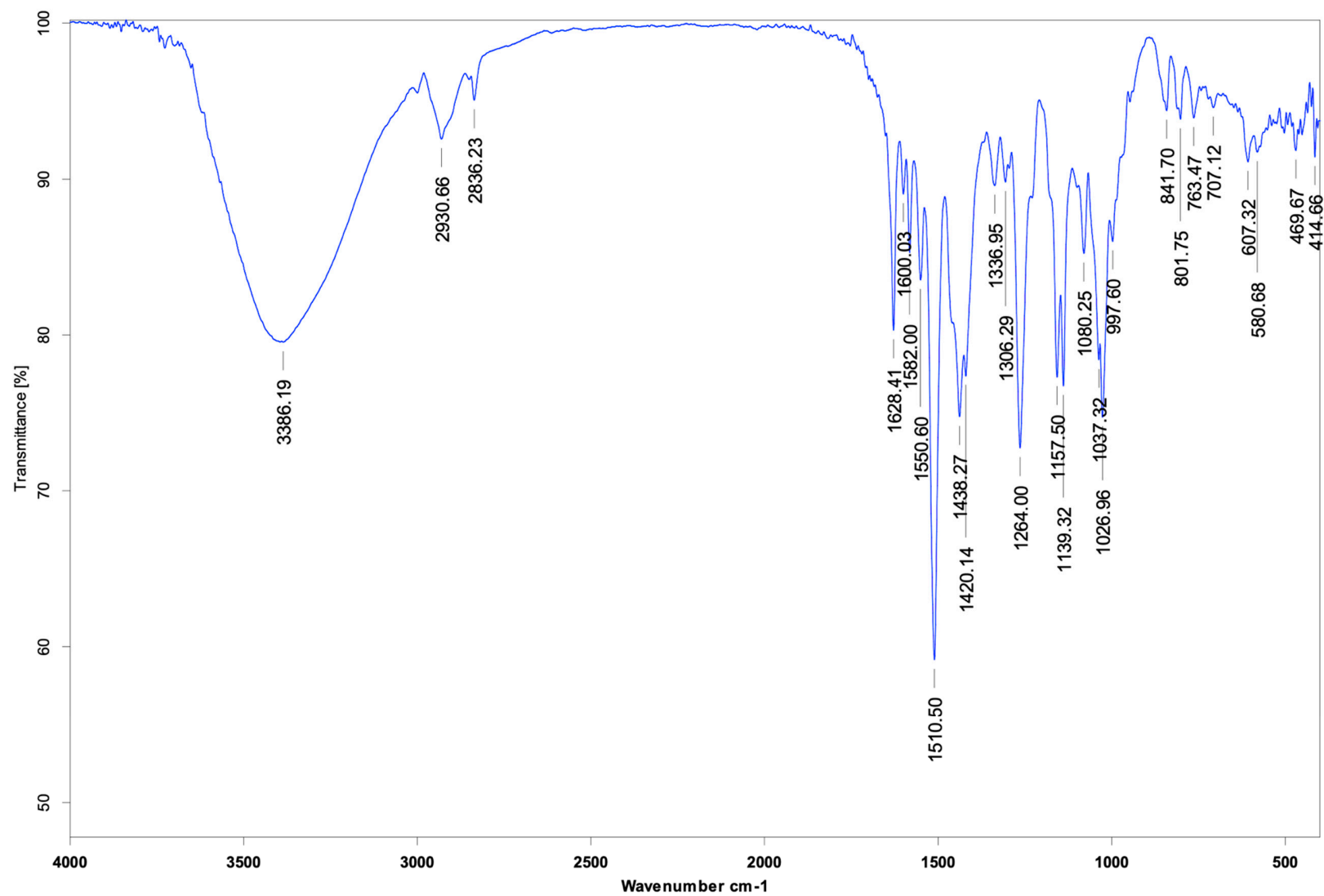
**Fig S19.**  $^{13}\text{C}$  NMR spectrum of DiMeOC-Mg-BCD (100 MHz,  $\text{DMSO}-d_6$ ).



**Fig S20.** HSQC NMR spectrum of DiMeOC-Mg-BCD (400 MHz,  $\text{DMSO-}d_6$ ).

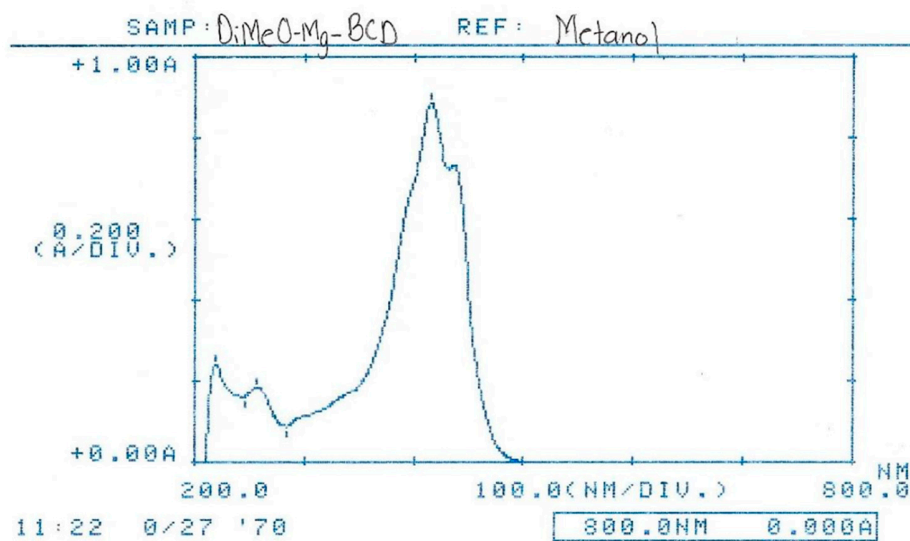


**Fig S21.** HMBC NMR spectrum of DiMeOC-Mg-BCD (400 MHz,  $\text{DMSO-}d_6$ ).

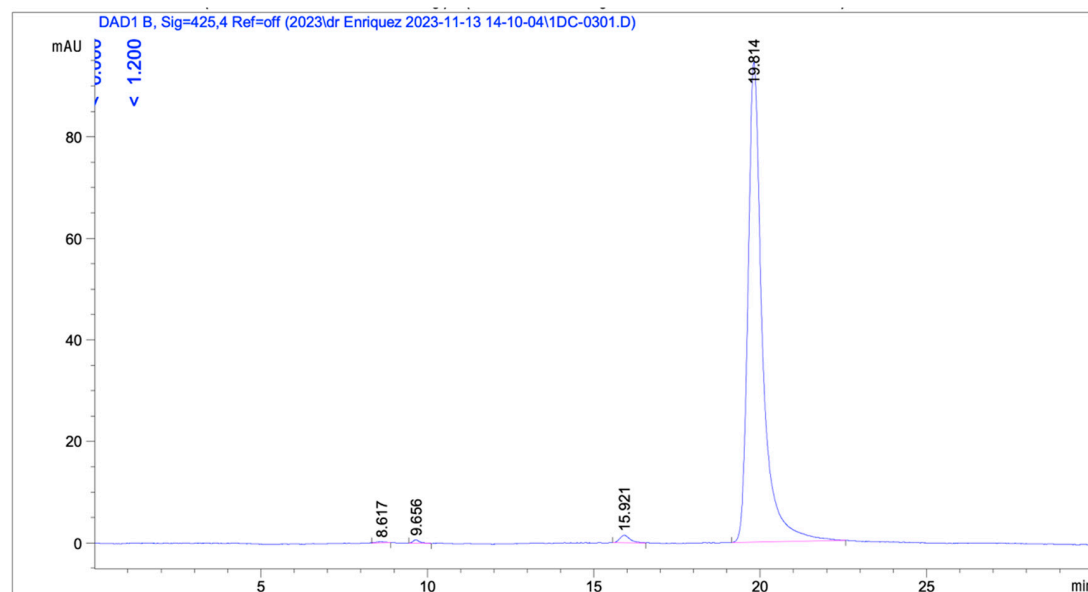


**Fig S22.** IR Spectrum of DiMeOC-Mg-BCD.

-- PEAK --		-- VALLEY --	
$\lambda$	ABS	$\lambda$	ABS
427.0	0.782		
416.0	0.888	640.0	-0.002
257.0	0.185	283.0	0.088
219.0	0.243	245.0	0.159

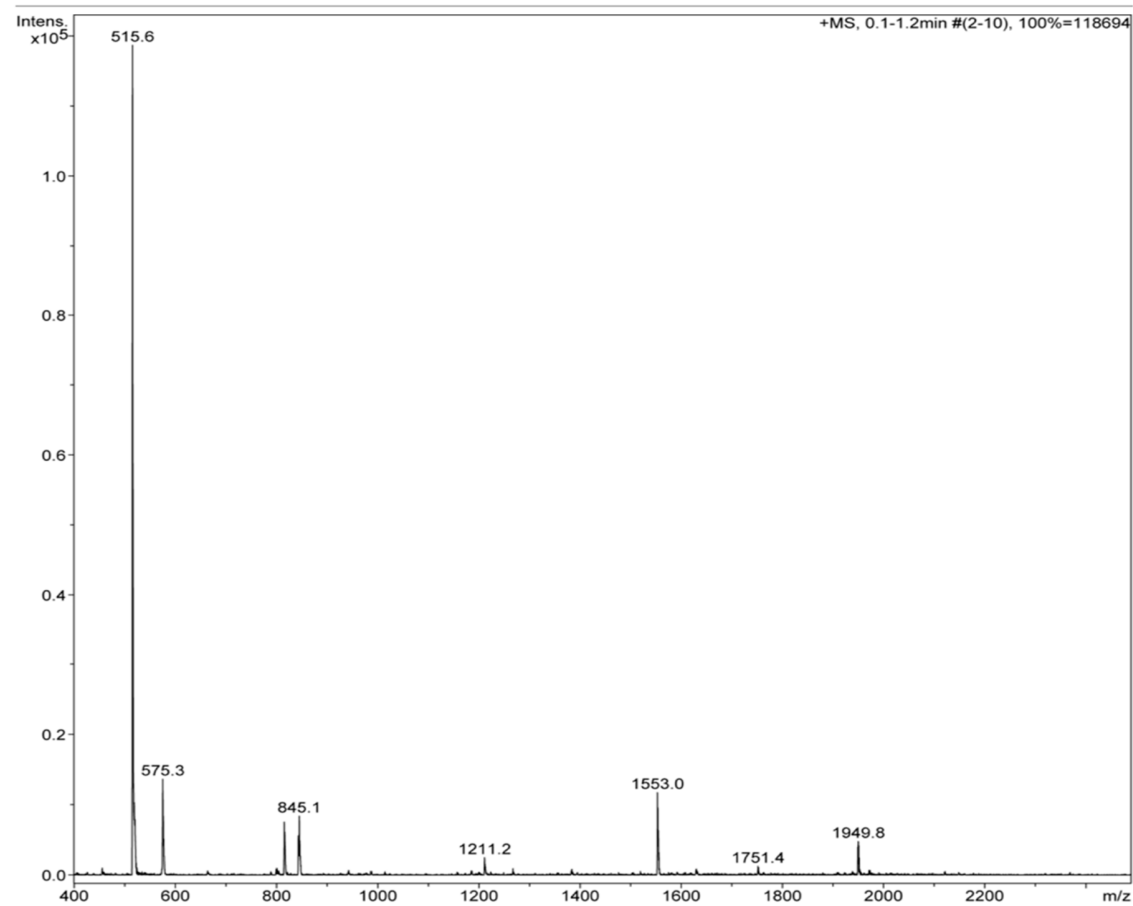


**Fig S23.** UV-VIS spectrum in methanol of DiMeOC-Mg-BCD .

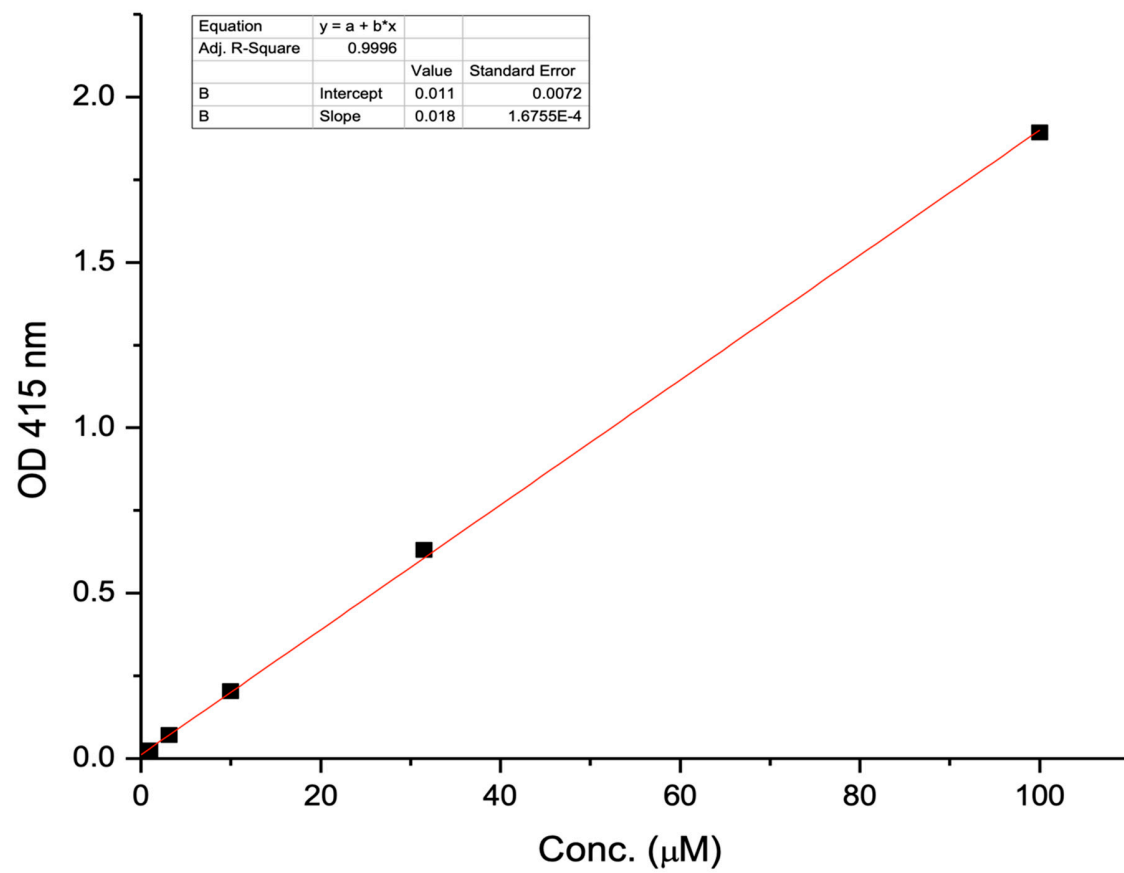


**Fig S24.** HPLC spectrum of DiMeOC-Mg-BCD (417nm, CH<sub>3</sub>CN/H<sub>2</sub>O (0.02% formic acid) 55:45).

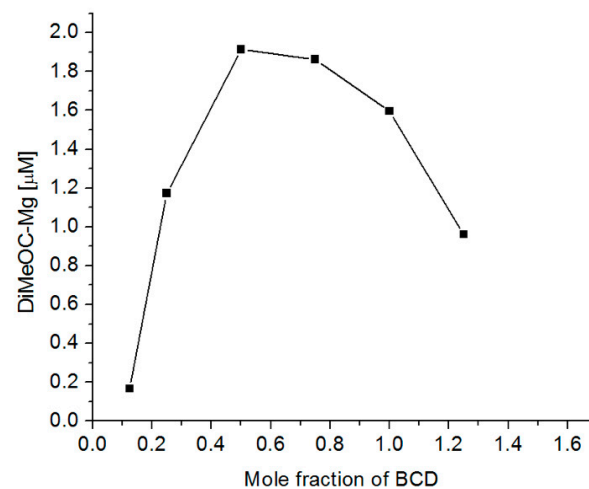
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.617	BB	0.1878	3.62682	2.37953e-1	0.1252
2	9.656	BB	0.1708	8.75976	6.51972e-1	0.3023
3	15.921	BB	0.2585	31.41060	1.49874	1.0841
4	19.814	BB	0.4463	2853.59155	94.51001	98.4884



**Fig S25.** Mass Spectrum of DiMeOC-Mg-BCD (ESI).

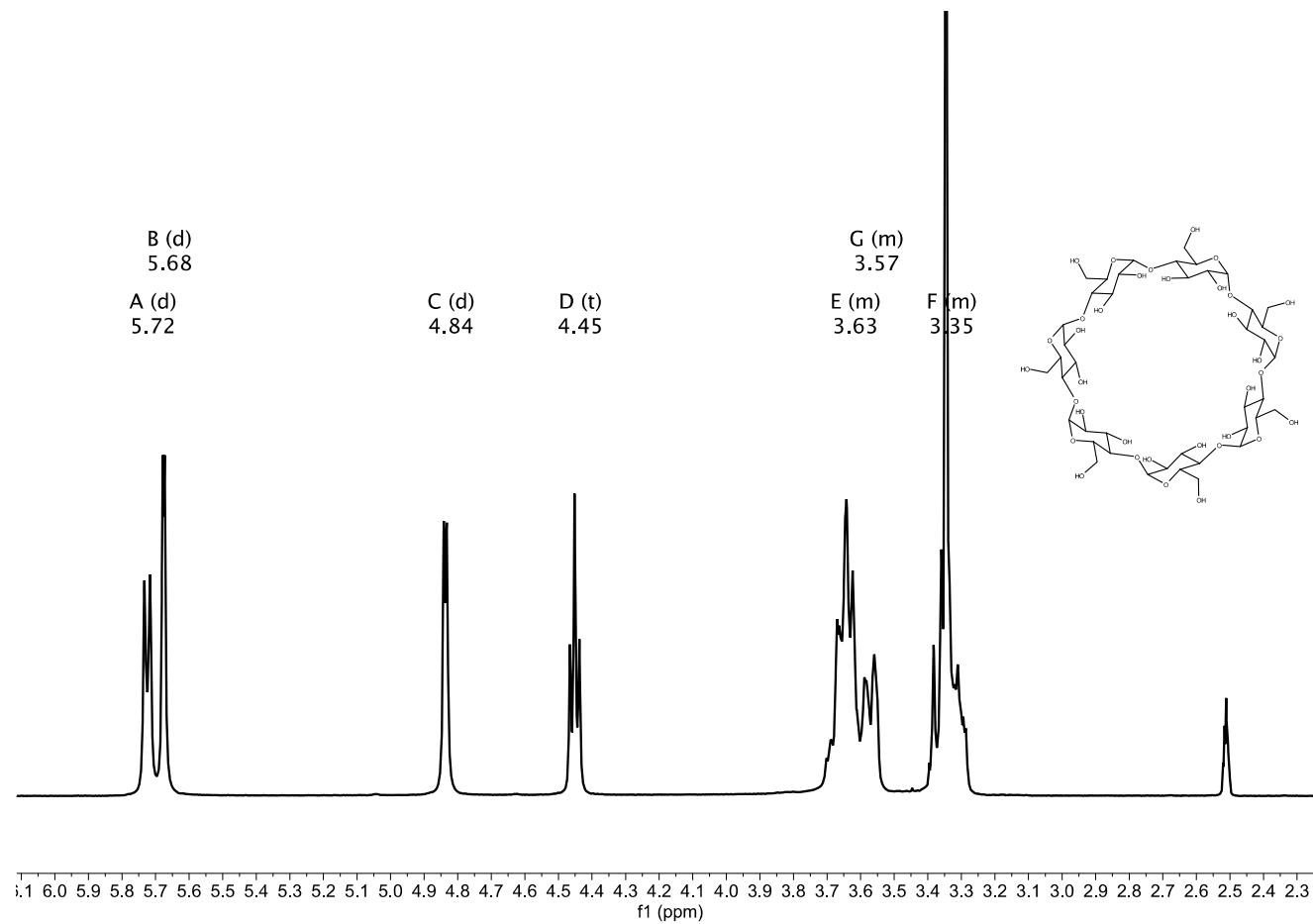


**Fig S26.** Standard curve of DiMeOC-Mg (415nm, 1-Octanol).

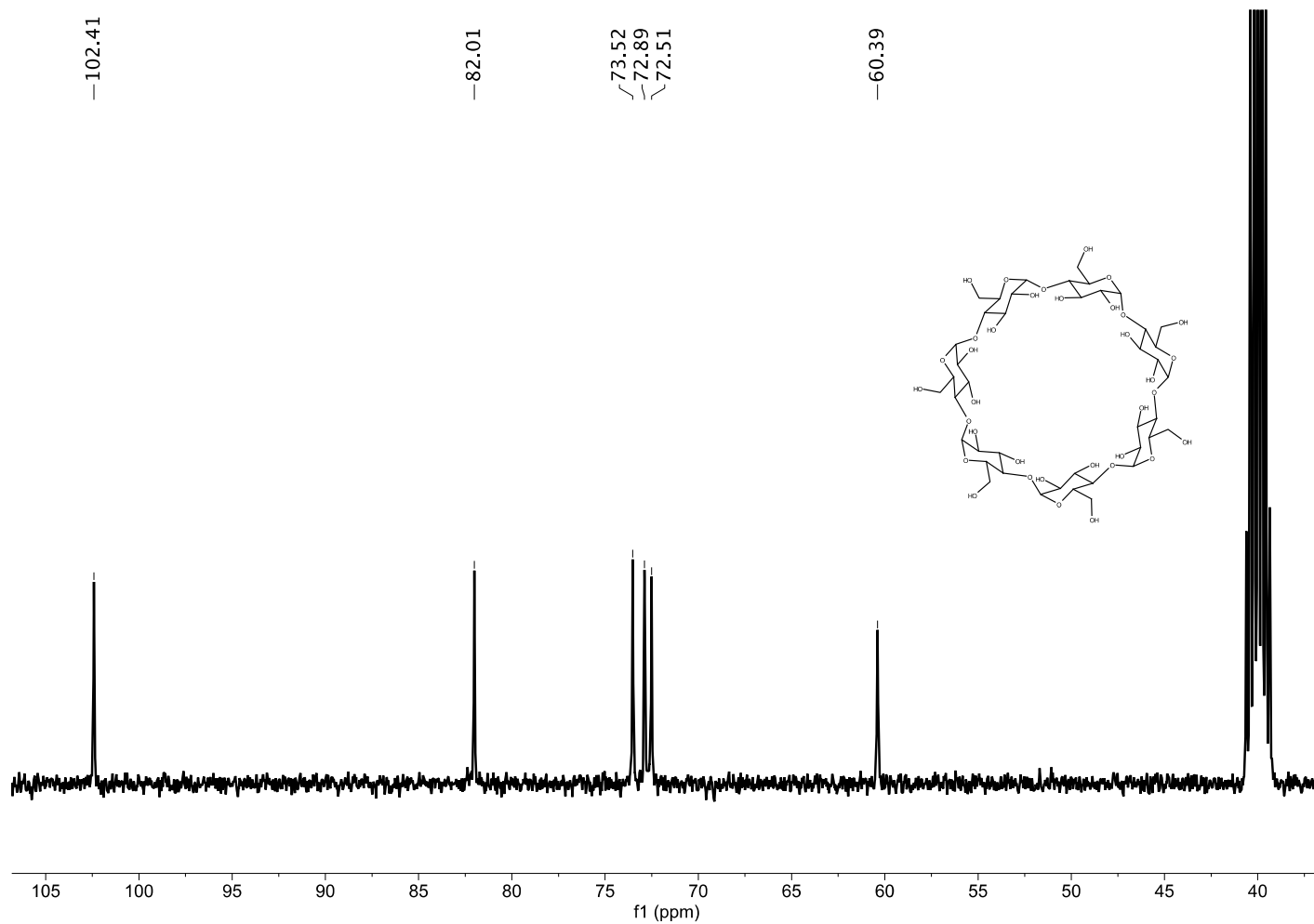


**Fig S27.** Inclusion ratio DiMeOC-Mg and BCD (PBS media).

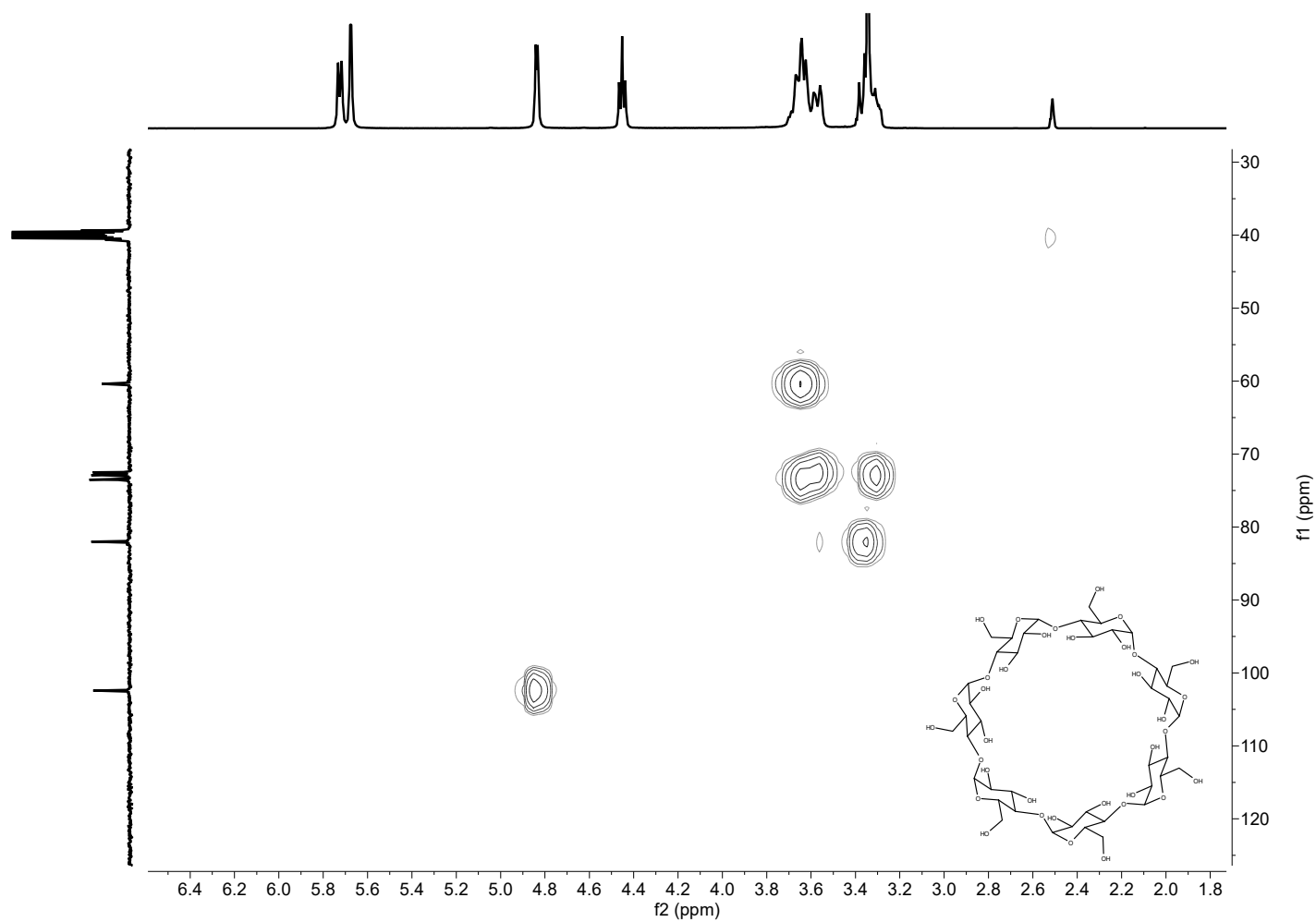
The inclusion ratio test results between DiMeOC-Mg and BCD are shown in Fig. s27. The mole fraction represents  $r$  of BCD in the mixture. when  $r = 0.5$ , the molar concentration value of DiMeOC-Mg was the largest, concluding that the inclusion complex was formed to the molar ratio of 1:1.



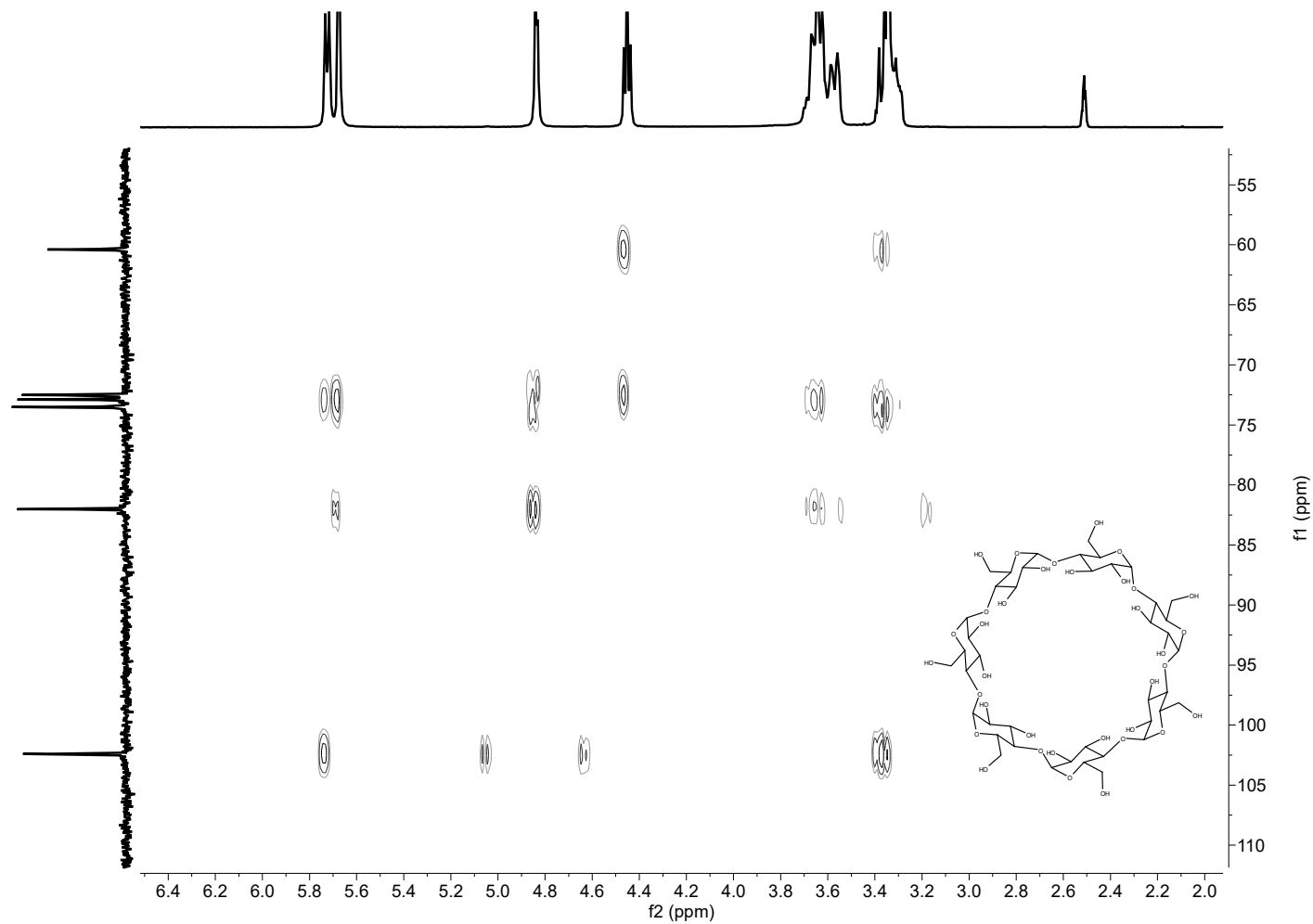
**Fig S28.**  $^1\text{H}$  NMR spectrum of Beta-cyclodextrin (BCD, 400 MHz,  $\text{DMSO-}d_6$ ).



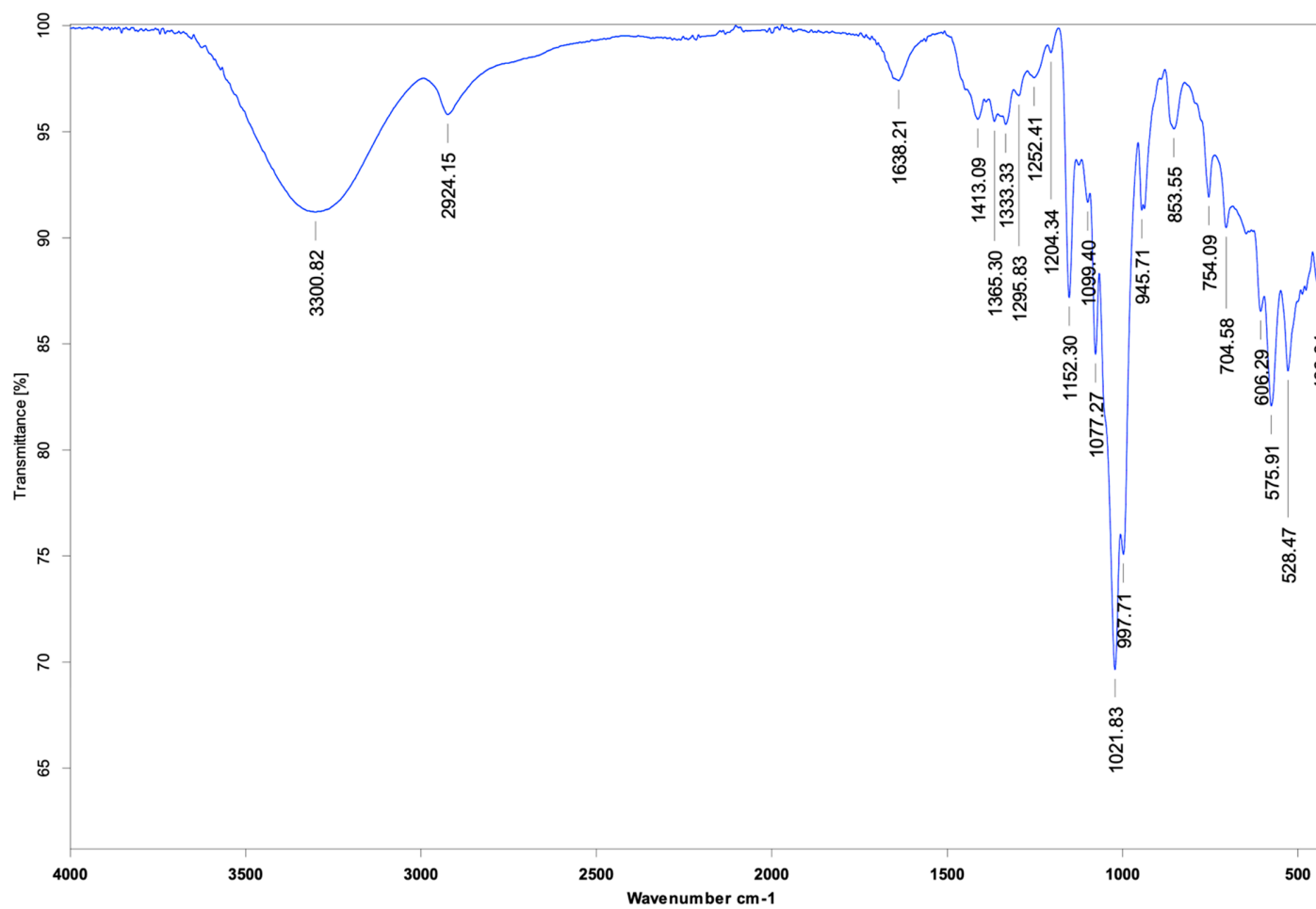
**Fig S29.**  $^{13}\text{C}$  NMR spectrum of BCD (100 MHz,  $\text{DMSO-}d_6$ ).



**Fig S30.** HSQC NMR spectrum of BCD (500 MHz, DMSO-*d*<sub>6</sub>).



**Fig S31.** HMBC NMR spectrum of BCD (500 MHz, DMSO- $d_6$ ).



**Fig S32.** IR Spectrum of BCD.