

1 **SUPPLEMENTARY DATA**

2 **Potential Anticancer Lipoxygenase Inhibitors from the Red Sea-Derived**
3 **Brown Algae *Sargassum cinereum*: An *In-Silico*-Supported *In-Vitro* Study**

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Table S1. Dereplicated metabolites using the Dictionary of Natural Products database from LC-HRESIMS analysis of *Sargassum cinnerum*

No.	Metabolites name	Original source	MF	RT(min.)	<i>m/z</i>	MS ² Fragmentation	Ionization Mode
1	(5R,7S,8S)-Communiol A	<i>Sargassum spp.</i>	C ₁₁ H ₂₀ O ₄	3.76288	215.1283	119.1183, 153.1283, 179.1075	[M-H] ⁻
2	Hedaol A	<i>Sargassum spp.</i>	C ₁₈ H ₃₀ O ₂	6.7354	277.2162	237.1864, 219.1752	[M-H] ⁻
3	Arachidonic acid	<i>Sargassum pallidum</i>	C ₂₀ H ₃₄ O ₂	6.6166	307.2624	289.2528, 271.2424, 245.2266	[M+H] ⁺
4	Sargachromanol A	<i>Sargassum siliquastrum</i>	C ₂₂ H ₃₀ O ₃	5.3686	343.2276	325.2158, 285.1853, 273.1850	[M+H] ⁺
5	2-Geranylgeranyl-6-methylbenzoquinone	<i>Sargassum micracanthum.</i>	C ₂₇ H ₃₈ O ₂	4.4710	395.2950	259.2425, 257.1534	[M+H] ⁺
6	24-Ethylcholesta-4,24(28)-dien-3,6-dione	<i>Sargassum carpophyllum</i>	C ₂₉ H ₄₄ O ₂	6.5544	425.3420	313.2157, 285.1854	[M+H] ⁺
7	Saringosterone	<i>Sargassum asperfolium</i>	C ₂₉ H ₄₆ O ₂	6.6324	427.3576	411.3262, 391.3363, 177.1277	[M+H] ⁺
8	Nahocol A	<i>Sargassum siliquastrum</i>	C ₂₉ H ₄₂ O ₆	6.6773	487.3060	459.3109, 373.2375	[M+H] ⁺
9	24xi-Hydroperoxy-24-vinylcholesterol	<i>Sargassum carpophyllum</i>	C ₂₉ H ₄₈ O ₃	6.5615	445.3682	373.2215	[M+H] ⁺
10	Sargathunbergol A	<i>Sargassum thunbergii</i>	C ₂₇ H ₃₈ O ₆	5.7502	459.2749	285.1855, 257.1534	[M+H] ⁺
11	1-O-(11-Hexadecenoyl)-3-O-(6'-sulfo-a-D-quinovopyranosyl) glycerol	<i>Sargassum hemiphyllum</i>	C ₂₅ H ₄₆ O ₁₁ S	4.4836	553.2681	-	[M-H] ⁻

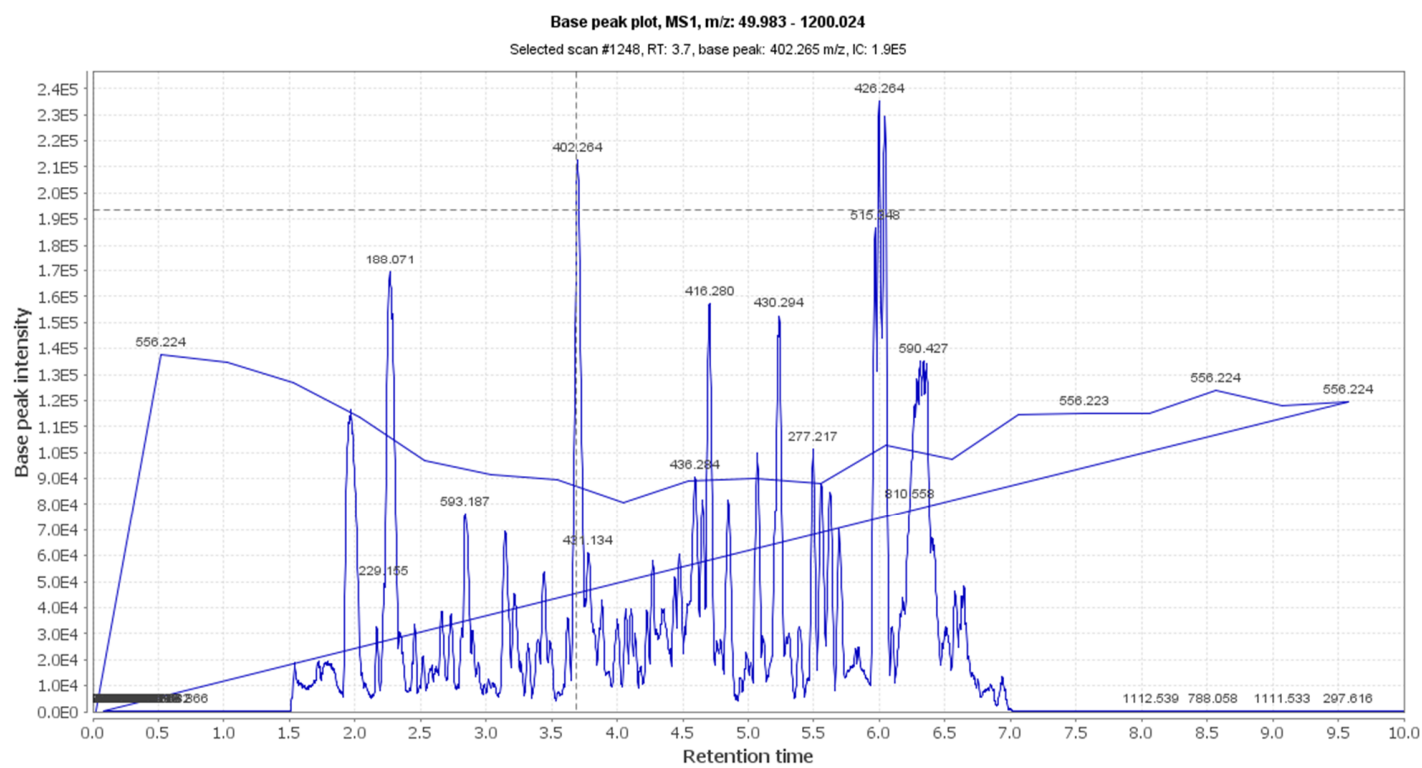


Figure S1. LC-HRESIMS Chromatogram of the dereplicated metabolites of *Sarragassum cinnerum* (positive)

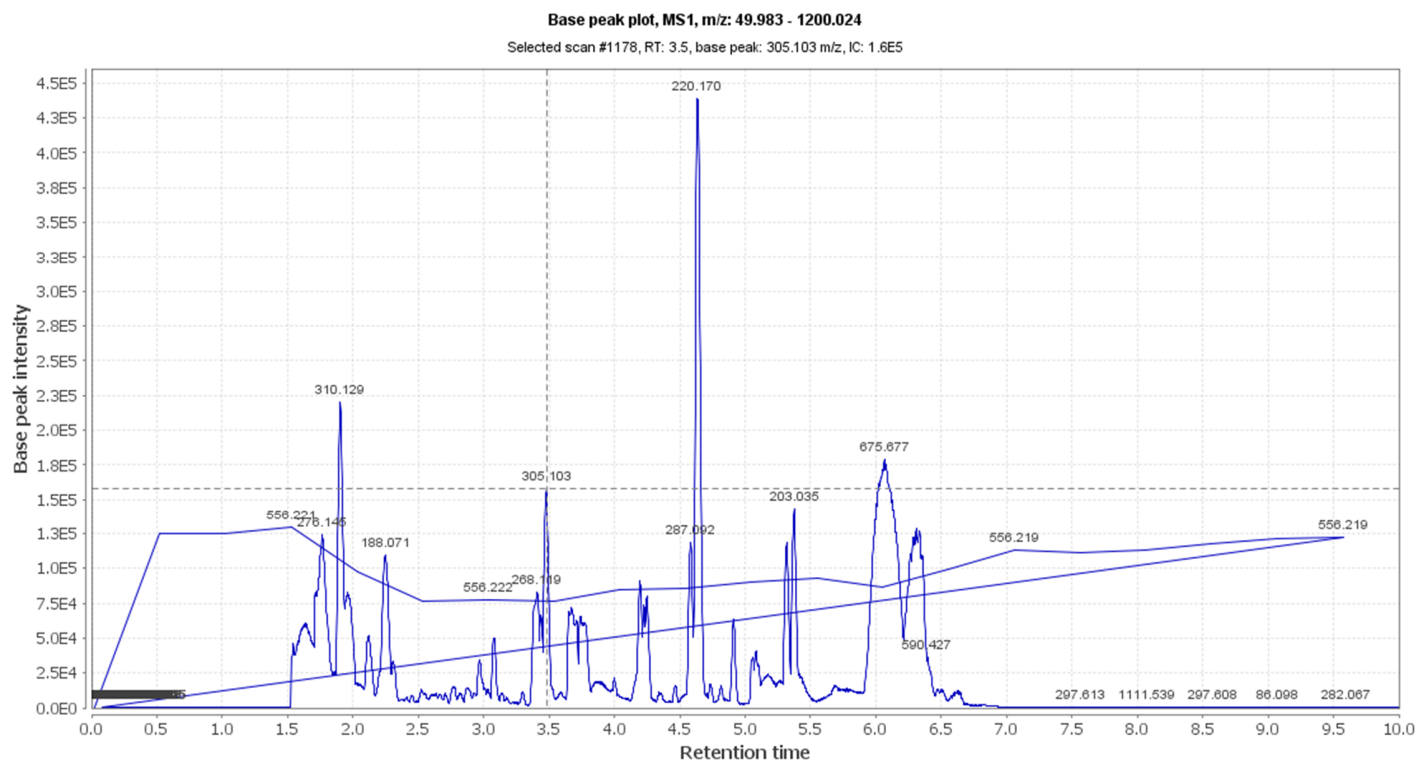


Figure S2. LC-HRESIMS Chromatogram of the dereplicated metabolites of *Sarragassum cinnerum* (negative)

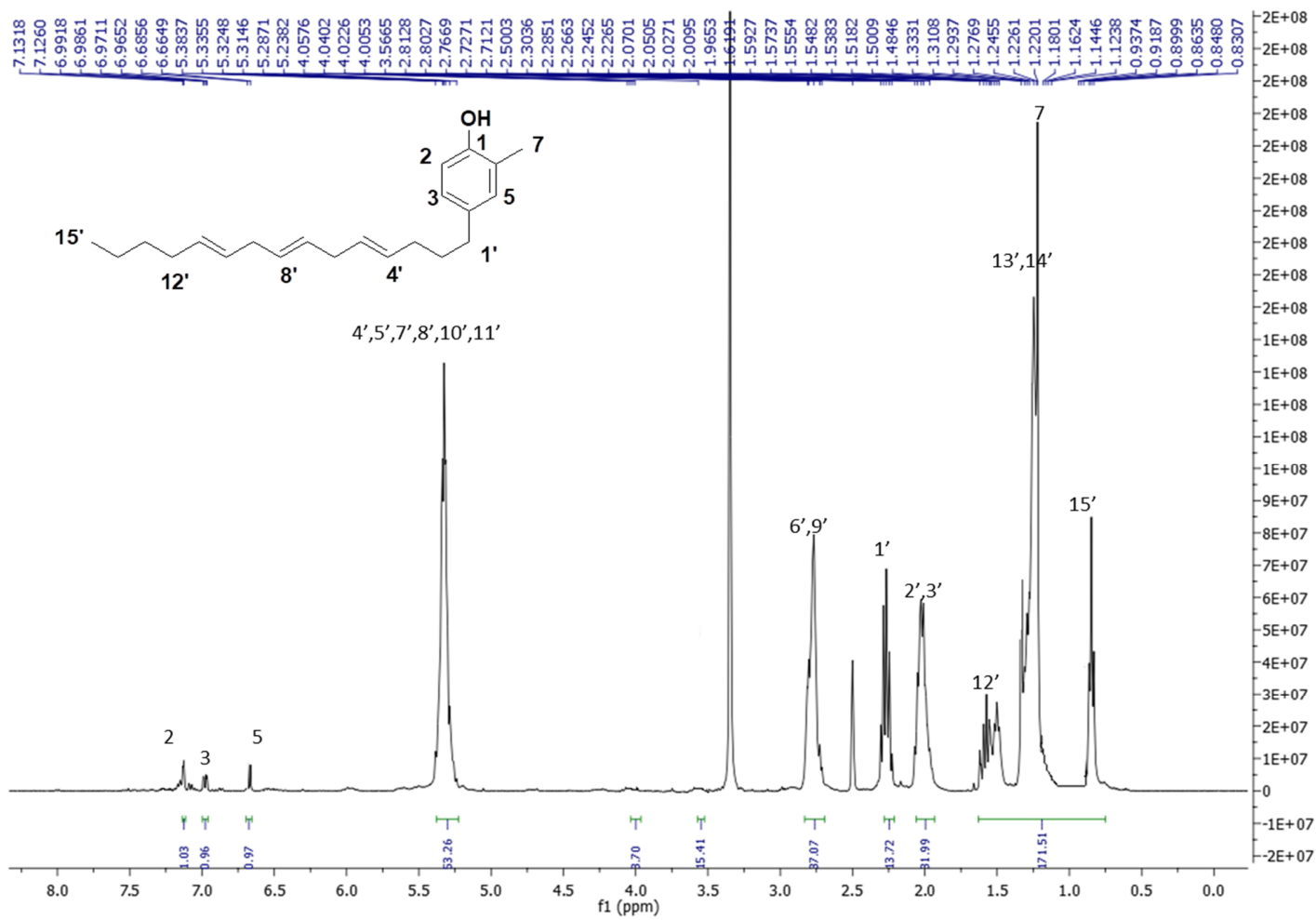


Figure S3. ¹H NMR spectrum of compound 12 measured in DMSO-*d*₆ at 400 MHz

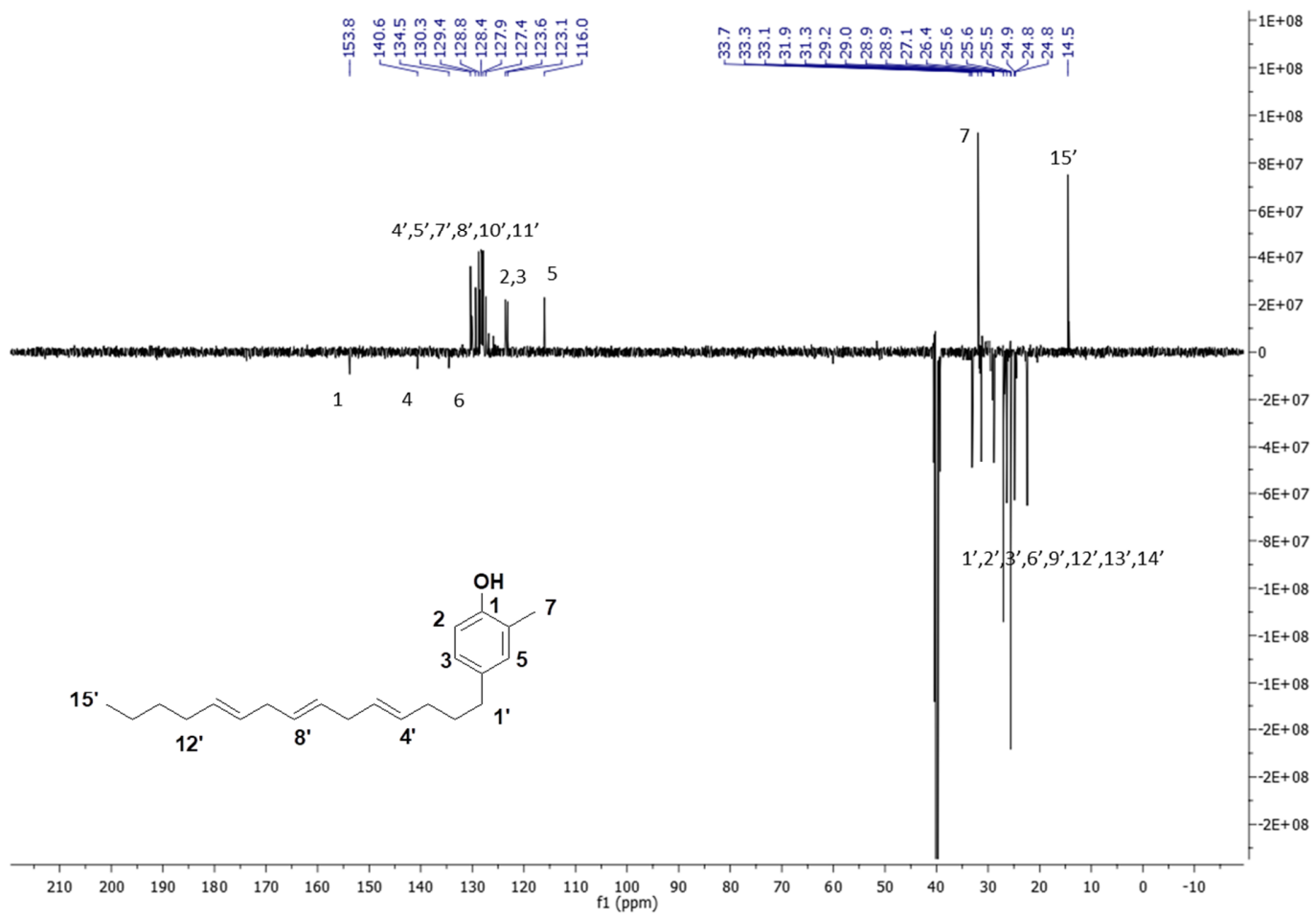


Figure S4. DEPT-Q NMR spectrum of compound **12** measured in DMSO-*d*₆ at 100 MHz.

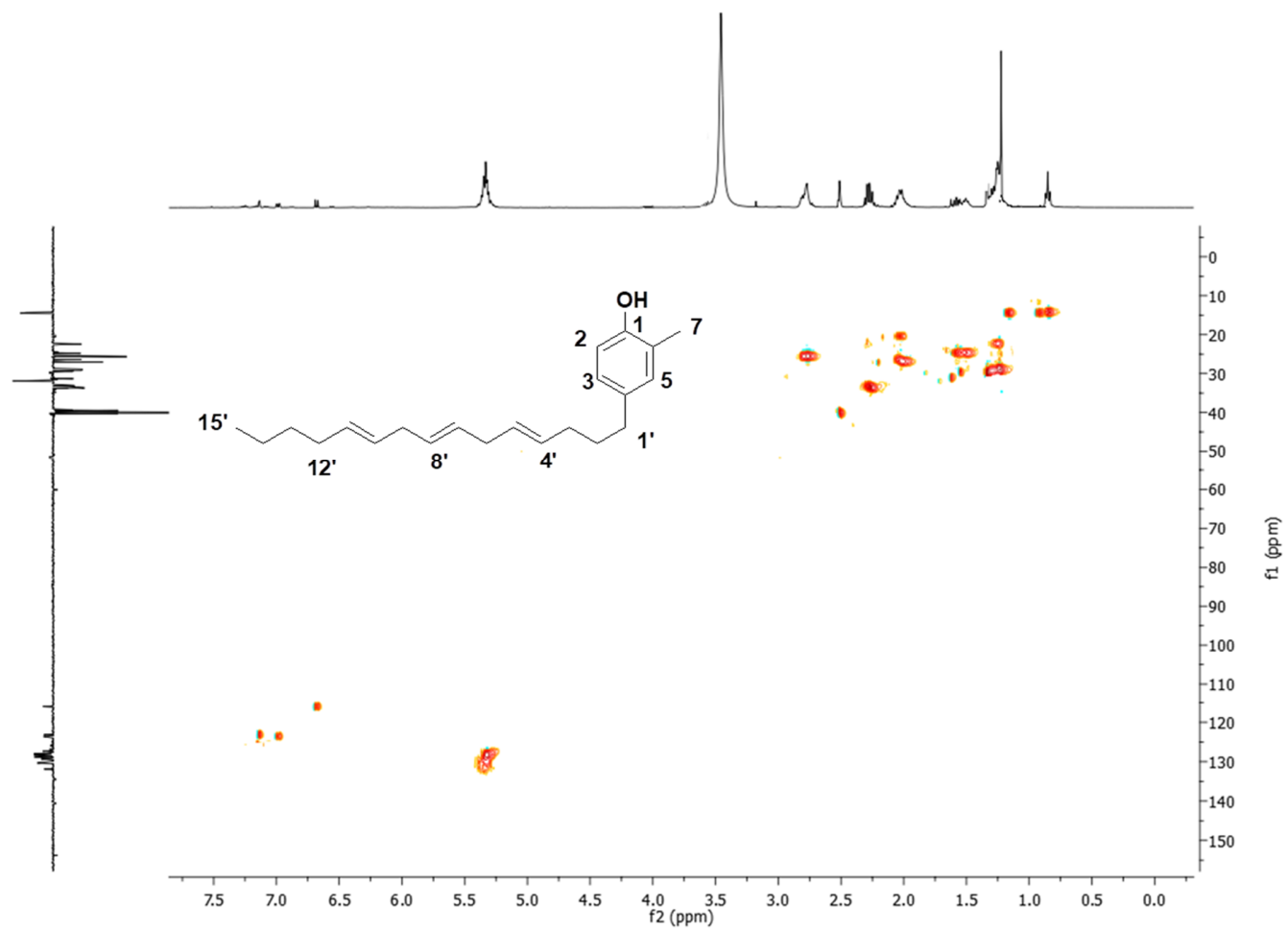


Figure S5. HSQC spectrum of compound **12** measured in $\text{DMSO-}d_6$

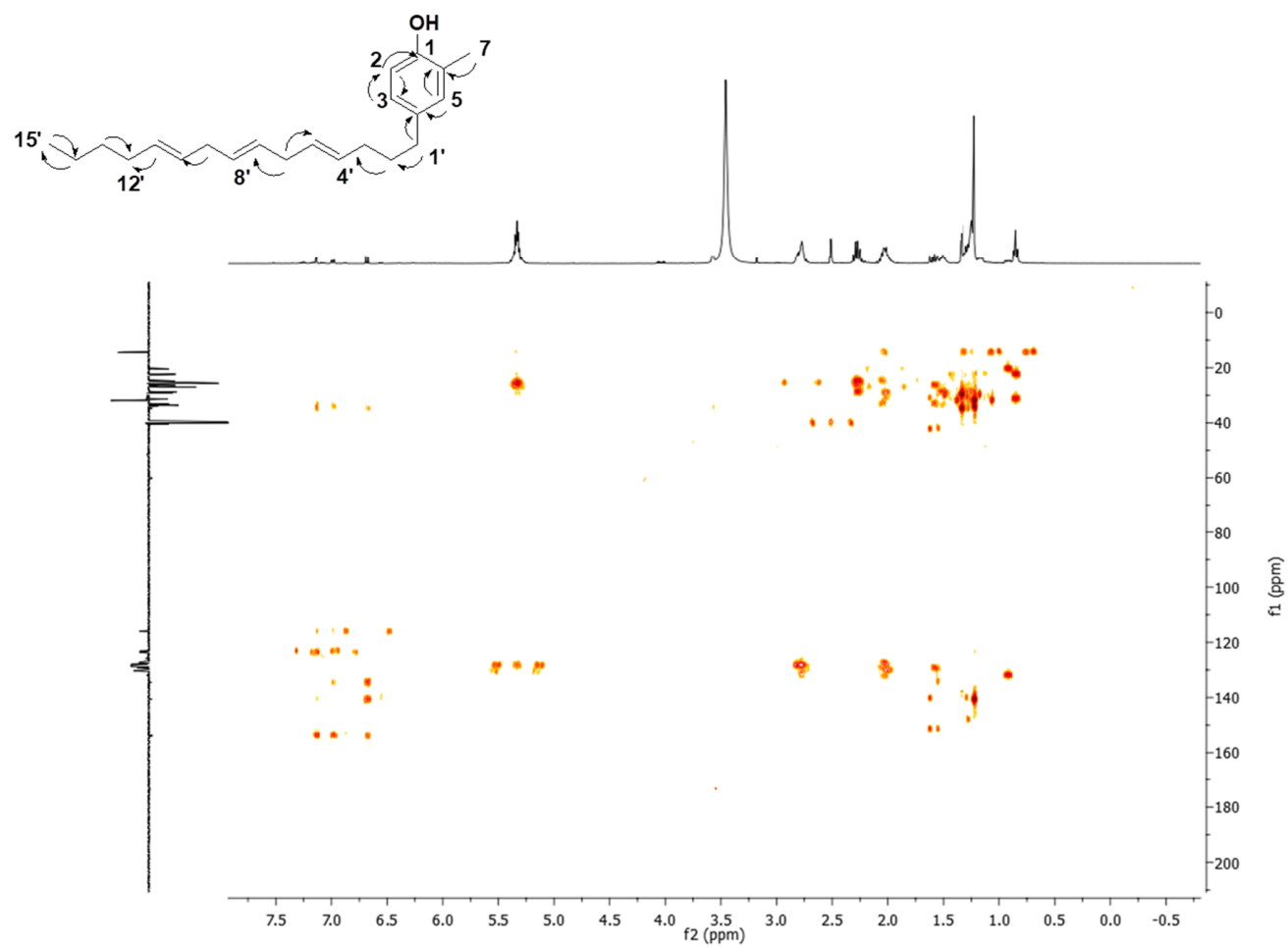


Figure S6. HMBC spectrum of compound 12 measured in DMSO-*d*₆

UR12_ESI_Positive_0311

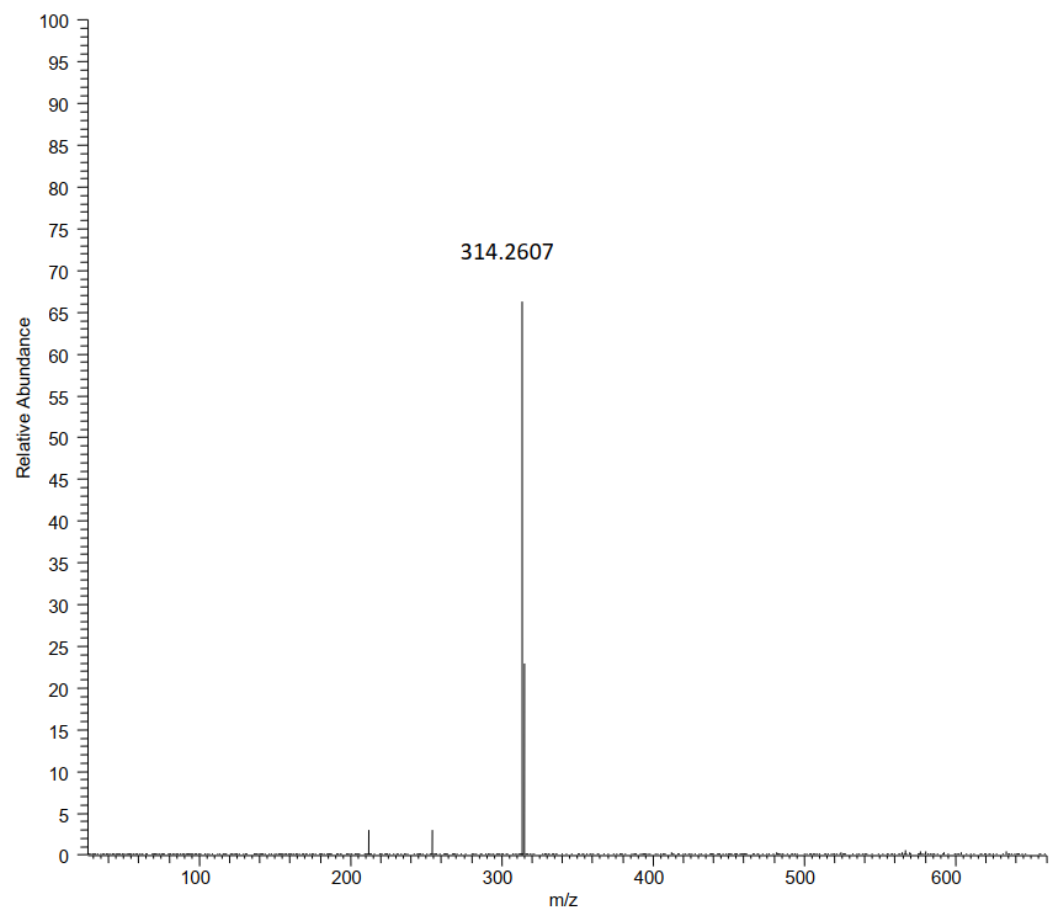


Figure S7. HRESIMS spectrum of compound **12**

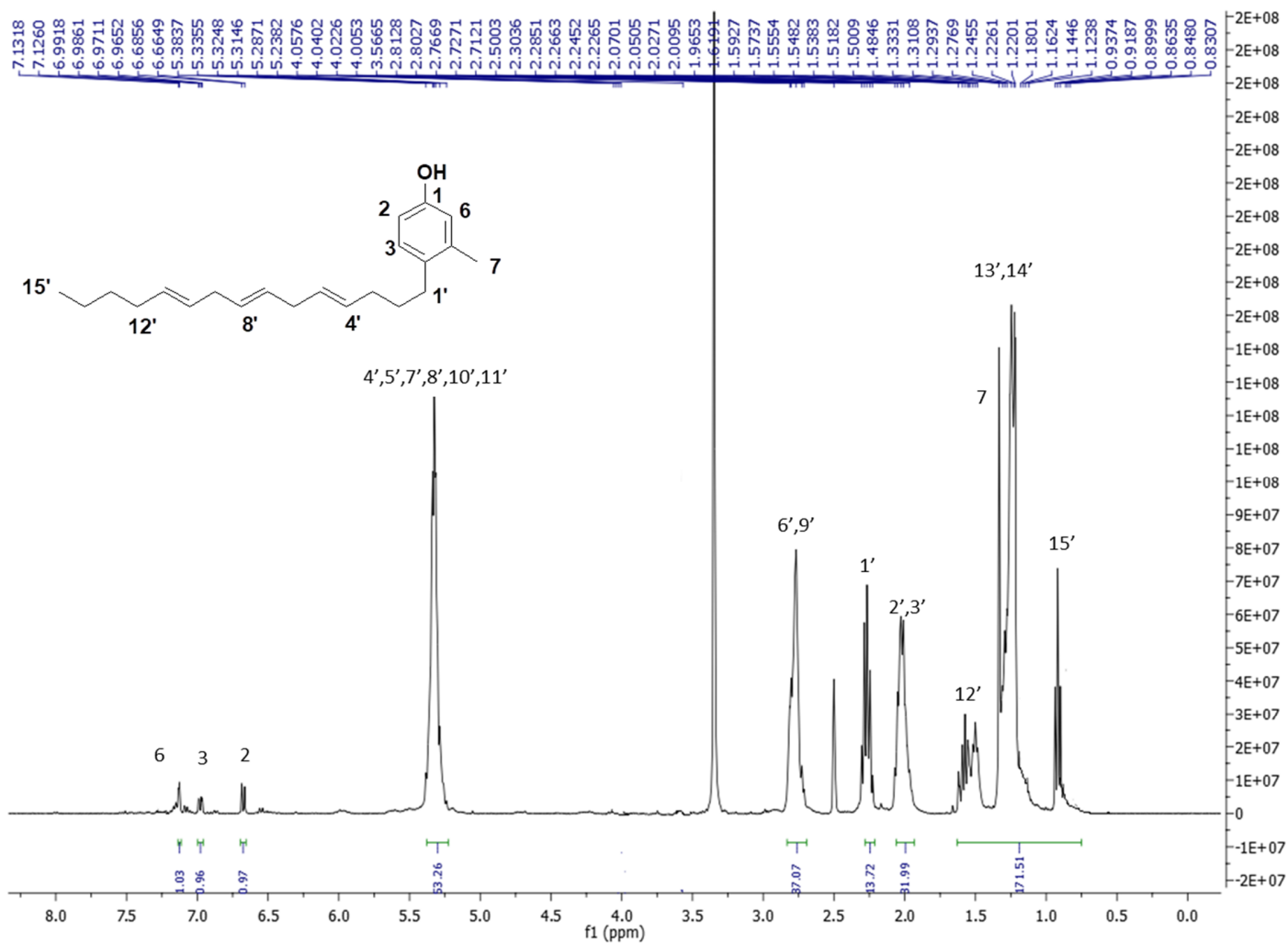


Figure S8. ¹H NMR spectrum of compound 13 measured in DMSO-*d*₆ at 400 MHz

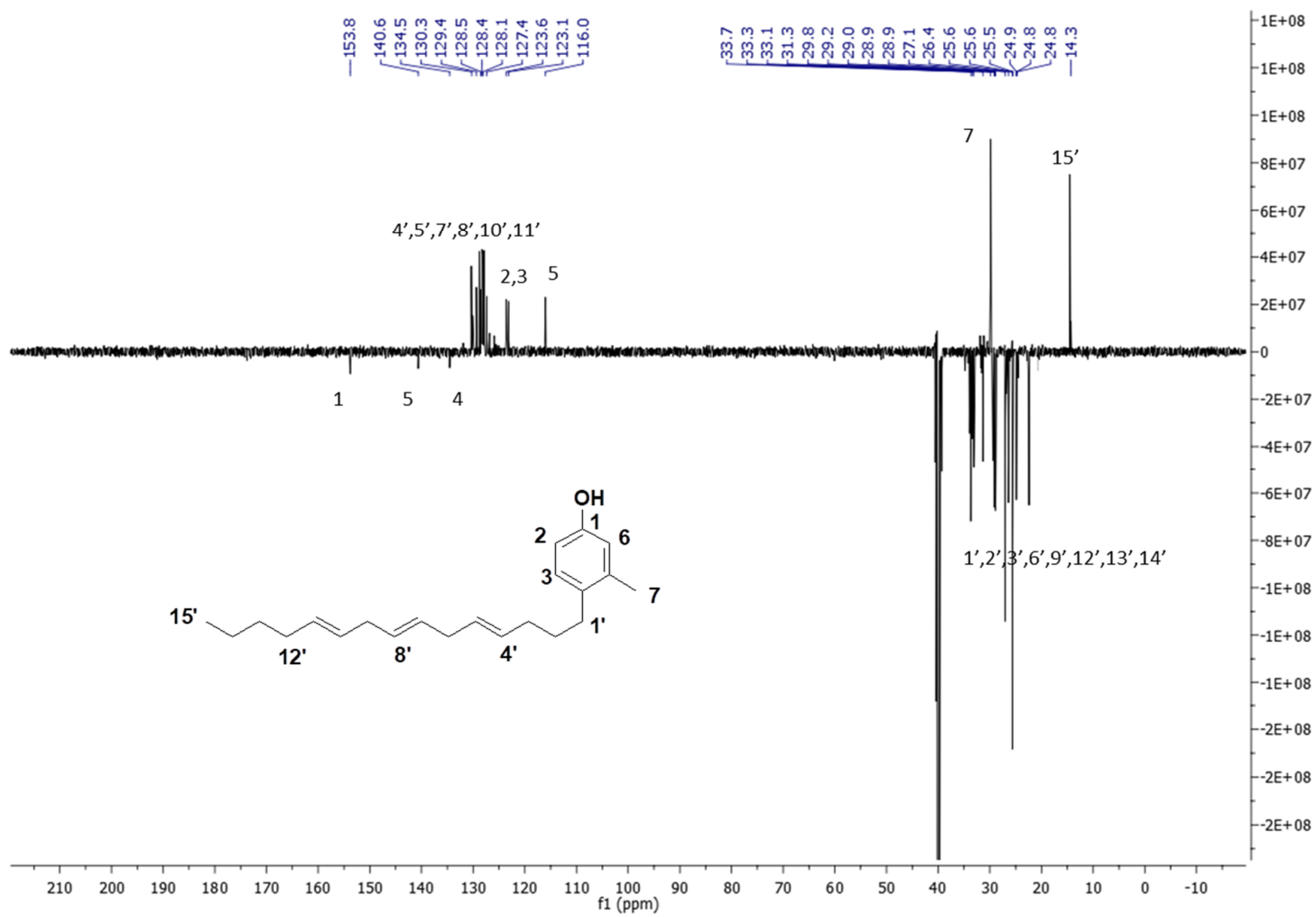


Figure S9. DEPT-Q NMR spectrum of compound **13** measured in DMSO- d_6 at 100 MHz.

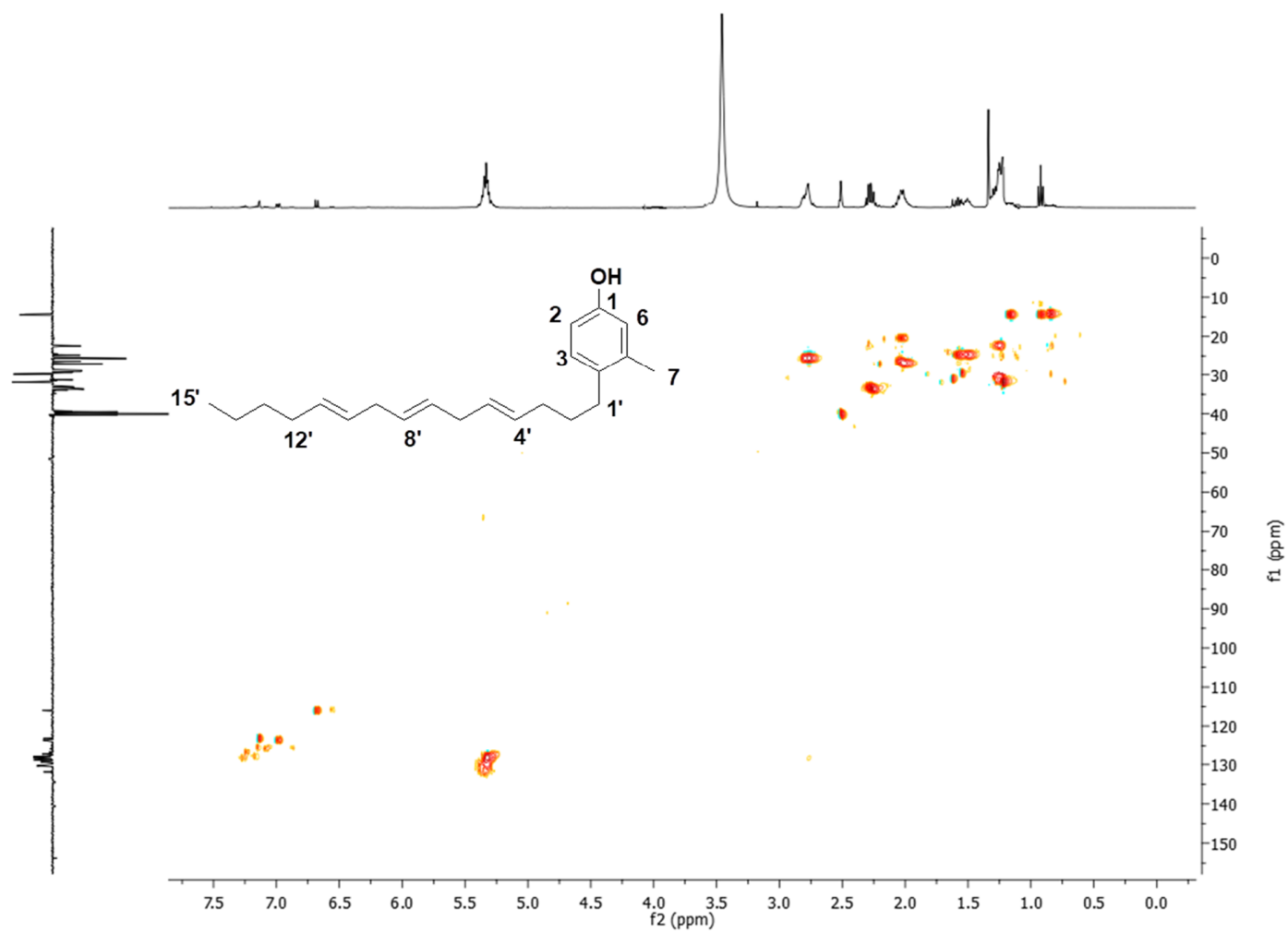


Figure S10. HSQC spectrum of compound **13** measured in DMSO-*d*₆

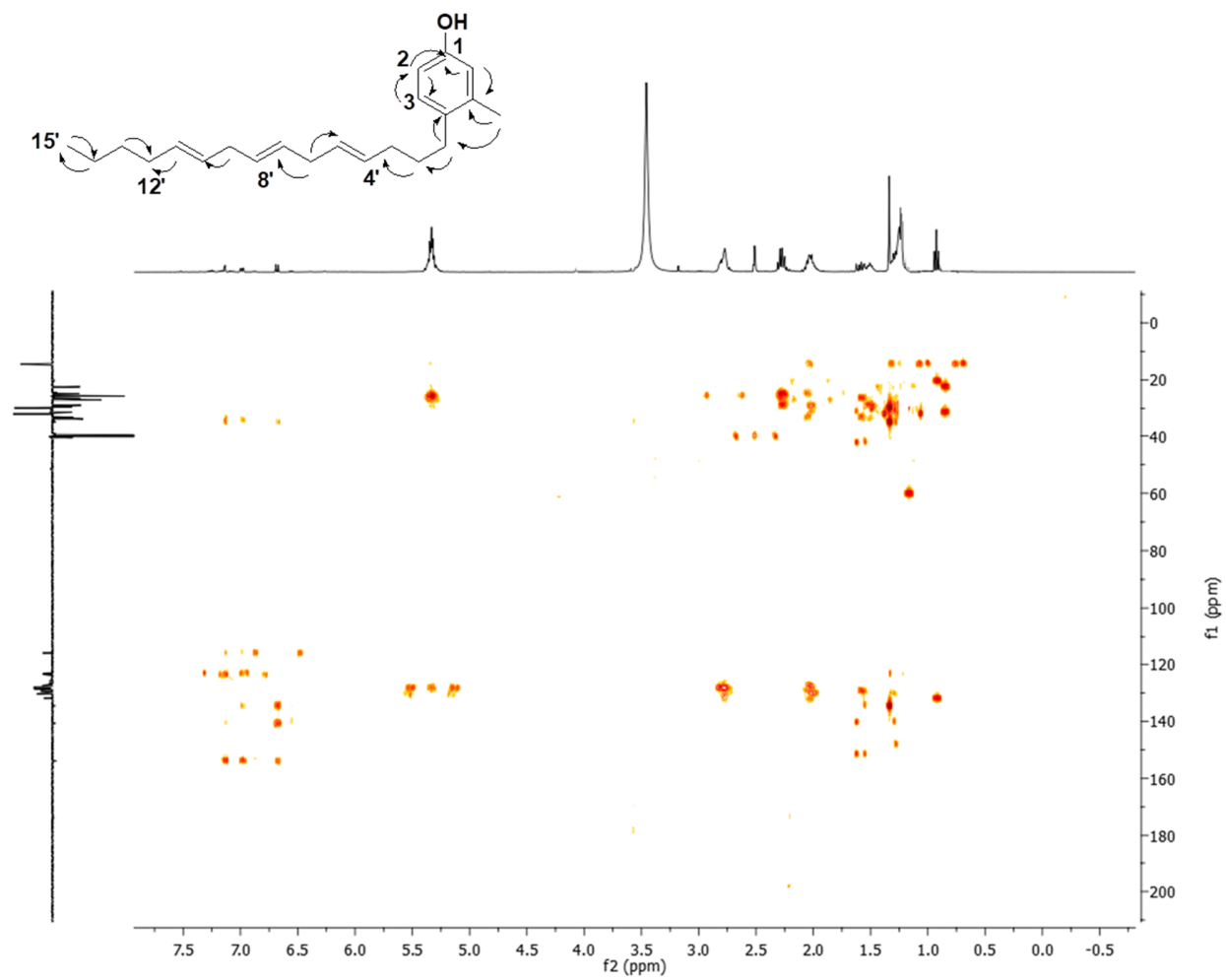


Figure S11. HMBC spectrum of compound **13** measured in DMSO- d_6

UR13_ESI_Positive_0311

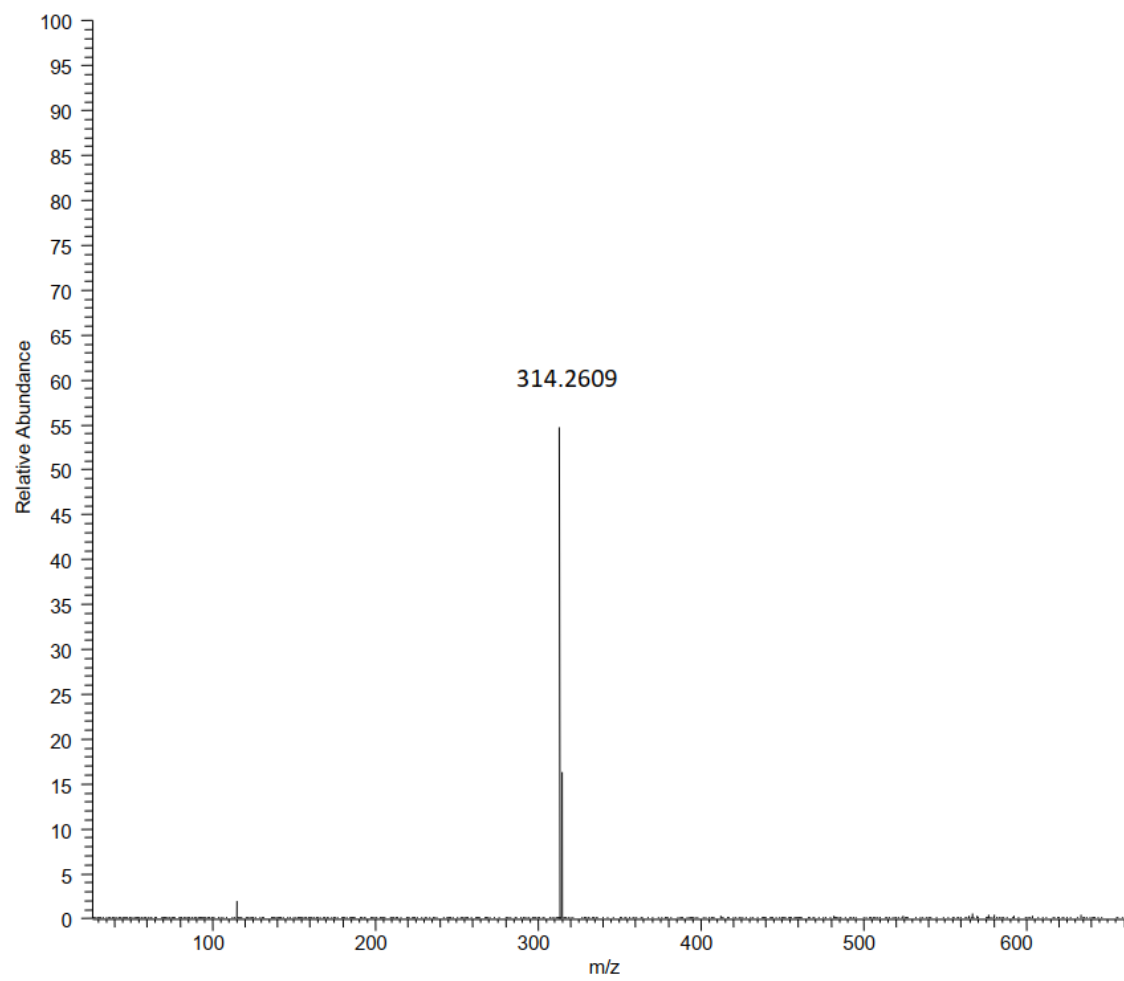


Figure S12. HRESIMS spectrum of compound **13**

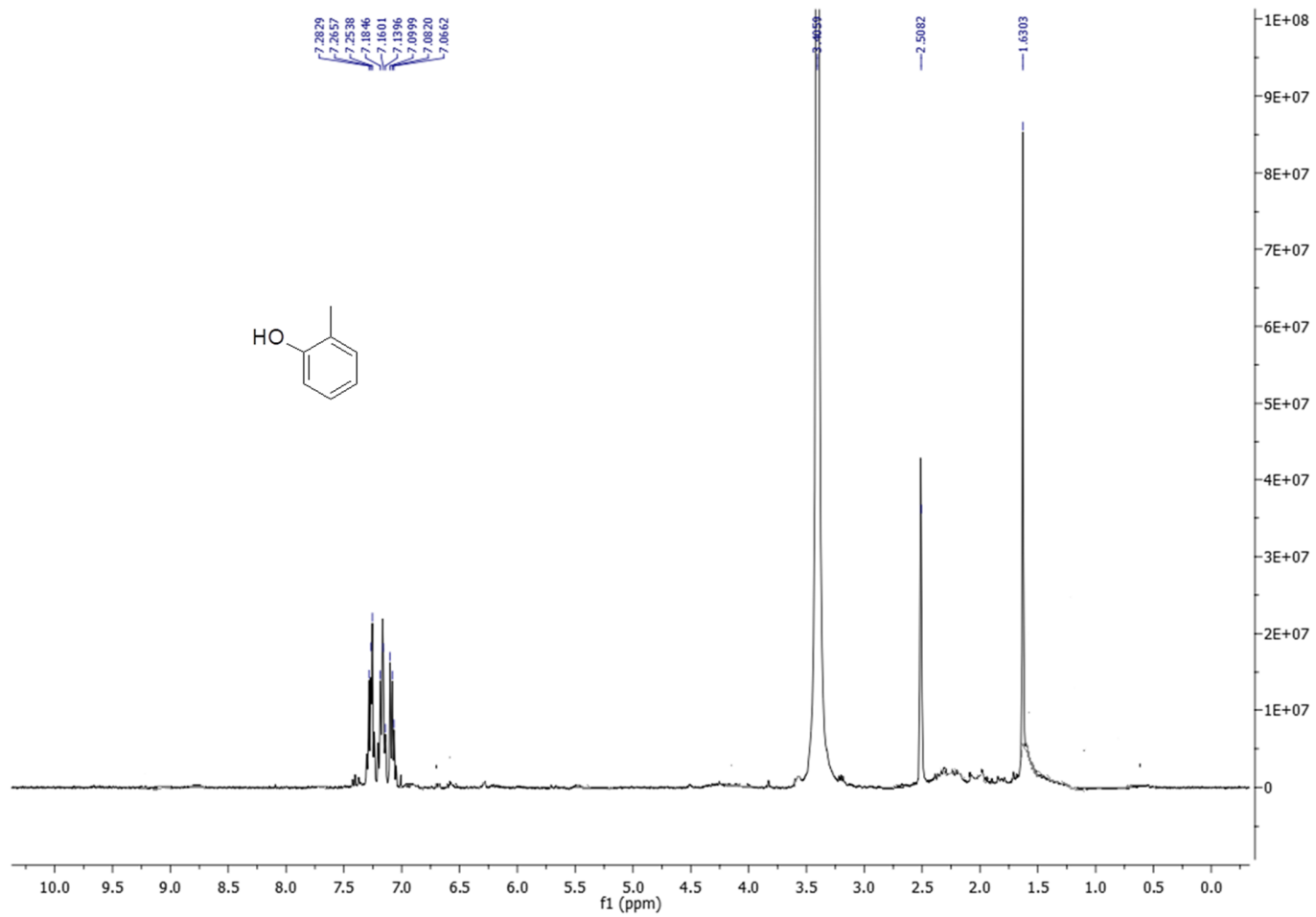


Figure S13. ¹H NMR spectrum of compound 14 measured in DMSO-*d*₆ at 400 MHz

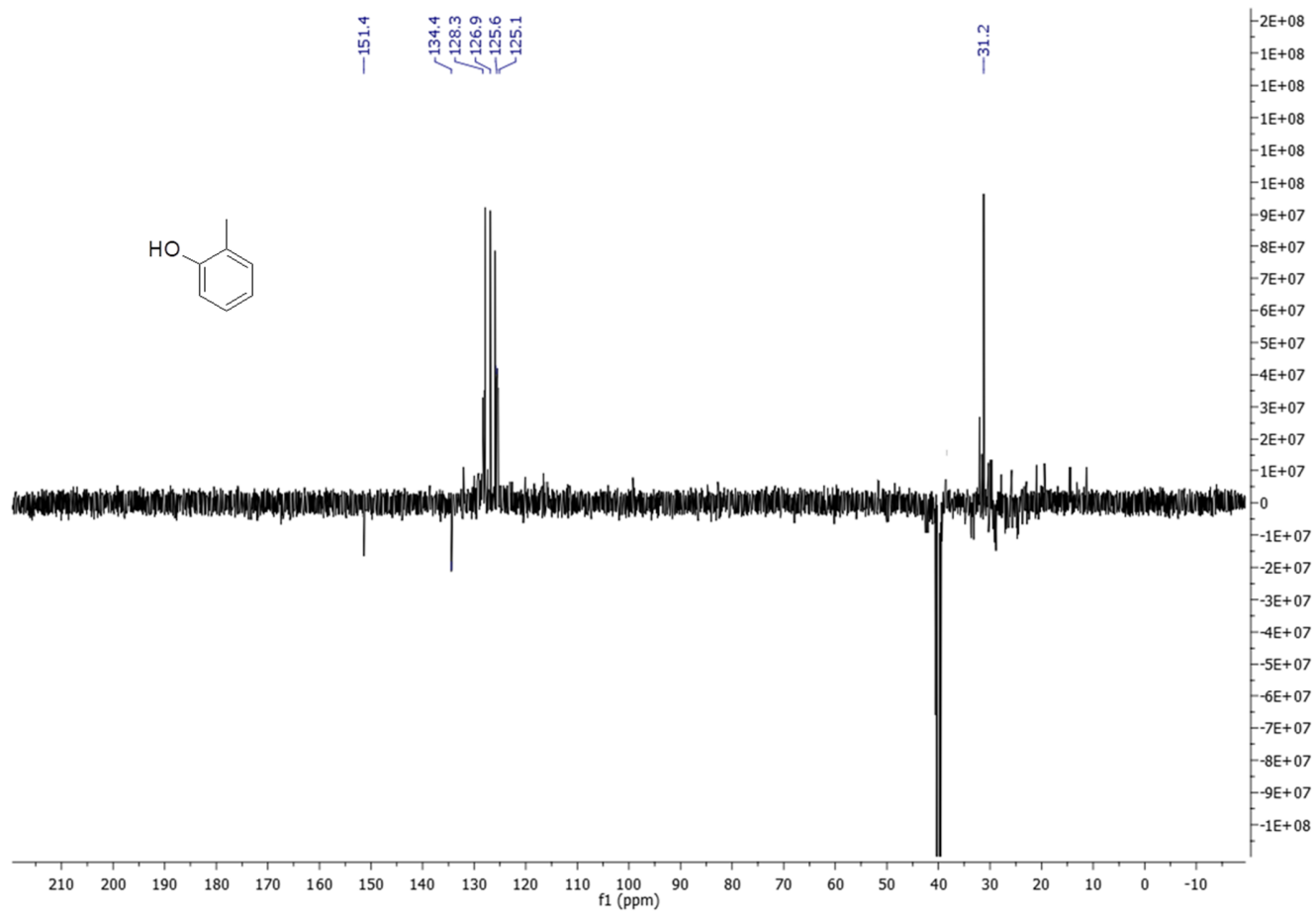


Figure S14. DEPT-Q NMR spectrum of compound **14** measured in DMSO- d_6 at 100 MHz.

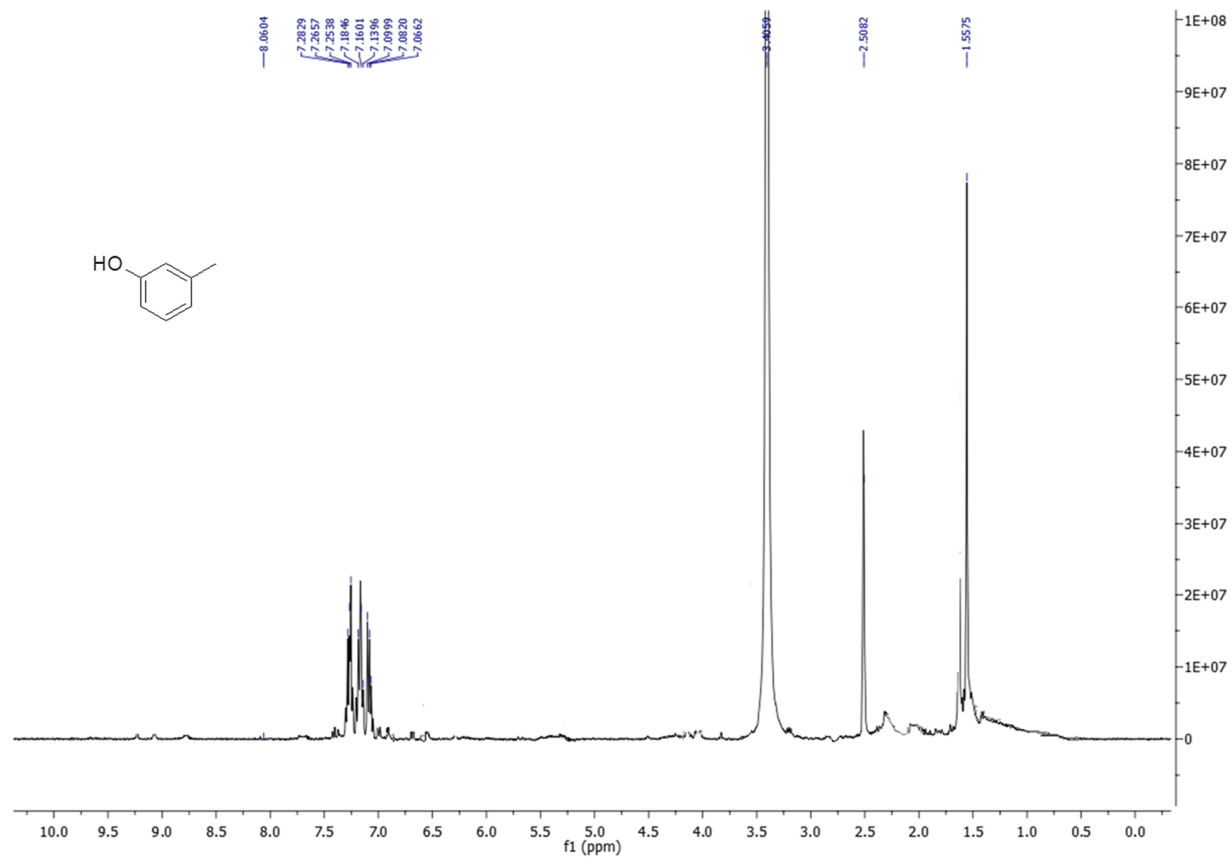


Figure S15. ^1H NMR spectrum of compound **15** measured in $\text{DMSO-}d_6$ at 400 MHz

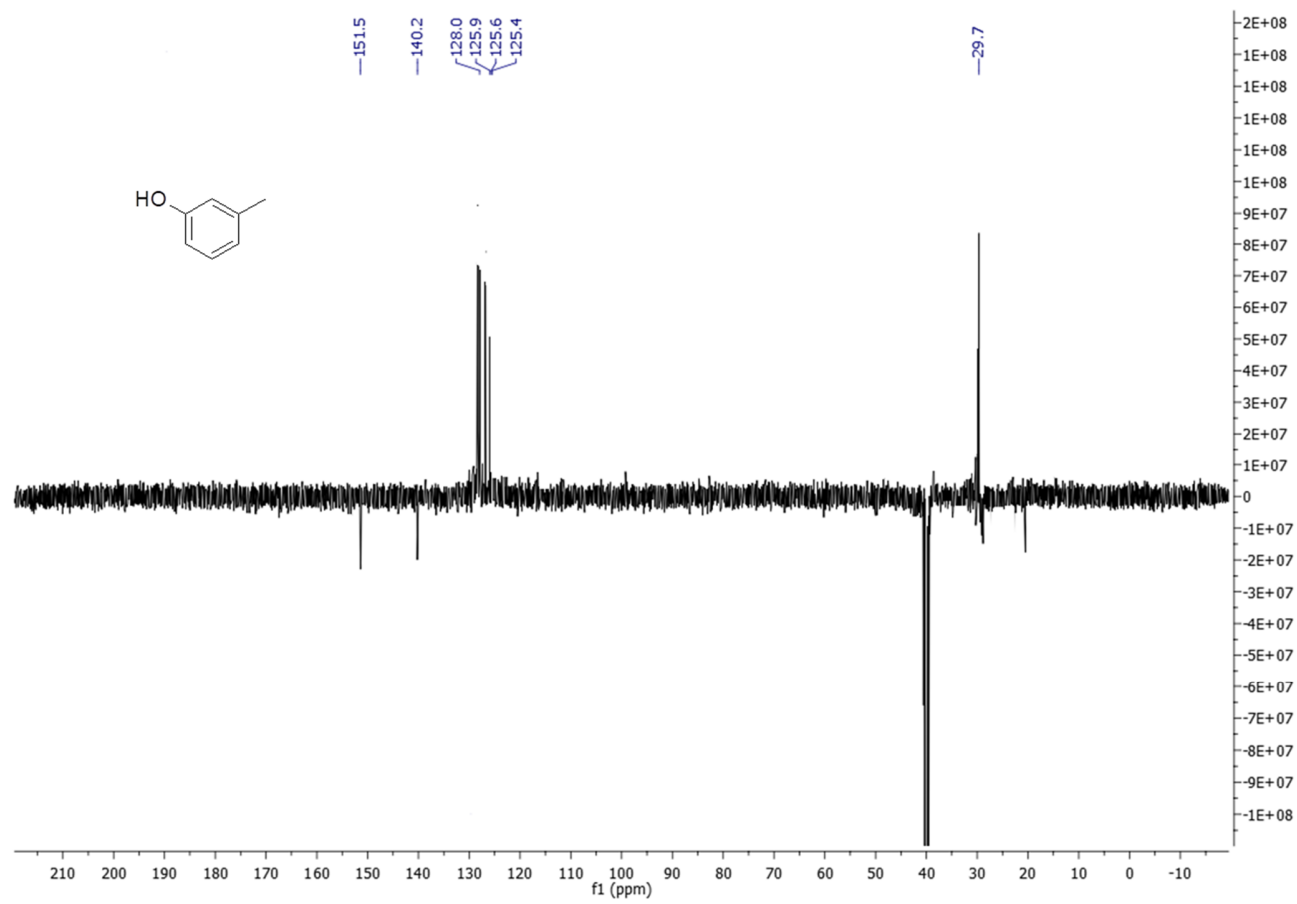


Figure S16. DEPT-Q NMR spectrum of compound **15** measured in DMSO- d_6 at 100 MHz

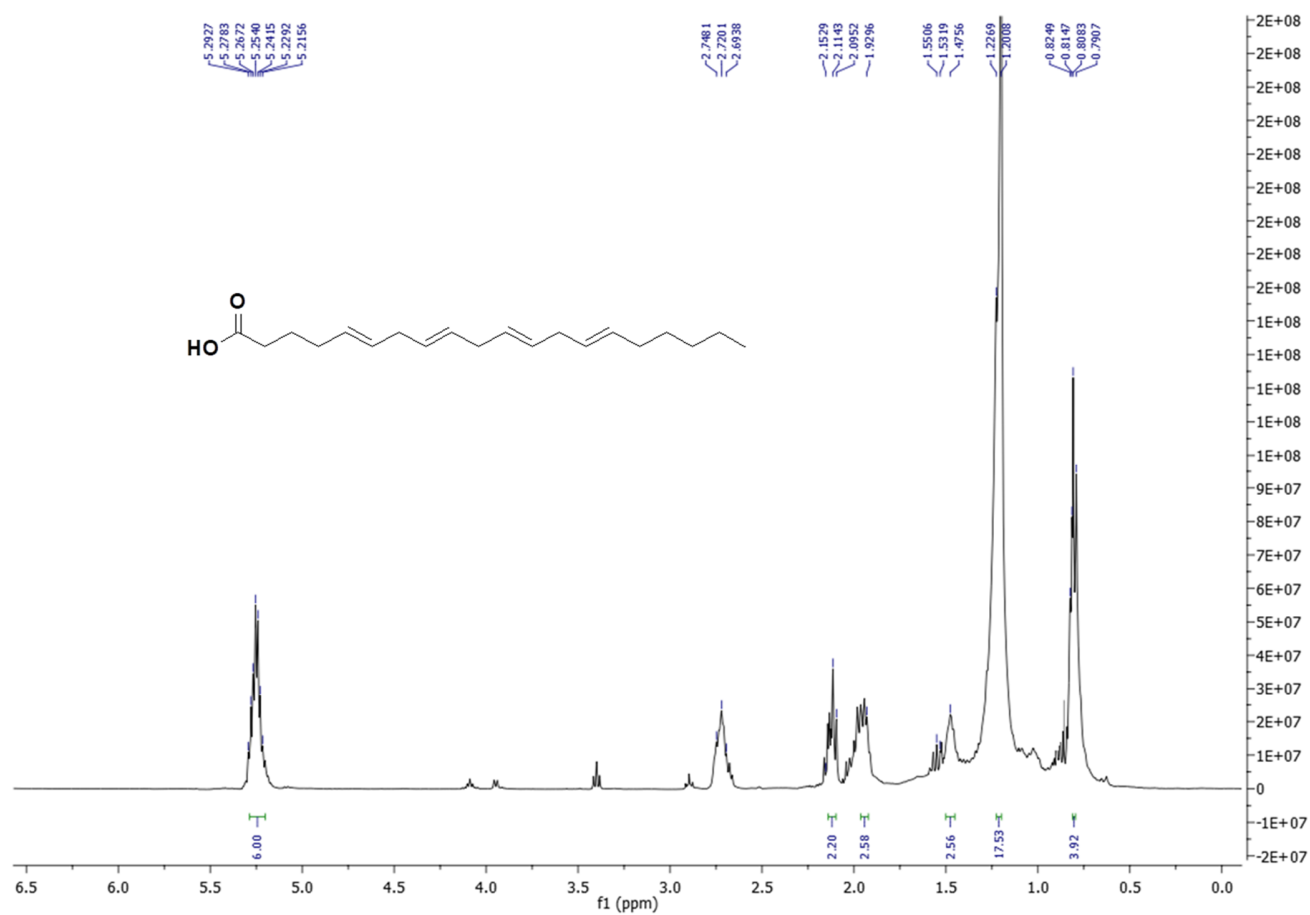


Figure S17. ¹H NMR spectrum of compound 16 measured in DMSO-*d*₆ at 400 MHz

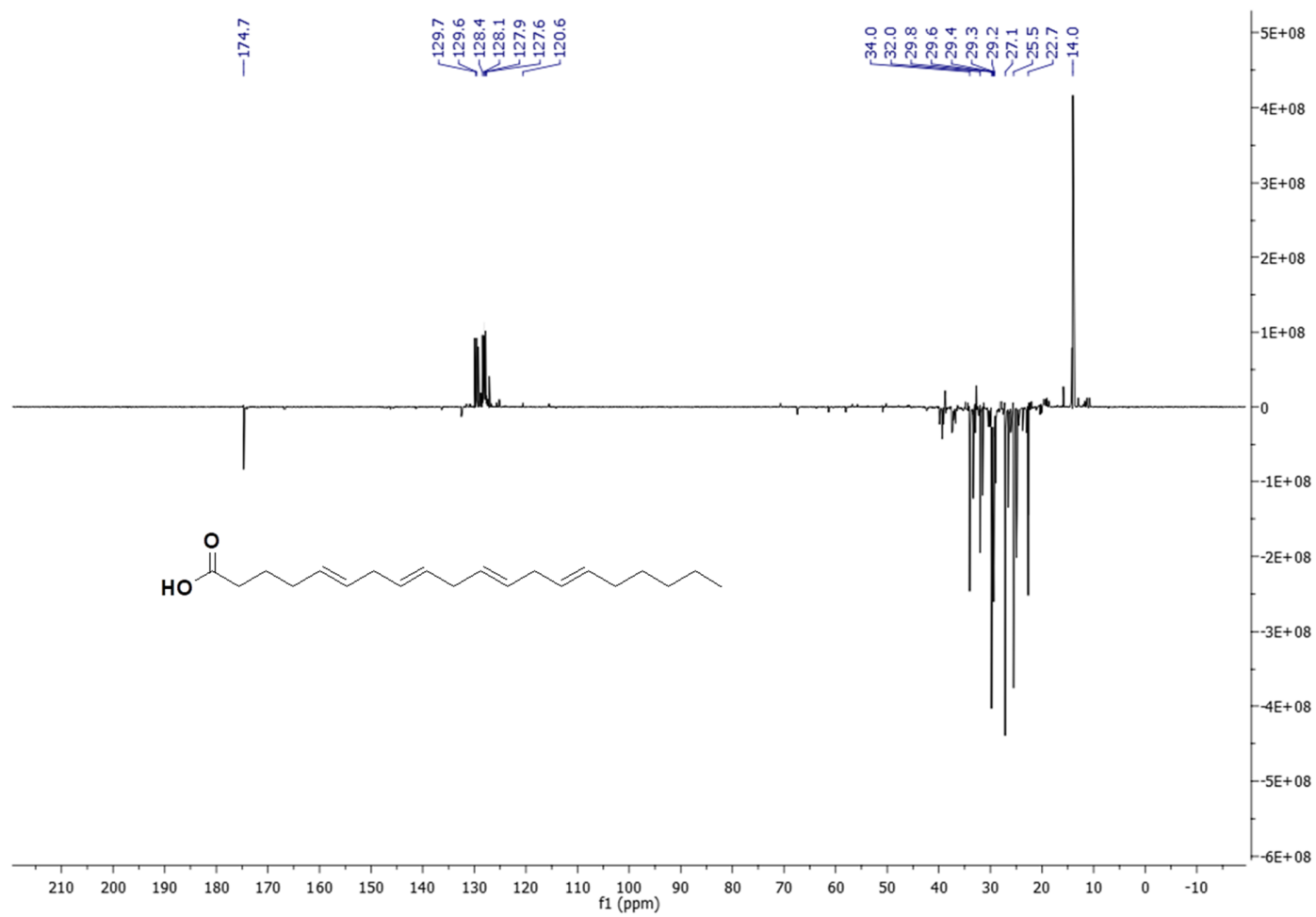


Figure S18. DEPT-Q NMR spectrum of compound **16** measured in DMSO-*d*₆ at 100 MHz

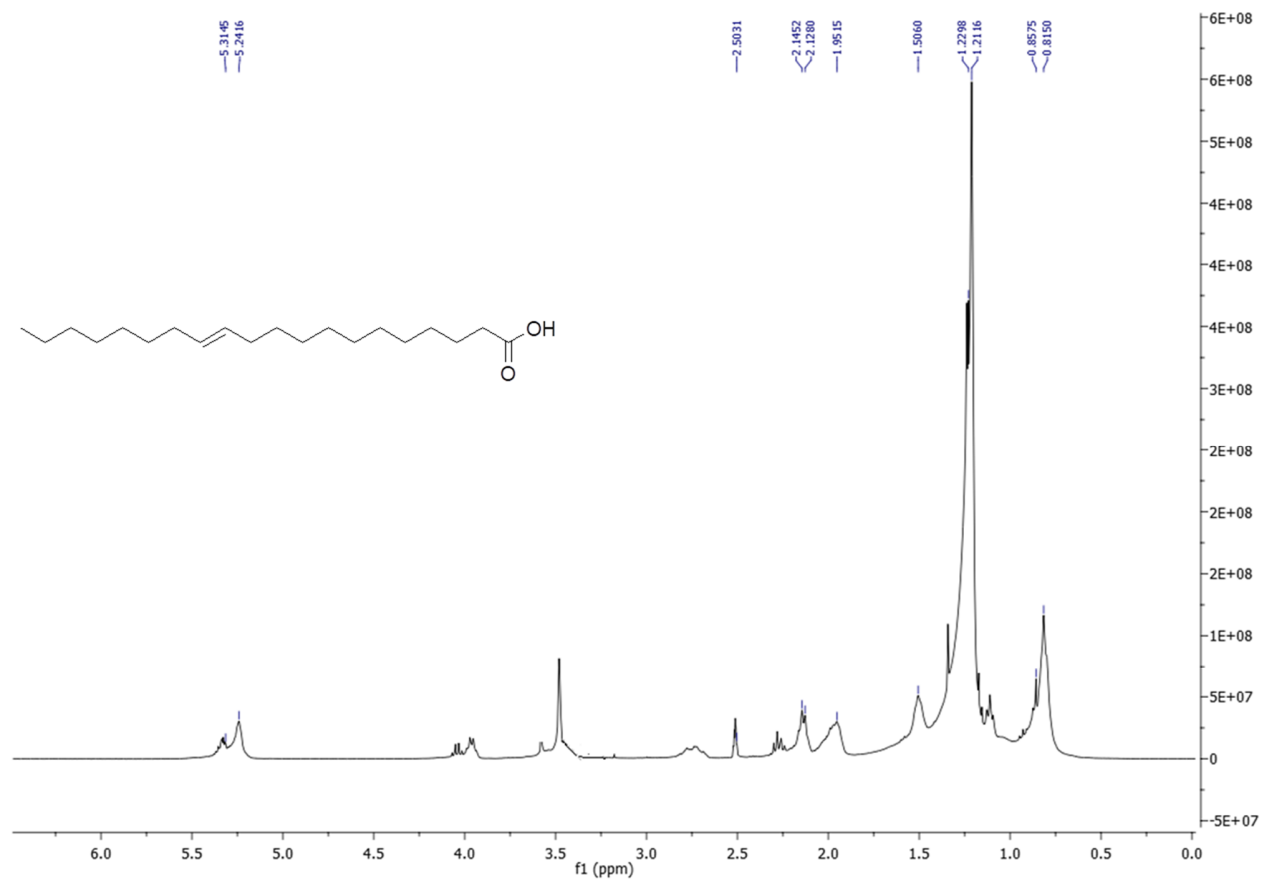


Figure S19. ¹H NMR spectrum of compound 17 measured in DMSO-*d*₆ at 400 MHz

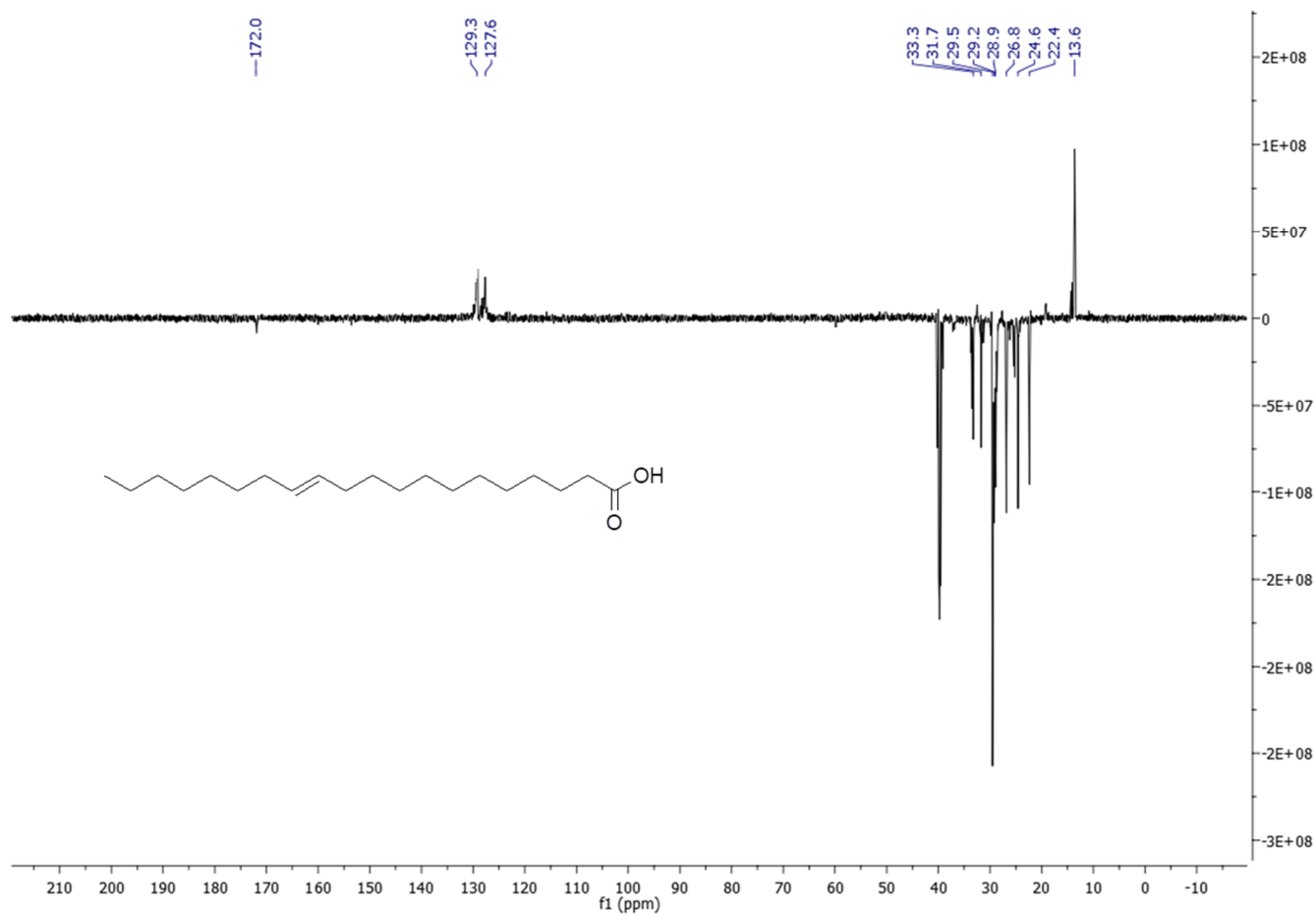


Figure S20. DEPT-Q NMR spectrum of compound 17 measured in DMSO- d_6 at 100 MHz

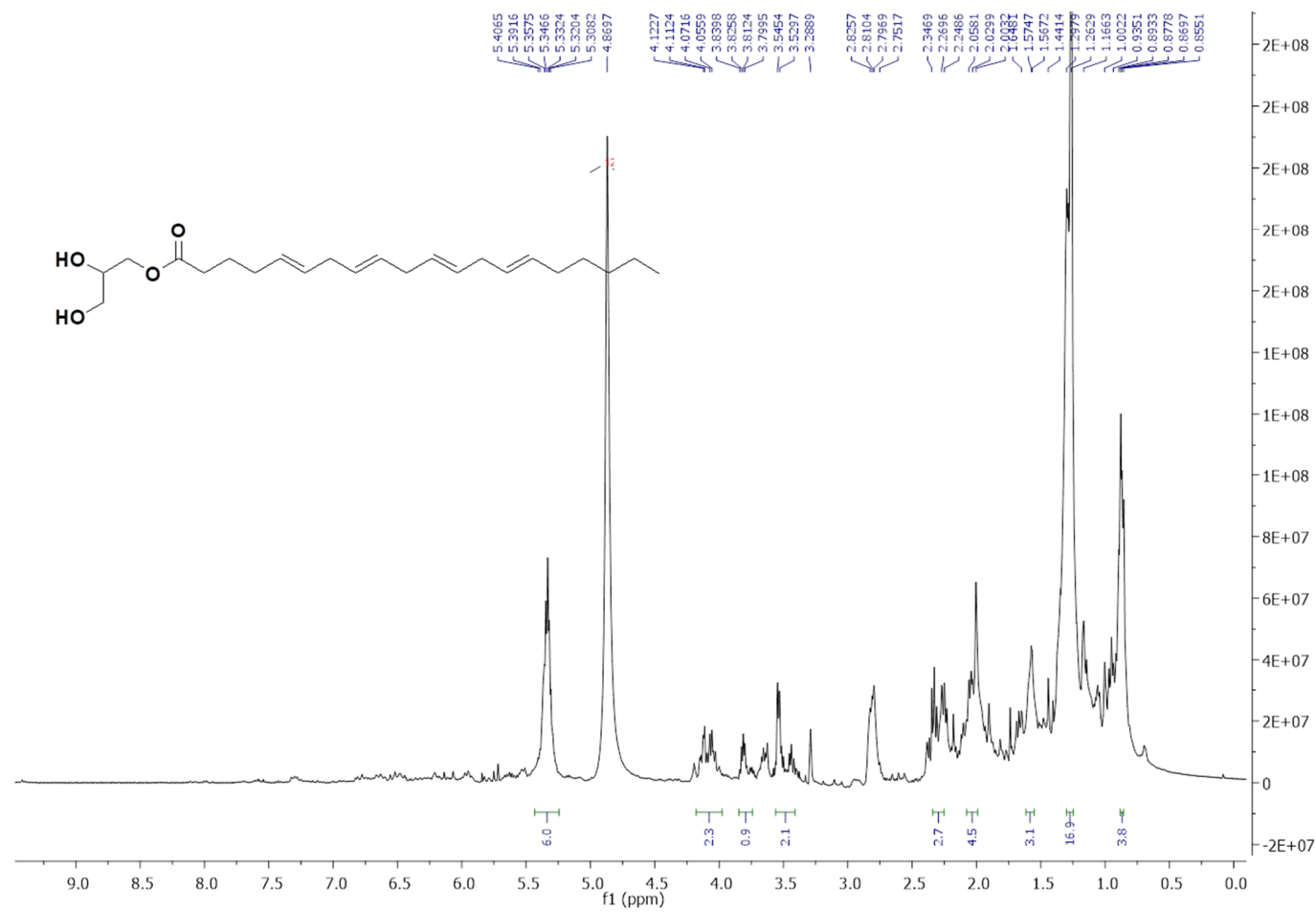


Figure S21. ^1H NMR spectrum of compound **18** measured in $\text{CD}_3\text{OD}-d_4$ at 400 MHz

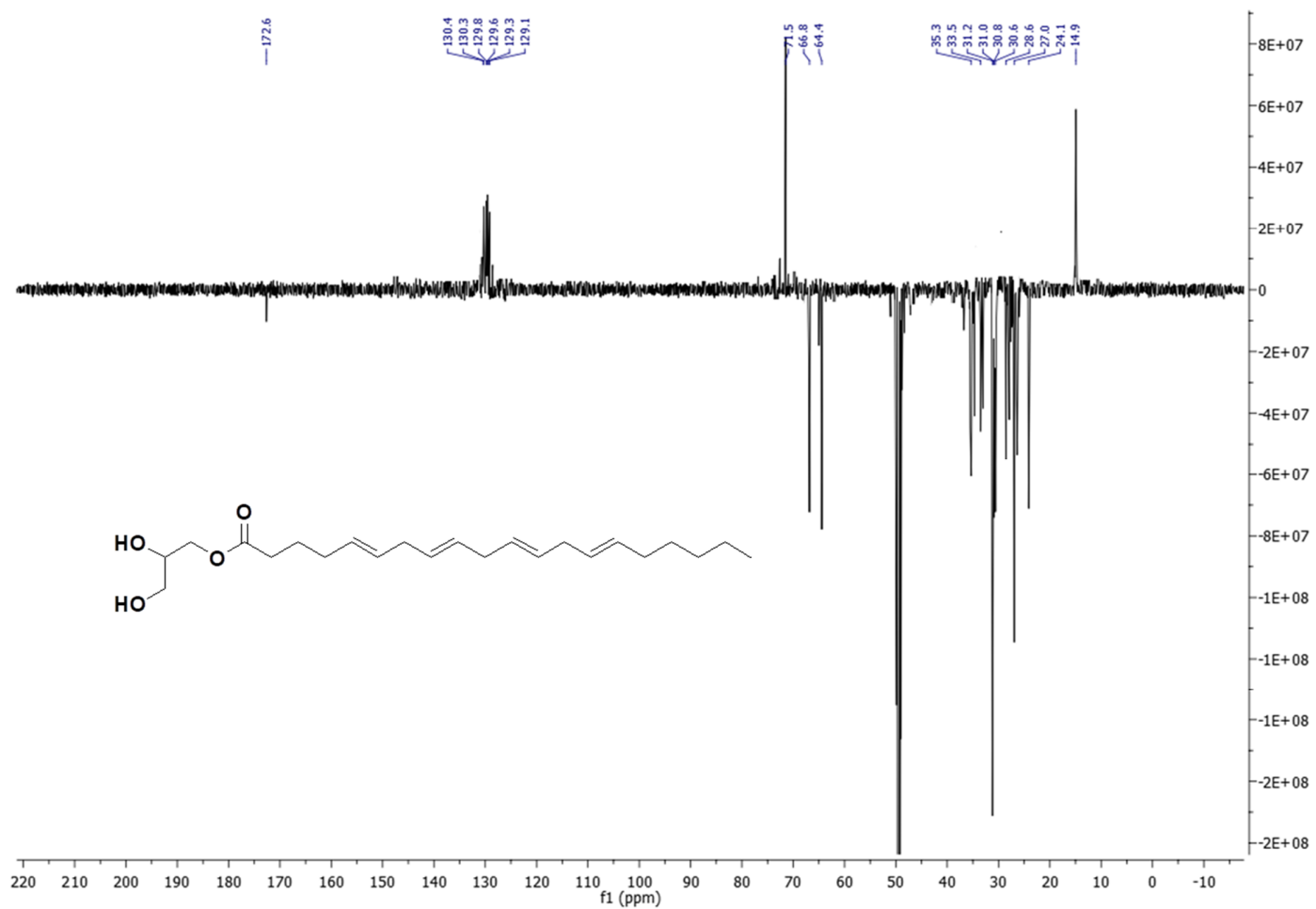


Figure S22. DEPT-Q NMR spectrum of compound 18 measured in CD₃OD-*d*₆ at 100 MHz

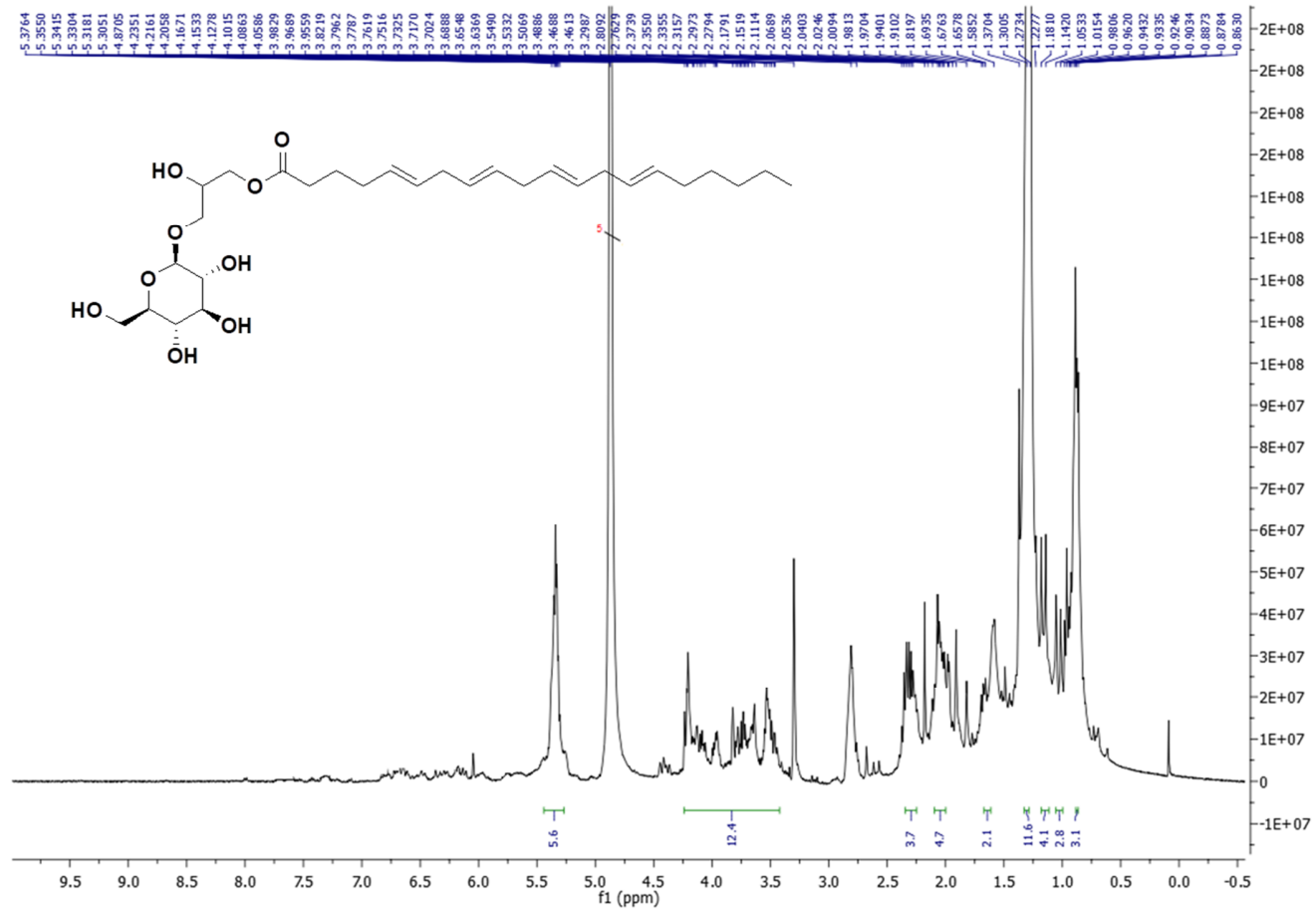


Figure S23. ¹H NMR spectrum of compound **19** measured in CD₃OD-*d*₄ at 400 MHz

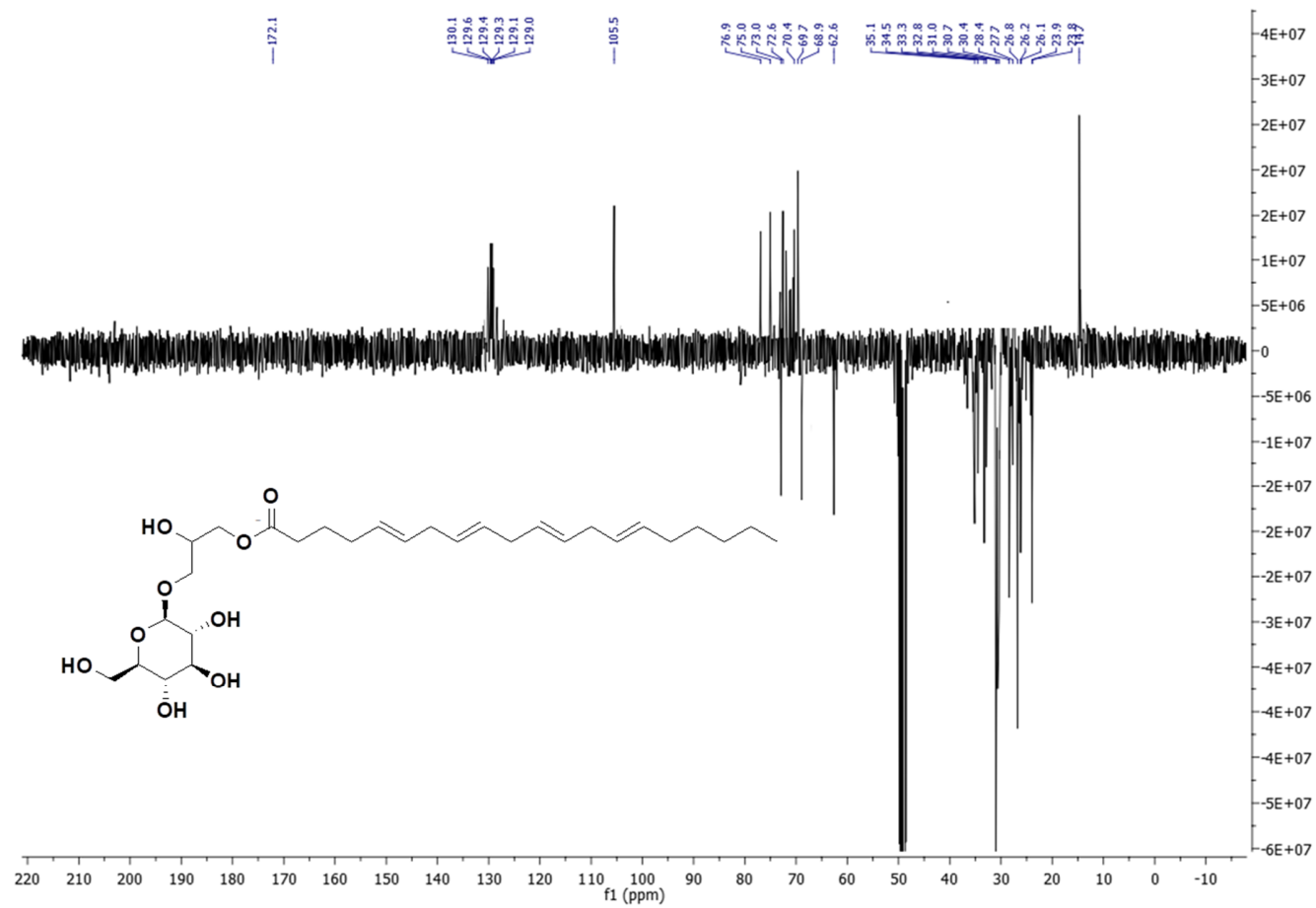


Figure S24. DEPT-Q NMR spectrum of compound **19** measured in $\text{CD}_3\text{OD}-d_6$ at 100 MHz

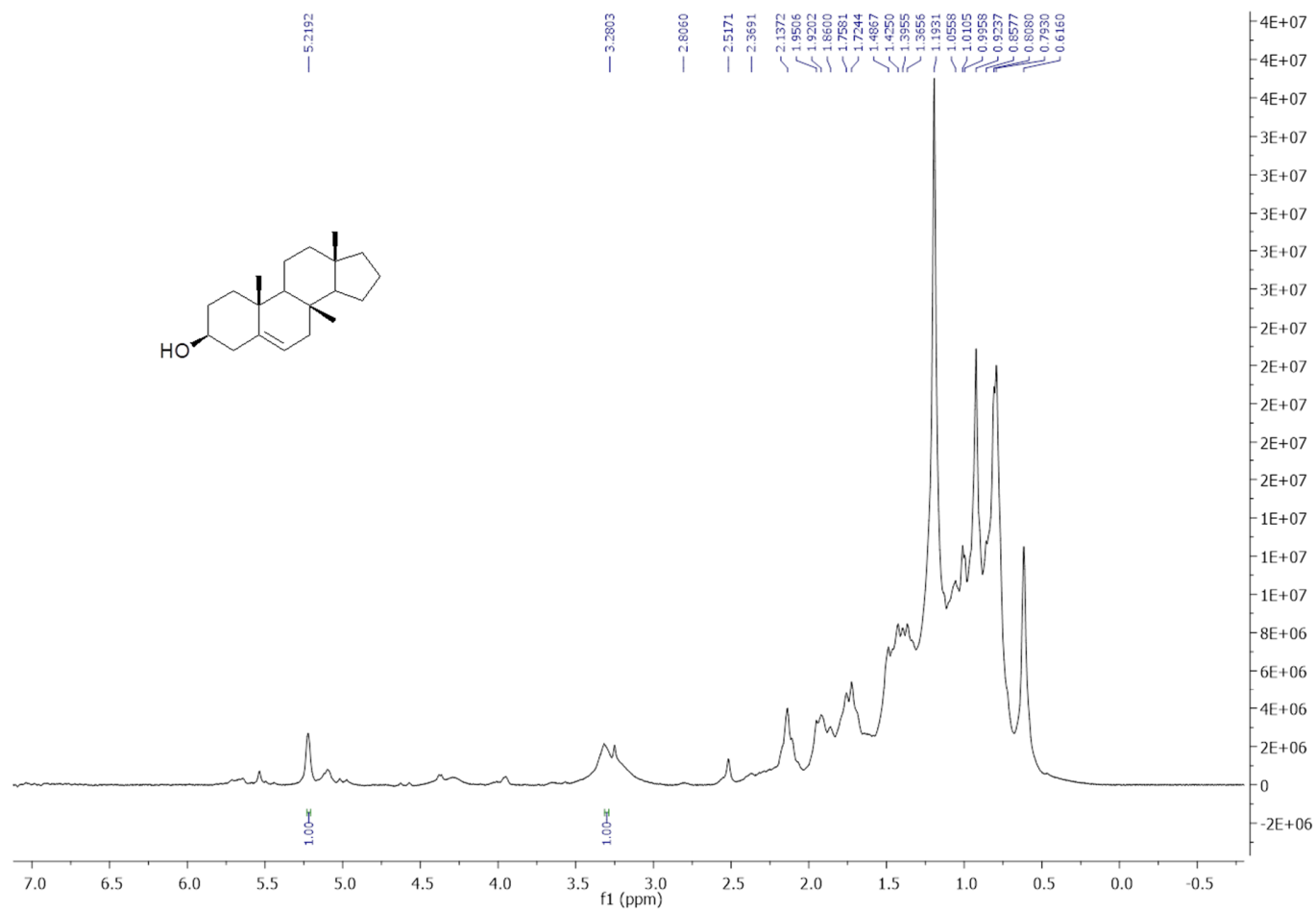


Figure S25. ^1H NMR spectrum of compound 20 measured in $\text{DMSO-}d_6$ at 400 MHz

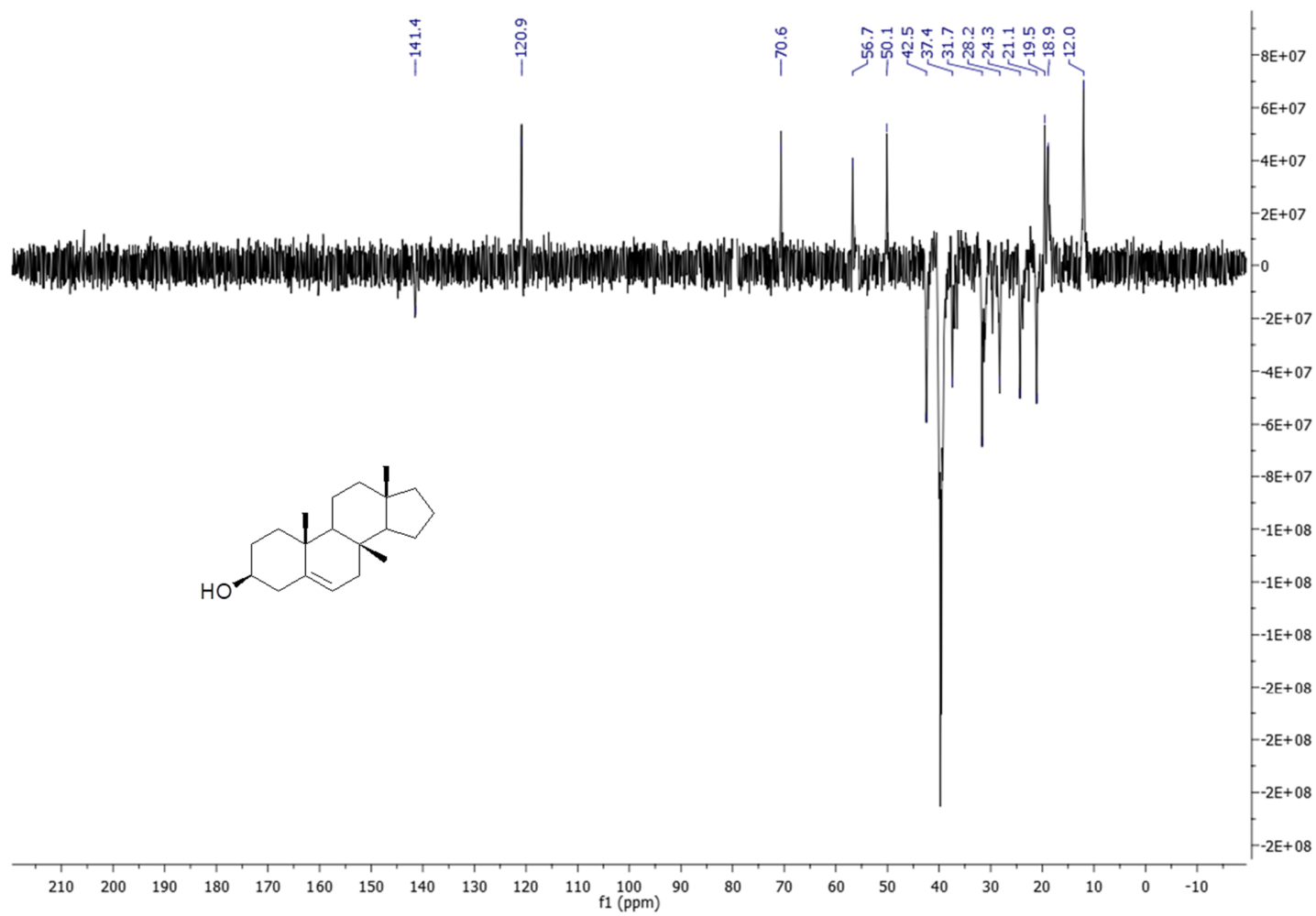


Figure S26. DEPT-Q NMR spectrum of compound **20** measured in DMSO- d_6 at 100 MHz

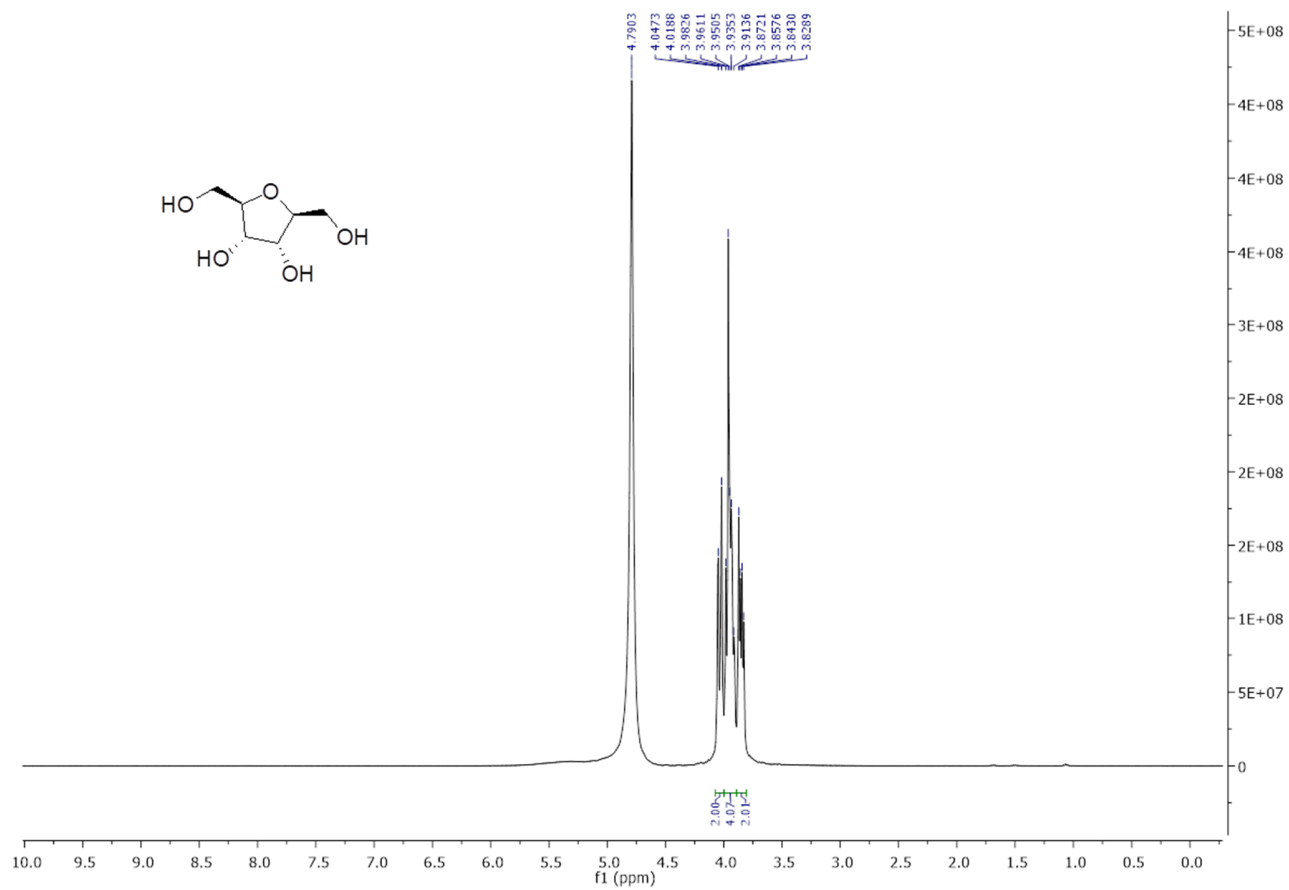


Figure S27. ¹H NMR spectrum of compound **21** measured in D₂O at 400 MHz

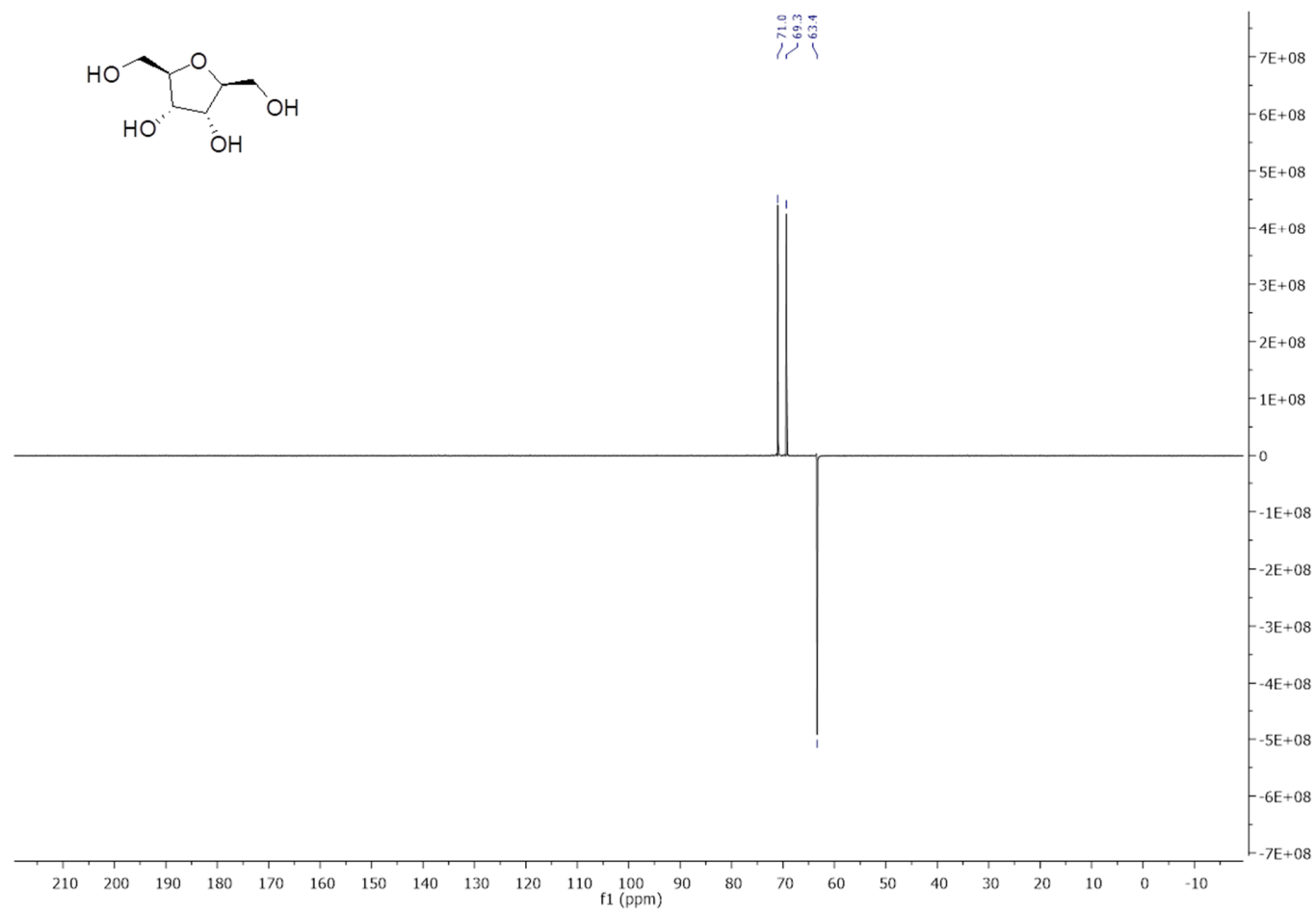


Figure S28. DEPT-Q NMR spectrum of compound **21** measured in D₂O at 100 MHz