

Supporting Information

Dimeric Polyphenols to Pave the Way for New Antimalarial Drugs.

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Synthesis propyl caffeate & gallate

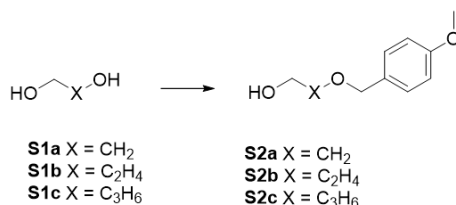
The carboxylic acid (1.0 g) was dissolved in 50 mL of *n*-propanol and a few drops of concentrated H₂SO₄ were cautiously added. The mixture was heated under reflux until the end of the reaction (monitored by TLC, ~ 6h). The reaction mixture was cooled before a part of the organic solvent was eliminated by evaporation under vacuo. After that, water (25 mL) was added, and the solution was extracted three times with ethyl acetate (50 mL). Then, the organic phase was washed with brine (50 mL) and dried over anhydrous magnesium sulfate (MgSO₄). The suspension was filtered, and the solvent was removed by evaporation under vacuo. The solid was placed overnight in a stove (30°C).

Propyl gallate, white solid, Yield 86 %, MP. 145°C/Lit. 145-146°C,¹ ¹H-NMR (in DMSO) δ 6.95 (2H, s), 4.12 (2H, t), 1.68 (2H, m), 0.95 (3H, t); ¹³C-NMR (in DMSO) δ 166.33, 146.02, 138.81, 120.02, 108.91, 65.89, 22.16, 10.86; EA Th C, 56.60%; H, 5.70%; Found: C, 56.93%; H, 6.10%.

Propyl caffeate, white solid, Yield 66 % after DCVC (DCM/MeOH (1/0 to 95/5), MP = 128 °C/Lit. 127 °C,² ¹H-NMR (in DMSO) δ 7.47 (1H, d), 7.04 (1H, d), 7.01 (1H, dd), 6.75 (1H, d), 6.26 (1H, d), 4.07 (2H, t), 1.64 (2H, m), 0.92 (3H, t); ¹³C-NMR (in DMSO) δ 167.09, 148.86, 146.03, 145.48, 125.96, 121.81, 116.19, 115.28, 114.46, 65.65, 22.15, 10.86; EA Th: C, 64.85%; H, 6.35%; Found: C, 64.84%; H, 6.39%.

Synthesis of (4-methoxybenzyl)oxydiol

The diol (13.0 mmol) was dispersed in DMSO (12 mL) at 0°C. Potassium hydroxide (13.0 mmol) was added to the reaction media and stirred until the solution was clear. Then, *para*-methoxybenzyl chloride (6.50 mmol) was poured in the mixture and stirred until the end of the reaction at RT. After that, 6 mL ether and 5 mL 5N HCl were poured to quench the reaction. The aqueous part was extracted 3 times with ether. The organic phase was dried with MgSO₄, filtrated, and evaporated. The oil was purified on DCVC (*n*-hexane/EtOAc, 1/0 to 0/1).



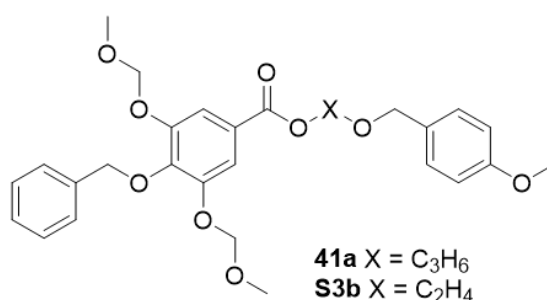
2-((4-methoxybenzyl)oxy)ethan-1-ol (S2a), colourless oil, ¹H-NMR (in CDCl₃) δ 7.27 (2H, d), 6.89 (2H, d), 4.49 (2H, s), 3.81 (3H, s), 3.74 (2H, t), 3.57 (2H, t); ¹³C-NMR (in CDCl₃) δ 159.34, 130.07, 129.46, 113.88, 72.97, 71.06, 61.92, 55.29.

3-((4-methoxybenzyl)oxy)propan-1-ol (S2b), colourless oil, ¹H-NMR (in CDCl₃) δ 7.25 (2H, d), 6.88 (2H, d), 4.45 (2H, s), 3.80 (3H, s), 3.77 (2H, t), 3.64 (2H, t), 1.85 (2H, m); ¹³C-NMR (in CDCl₃) δ 159.26, 130.16, 129.30, 113.85, 72.95, 69.20, 62.07, 55.29, 32.07.

4-((4-methoxybenzyl)oxy)butan-1-ol (S2c), colourless oil, $^1\text{H-NMR}$ (in CDCl_3) δ 7.25 (2H, d), 6.88 (2H, d), 4.44 (2H, s), 3.79 (3H, s), 3.62 (2H, t), 3.49 (2H, t), 1.71-1.64 (4H, m); $^{13}\text{C-NMR}$ (in CDCl_3) δ 159.22, 130.20, 129.37, 113.82, 72.71, 70.05, 62.66, 55.26, 30.19, 26.75.

Addition of hydroxybenzoic acid on (4-methoxybenzyl)oxydiol

To a solution of the protected alcohol (1.5 eq.) in CH_2Cl_2 (167 mL) were added the hydroxybenzoic acid (8.73 g, 25.1 mmol), DMAP (2.04 g, 16.7 mmol), and EDCI.HCl (6.41 g, 33.4 mmol). The mixture was stirred at rt until the term of the reaction (controlled by TLC). Then, the mixture was neutralized with 1 N aq. H_3PO_4 , and diluted with H_2O (25 mL). After, the solution was extracted with EtOAc. The organic layer was washed with H_2O and brine. After the general drying procedure and evaporation under vacuo, the resulting product was purified by flash chromatography to obtain a colourless oil.³



3-((4-methoxybenzyl)oxy)propyl 4-(benzyloxy)-3,5-bis(methoxymethoxy)benzoate (41a), colourless oil, $^1\text{H-NMR}$ (in CDCl_3) 7.50 (2H, s), 7.47 (2H, d), 7.36-7.31 (3H, m), 7.26 (2H, d), 6.86 (2H, d), 5.18 (4H, s), 5.13 (2H, s), 4.45 (2H, s), 4.40 (2H, t), 3.78 (3H, s), 3.59 (2H, t) 3.48 (6H, s), 2.05 (2H, m).

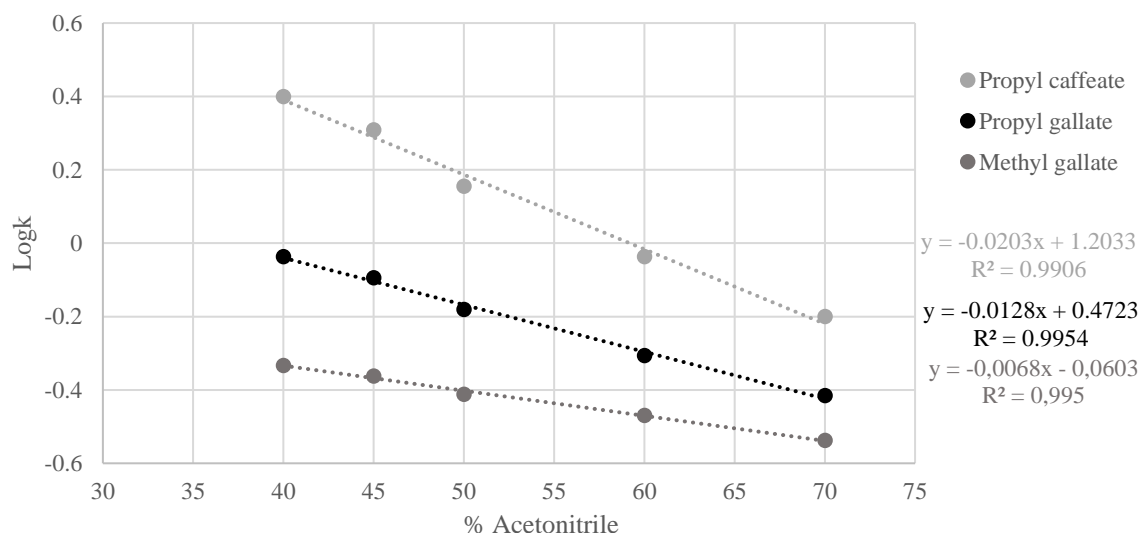
2-((4-methoxybenzyl)oxy)ethyl 4-(benzyloxy)-3,5-bis(methoxymethoxy)benzoate (S3b), colourless oil, $^1\text{H-NMR}$ (in CDCl_3) 7.54 (2H, s), 7.47 (2H, dd), 7.36-7.26 (5H, m), 6.87 (2H, d), 5.19 (4H, s), 5.13 (2H, s), 4.54 (2H, s), 4.46 (2H, t), 3.80 (3H, s), 3.76 (2H, t), 3.48 (6H, s).

Determination of LogP by HPLC

To confirm that the water solubility variation could be partially explained by the molecular behaviour in the solvent, we have experimentally measured the logP of three dimeric structures. Indeed, C_{\max} value of **22-24** showed a surprising trend as $24 > 22 > 23$, while their lipophilicity let expected a different situation with ethane more soluble than the corresponding propane (logP 1.13 and 1.23, respectively). Thus, as their estimated logP value were quite close, it could be possible that their experimental values will explain this situation.

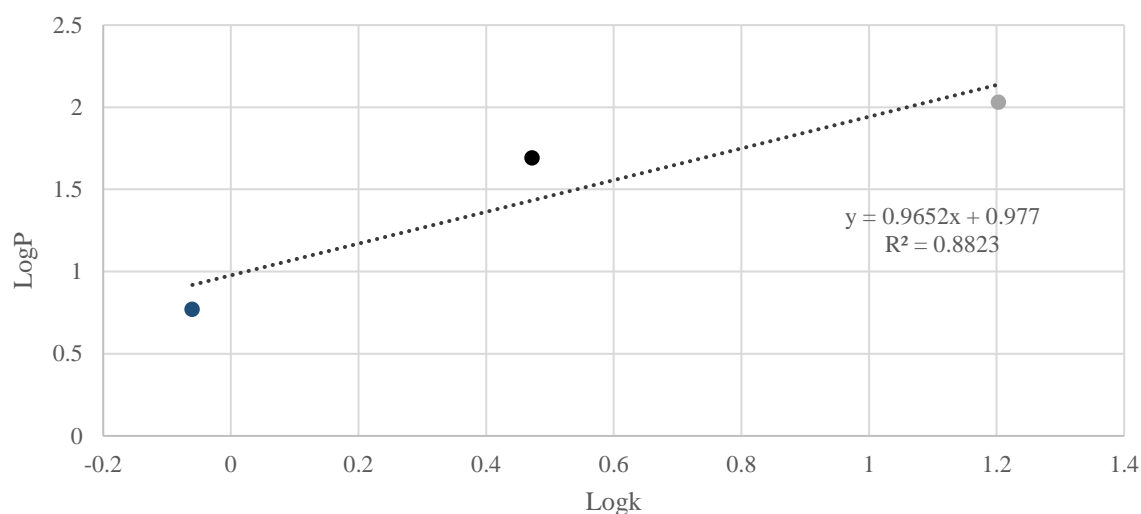
Therefore, we have employed an isocratic HPLC method inspired by the protocol reported by Liang *et al.* (2017).⁴ As our compounds belongs to the polyphenols' family, we have first selected references whose the logP value have already been experimentally determined and which are polyphenols. Consequently, we have chosen methyl and propyl gallate, as well as propyl caffeate (logP = 0.77, 1.69 & 2.03, respectively) to establish the calibration curve. All these compounds have been freshly prepared as previously reported and their purity controlled by elemental analysis.^{5,6}

Figure 1 Modification of retention time from polyphenolic references with percentage of acetonitrile.



Thanks to their retention time values obtained with several mobile phase (H_2O /Acetonitrile, from 70/30 to 20/80 + 0.05% TFA), we have first determined a graph of the $\log(T_R)$ following the organic modifier percentage (Fig. 1). Then, the linear regression allowed to estimate the $\log(T_R)$ value for 100% water and to draw a graph of $\log(T_R)$ following the logP value (Fig. 2).

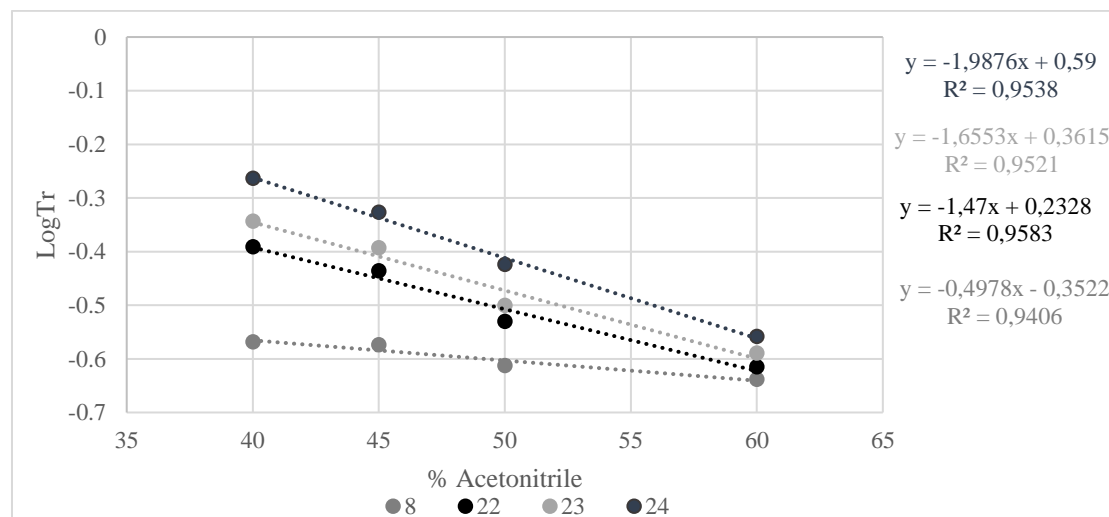
Figure 2 Calibration curve of LogP value with LogTr at 100% water.



After that, the test compounds have been injected in similar conditions to determine their own $\log(T_R)$ value in pure water (Fig. 3). Finally, the calibration curve was used to calculate the $\log P$ value of these compounds. These results were quite similar to the estimated ones according to Chemdraw 12.0 software.

In conclusion, the influence of other parameters that lipophilicity ($\log P$) in the water solubility of the dimeric structures seemed confirmed.

Figure 3 Modification of retention time with percentage of acetonitrile.



Biological activities of synthetic intermediates

Table 1 Pharmacological activities and Physical characterization of the reported compounds.

Compounds	3D7 ^a	FcB1 ^b	W2 ^c	HUVEC ^d	SI	Solubility ^e	Increment Solubility	cLogP ^f
9	2.8 ± 1.9	7.5 ± 2.8	8.9 ± 5.9	> 165	> 59	0.018 ± 0.003	1	1.1
8	68 ± 20	-	-	> 294	> 4	70 ± 8.2	3879	0.63 ^g
35	27 ± 1.8	-	-	171 ± 43	6	74 ± 7.7	4102	0.77 ^h
36	9.3 ± 3.0	-	-	> 161	> 17	0.59 ± 0.75	32	1.2
37a	56 ± 2.2	-	-	> 140	> 3	0.46 ± 0.22	26	3.6
37b	59 ± 0.49	-	-	> 129	> 2	0.074 ± 0.049	4	2.5
37d	> 262	-	-	> 131	-	-	-	0.5
38a	33 ± 5.4	-	-	> 182	> 6	3.7 ± 0.79	206	2.3
38c	17 ± 4	-	-	140 ± 4.3	8	0.005 ± 0.001	0.3	3.5
38b	95 ± 15	-	-	143 ± 14	1.5	0.20 ± 0.058	11	2.6
38d	> 353	-	-	-	-	-	-	0.6
39d	> 316	-	-	> 158	-	-	-	1.2
39f	70 ± 23	-	-	> 123	-	-	-	3.3
40a	29 ± 11	-	-	-	-	0.65 ± 0.15	36	3.2
40c	209 ± 42	-	-	> 126	-	-	-	4.2
40b	> 264	-	-	> 132	-	-	-	3.1
40d	> 269	-	-	-	-	-	-	1.1
40f	> 255	-	-	> 127	-	-	-	3
41a	> 190	-	-	-	-	-	-	5
42a	195 ± 39	-	-	-	-	-	-	4
11	4.5 ± 3.1	-	-	-	-	0.003 ± 0.00006	0.2	6.7
12	21 ± 1.1	-	-	-	-	-	-	-
17	1.8 ± 0.9	1.7 ± 1.1	1.9 ± 1.1	14 ± 5.8	8	0.026 ± 0.004	2	5.2
18	0.9 ± 0.4	0.9 ± 0.2	0.4 ± 0.2	6.9 ± 0.2	5	-	-	7.2
19	3.2 ± 0.96	-	-	15 ± 3.6	5	-	-	4.9
20	4.0 ± 0.7	1.1 ± 0.6	1.8 ± 1.0	9.7 ± 1.0	2.4	-	-	6.2
22	3.7 ± 1.1	3.7 ± 1.2	6.7 ± 3.2	69 ± 12	19	0.43 ± 0.25	24	1.04 ^g
23	5.8 ± 1.9	3.2 ± 1.4	4.1 ± 2.9	> 132	> 23	2.7 ± 0.64	150	1.13 ^g
24	3.7 ± 1.1	5.7 ± 3.4	5.0 ± 4.2	> 127	> 35	0.15 ± 0.05	8	1.30 ^g
25	5.5 ± 1	4.9 ± 2.5	7.6 ± 4.4	84 ± 5.4	41	0.28 ± 0.04	15	2.4
26	4.6 ± 0.6	3.8 ± 2.0	3.6 ± 1.2	-	> 21	1.2 ± 0.14	64	0.6
27	27 ± 1.9	11 ± 1.5	13 ± 2.4	78 ± 41	3	0.6 ± 0.014	33	2
28	> 352	-	-	-	-	0.007 ± 0.004	0.4	3.6
29	6.3 ± 4.8	4.7 ± 2.9	6.8 ± 3.2	59 ± 9.9	11	2.1 ± 0.27	114	1.6
30	9.9 ± 3.2	26 ± 6.7	12 ± 1.5	130 ± 6.8	28	0.61 ± 0.006	34	1.6
31	2.1 ± 1.0	3.7 ± 1.9	3.4 ± 0.9	54 ± 2.5	6	0.30 ± 0.11	16	2.0
32	3.9 ± 2.8	3.1 ± 1.1	2.9 ± 0.7	> 121	> 13	0.066 ± 0.003	4	-0.1
33	9.0 ± 4.3	-	-	> 144	> 42	0.033 ± 0.008	2	2
34	20 ± 3.0	4.3 ± 1.7	7.6 ± 4.5	> 118	> 14	-	-	0.98
Artemisinin (1)	13 ± 3.5 ^h	17 ± 6	24 ± 5	-	-	-	-	2.9
Quinine (6)	0.60 ± 0.12	-	-	-	-	-	86	3.4
Chloroquine (7)	0.5 ± 0.2	1.9 ± 0.3	1.5 ± 0.9	-	-	-	-	-

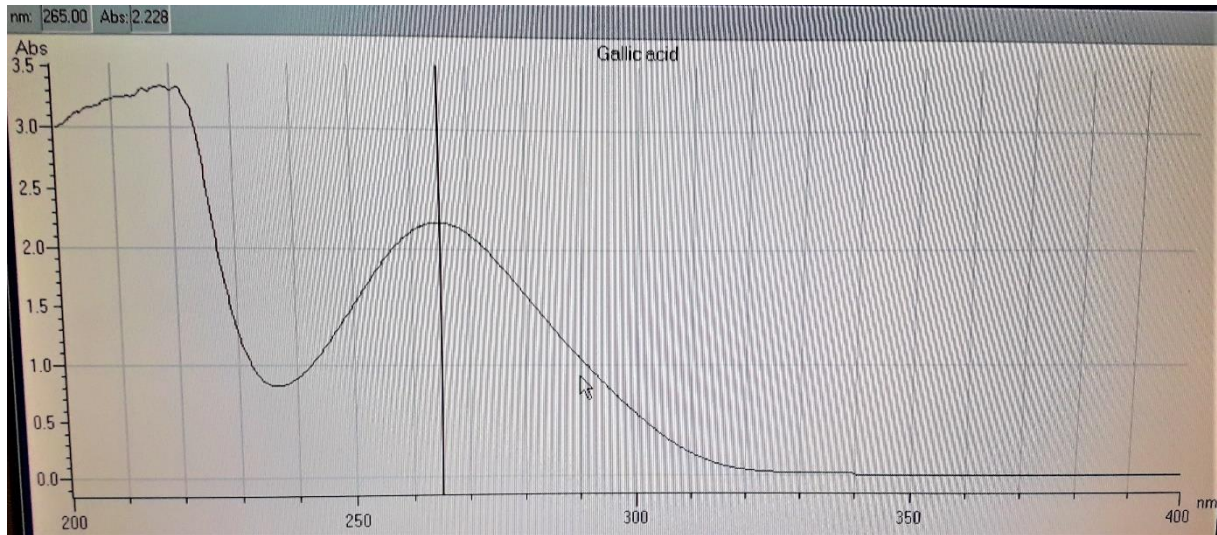
^a IC₅₀ value in μM against *Plasmodium falciparum* (chloroquine-sensitive) in triplicate with standard deviation; ^b IC₅₀ value in μM against *Plasmodium falciparum* (chloroquine-resistant) in triplicate with standard deviation; ^c IC₅₀ value in μM against *Plasmodium falciparum* (multi-resistant) in triplicate with standard deviation; ^d IC₅₀ value from cell toxicity assay in triplicate with standard deviation; ^e C_{max} value in mM in triplicate with standard deviation; ^f Calculated with ChemDraw 12.0; ^g experimental LogP (Supplementary); ^h IC₅₀ value in nM on *P. falciparum* in triplicate with standard deviation.

References

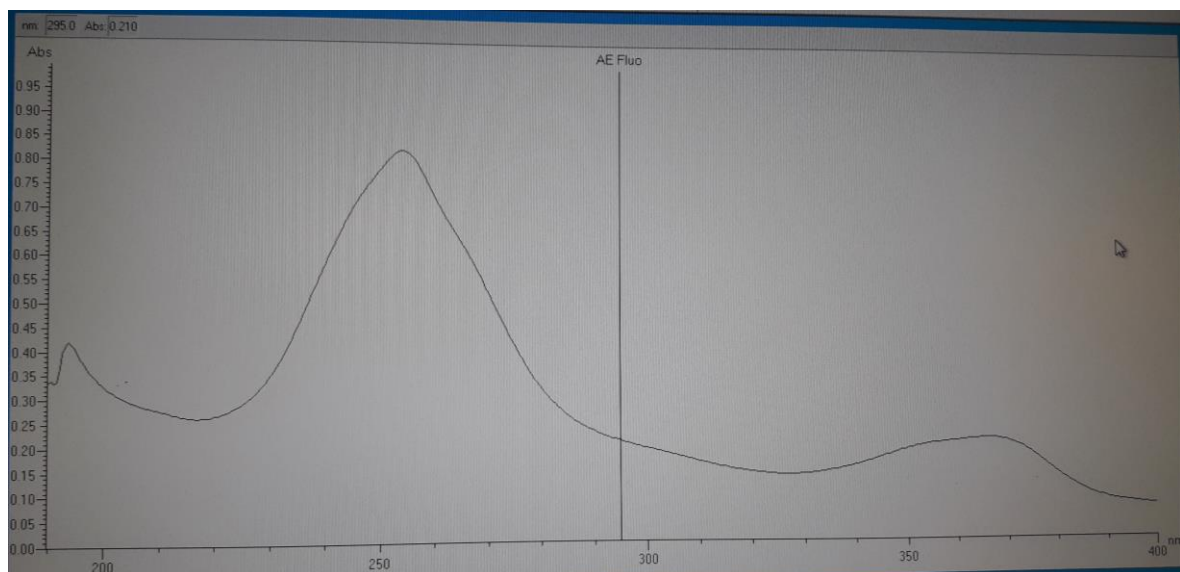
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- 3 T. Hirokane, Y. Hirata, T. Ishimoto, K. Nishii and H. Yamada, *Nat. Commun.*, 2014, **5**, 2017–2019.
- 4 C. Liang, J. qin Qiao and H. zhen Lian, *J. Chromatogr. A*, 2017, **1528**, 25–34.
- 5 G. Degotte, B. Pirotte, M. Frédérick and P. Francotte, *Arch. Pharm. (Weinheim)*, 2021, **354**, 2100190.
- 6 S. G. Alson, O. Jansen, E. Cieckiewicz, H. Rakotoarimanana, H. Rafatro, G. Degotte, P. Francotte and M. Frederich, *J. Pharm. Pharmacol.*, 2018, **70**, 1349–1356.

UV spectra

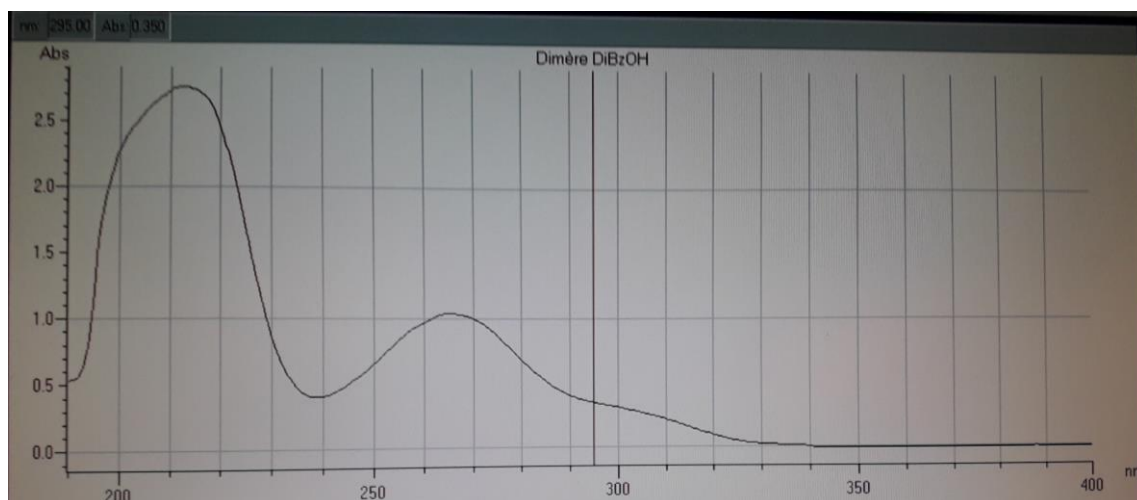
Gallic acid (8)



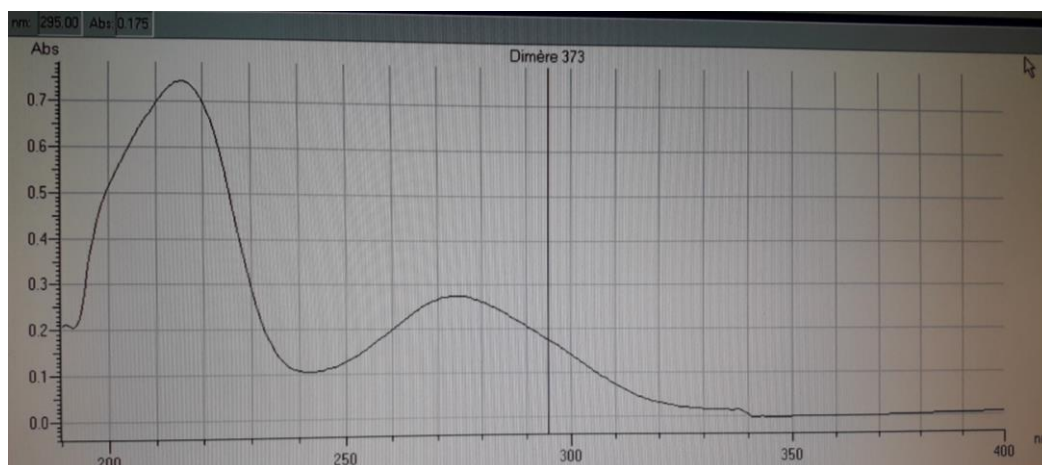
Ellagic acid (9)



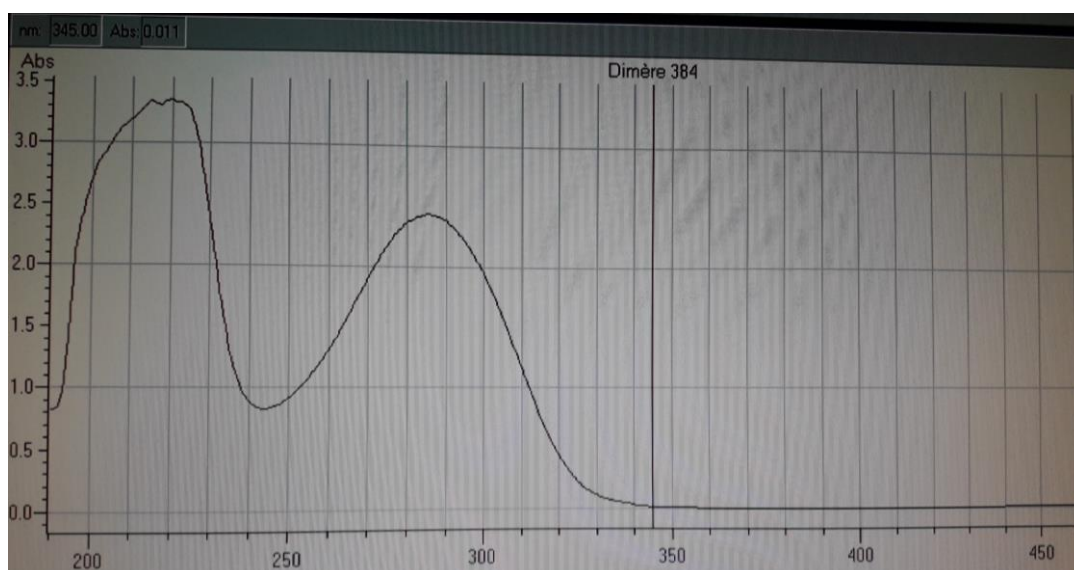
Propane-1,3-diyl bis(4-(benzyloxy)-3,5-dihydroxybenzoate) (**17**)



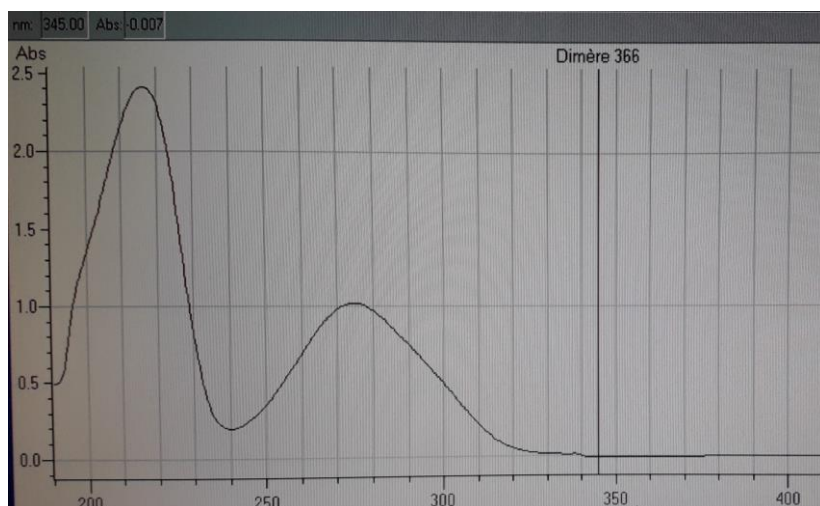
Ethane-1,2-diyl bis(3,4,5-trihydroxybenzoate) (**22**)



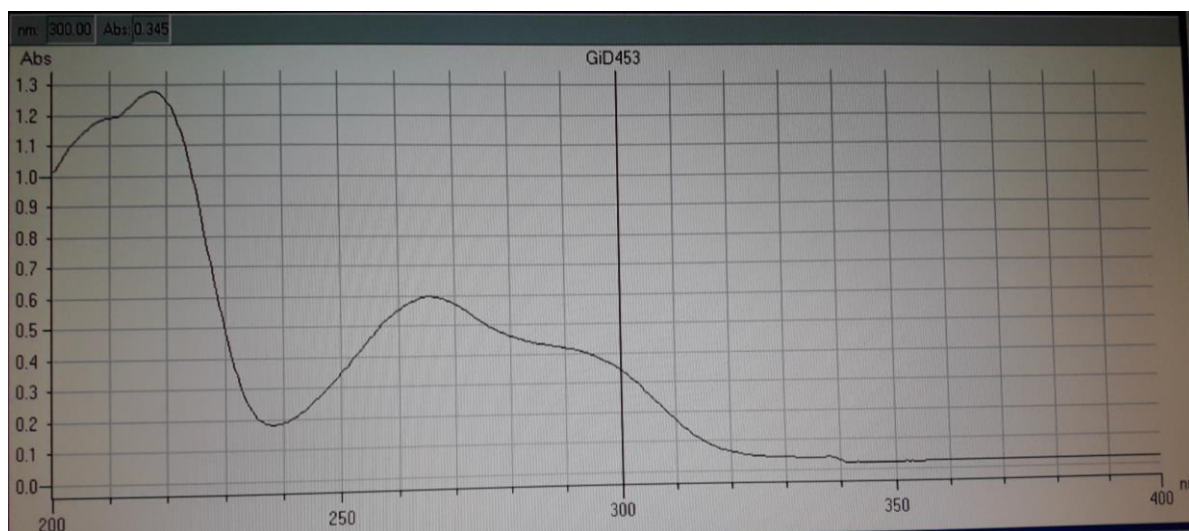
Propane-1,3-diyl bis(3,4,5-trihydroxybenzoate) (**23**)



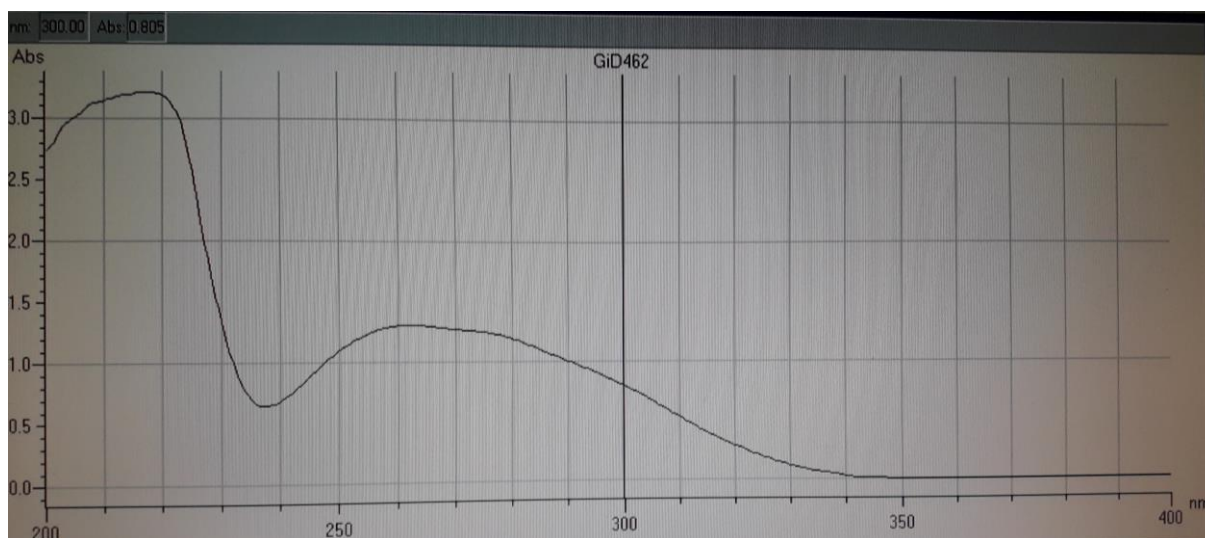
Butane-1,4-diyl bis(3,4,5-trihydroxybenzoate) (**24**)



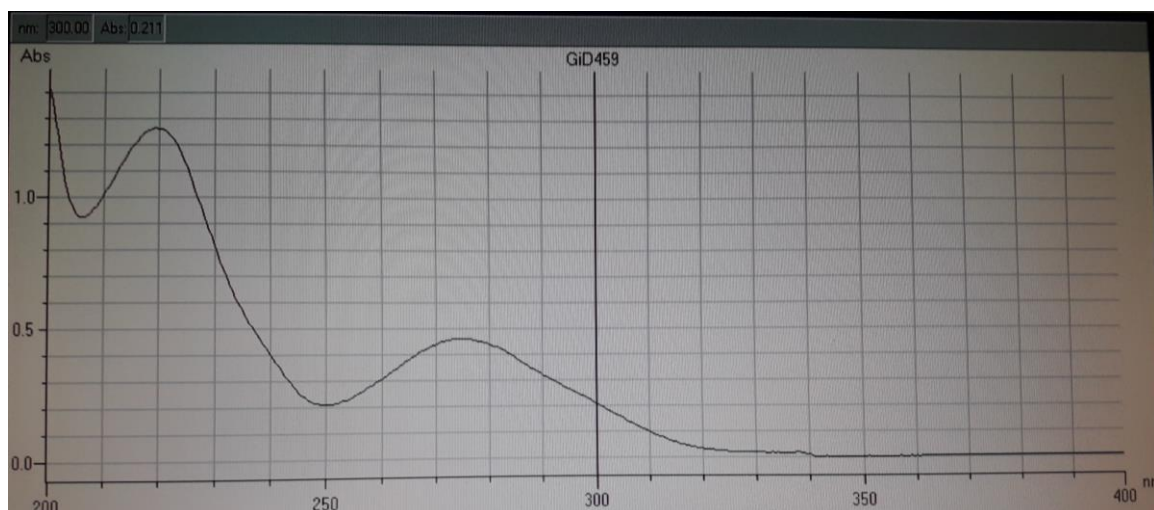
3-((3,4-dihydroxybenzoyl)oxy)propyl 3,4,5-trihydroxybenzoate (**25**)



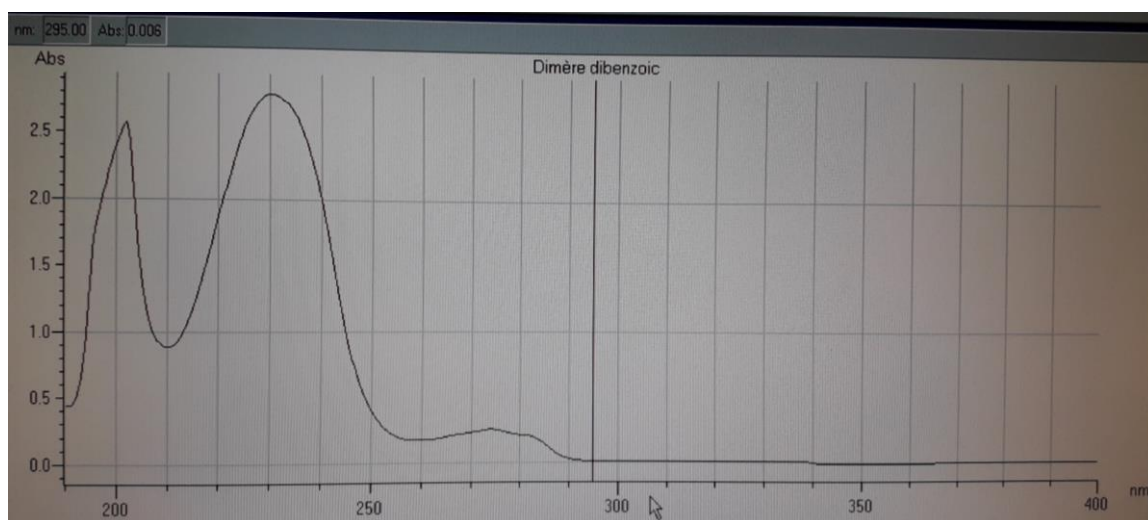
3-((3,5-dihydroxybenzoyl)oxy)propyl 3,4,5-trihydroxybenzoate (**26**)



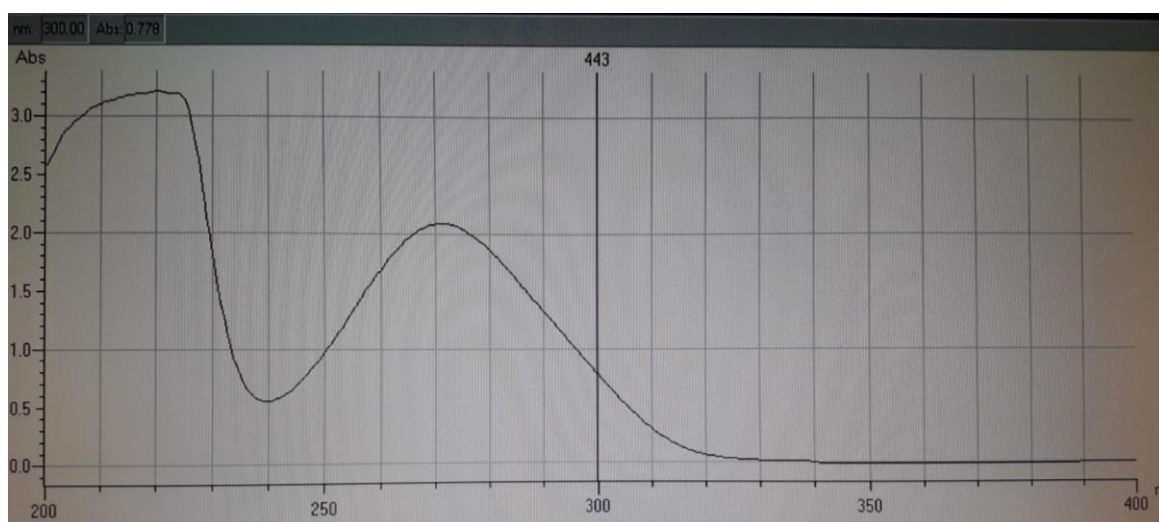
3-(benzyloxy)propyl-3,4,5-trihydroxybenzoate (**27**)



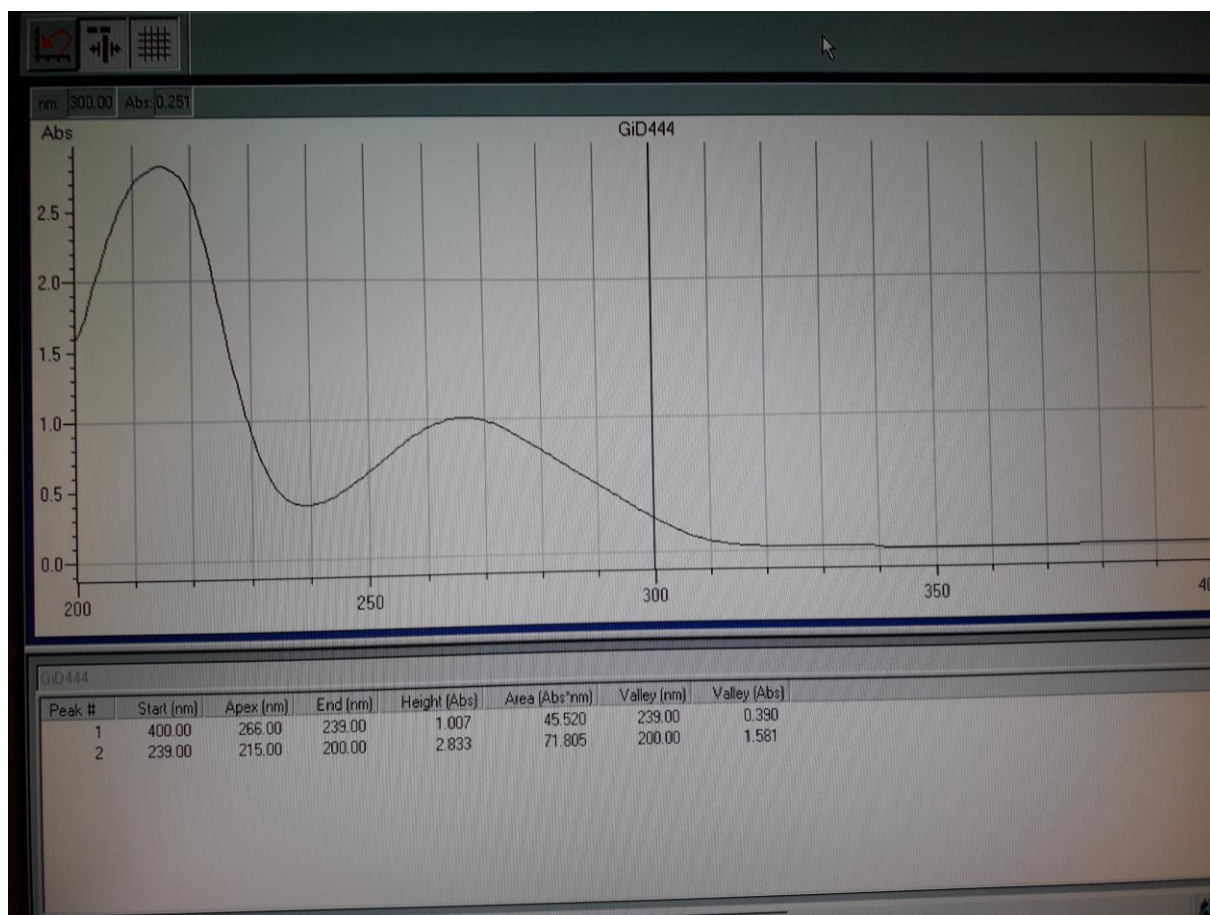
Propane-1,3-diyl dibenzoate (**28**)



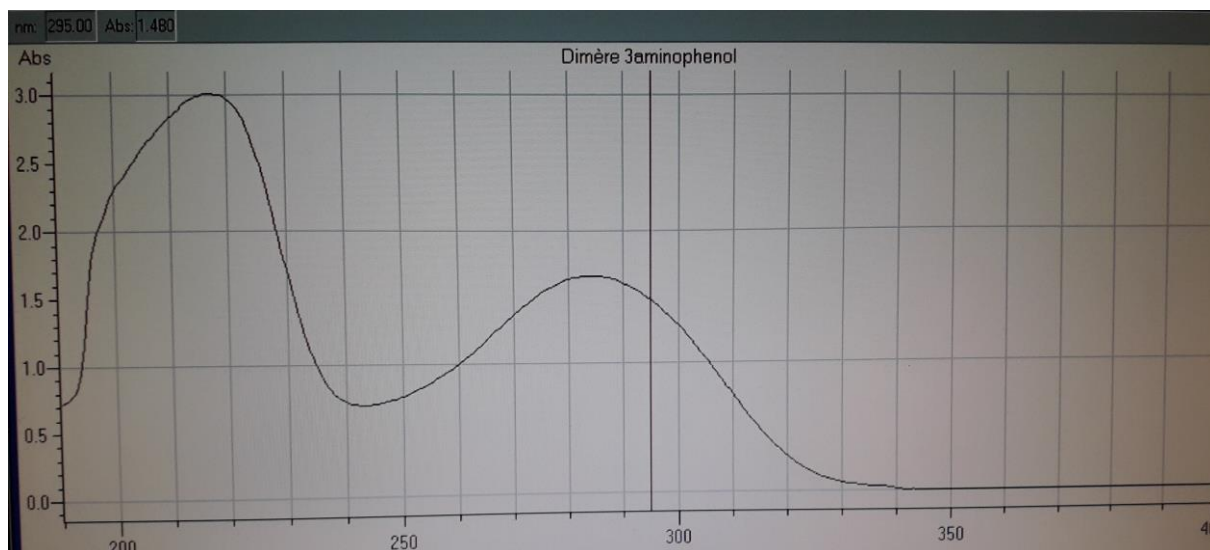
3-(3,4,5-trihydroxybenzamido)propyl 3,4,5-trihydroxybenzoate (**29**)



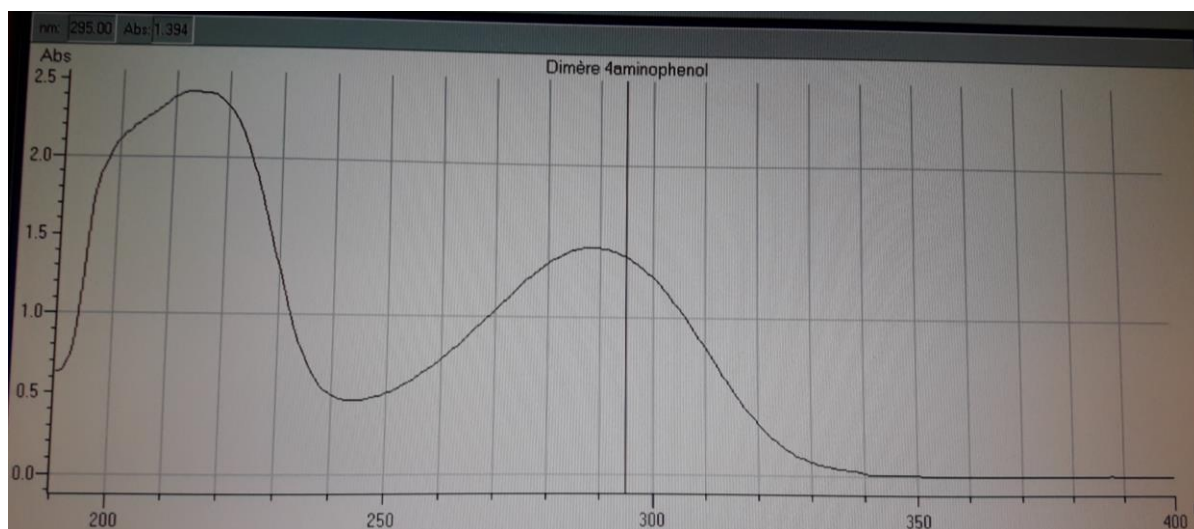
N,N'-(propane-1,3-diyl)bis(3,4,5-trihydroxybenzamide) (**30**)



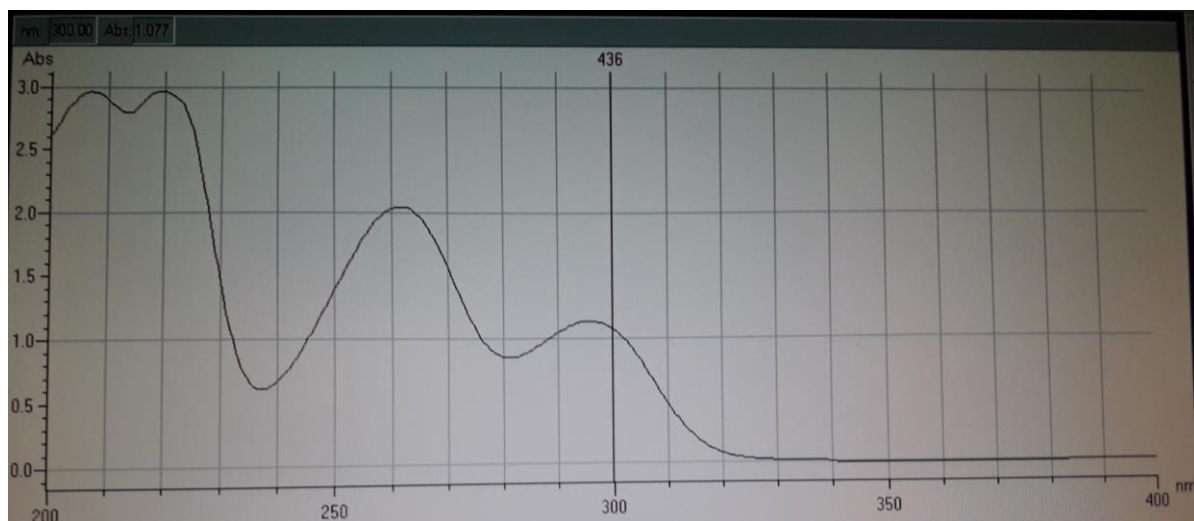
3-(3,4,5-trihydroxybenzamido)phenyl 3,4,5-trihydroxybenzoate (**31**)



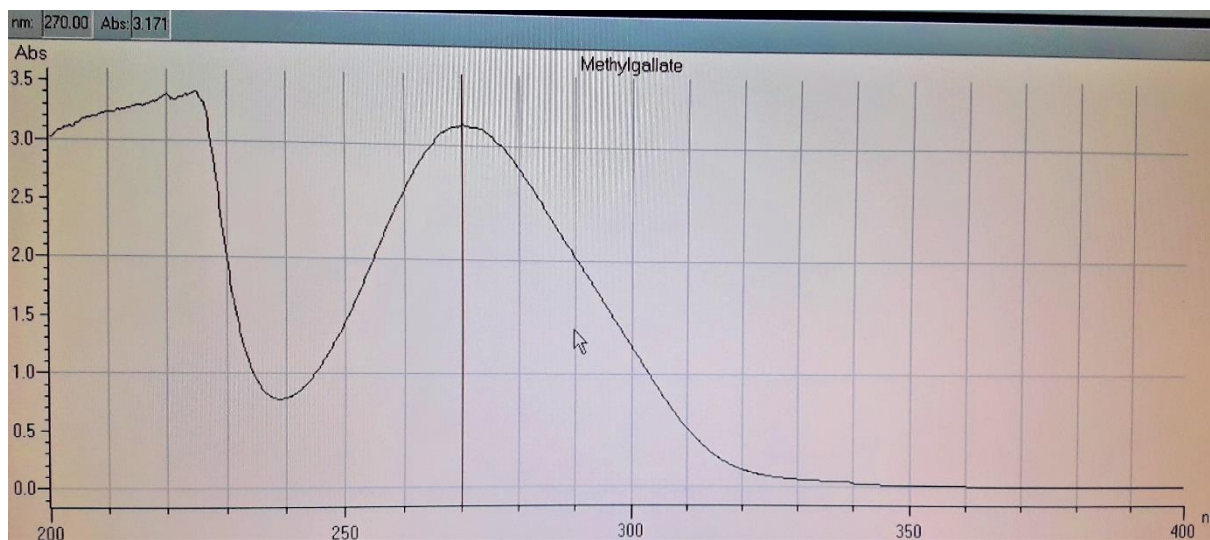
4-(3,4,5-trihydroxybenzamido)phenyl 3,4,5-trihydroxybenzoate (32)



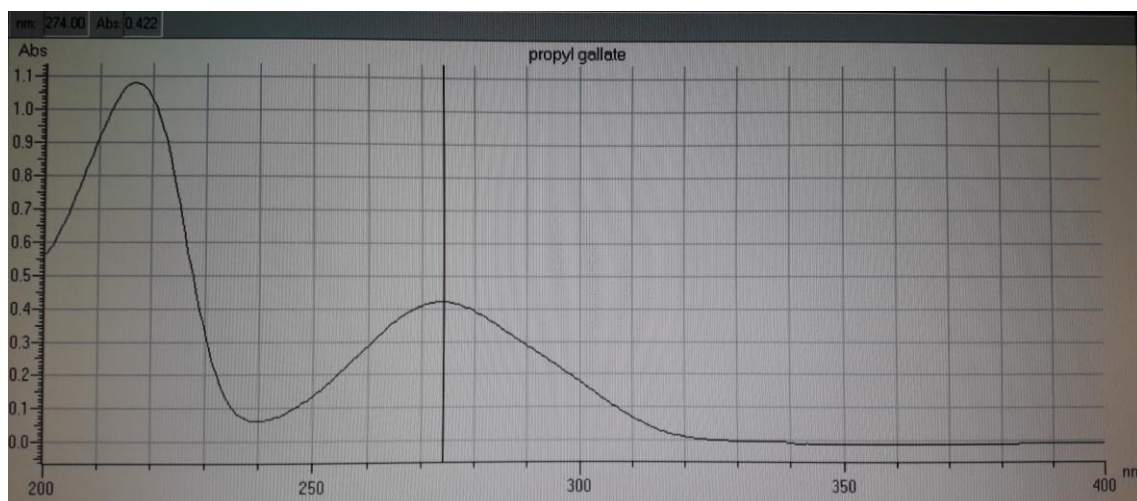
Propane-1,3-diyl bis(3,4-dihydroxybenzoate)(33)



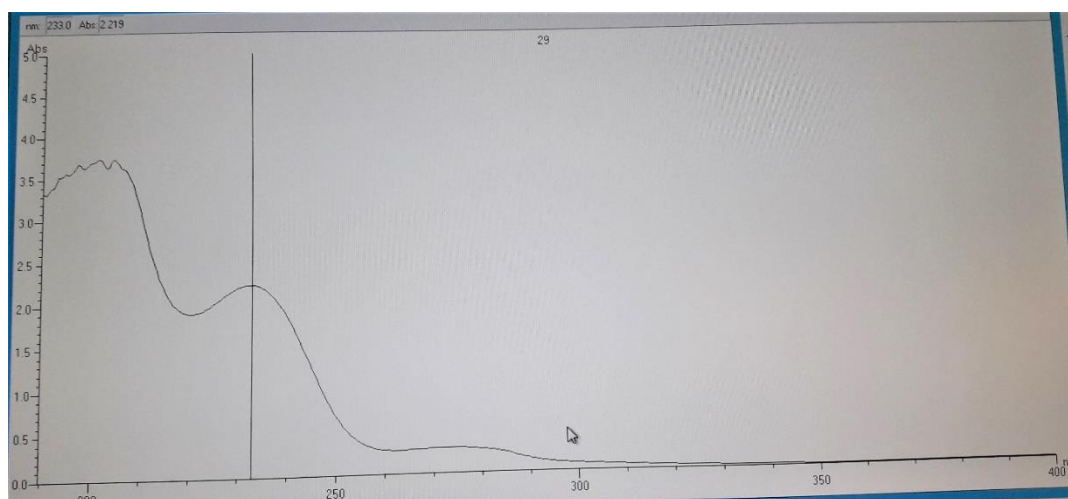
Methyl gallate (35)



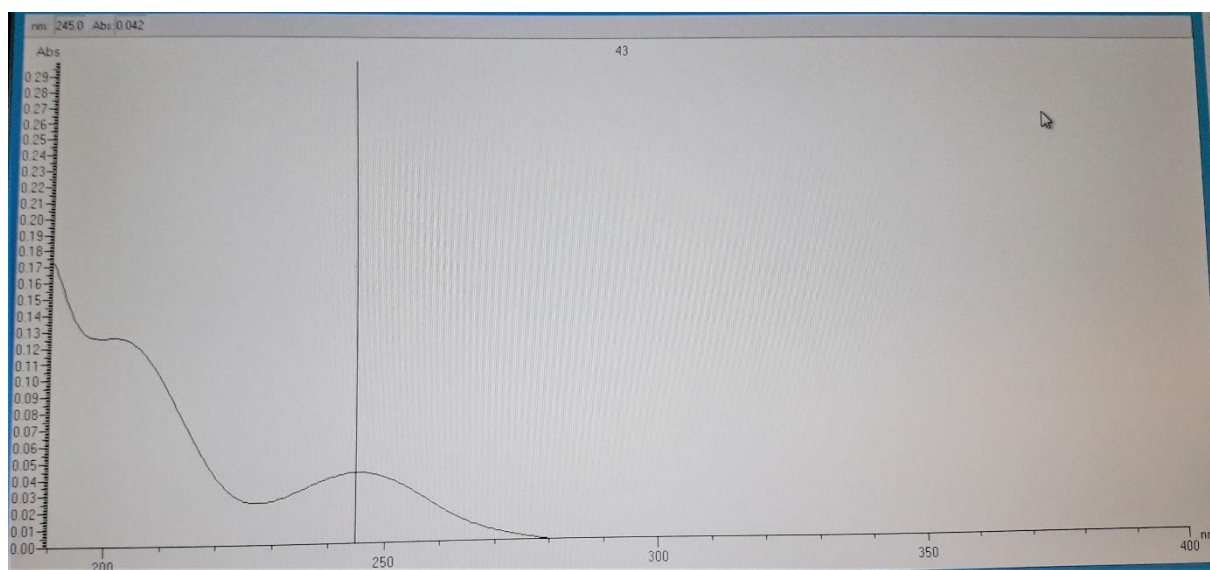
Propyl gallate



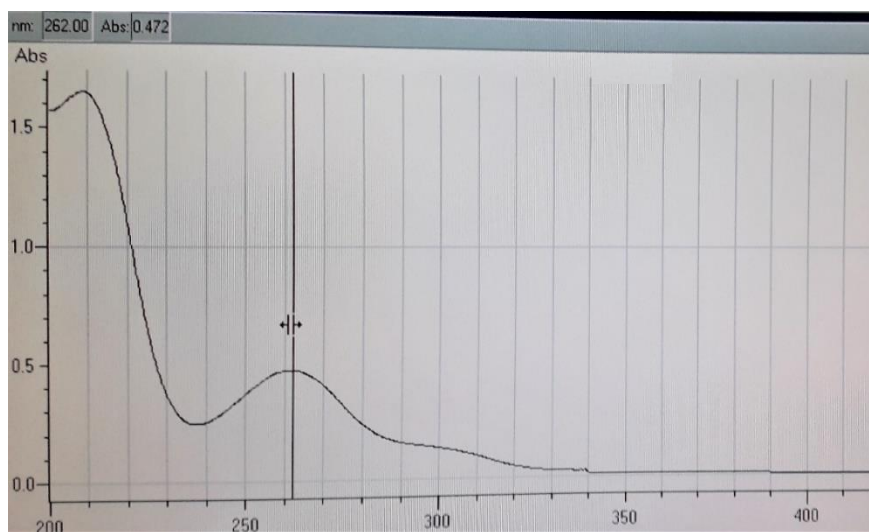
Methyl 3,4,5-triacetoxybenzoate (36)



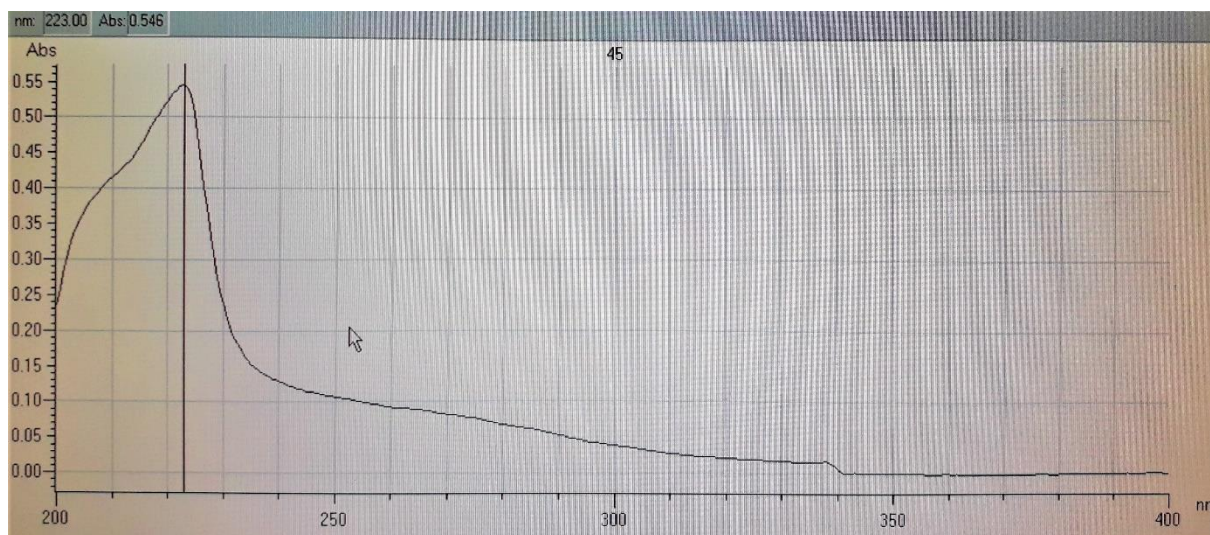
Methyl 4-benzyloxy-3,5-diacetoxybenzoate (37a)



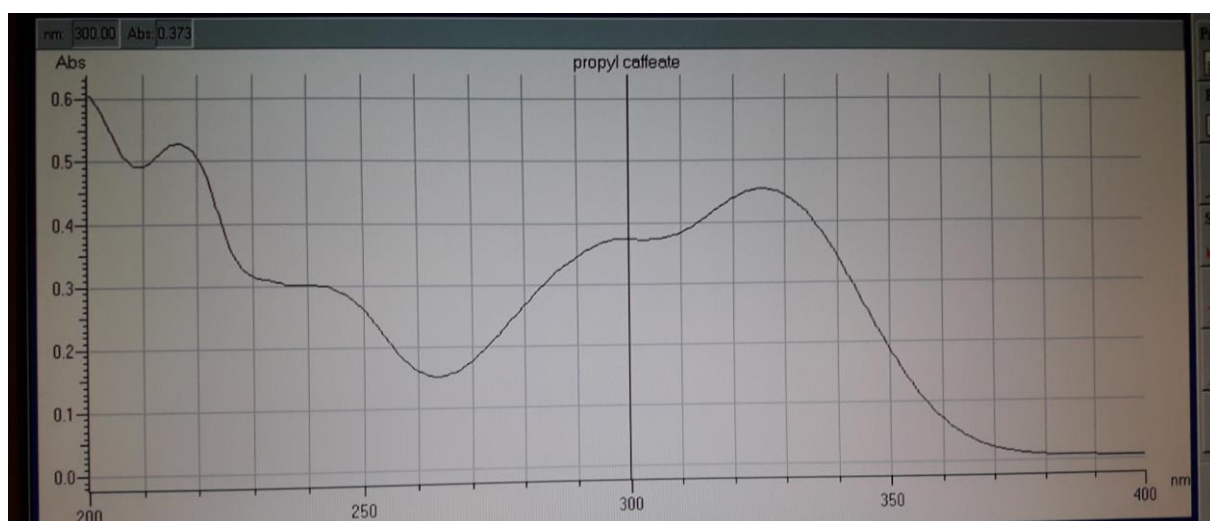
Methyl 4-benzoxy-3,5-dihydroxybenzoate (**38a**)



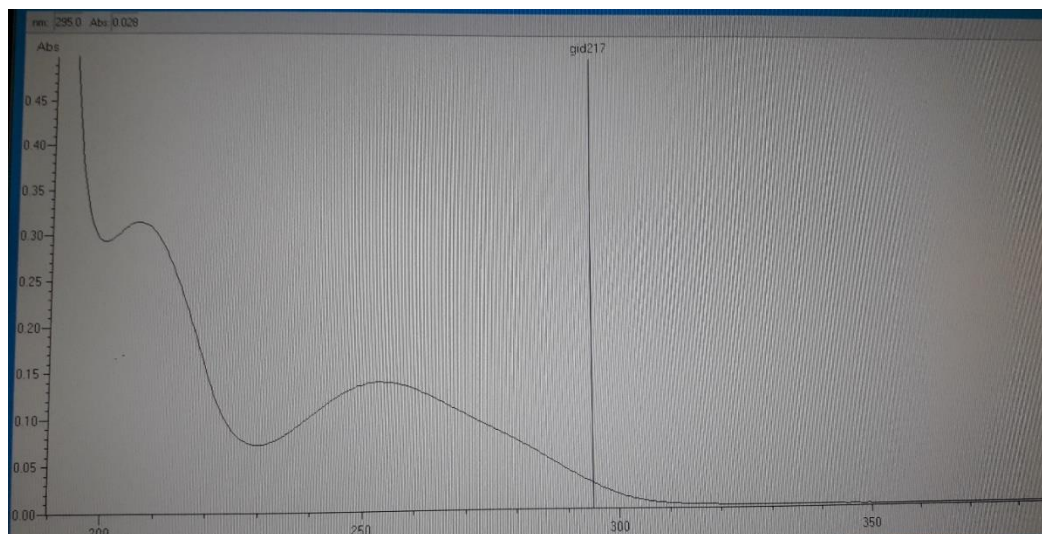
Methyl 4-naphthyl-3,5-dihydroxybenzoate (**38c**)



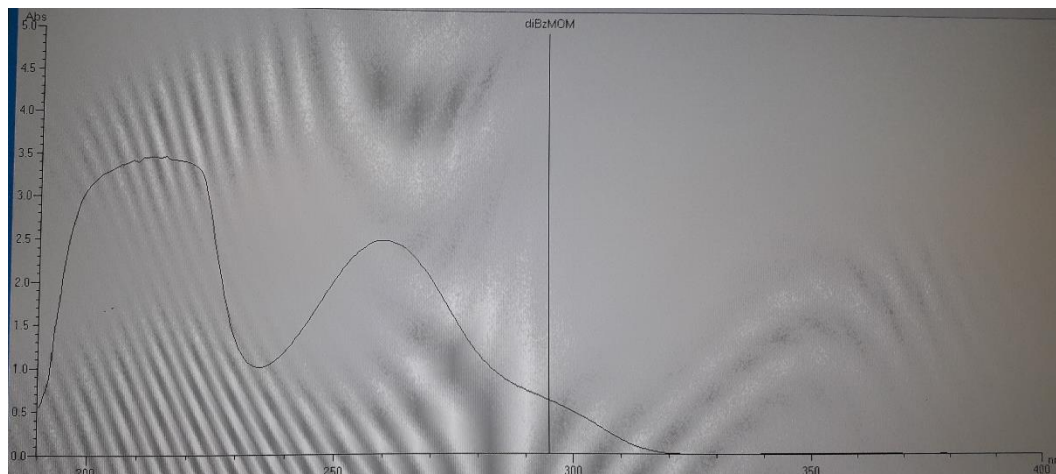
Propyl caffeate



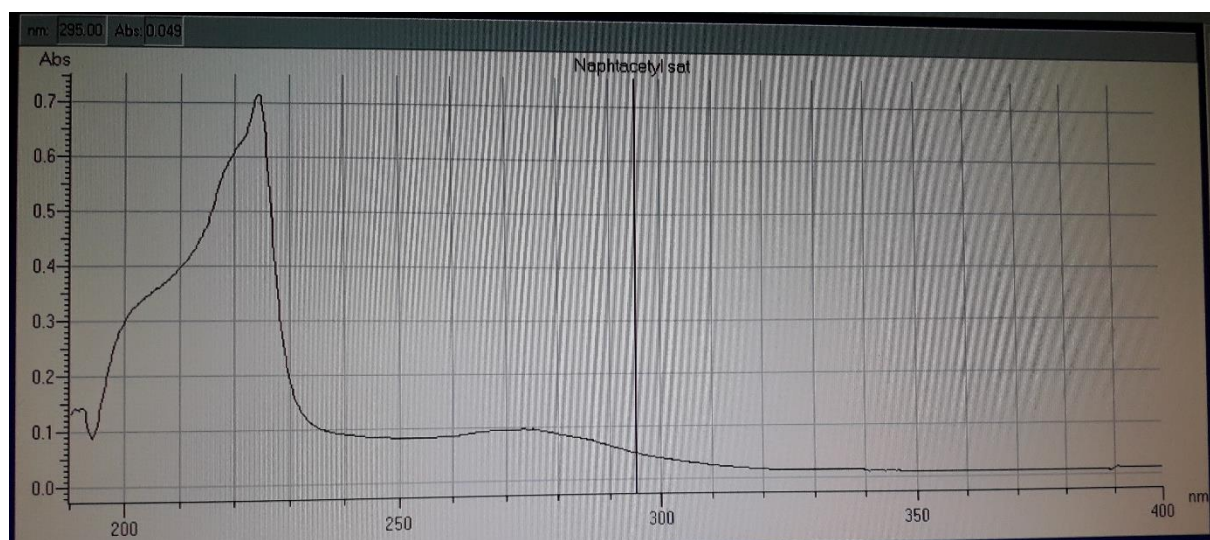
4-(benzyloxy)-3,5-bis(methoxymethoxy)benzoic acid (**40a**)



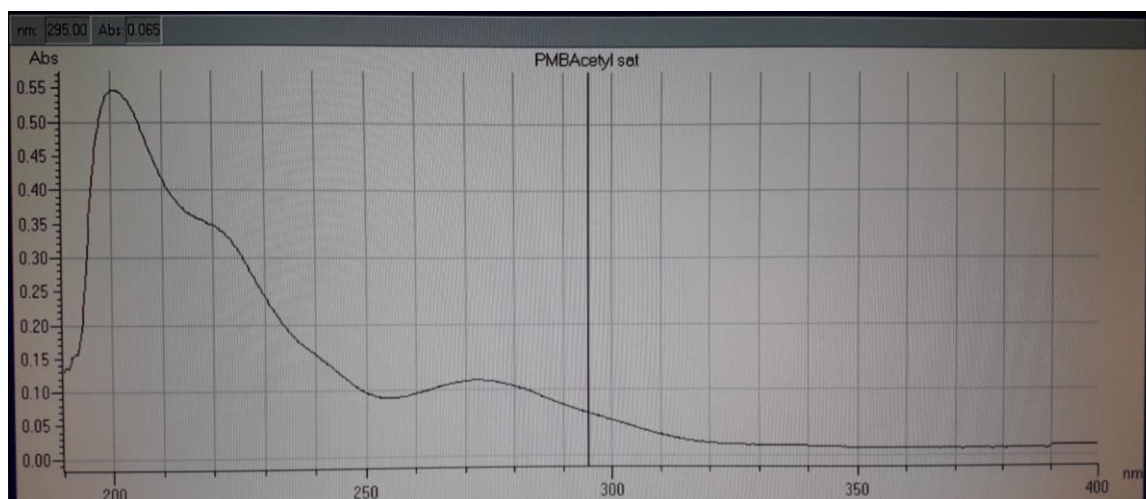
Propane-1,3-diyl bis(4-(benzyloxy)-3,5-bis(methoxymethoxy)benzoate) (**11**)



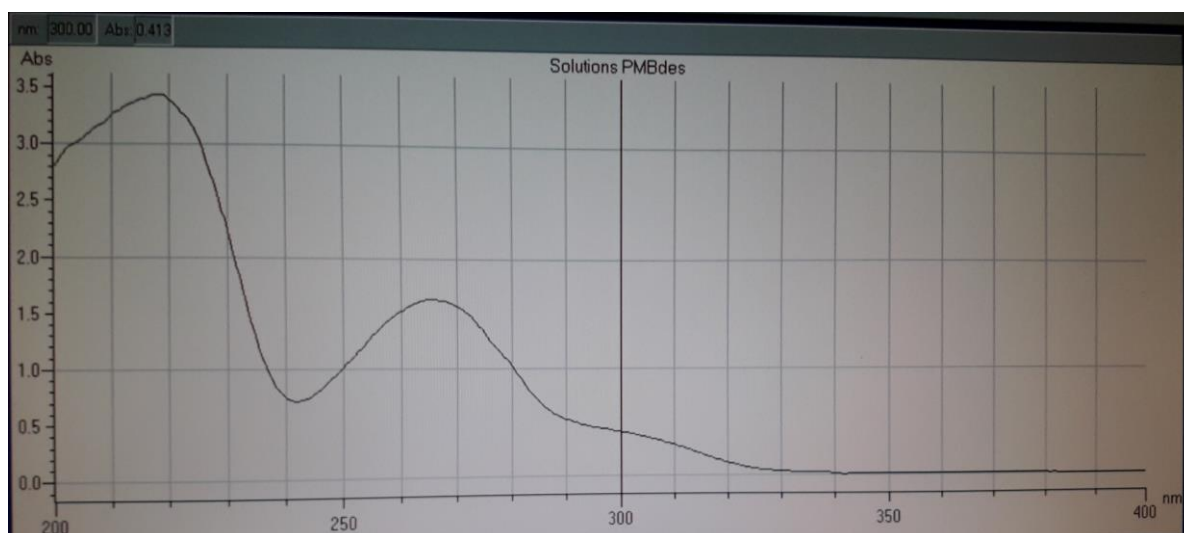
Methyl 4-naphth-2-ylmethoxy-3,5-diacetoxybenzoate (**37c**)



Methyl 4-(4-methoxybenzoxy)-3,5-diacetoxybenzoate (**37b**)

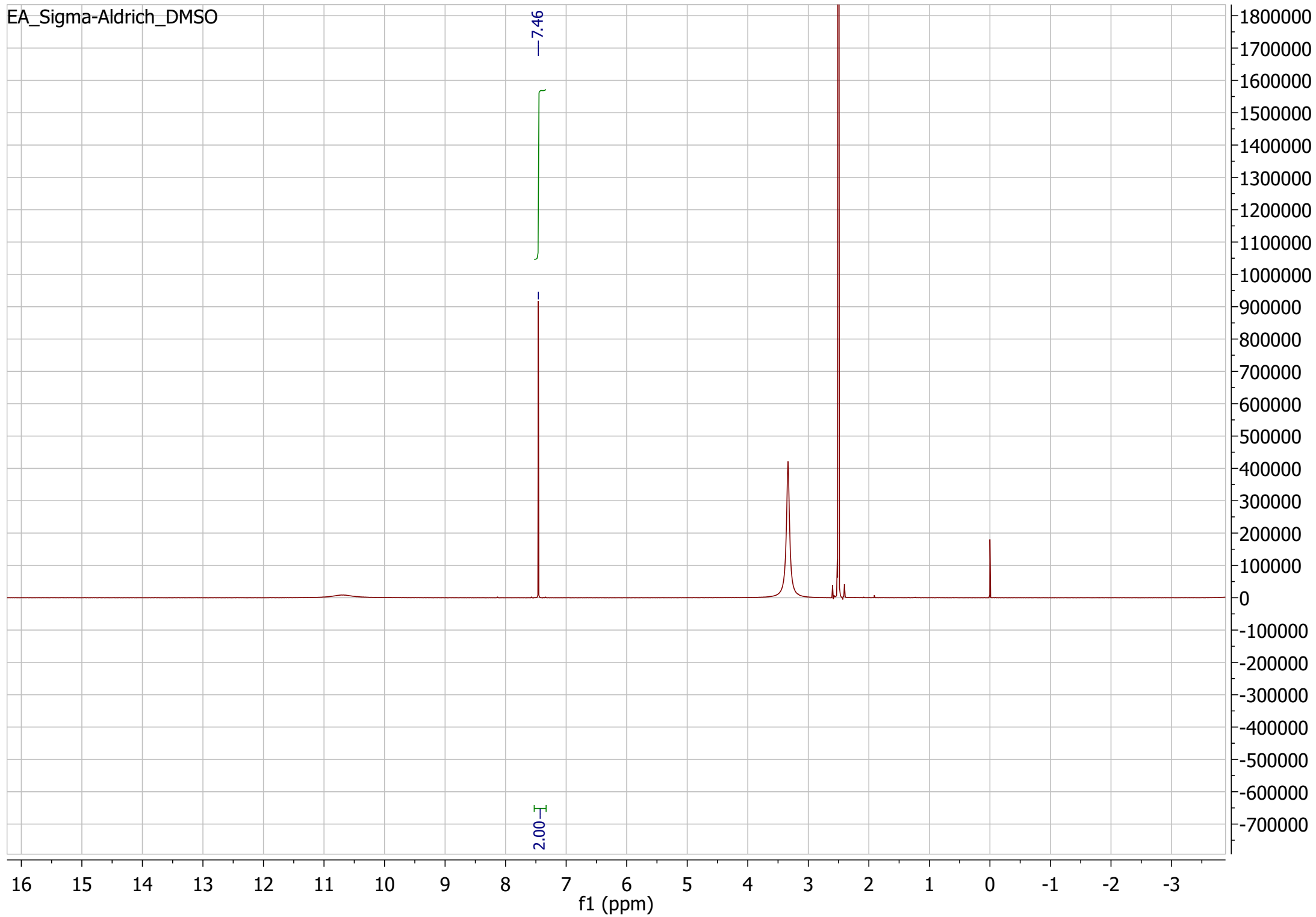


Methyl 4-(4-methoxybenzoxy)-3,5-dihydroxybenzoate (**38b**)

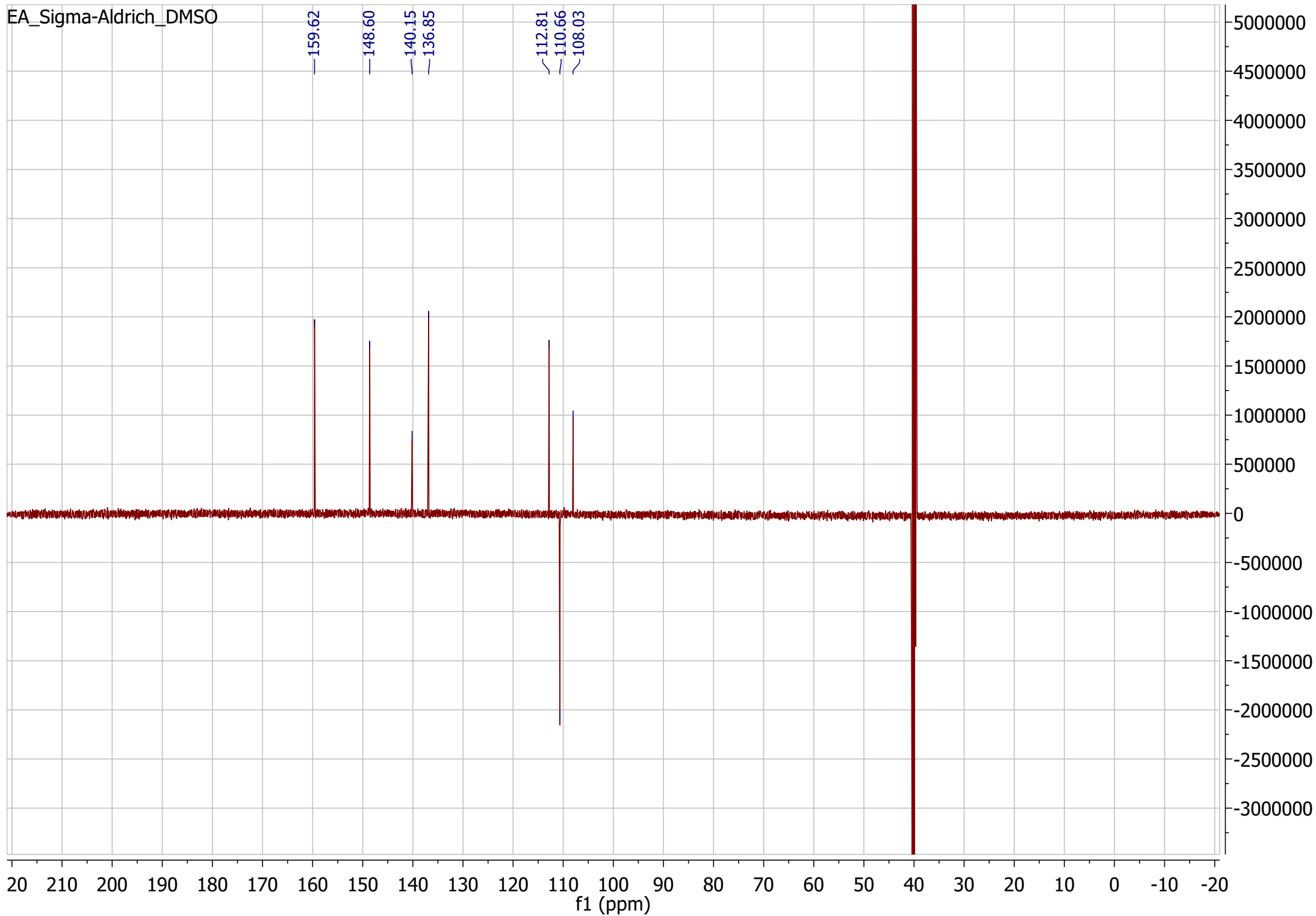


NMR Spectra

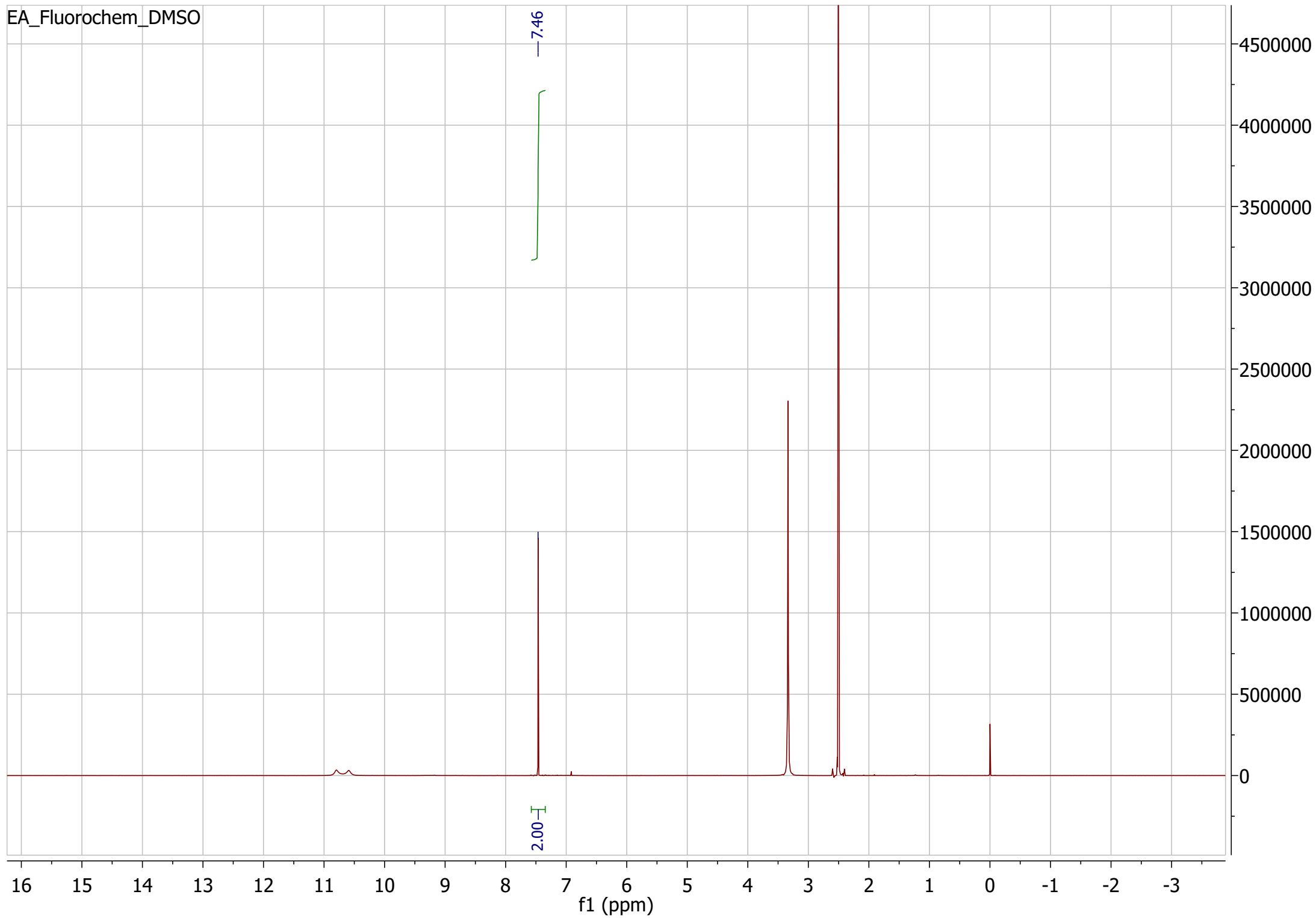
EA_Sigma-Aldrich_DMSO



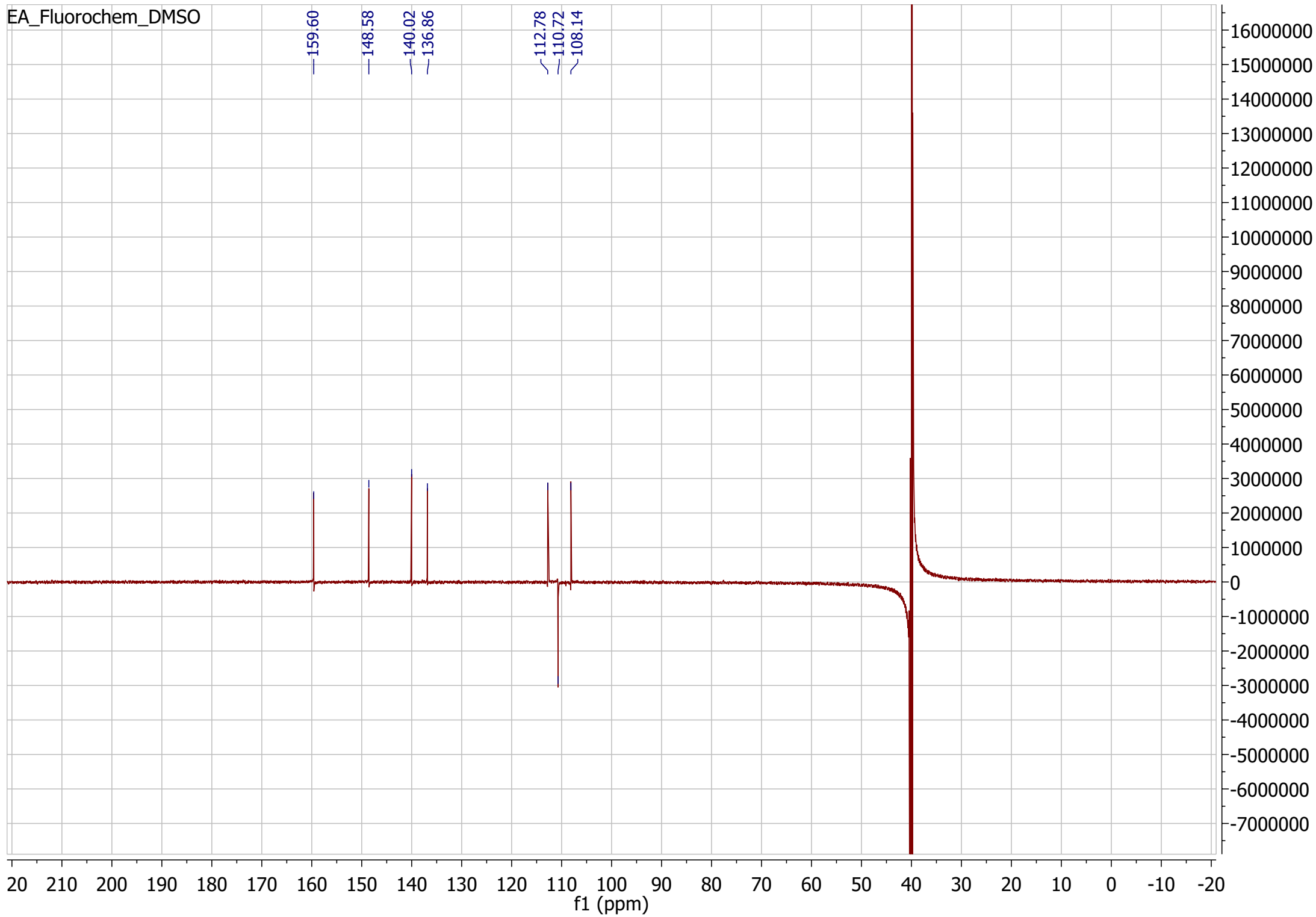
EA_Sigma-Aldrich_DMSO



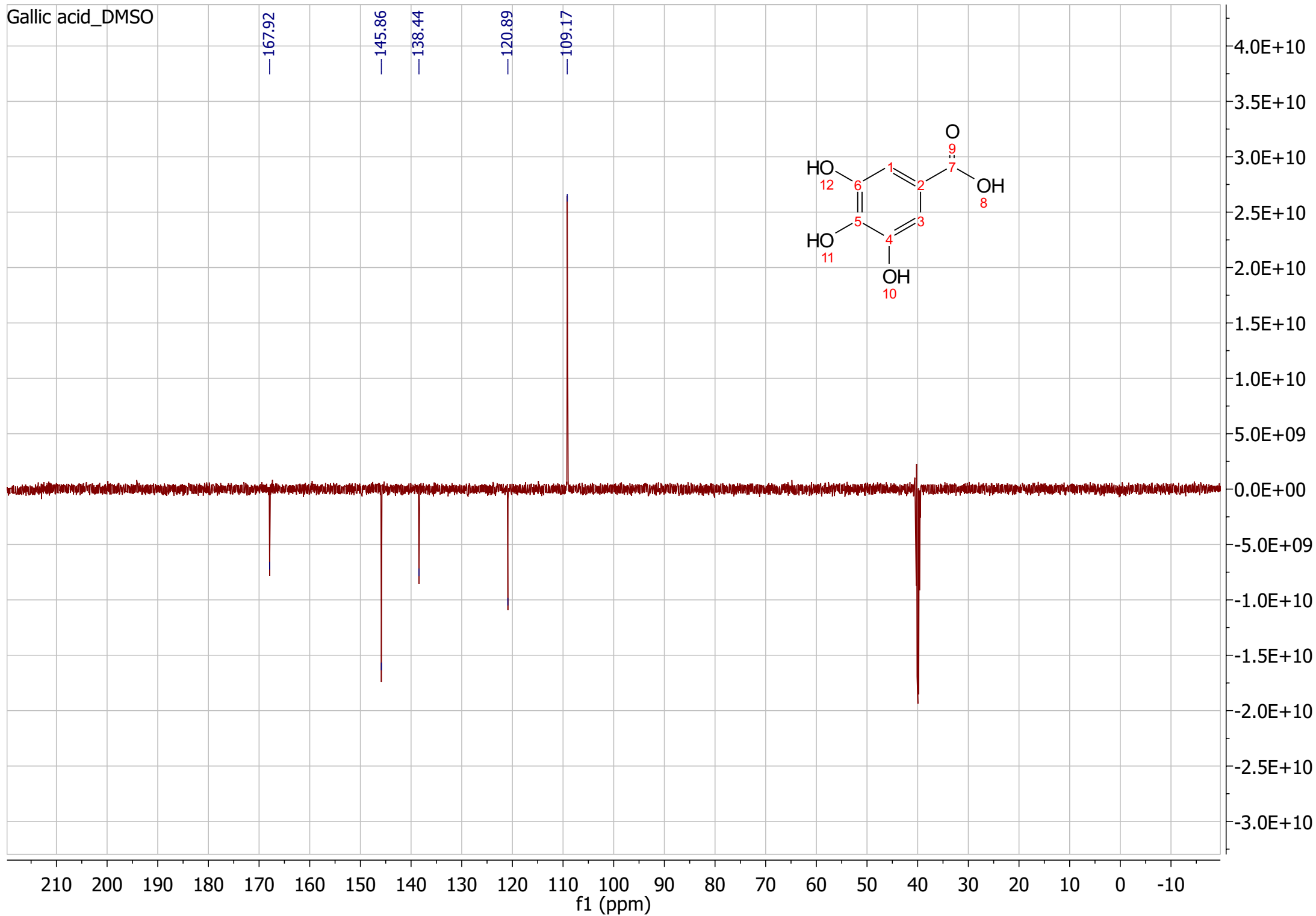
EA_Fluorochem_DMSO



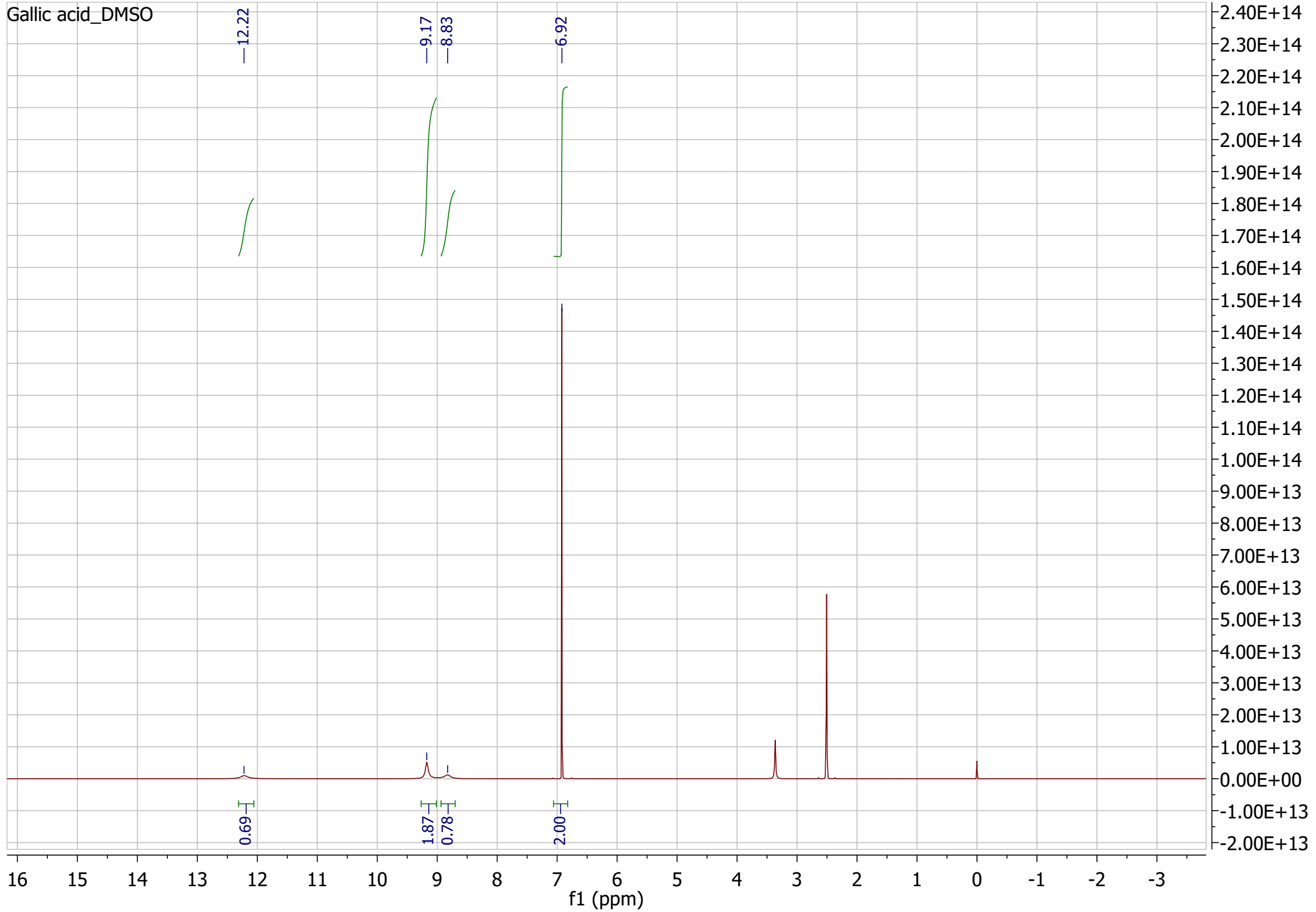
EA_Fluorochem_DMSO



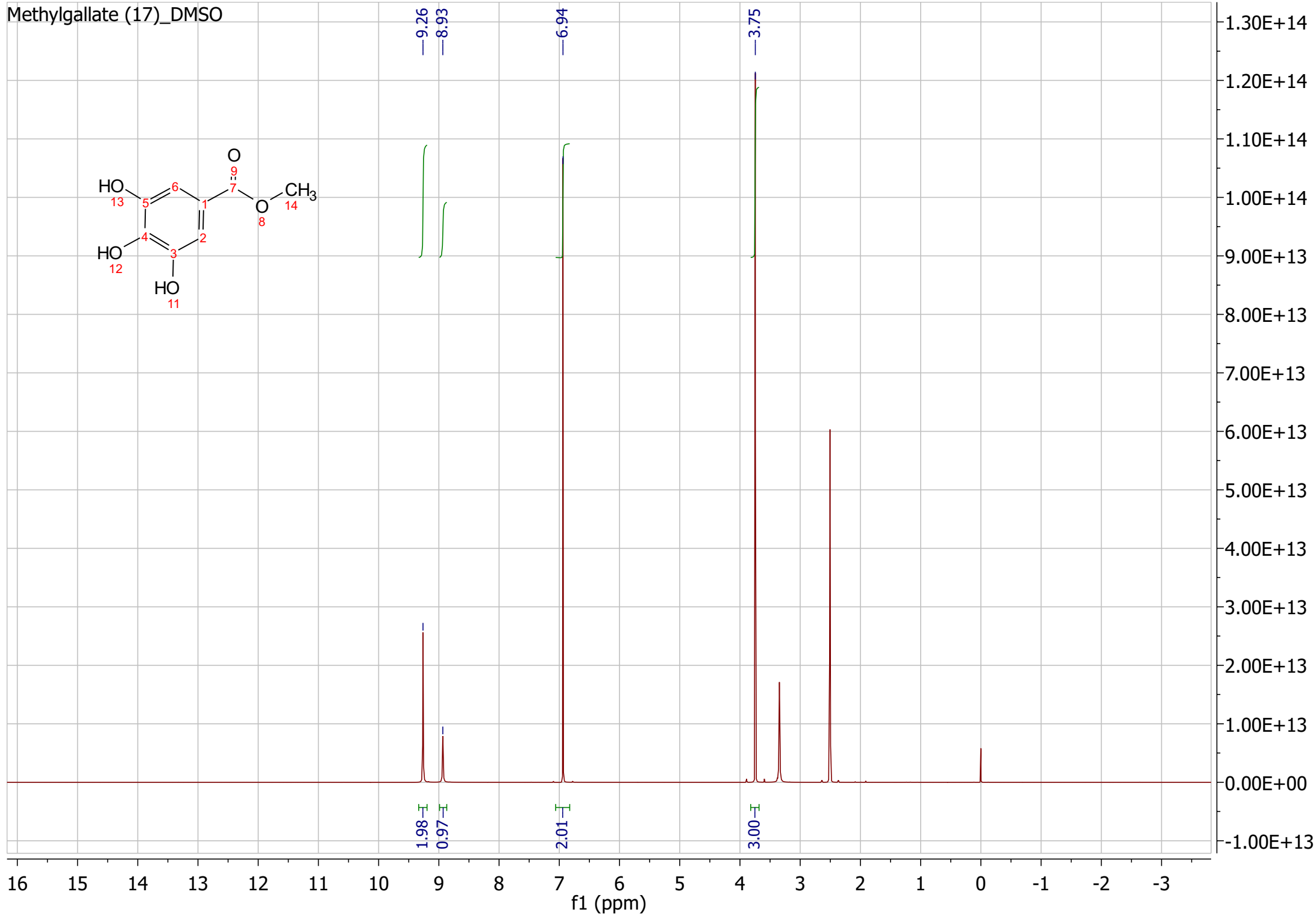
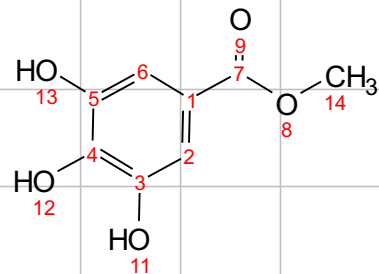
Gallic acid_DMSO



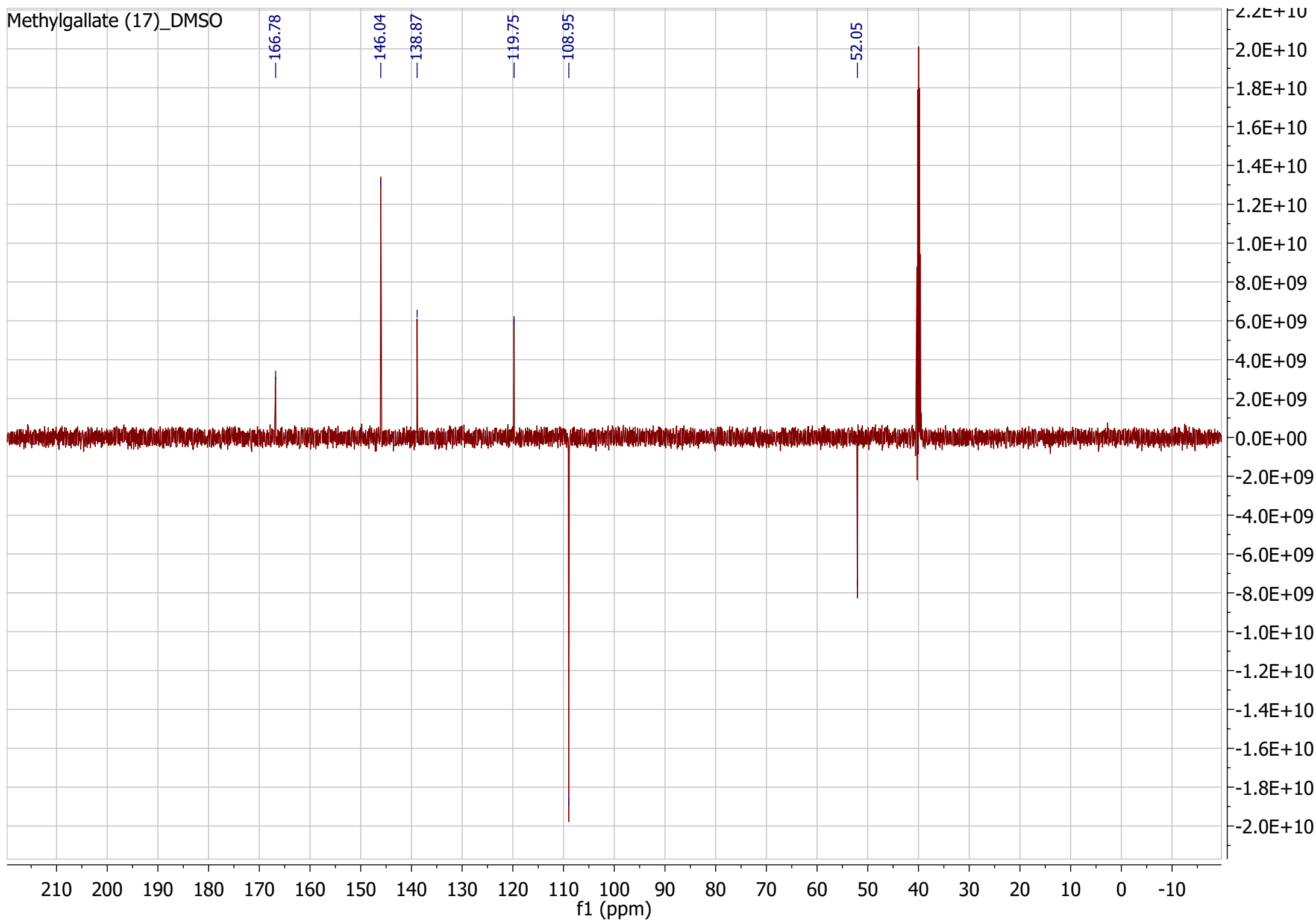
Gallic acid_DMSO



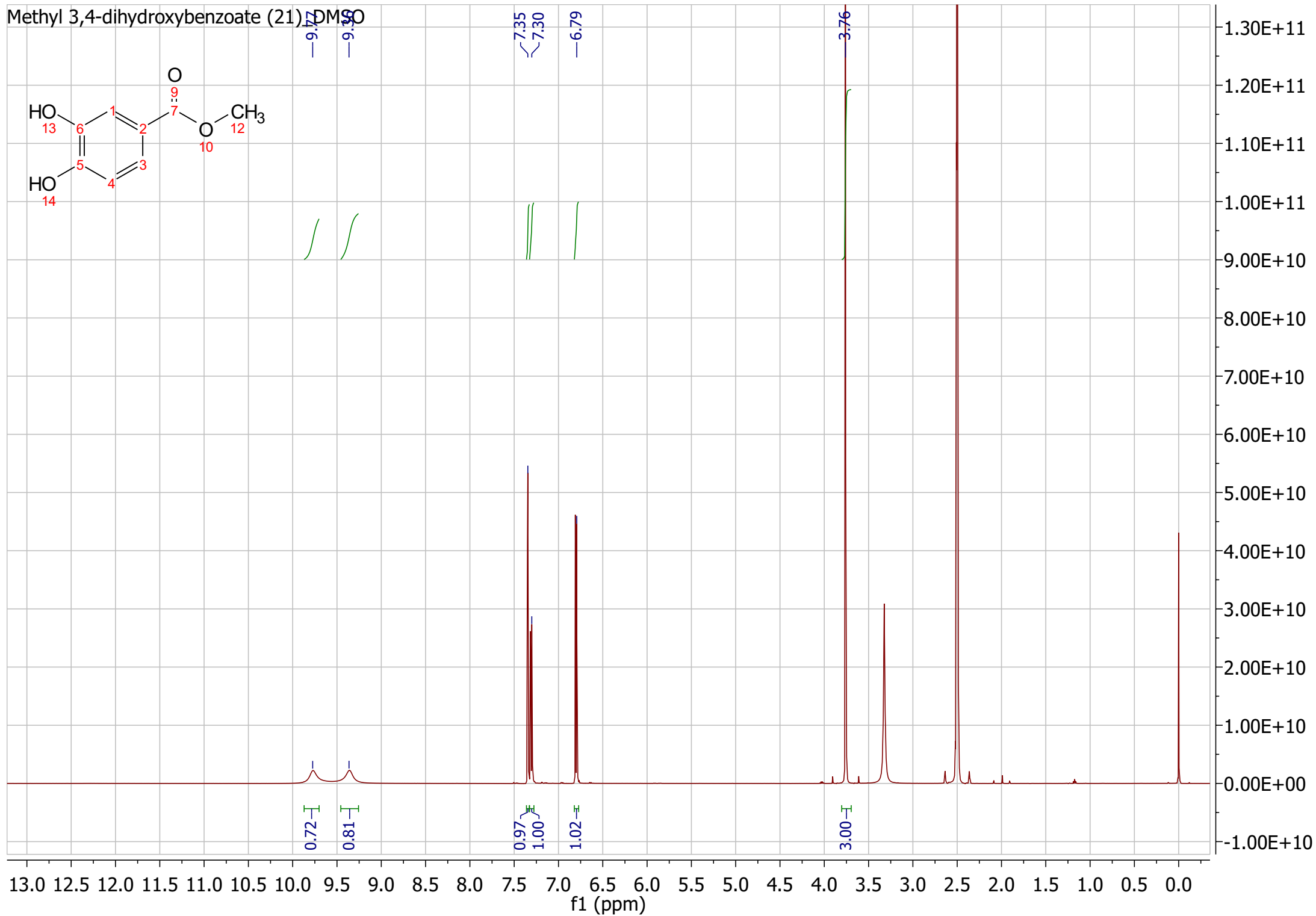
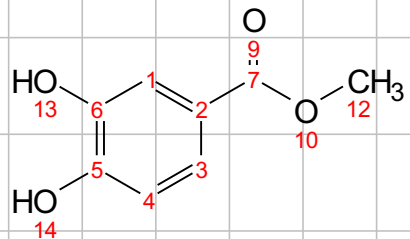
Methylgallate (17)_DMSO



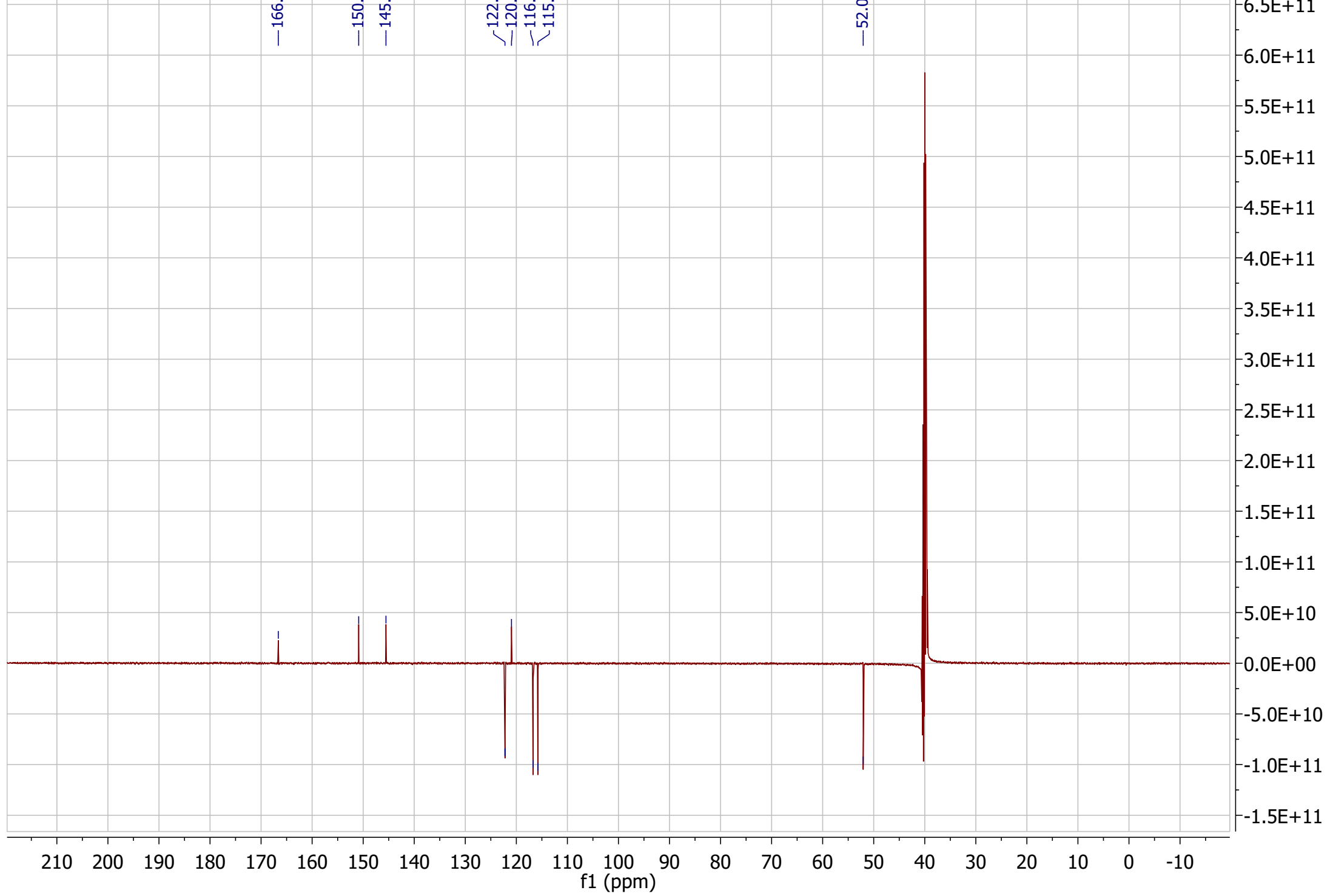
Methylgallate (17)_DMSO



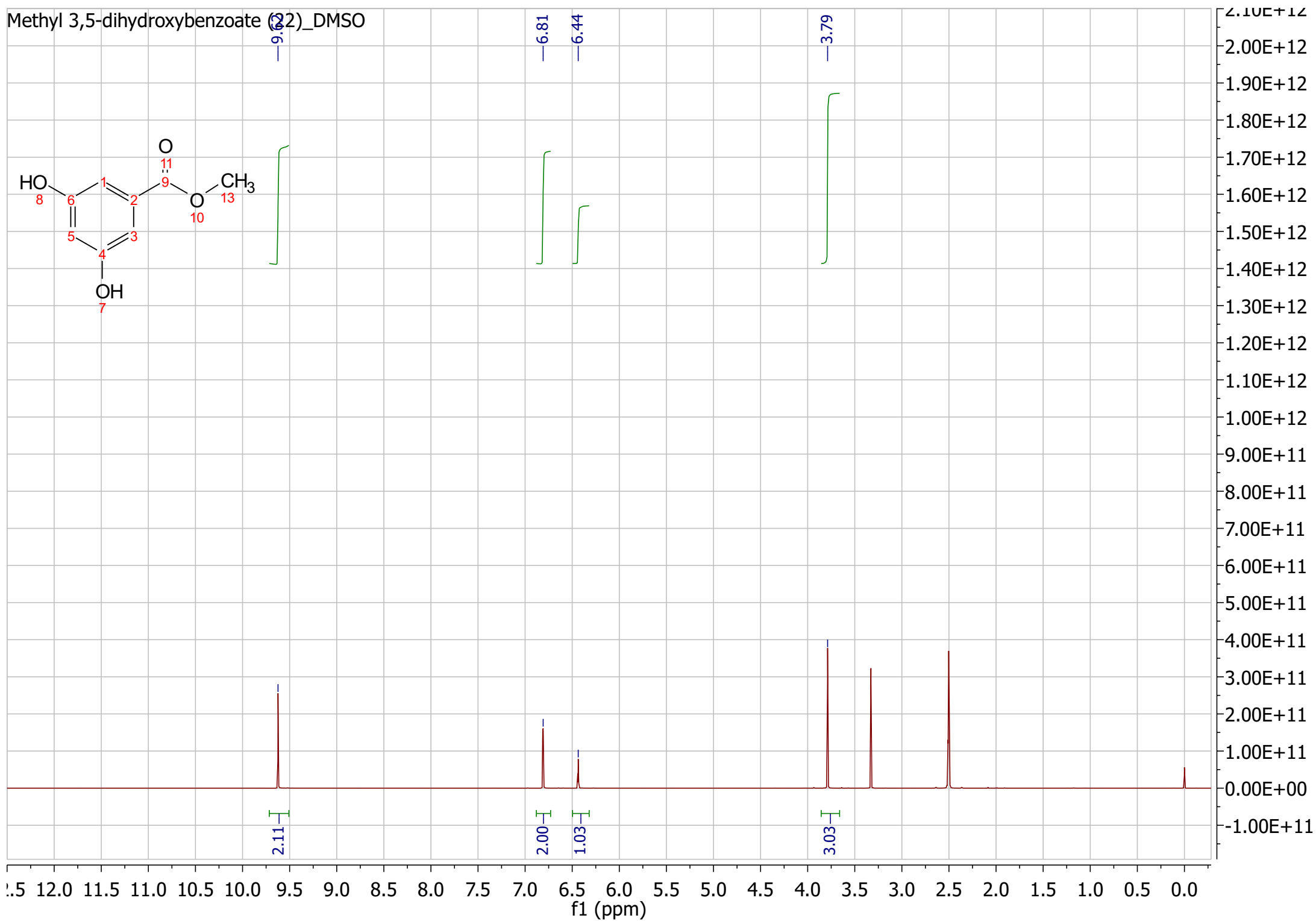
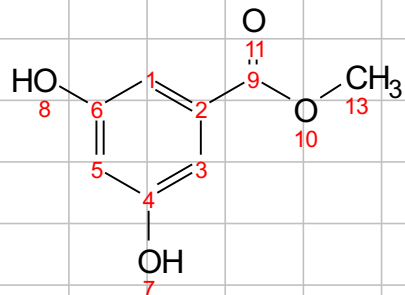
Methyl 3,4-dihydroxybenzoate (21) DMSO



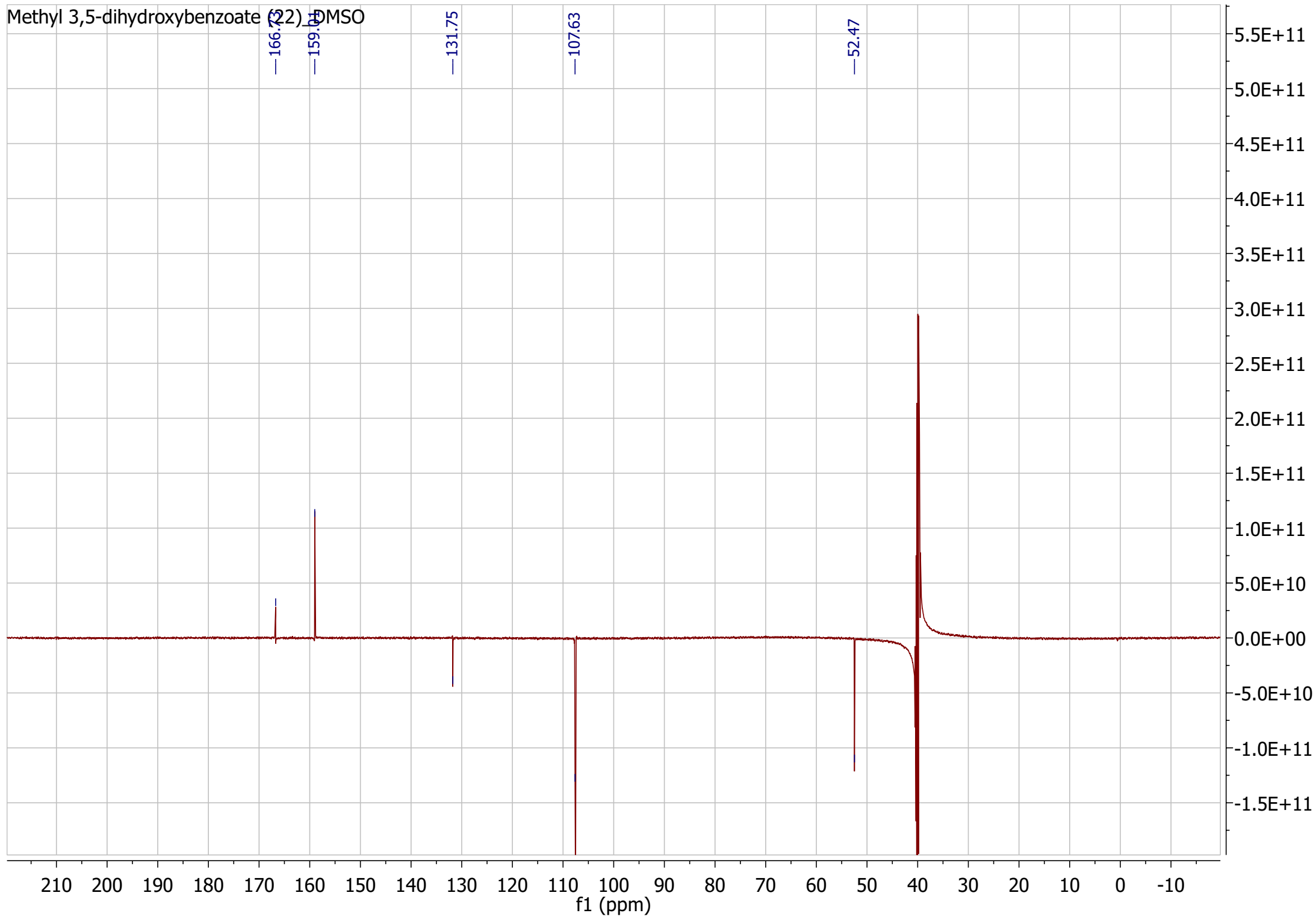
Methyl 3,4-dihydroxybenzoate (21)_DMSO



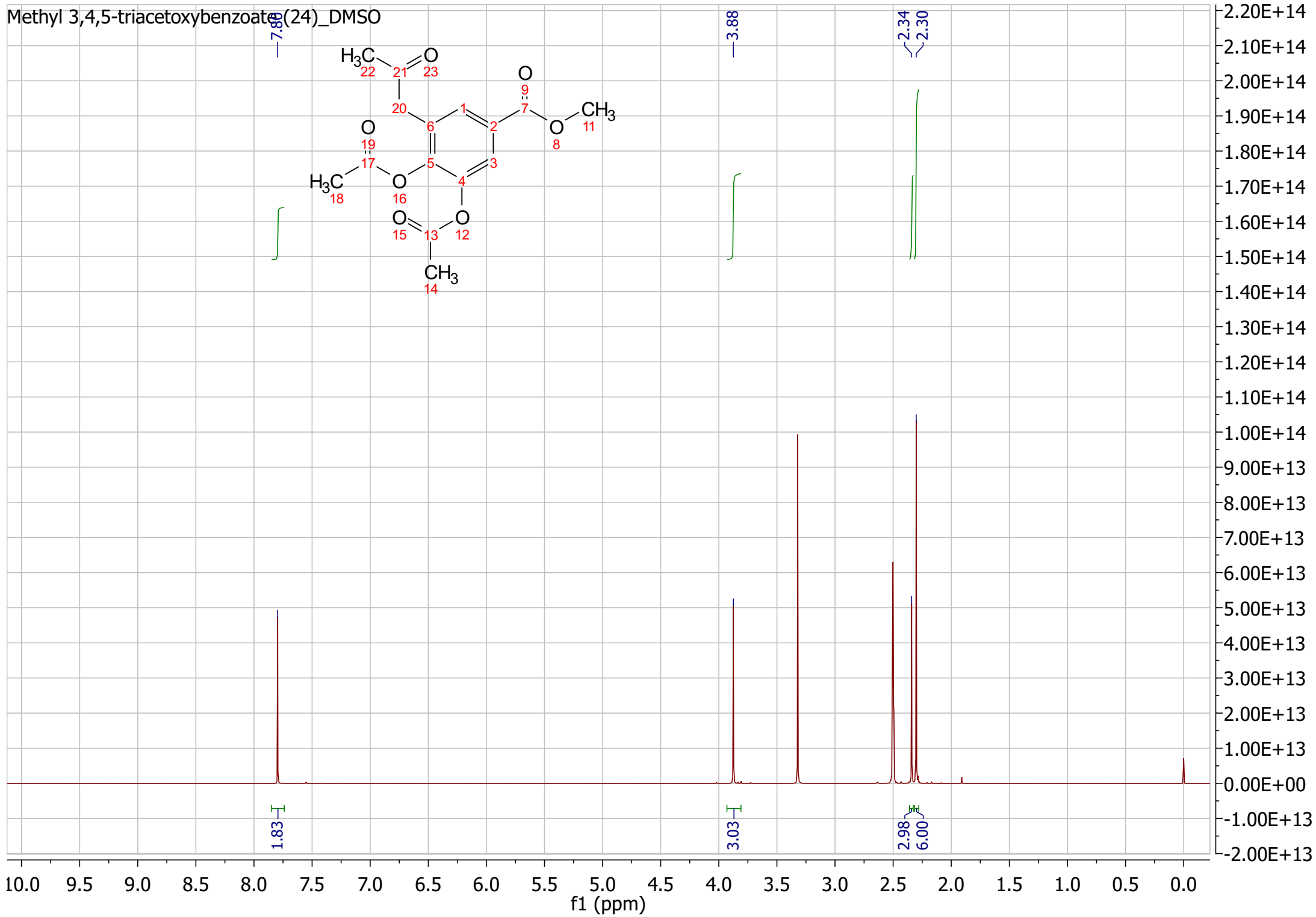
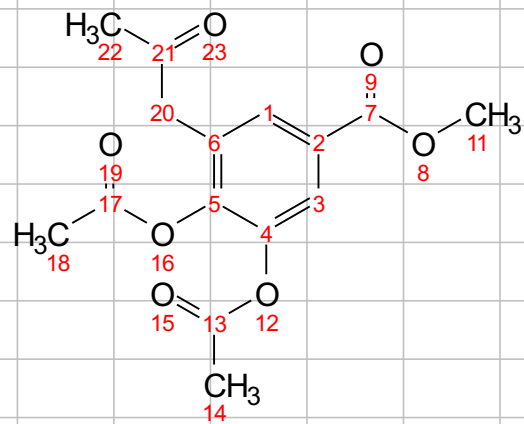
Methyl 3,5-dihydroxybenzoate (22)_DMSO



Methyl 3,5-dihydroxybenzoate (22) DMSO



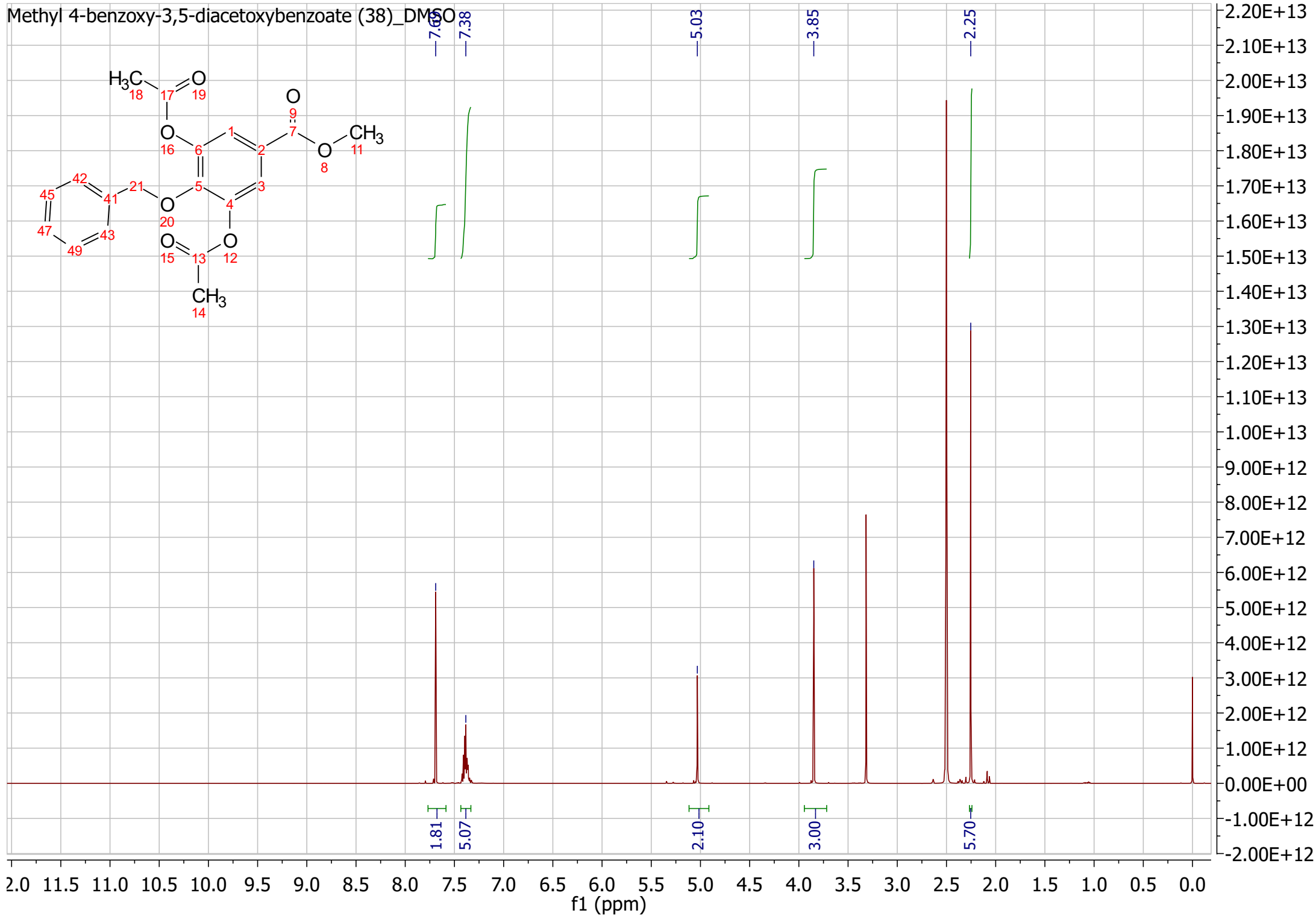
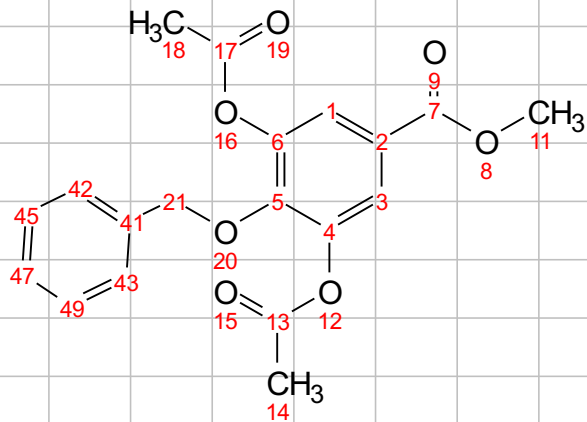
Methyl 3,4,5-triacetoxybenzoate(24)_DMSO



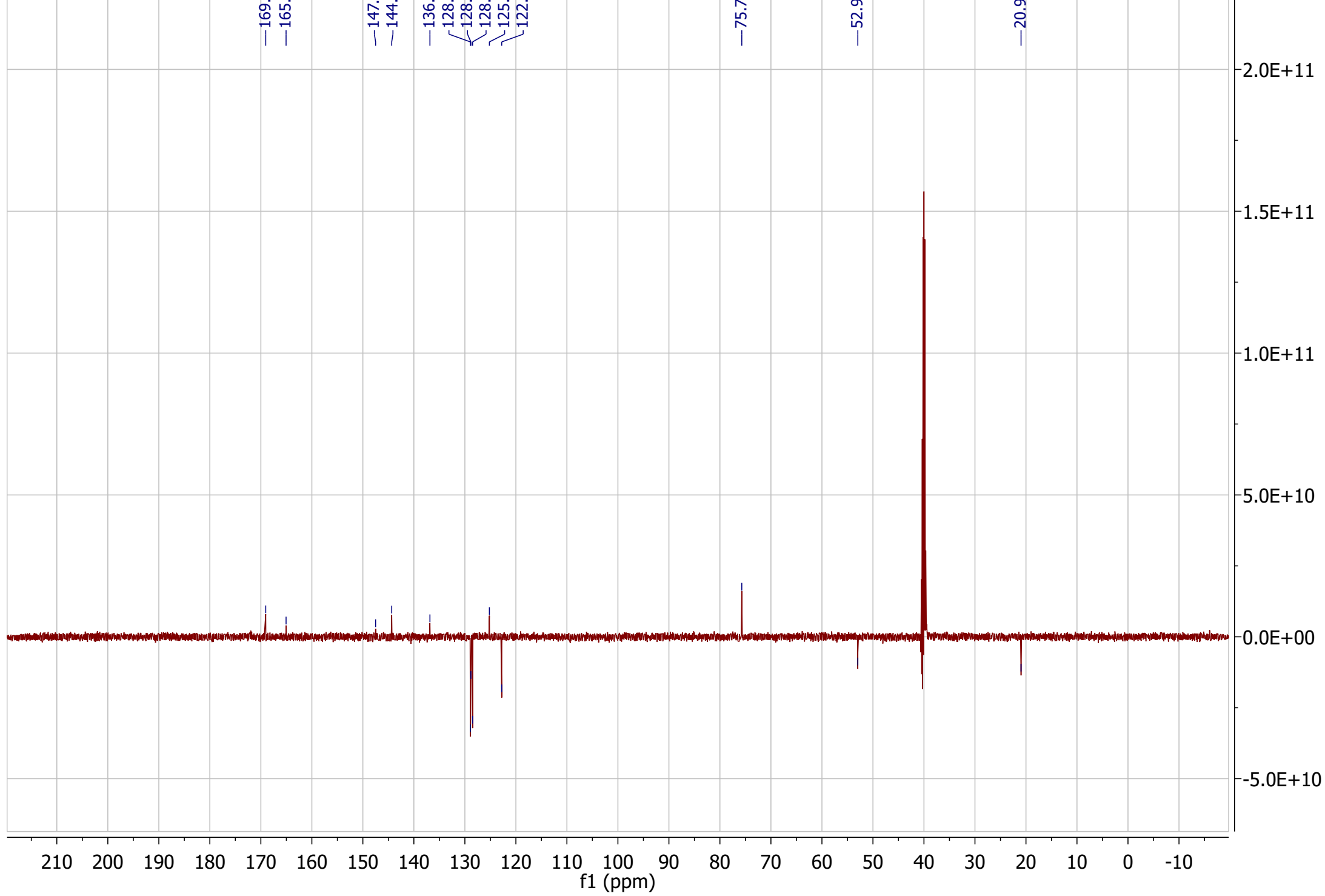
Methyl 3,4,5-triacetoxybenzoate (64)_DMSO



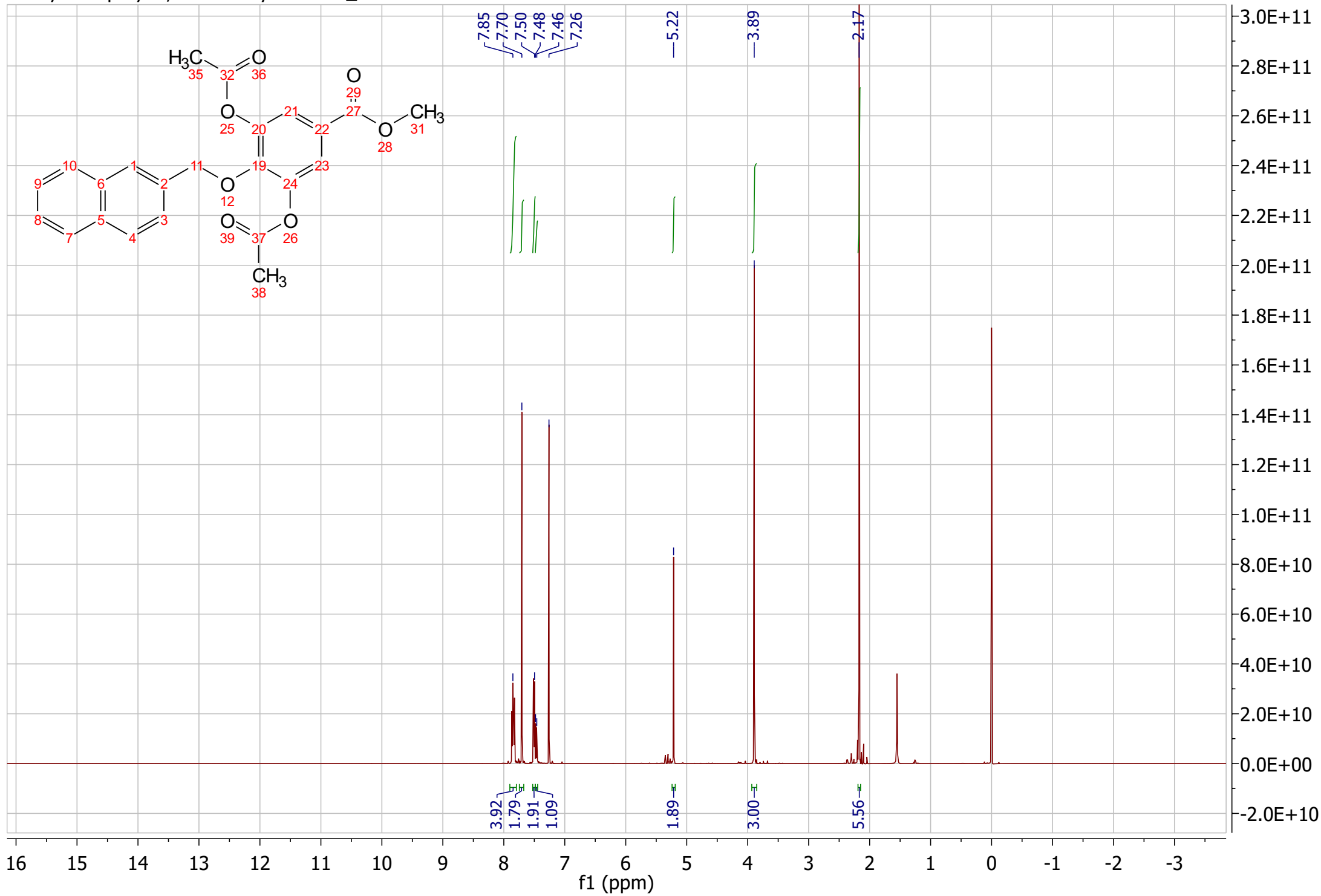
Methyl 4-benzoxy-3,5-diacetoxybenzoate (38)_DMSO



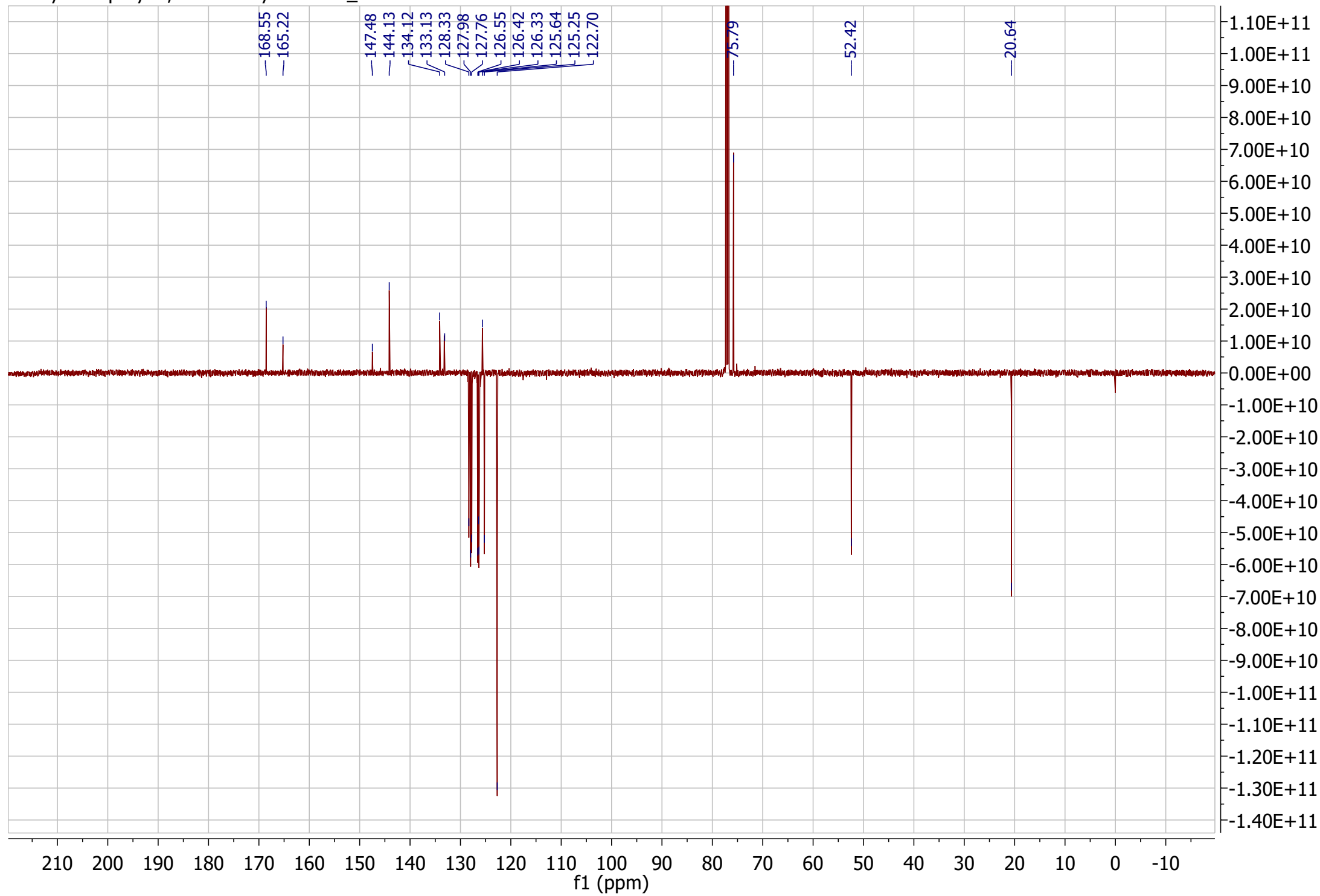
Methyl 4-benzyloxy-3,5-diacetoxybenzoate (88) DMSO



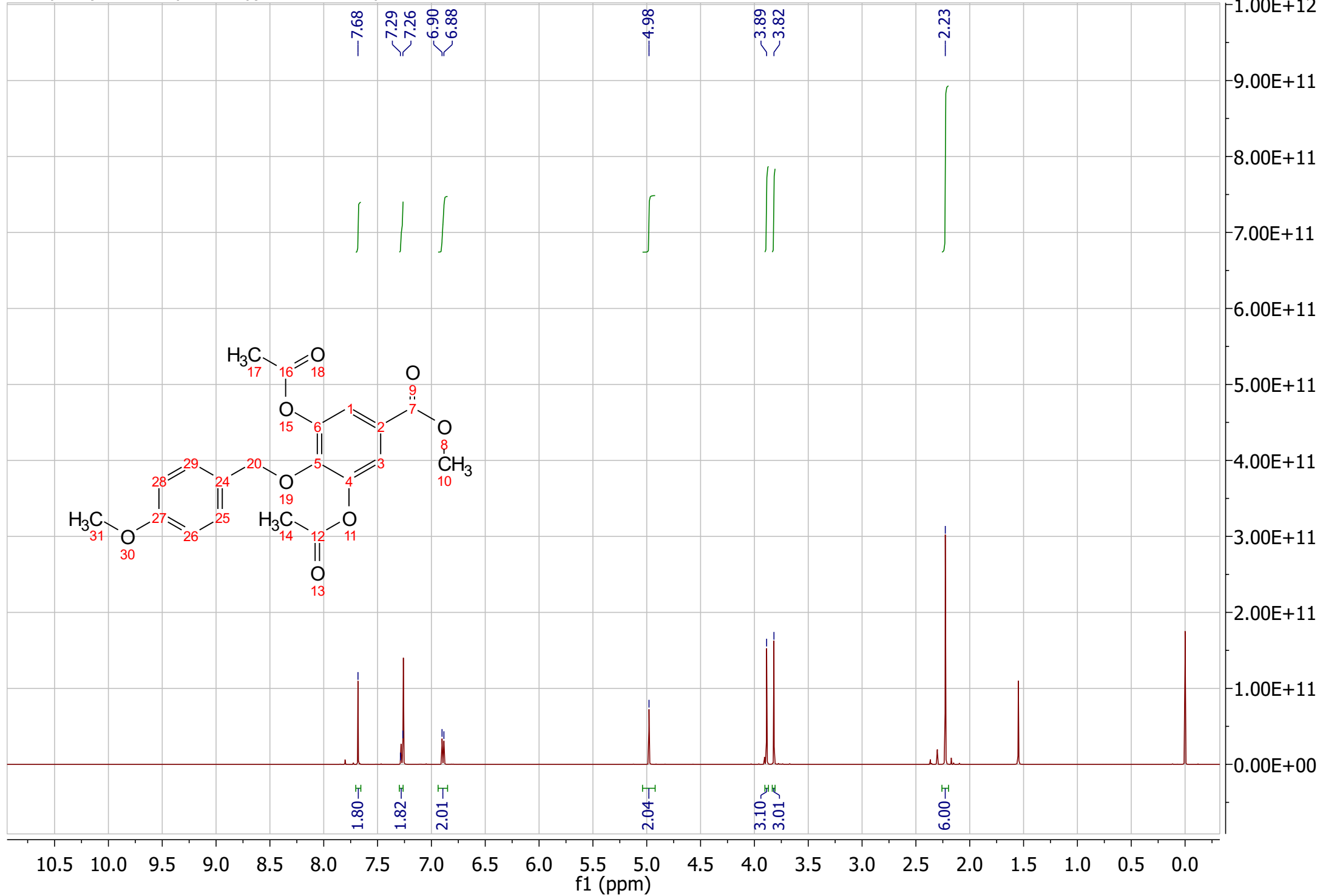
Methyl 4-naphtyl-3,5-diacetoxybenzoate_CDCI3



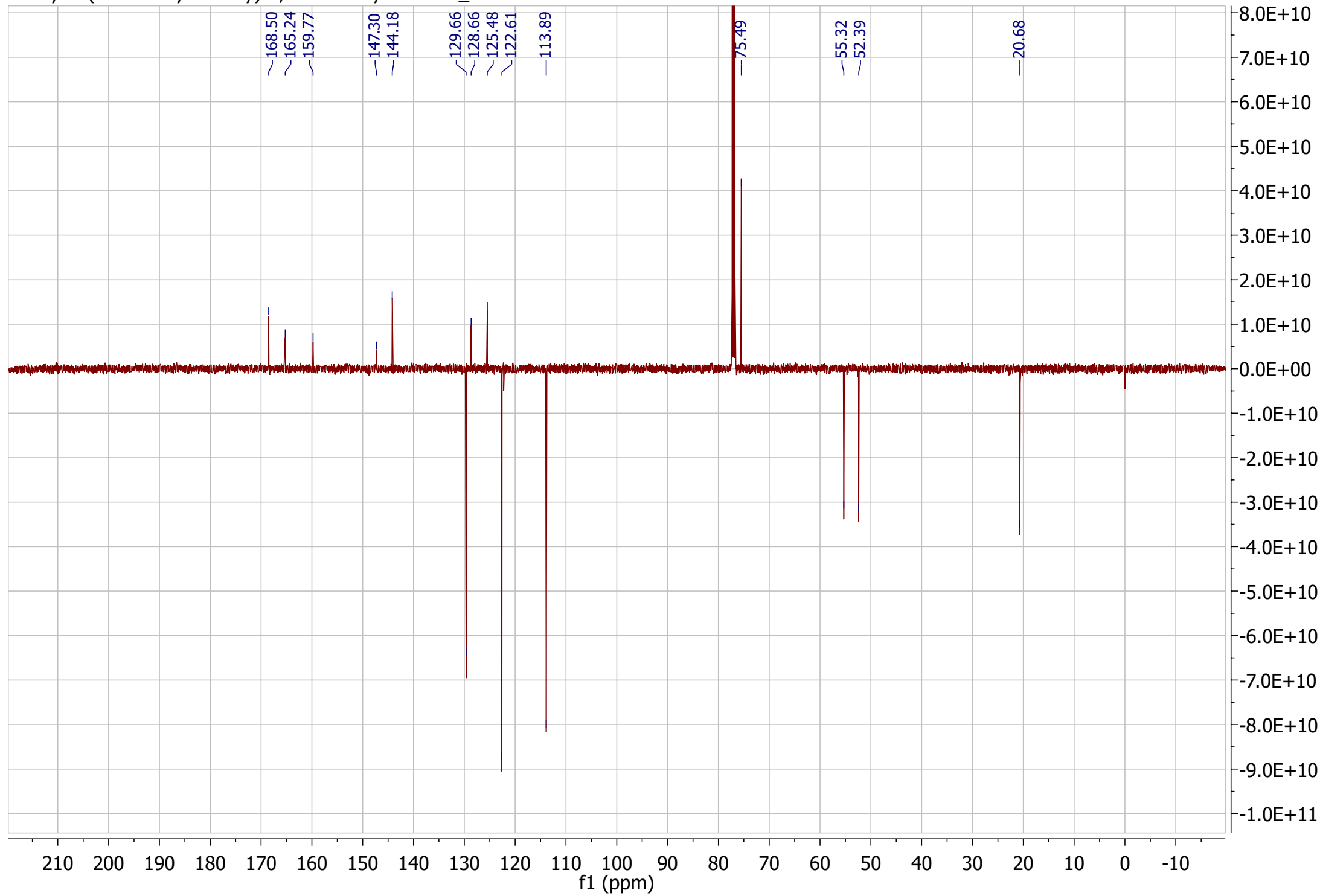
Methyl 4-naphtyl-3,5-diacetoxybenzoate_CDCl3



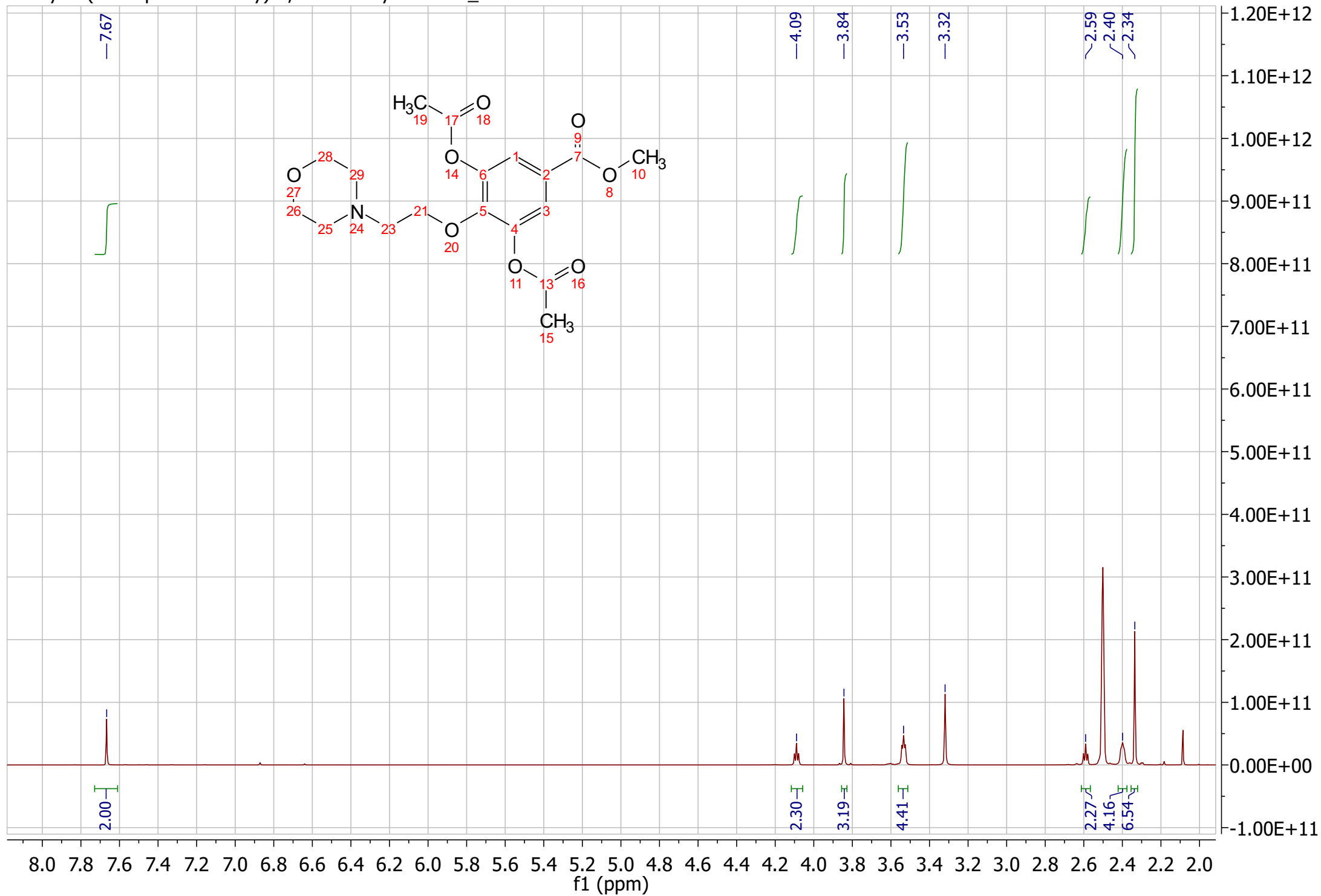
Methyl 4-(4-methoxybenzoxy)-3,5-diacetoxybenzoate_CDCl3



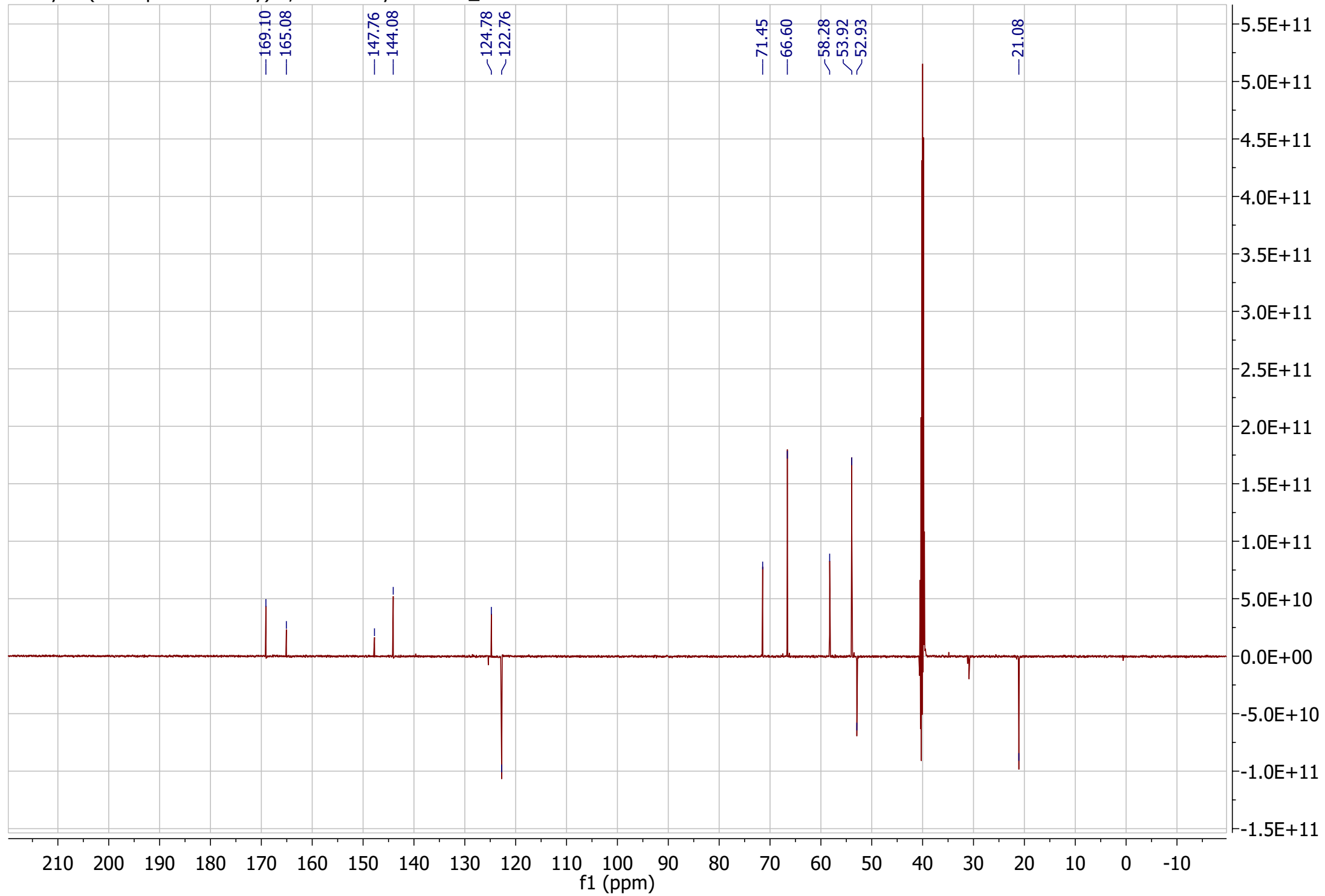
Methyl 4-(4-methoxybenzoxy)-3,5-diacetoxybenzoate_CDCl3



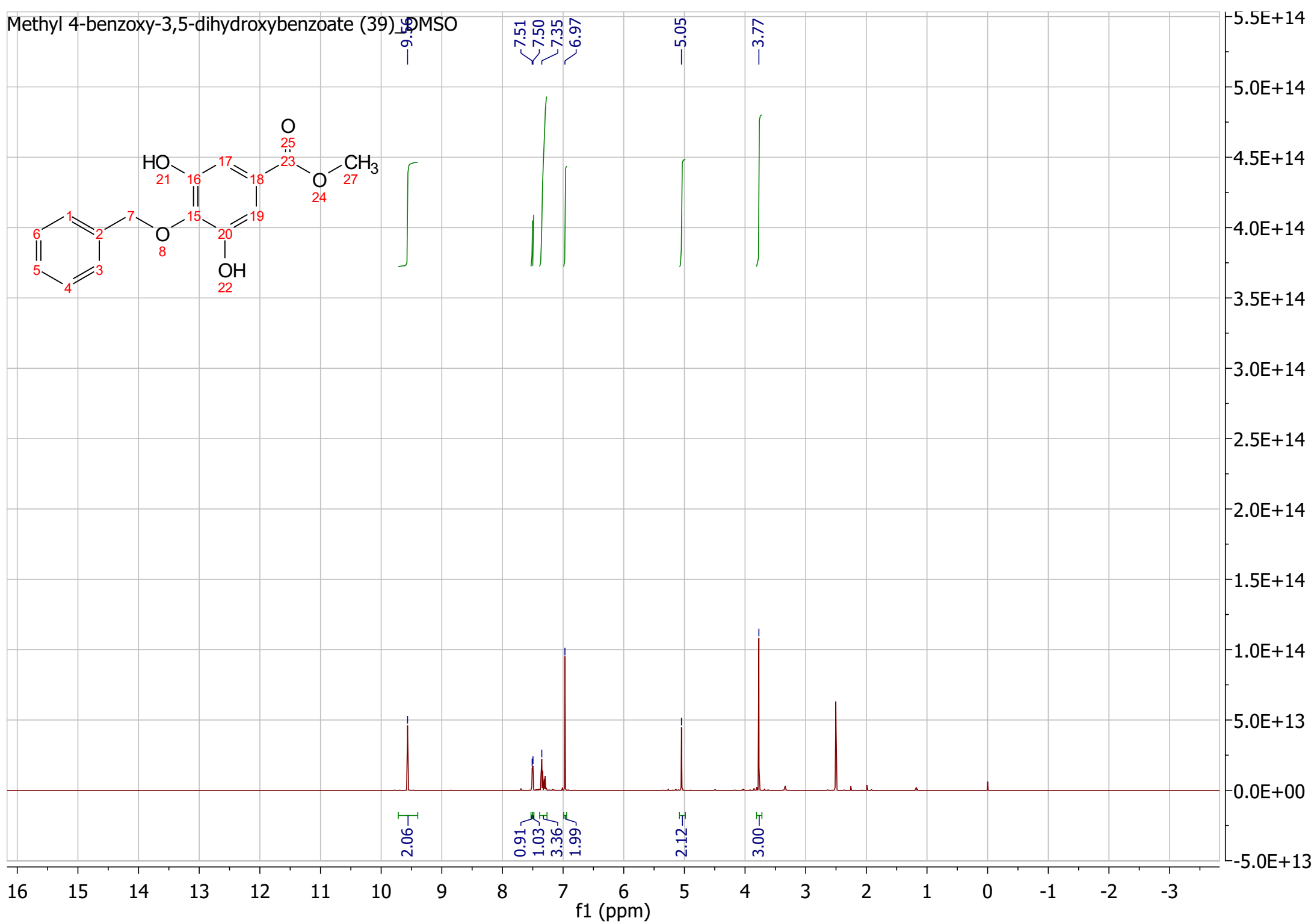
Methyl 4-(2-morpholinoethoxy)-3,5-diacetoxybenzoate_DMSO



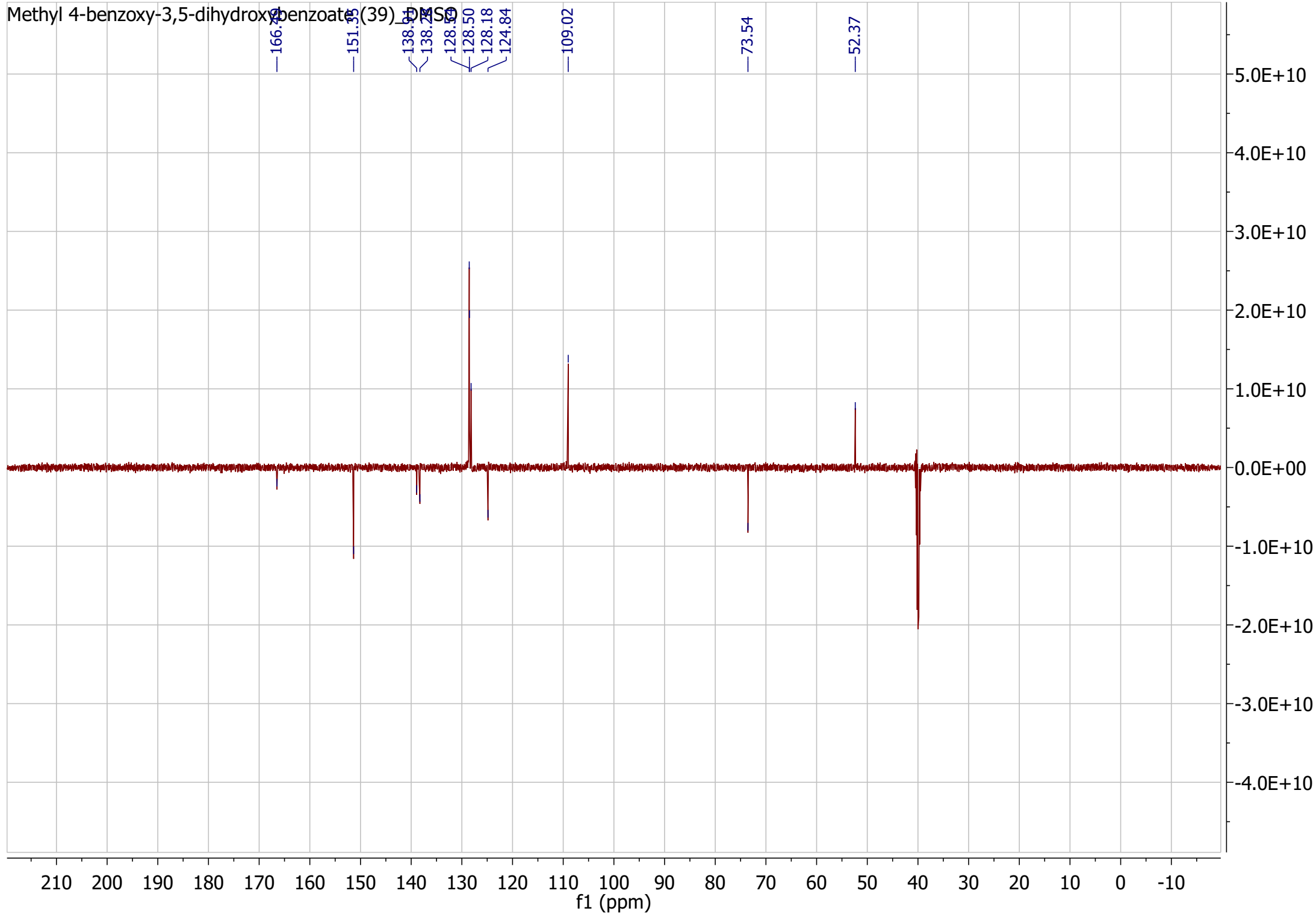
Methyl 4-(2-morpholinoethoxy)-3,5-diacetoxybenzoate_DMSO



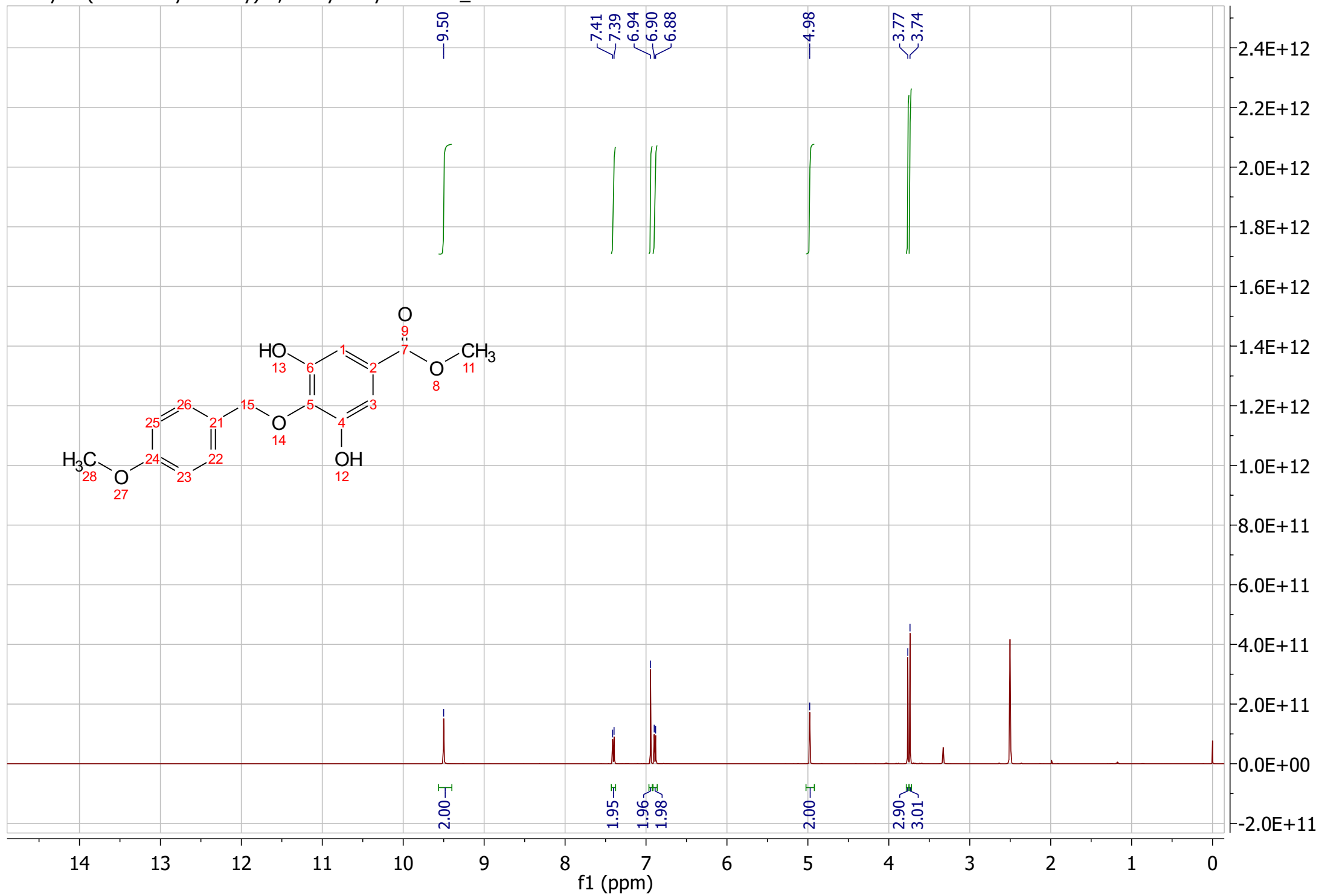
Methyl 4-benzoxy-3,5-dihydroxybenzoate (39) in DMSO



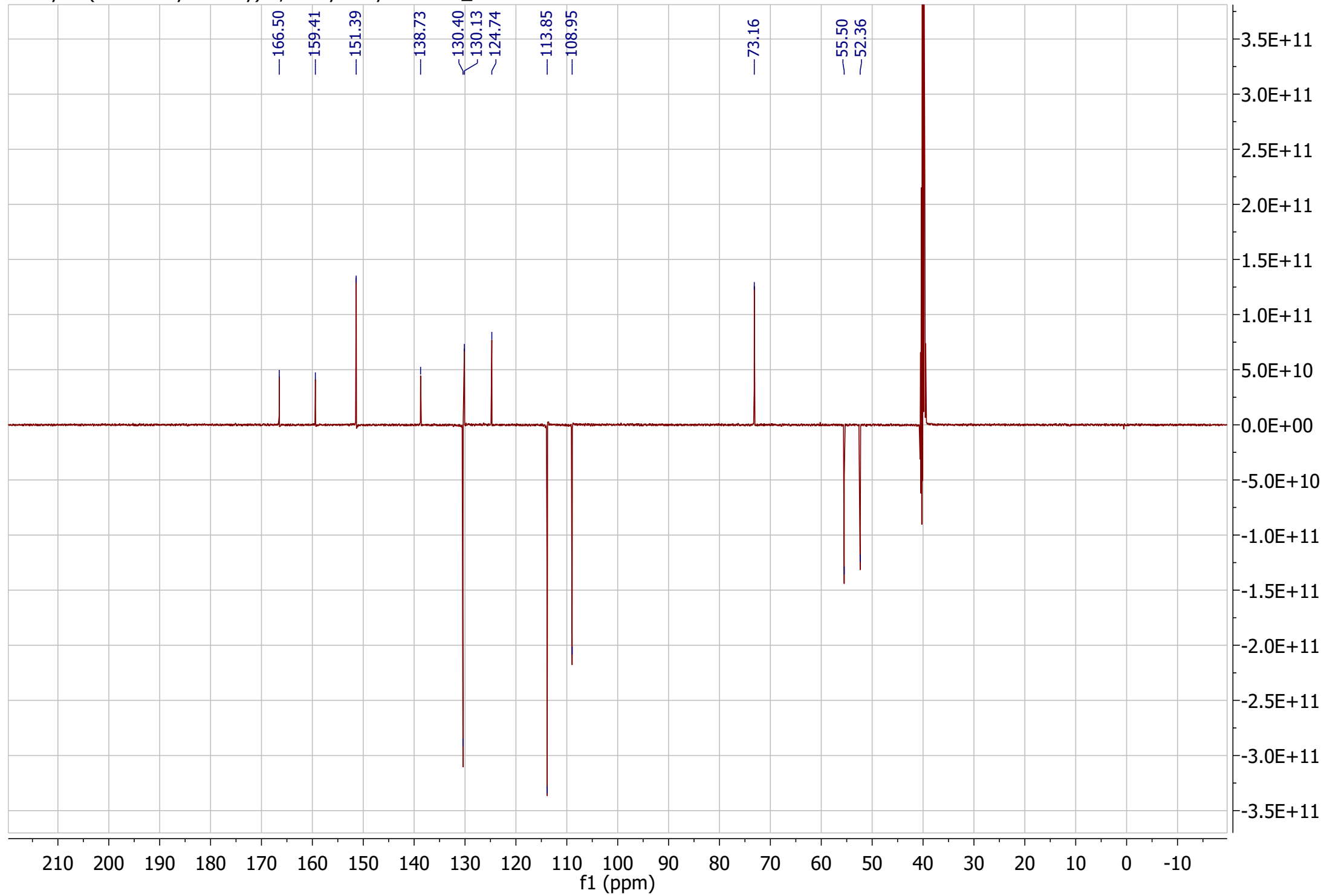
Methyl 4-benzyloxy-3,5-dihydroxybenzoate (39)



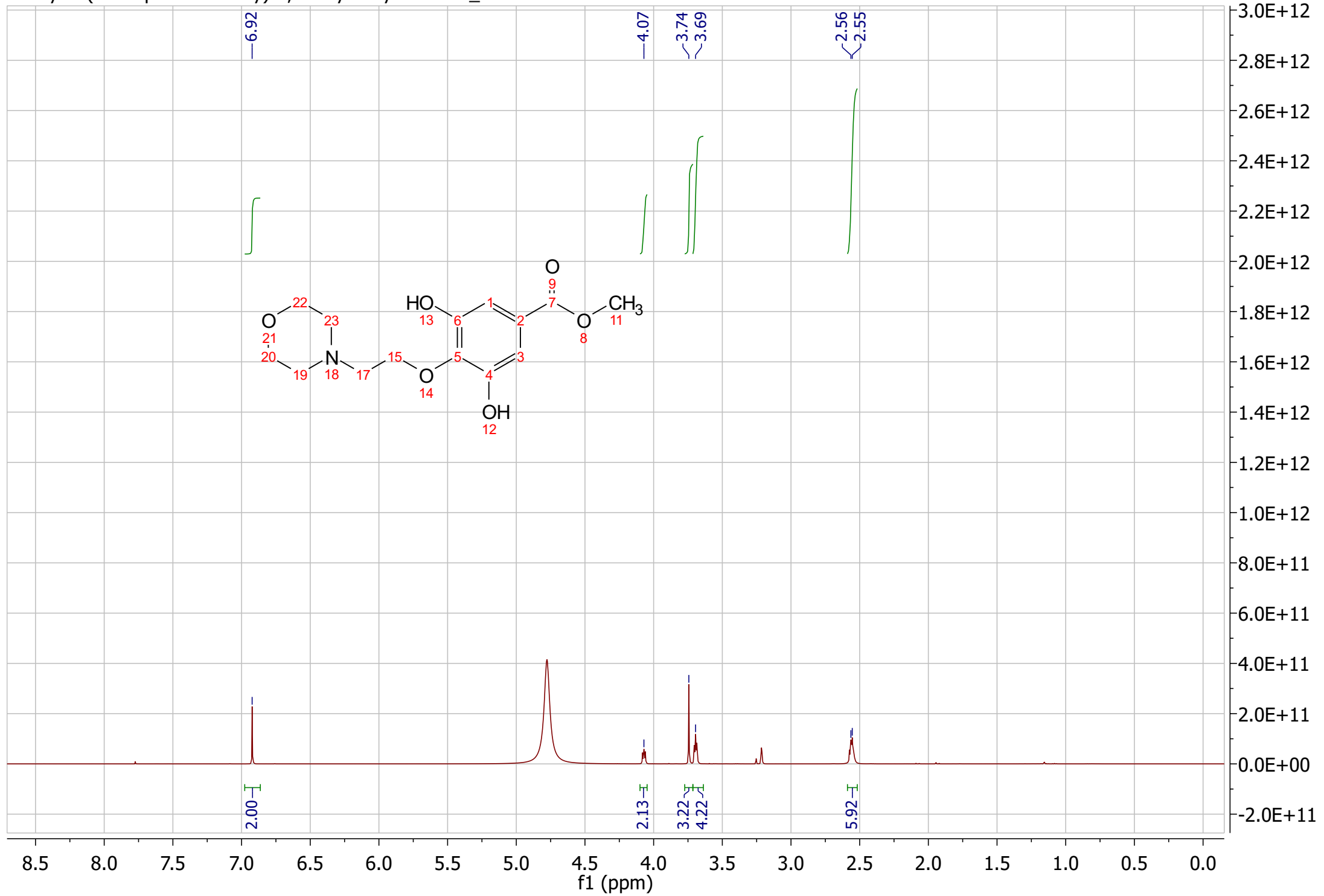
Methyl 4-(4-methoxybenzoxy)-3,5-dihydroxybenzoate_DMSO



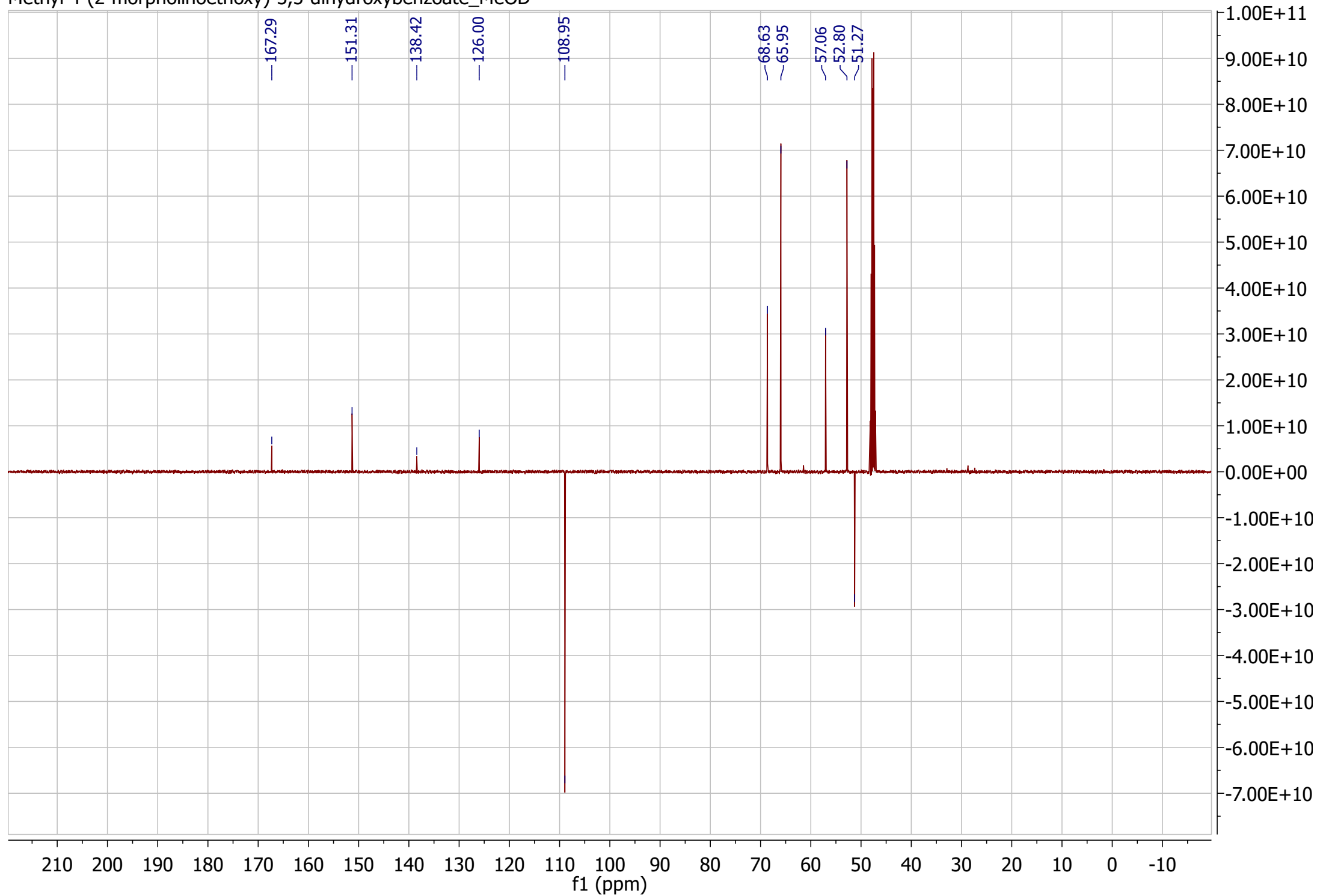
Methyl 4-(4-methoxybenzoxy)-3,5-dihydroxybenzoate_DMSO



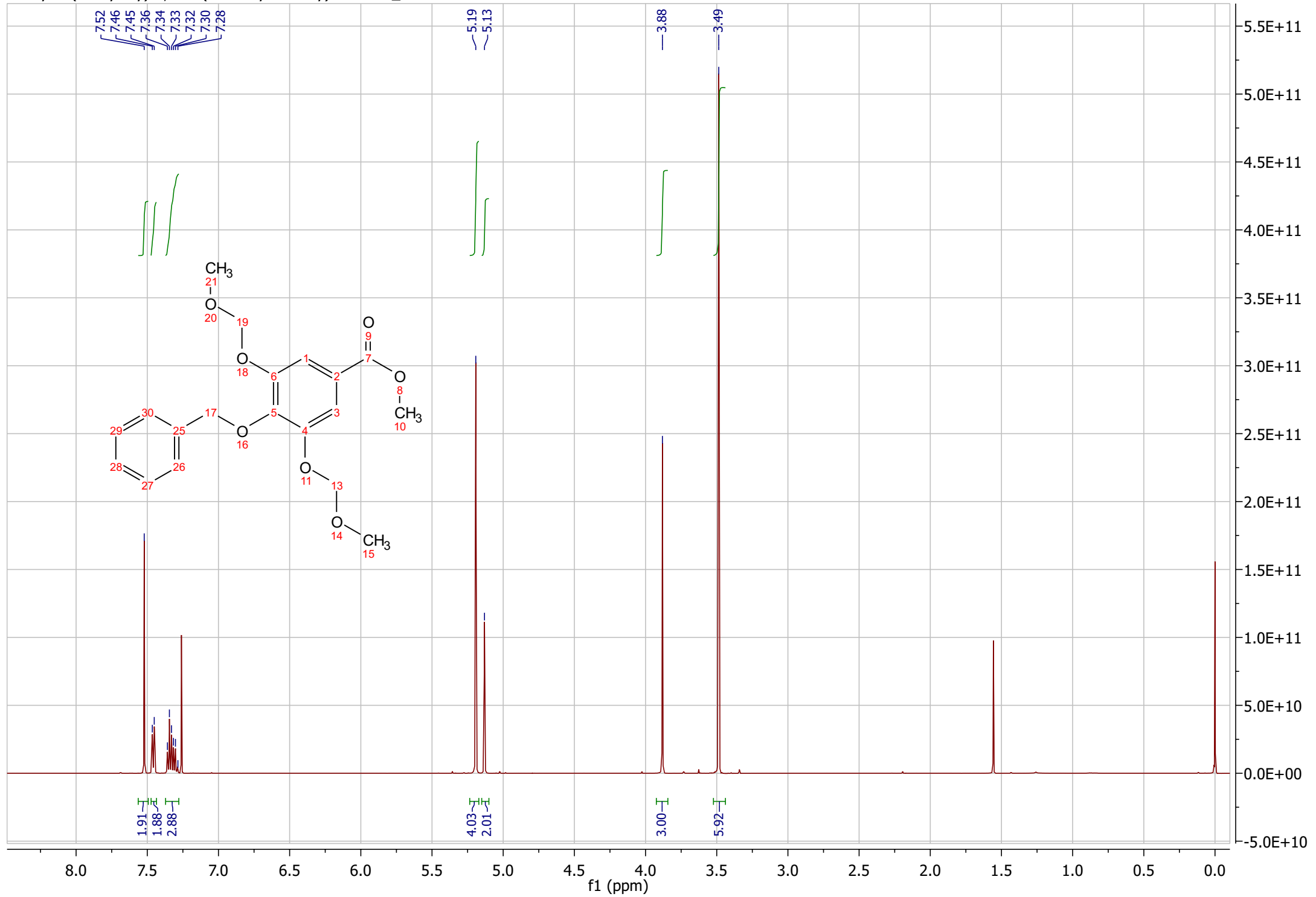
Methyl 4-(2-morpholinoethoxy)-3,5-dihydroxybenzoate_MeOD



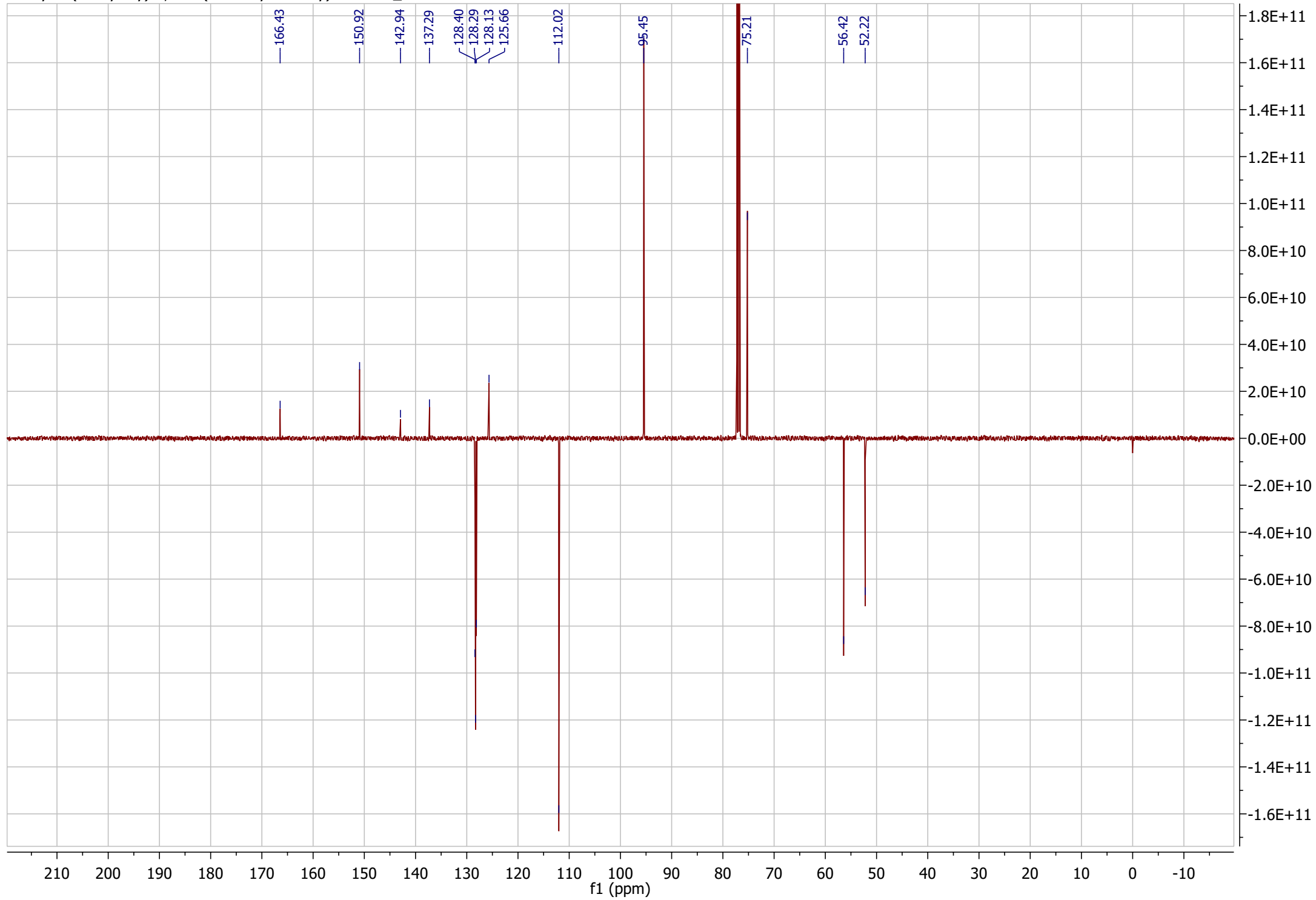
Methyl 4-(2-morpholinoethoxy)-3,5-dihydroxybenzoate_MeOD



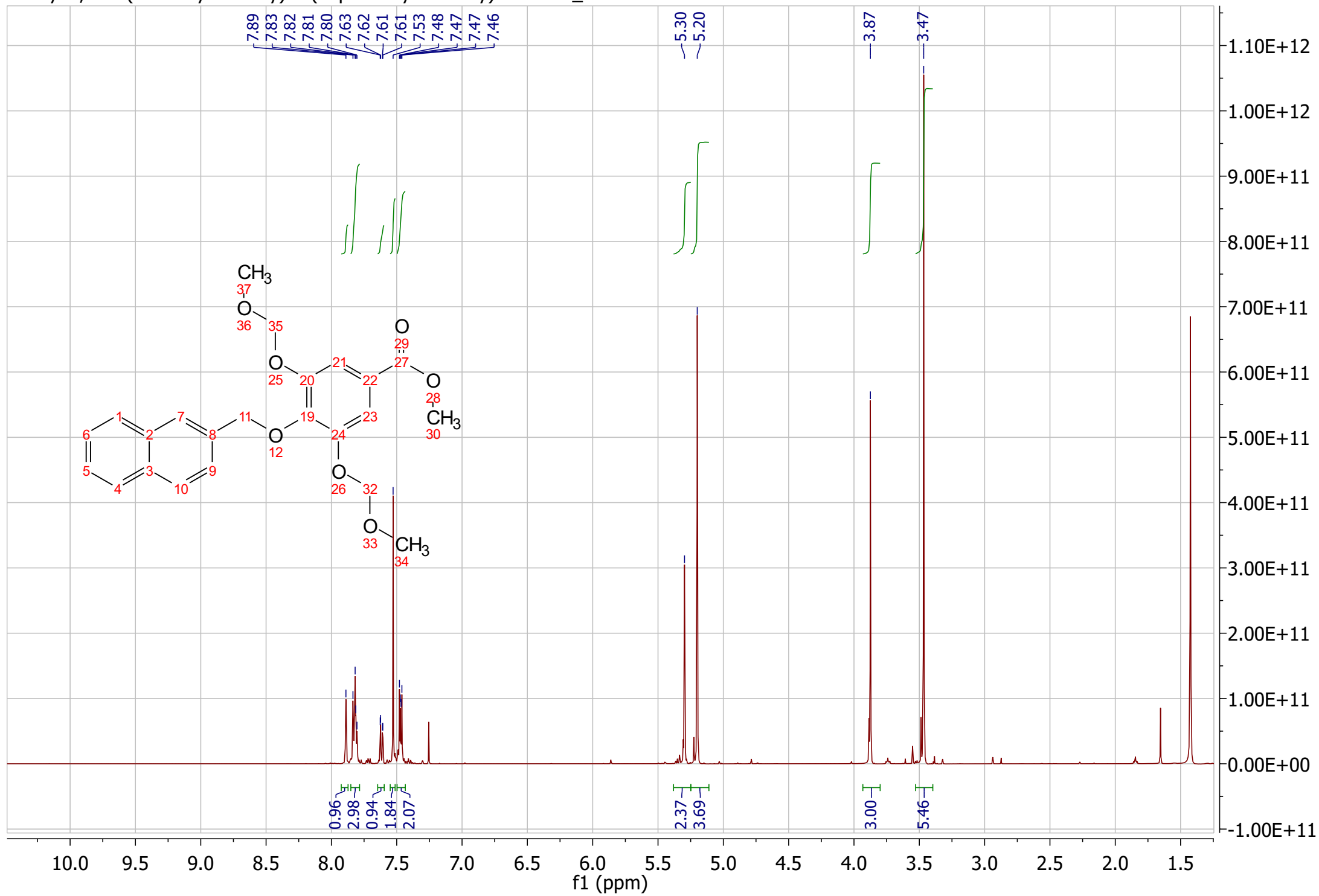
Methyl 4-(benzyloxy)-3,5-bis(methoxymethoxy)benzoate_CDCl3



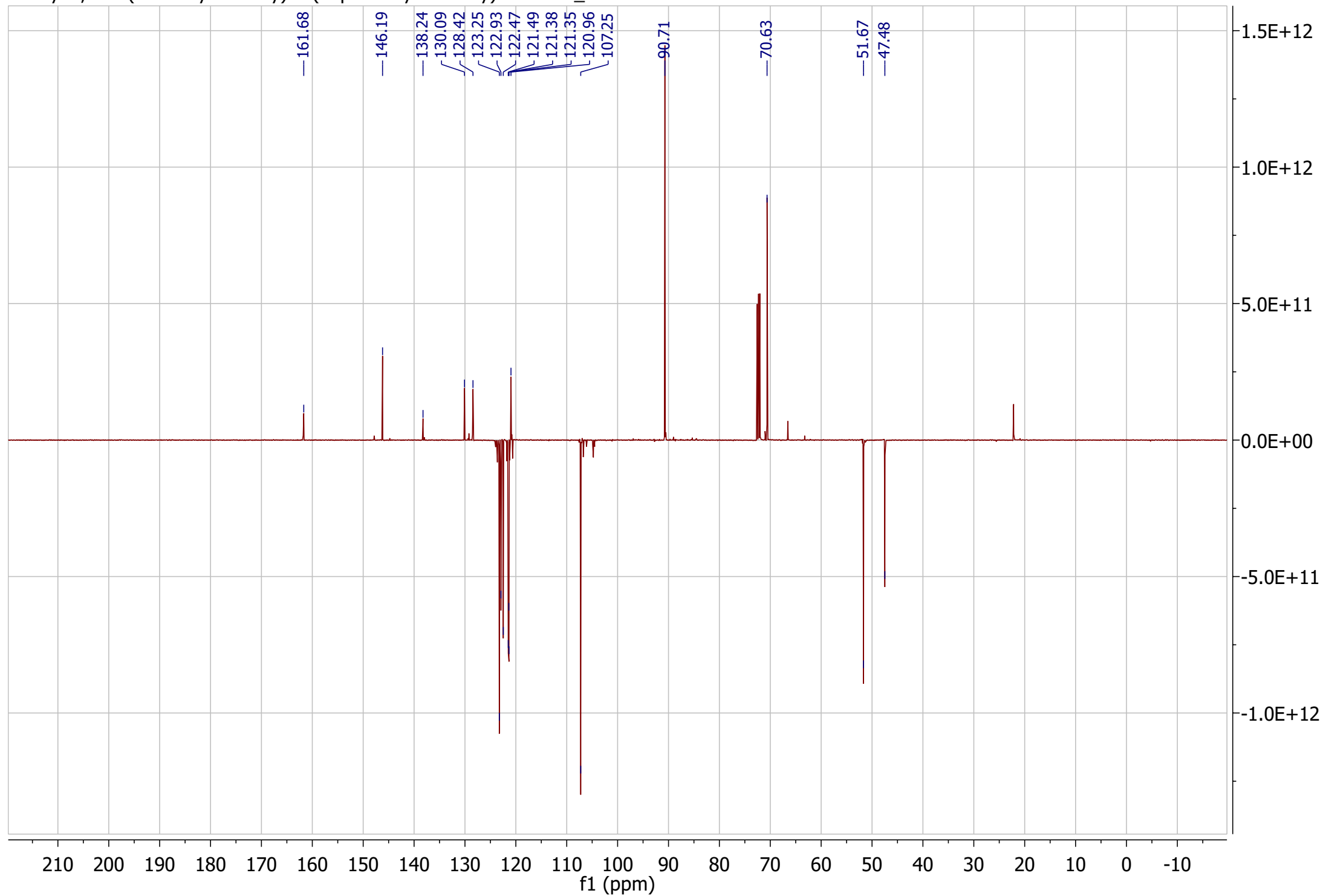
Methyl 4-(benzyloxy)-3,5-bis(methoxymethoxy)benzoate_CDCl3



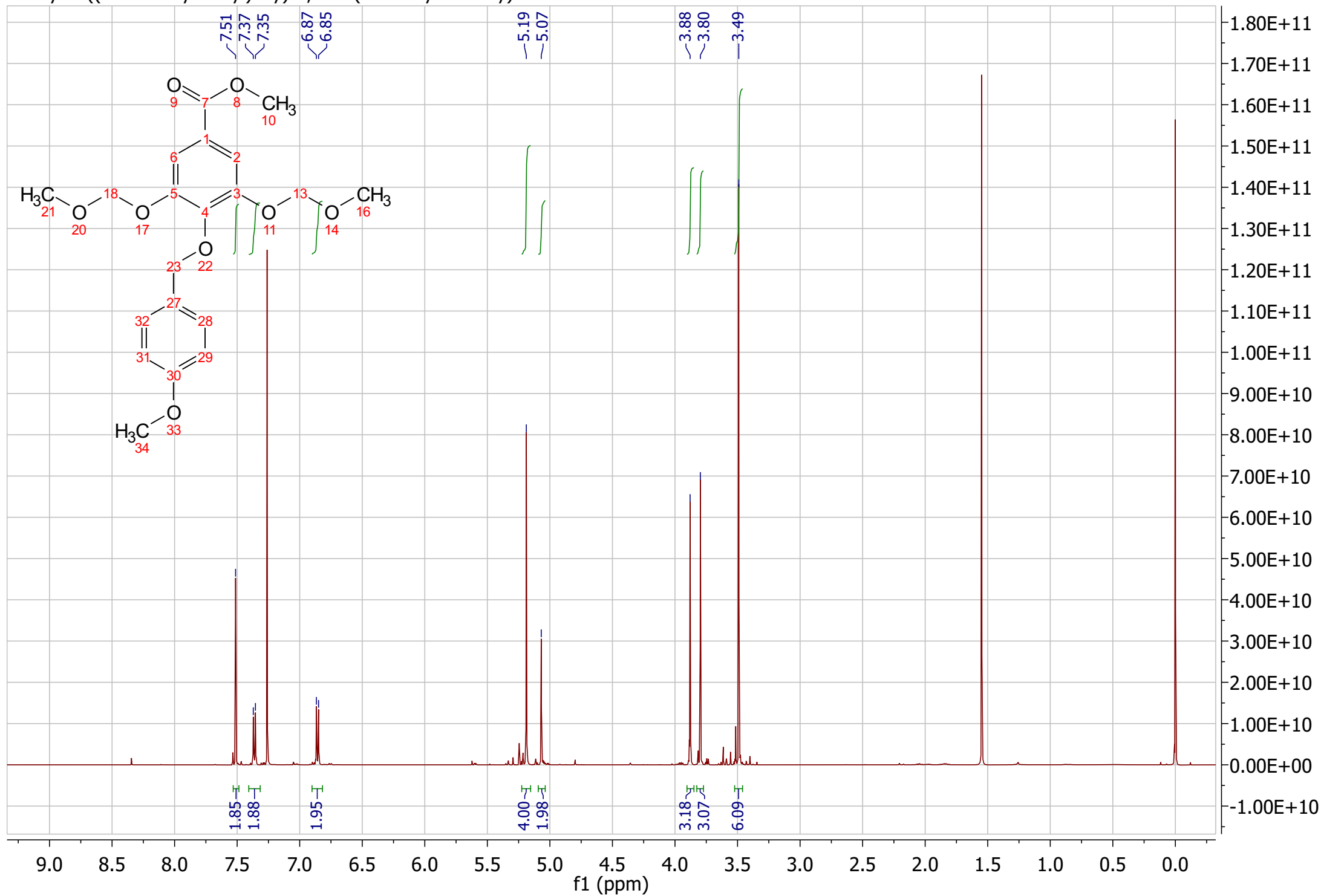
Methyl 3,5-bis(methoxymethoxy)-4-(naphth-2-ylmethoxy)benzoate_DMSO



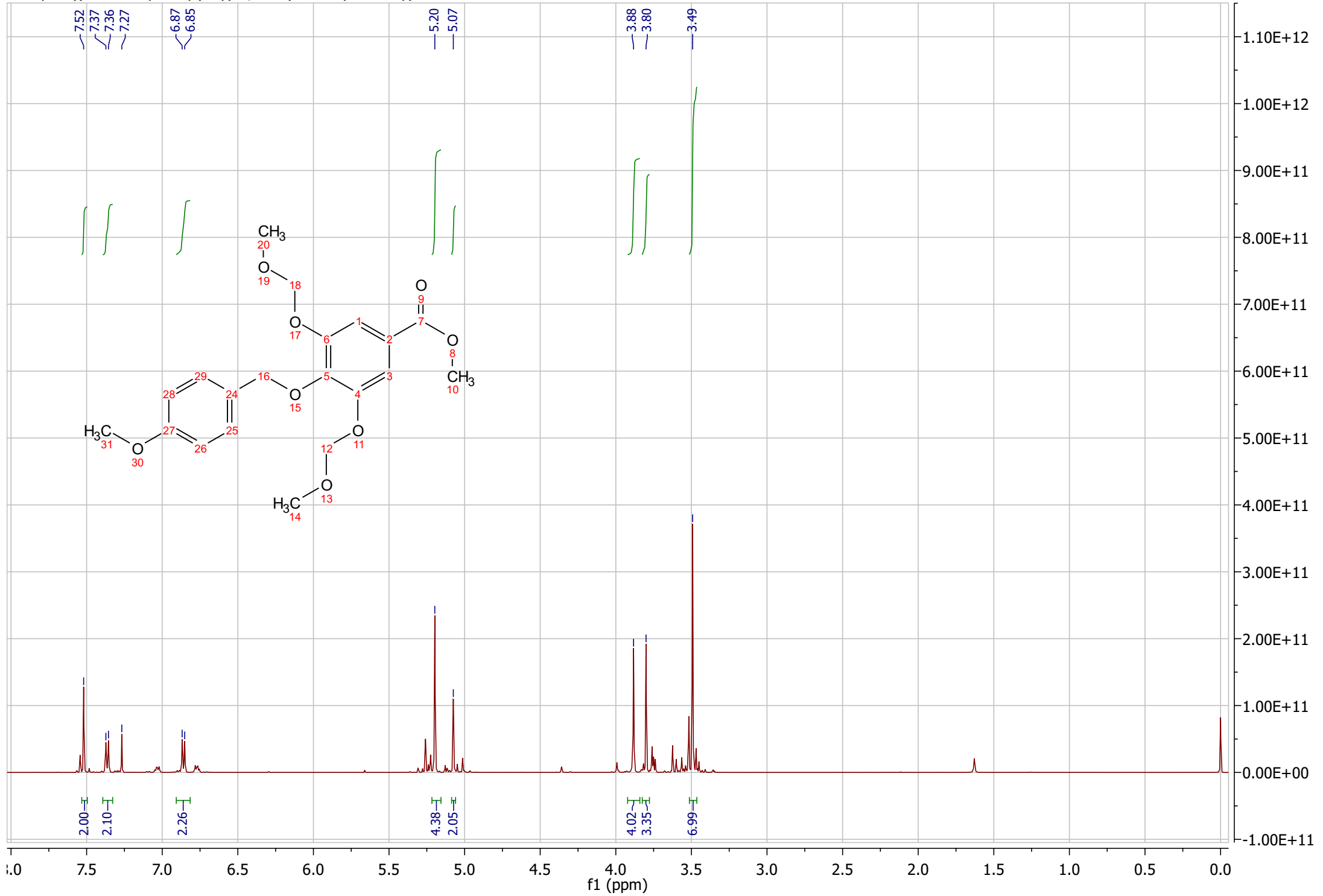
Methyl 3,5-bis(methoxymethoxy)-4-(naphth-2-ylmethoxy)benzoate_DMSO



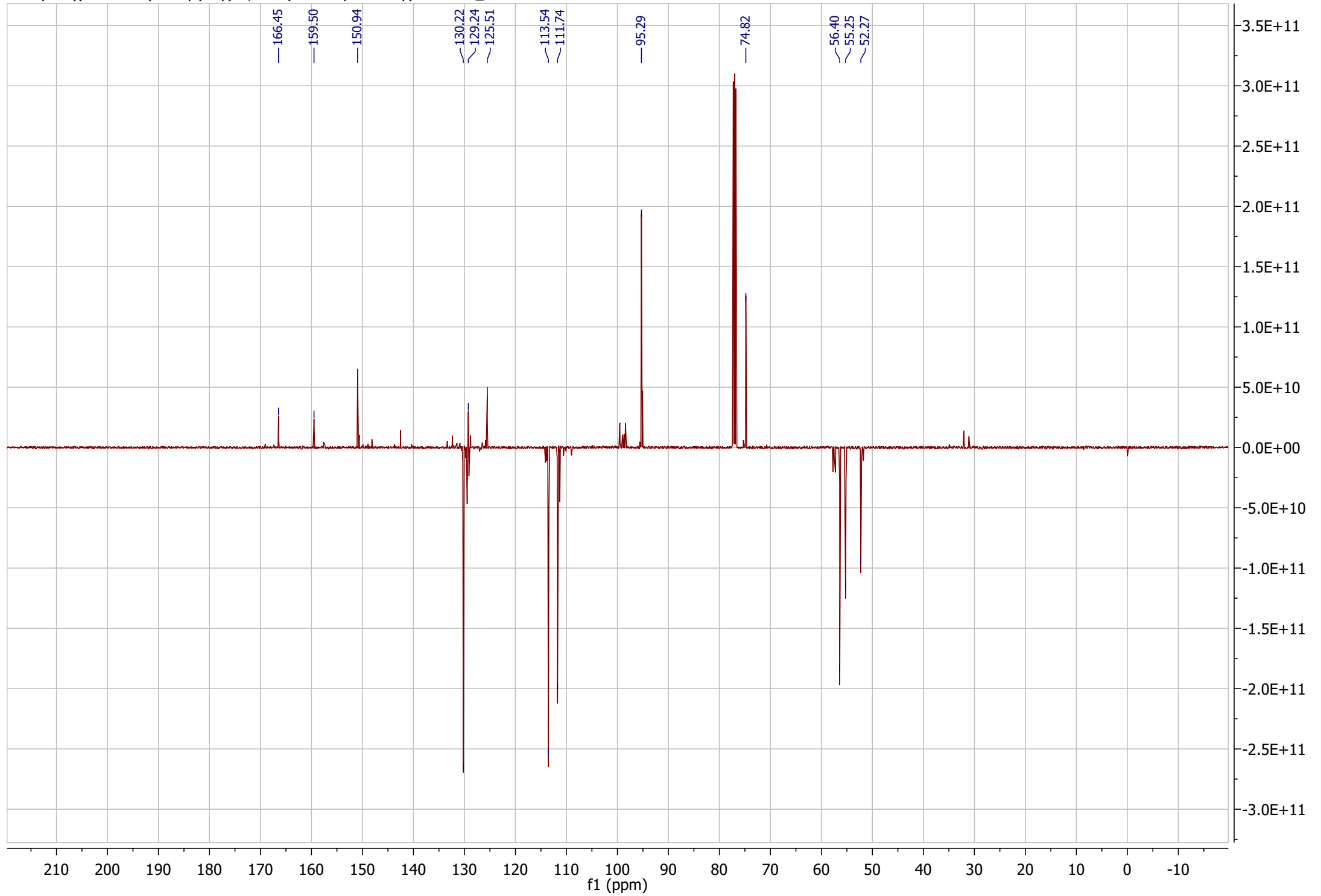
Methyl 4-((4-methoxybenzyl)oxy)-3,5-bis(methoxymethoxy)benzoate



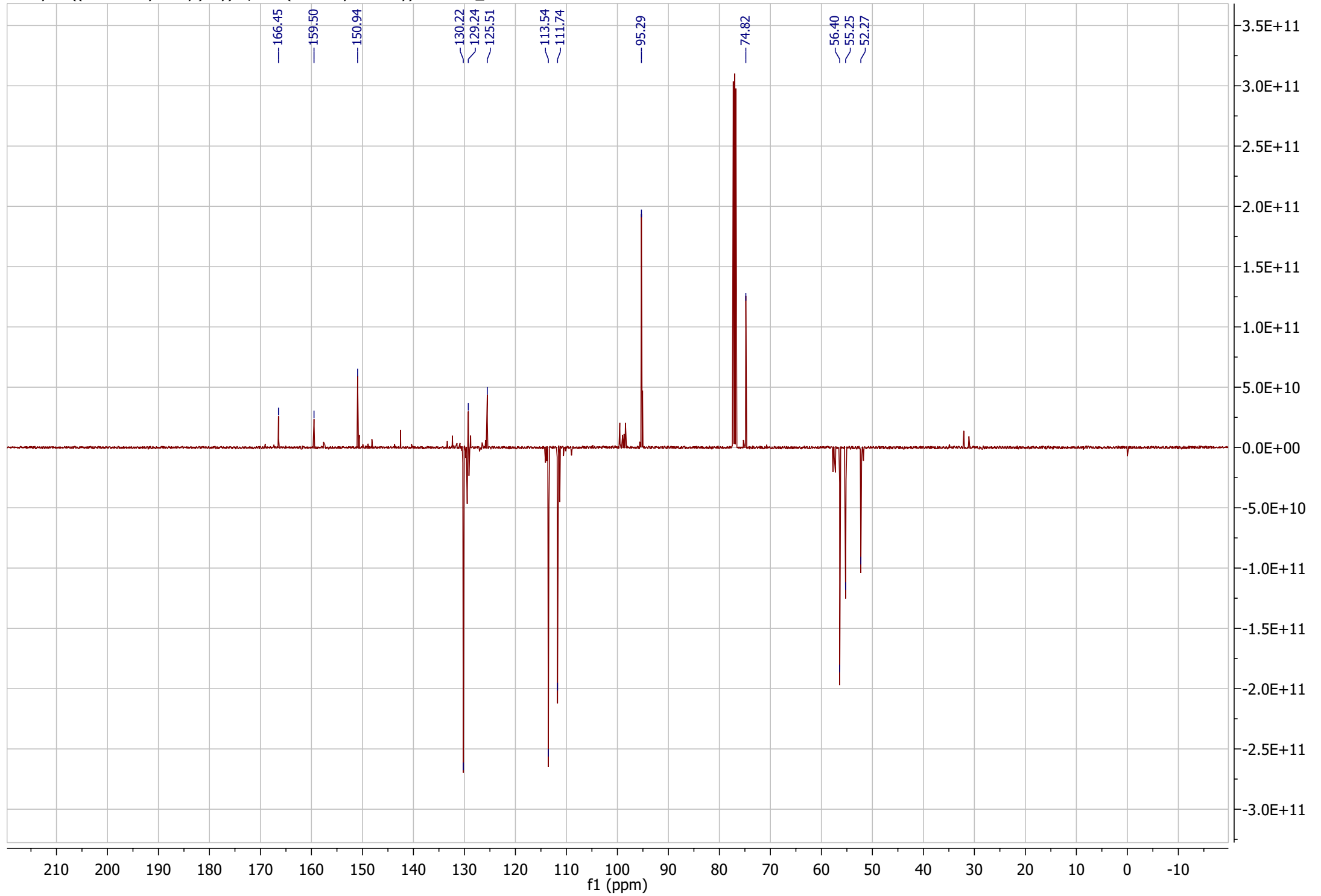
Methyl 4-((4-methoxybenzyl)oxy)-3,5-bis(methoxymethoxy)benzoate_CDCl3



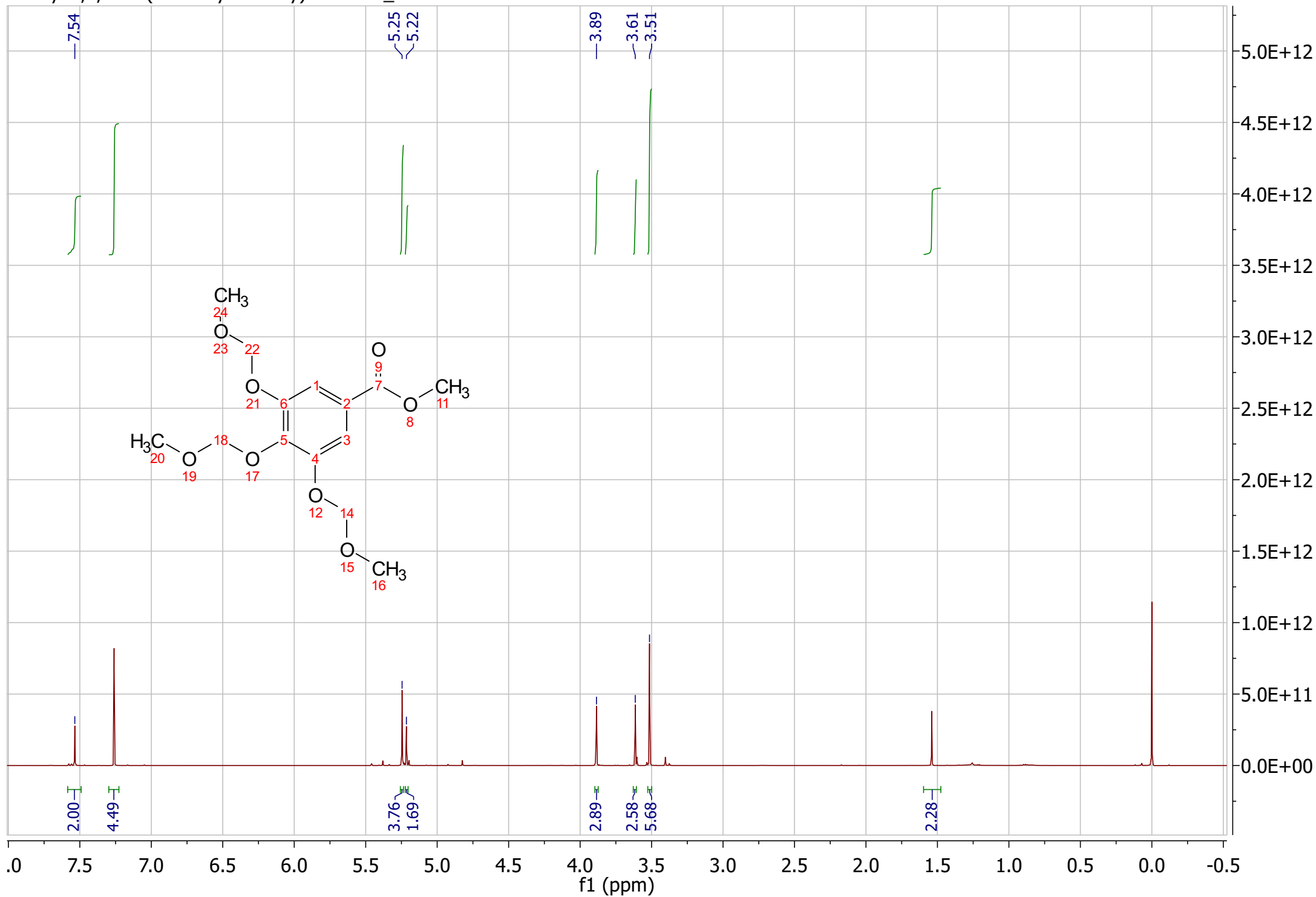
Methyl 4-((4-methoxybenzyl)oxy)-3,5-bis(methoxymethoxy)benzoate_CDCl3



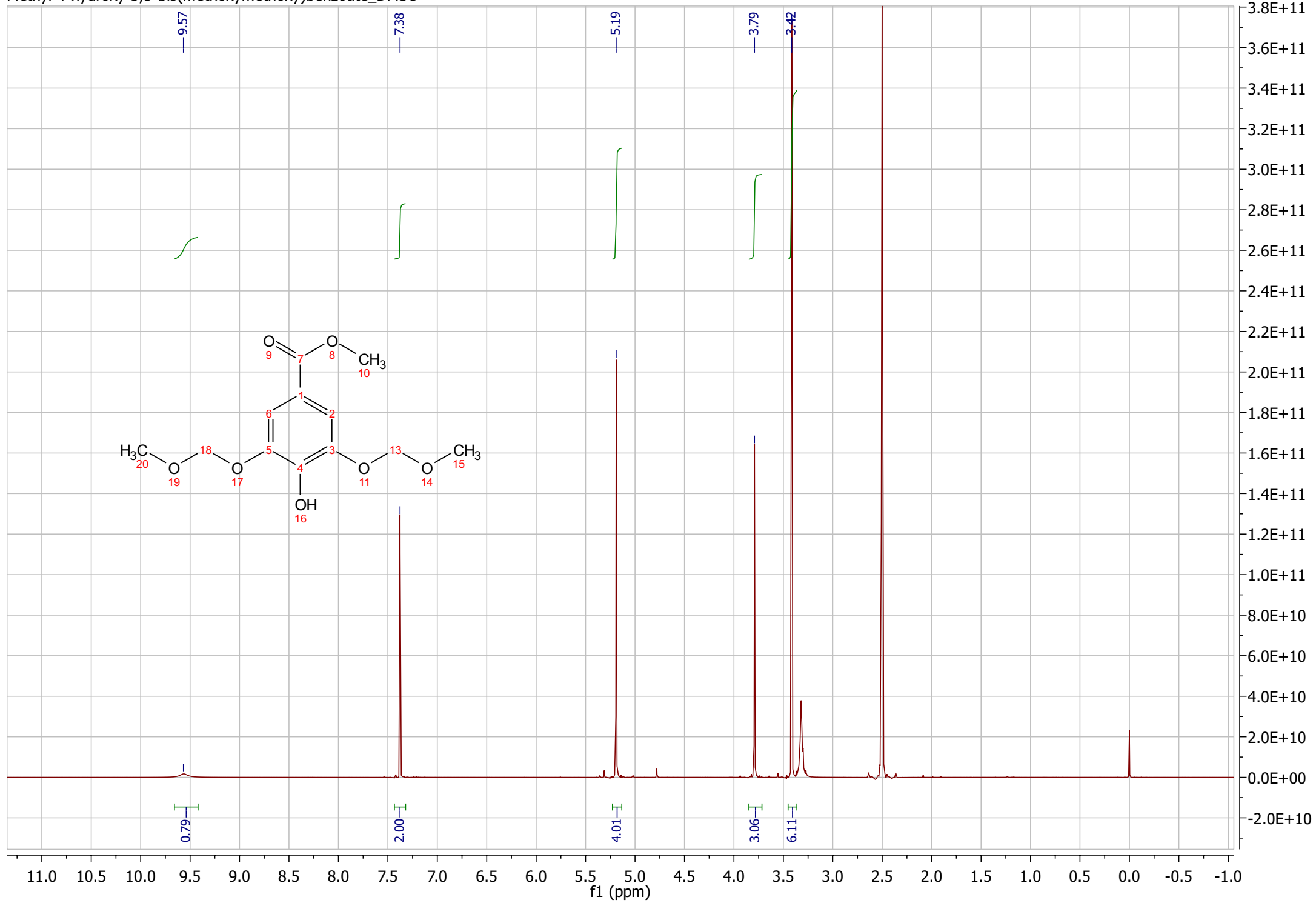
Methyl 4-((4-methoxybenzyl)oxy)-3,5-bis(methoxymethoxy)benzoate_CDCl3



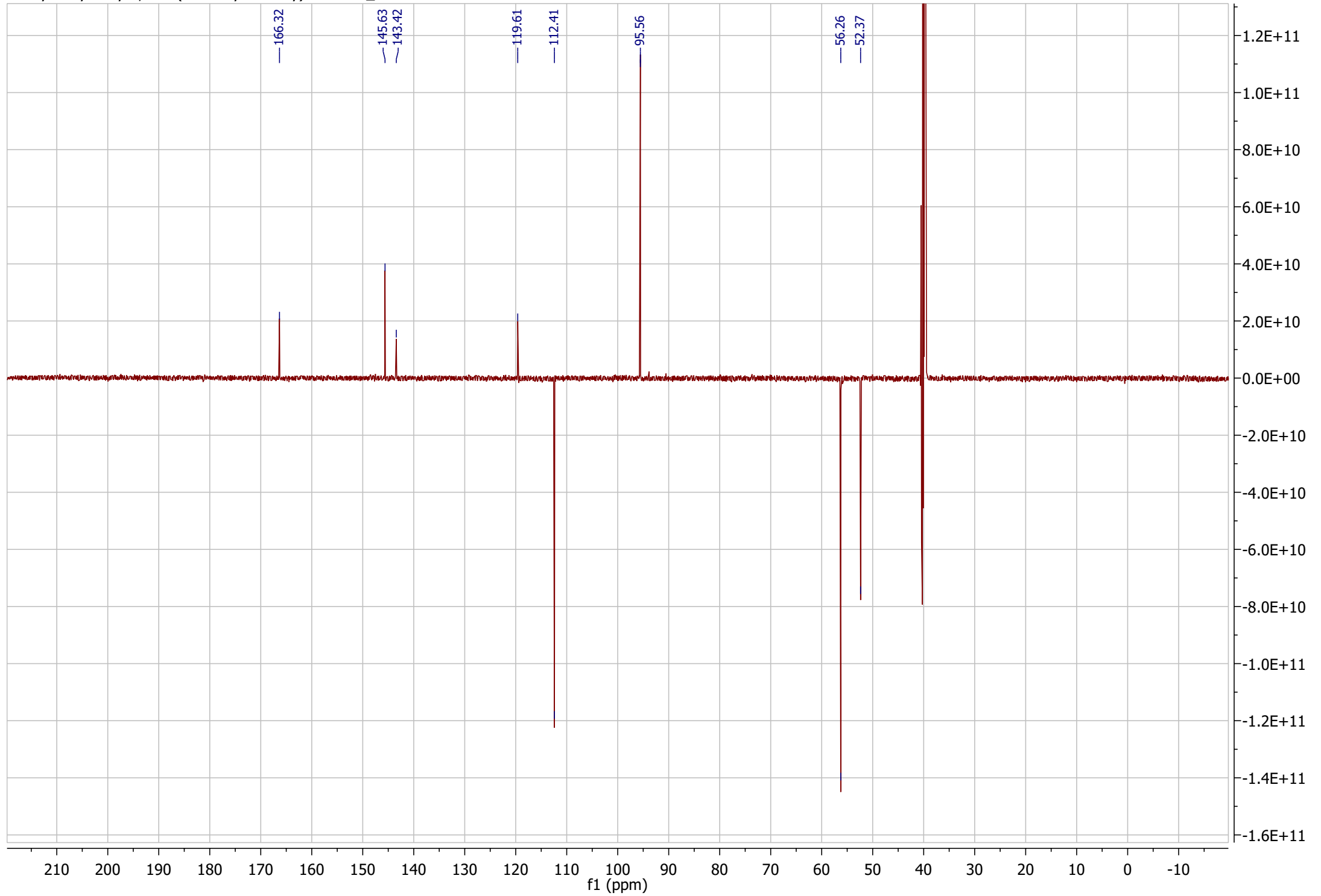
methyl 3,4,5-tris(methoxymethoxy)benzoate_CDCl3



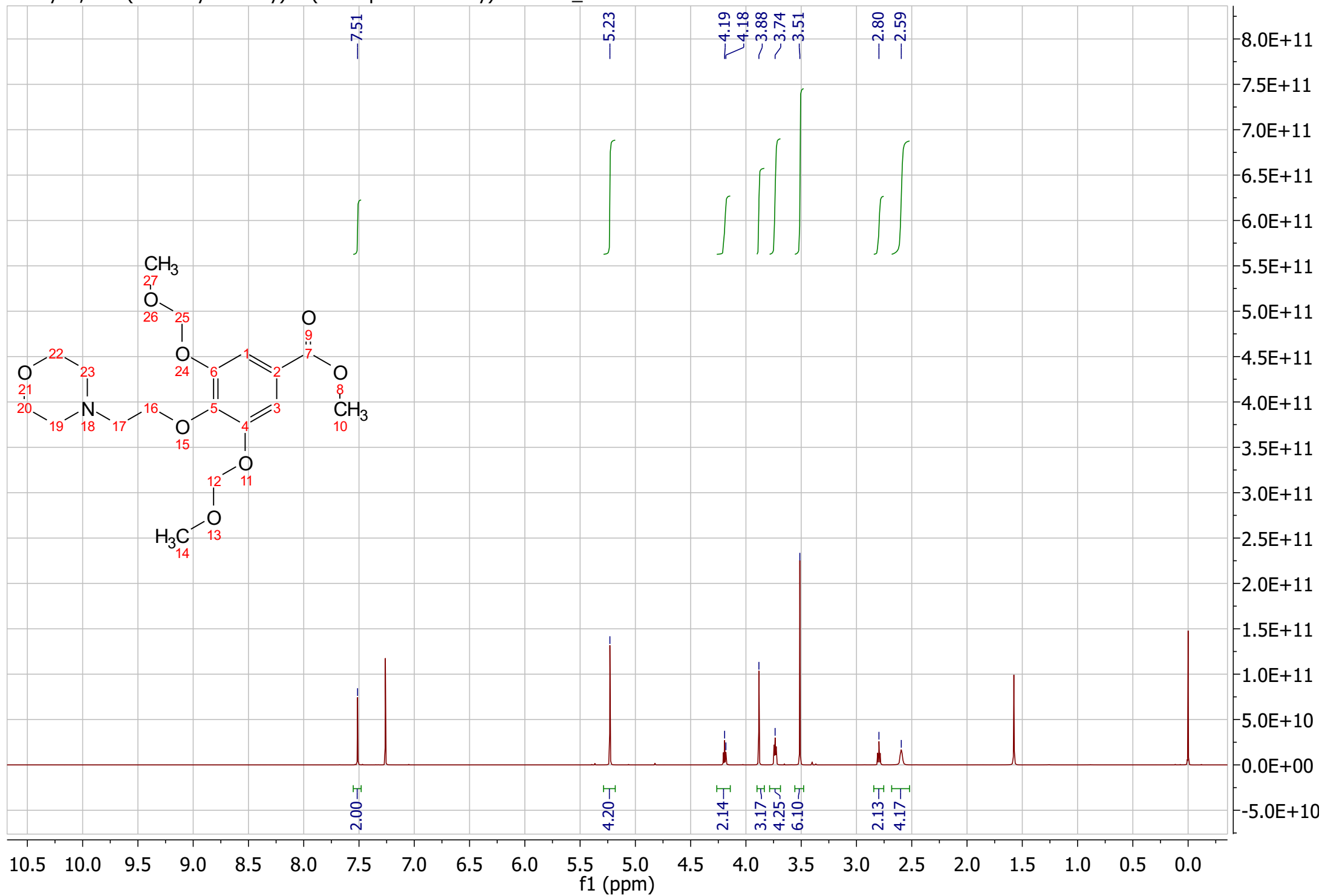
Methyl 4-hydroxy-3,5-bis(methoxymethoxy)benzoate_DMSO



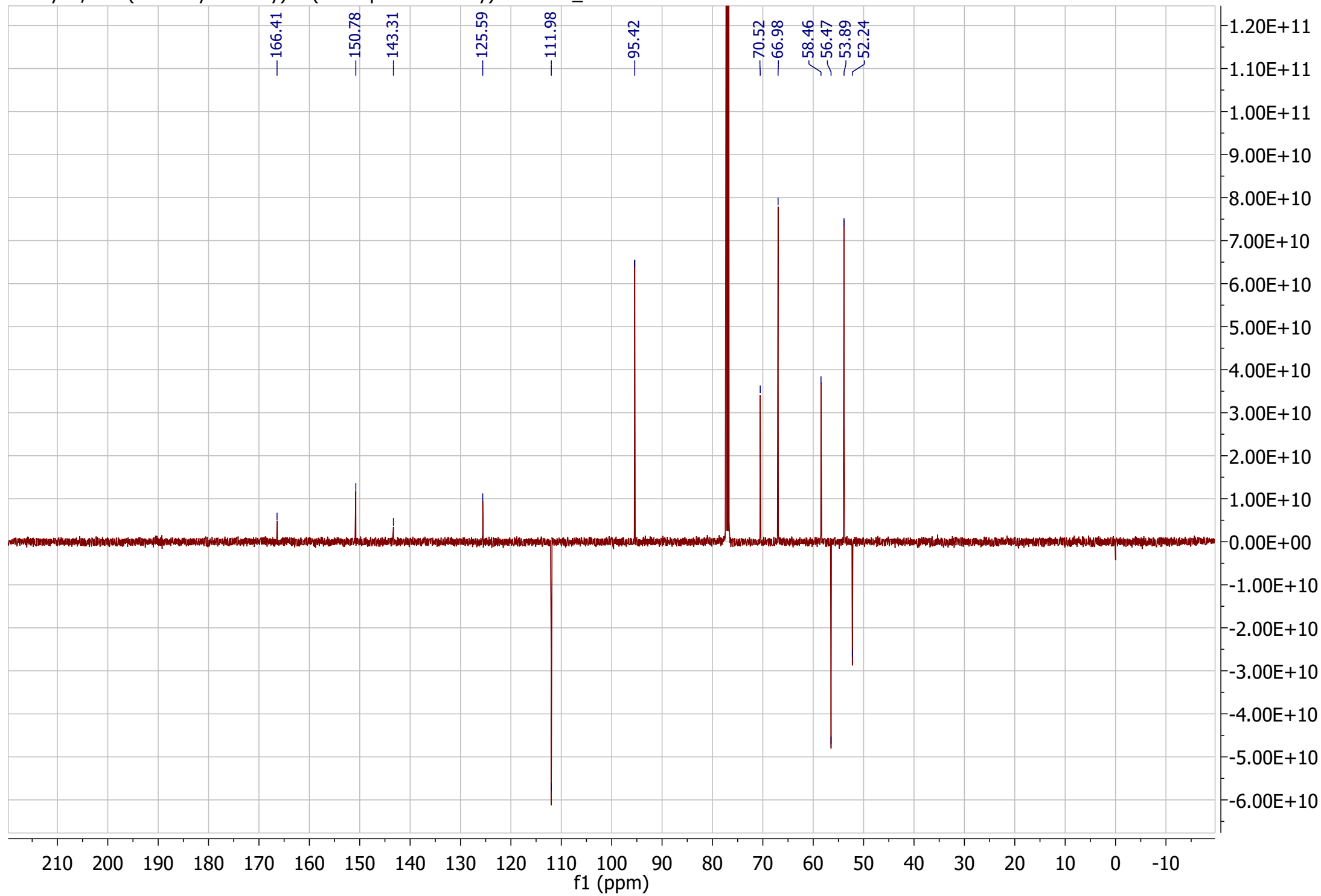
Methyl 4-hydroxy-3,5-bis(methoxymethoxy)benzoate_DMSO



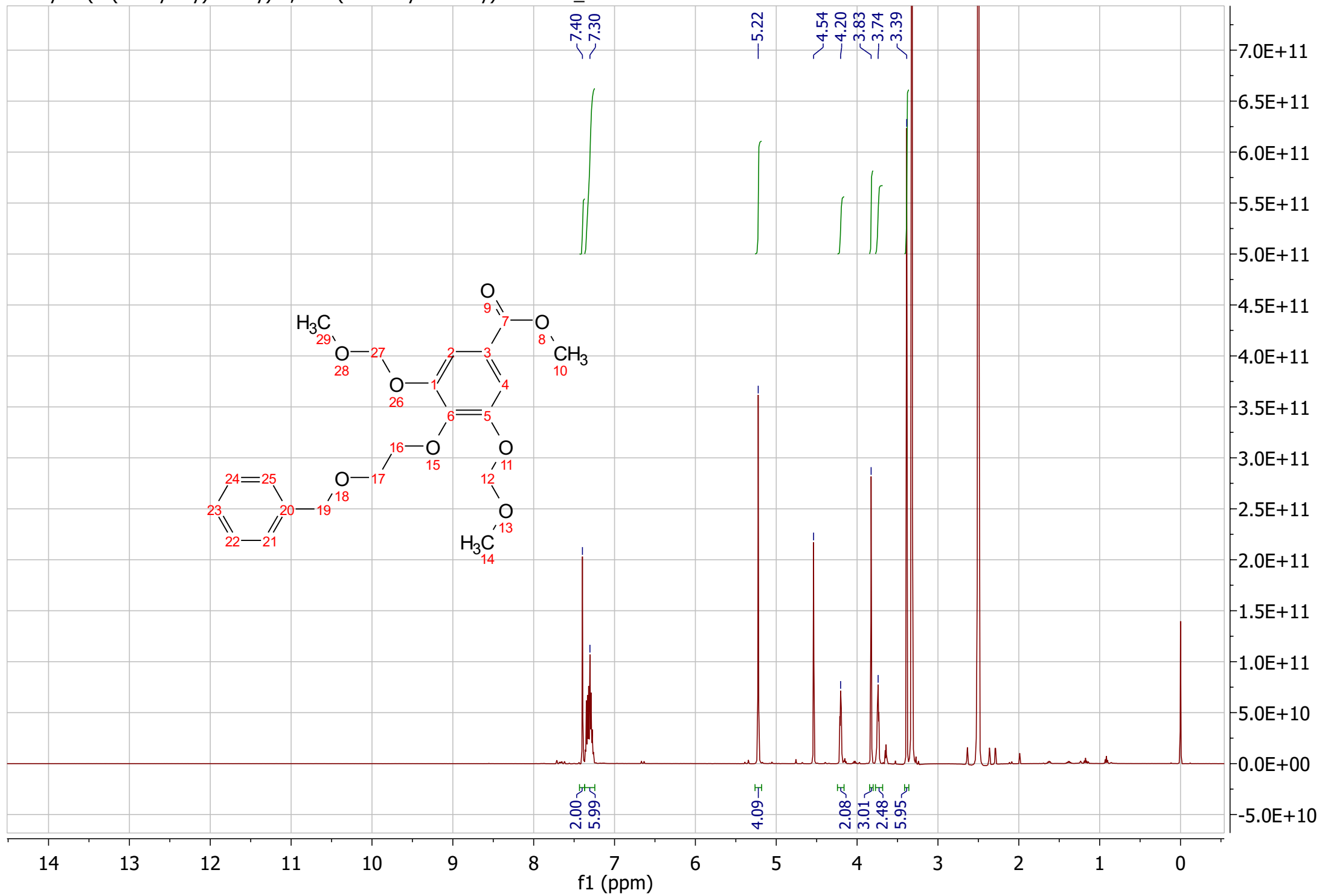
Methyl 3,5-bis(methoxymethoxy)-4-(2-morpholinoethoxy)benzoate_CDCI3



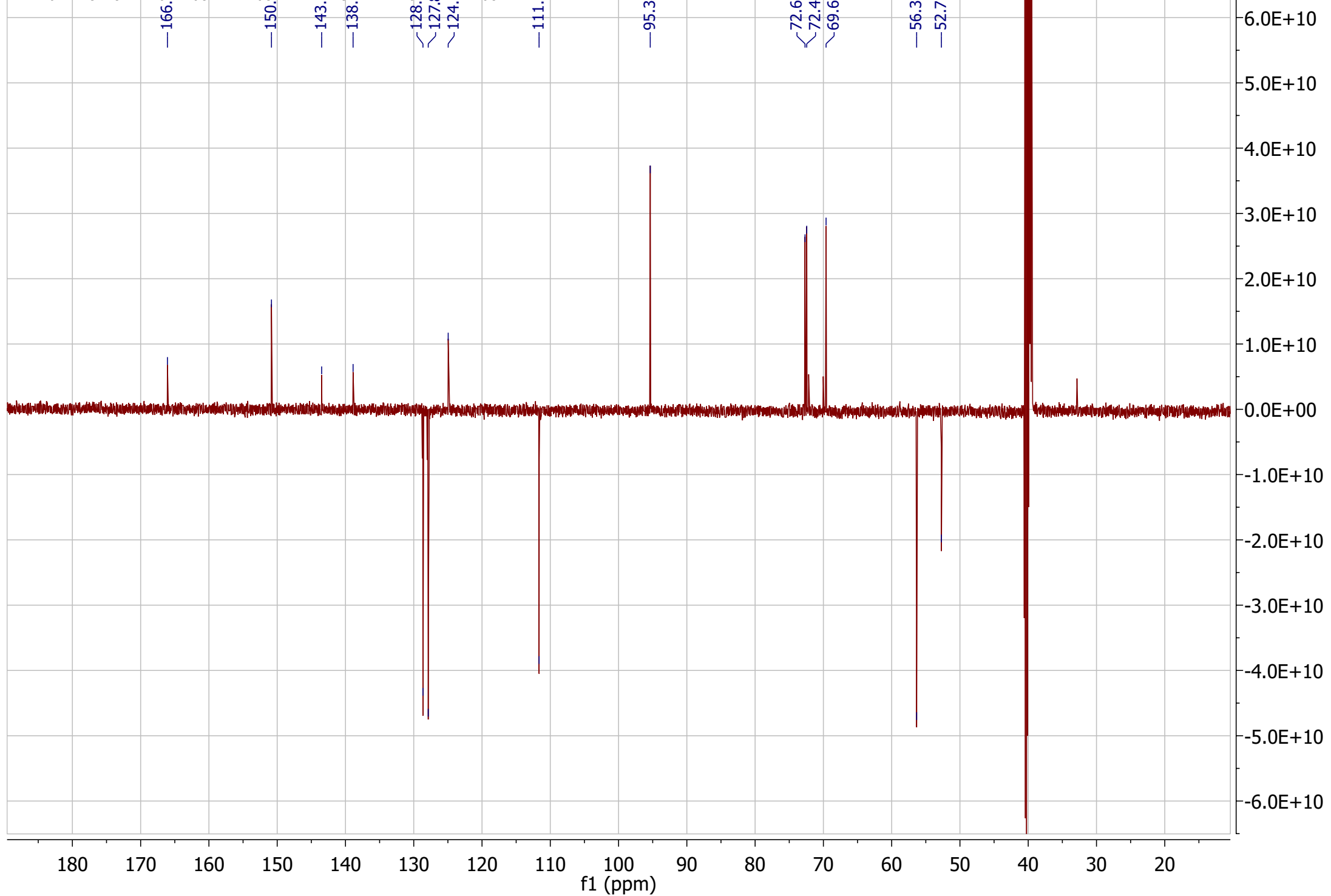
Methyl 3,5-bis(methoxymethoxy)-4-(2-morpholinoethoxy)benzoate_CDCl3



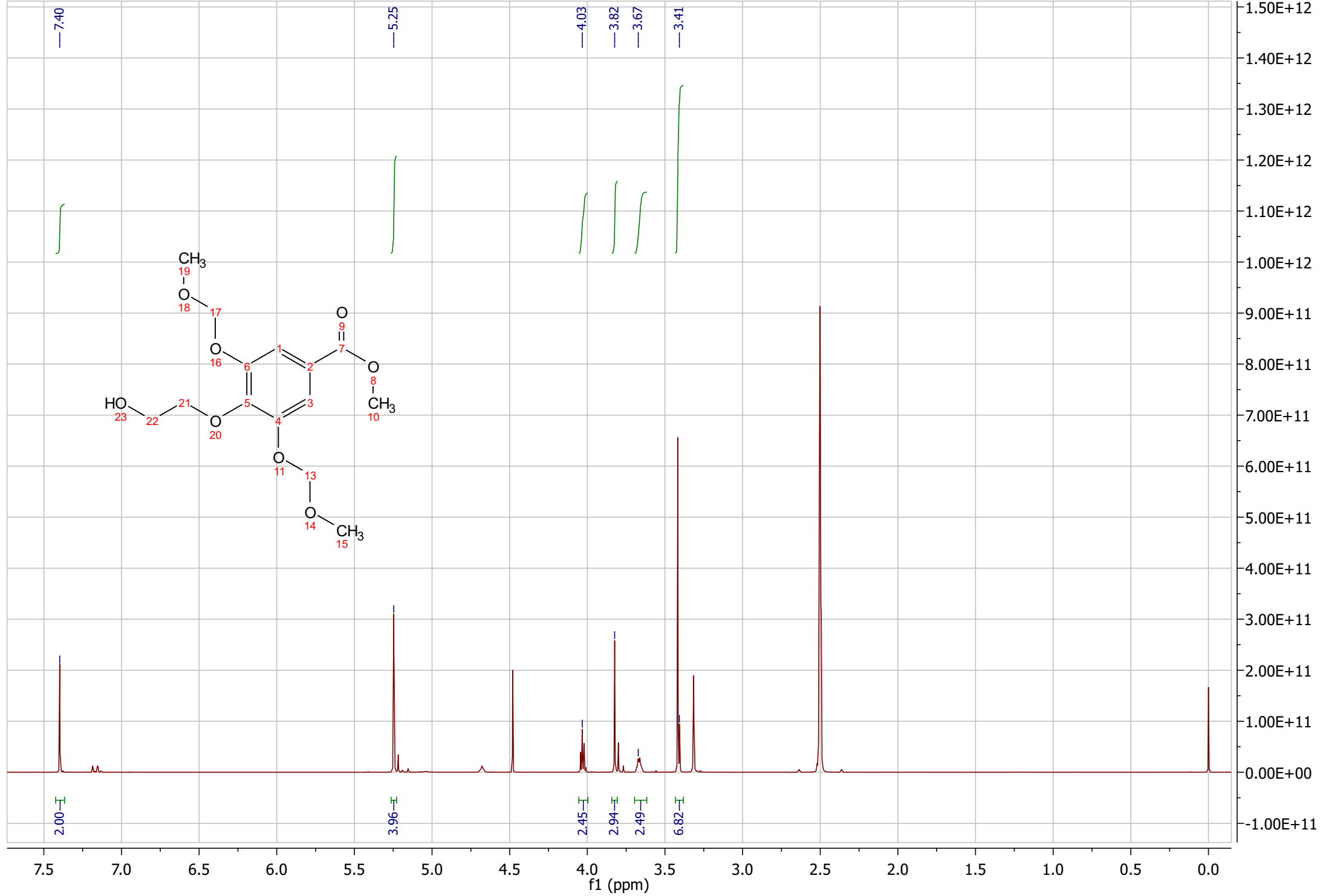
Methyl 4-(2-(benzyloxy)ethoxy)-3,5-bis(methoxymethoxy)benzoate_DMSO



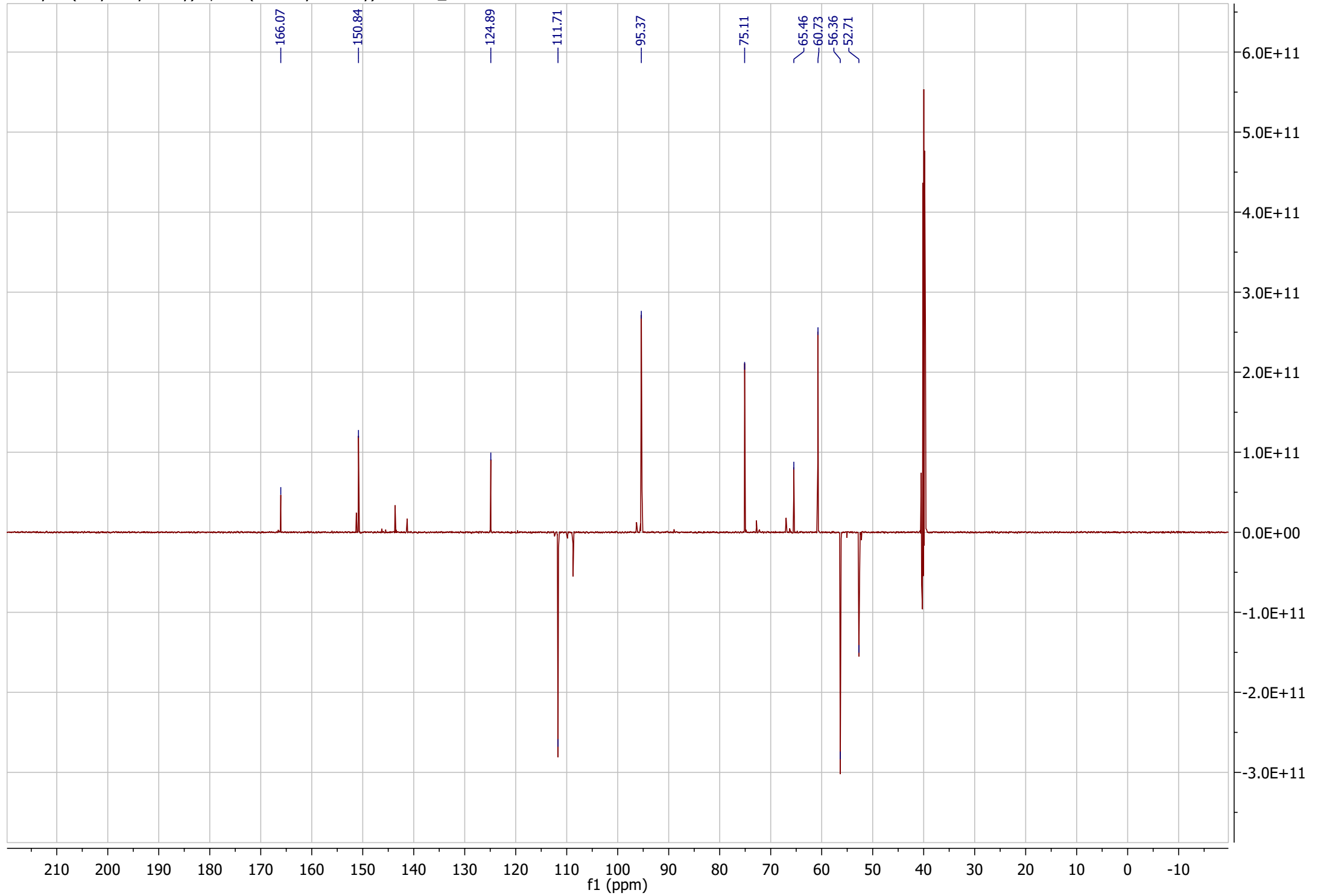
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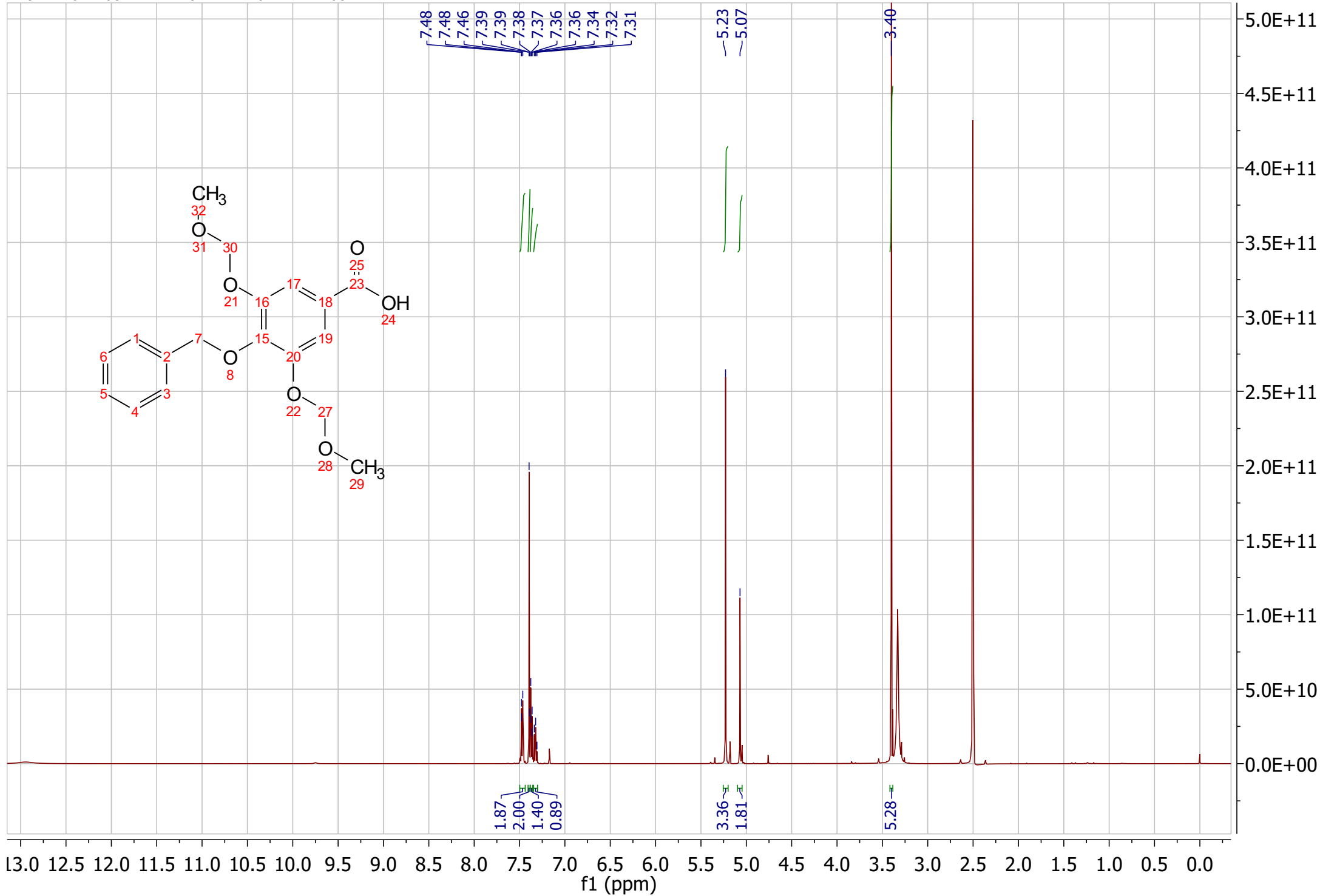
Methyl 4-(2-hydroxyethoxy)-3,5-bis(methoxymethoxy)benzoate_DMSO



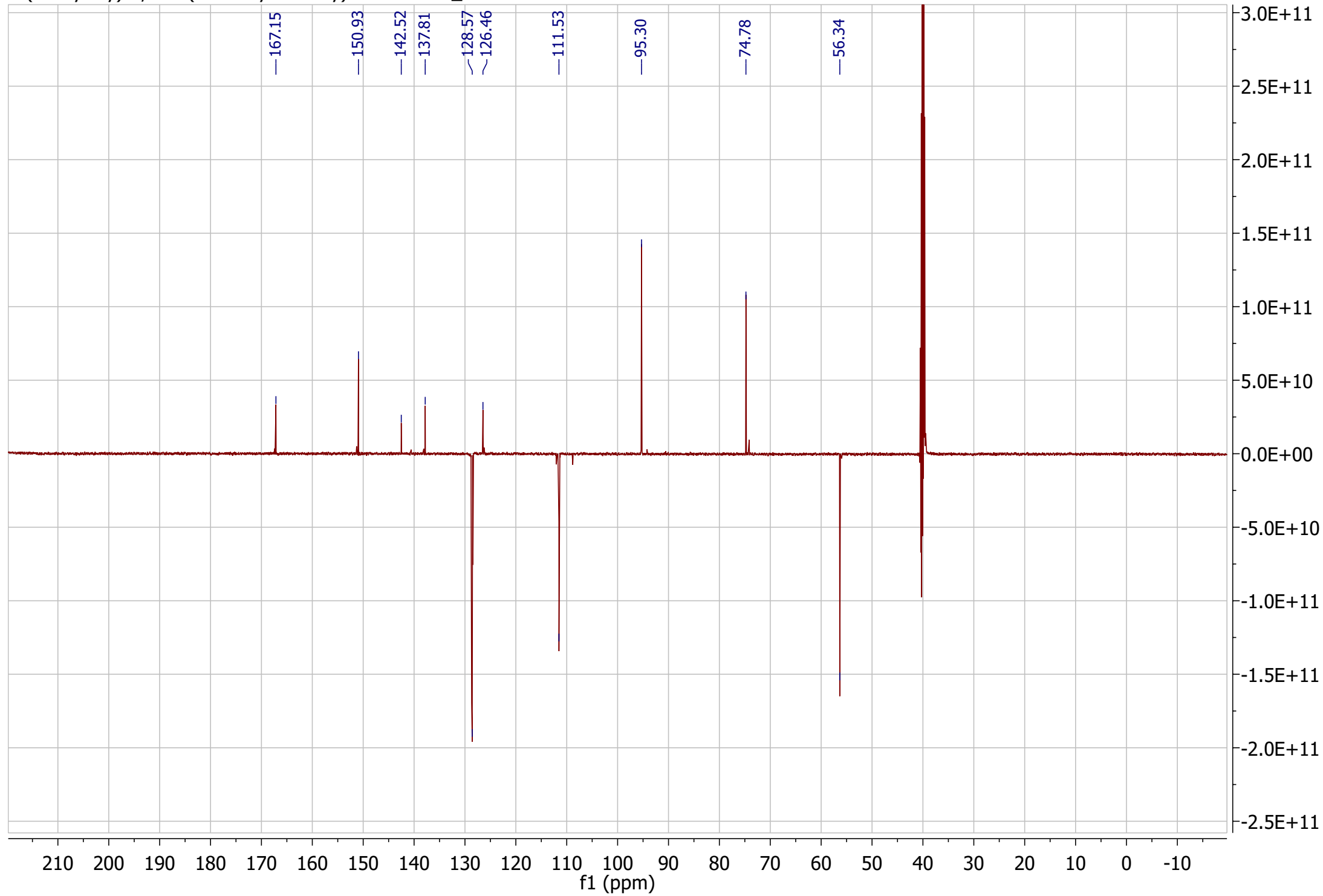
Methyl 4-(2-hydroxyethoxy)-3,5-bis(methoxymethoxy)benzoate_DMSO



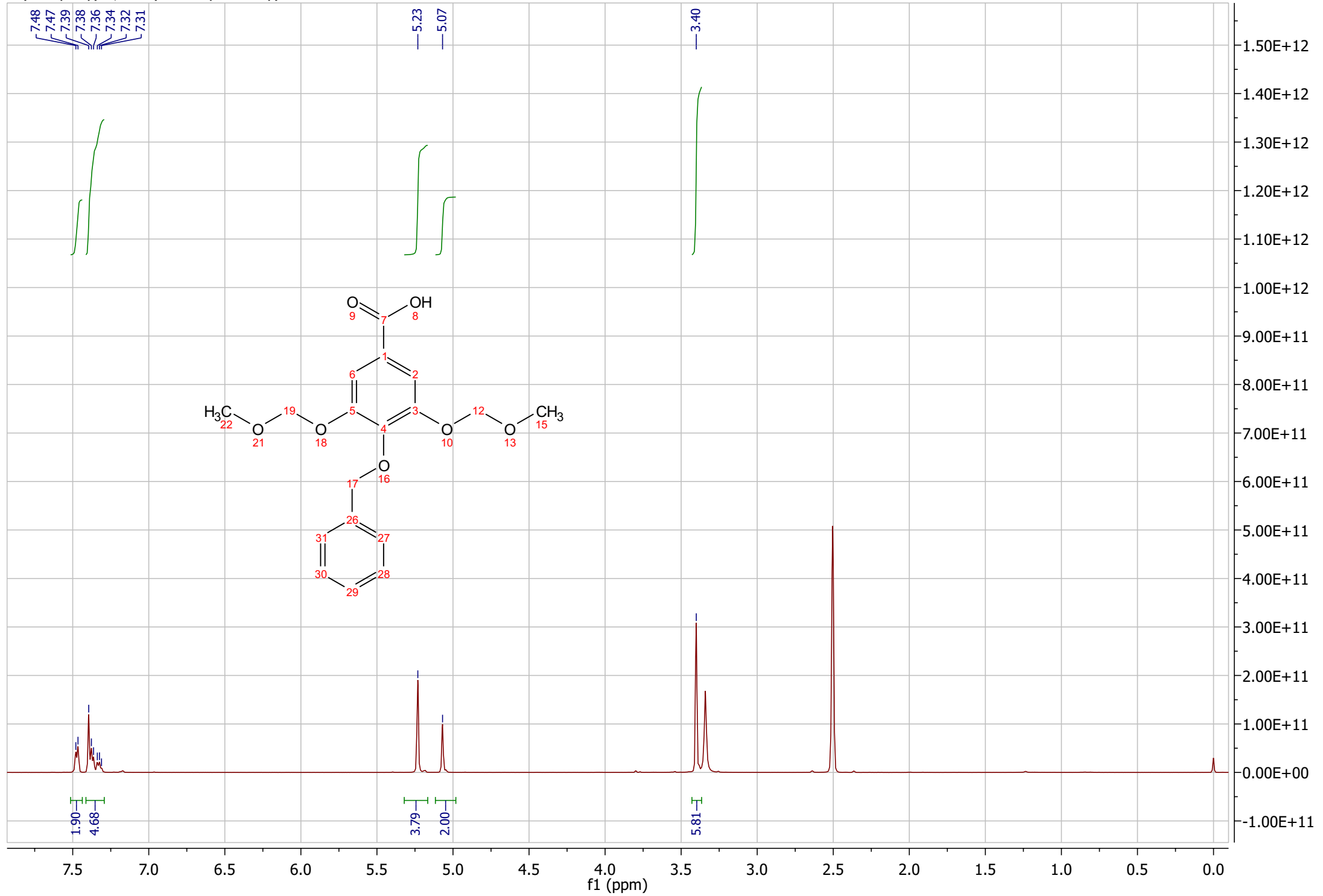
4-(benzyloxy)-3,5-bis(methoxymethoxy)benzoic acid_DMSO



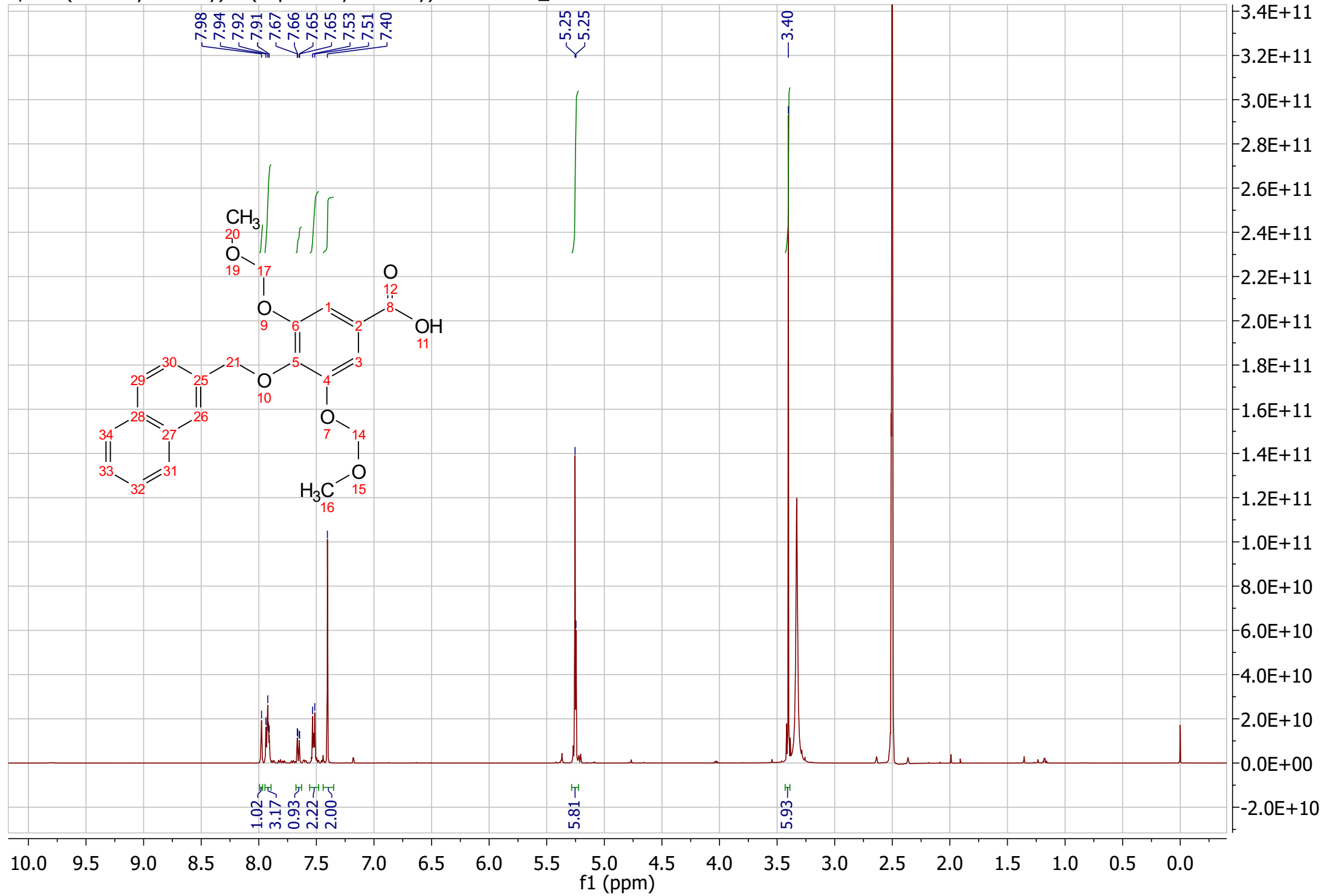
4-(benzyloxy)-3,5-bis(methoxymethoxy)benzoic acid_DMSO



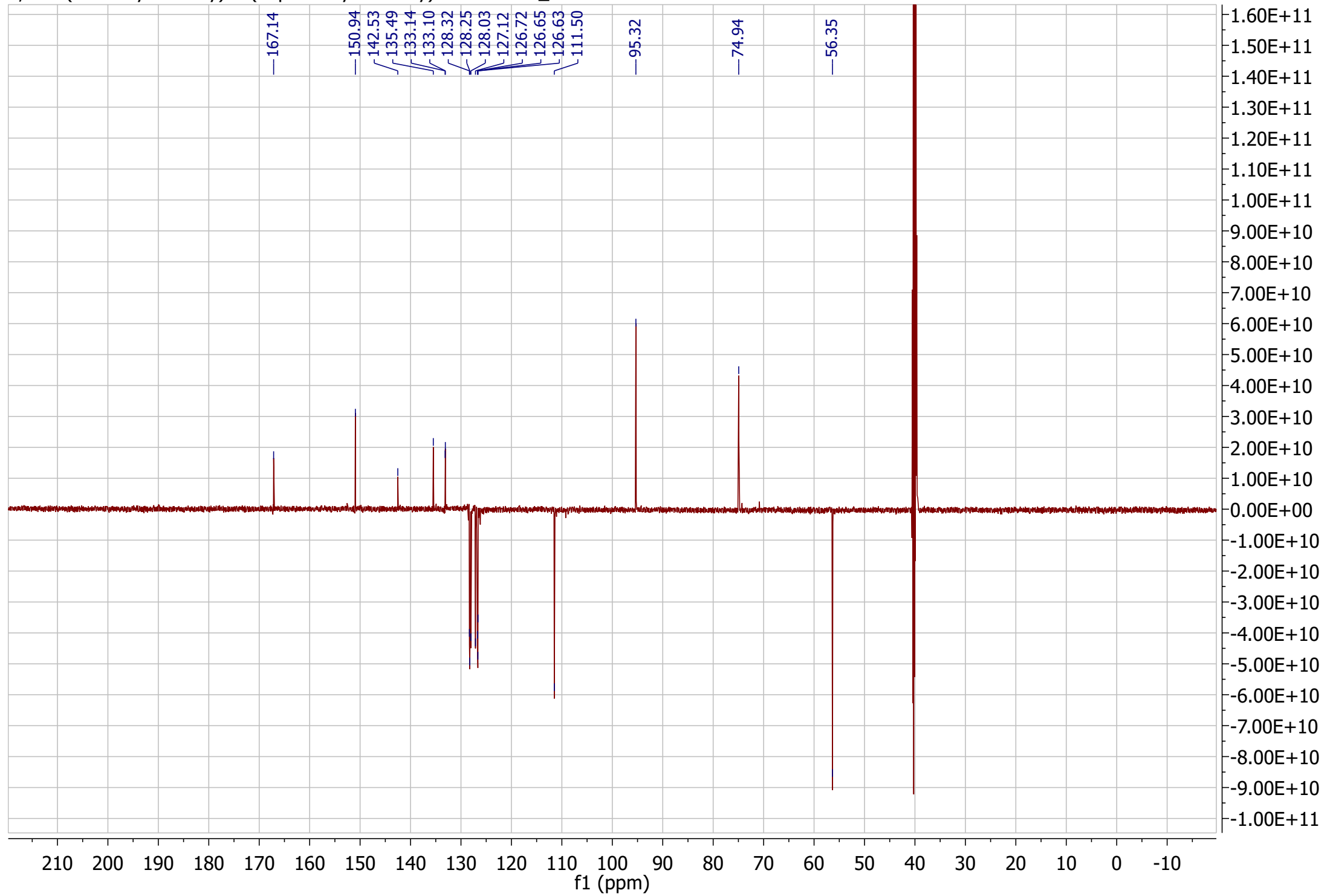
4-(benzyloxy)-3,5-bis(methoxymethoxy)benzoic acid_DMSO



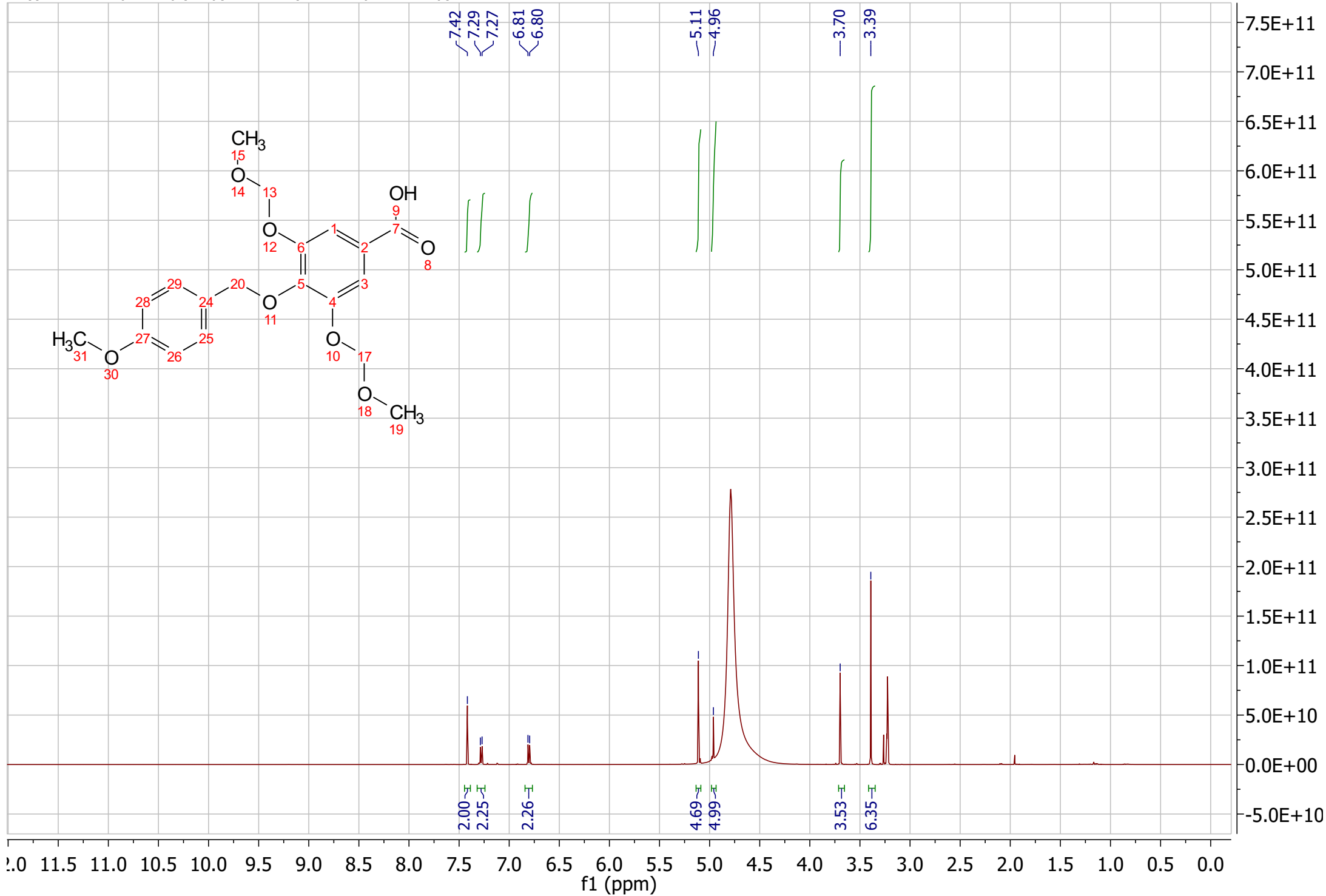
3,5-bis(methoxymethoxy)-4-(naphth-2-ylmethoxy)benzoic acid_DMSO



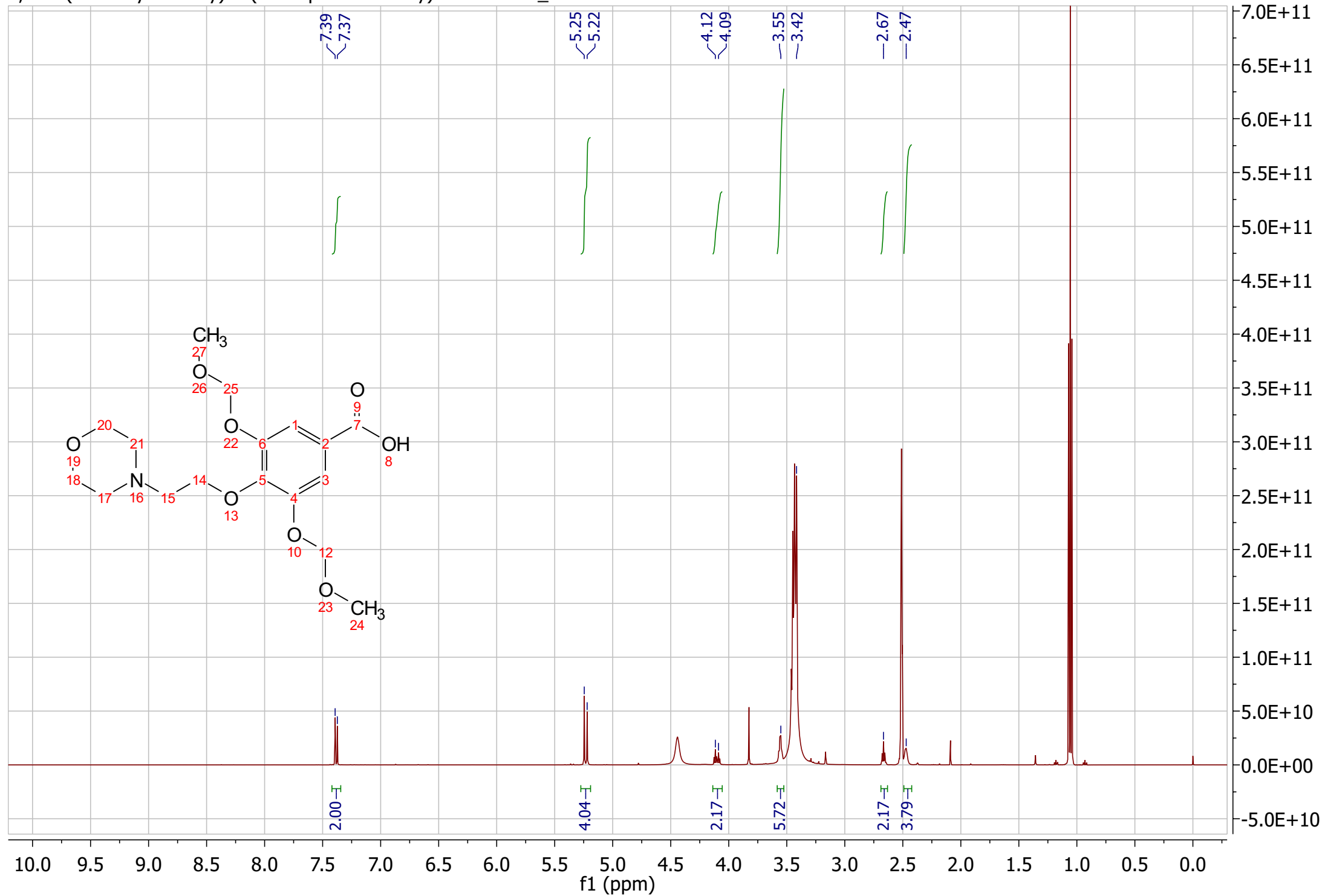
3,5-bis(methoxymethoxy)-4-(naphth-2-ylmethoxy)benzoic acid_DMSO



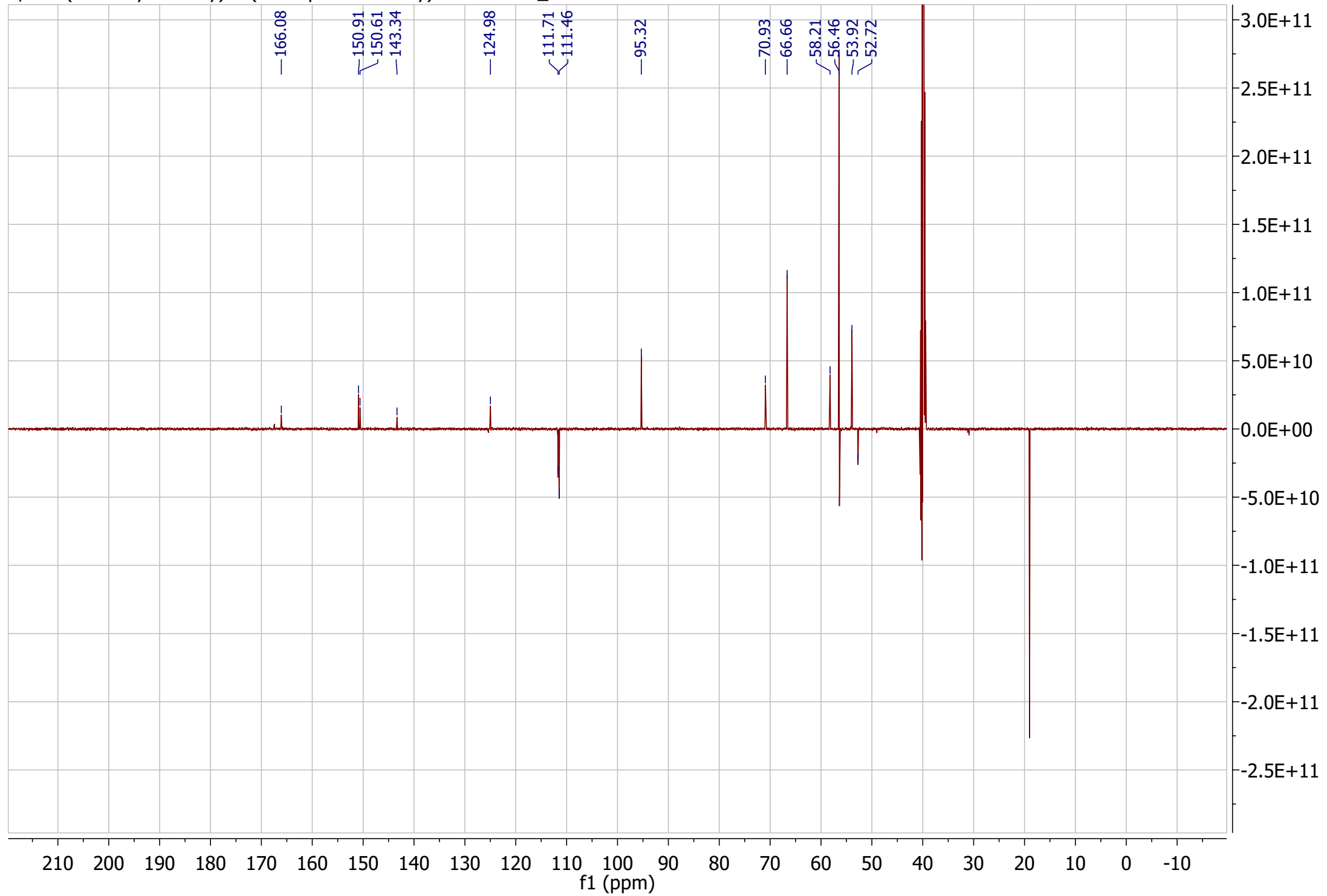
4-((4-methoxybenzyl)oxy)-3,5-bis(methoxymethoxy)benzoic acid_MeOD



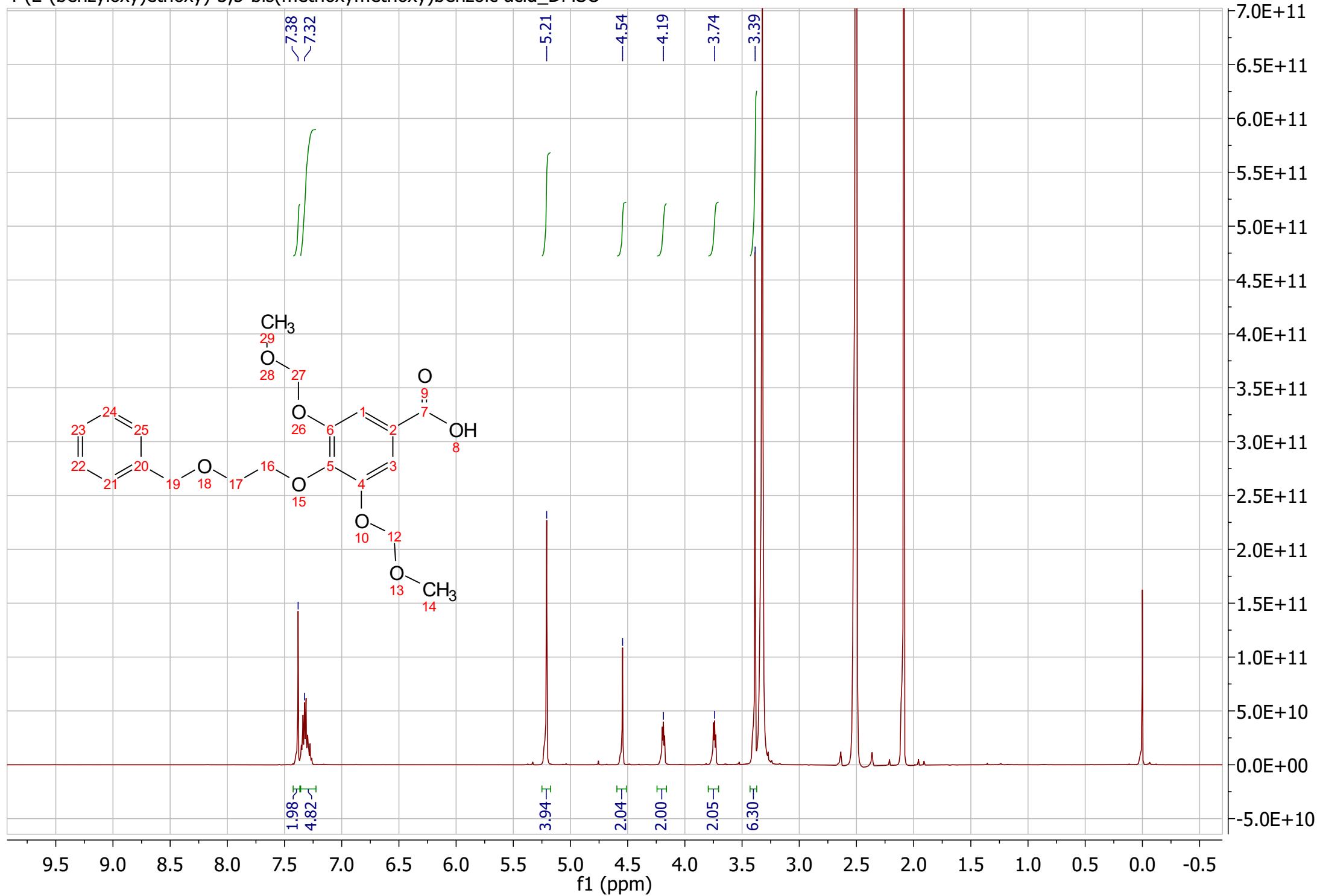
3,5-bis(methoxymethoxy)-4-(2-morpholinoethoxy)benzoic acid_DMSO



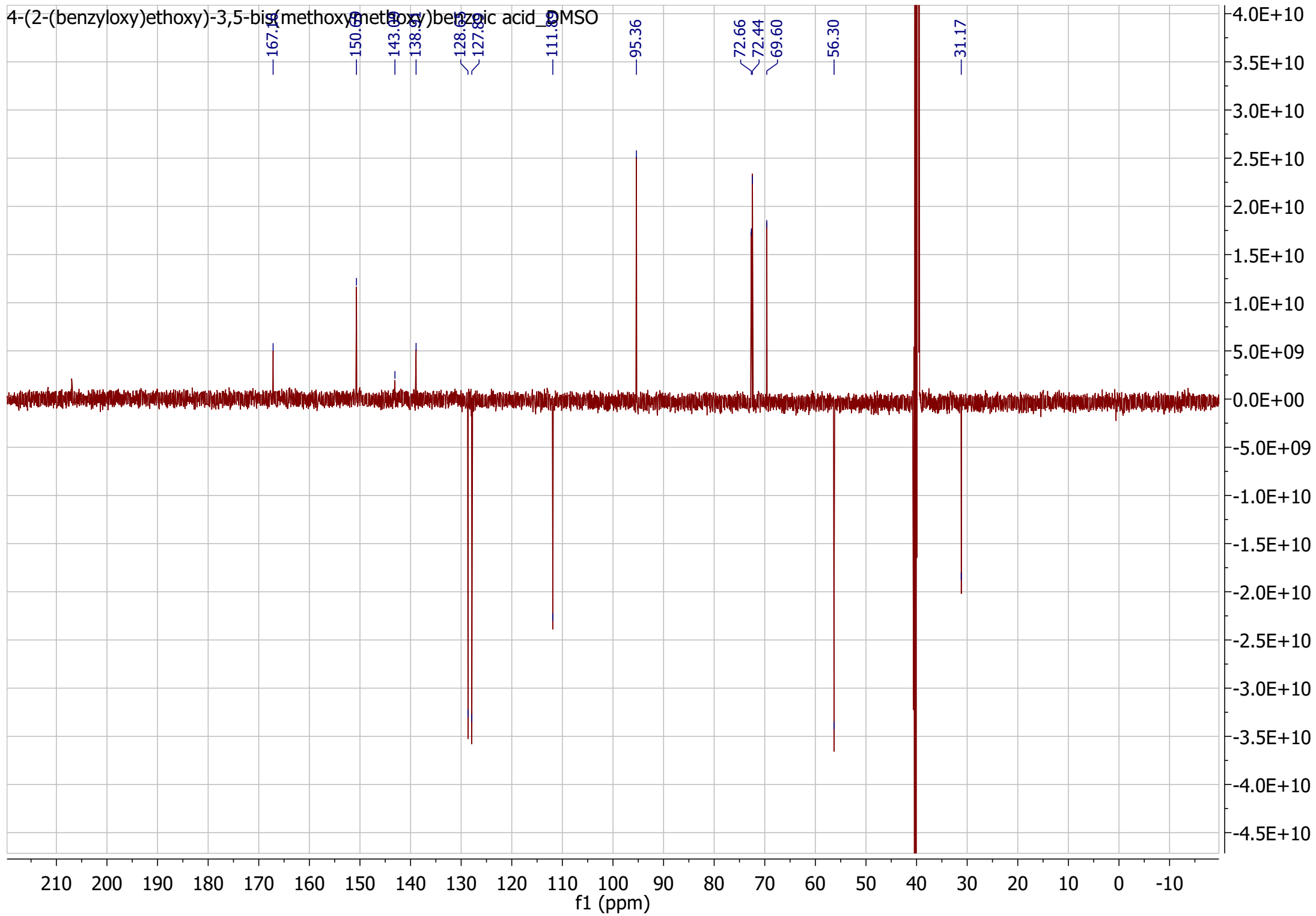
3,5-bis(methoxymethoxy)-4-(2-morpholinoethoxy)benzoic acid_DMSO



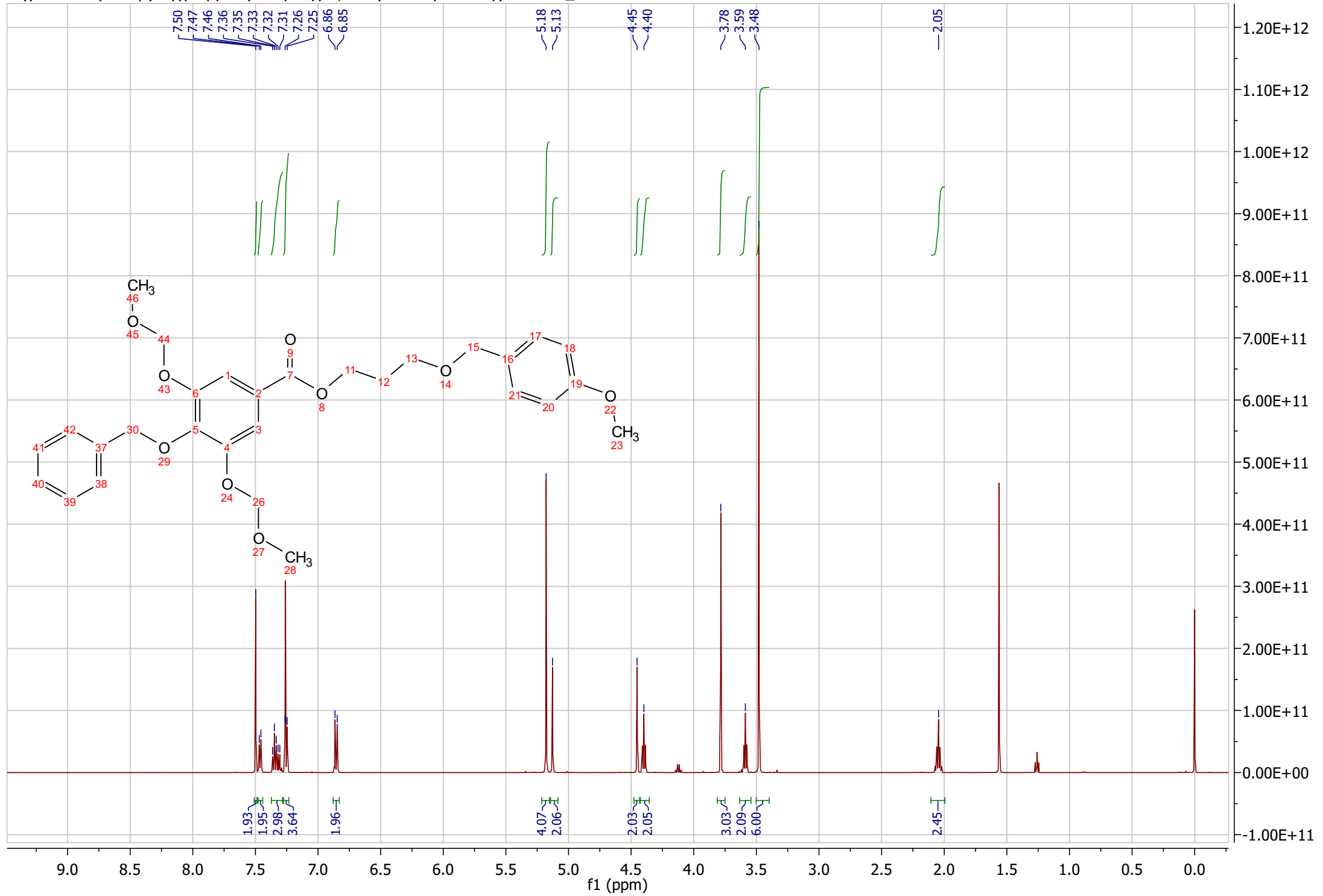
4-(2-(benzyloxy)ethoxy)-3,5-bis(methoxymethoxy)benzoic acid_DMSO



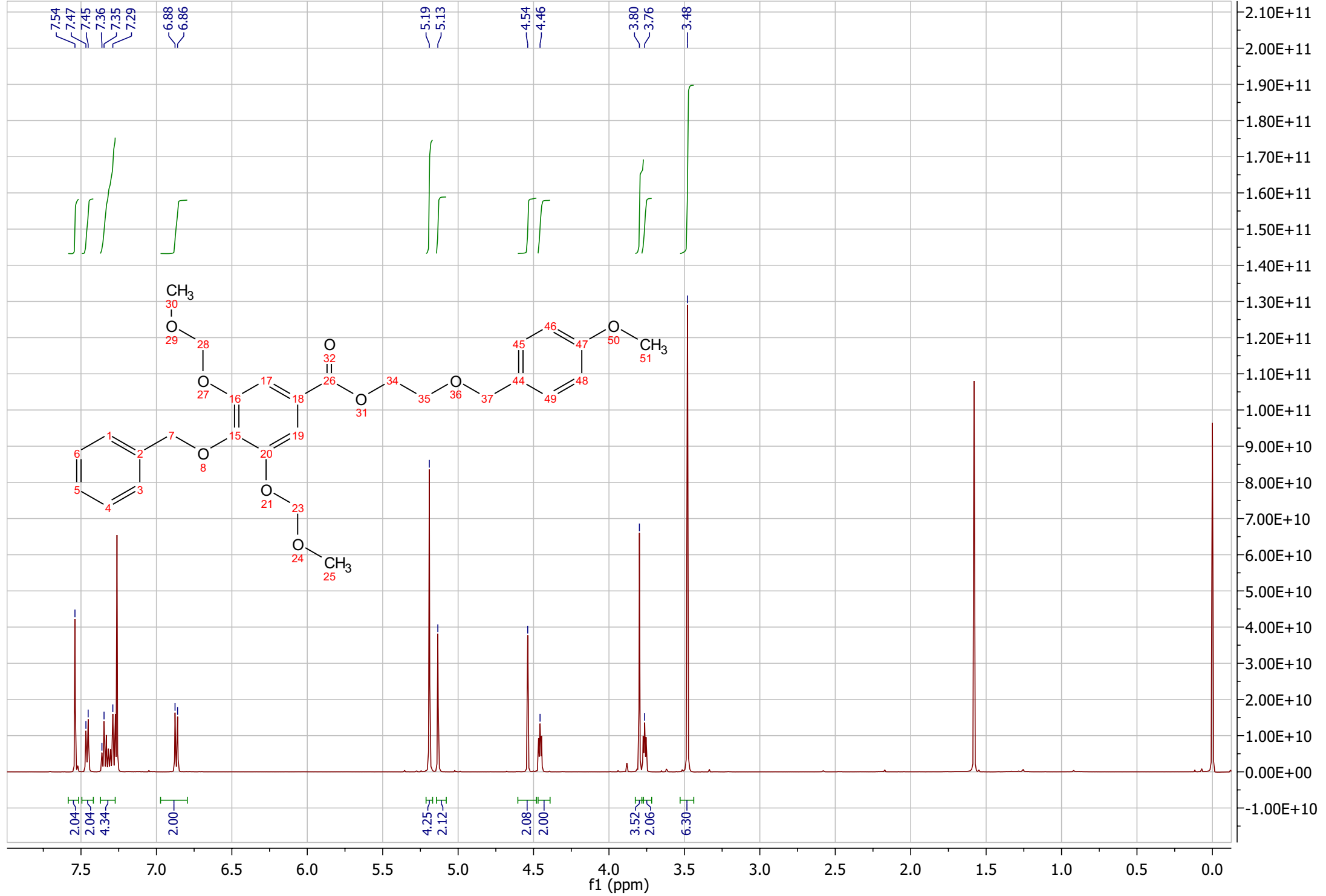
4-(2-(benzyloxy)ethoxy)-3,5-bis(methoxy)benzoic acid_DMSO



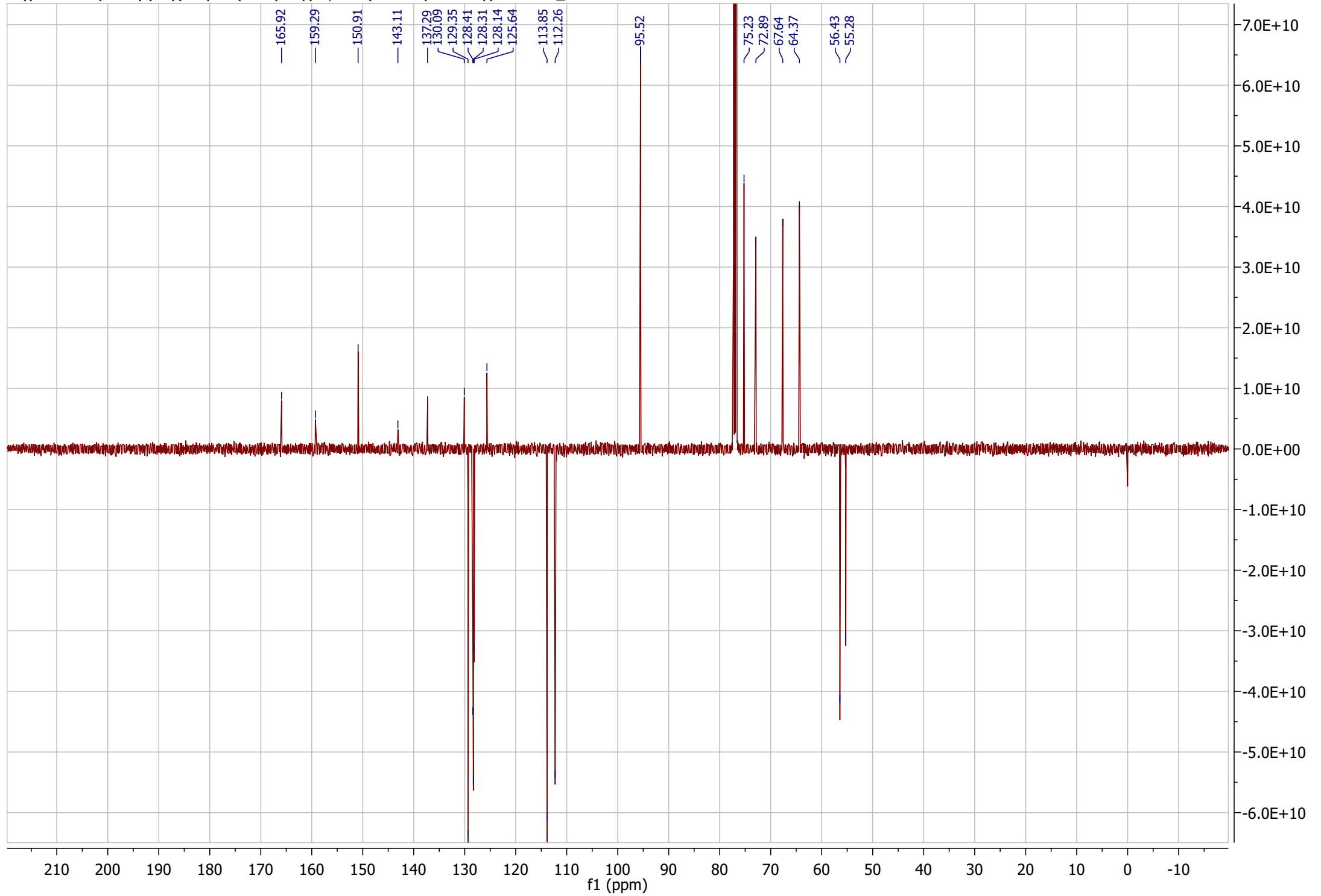
3-((4-methoxybenzyloxy)propyl 4-(benzyloxy)-3,5-bis(methoxymethoxy)benzoate_CDCl3



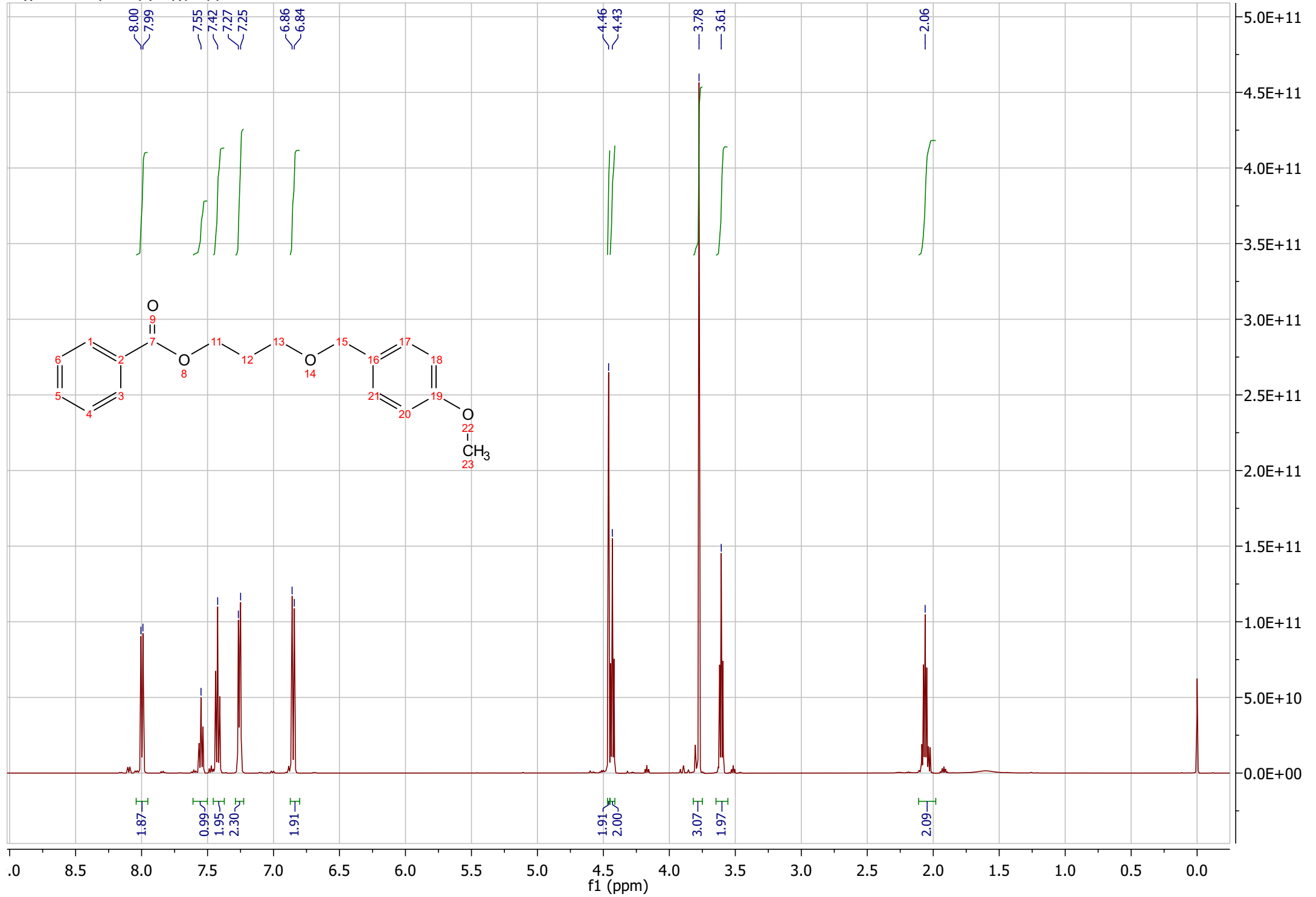
2-((4-methoxybenzyl)oxy)ethyl 4-(benzyloxy)-3,5-bis(methoxymethoxy)benzoate_CDCl3



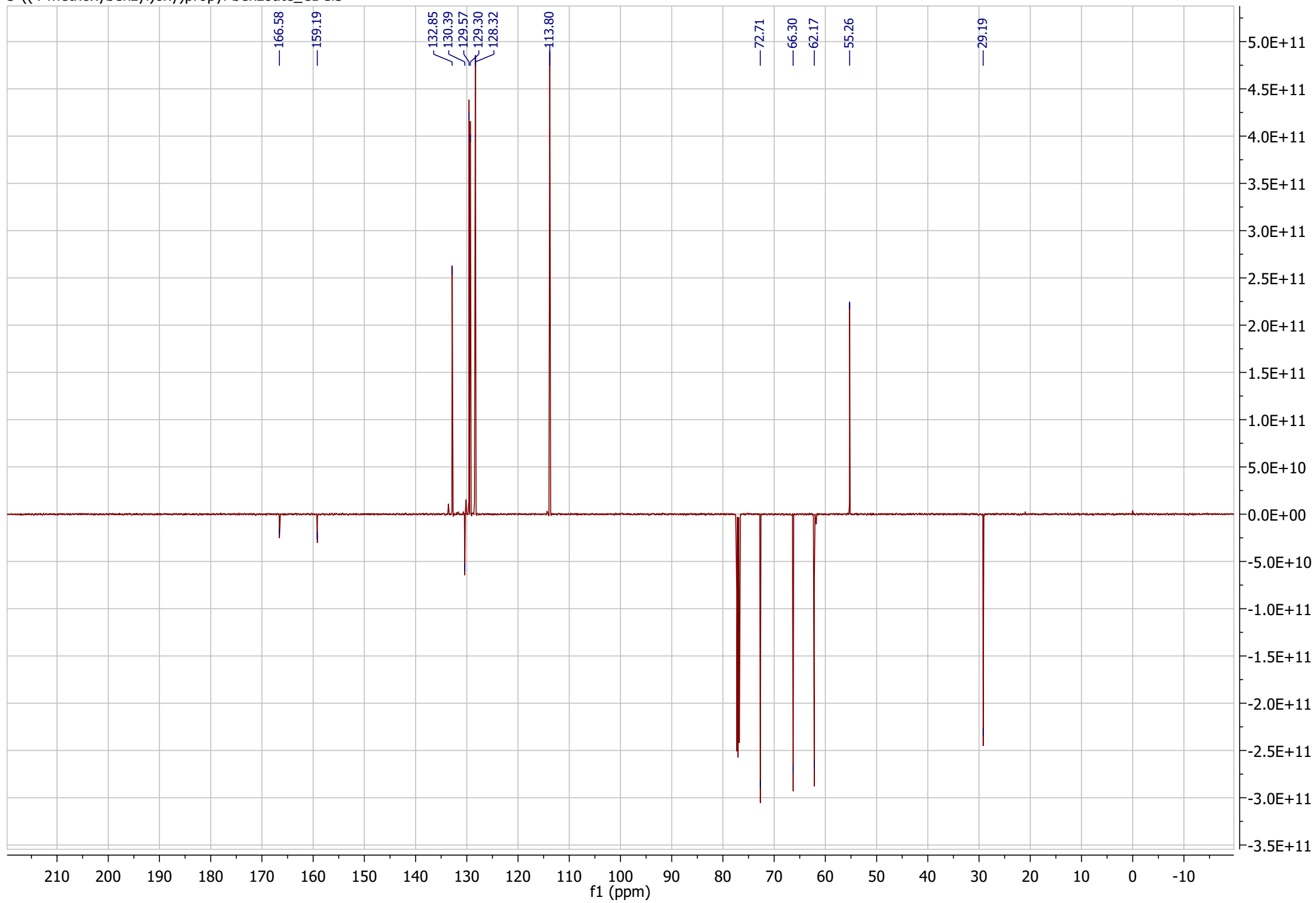
2-((4-methoxybenzyl)oxy)ethyl 4-(benzyloxy)-3,5-bis(methoxymethoxy)benzoate_CDCl3



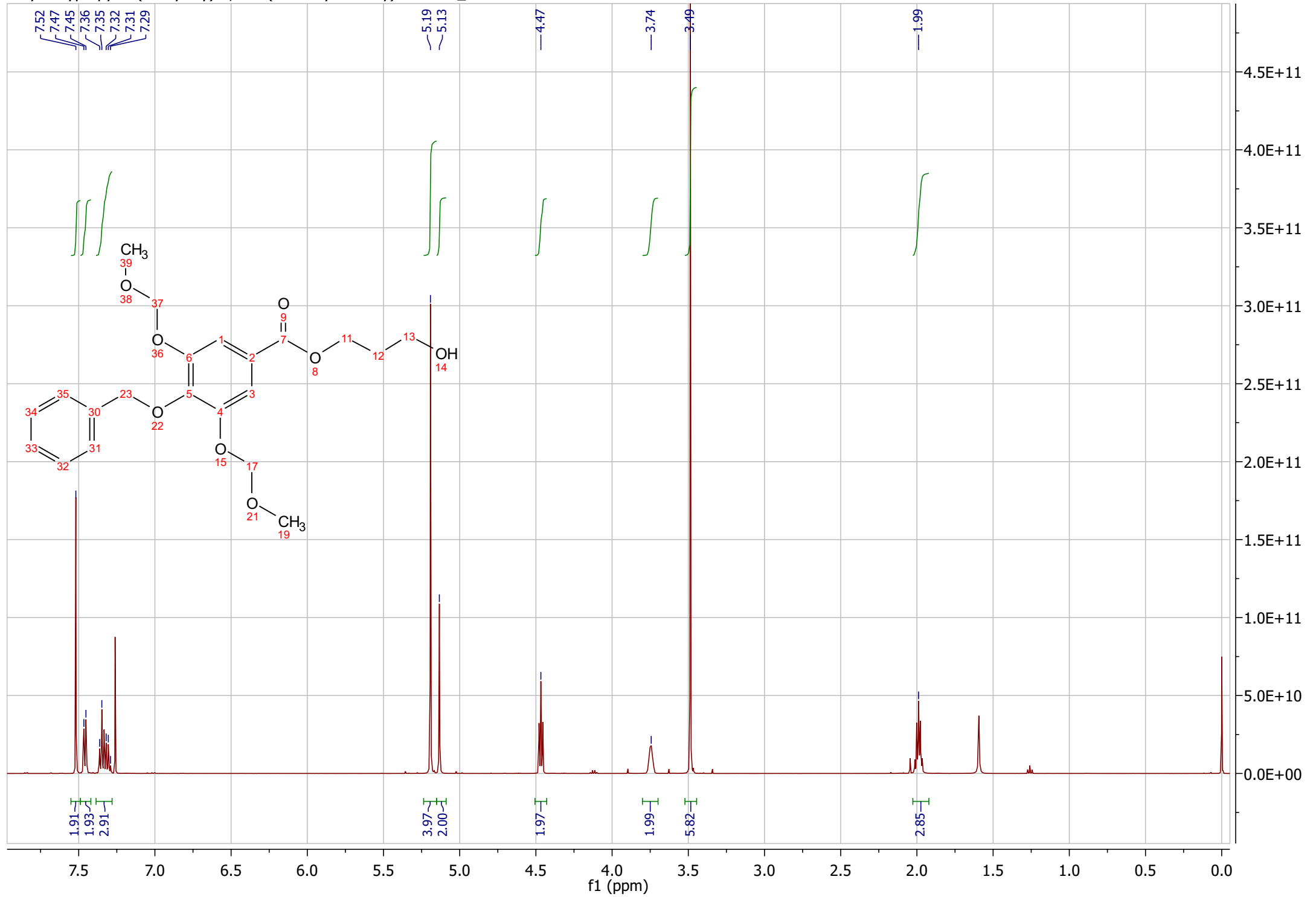
3-((4-methoxybenzyl)oxy)propyl benzoate_CDCl3



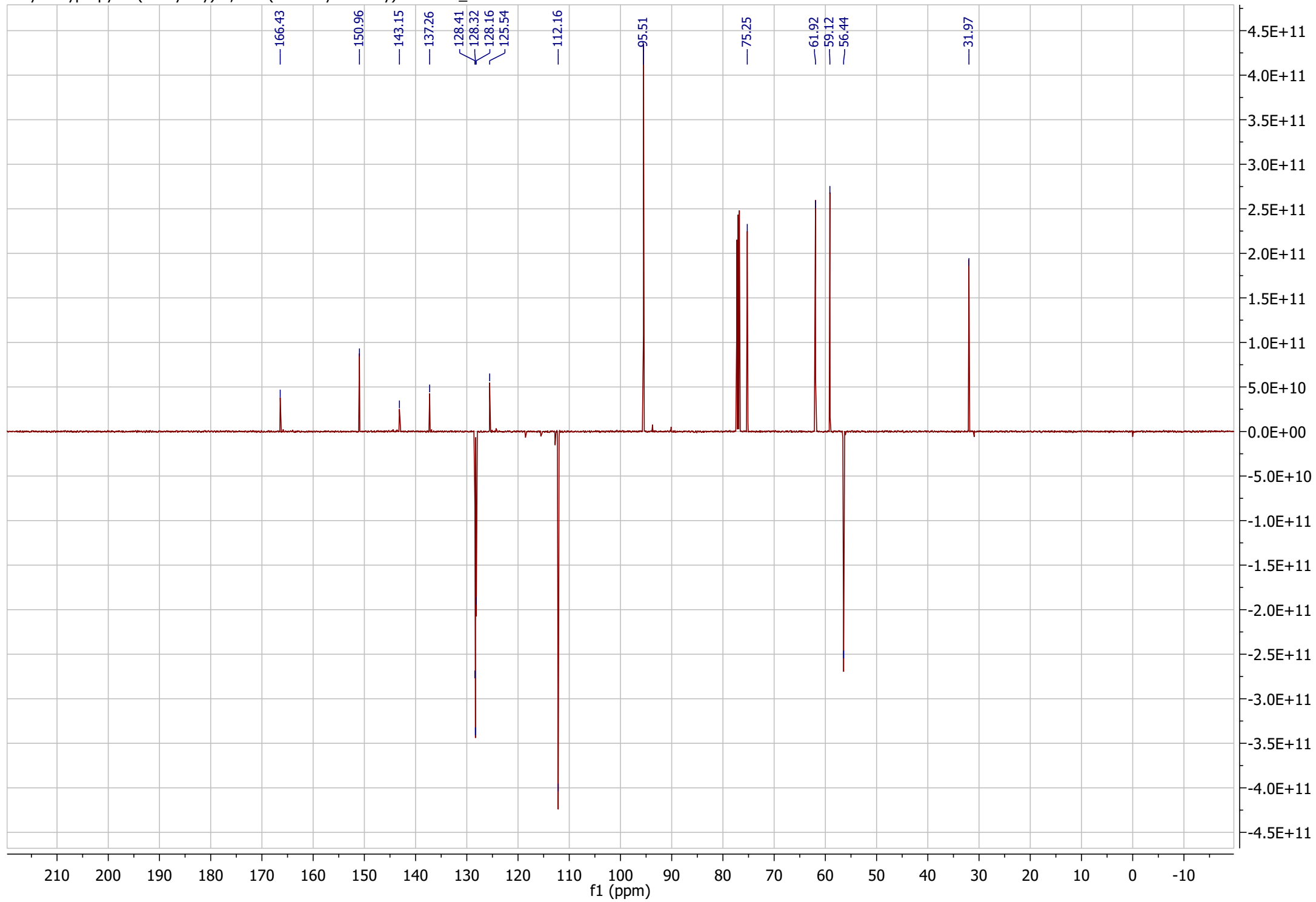
3-((4-methoxybenzyl)oxy)propyl benzoate_CDCl3



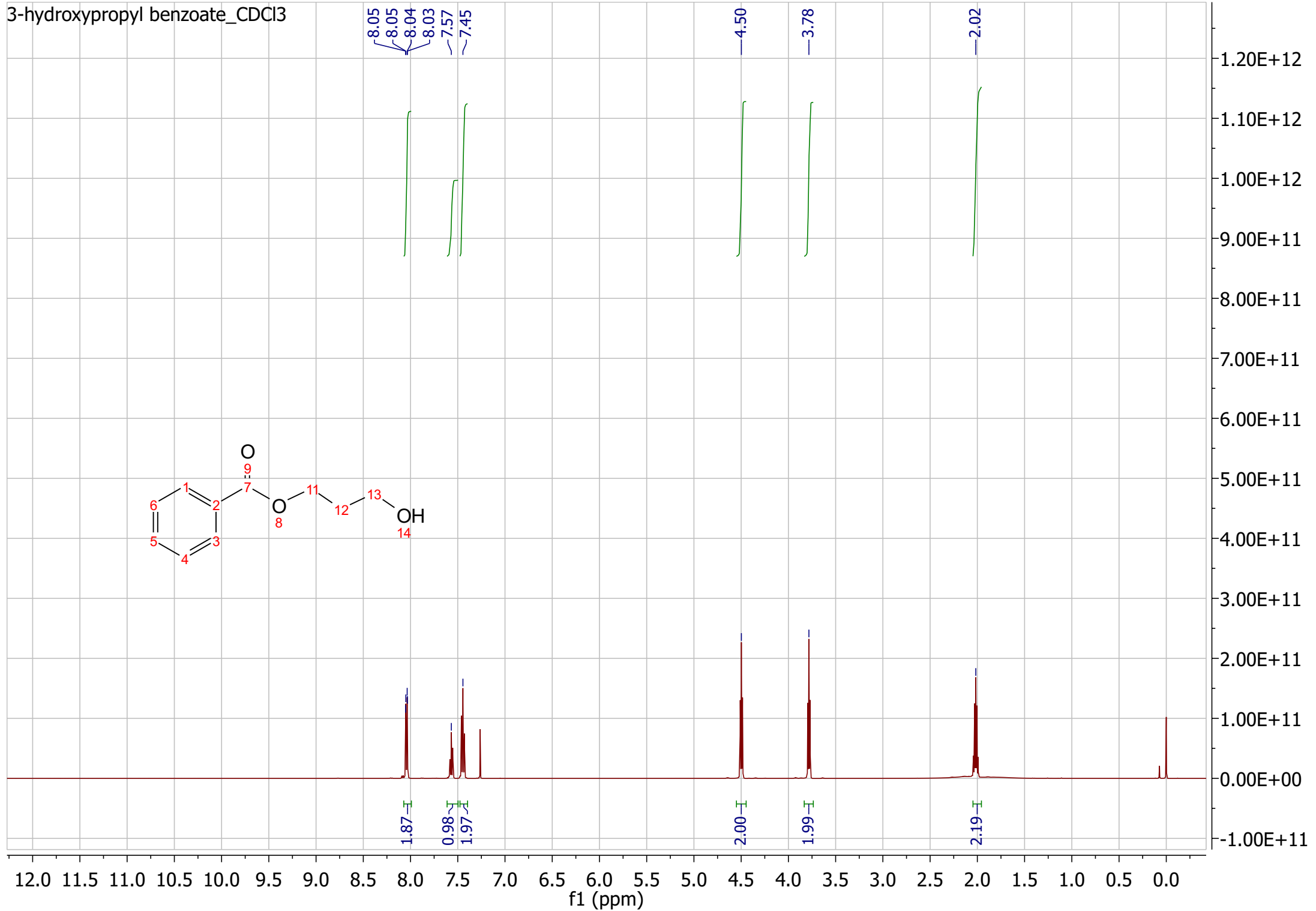
3-hydroxypropyl 4-(benzyloxy)-3,5-bis(methoxymethoxy)benzoate_CDCl3



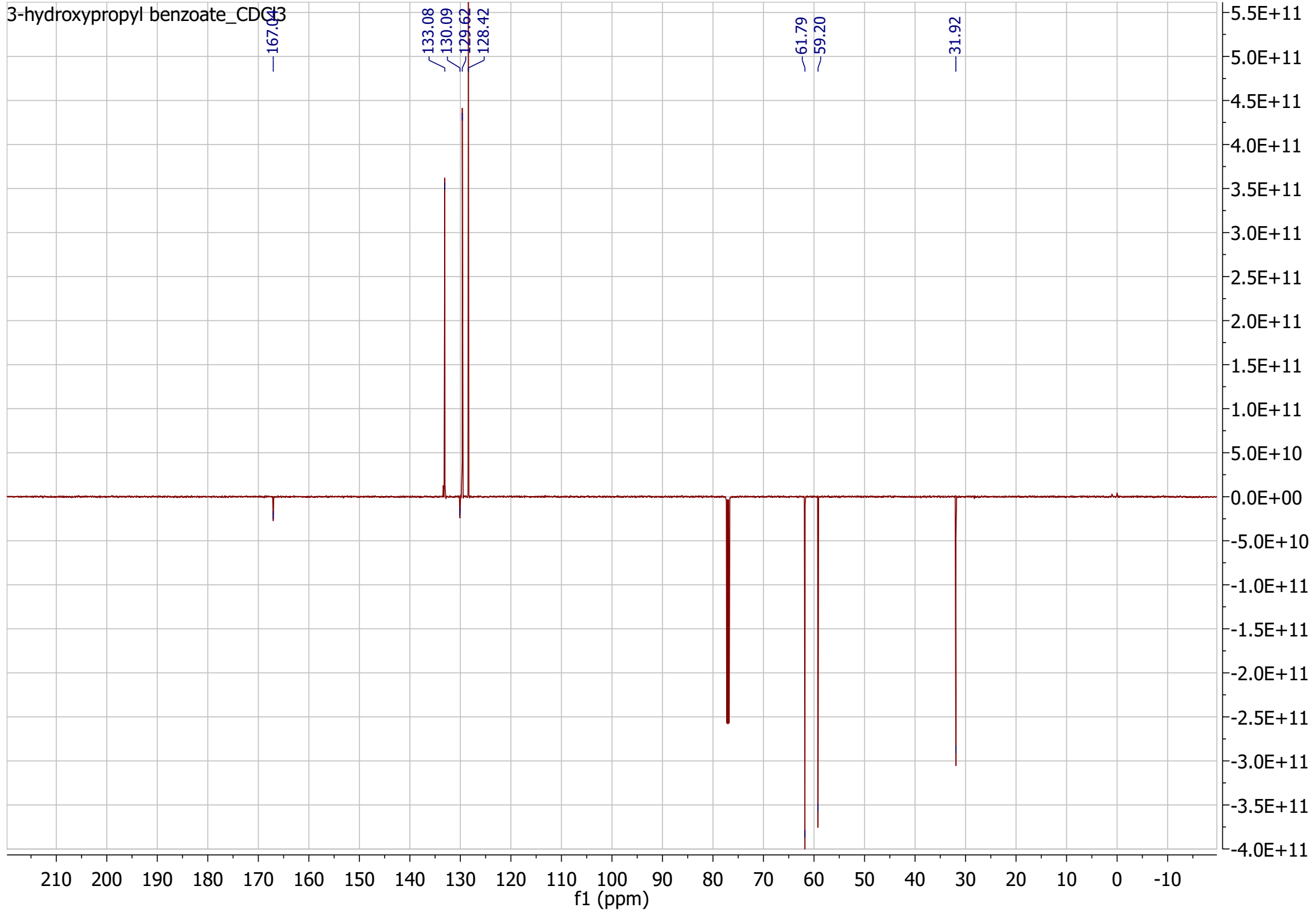
3-hydroxypropyl 4-(benzyloxy)-3,5-bis(methoxymethoxy)benzoate_CDCl3



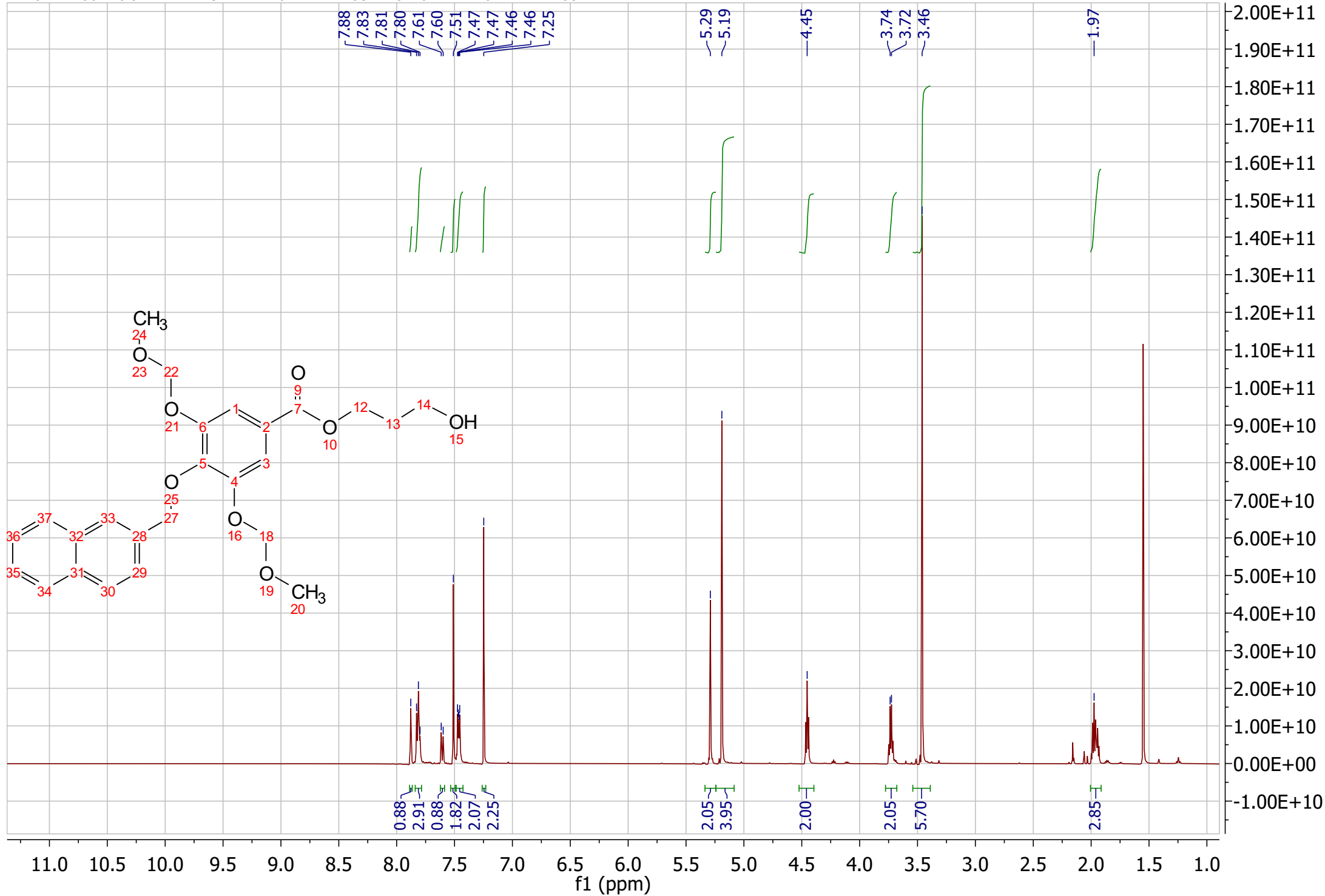
3-hydroxypropyl benzoate_CDCl3



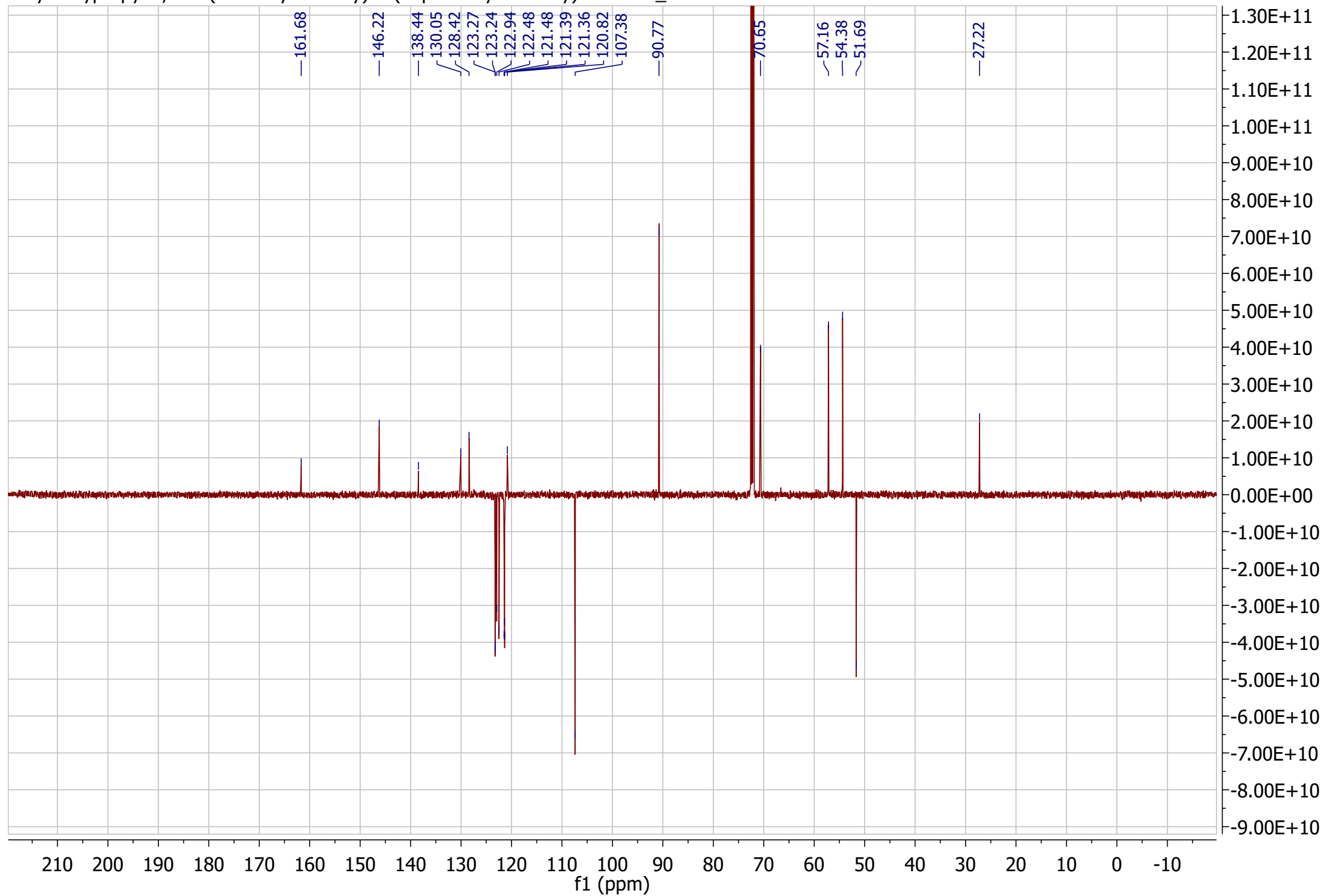
3-hydroxypropyl benzoate_CDCl3



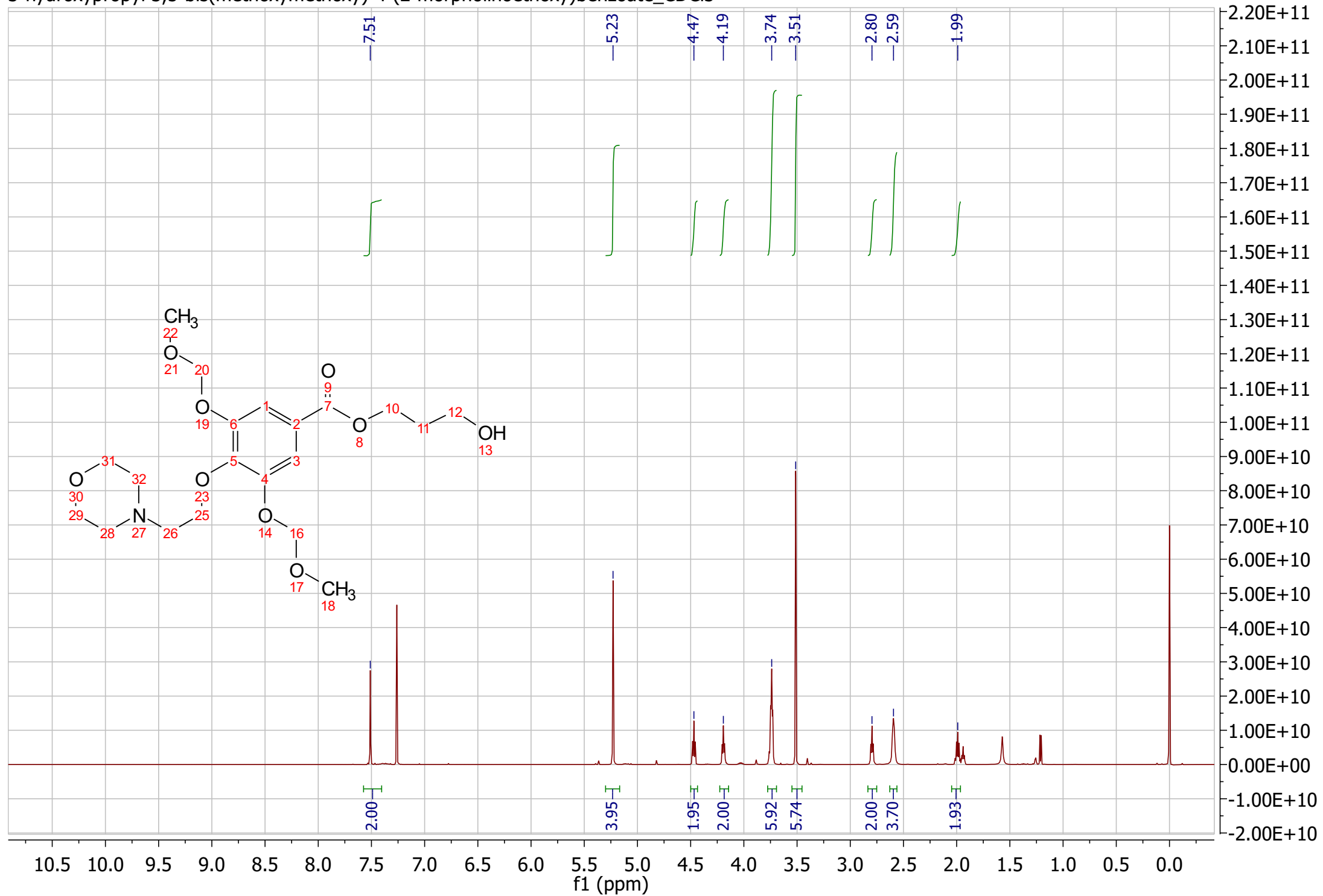
3-hydroxypropyl 3,5-bis(methoxymethoxy)-4-(naphth-2-ylmethoxy)benzoate_DMSO



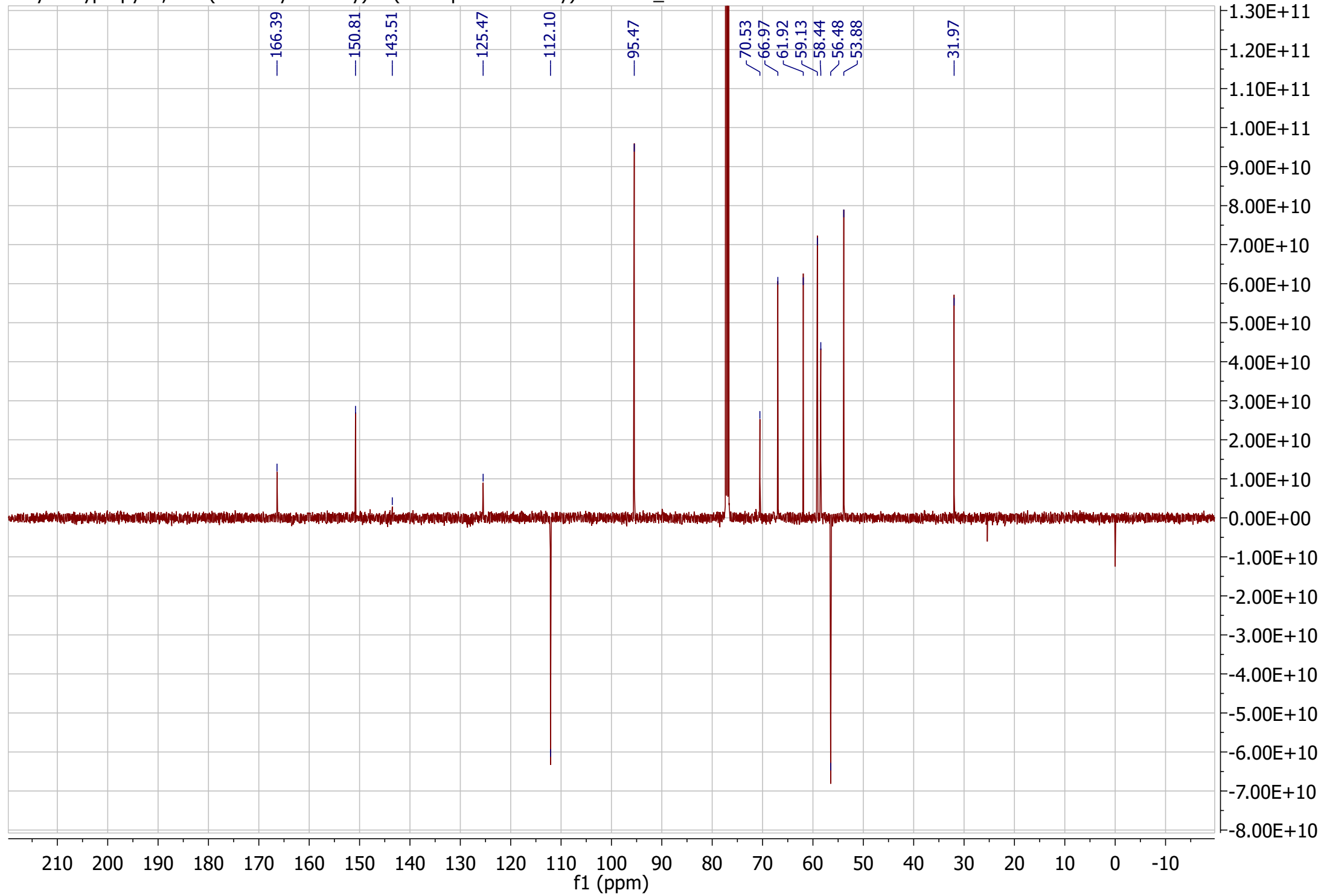
3-hydroxypropyl 3,5-bis(methoxymethoxy)-4-(naphth-2-ylmethoxy)benzoate_DMSO



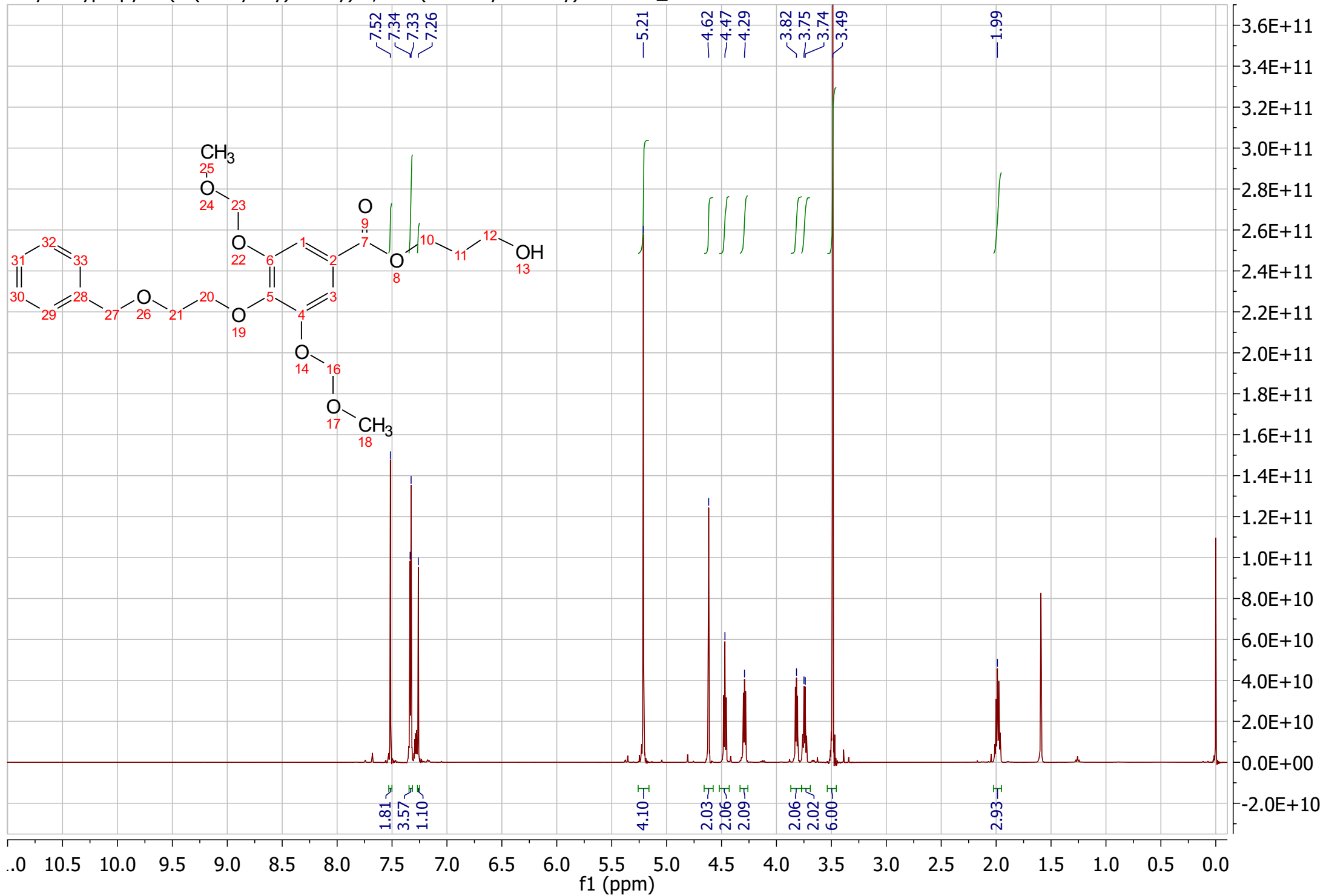
3-hydroxypropyl 3,5-bis(methoxymethoxy)-4-(2-morpholinoethoxy)benzoate_CDCl3



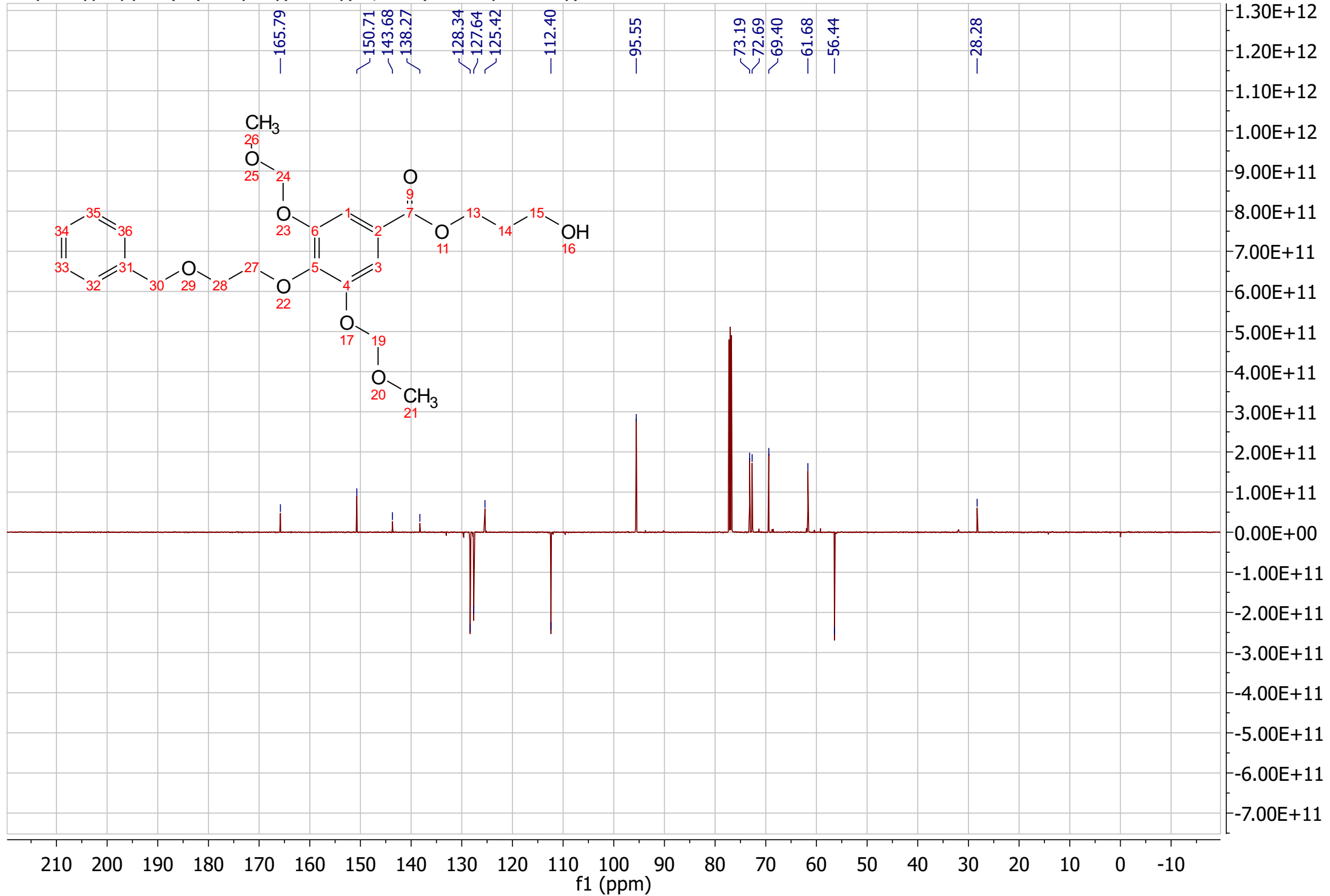
3-hydroxypropyl 3,5-bis(methoxymethoxy)-4-(2-morpholinoethoxy)benzoate_CDCl3



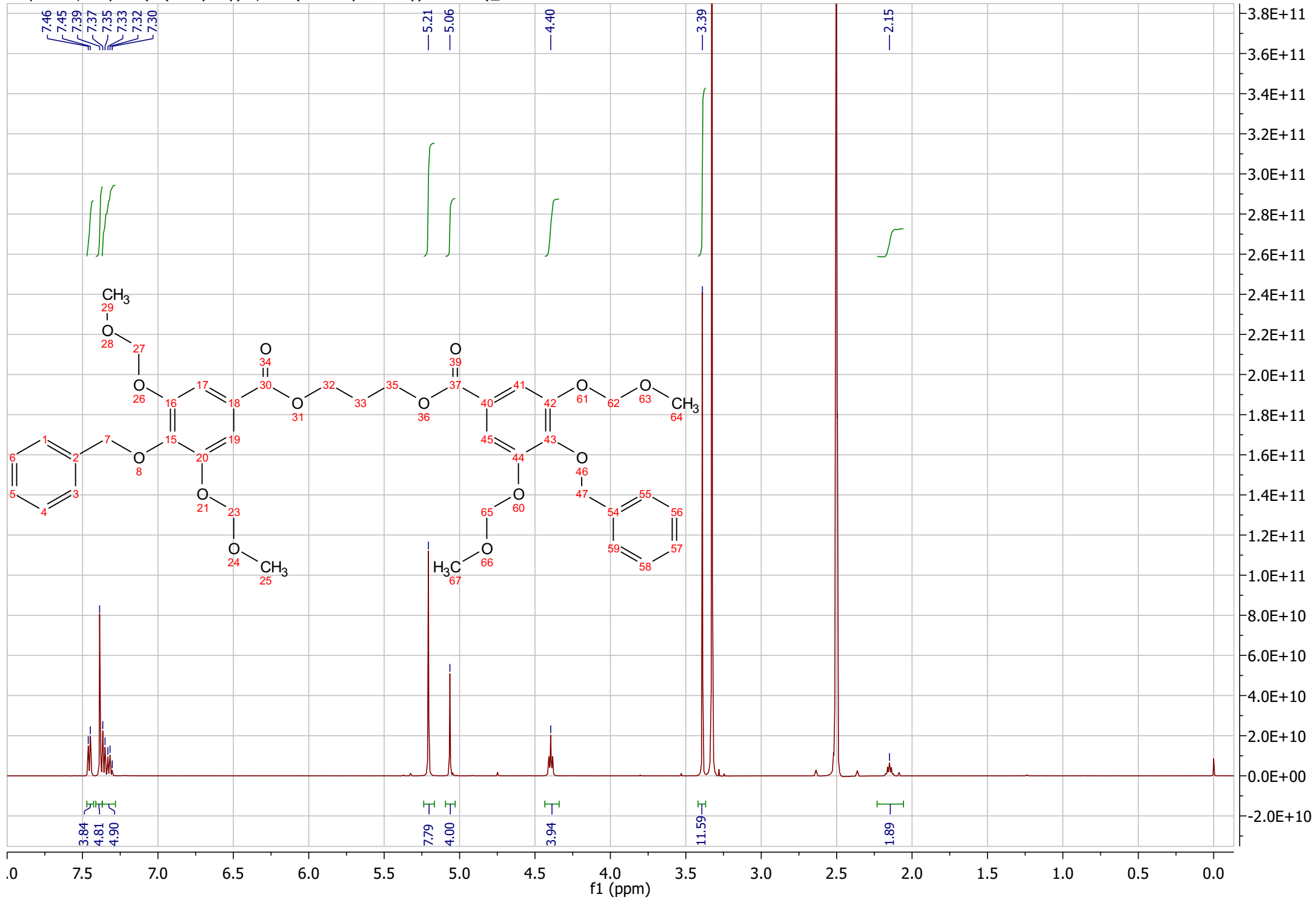
3-hydroxypropyl 4-(2-(benzyloxy)ethoxy)-3,5-bis(methoxymethoxy)benzoate_CDCl3



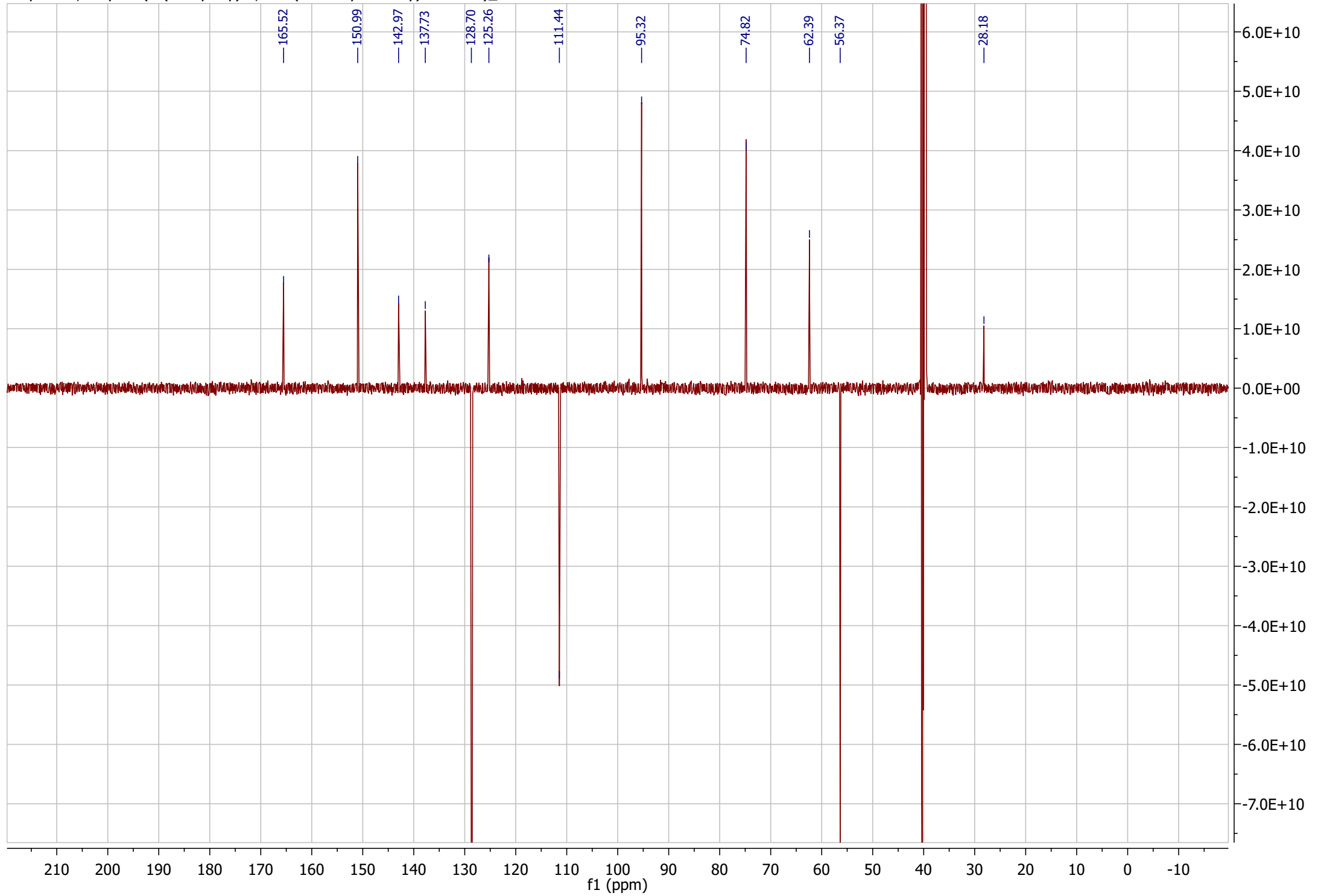
3-hydroxypropyl 4-(2-(benzyloxy)ethoxy)-3,5-bis(methoxymethoxy)benzoate_CDCl3



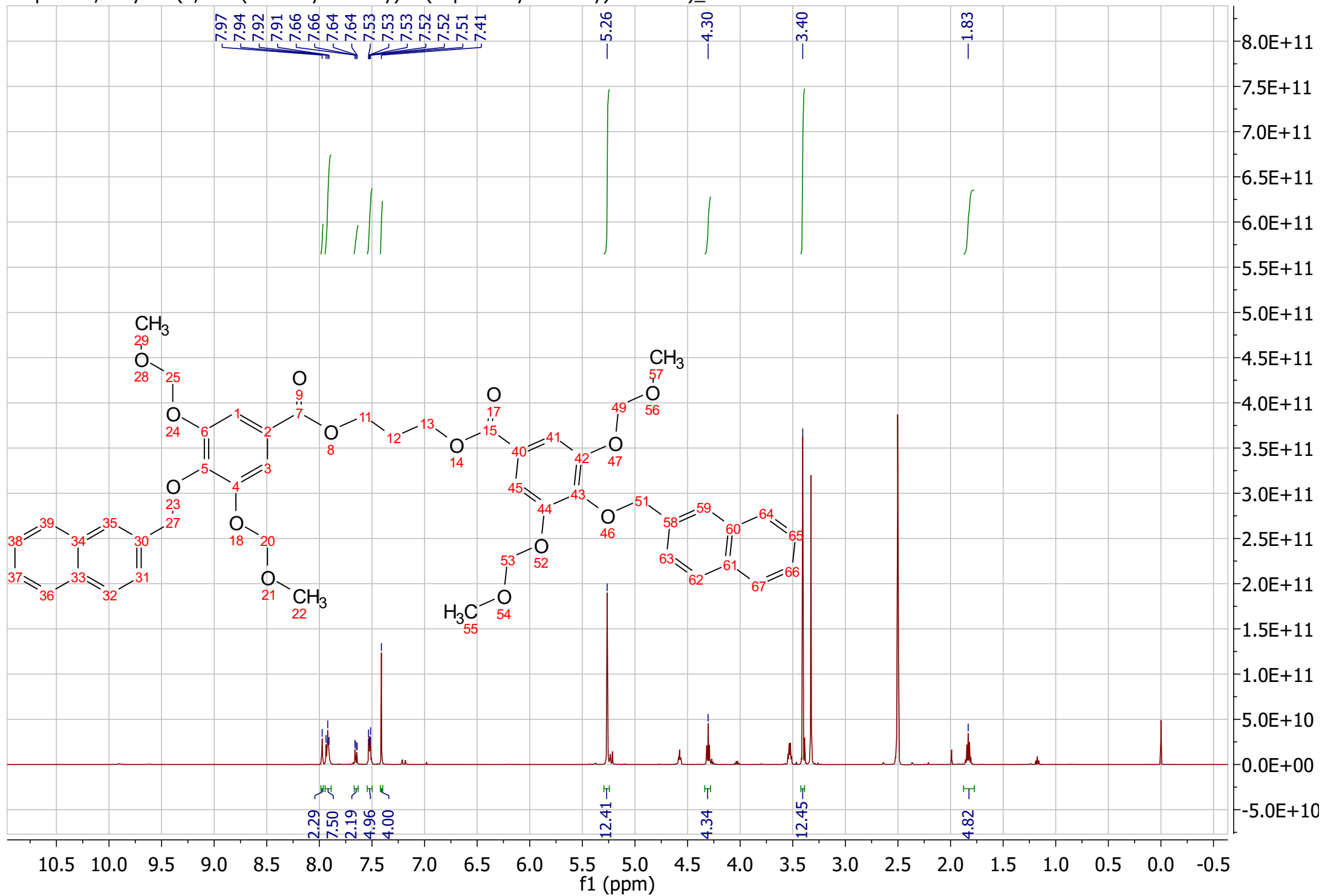
Propane-1,3-diyl bis(4-(benzyloxy)-3,5-bis(methoxymethoxy)benzoate)_DMSO



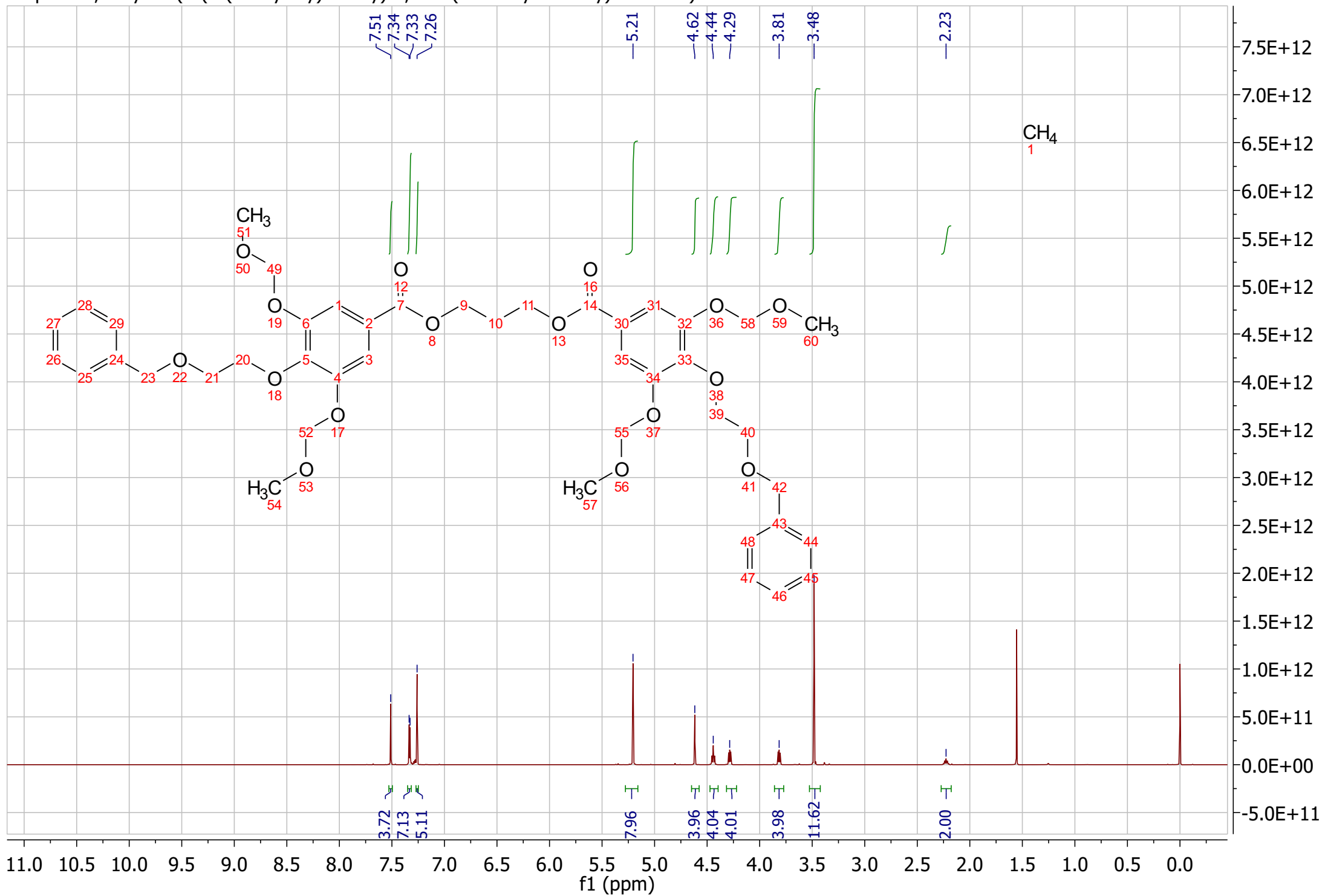
Propane-1,3-diyl bis(4-(benzyloxy)-3,5-bis(methoxymethoxy)benzoate)_DMSO



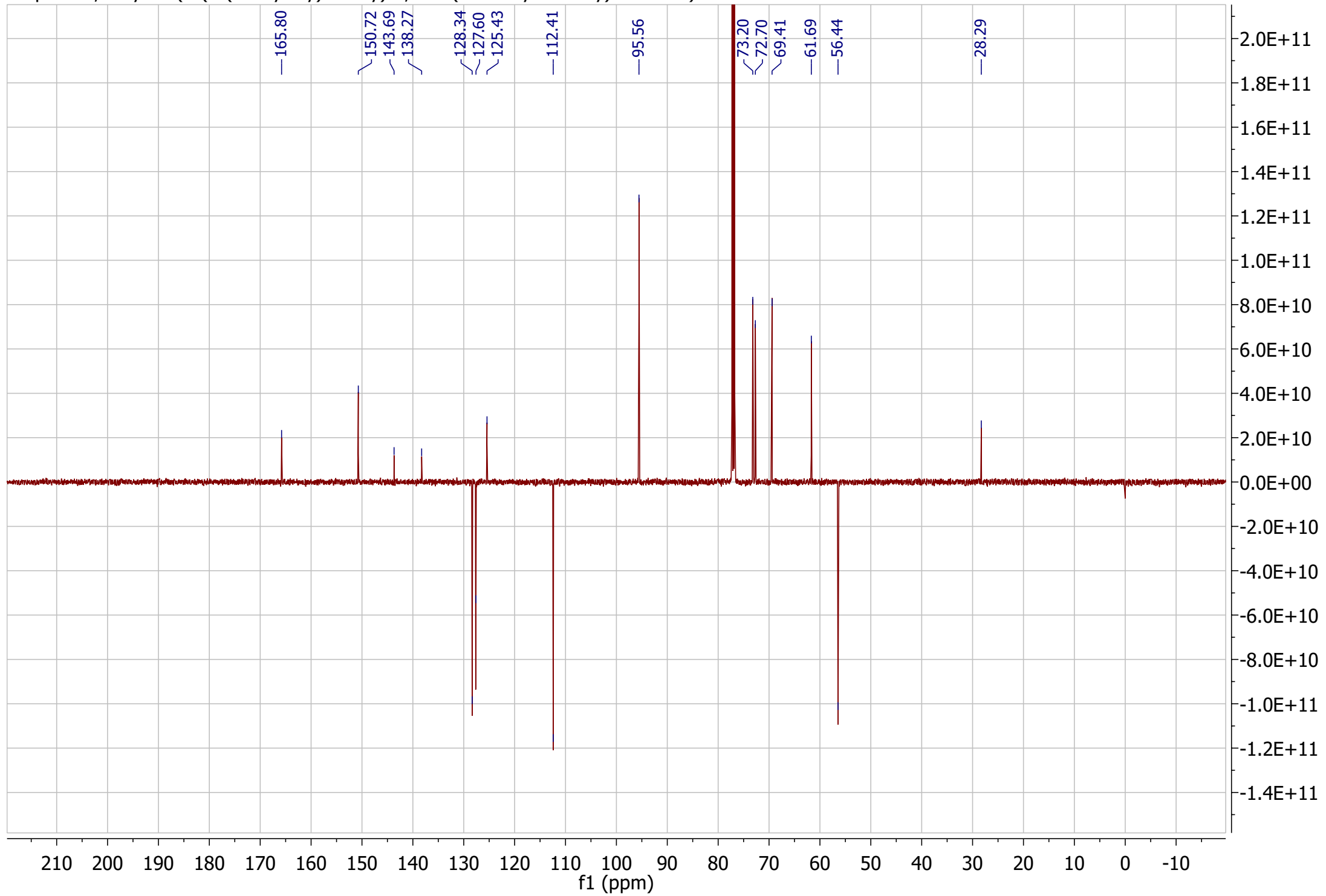
Propane-1,3-diyl bis(3,5-bis(methoxymethoxy)-4-(naphth-2-ylmethoxy)benzoate)_DMSO



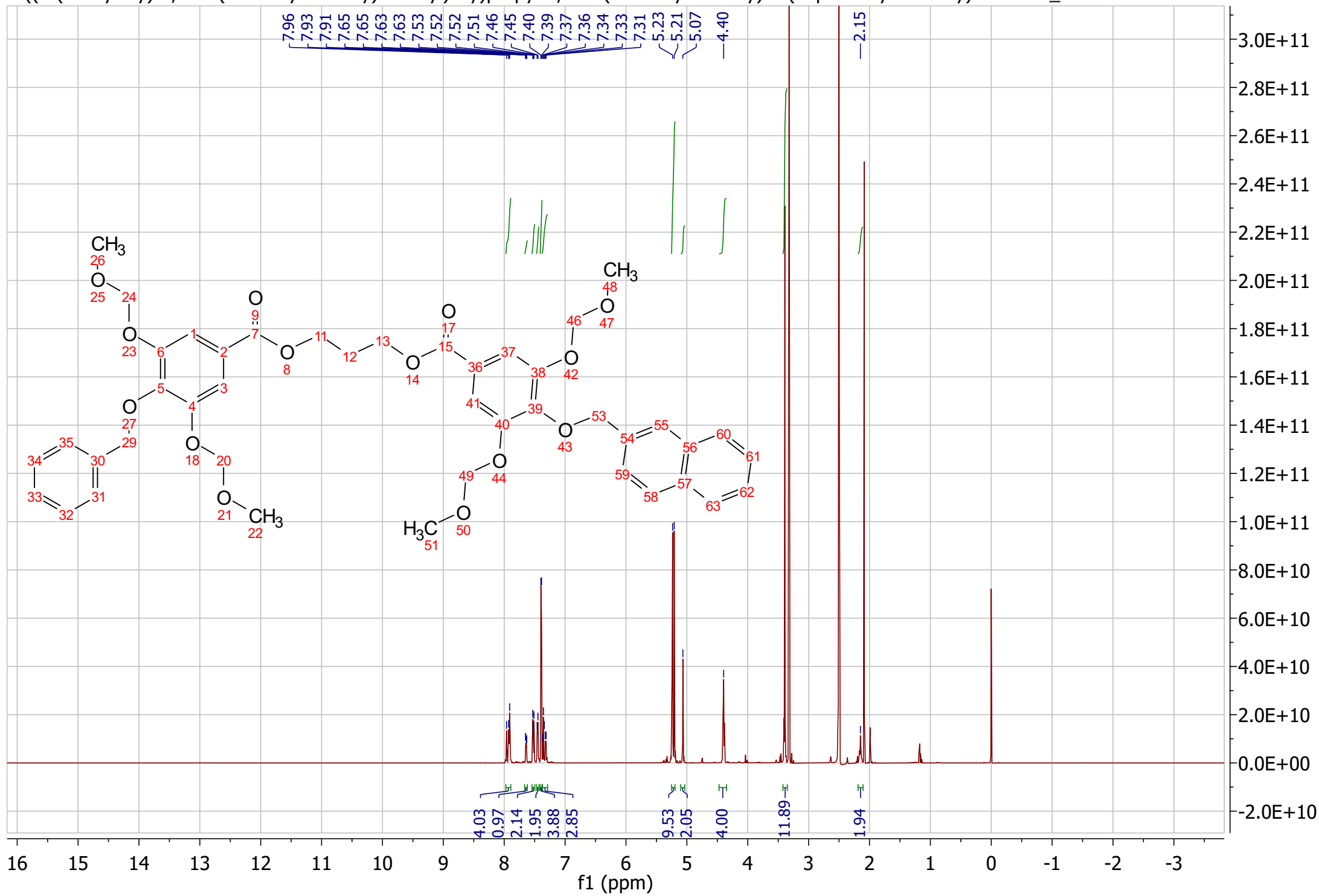
Propane-1,3-diyl bis(4-(2-(benzyloxy)ethoxy)-3,5-bis(methoxymethoxy)benzoate)



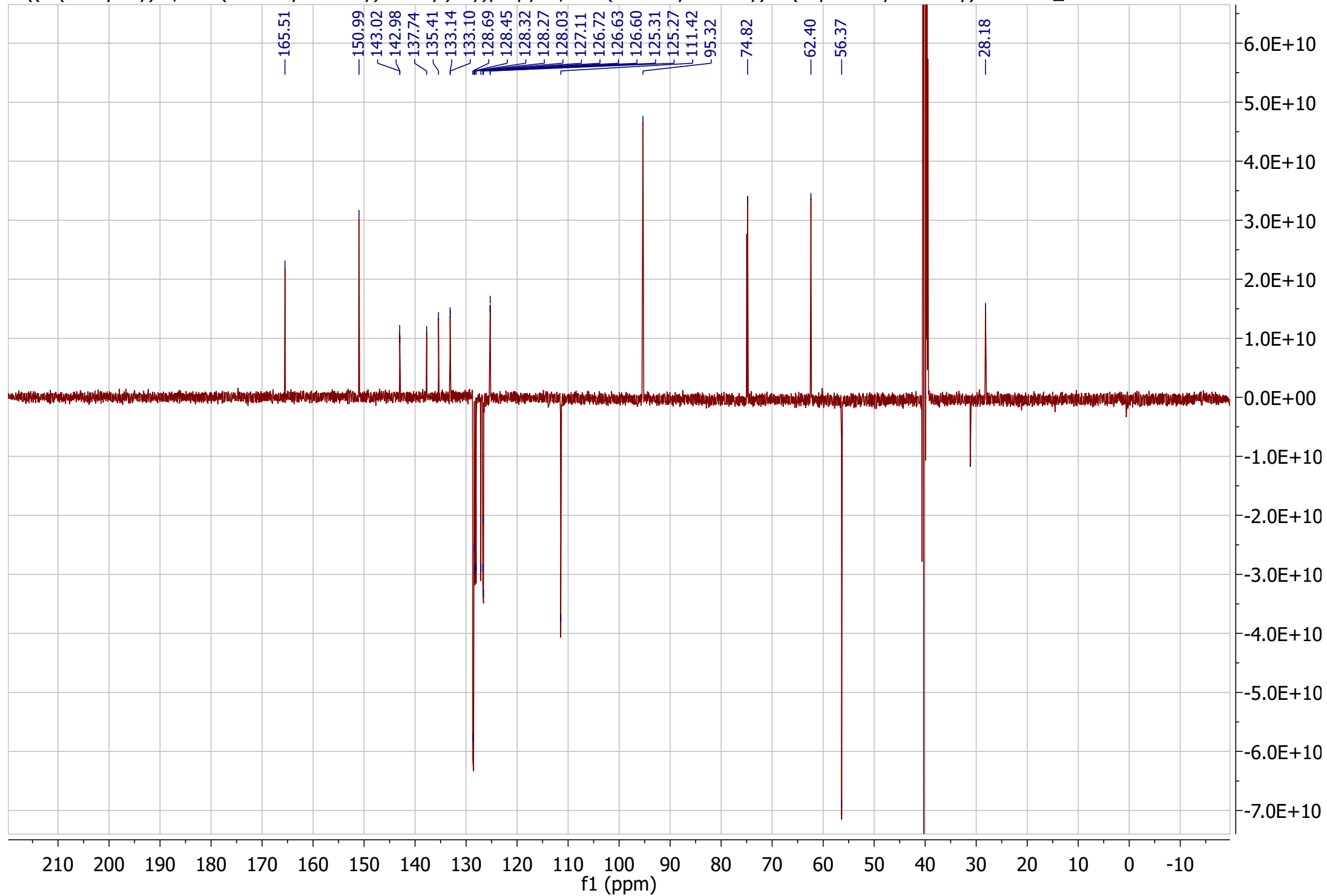
Propane-1,3-diyl bis(4-(2-(benzyloxy)ethoxy)-3,5-bis(methoxymethoxy)benzoate)



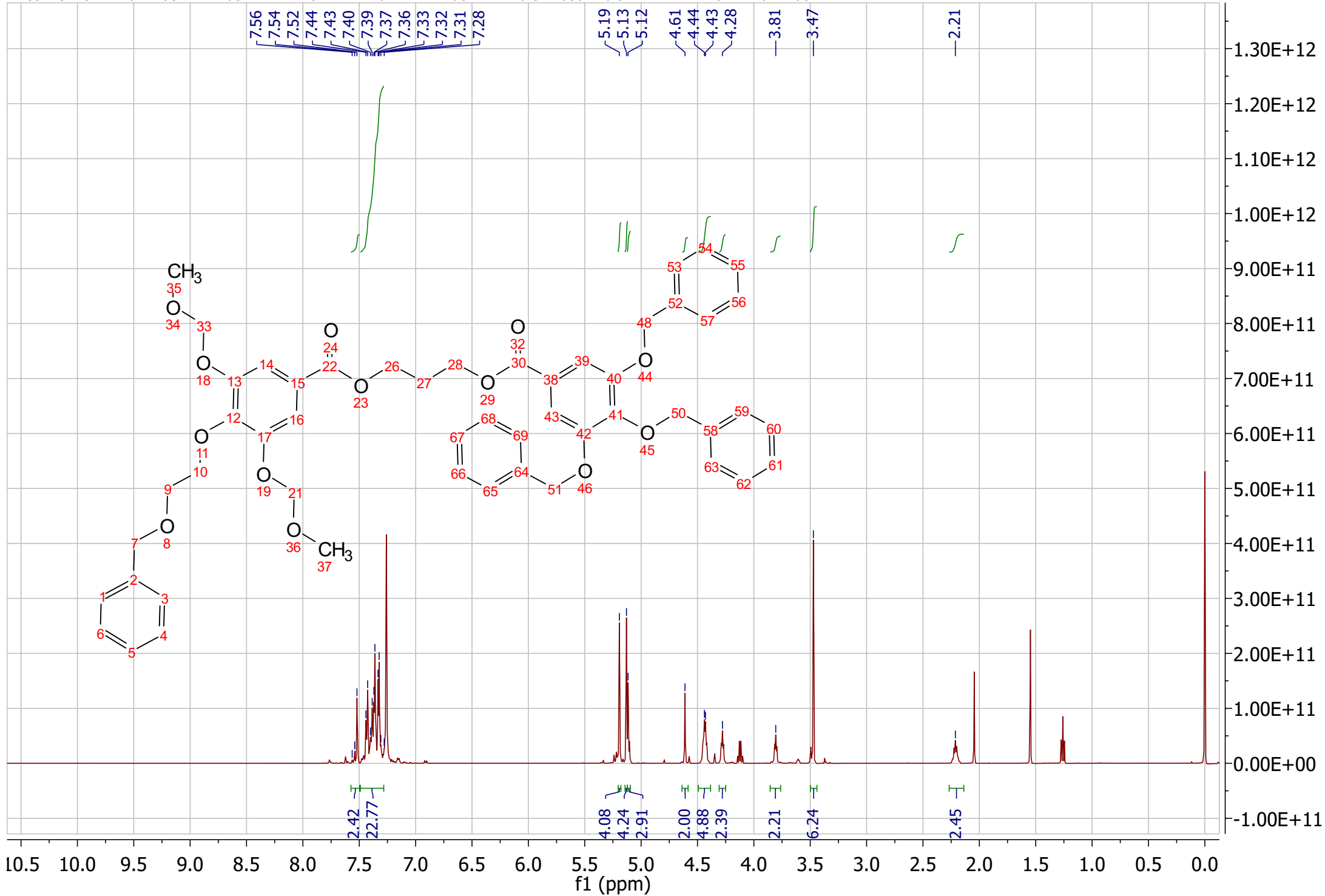
3-((4-(benzyloxy)-3,5-bis(methoxymethoxy)benzoyl)oxy)propyl-3,5-bis(methoxymethoxy)-4-(naphth-2-ylmethoxy)benzoate_DMSO



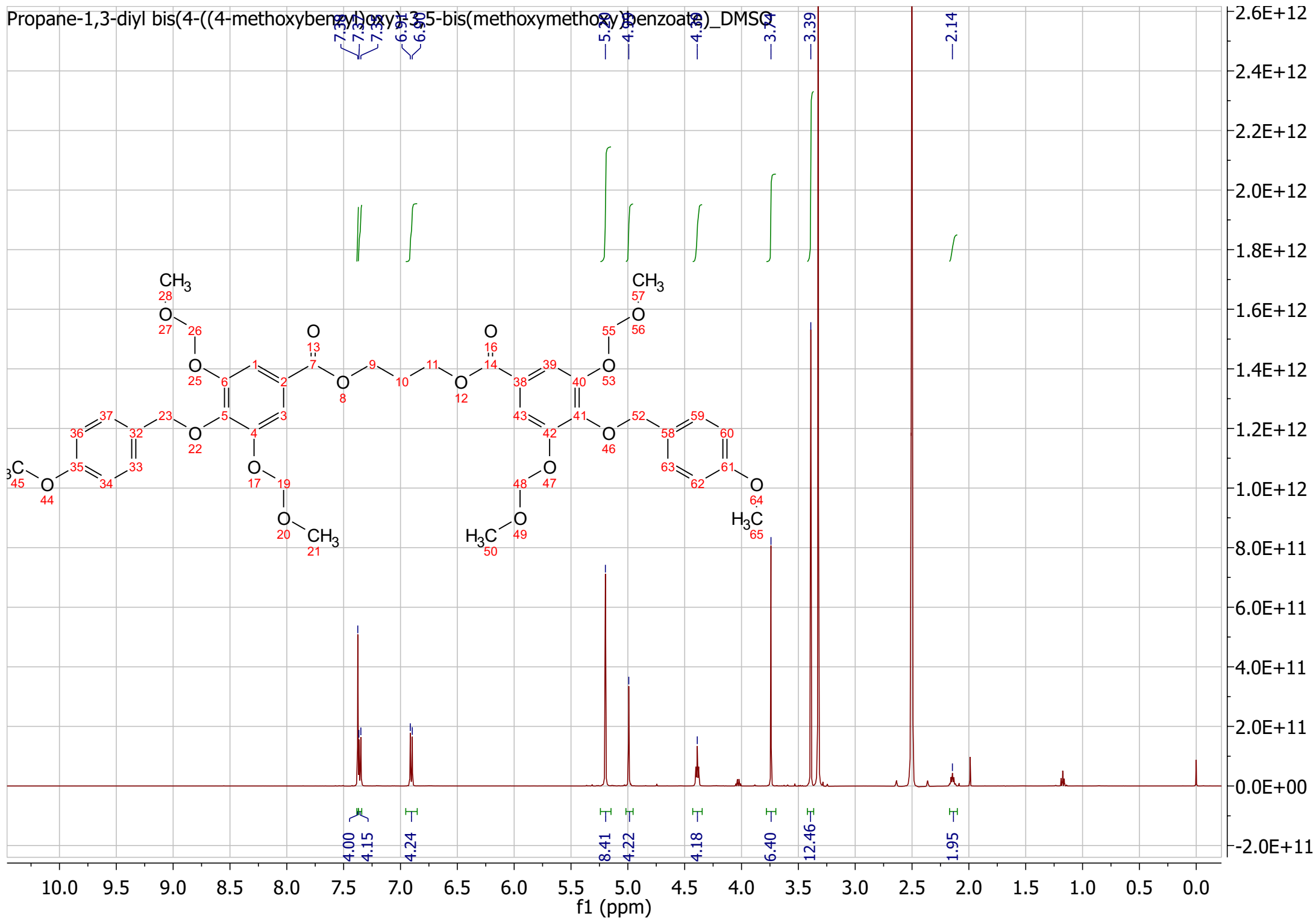
3-((4-(benzyloxy)-3,5-bis(methoxymethoxy)benzoyl)oxy)propyl-3,5-bis(methoxymethoxy)-4-(naphth-2-ylmethoxy)benzoate_DMSO



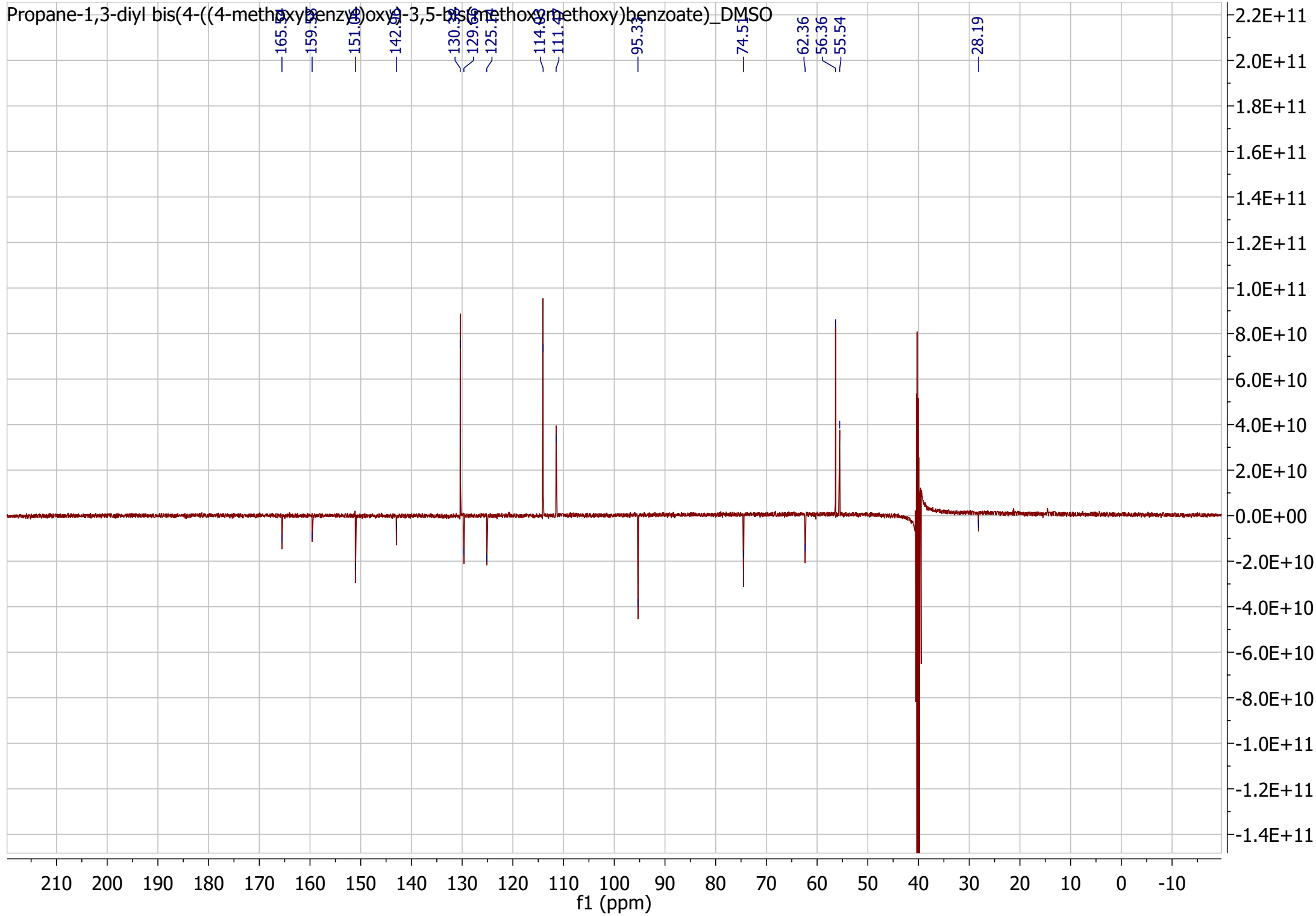
3-((4-(2-(benzyloxy)ethoxy)-3,5-bis(methoxymethoxy)benzoyl)oxy)propyl-3,4,5-tris(benzyloxy)benzoate_CDCl3



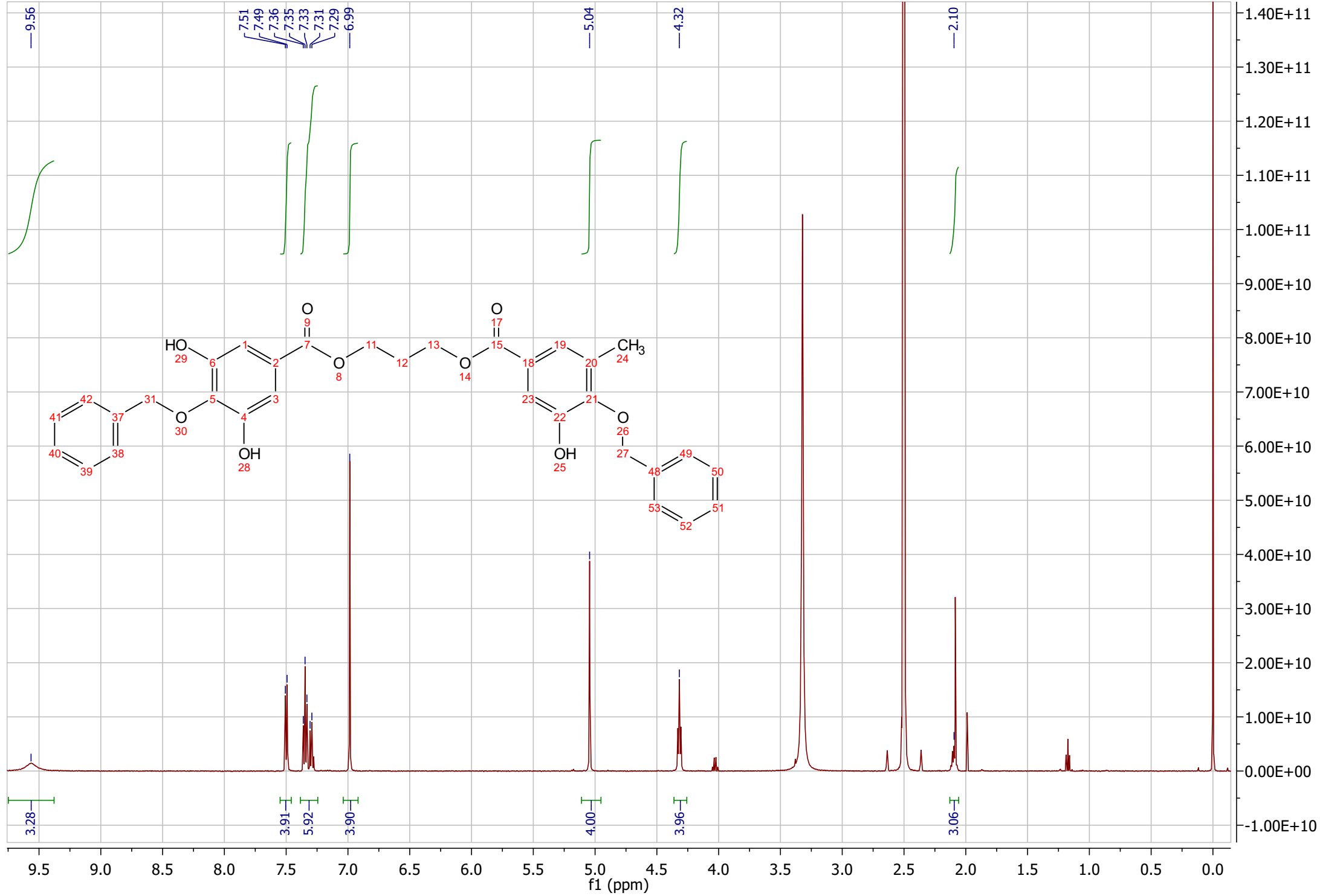
Propane-1,3-diyl bis(4-((4-methoxybenzyl)oxy)benzoate)_DMSO



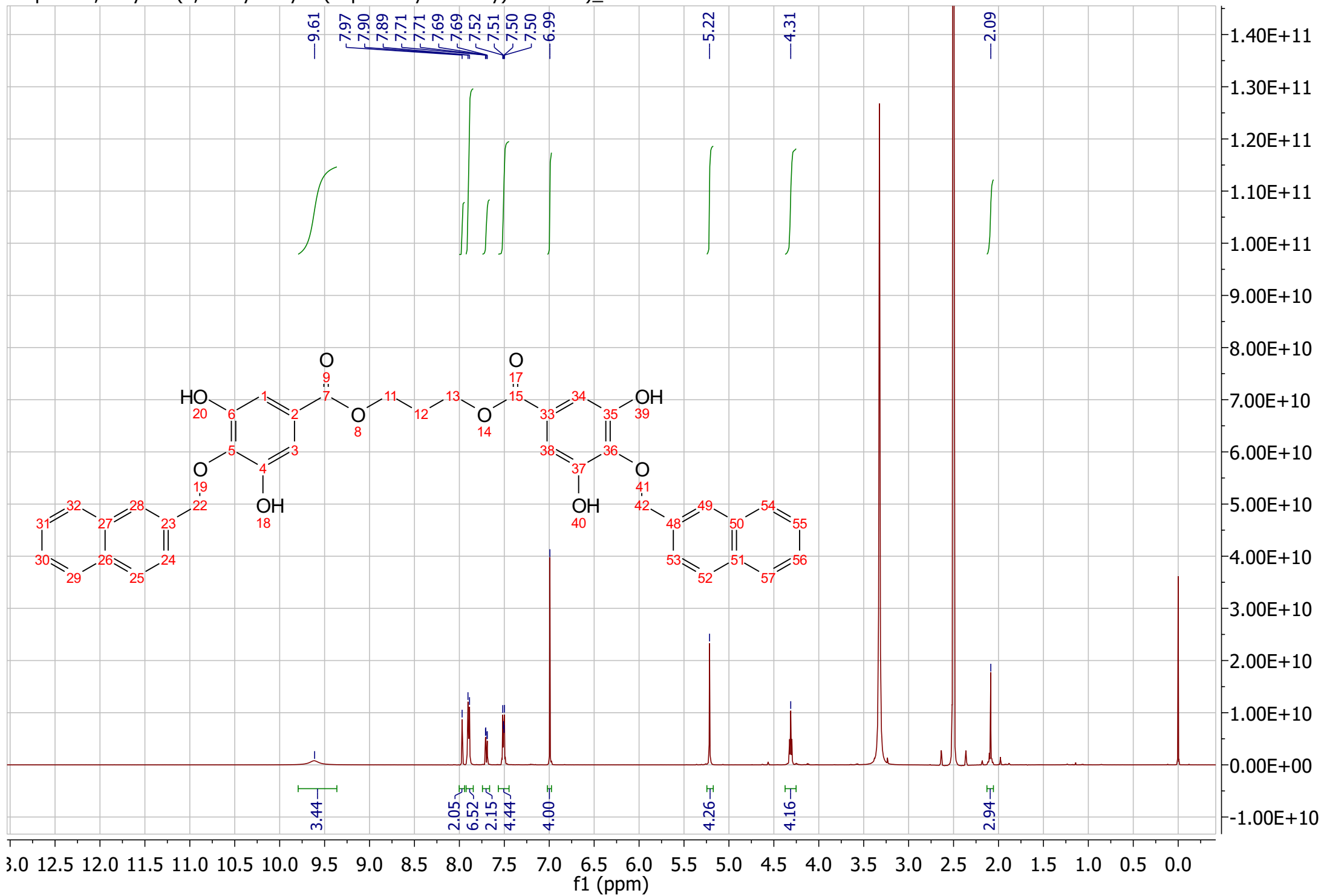
Propane-1,3-diyl bis(4-((4-methoxybenzoyloxy)-3,5-bis(methoxy)methoxy)benzoate)_DMSO



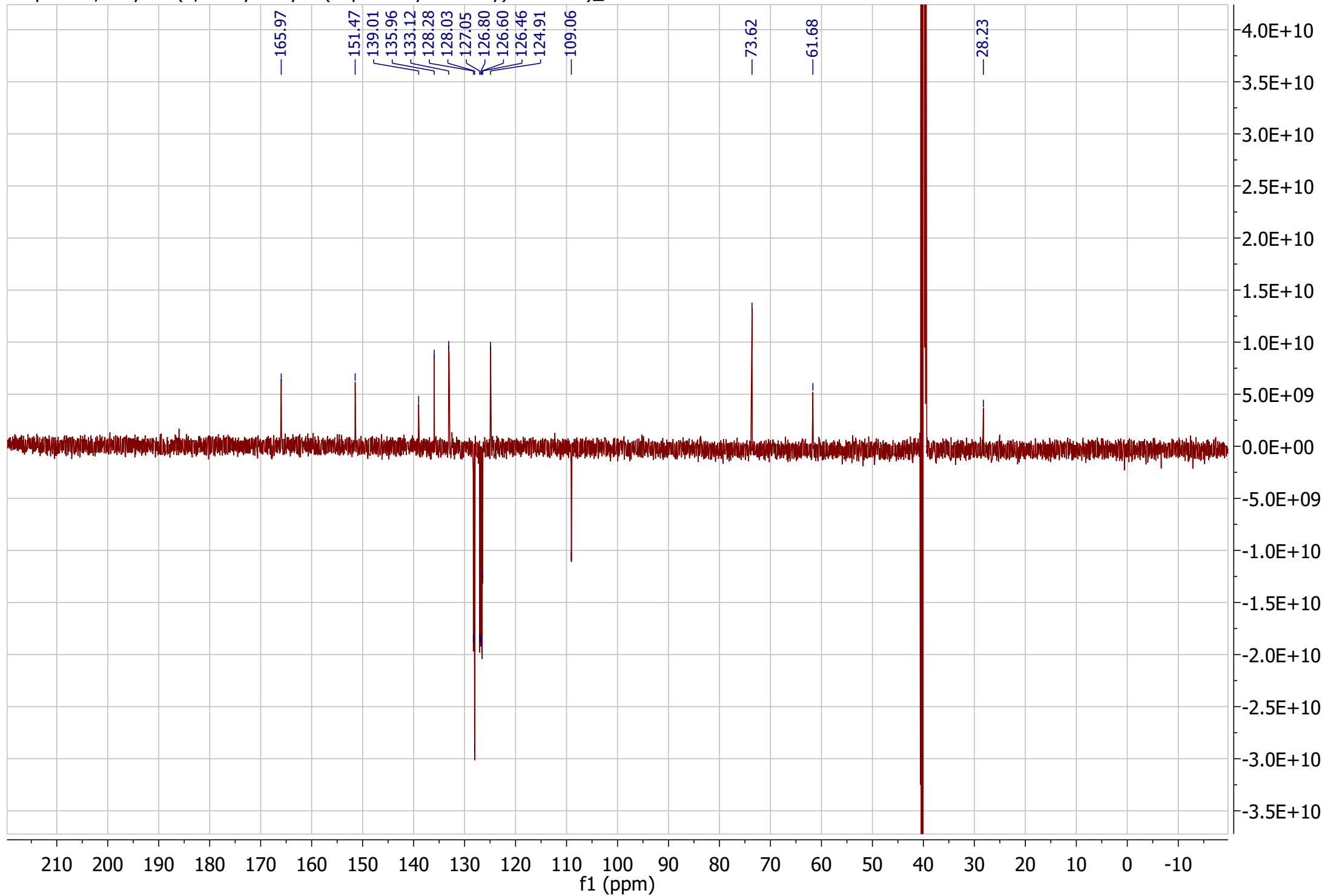
Propane-1,3-diyl bis(4-(benzyloxy)-3,5-dihydroxybenzoate)_DMSO



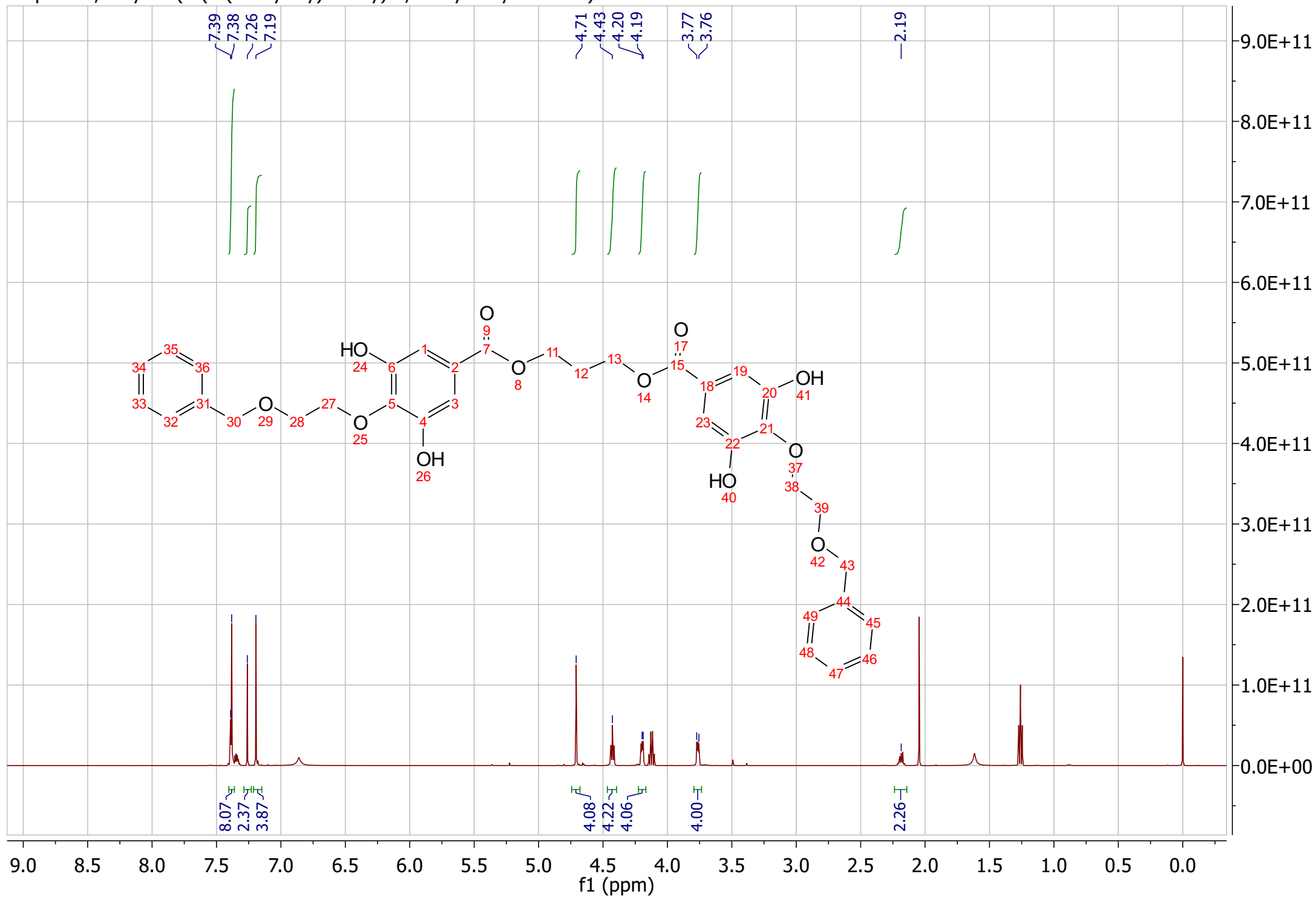
Propane-1,3-diyl bis(3,5-dihydroxy-4-(naphth-2-ylmethoxy)benzoate)_DMSO



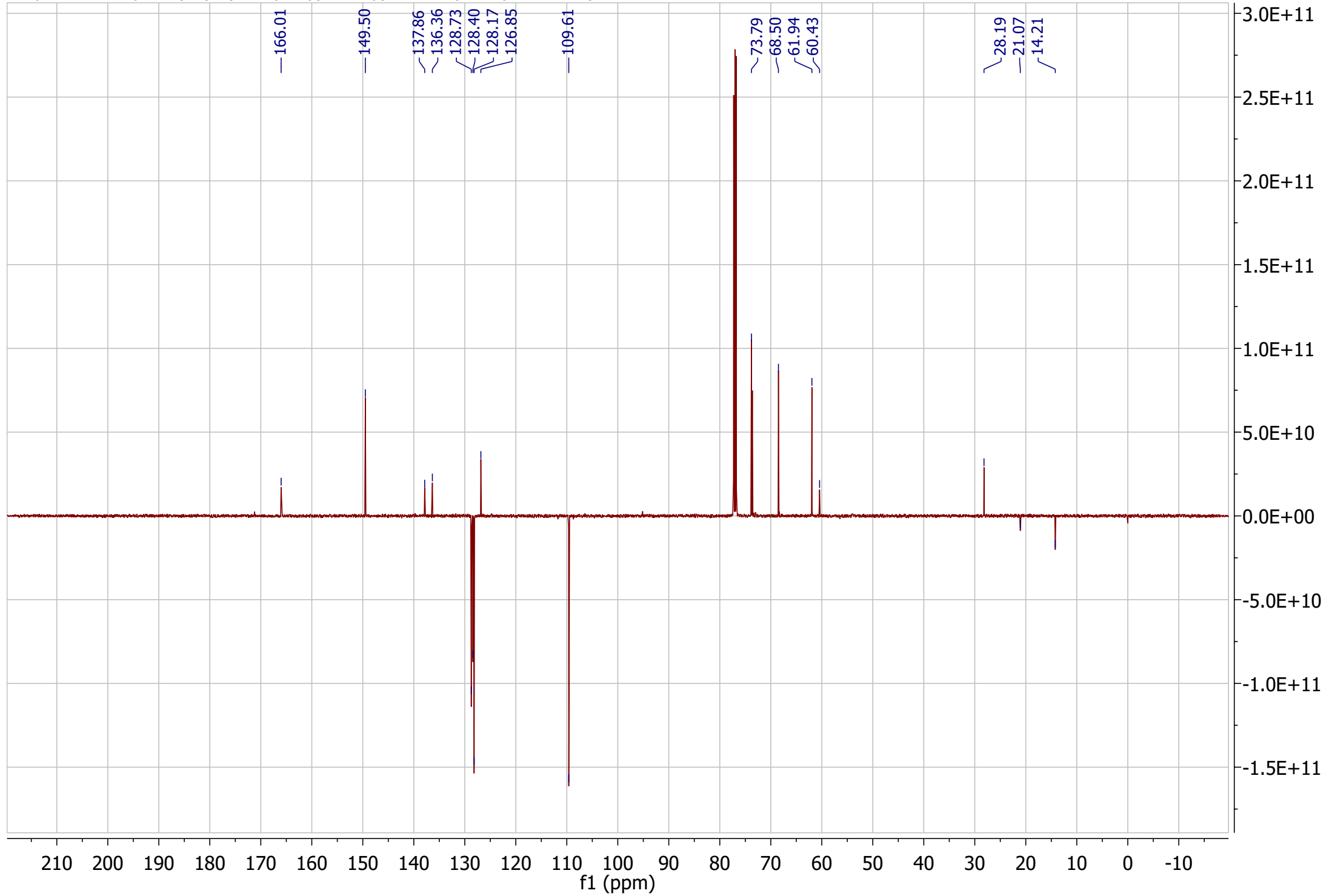
Propane-1,3-diyl bis(3,5-dihydroxy-4-(naphth-2-ylmethoxy)benzoate)_DMSO



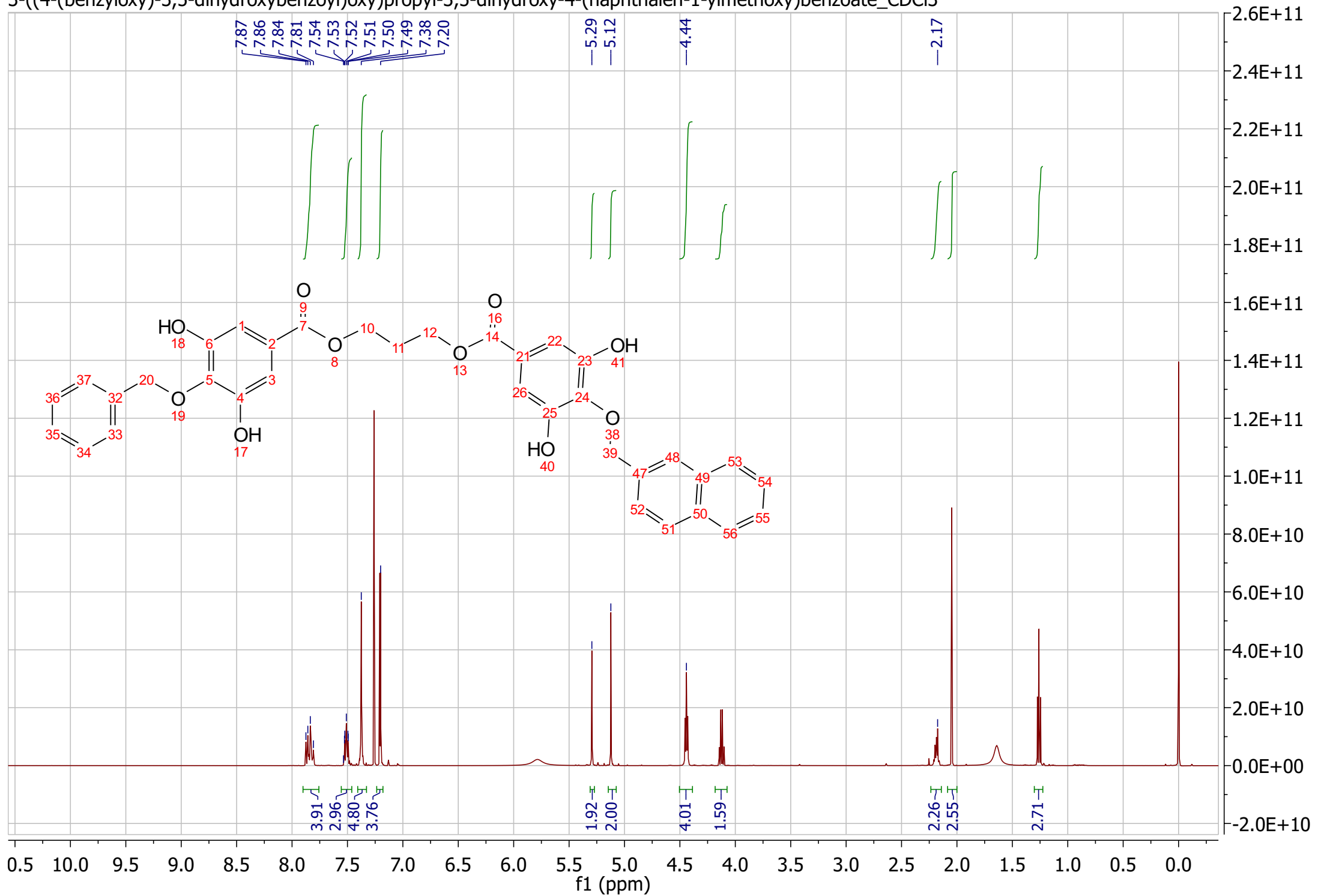
Propane-1,3-diyl bis(4-(2-(benzyloxy)ethoxy)-3,5-dihydroxybenzoate)



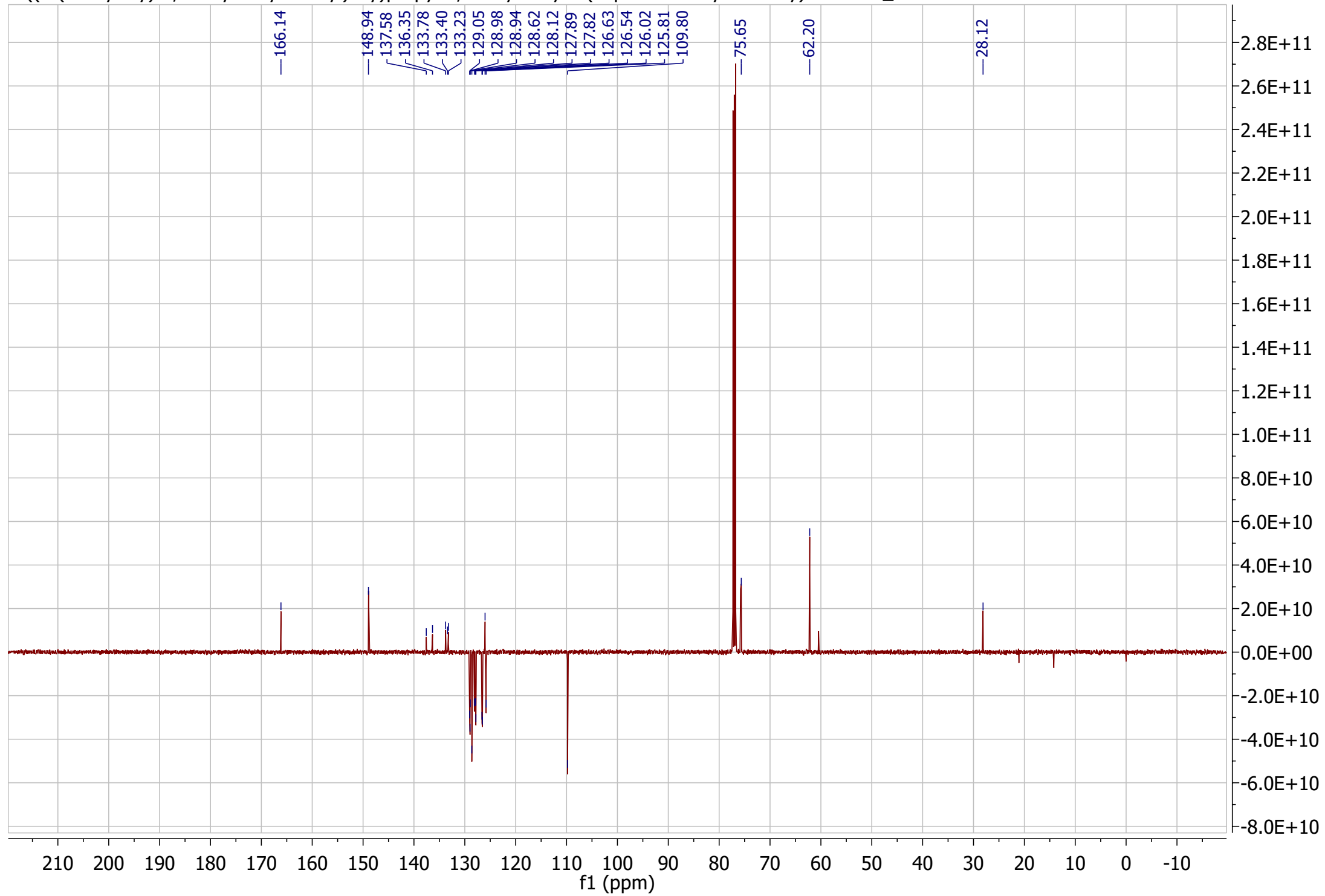
Propane-1,3-diyl bis(4-(2-(benzyloxy)ethoxy)-3,5-dihydroxybenzoate)



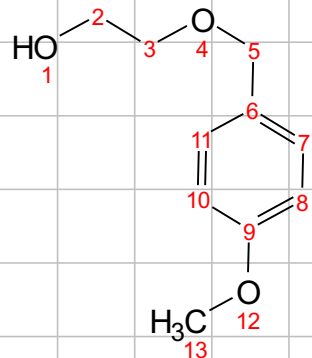
3-((4-(benzyloxy)-3,5-dihydroxybenzoyl)oxy)propyl-3,5-dihydroxy-4-(naphthalen-1-ylmethoxy)benzoate_CDCl3



3-((4-(benzyloxy)-3,5-dihydroxybenzoyl)oxy)propyl-3,5-dihydroxy-4-(naphthalen-1-ylmethoxy)benzoate_CDCl3



GID230_CCl3.10.1.1r
GID230_CDCI3



7.28
7.26
6.90
6.88

4.49

3.81
3.74
3.57

1.00

0.93

0.93

1.46

0.95

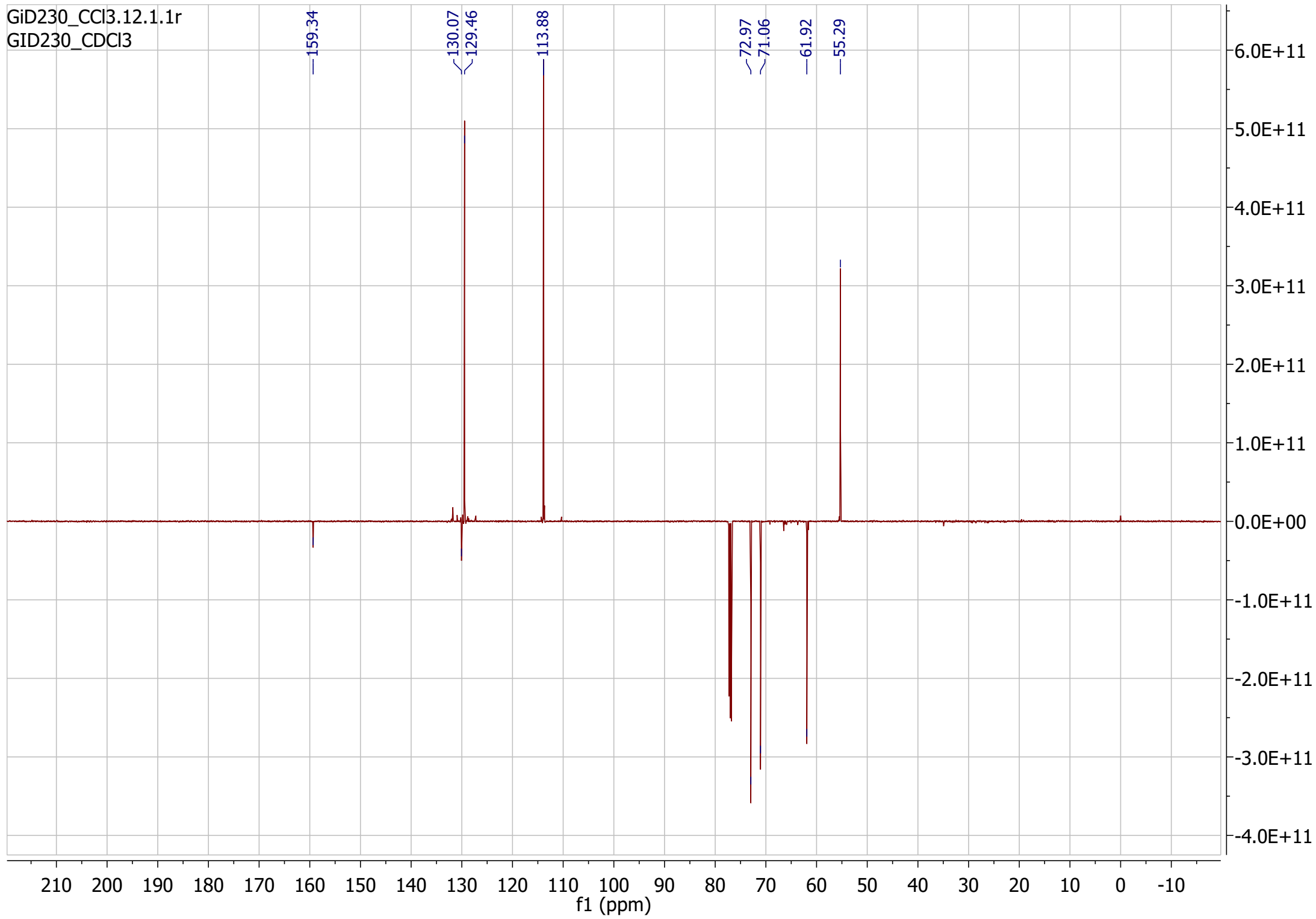
0.93

12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

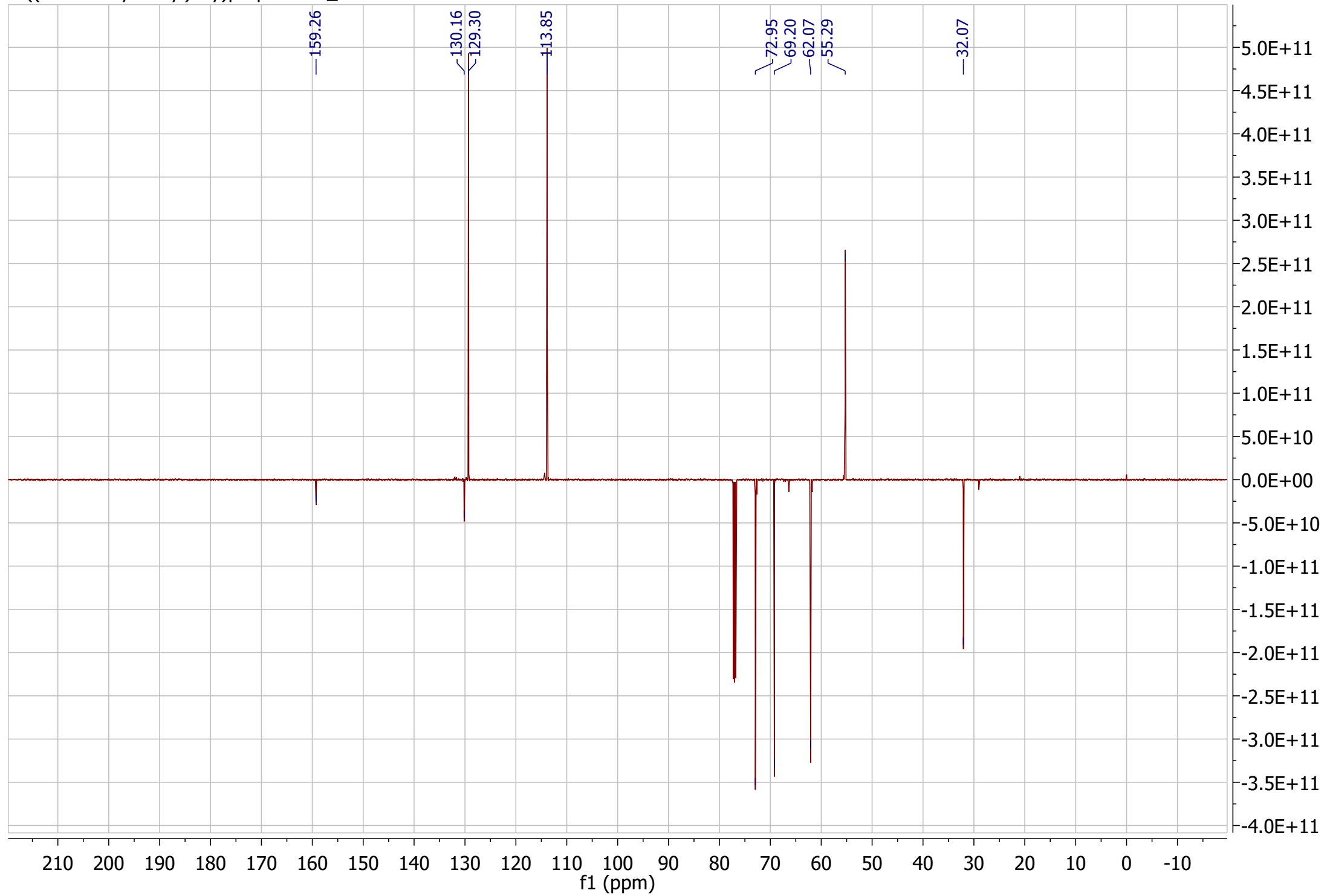
f1 (ppm)

1.70E+12
1.60E+12
1.50E+12
1.40E+12
1.30E+12
1.20E+12
1.10E+12
1.00E+12
9.00E+11
8.00E+11
7.00E+11
6.00E+11
5.00E+11
4.00E+11
3.00E+11
2.00E+11
1.00E+11
0.00E+00
-1.00E+11

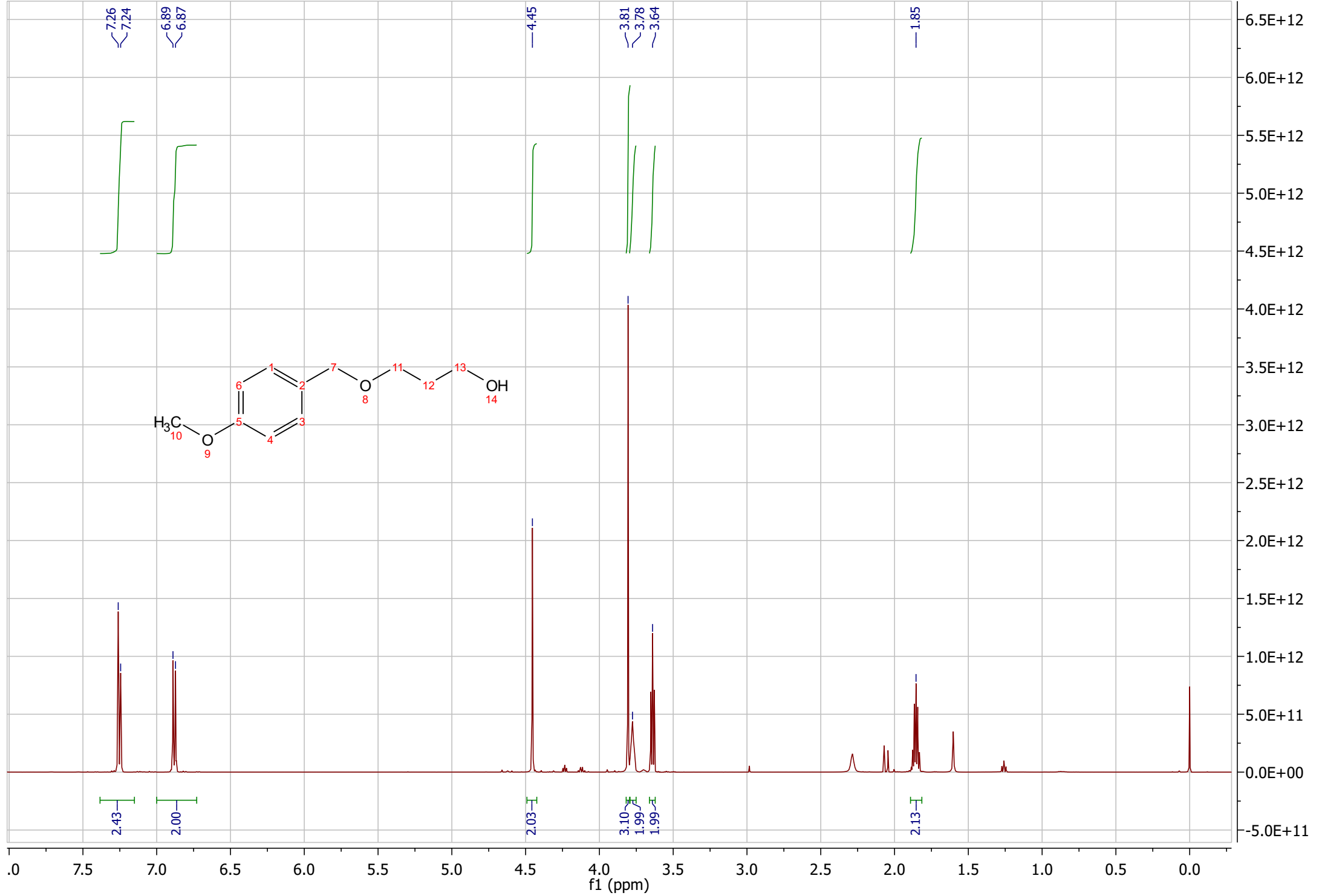
GID230_CCl3.12.1.1r
GID230_CDCl3



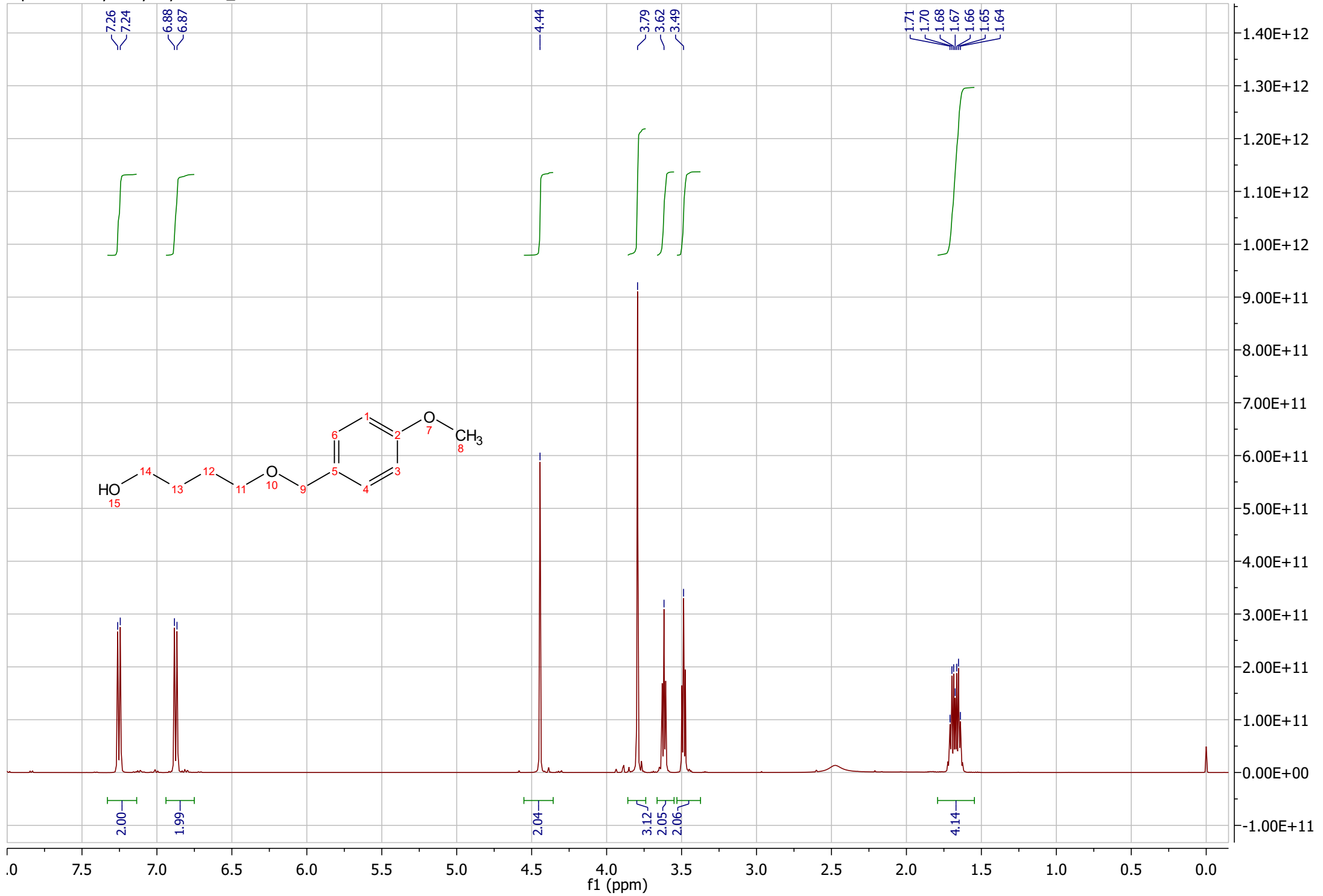
3-((4-methoxybenzyl)oxy)propan-1-ol_CDCl3

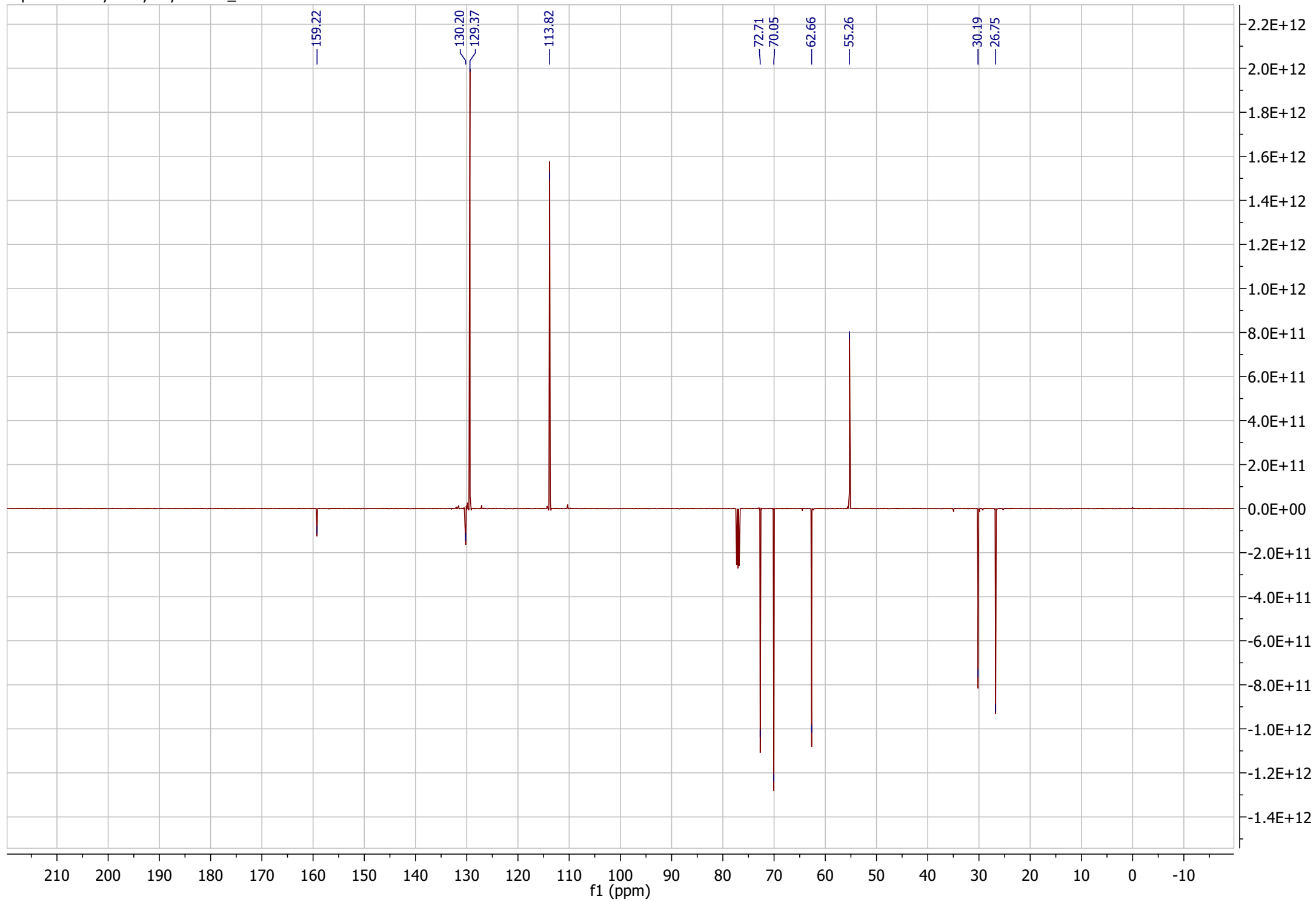


3-((4-methoxybenzyl)oxy)propan-1-ol_CDCI3

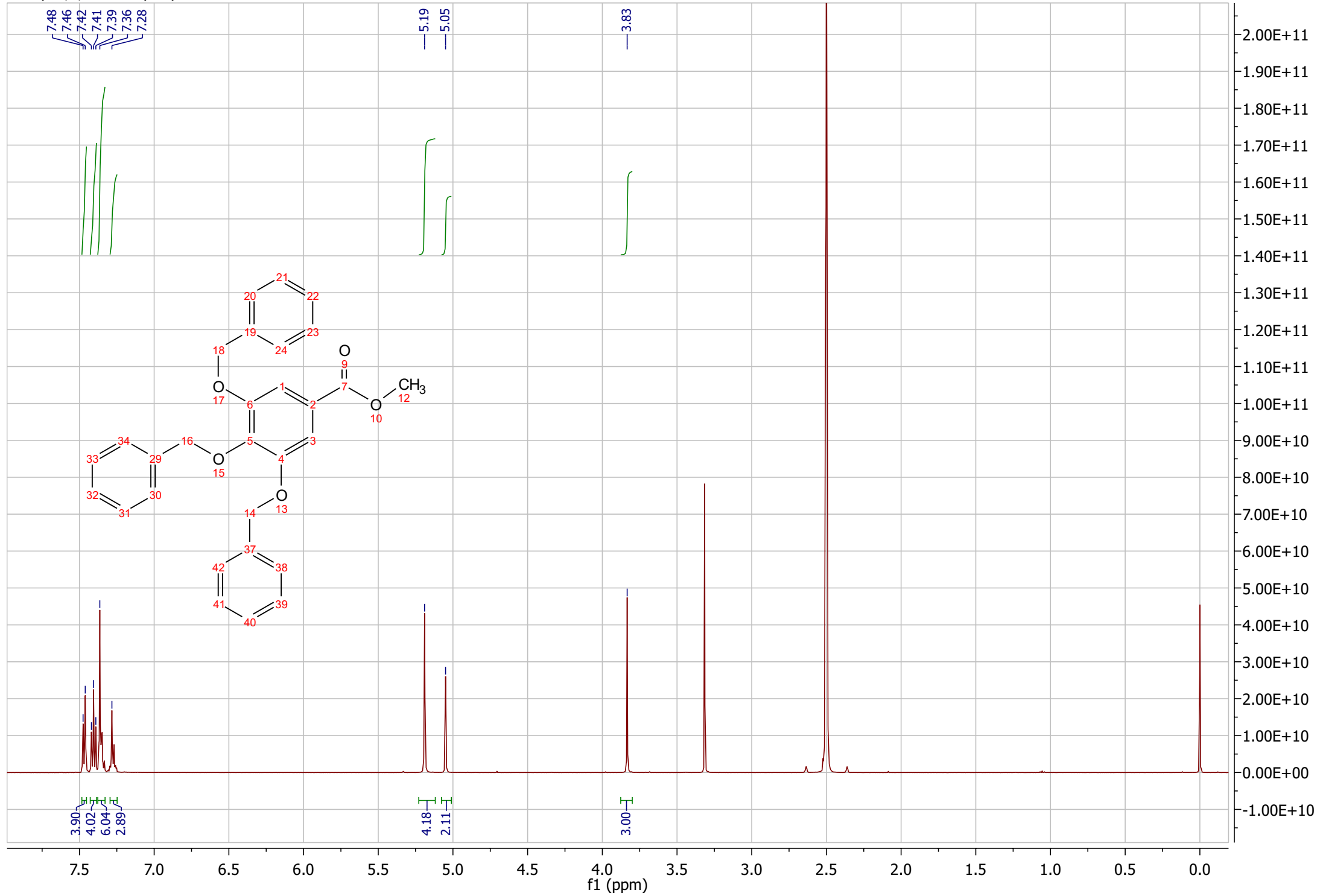


4-paramethoxybenzyloxybutanol_CDCI3

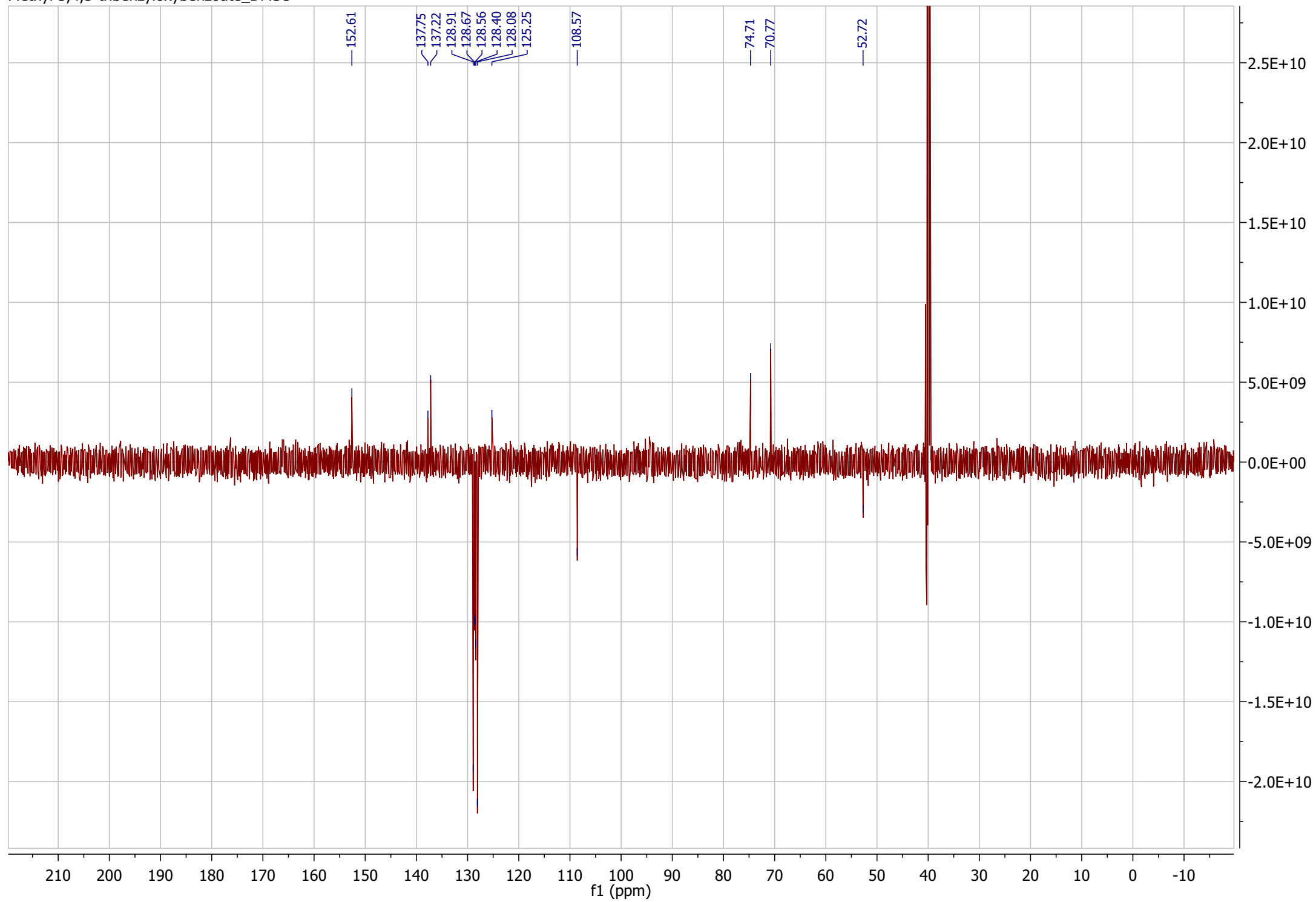




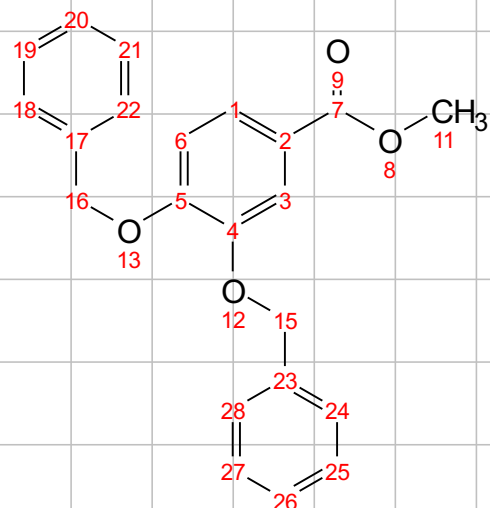
Methyl 3,4,5-tribenzyloxybenzoate_DMSO



Methyl 3,4,5-tribenzyloxybenzoate_DMSO



Methyl 3,4-dibenzyloxybenzoate_CDCl3



7.64
7.63
7.62
7.62
7.48
7.46
7.44
7.43
7.38
7.37
7.35
7.33
7.31
7.30

5.22
5.19

3.87

1.90

3.76

5.64

4.00

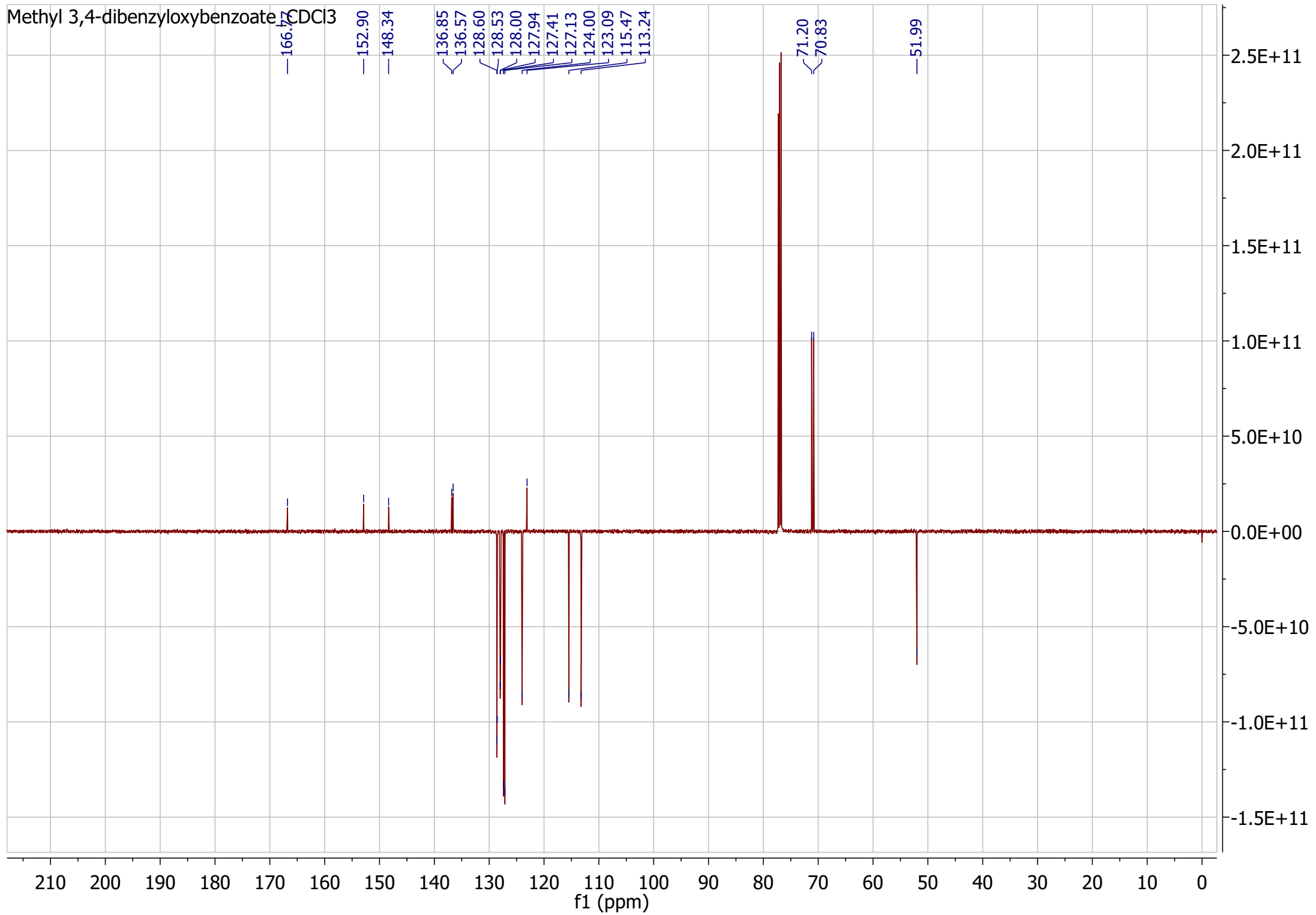
2.94

12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

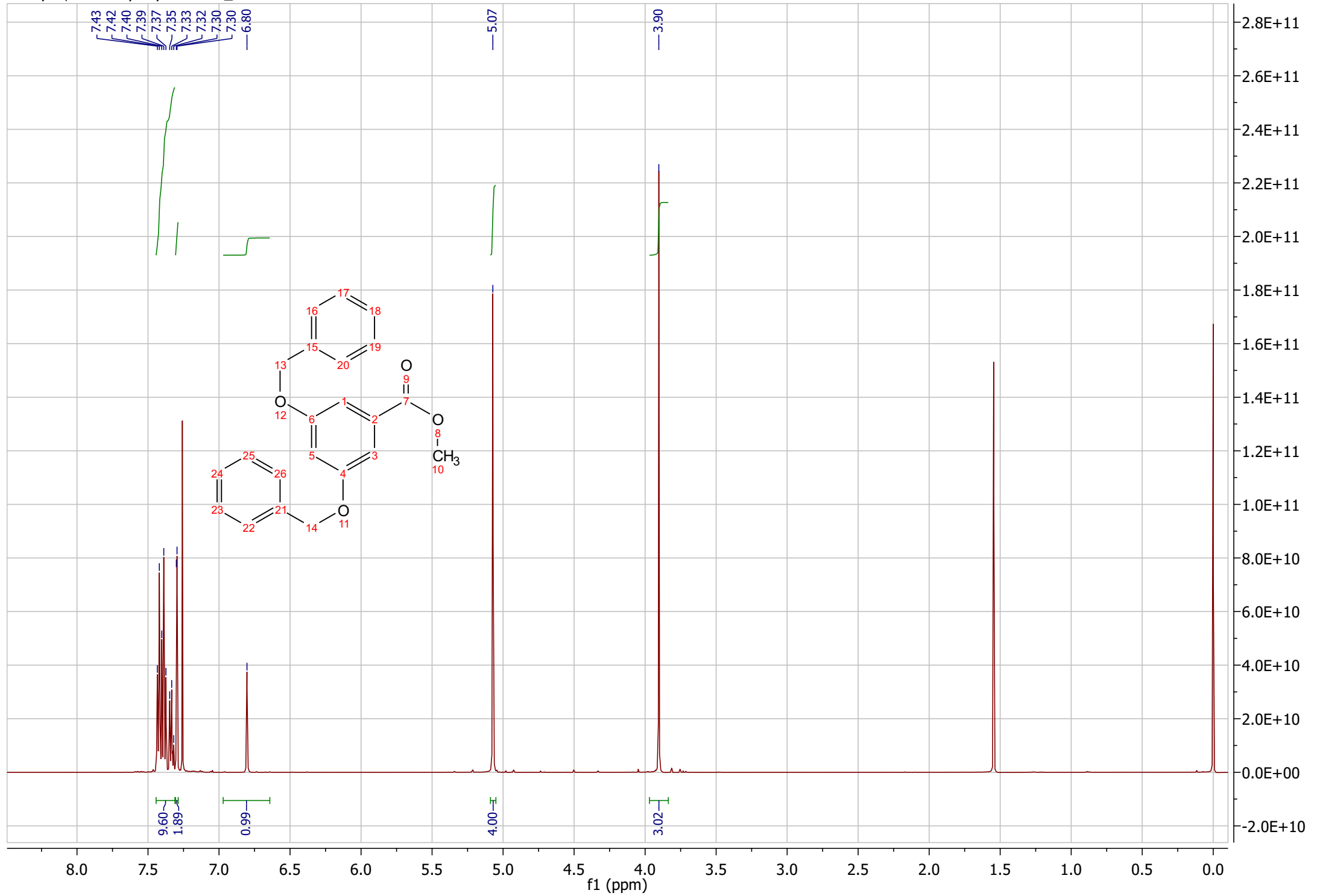
f1 (ppm)

3.0E+11
2.8E+11
2.6E+11
2.4E+11
2.2E+11
2.0E+11
1.8E+11
1.6E+11
1.4E+11
1.2E+11
1.0E+11
8.0E+10
6.0E+10
4.0E+10
2.0E+10
0.0E+00
-2.0E+10

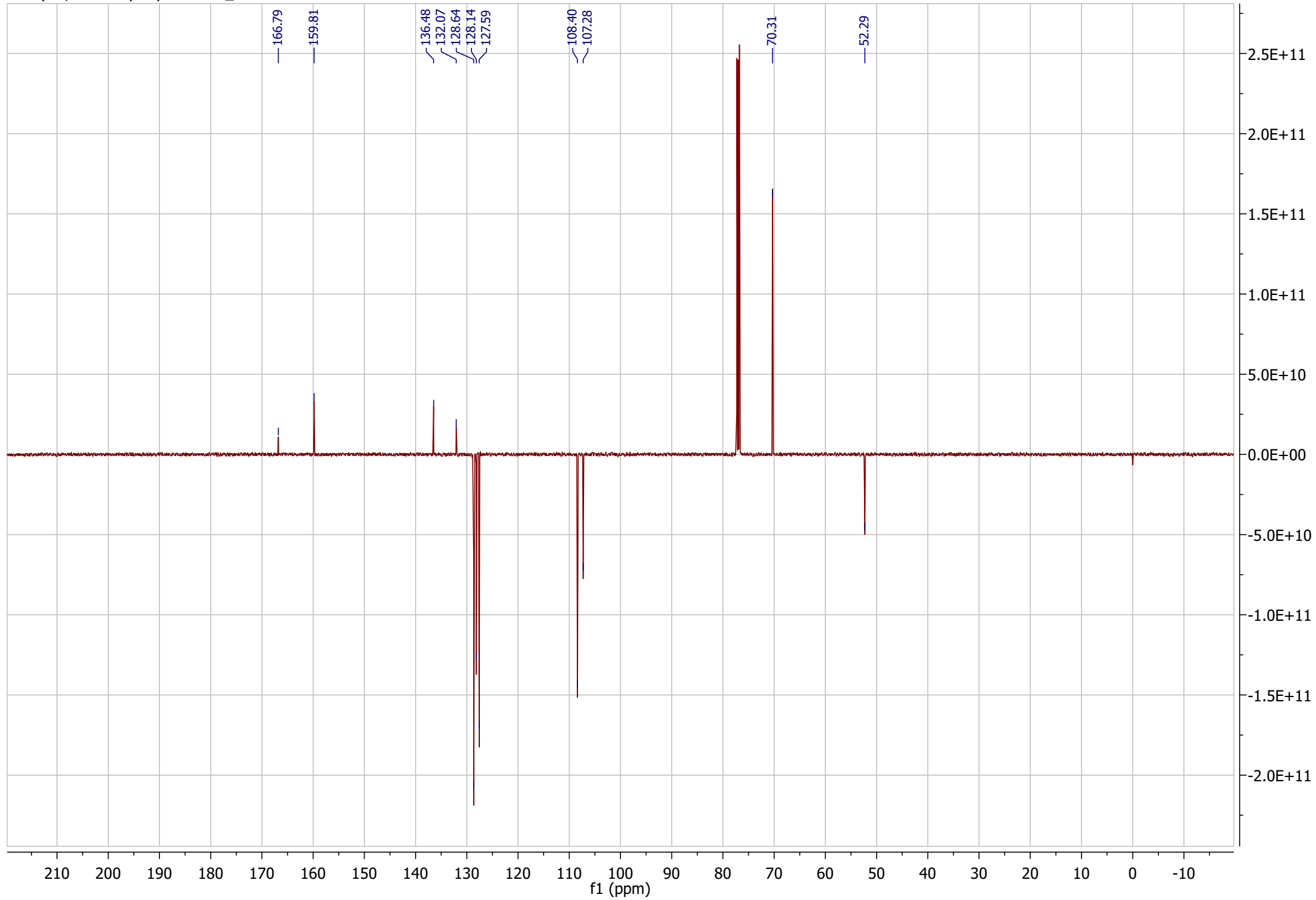
Methyl 3,4-dibenzyloxybenzoate CDCl₃



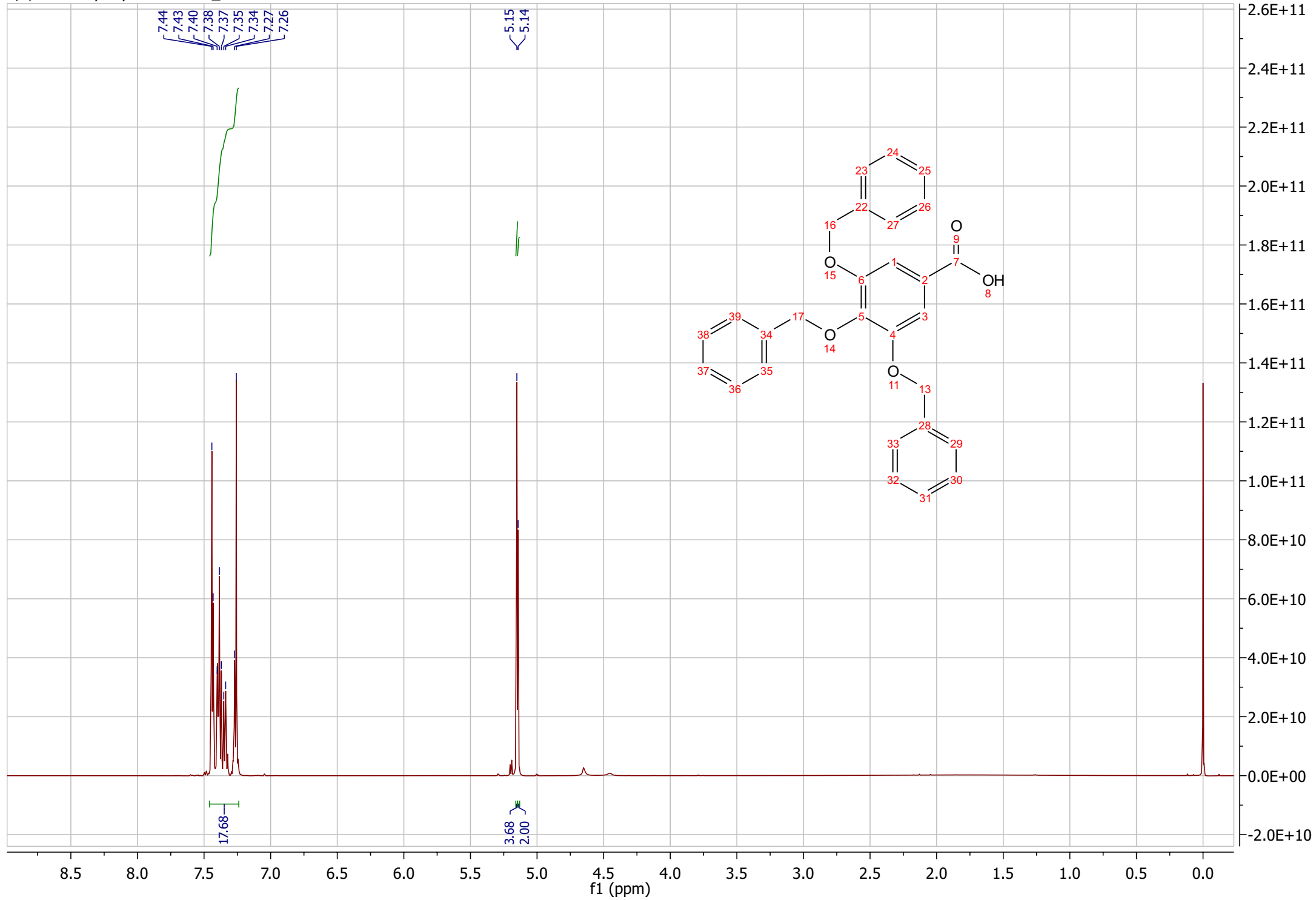
Methyl 3,5-dibenzyloxybenzoate_CDCl3



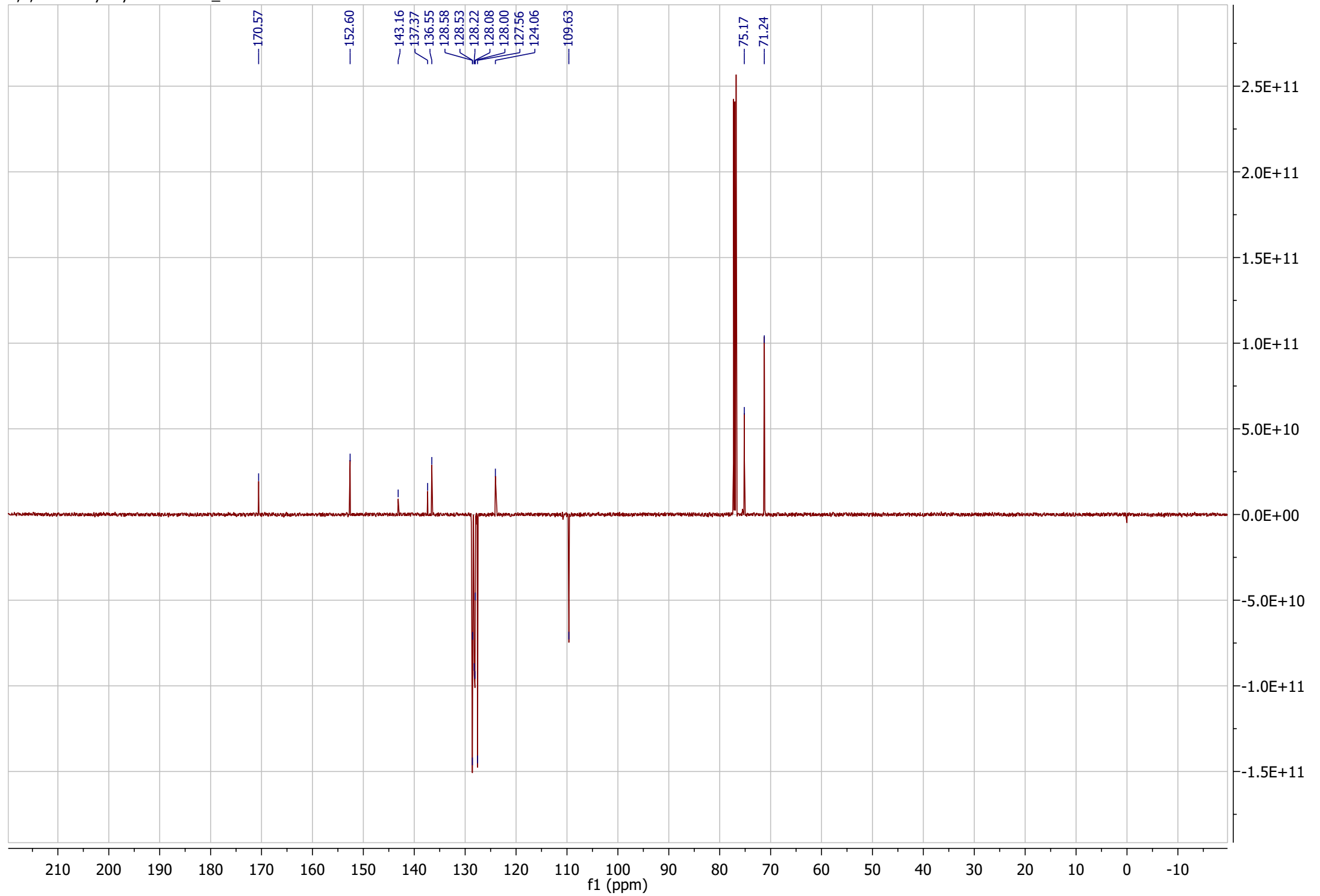
Methyl 3,5-dibenzyloxybenzoate_CDCl3



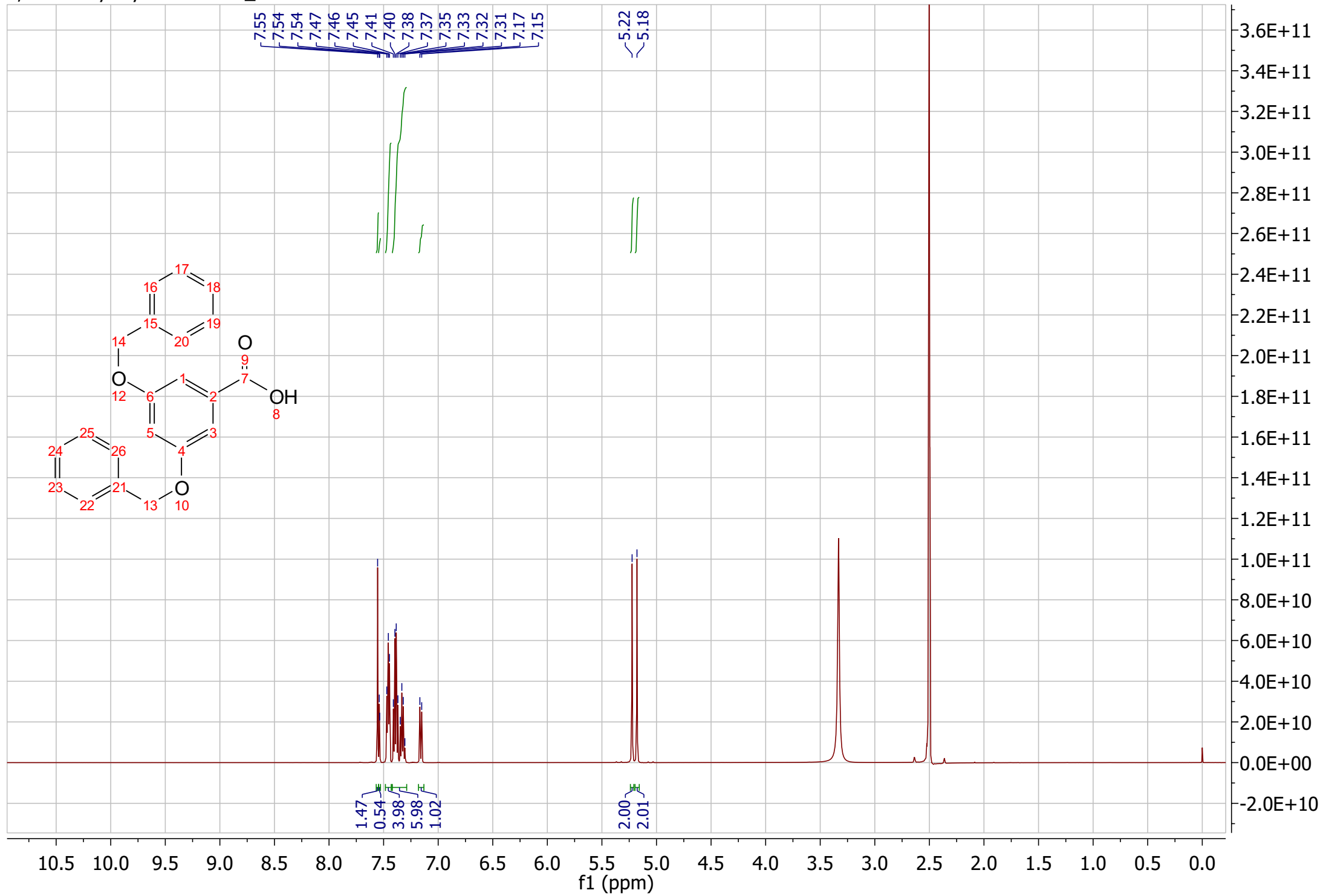
3,4,5-tribenzyloxybenzoic acid_CDCl3



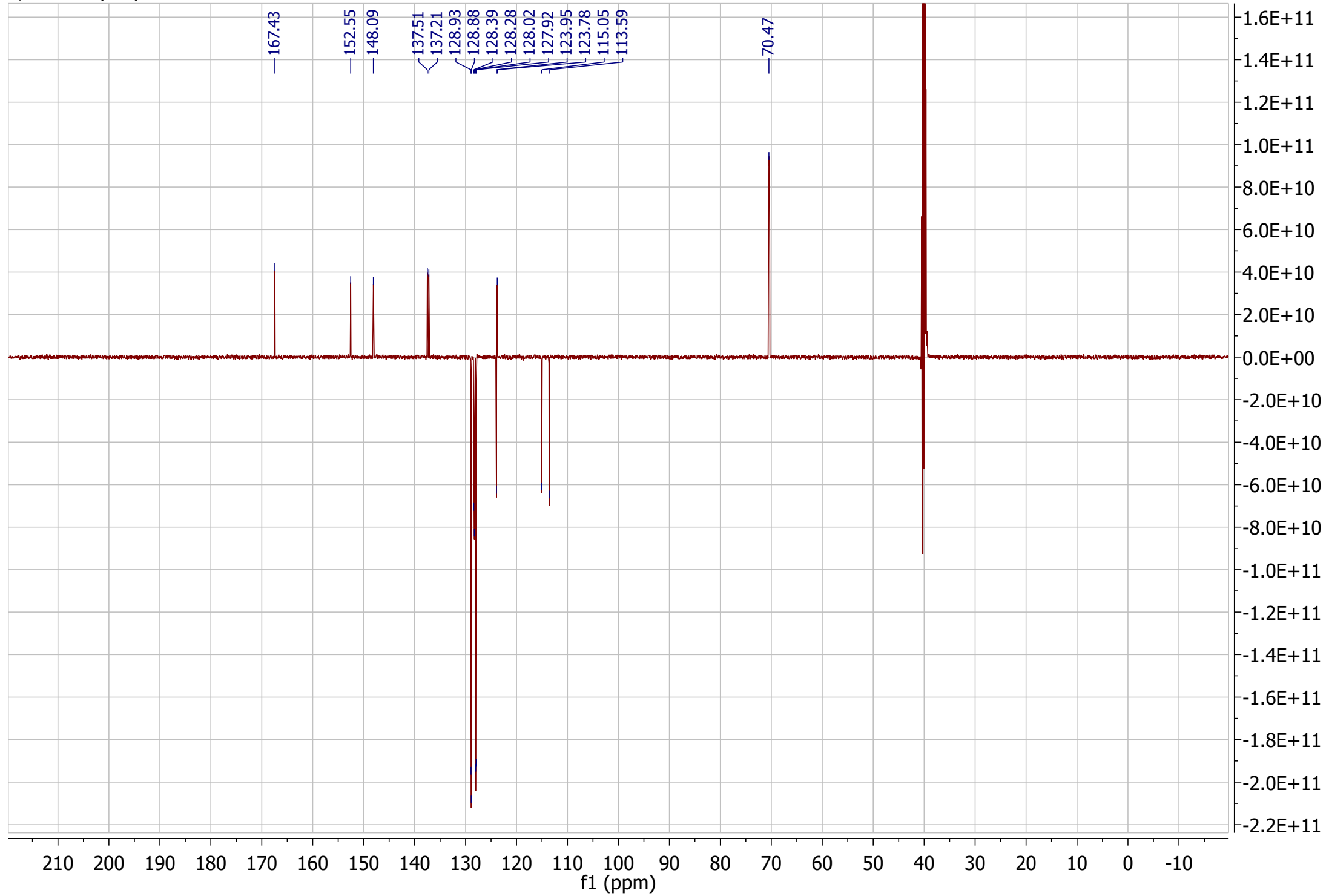
3,4,5-tribenzyloxybenzoic acid_CDCl3



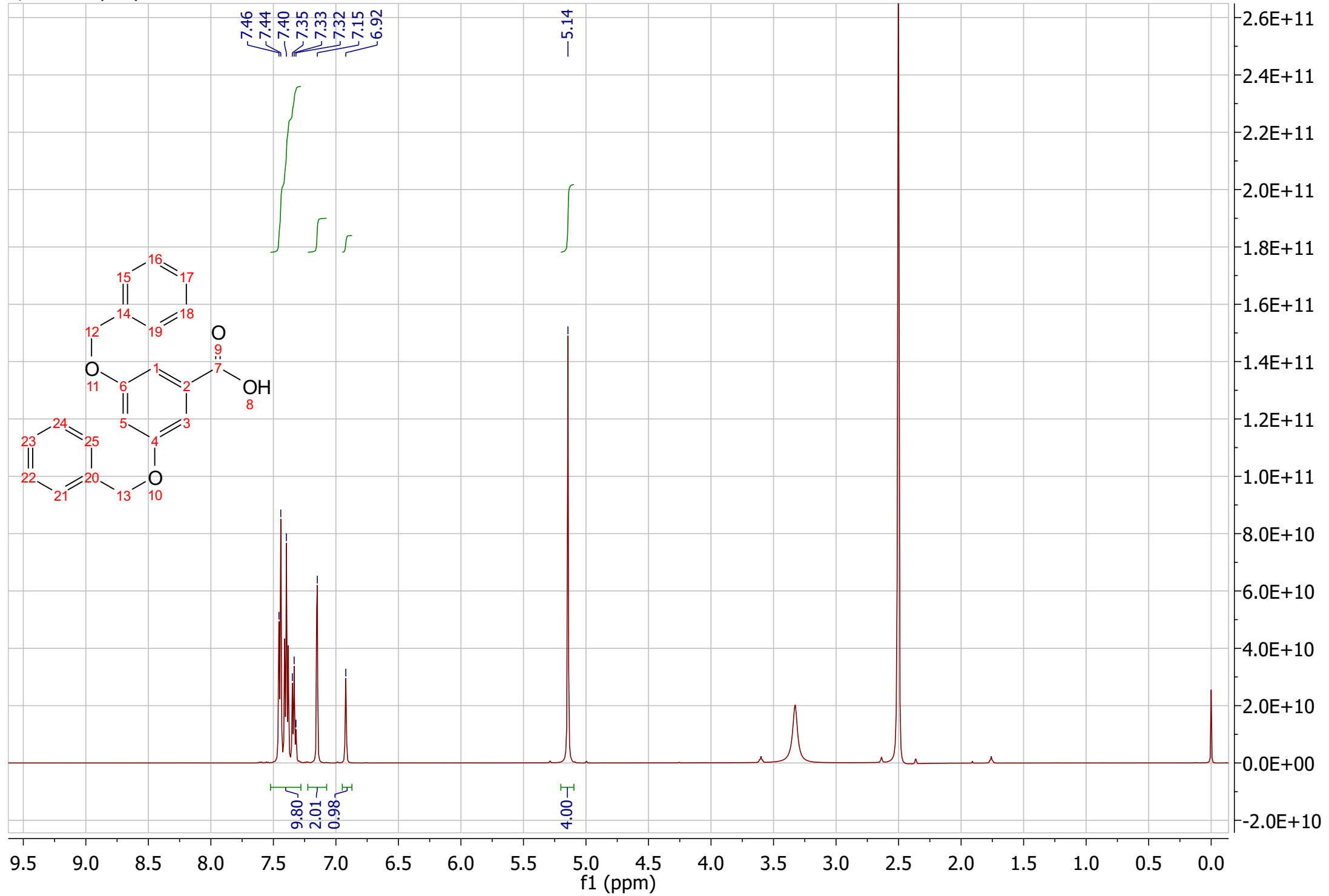
3,5-Dibenzoyloxybenzoic acid_DMSO



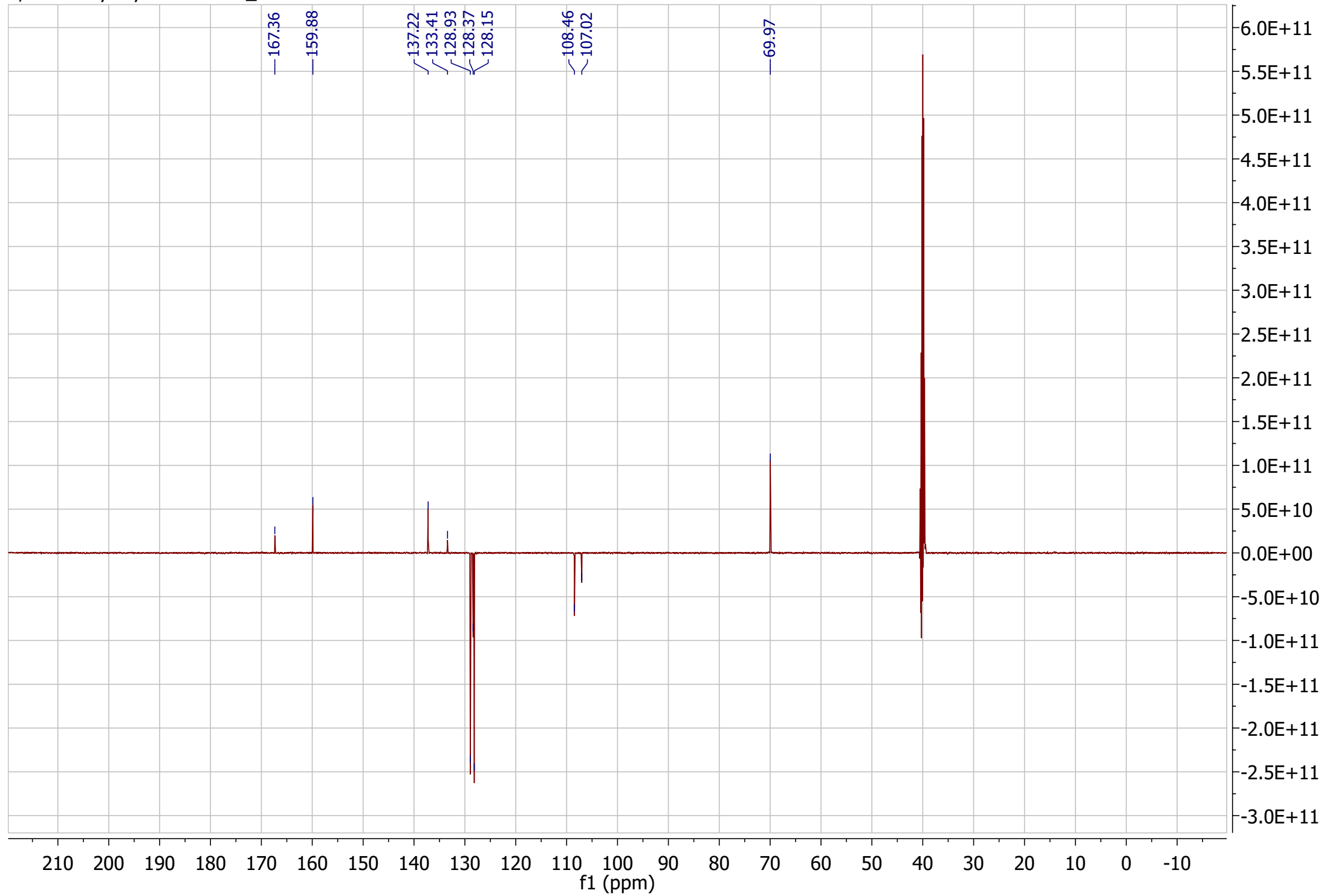
3,5-Dibenzyloxybenzoic acid_DMSO



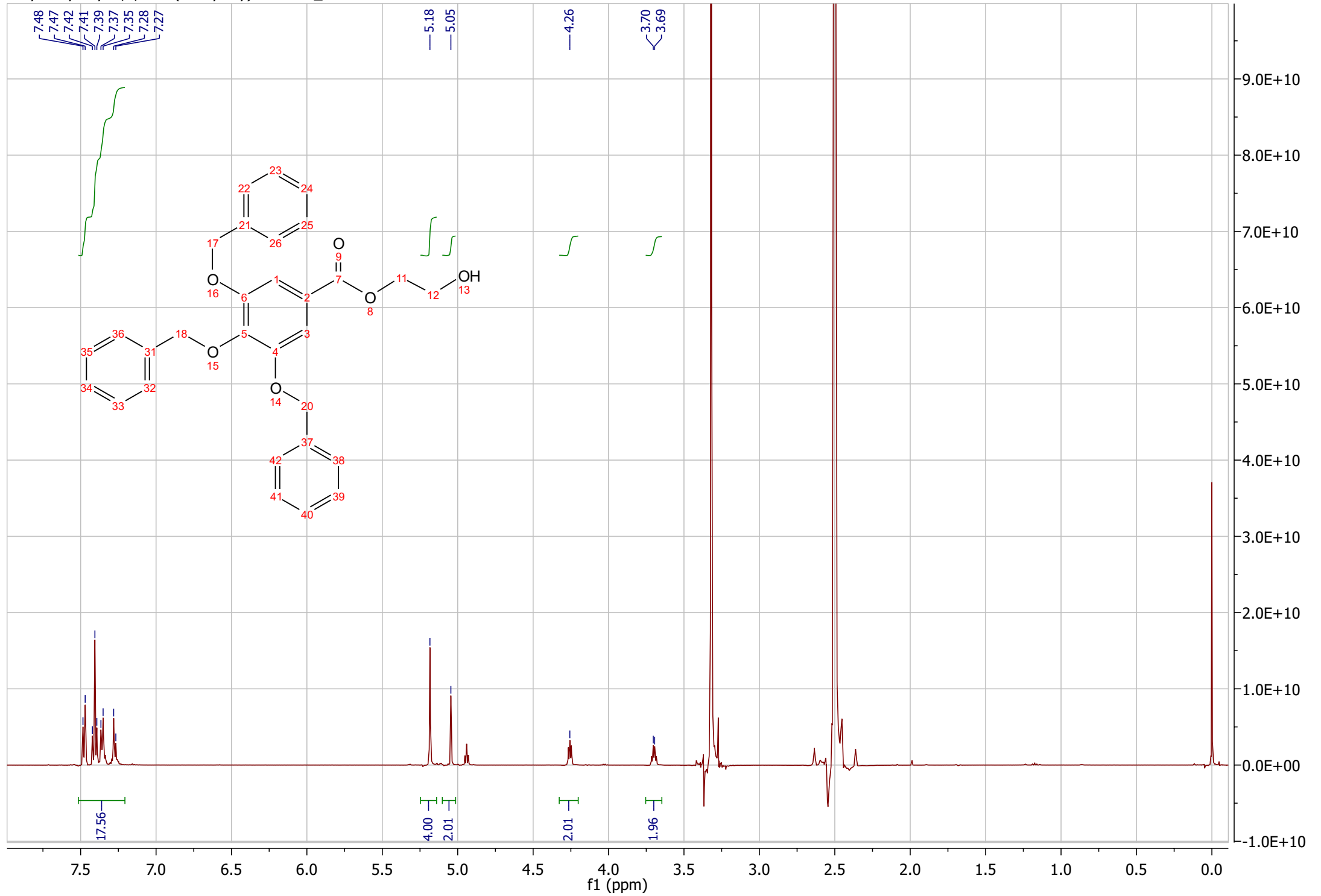
3,5-Dibenzoyloxybenzoic acid_DMSO



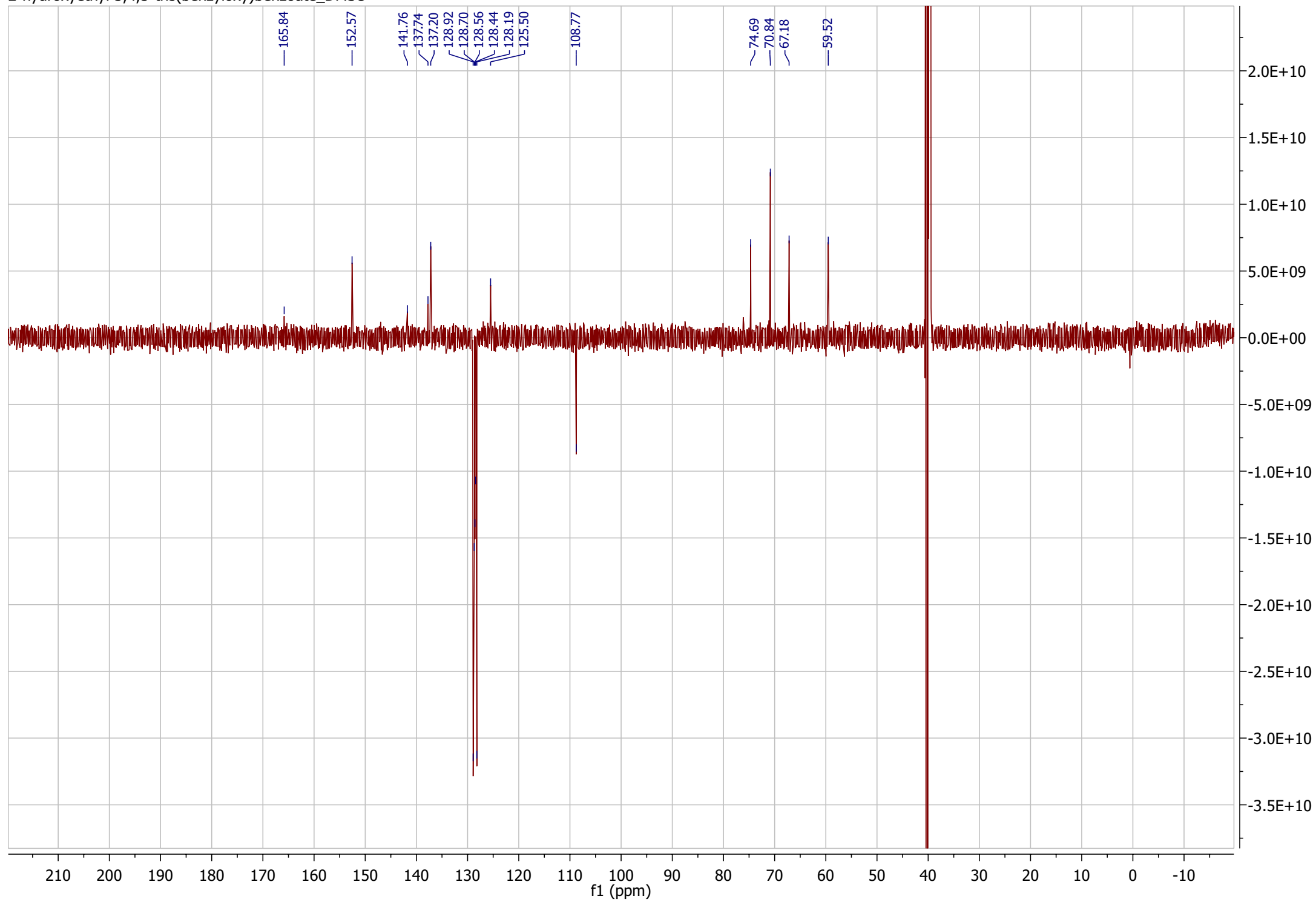
3,5-Dibenzyloxybenzoic acid_DMSO



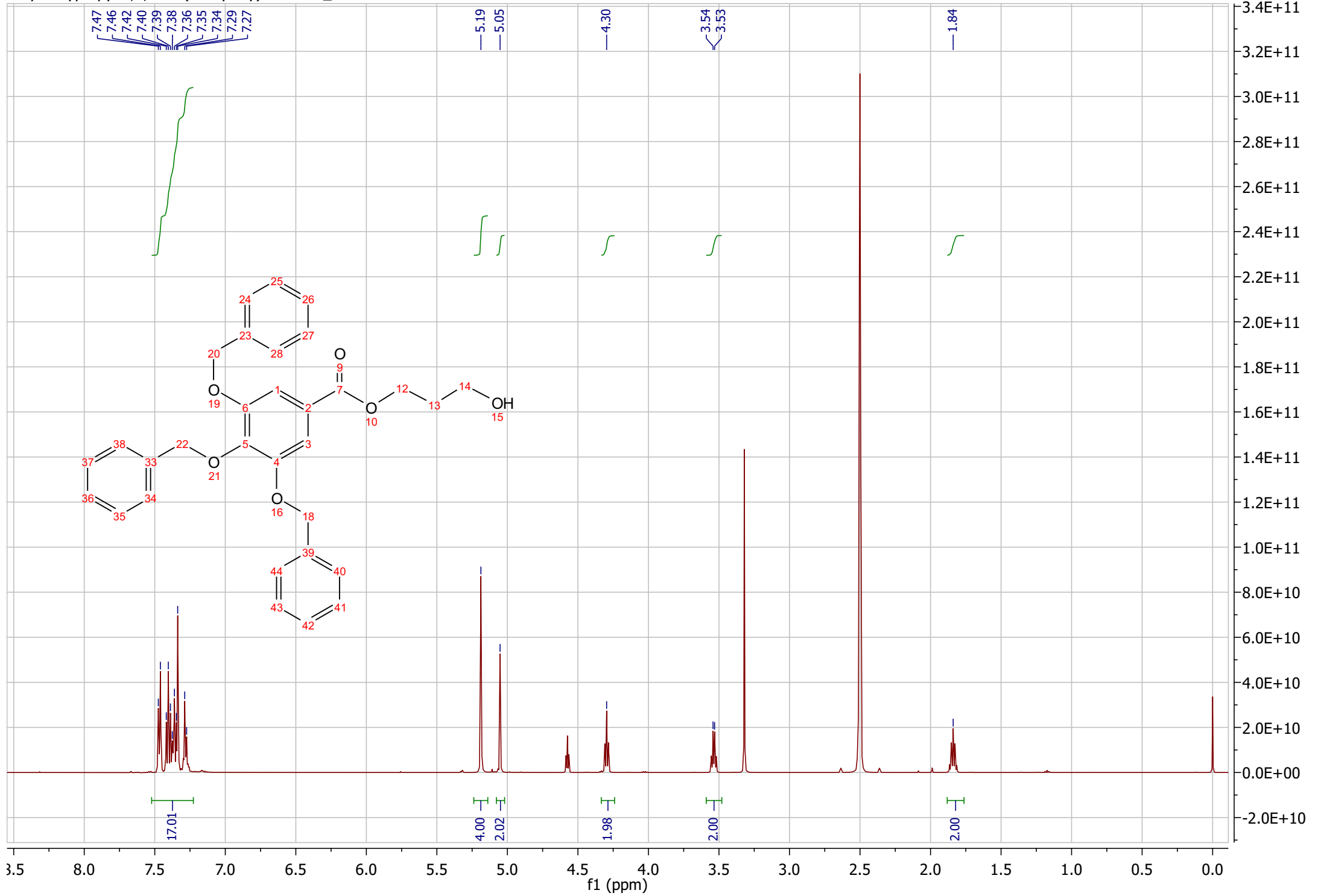
2-hydroxyethyl 3,4,5-tris(benzyloxy)benzoate_DMSO



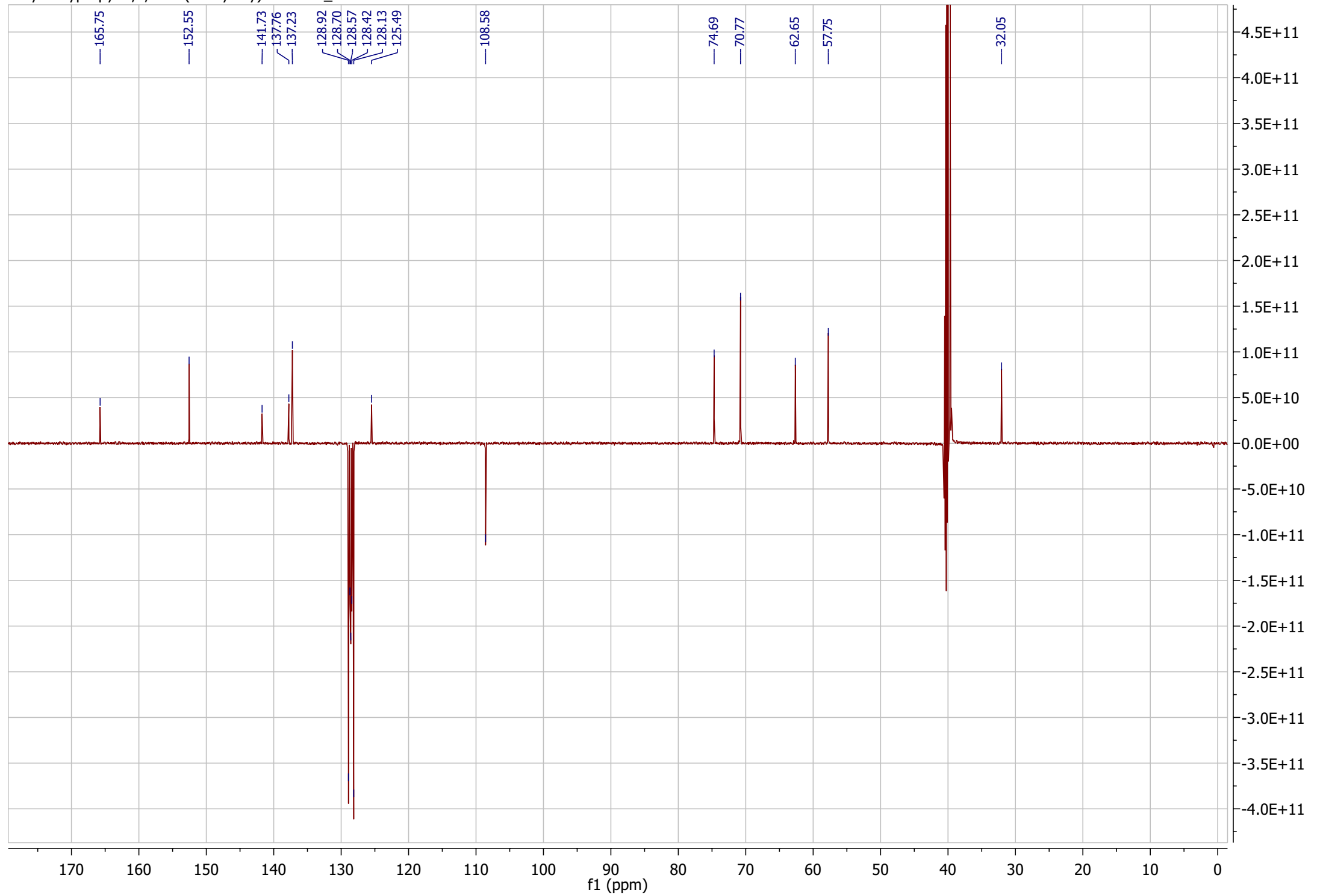
2-hydroxyethyl 3,4,5-tris(benzyloxy)benzoate_DMSO



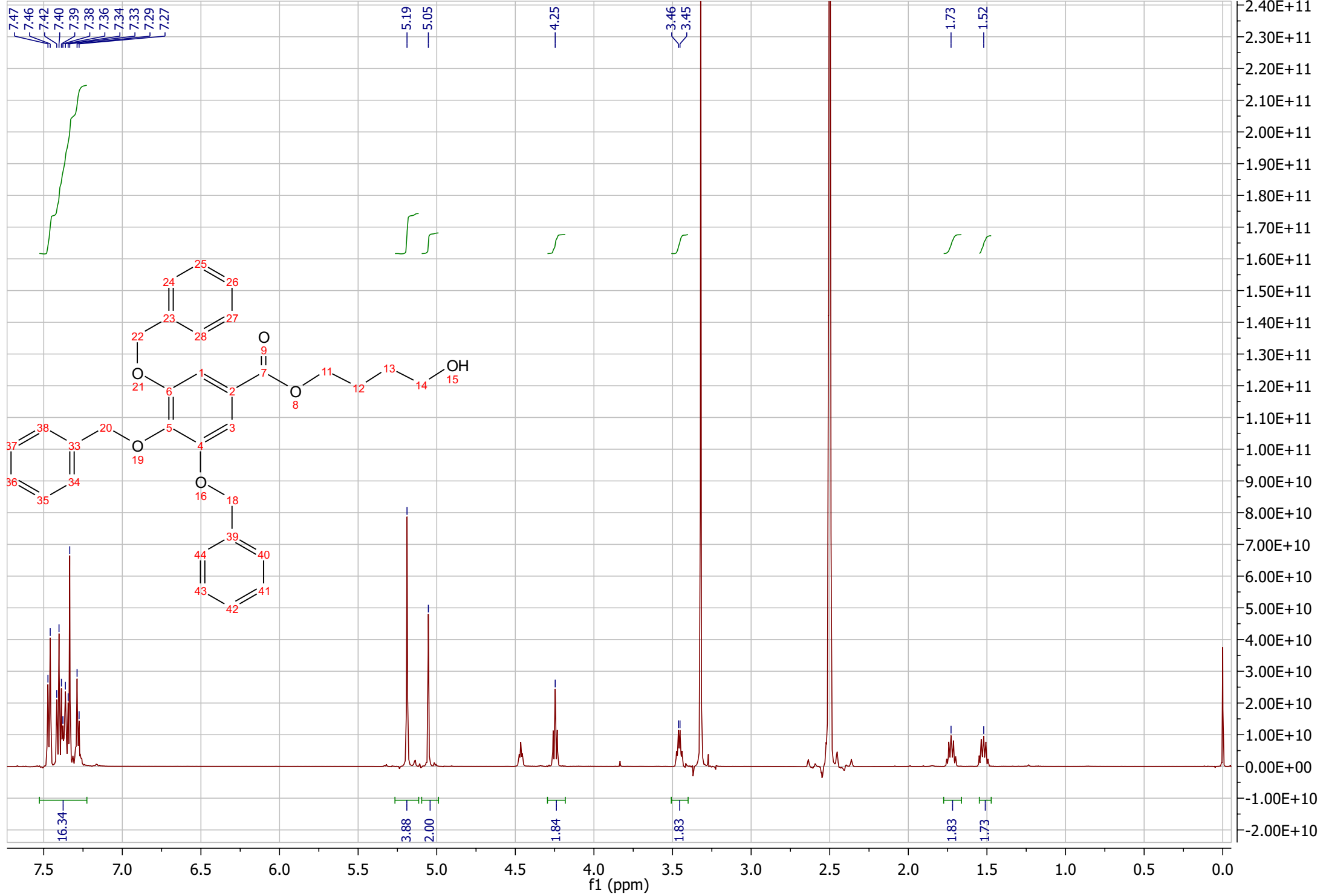
3-hydroxypropyl 3,4,5-tris(benzyloxy)benzoate_DMSO



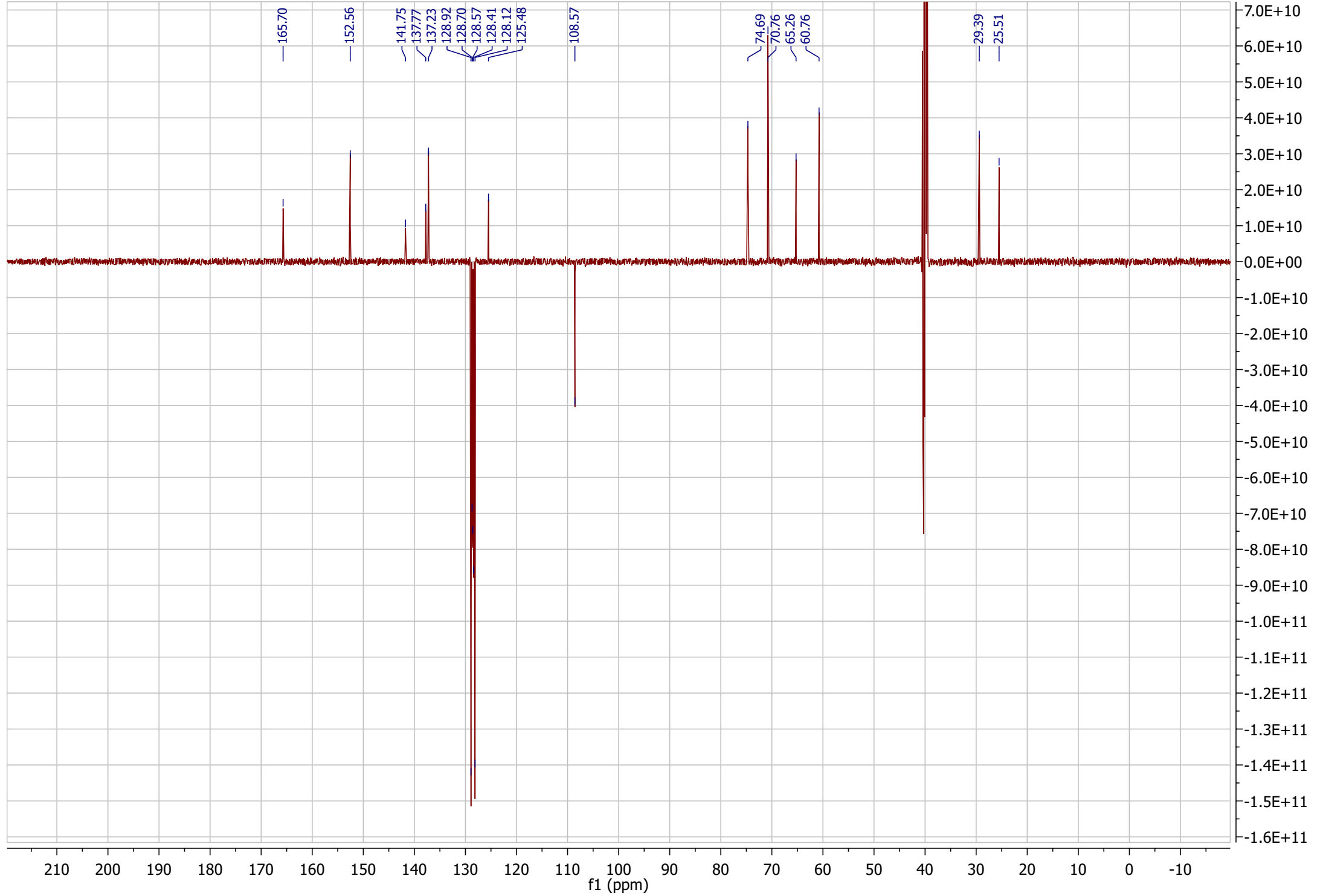
3-hydroxypropyl 3,4,5-tris(benzyloxy)benzoate_DMSO



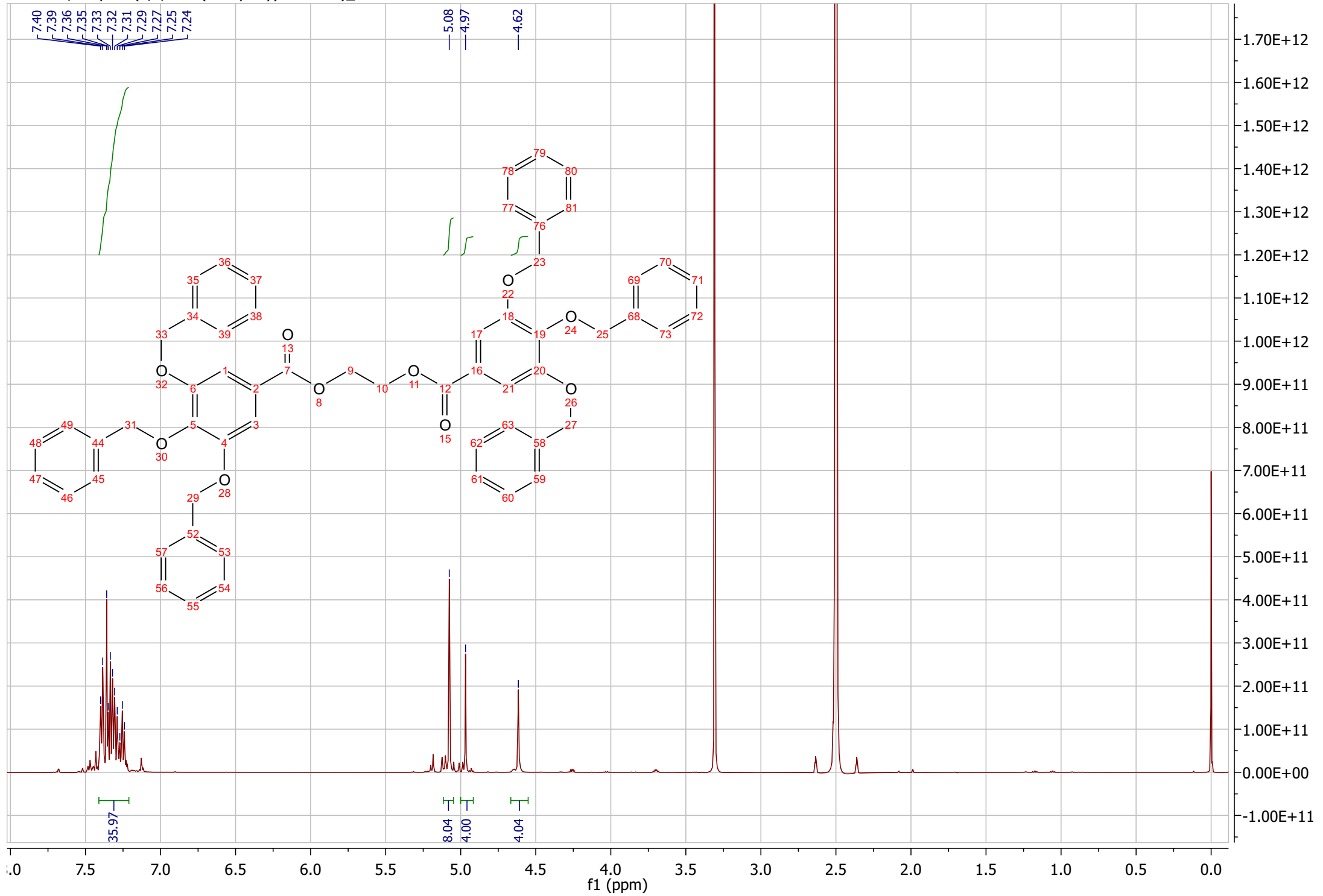
4-hydroxybutyl 3,4,5-tris(benzyloxy)benzoate_DMSO



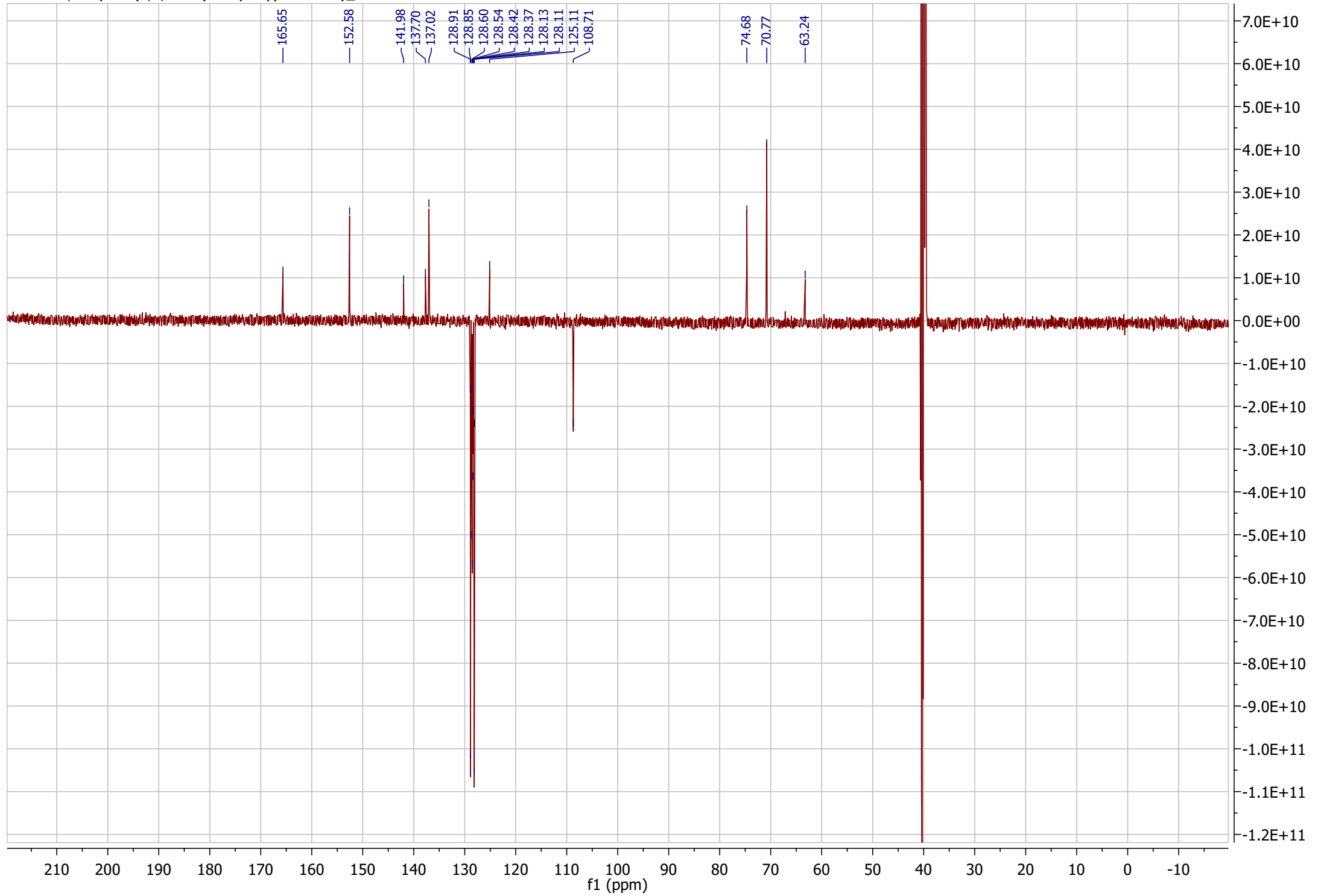
4-hydroxybutyl 3,4,5-tris(benzyloxy)benzoate_DMSO



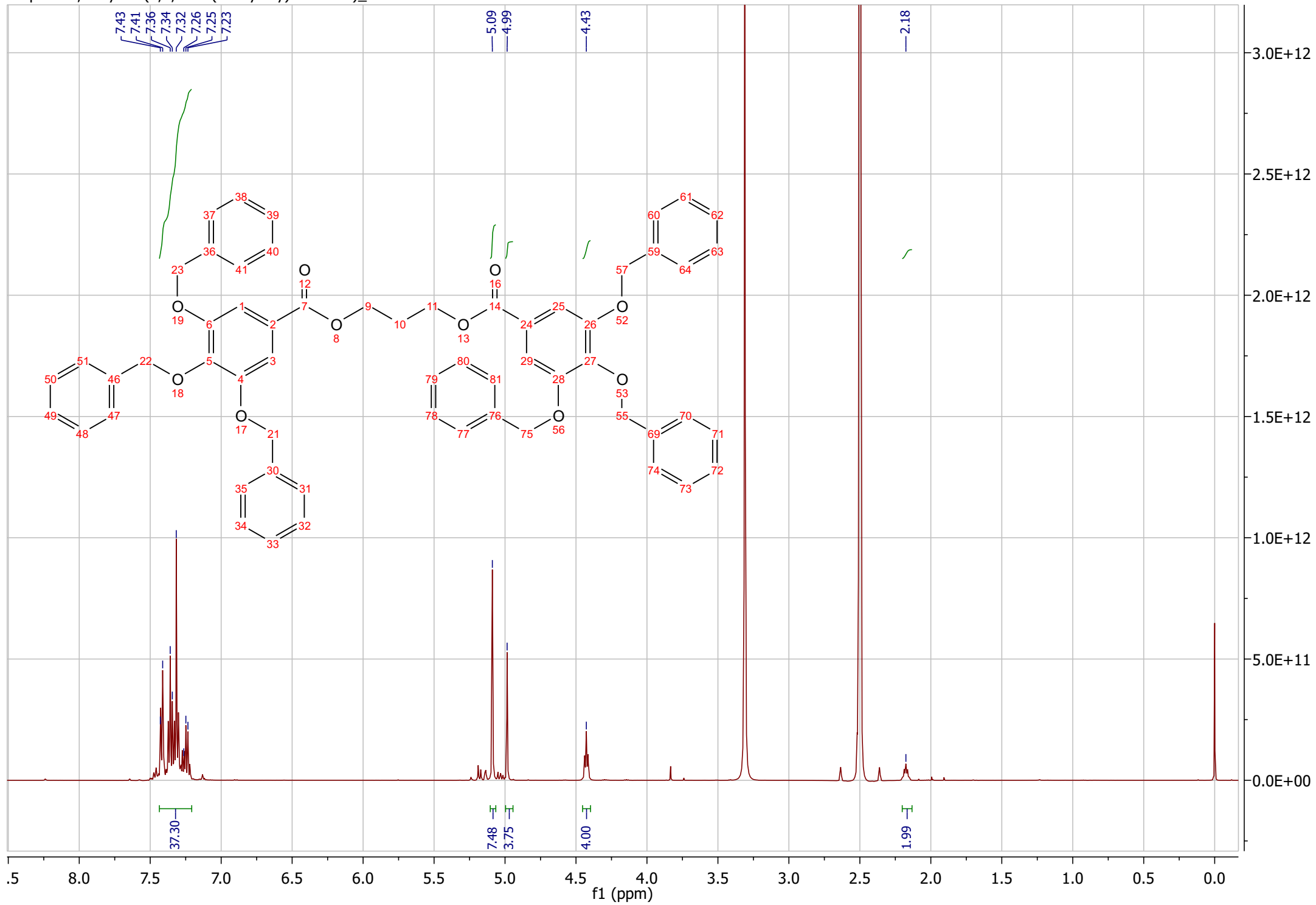
Ethane-1,2-diyl bis(3,4,5-tris(benzyloxy)benzoate)_DMSO



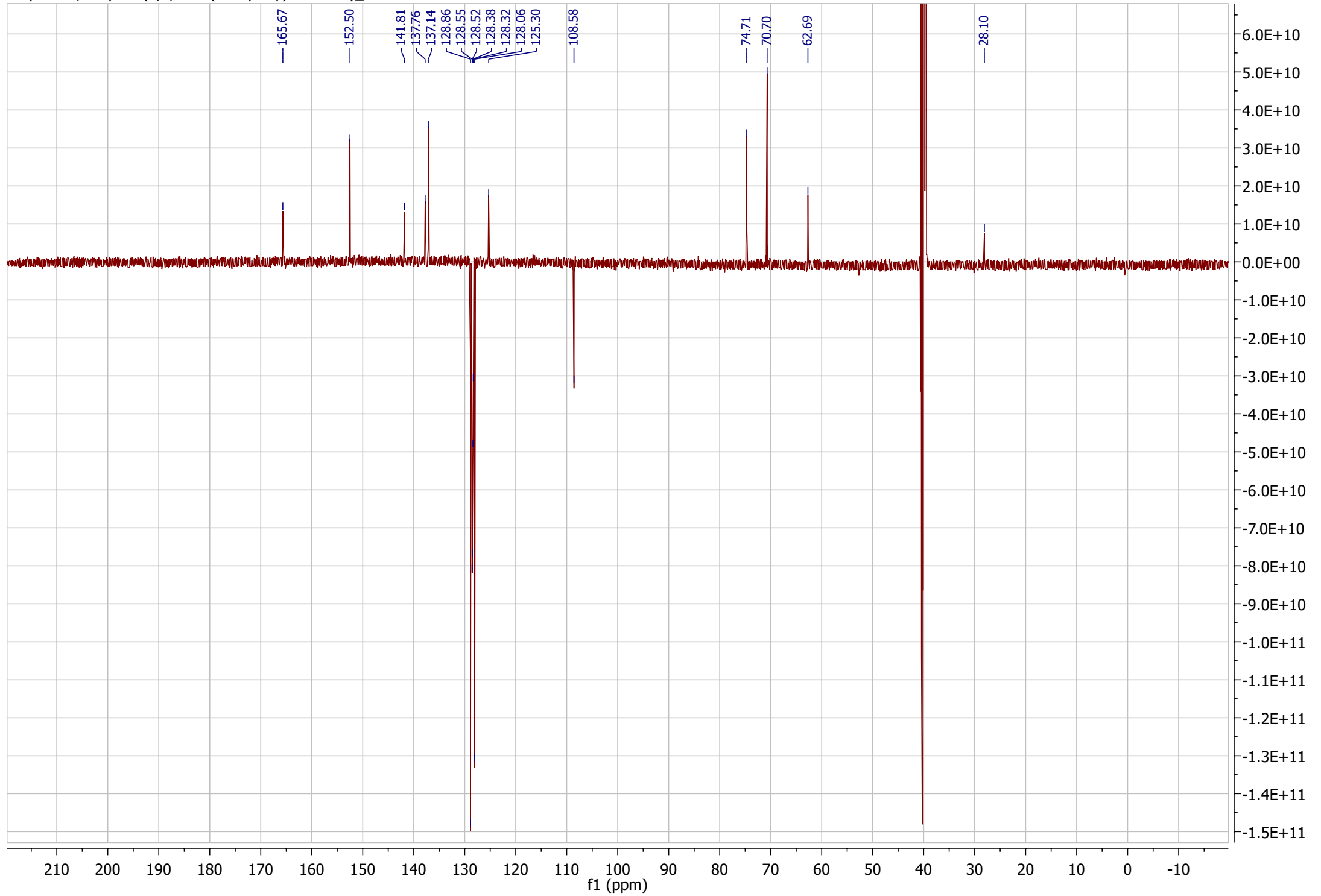
Ethane-1,2-diyl bis(3,4,5-tris(benzyloxy)benzoate)_DMSO



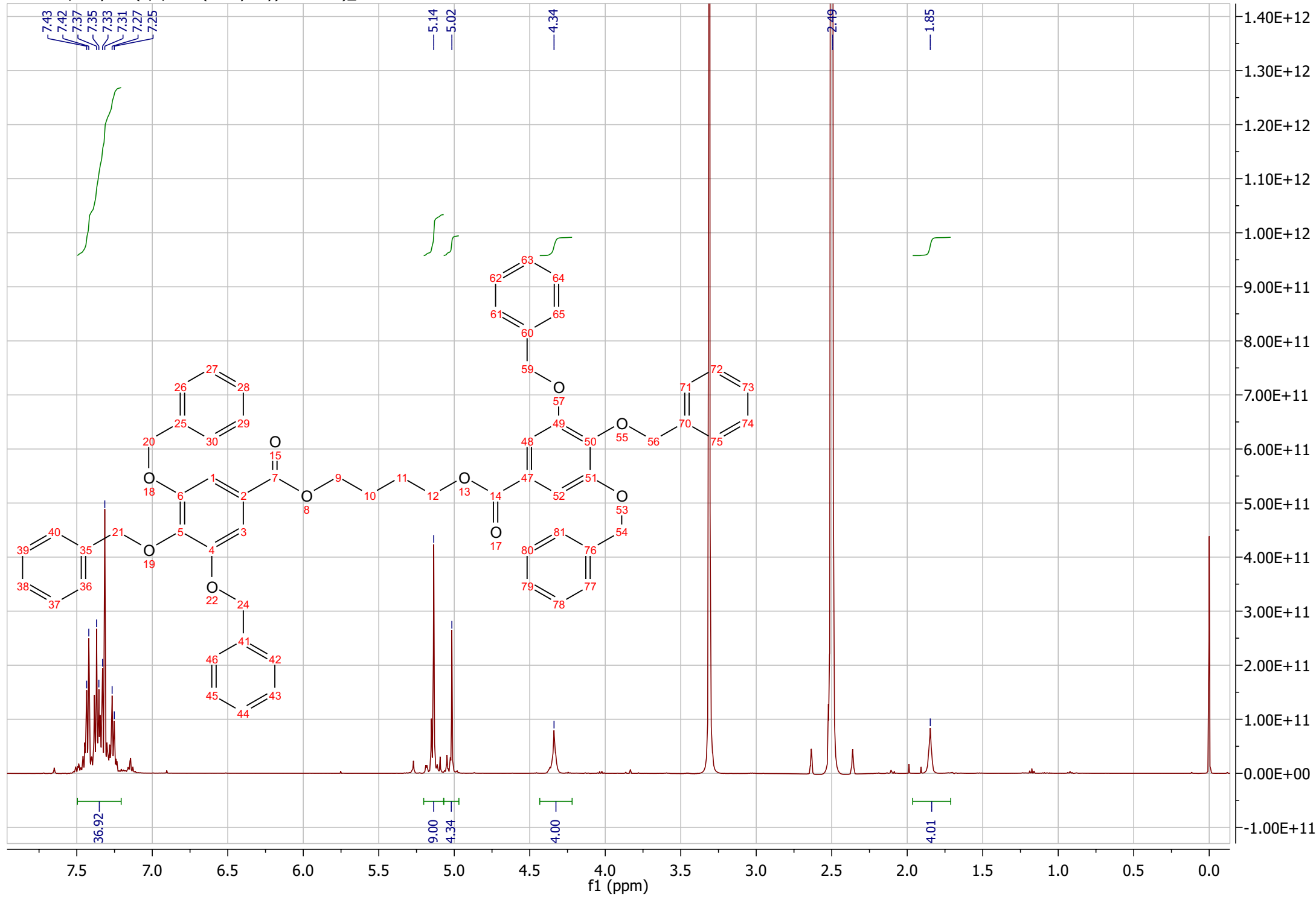
Propane-1,3-diyl bis(3,4,5-tris(benzyloxy)benzoate)_DMSO



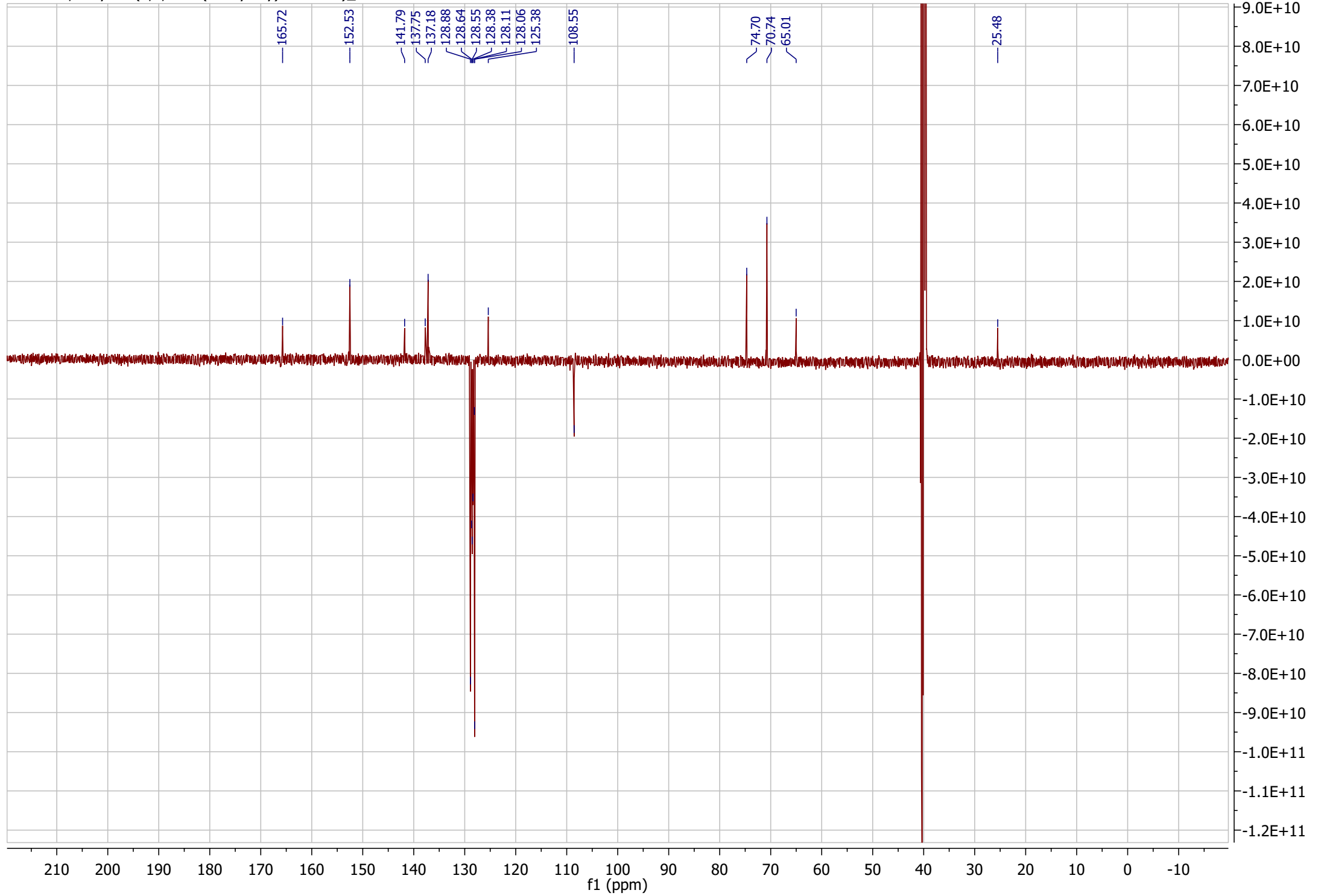
Propane-1,3-diyl bis(3,4,5-tris(benzyloxy)benzoate)_DMSO



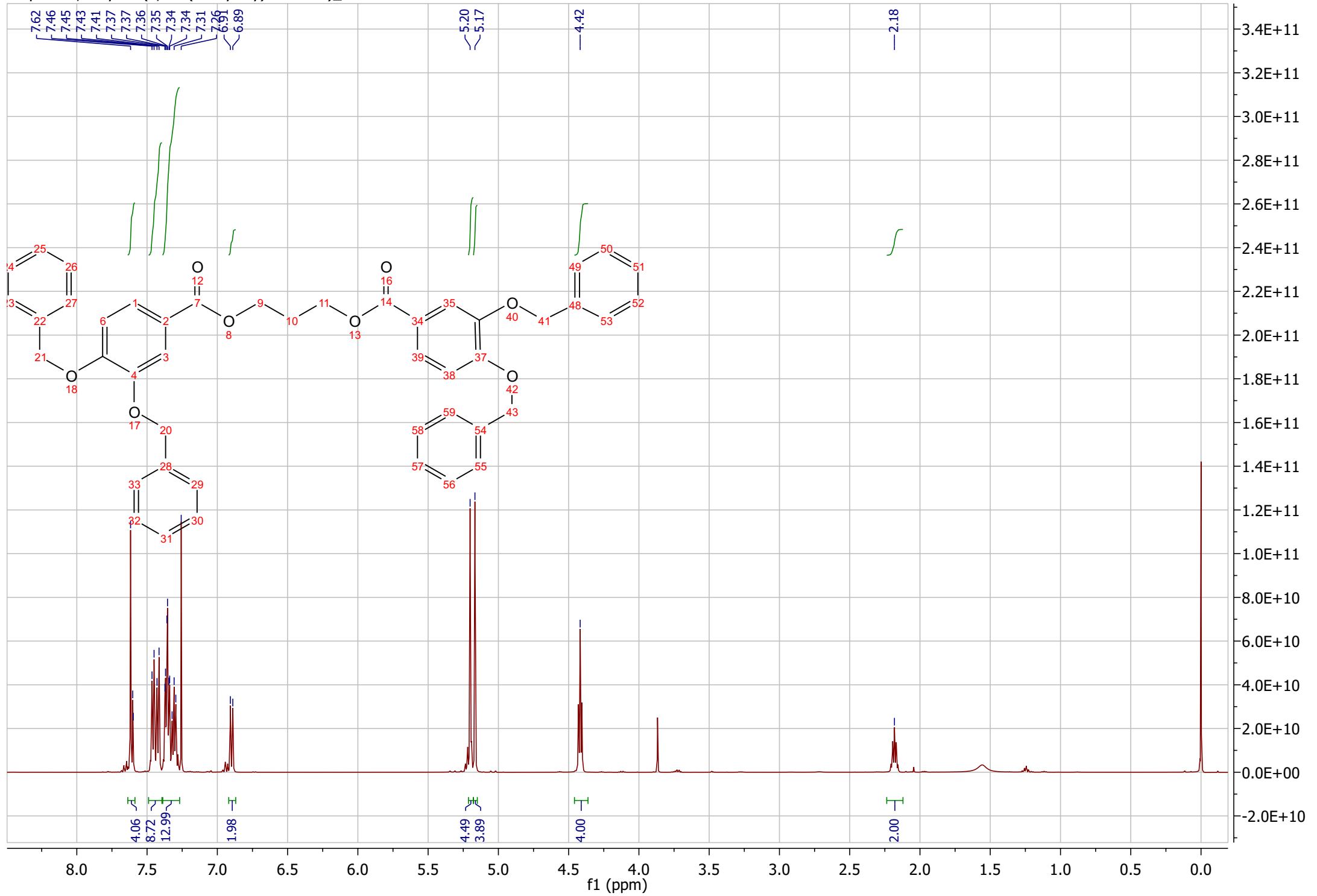
Butane-1,4-diyl bis(3,4,5-tris(benzyloxy)benzoate)_DMSO



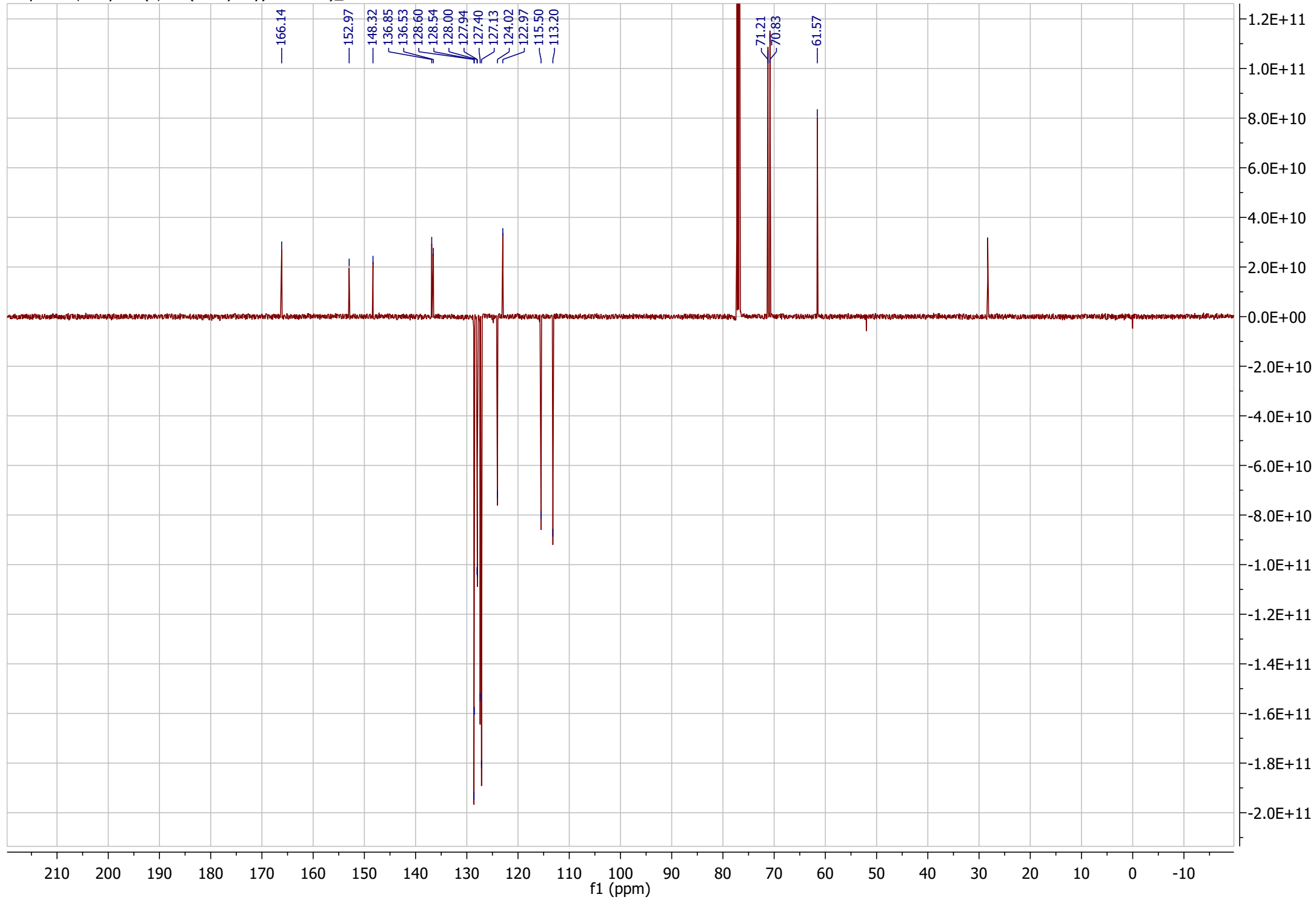
Butane-1,4-diyl bis(3,4,5-tris(benzyloxy)benzoate)_DMSO



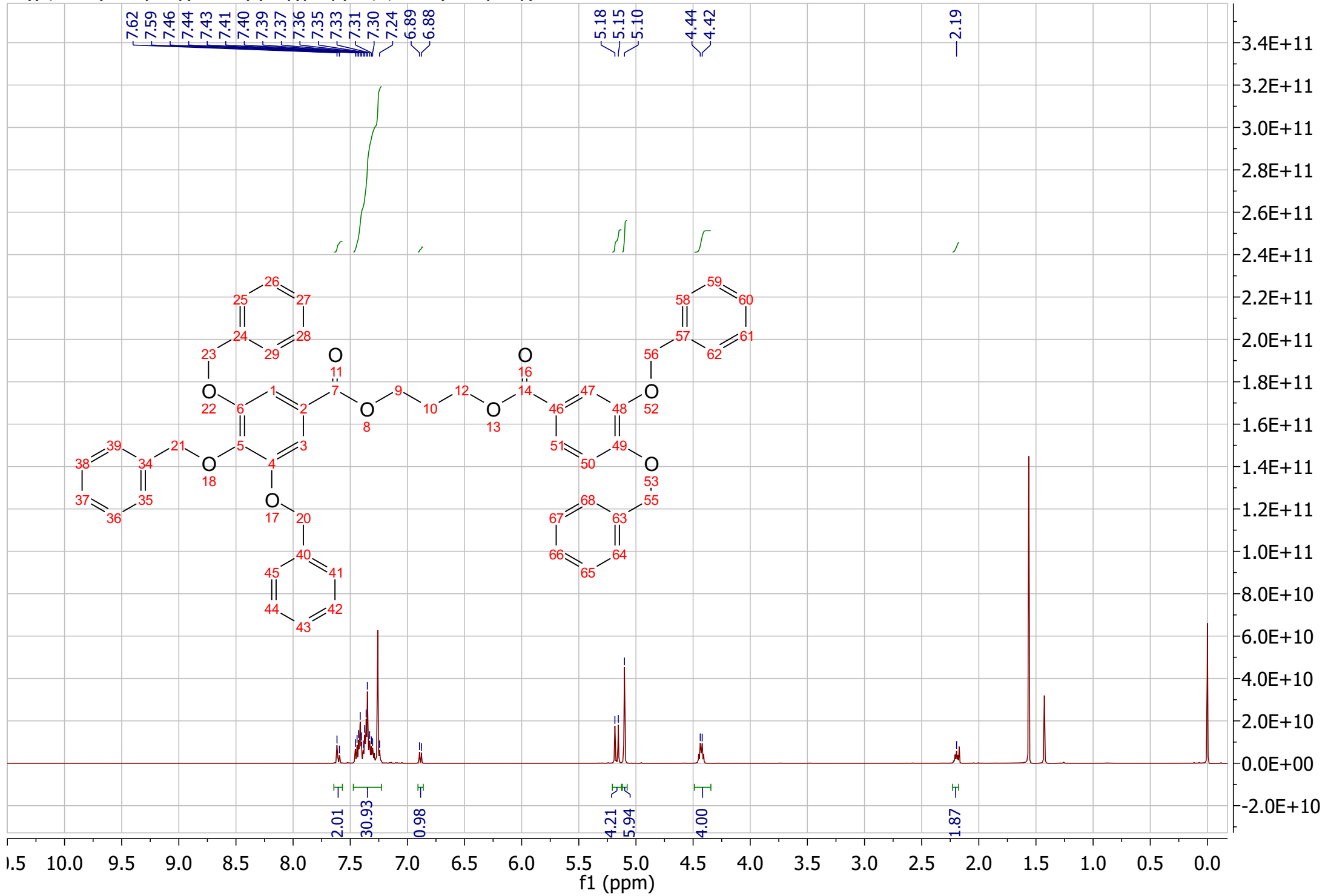
Propane-1,3-diyl bis(3,4-di(benzyloxy)benzoate)_CDCl3



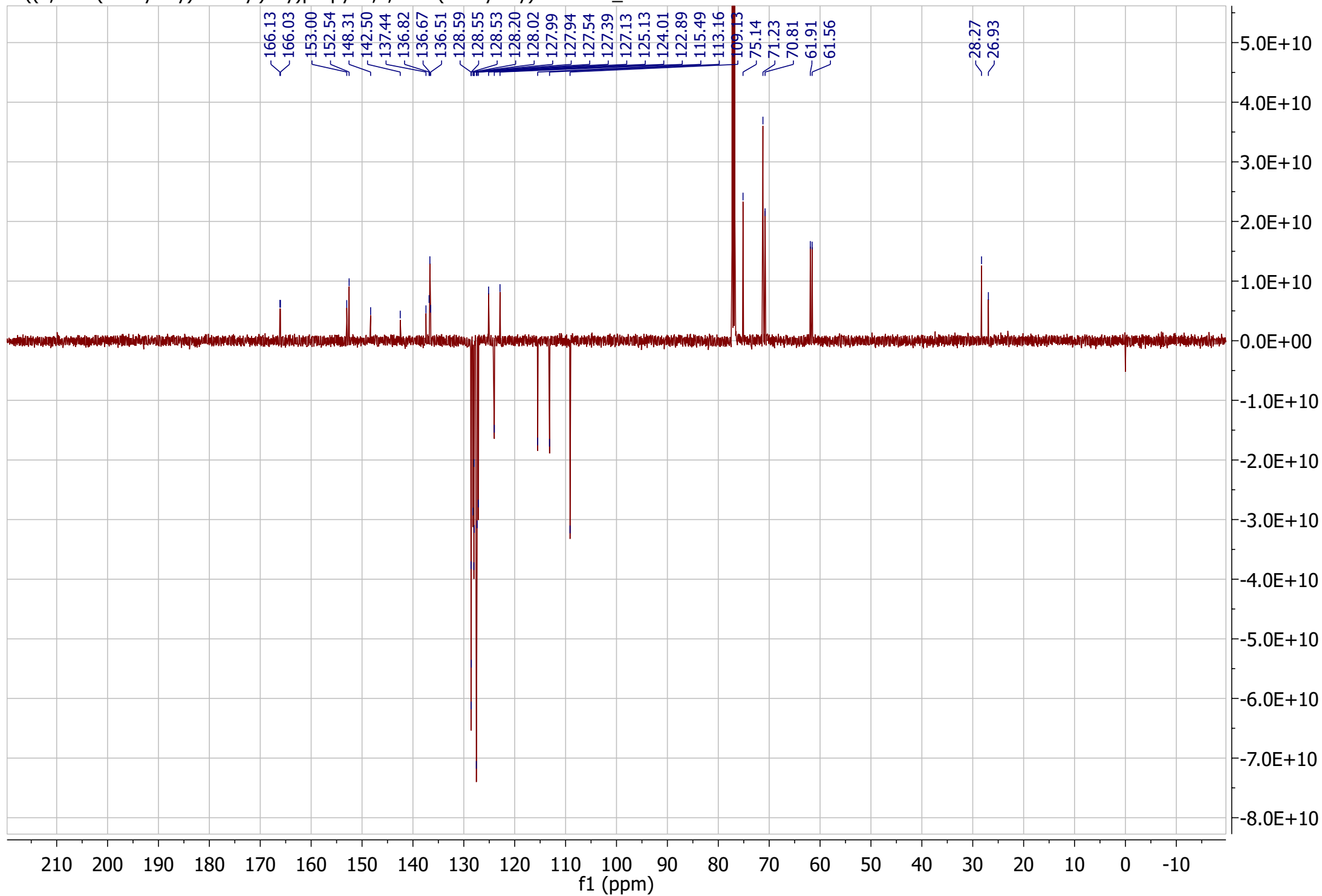
Propane-1,3-diyl bis(3,4-di(benzyloxy)benzoate)_CDCl3



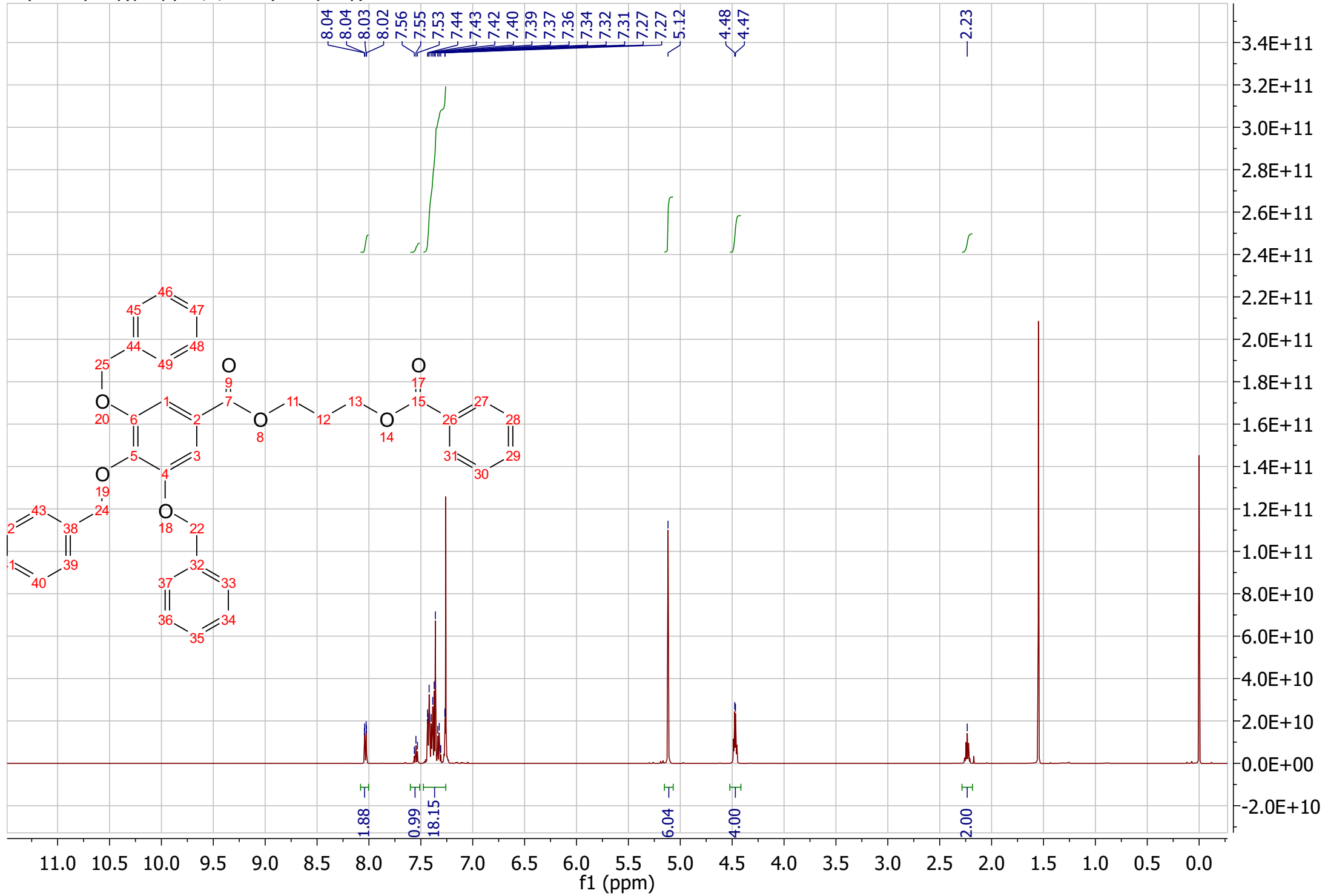
3-((3,5-bis(benzyloxy)benzoyl)oxy)propyl 3,4,5-tris(benzyloxy)benzoate_CDCl3



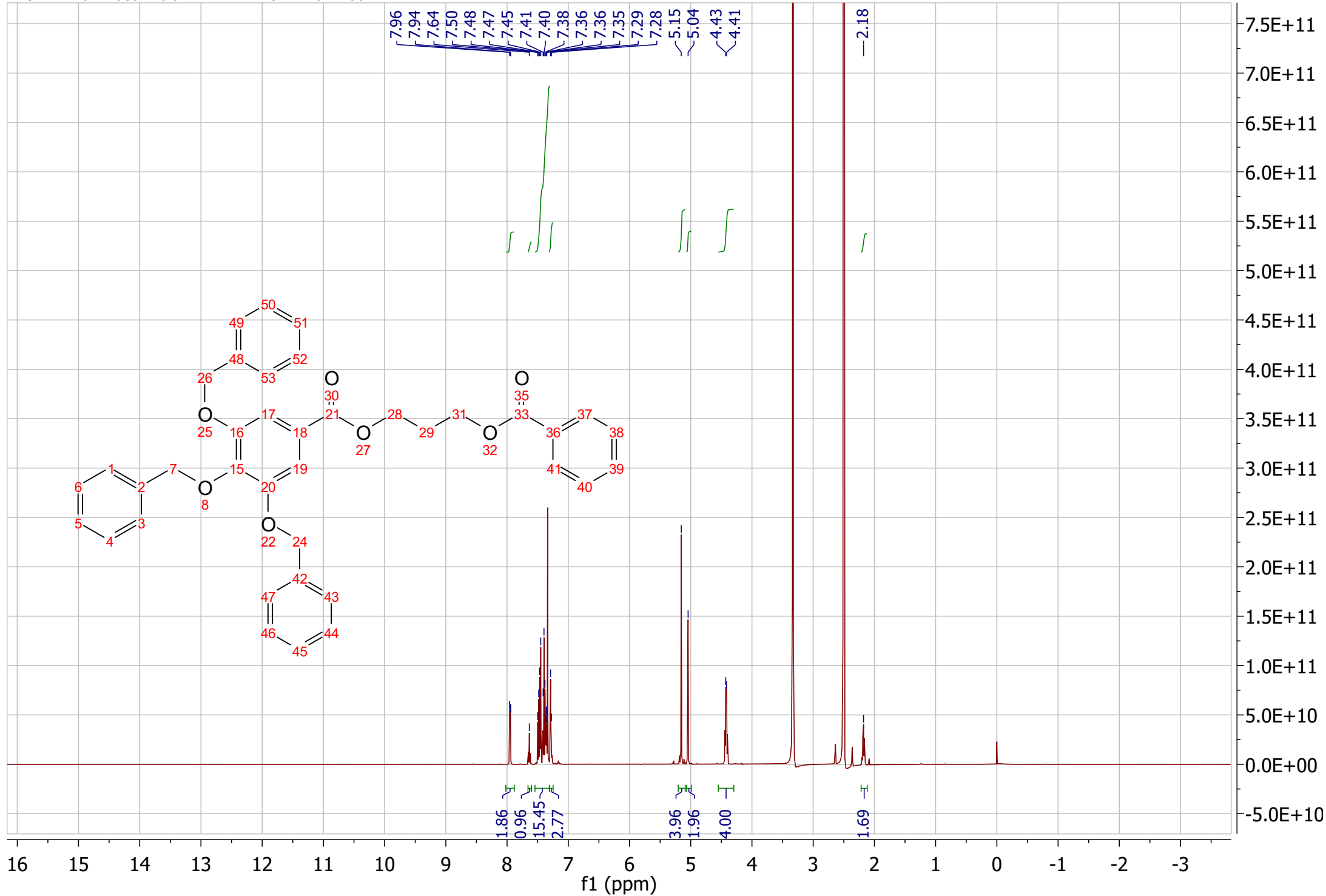
3-((3,5-bis(benzyloxy)benzoyl)oxy)propyl 3,4,5-tris(benzyloxy)benzoate_CDCl3



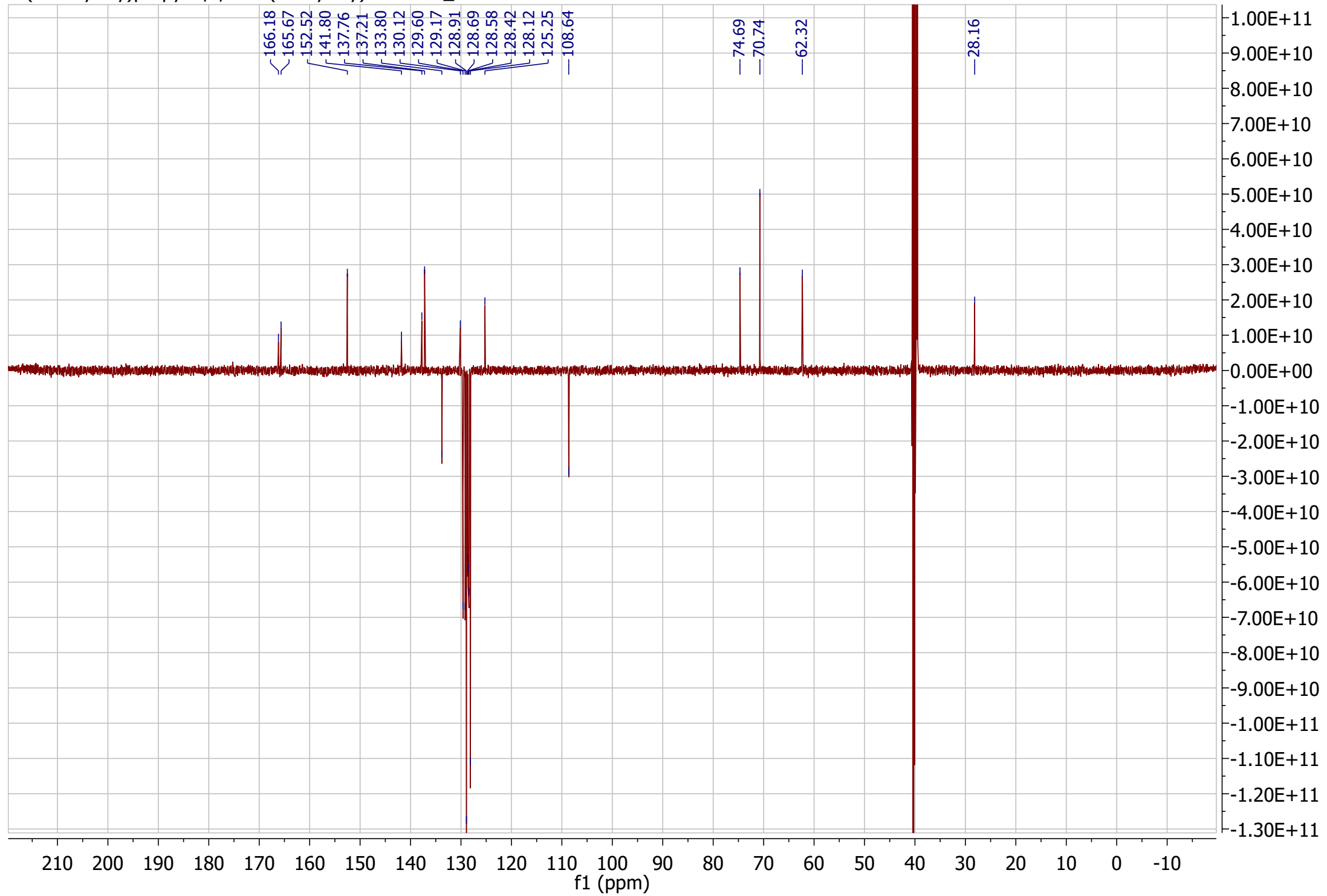
3-(benzyloxy)propyl 3,4,5-tris(benzyloxy)benzoate_CDCl3



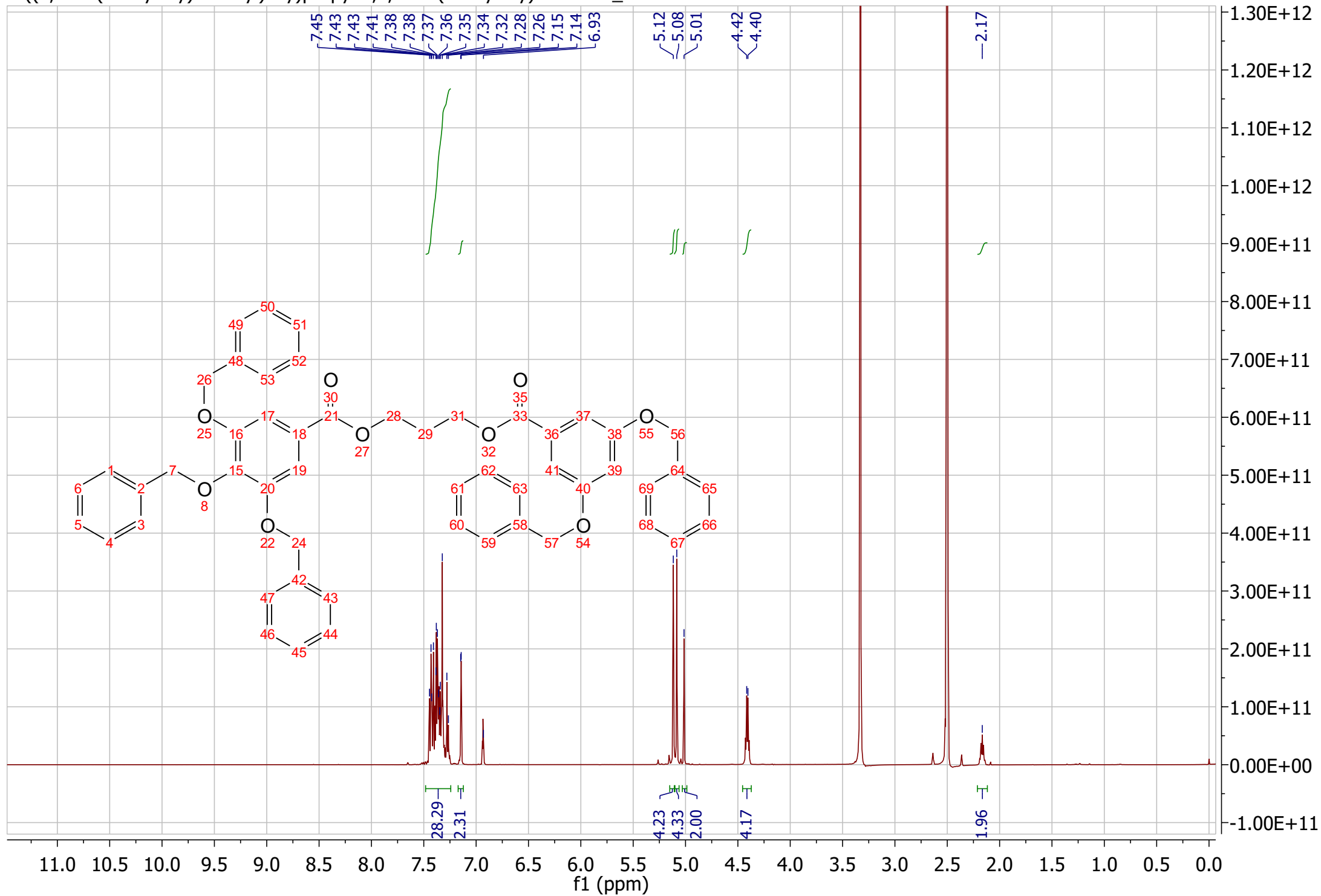
3-(benzyloxy)propyl 3,4,5-tris(benzyloxy)benzoate_DMSO



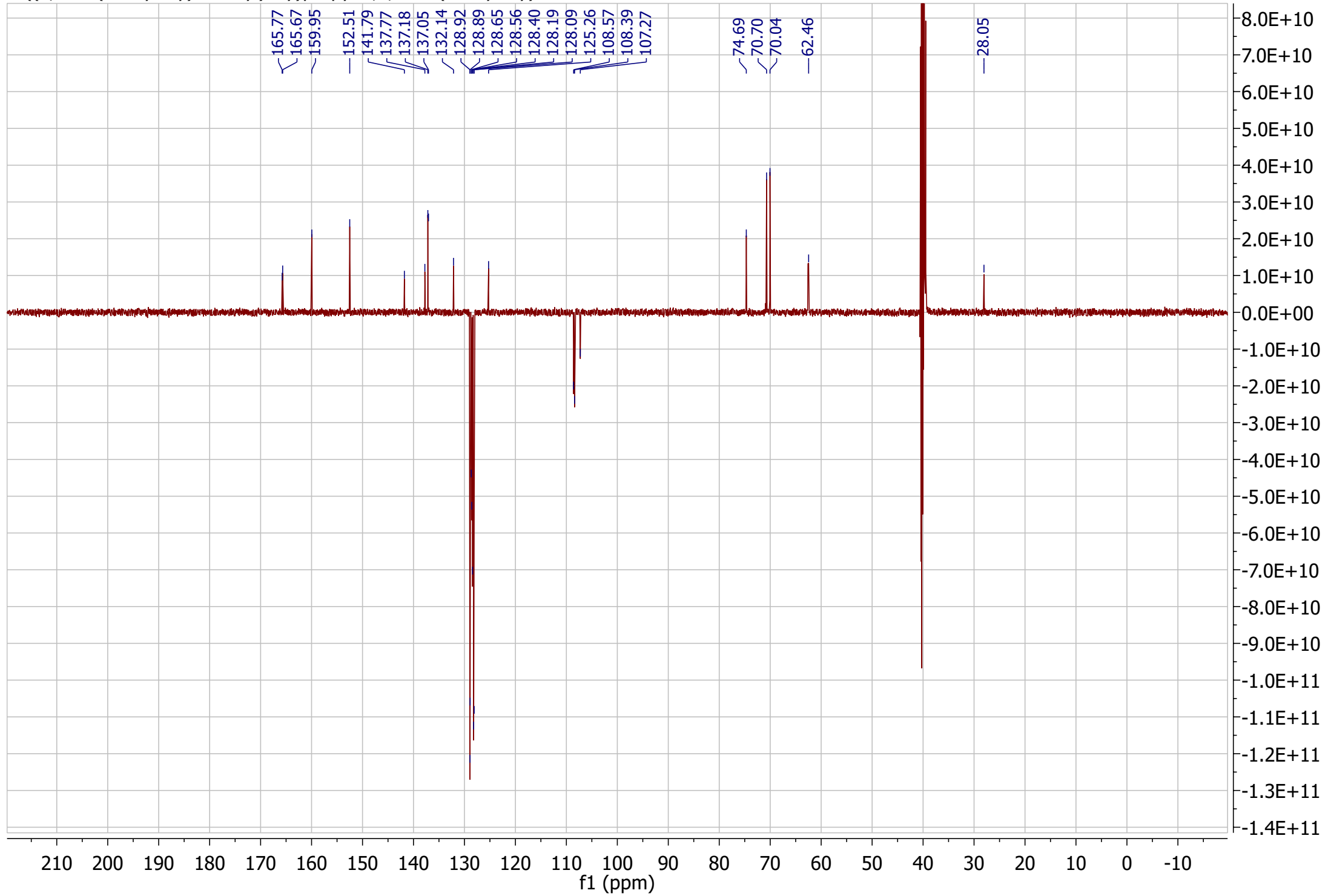
3-(benzyloxy)propyl 3,4,5-tris(benzyloxy)benzoate_DMSO



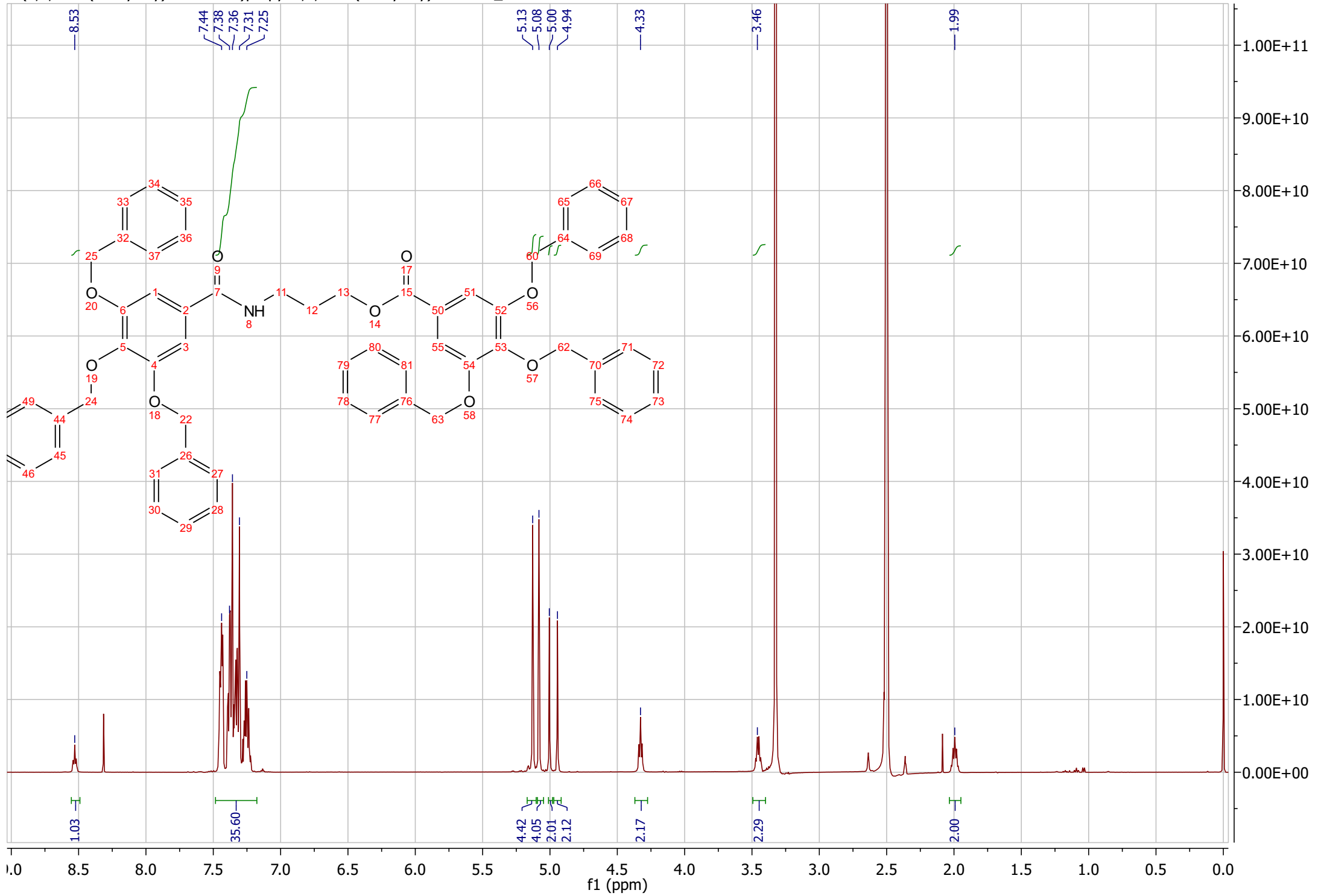
3-((3,5-bis(benzyloxy)benzoyl)oxy)propyl 3,4,5-tris(benzyloxy)benzoate_DMSO



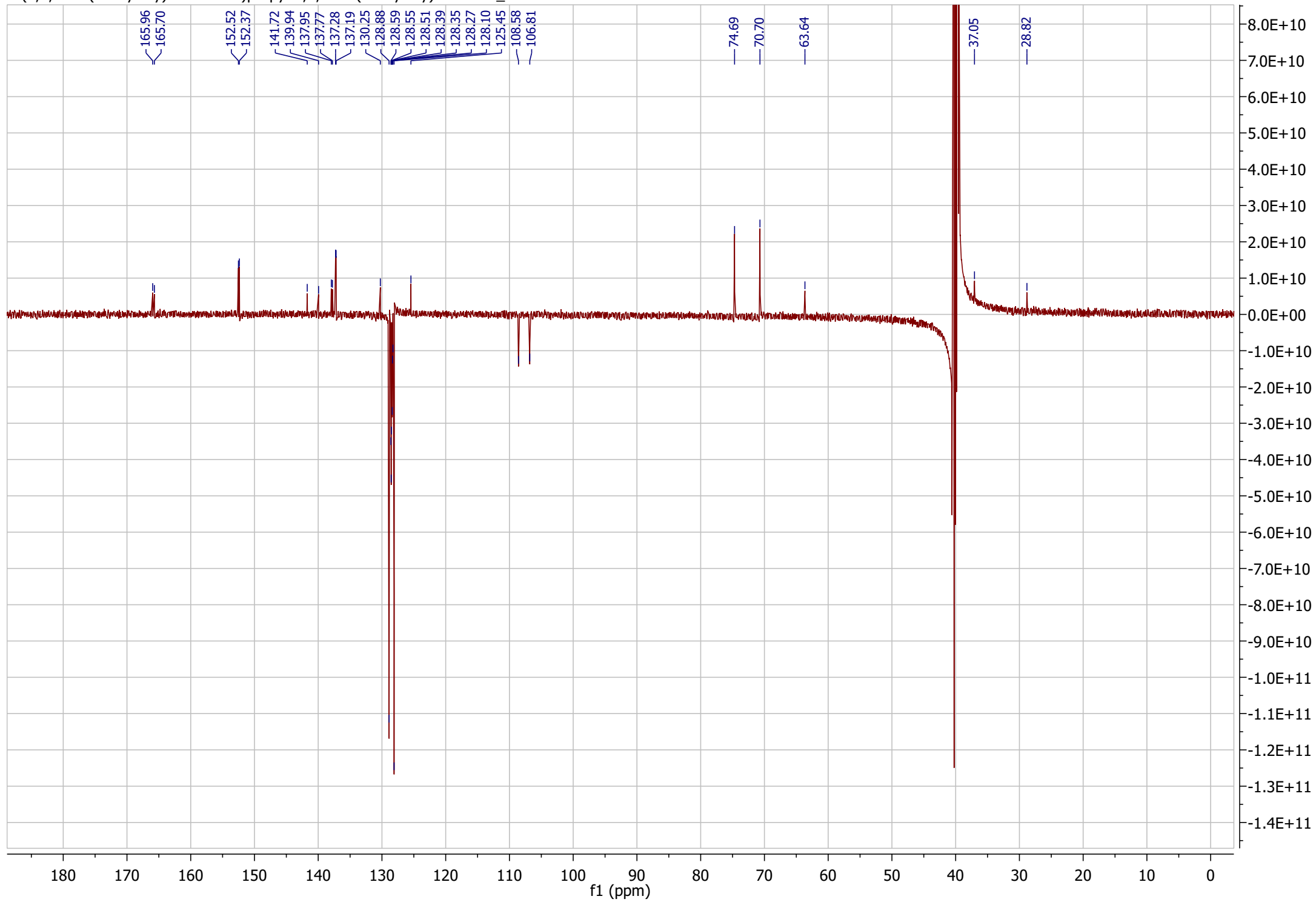
3-((3,5-bis(benzyloxy)benzoyl)oxy)propyl 3,4,5-tris(benzyloxy)benzoate_DMSO



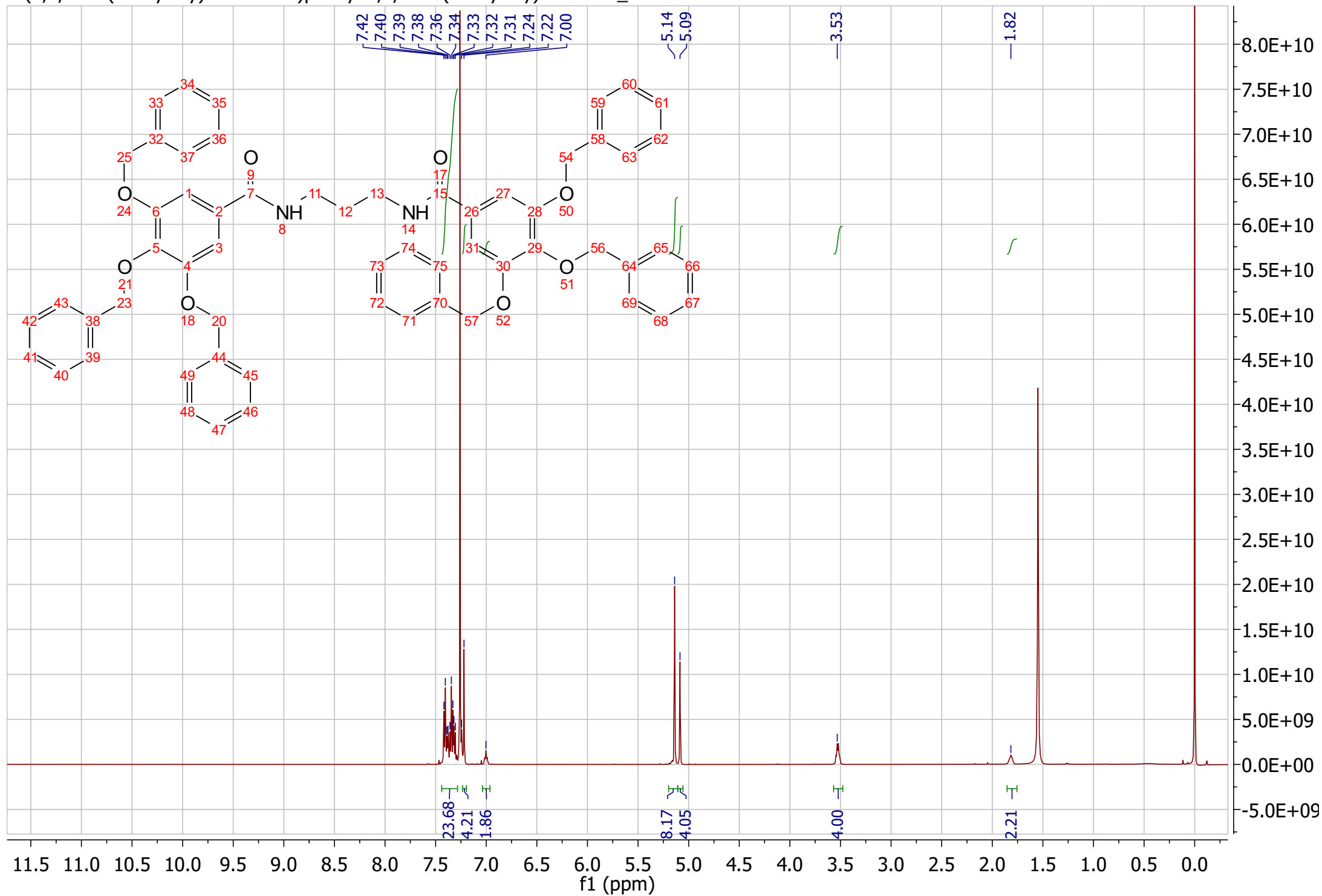
3-(3,4,5-tris(benzyloxy)benzamido)propyl 3,4,5-tris(benzyloxy)benzoate_DMSO



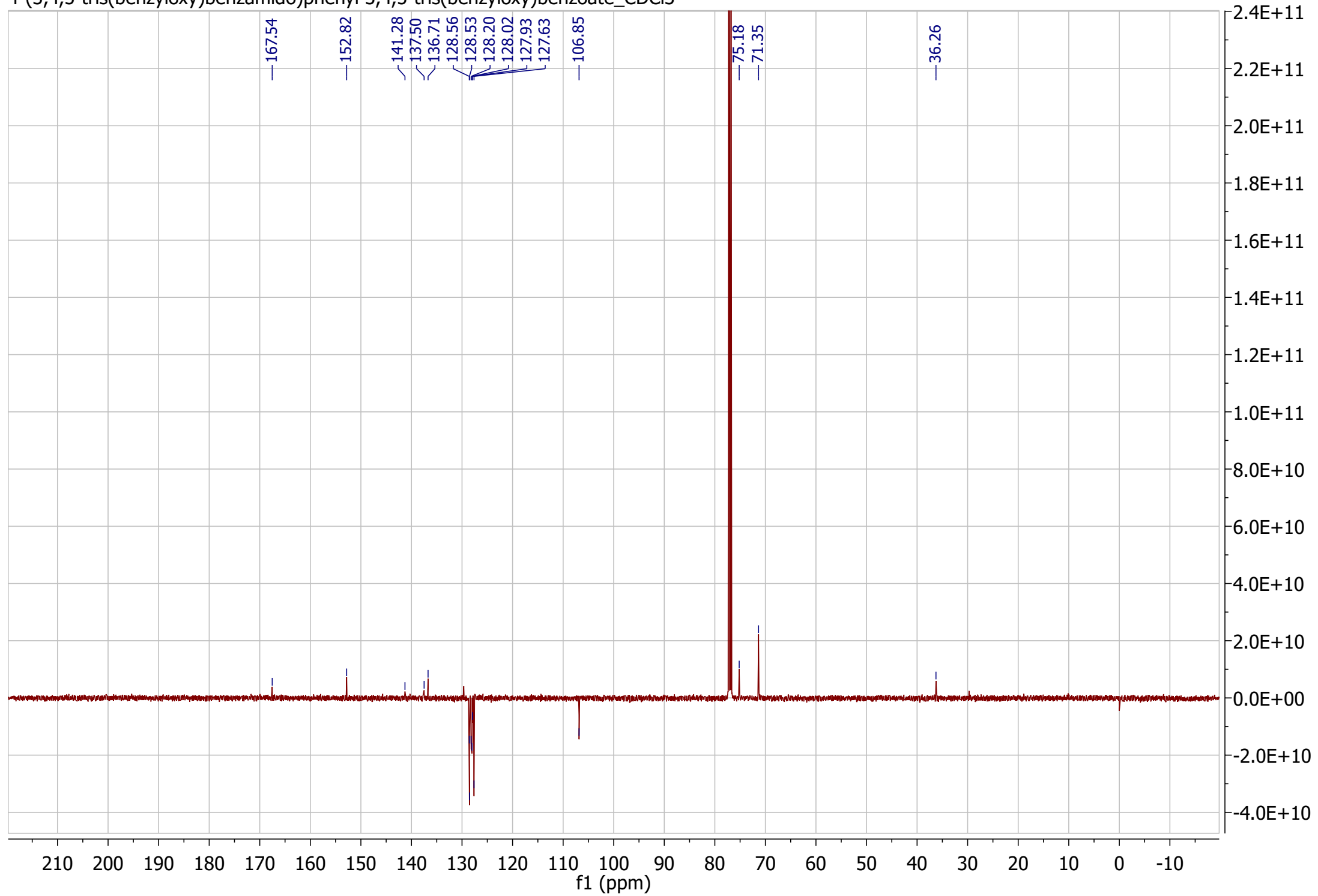
3-(3,4,5-tris(benzyloxy)benzamido)propyl 3,4,5-tris(benzyloxy)benzoate_DMSO



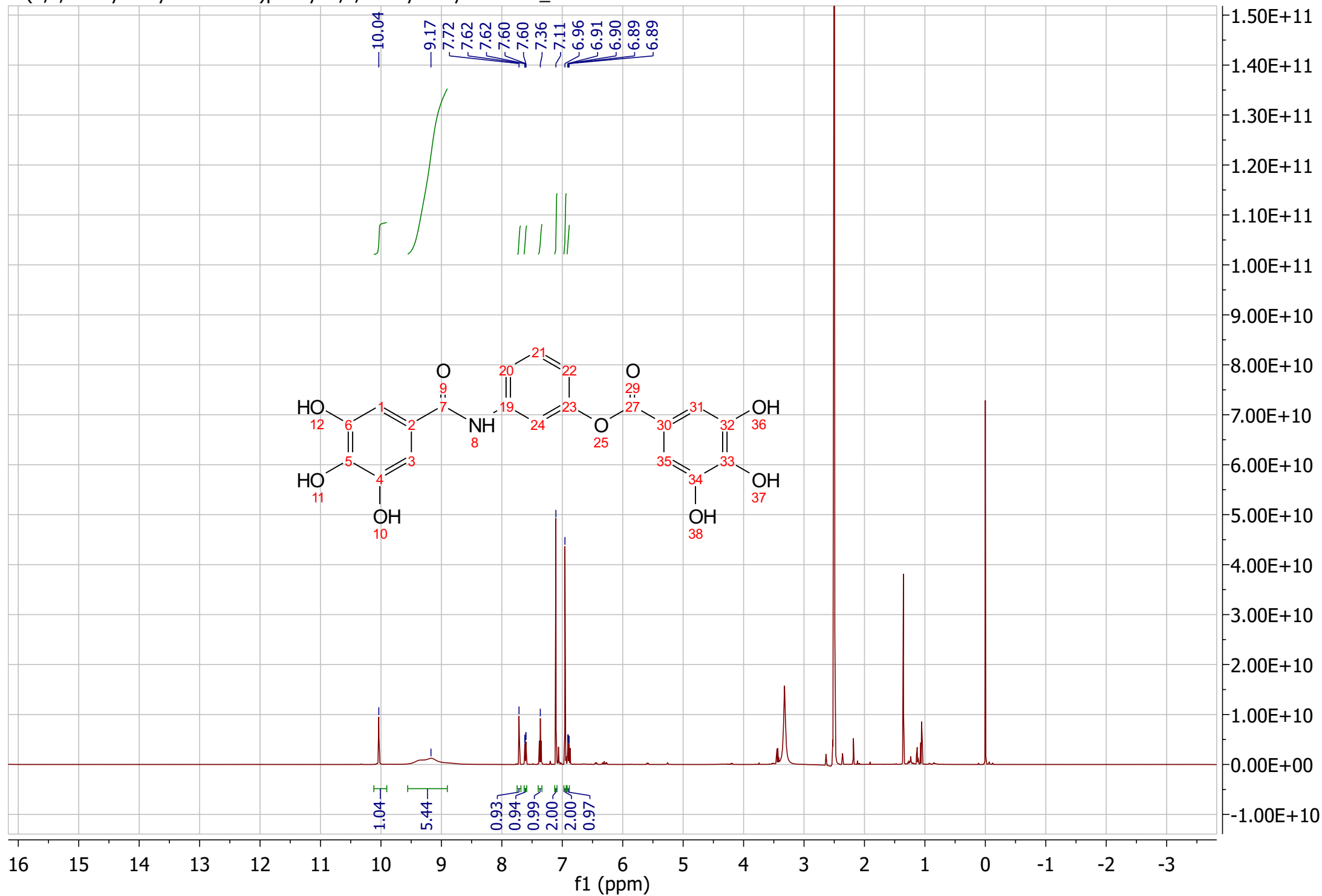
4-(3,4,5-tris(benzyloxy)benzamido)phenyl 3,4,5-tris(benzyloxy)benzoate_CDCl3



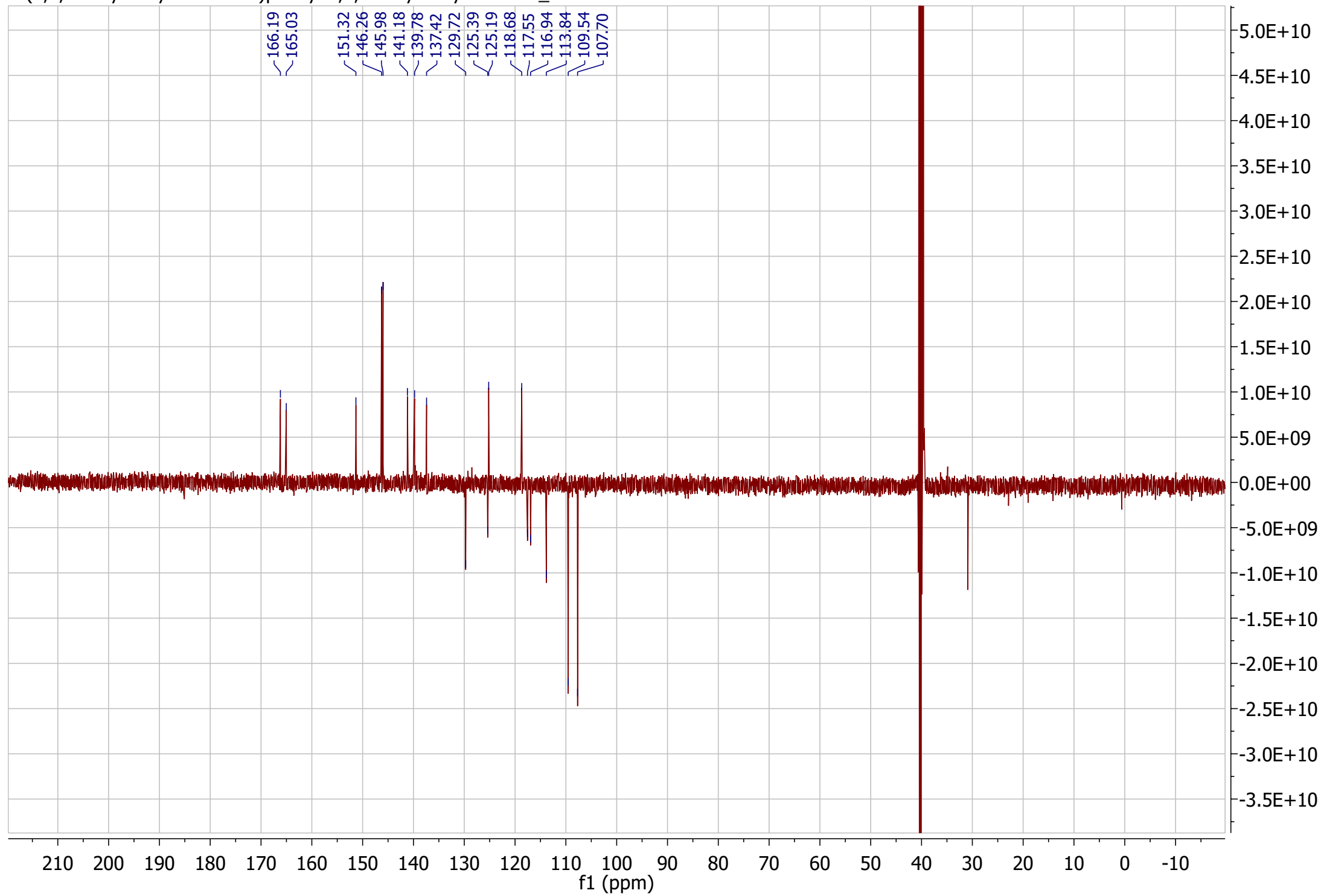
4-(3,4,5-tris(benzyloxy)benzamido)phenyl 3,4,5-tris(benzyloxy)benzoate_CDCl3



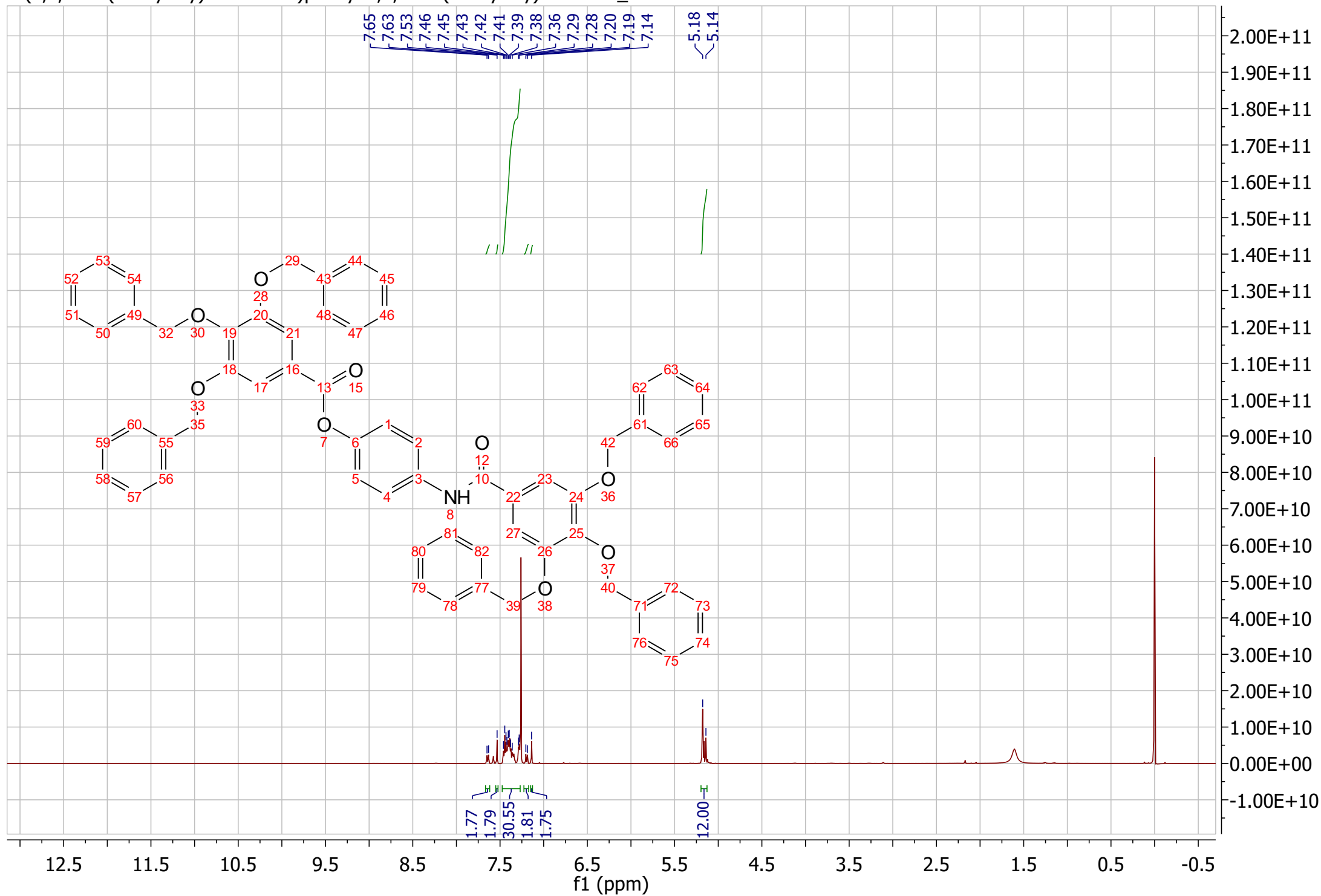
3-(3,4,5-trihydroxybenzamido)phenyl 3,4,5-trihydroxybenzoate_DMSO



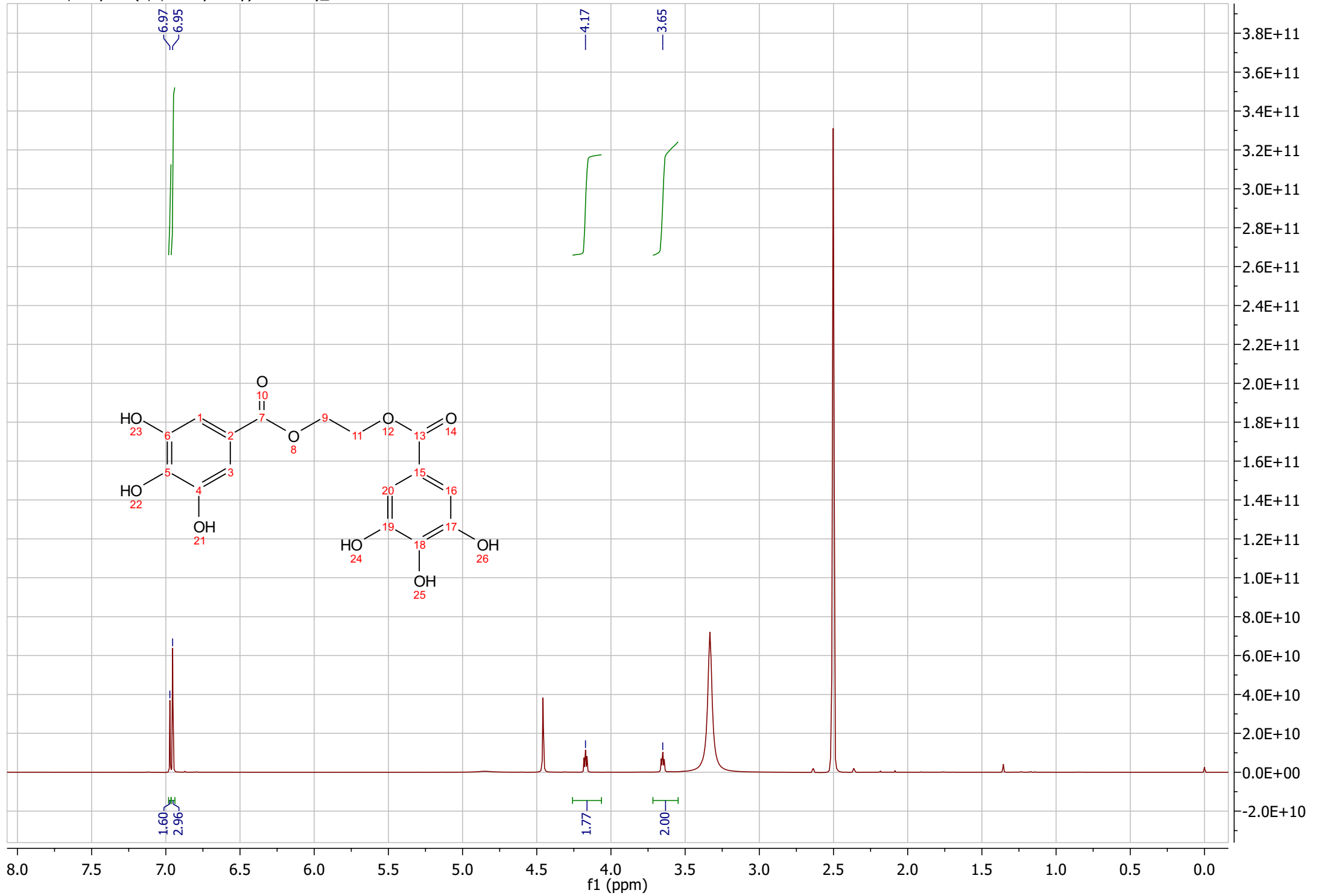
3-(3,4,5-trihydroxybenzamido)phenyl 3,4,5-trihydroxybenzoate_DMSO



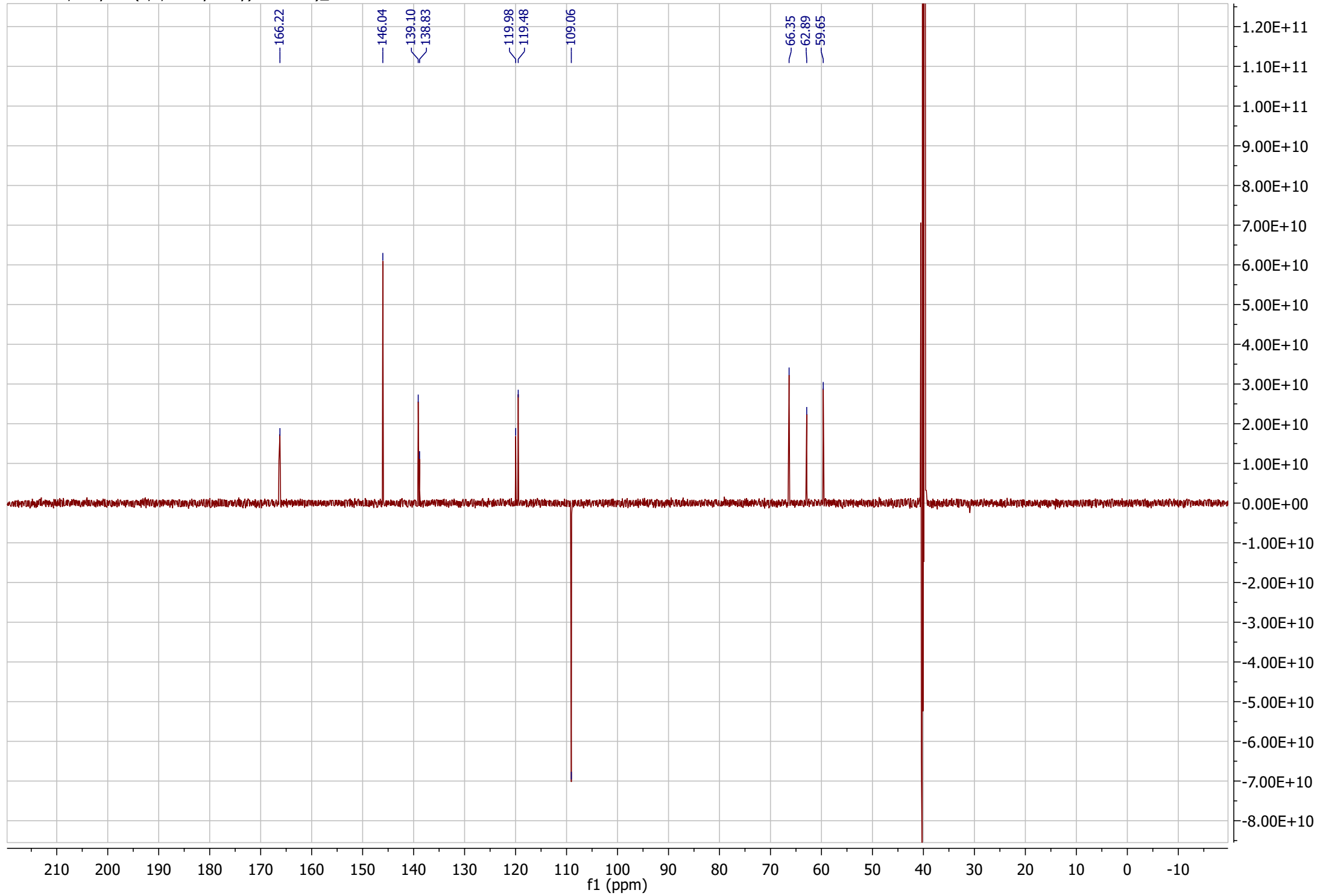
3-(3,4,5-tris(benzyloxy)benzamido)phenyl 3,4,5-tris(benzyloxy)benzoate_CDCl3



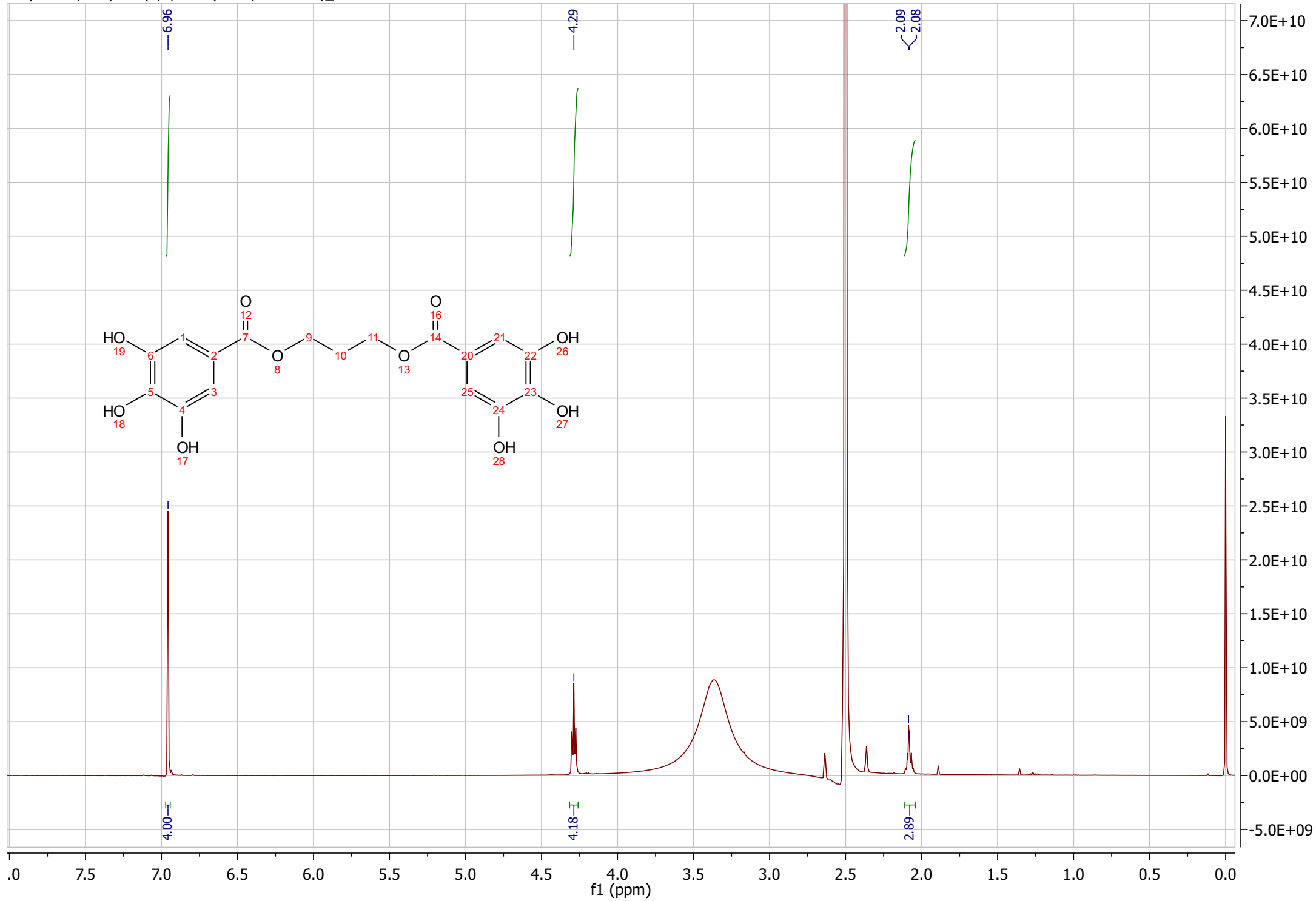
Ethane-1,2-diyl bis(3,4,5-trihydroxy)benzoate)_DMSO



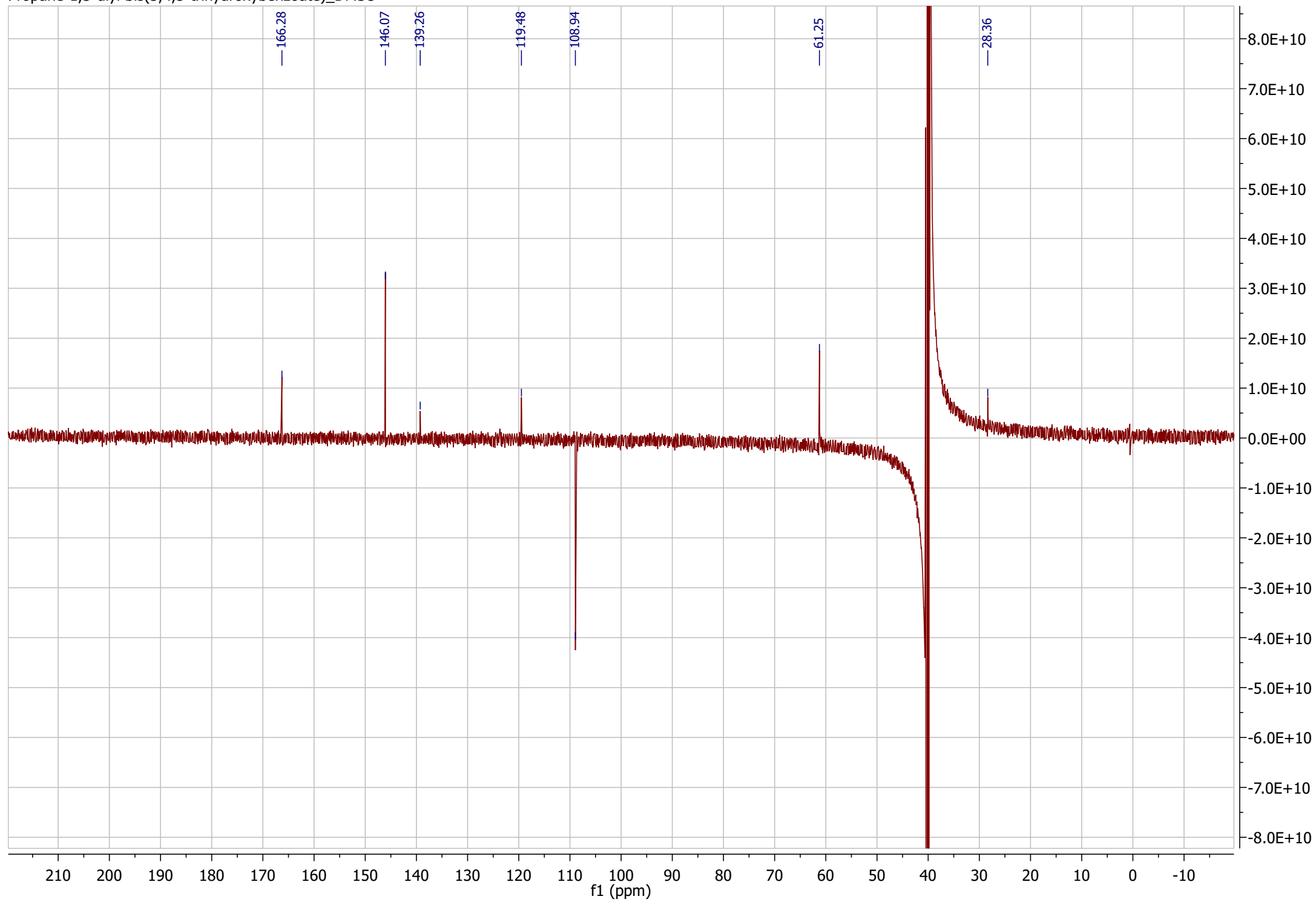
Ethane-1,2-diyl bis(3,4,5-trihydroxy)benzoate)_DMSO



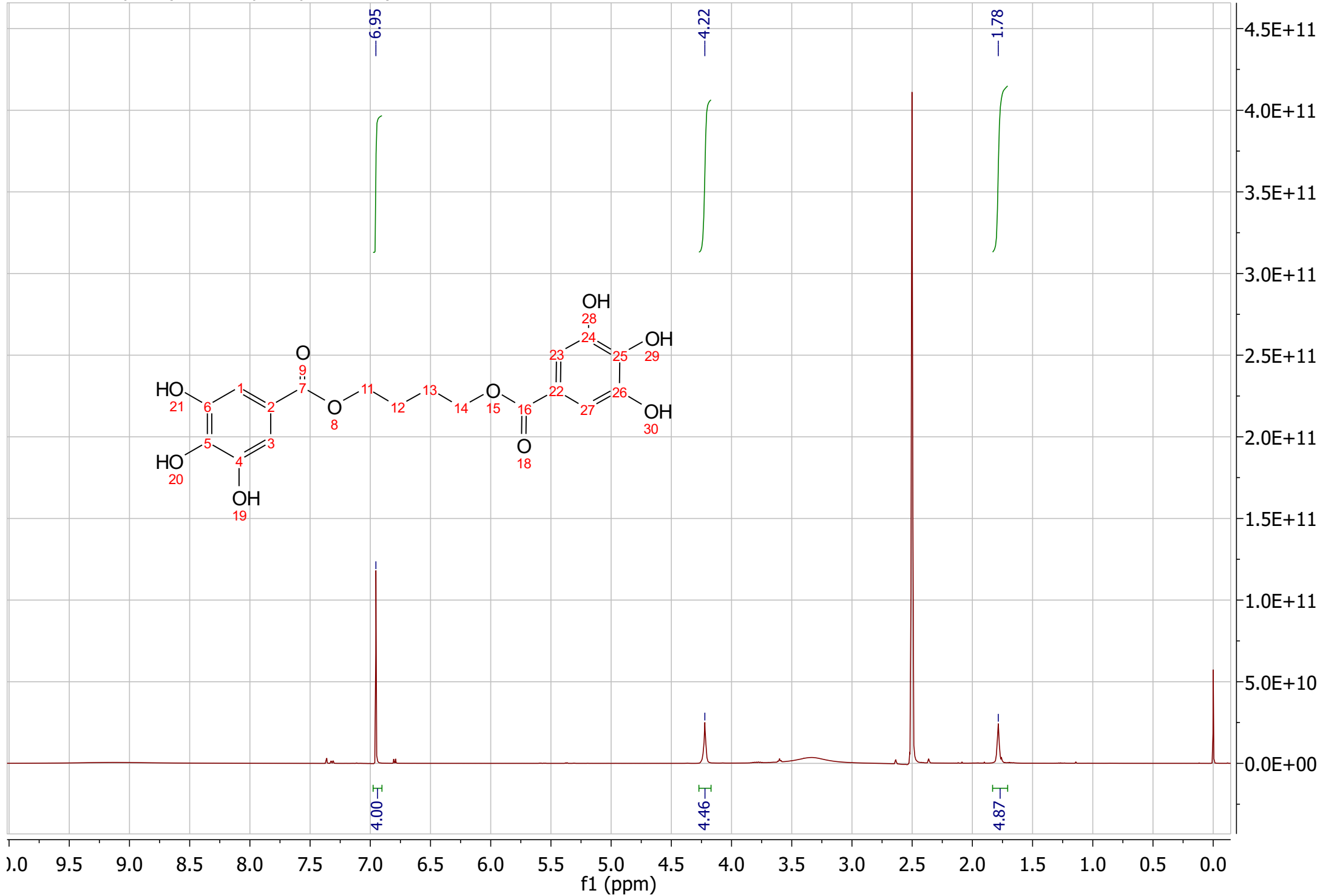
Propane-1,3-diyl bis(3,4,5-trihydroxybenzoate)_DMSO



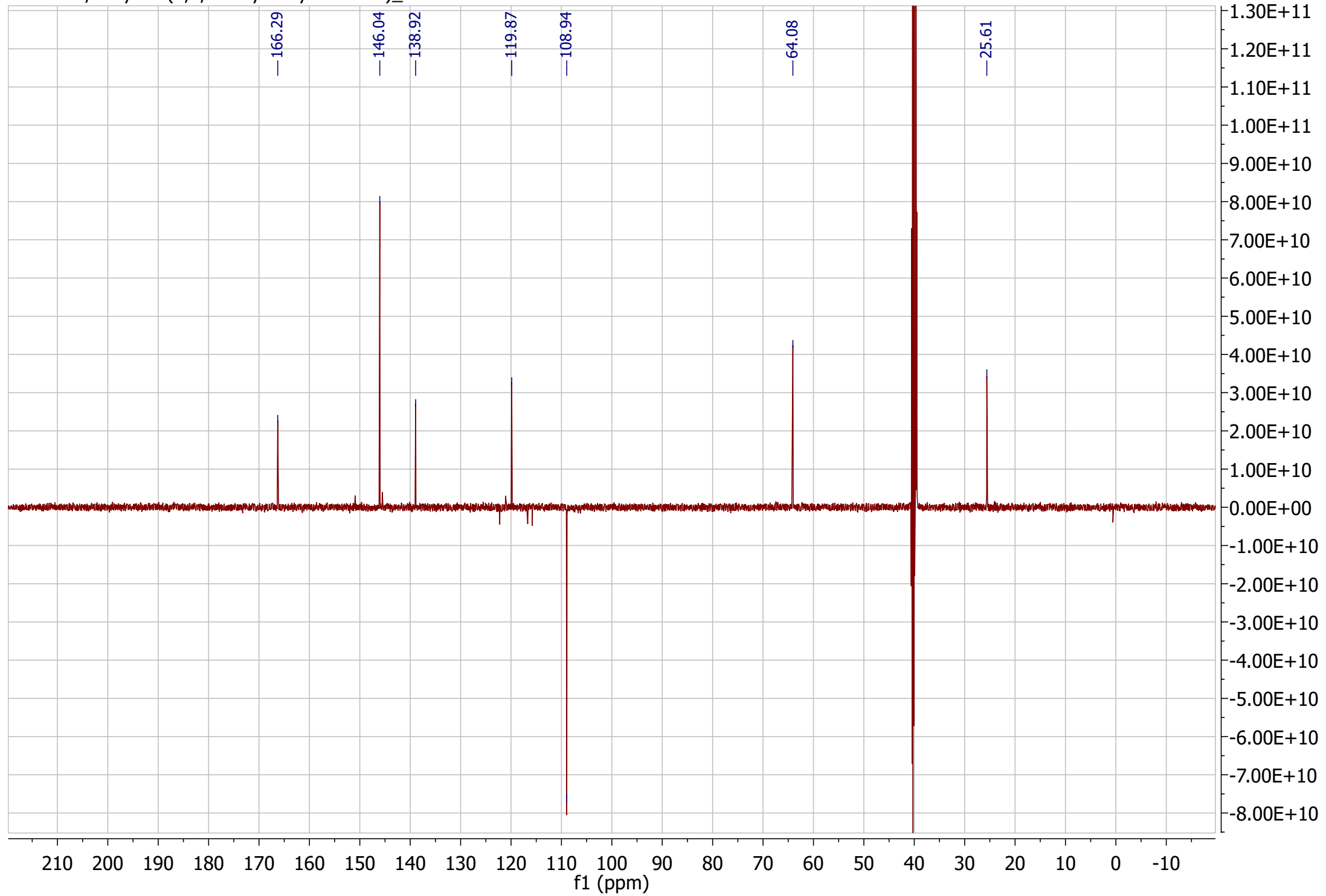
Propane-1,3-diyl bis(3,4,5-trihydroxybenzoate)_DMSO



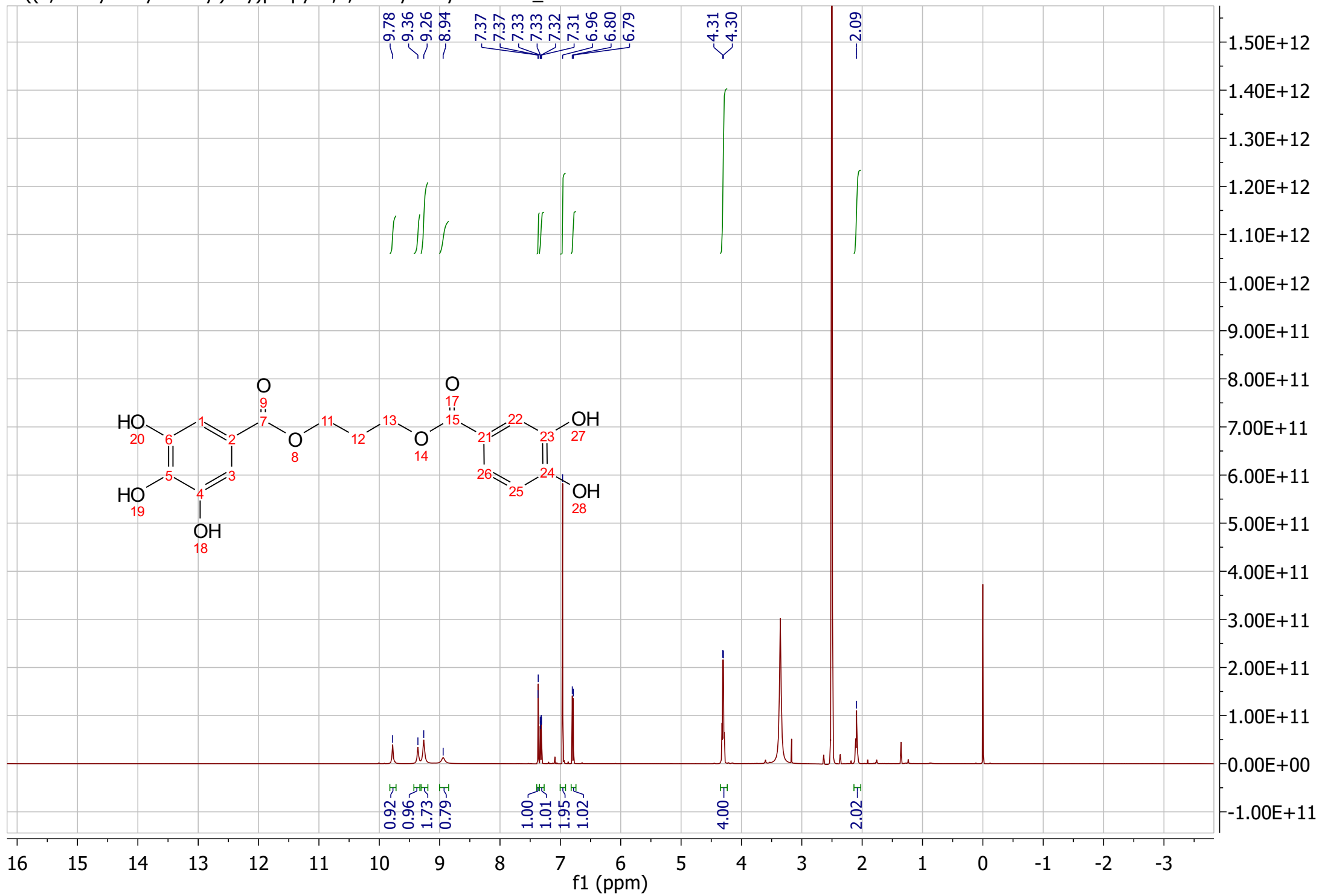
Butane-1,4-diyl bis(3,4,5-trihydroxybenzoate)_DMSO



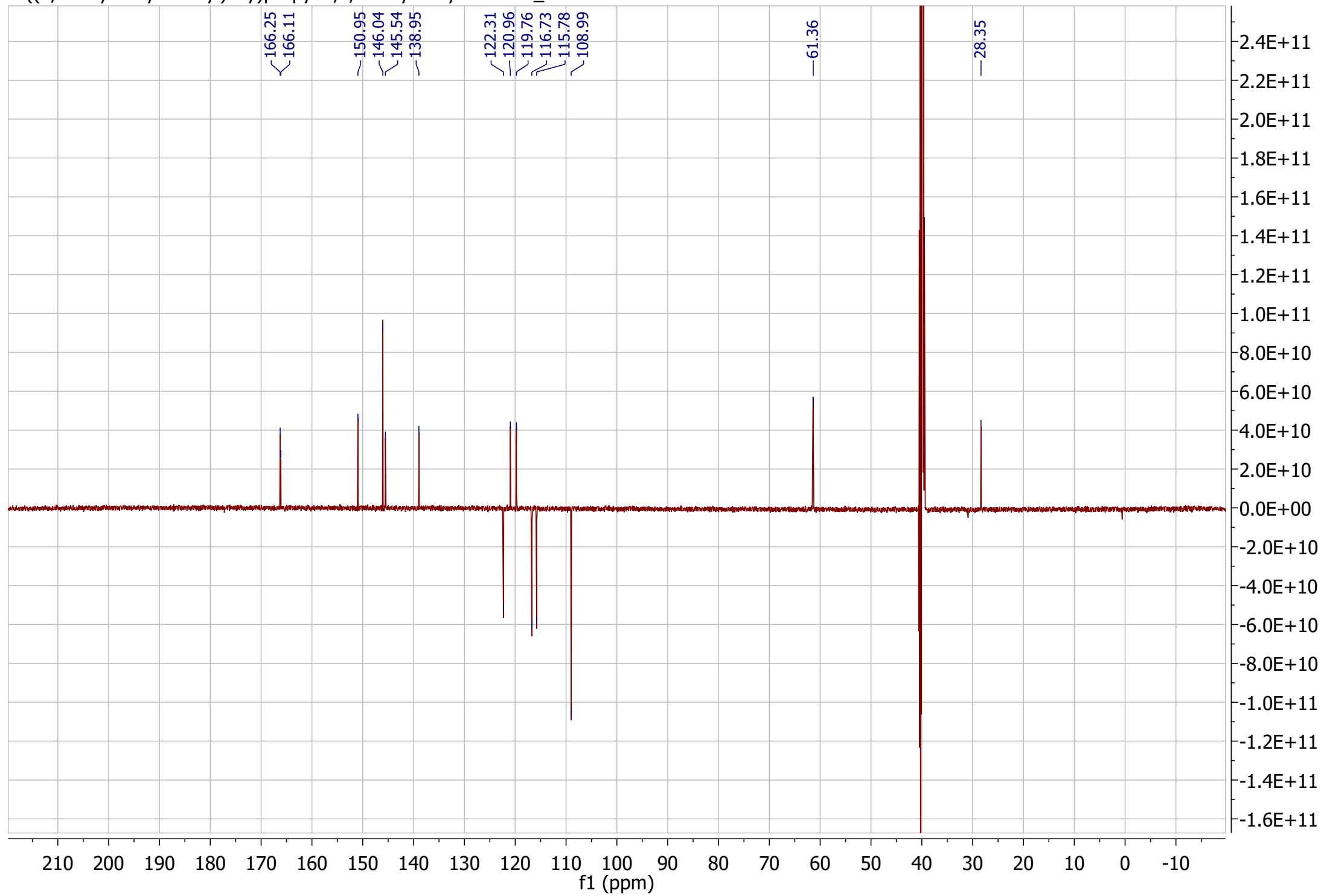
Butane-1,4-diyl bis(3,4,5-trihydroxybenzoate)_DMSO



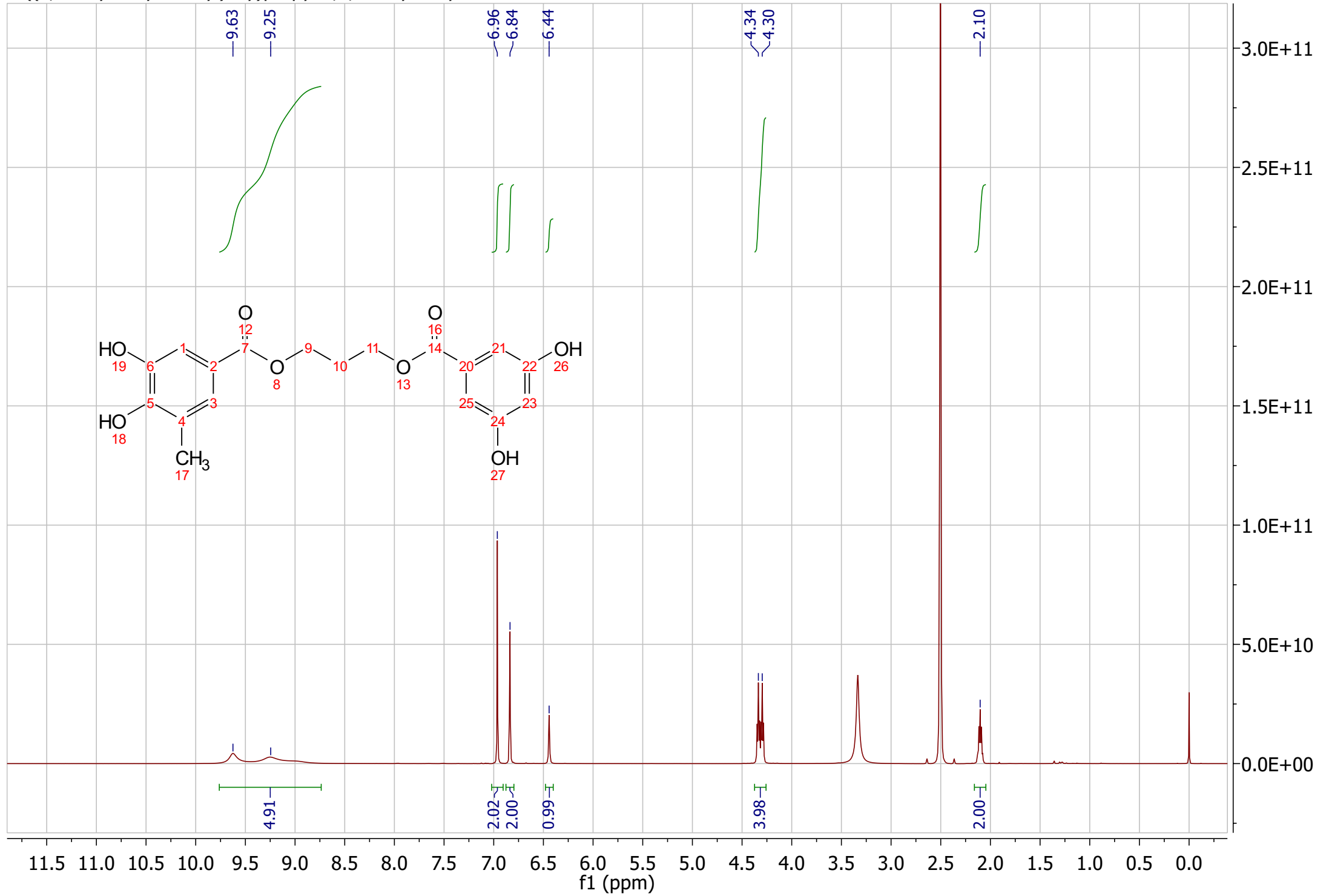
3-((3,4-dihydroxybenzoyl)oxy)propyl 3,4,5-trihydroxybenzoate_DMSO



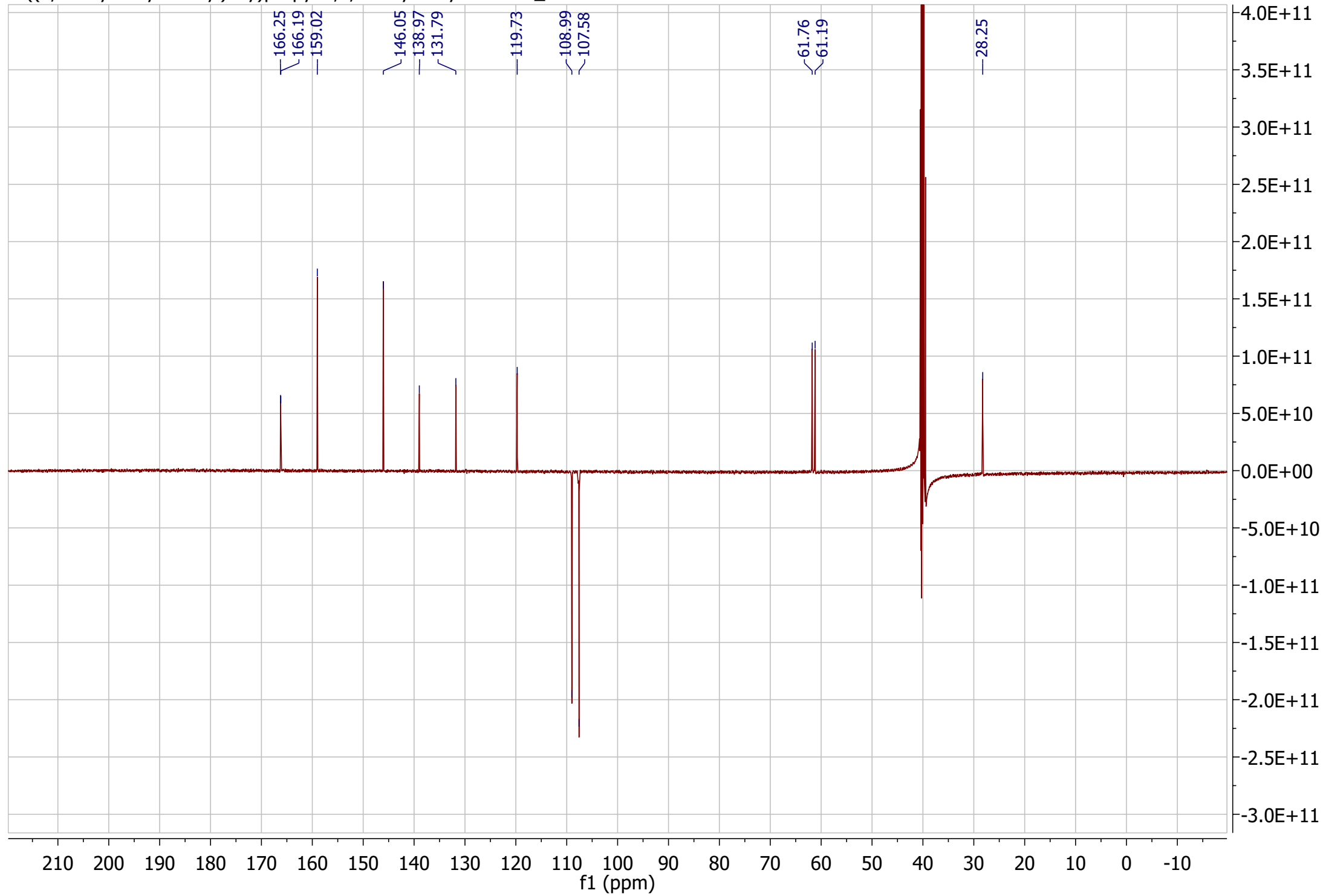
3-((3,4-dihydroxybenzoyl)oxy)propyl 3,4,5-trihydroxybenzoate_DMSO



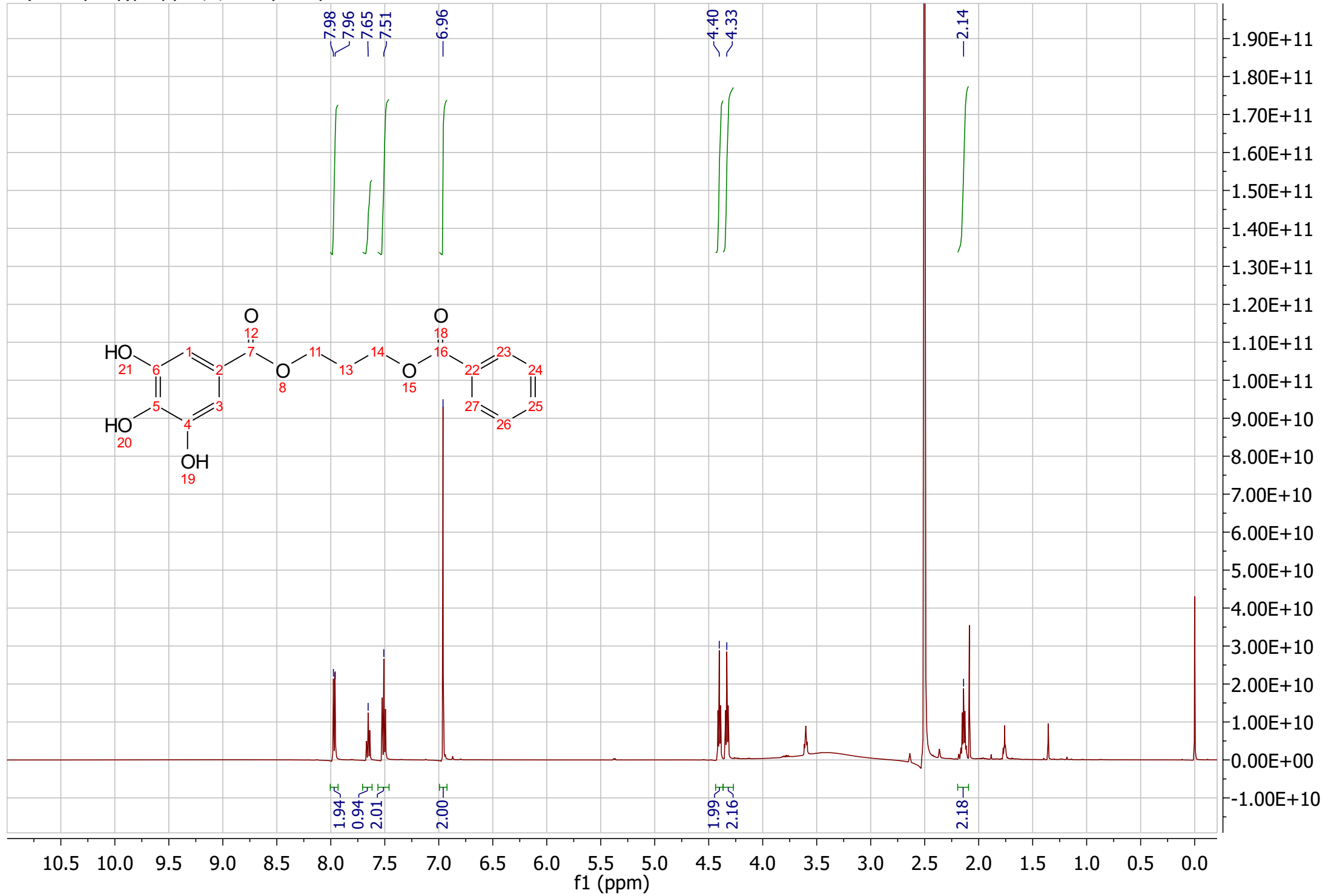
3-((3,5-dihydroxybenzoyl)oxy)propyl 3,4,5-trihydroxybenzoate_DMSO



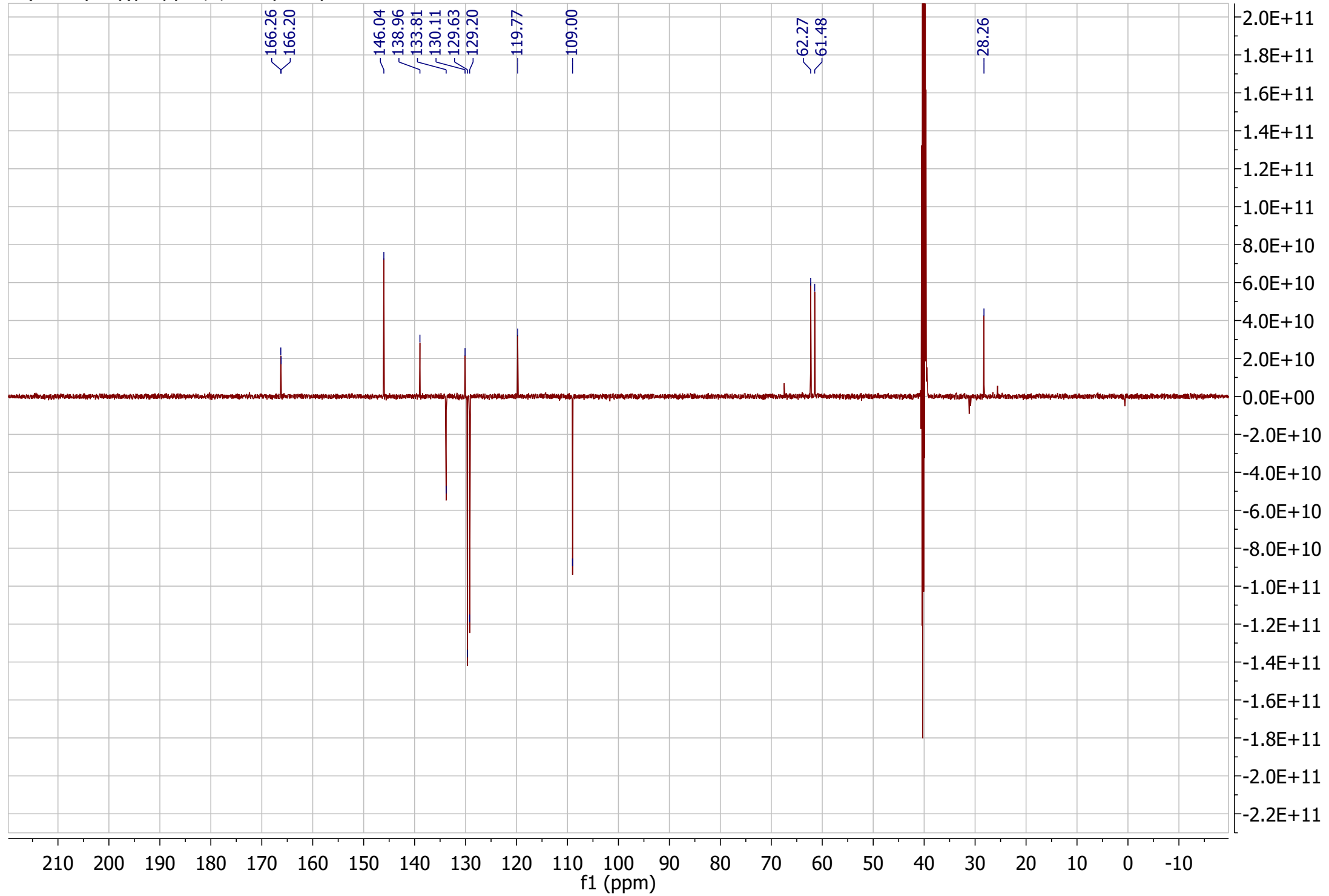
3-((3,5-dihydroxybenzoyl)oxy)propyl 3,4,5-trihydroxybenzoate_DMSO



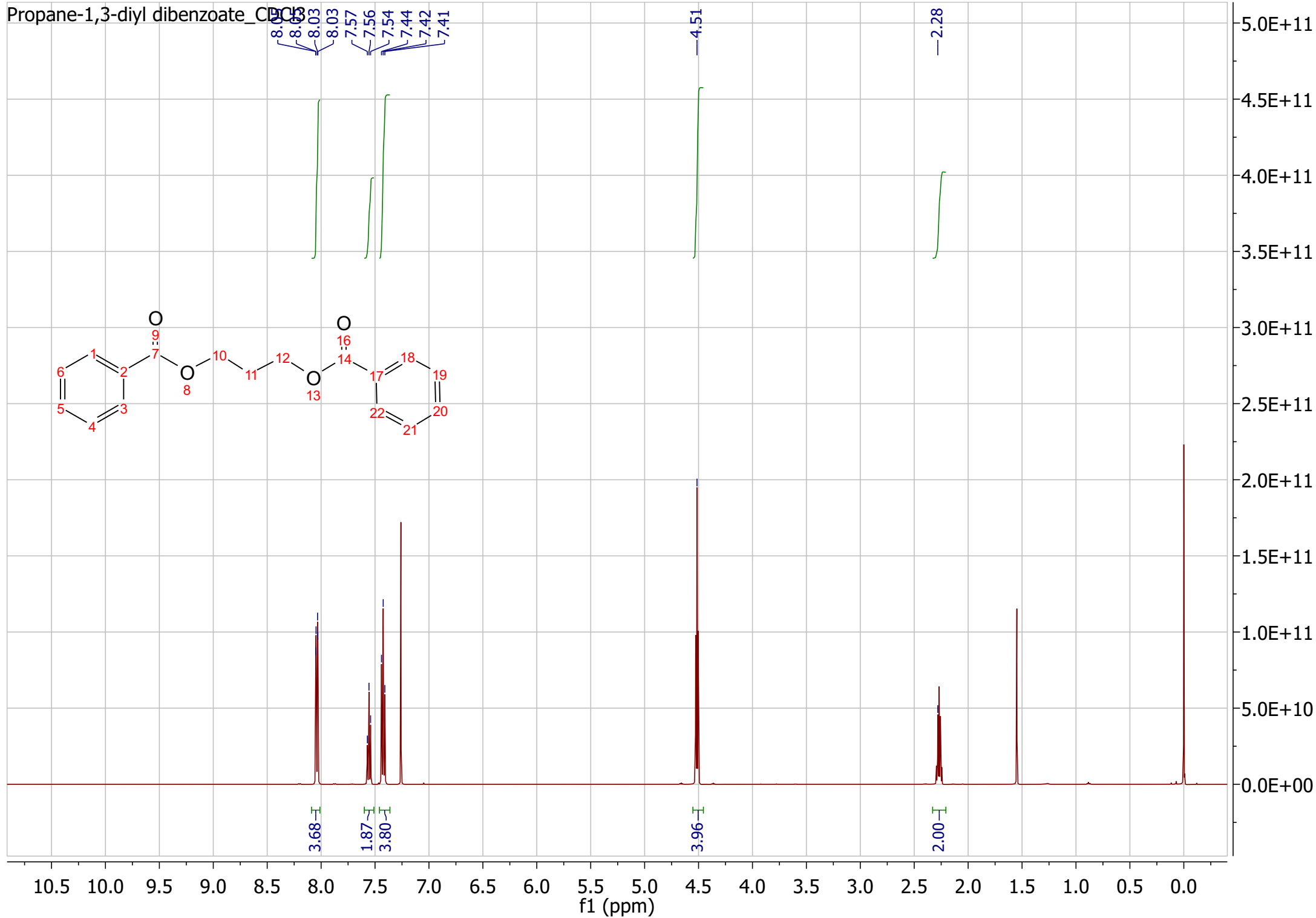
3-(benzyloxy)propyl-3,4,5-trihydroxybenzoate_DMSO



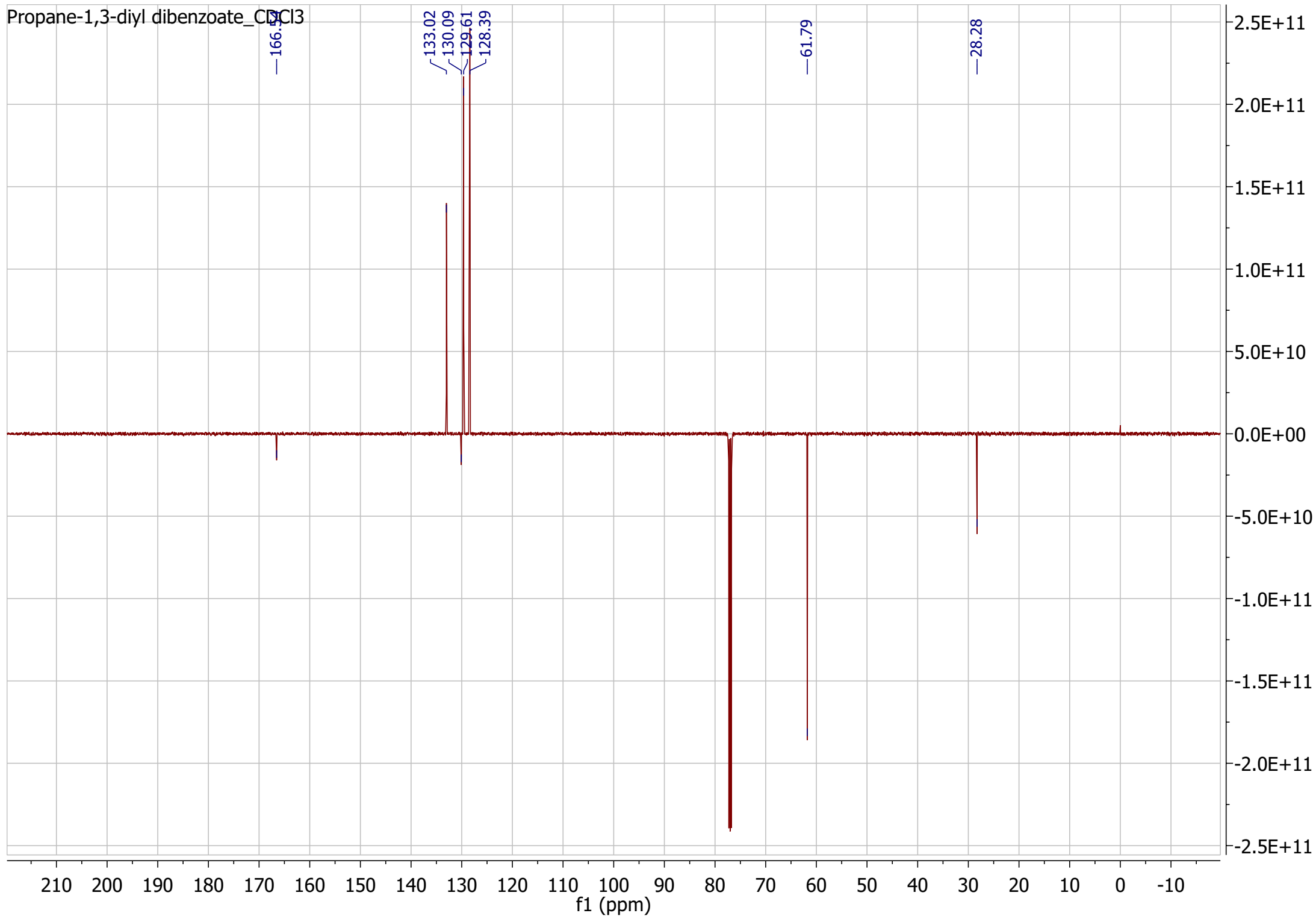
3-(benzyloxy)propyl-3,4,5-trihydroxybenzoate_DMSO



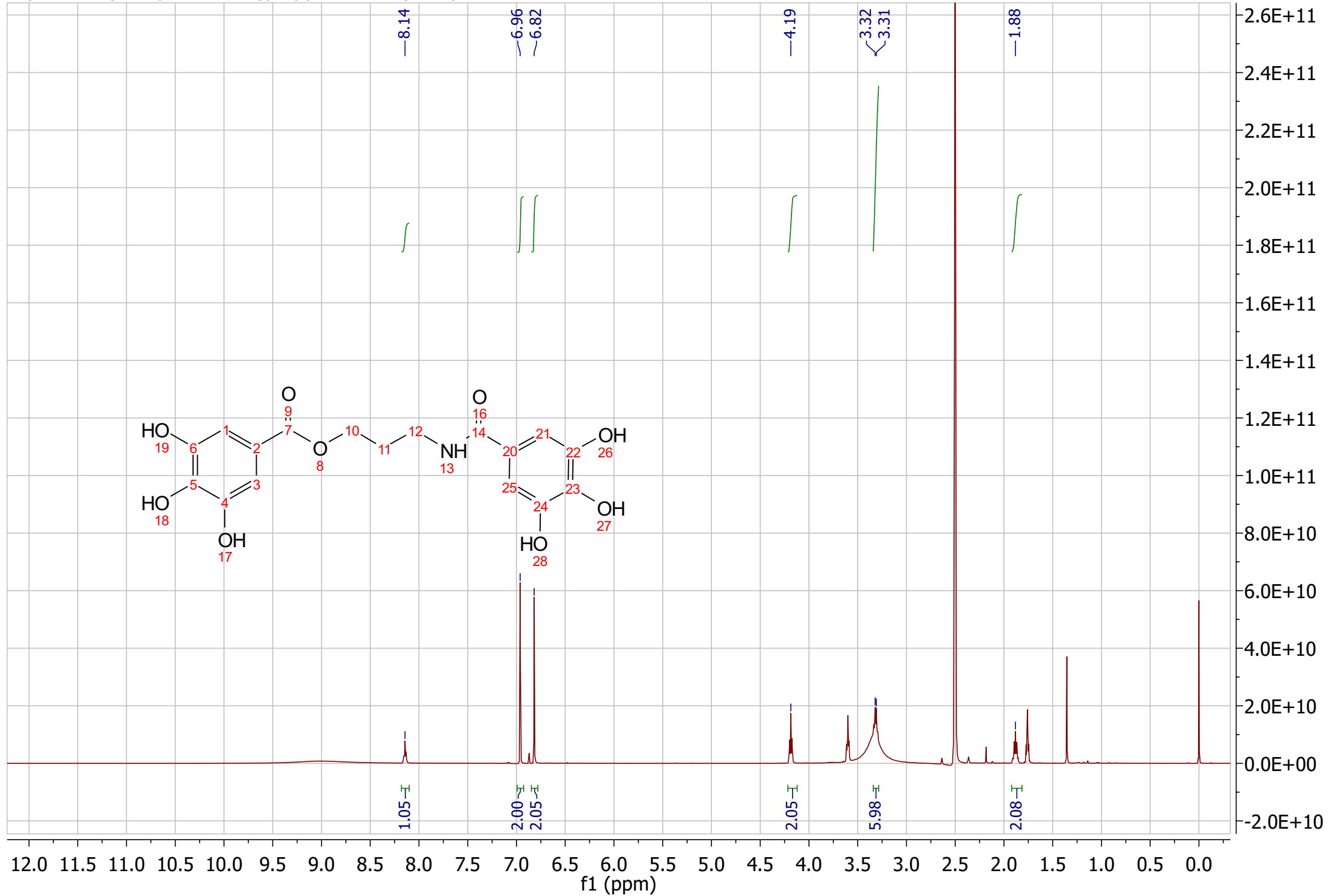
Propane-1,3-diyl dibenzoate_CDC3



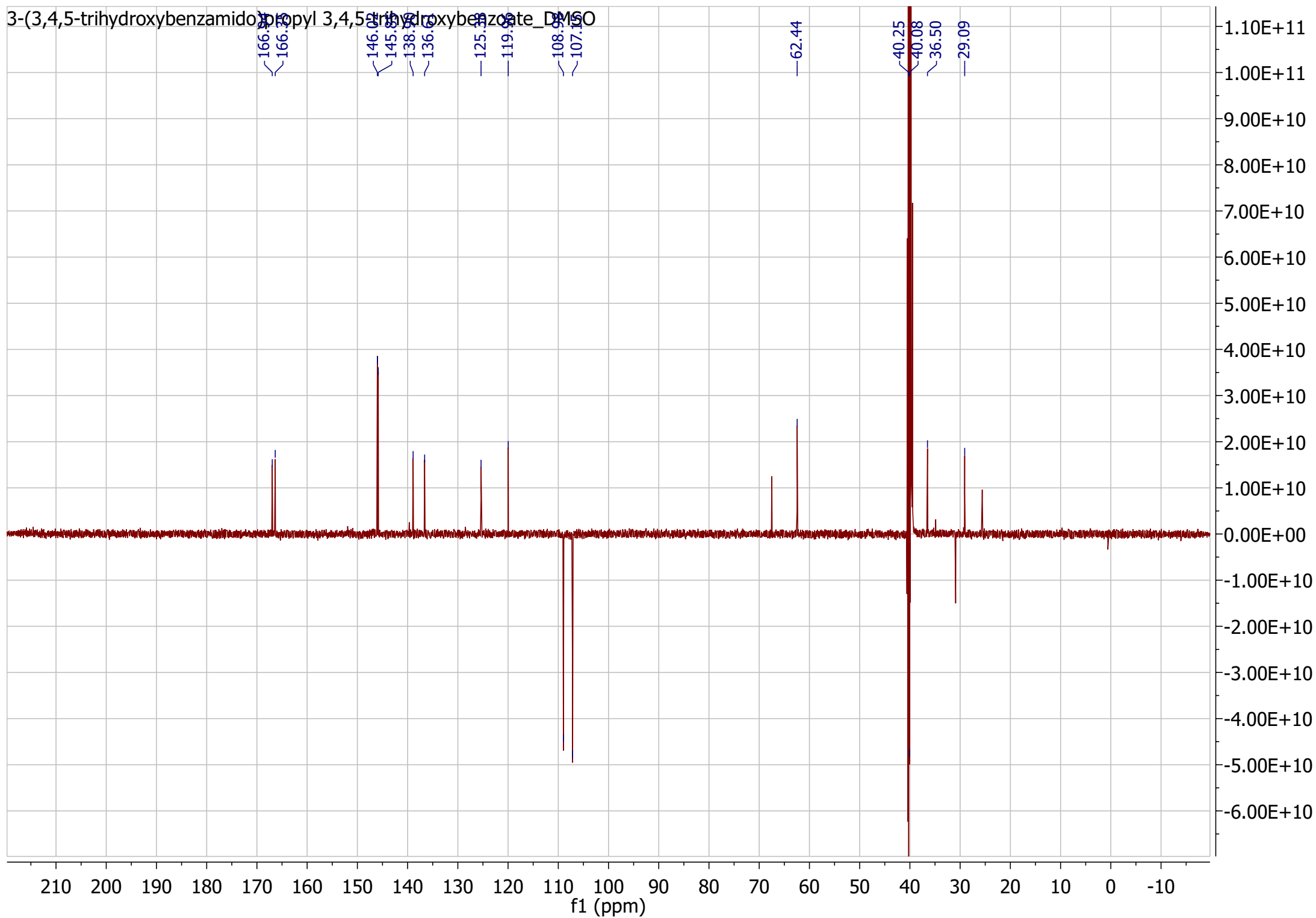
Propane-1,3-diyl dibenzoate_CDCl3



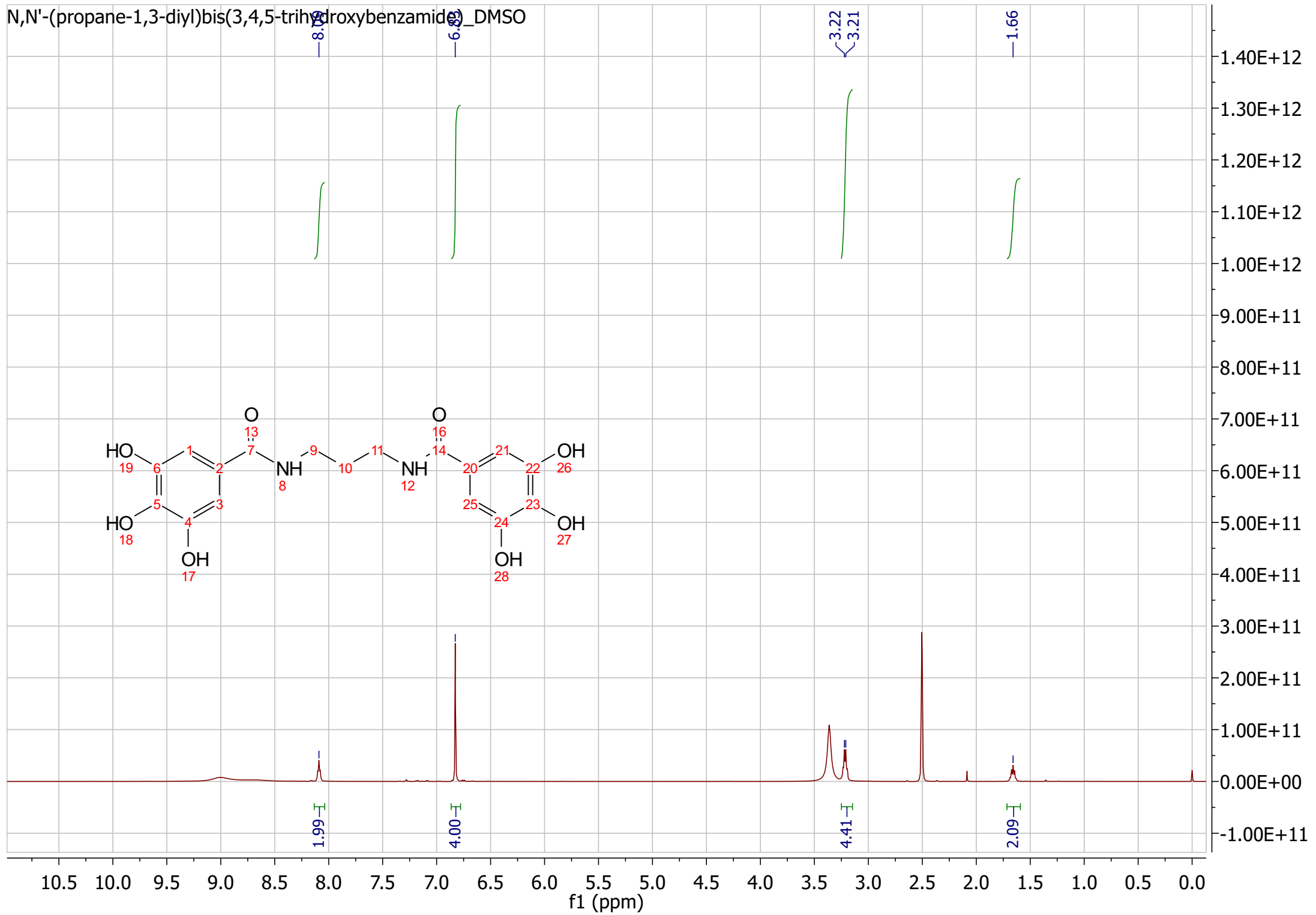
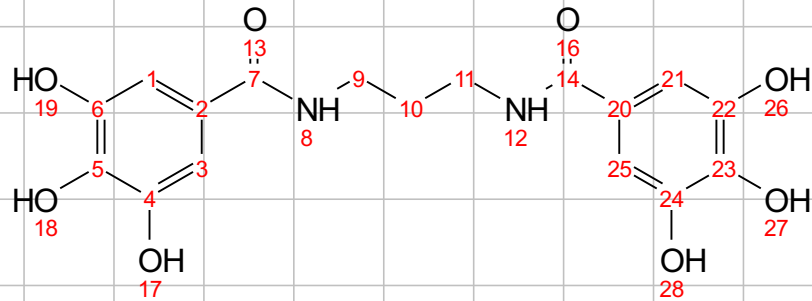
3-(3,4,5-trihydroxybenzamido)propyl 3,4,5-trihydroxybenzoate_DMSO



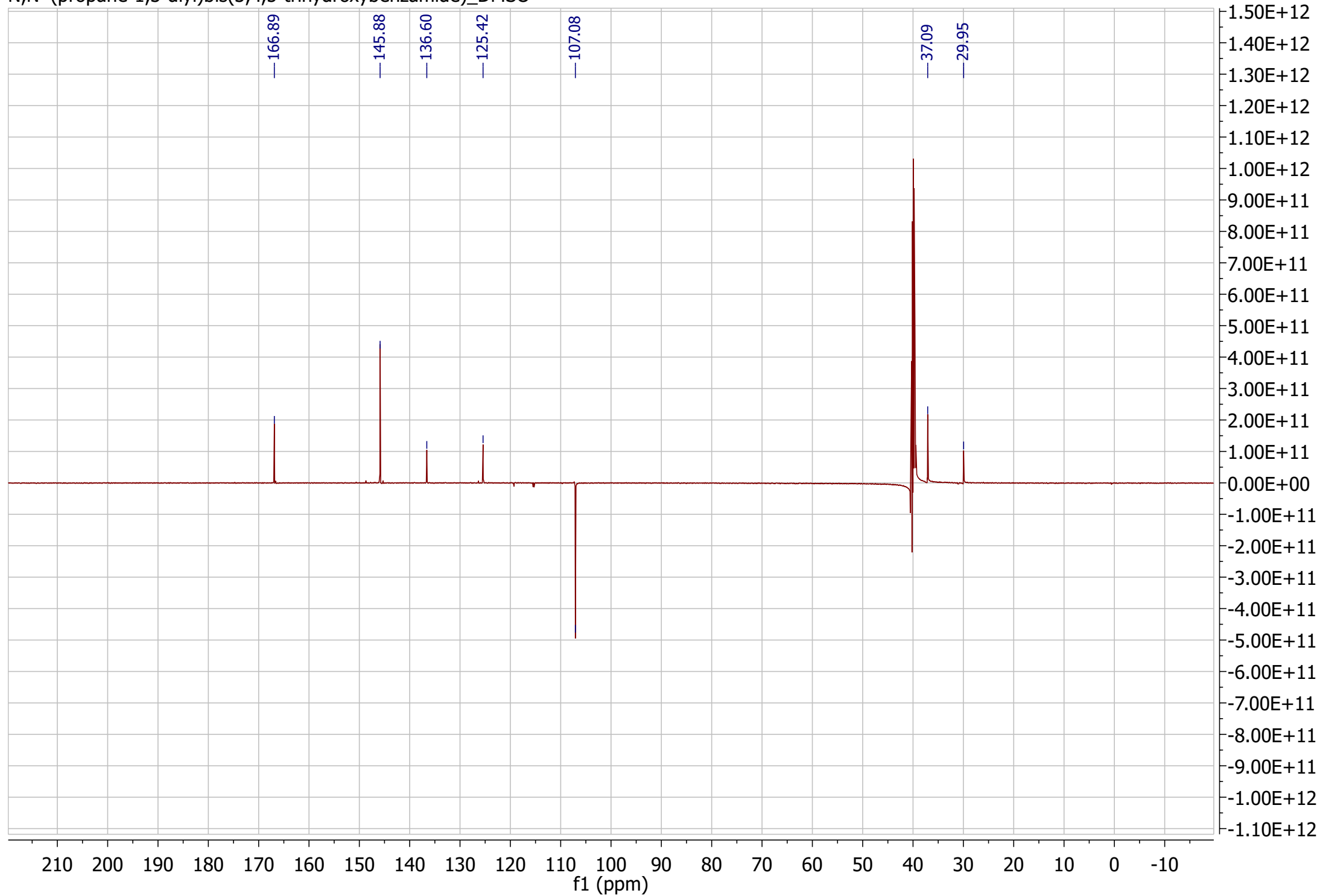
3-(3,4,5-trihydroxybenzamido)propyl 3,4,5-trihydroxybenzoate_DMSO



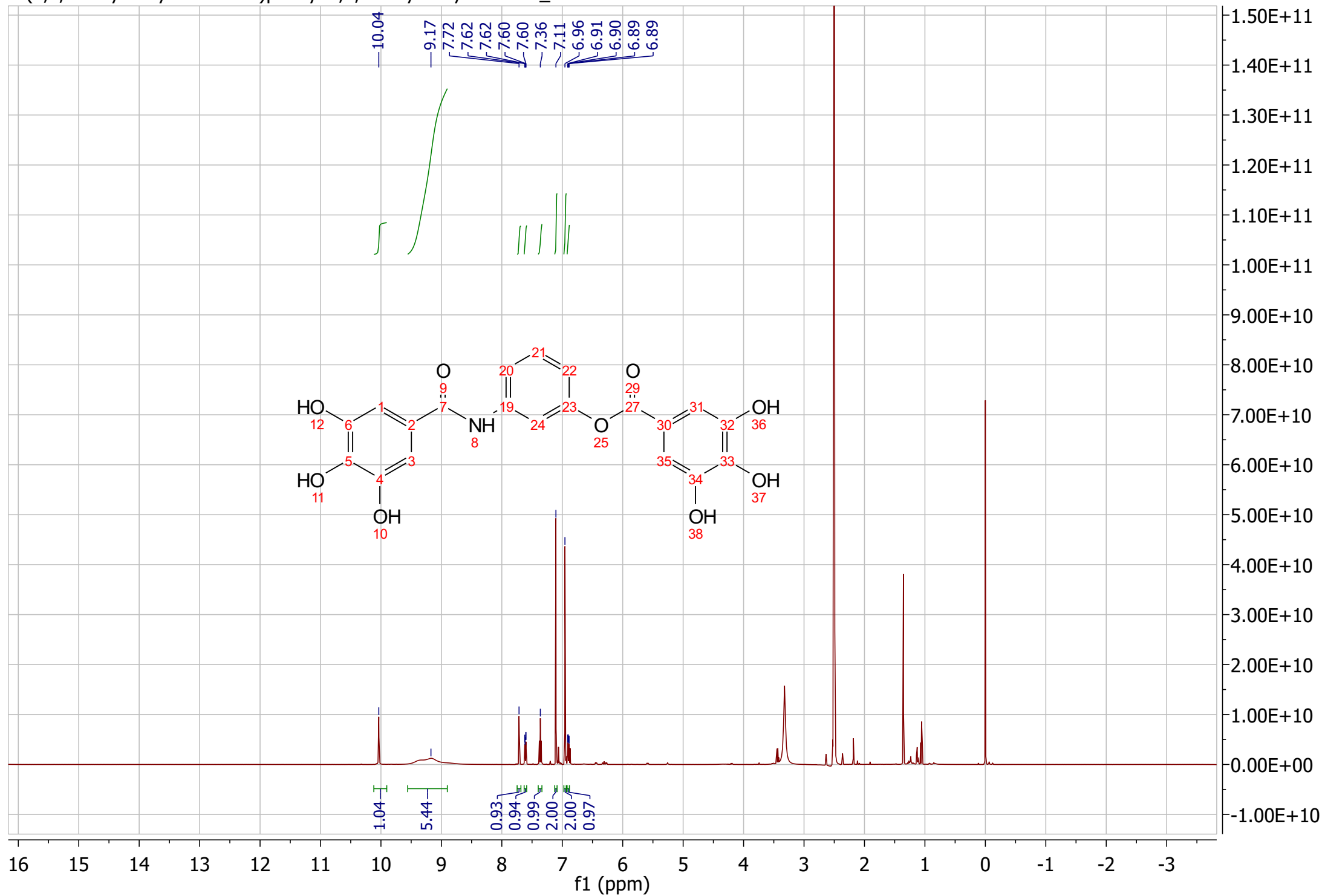
N,N'-(propane-1,3-diyl)bis(3,4,5-trihydroxybenzamide)_DMSO



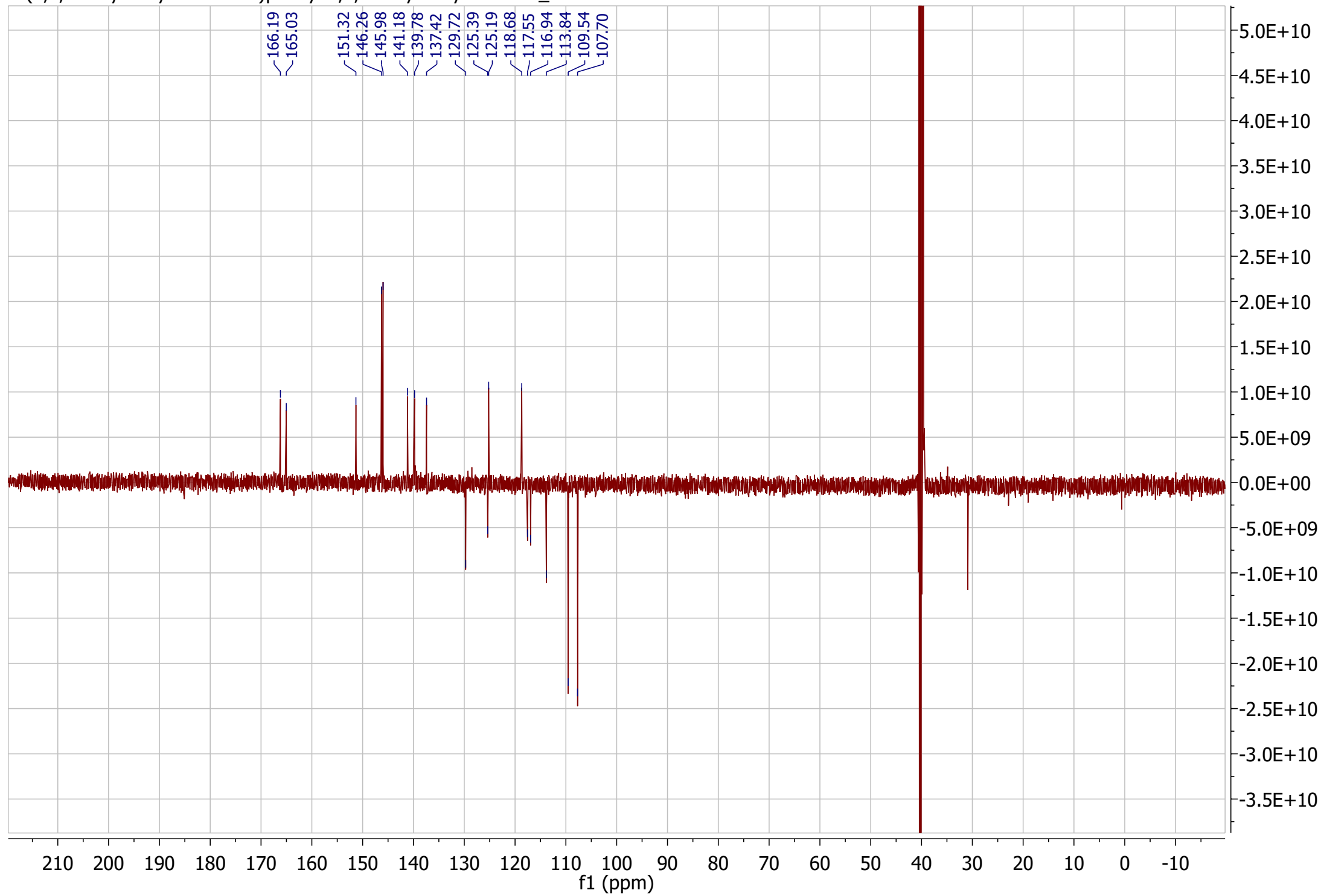
N,N'-(propane-1,3-diyl)bis(3,4,5-trihydroxybenzamide)_DMSO



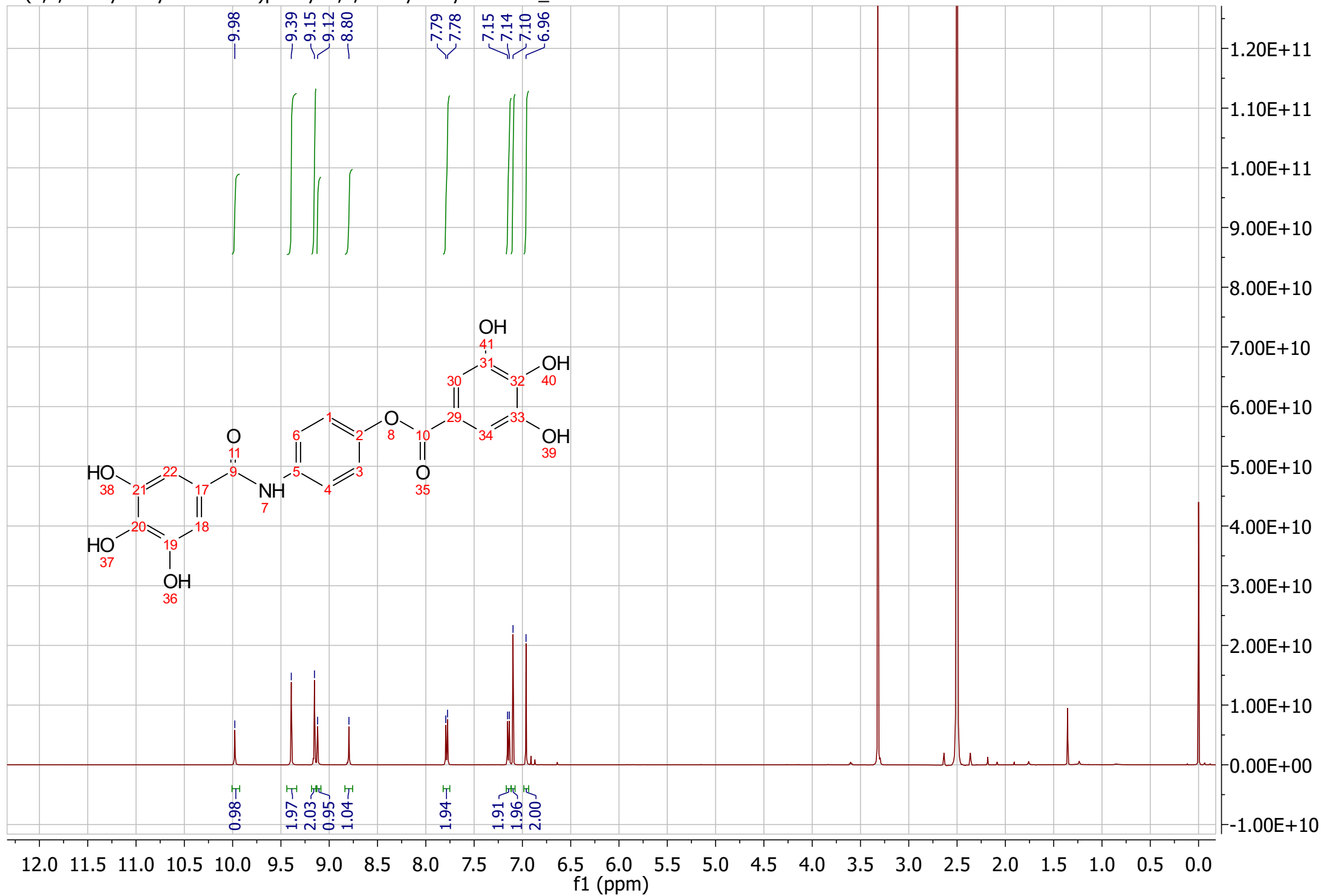
3-(3,4,5-trihydroxybenzamido)phenyl 3,4,5-trihydroxybenzoate_DMSO



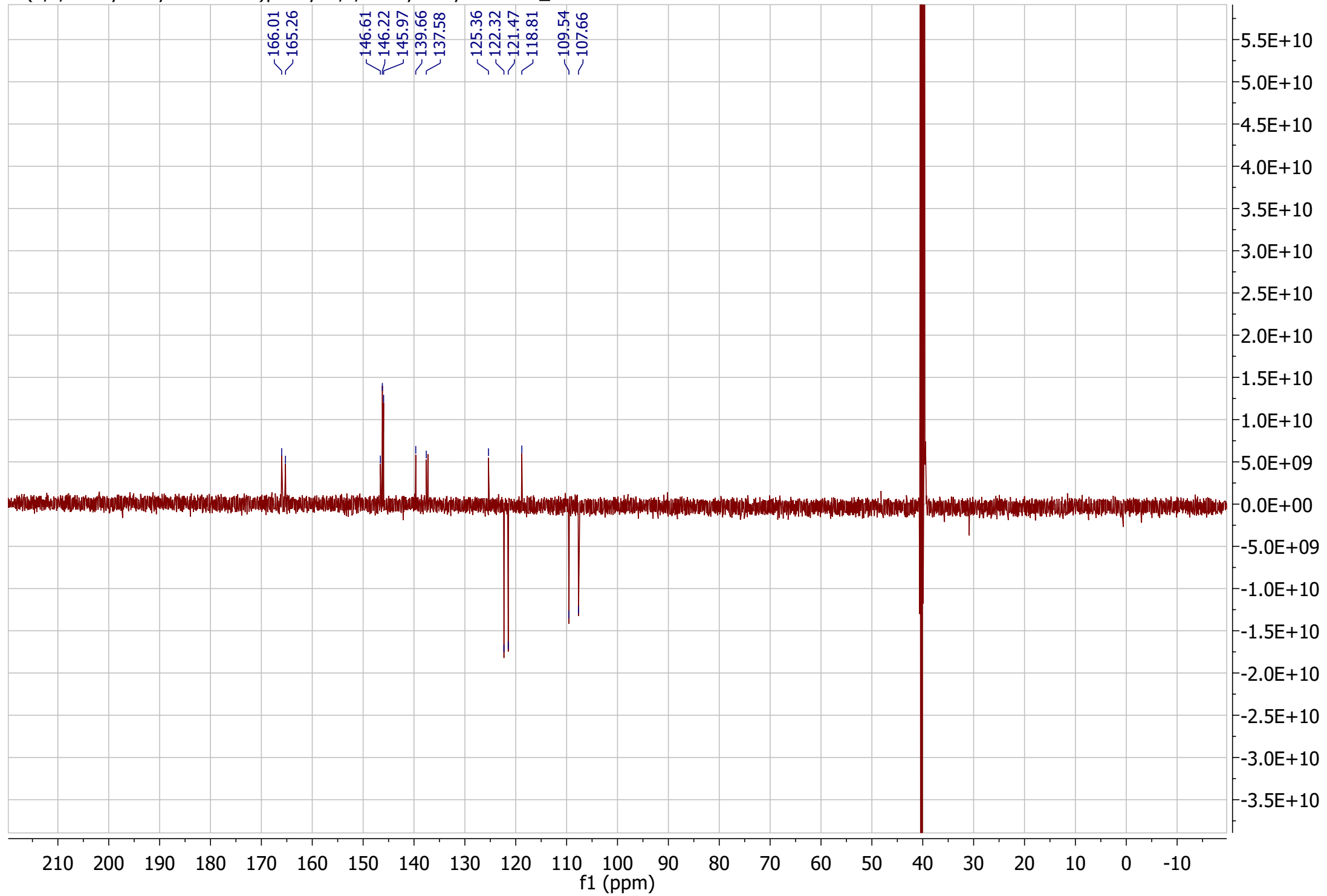
3-(3,4,5-trihydroxybenzamido)phenyl 3,4,5-trihydroxybenzoate_DMSO



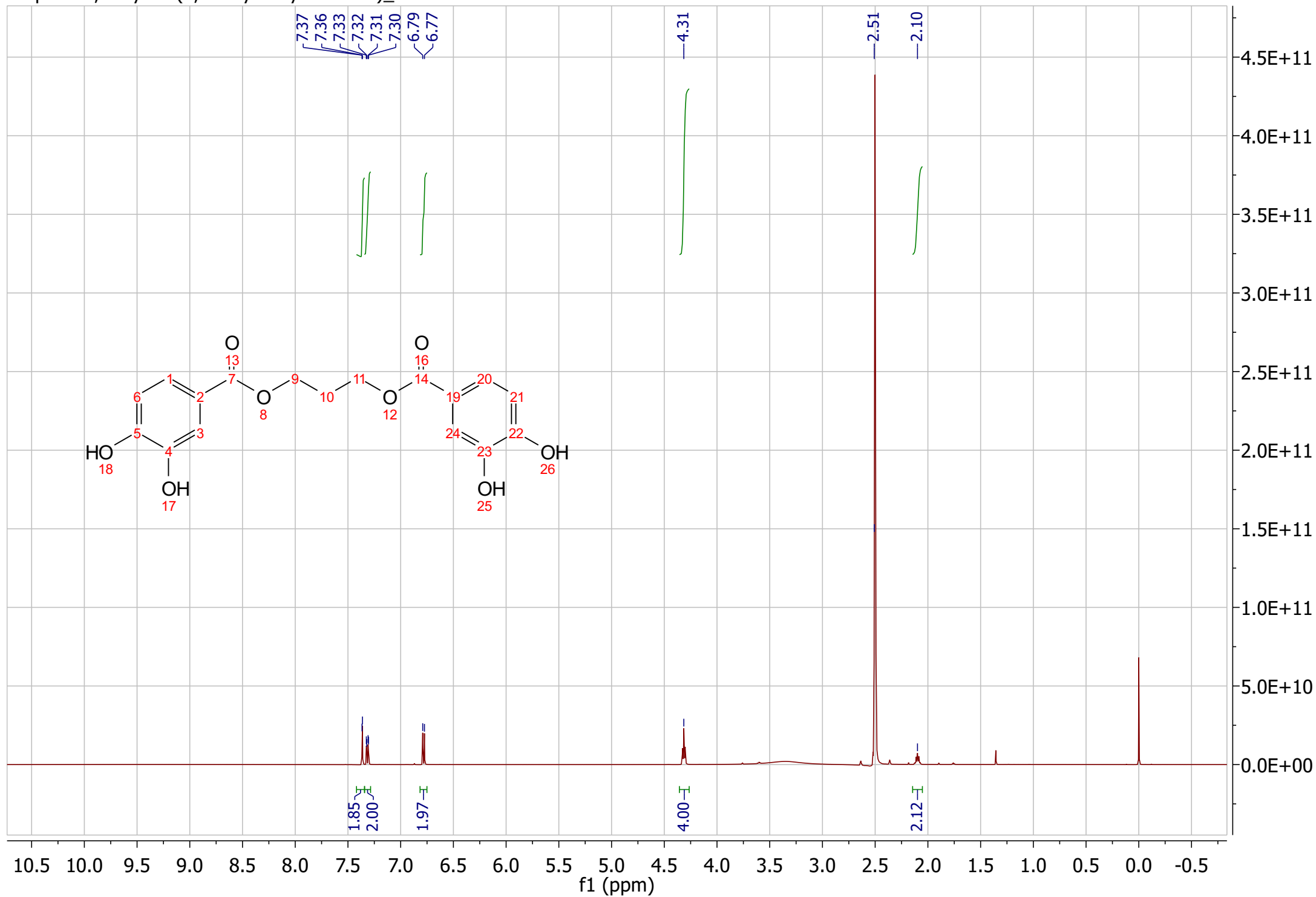
3-(3,4,5-trihydroxybenzamido)phenyl 3,4,5-trihydroxybenzoate_DMSO



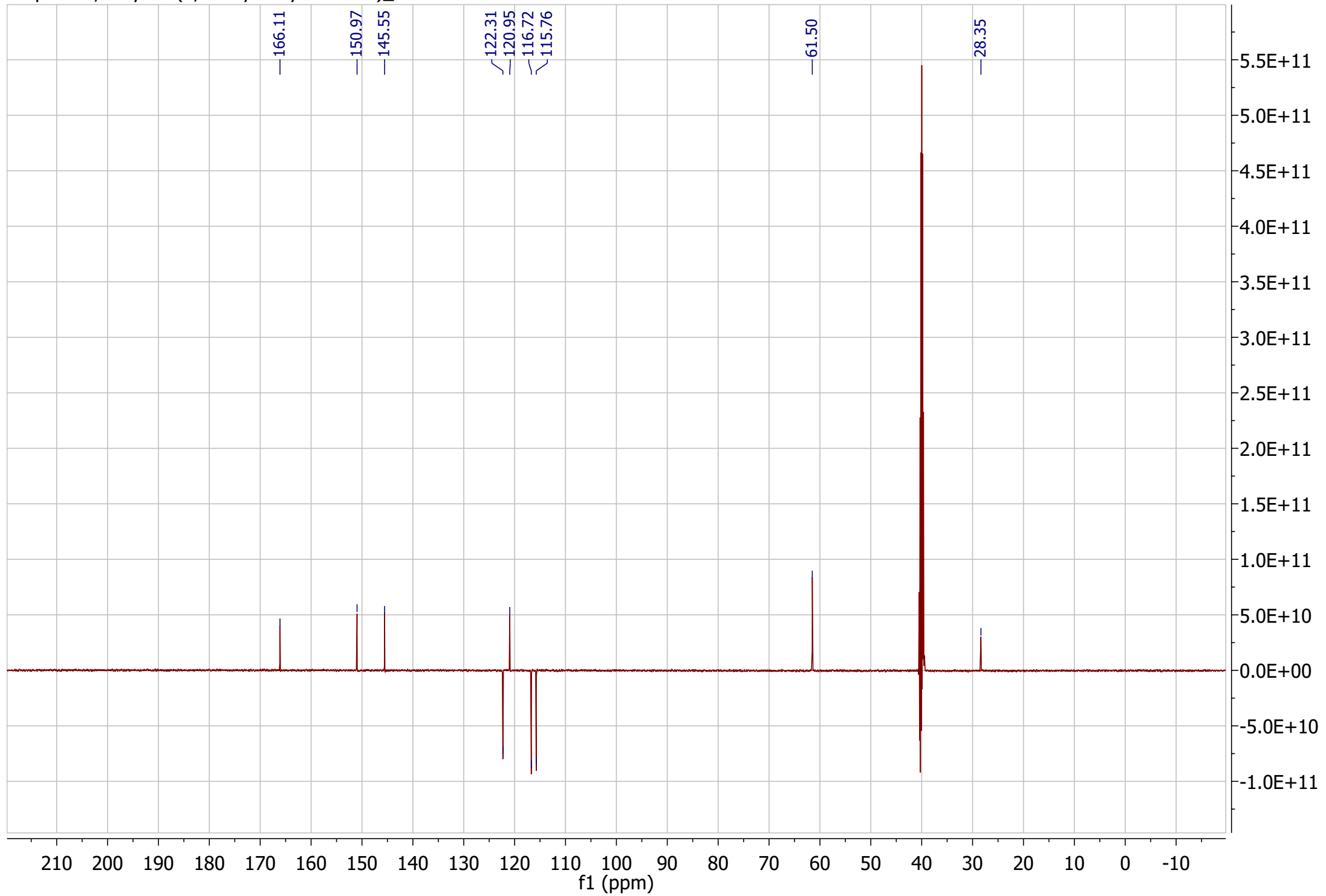
3-(3,4,5-trihydroxybenzamido)phenyl 3,4,5-trihydroxybenzoate_DMSO



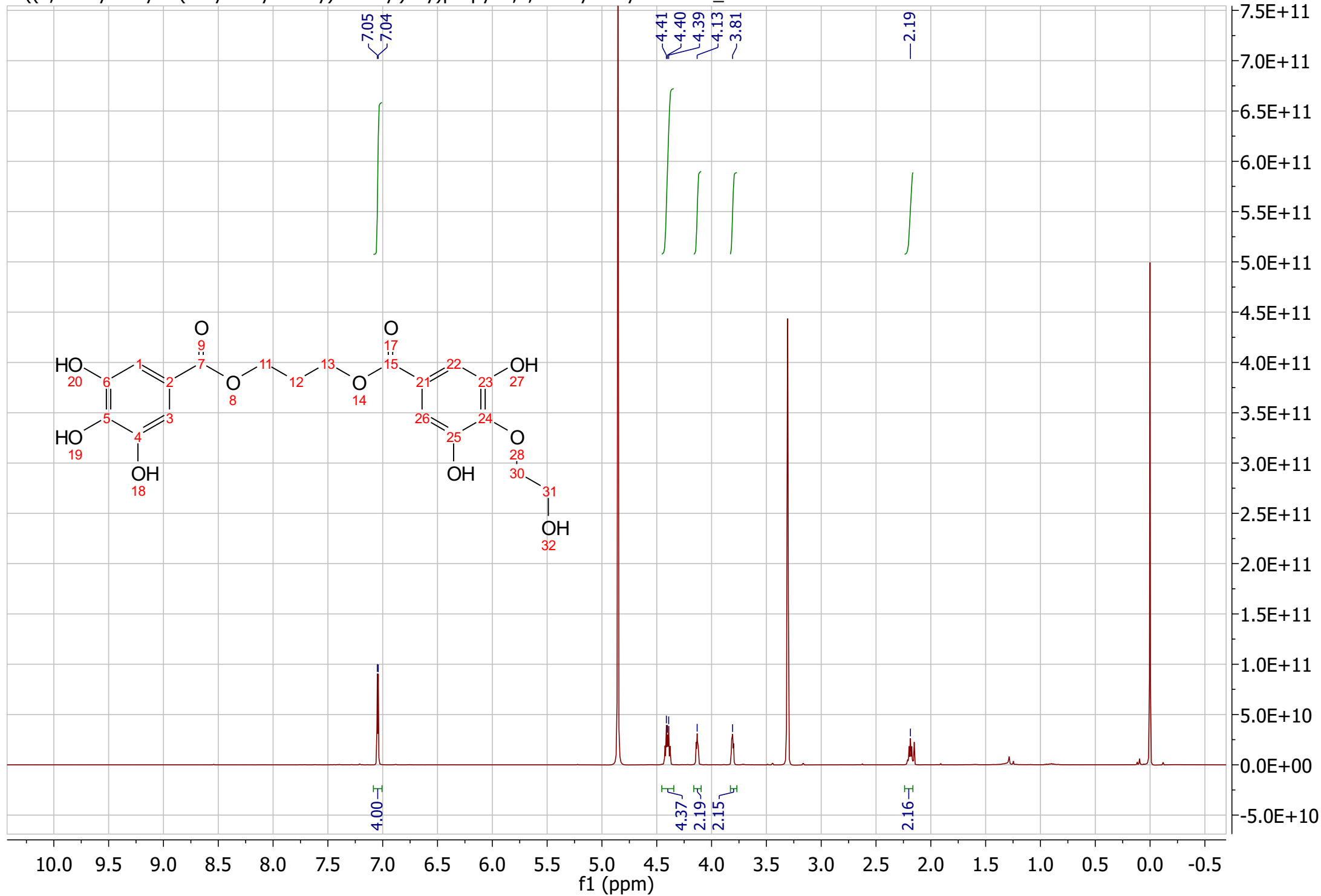
Propane-1,3-diyl bis(3,4-dihydroxybenzoate)_DMSO



Propane-1,3-diyl bis(3,4-dihydroxybenzoate)_DMSO



3-((3,5-dihydroxy-4-(2-hydroxyethoxy)benzoyl)oxy)propyl 3,4,5-trihydroxybenzoate_MeOD



3-((3,5-dihydroxy-4-(2-hydroxyethoxy)benzoyl)oxy)propyl 3,4,5-trihydroxybenzoate_MeOD

