An Improved Synthetic Method for Sensitive Iodine Containing Tricyclic Flavonoids

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Supplementary Material

1. Elemental analysis	**S2**
2. Nuclear magnetic resonance data	**S3-S4**
2. Copies of ^{13}C NMR spectra	**S5-S14**

1. Elemental analysis

Elemental analyses (C, H) were conducted using a CE440 Elemental Analyser; the results were found to be in good agreement (±0.3%) with the calculated values.

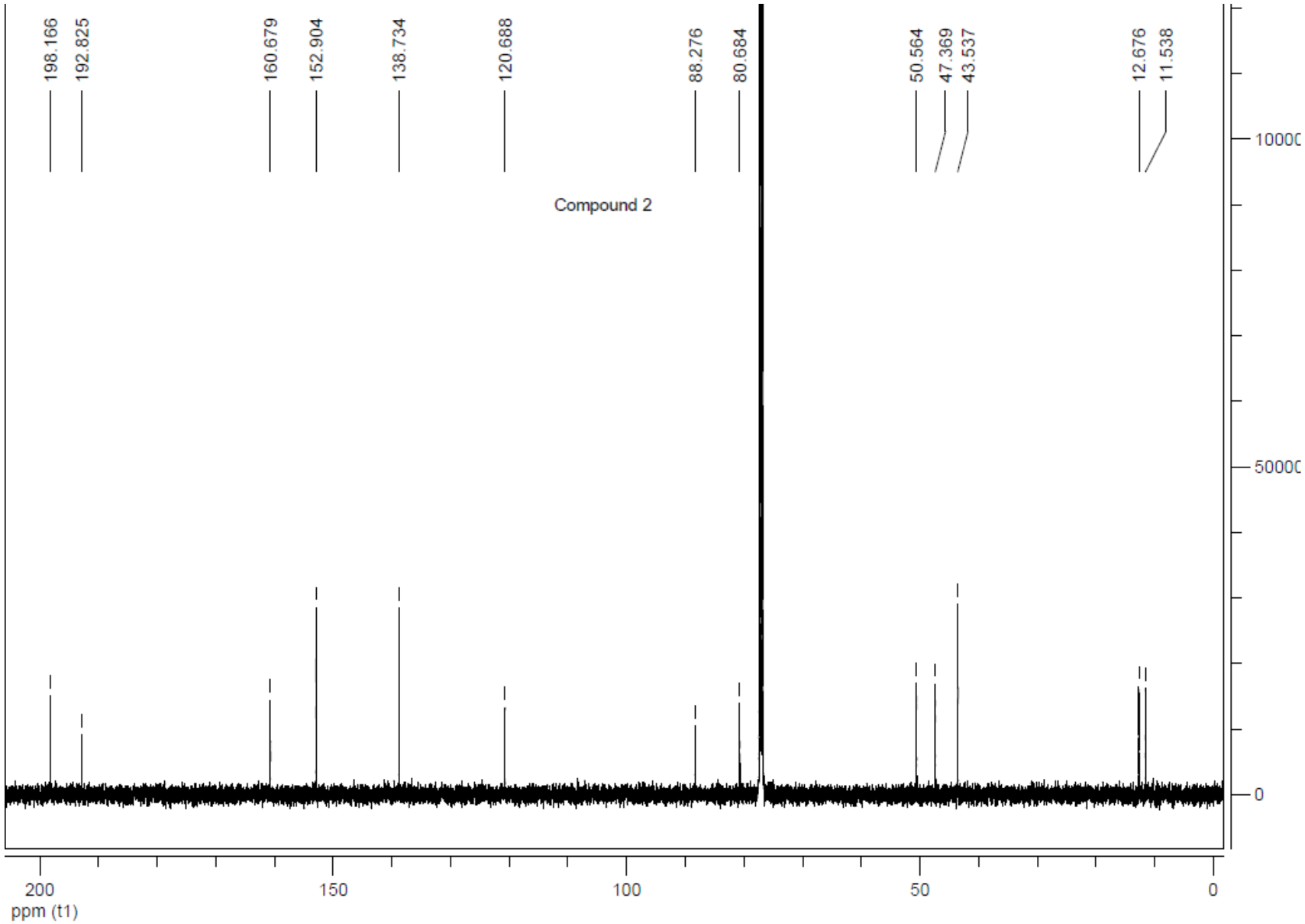
Table S1. Elemental analysis data for compounds **2**, **4a**–**e** and **5a**–**e**.

Compound	% C		% H	
	calcd.	found	calcd.	found
2	29.17	29.31	2.82	3.08
4a	39.57	39.74	3.32	3.47
4b	40.57	40.81	3.56	3.77
4c	37.46	37.65	2.83	3.02
4d	34.21	34.45	2.58	2.74
4e	38.61	38.85	3.24	3.41
5a	35.67	35.87	2.85	3.07
5b	36.64	36.88	3.07	3.31
5c	33.78	34.02	2.41	2.64
5d	31.12	31.40	2.22	2.47
5e	34.88	35.15	2.79	3.01

Table S2. Nuclear magnetic resonance data for compounds **2**, **4a**–**e** and **5a**–**e**.

Compound	**^{1}H NMR and ^{13}C NMR data**
2	^{1}H NMR ($CDCl_3$) δ 12.71 (s, 1H), 8.30 (d, *J* = 1.6 Hz, 1H), 8.25 (d, *J* = 1.7 Hz, 1H), 4.86 (s, 2H), 4.03 (q, *J* = 6.9 Hz, 2H), 3.83 (q, *J* = 6.9 Hz, 2H), 1.38 (t, *J* = 6.9 Hz, 3H), 1.30 (t, *J* = 6.9 Hz, 3H). ^{13}C NMR ($CDCl_3$) δ 198.1, 192.8, 160.6, 152.9, 138.7, 120.6, 88.2, 80.6, 50.5, 47.3, 43.5, 12.6, 11.5.
4a	^{1}H NMR ($CDCl_3$, selected data for the major isomer) δ 8.26 (d, *J* = 1.7 Hz, 1H), 8.13 (d, *J* = 1.7 Hz, 1H), 7.38 (d, *J* = 7.7 Hz, 2H), 7.16 (d, *J* = 7.7 Hz, 2H), 6.01 (d, *J* = 6.2 Hz, 1H), 5.75 (d, *J* = 6.2 Hz, 1H), 3.99 (m, 2H), 3.68 (m, 2H), 2.35 (s, 3H), 1.25 (t, *J* = 6.9 Hz, 6H). ^{13}C NMR ($CDCl_3$, selected data for the major isomer) δ 191.6, 186.2, 158.8, 152.6, 138.7, 136.3, 132.8, 129.3, 127.2, 122.9, 87.6, 84.7, 83.0, 57.8, 50.5, 47.3, 21.2, 12.6, 11.4.
4b	^{1}H NMR ($CDCl_3$, selected data for the major isomer) δ 8.26 (d, *J* = 1.8 Hz, 1H), 8.13 (d, *J* = 1.8 Hz, 1H), 7.4 (d, *J* = 7.9 Hz, 2H), 7.19 (d, *J* = 7.9 Hz, 2H), 6.01 (d, *J* = 6.3 Hz, 1H), 5.76 (d, *J* = 6.3 Hz, 1H), 3.98 (m, 2H), 3.69 (m, 2H), 2.65 (q, *J* = 7.5 Hz, 2H), 1.25 (t, *J* = 7.5 Hz, 3H), 1.23 (t, *J* = 7.6 Hz, 6H). ^{13}C NMR ($CDCl_3$, selected data for the major isomer) δ 191.2, 186.3, 158.8, 152.6, 144.9, 136.3, 133.0, 128.1, 127.2, 122.9, 87.6, 84.7, 83.0, 57.8, 50.5, 47.3, 28.5, 15.3, 12.6, 11.4.
4c	^{1}H NMR ($CDCl_3$, selected data for the major isomer) δ 8.27 (d, *J* = 1.9 Hz, 1H), 8.16 (d, *J* = 1.9 Hz, 1H), 7.49 (m, 2H), 7.06 (m, 2H), 5.96 (d, *J* = 7.3 Hz, 1H), 5.79 (d, *J* = 7.3 Hz, 1H), 3.95 (m, 2H), 3.71 (m, 2H), 1.24 (t, *J* = 6.8 Hz, 6H). ^{13}C NMR ($CDCl_3$, selected data for the major isomer) δ 190.9, 186.1, 162.9, 158.7, 152.7, 136.4, 131.7, 129.4, 122.4, 115.5, 87.4, 84.9, 82.6, 58.4, 50.7, 47.3, 12.6, 11.4.
4d	^{1}H NMR ($CDCl_3$, selected data for the major isomer) δ 8.28 (d, *J* = 1.9 Hz, 1H), 8.16 (d, *J* = 1.9 Hz, 1H), 7.52 (d, *J* = 8.2 Hz, 2H), 7.41 (d, *J* = 8.2 Hz, 2H), 5.95 (d, *J* = 7.1 Hz, 1H), 5.74 (d, *J* = 7.1, 1H), 3.92 (m, 2H), 3.66 (m, 2H), 1.24 (t, *J* = 6.7 Hz, 6H). ^{13}C NMR ($CDCl_3$, selected data for the major isomer) δ 190.8, 185.9, 158.7, 152.7, 136.5, 134.8, 131.7, 129.1, 123.1, 122.1, 87.4, 85.1, 82.6, 58.2, 50.7, 47.4, 12.6, 11.4.

4e	^{1}H NMR ($CDCl_3$, selected data for the major isomer) δ 8.26 (m, 1H), 8.14 (m, 1H), 7.42 (d, *J* = 8.2 Hz, 2H), 6.89 (d, *J* = 8.2 Hz, 2H), 5.96 (d, *J* = 6.7 Hz, 1H), 5.78 (d, *J* = 6.7 Hz, 1H), 3.97 (m, 2H), 3.81 (s, 3H), 3.65 (m, 2H), 1.25 (t, *J* = 6.7 Hz, 6H). ^{13}C NMR ($CDCl_3$, selected data for the major isomer) δ 191.2, 186.4, 159.9, 158.8, 152.6, 136.4, 128.7, 127.9, 122.8, 113.9, 87.7, 87.6, 84.7, 58.1, 55.3, 50.5, 47.3, 12.6, 11.4.
5a	^{1}H NMR (DMSO-*d*6) δ 8.04 (d, *J* = 1.8 Hz, 1H), 7.74 (d, *J* = 1.8 Hz, 1H), 7.37 (d, *J* = 8.0 Hz, 2H), 7.26 (d, *J* = 8.0 Hz, 2H), 6.89 (s, 1H), 3.89 (m, 4H), 2.31 (s, 3H), 1.40 (t, *J* = 7.1 Hz, 3H), 1.32 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (DMSO-*d*6) δ 184.9, 150.7, 147.8, 140.2, 133.8, 130.0, 129.7, 127.8, 126.8, 119.1, 88.7, 87.6, 76.2, 54.7, 54.6, 21.3, 10.8, 10.5.
5b	^{1}H NMR (DMSO-*d*6) δ 8.06 (d, *J* = 1.8 Hz, 1H), 7.73 (d, *J* = 1.8 Hz, 1H), 7.35 (d, *J* = 8.1 Hz, 2H), 7.24 (d, *J* = 8.1 Hz, 2H), 6.87 (s, 1H), 3.87 (m, 4H), 2.35 (q, *J* = 7.3 Hz, 2H), 1.40 (t, *J* = 7.1 Hz, 3H), 1.32 (t, *J* = 7.1 Hz, 3H), 1.26 (t, *J* = 7.3 Hz, 3H). ^{13}C NMR (DMSO-*d*6) δ 185, 150.5, 147.7, 140.1, 133.5, 129.9, 129.6, 127.5, 126.7, 119.0, 88.8, 87.5, 76.1, 54.8, 54.6, 25.4, 12.3, 10.7, 10.4.
5c	^{1}H NMR (DMSO-*d*6) δ 8.09 (d, *J* = 1.8 Hz, 1H), 7.80 (d, *J* = 1.8 Hz, 1H), 7.55 (dd, $^{3}J_{H\text{-}H}$ = 8.7 Hz, $^{4}J_{H\text{-}F}$ = 5.3 Hz, 2H), 7.30 (dd, $^{3}J_{H\text{-}H}$ = 8.8 Hz, $^{3}J_{H\text{-}F}$ = 8.7 Hz, 2H), 6.96 (s, 1H), 3.90 (m, 4H), 1.40 (t, *J* = 7.1 Hz, 3H), 1.33 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (DMSO-*d*6) δ 185.0, 164.2, 162.3, 150.4, 147.8, 133.0, 130.3, 129.2, 127.1, 119.0, 116.5, 88.7, 87.7, 75.5, 54.7, 54.6, 10.8, 10.5.
5d	^{1}H NMR (DMSO-*d*6) δ 8.09 (d, *J* = 1.7 Hz, 1H), 7.79 (d, *J* = 1.7 Hz, 1H), 7.66 (d, *J* = 8.4 Hz, 2H), 7.43 (d, *J* = 8.4 Hz, 2H), 6.92 (s, 1H), 3.87 (m, 4H), 1.39 (t, *J* = 7.1 Hz, 3H), 1.32 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (DMSO-*d*6) δ 185.0, 150.4, 147.9, 136.0, 133.1, 132.5, 130.0, 128.7, 127.2, 123.9, 119.0, 88.6, 87.8, 75.5, 54.7, 54.6, 10.7, 10.5.
5e	^{1}H NMR (DMSO-*d*6) δ 8.08 (d, *J* = 1.8 Hz, 1H), 7.78 (d, *J* = 1.8 Hz, 1H), 7.41 (d, *J* = 8.7 Hz, 2H), 6.99 (d, *J* = 8.7 Hz, 2H), 6.86 (s, 1H), 3.90 (m, 4H), 3.76 (s, 3H), 1.40 (t, *J* = 7.1 Hz, 3H), 1.32 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (DMSO-*d*6) δ 184.9, 160.9, 150.7, 147.7, 132.9, 129.9, 129.6, 128.6, 126.7, 119.0, 114.8, 88.7, 87.4, 76.1, 55.7, 54.7, 54.6, 10.8, 10.5.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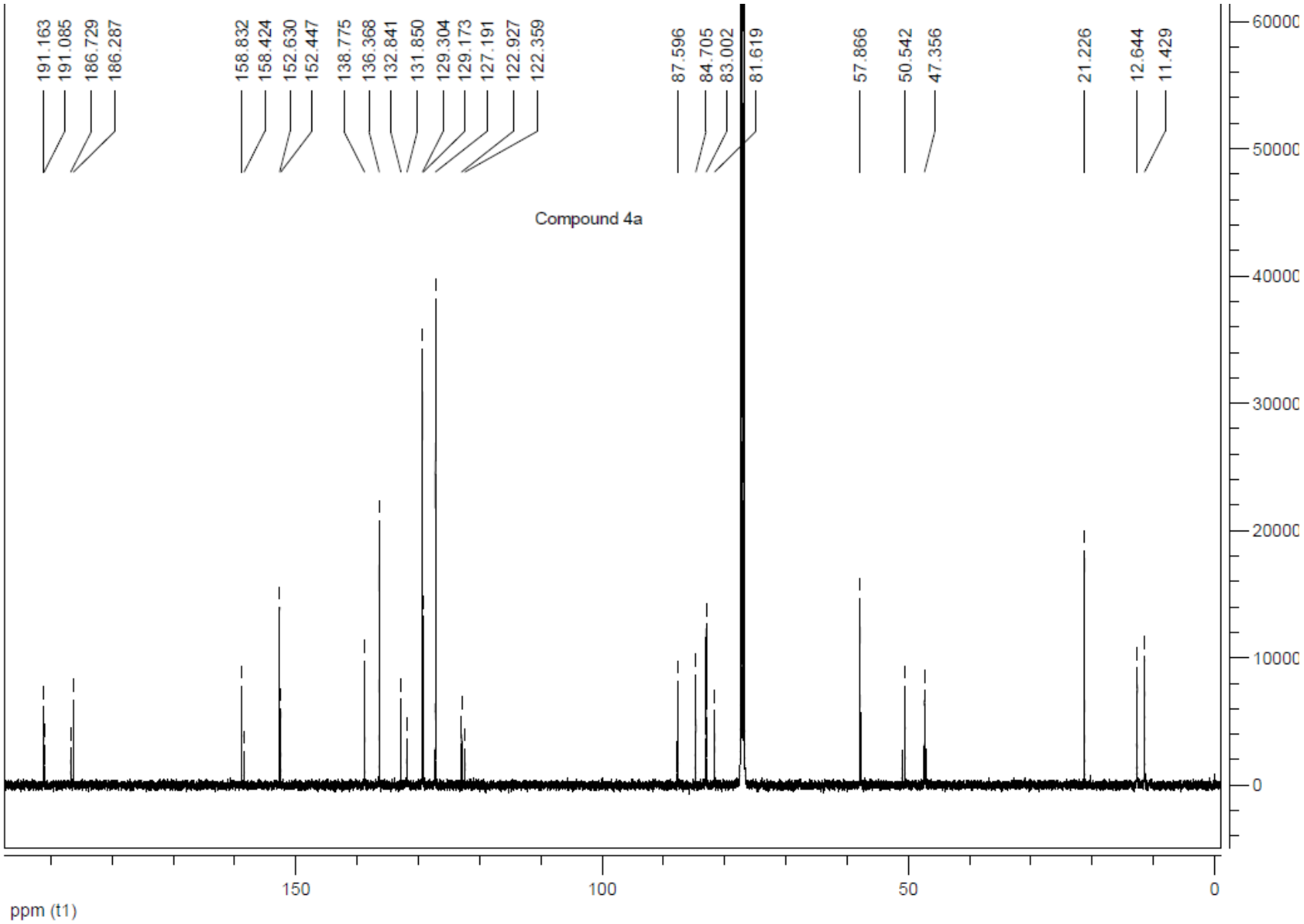
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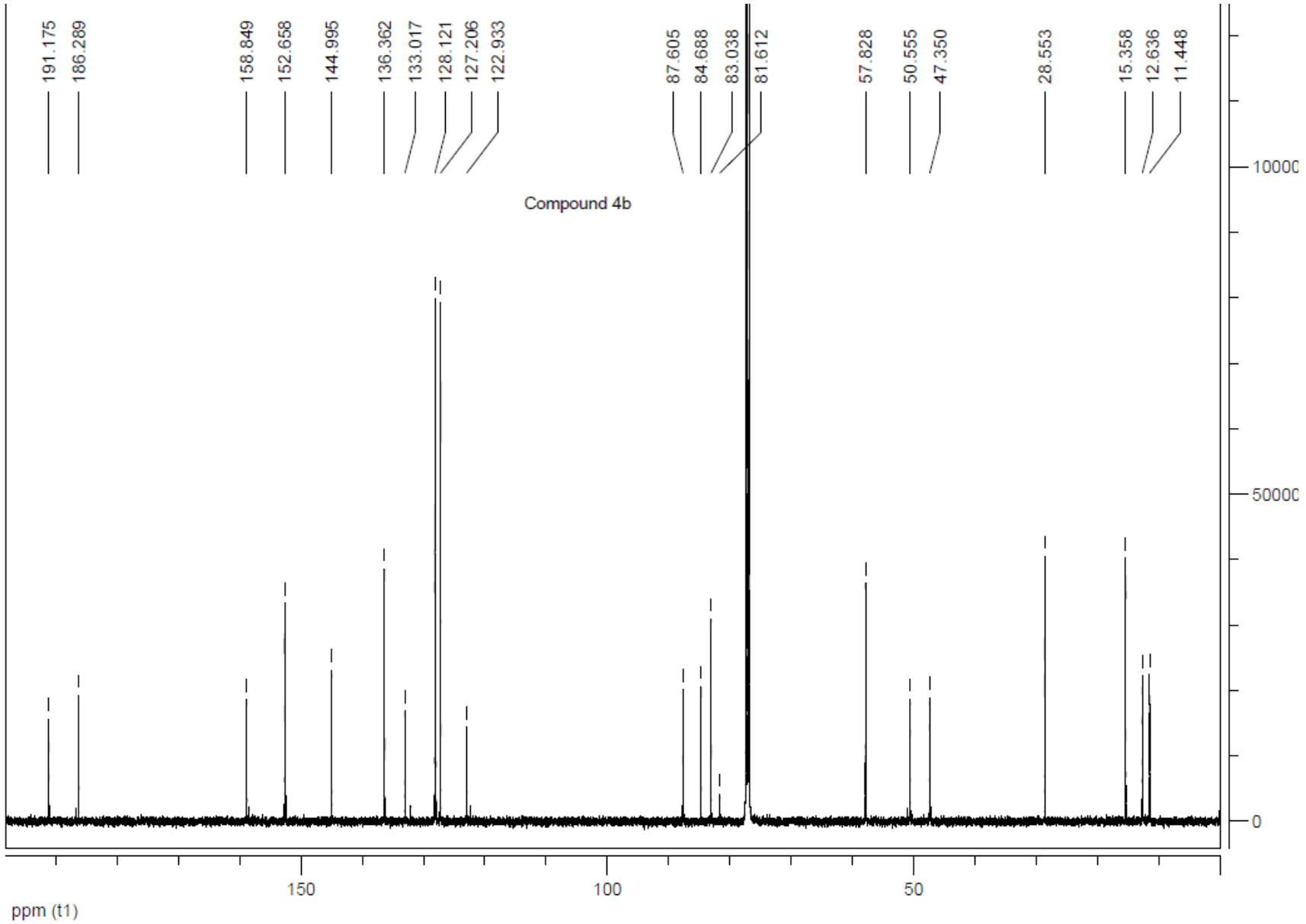
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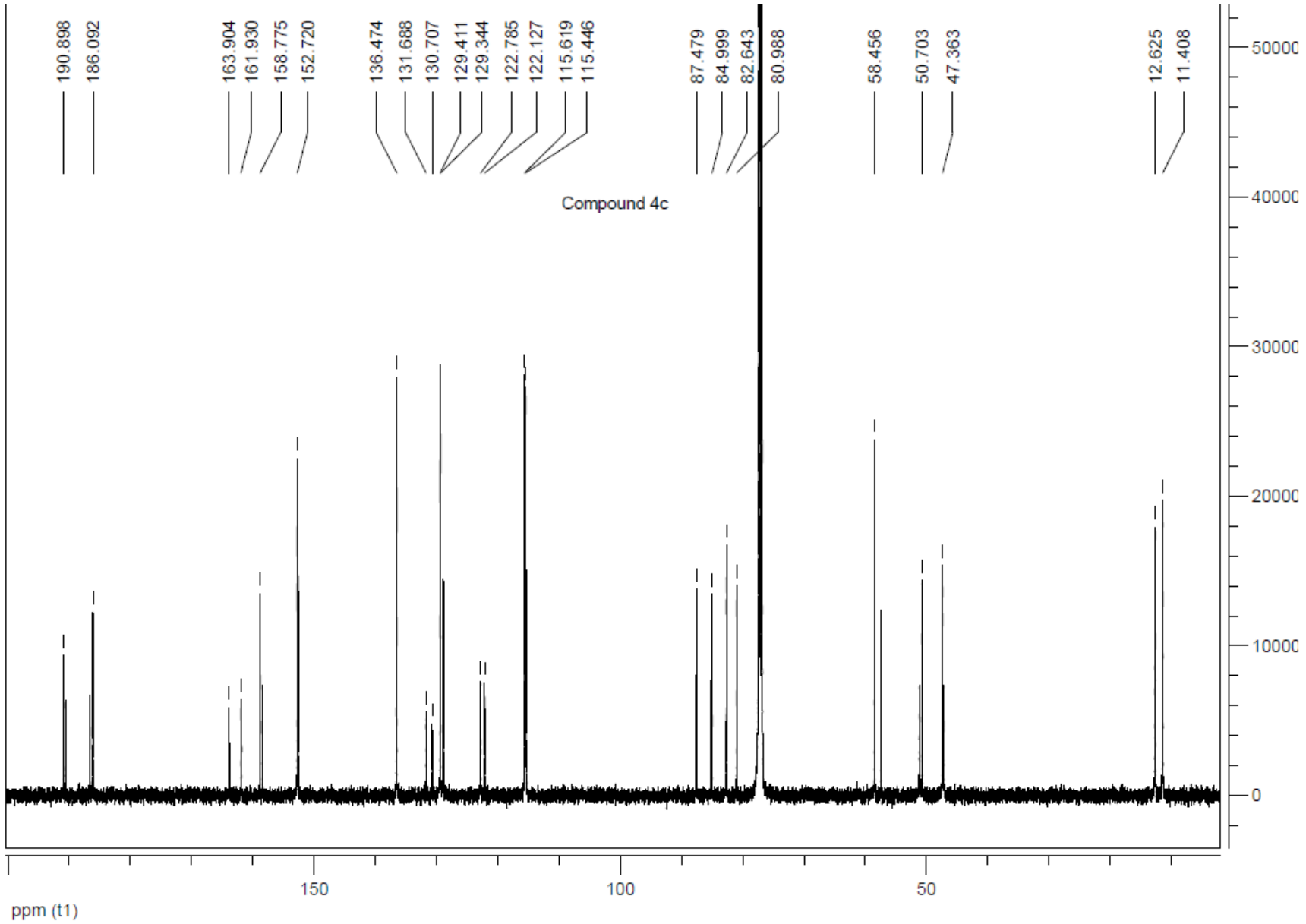
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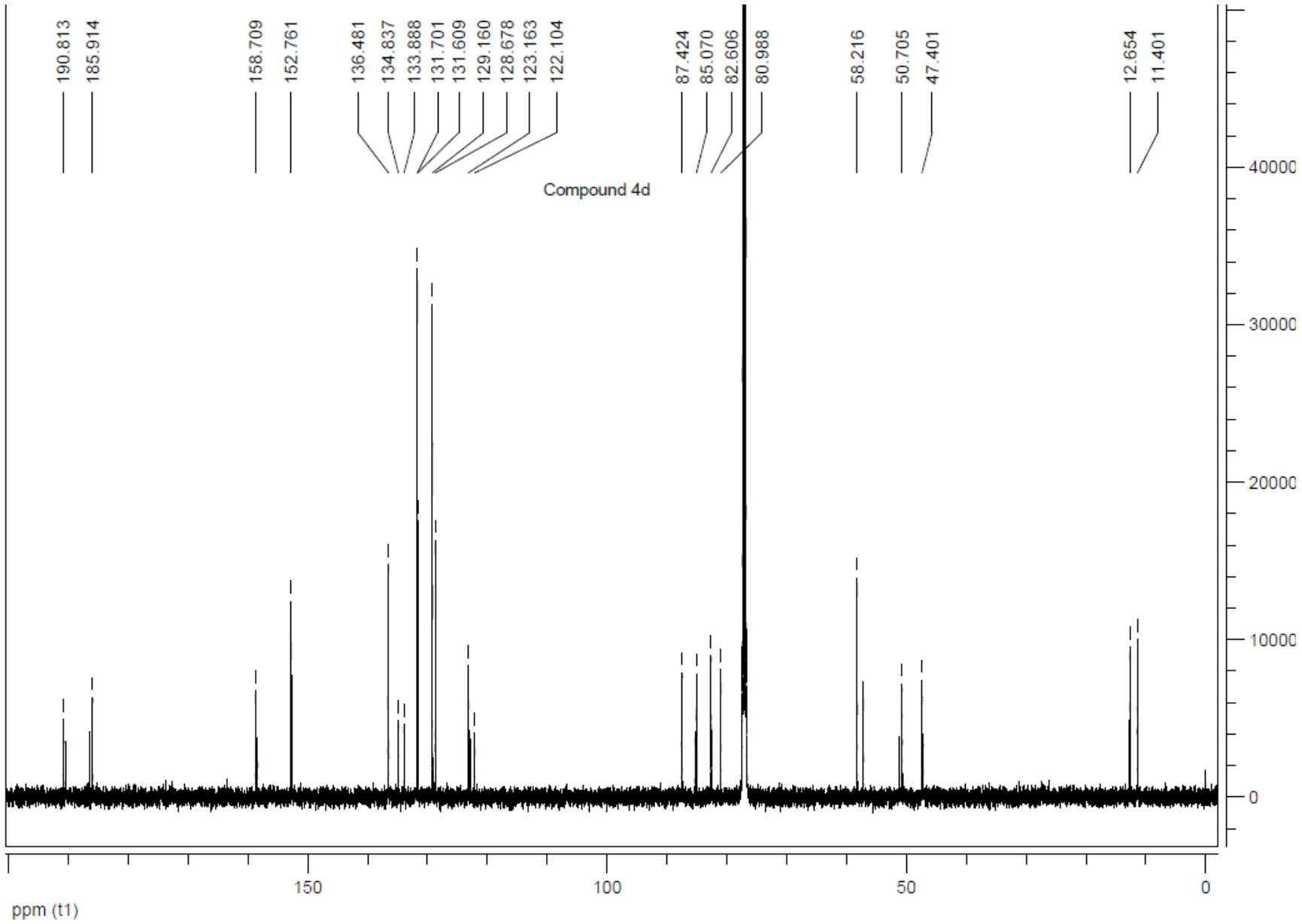
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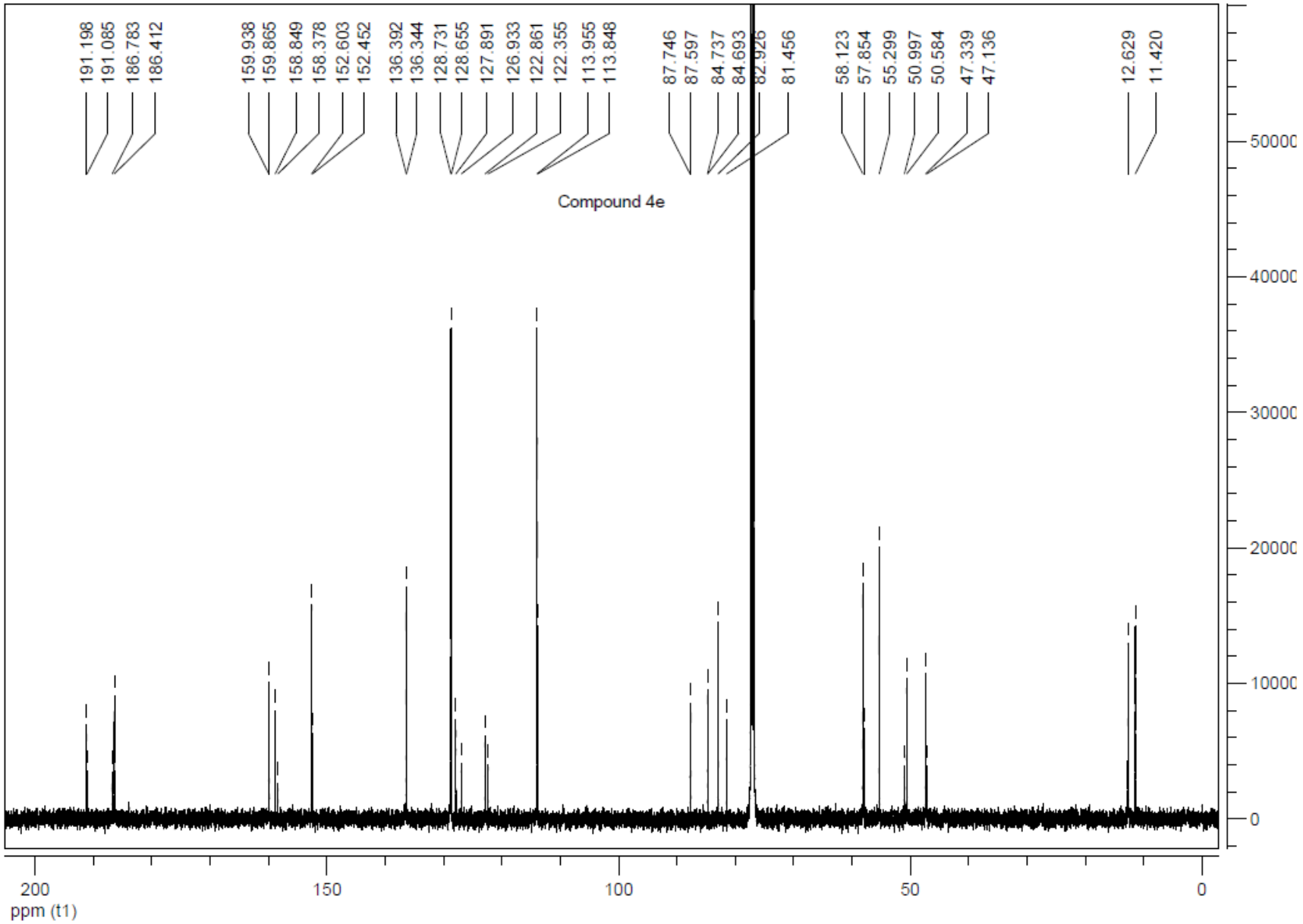
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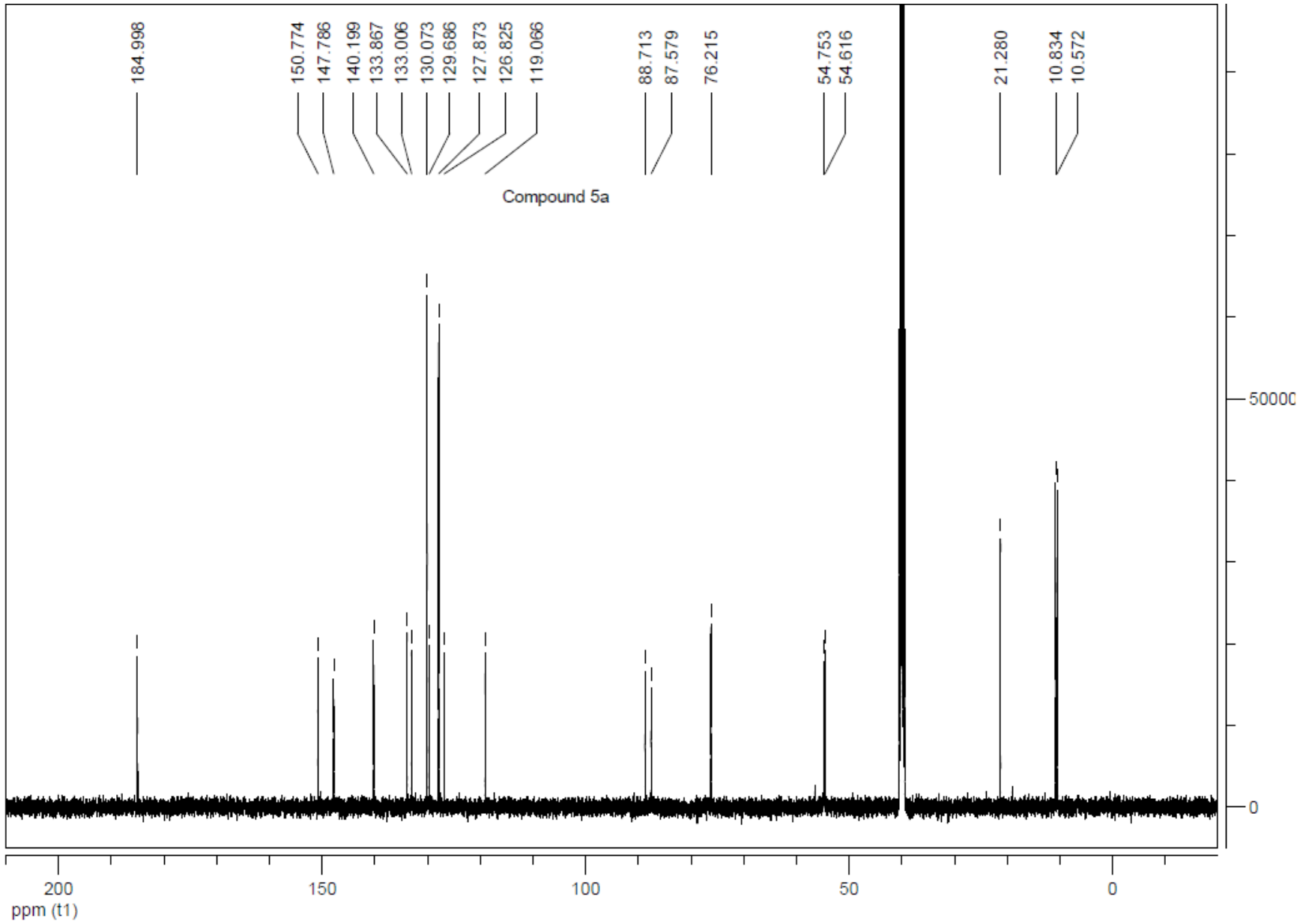
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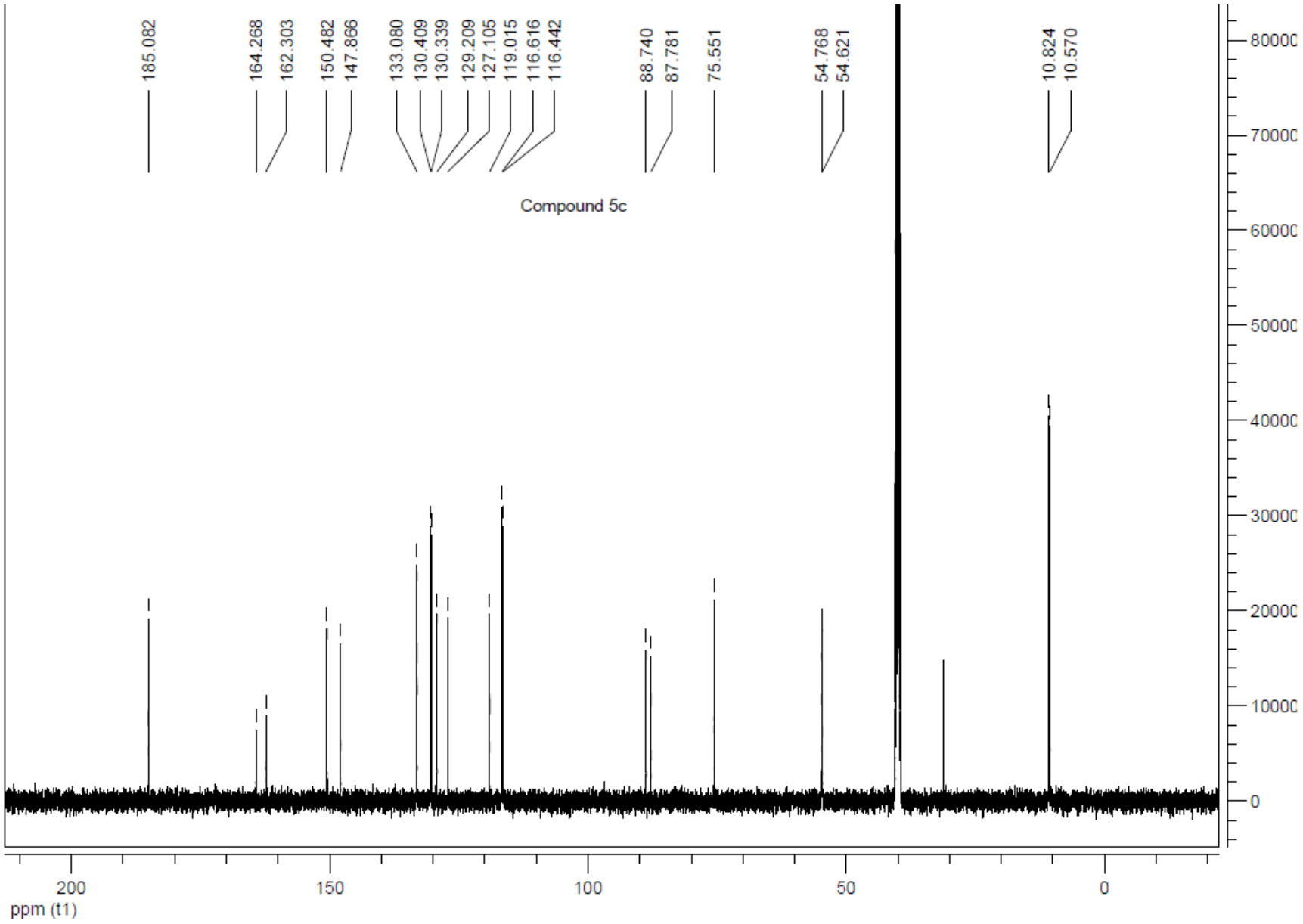
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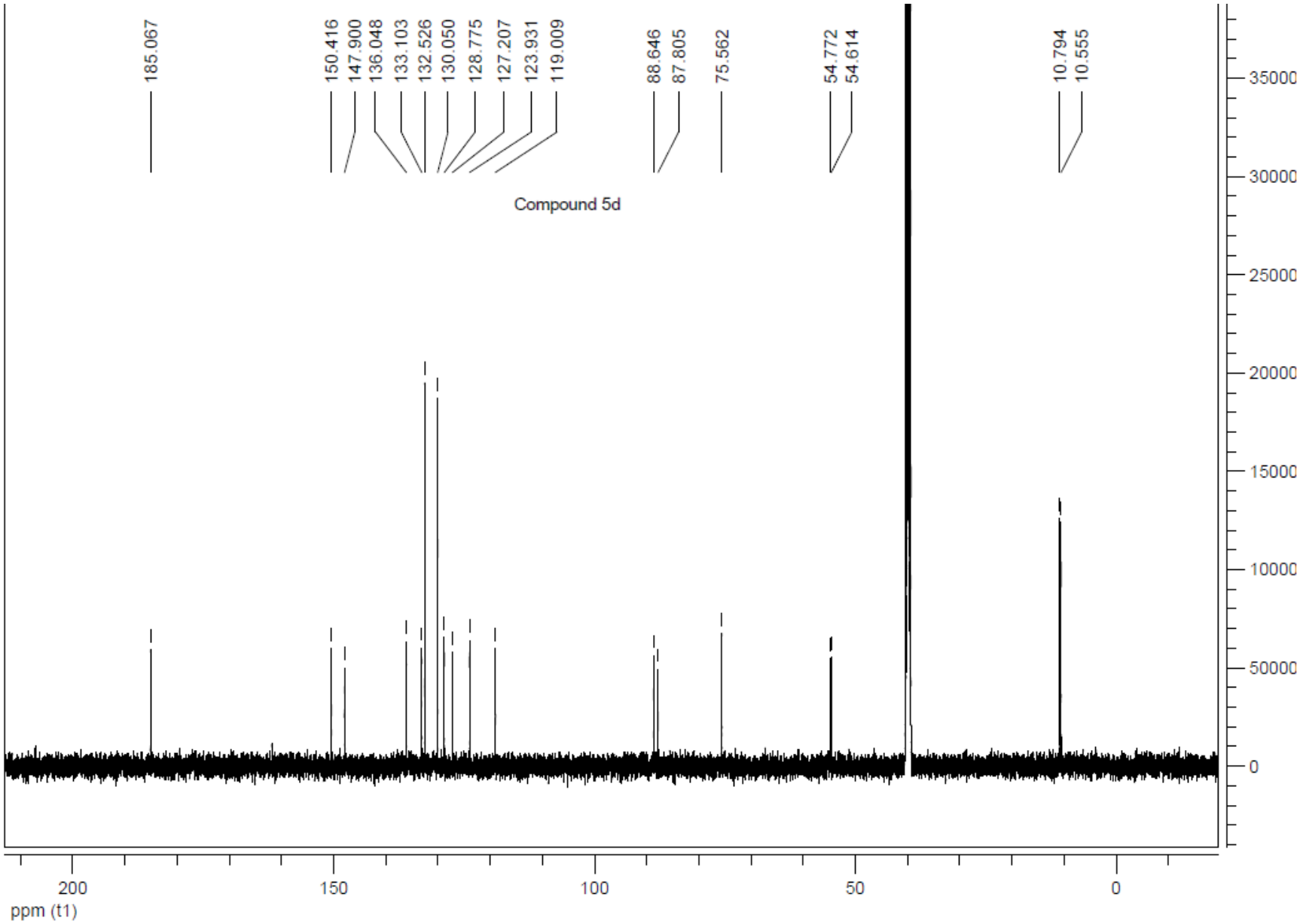
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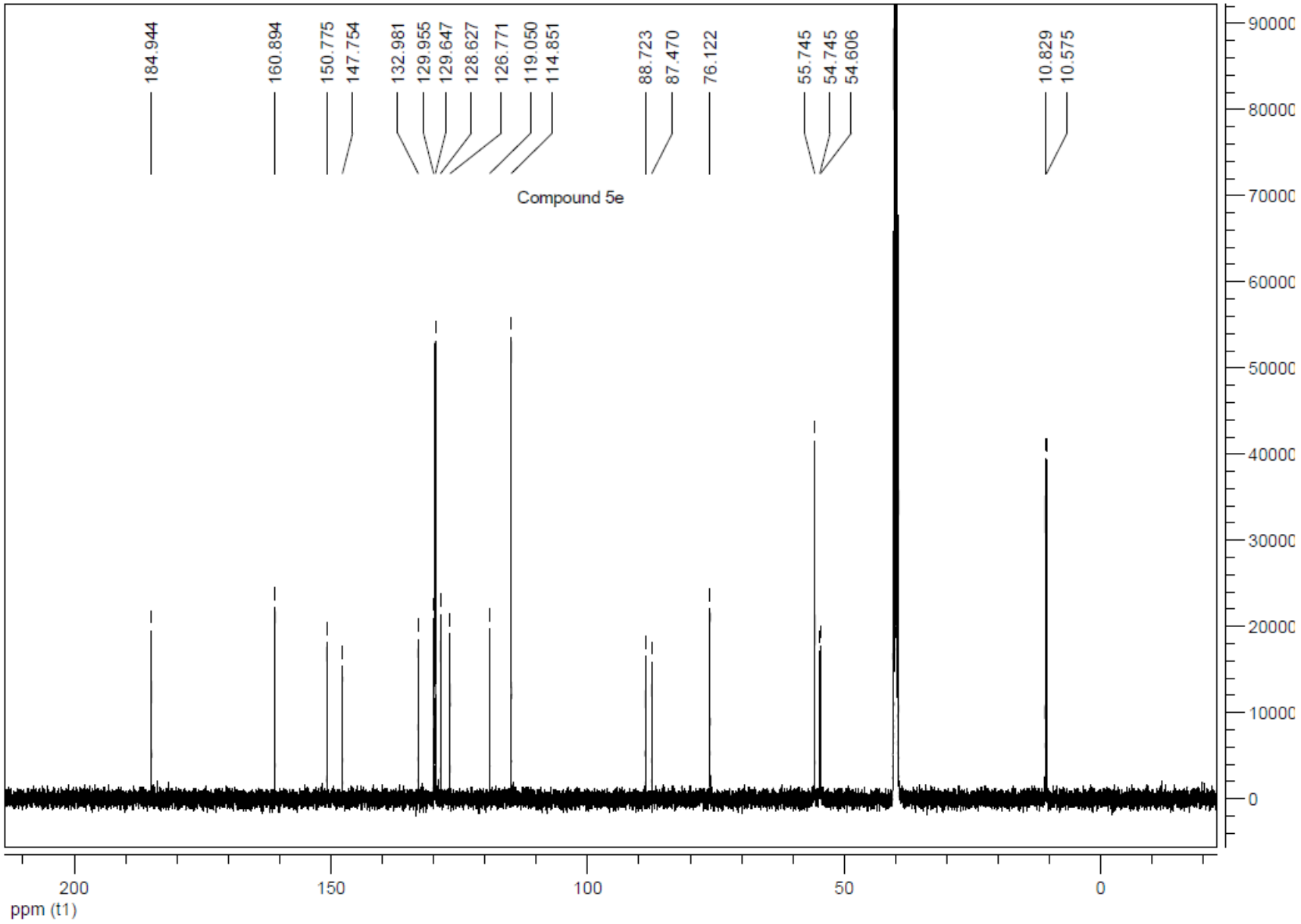
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