Supporting Information for

One-Pot Synthesis of Amine-Substituted Aryl Sulfides and Benzo[*b*]thiophene Derivatives

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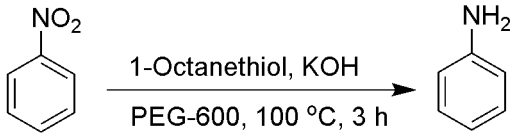
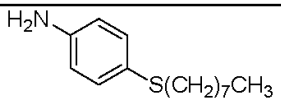
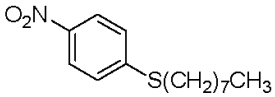
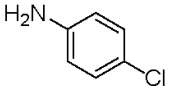
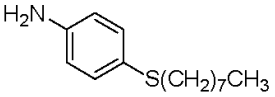
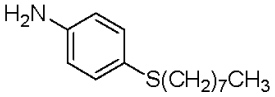
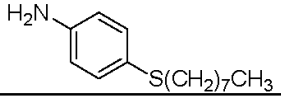
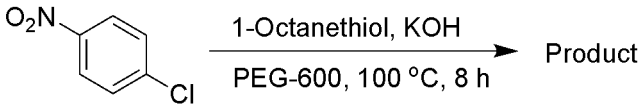
Table S1. The C-S Cross-Coupling of 1-Chloro-4-Nitrobenzene with Different Concentrations of 1-Octanethiol



entry	1-chloro-4-nitrobenzene	1-Octanethiol	KOH	product	yield [a]
1	0.5 mmol	0.75 mmol	3.0 equiv		98
2	0.5 mmol	0.75 mmol	---		7
3	0.5 mmol	---	3.0 equiv		80
4	0.5 mmol	0.4 mmol	3.0 equiv		80
5	0.5 mmol	0.5 mmol	3.0 equiv		90
6	0.5 mmol	0.6 mmol	3.0 equiv		92

[a] GC yield.

Table S2. Reduction of Nitrobenzene with 1-Octanethiol



entry	1-Octanethiol	KOH	yield [a]
1	1.5 equiv	3.0 equiv	71
2	1.5 equiv	---	< 2
3	0.5 equiv	3.0 equiv	36
4	0.25 equiv	3.0 equiv	19
5	0.025 equiv	3.0 equiv	13
6	---	3.0 equiv	12

[a] GC yield.

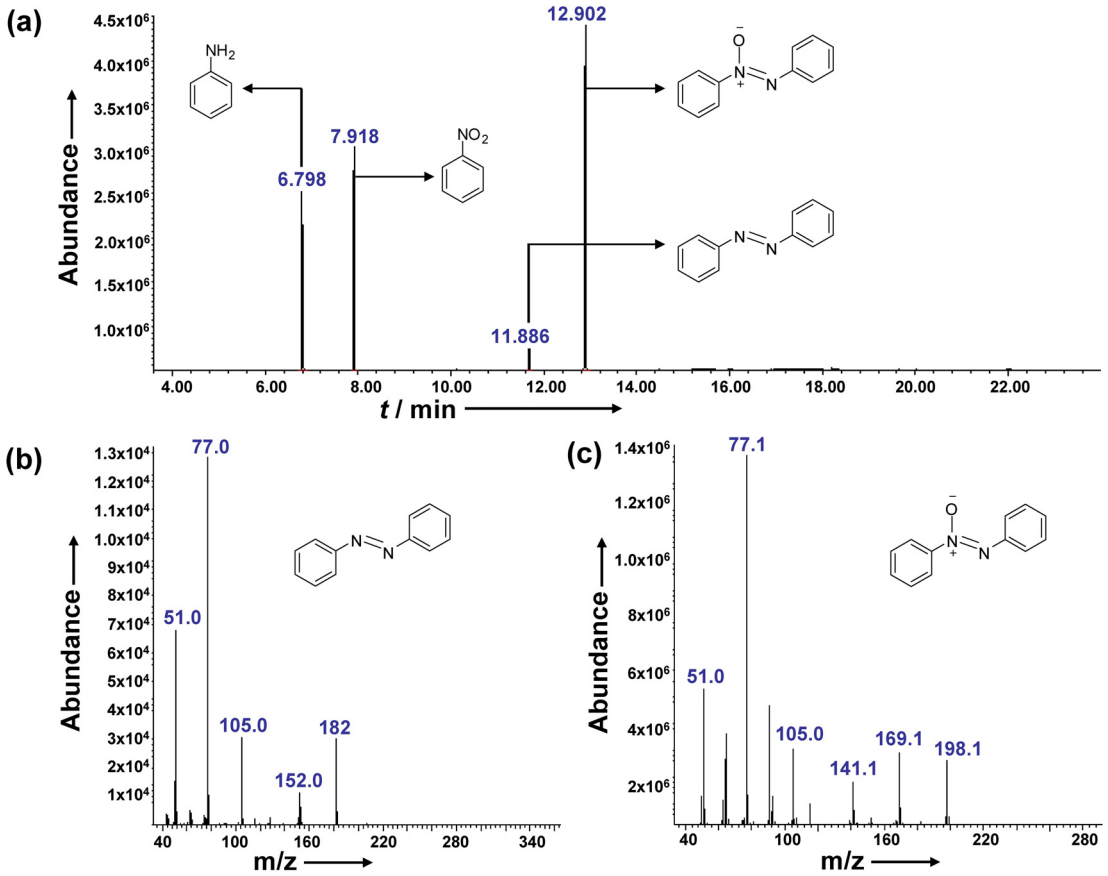


Figure S1. a) GC Analysis of Nitrobenzene Reduction with 1-Octanethiol in the presence of KOH and PEG-600. b) and c) Corresponding mass spectra of the peaks shown in GC spectrum at 11.88 and 12.90 minute, confirming the formation of azobenzene and azoxylbenzene, respectively.

Recycling Experiments of the PEG-600 for C-S Cross-Coupling

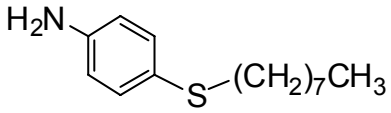
To a glass vial (20 mL) charged with PEG-600 (3 mL) was added 1-chloro-4-nitrobenzene (0.5 mmol), 1-octanethiol (0.75 mmol), and KOH (3 equiv). The resulting mixture was stirred at 100 °C for 2 h, at which time the product was extracted with diethyl ether (3×10 mL). The organic layers were combined, washed with water, dried over $NaSO_4$, and filtered. The solvent was removed *in vacuo* to afford the coupling product of 4-(octylthio)benzenamine. The separated mixture of KOH and PEG-600 was first treated *in vacuo* to remove unextracted diethyl ether and subsequently reused for recycling experiments with the same stoichiometric amounts of substrates and base.

runs	1	2	3
GC yield (%)	98	92	82

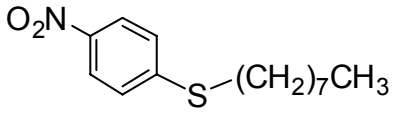
General Methods. Unless otherwise stated, all reactions were carried out without taking precautions to exclude air and moisture. All solvents were used as received. All the chemicals were purchased from commercial sources and used as received unless stated otherwise. Reactions were conducted in 20 mL of glass vials equipped with conventional screw caps. Column chromatography was carried out on silica gel (230-400 mesh). The yields of the coupling products listed in Tables 2 and 3 refer to isolated yields (average of two runs).

Physical Measurements. ^{1}H NMR and ^{13}C NMR spectra were recorded on a Bruker Avance 500 and 125 MHz FT-NMR spectrometers and referenced to solvent peaks. The coupling reaction of 1-chloro-4-nitrobenzene with 1-octanethiol shown in Table 1 was determined by using Hewlett- Packard Series 6890 GC (Santa Clara, CA, USA) coupled to a Hewlett Packard 5973 MS detector. High-resolution mass spectra were obtained using a Finnigan MAT95XL-T mass spectrometer.

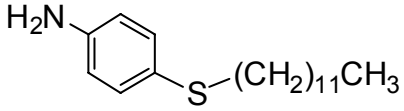
A General procedure for the one-pot C-S cross-coupling reaction. To a glass vial charged with PEG-600 (3 mL) was added nitroaryl halide (0.5 mmol), thiol (0.75 mmol), and KOH (84 mg, 3 equiv). The resulting mixture was stirred at 100 °C and monitored by TLC. Upon completion of the reaction (approx. 2 h), the mixture was cooled to room temperature, poured into water (10 mL), and extracted several times with ethyl acetate (15×3 mL). The combined organic layers were washed with water, dried over Na_2SO_4, and filtered. The solvent was removed *in vacuo* and the residue was purified by column chromatography (silica gel, eluent: hexane/ethyl acetate) to afford the aryl sulfide product.



4-(octylthio)benzenamine (**3a**). Obtained as a yellow oil in 92% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.26-7.22(td, 2 H), 6.62-6.60 (d, 2 H), 3.58 (br s, 2 H), 2.78-2.75(t, 2H), 1.59-1.53 (quint, 2 H), 1.40-1.37(m, 2H), 1.26(m, 8H), 0.90-0.87(t, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 145.6, 133.5, 123.7, 115.5, 36.3, 31.7, 29.3, 29.1, 29.0, 28.6, 22.5, 14.0 ppm; HR EIMS 237.1557 *m/z* (calcd. for $C_{14}H_{23}NS$: 237.1551).

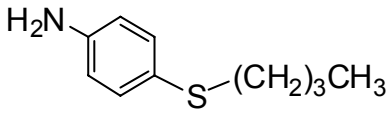


1-Nitro-4-(octylthio)benzene (**3a′**).[1] Obtained as a yellow oil in 89% yield. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.13-8.10(d, 2 H), 7.33-7.30 (d, 2 H), 3.05-3.00 (t, 2 H), 1.78-1.68 (quint, 2 H), 1.50-1.45 (m, 2H), 1.30 (m, 8H), 0.91-0.87 (t, 3H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 148.2, 144.7, 125.8, 123.8, 31.8, 31.7, 29.1, 29.0, 28.8, 28.4, 22.5, 14.0 ppm; HR EIMS 267.1296 *m/z* (calcd. for $C_{14}H_{21}O_2NS$: 267.1293).

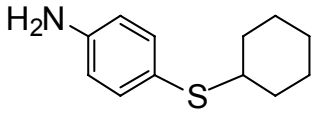


4-(dodecylthio)benzenamine (**3b**). Obtained as a yellow solid in 95% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.24-7.22 (td, 2 H), 6.63-6.61 (d, 2 H), 3.64 (br s, 2 H), 2.77-2.74 (t, 2H), 1.59-1.53 (quint, 2 H), 1.38-1.35 (m, 2H), 1.25 (m, 16H), 0.90-0.87 (t, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 145.6, 133.7, 124.0, 115.6, 36.4, 31.9,

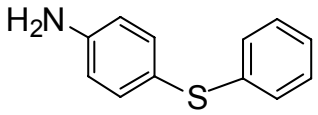
29.7, 29.65, 29.61, 29.5, 29.4, 29.3, 29.2, 28.7, 22.7, 14.1 ppm; HR EIMS 293.2176 *m/z* (calcd. for $C_{18}H_{31}NS$: 293.2177).



4-(butylthio)benzenamine (**3c**).[2] Obtained as a yellow oil in 96% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.24-7.22 (td, 2 H), 6.63-6.61 (td, 2 H), 3.50 (br s, 2 H), 2.78-2.75(t, 2H), 1.56-1.52 (quint, 2 H), 1.43-1.38 (m, 2H), 0.90-0.88 (t, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 145.6, 133.6, 123.9, 115.5, 36.0, 31.5, 21.8, 13.6 ppm; HR EIMS 181.0930 *m/z* (calcd. for $C_{10}H_{15}NS$: 181.0925).

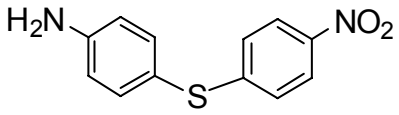


4-(cyclohexylthio)benzenamine (**3d**). Obtained as a yellow oil in 83% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.29-7.27(d, 2 H), 6.64-6.62 (d, 2 H), 3.76 (br s, 2 H), 2.88-2.83 (m, 1H), 1.96-1.93 (m, 2 H), 1.78-1.75(m, 2H), 1.62-1.59 (m, 1H), 1.36-1.20(m, 5H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 146.3, 136.1, 121.9, 115.3, 48.1, 33.4, 26.2, 25.8 ppm; HR EIMS 207.1092 *m/z* (calcd. for $C_{12}H_{17}NS$: 207.1082).

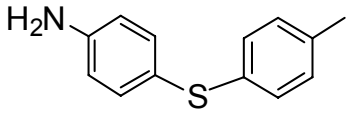


4-(phenylthio)benzenamine (**3e**).[3] Obtained as a light-yellow solid in 90% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.33-7.29(td, 2H), 7.23-7.20(t, 2H), 7.14-7.09 (m, 3H), 6.69-6.67 (td, 2H), 3.80(br s, 2 H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 147.09, 139.7,

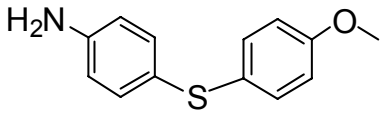
136.1, 128.8, 127.3, 125.2, 120.5, 115.8 ppm; HR EIMS 201.0613 *m/z* (calcd. for $C_{12}H_{11}NS$: 201.0612).



4-[(4-nitrophenyl)thio]benzenamine (**3f**). Obtained as yellow solid in 50% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.04-8.02(td, 2H), 7.35-7.32(td, 2H), 7.10-7.08 (td, 2 H), 6.75-6.73 (td, 2 H), 3.96 (s, 2 H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 151.0, 148.4, 144.8, 137.2, 125.3, 123.9, 116.5, 116.1 ppm; HR EIMS 246.0470 *m/z* (calcd. for $C_{12}H_{10}NO_2S$: 246.0463).

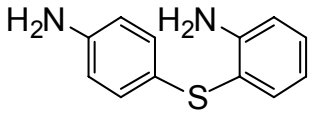


4-[(4-methylphenyl)thio]benzenamine (**3g**). Obtained as a yellow solid in 87% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.30-7.28 (td, 2H), 7.11-7.09 (d, 2H), 7.07-7.04 (d, 2H), 6.67-6.64 (td, 2H), 3.77(br s, 2 H), 2.30 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 146.7, 135.6, 135.5, 135.4, 129.7, 128.3, 121.7, 115.9, 21.0 ppm; HR EIMS 215.0777 *m/z* (calcd. for $C_{13}H_{13}NS$: 215.0769).

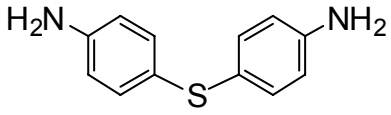


4-[(4-methoxyphenyl)thio]benzenamine (**3h**). Obtained as a yellow solid in 84% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.25-7.22(m, 4H), 6.83-6.81 (td, 2H), 6.63-6.61 (td, 2H), 3.77 (s, 5H, N*H*$_2$ and C*H*$_3$) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ158.4, 146.2,

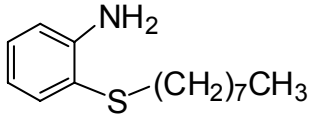
133.8, 131.3, 128.7, 123.3, 115.7, 114.5, 55.2 ppm; HR EIMS 231.0719 *m/z* (calcd. for $C_{13}H_{13}ONS$: 231.0718).



2-[(4-aminophenyl)thio]benzenamine (**3i**). Obtained as a yellow solid in 85% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.37-7.35 (dd, 1H), 7.16-7.13 (dt, 1H), 7.08-7.05(td, 2H), 6.72-6.69 (m, 2H), 6.60-6.57 (td, 2 H), 3.76 (br s, 4H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 147.6, 145.4, 135.5, 130.8, 129.9, 123.5, 118.7, 118.0, 116.0, 115.3 ppm; HR EIMS 216.0729 *m/z* (calcd. for $C_{12}H_{12}N_2S$: 216.0721).

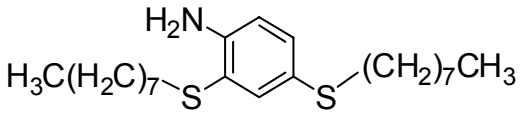


4, 4'-thiobisbenzenamine (**3j**). Obtained as a yellow solid in 87% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.26-7.15(m, 4 H), 6.61-6.57(t, 4H), 3.78(br s, 4 H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 147.1, 133.9, 125.7, 115.4 ppm; HR EIMS 216.0728 *m/z* (calcd. for $C_{12}H_{12}N_2S$: 216.0721).

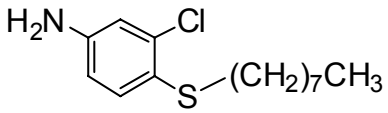


2-*n*-Octylsulfanylaniline (**3k**).[4] Obtained as a yellow liquid in 82% yield. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.39-7.36 (d, 1H), 7.14-7.08 (t, 1H), 6.74-6.67 (m, 2H), 4.34 (br s, 2H), 2.76-2.72 (t, 2H), 1.62-1.52 (quint, 2H), 1.40-1.36 (m, 2H), 1.26 (m, 8H), 0.90-0.86 (t, 3H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 148.0, 135.5, 129.3, 118.4,

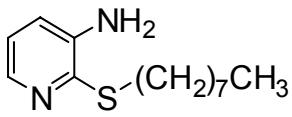
118.3, 114.7, 34.8, 31.7, 29.6, 29.1, 29.0, 28.6, 22.6, 14.0 ppm; HR EIMS: 237.1551 *m/z* (calcd. for $C_{14}H_{23}NS$: 237.1551).



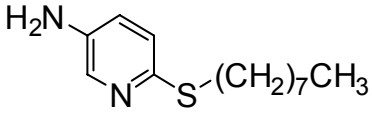
2,4-dioctylthio-benzenamine (**3l**). Obtained as a brown oil in 68% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.45(s, 1 H), 7.18-7.16(d, 1 H), 6.65-6.64(d, 1H), 4.36(br s, 2 H), 2.77-2.72(m, 4H), 1.57-1.54 (quint, 4 H), 1.37(s, 4H), 1.29 (m, 16H), 0.89-0.86 (t, 6H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 147.3, 139.3, 133.8, 123.6, 119.0, 115.2, 36.5, 34.9, 31.8, 29.6, 29.4, 29.2, 29.18, 29.16, 28.7, 22.7, 14.1 ppm; HR EIMS 381.2528 *m/z* (calcd. for $C_{22}H_{39}NS_2$: 381.2524).



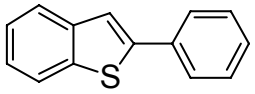
3-chloro-4-octylthio-benzenamine (**3m**). Obtained as a yellow oil in 80% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.25-7.23(d, 1 H), 6.75-6.74 (d, 1 H), 6.53-6.50 (dd, 1H), 3.77 (br s, 2 H), 2.81-2.78(t, 2H), 1.59-1.54 (quint, 2 H), 1.42-1.36 (quint, 2H), 1.25 (m, 8H), 0.89-0.86 (t, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 146.7, 137.7, 134.7, 122.3, 116.1, 113.9, 34.9, 31.8, 29.1, 29.0, 28.7, 22.6, 14.1 ppm; HR EIMS: 271.1162 *m/z* (calcd. for $C_{14}H_{22}NClS$: 271.1161).



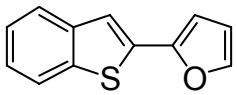
2-octylthio-3-pyridinamine (**3n**). Obtained as a brown oil in 75% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.96-7.94(m, 1 H), 6.89-6.84 (m, 2 H), 3.86 (br s, 2 H), 3.23-3.19 (t, 2H), 1.72-1.66 (quint, 2 H), 1.46-1.40 (quint, 2H), 1.26 (m, 8H), 0.89-0.86(t, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ143.7, 140.6, 139.7, 120.4, 120.1, 31.8, 30.8, 29.7, 29.2, 29.1, 28.9, 22.7, 14.1 ppm; HR EIMS: 238.1512 *m/z* (calcd. for $C_{13}H_{22}N_2S$: 238.1504).



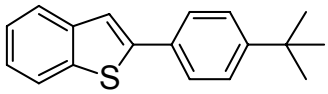
6-octylthio-3-pyridinamine (**3o**). Obtained as a brown oil in 61% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.99(s, 1 H), 7.04-7.02 (d, 1H), 6.90-6.87(d, 1H), 3.94 (br s, 2 H), 3.08-3.04(t, 2H), 1.68-1.62 (quint, 2 H), 1.44-1.38(quint, 2H), 1.25(m, 8H), 0.89-0.86(t, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ147.3, 139.7, 137.1, 123.7, 123.3, 31.8, 31.7, 29.6, 29.2, 29.0, 28.9, 22.6, 14.1 ppm; HR EIMS: 238.1497 *m/z* (calcd. for $C_{13}H_{22}N_2S$: 238.1504).



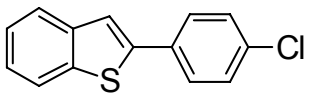
2-phenylbenzo[*b*]thiophene (**3p**).[5] Obtained as a white solid in 81% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.85-7.83 (d, 1H), 7.79-7.77 (d, 1H), 7.74-7.72 (td, 2H), 7.56 (s, 1H), 7.45-7.42(t, 2H), 7.38-7.30(m, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 144.3, 140.7, 139.5, 134.3, 129.0, 128.3, 126.5, 124.5, 124.3, 123.6, 122.3, 119.5; HR EIMS: 210.0499 *m/z* (calcd. for $C_{14}H_{10}S$: 210.0503).



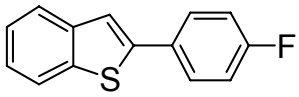
2-(2-furanyl)benzo[*b*]thiophene(3q). Obtained as a white solid in 86% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.81-7.79 (d, 1H), 7.76-7.74 (d, 1H), 7.48 (s, 2H), 7.37-7.29(m, 2H), 6.65-6.64 (d, 1H), 6.50-6.49 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 149.3, 142.5, 140.2, 138.9, 133.3, 124.6, 124.4, 123.6, 122.2, 118.6, 111.9, 107.0; HR EIMS: 200.0305 *m/z* (calcd. for $C_{12}H_8OS$: 200.0296).



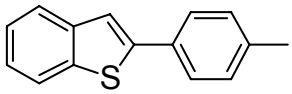
2-(4 -tert-butylphenyl)benzo[*b*]thiophene (**3r**). Obtained as a white solid in 87% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.83-7.81 (d, 1H), 7.77-7.75 (d, 1H), 7.67-7.65 (d, 2H), 7.51 (s, 1H), 7.46-7.44(d, 2H), 7.35-7.30(m, 2H), 1.37 (s, 9H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 151.5, 144.3, 140.8, 139.4, 131.5, 126.2, 125.9, 124.4, 124.1, 123.4, 122.2, 118.9, 34.7, 31.3; HR EIMS: 266.1131 *m/z* (calcd. for $C_{18}H_{18}S$: 266.1129).



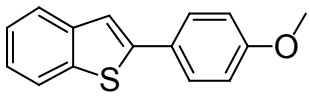
2-(4-chlorophenyl)benzo[*b*]thiophene(3s).[5] Obtained as a white solid in 75% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.84-7.82 (d, 1H), 7.78-7.76 (d, 1H), 7.65-7.63 (d, 2H), 7.52 (s, 1H), 7.41-7.32(m, 4H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 142.8, 140.6, 139.5, 134.1, 132.8, 129.1, 127.6, 124.7, 124.6, 123.6, 122.3, 119.9; HR EIMS: 244.0122 *m/z* (calcd. for $C_{14}H_9ClS$: 244.0113).



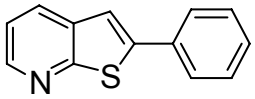
2-(4-fluorophenyl)benzo[*b*]thiophene (**3t**).[5] Obtained as a white solid in 74% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.83-7.81 (d, 1H), 7.78-7.76 (d, 1H), 7.70-7.66 (m, 2H), 7.47 (s, 1H), 7.36-7.31(m, 2H), 7.14-7.11(t, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 143.1, 140.7, 139.4, 130.6, 128.1, 124.6, 124.4, 123.5, 122.2, 119.4, 116.0, 115.9; HR EIMS: 228.0410 *m/z* (calcd. for $C_{14}H_9FS$: 228.0409).



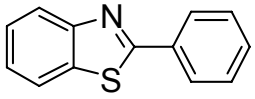
2-(4-methylphenyl)benzo[*b*]thiophene(**3u**).[5] Obtained as a white solid in 85% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.83-7.81 (d, 1H), 7.77-7.75 (d, 1H), 7.63-7.60 (d, 2H), 7.51 (s, 1H), 7.36-7.28 (m, 2H), 7.25-7.23 (d, 2H), 2.40 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 144.4, 140.8, 139.3, 138.3, 131.5, 129.6, 126.4, 124.4, 124.1, 123.4, 122.2, 118.8, 21.2; HR EIMS: 224.0655 *m/z* (calcd. for $C_{15}H_{12}S$: 224.0660).



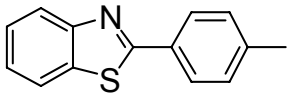
2-(4-Methoxyphenyl)benzo[*b*]thiophene (**3v**).[5, 6] Obtained as a white solid in 82% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.82-7.80 (d, 1H), 7.75-7.73 (d, 1H), 7.67-7.64 (td, 2H), 7.43 (s, 1H), 7.35-7.32(t, 1H), 7.30-7.27(t, 1H), 6.98-6.95 (td, 2H); 3.86(s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 159.8, 144.2, 140.9, 139.2, 127.8, 127.1, 124.5, 124.0, 123.3, 122.2, 118.2, 114.4, 55.4; HR EIMS: 240.0610 *m/z* (calcd. for $C_{15}H_{12}OS$: 240.0609).



2-phenyl-thieno[2,3-*b*]pyridine (**3w**). Obtained as a white solid in 70% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.53-8.51 (dd, 1H), 8.02-8.00 (dd, 1H), 7.74-7.72 (d, 2H), 7.46-7.43(m, 3H), 7.40-7.37(m, 1H), 7.30-7.27(m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 161.6, 146.3, 144.6, 134.3, 133.9, 130.7, 129.1, 128.8, 126.6, 119.8, 116.7; HR EIMS: 211.0458 *m/z* (calcd. for $C_{13}H_9NS$: 211.0456).



2-Phenylbenzothiazole (**3x**)**.** Obtained as a white solid in 46% yield. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.12-8.07 (3H, m, aromatic), 7.93-7.90 (1H, d, aromatic), 7.52-7.47 (4H, m, aromatic), 7.42-7.39 (1H, t, aromatic); ^{13}C NMR (75 MHz, $CDCl_3$) δ 168.1, 154.1, 135.1, 133.6, 131.0, 129.0, 127.6, 126.3, 125.2, 123.2, 121.6; HR EIMS: 211.0453 m/z (calcd. for $C_{13}H_9NS$: 211.0456).



2-(4-Methylphenyl)benzothiazole (**3y**)**.**[7] Obtained as a white solid in 40% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.08-8.06 (1H, d, aromatic), 8.00-7.98 (2H, d, aromatic), 7.89-7.87 (1H, d, aromatic), 7.50-7.47 (1H, t, aromatic), 7.39-7.35(1H, t, aromatic), 7.30-7.28(2H, d, aromatic), 2.42(3H, s, C*H*$_3$); ^{13}C NMR (125 MHz, $CDCl_3$) δ 168.3,

154.2, 141.4, 135.0, 131.0, 129.7, 127.5, 126.3, 125.0, 123.1, 121.6, 21.5; HR EIMS: 225.0612 m/z (calcd. for $C_{14}H_{11}NS$: 225.0612).

References:

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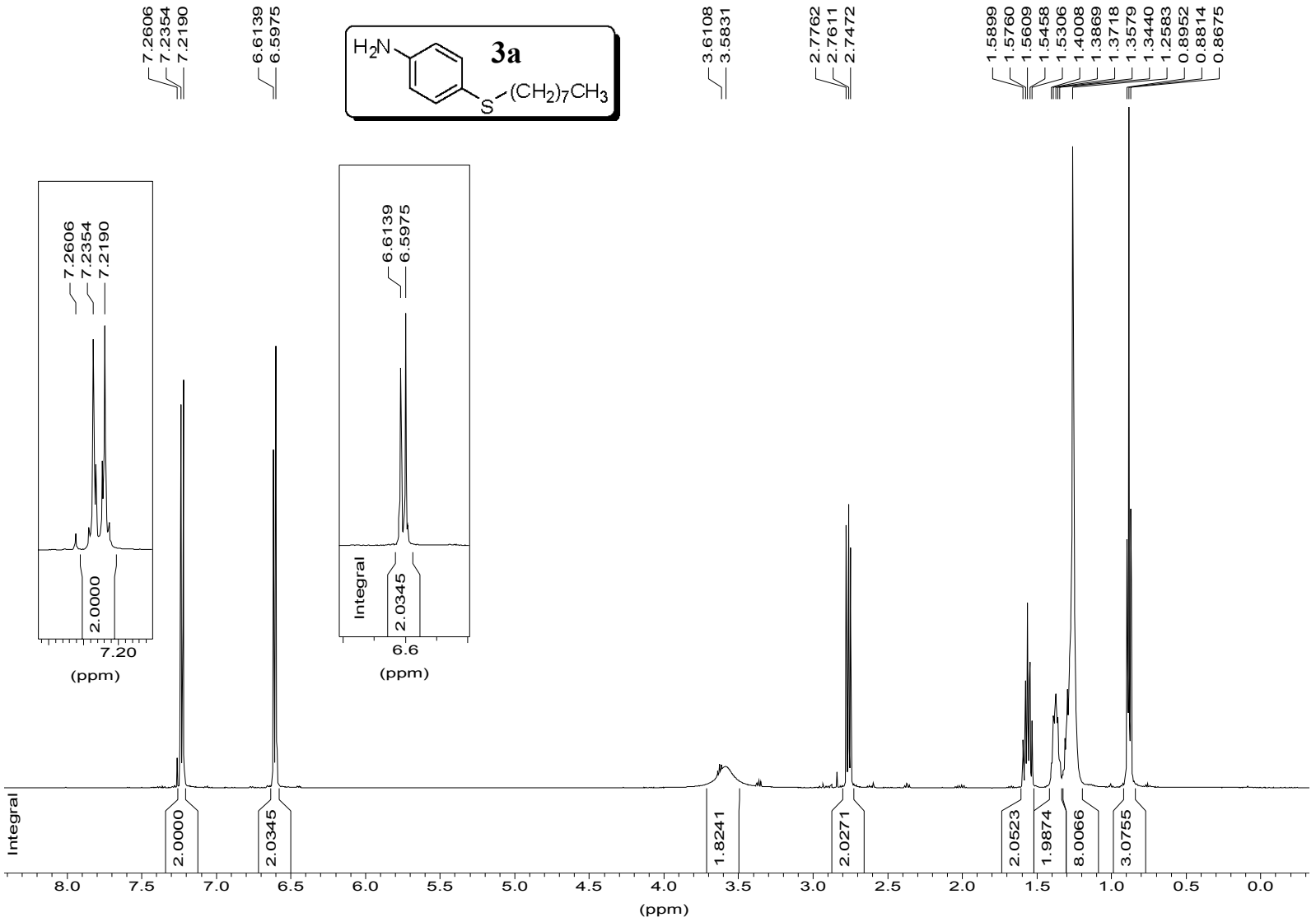
7. Chakraborti, A. K.; Rudrawar, S.; Jadhav, K. B; Kaur, G.; Chankeshwara, S. V. *Green Chem.* **2007**, *9*, 1335–1340.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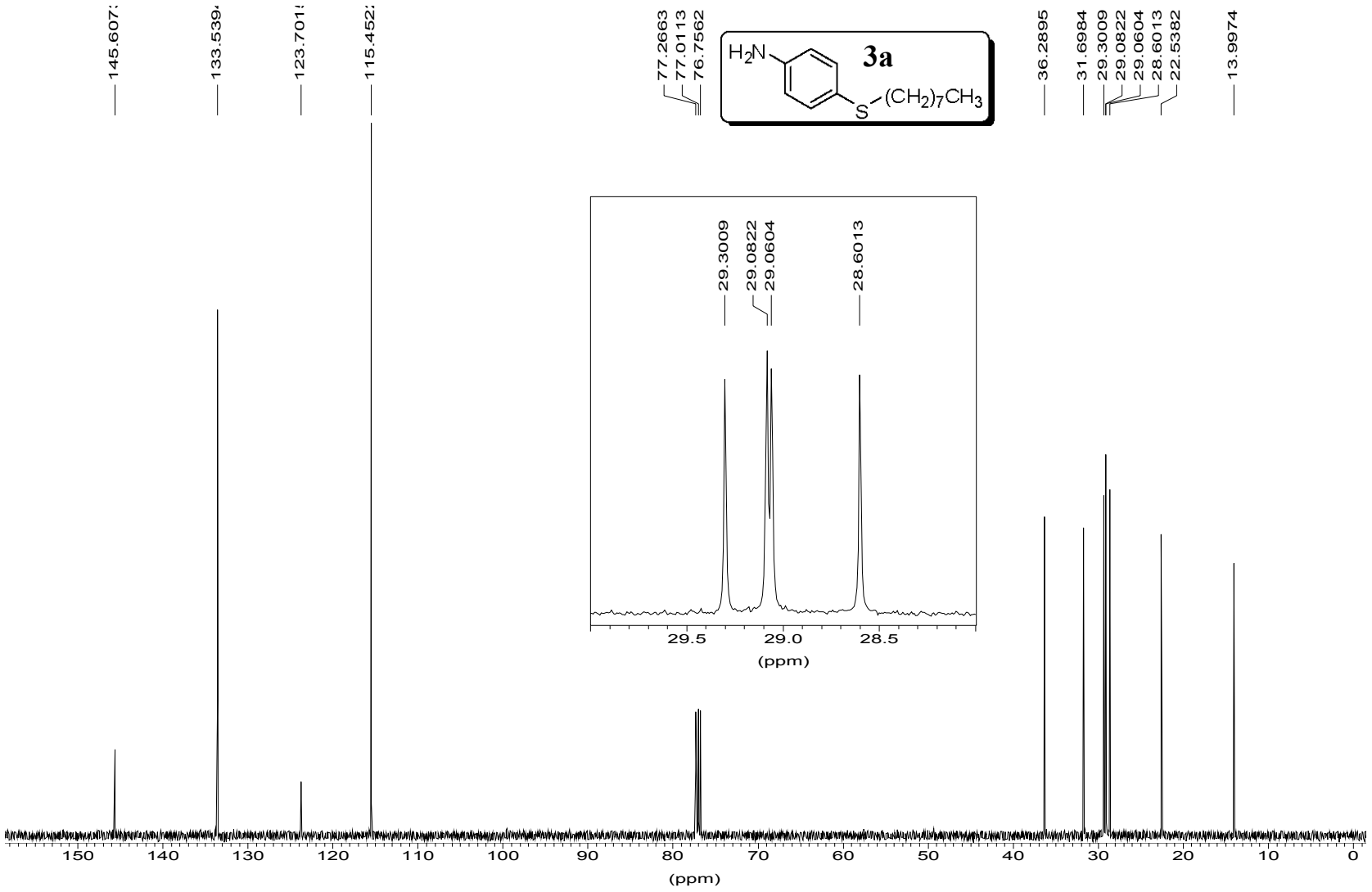
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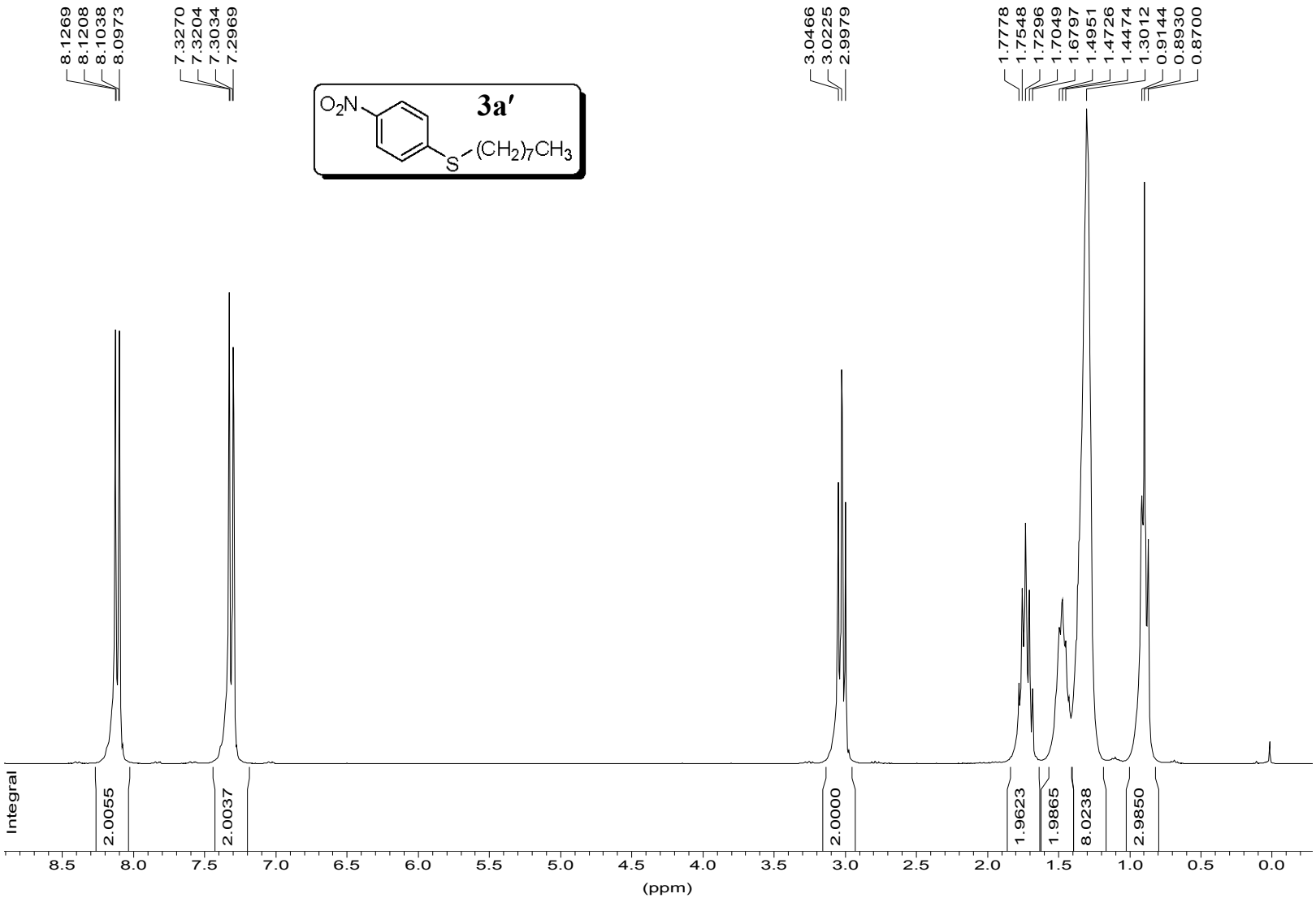
(ppm)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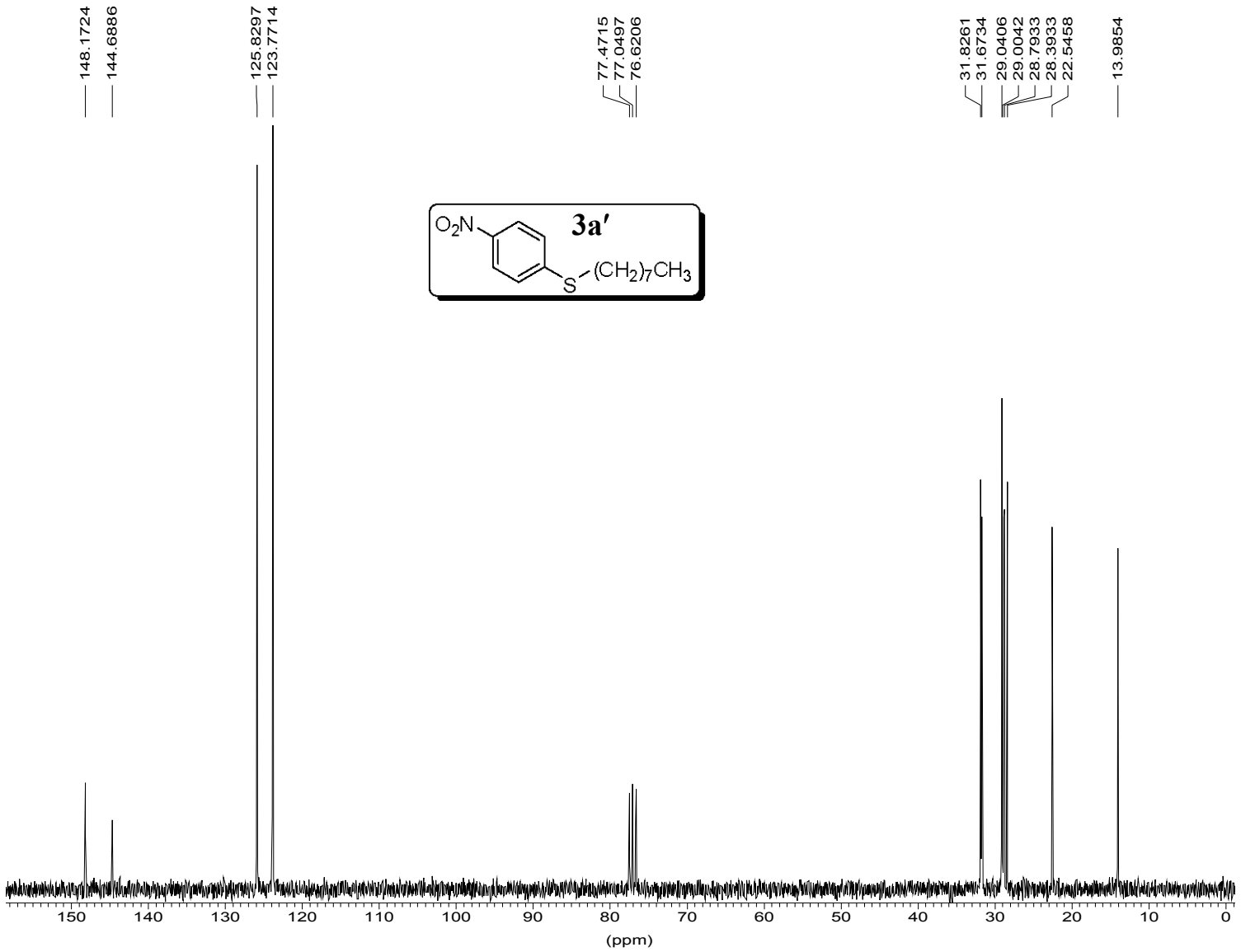
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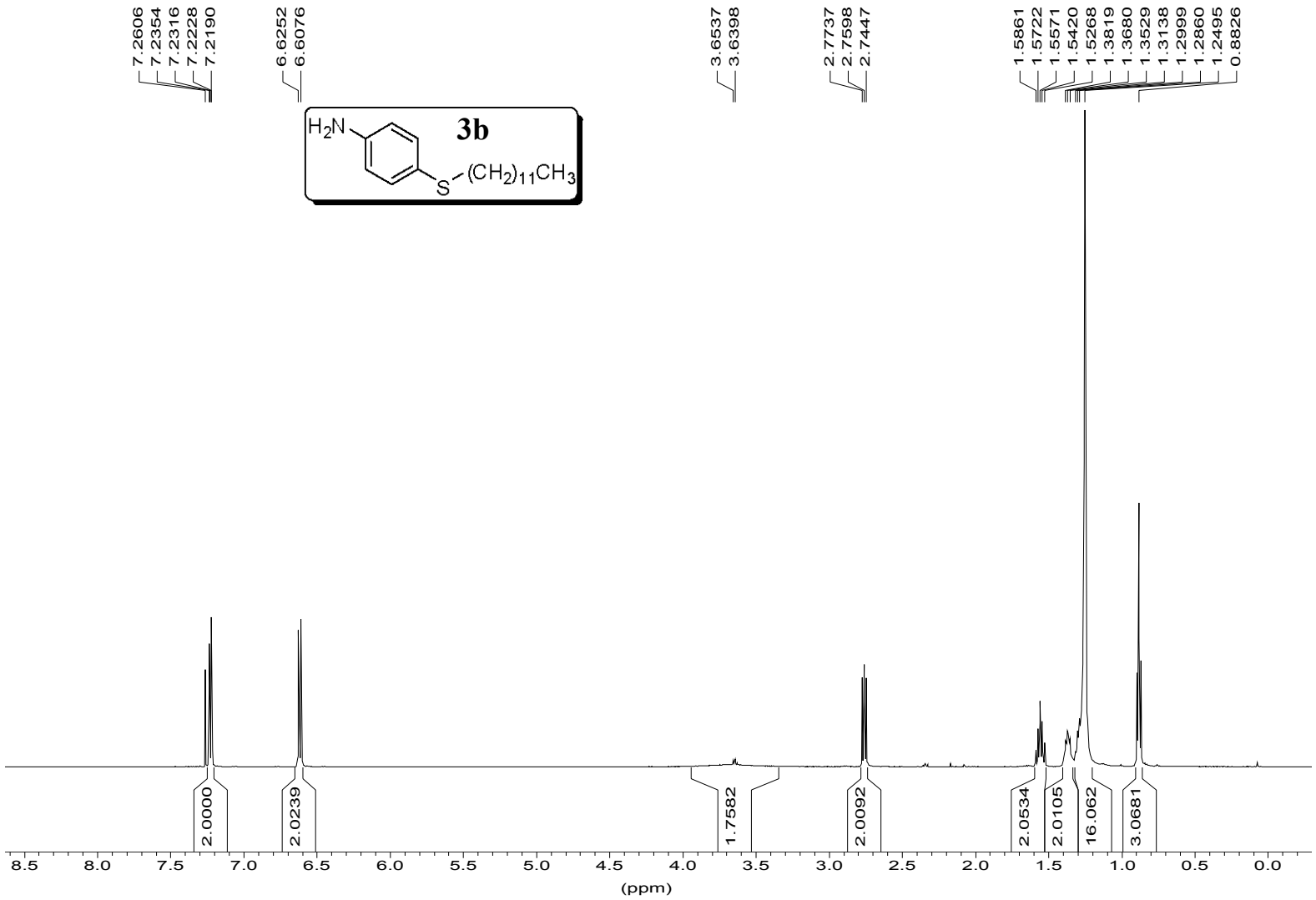
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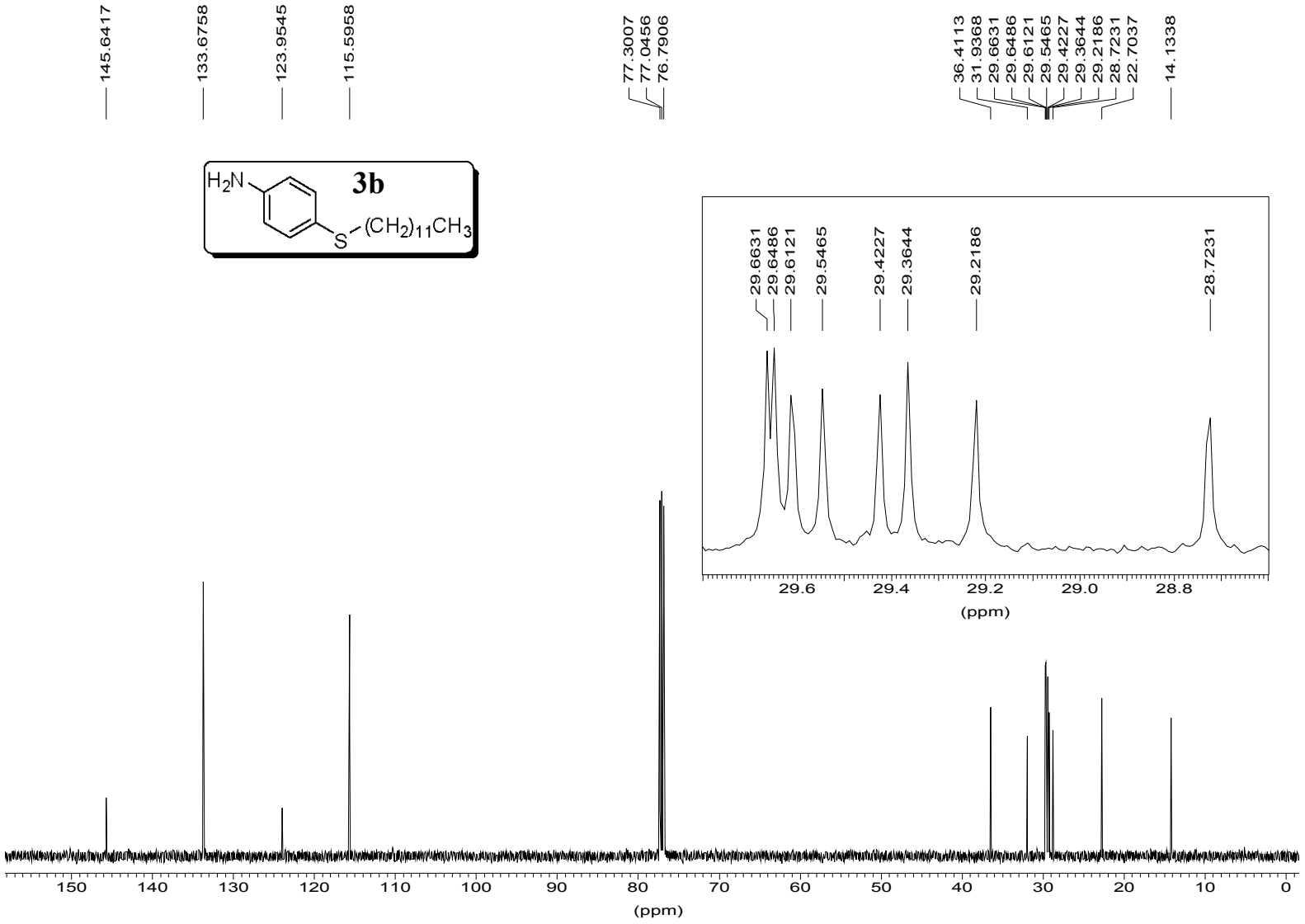
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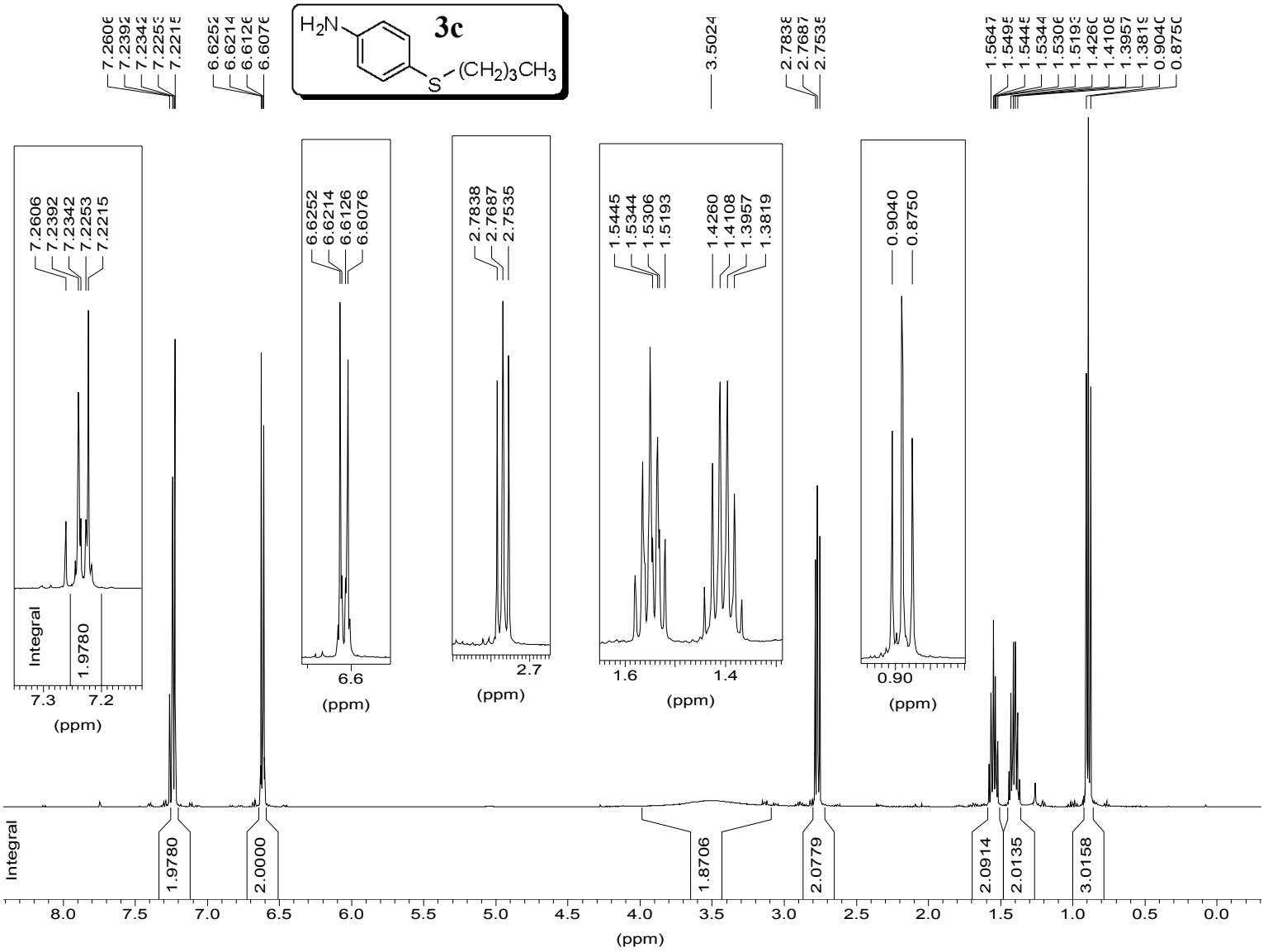
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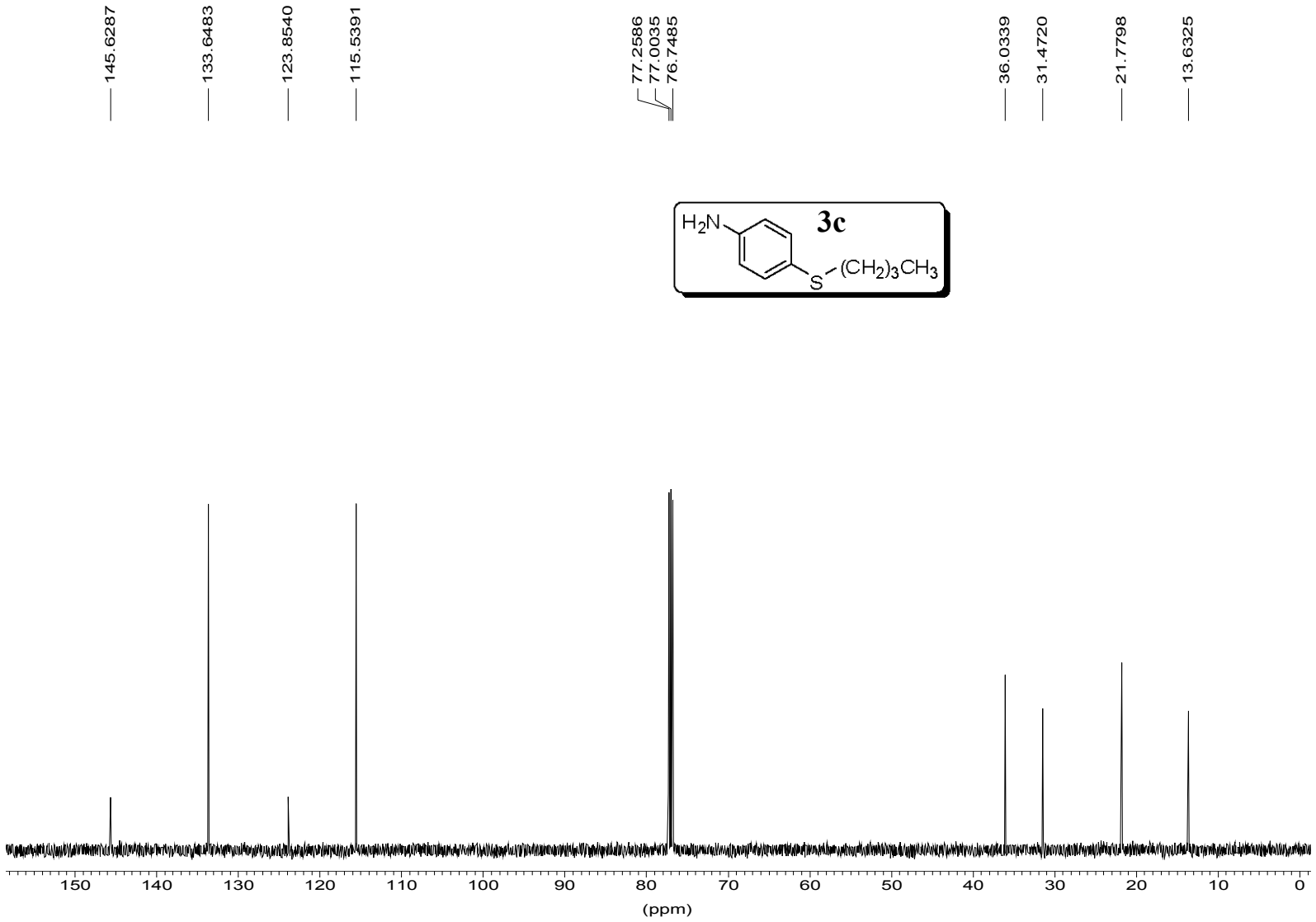
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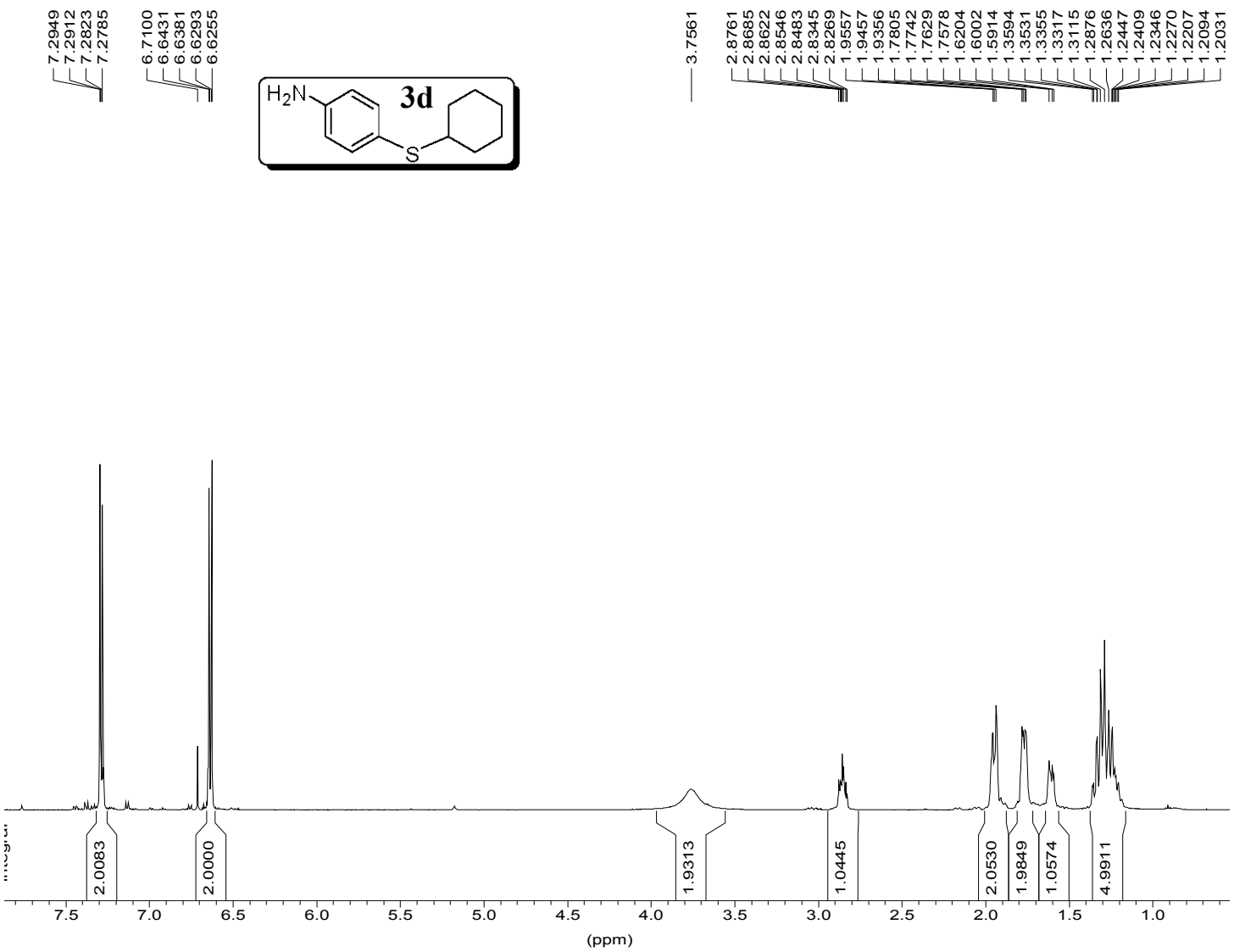
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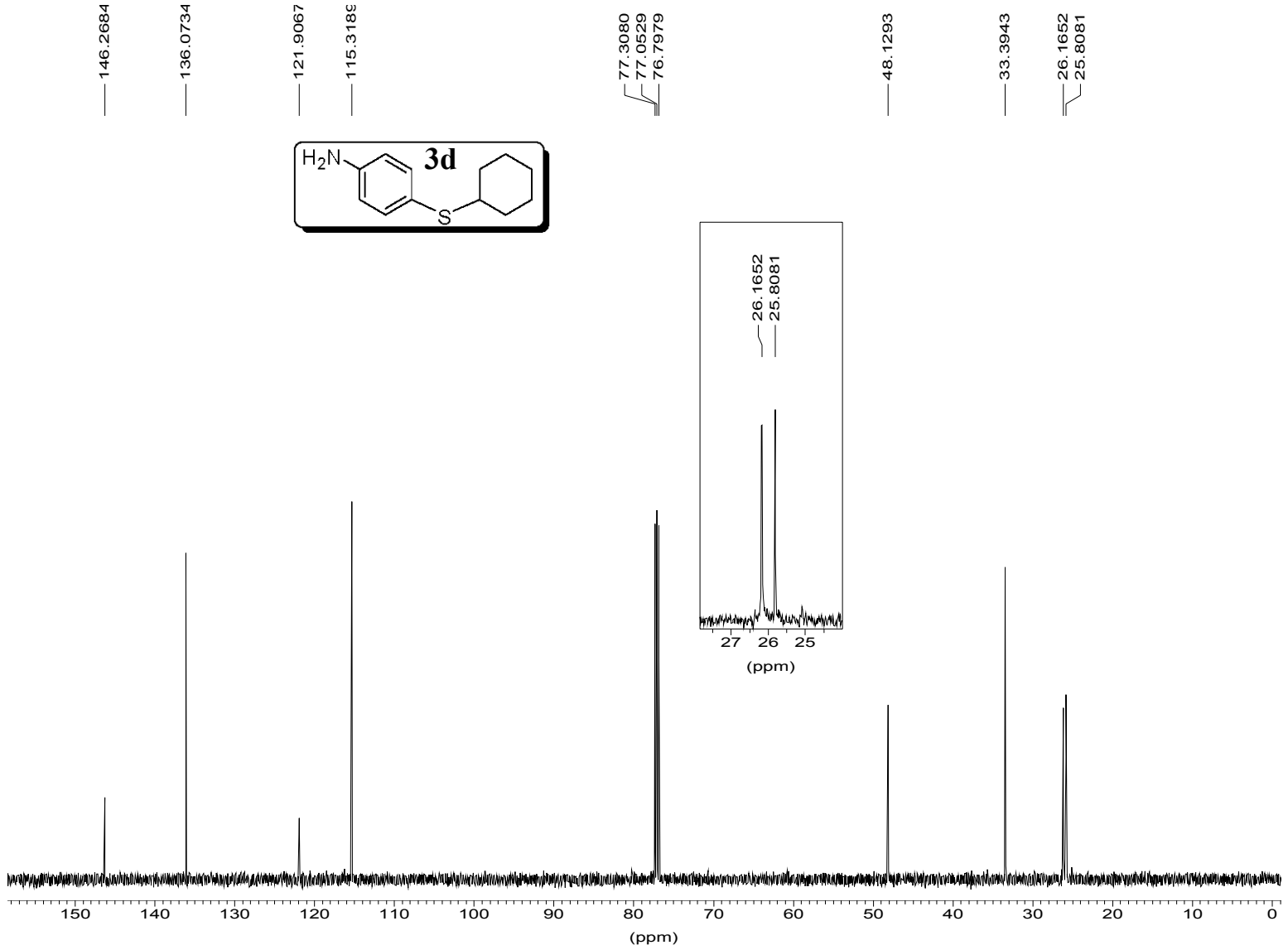
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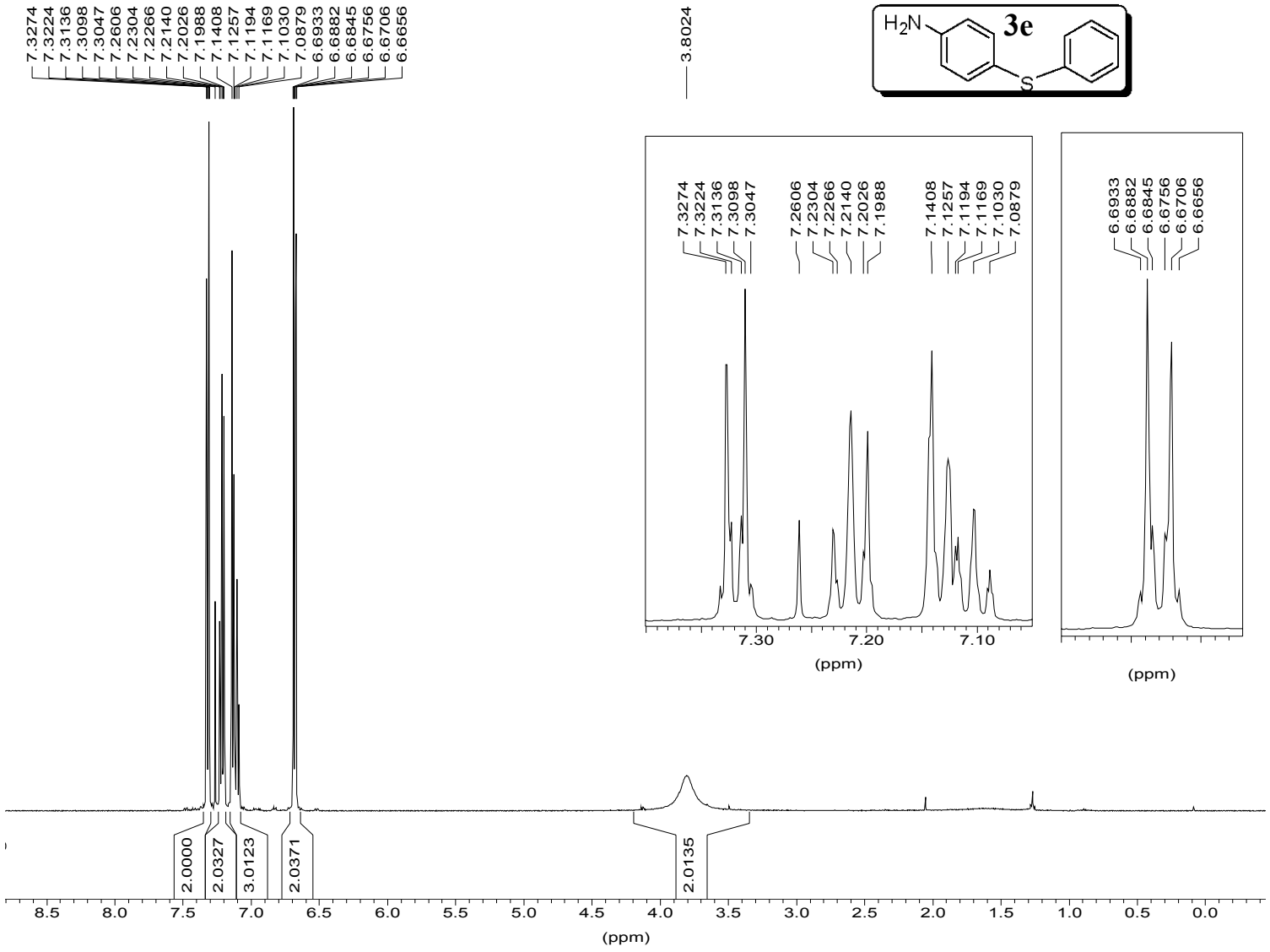
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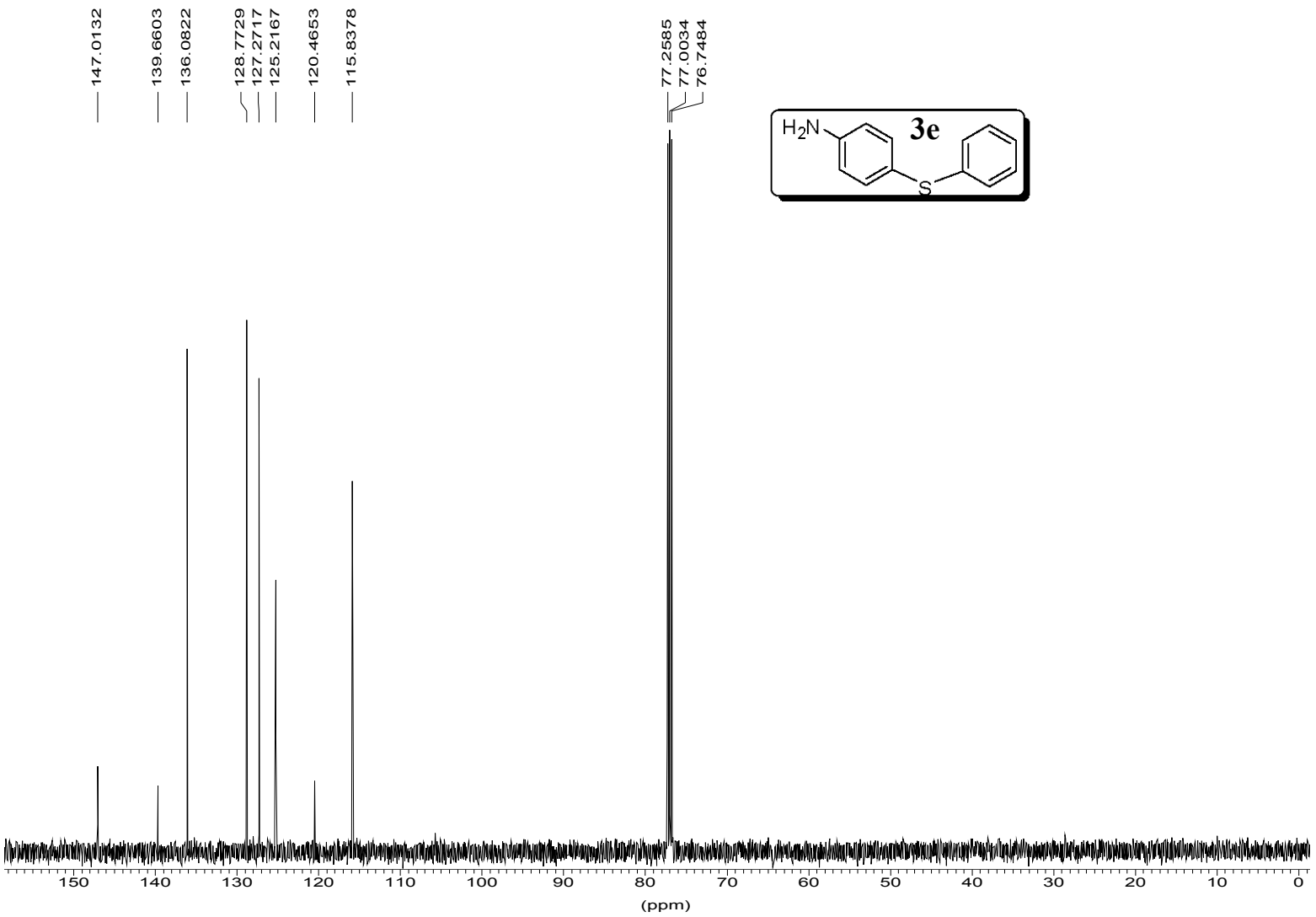
7.0879
6.6933
6.6882
6.6845
6.6756
6.6706
6.6656
3.8024
H2N
3e
S
7.30
7.20
7.10
(ppm)
(ppm)
2.0000
2.0327
3.0123
2.0371
2.0135
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
(ppm)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136.0822
128.7729
127.2717
125.2167
120.4653
115.8378
77.2585
77.0034
76.7484
H2N
S
3e
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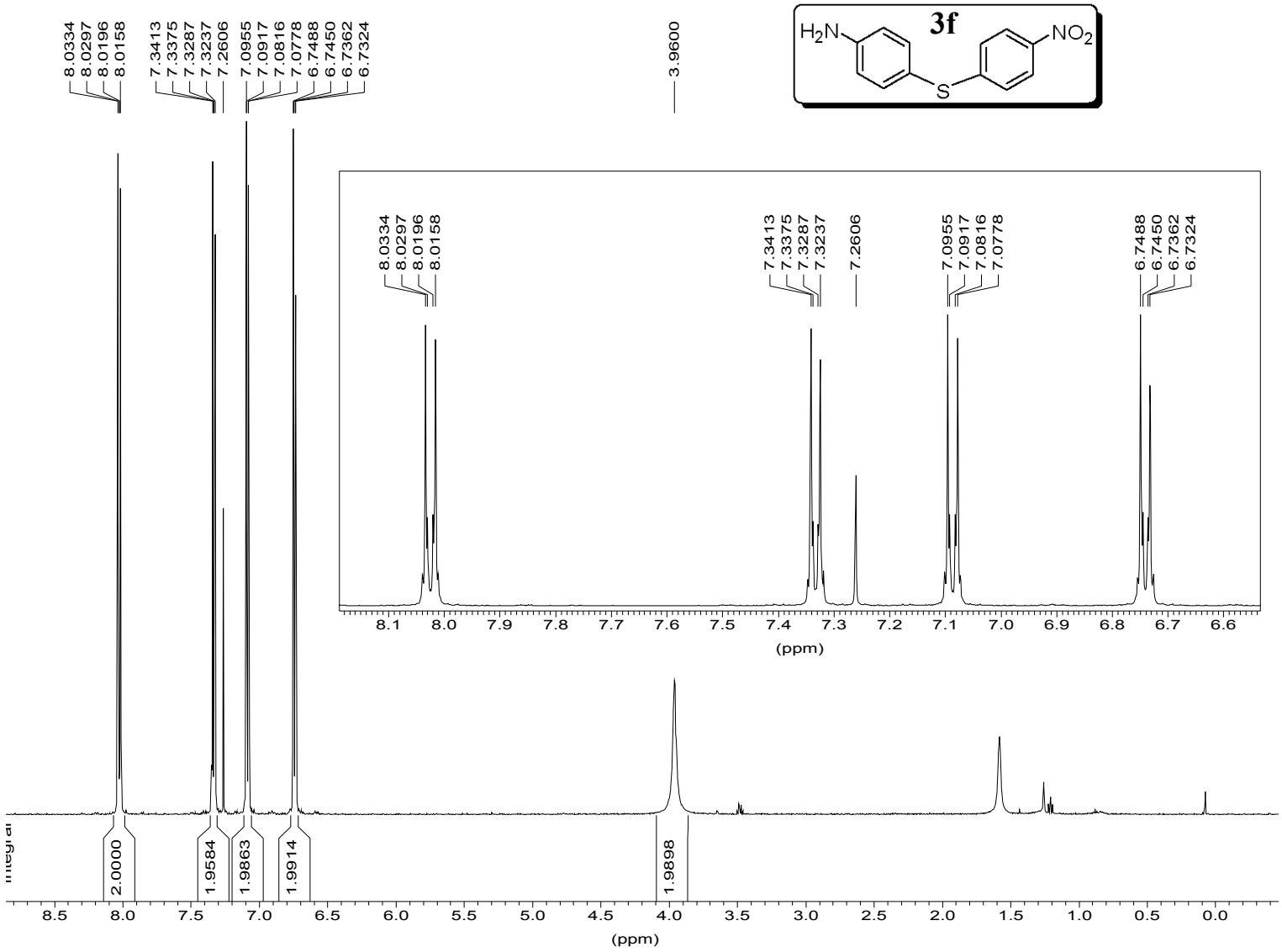
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
(ppm)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H_2N
NO_2
S
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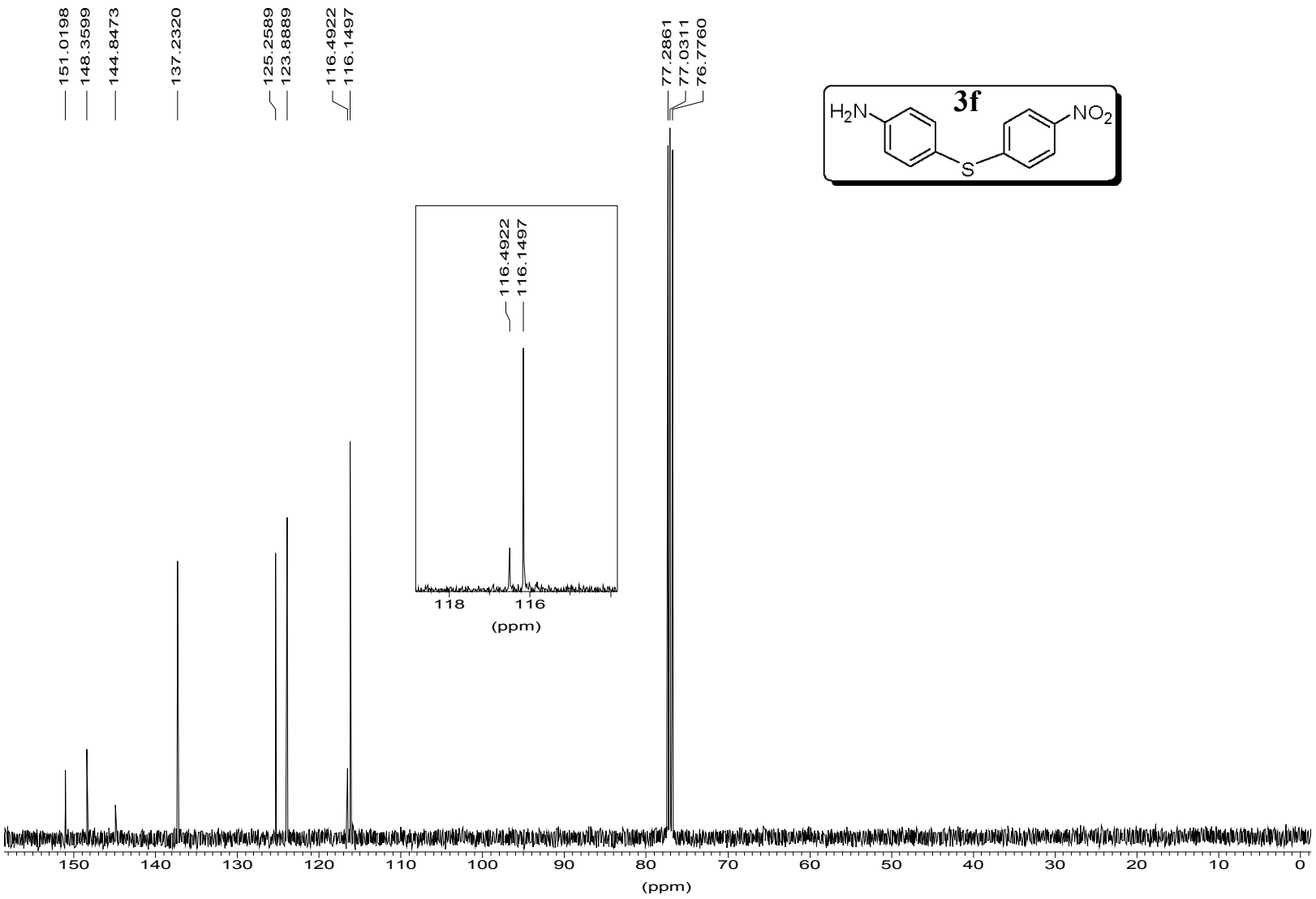
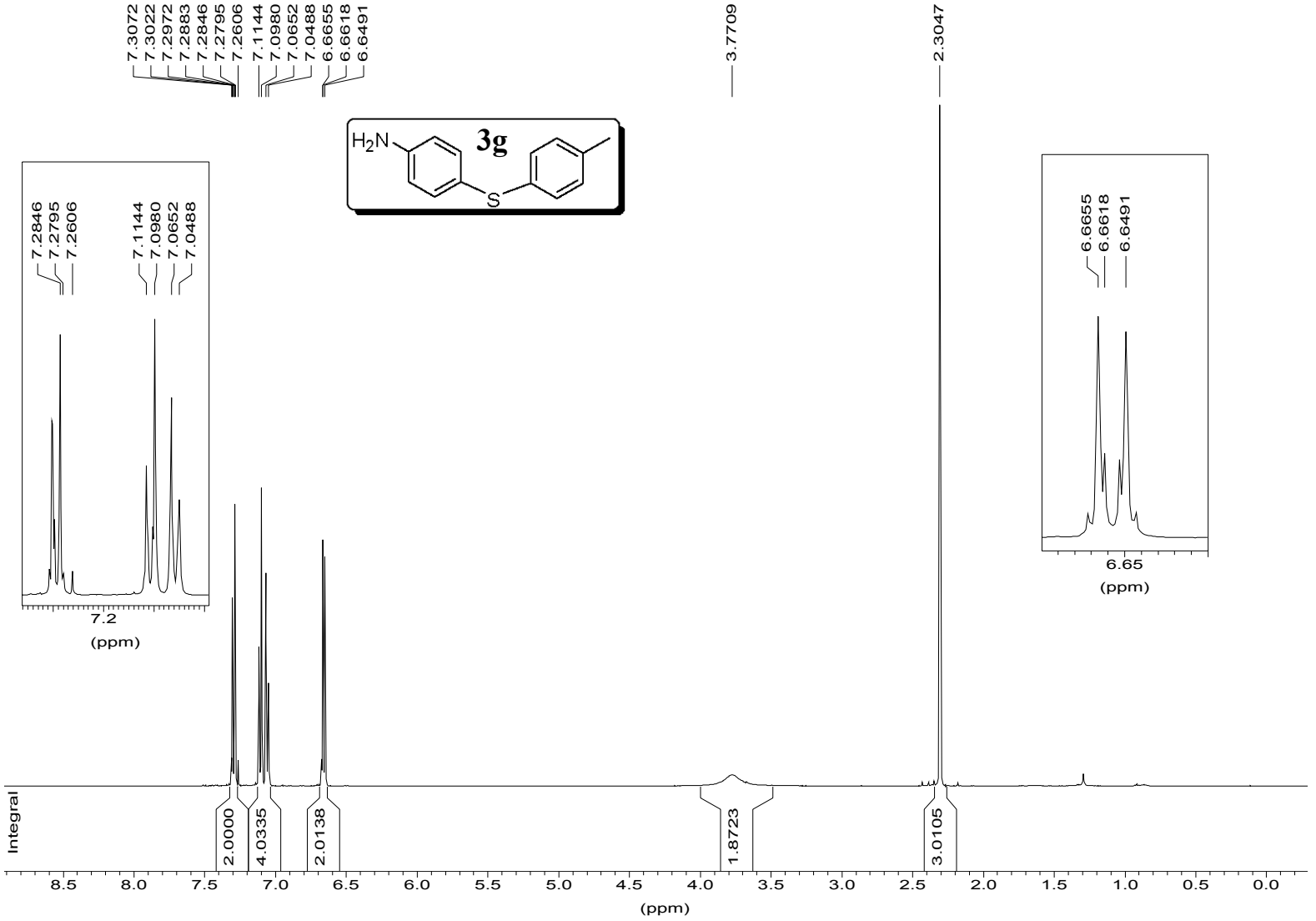
8.0297
8.0196
8.0158
7.3413
7.3375
7.3287
7.3237
7.2606
7.0955
7.0917
7.0816
7.0778
6.7488
6.7450
6.7362
6.7324
3.9600
2.0000
1.9584
1.9863
1.9914
1.9898
(ppm)


151.0198
148.3599
144.8473
137.2320
125.2589
123.8889
116.4922
116.1497
77.2861
77.0311
76.7760
3f
H2N
NO2
S
116.4922
116.1497
118
116
(ppm)
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
(ppm)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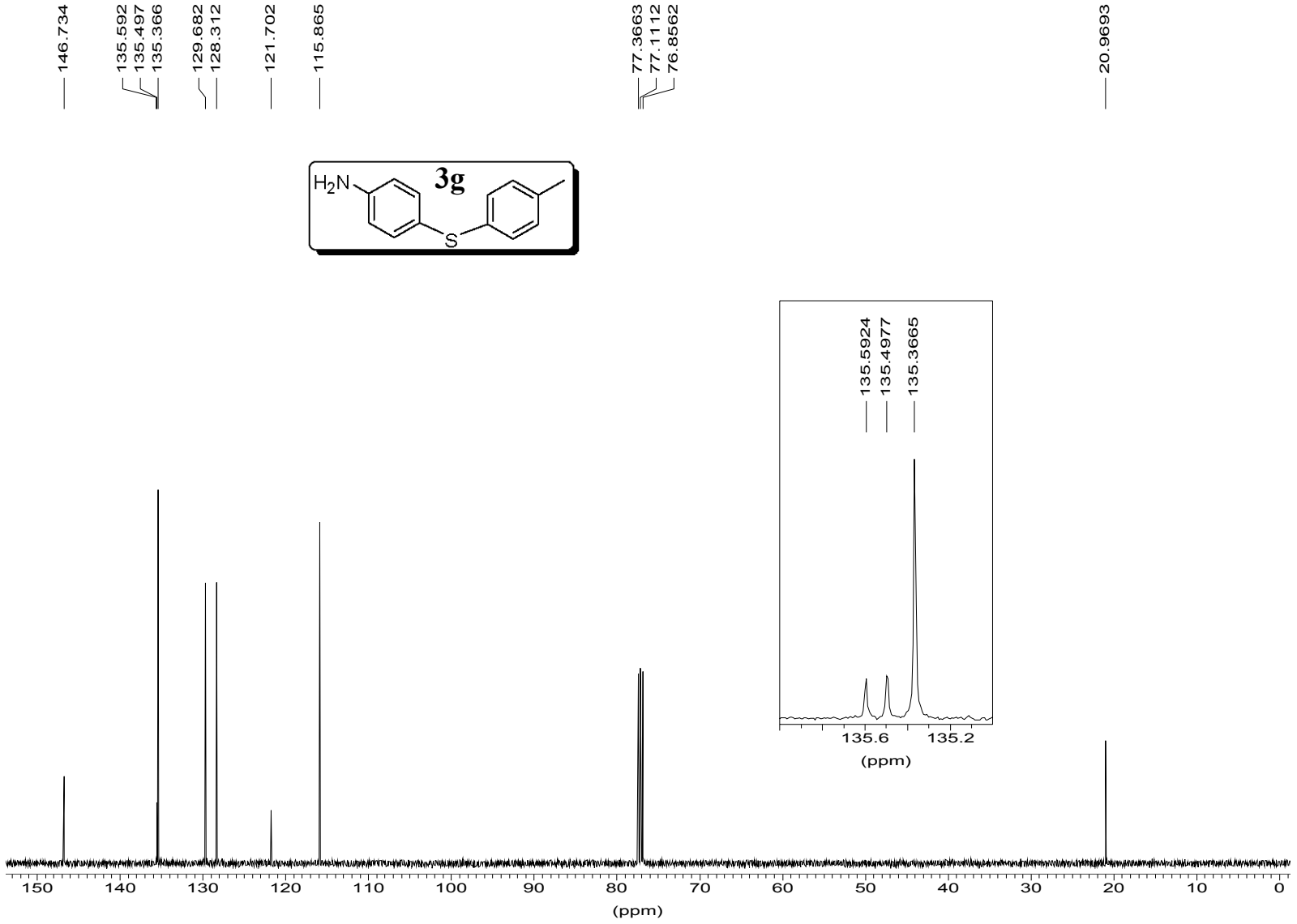
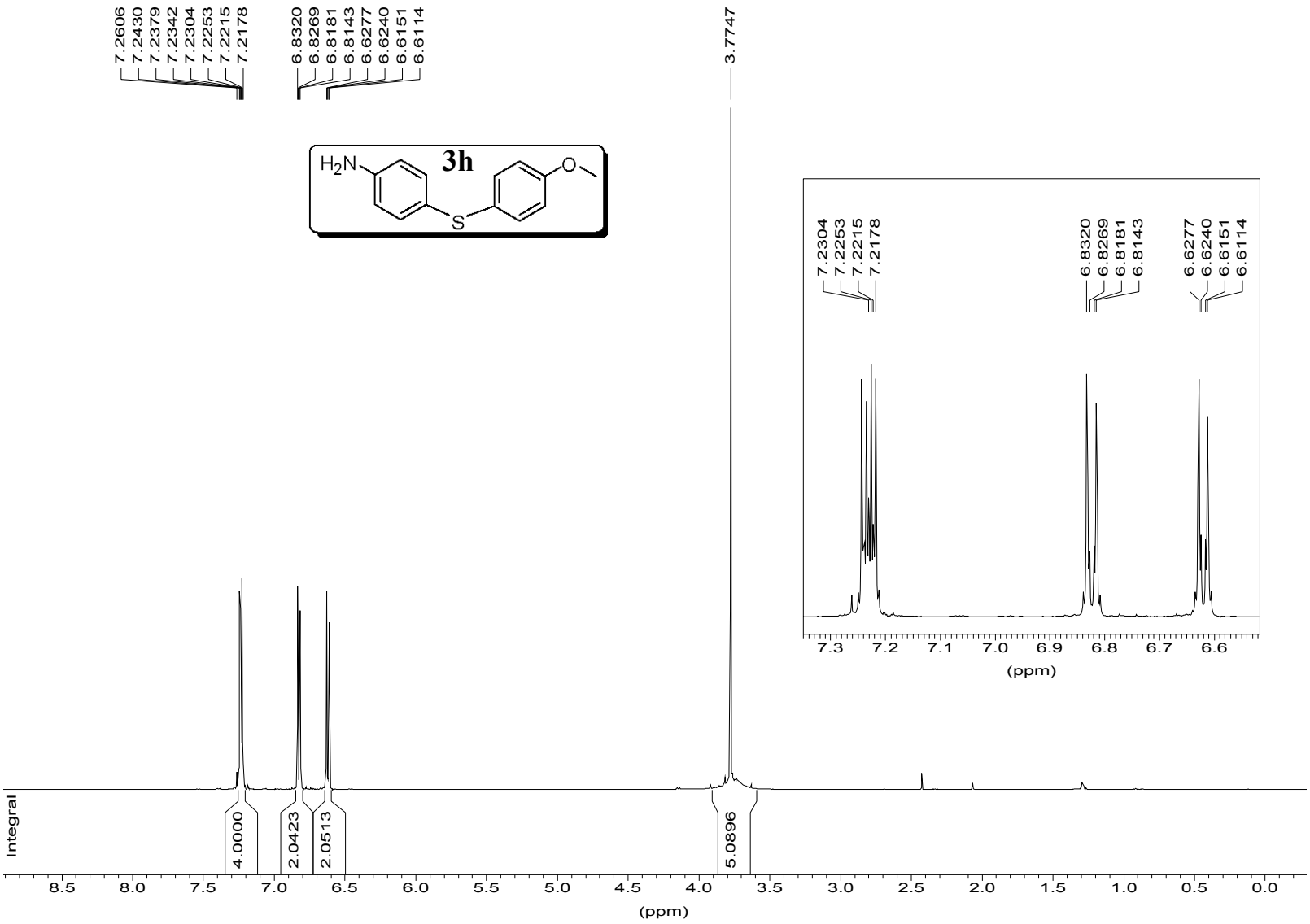
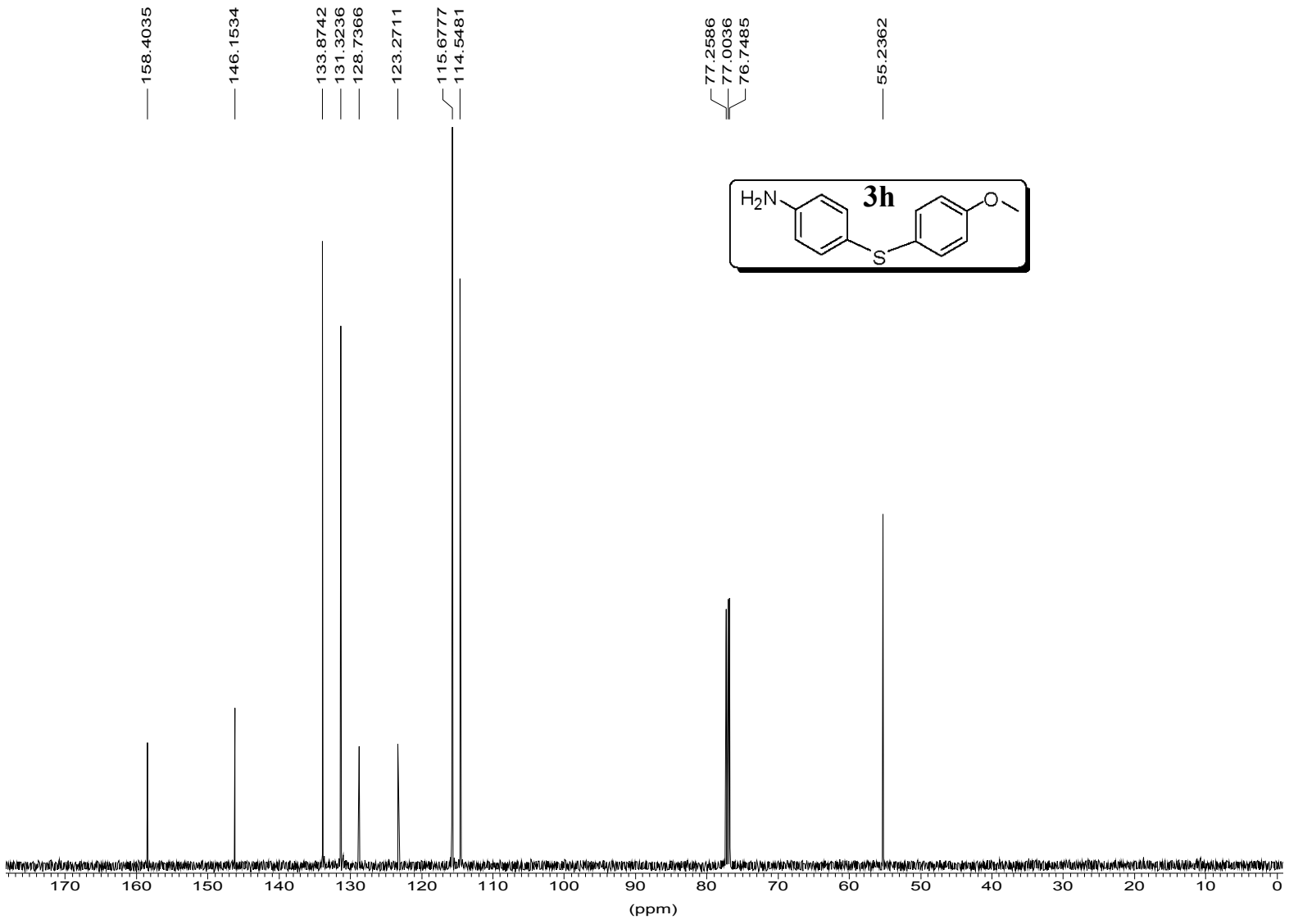
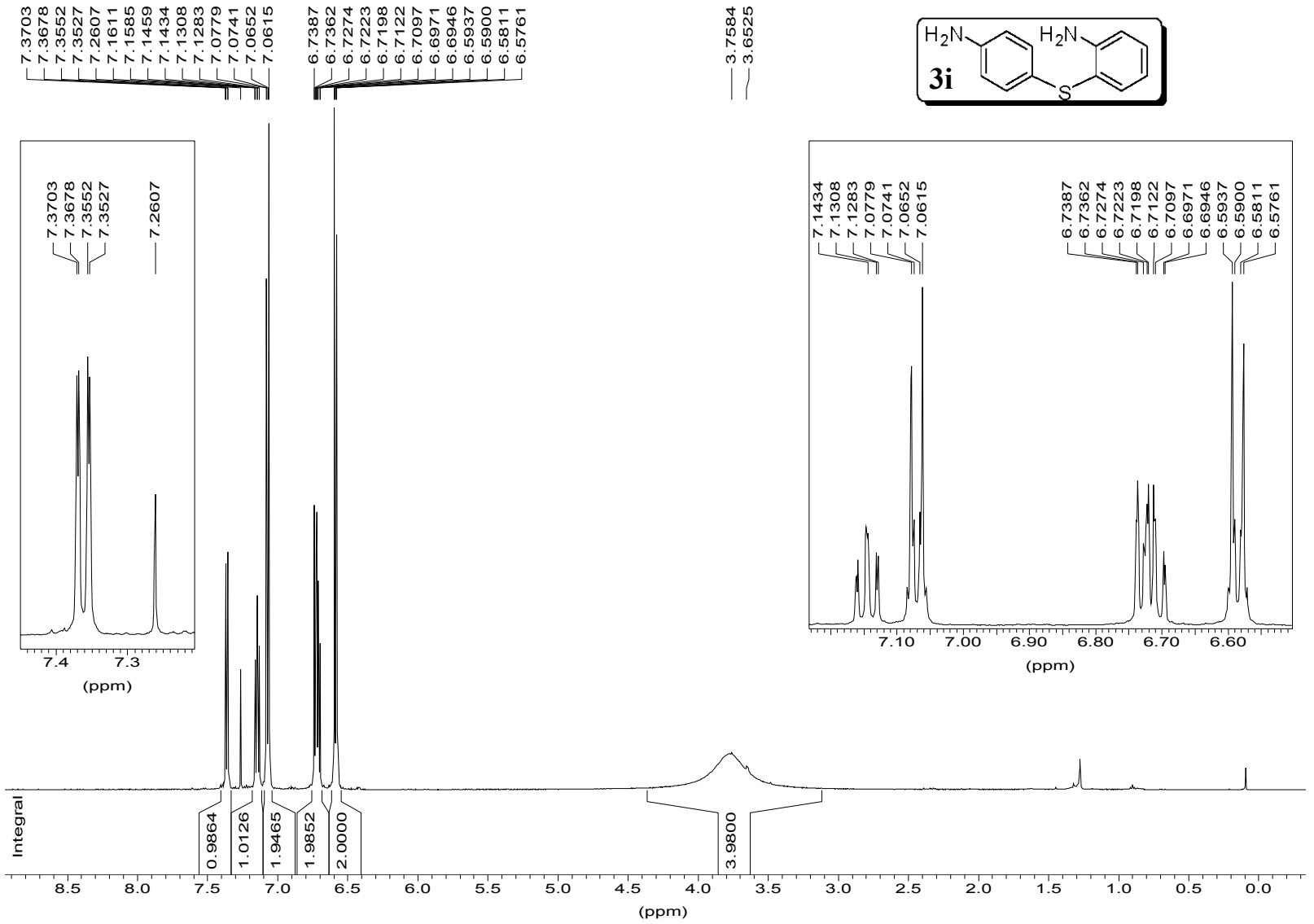
7.3022
7.2972
7.2883
7.2846
7.2795
7.2606
7.1144
7.0980
7.0652
7.0488
6.6655
6.6618
6.6491
3.7709
2.3047
3g
H2N
S
7.2
(ppm)
6.65
(ppm)
Integral
2.0000
4.0335
2.0138
1.8723
3.0105
(ppm)


146.734
135.592
135.497
135.366
129.682
128.312
121.702
115.865
77.3663
77.1112
76.8562
20.9693
3g
H2N
S
135.5924
135.4977
135.3665
135.6
135.2
(ppm)
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
(ppm)


7.2606
7.2430
7.2379
7.2342
7.2304
7.2253
7.2215
7.2178
6.8320
6.8269
6.8181
6.8143
6.6277
6.6240
6.6151
6.6114
3.7747
3h
H2N
O
S
Integral
4.0000
2.0423
2.0513
5.0896
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
(ppm)
7.3 7.2 7.1 7.0 6.9 6.8 6.7 6.6
(ppm)


158.4035
146.1534
133.8742
131.3236
128.7366
123.2711
115.6777
114.5481
77.2586
77.0036
76.7485
55.2362
3h
H2N
O
S
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
(ppm)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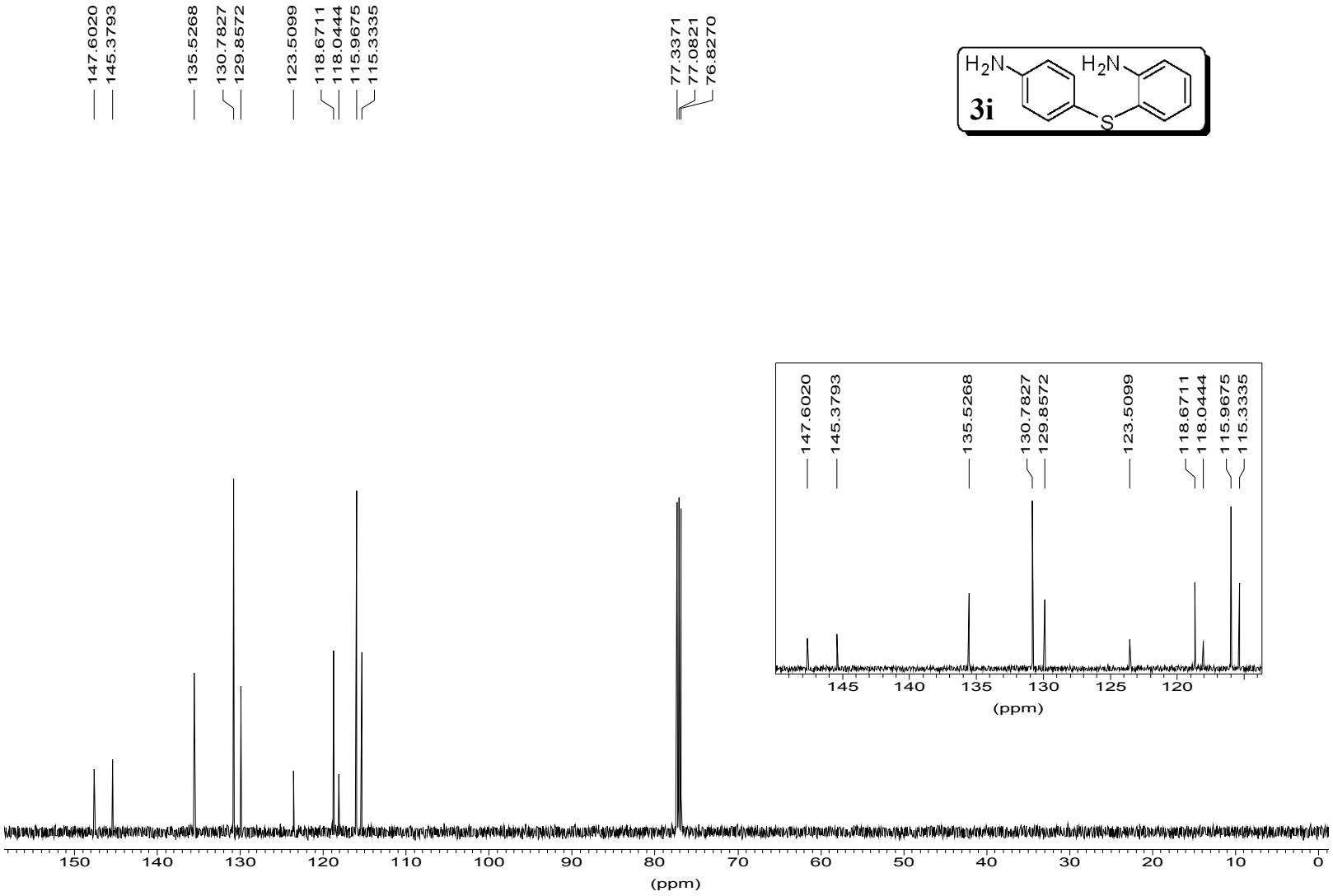
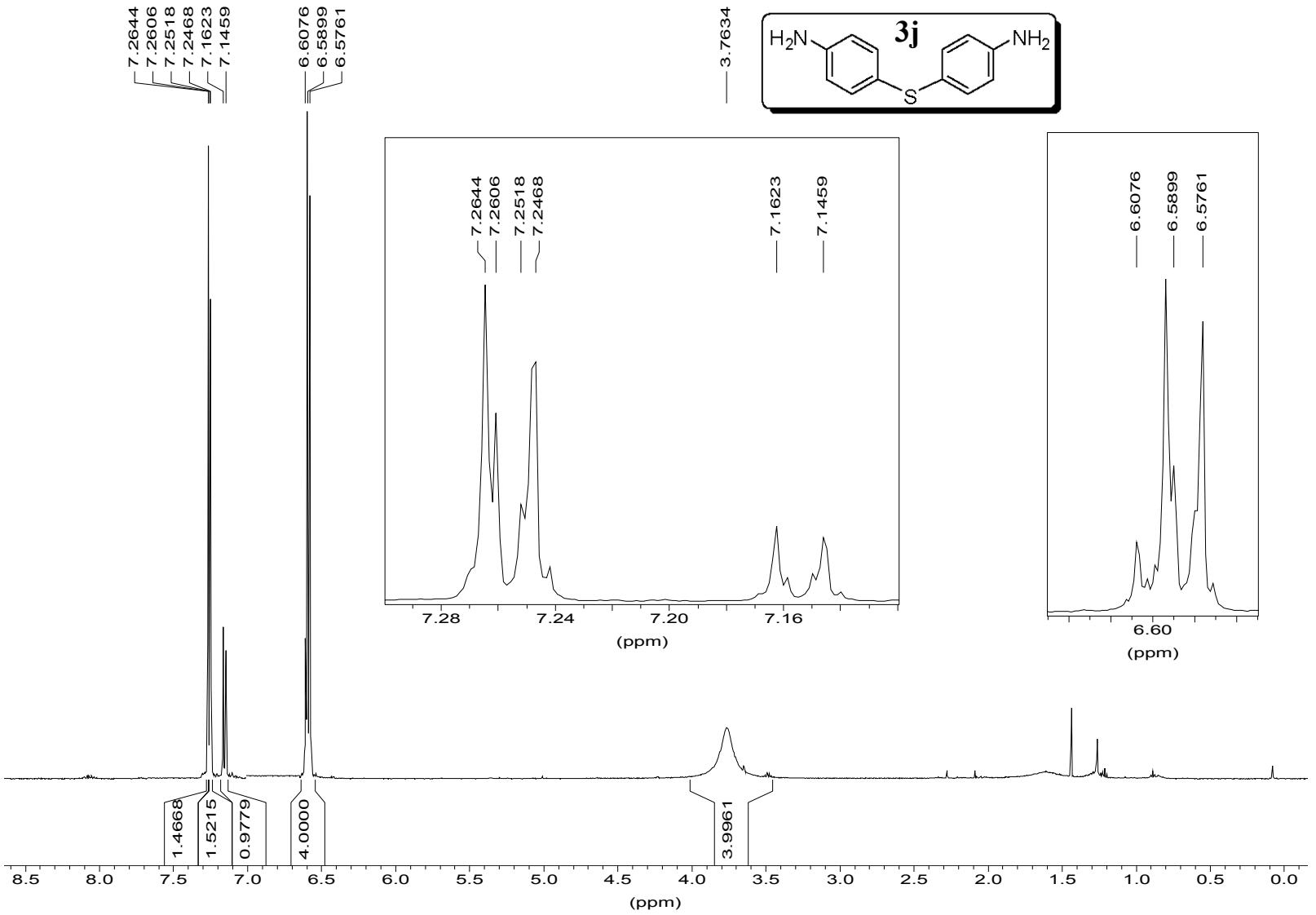
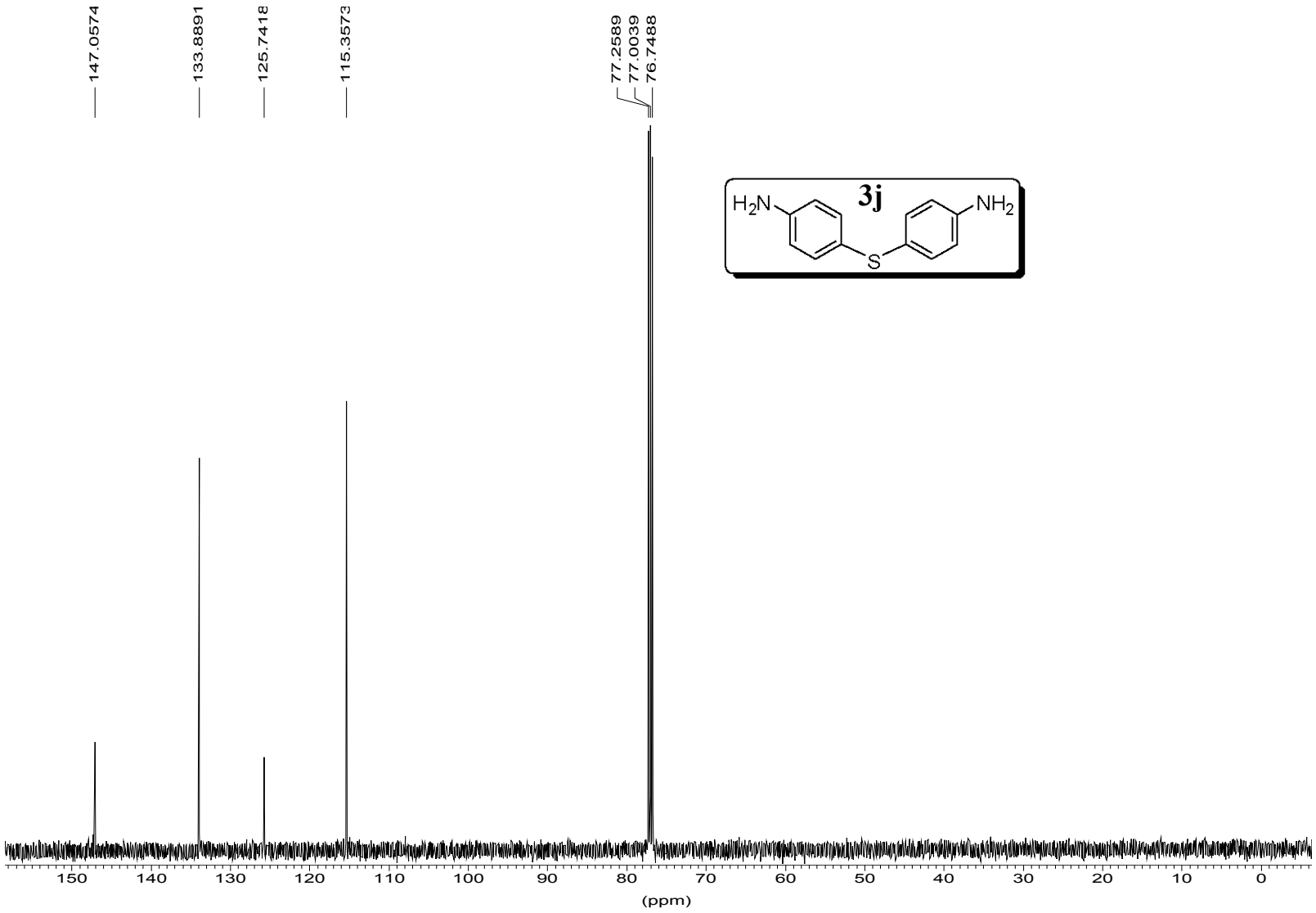
7.3678
7.3552
7.3527
7.2607
7.1611
7.1585
7.1459
7.1434
7.1308
7.1283
7.0779
7.0741
7.0652
7.0615
6.7387
6.7362
6.7274
6.7223
6.7198
6.7122
6.7097
6.6971
6.6946
6.5937
6.5900
6.5811
6.5761
3.7584
3.6525
3i
Integral
0.9864
1.0126
1.9465
1.9852
2.0000
3.9800
(ppm)


147.6020
145.3793
135.5268
130.7827
129.8572
123.5099
118.6711
118.0444
115.9675
115.3335
77.3371
77.0821
76.8270
H2N
H2N
S
3i
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
(ppm)
145
140
135
130
125
120
(ppm)


7.2644
7.2606
7.2518
7.2468
7.1623
7.1459
6.6076
6.5899
6.5761
3.7634
3j
H2N
NH2
S
7.28
7.24
7.20
7.16
(ppm)
6.60
(ppm)
1.4668
1.5215
0.9779
4.0000
3.9961
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
(ppm)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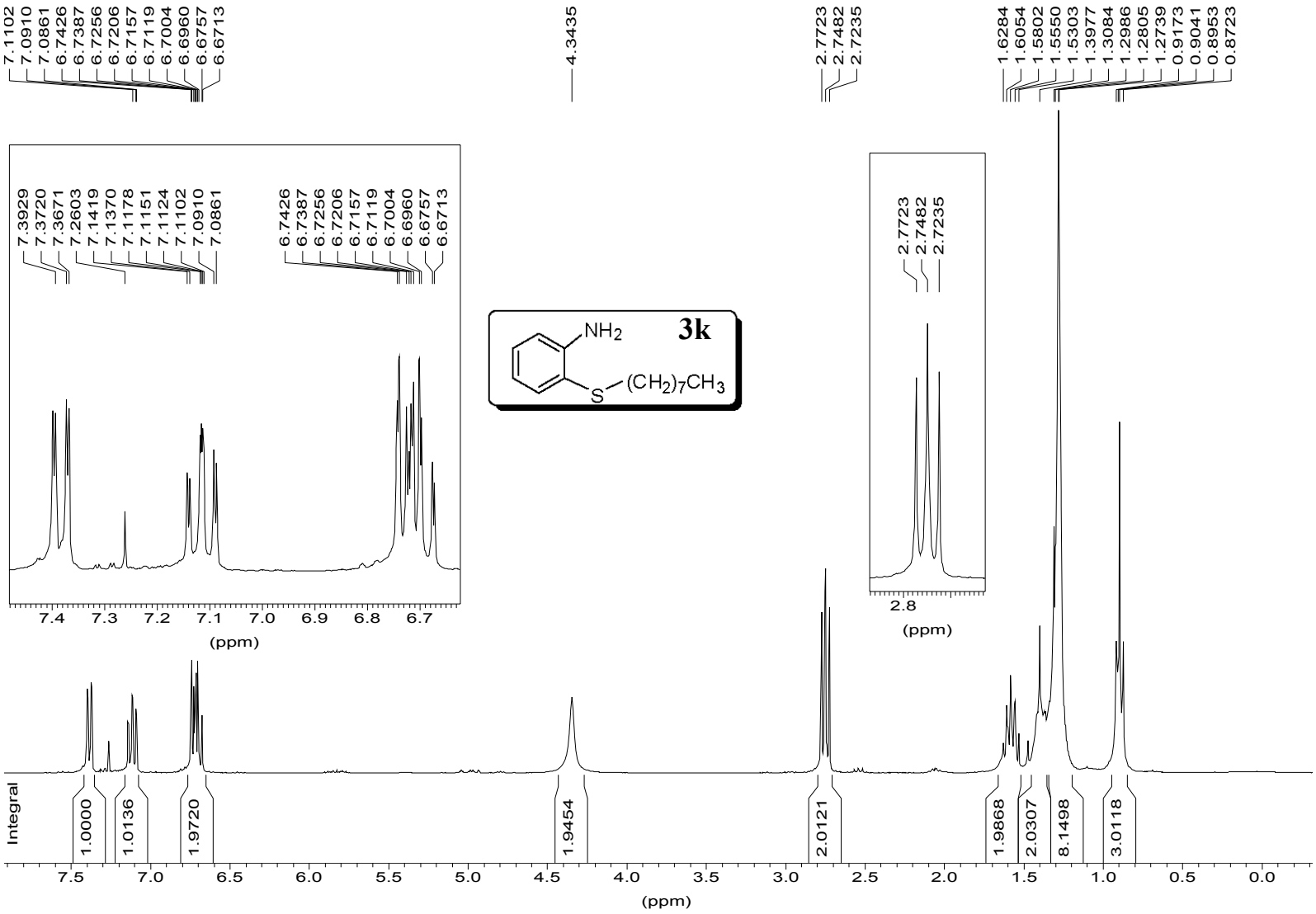
133.8891
125.7418
115.3573
77.2589
77.0039
76.7488
3j
H2N
NH2
S
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
(ppm)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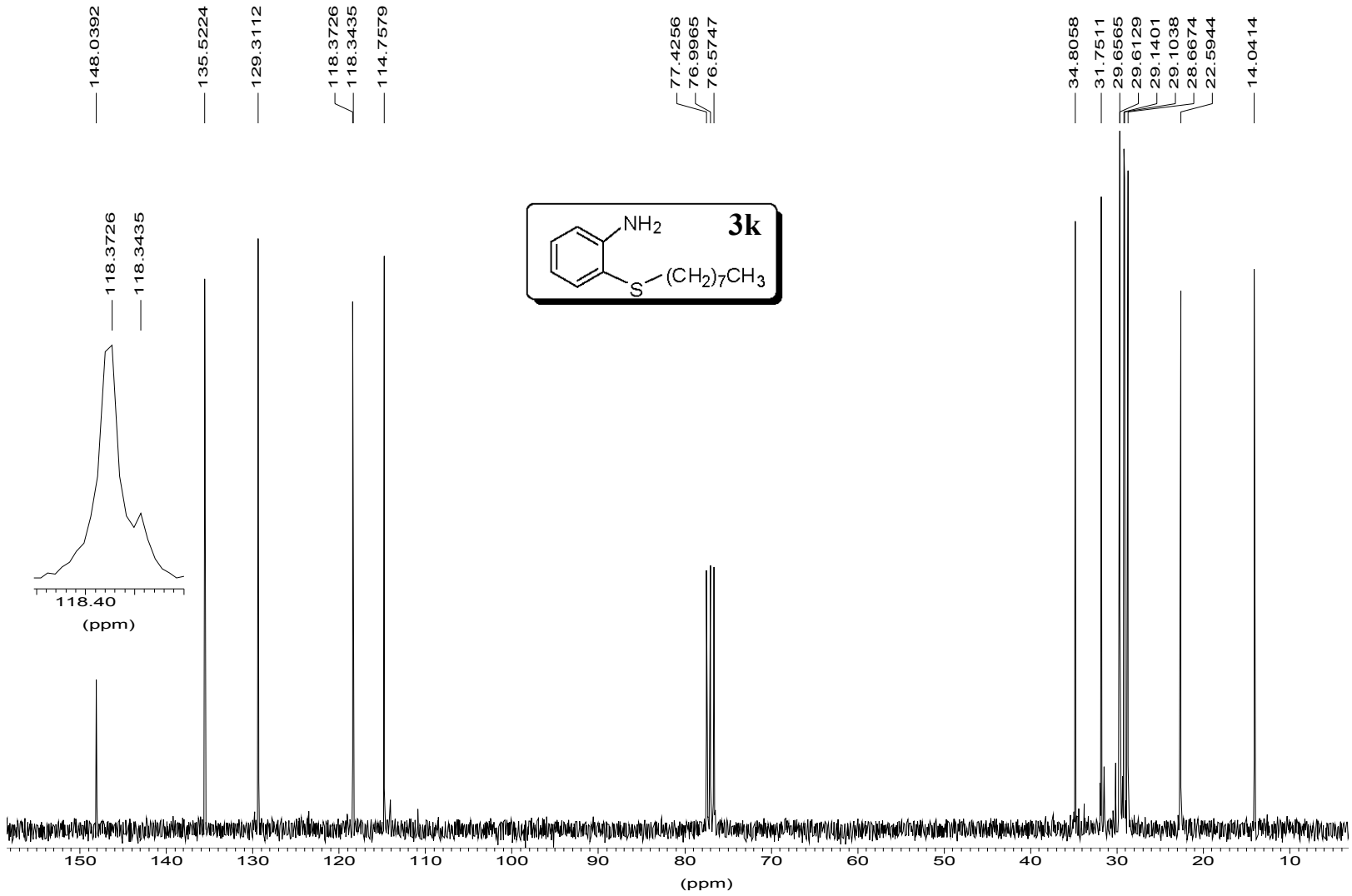
7.0861
6.7426
6.7387
6.7256
6.7206
6.7157
6.7119
6.7004
6.6960
6.6757
6.6713
4.3435
2.7723
2.7482
2.7235
1.6284
1.6054
1.5802
1.5550
1.5303
1.3977
1.3084
1.2986
1.2805
1.2739
0.9173
0.9041
0.8953
0.8723
7.3929
7.3720
7.3671
7.2603
7.1419
7.1370
7.1178
7.1151
7.1124
7.1102
7.0910
7.0861
6.7426
6.7387
6.7256
6.7206
6.7157
6.7119
6.7004
6.6960
6.6757
6.6713
7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7
(ppm)
2.7723
2.7482
2.7235
2.8
(ppm)
NH2
3k
S
(CH2)7CH3
Integral
1.0000
1.0136
1.9720
1.9454
2.0121
1.9868
2.0307
8.1498
3.0118
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
(ppm)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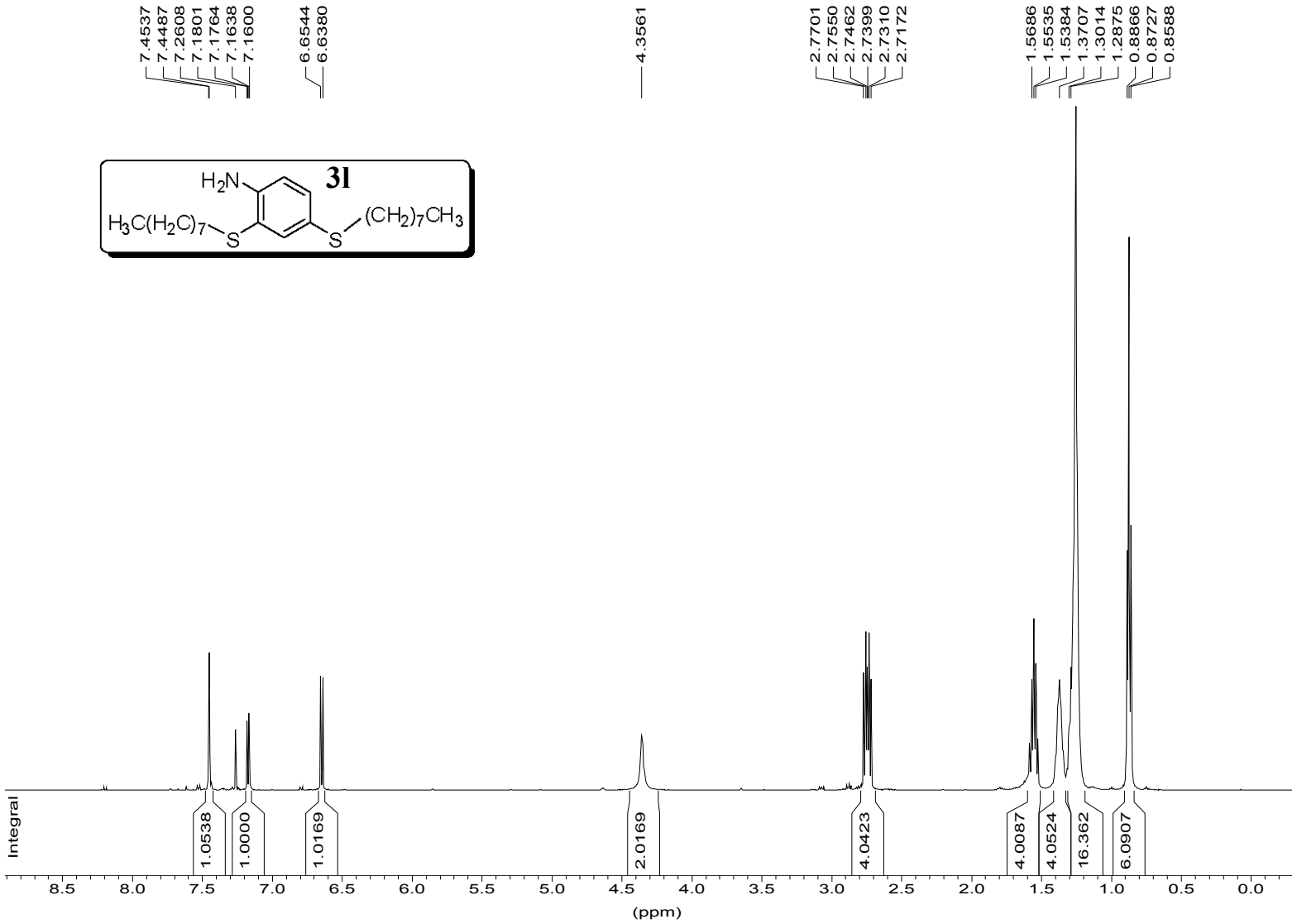
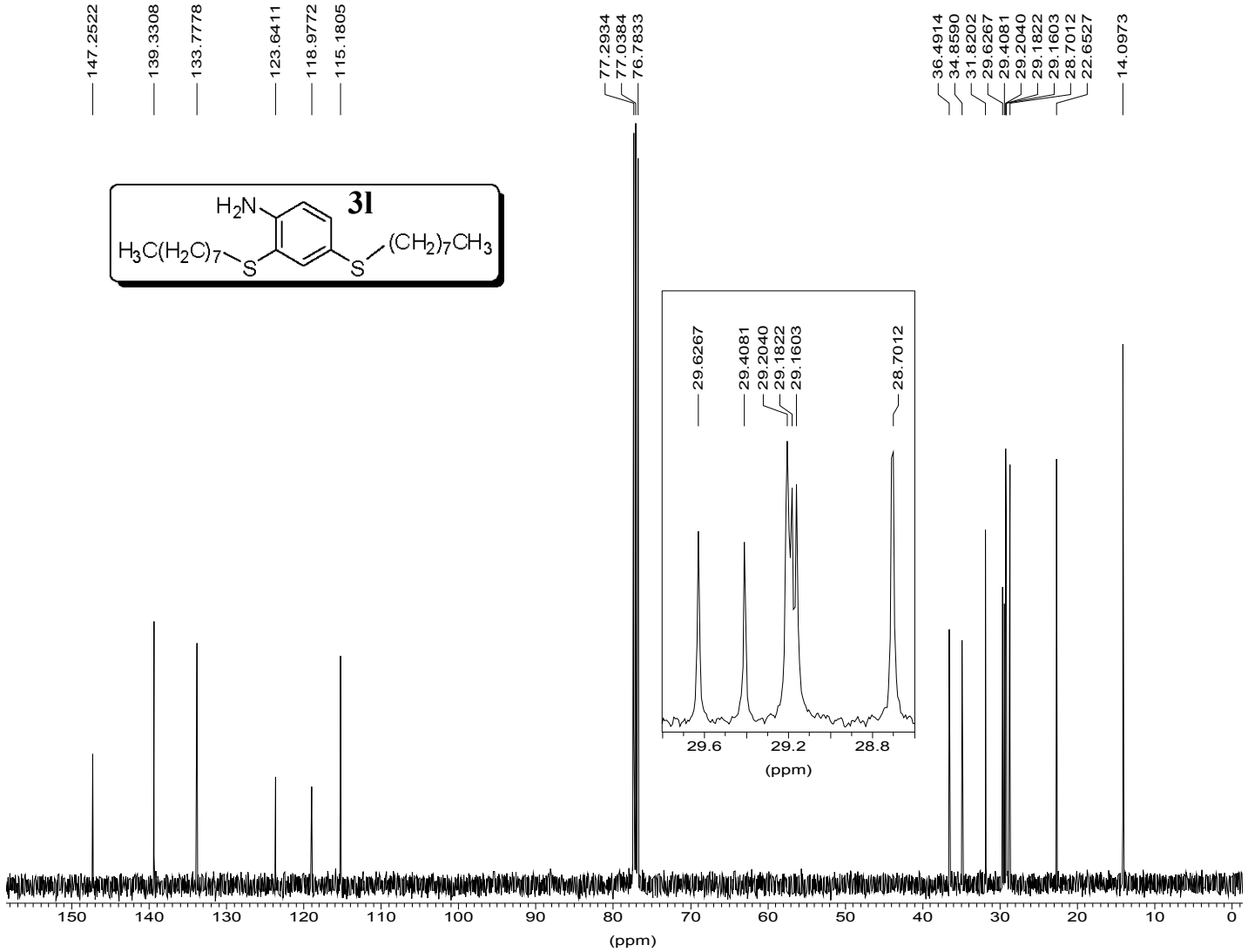
135.5224
129.3112
118.3726
118.3435
114.7579
77.4256
76.9965
76.5747
34.8058
31.7511
29.6565
29.6129
29.1401
29.1038
28.6674
22.5944
14.0414
3k
NH2
S
(CH2)7CH3
118.40
(ppm)
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
(ppm)


7.4537
7.4487
7.2608
7.1801
7.1764
7.1638
7.1600
6.6544
6.6380
4.3561
2.7701
2.7550
2.7462
2.7399
2.7310
2.7172
1.5686
1.5535
1.5384
1.3707
1.3014
1.2875
0.8866
0.8727
0.8588
3l
H2N
H3C(H2C)7
S
S
(CH2)7CH3
Integral
1.0538
1.0000
1.0169
2.0169
4.0423
4.0087
4.0524
16.362
6.0907
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
(ppm)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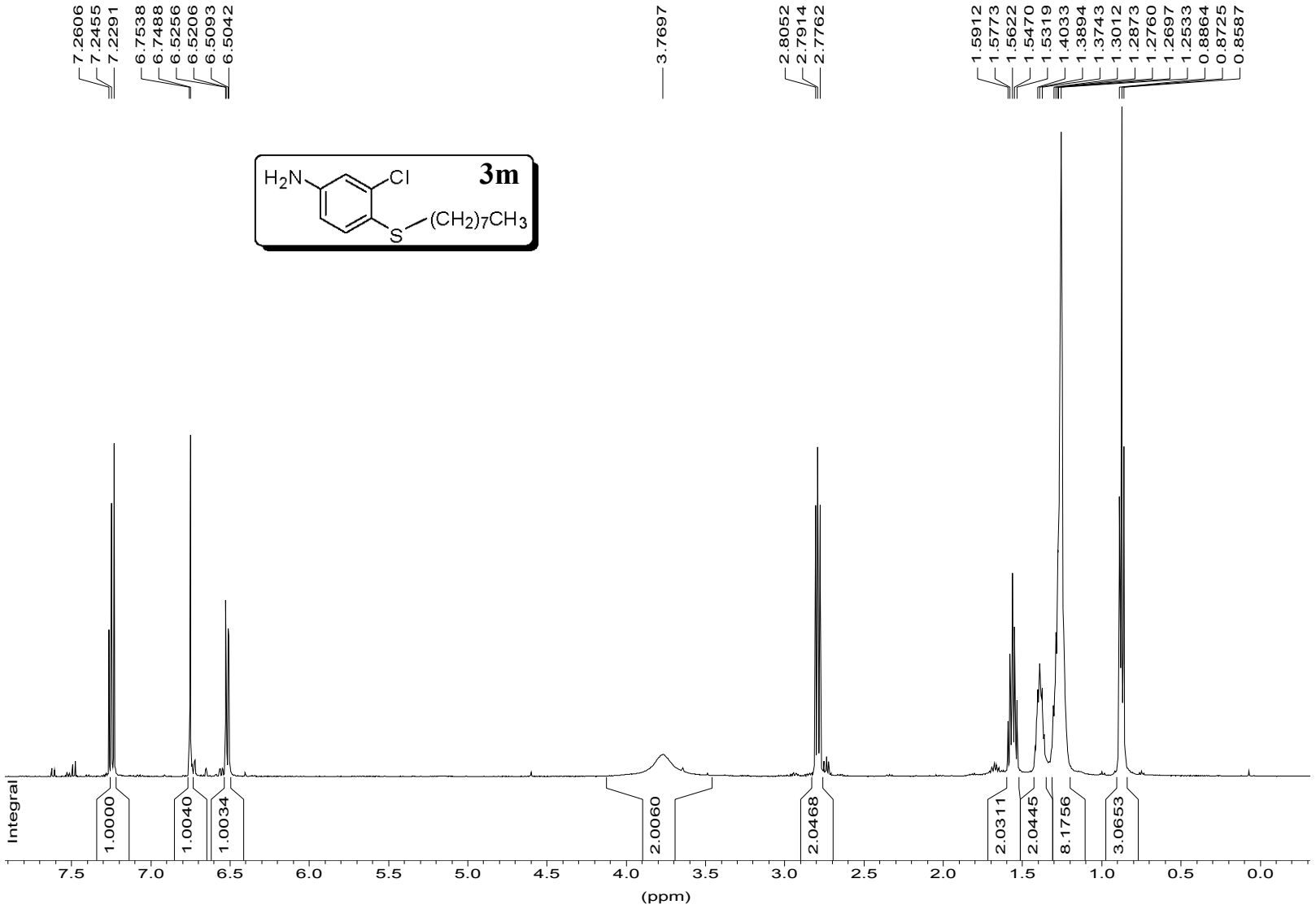
133.7778
123.6411
118.9772
115.1805
77.2934
77.0384
76.7833
36.4914
34.8590
31.8202
29.6267
29.4081
29.2040
29.1822
29.1603
28.7012
22.6527
14.0973
3l
H2N
H3C(H2C)7
S
S
(CH2)7CH3
29.6267
29.4081
29.2040
29.1822
29.1603
28.7012
29.6
29.2
28.8
(ppm)
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
(ppm)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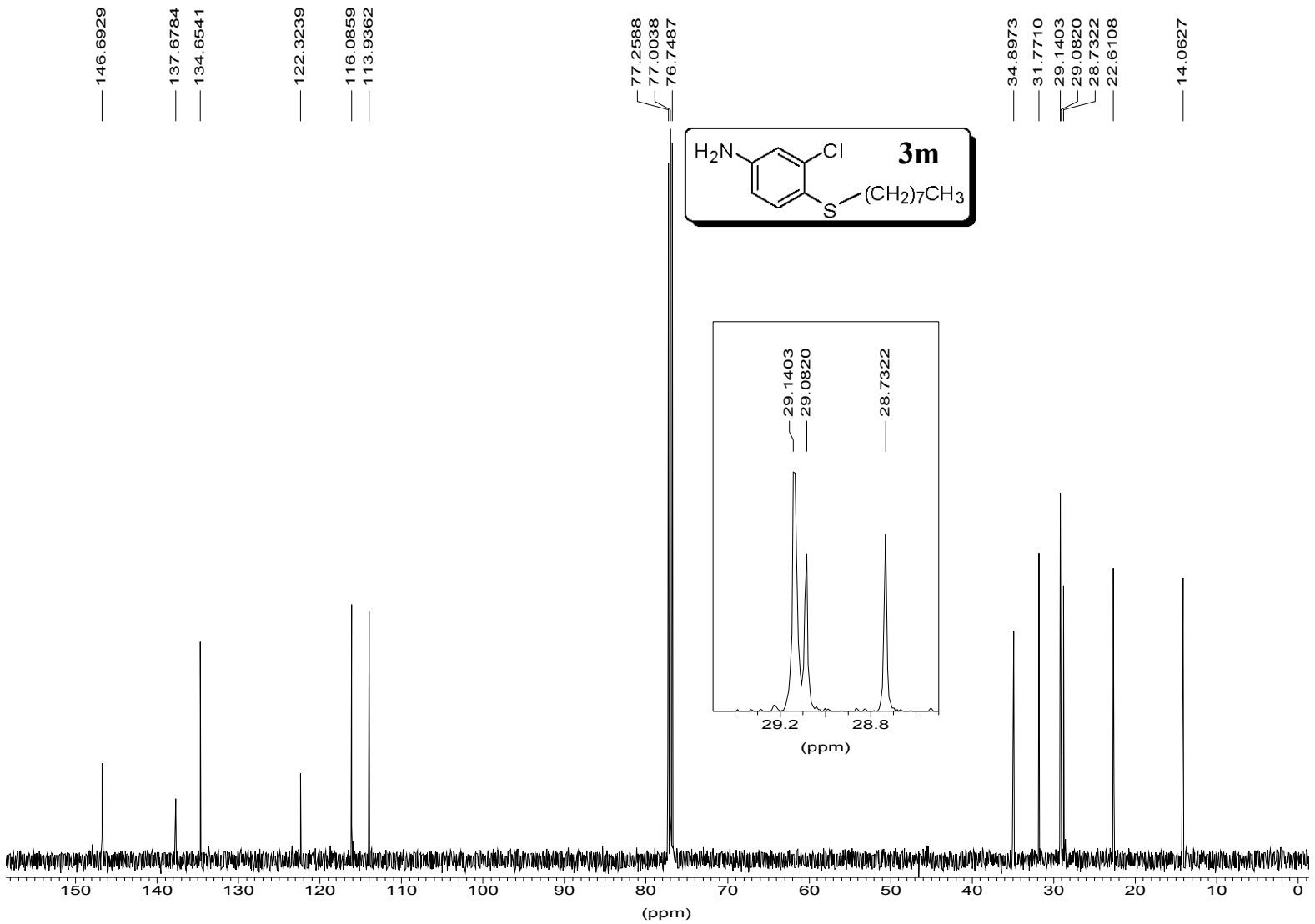
7.2291
6.7538
6.7488
6.5256
6.5206
6.5093
6.5042
3.7697
2.8052
2.7914
2.7762
1.5912
1.5773
1.5622
1.5470
1.5319
1.4033
1.3894
1.3743
1.3012
1.2873
1.2760
1.2697
1.2533
0.8864
0.8725
0.8587
H2N
Cl
S
(CH2)7CH3
3m
Integral
1.0000
1.0040
1.0034
2.0060
2.0468
2.0311
2.0445
8.1756
3.0653
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
(ppm)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77.2588
77.0038
76.7487
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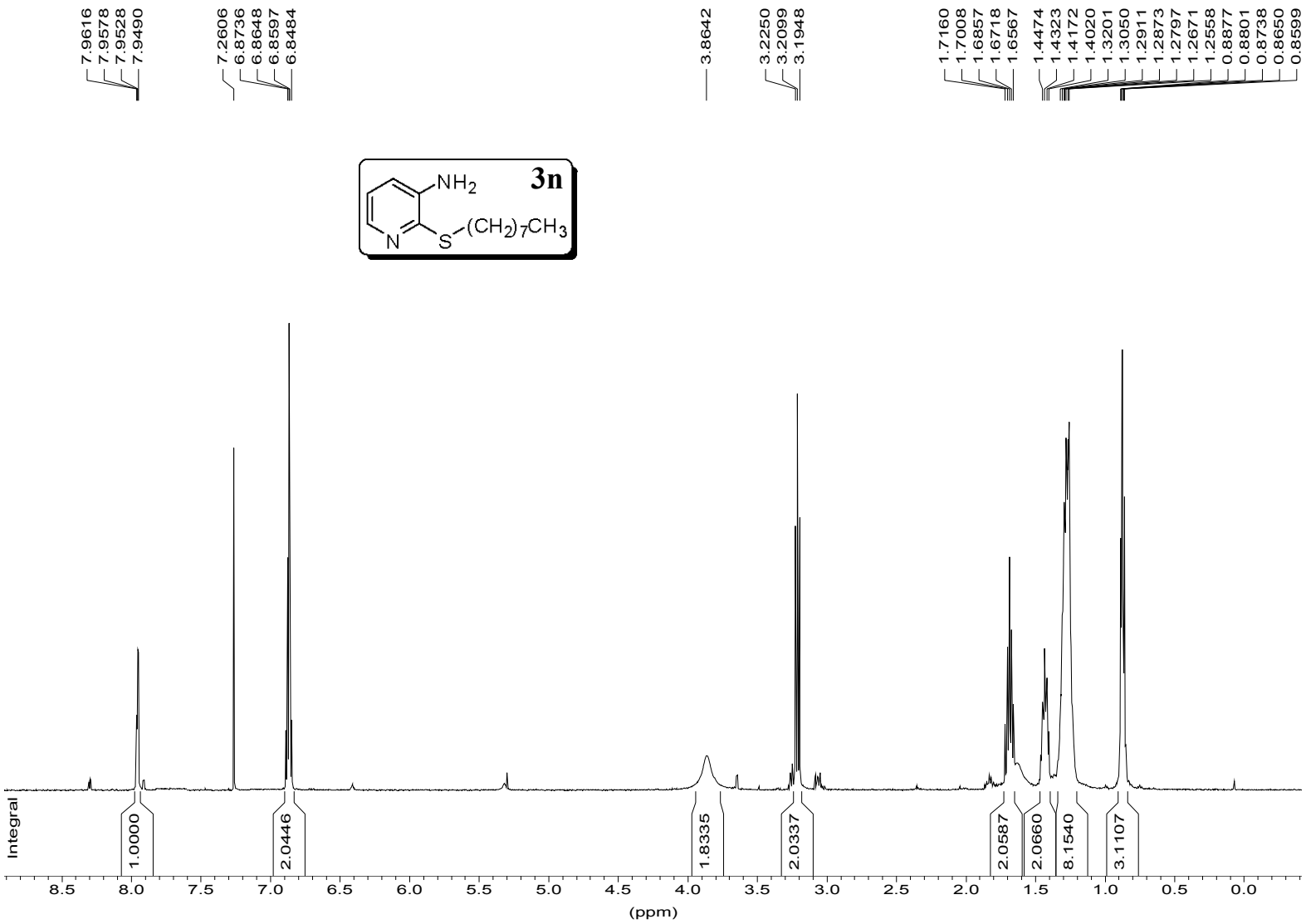
31.7710
29.1403
29.0820
28.7322
22.6108
14.0627
H2N
Cl
S
(CH2)7CH3
3m
29.1403
29.0820
28.7322
29.2
28.8
(ppm)
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
(ppm)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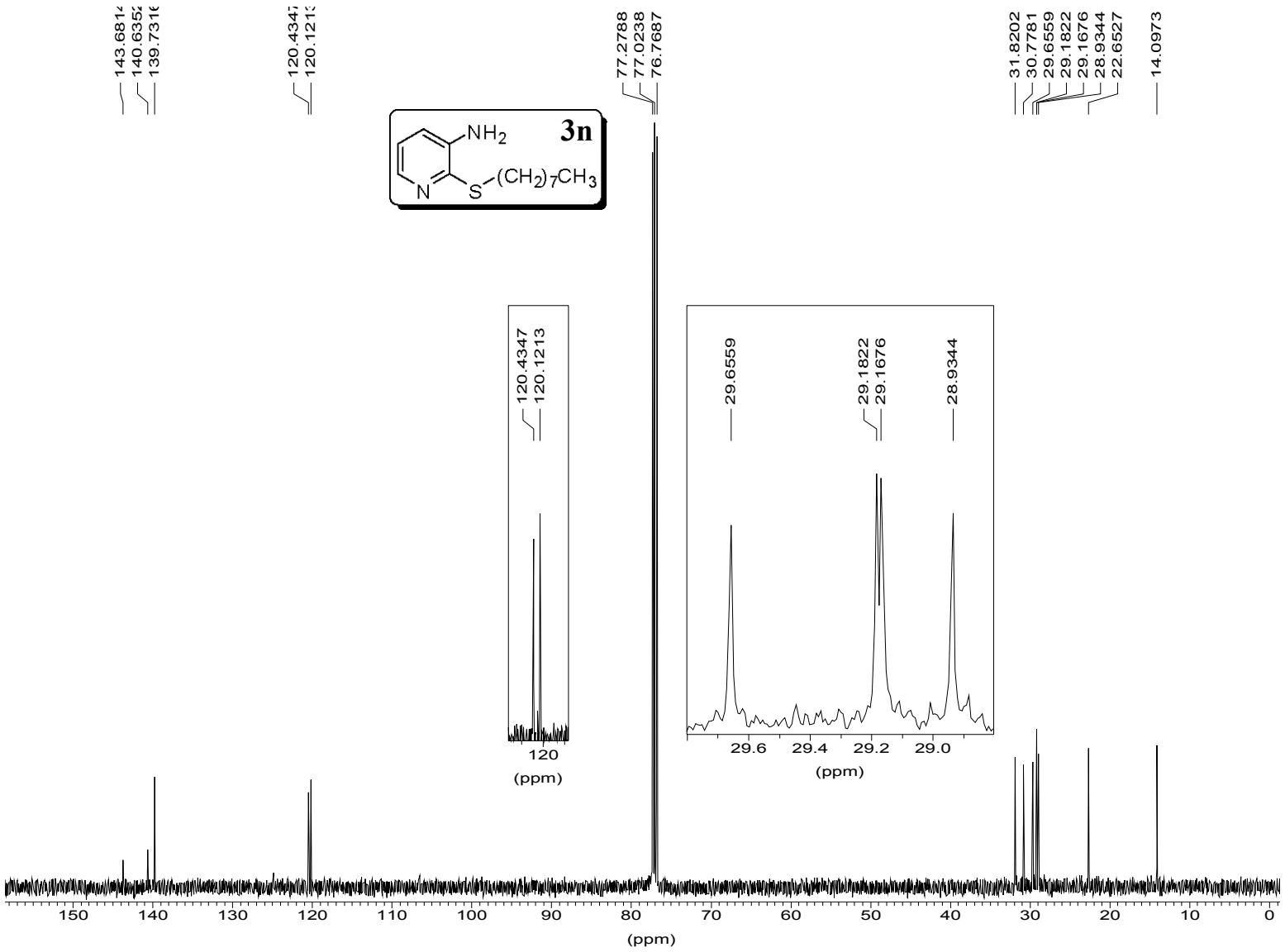
7.9578
7.9528
7.9490
7.2606
6.8736
6.8648
6.8597
6.8484
3.8642
3.2250
3.2099
3.1948
1.7160
1.7008
1.6857
1.6718
1.6567
1.4474
1.4323
1.4172
1.4020
1.3201
1.3050
1.2911
1.2873
1.2797
1.2671
1.2558
0.8877
0.8801
0.8738
0.8650
0.8599
NH2
3n
N
S
(CH2)7CH3
Integral
1.0000
2.0446
1.8335
2.0337
2.0587
2.0660
8.1540
3.1107
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
(ppm)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29.6559
29.1822
29.1676
28.9344
22.6527
14.0973
NH2
3n
N
S
(CH2)7CH3
120.4347
120.1213
120
(ppm)
29.6559
29.1822
29.1676
28.9344
29.6
29.4
29.2
29.0
(ppm)
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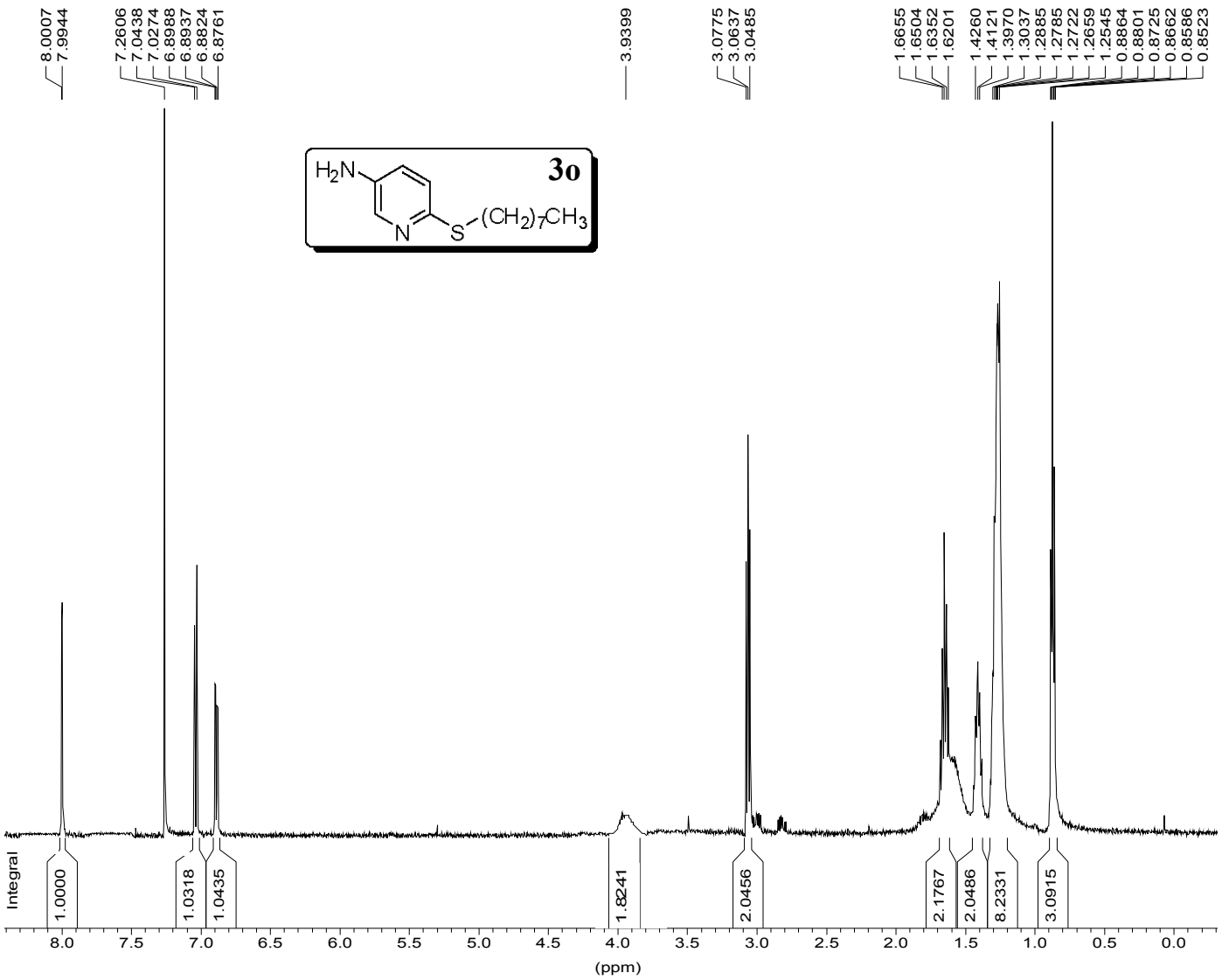
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
(ppm)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7.2606
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7.0274
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6.8937
6.8824
6.8761
3.9399
3.0775
3.0637
3.0485
1.6655
1.6504
1.6352
1.6201
1.4260
1.4121
1.3970
1.3037
1.2885
1.2785
1.2722
1.2659
1.2545
0.8864
0.8801
0.8725
0.8662
0.8586
0.8523
3o
Integral
1.0000
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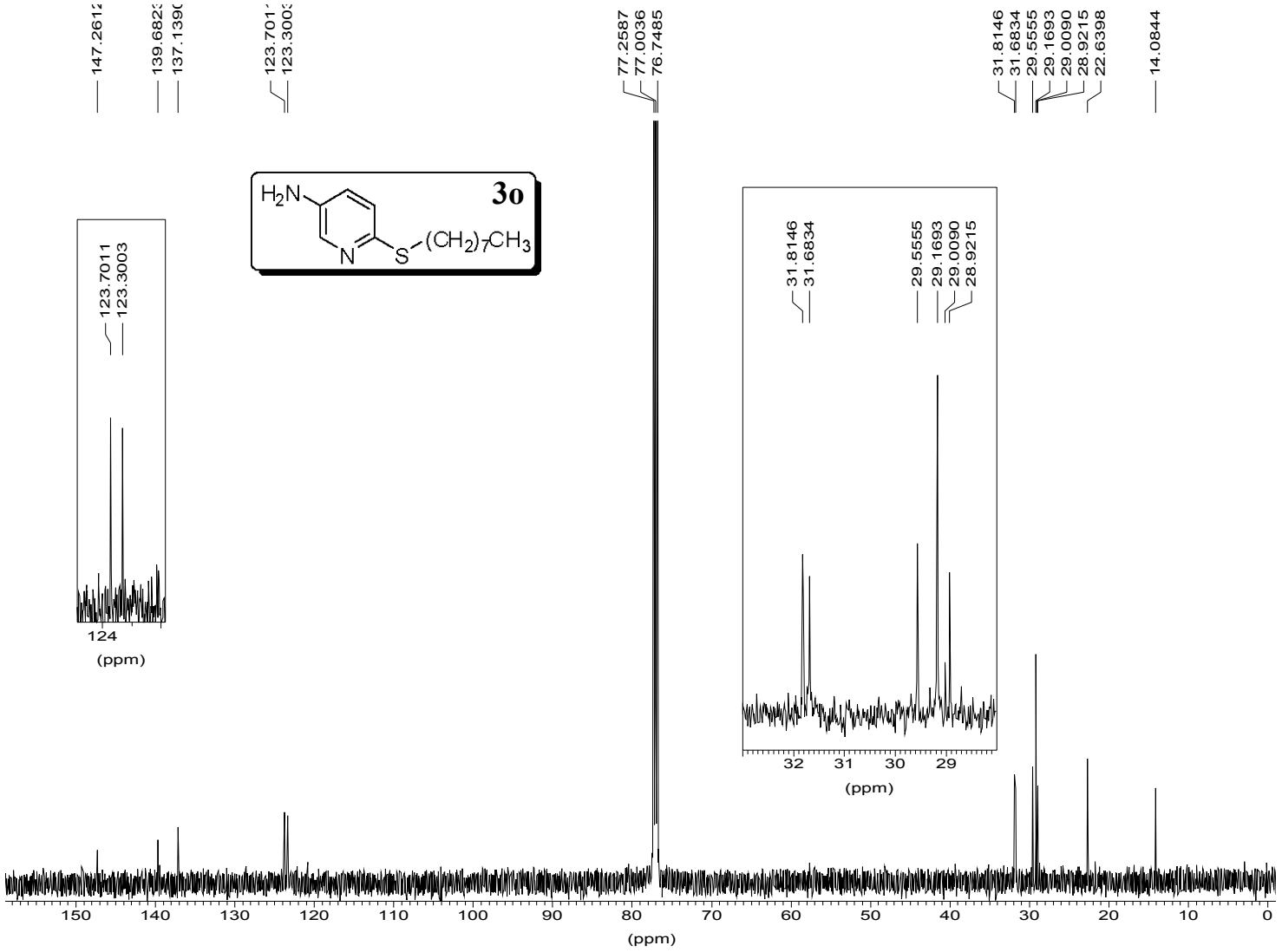
1.0435
1.8241
2.0456
2.1767
2.0486
8.2331
3.0915
(ppm)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137.1396
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123.3003
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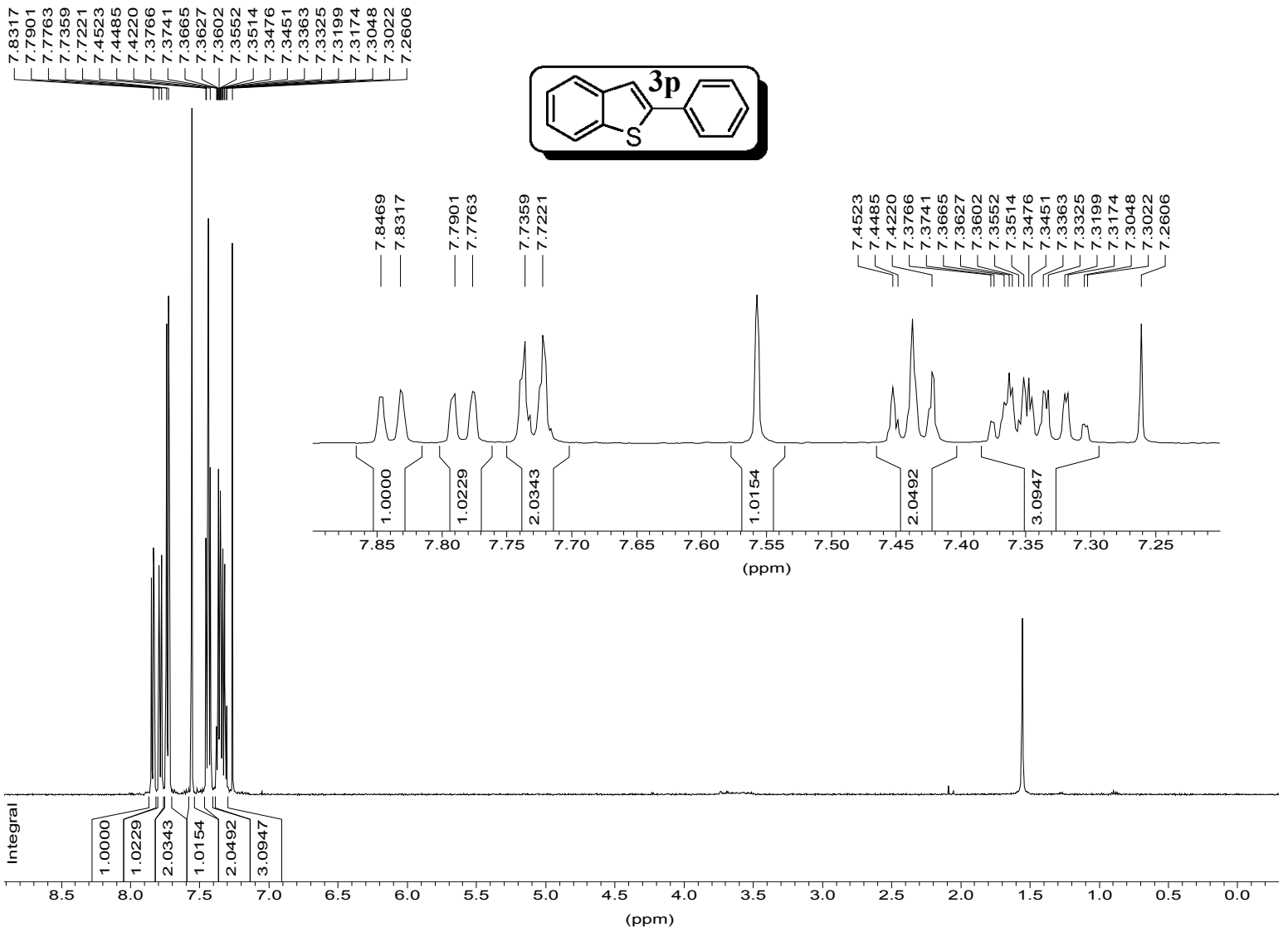
77.0036
76.7485
31.8146
31.6834
29.5555
29.1693
29.0090
28.9215
22.6398
14.0844
3o
H_2N
N
S
$(CH_2)_7CH_3$
123.7011
123.3003
124
(ppm)
31.8146
31.6834
29.5555
29.1693
29.0090
28.9215
32
31
30
29
(ppm)
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
(ppm)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7.4485
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7.3766
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7.3665
7.3627
7.3602
7.3552
7.3514
7.3476
7.3451
7.3363
7.3325
7.3199
7.3174
7.3048
7.3022
7.2606
3p
S
7.8469
7.8317
7.7901
7.7763
7.7359
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7.4220
7.3766
7.3741
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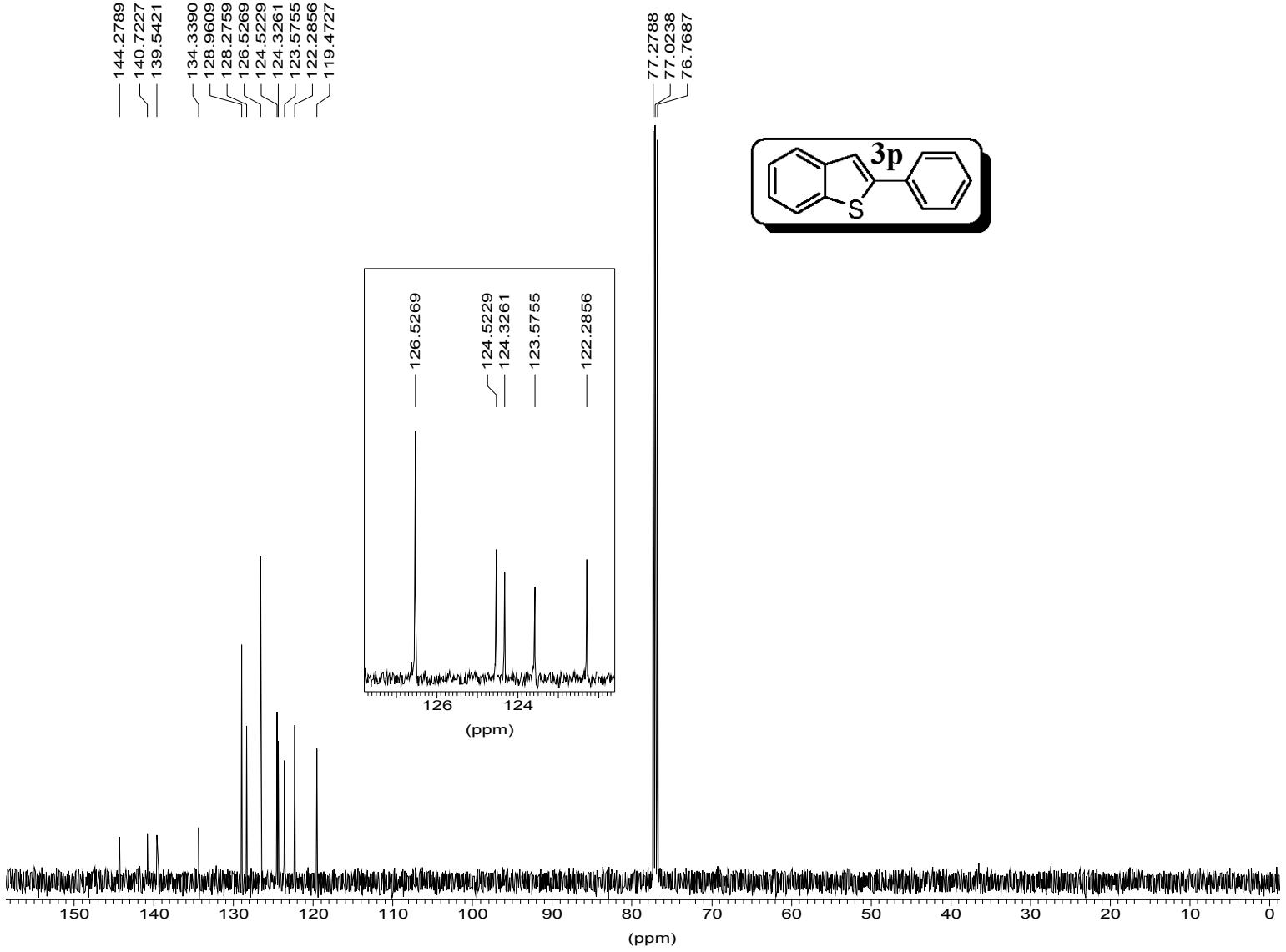
7.3627
7.3602
7.3552
7.3514
7.3476
7.3451
7.3363
7.3325
7.3199
7.3174
7.3048
7.3022
7.2606
1.0000
1.0229
2.0343
1.0154
2.0492
3.0947
7.85 7.80 7.75 7.70 7.65 7.60 7.55 7.50 7.45 7.40 7.35 7.30 7.25
(ppm)
Integral
1.0000
1.0229
2.0343
1.0154
2.0492
3.0947
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
(ppm)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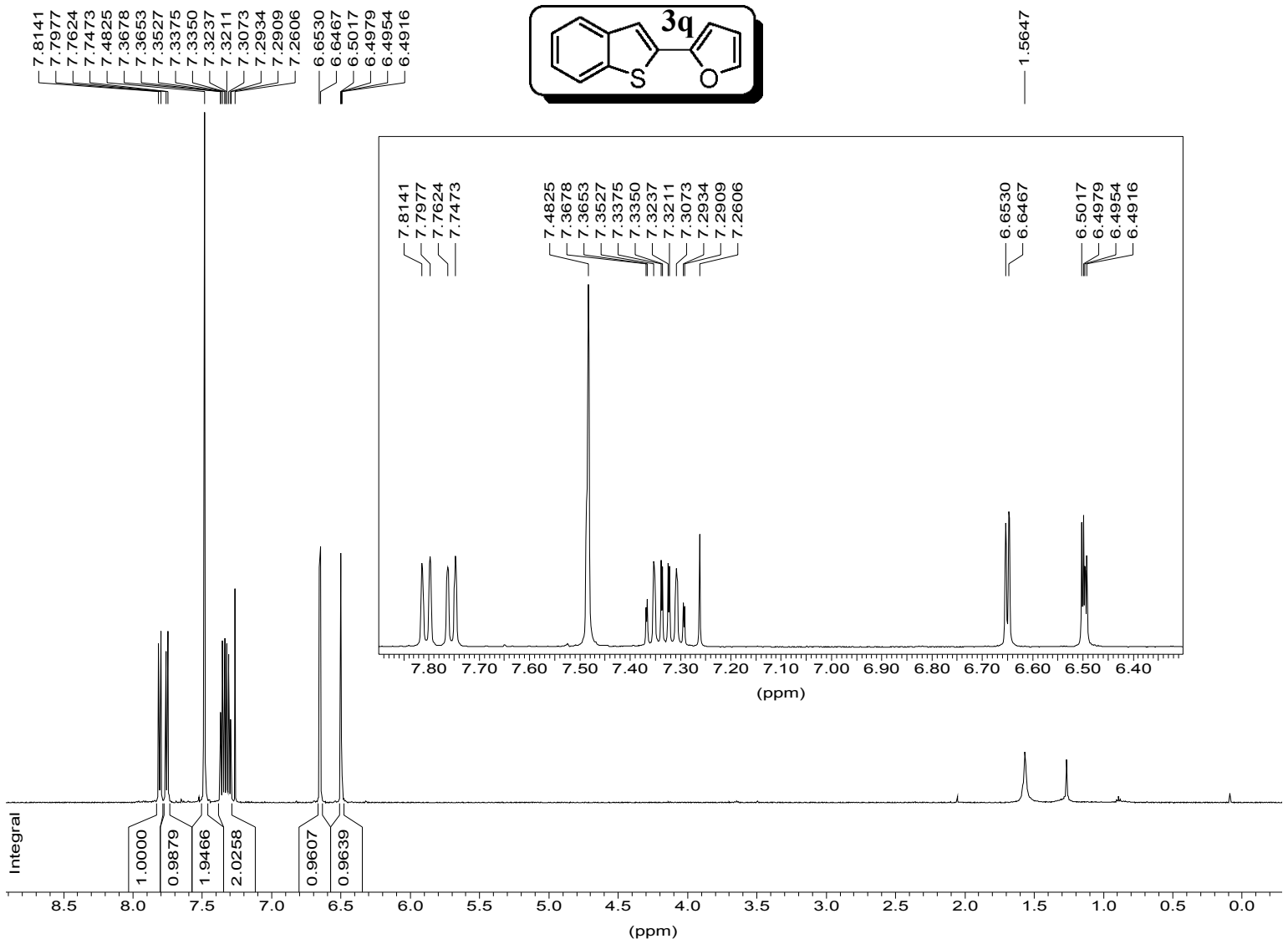
140.7227
139.5421
134.3390
128.9609
128.2759
126.5269
124.5229
124.3261
123.5755
122.2856
119.4727
77.2788
77.0238
76.7687
3p
S
126.5269
124.5229
124.3261
123.5755
122.2856
126
124
(ppm)
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
(ppm)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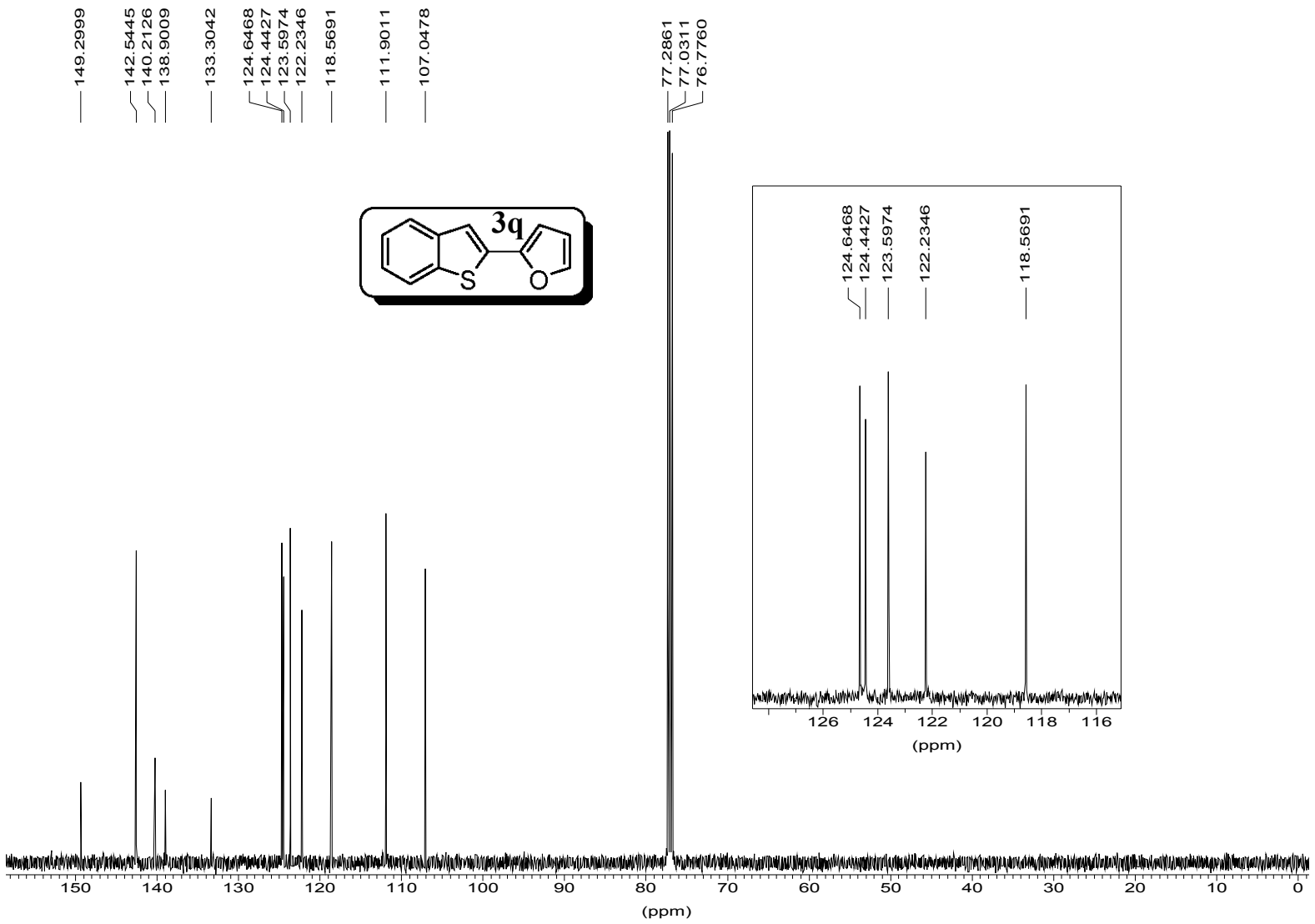
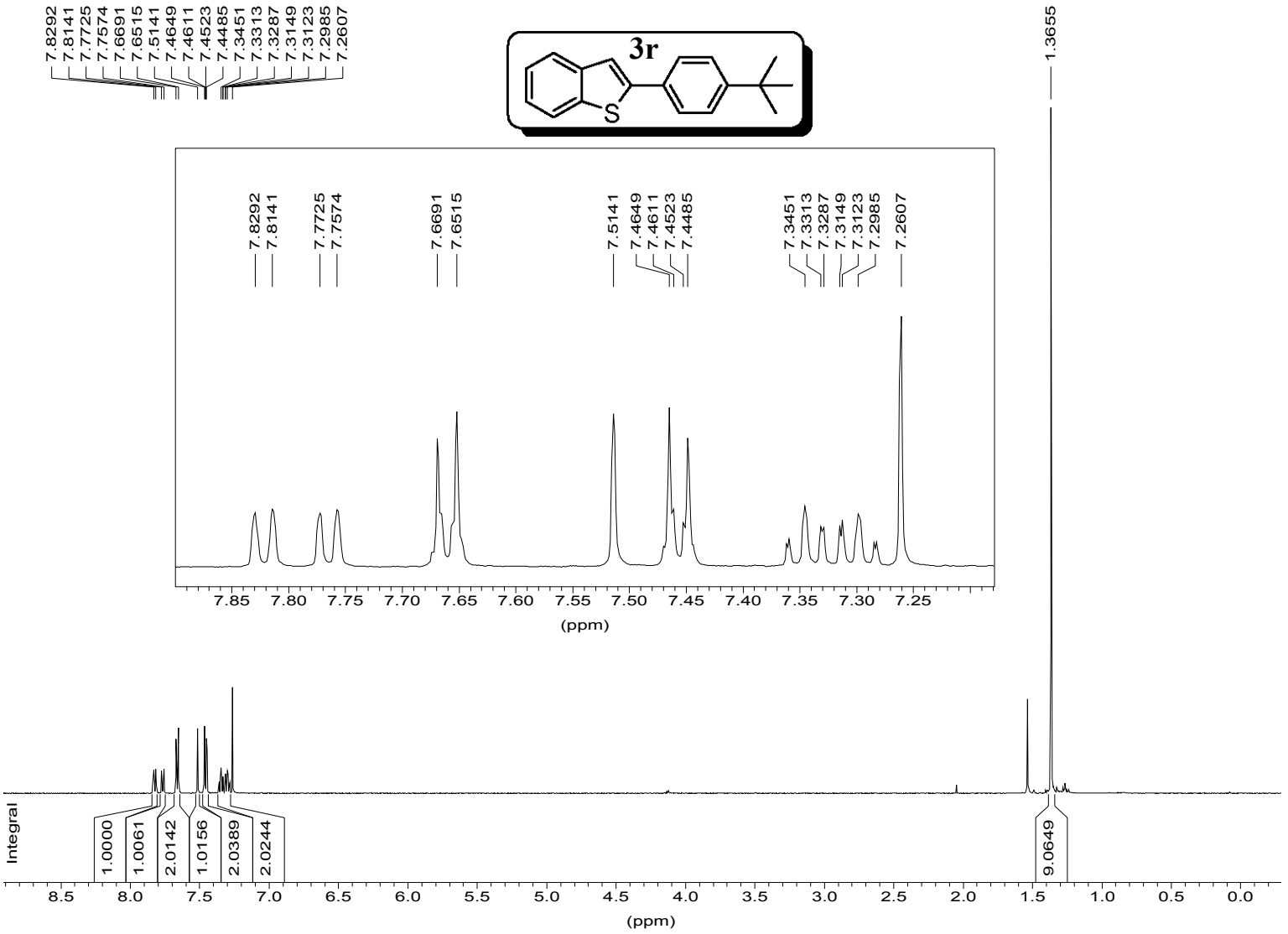
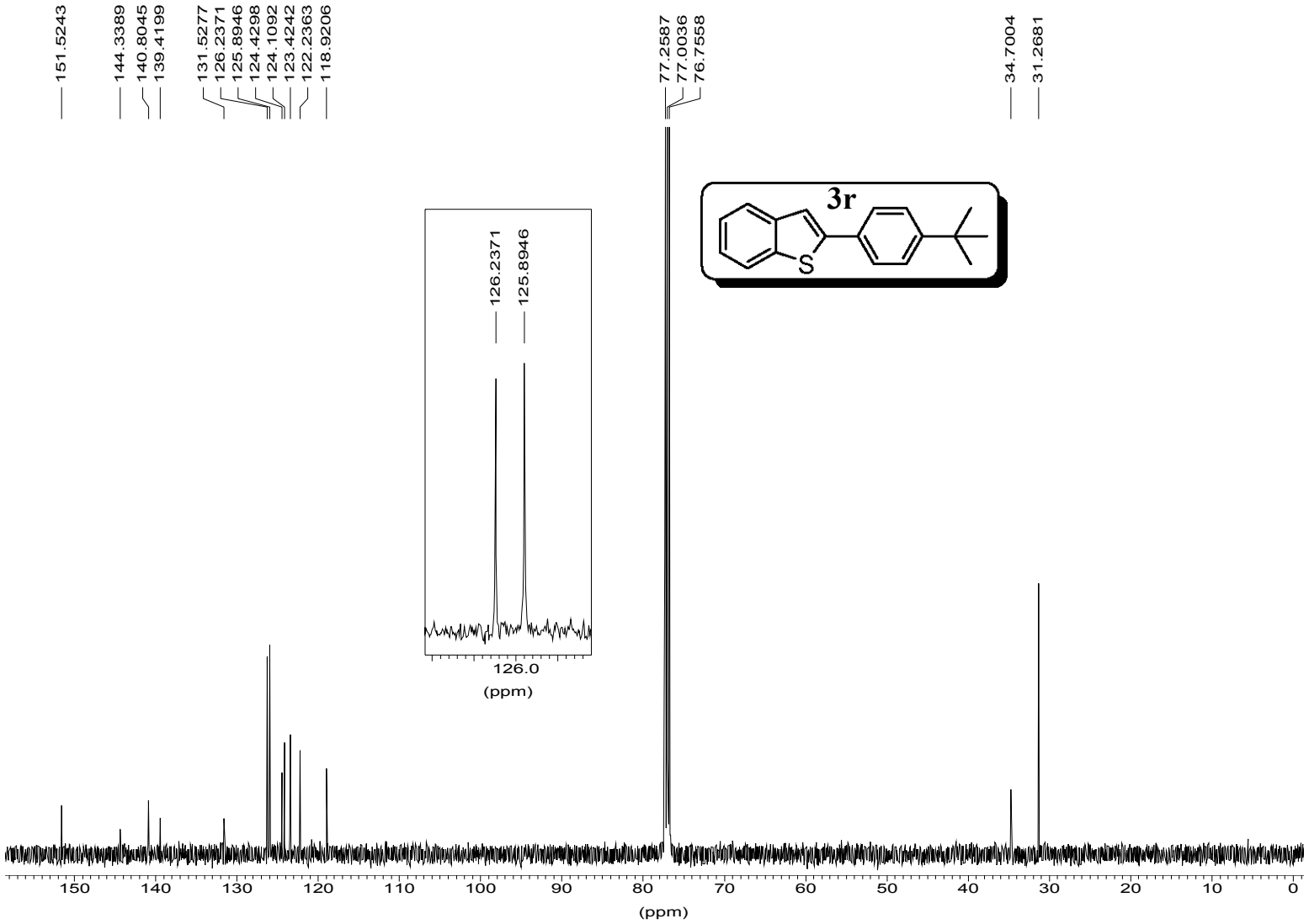
7.7977
7.7624
7.7473
7.4825
7.3678
7.3653
7.3527
7.3375
7.3350
7.3237
7.3211
7.3073
7.2934
7.2909
7.2606
6.6530
6.6467
6.5017
6.4979
6.4954
6.4916
1.5647
3q
S
O
Integral
1.0000
0.9879
1.9466
2.0258
0.9607
0.9639
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
(ppm)
7.80 7.70 7.60 7.50 7.40 7.30 7.20 7.10 7.00 6.90 6.80 6.70 6.60 6.50 6.40
(ppm)


149.2999
142.5445
140.2126
138.9009
133.3042
124.6468
124.4427
123.5974
122.2346
118.5691
111.9011
107.0478
77.2861
77.0311
76.7760
3q
S
O
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
(ppm)
126
124
122
120
118
116
(ppm)


7.8292
7.8141
7.7725
7.7574
7.6691
7.6515
7.5141
7.4649
7.4611
7.4523
7.4485
7.3451
7.3313
7.3287
7.3149
7.3123
7.2985
7.2607
3r
S
1.3655
7.85 7.80 7.75 7.70 7.65 7.60 7.55 7.50 7.45 7.40 7.35 7.30 7.25
(ppm)
Integral
1.0000
1.0061
2.0142
1.0156
2.0389
2.0244
9.0649
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
(ppm)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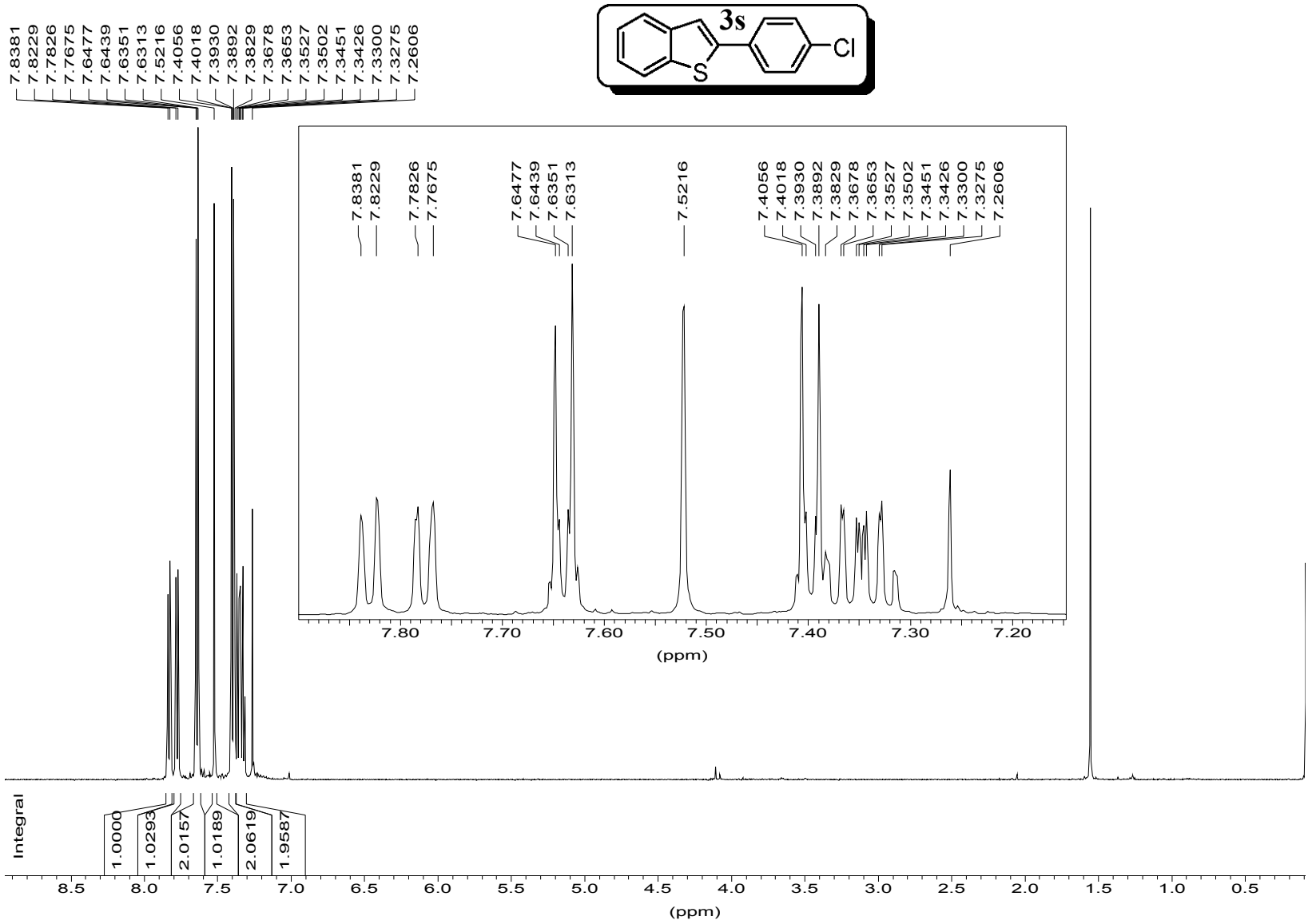
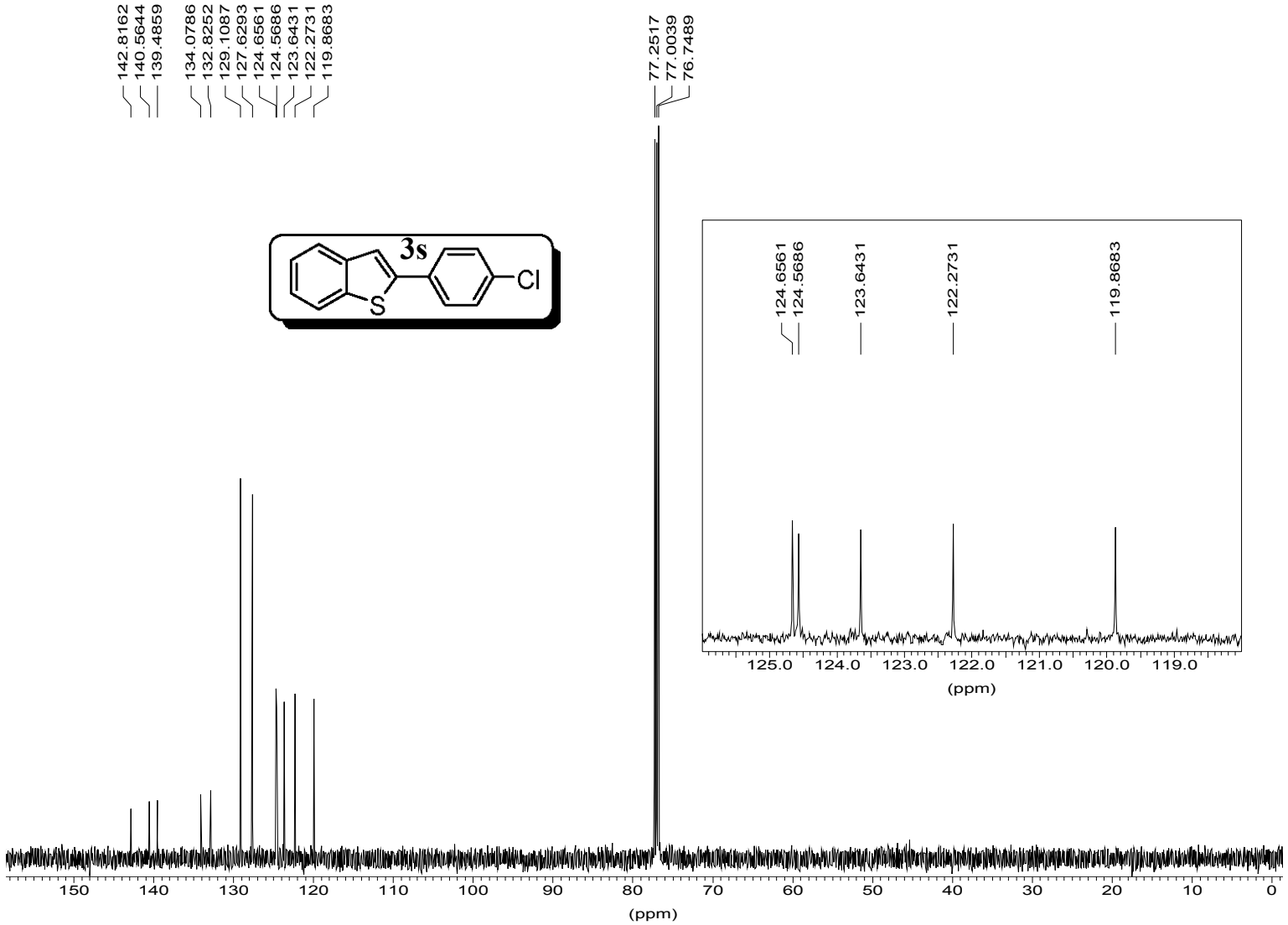
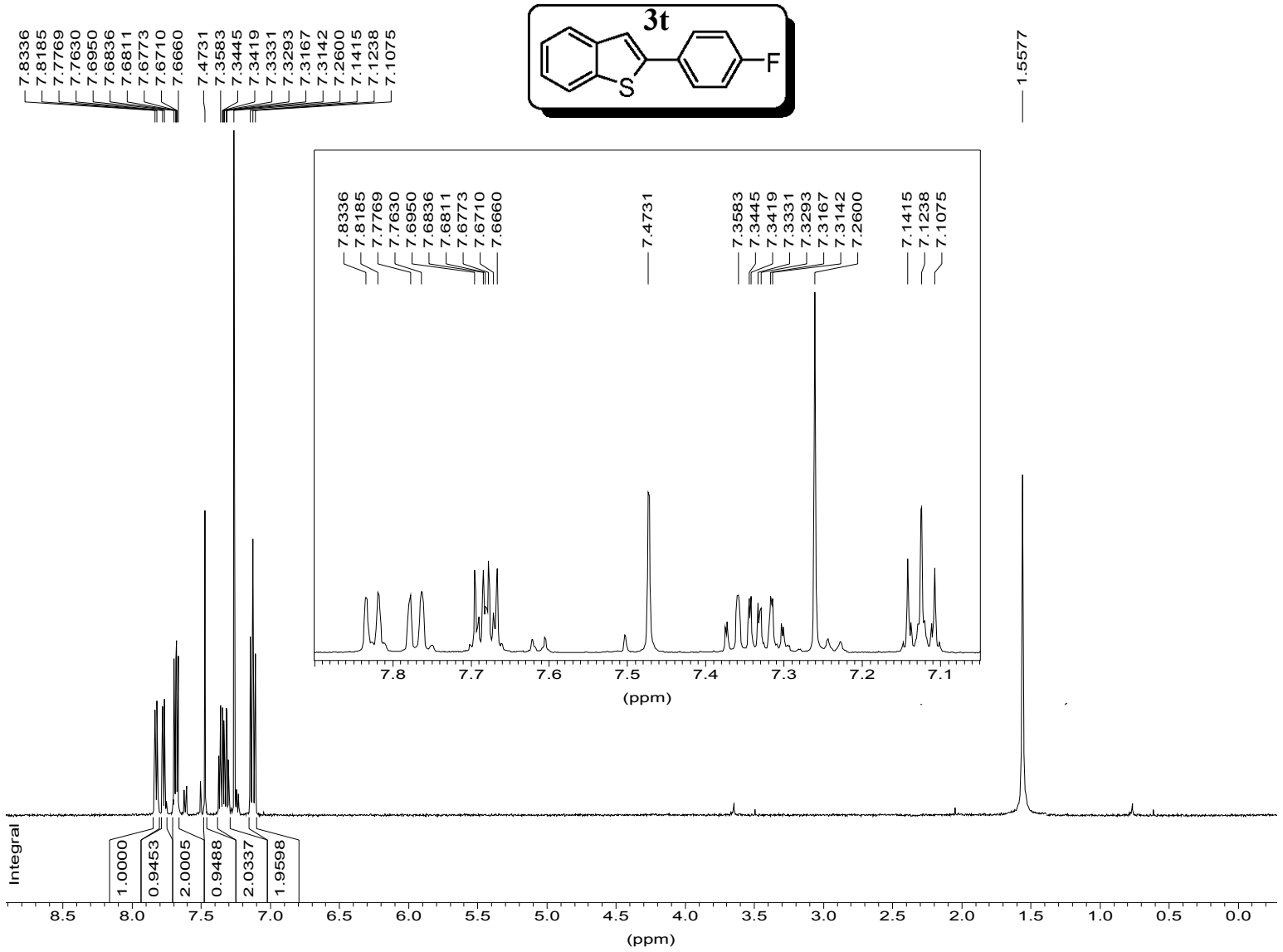
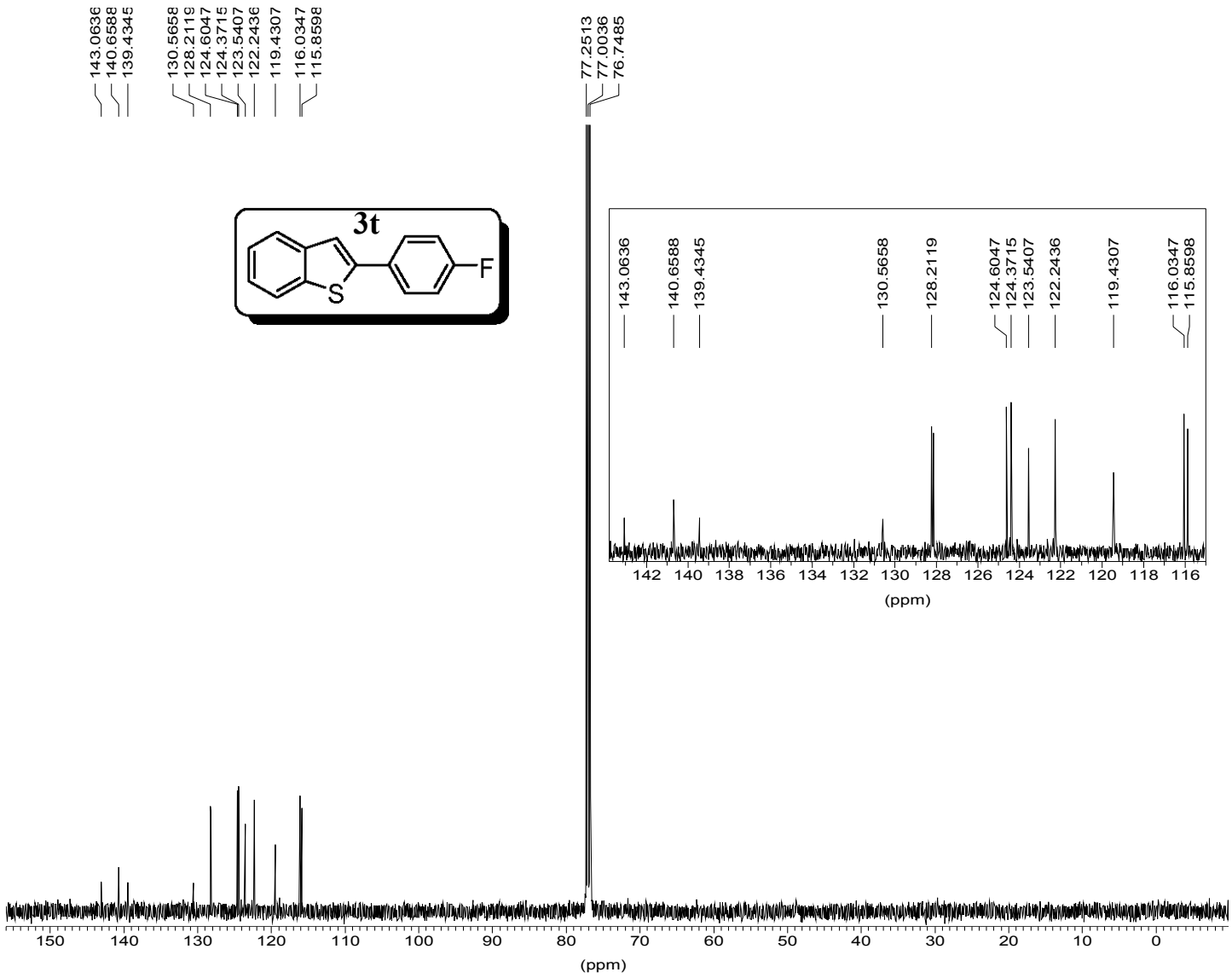
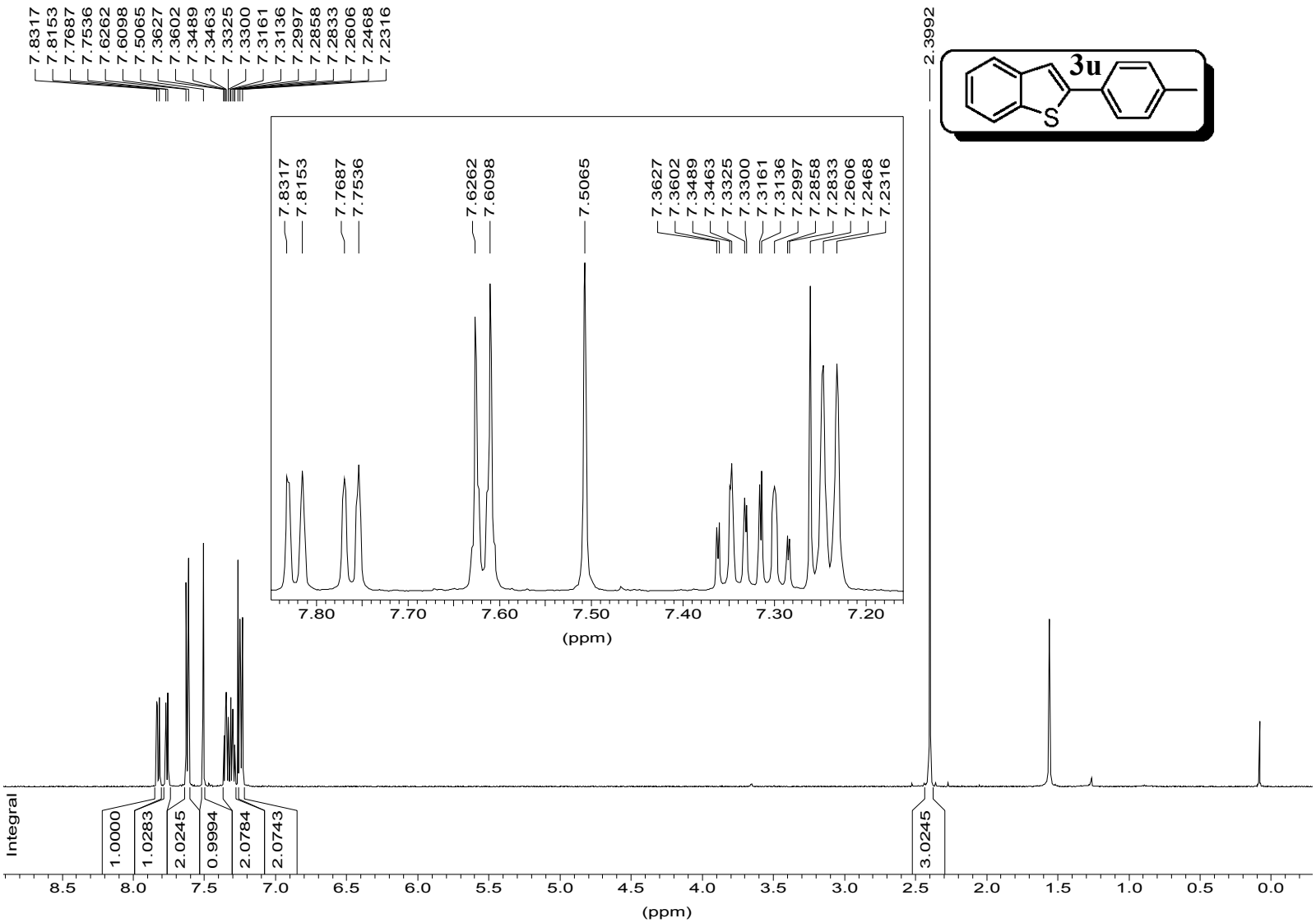
144.3389
140.8045
139.4199
131.5277
126.2371
125.8946
124.4298
124.1092
123.4242
122.2363
118.9206
77.2587
77.0036
76.7558
34.7004
31.2681
3r
S
126.2371
125.8946
126.0
(ppm)
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
(ppm)

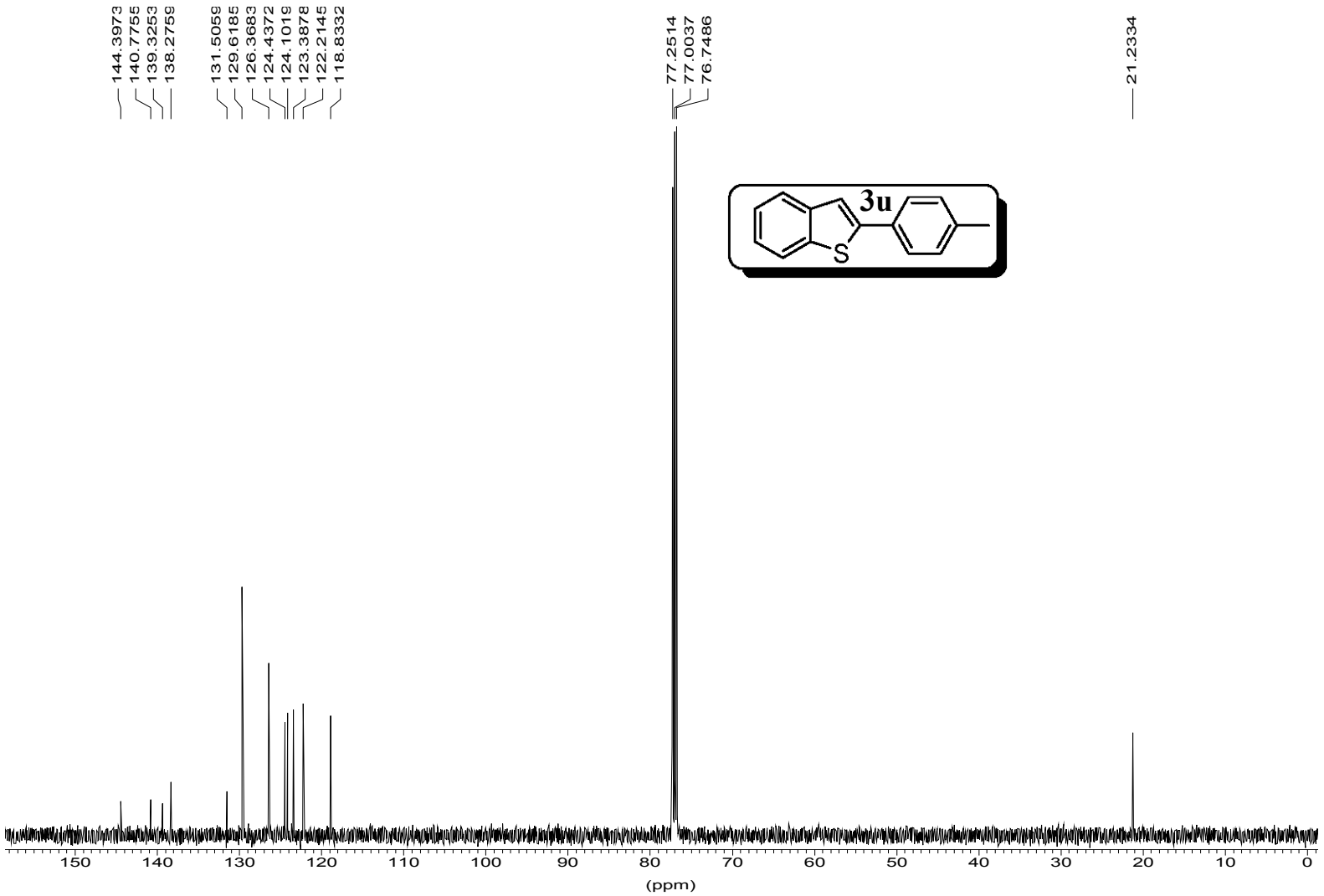

3s
Cl
S
7.8381
7.8229
7.7826
7.7675
7.6477
7.6439
7.6351
7.6313
7.5216
7.4056
7.4018
7.3930
7.3892
7.3829
7.3678
7.3653
7.3527
7.3502
7.3451
7.3426
7.3300
7.3275
7.2606
7.80
7.70
7.60
7.50
7.40
7.30
7.20
(ppm)
Integral
1.0000
1.0293
2.0157
1.0189
2.0619
1.9587
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
(ppm)

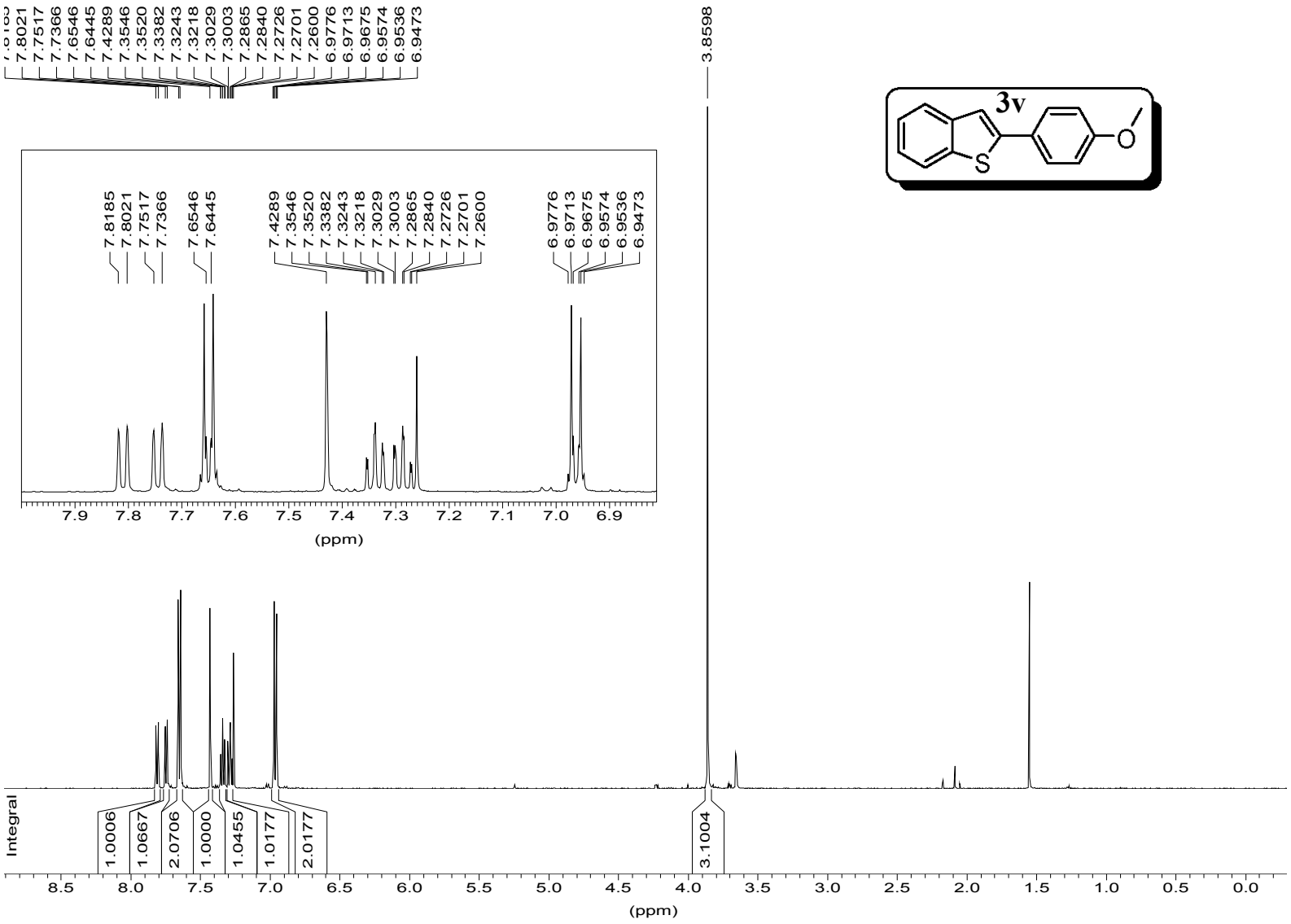

142.8162
140.5644
139.4859
134.0786
132.8252
129.1087
127.6293
124.6561
124.5686
123.6431
122.2731
119.8683
77.2517
77.0039
76.7489
3s
Cl
S
124.6561
124.5686
123.6431
122.2731
119.8683
125.0
124.0
123.0
122.0
121.0
120.0
119.0
(ppm)
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
(ppm)


3t
F
S
7.8336
7.8185
7.7769
7.7630
7.6950
7.6836
7.6811
7.6773
7.6710
7.6660
7.4731
7.3583
7.3445
7.3419
7.3331
7.3293
7.3167
7.3142
7.2600
7.1415
7.1238
7.1075
1.5577
Integral
1.0000
0.9453
2.0005
0.9488
2.0337
1.9598
(ppm)
(ppm)


143.0636
140.6588
139.4345
130.5658
128.2119
124.6047
124.3715
123.5407
122.2436
119.4307
116.0347
115.8598
77.2513
77.0036
76.7485
3t
S
F
(ppm)
(ppm)


7.8317
7.8153
7.7687
7.7536
7.6262
7.6098
7.5065
7.3627
7.3602
7.3489
7.3463
7.3325
7.3300
7.3161
7.3136
7.2997
7.2858
7.2833
7.2606
7.2468
7.2316
2.3992
3u
S
Integral
1.0000
1.0283
2.0245
0.9994
2.0784
2.0743
3.0245
(ppm)


144.3973
140.7755
139.3253
138.2759
131.5059
129.6185
126.3683
124.4372
124.1019
123.3878
122.2145
118.8332
77.2514
77.0037
76.7486
21.2334
3u
S
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
(ppm)


7.8185
7.8021
7.7517
7.7366
7.6546
7.6445
7.4289
7.3546
7.3520
7.3382
7.3243
7.3218
7.3029
7.3003
7.2865
7.2840
7.2726
7.2701
7.2600
6.9776
6.9713
6.9675
6.9574
6.9536
6.9473
3.8598
3v
O
S
(ppm)
Integral
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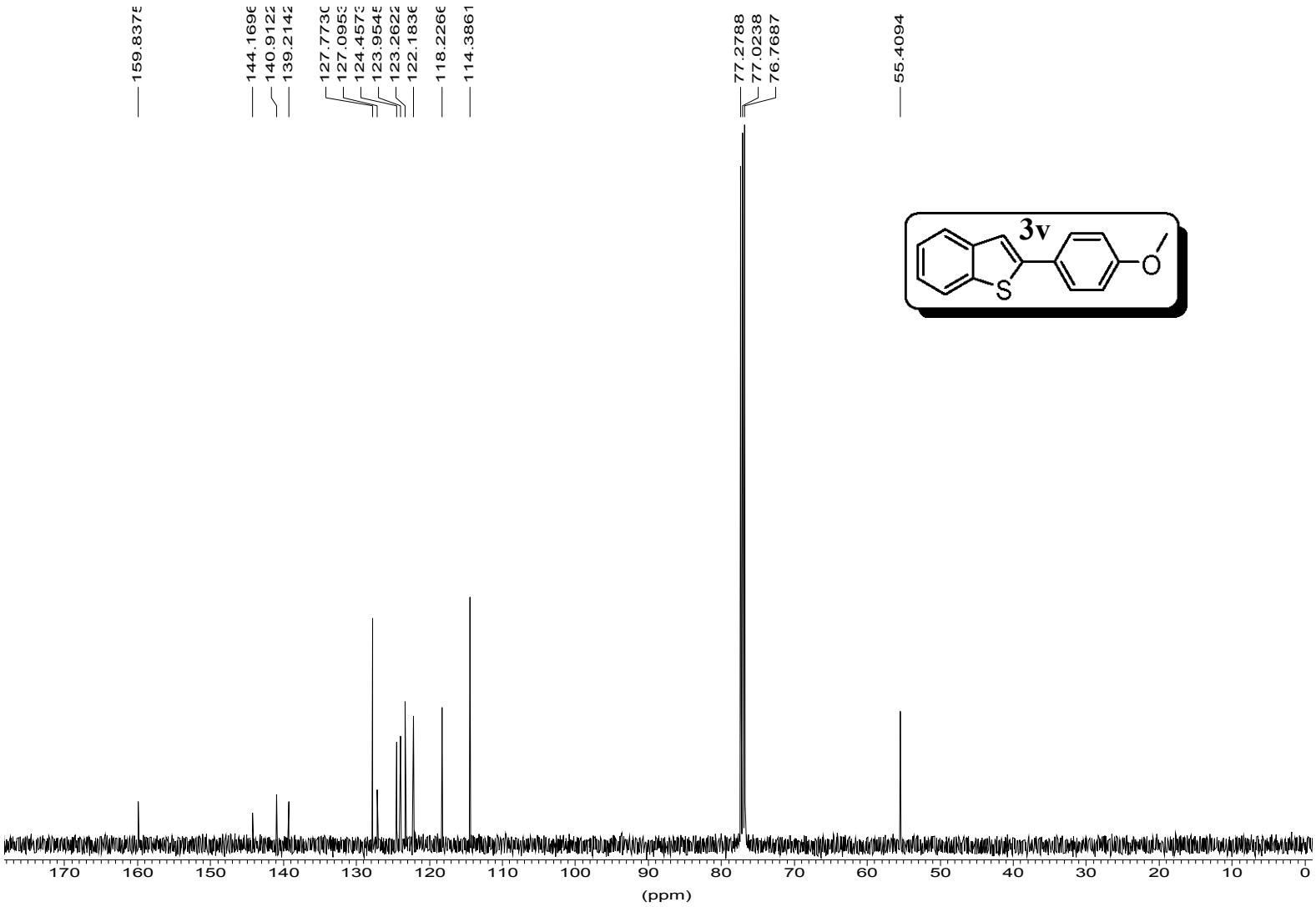
1.0667
2.0706
1.0000
1.0455
1.0177
2.0177
3.1004
(ppm)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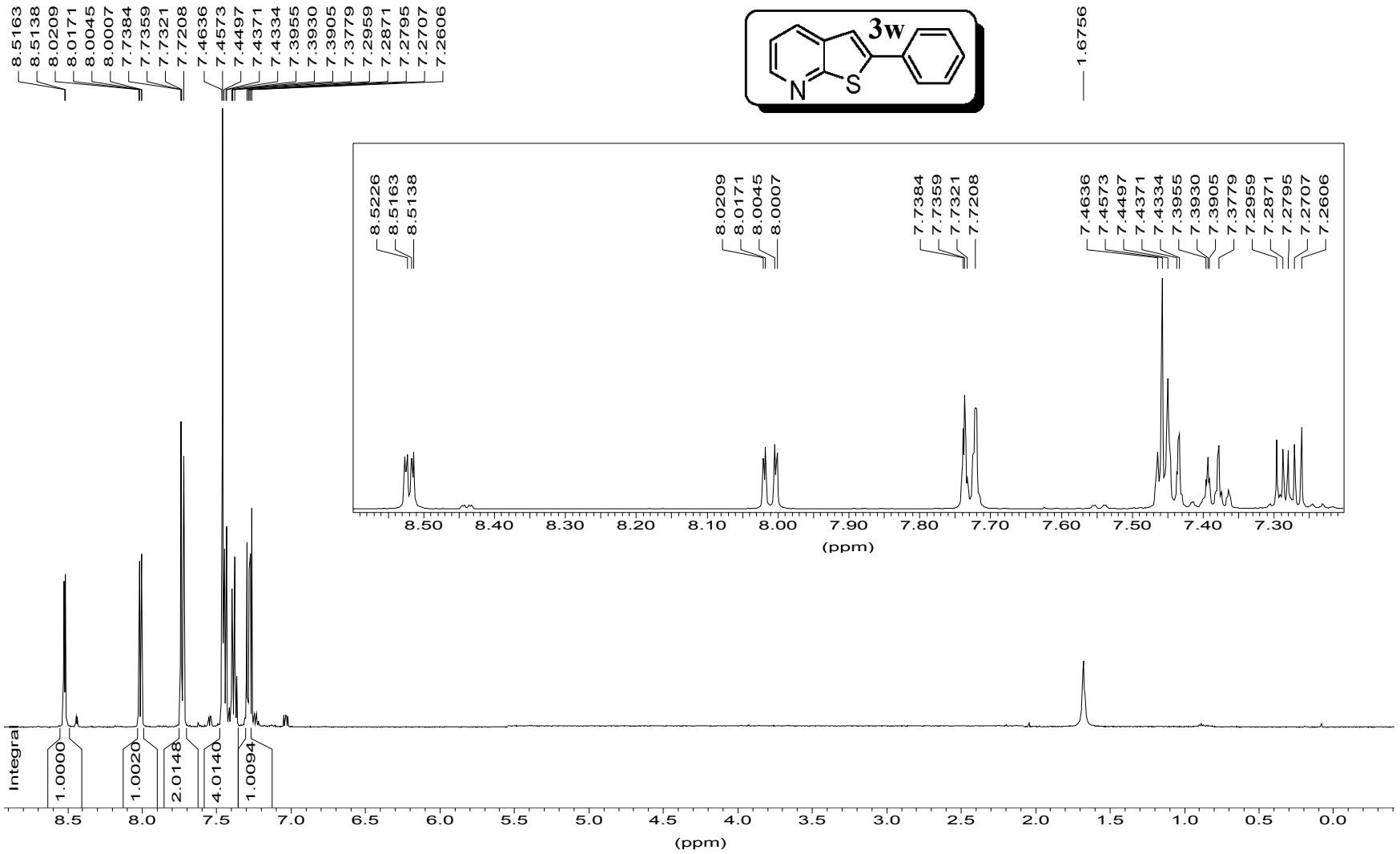
140.9122
139.2142
127.7730
127.0953
124.4573
123.9545
123.2622
122.1836
118.2266
114.3861
77.2788
77.0238
76.7687
55.4094
3v
S
O
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
(ppm)


8.5163
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8.0209
8.0171
8.0045
8.0007
7.7384
7.7359
7.7321
7.7208
7.4636
7.4573
7.4497
7.4371
7.4334
7.3955
7.3930
7.3905
7.3779
7.2959
7.2871
7.2795
7.2707
7.2606
1.6756
3w
N
S
Integral
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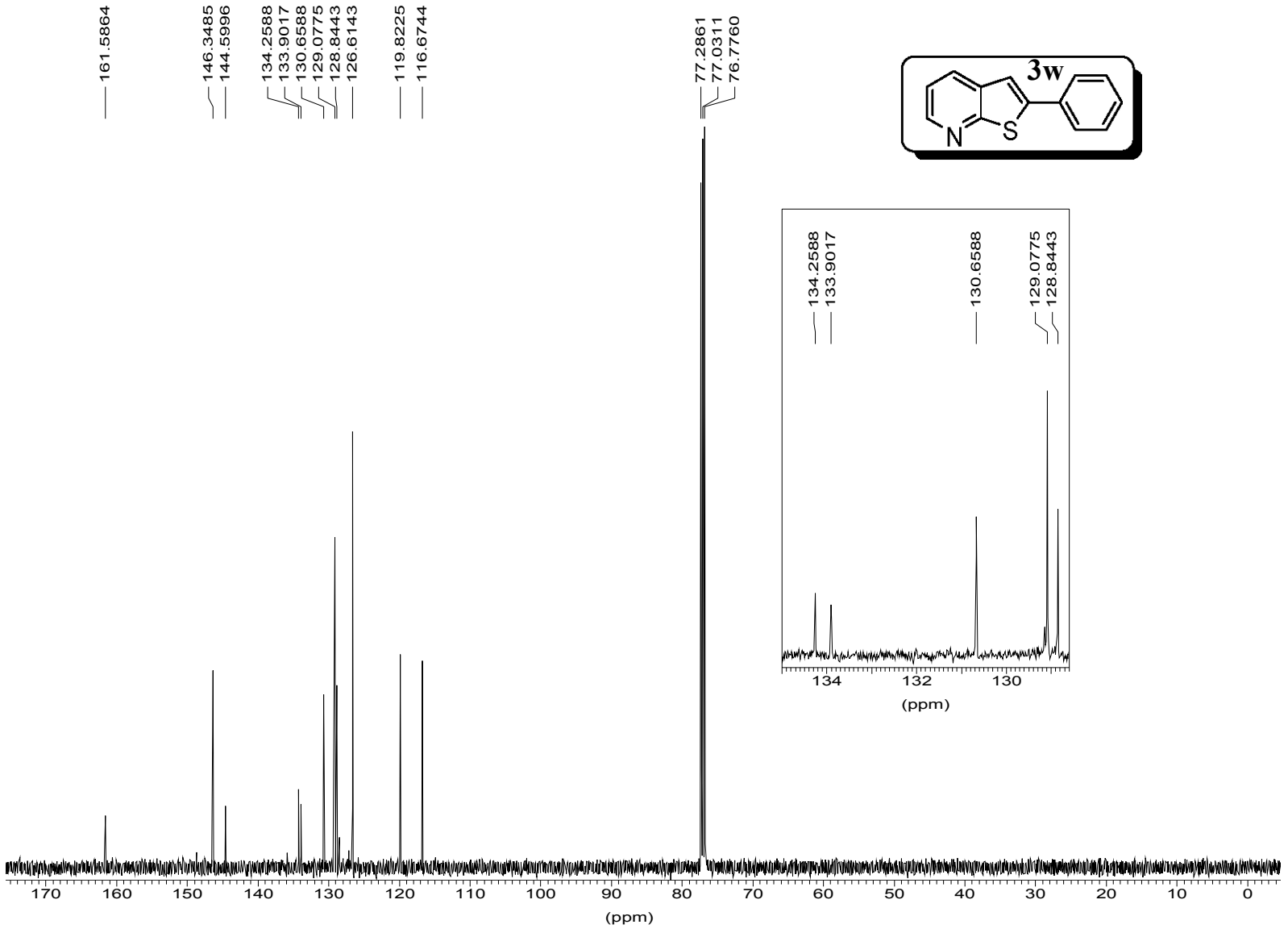
1.0020
2.0148
4.0140
1.0094
(ppm)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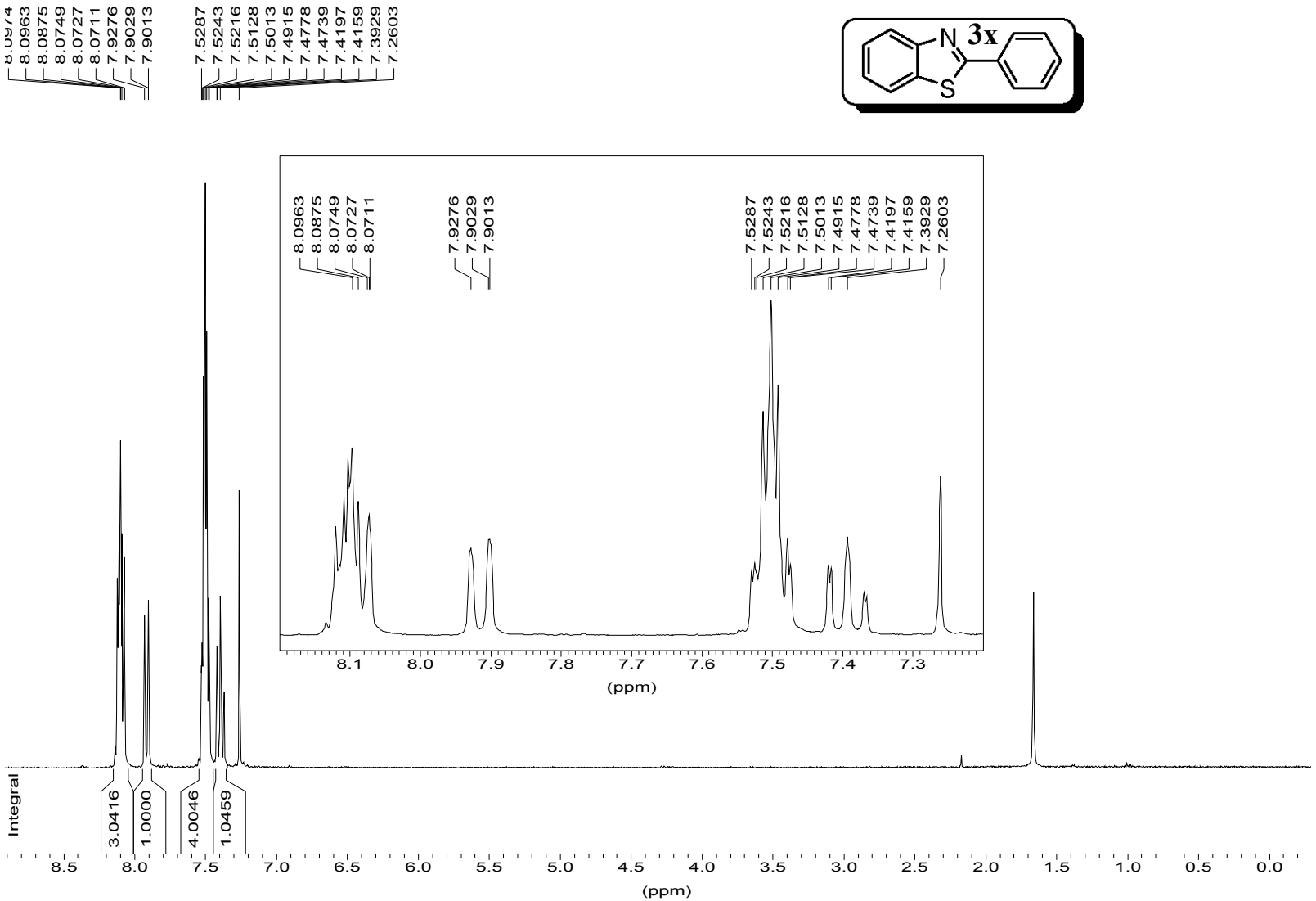
129.0775
128.8443
126.6143
119.8225
116.6744
77.2861
77.0311
76.7760
3w
N
S
134.2588
133.9017
130.6588
129.0775
128.8443
134
132
130
(ppm)
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
(ppm)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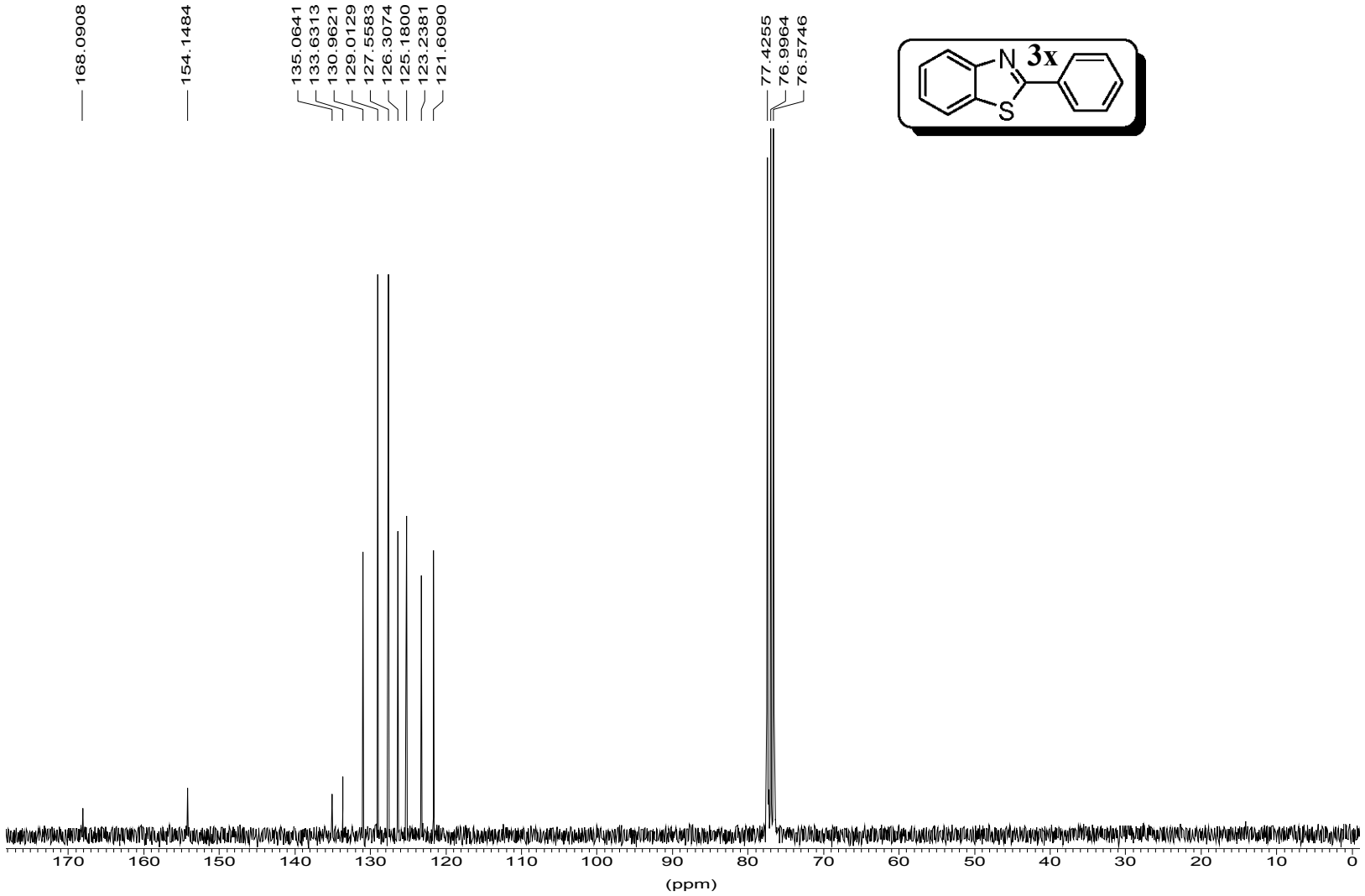
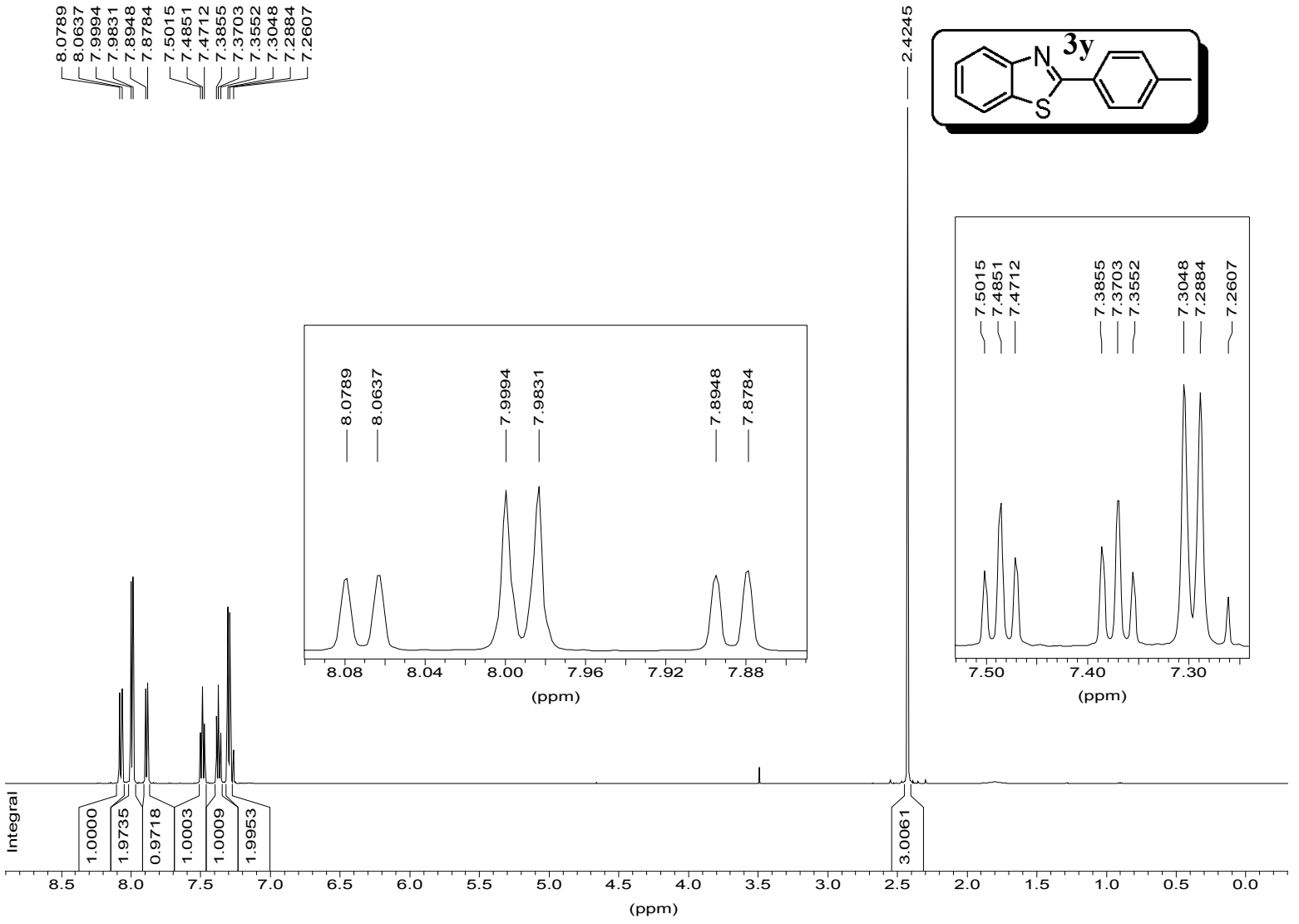
8.0963
8.0875
8.0749
8.0727
8.0711
7.9276
7.9029
7.9013
7.5287
7.5243
7.5216
7.5128
7.5013
7.4915
7.4778
7.4739
7.4197
7.4159
7.3929
7.2603
3x
N
S
Integral
3.0416
1.0000
4.0046
1.0459
(ppm)


168.0908
154.1484
135.0641
133.6313
130.9621
129.0129
127.5583
126.3074
125.1800
123.2381
121.6090
77.4255
76.9964
76.5746
N
S
3x
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
(ppm)


8.0789
8.0637
7.9994
7.9831
7.8948
7.8784
7.5015
7.4851
7.4712
7.3855
7.3703
7.3552
7.3048
7.2884
7.2607
2.4245
3y
N
S
Integral
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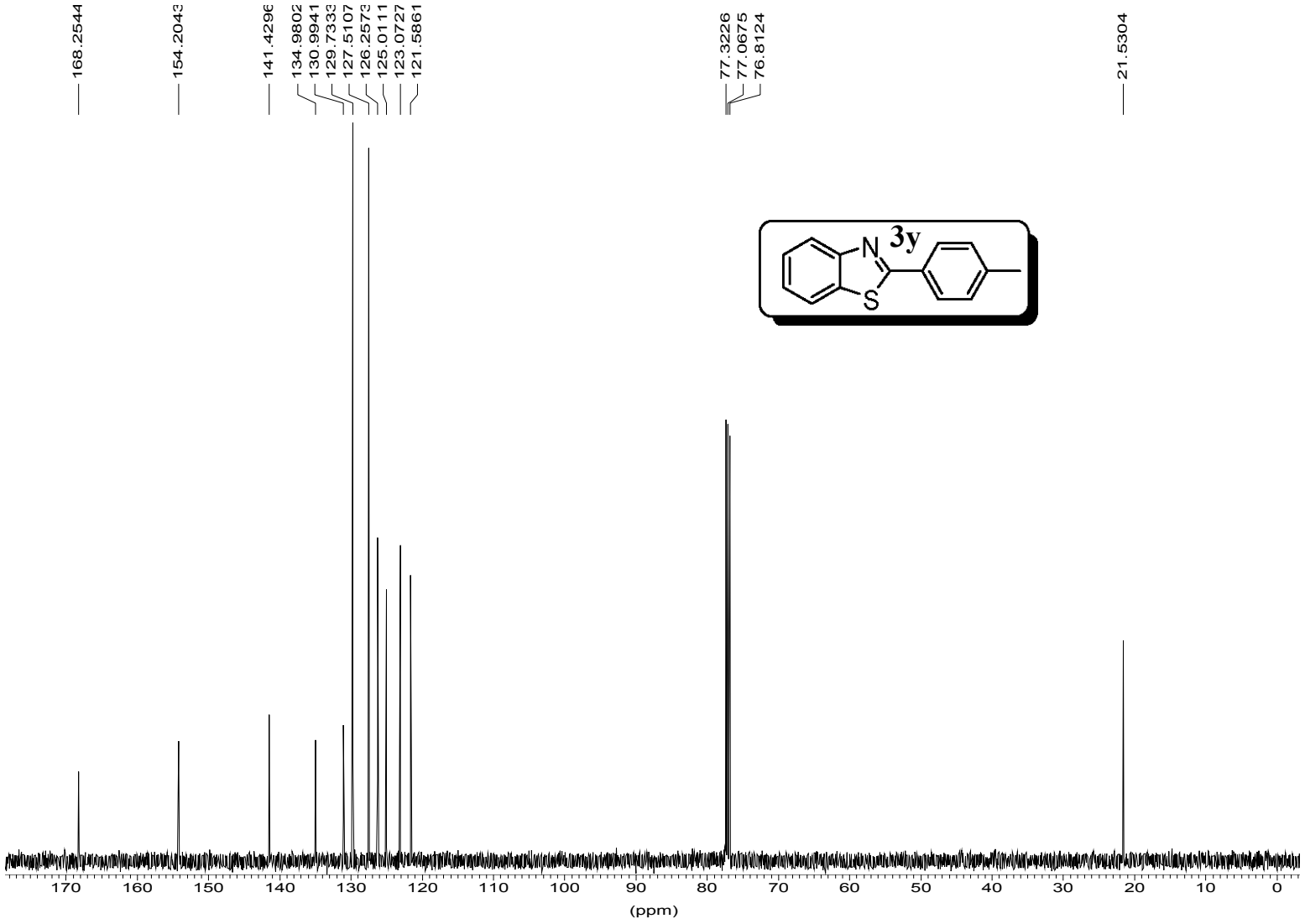
0.9718
1.0003
1.0009
1.9953
3.0061
(ppm)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141.4296
134.9802
130.9941
129.7333
127.5107
126.2573
125.0111
123.0727
121.5861
77.3226
77.0675
76.8124
21.5304
3y
N
S
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
(ppm)