Facile *N*-Arylation of Amines and Sulfonamides and *O*-Arylation of Phenols and Arenecarboxylic Acids

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Supporting Information

General. The ^{1}H and ^{13}C NMR spectra were recorded at 300 and 75.5 MHz or 400 and 100 MHz respectively. All melting points are uncorrected. High resolution mass spectra were recorded on a Kratos MS50TC double focusing magnetic sector mass spectrometer using EI at 70 eV. All reagents were used directly as obtained commercially unless otherwise noted. All yields reported represent an average of at least two independent runs. The substituted silylaryl triflates (**1b**, **1c**, **1d**, and **1e**) were prepared according to a literature procedure.[1] The product characterization data, and ^{1}H and ^{13}C NMR spectra for compounds **1**, **2**, **9**, **14**, **21**, **22**, **32**, **35**, **36**, **37**, **38**, **44**, **46**, **48**, and **53** have been reported in our previous communication.[2] The product characterization data, and ^{1}H and ^{13}C NMR spectra for compounds **62**, **63**, **64**, **67**, **68**, **69**, **70**, **71**, **75**, **76**, **83**, **84**, **85**, **86**, **89**, and **91** have been reported in our previous communication.[3]

General Procedure for the Mono *N*-Arylation of Aromatic Amines (Table 1).

For this experimental procedure, see the text.

General Procedure for the Mono *N*-Arylation of Alkylamines (Table 2).

For this experimental procedure, see the text.

General Procedure for the Diarylation of Amines and Sulfonamides (Tables 2 and 3).

For this experimental procedure, see the text.

General Procedure for the *O*-Arylation of Phenols (Table 4).

For this experimental procedure, see the text.

General Procedure for the *O*-Arylation of Carboxylic Acids (Table 5).

For this experimental procedure, see the text.

Characterization Data:

***N*-(4-Nitrophenyl)aniline (3).** The indicated compound was obtained in an 85% yield as a light yellow solid: mp 135-136 ^{o}C (lit.[4] 134-135 ^{o}C); the ^{1}H and ^{13}C NMR spectra match the literature data.[5]

4-(Phenylamino)benzonitrile (4). The indicated compound was obtained in a 90% yield as a white solid: mp 99-100 ^{o}C (lit.[6] 101-102 ^{o}C); the ^{1}H and ^{13}C NMR spectra match the literature data.[5]

Ethyl 4-(phenylamino)benzoate (5). The indicated compound was obtained in a 92% yield as light yellow oil. The ^{1}H and ^{13}C NMR spectra match the literature data.[7]

***N*-(4-Acetylphenyl)aniline (6).** The indicated compound was obtained in a 94% yield as a light yellow solid: mp 105-106 ^{o}C (lit.[8] 104-105 ^{o}C); the ^{1}H and ^{13}C NMR spectra match the literature data.[9]

***N*-[(3-(Phenylamino)phenyl]acetamide (7).** The indicated compound was obtained in a 95% yield as a light yellow oil: ^{1}H NMR (300 MHz, $CDCl_3$) δ 2.04 (s, 3H), 5.79 (s, 1H), 6.77 (dd, J = 8.1, 1.5 Hz, 1H), 6.88 (t, J = 7.2 Hz, 1H), 6.94-7.01 (m, 3H), 7.09 (t, J = 7.8 Hz, 1H), 7.19 (t, J = 7.8 Hz, 2H), 7.29 (t, J = 1.8 Hz, 1H), 8.15 (s, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 24.7, 109.4, 112.6, 113.2, 118.6, 121.5, 129.6, 129.9, 139.4, 142.9, 144.3, 169.5; HRMS m/z 226.1109 (calcd $C_{14}H_{14}N_2O$, 226.1106).

***N*-(4-Methoxyphenyl)aniline (8).** The indicated compound was obtained in an 89% yield as a white solid: mp 101-102 ^{o}C (lit.[10] 102-103 ^{o}C); the ^{1}H and ^{13}C NMR spectra match the literature data.[9]

***N*-Phenyl-4-iodoaniline (10).** The indicated compound was obtained in a 92% yield as a light yellow solid: mp 100-102 ^{o}C (lit.[11] 102-104 ^{o}C); the ^{1}H and ^{13}C NMR spectra match the literature data.[11]

***N*-Phenyl-4-bromoaniline (11).** The indicated compound was obtained in a 91% yield as a light yellow solid: mp 87-89 ^{o}C (lit.[8] 87-89 ^{o}C); the ^{1}H and ^{13}C NMR spectra match the literature data.[12]

***N*-Phenyl-2-*tert*-butylaniline (12).** The indicated compound was obtained in a 77% yield as a yellow solid: mp 64-65 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 1.46 (s, 9H), 5.42 (s, 1H), 6.82-6.86 (m, 3H), 7.09-7.47 (m, 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 30.8, 35.1, 116.2, 119.4, 124.2, 126.2, 127.1, 127.3, 129.5, 141.4, 143.6, 146.2; IR ($CDCl_3$, cm^{-1}) 3454, 3047, 2962, 2097, 2870, 1595, 1497; HRMS m/z 225.1520 (calcd $C_{16}H_{19}N$, 225.1517).

***N*-Phenyl-2,4,6-trimethylaniline (13).** The indicated compound was obtained in a 90% yield as a yellow solid: mp 54-56 ^{o}C (lit.[13] 56 ^{o}C); the ^{1}H and ^{13}C NMR spectra match the literature data.[13]

***N*-Methyl-*N*-phenyl-3,4-dimethylaniline (15).** The indicated compound was obtained in a 97% yield as a yellow oil; ^{1}H NMR (300 MHz, $CDCl_3$) δ 2.75 (s, 3H), 2.28 (s, 3H), 3.33 (s, 3H), 6.87-6.98 (m, 5H), 7.12 (d, J = 8.1 Hz, 1H), 7.24-7.30 (m, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 19.4, 20.3, 40.6, 118.1, 119.8, 120.6, 124.5, 129.2, 130.7, 131.3, 137.8, 147.2, 149.7; IR ($CDCl_3$, cm^{-1}) 3021, 2920, 2863, 1595, 1497; HRMS m/z 211.1364 (calcd $C_{15}H_{17}N$, 211.1361).

***N*-Methyl-*N*-phenyl-3-methoxyaniline (16).** The indicated compound was obtained in a 47% yield as a yellow oil; the ^{1}H and ^{13}C NMR spectra match the literature data.[14]

***N*-Methyl-*N*-phenyl-4-methoxyaniline (17).** The indicated compound was obtained in a 47% yield as a yellow oil; the ^{1}H and ^{13}C NMR spectra match the literature data.[14]

***N*-Methyl-*N*-phenyl-2-iodoaniline (18).** The indicated compound was obtained in a 97% yield as a white solid: mp 31-33 ^{o}C; ^{1}H NMR (300 MHz, CDCl3) δ 3.20 (s, 3H), 6.54 (d, J = 8.8 Hz, 2H), 6.75 (t, J = 7.2 Hz, 1H), 6.95-7.00 (m, 3H), 7.35 (t, J = 7.2 Hz, 1H), 7.94 (d, J = 8.8 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 39.3, 101.4, 113.6, 117.9, 128.3,

129.1, 129.9, 130.2, 140.5, 148.7, 150.7; IR ($CDCl_3$, cm^{-1}) 3054, 3035, 2918, 2881, 2811, 1609, 1497; HRMS m/z 309.0019 (calcd $C_{13}H_{12}IN$, 309.0014).

***N*-Allyl-*N*-phenylaniline (19).** The indicated compound was obtained in a 97% yield as a yellow oil; the ^1H and ^{13}C NMR spectra match the literature data.[15]

1-Phenylindoline (20). The indicated compound was obtained in a 97% yield as a yellow oil; the ^1H and ^{13}C NMR spectra match the literature data.[15]

***N*-(3,4-Dimethylphenyl)-*N*-(4-methoxyphenyl)-3,4-dimethylaniline (23).** The indicated compound was obtained in a 93% yield as a white solid: mp 110-111 ^oC; ^1H NMR (300 MHz, $CDCl_3$) δ 2.14 (s, 6H), 2.19 (s, 6H), 6.74-6.82 (m, 6H), 6.95-7.03 (m, 4H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 19.3, 20.2, 55.7, 114.8, 120.9, 124.7, 126.6, 130.2, 130.4, 137.4, 141.7, 146.5, 155.7; IR ($CDCl_3$, cm^{-1}) 3017, 2963, 2932, 2918, 2858, 1606, 1501; HRMS m/z 331.1942 (calcd $C_{23}H_{25}NO$, 331.1936).

***N,N*-Diphenyl-4-methoxyaniline (24).** The indicated compound was obtained in a 90% yield as a yellow solid: mp 98-100 ^oC (lit.[16] 98-100 ^oC); the ^1H and ^{13}C NMR spectra match the literature data.[17]

***N,N*-Diphenyl-4-nitroaniline (25).** The indicated compound was obtained in a 55% yield as a yellow solid: mp 139-141 ^oC (lit.[18] 138-139 ^oC); the ^1H and ^{13}C NMR spectra match the literature data.[19]

1-Phenyl-1*H*-imidazole (26). The indicated compound was obtained in a 76% yield as a yellow oil; the ^1H and ^{13}C NMR spectra match the literature data.[20]

***N,N*-Diphenylnaphthalen-1-amine (27).** The indicated compound was obtained in an 81% yield as a white solid: mp 135-137 ^oC (lit.[16] 136-137 ^oC); the ^1H and ^{13}C NMR spectra match the literature data.[16]

2-Phenyl-2*H*-benzo[*d*][1,2,3]triazole (28). The indicated compound was obtained in a 20% yield as a white solid: mp 109-110 ^{o}C (lit.[21] 108-110 ^{o}C); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.40-7.49 (m, 3H), 7.54-7.60 (m, 2H), 7.92-7.96 (m, 2H), 8.36 (dd, J = 9.0, 1.2 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 118.6, 120.8, 127.4, 129.2, 129.6, 140.6, 145.2.

1-Phenyl-1*H*-benzo[*d*][1,2,3]triazole (29). The indicated compound was obtained in a 72% yield as a white solid: mp 85-86 ^{o}C (lit.[22] 85-87 ^{o}C); the ^{1}H and ^{13}C NMR spectra match the literature data.[23]

***N*-Benzylaniline (30).** The indicated compound was obtained in a 70% yield as a yellow oil; the ^{1}H NMR spectrum matches the literature data.[24]

***N*-Benzyl-3-methoxyaniline (31).** The indicated compound was obtained in a 71% yield as a yellow oil; the ^{1}H and ^{13}C NMR spectra match the literature data.[25]

***N*-(2-Phenylethyl)aniline (33).** The indicated compound was obtained in a 66 % yield as a yellow oil; the ^{1}H and ^{13}C NMR spectra match the literature data.[26]

***N*,*N*-Diphenylaniline (34).** The indicated compound was obtained in a 97% yield as a yellow solid: mp 86-87 ^{o}C (lit.[27] 88-89 ^{o}C); the ^{1}H and ^{13}C NMR spectra match the literature data.[27]

1-Phenylpyrrolidine (39). The indicated compound was obtained in a 95% yield as a yellow oil; the ^{1}H and ^{13}C NMR spectra match the literature data.[28]

***N*-(3-Methoxyphenyl)pyrrolidine (40).** The indicated compound was obtained in a 97% yield as a yellow oil; the ^{1}H and ^{13}C NMR spectra match the literature data.[29]

4-Phenylmorpholine (41). The indicated compound was obtained in an 81% yield as a yellow oil; the ^{1}H and ^{13}C NMR spectra match the literature data.[30]

***N,N*-Dibenzylaniline (42).** The indicated compound was obtained in a 99% yield as a yellow oil; The ^{1}H and ^{13}C NMR spectra match the literature data.[31]

***N*-Phenylphenylalanine ethyl ester (43).** The indicated compound was obtained in a 65% yield as a colorless oil; The ^{1}H and ^{13}C NMR spectra match the literature data.[32]

***N,N*-Diphenyltrifluoromethanesulfonamide (45).** The indicated compound was obtained in a 78% yield as a white solid: mp 105-106 ^{o}C; ^{1}H NMR ($CDCl_3$, 300 MHz) δ 7.33-7.49 (m, 10H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 120.6 (q, J = 322 Hz), 128.6, 129.1, 130.0, 140.1; IR ($CDCl_3$, cm^{-1}) 3087, 3071, 3017, 1589, 1492; HRMS m/z 301.0388 (calcd $C_{13}H_{10}F_3NO_2S$, 301.0384).

***N,N*-Diphenyl-4-methylbenzenesulfonamide (47).** The indicated compound was obtained in a 100% yield as a yellow solid: mp 138-139 ^{o}C; ^{1}H NMR ($CDCl_3$, 300 MHz) δ 2.43 (s, 3H), 7.25-7.32 (m, 12H), 7.60 (d, J = 7.2 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 21.8, 127.6, 128.0, 128.6, 129.5, 129.8, 137.8, 141.8, 143.8; IR ($CDCl_3$, cm^{-1}) 3098, 3067, 2922, 1592, 1345; HRMS m/z 323.0986 (calcd $C_{19}H_{17}NO_2S$, 323.0980).

***N,N*-Diphenyl-2-methylbenzenesulfonamide (49).** The indicated compound was obtained in a 99% yield as a yellow solid: mp 65-67 ^{o}C; ^{1}H NMR ($CDCl_3$, 300 MHz) δ 2.51 (s, 3H), 7.20-7.33 (m, 12H), 7.44 (td, J = 7.2, 0.9 Hz, 1H), 7.83 (d, J = 7.8 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 21.0, 126.3, 127.7, 128.8, 129.5, 130.9, 132.8, 133.3, 138.4, 138.5, 141.7; IR ($CDCl_3$, cm^{-1}) 3062, 3037, 2933, 1589, 1487; HRMS m/z 323.0986 (calcd $C_{19}H_{17}NO_2S$, 323.0980).

***N,N*-Diphenyl-4-methoxybenzenesulfonamide (50).** The indicated compound was obtained in a 100% yield as a yellow solid: mp 122-123 ^{o}C; ^{1}H NMR ($CDCl_3$, 300 MHz) δ 3.86 (s, 3H), 6.93 (dd, J = 6.9, 2.1 Hz, 2H), 7.22-7.34 (m, 10H), 7.32 (dd, J = 6.9, 2.1 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 55.8, 114.3, 127.6, 128.6, 129.5, 130.1, 132.4, 141.8, 163.2; IR ($CDCl_3$, cm^{-1}) 3076, 3006, 2985, 2945, 2844, 1594, 1493; HRMS m/z 339.0934 (calcd $C_{19}H_{17}NO_3S$, 339.0929).

***N,N*-Diphenyl-4-(trifluoromethyl)benzenesulfonamide (51).** The indicated compound was obtained in a 91% yield as a white solid: mp 128-129 ^{o}C; ^{1}H NMR ($CDCl_3$, 300 MHz) δ 7.24-7.37 (m, 10H), 7.75 (d, J = 8.7 Hz, 2H), 7.82 (d, J = 8.7 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 123.5 (q, J = 271.4 Hz), 126.3 (q, J = 3.7 Hz), 128.2, 128.4, 128.6, 129.7, 134.7 (q, J = 32.9 Hz), 141.2, 144.2 (q, J = 1.3 Hz); IR ($CDCl_3$, cm^{-1}) 3063, 2919, 1587, 1490; HRMS m/z 337.0700 (calcd $C_{19}H_{14}F_3NO_2S$, 337.0697).

***N,N*-Diphenyl-4-(phenylamino)benzenesulfonamide (52).** The indicated compound was obtained in a 75% yield as a pale yellow solid: mp 206-208 ^{o}C; ^{1}H NMR (acetone-d_6, 300 MHz) δ 7.03-7.17 (m, 3H), 7.25-7.39 (m, 14H), 7.54 (dt, J = 9.0, 2.7 Hz, 2H), 8.11 (s, 1H); ^{13}C NMR (75 MHz, acetone-d_6) δ 114.2, 120.6, 123.0, 127.3, 128.6, 129.3, 129.5, 129.6, 129.9, 141.3, 142.3, 149.0; IR ($CDCl_3$, cm^{-1}) 3367, 3055, 3034, 1743, 1591, 1145; HRMS m/z 400.1252 (calcd $C_{24}H_{20}N_2O_2S$, 400.1245).

***N*-(3-Methoxyphenyl)-*N*-methyl-4-methylbenzenesulfonamide (54).** The indicated compound was obtained in a 91% yield as a colorless oil; ^{1}H NMR ($CDCl_3$, 300 MHz) δ 2.41 (s, 3H), 3.14 (s, 3H), 3.76 (s, 3H), 6.61-6.64 (m, 1H), 6.71 (t, J = 2.4 Hz, 1H), 6.79-6.82 (m, 1H), 7.18 (t, J = 8.4 Hz, 1H), 7.24 (d, J = 8.1 Hz, 2H), 7.46 (d, J = 8.4 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 21.8, 38.4, 55.6, 112.9, 113.3, 118.6, 128.1, 129.5, 133.7, 143.0, 143.8, 160.0; IR ($CDCl_3$, cm^{-1}) 3058, 3027, 2932, 1589, 1485; HRMS m/z 291.0932 (calcd $C_{15}H_{16}NO_3S$, 291.0929).

***N*-Benzyl-*N*-phenyl-4-methylbenzenesulfonamide (55).** The indicated compound was obtained in a 94% yield as a yellow solid: mp 139-140 ^{o}C; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.44 (s, 3H), 4.74 (s, 2H), 6.98-7.01 (m, 2H), 7.18-7.29 (m, 10H), 7.55 (d, J = 8.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 21.9, 54.9, 127.8, 127.9, 128.0, 128.6, 128.7, 129.1, 129.2, 129.7, 135.7, 136.2, 139.2, 143.8; IR ($CDCl_3$, cm^{-1}) 3062, 3027, 2918, 1595, 1491; HRMS m/z 337.1140 (calcd $C_{20}H_{19}NO_2S$, 337.1136).

Methyl 3-iodo-4-(*N*-phenylmethanesulfonylamino)benzoate (56). The indicated compound was obtained in a 98% yield as a pale yellow solid: mp 135-137 ^{o}C; ^{1}H NMR

($CDCl_3$, 400 MHz) δ 3.27 (s, 3H), 3.92 (s, 3H), 7.25-7.27 (m, 1H), 7.36 (t, J = 7.2 Hz, 2H), 7.46 (d, J = 7.6 Hz, 2H), 7.69 (d, J = 8.0 Hz, 1H), 8.10 (dd, J = 8.0, 1.2 Hz, 1H), 8.58 (d, J = 2.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 41.7, 52.9, 101.7, 126.0, 127.1, 129.6, 130.7, 131.8, 132.0, 140.0, 146.5, 164.9; IR ($CDCl_3$, cm^{-1}) 3065, 3026, 2952, 2930, 2849, 2256, 1724, 1351; HRMS m/z 430.9693 (calcd $C_{15}H_{14}INO_4S$, 430.9688).

***N*-Phenylsaccharin (57).** The indicated compound was obtained in a 72% yield as a white solid: mp 187-189 ^{o}C (lit.[33] 189-191 ^{o}C); the ^{1}H and ^{13}C NMR spectra match the literature data.[33]

***N*-Phenylphthalimide (59).** The indicated compound was obtained in a 60% yield as a white solid: mp 207-209 ^{o}C (lit.[34] 207.9-209.9 ^{o}C); the ^{1}H and ^{13}C NMR spectra match the literature data.[35]

Ethyl *N*,*N*-diphenylcarbamate (60). The indicated compound was obtained in a 96% yield as a white solid: mp 69-70 ^{o}C (lit.[36] 69-70 ^{o}C); the ^{1}H NMR spectrum matches the literature data.[36]

Ethyl *N*-(4-chloro-2-iodophenyl)-*N*-phenylcarbamate (61). The indicated compound was obtained in a 93% yield as a colorless oil; ^{1}H NMR ($CDCl_3$, 300 MHz) δ 1.25 (t, J = 7.2 Hz, 3H), 4.21-4.26 (m, 2H), 7.13-7.19 (m, 2H), 7.25-7.35 (m, 5H), 7.90 (d, J = 2.4 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 14.8, 62.8, 100.9, 125.2, 125.8, 128.9, 129.8, 130.7, 133.9, 139.5, 141.5, 143.6, 153.9; IR ($CDCl_3$, cm^{-1}) 3065, 2980, 2932, 2906, 1721, 1493, 1308; HRMS m/z 440.9684 (calcd $C_{15}H_{13}ClINO_2$, 440.9679).

(4-*tert*-Butylphenyl) phenyl ether (65). The indicated compound was obtained in an 85% yield as a colorless oil; the ^{1}H and ^{13}C NMR spectra match the literature data.[37]

***N*-(4-Phenoxyphenyl)acetamide (66).** The indicated compound was obtained in a 91% yield as a white solid: mp 130-131^{o}C (lit.[38] 128-129 ^{o}C); the ^{1}H and ^{13}C NMR spectra match the literature data.[39]

2,4-Dimethylphenyl 4-iodophenyl ether (72) and 3,5-dimethylphenyl 4-iodophenyl ether (73). The indicated compounds were obtained as a 1:1.5 mixture in a 92% yield as a colorless oil; ^{1}H NMR ($CDCl_3$, 300 MHz) δ 2.18 (s, 3H), 2.32 (s, 8H), 2.35 (s, 3H), 6.66-6.69 (m, 5H), 6.76-6.80 (m, 4H), 6.85 (d, J = 8.1 Hz, 1H), 7.02 (d, J = 8.1 Hz, 1H), 7.09 (s, 1H), 7.55-7.65 (m, 5H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 16.3, 21.1, 21.6, 84.6, 85.9, 117.1, 119.1, 120.6, 121.1, 125.8, 128.1, 130.2, 132.5, 134.5, 138.7, 138.8, 140.0, 151.5, 156.7, 157.9, 158.7.

2-Iodophenyl phenyl ether (74). The indicated compound was obtained in a 90% yield as a pale yellow solid: mp 52-54 ^{o}C (lit.[40] 53-54 ^{o}C); the ^{1}H and ^{13}C NMR spectra match the literature data.[40]

2-Naphthyl phenyl ether (77). The indicated compound was obtained in an 84% yield as a pale yellow solid: mp 46-47 ^{o}C (lit.[41] 45-46 ^{o}C); ^{1}H NMR ($CDCl_3$, 300 MHz) δ 7.07 (d, J = 7.8 Hz, 2H), 7.14 (t, J = 7.5 Hz, 1H), 7.24-7.47 (m, 6H), 7.69 (d, J = 7.8 Hz, 1H), 7.80-7.84 (m, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 114.3, 119.4, 120.2, 123.7, 124.9, 126.7, 127.4, 127.9, 130.0, 130.1, 130.4, 134.5, 155.3, 157.4.

Benzyl phenyl ether (78). The indicated compound was obtained in a 25% yield as a colorless oil; the ^{1}H and ^{13}C NMR spectra match the literature data.[42]

2-Bromobenzyl phenyl ether (79). The indicated compound was obtained in a 36% yield as a pale yellow solid: mp 35-37 ^{o}C (lit.[43] 34-36 ^{o}C); the ^{1}H and ^{13}C NMR spectra match the literature data.[44]

4-Phenoxybenzyl alcohol (80). The indicated compound was obtained in a 36% yield as a white solid: mp 54-55 ^{o}C (lit.[45] 54.5 ^{o}C); ^{1}H NMR ($CDCl_3$, 300 MHz) δ 1.93 (s, 1H), 4.64 (s, 2H), 7.00 (dd, J = 9.0, 2.1 Hz, 4H), 7.09 (t, J = 7.2 Hz, 1H), 7.30-7.35 (m, 4H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 65.1, 119.1, 119.2, 123.5, 128.9, 130.0, 135.9, 157.0,

157.4; IR ($CDCl_3$, cm^{-1}) 3385, 063, 3053, 2949, 2887, 1591, 1491; HRMS m/z 200.0840 (calcd $C_{13}H_{12}O_2$, 200.0836).

Diphenyl sulfide (81). The indicated compound was obtained in a 70% yield as a colorless oil; the ^1H and ^{13}C NMR spectra match the literature data.[46]

3-Methoxyphenyl phenyl sulfide (82). The indicated compound was obtained in a 66% yield as a colorless oil; ^1H NMR ($CDCl_3$, 300 MHz) δ 3.74 (s, 3H), 6.74-6.78 (m, 1H), 6.85-6.92 (m, 2H), 7.17-7.38 (m, 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 55.5, 113.0, 116.1, 123.2, 127.5, 129.5, 130.2, 131.7, 135.5, 137.5, 160.3; IR ($CDCl_3$, cm^{-1}) 3059, 3002, 2957, 2935, 2833, 1588, 1476; HRMS m/z 216.0611 (calcd $C_{13}H_{12}OS$, 216.0608).

Phenyl 2-methoxybenzoate (87). The indicated compound was obtained in an 84% yield as a pale yellow solid: mp 54-56 ^oC; ^1H NMR ($CDCl_3$, 300 MHz) δ 3.92 (s, 3H), 7.01-7.06 (m, 2H), 7.20-7.27 (m, 3H), 7.38-7.56 (m, 3H), 8.00 (d, J = 7.2 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 56.3, 112.5, 120.4, 122.1, 125.9, 129.6, 132.4, 134.5, 151.2, 160.1, 164.6; IR ($CDCl_3$, cm^{-1}) 3071, 2963, 2941, 2839, 1743, 1487; HRMS m/z 228.0789 (calcd $C_{14}H_{12}O_3$, 228.0786).

3,4-Dimethylphenyl 4-iodobenzoate (88). The indicated compound was obtained in an 81% yield as a pale yellow solid: mp 79-80 ^oC; ^1H NMR ($CDCl_3$, 300 MHz) δ 2.28 (s, 3H), 2.29 (s, 3H), 6.93 (dd, J = 6.1, 2.4 Hz, 1H), 6.99 (d, J = 2.4 Hz, 1H), 7.18 (d, J = 8.1 Hz, 1H), 7.85-7.93 (m, 4H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 19.5, 20.2, 101.7, 118.8, 122.7, 129.5, 130.7, 131.7, 134.6, 138.1, 138.3, 148.9, 165.3; IR ($CDCl_3$, cm^{-1}) 3085, 2970, 2935, 1728; HRMS m/z 351.9965 (calcd $C_{15}H_{13}IO_2$, 351.9960).

Phenyl 2-iodo-5-methylbenzoate (90). The indicated compound was obtained in an 89% yield as a yellow oil; ^1H NMR ($CDCl_3$, 300 MHz) δ 2.37 (s, 3H), 7.01-7.05 (m, 1H), 7.24-7.29 (m, 3H), 7.40-7.45 (m, 2H), 7.83 (d, J = 1.8 Hz, 1H), 7.91 (d, J = 8.1 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 21.1, 90.7, 121.8, 126.3, 129.7, 132.5, 134.5, 138.5, 141.6,

151.0, 165.3; IR ($CDCl_3$, cm^{-1}) 3059, 3042, 2952, 2921, 2854, 1742, 1591; HRMS m/z 337.9808 (calcd $C_{14}H_{11}IO_2$, 337.9803).

Phenyl phenylacetate (92). The indicated compound was obtained in a 45% yield as a white solid: mp 39-40 ^oC (lit.[47] 40-41.5 ^oC); the ^1H NMR spectrum matches the literature data.[47]

Phenyl benzenesulfonate (93). The indicated compound was obtained in a 33 % yield as a colorless oil: ^{13}C NMR (75 MHz, $CDCl_3$) δ 120.7, 122.6, 127.4, 128.7, 129.3, 129.8, 134.4, 149.8. The ^1H NMR spectrum matches the literature data.[48]

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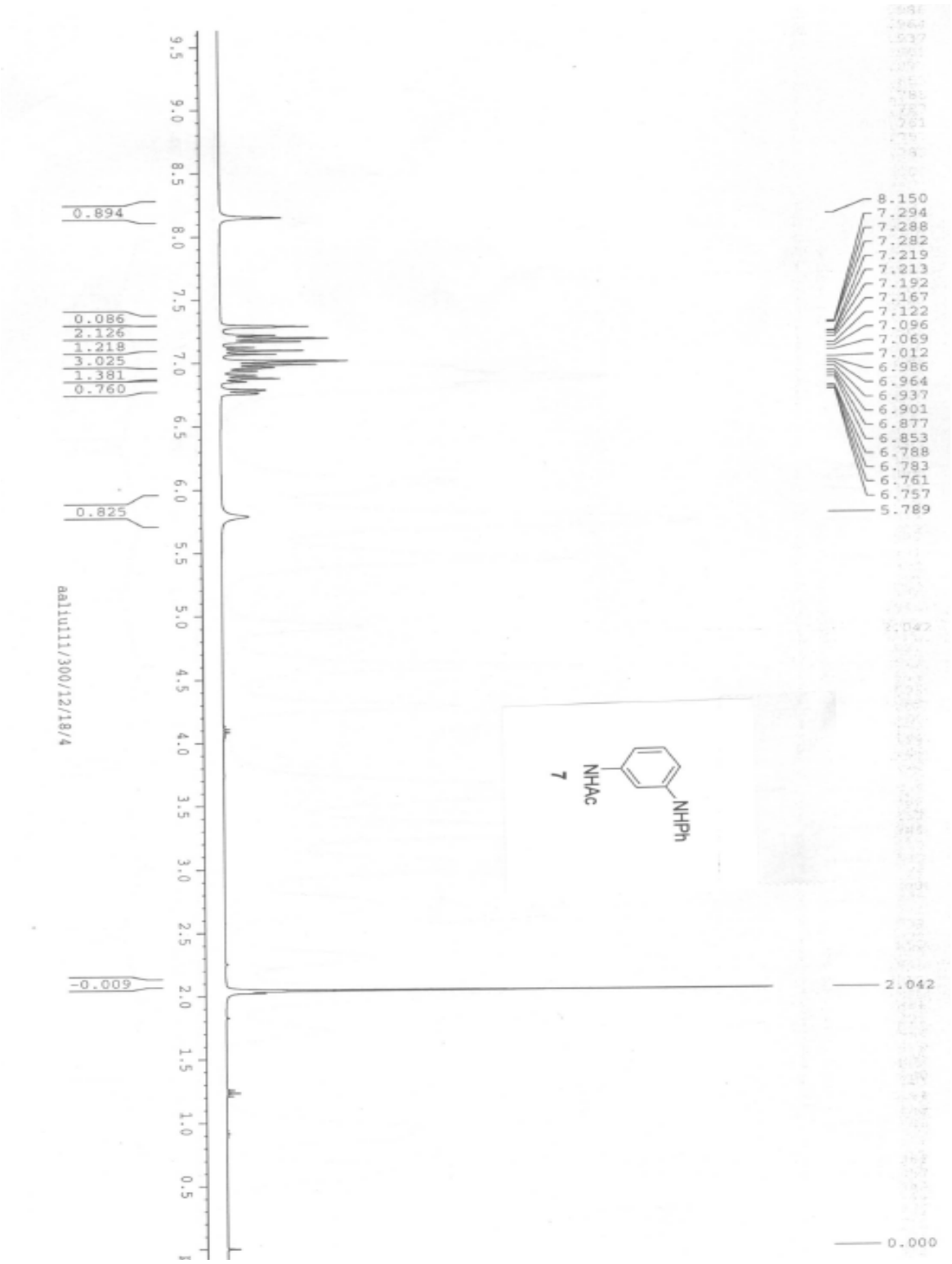
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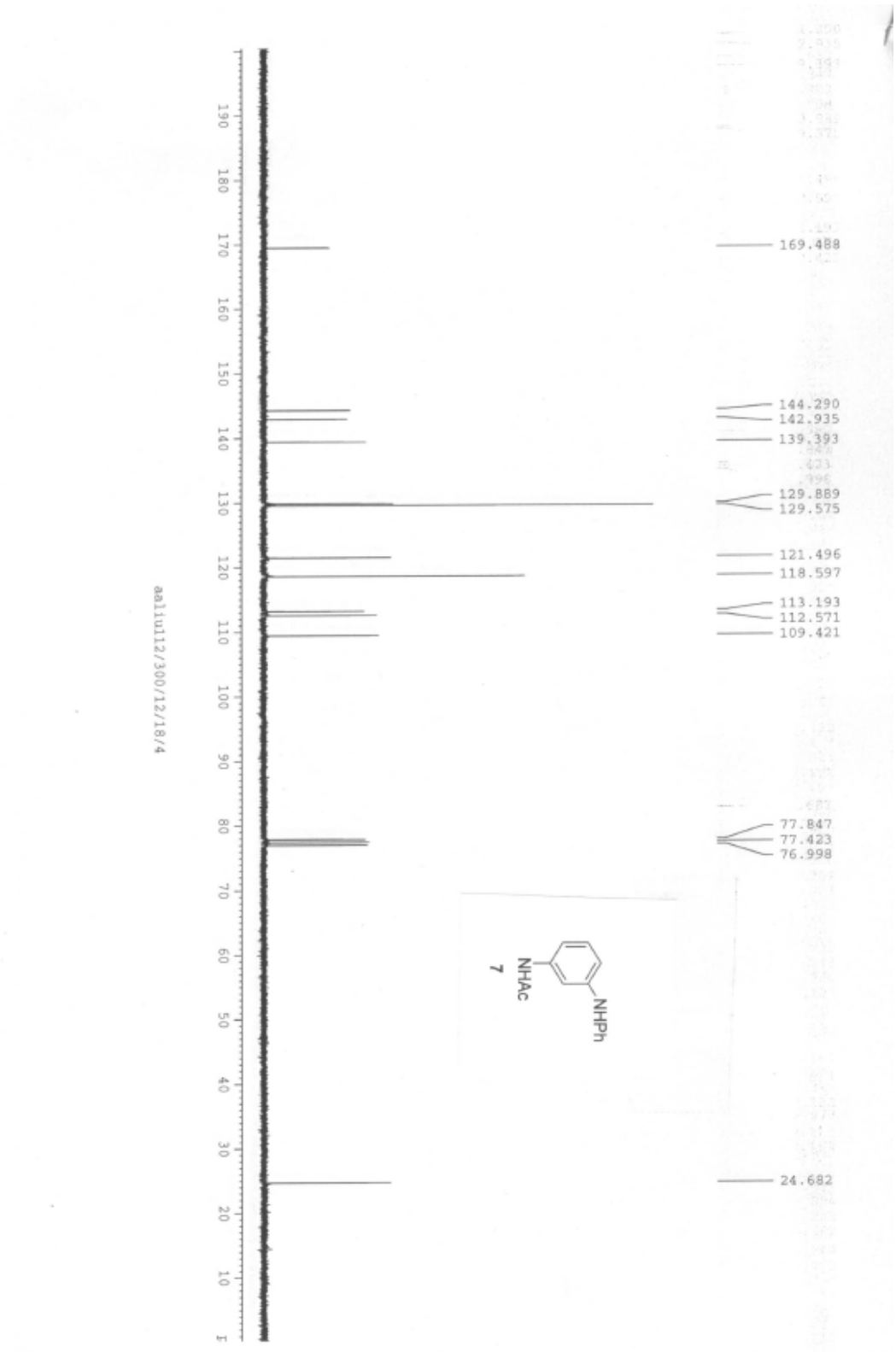
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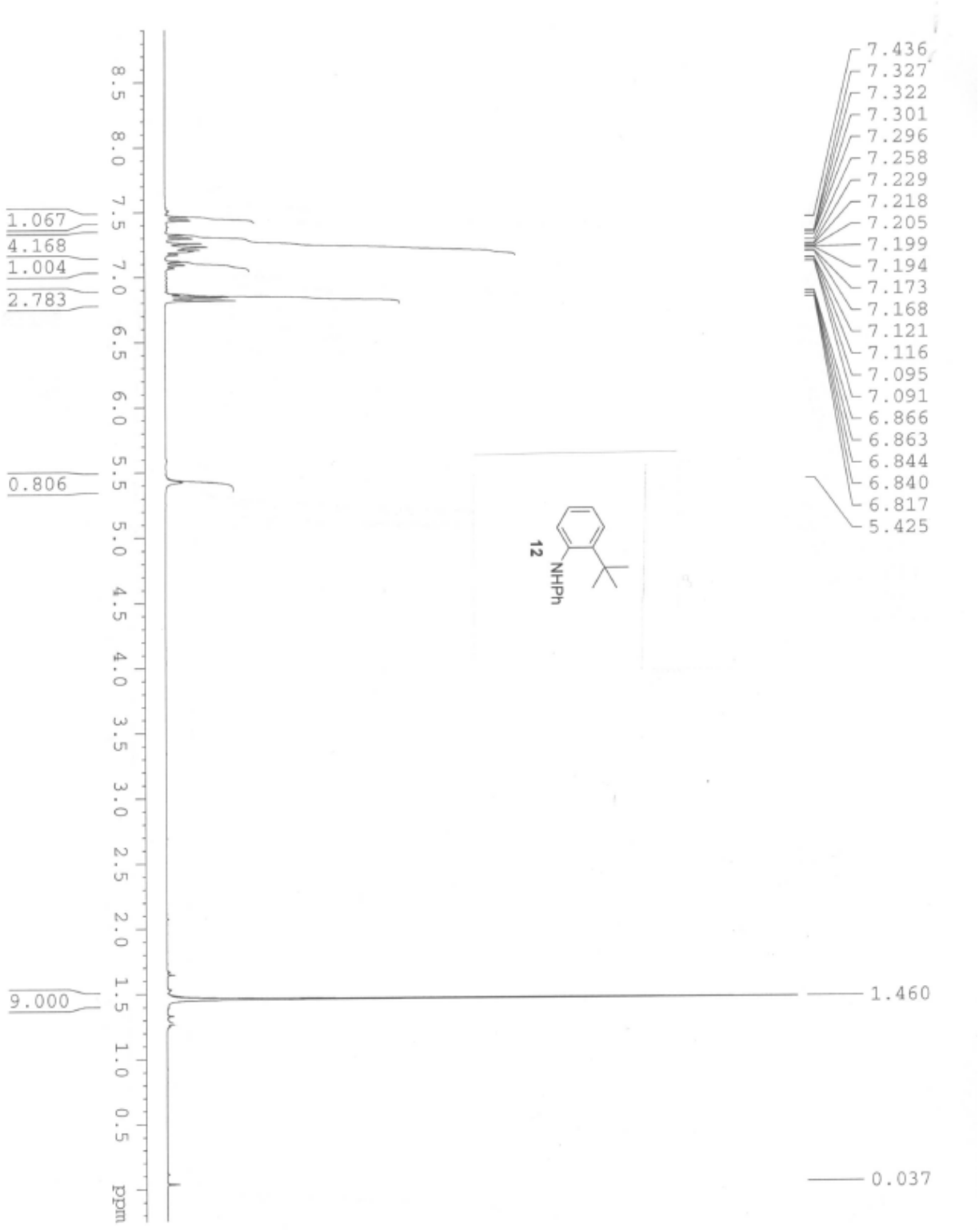
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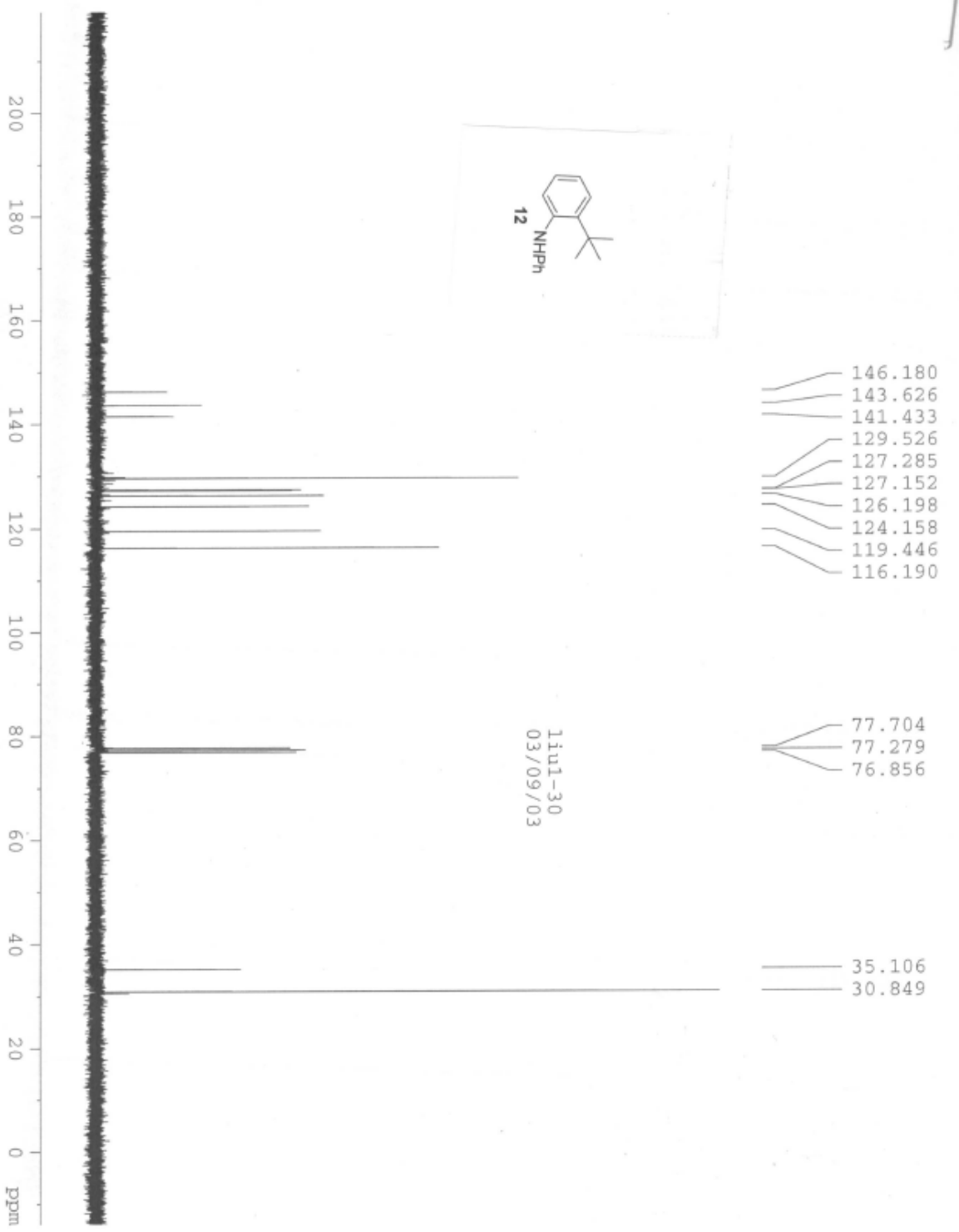
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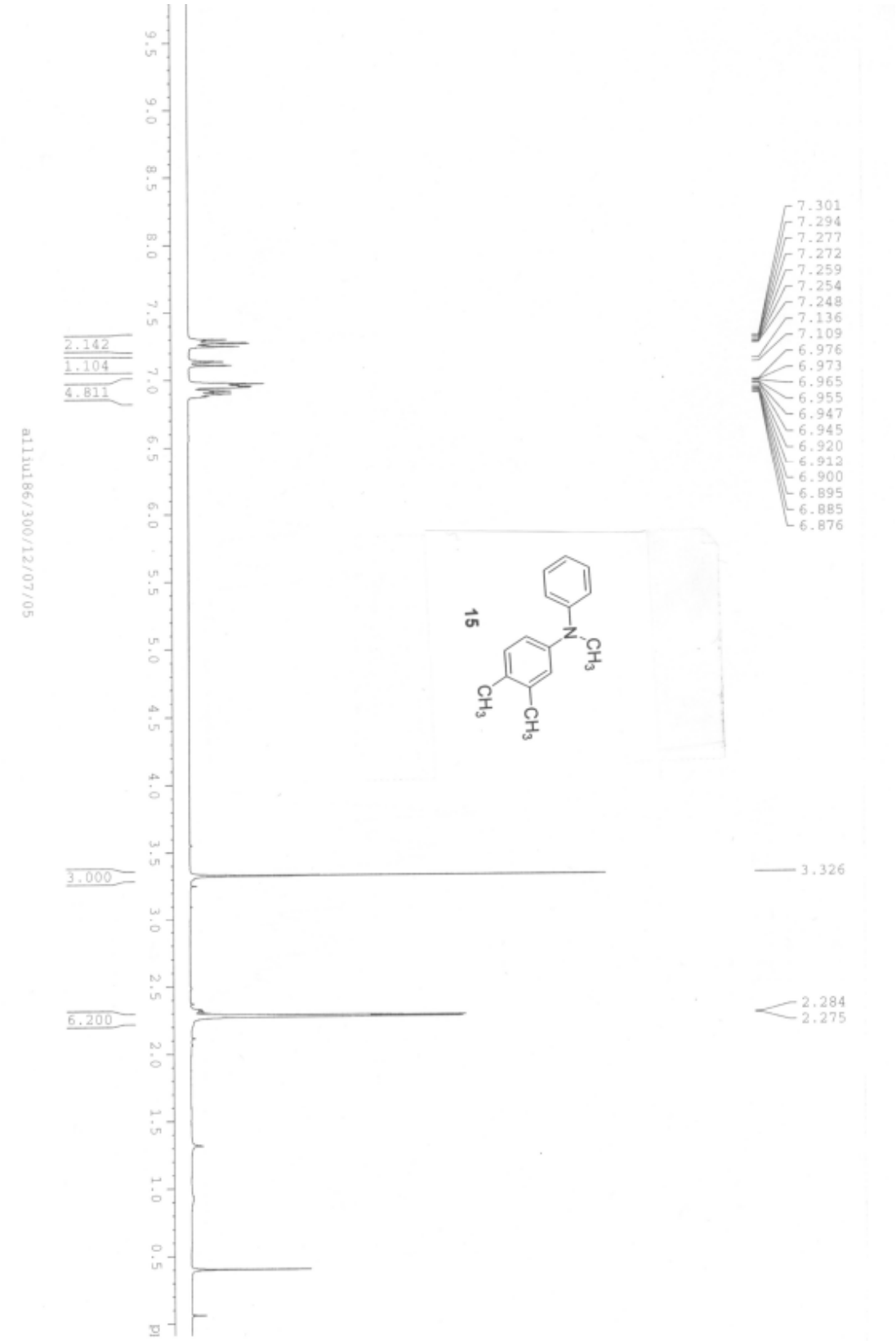
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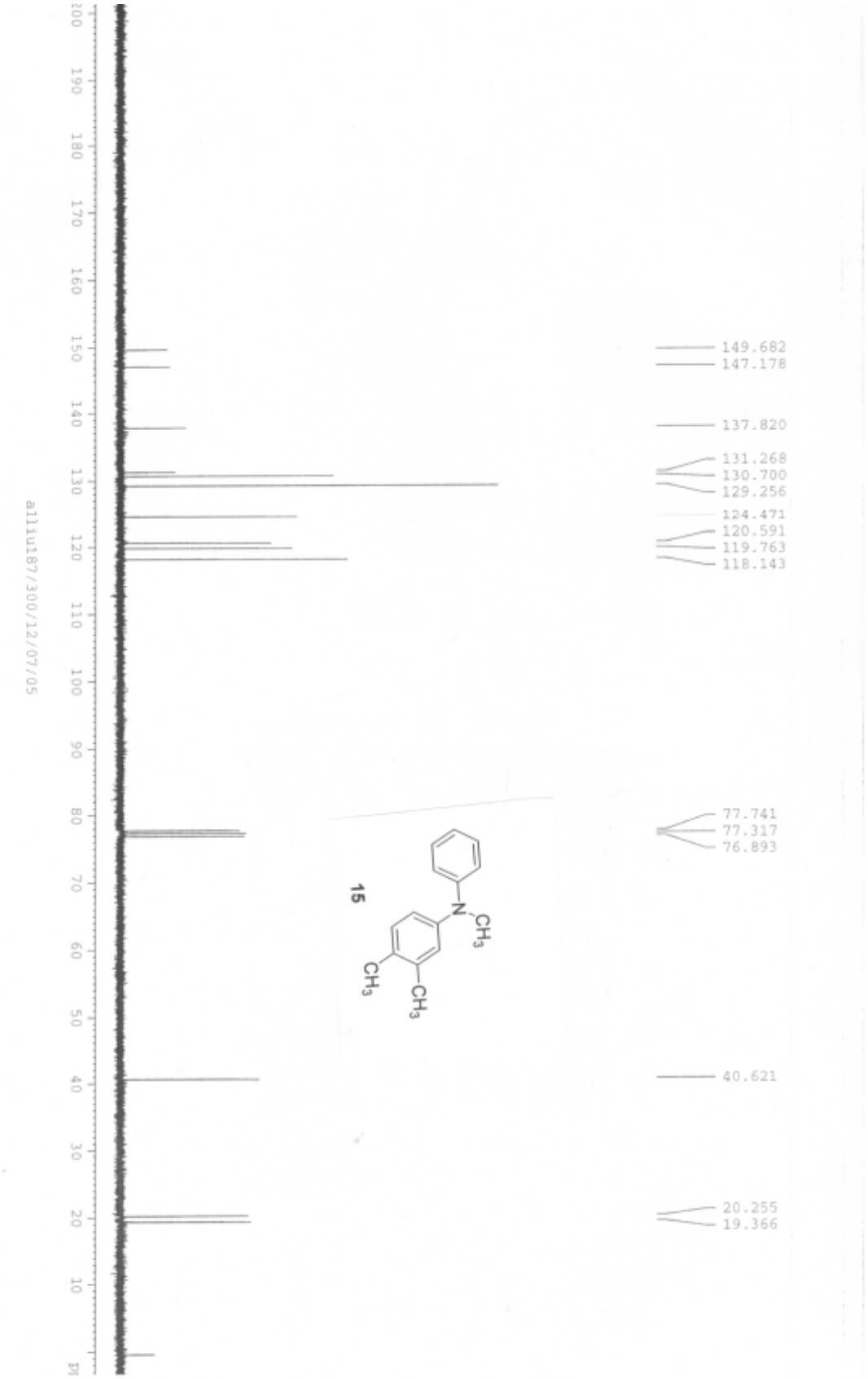
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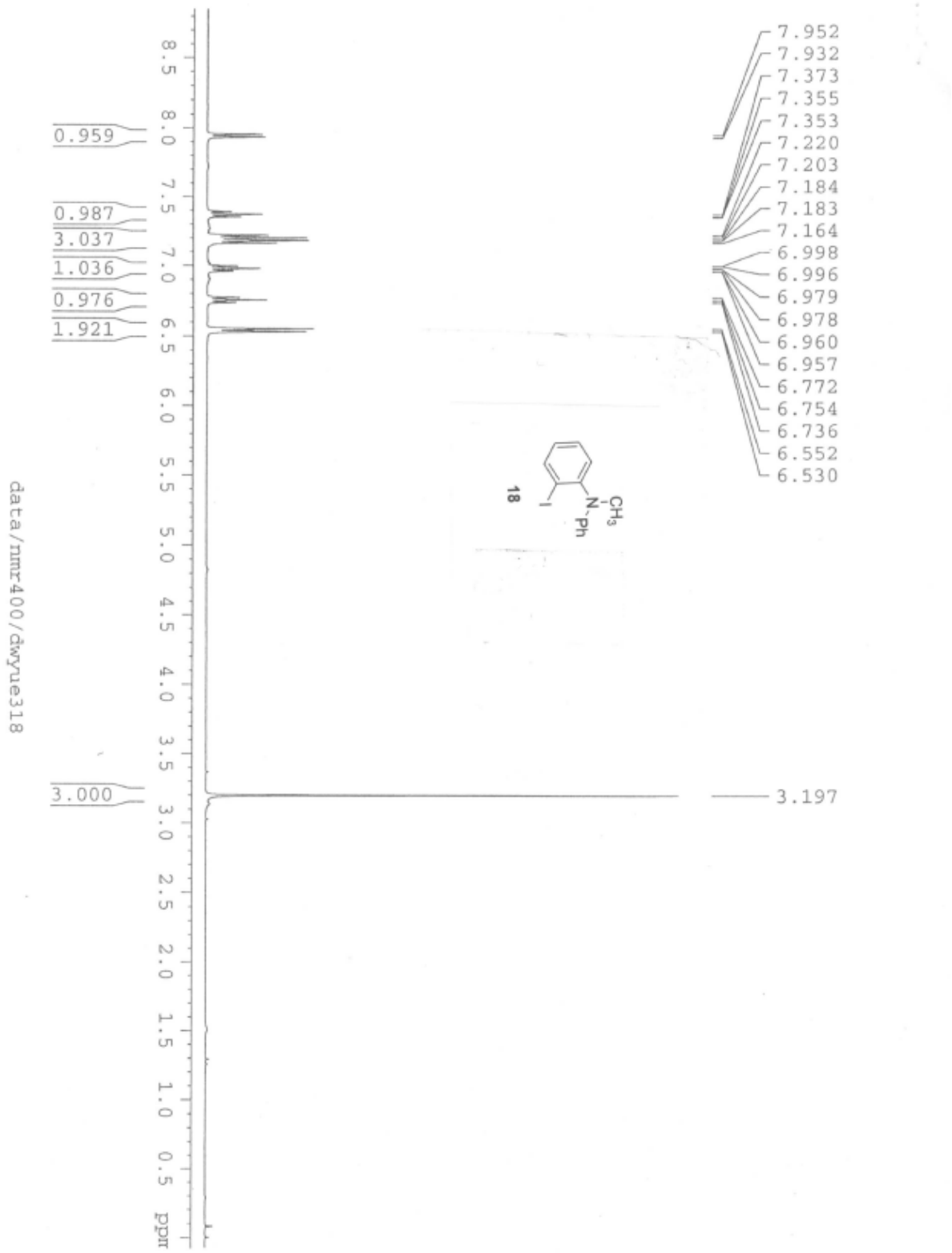
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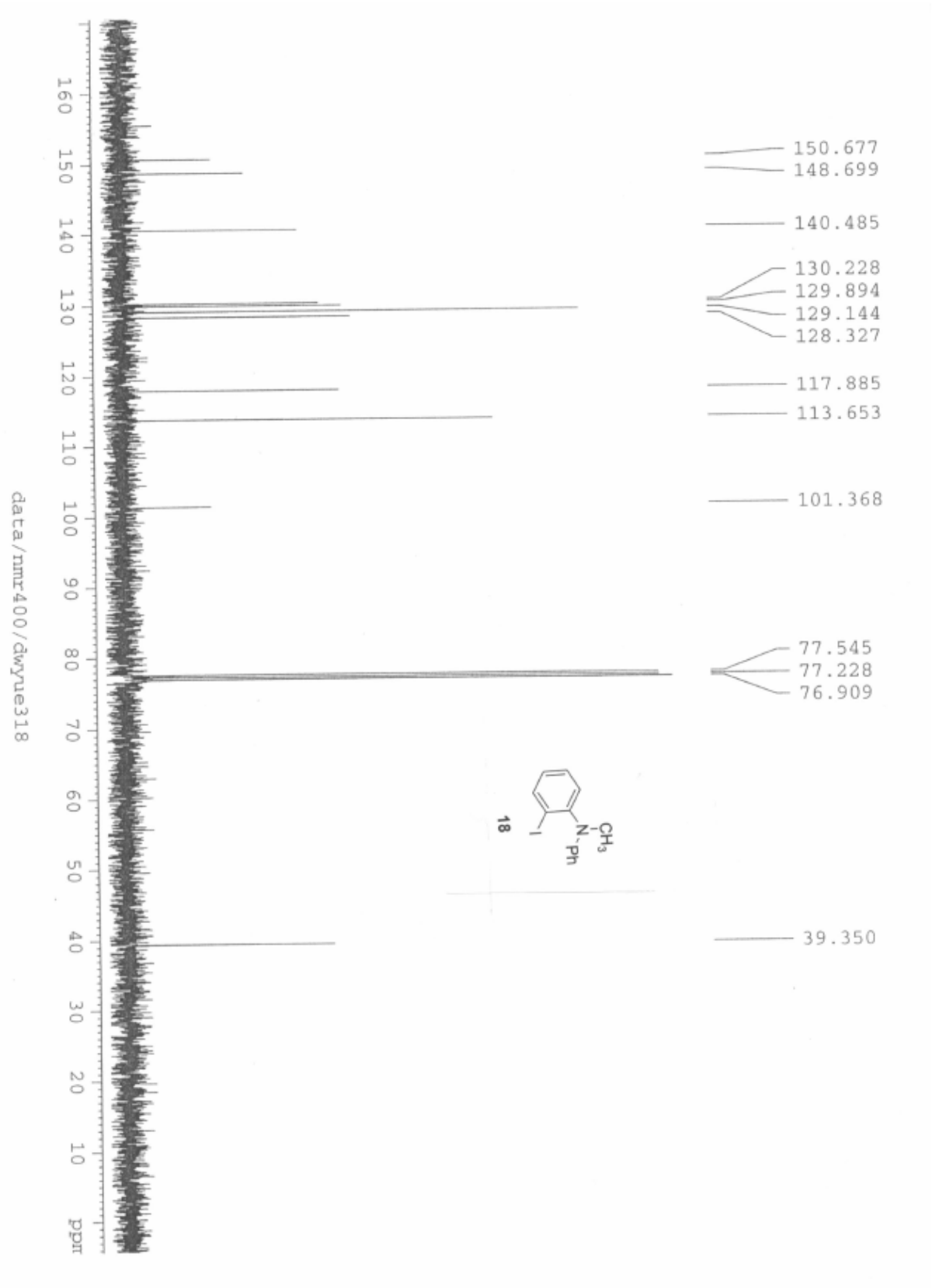
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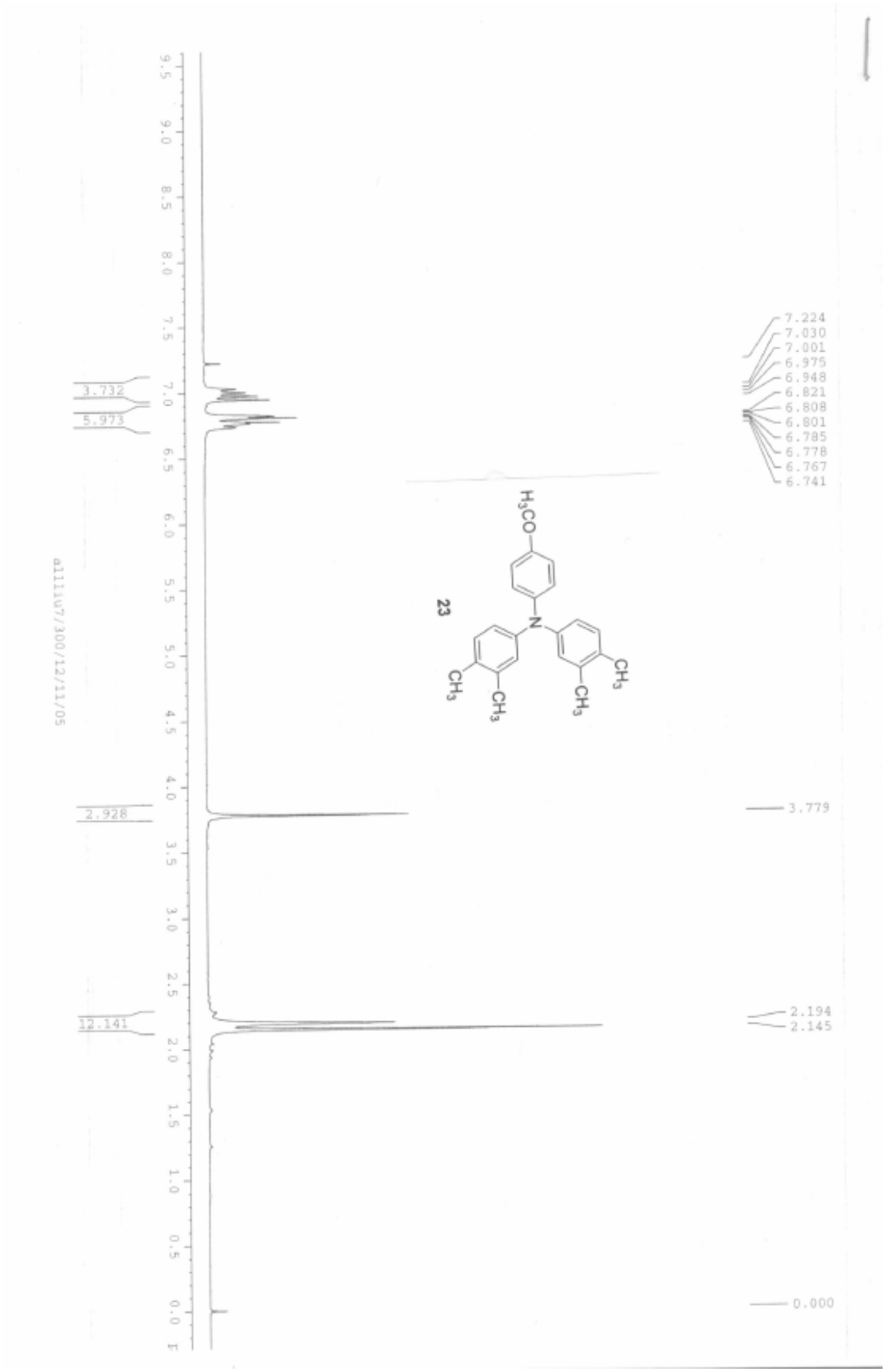
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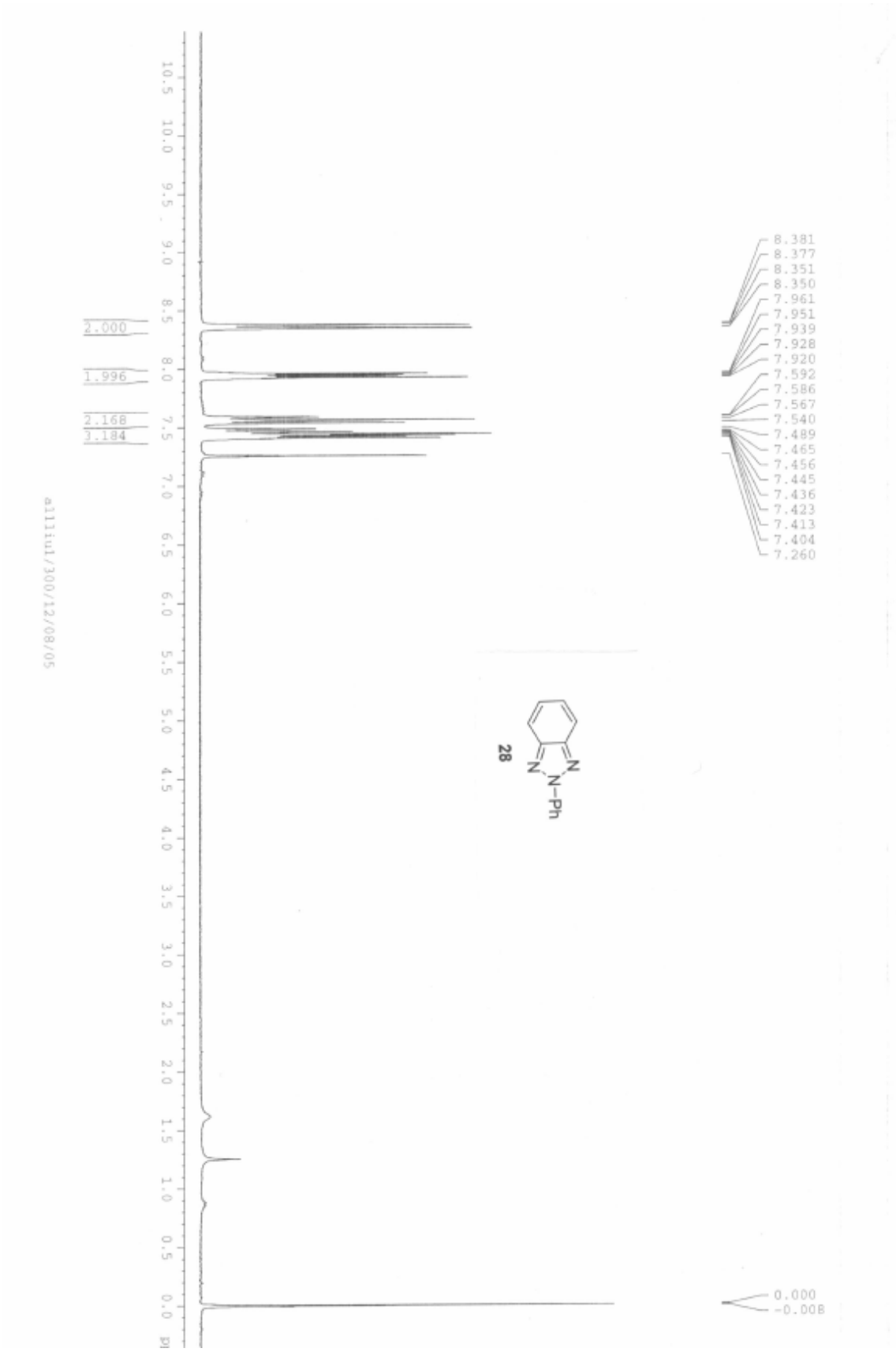
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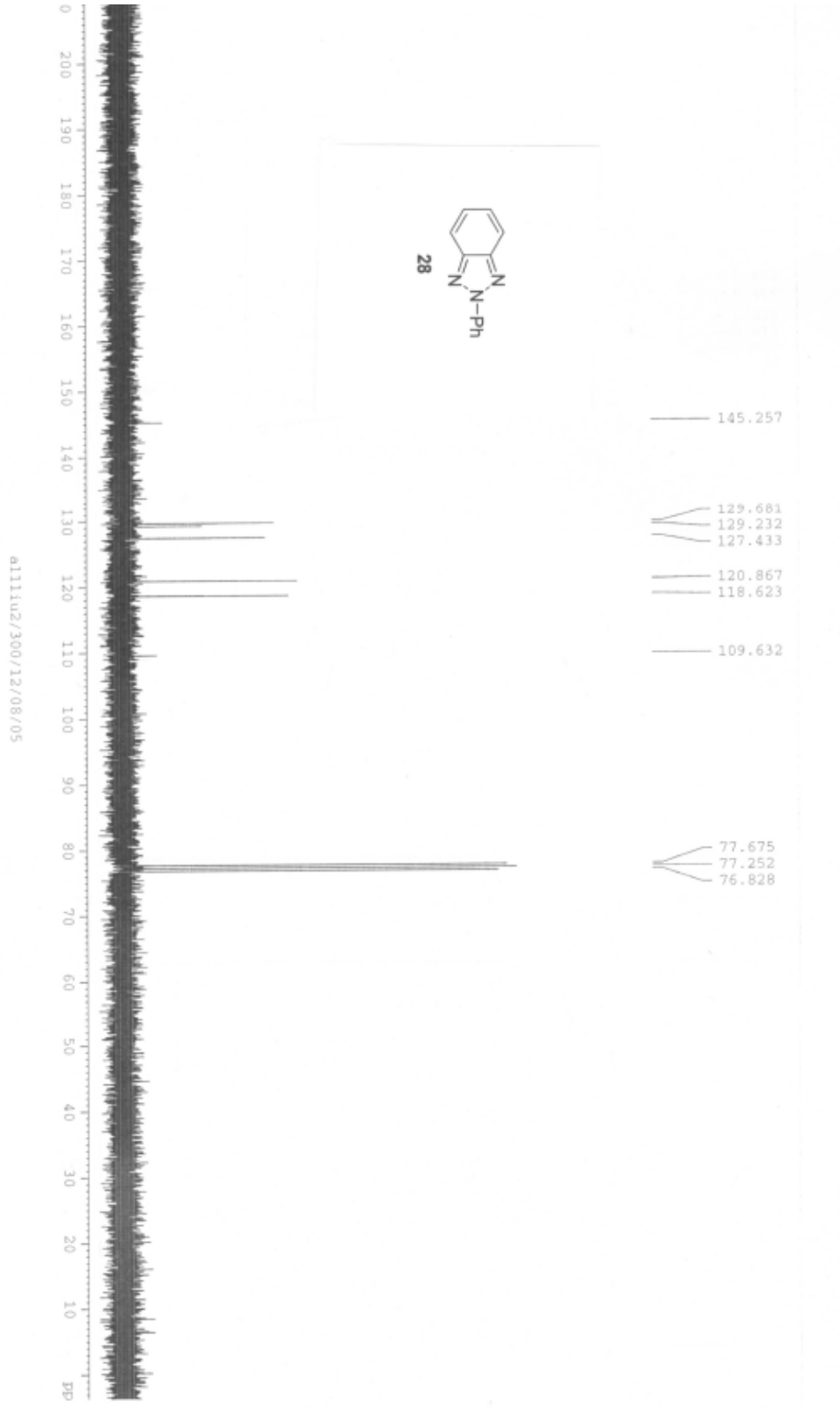
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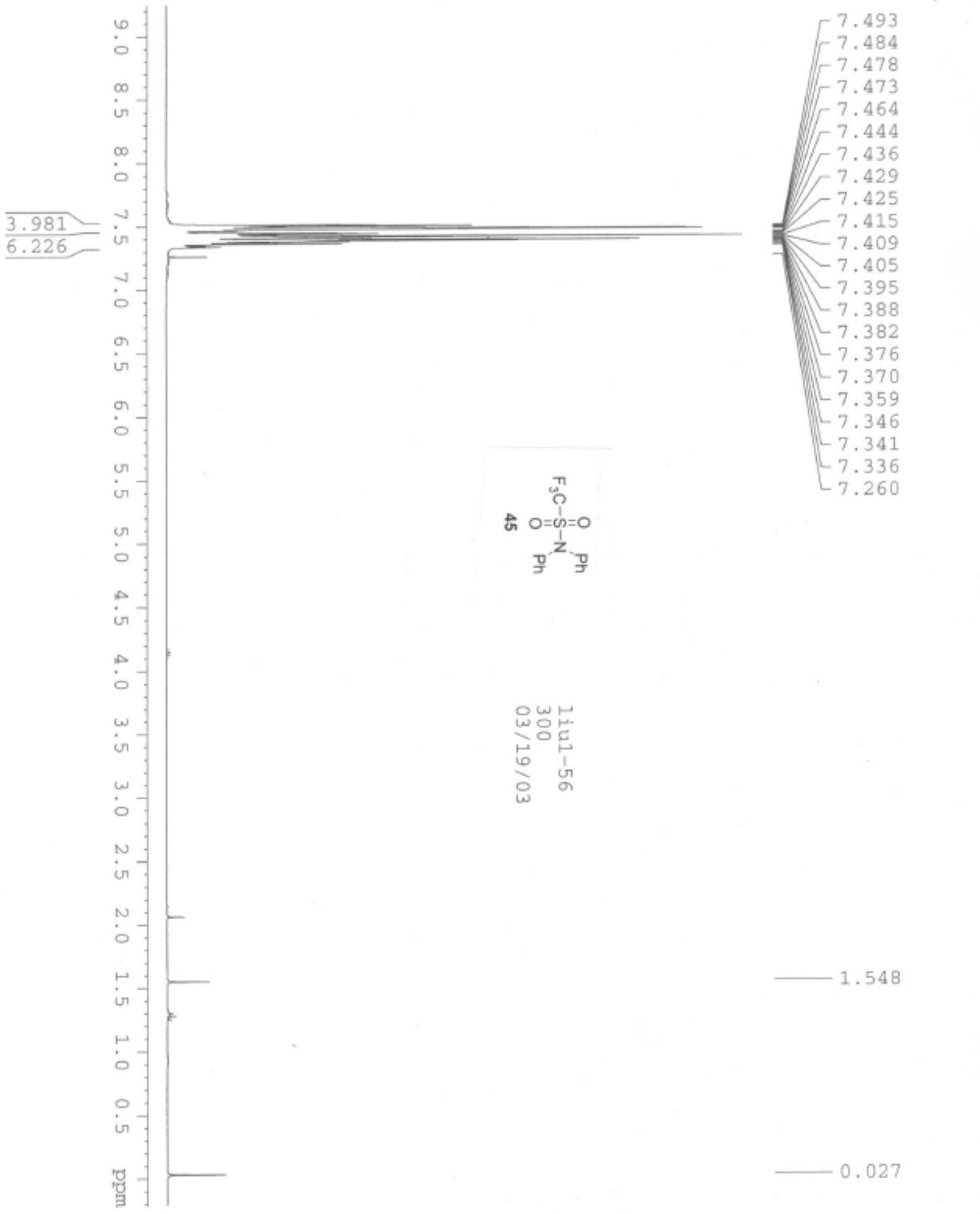
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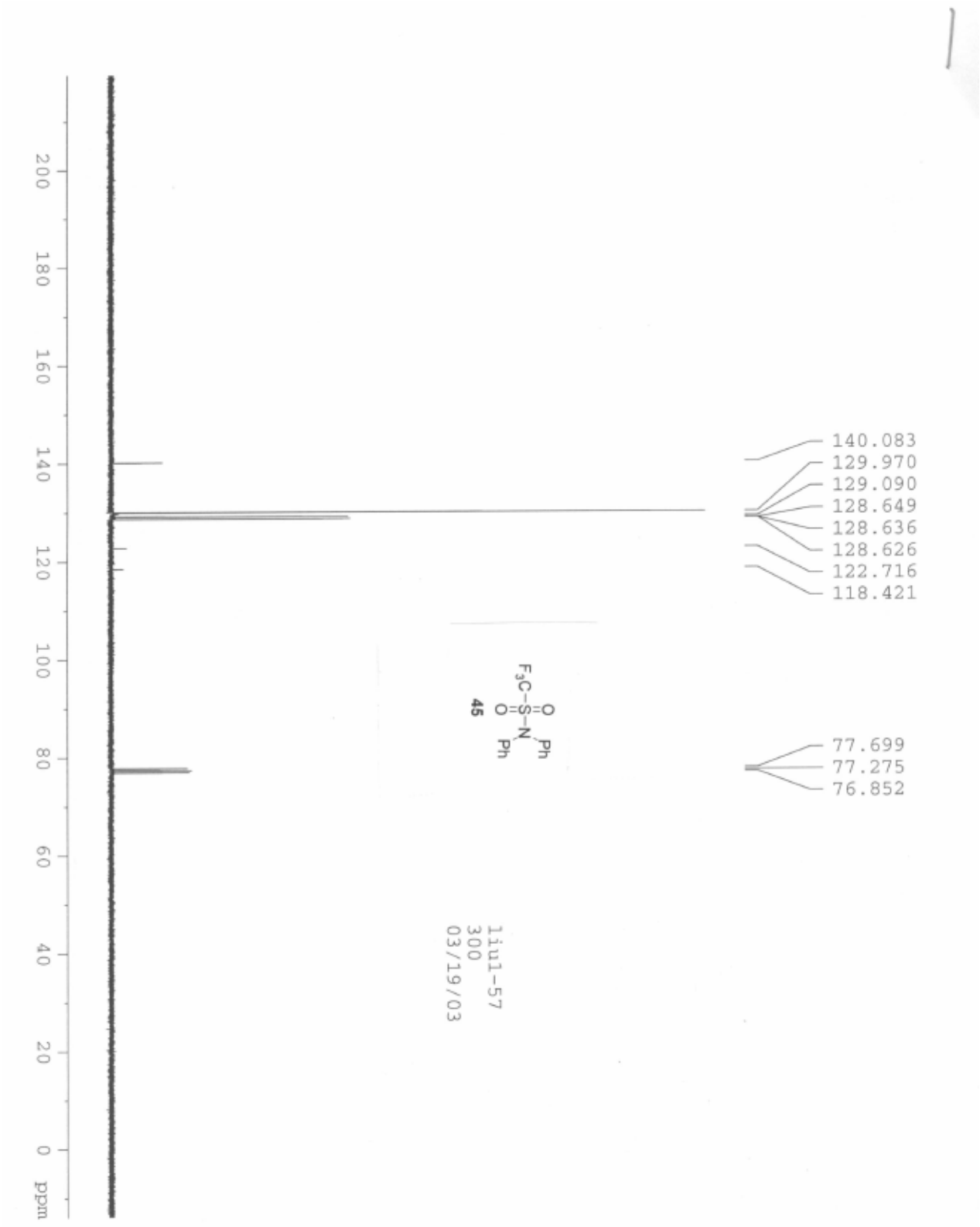
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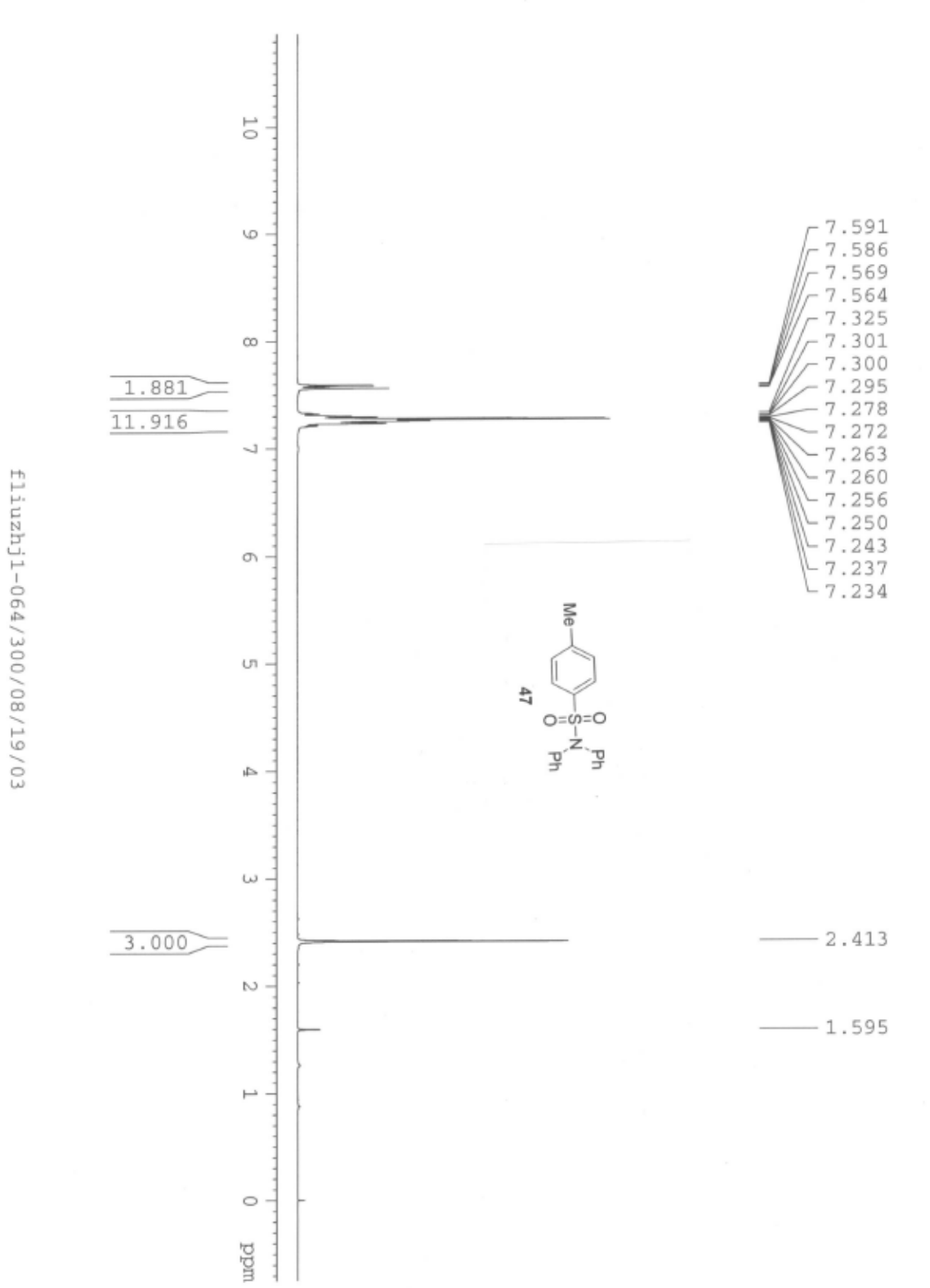
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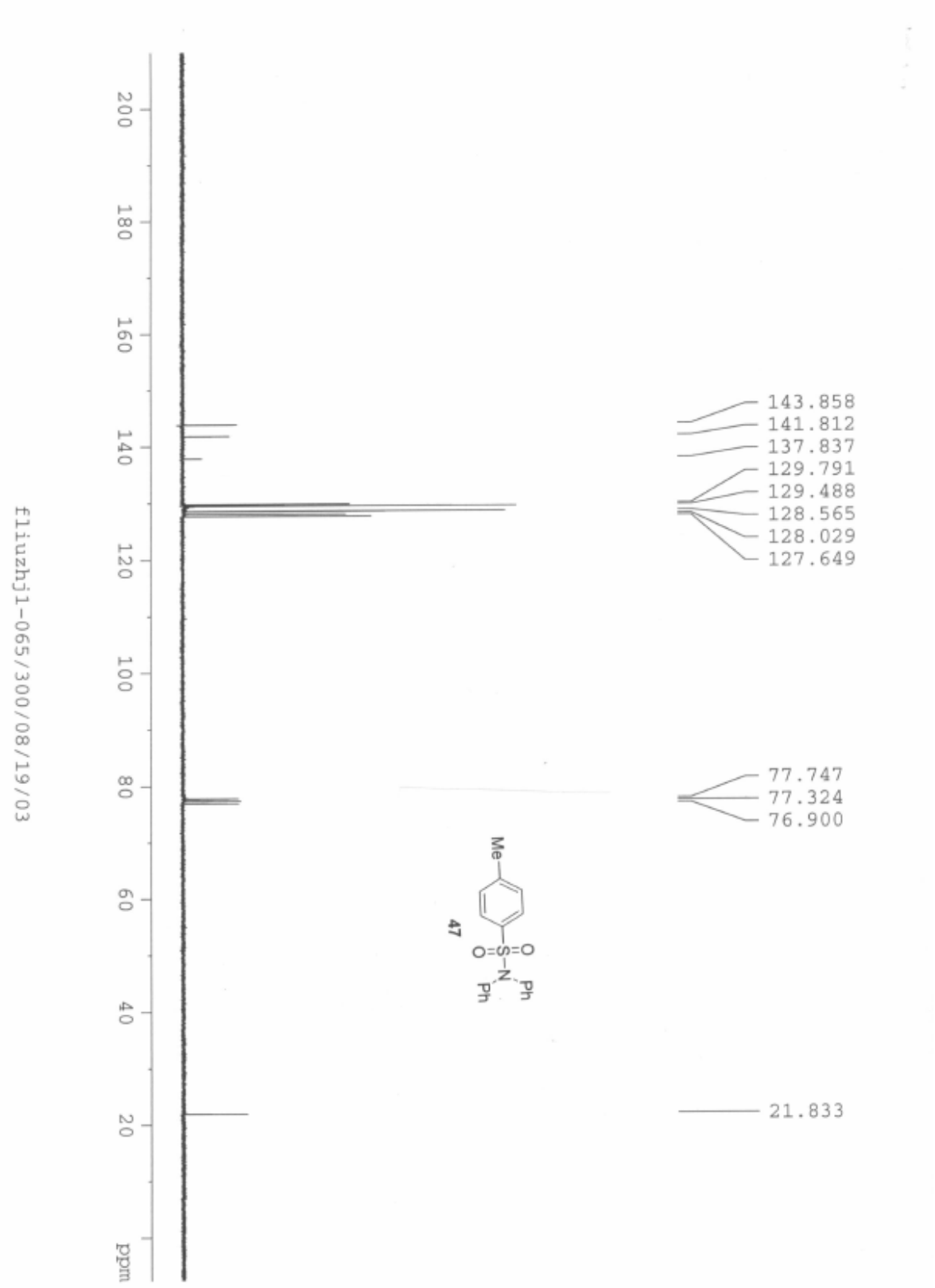
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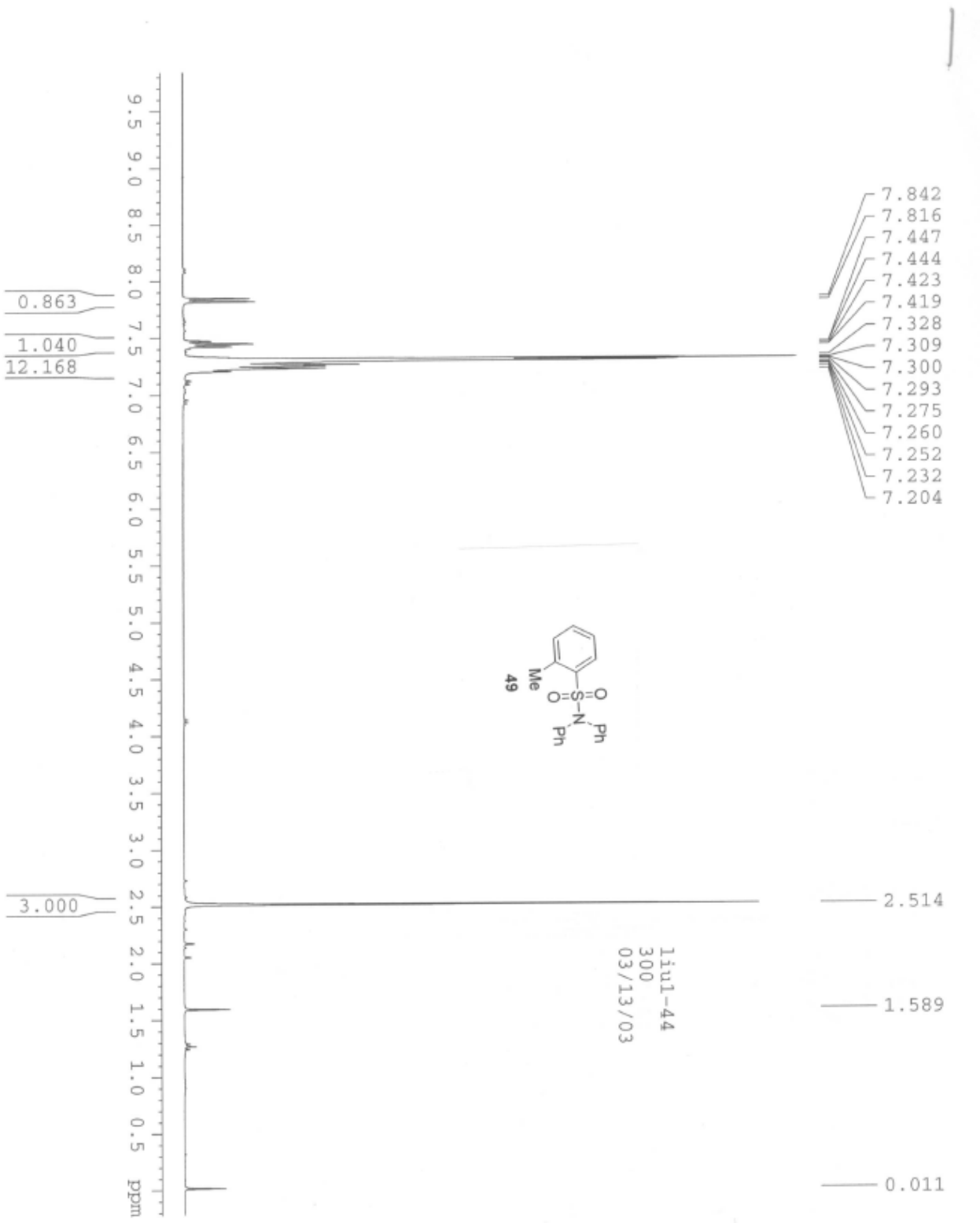
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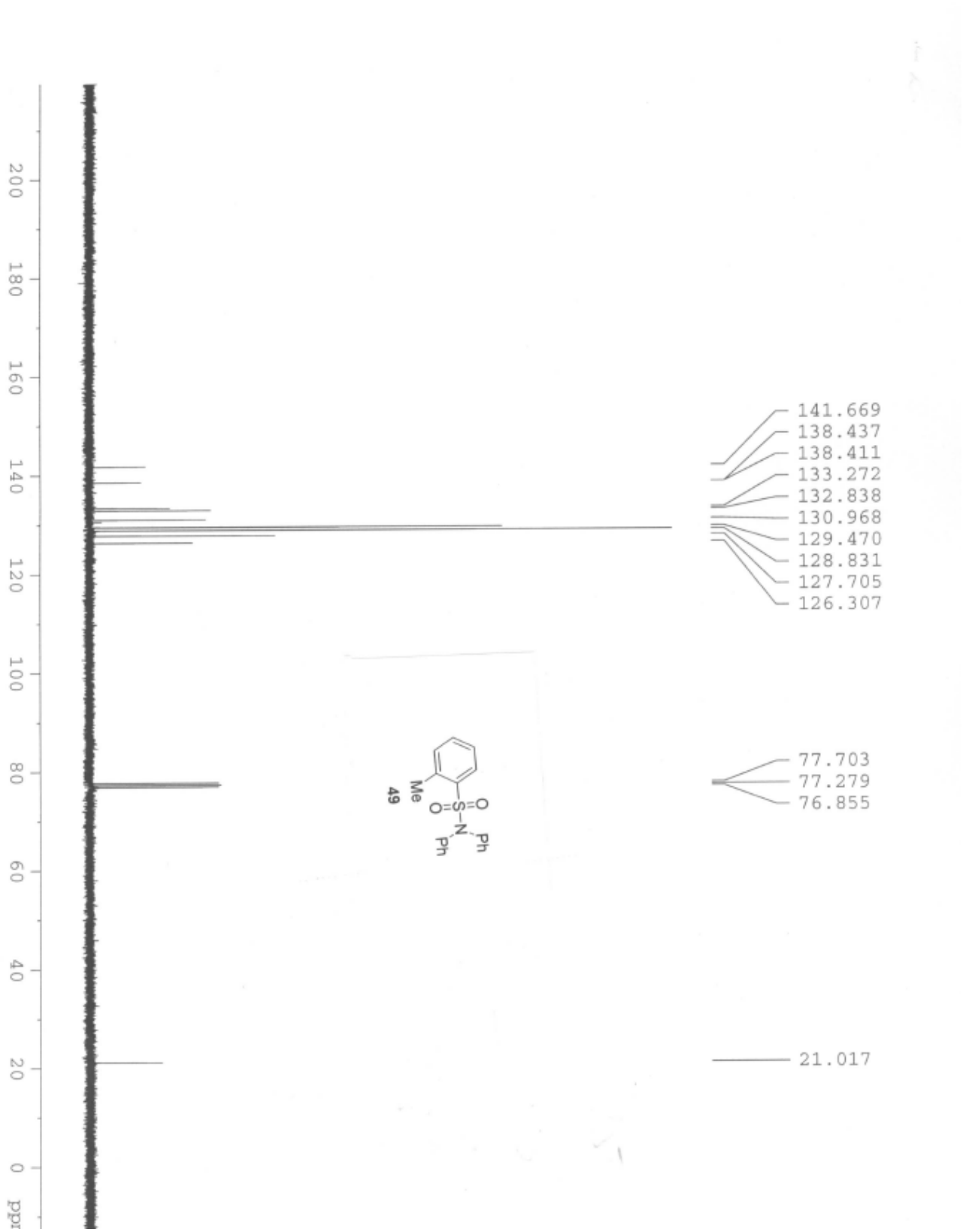
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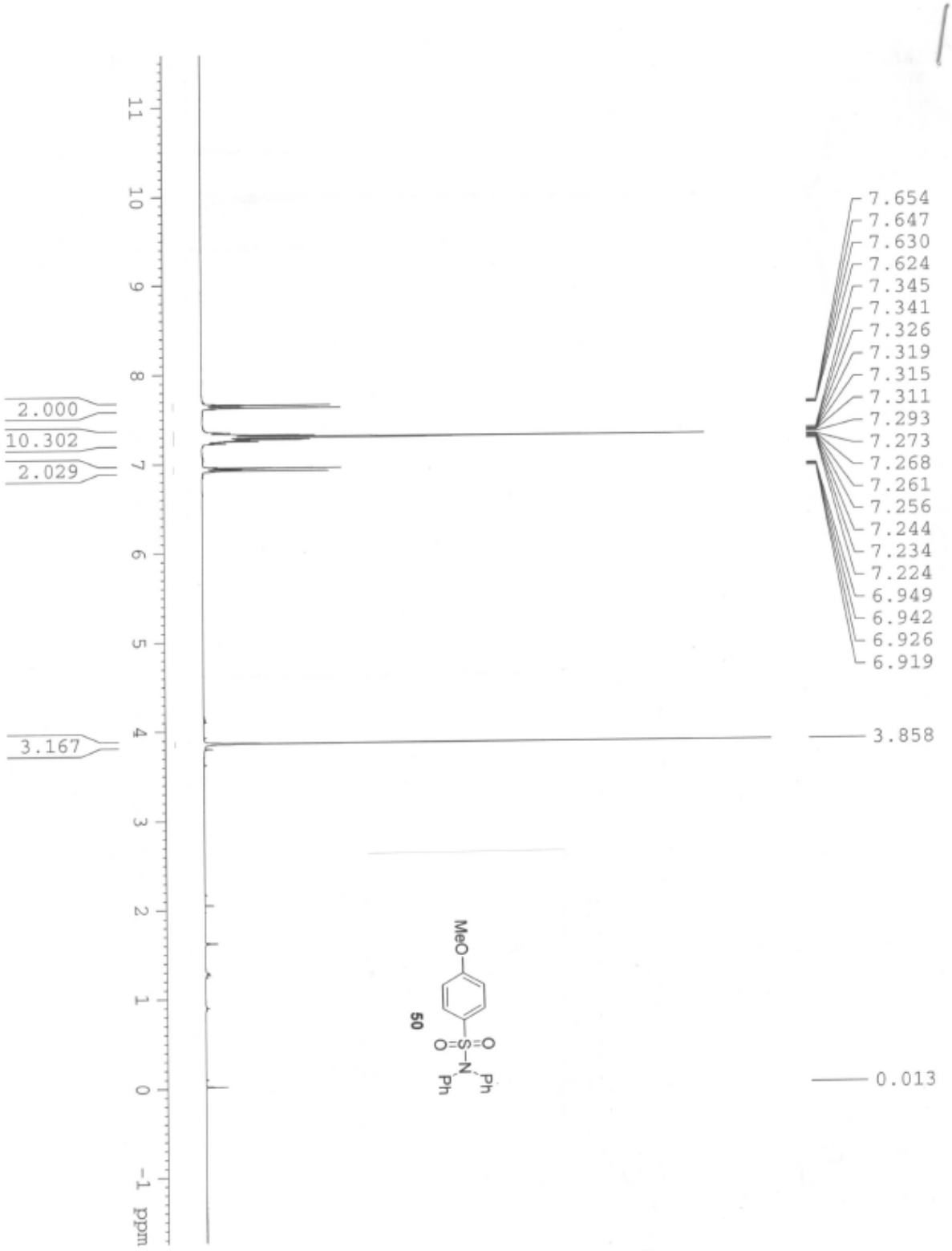
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7.319
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7.293
7.273
7.268
7.261
7.256
7.244
7.234
7.224
6.949
6.942
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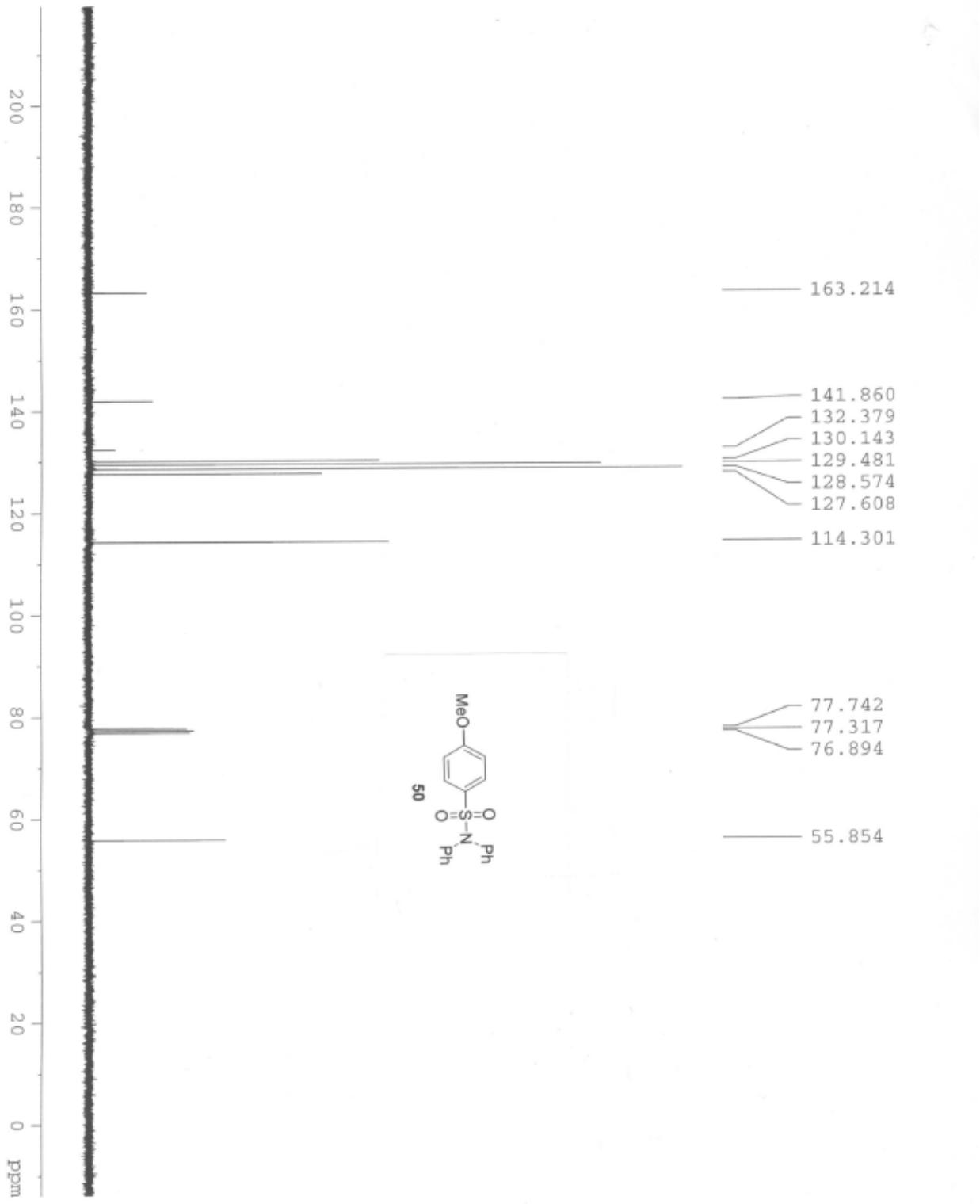
10.302
2.029
3.167
3.858
0.013
MeO
50
Ph
Ph
ppm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20
0
ppm
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132.379
130.143
129.481
128.574
127.608
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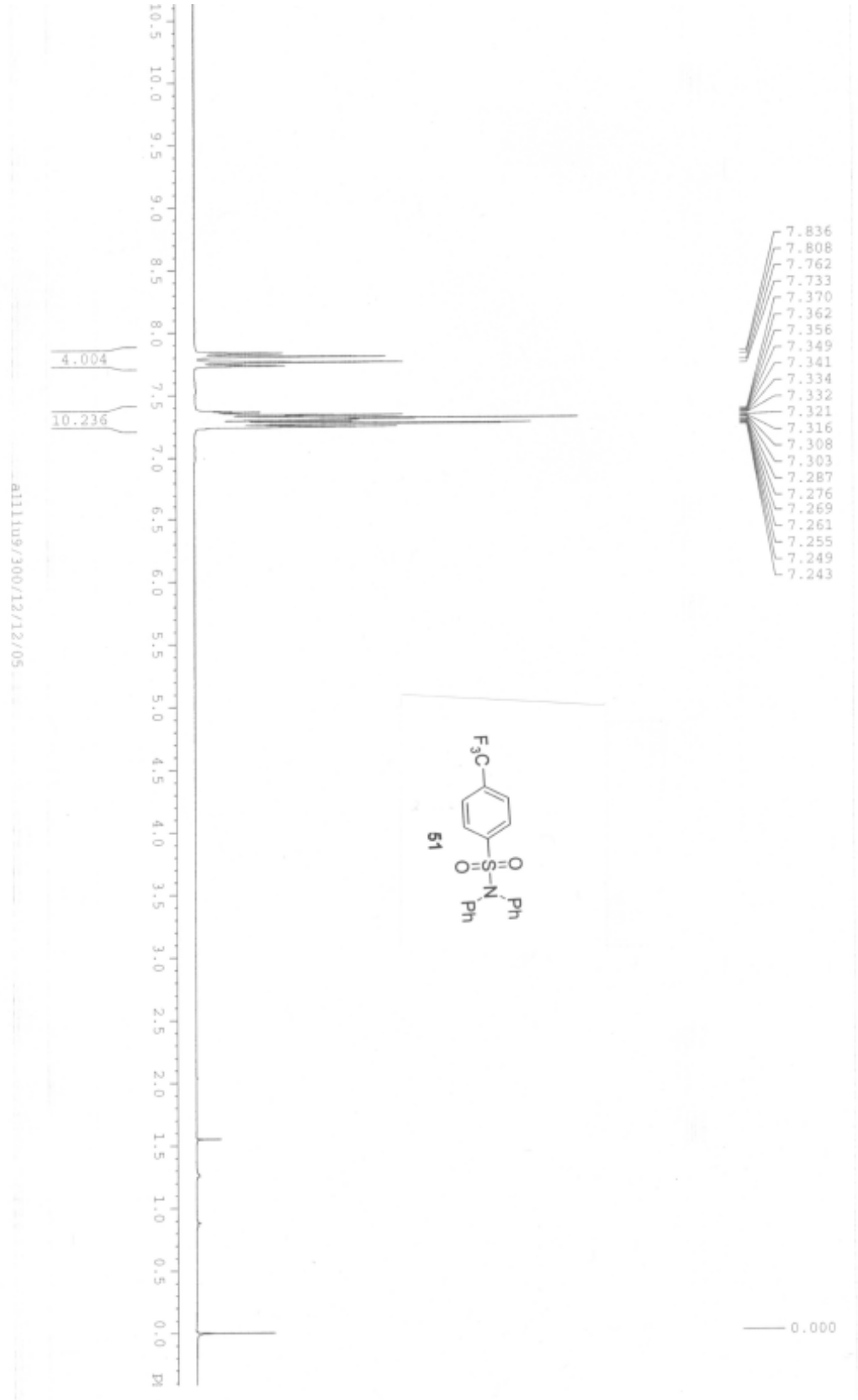
77.742
77.317
76.894
55.854
MeO
O
S
O
N
Ph
Ph
50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7.332
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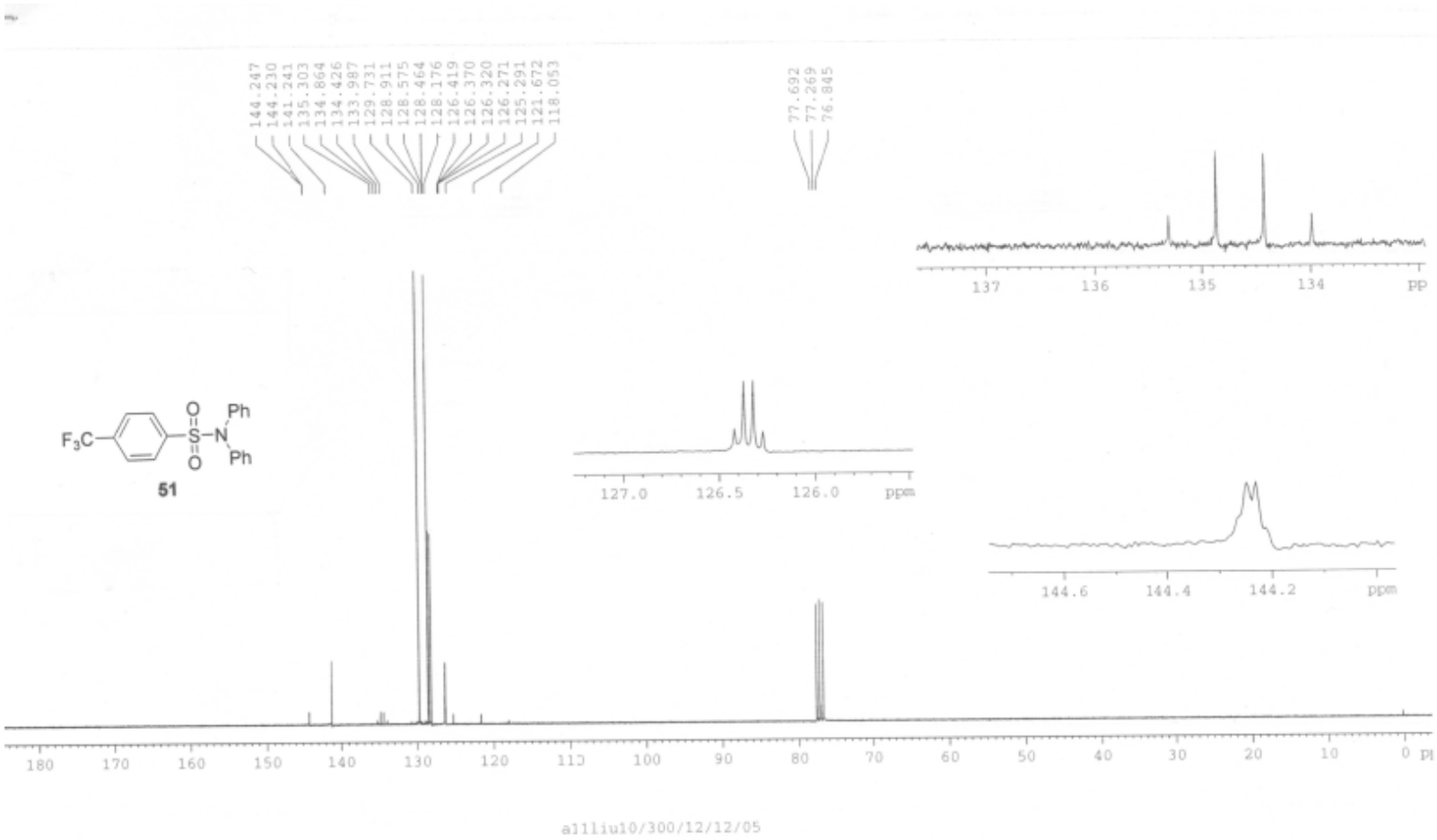
7.316
7.308
7.303
7.287
7.276
7.269
7.261
7.255
7.249
7.243
4.004
10.236
51
F3C
O
S
N
Ph
Ph
0.000
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
all11u9/300/12/12/05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126.419
126.370
126.320
126.271
125.291
121.672
118.053
77.692
77.269
76.845
137
136
135
134
127.0
126.5
126.0
144.6
144.4
144.2
ppm
180
170
160
150
140
130
120
100
90
80
70
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50
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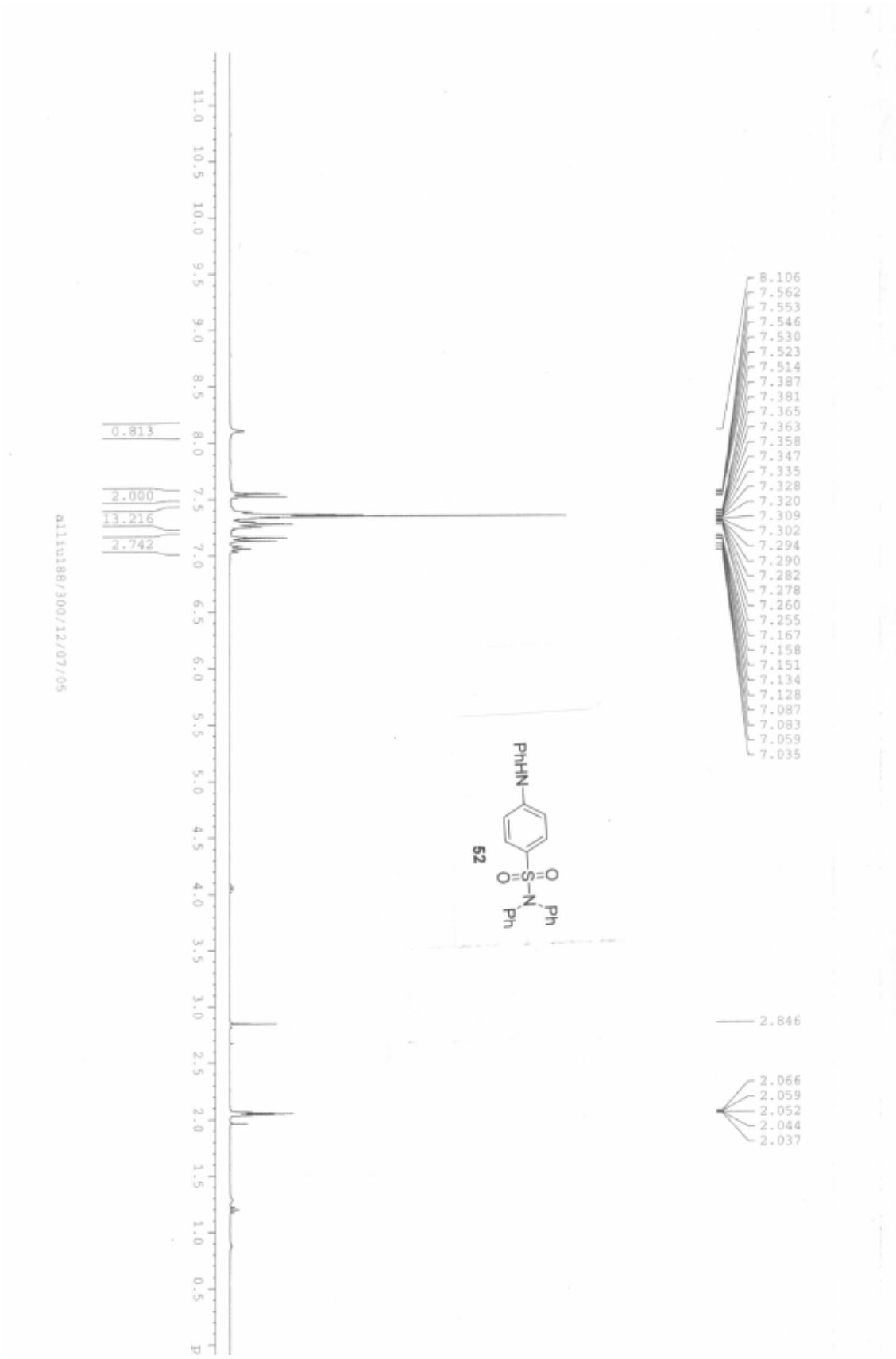
30
20
10
0
alliu10/300/12/12/05

O
Ph
F3C
S
N
O
Ph

51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7.358
7.347
7.335
7.328
7.320
7.309
7.302
7.294
7.290
7.282
7.278
7.260
7.255
7.167
7.158
7.151
7.134
7.128
7.087
7.083
7.059
7.035
PhHN
52
O
S
N
Ph
Ph
2.846
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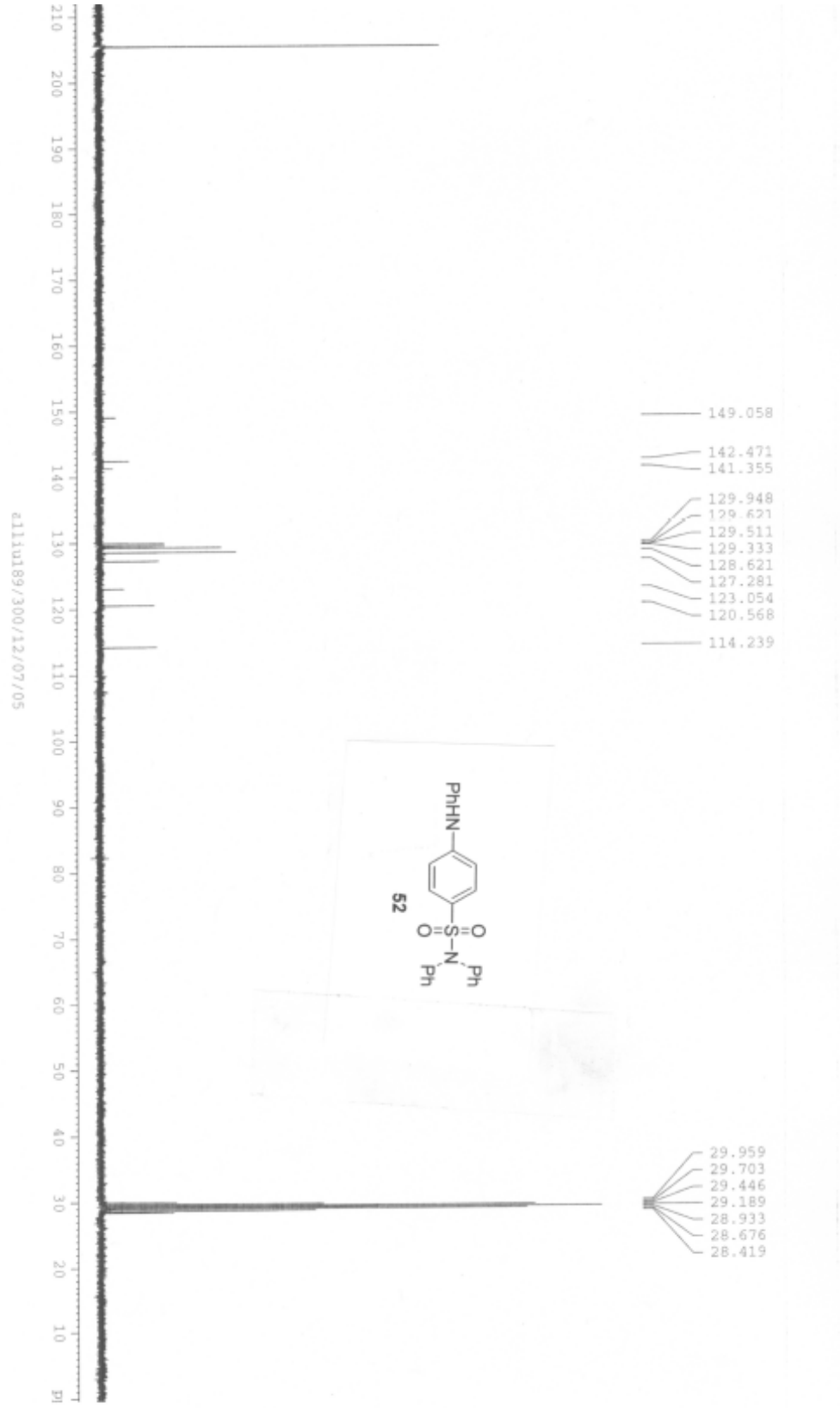
2.059
2.052
2.044
2.037
0.813
2.000
13.216
2.742
allin188/300/12/07/05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142.471
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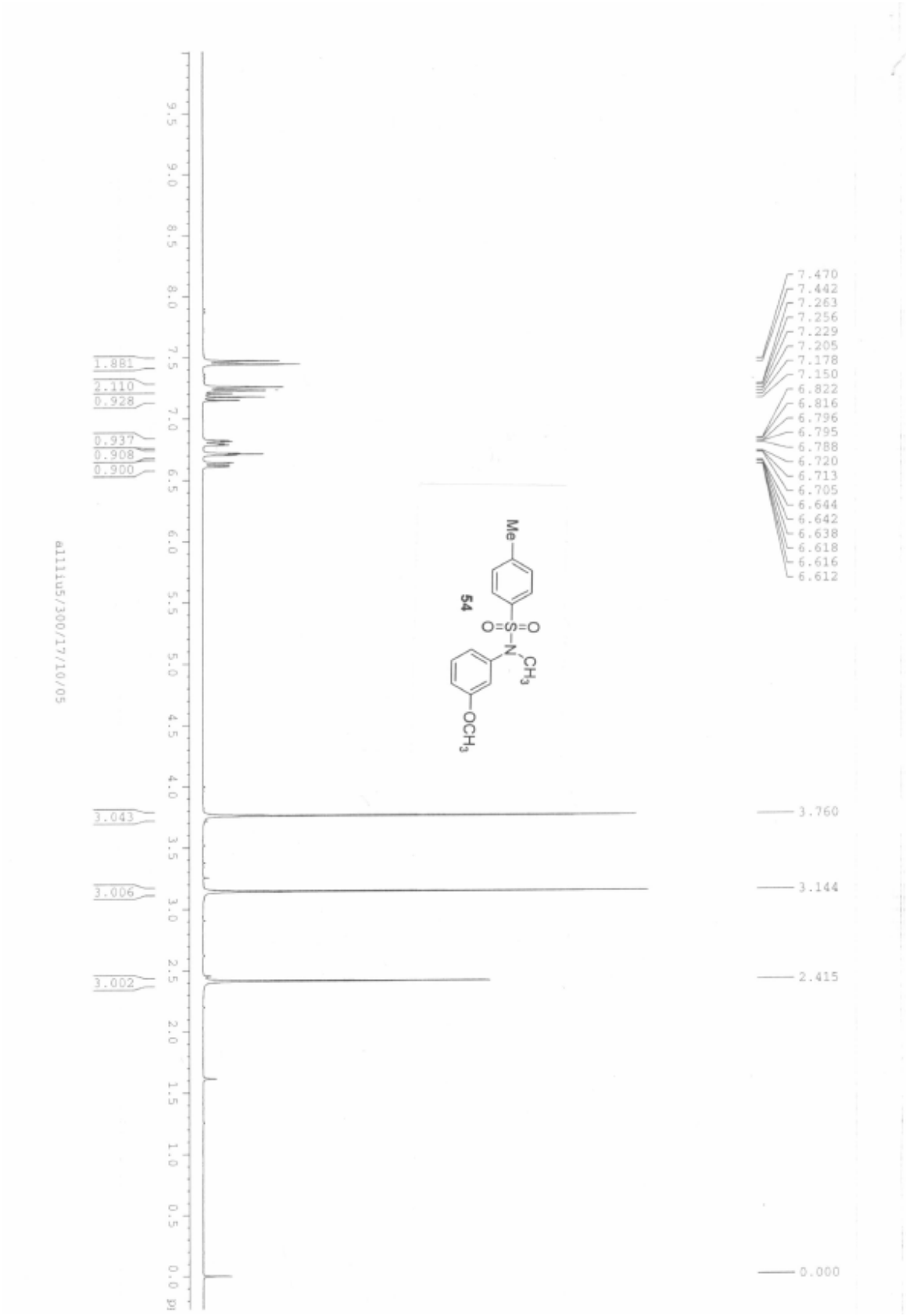
127.281
123.054
120.568
114.239
29.959
29.703
29.446
29.189
28.933
28.676
28.419
PhHN
O
S
N
Ph
Ph
52
elliu189/300/12/07/05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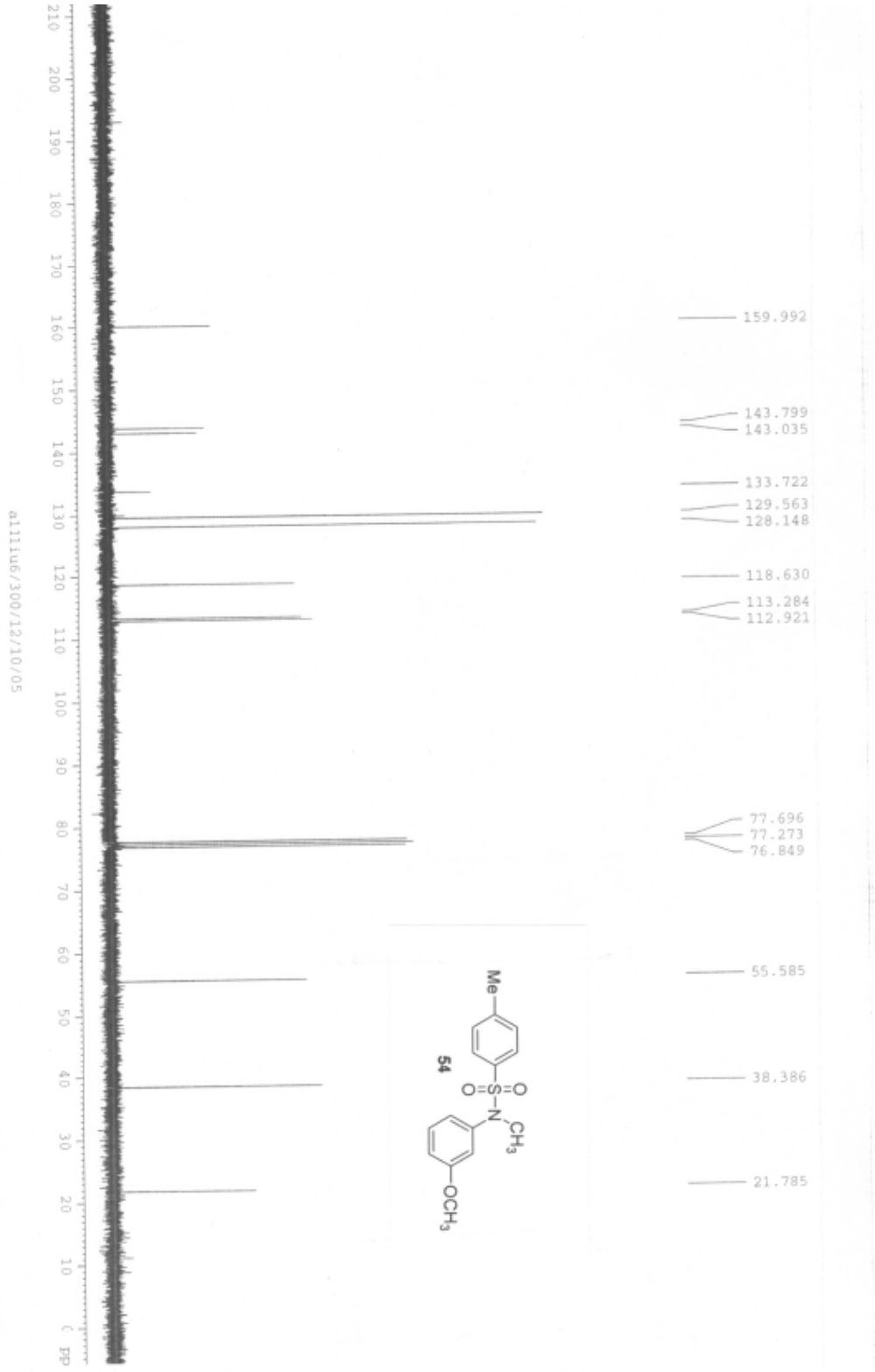
7.205
7.178
7.150
6.822
6.816
6.796
6.795
6.788
6.720
6.713
6.705
6.644
6.642
6.638
6.618
6.616
6.612
1.881
2.110
0.928
0.937
0.908
0.900
3.043
3.006
3.002
3.760
3.144
2.415
0.000
Me
54
O=S=O
N
CH3
OCH3
a1111u5/300/17/10/05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143.035
133.722
129.563
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118.630
113.284
112.921
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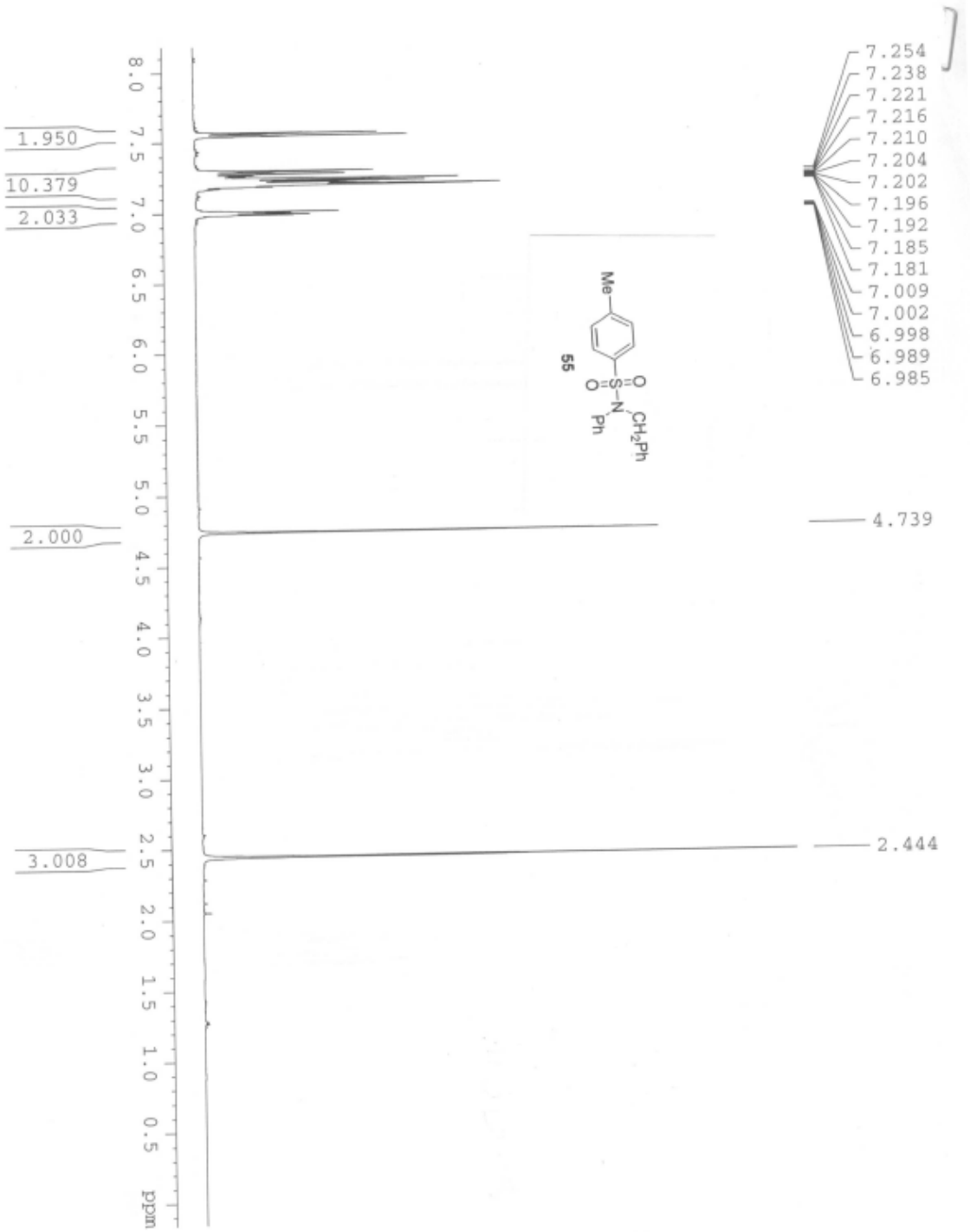
77.273
76.849
55.585
38.386
21.785
54
Me
CH3
OCH3
a111u6/300/12/10/05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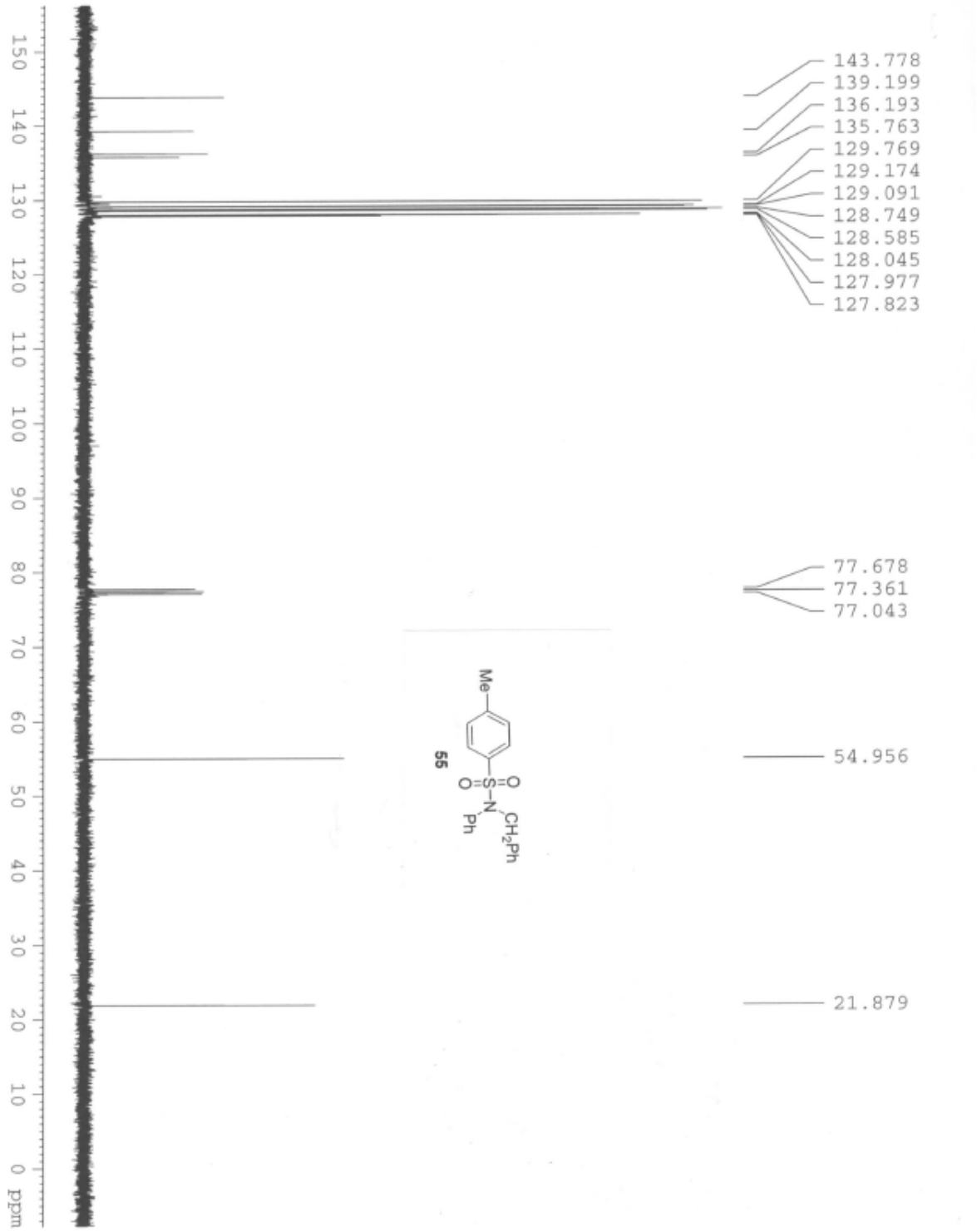
7.238
7.221
7.216
7.210
7.204
7.202
7.196
7.192
7.185
7.181
7.009
7.002
6.998
6.989
6.985
1.950
10.379
2.033
2.000
3.008
4.739
2.444
55
Me
O
O
S
N
Ph
CH2Ph
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm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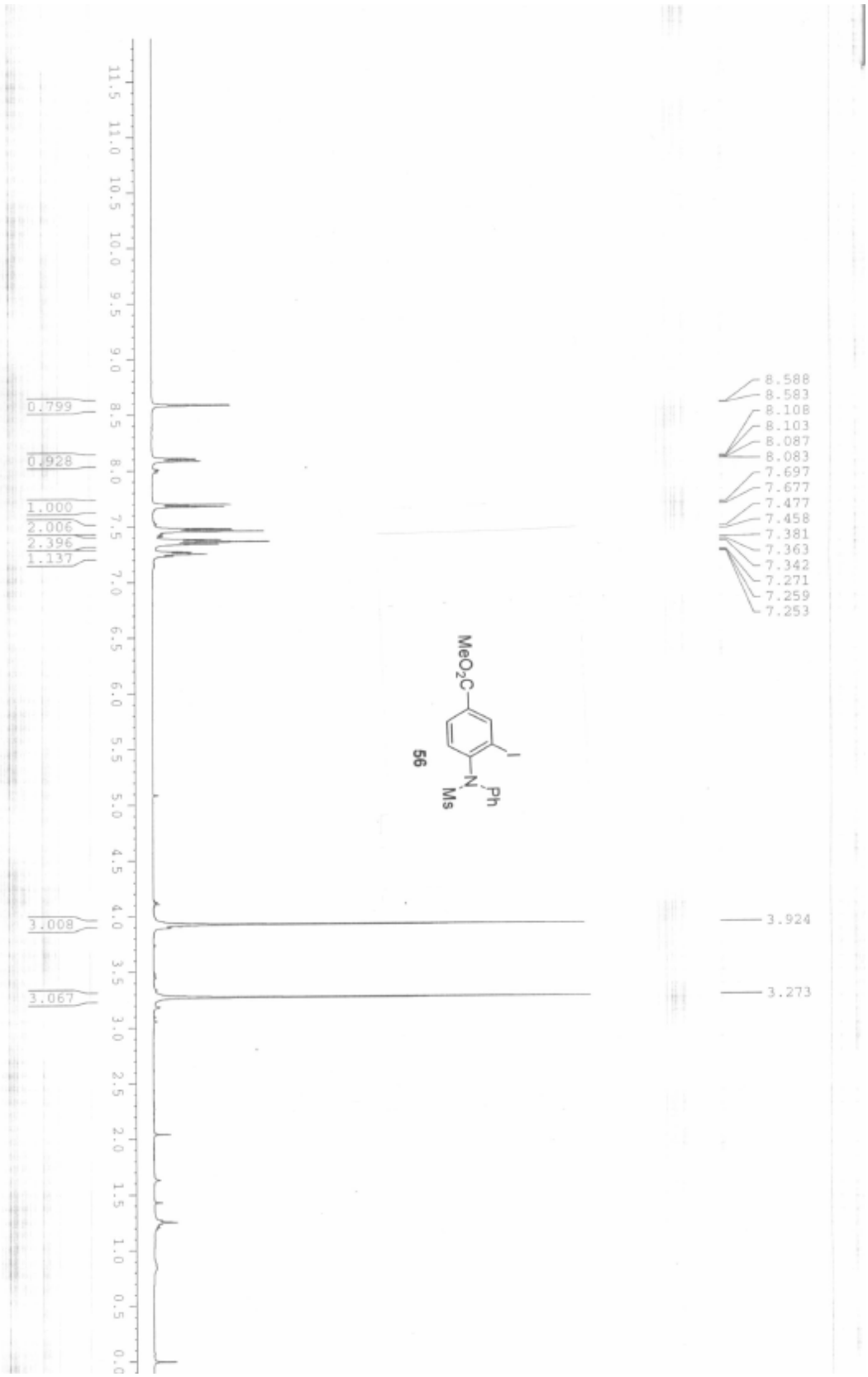
129.174
129.091
128.749
128.585
128.045
127.977
127.823
77.678
77.361
77.043
54.956
21.879
Me
55
Ph
CH2Ph
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm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8.103
8.087
8.083
7.697
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7.458
7.381
7.363
7.342
7.271
7.259
7.253
MeO2C
I
N
Ph
Ms
56
3.924
3.273
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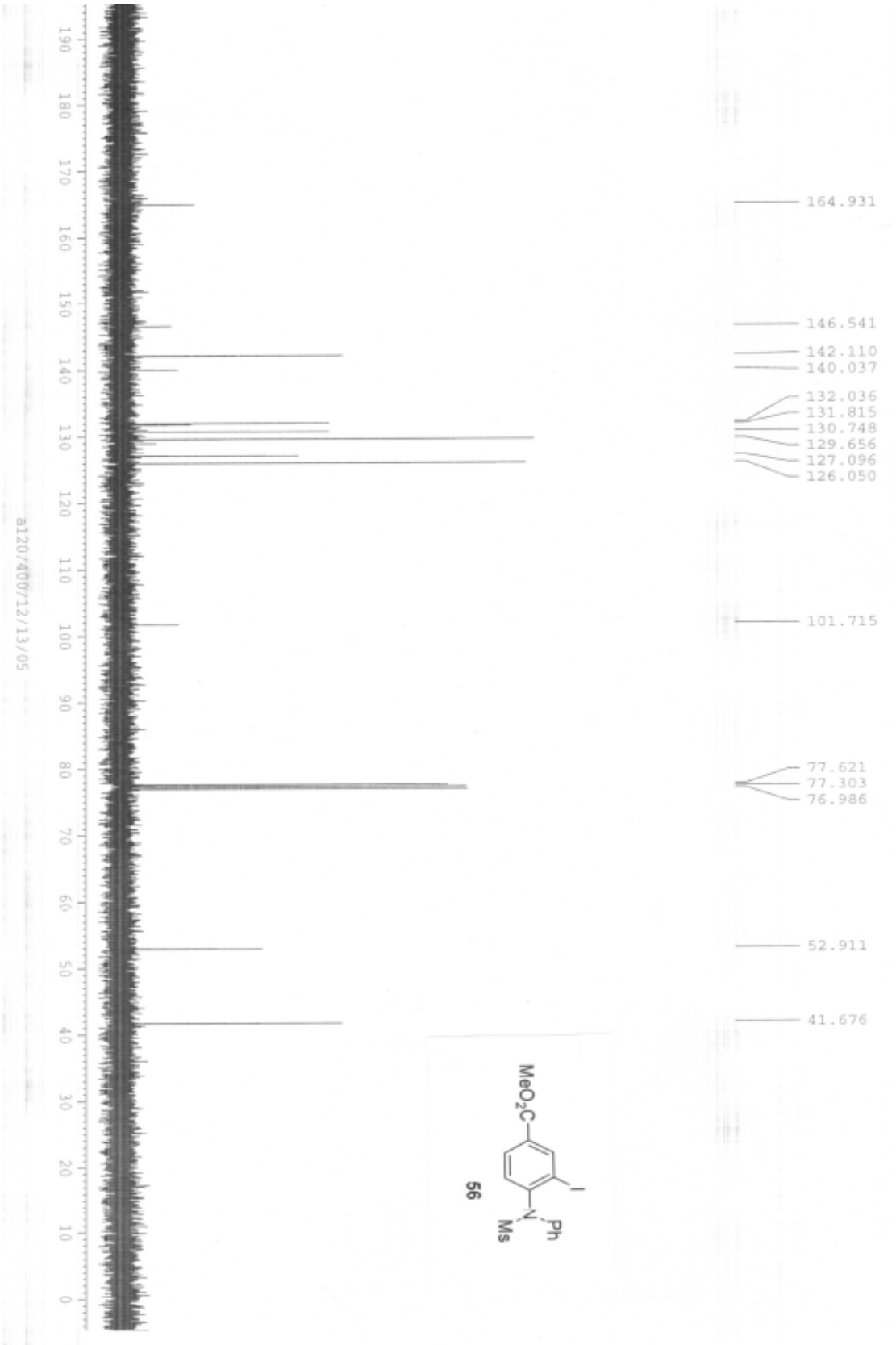
0.928
1.000
2.006
2.396
1.137
3.008
3.067
a119/400/12/13/05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126.050
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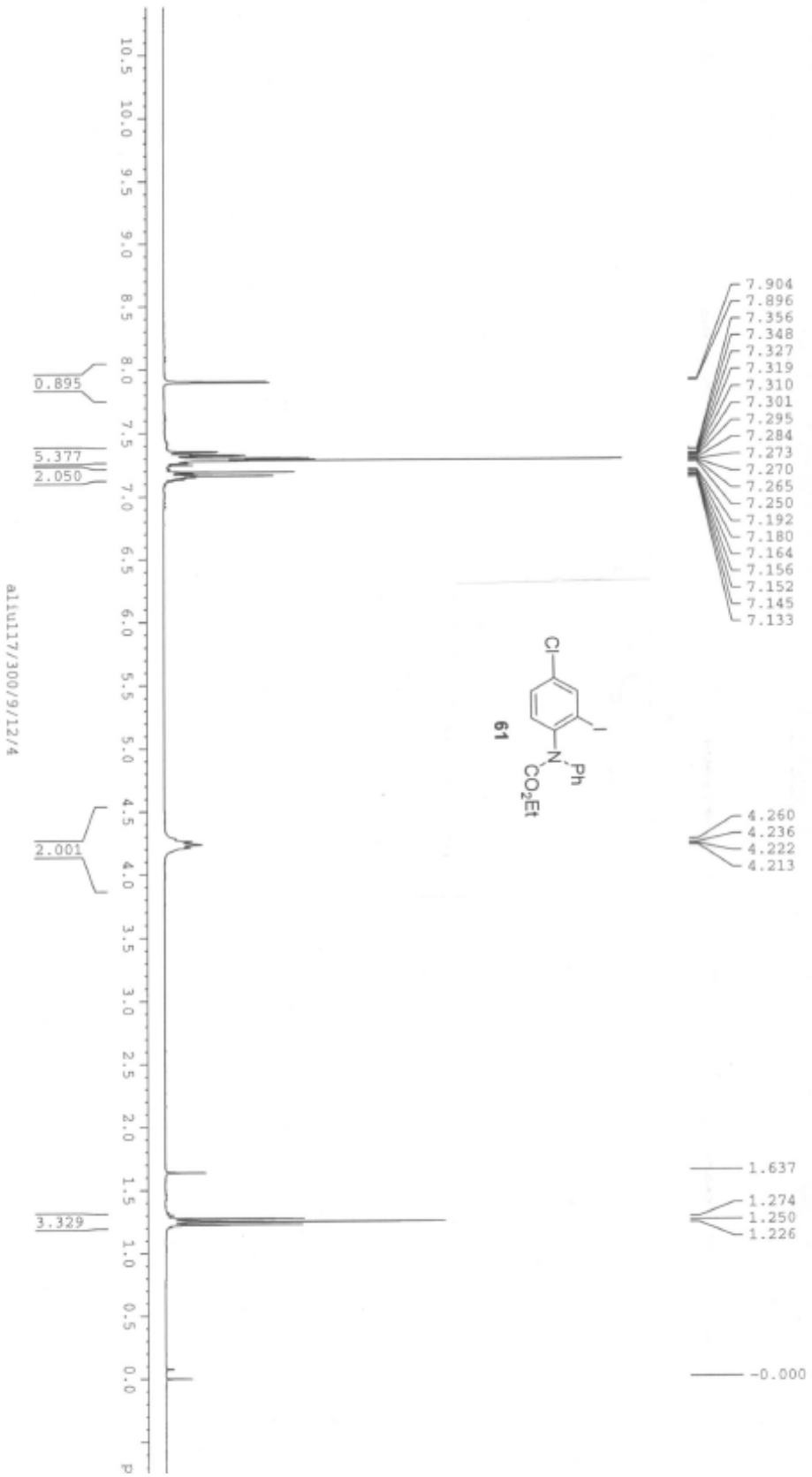
76.986
52.911
41.676
a120/400/12/13/05
MeO2C
I
N
Ph
Ms
56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7.301
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7.284
7.273
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7.265
7.250
7.192
7.180
7.164
7.156
7.152
7.145
7.133
4.260
4.236
4.222
4.213
1.637
1.274
1.250
1.226
-0.000
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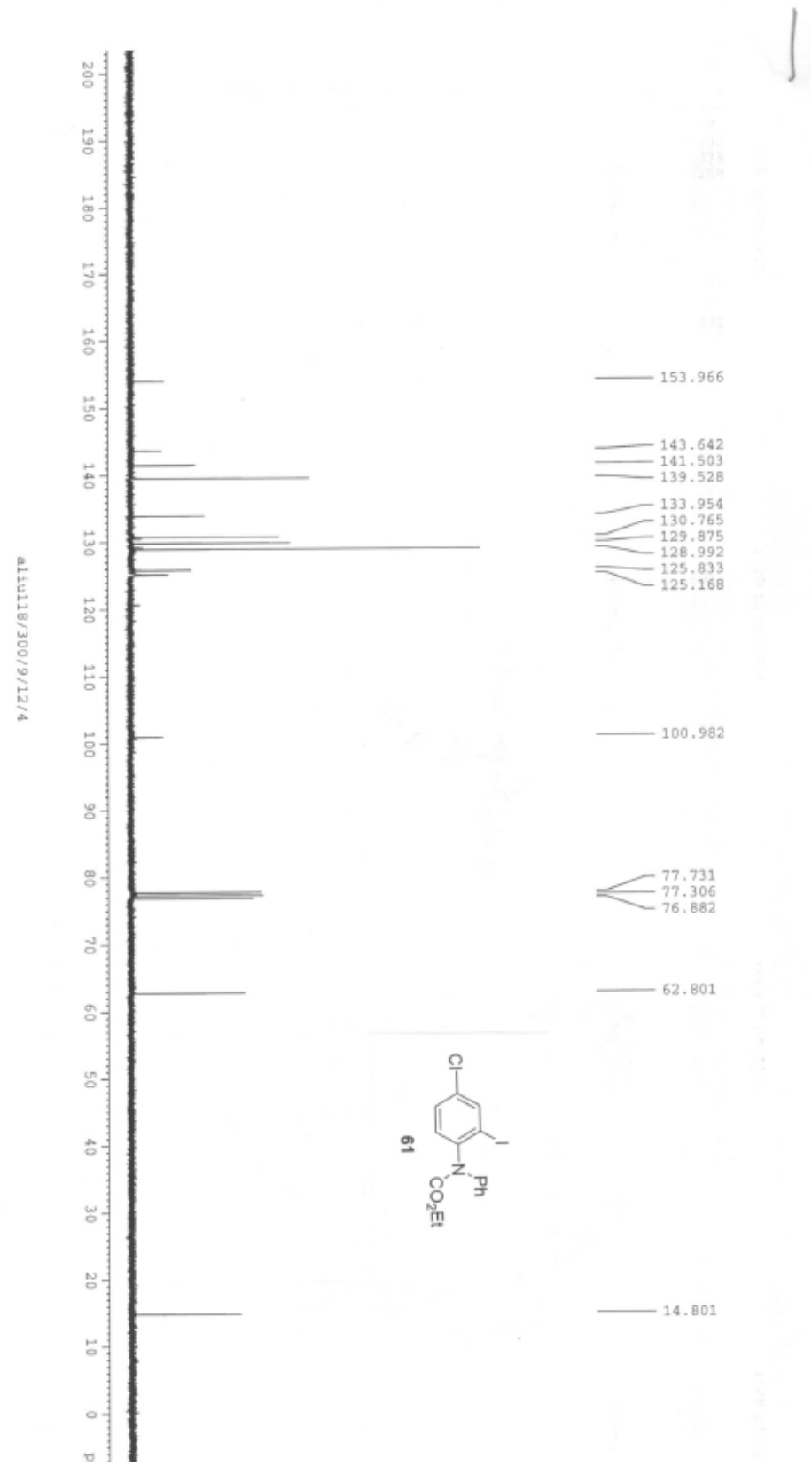
2.050
2.001
3.329
Cl
I
N
Ph
CO2Et
61
altu117/300/9/12/4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128.992
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125.168
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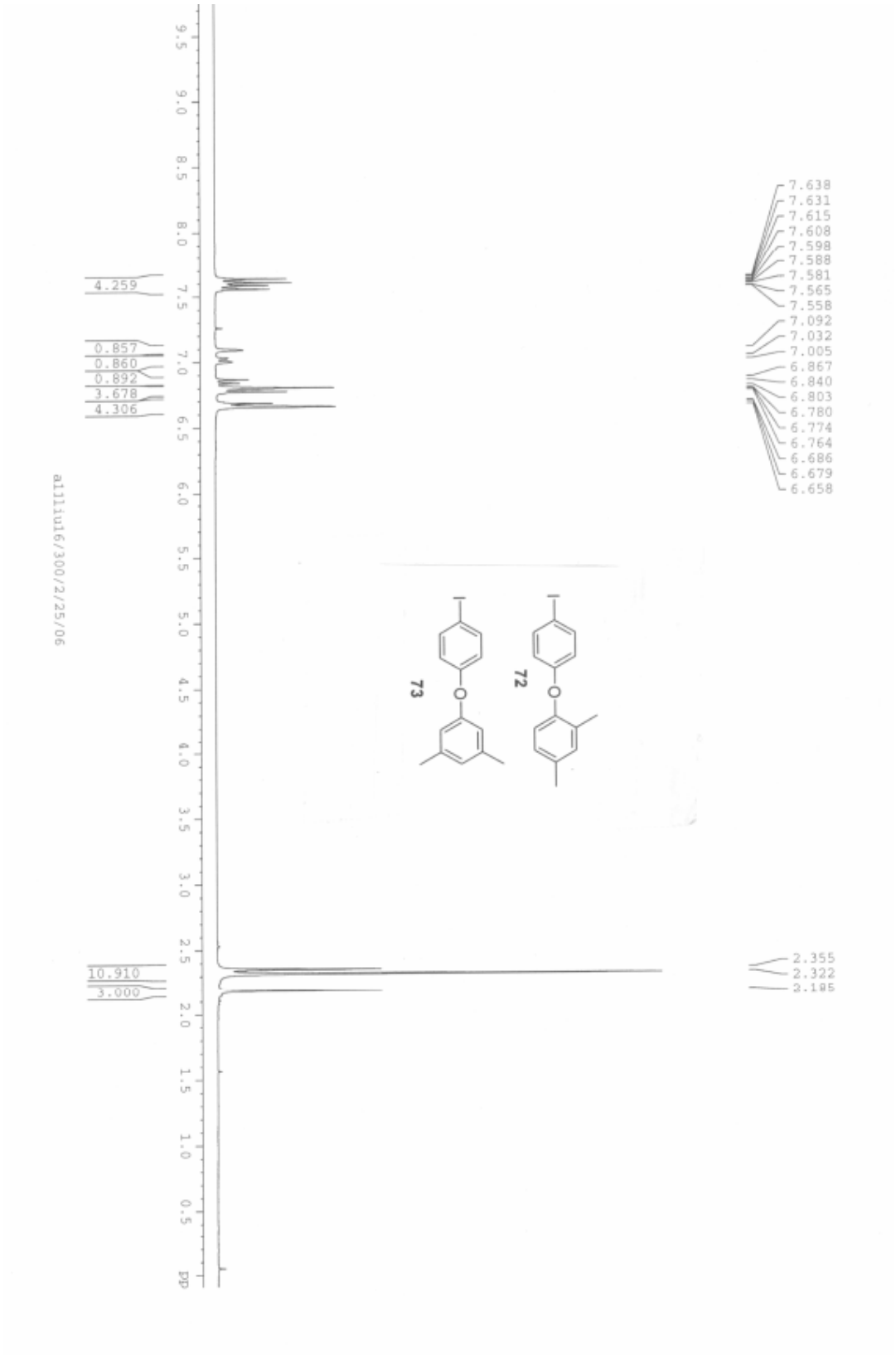
76.882
62.801
14.801
Cl
I
Ph
N
CO2Et
61
aliu118/300/9/12/4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7.615
7.608
7.598
7.588
7.581
7.565
7.558
7.092
7.032
7.005
6.867
6.840
6.803
6.780
6.774
6.764
6.686
6.679
6.658
2.355
2.322
2.195
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0.892
3.678
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3.000
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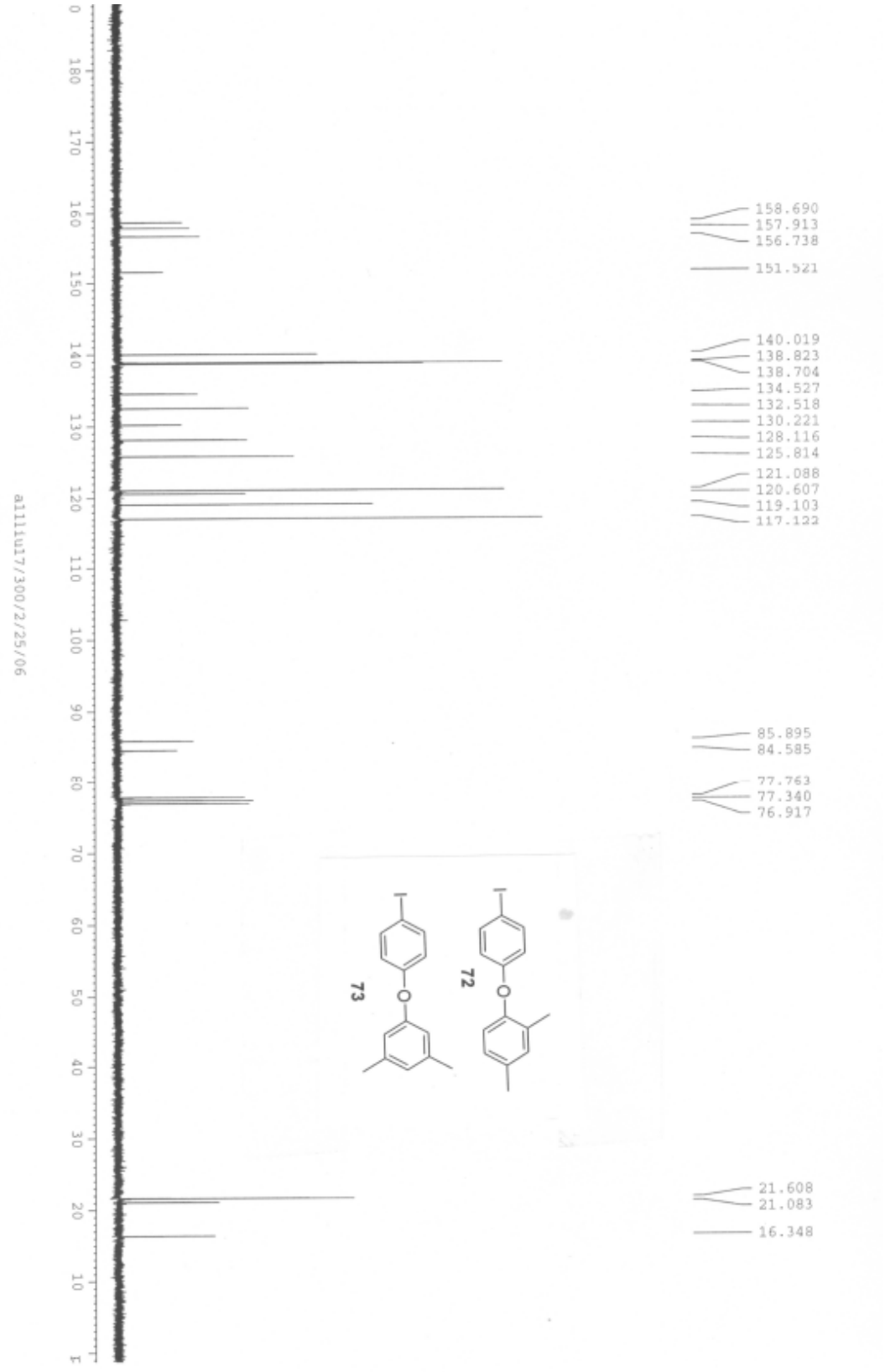
73
72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130.221
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125.814
121.088
120.607
119.103
117.122
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84.585
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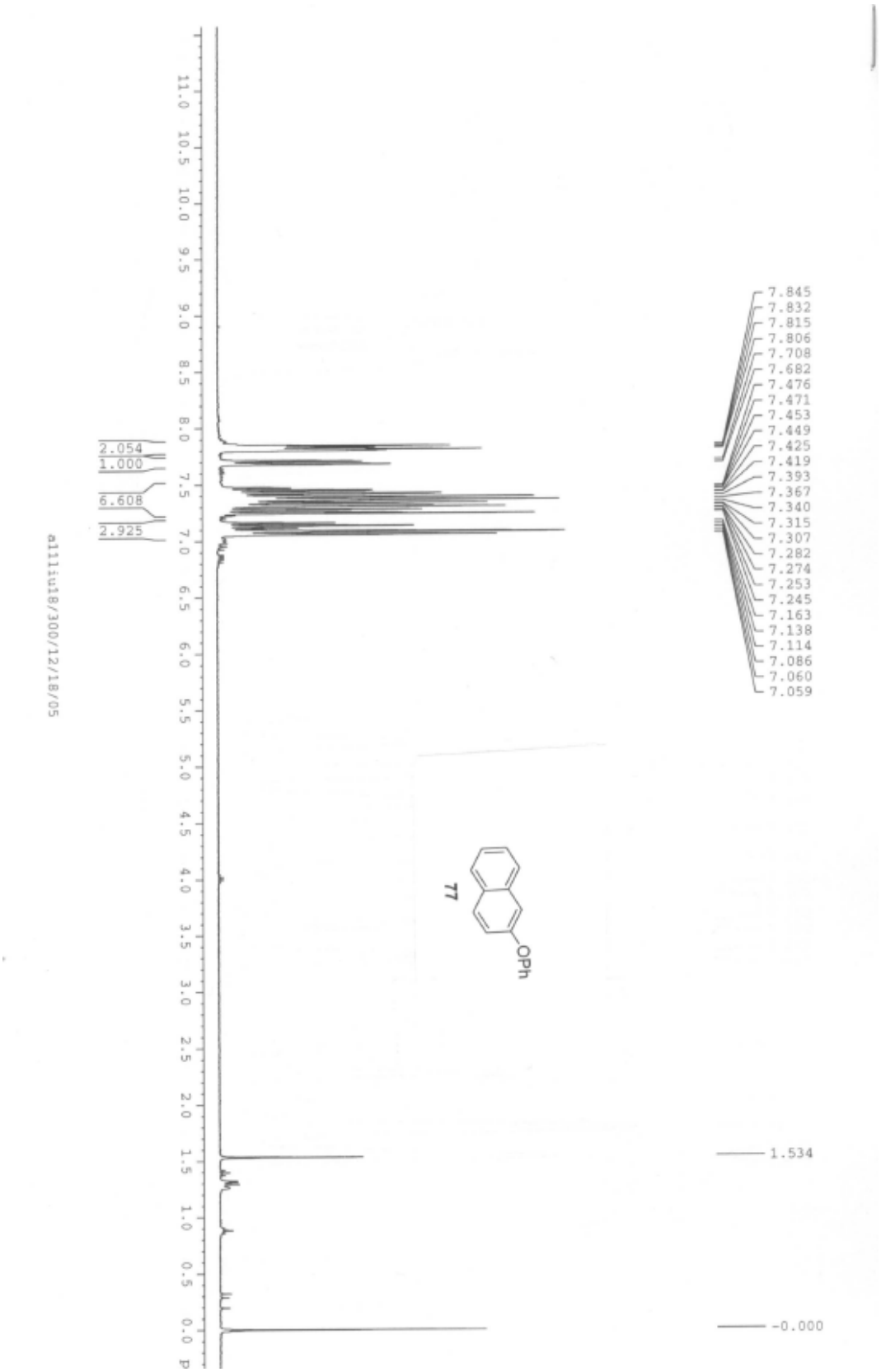
77.340
76.917
21.608
21.083
16.348
73
72
allilu17/300/2/25/06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7.806
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7.682
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7.471
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7.449
7.425
7.419
7.393
7.367
7.340
7.315
7.307
7.282
7.274
7.253
7.245
7.163
7.138
7.114
7.086
7.060
7.059
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1.000
6.608
2.925
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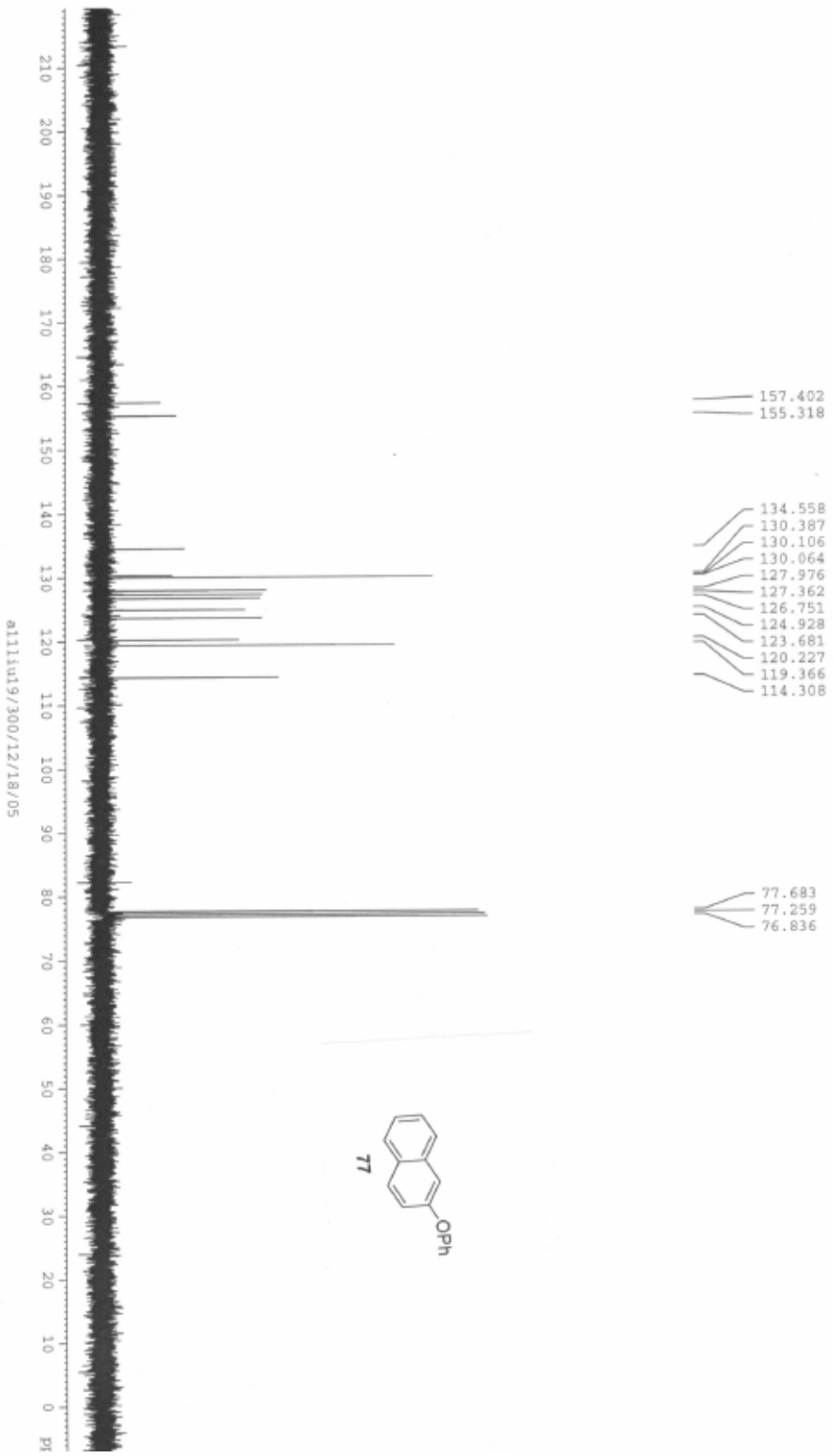
OPh
77
a111u18/300/12/18/05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119.366
114.308
77.683
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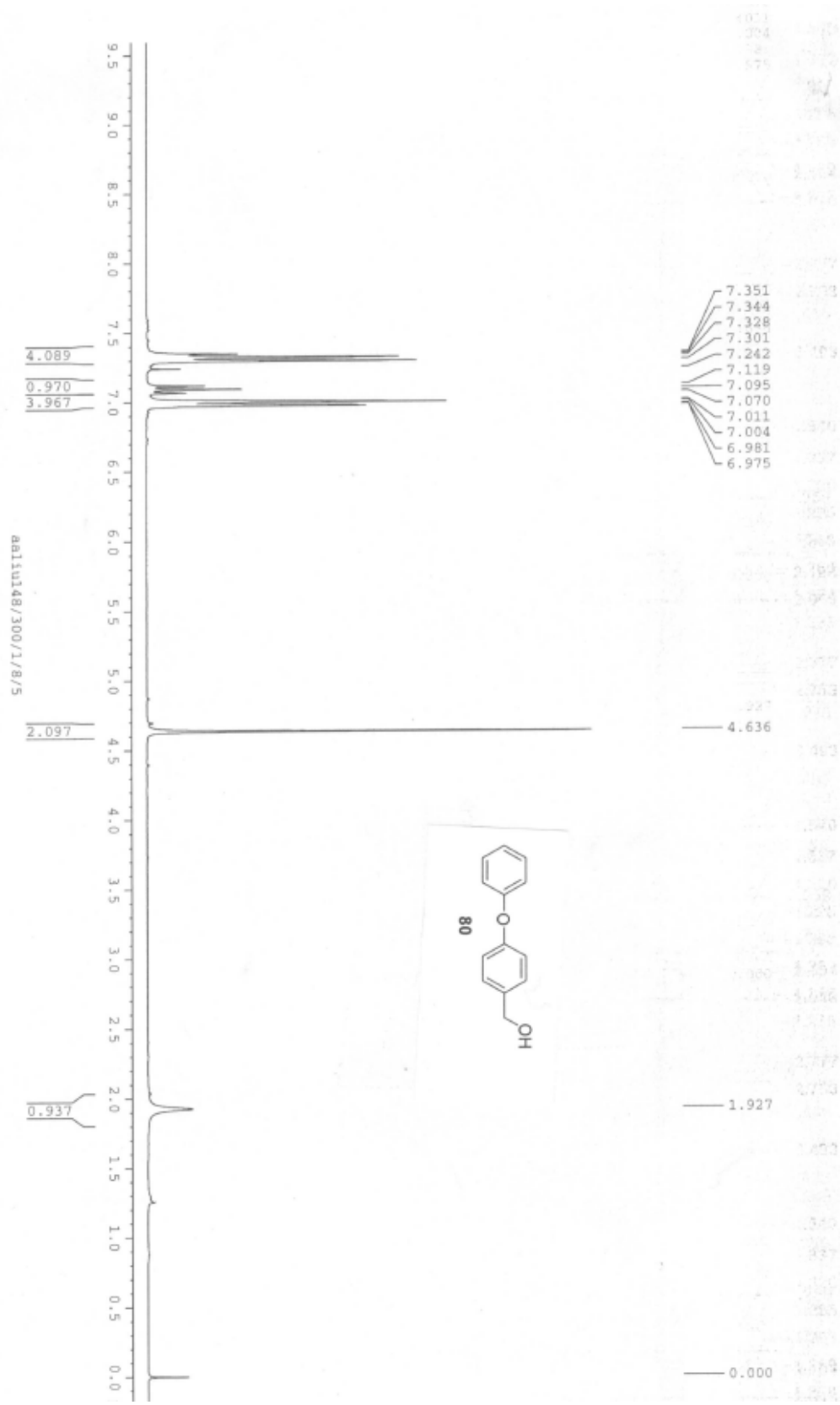
76.836
77
OPh
a111iu19/300/12/18/05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7.242
7.119
7.095
7.070
7.011
7.004
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6.975
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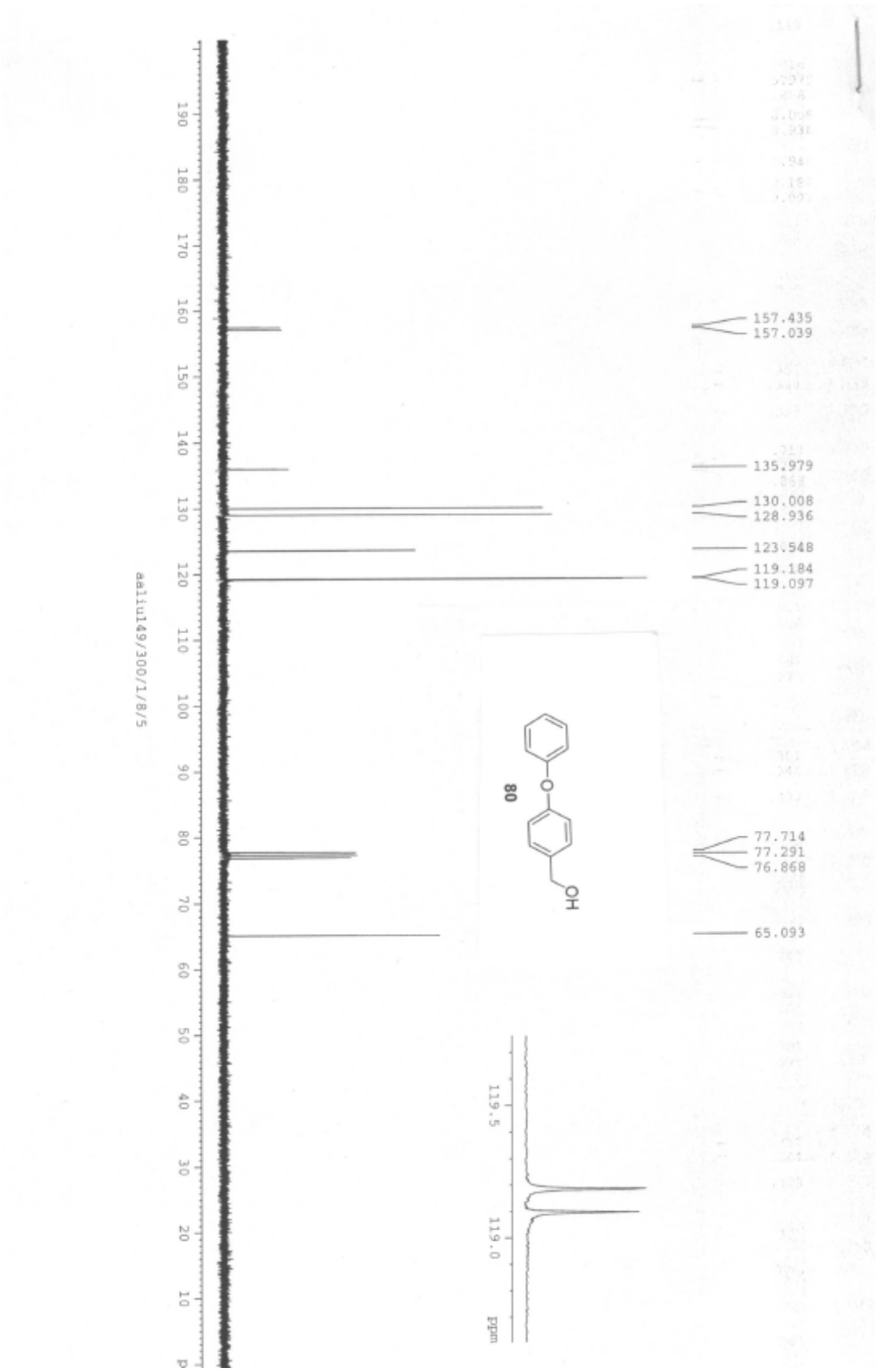
2.097
0.937
4.636
1.927
0.000
80
OH
aaliu148/300/1/8/5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119.0
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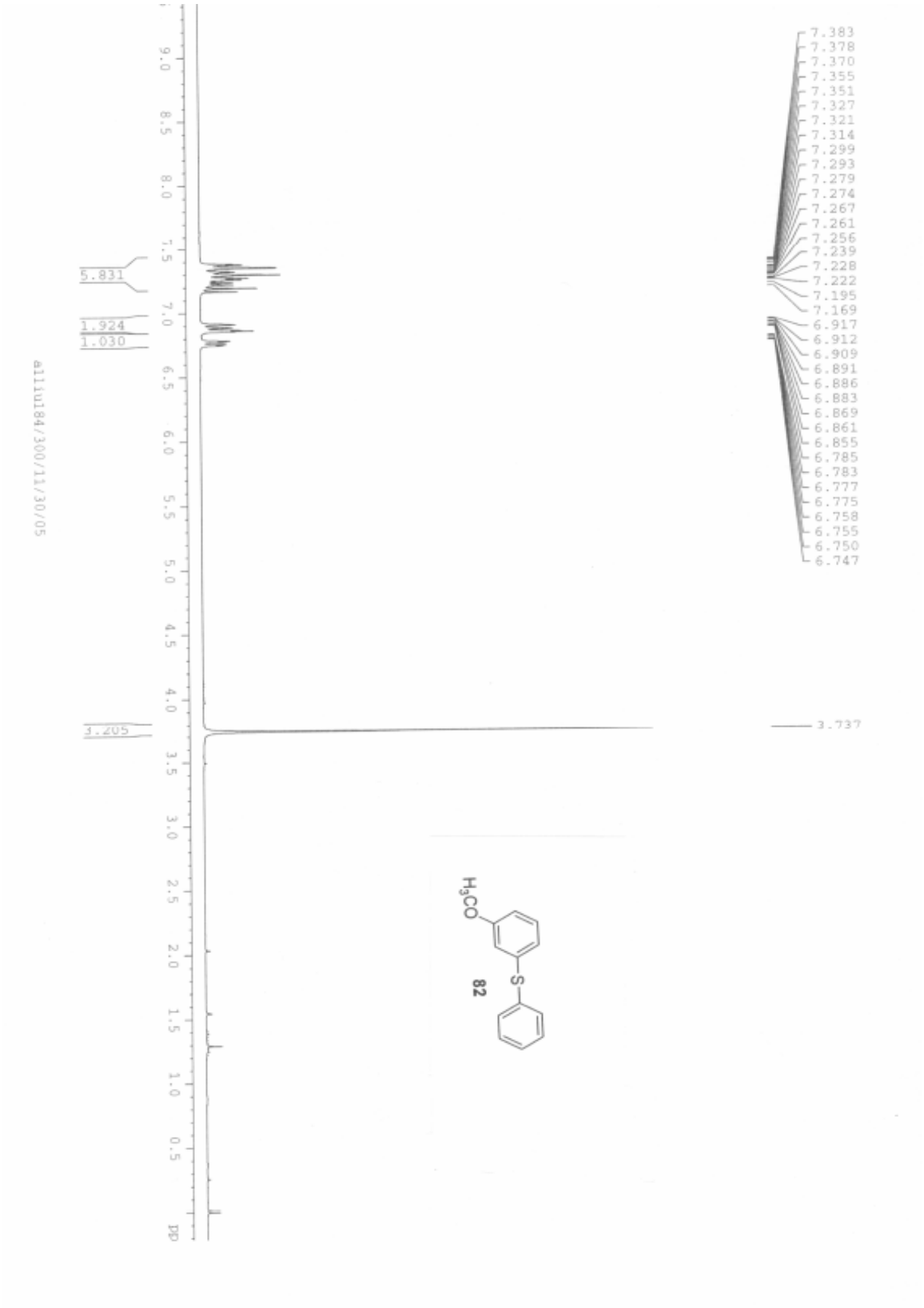
aaliu149/300/1/8/5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7.293
7.279
7.274
7.267
7.261
7.256
7.239
7.228
7.222
7.195
7.169
6.917
6.912
6.909
6.891
6.886
6.883
6.869
6.861
6.855
6.785
6.783
6.777
6.775
6.758
6.755
6.750
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3.205
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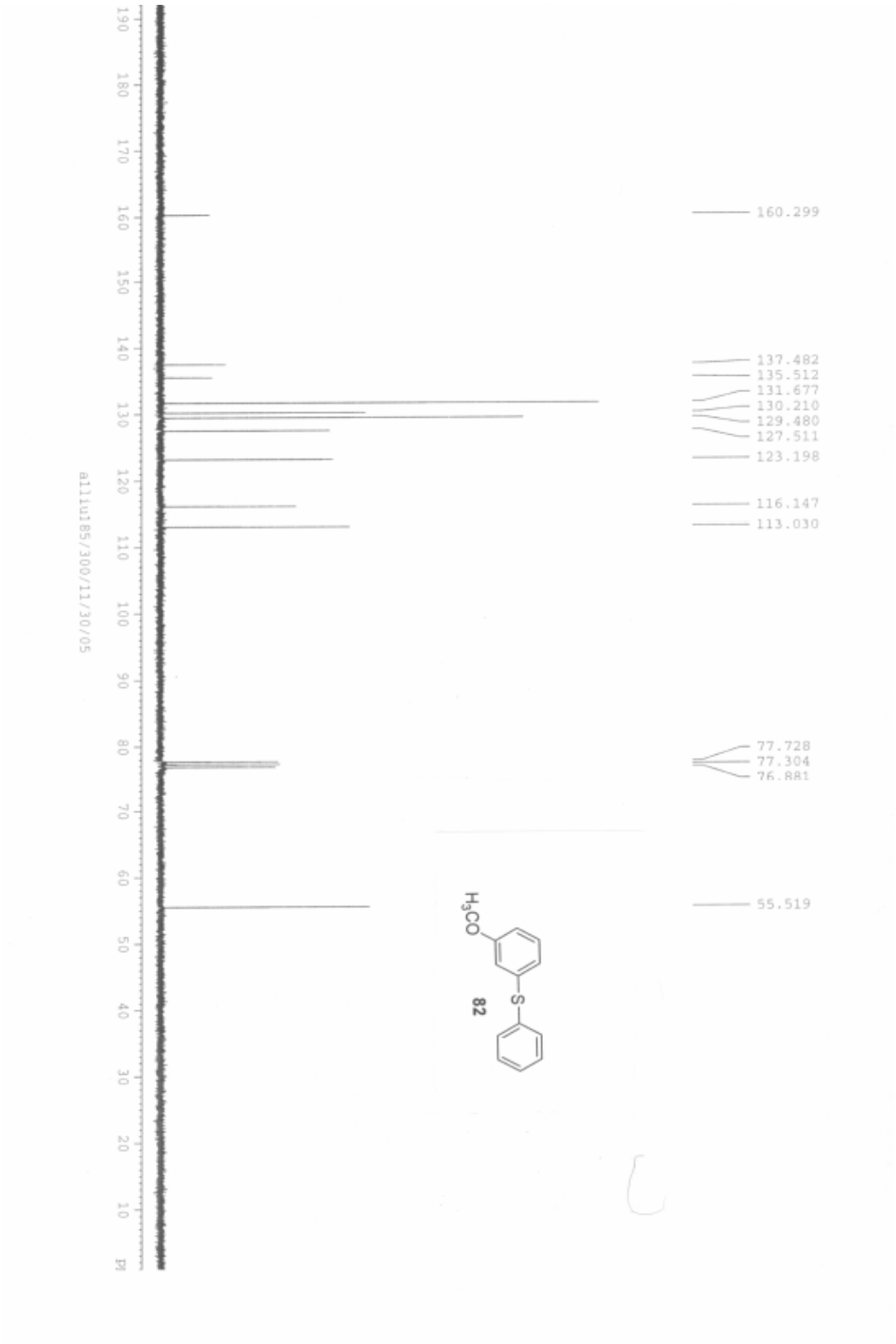
allu184/300/11/30/05
H3CO
S
82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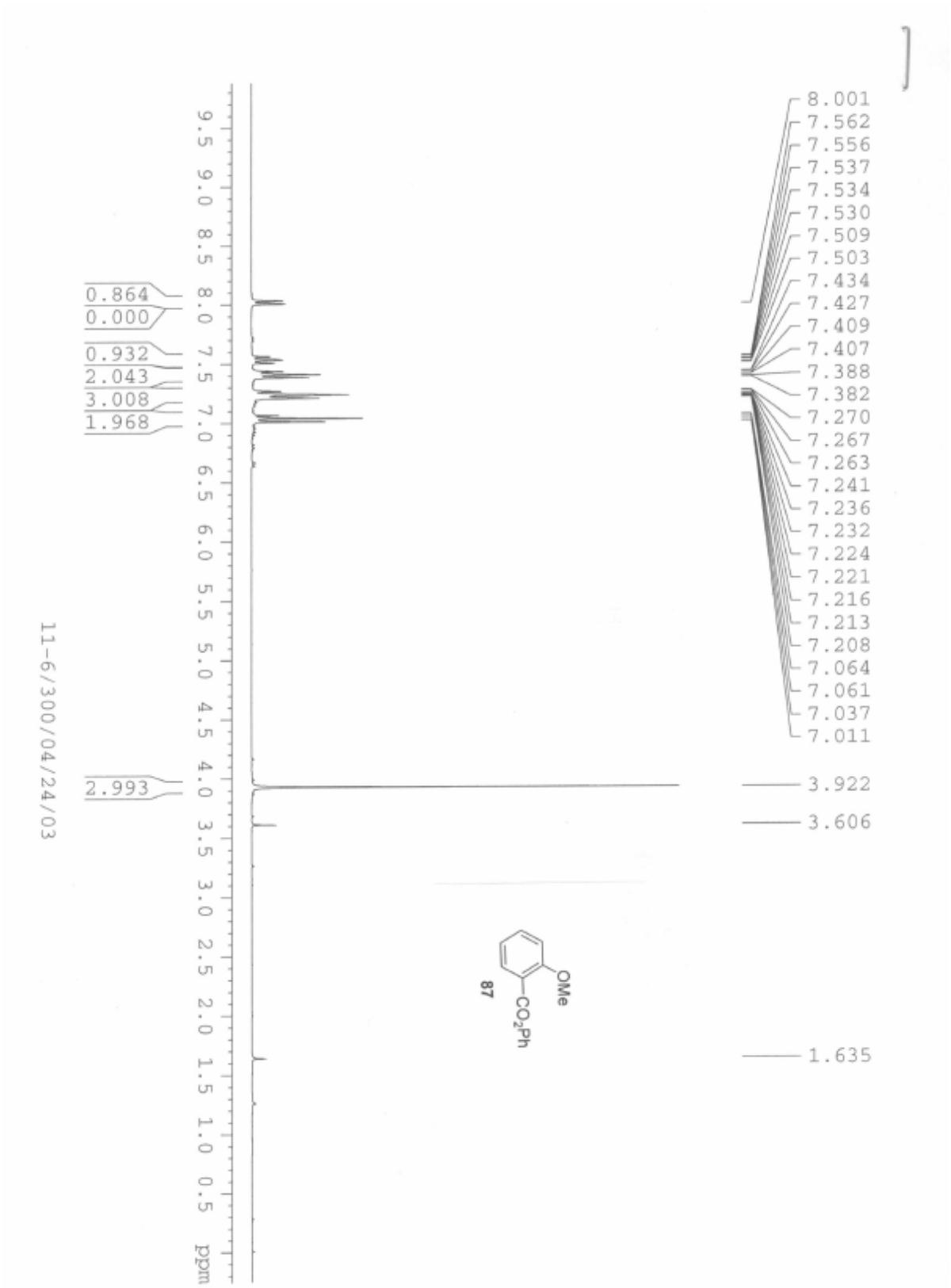
H3CO
S
82
allu185/300/11/30/05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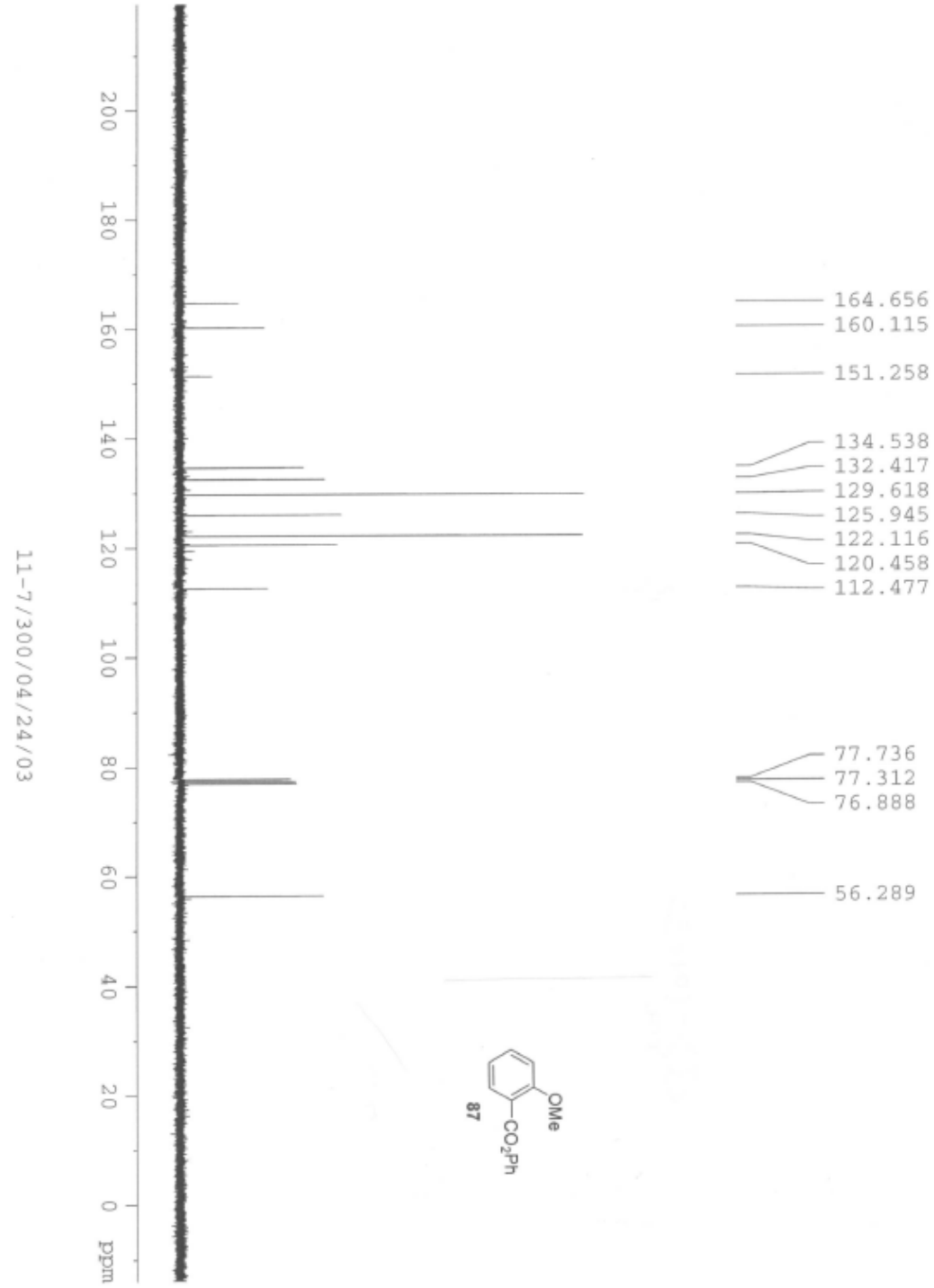
7.382
7.270
7.267
7.263
7.241
7.236
7.232
7.224
7.221
7.216
7.213
7.208
7.064
7.061
7.037
7.011
3.922
3.606
1.635
OMe
CO2Ph
87
0.864
0.000
0.932
2.043
3.008
1.968
2.993
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
11-6/300/04/24/03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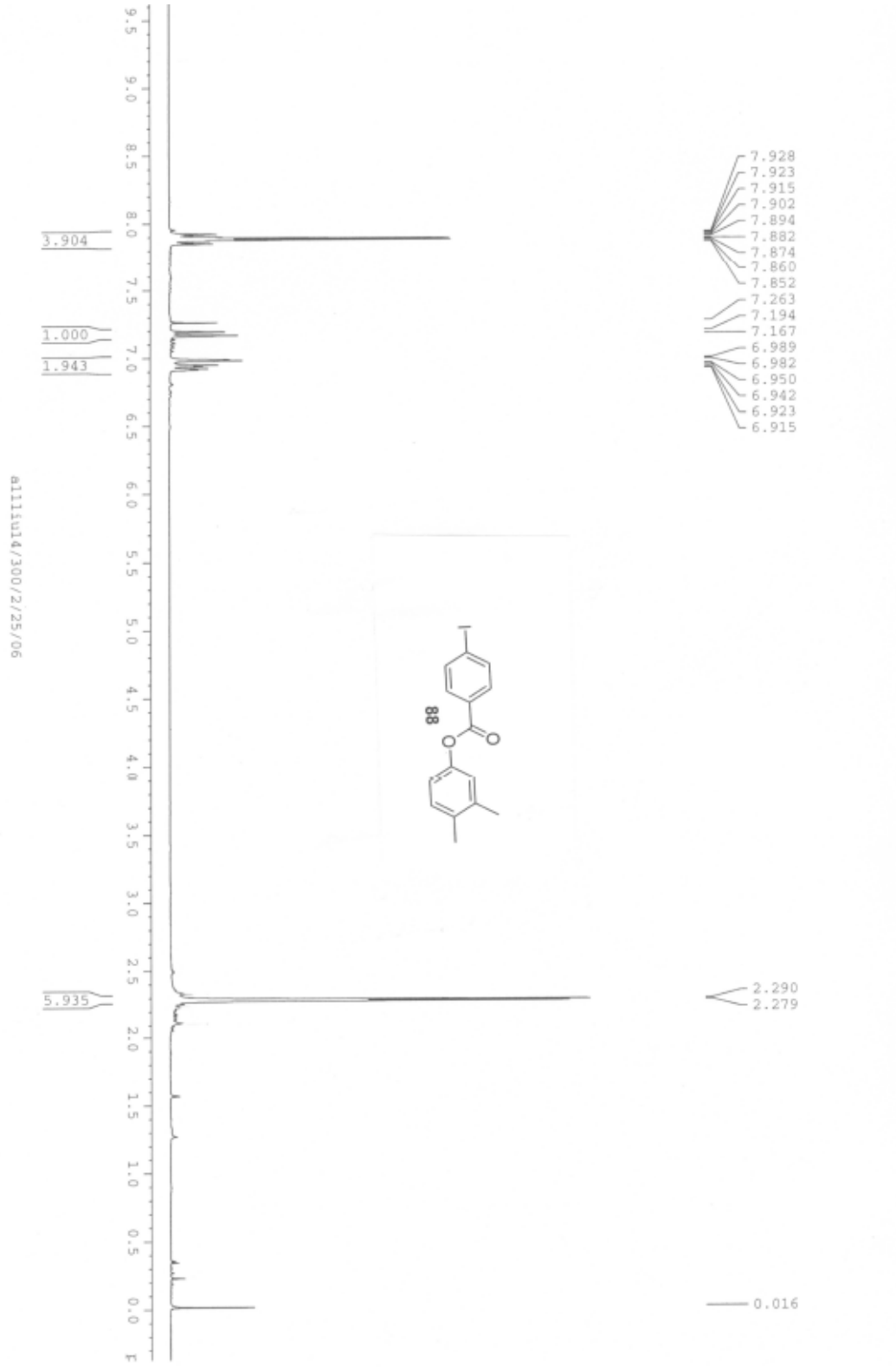
151.258
134.538
132.417
129.618
125.945
122.116
120.458
112.477
77.736
77.312
76.888
56.289
200
180
160
140
120
100
80
60
40
20
0
ppm
11-7/300/04/24/03
OMe
CO2Ph
87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7.902
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7.194
7.167
6.989
6.982
6.950
6.942
6.923
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3.904
1.000
1.943
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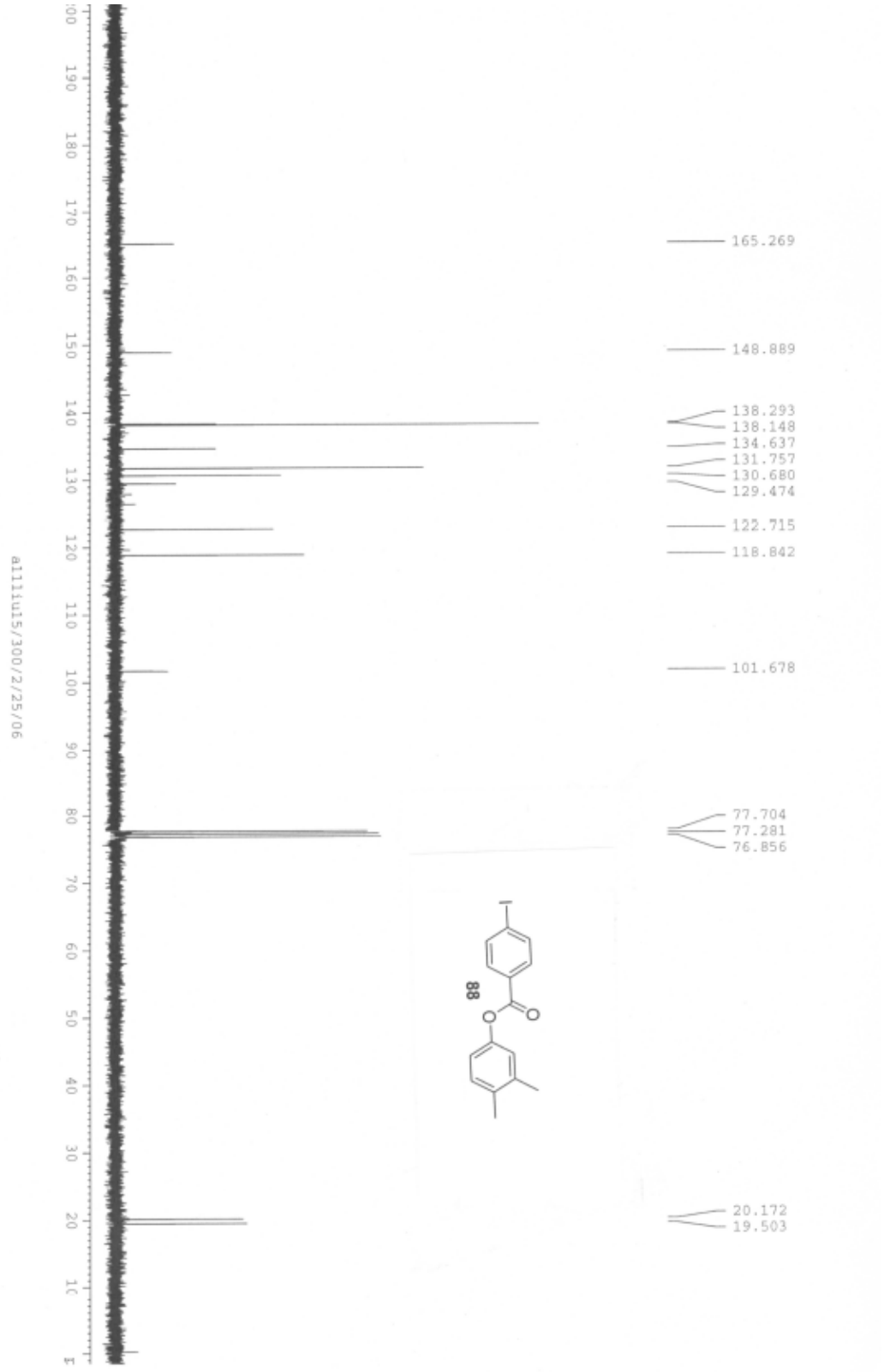
88
a111u14/300/2/25/06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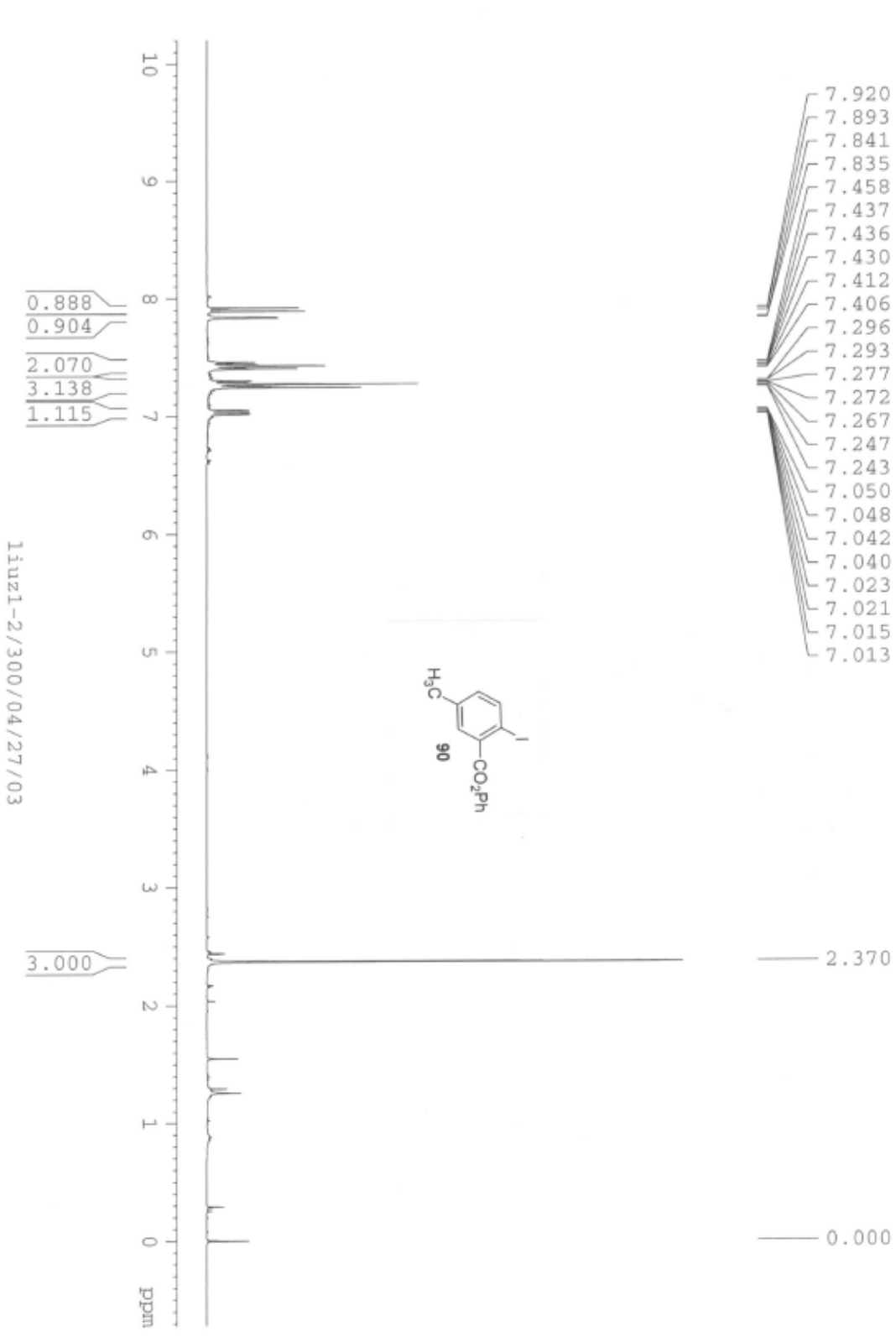
19.503
88
allius15/300/2/25/06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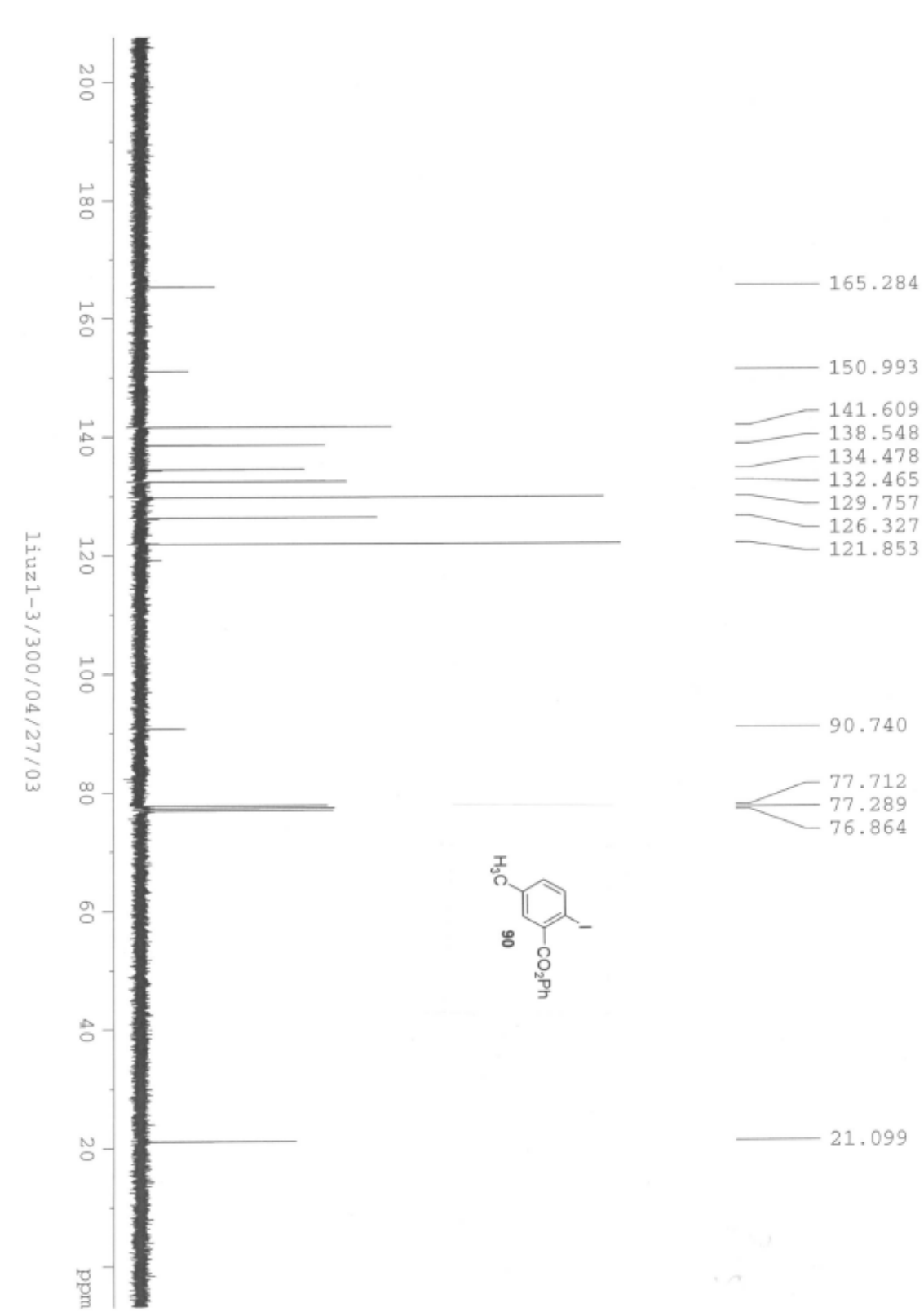
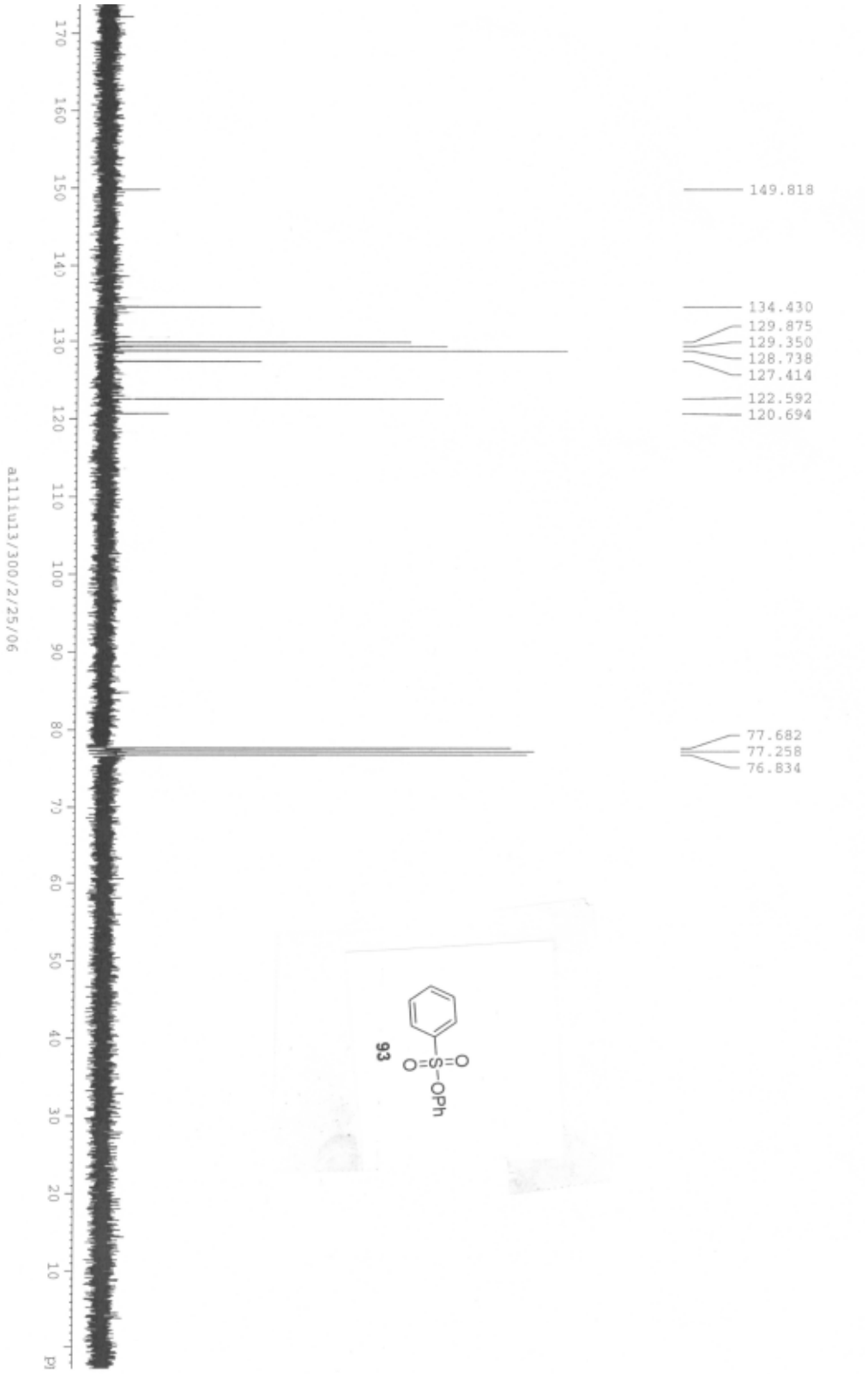
7.406
7.296
7.293
7.277
7.272
7.267
7.247
7.243
7.050
7.048
7.042
7.040
7.023
7.021
7.015
7.013
0.888
0.904
2.070
3.138
1.115
3.000
2.370
0.000
ppm
liuz1-2/300/04/27/03
H3C
I
CO2Ph
90


165.284
150.993
141.609
138.548
134.478
132.465
129.757
126.327
121.853
90.740
77.712
77.289
76.864
21.099
200
180
160
140
120
100
80
60
40
20
ppm
liuzl-3/300/04/27/03
H3C
I
CO2Ph
90


149.818
134.430
129.875
129.350
128.738
127.414
122.592
120.694
77.682
77.258
76.834
allliul3/300/2/25/06
93
O=S=O
OPh