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SUPPORTING INFORMATION

Title: Efficient and Copper-Free Sonogashira Cross-Coupling Reaction Catalyzed by $Pd(OAc)_2$/Pyrimidines Catalytic System

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Ref. No.: O200500519

(A) Analytical data for 3─14

1-Methoxy-4-(2-phenylethynyl)benzene (3): ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.52–7.51 (m, 2H), 7.48 (d, *J* = 9.0 Hz, 2H), 7.34–7.32 (m, 3H), 6.88 (d, *J* = 8.8 Hz, 2H), 3.83 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 159.6, 133.0, 131.4, 128.3, 127.9, 123.6, 115.4, 114.0, 89.4, 88.1, 55.3.

1-(Dec-1-ynyl)-4-methoxybenzene (4): ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.33 (d, *J* = 8.8 Hz, 2H), 6.81 (d, *J* = 8.8 Hz, 2H), 3.80 (s, 3H), 2.38 (t, *J* = 7.6 Hz, 2H), 1.61–1.57 (m, 2H), 1.45–1.40 (m, 2H), 1.31–1.24 (m, 8H), 0.88 (t, *J* = 6.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ:158.9, 132.8, 116.1, 113.7, 88.8, 80.1, 55.2, 31.8, 29.2, 29.1, 28.9, 28.8, 22.7, 19.4, 14.1.

1-(2-(4-Nitrophenyl)ethynyl)benzene (5): ^{1}H NMR (300 MHz, $CDCl_3$) δ: 8.21 (d, *J* = 8.8 Hz, 2H), 7.65 (d, *J* = 8.8 Hz, 2H), 7.58─7.54 (m, 2H), 7.40─7.38 (m, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ: 141.3, 132.6, 132.2, 130.6, 129.6, 128.8, 124.0, 122.5, 95.0, 87.9.

1-(Dec-1-ynyl)-4-nitrobenzene (6): ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.15 (d, *J* = 8.8 Hz, 2H), 7.51 (d, *J* = 8.8 Hz, 2H), 2.44 (t, *J* = 7.2 Hz, 2H), 1.74–1.59 (m, 2H), 1.47–1.43 (m, 2H), 1.31–1.26 (m, 8H), 0.89 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 132.6, 131.6, 123.8, 118.5, 97.2, 79.6, 32.2, 29.5, 29.4, 29.3, 28.7, 23.0, 19.9, 14.4.

3-(4-Nitrophenyl)prop-2-yn-1-ol (7): ^{1}H NMR (300 MHz, $CDCl_3$) δ: 8.19 (d, *J* = 8.8 Hz, 2H), 7.58 (d, *J* = 8.8 Hz, 2H), 4.54 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 147.3, 132.4, 129.4, 123.6, 92.5, 83.8, 51.5.

1-(2-(2-Nitrophenyl)ethynyl)benzene (8): ^{1}H NMR (300 MHz, $CDCl_3$) δ: 8.10 (d, *J* = 8.4 Hz, 1H), 7.73 (d, *J* = 7.6 Hz, 1H), 7.64─7.60 (m, 3H), 7.48 (t, *J* = 8.4 Hz, 1H), 7.40─7.38 (m, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ: 149.5, 134.6, 132.9, 132.0, 129.2, 128.5, 128.4, 124.7, 122.3, 118.7, 97.1, 84.8.

1,2-Diphenylethyne (9): ^{1}H NMR (300 MHz, $CDCl_3$) δ: 7.60─7.51 (m, 4H), 7.39─7.26 (m, 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ: 132.0, 128.7, 128.6, 123.7, 89.7.

1-(2-*p*-Tolylethynyl)benzene (10): ^{1}H NMR (300 MHz, $CDCl_3$) δ: 7.54–7.50 (m, 2H), 7.43 (d, *J* = 8.1 Hz, 2H), 7.35–7.31 (m, 3H), 7.15 (d, *J* = 7.8 Hz, 2H), 2.36 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 138.7, 132.9, 131.9, 129.6, 129.5, 128.8, 128.7, 128.4, 89.1, 83.4, 21.9.

1-(2-*o*-Tolylethynyl)benzene (11): ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.53–7.52 (m, 3H), 7.35–7.33 (m, 4H), 7.23–7.22 (m, 2H) 2.52 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 140.2, 132.6, 131.9, 131.6, 129.5, 129.2, 128.4, 128.3, 128.2, 125.6, 88.4, 81.7, 20.7.

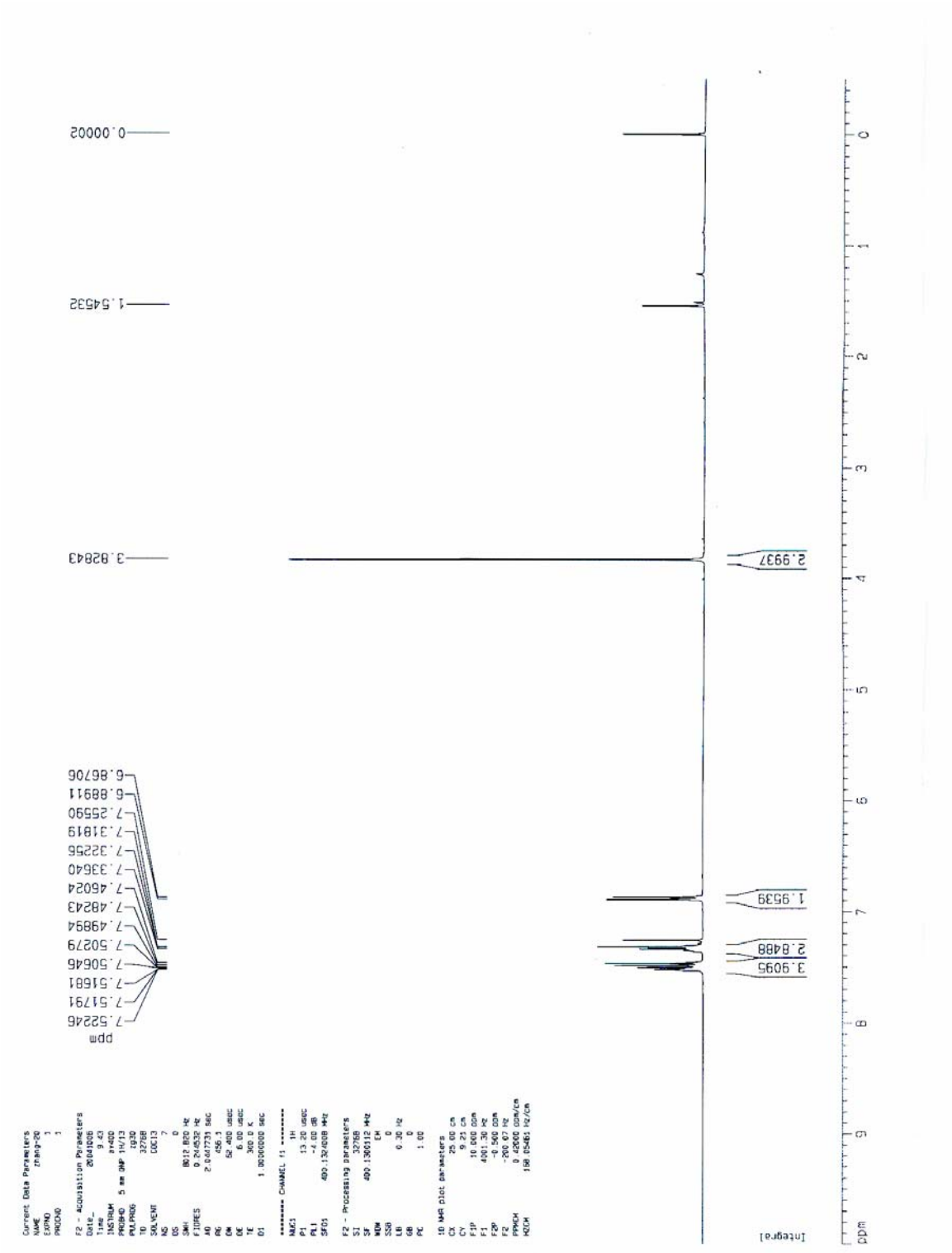
1-Fluoro-4-(2-(4-nitrophenyl)ethynyl)benzene (12): ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.23 (d, *J* = 8.0 Hz, 2H), 7.66 (d, *J* = 8.4 Hz, 2H), 7.57─7.54 (m, 2H), 7.10 (t, *J* = 8.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 164.3, 161.8, 146.9, 133.8, 132.2, 130.0, 123.7, 116.0 (d, J = 22 Hz, 1C), 93.6, 87.3.

1-(2-(4-Methoxyphenyl)ethynyl)-4-nitrobenzene (13): ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.20 (d, *J* = 8.4 Hz, 2H), 7.63 (d, *J* = 8.8 Hz, 2H), 7.50 (d, *J* = 8.4 Hz, 2H), 6.90 (d, *J* = 8.4 Hz, 2H), 3.84 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 160.4, 146.7, 134.0, 133.4, 132.0, 123.6, 114.2, 114.1, 95.1, 86.6, 55.3.

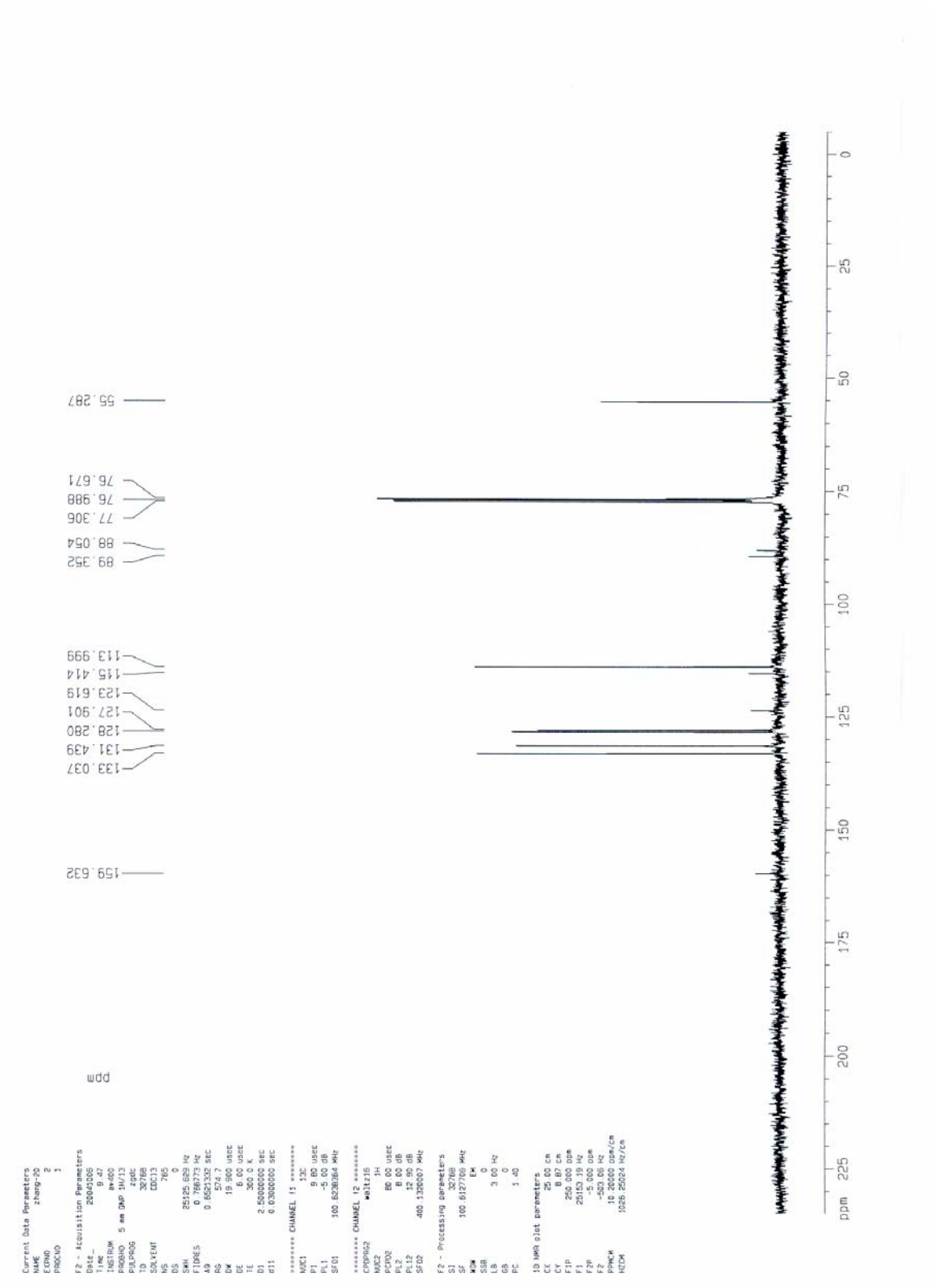
1-(Dec-1-ynyl)-4-methylbenzene (14): ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.28 (d, *J* = 8.0 Hz, 2H), 7.08 (d, *J* = 8.0 Hz, 2H), 2.38 (t, *J* = 7.2 Hz, 2H), 2.32 (s, 3H), 1.61–1.55 (m, 2H), 1.46–1.42 (m, 2H), 1.31–1.29 (m, 8H), 0.89 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 137.4, 131.4, 128.9, 121.0, 89.6, 80.6, 31.9, 29.2, 29.1, 28.9, 28.8, 23.7, 21.4, 18.4, 14.1.

(B) Spectra

1-methoxy-4-(2-phenylethynyl)benzene (3)



1-methoxy-4-(2-phenylethynyl)benzene (3)



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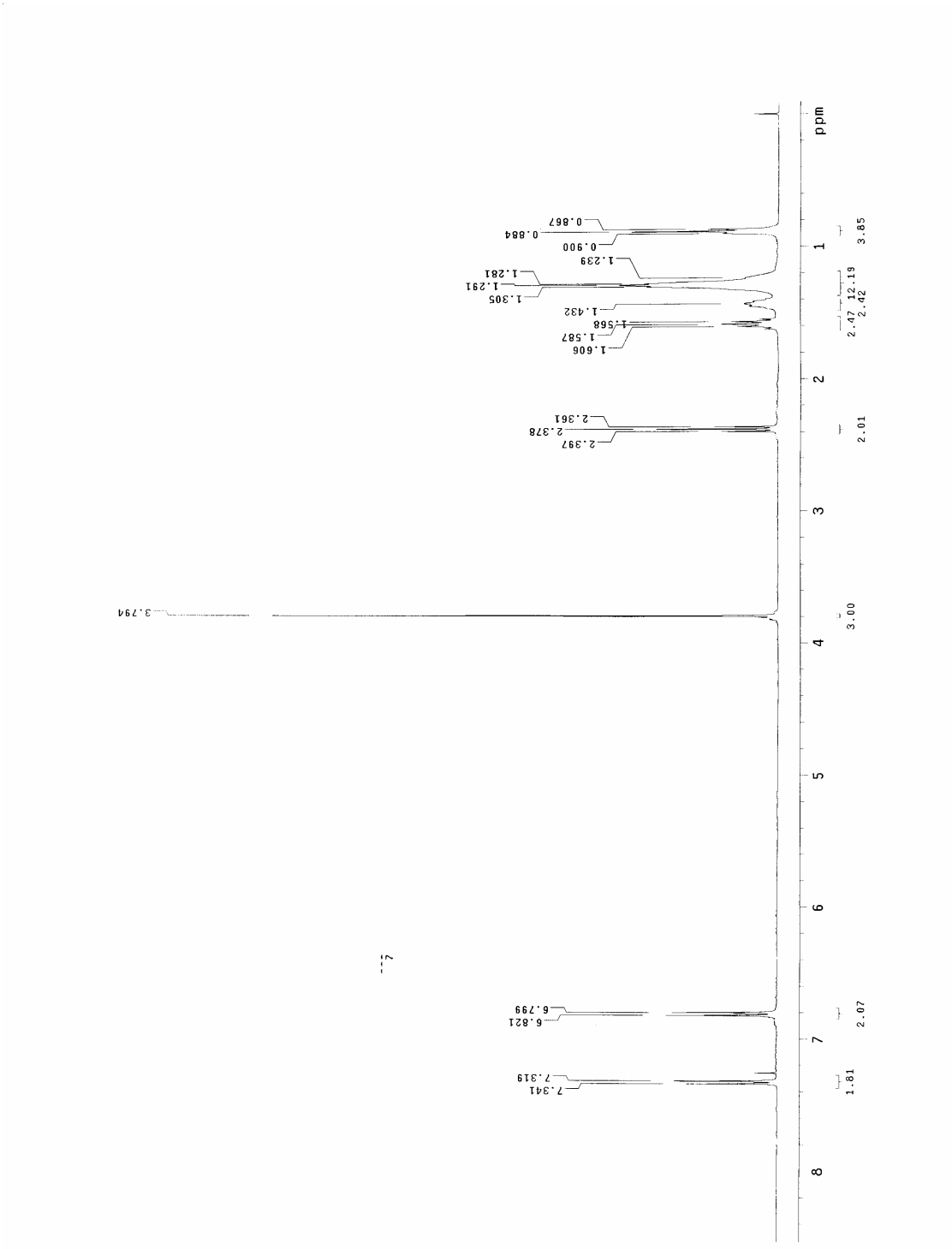

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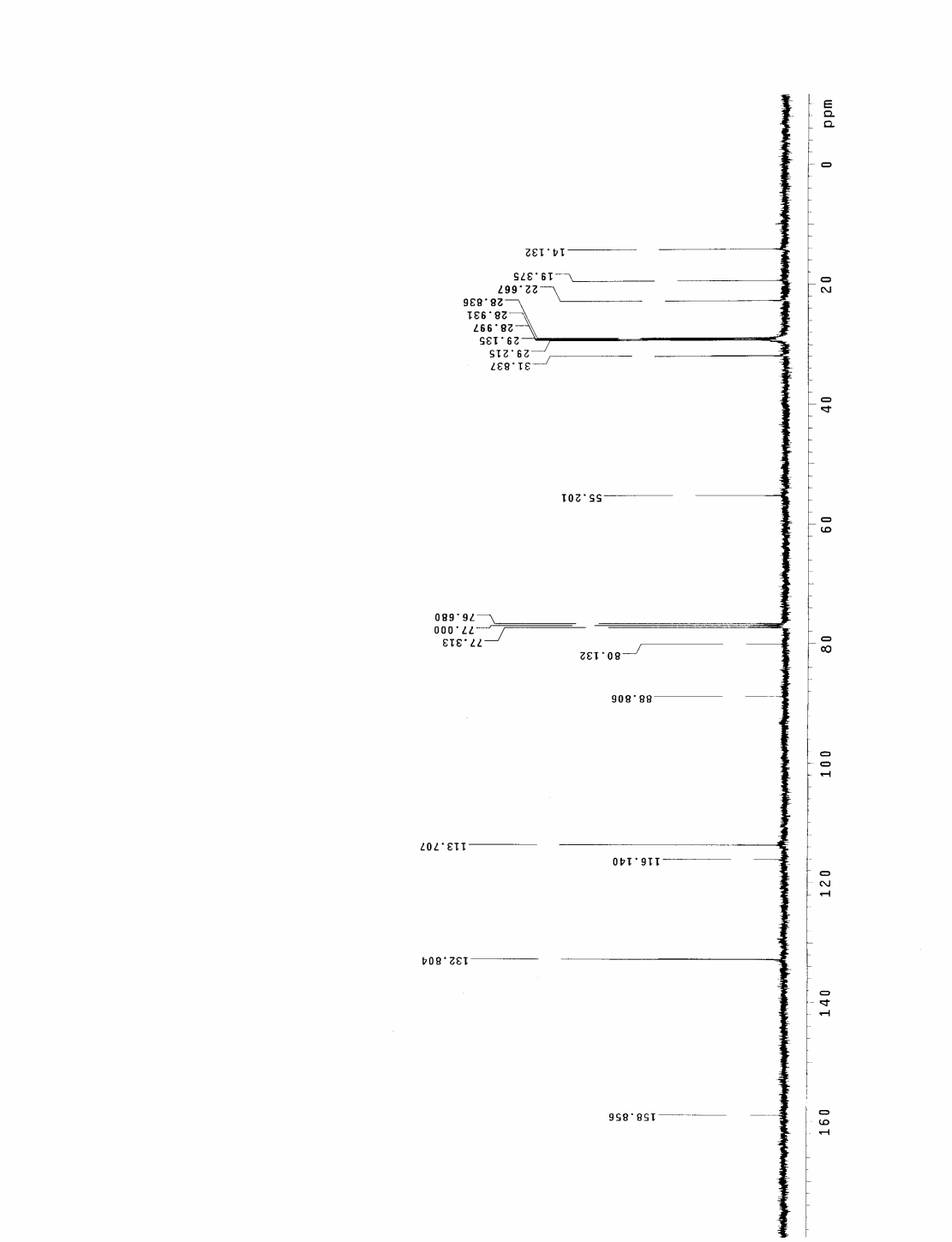

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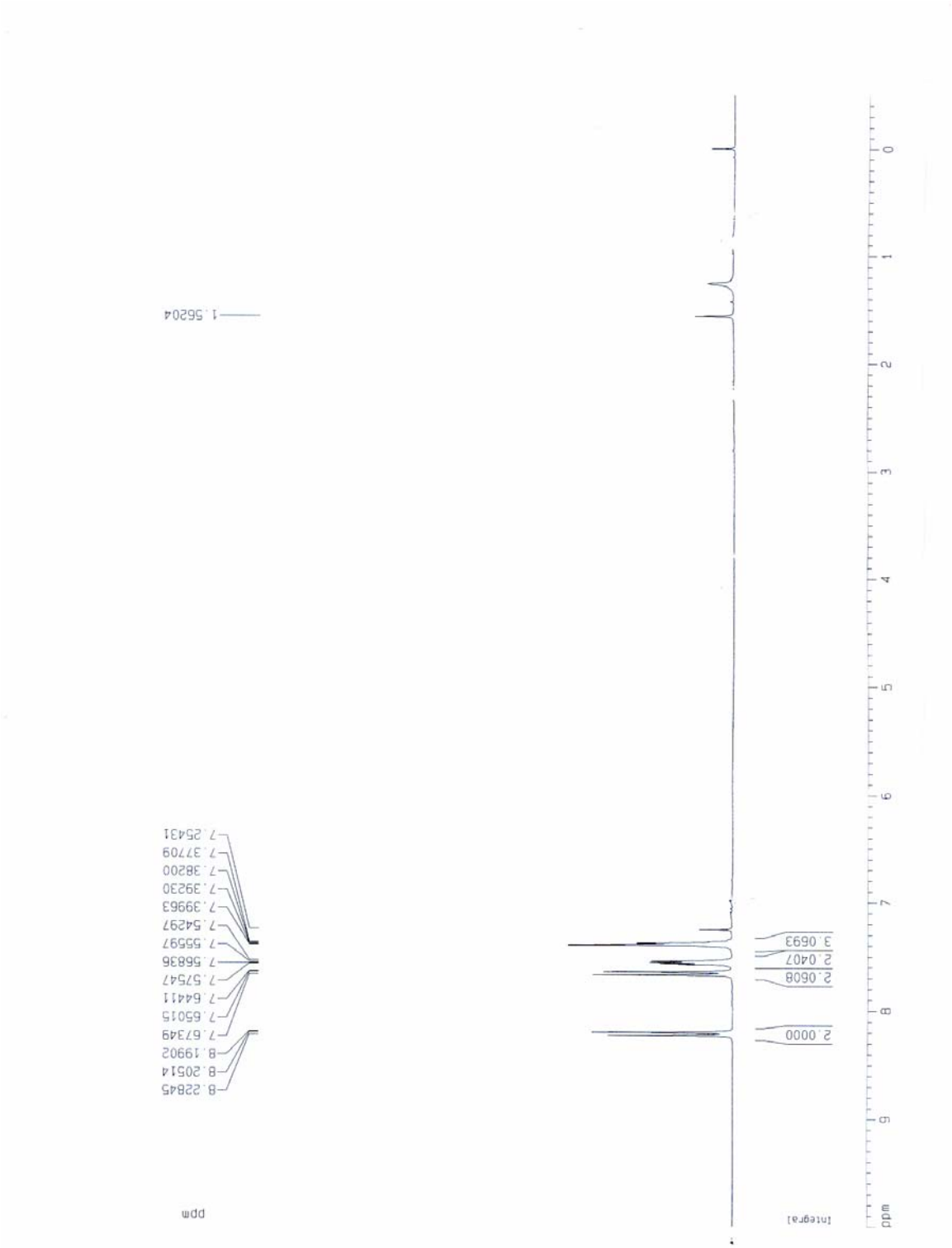

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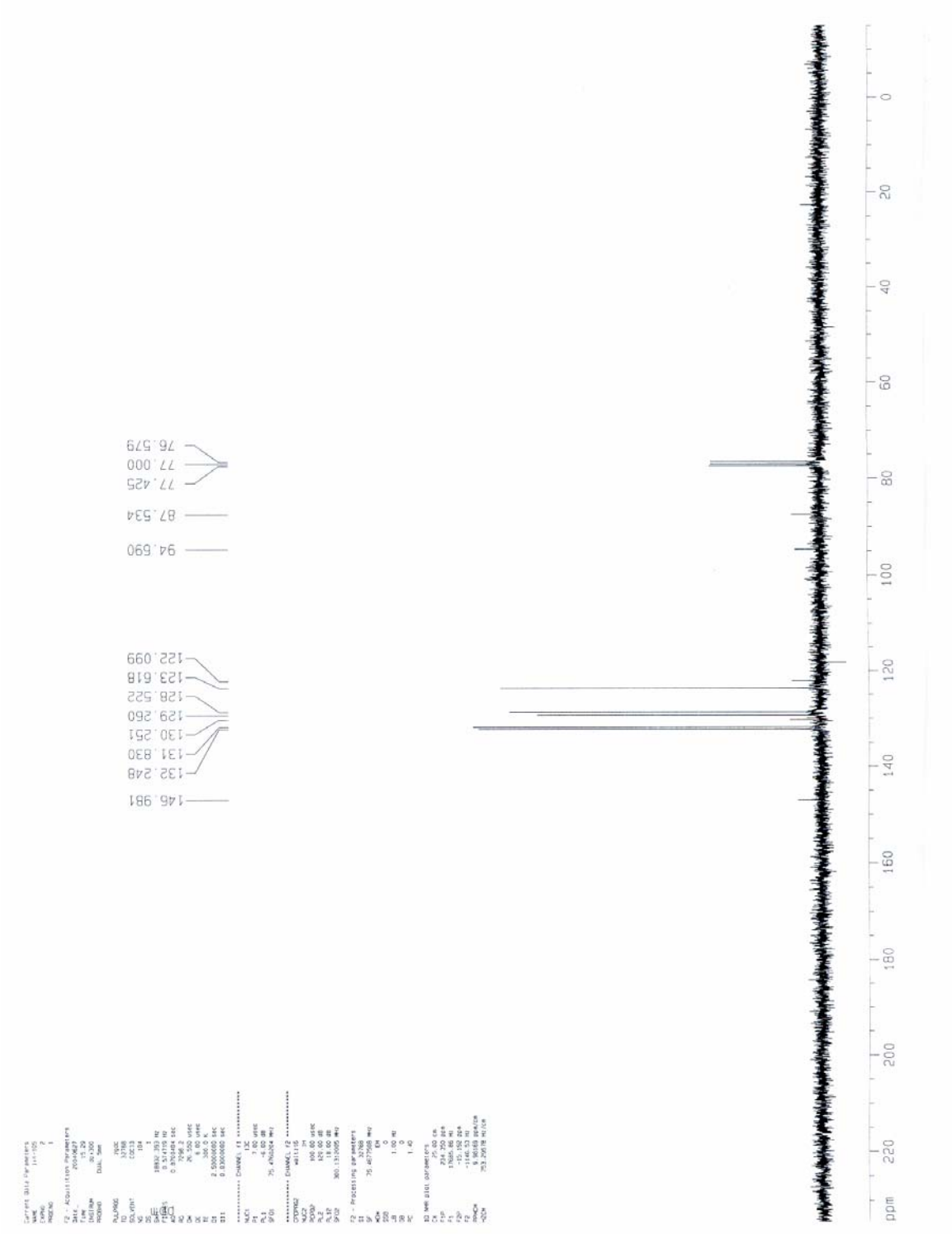

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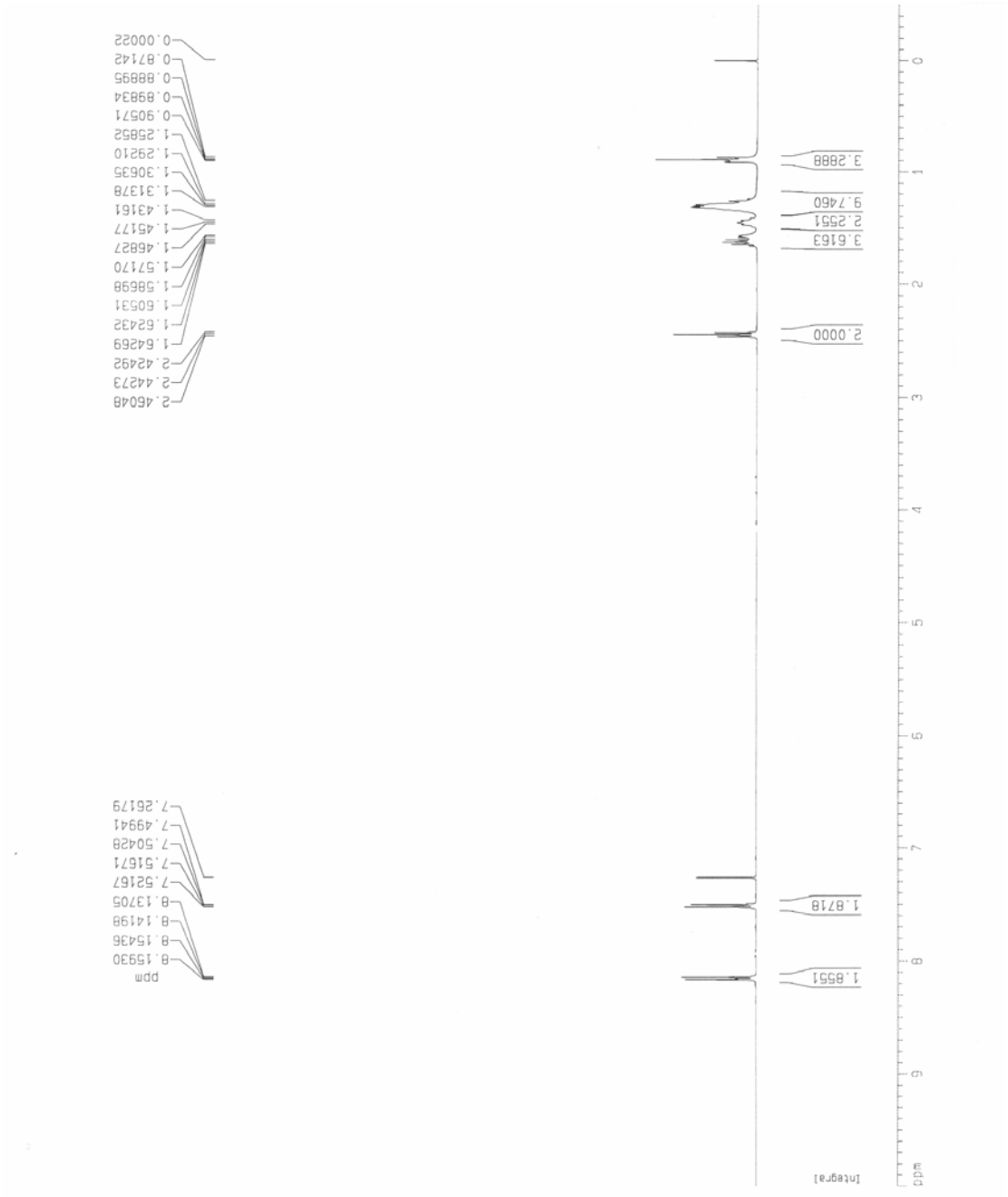

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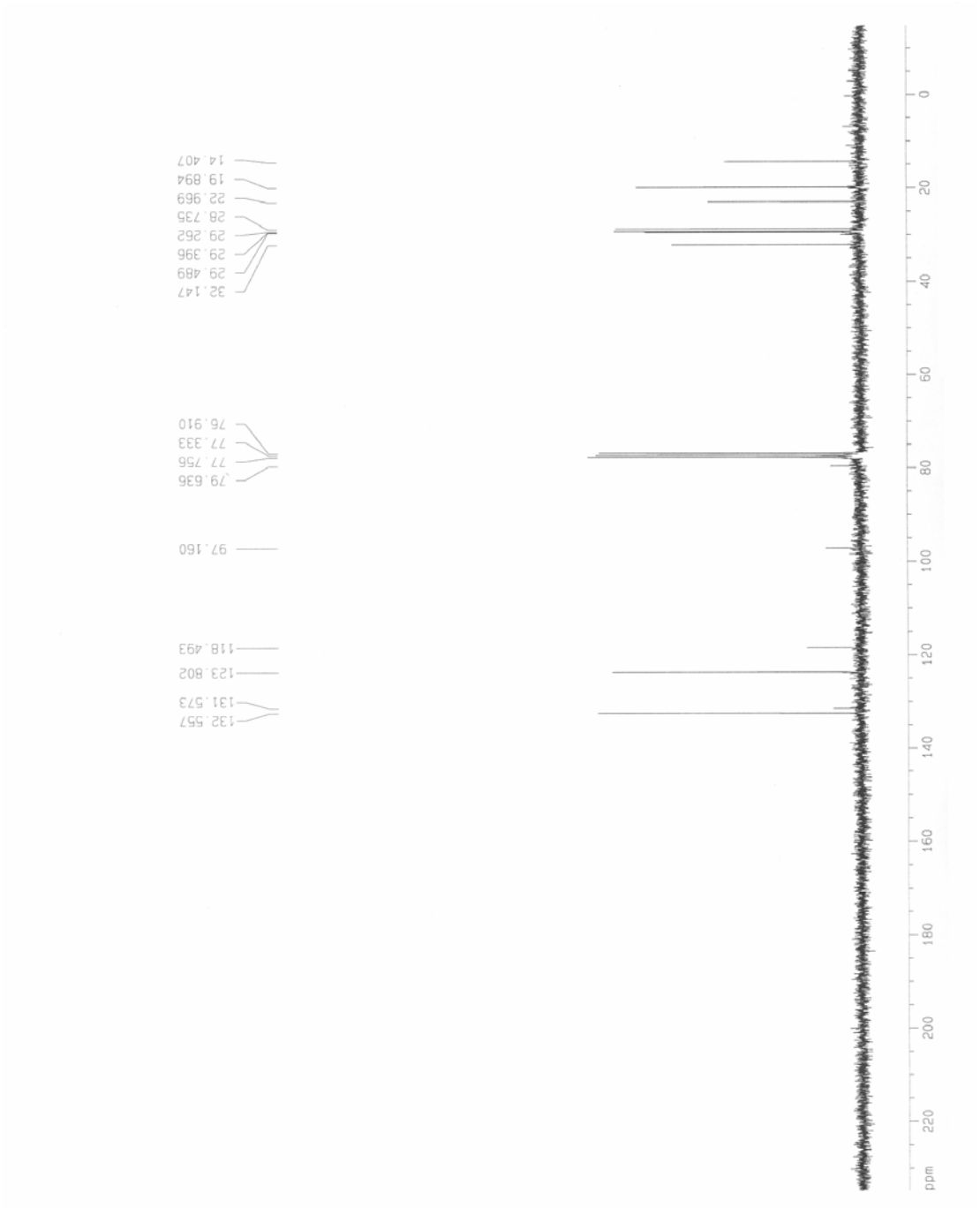

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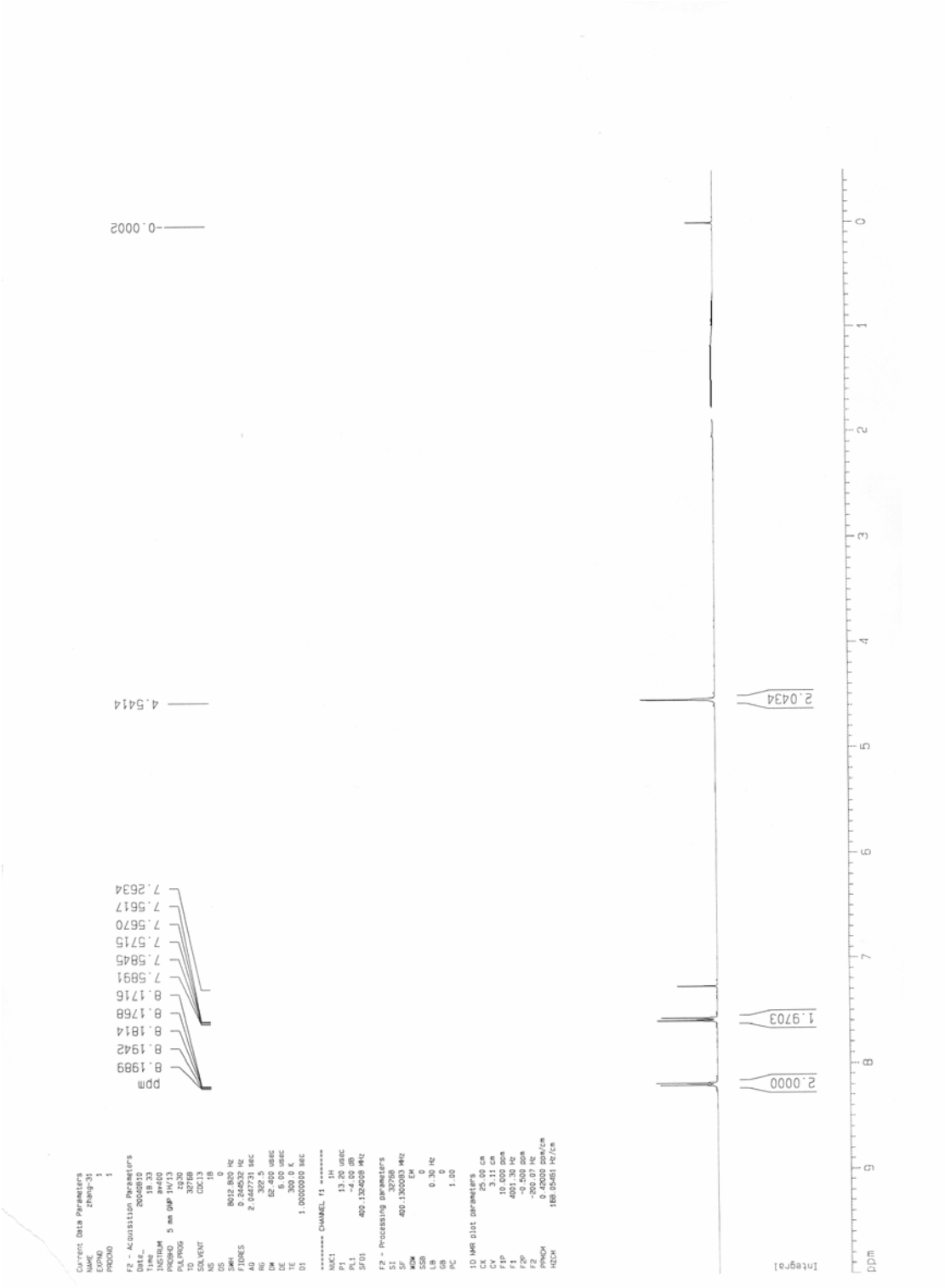
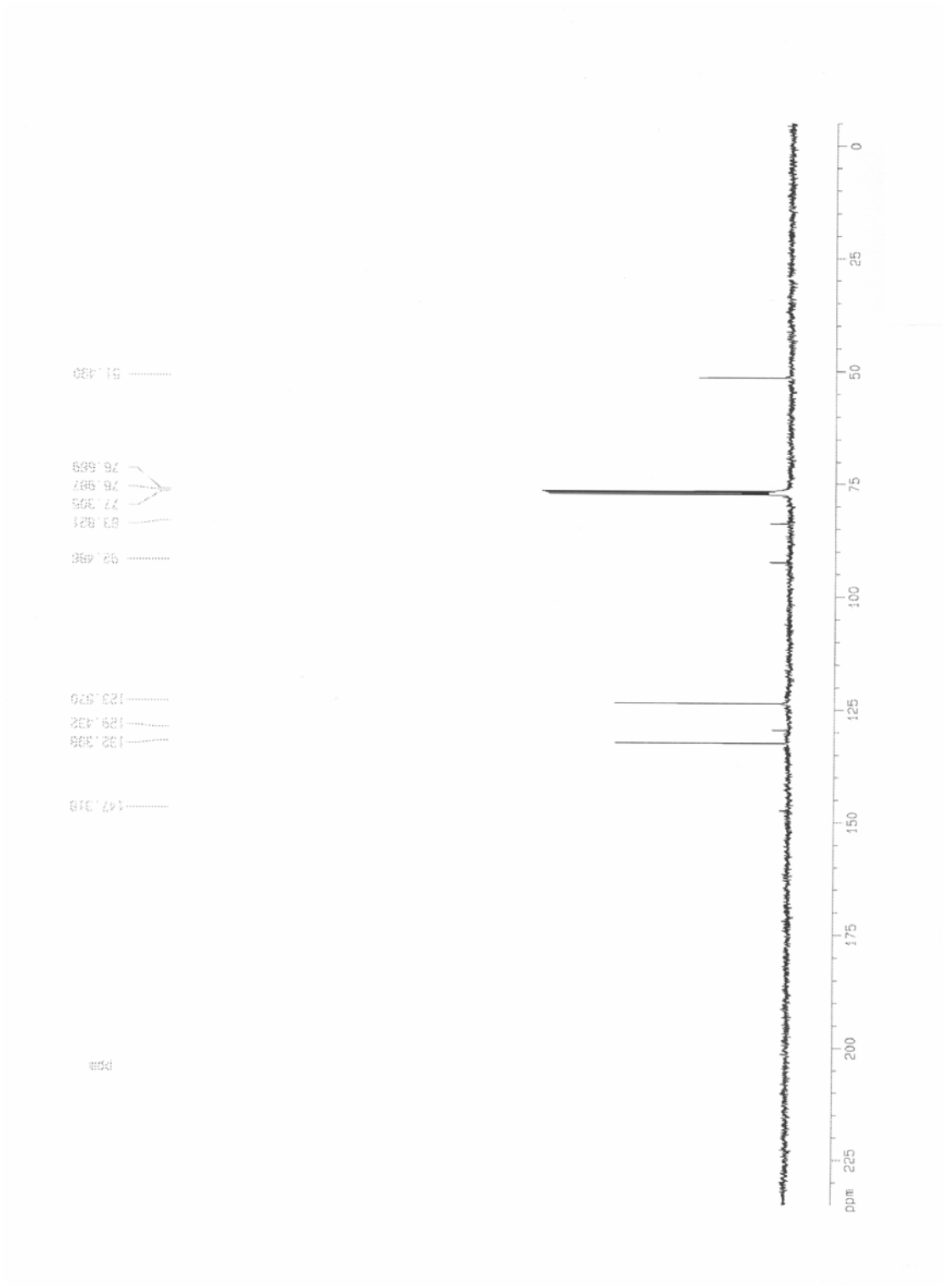


3-(4-nitrophenyl)prop-2-yn-1-ol (7)



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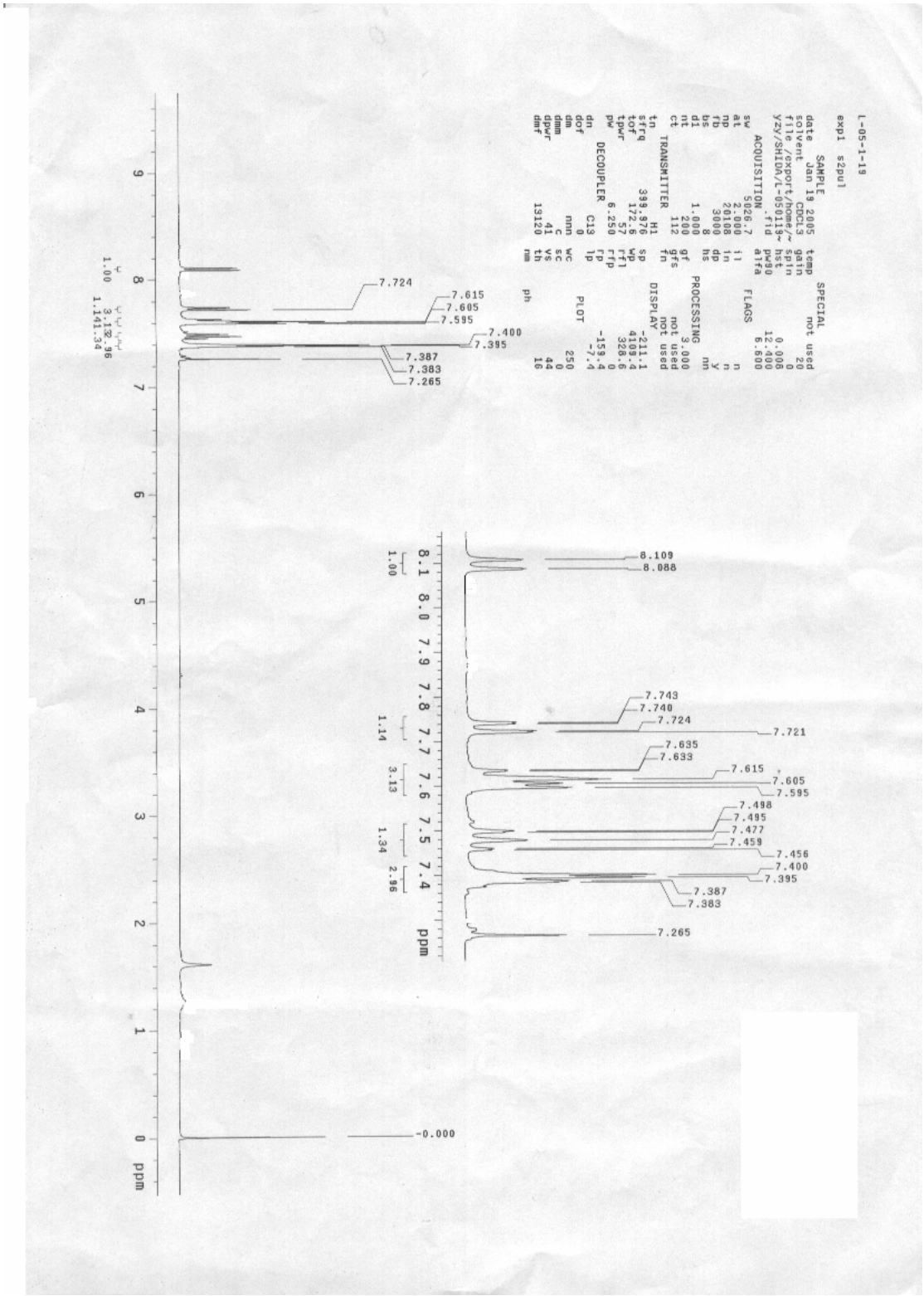

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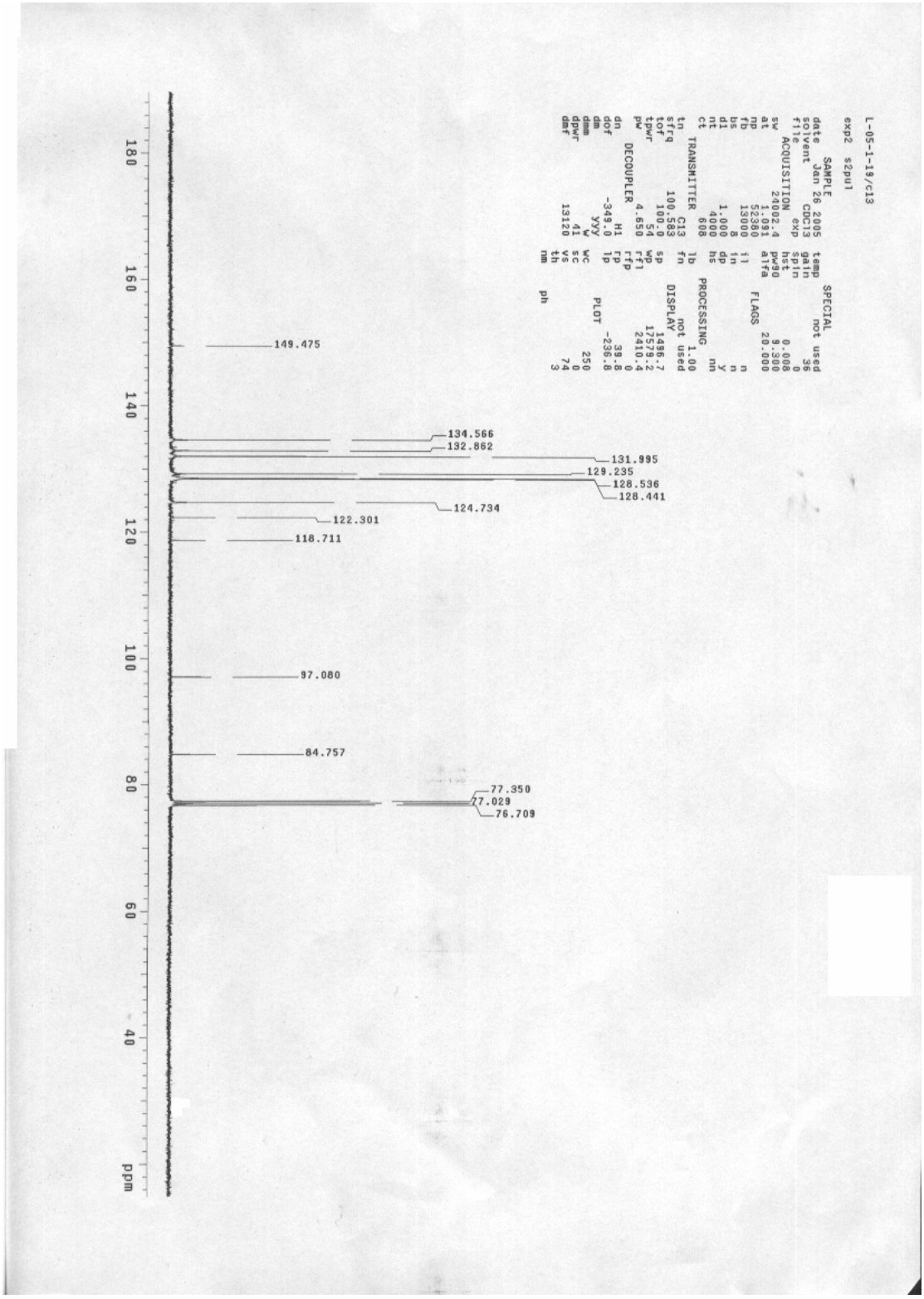

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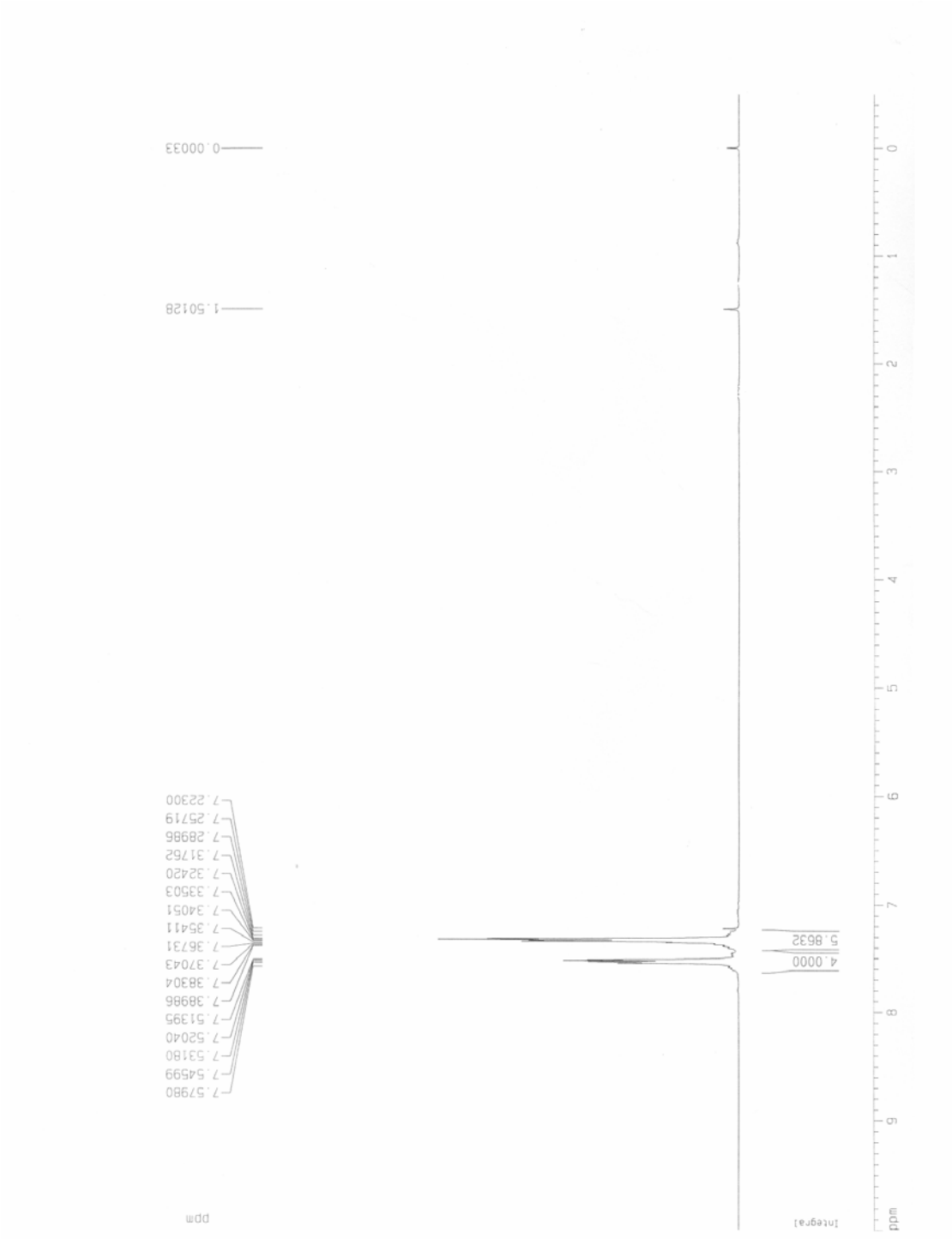
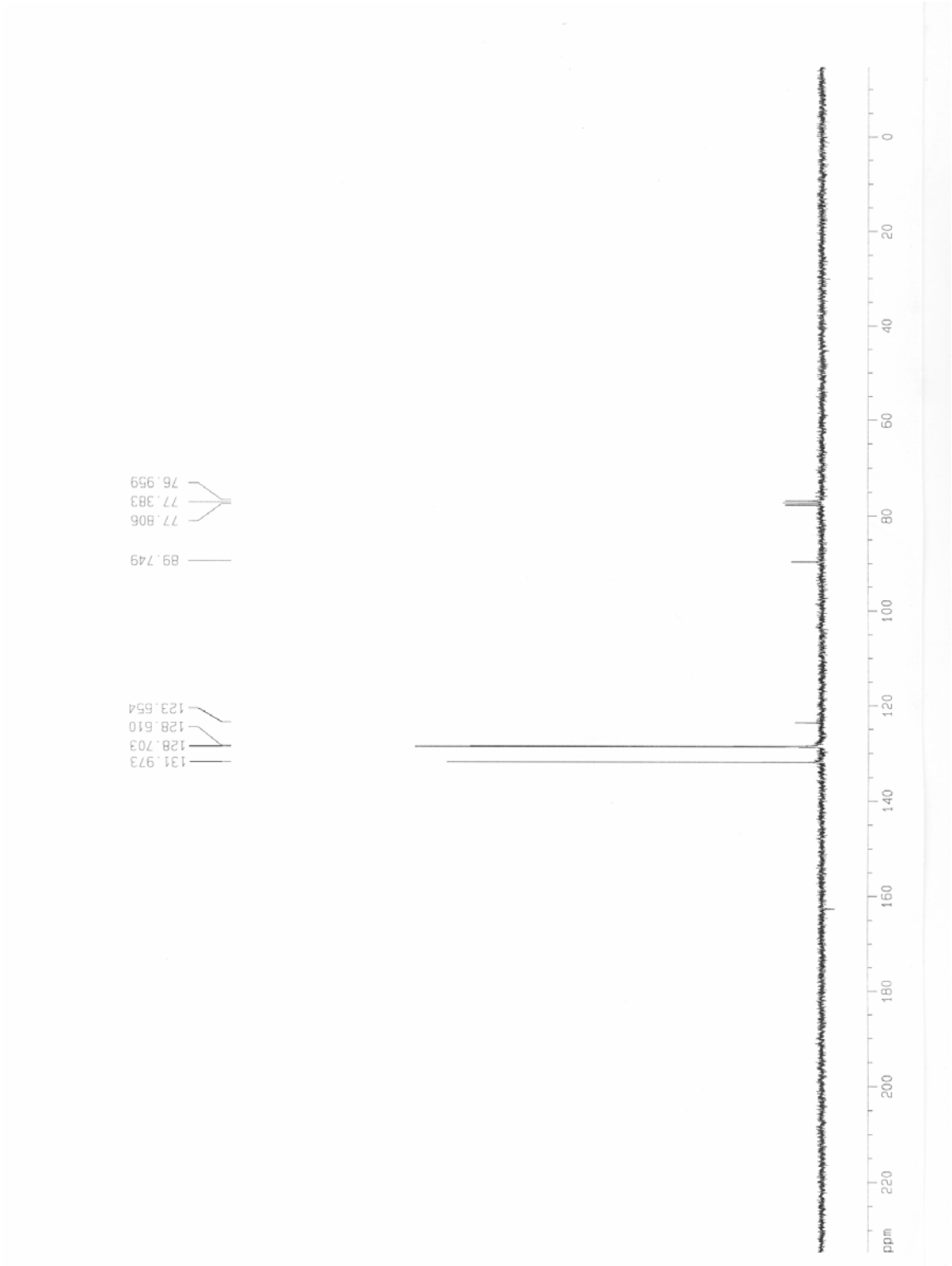


1,2-diphenylethyn (9)



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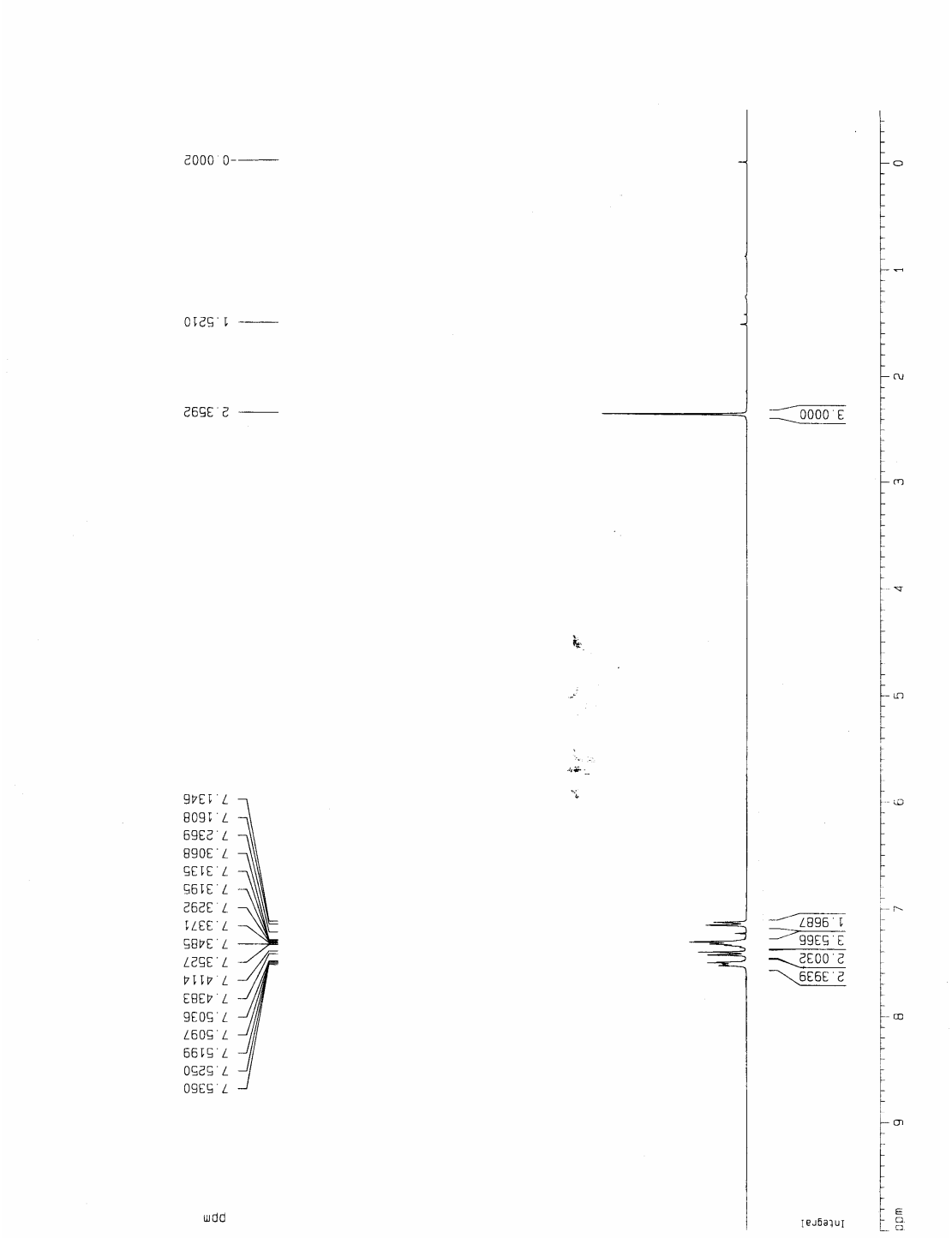
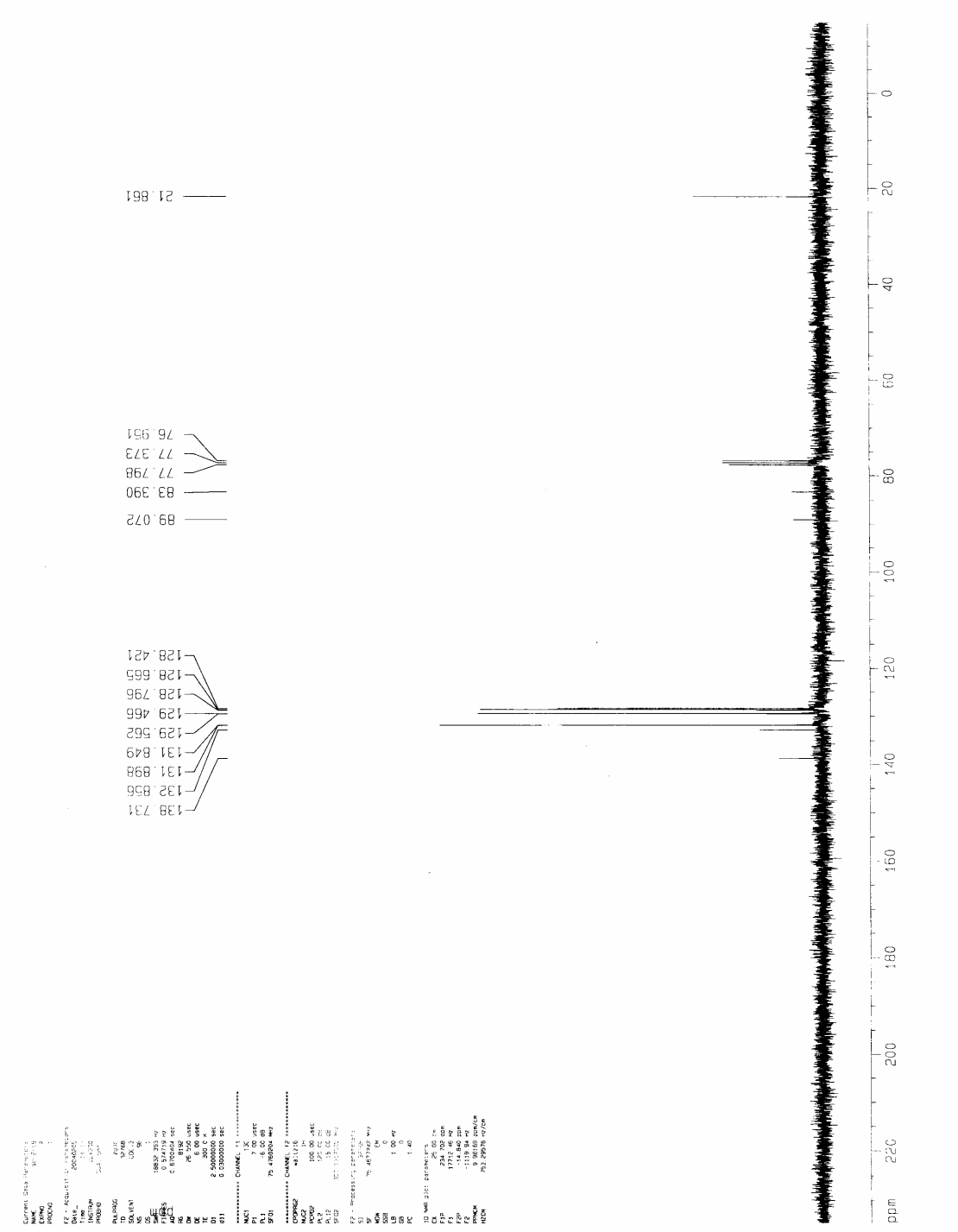
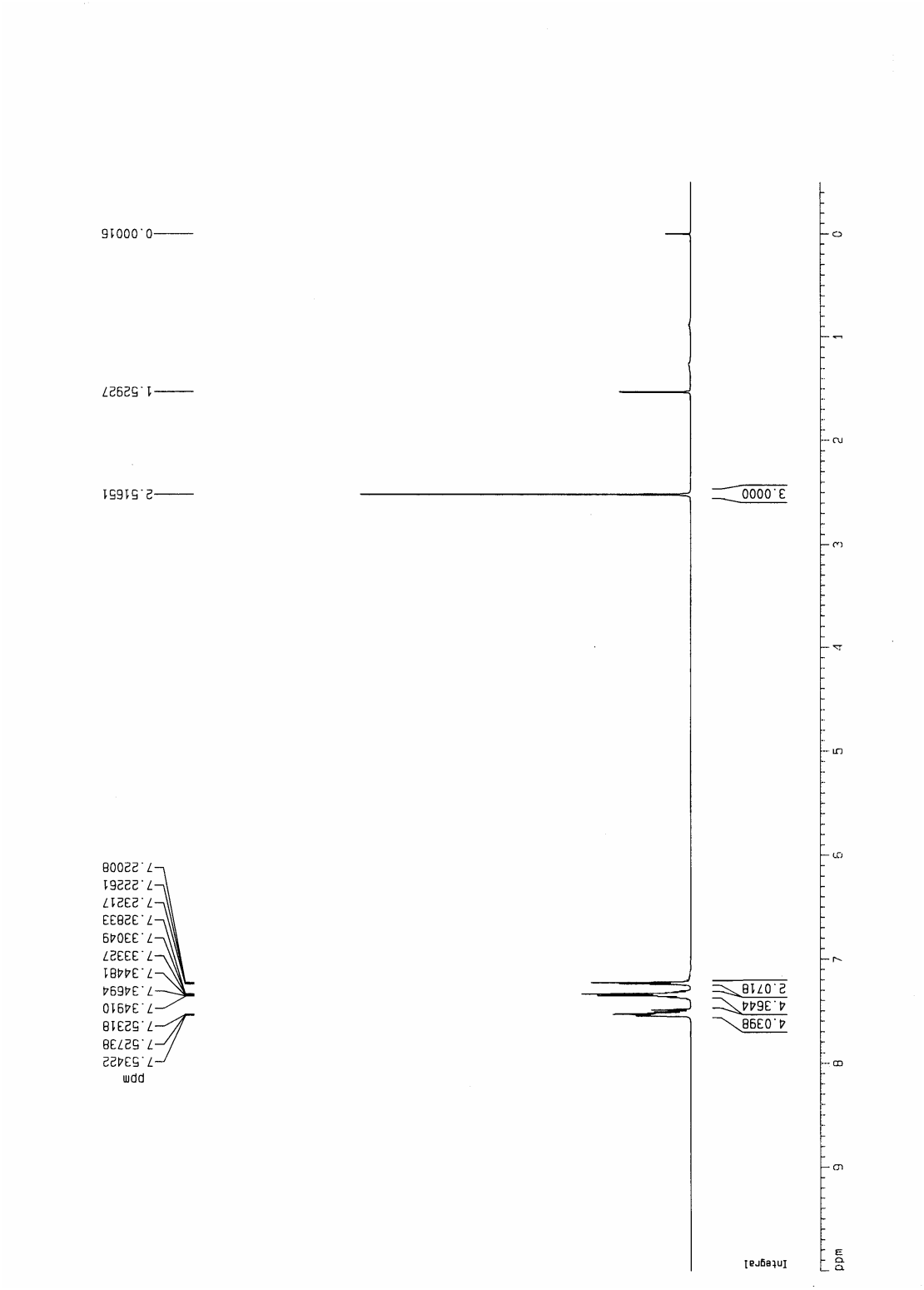


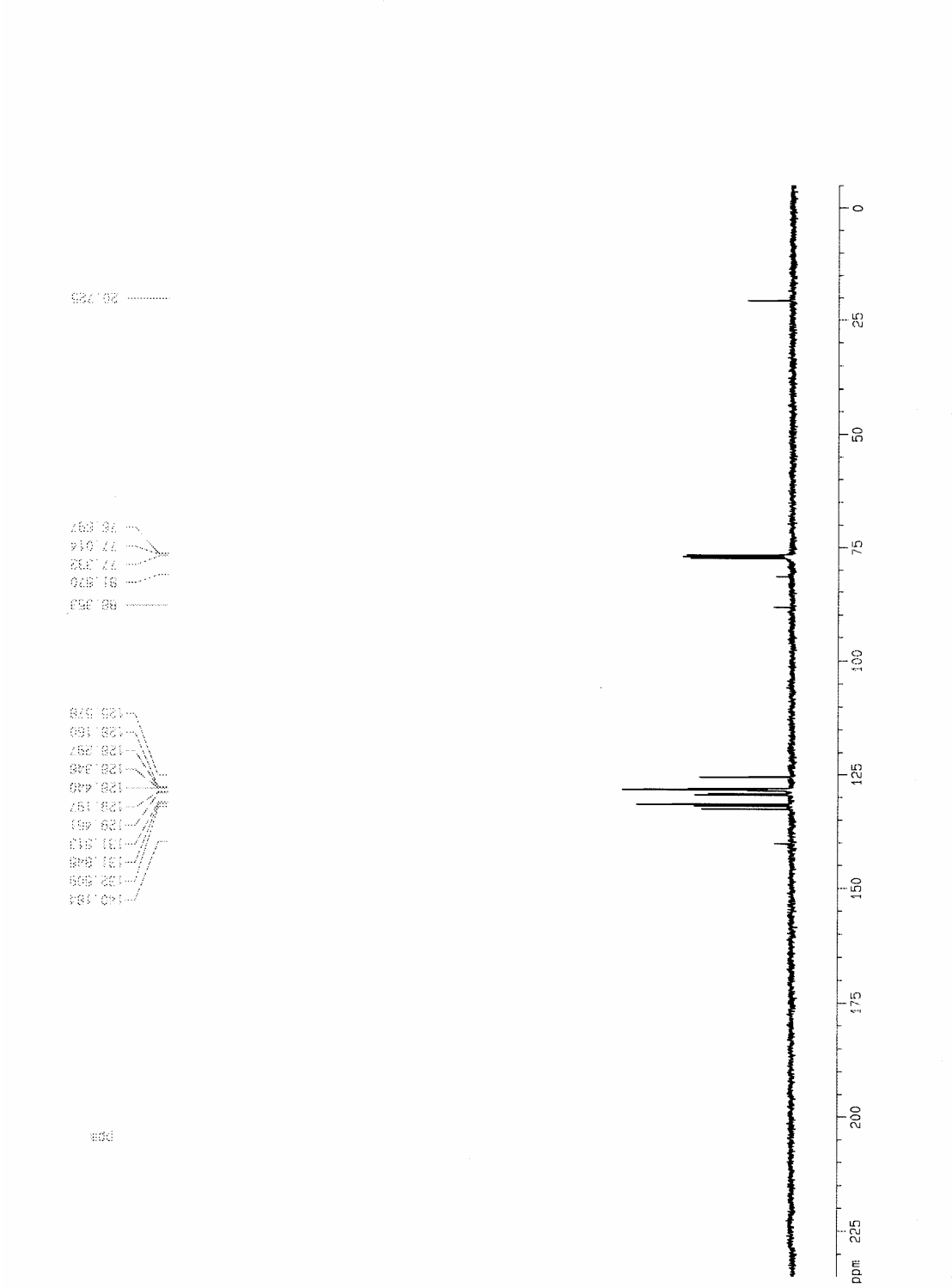
1-(2-*p*-tolylethynyl)benzene (10)



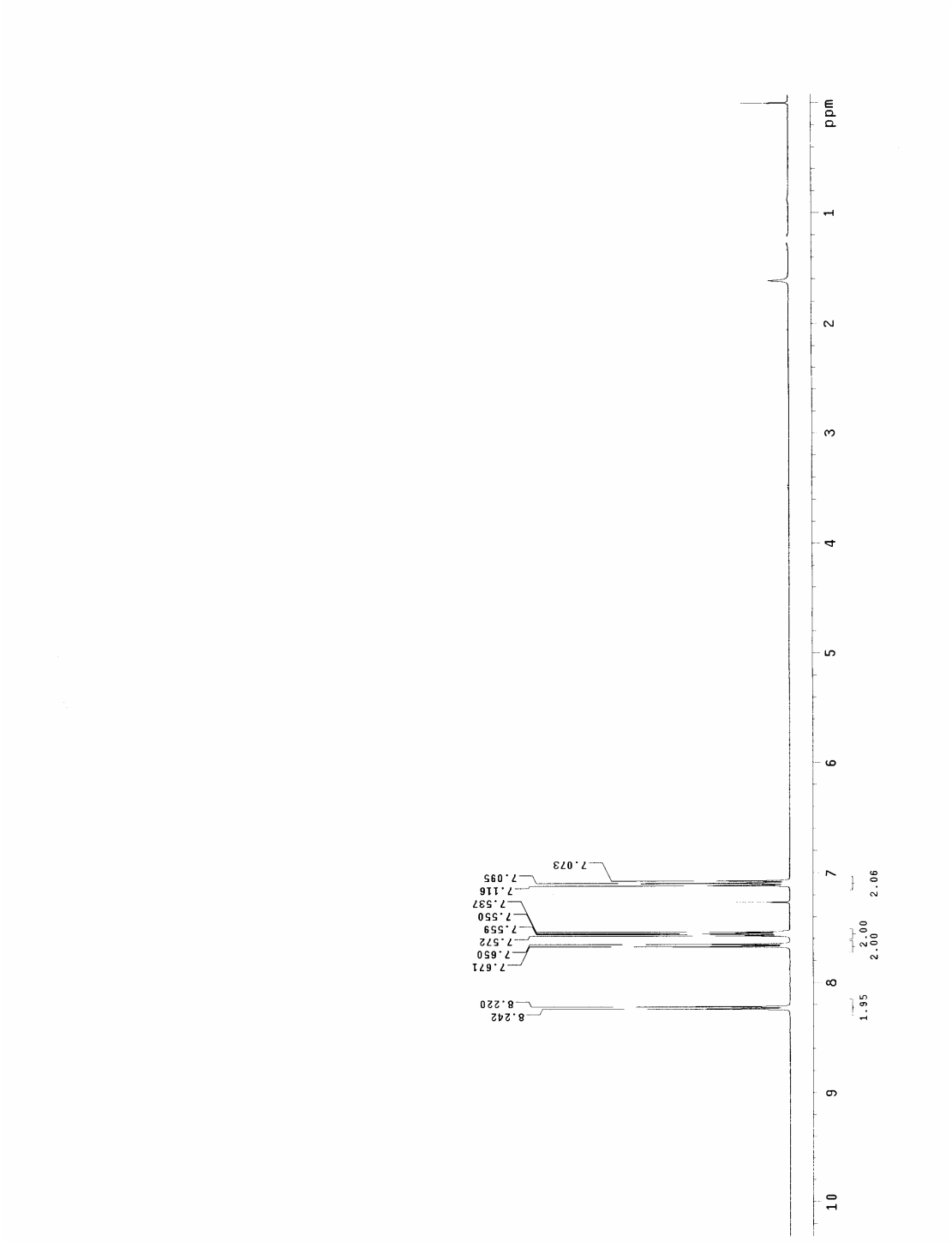
1-(2-*o*-tolylethynyl)benzene (11)



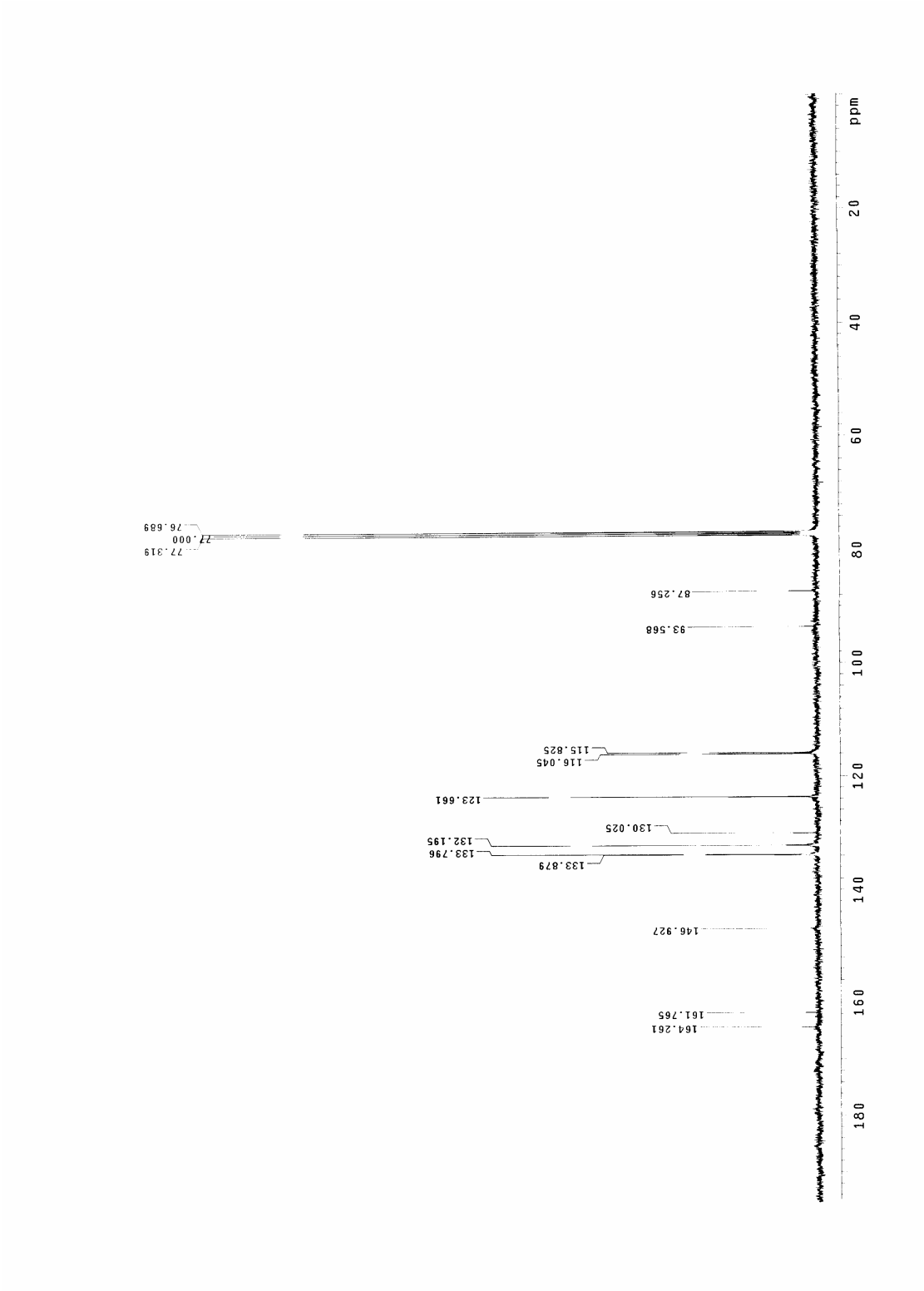
1-(2-*o*-tolylethynyl)benzene (11)



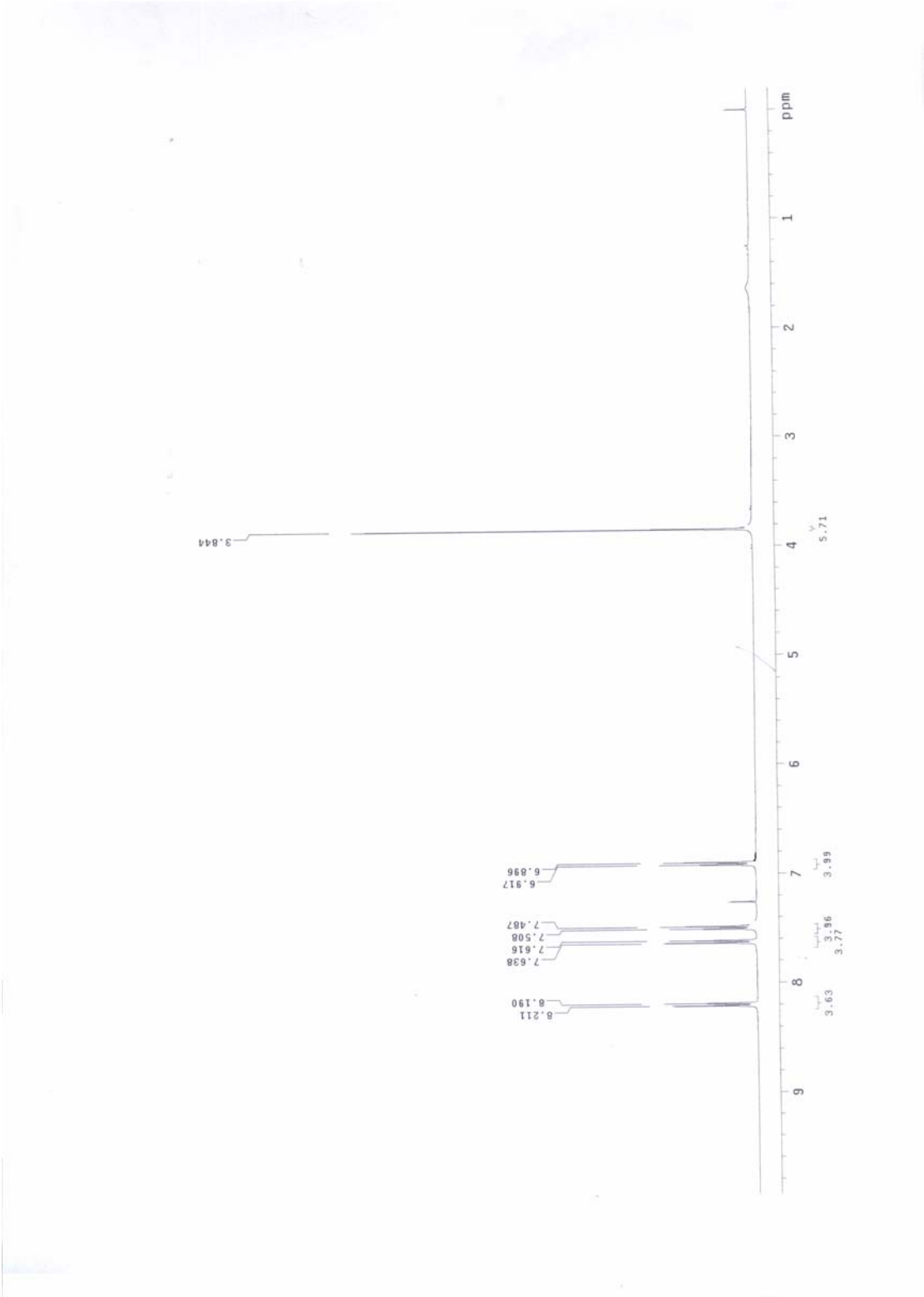
1-fluoro-4-(2-(4-nitrophenyl)ethynyl)benzene (12)



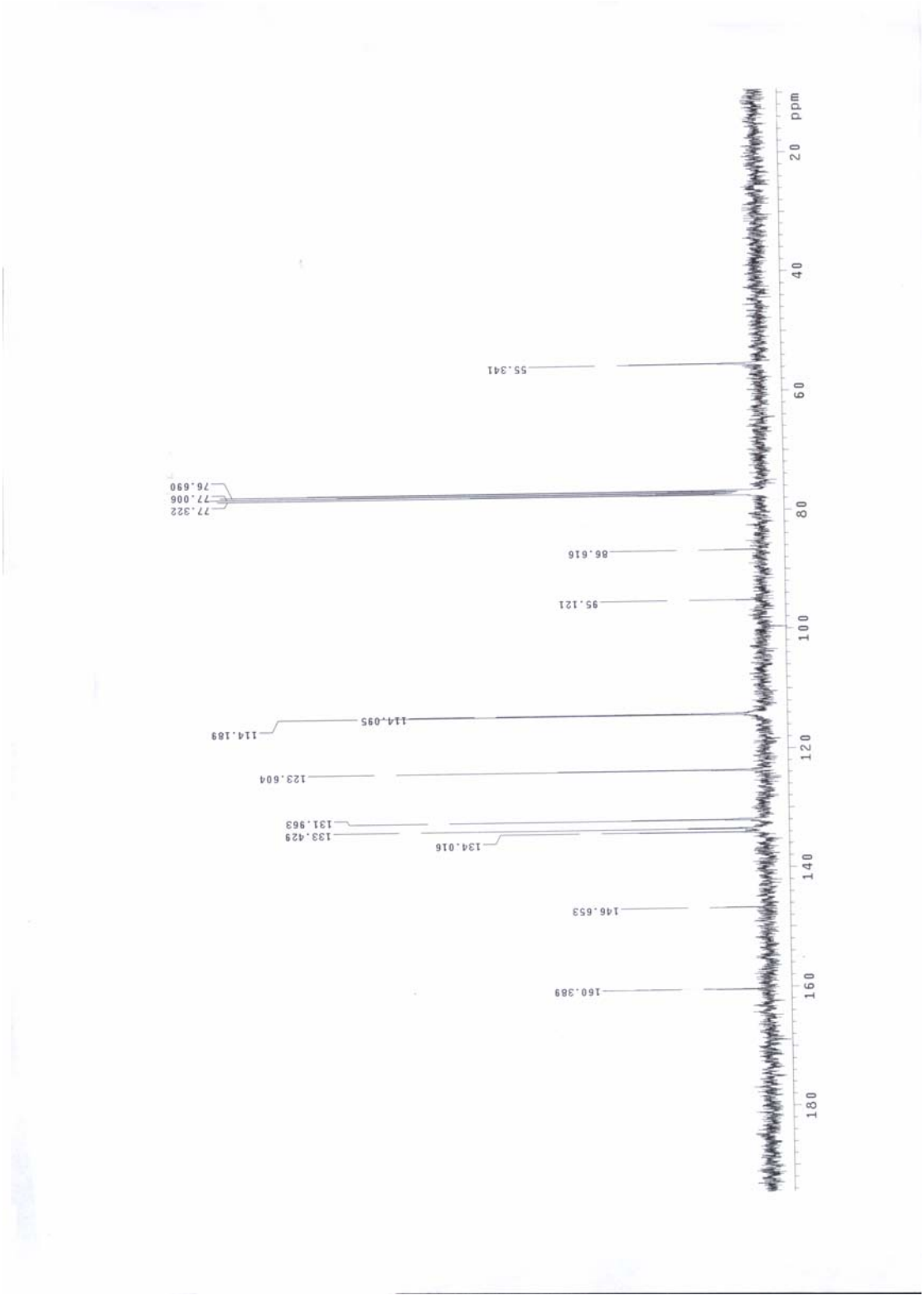
1-fluoro-4-(2-(4-nitrophenyl)ethynyl)benzene (12)



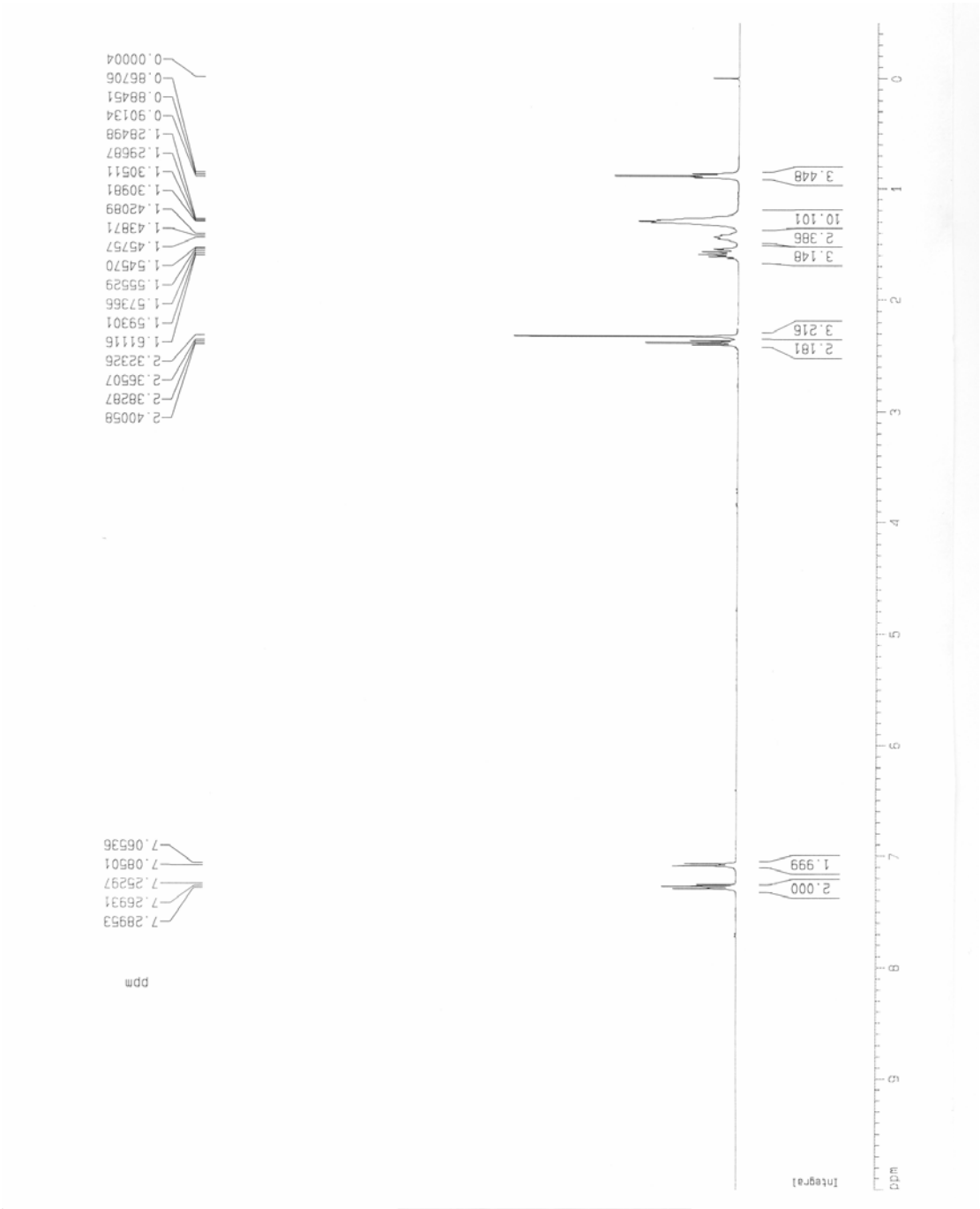
1-(2-(4-Methoxyphenyl)ethynyl)-4-nitrobenzene (13)



1-(2-(4-Methoxyphenyl)ethynyl)-4-nitrobenzene (13)



1-(dec-1-ynyl)-4-methylbenzene (14)



1-(dec-1-ynyl)-4-methylbenzene (14)