Supporting Information for:

Synthesis of α-Ketoester- and α-Hydroxyester-Substituted Isoindazoles via the Thermodynamic Coarctate Cyclization of Ester-Terminated Azo-Ene-Yne Systems

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Experimental Details

Ester 6b. Triazene **8b** was reacted according to General Procedure B to give **6b** (0.440 g, 68%) as a orange oil. ^{1}H NMR ($CDCl_3$) δ 7.72 (d, *J* = 1.5 Hz, 1H), 7.50 (m, 2H), 3.81 (q, *J* = 7.2 Hz, 4H), 3.78 (s, 3H), 1.33, (t, *J* = 7.2 Hz, 3H), 1.25 (t, *J* = 7.0 Hz, 3H). ^{13}C NMR ($CDCl_3$) δ 156.8, 154.1, 137.5, 133.9, 118.1, 117.4, 114.9, 107.0, 85.0, 82.8, 52.5, 49.9, 42.8, 14.1, 10.4. IR (NaCl) ν 3309, 2979, 2938, 2876, 2110, 1607, 1396, 1327, 1266, 1102, 1072 cm^{-1}. HRMS (EI+) for $C_{15}H_{16}N_3O_2F_3$: calc 327.11946, found 327.12051.

Ester 6c. Triazene **8c** was reacted according to General Procedure A to give **6c** (0.955 g, 85%) as a tan solid. ^{1}H NMR ($CDCl_3$) δ 7.79 (d, *J* = 1.2 Hz, 1H), 7.55 (m, 2H), 3.84 (q, *J* = 7.5 Hz, 4H), 3.82 (s, 3H), 1.36 (t, *J* = 7.2 Hz, 3H), 1.30 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR ($CDCl_3$) δ 156.2, 154.5, 131.1, 131.0 127.8, 127.7, 117.4, 114.4, 84.7, 84.2, 52.7, 49.7, 42.6, 14.4, 10.6. IR (NaCl) ν 2979, 2938, 2875, 2224, 1712, 1597, 1327, 1269, 1205, 1107 cm^{-1}. HRMS (EI+) for $C_{15}H_{16}N_4O_2$: calc 284.12732, found 284.12726.

Ester 6d. Triazene **8d** was reacted according to General Procedure A to give **6d** (1.01 g, 82%) as a yellow oil. ^{1}H NMR ($CDCl_3$) δ 7.49 (d, *J* = 2.4 Hz, 1H), 7.38 (d, *J* = 8.9 Hz, 1H), 7.28 (dd, *J* = 8.9, 2.4 Hz), 3.80 (s, 3H), 3.79 (q, *J* = 6.9 Hz, 4H), 1.30 (br t, 6H). ^{13}C NMR ($CDCl_3$) δ 154.5, 152.8, 133.0, 131.3, 129.3, 118.3, 115.4, 84.7, 84.2, 52.6, 49.4, 42.2, 14.4, 10.6. IR (NaCl) ν 2977, 2936, 2874, 2223, 1712, 1389, 1331, 1270, 1168, 1105 cm^{-1}. HRMS (EI+) for $C_{14}H_{16}N_3O_2Cl$: calc 293.09310, found 293.09350.

Ester 6e. Triazene **8e** was reacted according to General Procedure A to give **6e** (1.06 g, 75%) as an orange solid. ^{1}H NMR ($CDCl_3$) δ 7.54 (dd, *J* = 7.8, 0.9 Hz, 1H), 7.43 (dd, *J* = 8.1, 0.9 Hz, 1H), 7.36 (dt, *J* = 7.6, 1.3 Hz, 1H), 7.07 (dt, *J* = 7.8, 1.3 Hz, 1H), 3.81 (s, 3H), 3.80 (q, *J* = 6.9 Hz, 4H), 1.32 (br t, 6H). ^{13}C NMR ($CDCl_3$) δ 154.9, 154.4, 133.9, 131.3, 124.5, 117.2, 114.2, 86.1, 84.1, 52.5, 49.3, 42.1, 14.5, 10.8. IR (NaCl) ν 2976, 2936, 2874, 2218, 1710, 1302, 1268, 1198, 1094 cm^{-1}. HRMS (EI+) for $C_{14}H_{17}N_3O_2$: calc 259.13208, found 259.13201.

Ester 6f. Triazene **8f** was reacted according to General Procedure A to give **6f** (1.75 g, 68%) as a red oil. ^{1}H NMR ($CDCl_3$) δ 7.35 (d, *J* = 1.3 Hz, 1H), 7.33 (d, *J* = 8.5 Hz, 1H), 7.16 (dd, *J* =

8.5, 1.3 Hz, 1H), 3.81 (s, 3H), 3.79 (q, *J* = 7.2 Hz, 4H), 1.31 (br t, 6H). ^{13}C NMR ($CDCl_3$) δ 154.8, 152.1, 134.2, 134.0, 132.2, 117.0, 113.9, 86.3, 83.8, 52.4, 49.1, 41.9, 20.6, 14.4, 10.9. IR (NaCl) ν 2975, 2935, 2214, 1709, 1215, 1148, 1102 cm^{-1}. HRMS (EI+) for $C_{15}H_{19}N_3O_2$: calc 273.14773, found 273.14705.

Ester 6g. Triazene **8g** was reacted according to General Procedure A to give **6g** (0.125 g, 65%) as a red oil. ^{1}H NMR ($CDCl_3$) δ 7.56 (d, *J* = 2.1 Hz, 1H), 7.40 (dd, *J* = 8.7, 2.1 Hz, 1H), 7.35 (d, *J* = 8.7 Hz, 1H), 3.81 (s, 3H), 3.79 (q, *J* = 7.5 Hz, 4H), 1.30 (m, 15H). ^{13}C NMR ($CDCl_3$) δ 154.9, 152.1, 147.5, 130.6, 128.8, 116.9, 113.4, 86.8, 85.5, 52.5, 49.0, 41.9, 34.3, 31.1, 14.4, 10.8. IR (NaCl) ν 2964, 2871, 2214, 1711, 1465, 1392, 1271, 1205, 1169, 1106 cm^{-1}. HRMS (EI+) for $C_{18}H_{25}N_3O_2$: calc 315.19468, found 315.19524.

Ester 6h. Triazene **8h** was reacted according to General Procedure A to give **6h** (0.083 g, 65%) as a red oil. ^{1}H NMR ($CDCl_3$) δ 7.28 (d, *J* = 9.1 Hz, 1H), 7.03 (d, *J* = 2.7 Hz, 1H), 6.94 (dd, *J* = 9.1, 2.7 Hz, 1H), 3.80 (s, 3H), 3.78 (s, 3H), 3.76 (q, *J* = 6.9 Hz, 4H), 1.29 (t, *J* = 6.9 Hz, 6H). ^{13}C NMR ($CDCl_3$) δ 156.4, 154.7, 148.5, 119.1, 118.2, 116.5, 114.5, 85.9, 83.9, 55.5, 52.5, 49.1 (br), 41.8 (br), 14.6 (br), 11.0 (br). IR (NaCl) ν 2973, 2936, 2872, 2213, 1709, 1456, 1226, 1153, 1034 cm^{-1}. HRMS for $C_{15}H_{19}N_3O_3$: calc 289.14265, found 289.14288.

α-Ketoester 9b. Ester **6b** was cyclized according to General Procedure C to give **9b** (20 mg, 85%) as a yellow solid. ^{1}H NMR ($CDCl_3$) δ 8.62 (d, *J* = 1.4 Hz, 1H), 7.88 (d, *J* = 8.9 Hz, 1H), 7.57 (dd, *J* = 8.9, 1.4 Hz, 1H), 3.97 (s, 3H), 3.30 (q, *J* = 7.2 Hz, 4H), 0.94 (t, *J* = 7.2 Hz, 6H). ^{13}C NMR ($CDCl_3$) δ 177.2, 163.7, 146.3, 129.8, 128.6, 128.3, 120.5, 120.0, 118.6, 110.1, 52.6, 52.2, 11.1. IR (NaCl) ν 2983, 2955, 2878, 2228, 1747, 1662, 1327, 1251, 1167, 1015 cm^{-1}. HRMS (EI+) for $C_{15}H_{16}N_3O_3F_3$: calc 343.11438, found 343.11417.

α-Ketoester 9c. Ester **6c** was cyclized according to General Procedure C to give **9c** (61 mg, 92%) as a orange solid. ^{1}H NMR ($CDCl_3$) δ 8.55 (d, *J* = 1.2 Hz, 1H), 7.91 (d, *J* = 9.0 Hz, 1H), 7.62 (dd, *J* = 9.0, 1.2 Hz, 1H), 3.98 (s, 3H), 3.31 (q, *J* = 7.5 Hz, 4H), 0.95 (t, *J* = 7.5 Hz, 6H). ^{13}C NMR ($CDCl_3$) δ 177.2, 163.7, 146.3, 129.8, 128.6, 128.3, 120.5, 120.0, 118.9, 110.1, 52.6,

52.2, 11.1. IR (NaCl) ν 2981, 2954, 2876, 2228, 1745, 1662, 1653, 1507, 1456, 1213, 1017 cm^{-1}. HRMS (EI+) for $C_{15}H_{16}N_4O_3$: calc 300.12224, found 300.12269.

α-Ketoester 9d. Ester **6d** was cyclized according to General Procedure C to give **9d** (15 mg, 60%) as a orange solid. ^1H NMR ($CDCl_3$) δ 8.25 (d, *J* = 1.8 Hz, 1H), 7.77 (d, *J* = 9.0 Hz, 1H), 7.42 (dd, *J* = 9.0, 1.8 Hz, 1H), 3.99 (s, 3H), 3.30 (m, 4H), 0.96 (t, *J* = 7.2 Hz, 6H). ^{13}C NMR ($CDCl_3$) δ 177.3, 164.3, 144.5, 133.2, 129.0, 133.3, 120.5, 120.3, 120.0, 52.3, 52.2, 29.1, 11.1. IR (NaCl) ν 2980, 2952, 2873, 1744, 1653, 1506, 1153, 1015 cm^{-1}. HRMS (EI+) for $C_{14}H_{17}N_3O_3Cl$: calc 310.09585, found 310.09675.

α-Ketoester 9e. Ester **6e** was cyclized according to General Procedure C to give **9e** (19 mg, 75%) as a orange oil. ^1H NMR ($CDCl_3$) δ 8.21 (dd, *J* = 7.5, 2.1 Hz, 1H), 7.81 (dd, *J* = 7.8, 1.8 Hz, 1H), 7.43 (m, 2H), 3.96 (s, 3H), 3.30 (m, 4H), 0.94 (t, *J* = 7.5 Hz, 6H). ^{13}C NMR ($CDCl_3$) δ 177.5, 164.5, 146.2, 127.5, 127.0, 121.8, 121.4, 118.5, 52.3, 52.1, 11.1. IR (NaCl) ν 2980, 2941, 2871, 1743, 1652, 1456, 1254, 1018 cm^{-1}. HRMS (EI+) for $C_{14}H_{17}N_3O_3$: calc 275.12700, found 275.12711.

α-Ketoester 9f. Ester **6f** was cyclized according to General Procedure C to give **9f** (22 mg, 88%) as a orange oil. ^1H NMR ($CDCl_3$) δ 7.99 (d, *J* = 1.2 Hz, 1H), 7.70 (d, *J* = 8.7 Hz, 1H), 7.28 (dd, *J* = 8.7, 1.2 Hz, 1H), 3.95 (s, 3H), 3.27 (m, 4H), 2.49 (s, 3H), 0.94 (t, *J* = 7.2 Hz, 6H). ^{13}C NMR ($CDCl_3$) δ 177.5, 164.7, 145.0, 137.4, 130.2, 128.1, 122.2, 119.8, 118.2, 52.2, 52.1, 22.1, 11.1. IR (NaCl) ν 2979, 2979, 2868, 1744, 1651, 1627, 1523, 1455, 1256, 1198, 1121, 1018 cm^{-1}. HRMS (EI+) for $C_{15}H_{19}N_3O_3$: calc 289.14265, found 289.14201.

α-Ketoester 9g. Ester **6g** was cyclized according to General Procedure C to give **9g** (23 mg, 88%) as a orange oil. ^1H NMR ($CDCl_3$) δ 8.14 (d, *J* = 1.8 Hz, 1H), 7.77 (d, *J* = 9.0 Hz, 1H), 7.57 (dd, *J* = 9.0, 1.8 Hz, 1H), 3.96 (s, 3H), 3.28 (m, 4H), 1.40 (s, 9H), 0.93 (t, *J* = 7.2 Hz, 6H). ^{13}C NMR ($CDCl_3$) δ 177.6, 164.7, 150.5, 144.9, 128.8, 127.0, 122.0, 118.0, 115.9, 52.2, 52.1, 35.3, 31.2, 11.1. IR (NaCl) ν 2964, 2870, 1744, 1652, 1457, 1259, 1156, 1016 cm^{-1}. HRMS (EI+) for $C_{18}H_{25}N_3O_3$: calc 331.18960, found 331.19006.

α-Ketoester 9h. Ester **6h** was cyclized according to General Procedure C to give **9h** (15 mg, 69%) as a orange solid. ^{1}H NMR ($CDCl_3$) δ 7.68 (d, *J* = 9.3 Hz, 1H), 7.74 (d, *J* = 2.4 Hz, 1H), 7.11 (dd, *J* = 9.3, 2.4 Hz, 1H), 3.96 (s, 3H), 3.91 (s, 3H), 3.26 (m, 4H), 0.94 (t, *J* = 7.5 Hz, 6H). ^{13}C NMR ($CDCl_3$) δ 177.5, 164.8, 159.5, 142.4, 123.1, 122.1, 120.0, 99.9, 98.1, 55.7, 52.2, 52.0, 11.1. IR (NaCl) ν 2977, 2950, 2870, 1742, 1652, 1526, 1216, 1018 cm^{-1}. HRMS (EI+) for HRMS (EI+) for $C_{15}H_{19}N_3O_4$: calc 305.13756, found 305.13759.

α-Hydroxyester 10b. Ester **6b** cyclized according to General Procedure D to give **10b** (26 mg, 99%) as a white solid. ^{1}H NMR ($CDCl_3$) δ 8.09 (d, *J* = 1.0 Hz, 1H), 7.71 (d, *J* = 9.0 Hz, 1H), 7.40 (dd, *J* = 9.0, 1.0 Hz, 1H), 5.93 (s, 1H), 4.3 (br s, 1H), 3.76 (s, 3H), 3.5-3.1 (m, 4H), 0.88 (br t, 6H). ^{13}C NMR ($CDCl_3$) δ 172.2, 146.4, 133.3, 124.7, 122.4, 118.8, 118.4, 118.2, 116.1, 64.6, 53.4, 52.5, 52.3, 11.8. IR (NaCl) ν 3324, 2977, 2955, 2933, 2879, 1751, 1313, 1118, 1081 cm^{-1}. HRMS (EI+) for $C_{15}H_{18}N_3O_3F_3$: calc 345.13003, found 345.12974.

α-Hydroxyester 10c. Ester **6c** cyclized according to General Procedure D to give **10c** (24 mg, 92%) as a tan solid. ^{1}H NMR ($CDCl_3$) δ 7.94 (d, *J* = 1.5 Hz, 1H), 7.77 (d, *J* = 9.0 Hz, 1H), 7.47 (dd, *J* = 9.0, 1.5 Hz, 1H), 5.94 (d, *J* = 6.3 Hz, 1H), 4.19 (d, *J* = 6.3 Hz, 1H), 3.78 (s, 3H), 3.6-3.2 (m, 4H), 0.92 (t, *J* = 6.9 Hz, 3H), 0.90 (t, *J* = 6.9 Hz, 3H). ^{13}C NMR ($CDCl_3$) δ 172.2. 146.5, 133.3, 122.5, 122.4, 118.8, 118.4, 118.3, 116.1, 64.6, 53.3, 52.5, 52.3, 11.8. IR (NaCl) ν 3420, 1977, 2937, 2875, 2223, 1750, 1436, 1216, 1094 cm^{-1}. HRMS (EI+) for $C_{15}H_{18}N_4O_3$: calc 302.13789, found 302.13800.

α-Hydroxyester 10d. Ester **6d** was cyclized according to General Procedure D to give **10d** (28 mg, 95%) as a white solid. ^{1}H NMR ($CDCl_3$) δ 7.61 (d, *J* = 9.0 Hz, 1H), 7.56 (d, *J* = 2.1 Hz, 1H), 7.24 (dd, *J* = 9.0, 2.1 Hz, 1H), 5.87 (d, *J* = 6.6 Hz, 1H), 4.13 (d, *J* = 6.6 Hz, 1H), 3.77 (m, 3H), 3.5-3.1 (m, 4H), 0.90 (br t, 6H). ^{13}C NMR ($CDCl_3$) δ 172.4, 144.2, 131.0, 128.0, 127.8, 119.2, 118.2, 117.8, 64.5, 53.3, 52.5, 52.2, 11.8. IR (NaCl) ν 3365, 2977, 2954, 2875, 1749, 1212, 1114, 1079 cm^{-1}. HRMS (EI+) for $C_{14}H_{18}N_3O_3Cl$: calc 311.10367, found 311.10367.

α-Hydroxyester 10e. Ester **6e** was cyclized according to General Procedure D to give **10e** (29 mg, 95%) as a orange solid. ^{1}H NMR ($CDCl_3$) δ 7.68 (d, *J* = 9.0 Hz, 1H), 7.58 (d, *J* = 8.7 Hz,

1H), 7.31 (t, *J* = 6.6 Hz, 1H), 7.10 (t, *J* = 7.8 Hz, 1H), 5.91 (d, *J* = 6.9 Hz, 1H), 4.21 (d, *J* = 6.9 Hz, 1H), 3.75 (s, 3H), 3.5-3.1 (m, 4H), 0.91 (t, *J* = 7.2 Hz, 6H). ^{13}C NMR ($CDCl_3$) δ 172.7, 145.9, 126.4, 122.3, 119.4, 117.6, 117.4, 64.6, 53.1, 52.6, 52.2, 11.9. IR (NaCl) ν 3392, 2977, 2872, 1750, 1211, 1103, 1074 cm^{-1}. HRMS (EI+) for $C_{14}H_{19}N_3O_3$: calc 277.14265, found 277.14273.

α-Hydroxyester 10f. Ester **6f** was cyclized according to General Procedure D to give **10f** (21 mg, 90%) as a tan solid. ^{1}H NMR ($CDCl_3$) δ 7.58 (d, *J* = 8.7 Hz, 1H), 7.32 (d, *J* = 1.5 Hz, 1H), 7.15 (dd, *J* = 8.7, 1.5 Hz, 1H), 5.89 (d, *J* = 7.0 Hz, 1H), 4.14 (d, *J* = 7.0 Hz, 1H), 3.76 (s, 3H), 3.5-3.3 (m, 2H), 3.28-3.12 (m, 2H), 2.41 (s, 3H), 0.90 (t, *J* = 7.5 Hz). ^{13}C NMR ($CDCl_3$) δ 172.8, 144.7, 131.7, 130.1, 129.3, 117.6, 117.4, 117.3, 64.6, 53.0, 52.5, 52.1, 21.7, 11.9 IR (NaCl) ν 3333, 2977, 2868, 1750, 1528, 1435, 1214, 1098, 1066 cm^{-1}. HRMS (EI+) for $C_{15}H_{21}N_3O_3$: calc 291.15830, found 291.15884.

α-Hydroxyester 10g. Ester **6g** was cyclized according to General Procedure D to give **10g** (20 mg, 95%) as a tan solid. ^{1}H NMR ($CDCl_3$) δ 7.63 (d, *J* = 8.7 Hz, 1H), 7.44 (m, 2H), 5.90 (d, *J* = 7.1 Hz, 1H), 4.22 (d, *J* = 7.1 Hz, 1H), 3.76 (s, 3H), 3.5-3.1 (m, 4H), 1.36 (s, 9H), 0.92 (t, *J* = 6.9 Hz, 6H). ^{13}C NMR ($CDCl_3$) δ 172.8, 144.9, 144.7, 130.7, 126.2, 117.3, 117.2, 113.4, 64.7, 53.1, 52.5, 52.1, 34.9, 31.2, 11.9, 11.8. IR (NaCl) ν 3274, 2963, 2869, 1750, 1456, 1256, 1206, 1120, 1083 cm^{-1}. HRMS (EI+) for $C_{18}H_{27}N_3O_3$: calc 333.20525, found 333.20535.

α-Hydroxyester 10h. Ester **6h** was cyclized according to General Procedure D to give **10a** (22 mg, 88%) as a orange solid. ^{1}H NMR ($CDCl_3$) δ 7.57 (d, *J* = 9.3 Hz, 1H), 7.00 (dd, *J* = 9.3, 2.4 Hz, 1H), 6.76 (d, *J* = 2.4 Hz, 1H), 5.88 (d, *J* = 6.9 Hz, 1H), 4.18 (d, *J* = 6.9 Hz, 1H), 3.82 (s, 3H), 3.76 (s, 3H), 3.5-3.1 (m, 4H), 0.90 (t, *J* = 7.2 Hz, 6H). ^{13}C NMR ($CDCl_3$) δ 172.8, 155.5, 142.5, 129.9, 121.3, 119.1, 117.3, 95.6, 64.7, 55.4, 53.0, 52.5, 52.1, 11.9. IR (NaCl) ν 3291, 2962, 2906, 2869, 1750, 1457, 1256, 1207, 1083 cm^{-1}. HRMS (EI+) for $C_{15}H_{21}N_3O_4$: calc 307.15321, found 307.15356.

α-Methoxyester 11a. To a flame dried RBF was added **6f** (25 mg, 0.09 mmol), $Rh(OAc)_2]_2$ (2 mg, 0.004), distilled MeOH (0.1 mL) and distilled DCE (5 mL). The reaction was stirred under

Ar at rt until complete by TLC. The resulting solution was filtered through a plug of silica eluting with 1:1 hexanes:ethyl acetate. Purification by preparative TLC afforded **11a** (10 mg, 40 %) as a tan solid. . ^{1}H NMR ($CDCl_3$) δ 7.58 (d, *J* = 9.0 Hz, 1H), 7.48 (d, *J* = 1.2 Hz, 1H), 7.14 (dd, *J* = 9.0, 1.2 Hz, 1H), 5.63 (s, 1H), 3.74 (s, 3H), 3.47 (s, 3H), 3.4-3.1 (m, 4H), 2.40 (s, 3H), 0.90 (m, 6H). ^{13}C NMR ($CDCl_3$) δ169.7, 144.8, 131.8, 129.3, 128.8, 118.8, 188.1, 117.2, 73.5, 57.7, 52.6, 52.2, 52.9, 29.6, 21.8, 12.1. IR (NaCl) ν 2976, 2936, 2866, 2825, 1751, 1652, 1558, 1456, 1105. HRMS (EI+) for $C_{16}H_{23}N_3O_3$: calc 305.17395, found 305.17368.

α-Deuteroxyester 11b. To a flame dried RBF was added **6d** (25 mg, 0.08 mmol), $Rh(OAc)_2]_2$ (2 mg, 0.004), D_2O (0.1 mL) and distilled DCE (5 mL). The reaction was stirred under Ar at rt until complete by TLC. The resulting solution was filtered through a plug of silica eluting with 1:1 hexanes:ethyl acetate to give **11b** as a tan solid (22 mg, 87 %). The product was a mixture of the D-OD, H-OD and D-OH trapped products. ^{1}H NMR ($CDCl_3$) δ 7.61 (d, *J* = 5.4 Hz, 1H), 7.57 (d, *J* = 0.9 Hz, 1H), 7.23 (dd, *J* = 9.0, 1.2 Hz, 1H), 5.86 (m, 0.3H), 4.09, (m, .8H), 3.77 (s, 3H), 3.4-3.1 (m, 4H), 0.90 (m, 6H). ^{13}C NMR ($CDCl_3$) 172.4, 144.3, 130.9, 128.0, 127.8, 119.2, 118.1, 117.7, 64.4, 53.2, 52.5, 52.2, 11.8. δ IR (NaCl) ν 3446, 2977, 2873, 1748, 1652, 1263. HRMS (EI+) for $C_{14}H_{15}N_3O_3ClD_2$: calc 311.10212, found 311.10403; for $C_{14}H_{16}N_3O_3ClD$: calc 312.10840, found 312.10974.

α-Aminoester 11c. To a flame dried RBF was added **6d** (50 mg, 0.18 mmol), $Rh(OAc)_2]_2$ (4 mg, 0.008), H_2NPr (0.1 mL) and distilled DCE (10 mL). The reaction was stirred under Ar at rt until complete by TLC. The resulting solution was filtered through a plug of silica eluting with 1:1 hexanes:ethyl acetate. Purification by preparative TLC yielded **11c** as a yellow oil (34 mg, 56%). ^{1}H NMR ($CDCl_3$) δ 8.66 (m, 1H) 7.37 (d, *J* = 8.7 Hz, 1H), 7.27 (dd, *J* = 8.7, 2.1 Hz, 1H), 7.20 (d, *J* = 2.1 Hz, 1H), 4.43 (s, 1H), 3.70 (n, 7H), 2.87 (m, 2H), 1.45 (q, *J* = 7.5Hz, 2H), 1.2 (m, 6H), 0.90 (t, *J* = 7.5 Hz, 6H). ^{13}C NMR ($CDCl_3$) δ 171.0, 165.0, 145.8, 134.4, 130.4, 130.1, 129.2, 116.7, 82.3, 52.6, 49.9, 45.9, 23.5, 20.8, 11.3 IR (NaCl) ν 3243, 3066, 2973, 2935, 2874, 1733, 1652, 1456. HRMS (EI+) for $C_{17}H_{25}N_4O_2Cl$: calc 352.16660, found 352.16759.

Transition State Analysis for Cyclizations

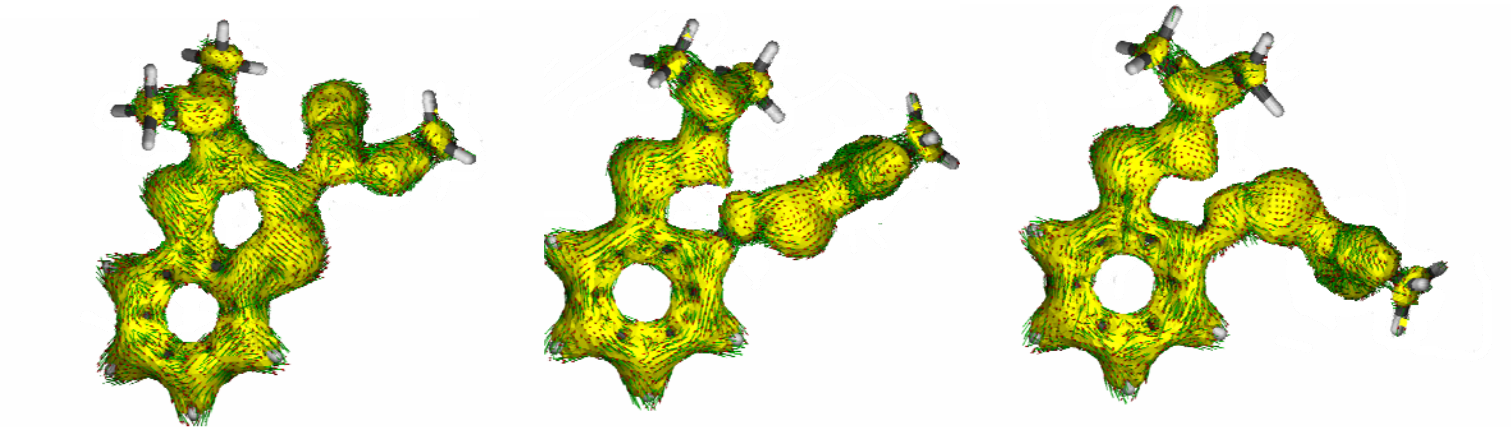
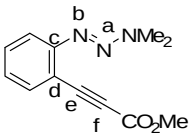


FIGURE S1. Electron flow in the non-planar TS of the pericyclic (**4 peri**, left) and coarctate (**4 anti**, middle and **4 syn**, right) reaction of **4** (Figure 2) with ACID plots taken at isosurface value of 0.05. The vector field of the induced current density depends on the relative orientation of the molecule with respect to the magnetic field. The magnetic field in all plots is orthogonal with respect to the benzene ring. The scale (length of the arrows) is a function of the strength of the induced current at the point of origin of the arrow.

TABLE S1. Transition state analysis for the dual cyclization of triazene **4**.

	CIV	angle[a]
4 peri	0.0812	2.9
4 syn	0.0277	5.8
4 anti	0.0497	6.3

[a]Dihedral angle defined as ∠a-b-d-e



ACID (Anisotropy of the Induced Current Density) is a method developed by the Herges group to visualize the density of electrons which are not localized at an atom or bond but are "mobile" within a molecule if subjected to a magnetic field.[1] ACID is interpreted as the density of delocalized electrons and plotted as an isosurface. Further information about the delocalization of electrons is obtained by plotting the current density on top of the ACID isosurface. The arrows (green arrows with red arrow head) represent strength and direction of the induced current and thus allow one to differentiate diatropic (aromatic) and paratropic (antiaromatic) ring currents. A coarctate reaction is characterized by a hairpin-like pinched cycle

in bond making and bond breaking. By visualizing the response of the electrons to the external magnetic field, it is possible to see this 'looping' of electrons in an ACID diagram (Figure S1). Previously the ACID method to distinguish between pericyclic/pseudopericyclic and coarctate/ pseudocoarctate by others as well as ourselves.[2,3] The "disconnection" in the otherwise contiguous cyclic (pericyclic) or constricted (coarctate) system of delocalized electrons in the transition state, which is characteristic to a pseudo (pericyclic or coarctate) reaction, is clearly visible in the ACID plot as a disconnection of the isosurface. To quantify the "degree" of electron delocalization we defined the so called "critical isosurface value" (CIV). The CIV is the ACID value (density of delocalized electrons) at the point of the lowest delocalization in a conjugated system. Applied to transition states of pericyclic and coarctate reactions, the CIV gives a number that determines the "degree" of disconnection (a CIV of zero would imply a perfect disconnection of electron delocalization and thus a perfect pseudo type reaction). We previously defined pericyclic and coarctate reactions with a CIV value below 0.025 as a pseudo type reaction while values above 0.03 are taken as the true form.[3] Values in between are classified as borderline. Additionally, true pericyclic/coarctate transition states would be non-planar to allow for the to allow for the orbital overlap necessary for an aromatic transition state. Alternatively, if the lone pair electrons are participating in the cyclication (pseudpericyclic/pseudocoarctate), the transition states would be planar.

Analysis of the ACID plots reveal that the 5 membered ring formation does proceed through a coarctate mechanism. In the TS it is possible to see the hallmark 'looping' of the electrons at the carbene carbon. The transition states for **4 peri**, **4 syn** and **4 anti** are all non planar indicating that they are the "true" reactions. The CIV for **4 peri** and **4 anti** are well above the 0.03 threshold, and coupled with the non-planar transition states they can be labled as true pericyclic/coarctate cyclizations. The CIV of **4 syn** is in the borderline region, however

together with the non-planar transition state it would be more likely that it is a true coarctate cyclization.

Cartesian Coordinates of Stationary Points

1

B3LYP/6-31G* = -551.816091083 au
B3LYP/6-31G* Zero Point Corrected Energy = -551.623981 au
NIMAG = 0

N	0.67959700	0.19300800	-0.10283600
C	-0.63690200	-0.31174300	-0.05496700
C	-3.32844100	-1.12964500	0.02779900
C	-1.67150400	0.65383800	0.02564800
C	-0.97412700	-1.67453500	-0.10245300
C	-2.30332400	-2.07872300	-0.05849800
C	-3.01116700	0.22307000	0.06817600
C	-1.38450500	2.05306300	0.06970100
H	-0.17496400	-2.40343300	-0.17666300
H	-2.54414000	-3.13800700	-0.09768300
H	-3.79467000	0.97178500	0.13195400
H	-4.36759700	-1.44489600	0.05782300
N	1.57761200	-0.69762300	0.01305900
N	2.81865100	-0.23022300	-0.11446100
C	-1.21268200	3.25037000	0.11150900
H	-1.04077200	4.30173500	0.14606900
C	3.07594000	1.19762000	-0.23548600
H	2.49093500	1.60808600	-1.06176600
H	2.78038200	1.73361600	0.67654500
H	4.14310100	1.33818500	-0.42074300
C	3.87272300	-1.13344900	0.30591200
H	3.47068100	-2.14763700	0.29248900
H	4.72106500	-1.06924400	-0.38396100
H	4.22888900	-0.90551600	1.32154900

1 reactive conf.

B3LYP/6-31G* = -551.812461679 au
B3LYP/6-31G* Zero Point Corrected Energy = -551.62057 au
NIMAG = 0

N	-0.59636400	-0.86559400	-0.23862300
C	0.77030000	-0.55898800	-0.07092000
C	3.55564800	-0.24223900	0.21590500
C	1.33604900	0.74516800	-0.06070100
C	1.62160500	-1.67014000	0.02441700
C	2.99530800	-1.52226000	0.17782900
C	2.73232100	0.87077900	0.08856000
C	0.57962900	1.94322900	-0.25377200

H	1.16473100	-2.65437600	-0.01317000
H	3.62785300	-2.40161800	0.26397700
H	3.15776800	1.86971200	0.09201500
H	4.62819900	-0.11240100	0.32910900
N	-1.38265300	-0.00694800	0.26913200
N	-2.66994700	-0.23773900	0.02737900
C	0.05005300	3.01619400	-0.43979600
H	-0.45148200	3.94305300	-0.59918900
C	-3.60091400	0.53594500	0.82683700
H	-3.06452900	1.40333800	1.21391600
H	-4.44050400	0.87200200	0.20854800
H	-3.99854300	-0.04536200	1.67186600
C	-3.10994100	-1.43329200	-0.67520300
H	-2.57726700	-1.51778200	-1.62563900
H	-2.89944500	-2.34045600	-0.09237400
H	-4.18437800	-1.35052100	-0.85321400

1 pericyclic prod

B3LYP/6-31G* = -551.792314552 au

B3LYP/6-31G* Zero Point Corrected Energy = -551.596655 au

NIMAG = 0

N	0.52266000	-0.69031700	0.00010300
C	-0.80867600	-0.44677500	-0.00049600
C	-3.57863800	-0.06670100	0.01126800
C	-1.33173700	0.89384800	-0.00927500
C	-1.67594900	-1.57854500	0.01196800
C	-3.03356300	-1.38205900	0.01734500
C	-2.75247300	1.03164000	-0.00131600
H	1.70156500	2.35747100	-0.05290200
H	-1.23665400	-2.57177100	0.01691800
H	-3.70464700	-2.23692500	0.02653000
H	-3.14350800	2.04464200	-0.00708100
H	-4.65822300	0.05846300	0.01641000
N	1.28588400	0.37121000	-0.01764200
C	0.86033100	1.66848300	-0.03362100
N	2.70124600	0.13453800	-0.01476300
C	-0.48795500	2.04923500	-0.02625800
C	3.09536600	-0.51491000	1.24113400
H	4.18708600	-0.57909900	1.24867700
H	2.77918300	0.10979800	2.08077500
H	2.67054700	-1.52244200	1.35572000
C	3.08570400	-0.63926700	-1.20103300
H	2.66895700	-1.65612600	-1.20600300
H	2.75482100	-0.10714500	-2.09688600

H	4.17788100	-0.69456800	-1.21434600

1 pericyclic TS

B3LYP/6-31G* = -551.764712103 au

B3LYP/6-31G* Zero Point Corrected Energy = -551.572291 au

NIMAG = 1

N	0.48817200	-0.72575400	0.03890200
C	-0.86576300	-0.40396700	0.11608000
C	-3.63999700	-0.05729500	-0.03900400
C	-1.39936100	0.89916900	-0.09560600
C	-1.73074300	-1.50671300	0.27625300
C	-3.10340000	-1.33101500	0.21909300
C	-2.79752900	1.03299200	-0.20581500
H	1.66099400	2.52697300	0.04097500
H	-1.29085200	-2.48529000	0.44659300
H	-3.76481800	-2.18178700	0.35823900
H	-3.19632900	2.02570400	-0.39332600
H	-4.71697800	0.07258900	-0.10384500
N	1.35699400	0.19980300	0.11356700
C	0.76824600	1.94198400	-0.08026700
N	2.62961000	-0.17303700	-0.23846800
C	-0.50167700	2.01777700	-0.19408500
C	3.65477800	0.44886900	0.59382700
H	4.60901300	0.41571000	0.06131300
H	3.39694300	1.49160100	0.78287400
H	3.76789000	-0.06237100	1.56253300
C	2.85691300	-1.56764000	-0.59922300
H	2.70721300	-2.25056700	0.24970100
H	2.16778000	-1.85617200	-1.39409400
H	3.88691000	-1.64843900	-0.95648500

1 syn product

B3LYP/6-31G* = -551.773463245 au

B3LYP/6-31G* Zero Point Corrected Energy = -551.579031 au

NIMAG = 0

H	4.21868500	-1.53893200	0.20042500
C	3.31335600	-0.94311500	0.12843300
C	2.07555700	-1.57044400	0.11924300
C	3.41717400	0.46322700	0.04469100

C	2.29057200	1.27372200	-0.04446000
H	4.40336800	0.91951400	0.05002200
H	1.97501700	-2.64929400	0.18538900
C	1.03527200	0.65589500	-0.05940700
C	0.94434300	-0.74748400	0.02437900
H	2.37908500	2.35487700	-0.10664600
N	-0.37603500	-1.15455700	0.01053200
C	-0.31909000	1.16280800	-0.14544100
N	-2.44973800	-0.19115800	-0.24018200
N	-1.08818500	-0.07266700	-0.07146200
C	-0.91337600	2.39265700	-0.26058400
H	-0.10638300	3.14306000	-0.35020900
C	-3.26027600	0.68329100	0.62446200
H	-3.22822300	0.34915400	1.67347400
H	-2.88517700	1.70221800	0.52056300
H	-4.28887100	0.62555500	0.26040300
C	-2.90897100	-1.57372900	-0.31392200
H	-3.97608700	-1.53216500	-0.54286100
H	-2.38456100	-2.10091900	-1.11237300
H	-2.75650700	-2.12537000	0.62523300

1 syn TS

B3LYP/6-31G* = -551.763911839 au

B3LYP/6-31G* Zero Point Corrected Energy = -551.571807 au

NIMAG = 1

H	4.17107800	-1.66581200	0.15015800
C	3.29786500	-1.02214300	0.09559800
C	2.02329100	-1.58351300	0.08739600
C	3.46175400	0.37111200	0.03287600
C	2.36037600	1.22371900	-0.03124700
H	4.46328900	0.79254800	0.03248300
H	1.86917600	-2.65707500	0.13828100
C	1.07395400	0.67310800	-0.04840600
C	0.92653600	-0.72350900	0.01564300
H	2.49031900	2.30118800	-0.07731600
N	-0.40415300	-1.15666400	-0.00626000
C	-0.17835100	1.38432900	-0.11584400
N	-2.46299600	-0.27906900	-0.15369000
N	-1.14682500	-0.12353400	0.02391200

C	-0.81110300	2.51002700	-0.18855200
H	-0.25104500	3.42677200	-0.37337200
C	-3.31538700	0.75096100	0.44176600
H	-3.50994000	0.53821300	1.50325100
H	-2.80528000	1.71315000	0.33252700
H	-4.26335500	0.76127200	-0.10227200
C	-2.96681600	-1.64163600	-0.25490700
H	-4.03367300	-1.57626900	-0.47768600
H	-2.44883700	-2.17050800	-1.05776000
H	-2.81662800	-2.20335100	0.67803900

1 anti product

B3LYP/6-31G* = -551.768676909 au

B3LYP/6-31G* Zero Point Corrected Energy = -551.574842 au

NIMAG = 0

H	4.16385500	-1.61652900	0.18977700
C	3.27094800	-1.00172800	0.12029500
C	2.02579100	-1.60126000	0.11350300
C	3.41226900	0.40938400	0.03754300
C	2.31474000	1.24968800	-0.05347300
H	4.41249300	0.83425700	0.04590500
H	1.90134400	-2.67776400	0.17493400
C	1.04191900	0.66017700	-0.05958800
C	0.90686300	-0.74874900	0.02512600
H	2.41260300	2.32848300	-0.12014800
N	-0.41585900	-1.11084900	0.02083400
C	-0.28670000	1.19557400	-0.15704300
N	-2.47918200	0.02268700	-0.11996900
N	-1.08058500	0.00893400	-0.09406800
C	-0.68943600	2.51569800	-0.31065500
H	-1.79161200	2.53150500	-0.41351200
C	-3.02019900	0.04865500	1.24625800
H	-2.81698800	-0.88434600	1.79500800
H	-2.58505700	0.89137300	1.78720700
H	-4.10100400	0.19834000	1.17651500
C	-3.01904600	-1.07011600	-0.93350300
H	-4.09473100	-0.89845500	-1.03036100
H	-2.56734200	-1.03303700	-1.92751200
H	-2.84707500	-2.06317000	-0.49618000

1 anti TS

B3LYP/6-31G* = -551.762404026 au

B3LYP/6-31G* Zero Point Corrected Energy = -551.570249 au

NIMAG = 1

H	4.17243800	-1.64445500	0.20600300
C	3.29278700	-1.01117800	0.13571900
C	2.02765400	-1.58589500	0.11201200
C	3.44666300	0.38783700	0.06358800
C	2.34670300	1.23678400	-0.02159200
H	4.44763400	0.81107000	0.06888200
H	1.88224300	-2.66050200	0.16491400
C	1.06680000	0.67257300	-0.04480300
C	0.92691400	-0.72664200	0.02415200
H	2.45644100	2.31462400	-0.08572700
N	-0.40384000	-1.13837300	-0.01822500
C	-0.21512800	1.32461700	-0.15749800
N	-2.46832400	-0.18767100	-0.18918400
N	-1.12466700	-0.08521000	0.01625100
C	-0.61139200	2.55180100	-0.41843700
H	-1.67053600	2.81410700	-0.42426600
C	-3.25340700	0.59056400	0.77443000
H	-3.36748900	0.05199900	1.72792800
H	-2.75557000	1.54069900	0.95768400
H	-4.24174000	0.77761100	0.34694400
C	-2.96748400	-1.52935300	-0.46563000
H	-4.02779800	-1.43425600	-0.71293200
H	-2.42900900	-1.95190400	-1.31559200
H	-2.84944700	-2.20686000	0.39261800

4

B3LYP/6-31G* = -779.6954003 au

B3LYP/6-31G* Zero Point Corrected Energy = -779.459158 au

NIMAG = 0

N	-1.42516100	-0.49407600	-0.12850700
C	-1.50716100	0.90743800	-0.06157900
C	-1.44748700	3.72424000	0.03593800
C	-0.26740500	1.59898700	-0.01693800

C	-2.69952000	1.64975800	-0.06343100
C	-2.66810600	3.03863000	-0.01213100
C	-0.25802700	3.00687600	0.03273800
C	0.96072900	0.88132100	-0.00963100
H	-3.64263100	1.11688500	-0.10895900
H	-3.60186200	3.59518500	-0.01604700
H	0.69807600	3.51972200	0.06874300
H	-1.42866900	4.80955400	0.07073000
N	-2.53398300	-1.08961200	0.06493800
N	-2.45540100	-2.40609600	-0.06457300
C	2.02738400	0.30000500	0.00285400
C	3.22796200	-0.49195300	0.01830400
O	3.25793900	-1.70789900	0.00737100
O	4.33414400	0.28974000	0.04800100
C	5.57799600	-0.42751200	0.06722300
H	6.35358200	0.33876200	0.08893700
H	5.64245900	-1.06530500	0.95318400
H	5.67817000	-1.05116600	-0.82541800
C	-3.62428400	-3.16144200	0.34283300
H	-4.45546600	-2.46233700	0.44504300
H	-3.87356400	-3.91539800	-0.41229800
H	-3.46300000	-3.66881300	1.30440900
C	-1.18287300	-3.06784000	-0.32503400
H	-0.74044200	-2.67785300	-1.24578600
H	-0.46822300	-2.87708300	0.48457200
H	-1.36852700	-4.13945200	-0.41997000

4 reactive conf.

B3LYP/6-31G* = -779.6938541 au

B3LYP/6-31G* Zero Point Corrected Energy = -779.45747 au

NIMAG = 0

N	-1.70931800	1.29508700	-0.22364100
C	-2.15671700	-0.02814300	-0.06626300
C	-3.23609300	-2.62825600	0.12172900
C	-1.29316600	-1.15643400	0.04294500
C	-3.54162900	-0.24036100	-0.11923200
C	-4.07844100	-1.51865700	-0.01489500
C	-1.85957100	-2.44473100	0.14106000
C	0.12201700	-1.03137100	-0.01411000
H	-4.18198000	0.62920500	-0.23046600
H	-5.15647400	-1.65301100	-0.04139600
H	-1.19130800	-3.29676300	0.22063600
H	-3.65178900	-3.62866600	0.19738900
N	-0.67959800	1.55864700	0.47850300
N	-0.17447000	2.76687000	0.29394400
C	1.33414800	-0.98322500	-0.10176700
C	2.74471900	-0.72839900	-0.17818800
O	3.23908700	0.36475700	-0.39719000
O	3.46987300	-1.85230100	0.02399500
C	4.89401800	-1.67326300	-0.02996700

H	5.31645900	-2.66188500	0.15199800
H	5.19896300	-1.29895700	-1.01103600
H	5.22372100	-0.96703800	0.73701100
C	1.14849800	2.96310100	0.87423700
H	1.94261600	2.63945800	0.18927500
H	1.28080900	4.01888500	1.12735800
H	1.21056600	2.36099700	1.78190300
C	-0.64657700	3.62064100	-0.78819500
H	-0.46067200	3.15524500	-1.76540000
H	-1.72369600	3.77720600	-0.69136100
H	-0.12242000	4.57603300	-0.72612600

4 pericyclic prod

B3LYP/6-31G* = -779.6611048 au

B3LYP/6-31G* Zero Point Corrected Energy = -779.422727 au

NIMAG = 0

N	-0.86756800	1.29965400	-0.05364900
C	-1.89605900	0.42240700	0.00570900
C	-4.09371800	-1.30276400	-0.00338800
C	-1.67248000	-0.99754400	0.02836700
C	-3.21470200	0.96308800	0.00094400
C	-4.28750200	0.10741500	0.00186600
C	-2.82605700	-1.83539200	0.00458300
H	-3.33675800	2.04208300	-0.00378100
H	-5.29841600	0.50614000	0.00164400
H	-2.65373300	-2.90733900	0.00917700
H	-4.96232300	-1.95581500	-0.01076200
N	0.33077900	0.78248500	-0.02258900
C	0.61369700	-0.55561100	0.07880200
N	1.42247100	1.70040300	-0.15947400
C	-0.35975600	-1.55785800	0.06742800
C	2.06597800	-0.89047800	0.31203500
O	2.66596900	-0.63288400	1.33617900
O	2.58324700	-1.57998300	-0.71449600
C	3.92759200	-2.05139700	-0.52004600
H	3.97329000	-2.72740400	0.33767800
H	4.18551100	-2.57888200	-1.43855200
H	4.60840500	-1.21271600	-0.35120700
C	1.21581500	2.59281500	-1.30476100
H	2.14217400	3.15883600	-1.43686300
H	1.04566100	1.99127400	-2.20156500

H	0.37833300	3.28984100	-1.17009200
C	1.62913900	2.41385100	1.10849700
H	0.77095000	3.04663700	1.37928500
H	1.82492400	1.68019300	1.89233300
H	2.51679300	3.04110900	0.98900200

4 pericyclic TS

B3LYP/6-31G* = -779.6402139 au

B3LYP/6-31G* Zero Point Corrected Energy = -779.404093 au

NIMAG = 1

N	0.95922200	1.27808700	-0.22609700
C	1.87022500	0.25128800	-0.28724300
C	3.95964700	-1.57277700	0.14337800
C	1.58802900	-1.05570700	0.21947000
C	3.19448200	0.59004400	-0.65280300
C	4.21538100	-0.32139000	-0.45632800
C	2.66559100	-1.92770100	0.48456000
H	3.38505100	1.57164800	-1.07619400
H	5.22973300	-0.06281500	-0.74805900
H	2.44265300	-2.90139500	0.91077000
H	4.77930700	-2.26359400	0.31910300
N	-0.30851600	1.08842900	-0.16359300
C	-0.80525400	-0.64186500	0.17924500
N	-0.98042800	2.15490500	0.39065900
C	0.22206400	-1.38968100	0.38466200
C	-2.20449800	-0.88947800	-0.17756200
O	-2.92461100	-0.18697600	-0.86466500
O	-2.62108000	-2.05612400	0.36072100
C	-3.96768100	-2.42810300	0.03021900
H	-4.08251800	-2.54934100	-1.05049700
H	-4.13672800	-3.37598300	0.54204700
H	-4.67549700	-1.67096600	0.37895300
C	-0.18012100	3.18822900	1.04012800
H	-0.87516100	3.82938900	1.58990000
H	0.52279400	2.72839900	1.73726800
H	0.38895900	3.79876400	0.32513200
C	-2.09077500	2.66455400	-0.41855400
H	-1.72671100	3.38815800	-1.16506300
H	-2.57842700	1.83045000	-0.91642800

H	-2.80241300	3.16764700	0.24279600

4 syn product

B3LYP/6-31G* = -779.664807 au

B3LYP/6-31G* Zero Point Corrected Energy = -779.426673 au

NIMAG = 0

H	1.52298800	4.68550100	-0.03149700
C	1.17096700	3.65855300	0.00095600
C	2.07515400	2.61658900	-0.14889000
C	-0.20343900	3.40619900	0.20510400
C	-0.71097700	2.11173800	0.26189400
H	-0.88020600	4.24753100	0.32584200
H	3.13701500	2.78880400	-0.29319600
C	0.18703000	1.05229300	0.09298800
C	1.55887300	1.31454500	-0.09510500
H	-1.76391300	1.92626000	0.44497600
N	2.27795400	0.13784800	-0.19056700
C	0.03813100	-0.38910300	0.08560600
N	1.83364800	-2.12601000	-0.23800000
N	1.41976100	-0.82381800	-0.05702500
C	-0.99175100	-1.26684300	0.15095200
C	-2.35223000	-0.81383900	0.26601000
O	-2.88875900	-0.53971600	1.33412100
O	-3.02024700	-0.84042300	-0.92104400
C	-4.42066600	-0.54579700	-0.83514000
H	-4.58918500	0.46811700	-0.45910300
H	-4.80036700	-0.63766400	-1.85395200
H	-4.92904200	-1.25301600	-0.17365200
C	1.43399800	-3.04149100	0.84460000
H	1.98473200	-2.83015500	1.77393500
H	0.35991300	-2.95167100	0.99766700
H	1.66780200	-4.05440900	0.50925100
C	3.23136400	-2.23895200	-0.64232300
H	3.40618900	-3.29536900	-0.85788300
H	3.40664200	-1.64981300	-1.54386700
H	3.93121900	-1.90249300	0.13610200

4 syn TS

B3LYP/6-31G* = -779.654868 au

B3LYP/6-31G* Zero Point Corrected Energy = -779.418723 au
NIMAG = 1

H	-3.33777500	-3.86085900	-0.13798800
C	-2.59633700	-3.06975200	-0.07485500
C	-2.99483800	-1.73915000	-0.18126700
C	-1.24432200	-3.39704800	0.11658300
C	-0.26780000	-2.40540000	0.20851700
H	-0.95261600	-4.44064800	0.19396500
H	-4.03476800	-1.46097000	-0.32137800
C	-0.65494000	-1.06721500	0.08819600
C	-2.01216300	-0.75251500	-0.09481600
H	0.77609900	-2.65782600	0.36701200
N	-2.27330900	0.62078800	-0.18242100
C	0.19539100	0.09474800	0.14786600
N	-1.13890300	2.56035400	-0.14560800
N	-1.18734400	1.23787800	0.05398000
C	1.38890000	0.54656100	0.25157800
C	2.70665100	-0.00875000	0.31515100
O	3.24804100	-0.41501700	1.33266600
O	3.33341600	0.03461500	-0.89773400
C	4.68325800	-0.44531400	-0.88972100
H	4.72708200	-1.49615600	-0.58759600
H	5.03825600	-0.33218500	-1.91554200
H	5.30380900	0.14043500	-0.20516600
C	-0.17499100	3.28862200	0.68106500
H	-0.58692400	3.50336900	1.67758600
H	0.72865100	2.68387800	0.77079400
H	0.06013800	4.22937000	0.17763400
C	-2.38038400	3.22403000	-0.52108800
H	-2.13982900	4.26850900	-0.72888000
H	-2.79542100	2.75181200	-1.41375700
H	-3.13201300	3.16842600	0.27895600

4 anti product
B3LYP/6-31G* = -779.6635691 au
B3LYP/6-31G* Zero Point Corrected Energy = -779.425541 au
NIMAG = 0

H	-5.45373200	-0.29112400	-0.26837100
C	-4.37519200	-0.37894200	-0.17511300

C	-3.58439200	0.75270400	-0.26955400
C	-3.80497500	-1.65885400	0.04180300
C	-2.43484500	-1.83801400	0.16913800
H	-4.46434100	-2.51993700	0.10865700
H	-4.00353700	1.73984500	-0.43601400
C	-1.62057400	-0.70264800	0.07895800
C	-2.19564700	0.57192800	-0.13512000
H	-1.99260000	-2.81582900	0.33099700
N	-1.22493000	1.54532700	-0.16555500
C	-0.19566300	-0.50375000	0.13238100
N	1.11840100	1.61257200	-0.00629100
N	-0.09185700	0.92262000	-0.01730600
C	0.79888100	-1.43125200	0.21206800
C	2.20412100	-1.17864800	0.25160900
O	2.80357100	-0.97586700	1.30795700
O	2.82849100	-1.34508900	-0.94282700
C	4.25883600	-1.26339800	-0.89590400
H	4.67107800	-2.00391500	-0.20489300
H	4.59491000	-1.46528000	-1.91421600
H	4.58577200	-0.26759700	-0.58088400
C	1.54709800	1.90320900	1.37451400
H	0.85173800	2.59428200	1.87552000
H	1.64079400	0.97038800	1.93094200
H	2.53761000	2.36079900	1.31854500
C	1.08260700	2.79856000	-0.86520400
H	2.10781400	3.17161600	-0.93142800
H	0.74507800	2.51189500	-1.86362100
H	0.43008600	3.59350100	-0.47966900

4 anti TS

B3LYP/6-31G* = -779.6565061 au

B3LYP/6-31G* Zero Point Corrected Energy = -779.420238 au

NIMAG = 1

H	-5.42156000	-0.73590900	-0.25518400
C	-4.34002000	-0.73033800	-0.15712300
C	-3.64179000	0.46841400	-0.26791200
C	-3.65665100	-1.93695700	0.07861400
C	-2.26952400	-1.97190000	0.21317800
H	-4.22200400	-2.86191600	0.15213000
H	-4.14504400	1.41338000	-0.44726700
C	-1.55744400	-0.77522200	0.10149800
C	-2.25247500	0.42421700	-0.13186400
H	-1.73698200	-2.90153100	0.38720700
N	-1.41526000	1.54298500	-0.19868200

C	-0.13139600	-0.56024200	0.16151300
N	0.80497600	2.01040300	-0.06184900
N	-0.23373900	1.15211600	0.06159100
C	0.94404700	-1.27523700	0.15112400
C	2.35589900	-1.19576100	0.24436600
O	2.98307800	-1.09183300	1.29745200
O	2.96618300	-1.32792200	-0.96935300
C	4.39747500	-1.34017700	-0.92506700
H	4.76392700	-2.18290900	-0.33161700
H	4.71908600	-1.43967800	-1.96319100
H	4.78977800	-0.41383100	-0.49397100
C	1.74720600	1.98464500	1.06728900
H	1.36356400	2.58746400	1.90415000
H	1.92375300	0.96432000	1.40376900
H	2.69456400	2.40767000	0.72542200
C	0.47076300	3.33677500	-0.56918300
H	1.41198000	3.86563700	-0.73501500
H	-0.07069500	3.24138400	-1.51210400
H	-0.15283300	3.90611400	0.13486900

Crystal Structure Data for 10a (see cif file for full data)

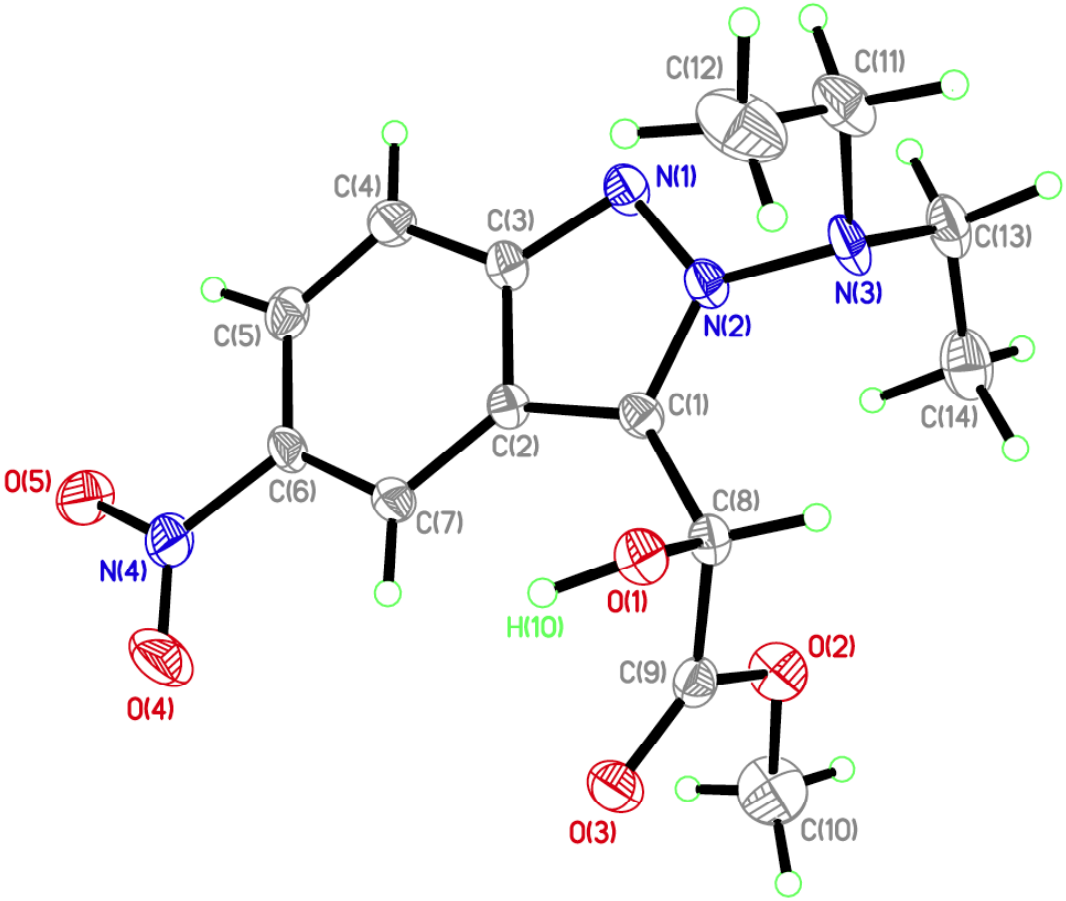


Figure S1. X-ray crystal structure of **10a**; ellipsoids drawn at the 50% probability level.

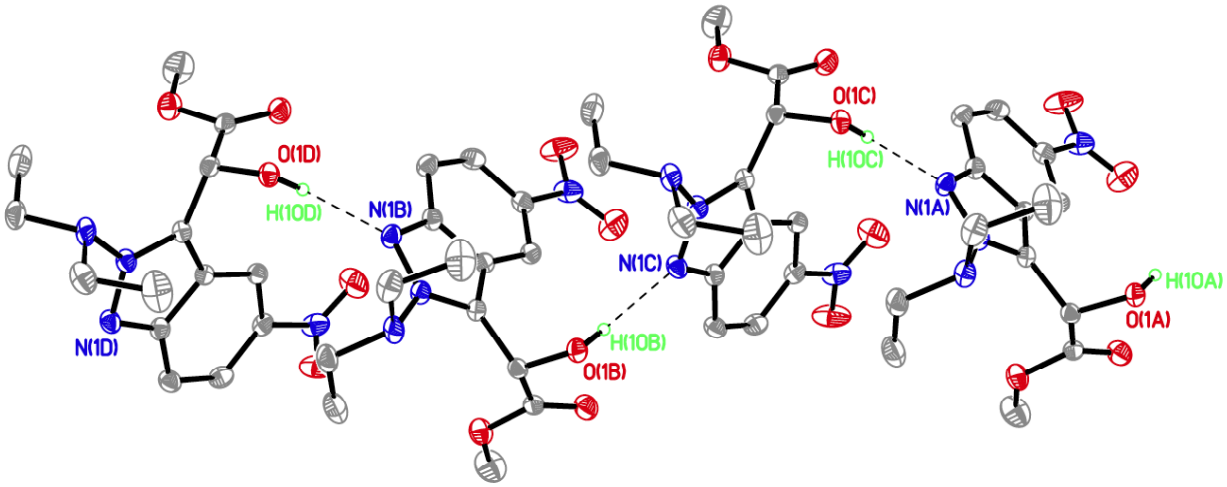


Figure S2. Intermolecular H-bonding in crystal lattice of **10a**.

Table 1. Crystal data and structure refinement for **10a**.

Empirical formula	C14 H18 N4 O5	
Formula weight	322.32	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 9.739(2) Å	α= 90°.
	b = 14.681(3) Å	β= 92.569(4)°.
	c = 11.462(3) Å	γ = 90°.
Volume	1637.0(6) $Å^3$	
Z	4	
Density (calculated)	1.308 Mg/m^3	
Absorption coefficient	0.101 mm^{-1}	
F(000)	680	
Crystal size	0.35 x 0.07 x 0.05 mm^3	
Theta range for data collection	2.09 to 25.00°.	
Index ranges	-11<=h<=11, -17<=k<=17, -13<=l<=13	
Reflections collected	13040	
Independent reflections	2880 [R(int) = 0.0941]	
Completeness to theta = 25.00°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9950 and 0.9655	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2880 / 0 / 280	
Goodness-of-fit on F^2	0.999	
Final R indices [I>2sigma(I)]	R1 = 0.0546, wR2 = 0.0927	
R indices (all data)	R1 = 0.1172, wR2 = 0.1187	
Largest diff. peak and hole	0.186 and -0.199 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **10a**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	13(2)	1120(1)	389(2)	34(1)
O(2)	-2580(2)	6(1)	-1401(2)	45(1)
O(3)	-2436(2)	211(1)	543(2)	46(1)
O(4)	-5028(3)	2749(2)	1491(2)	69(1)
O(5)	-5840(3)	3952(2)	624(2)	74(1)
N(1)	-1149(3)	2901(2)	-2649(2)	35(1)
N(2)	-621(2)	2096(2)	-2223(2)	31(1)
N(3)	491(3)	1658(2)	-2727(2)	38(1)
N(4)	-5031(3)	3308(2)	697(3)	49(1)
C(1)	-1233(3)	1771(2)	-1280(2)	28(1)
C(2)	-2256(3)	2398(2)	-1042(2)	27(1)
C(3)	-2155(3)	3086(2)	-1908(2)	32(1)
C(4)	-3030(3)	3854(2)	-1908(3)	37(1)
C(5)	-3959(3)	3901(2)	-1062(3)	39(1)
C(6)	-4044(3)	3206(2)	-215(2)	33(1)
C(7)	-3218(3)	2462(2)	-177(3)	31(1)
C(8)	-768(3)	923(2)	-655(2)	29(1)
C(9)	-2010(3)	339(2)	-410(3)	33(1)
C(10)	-3780(5)	-564(4)	-1281(5)	67(1)
C(11)	1707(4)	2260(3)	-2699(3)	49(1)
C(12)	2161(5)	2514(5)	-1481(4)	72(1)
C(13)	95(4)	1344(3)	-3916(3)	47(1)
C(14)	-1004(5)	625(3)	-3905(3)	57(1)

Table 3. Bond lengths [Å] and angles [°] for **10a**.

O(1)-C(8)	1.418(3)
O(1)-H(1O)	0.89(4)
O(2)-C(9)	1.334(3)
O(2)-C(10)	1.449(5)
O(3)-C(9)	1.200(3)
O(4)-N(4)	1.226(3)
O(5)-N(4)	1.230(3)
N(1)-C(3)	1.353(3)
N(1)-N(2)	1.370(3)
N(2)-C(1)	1.345(3)
N(2)-N(3)	1.405(3)
N(3)-C(13)	1.474(4)
N(3)-C(11)	1.477(4)
N(4)-C(6)	1.459(4)
C(1)-C(2)	1.392(4)
C(1)-C(8)	1.496(4)
C(2)-C(7)	1.398(4)
C(2)-C(3)	1.422(4)
C(3)-C(4)	1.414(4)
C(4)-C(5)	1.357(4)
C(4)-H(4)	0.94(3)
C(5)-C(6)	1.413(4)
C(5)-H(5)	0.94(3)
C(6)-C(7)	1.356(4)
C(7)-H(7)	0.92(2)
C(8)-C(9)	1.519(4)
C(8)-H(8)	0.96(2)
C(10)-H(10A)	0.94(4)
C(10)-H(10B)	0.99(4)
C(10)-H(10C)	0.93(4)
C(11)-C(12)	1.492(5)
C(11)-H(11A)	0.98(3)
C(11)-H(11B)	1.00(3)
C(12)-H(12A)	0.99(4)
C(12)-H(12B)	0.92(4)
C(12)-H(12C)	1.02(4)
C(13)-C(14)	1.504(5)
C(13)-H(13A)	1.00(3)

C(13)-H(13B)	1.03(3)
C(14)-H(14A)	0.99(3)
C(14)-H(14B)	1.03(4)
C(14)-H(14C)	1.07(4)

C(8)-O(1)-H(1O)	110(3)
C(9)-O(2)-C(10)	116.0(3)
C(3)-N(1)-N(2)	102.7(2)
C(1)-N(2)-N(1)	114.8(2)
C(1)-N(2)-N(3)	123.1(2)
N(1)-N(2)-N(3)	122.1(2)
N(2)-N(3)-C(13)	110.4(2)
N(2)-N(3)-C(11)	110.4(3)
C(13)-N(3)-C(11)	112.5(3)
O(4)-N(4)-O(5)	123.0(3)
O(4)-N(4)-C(6)	118.9(3)
O(5)-N(4)-C(6)	118.1(3)
N(2)-C(1)-C(2)	105.7(2)
N(2)-C(1)-C(8)	123.0(3)
C(2)-C(1)-C(8)	131.3(3)
C(1)-C(2)-C(7)	133.8(3)
C(1)-C(2)-C(3)	105.1(2)
C(7)-C(2)-C(3)	121.1(3)
N(1)-C(3)-C(4)	127.9(3)
N(1)-C(3)-C(2)	111.7(2)
C(4)-C(3)-C(2)	120.4(3)
C(5)-C(4)-C(3)	117.5(3)
C(5)-C(4)-H(4)	125.1(19)
C(3)-C(4)-H(4)	117.3(19)
C(4)-C(5)-C(6)	121.0(3)
C(4)-C(5)-H(5)	120.4(17)
C(6)-C(5)-H(5)	118.6(17)
C(7)-C(6)-C(5)	123.5(3)
C(7)-C(6)-N(4)	117.9(3)
C(5)-C(6)-N(4)	118.6(3)
C(6)-C(7)-C(2)	116.5(3)
C(6)-C(7)-H(7)	119.7(15)
C(2)-C(7)-H(7)	123.7(15)
O(1)-C(8)-C(1)	111.9(2)
O(1)-C(8)-C(9)	111.2(2)

C(1)-C(8)-C(9)	109.4(2)
O(1)-C(8)-H(8)	105.5(16)
C(1)-C(8)-H(8)	109.1(15)
C(9)-C(8)-H(8)	109.8(15)
O(3)-C(9)-O(2)	124.7(3)
O(3)-C(9)-C(8)	124.6(3)
O(2)-C(9)-C(8)	110.7(3)
O(2)-C(10)-H(10A)	103(3)
O(2)-C(10)-H(10B)	111(2)
H(10A)-C(10)-H(10B)	113(3)
O(2)-C(10)-H(10C)	109(3)
H(10A)-C(10)-H(10C)	109(4)
H(10B)-C(10)-H(10C)	111(4)
N(3)-C(11)-C(12)	111.9(3)
N(3)-C(11)-H(11A)	104.5(19)
C(12)-C(11)-H(11A)	110.0(19)
N(3)-C(11)-H(11B)	108.5(17)
C(12)-C(11)-H(11B)	114.6(17)
H(11A)-C(11)-H(11B)	107(2)
C(11)-C(12)-H(12A)	116(3)
C(11)-C(12)-H(12B)	111(3)
H(12A)-C(12)-H(12B)	109(3)
C(11)-C(12)-H(12C)	112(2)
H(12A)-C(12)-H(12C)	100(3)
H(12B)-C(12)-H(12C)	109(3)
N(3)-C(13)-C(14)	111.6(3)
N(3)-C(13)-H(13A)	109.6(17)
C(14)-C(13)-H(13A)	111.2(18)
N(3)-C(13)-H(13B)	106.0(17)
C(14)-C(13)-H(13B)	112.1(17)
H(13A)-C(13)-H(13B)	106(2)
C(13)-C(14)-H(14A)	111.9(18)
C(13)-C(14)-H(14B)	112.1(19)
H(14A)-C(14)-H(14B)	102(3)
C(13)-C(14)-H(14C)	112(2)
H(14A)-C(14)-H(14C)	109(3)
H(14B)-C(14)-H(14C)	109(3)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for **10a**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	33(1)	39(1)	29(1)	0(1)	-2(1)	1(1)
O(2)	39(2)	54(1)	40(1)	-6(1)	-7(1)	-7(1)
O(3)	53(2)	47(1)	39(1)	-3(1)	13(1)	-11(1)
O(4)	69(2)	74(2)	67(2)	18(2)	41(1)	19(2)
O(5)	70(2)	41(1)	115(2)	5(2)	57(2)	17(1)
N(1)	38(2)	38(2)	29(1)	5(1)	5(1)	12(1)
N(2)	29(2)	38(2)	28(1)	2(1)	5(1)	7(1)
N(3)	34(2)	53(2)	28(1)	1(1)	12(1)	17(1)
N(4)	41(2)	40(2)	66(2)	-6(2)	24(2)	3(2)
C(1)	28(2)	33(2)	24(2)	2(1)	1(1)	1(2)
C(2)	25(2)	30(2)	26(2)	-1(1)	0(1)	3(1)
C(3)	29(2)	37(2)	28(2)	-1(1)	2(1)	5(2)
C(4)	39(2)	35(2)	37(2)	6(2)	4(2)	6(2)
C(5)	34(2)	34(2)	48(2)	-4(2)	3(2)	9(2)
C(6)	28(2)	38(2)	36(2)	-6(2)	13(1)	0(2)
C(7)	29(2)	33(2)	31(2)	0(2)	6(2)	1(2)
C(8)	31(2)	31(2)	26(2)	-3(1)	2(1)	4(2)
C(9)	37(2)	29(2)	32(2)	-1(2)	0(2)	6(2)
C(10)	51(3)	77(3)	74(3)	-15(3)	-5(3)	-25(3)
C(11)	35(3)	68(3)	45(2)	11(2)	11(2)	10(2)
C(12)	49(3)	110(4)	57(3)	3(3)	0(2)	-23(3)
C(13)	54(3)	57(2)	29(2)	-2(2)	11(2)	19(2)
C(14)	63(3)	71(3)	37(2)	-13(2)	0(2)	11(3)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **10a**.

	x	y	z	U(eq)
H(1O)	-530(40)	1350(30)	910(30)	105(16)
H(4)	-2900(30)	4300(20)	-2470(30)	56(10)
H(5)	-4550(30)	4401(18)	-1020(20)	36(8)
H(7)	-3290(20)	2044(15)	412(19)	17(7)
H(8)	-160(30)	591(16)	-1140(20)	29(8)
H(10A)	-3930(40)	-800(30)	-2040(40)	110(17)
H(10B)	-3610(40)	-1040(30)	-680(30)	91(16)
H(10C)	-4520(50)	-200(30)	-1100(40)	107(19)
H(11A)	2420(30)	1900(20)	-3060(30)	62(11)
H(11B)	1510(30)	2790(20)	-3230(30)	56(10)
H(12A)	1560(50)	2940(30)	-1080(40)	117(19)
H(12B)	2280(40)	2000(30)	-1020(30)	96(18)
H(12C)	3050(40)	2880(20)	-1460(30)	86(13)
H(13A)	-210(30)	1870(20)	-4410(30)	58(10)
H(13B)	980(30)	1110(20)	-4260(30)	62(10)
H(14A)	-1320(30)	443(19)	-4710(30)	59(10)
H(14B)	-1900(40)	870(20)	-3570(30)	73(12)
H(14C)	-680(40)	30(20)	-3420(30)	84(13)

Table 6. Hydrogen bonds for **10a** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(1O)...N(1)#1	0.89(4)	2.09(4)	2.938(3)	160(4)

Symmetry transformations used to generate equivalent atoms:

#1 x,-y+1/2,z+1/2

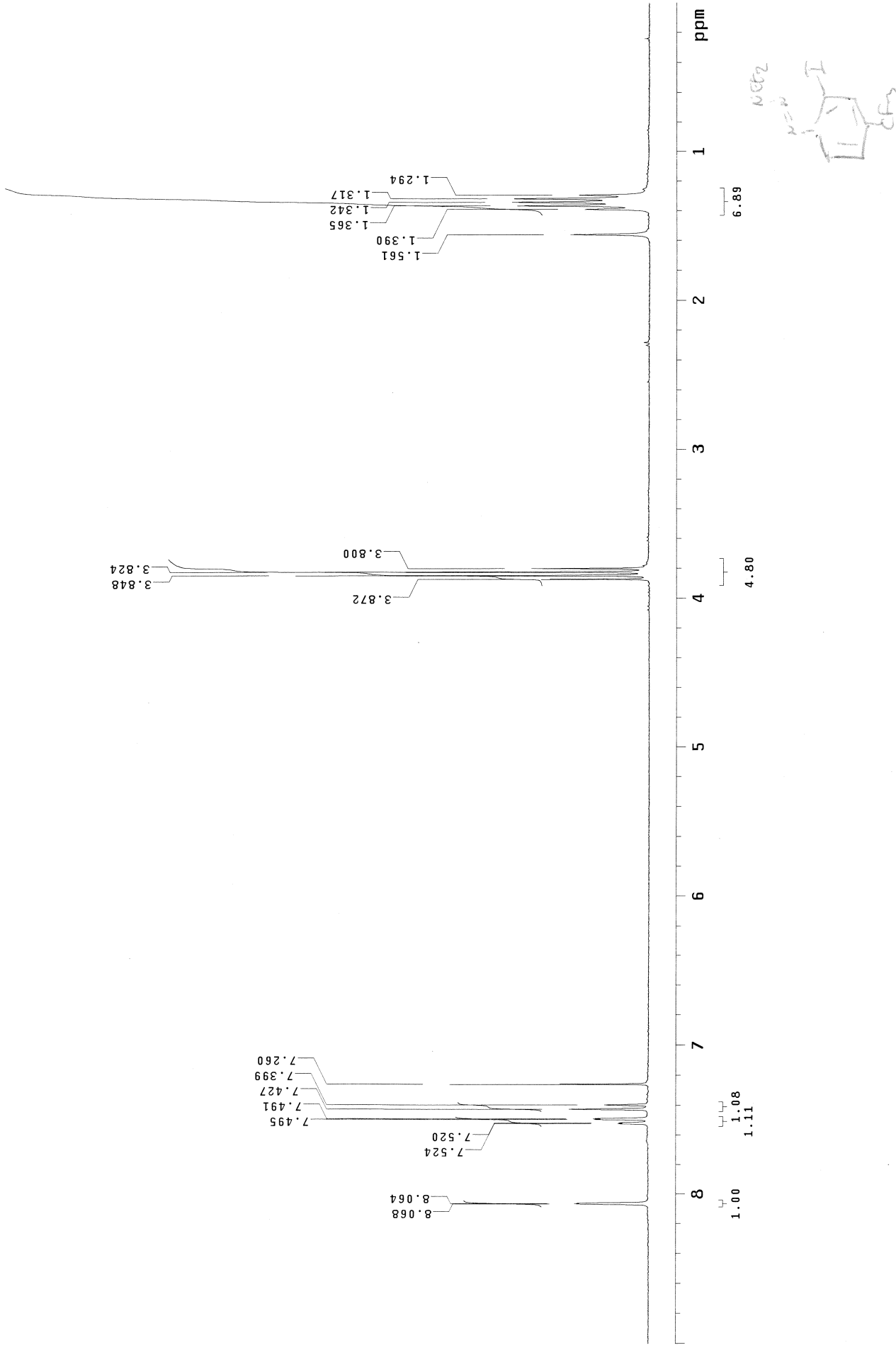
References:

1) (a) Herges, R.; Geuenich, D. *J. Phys. Chem. A* **2001**, *105*, 3214-3220. (b) Geuenich, D.; Hess, K.; Kohler, F.; Herges, R. *Chem. Rev*. **2005**, *105*, 3758-3772.

2) (a) Pena-Gallego, A.; Rodriguez-Otero, J.; Cabaleiro-Lago, E. M. *J. Org. Chem*. **2004**, *69*, 7013-7017. (b) Rodriguez-Otero, J.; Cabaleiro-Lago, E. M.; Hermida-Ramon, J. M.; Pena-Gallego, A. *J. Org. Chem*. **2003**, *68*, 8823-8830. (c) Subbotina, J. O.; Bakulev, V. A.; Herges, R.; Fabian, W. M. F. *Int. J. Quant. Chem*. **2006**, *106*, 2229-2235.

3) (a) Shirtcliff, L. D.; Hayes, A. G.; Haley, M. M.; Kohler, F.; Hess, K.; Herges, R. *J. Am. Chem. Soc*. **2006**, *128*, 9711-9721. (b) McClintock, S. P.; Shirtcliff, L. D.; Haley, M. M. *J. Org. Chem.* **2008**, *73*, 8755-8762. (c) Kimball, D. B.; Weakley, T. J. R.; Herges, R.; Haley, M. M. *J. Am. Chem. Soc.* **2002**, *124*, 13463-13473. (d) Shirtcliff, L. D.; Hayes, A. G.; Haley, M. M; Kohler, F.; Hess, K.; Herges, R. *J. Am. Chem Soc.* **2006**, *128,* 9711-9721.

5b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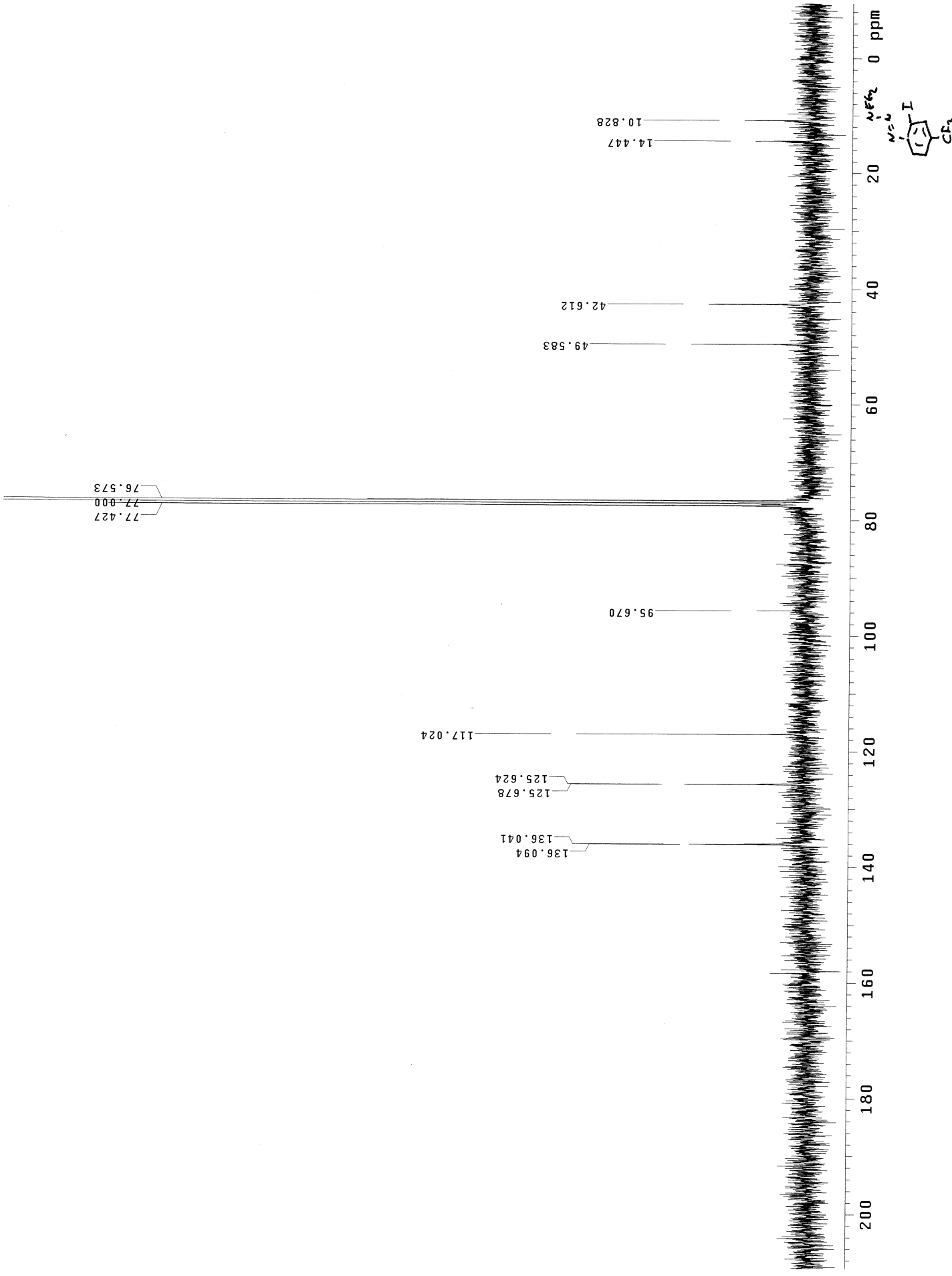
5b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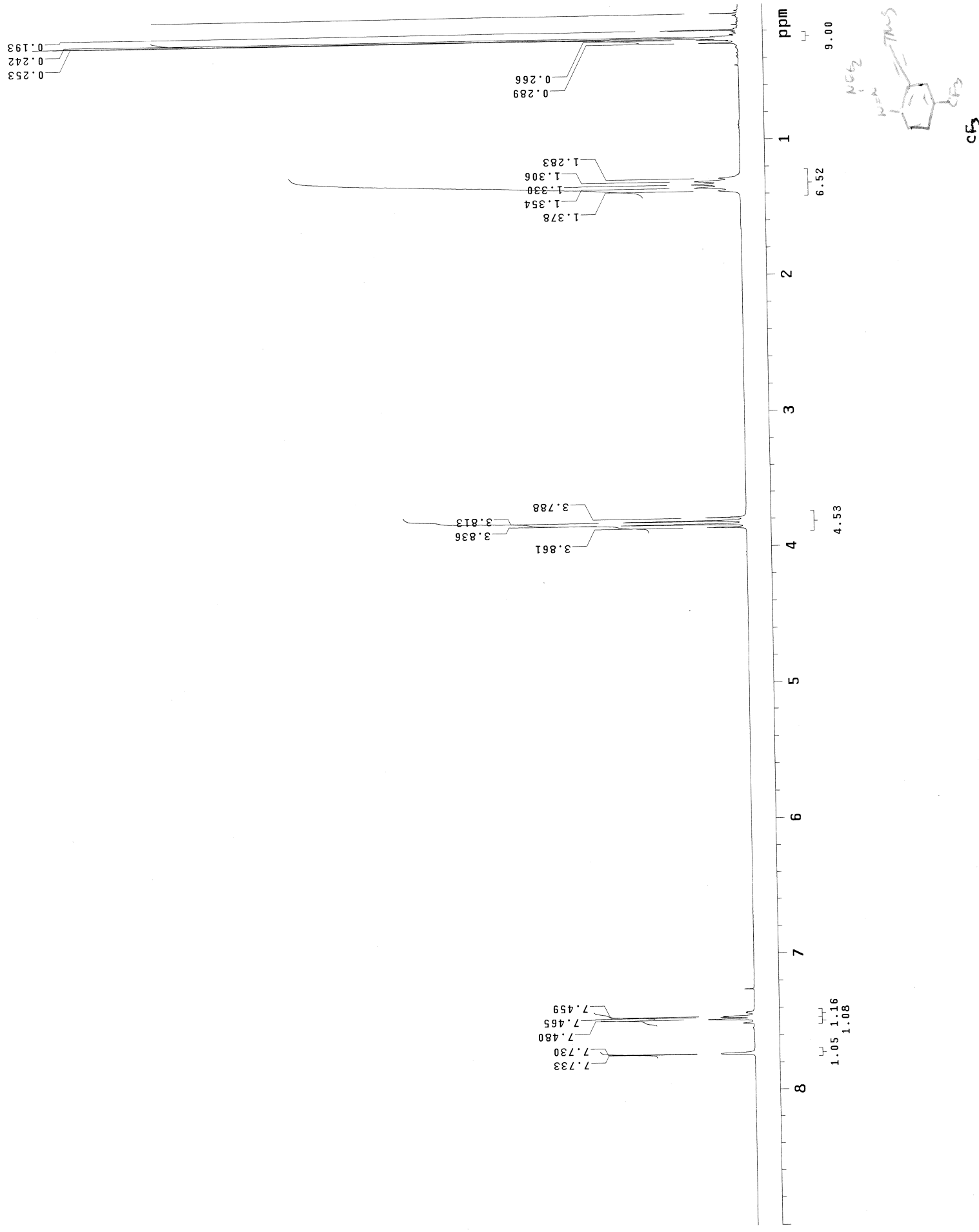
7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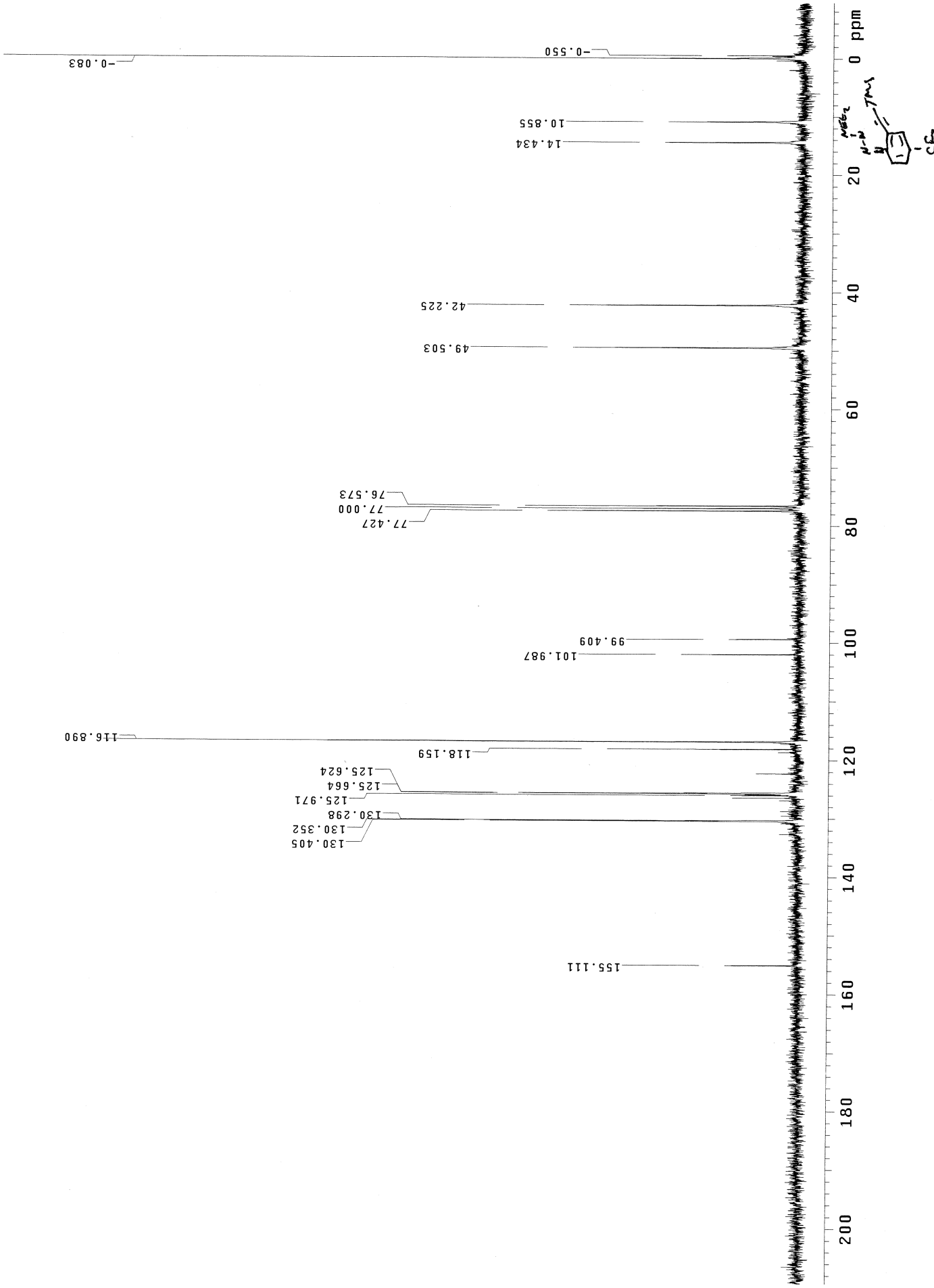
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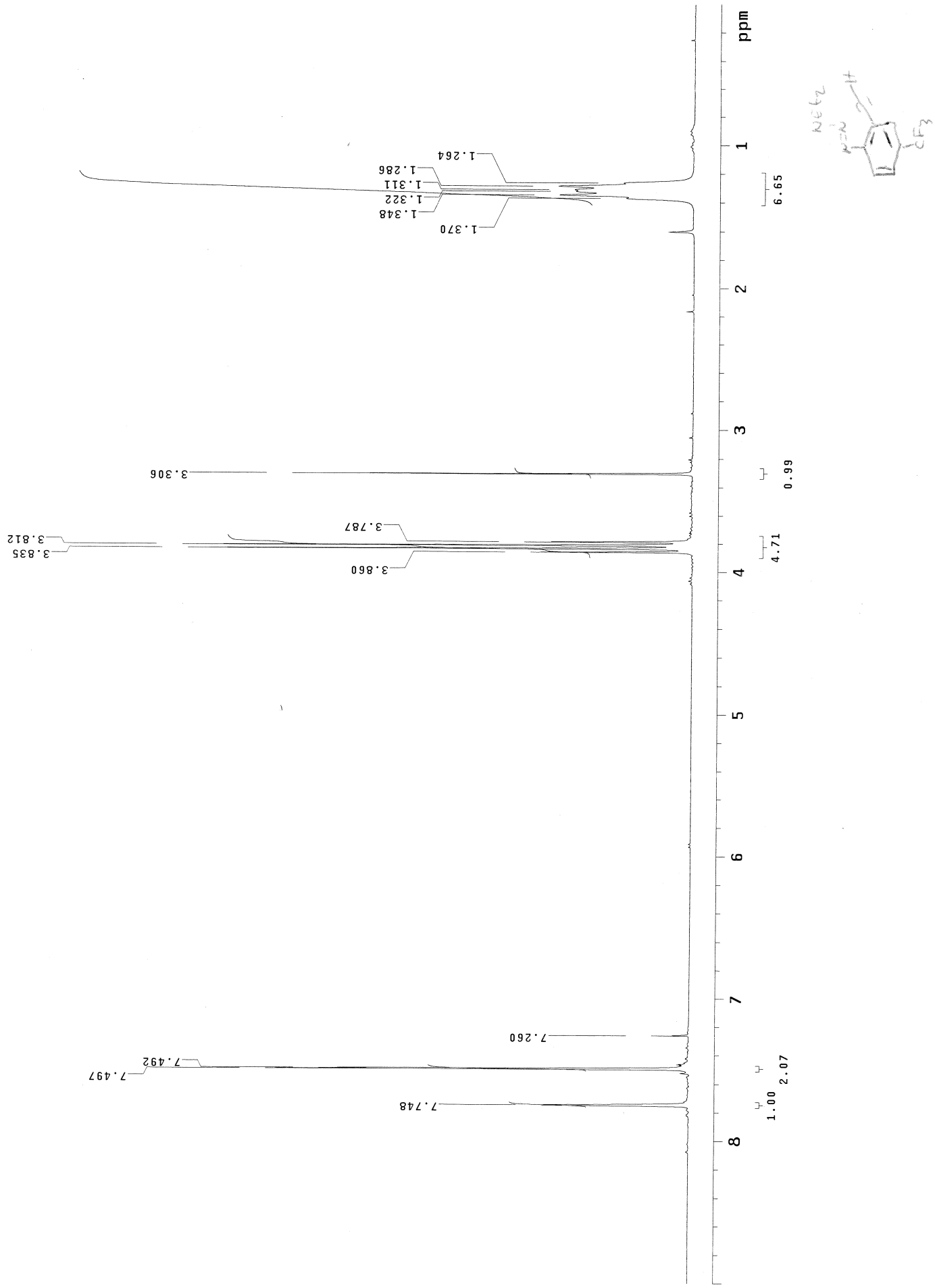
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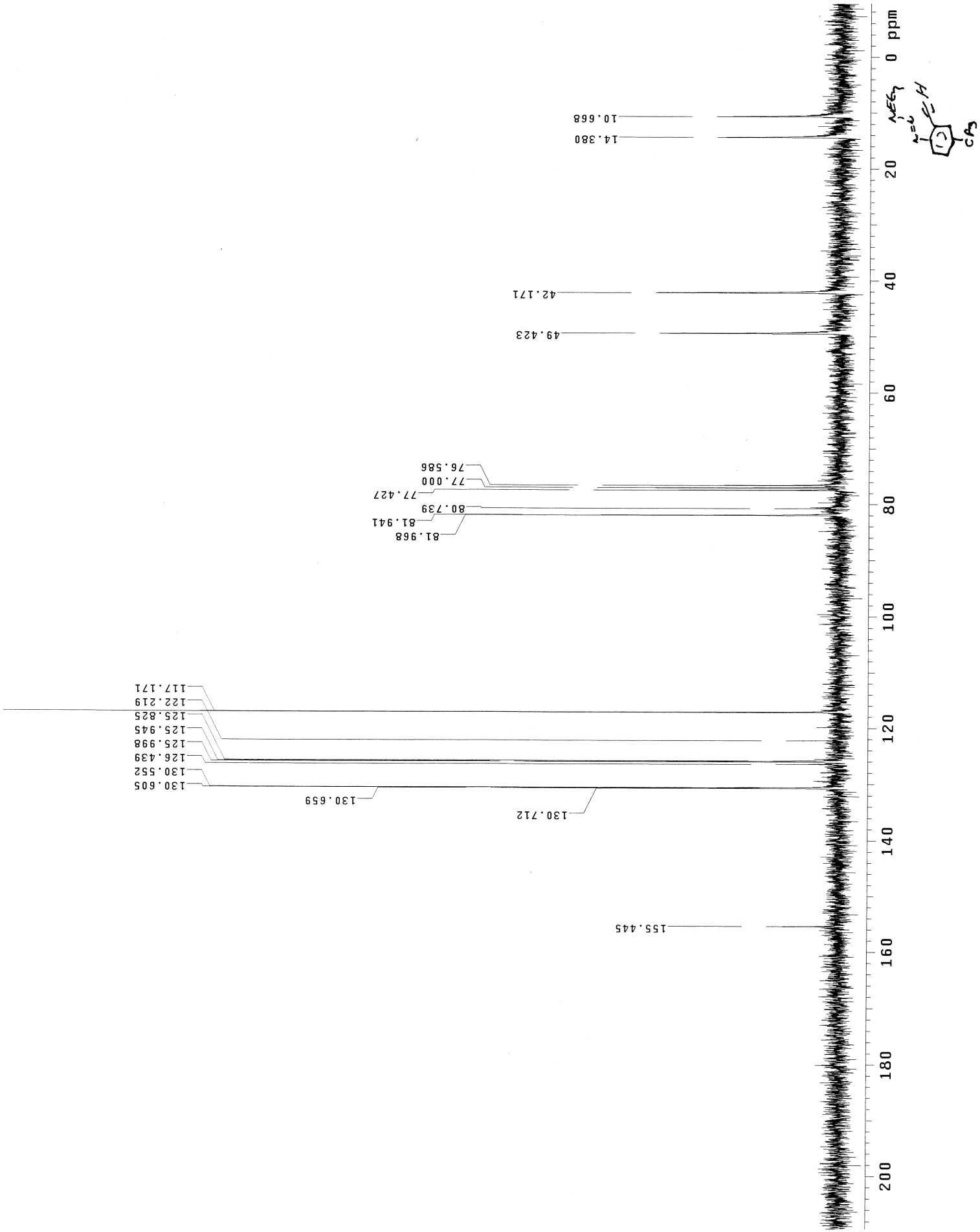
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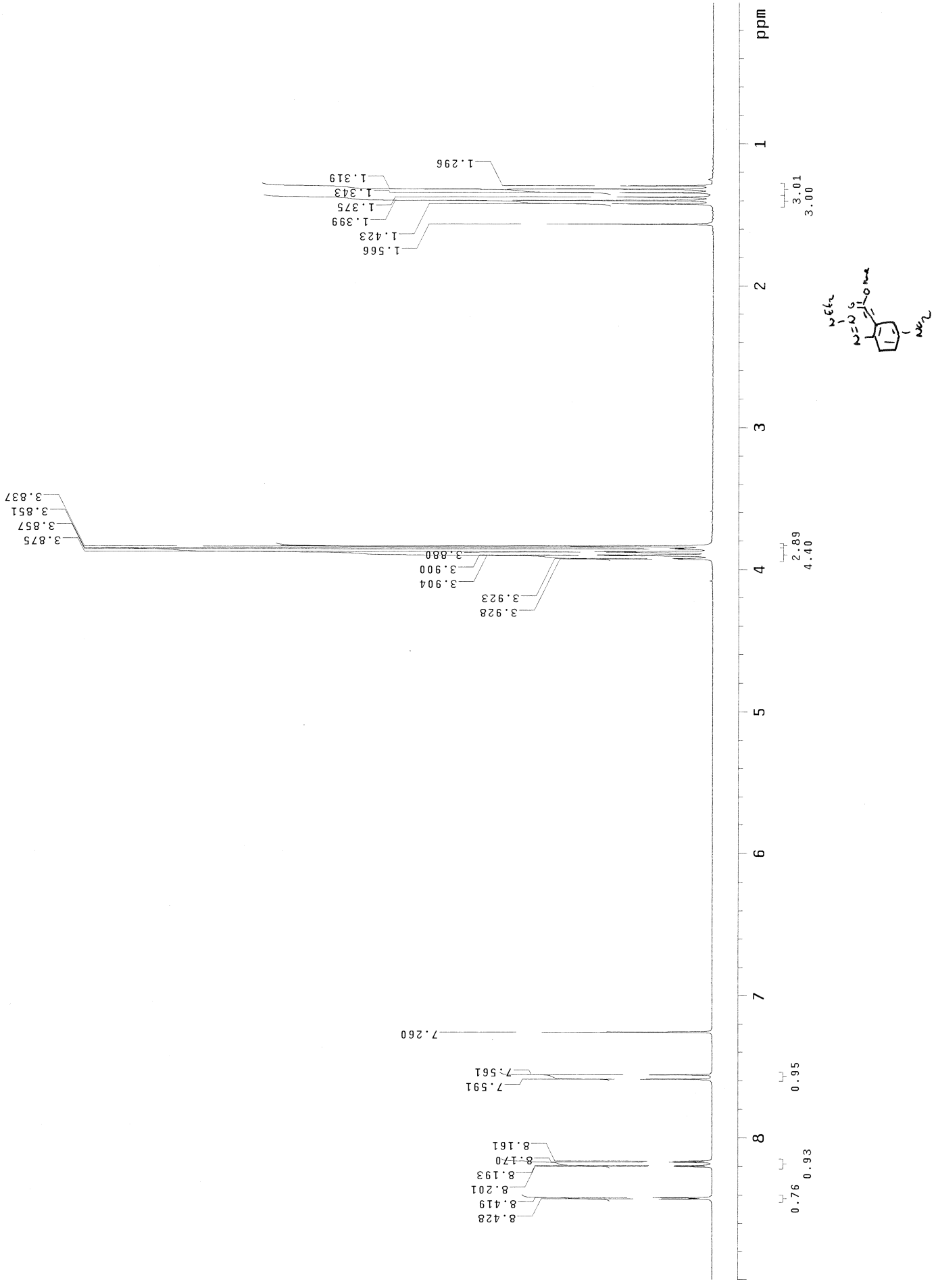
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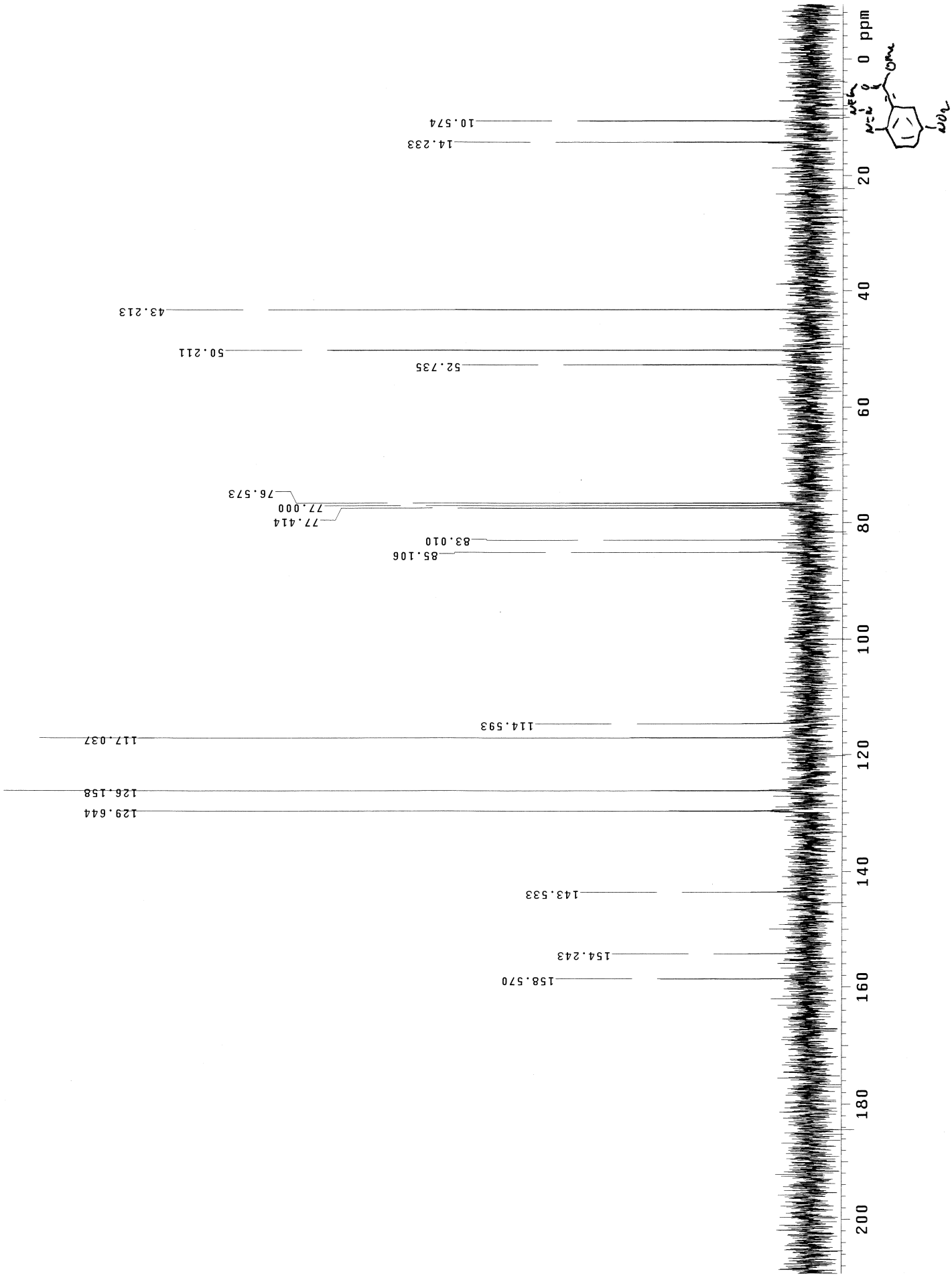
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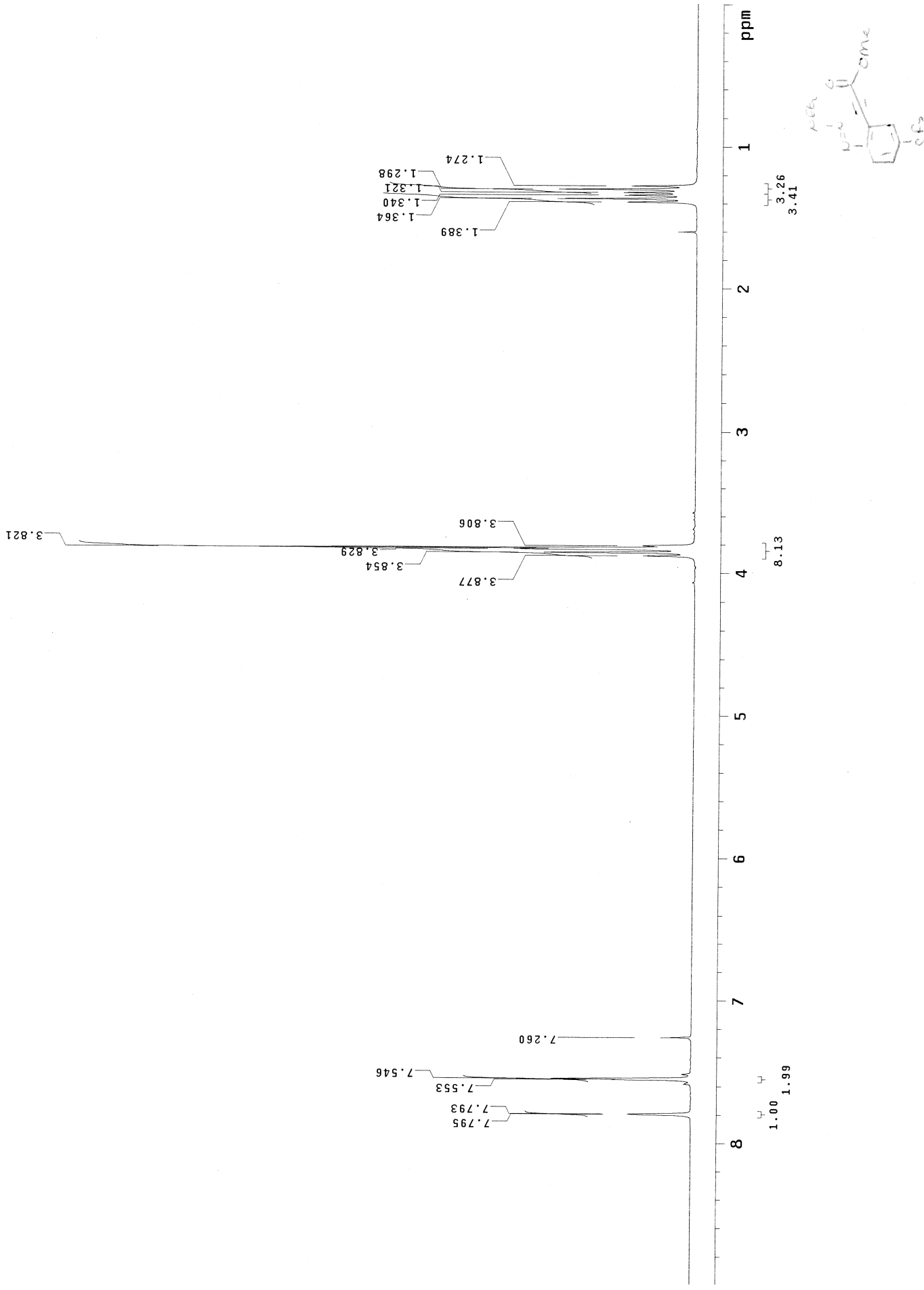
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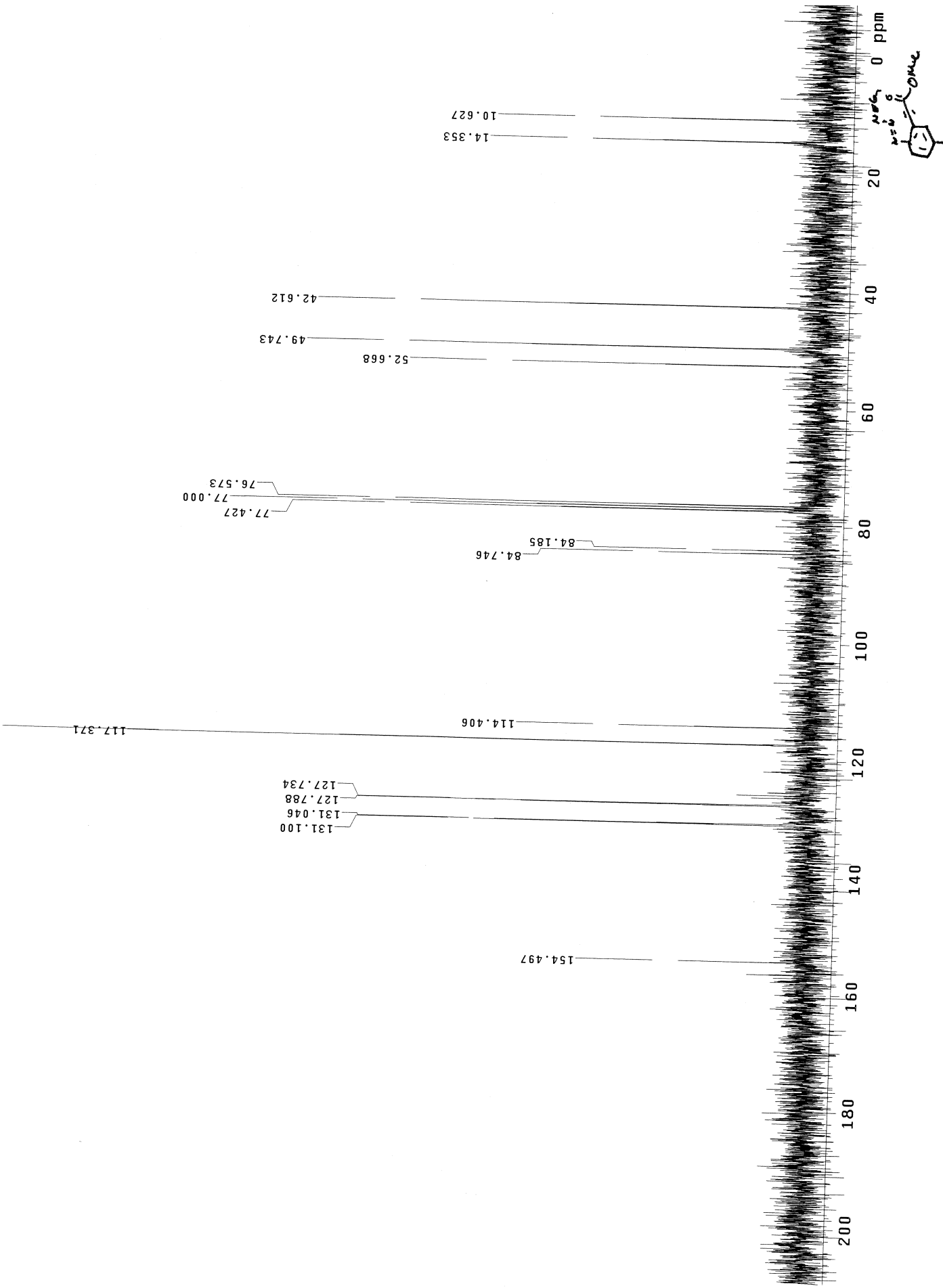
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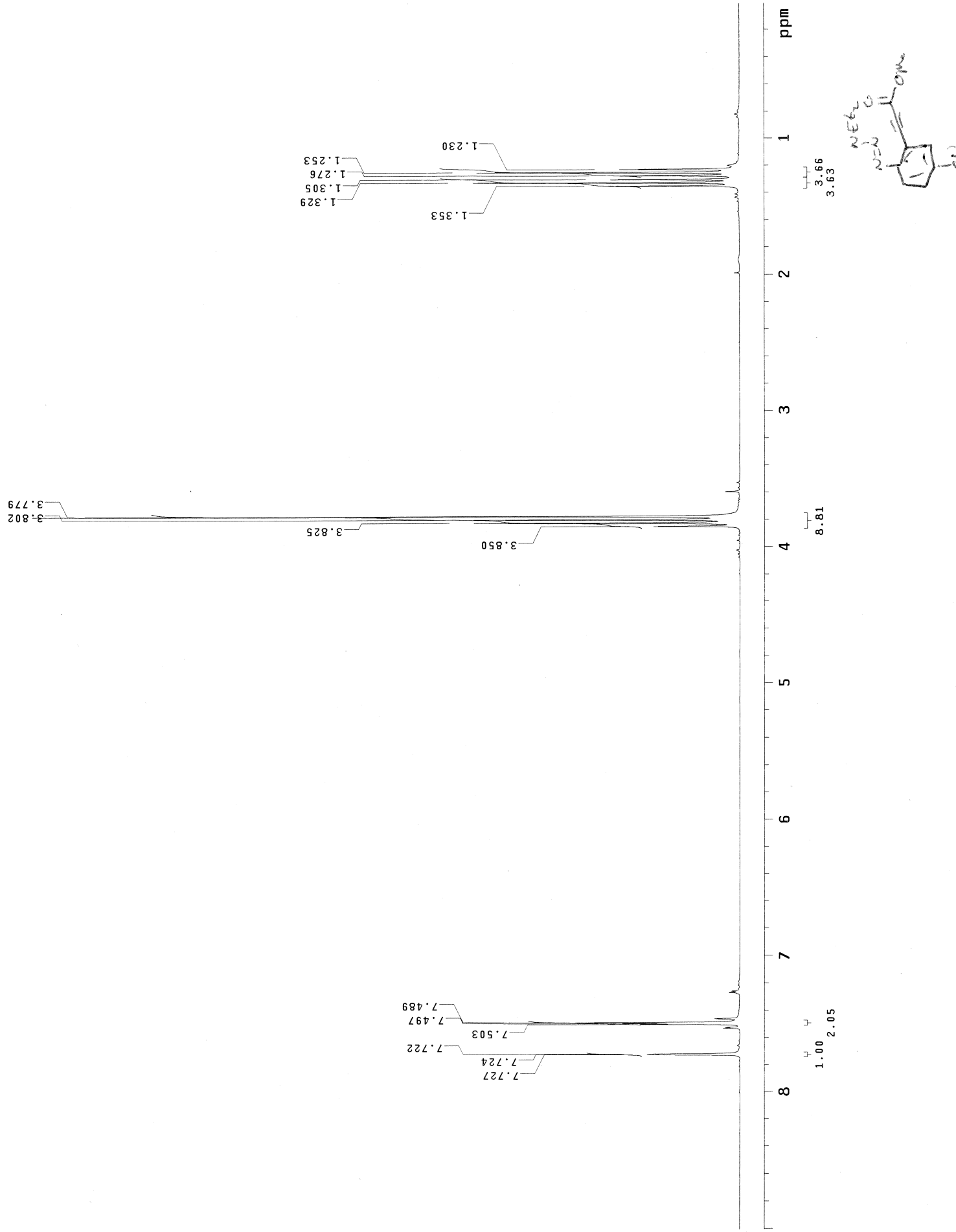
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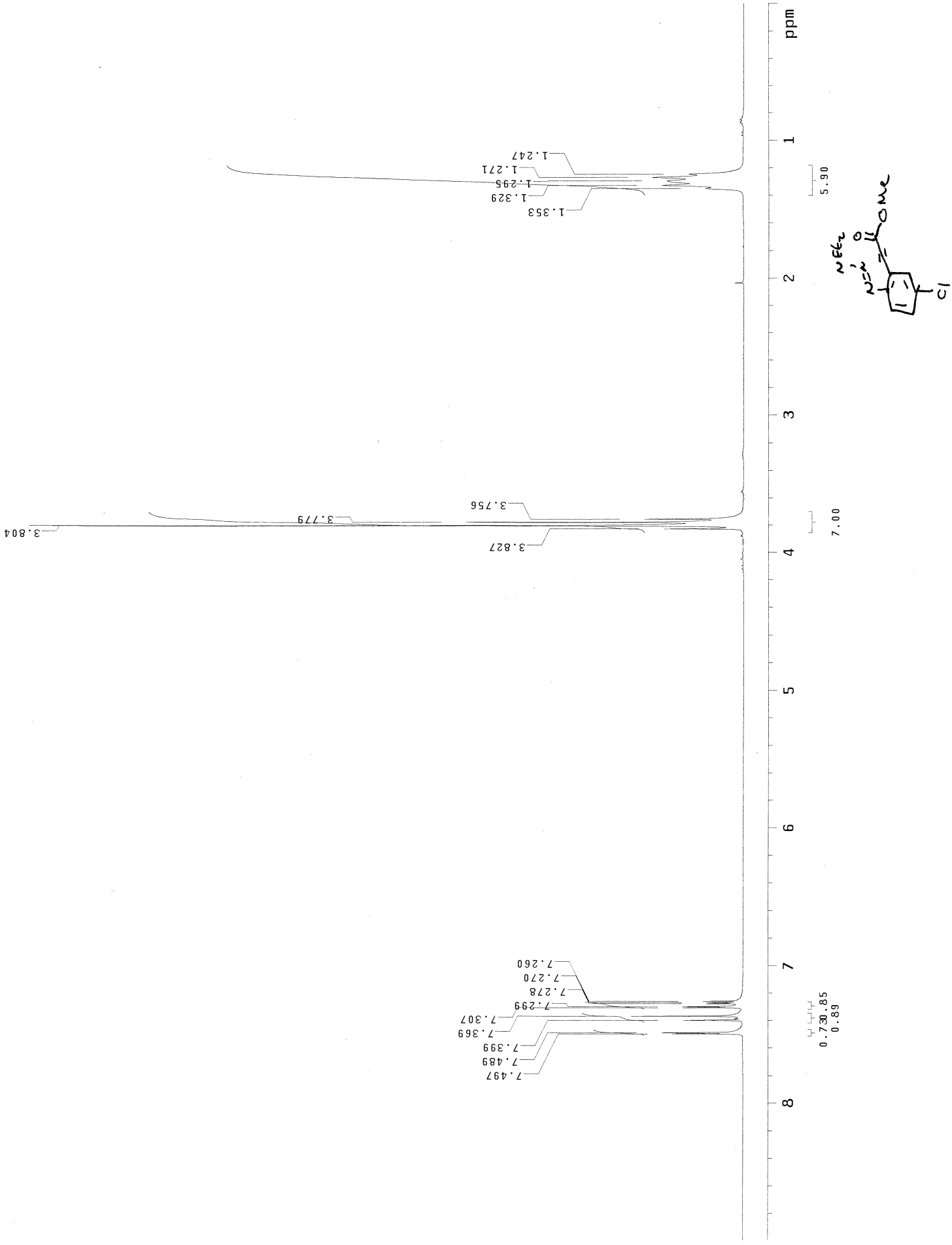
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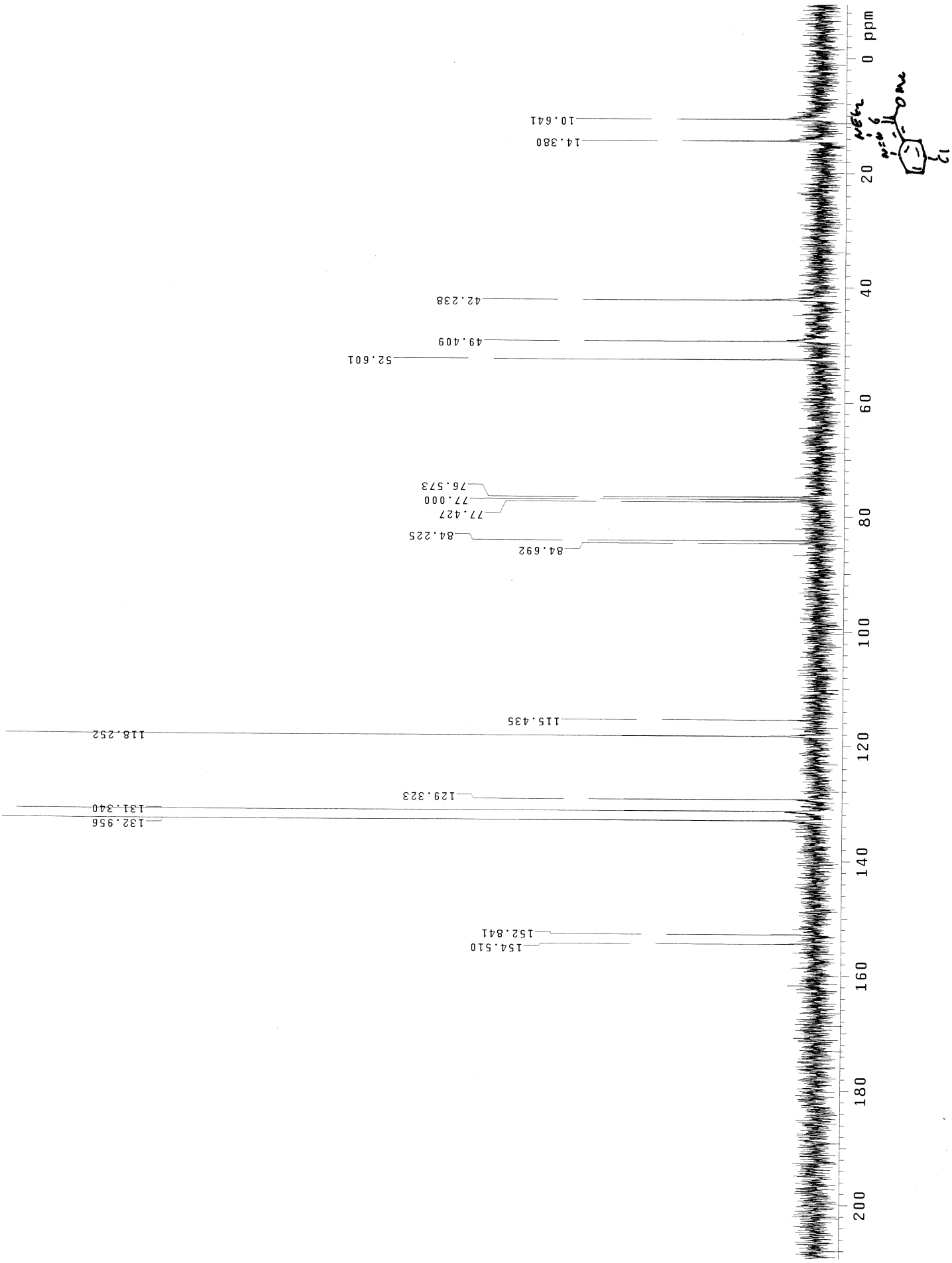
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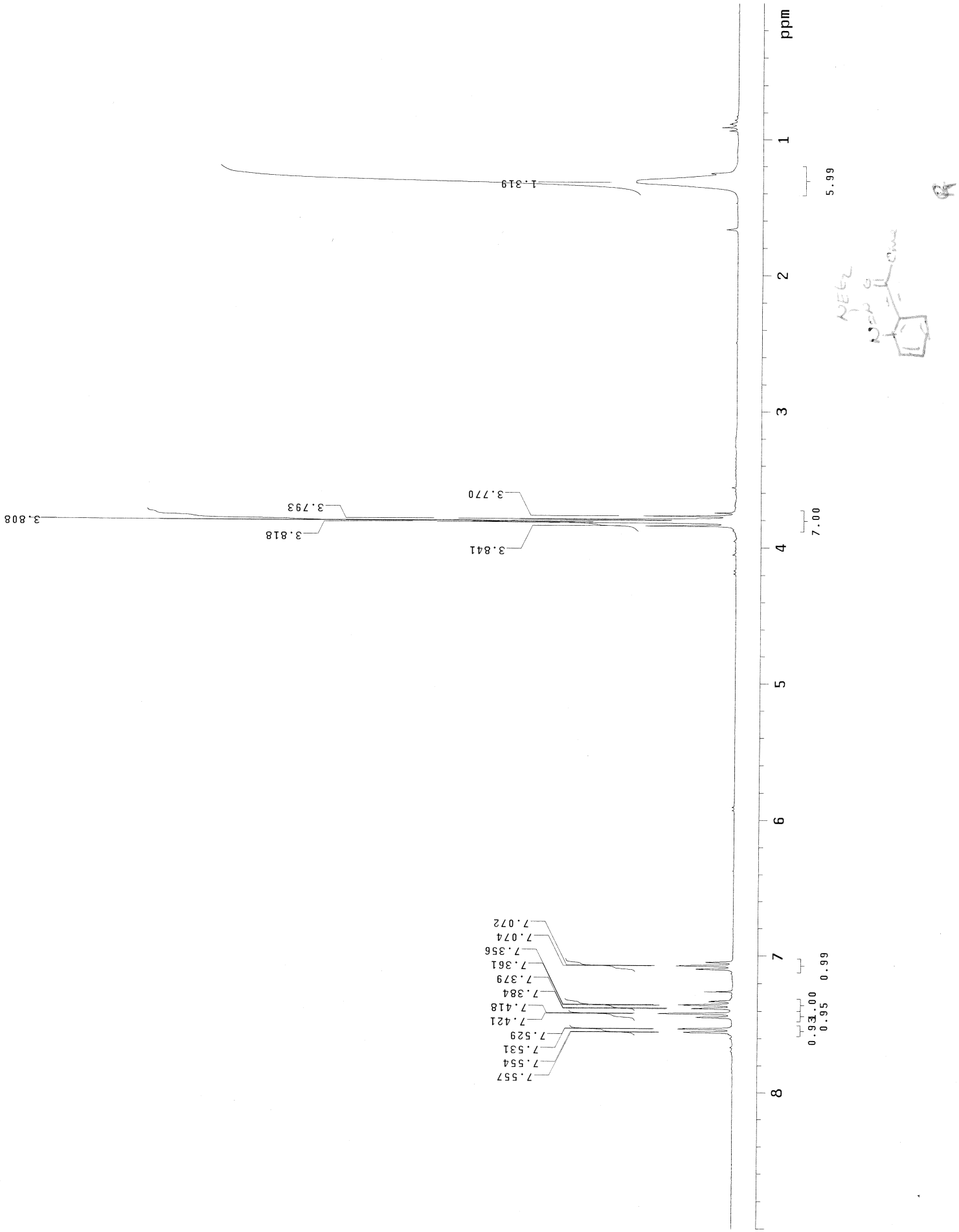
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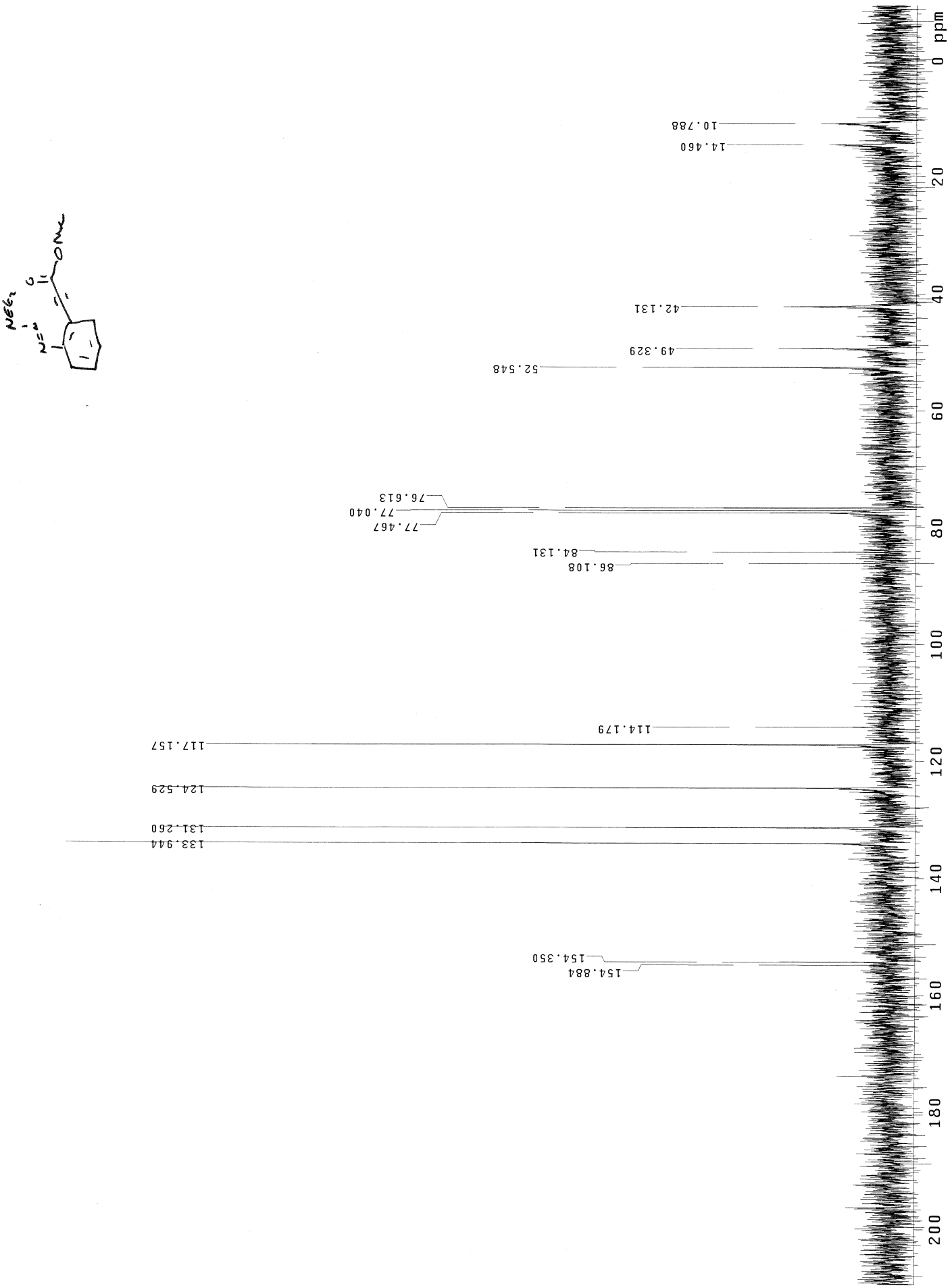
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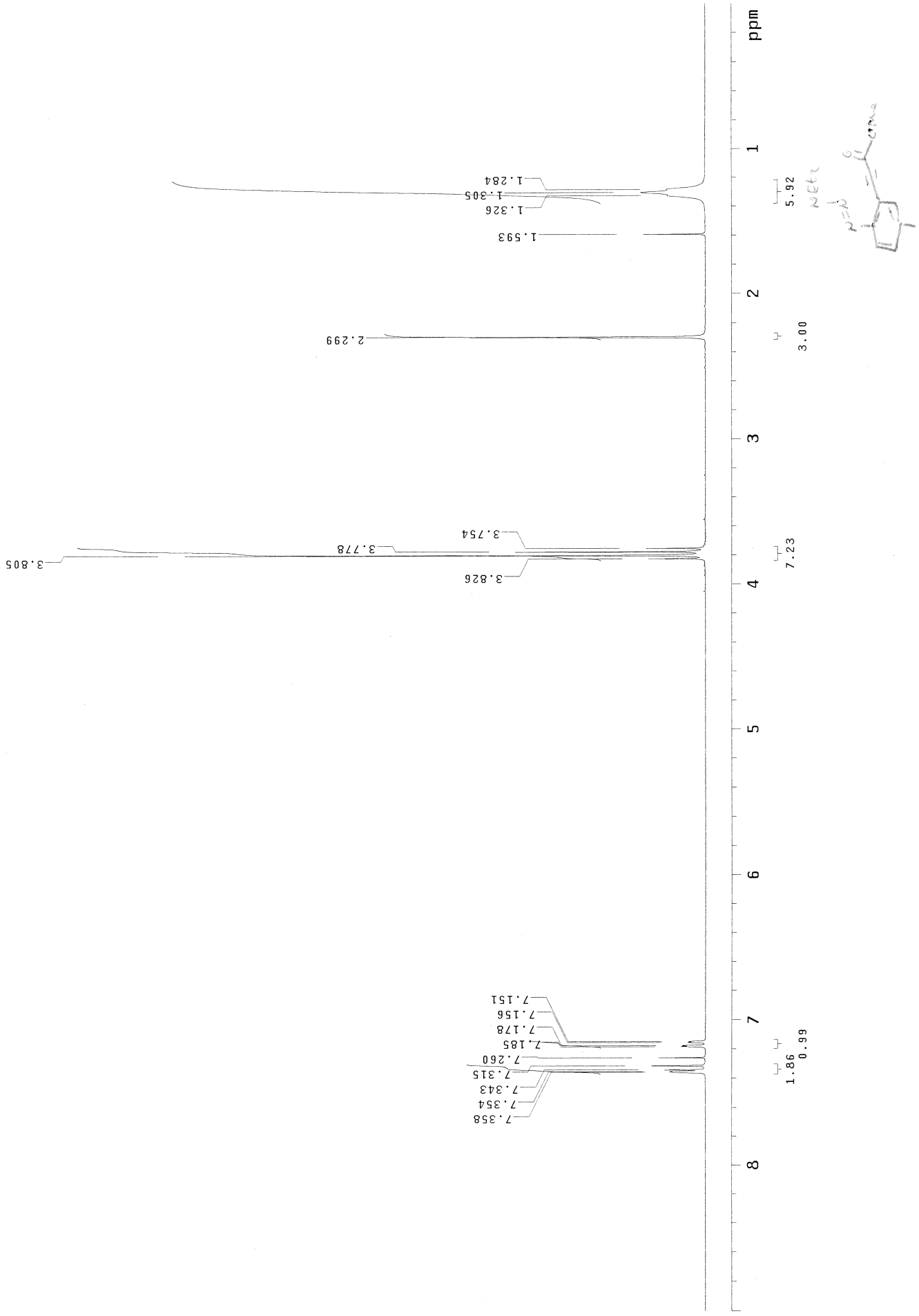
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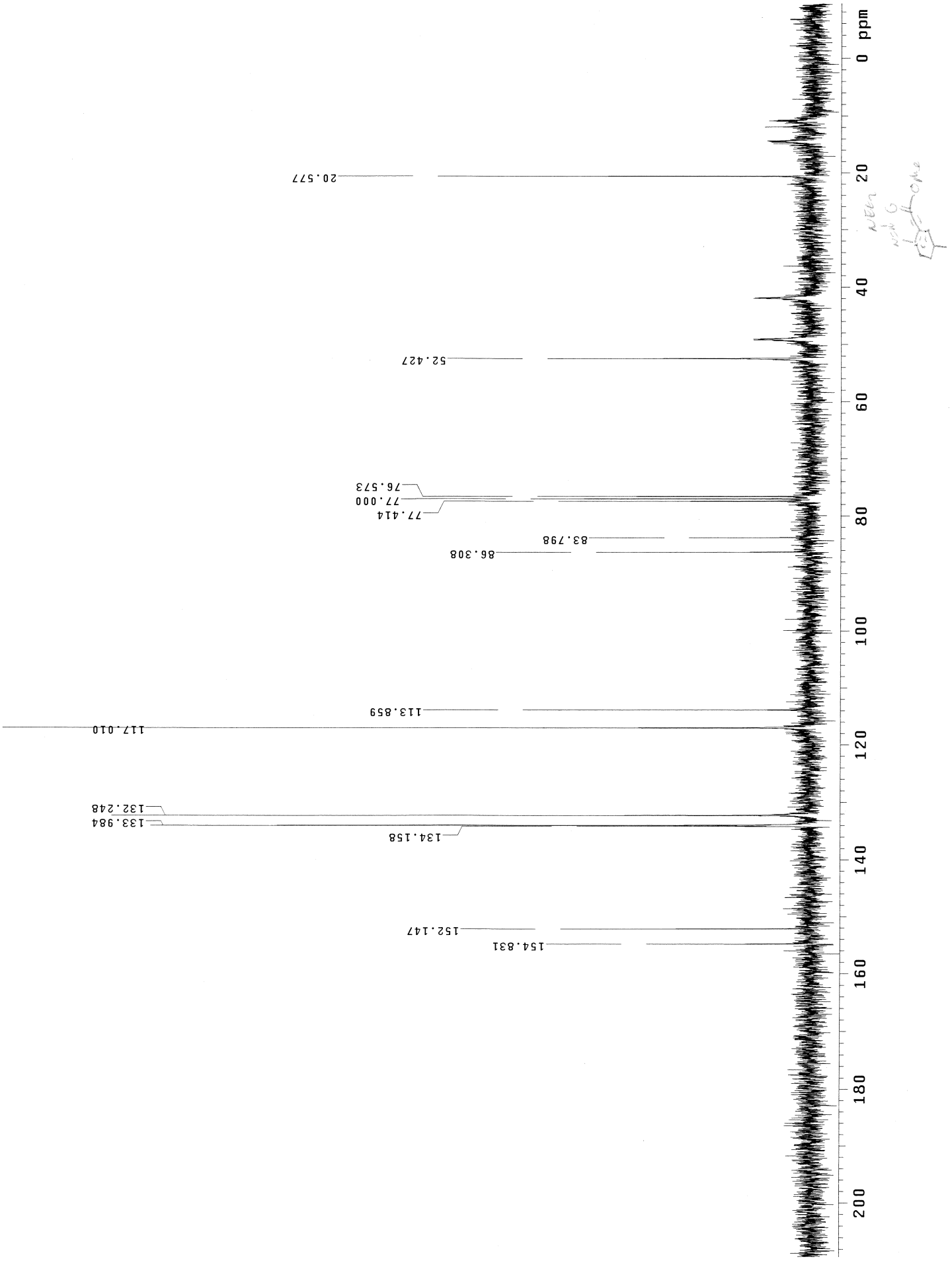
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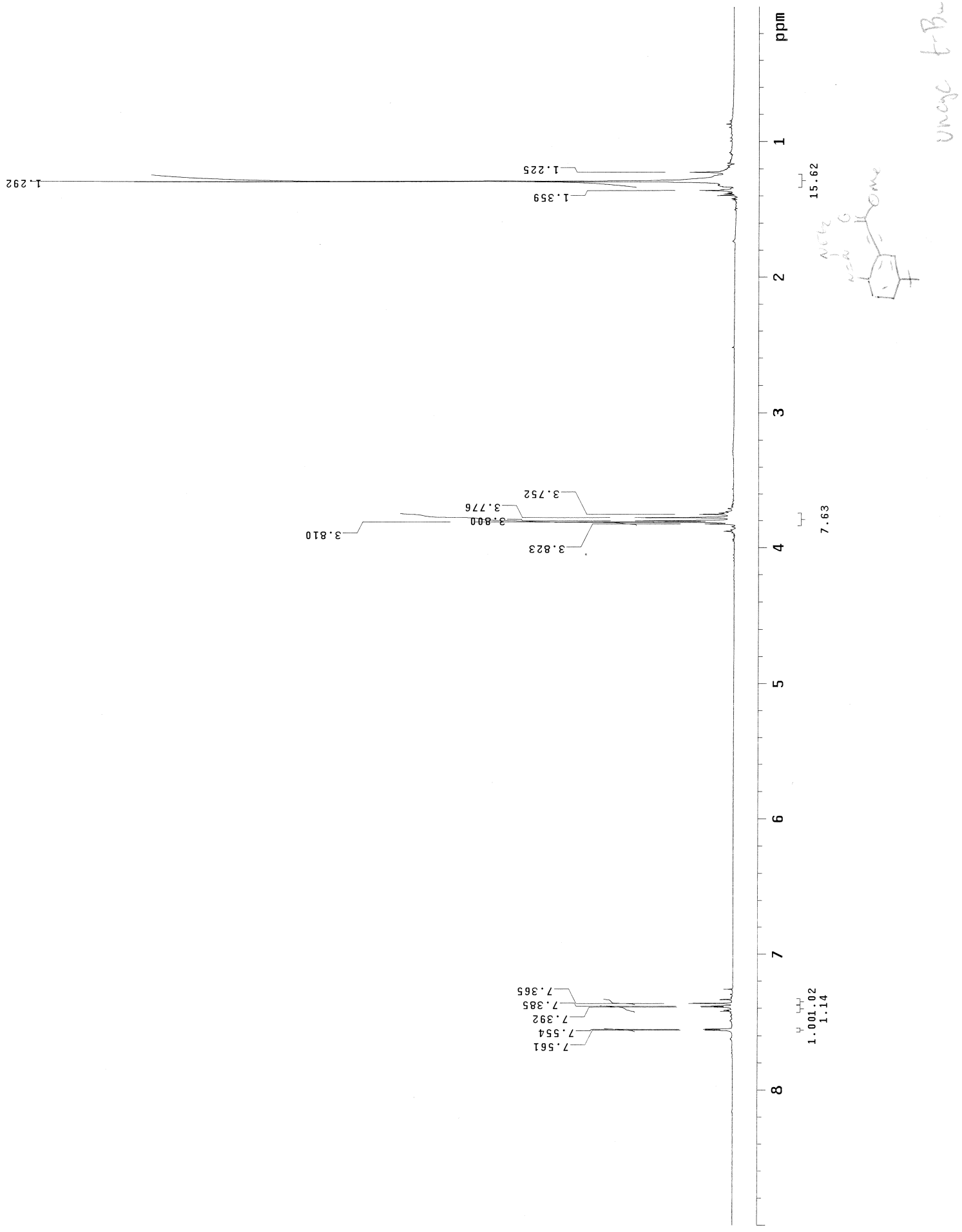
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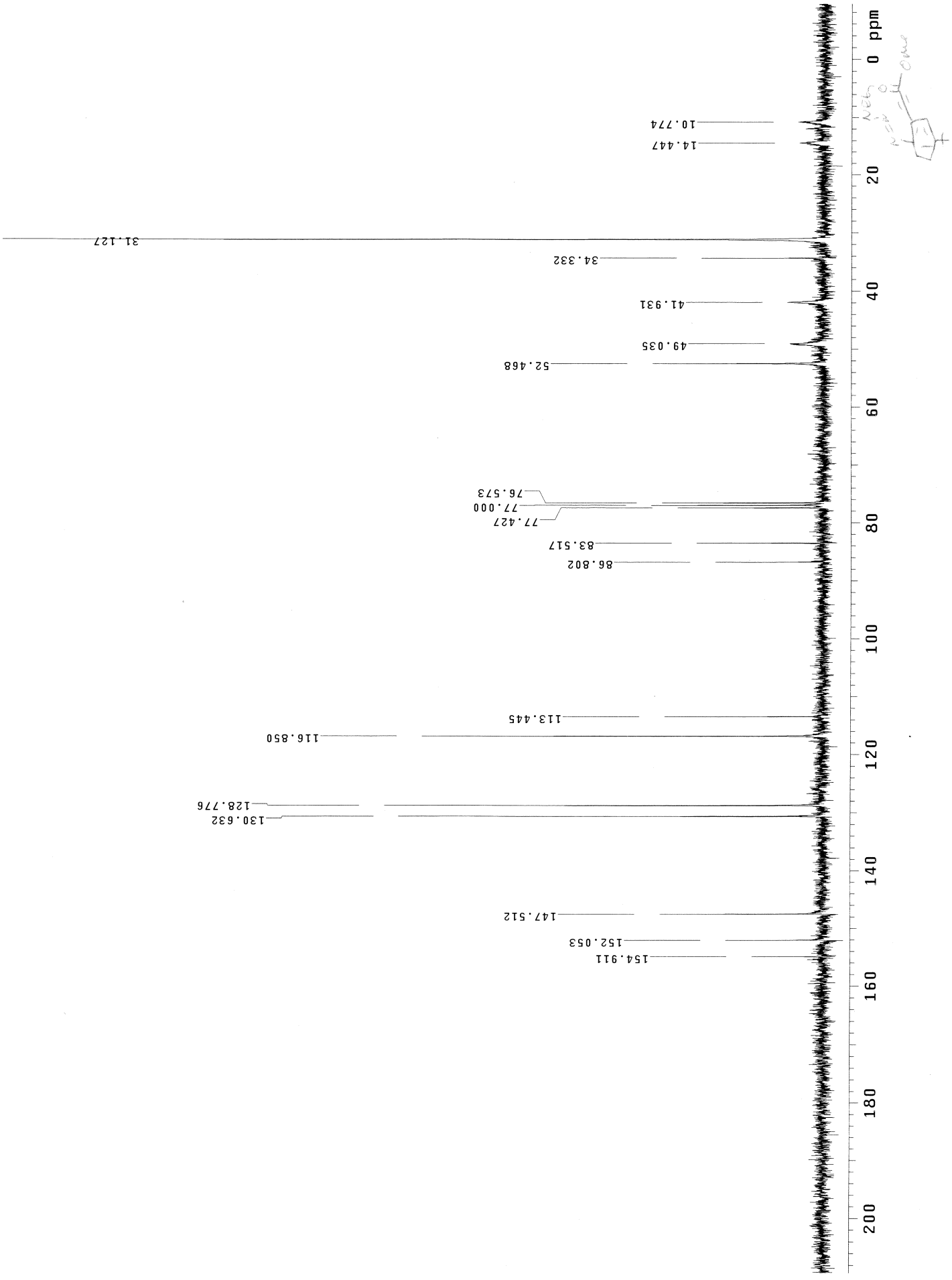
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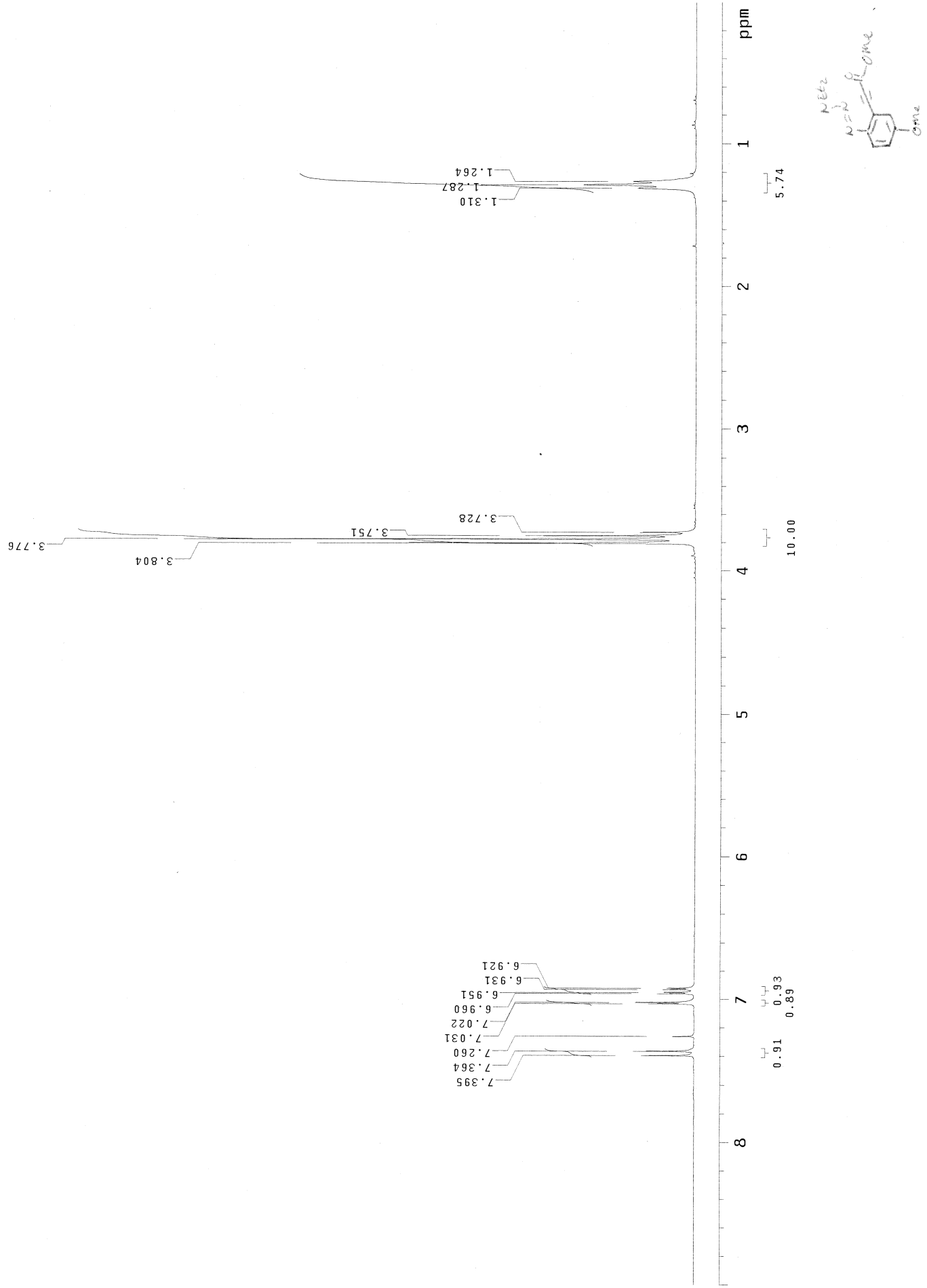
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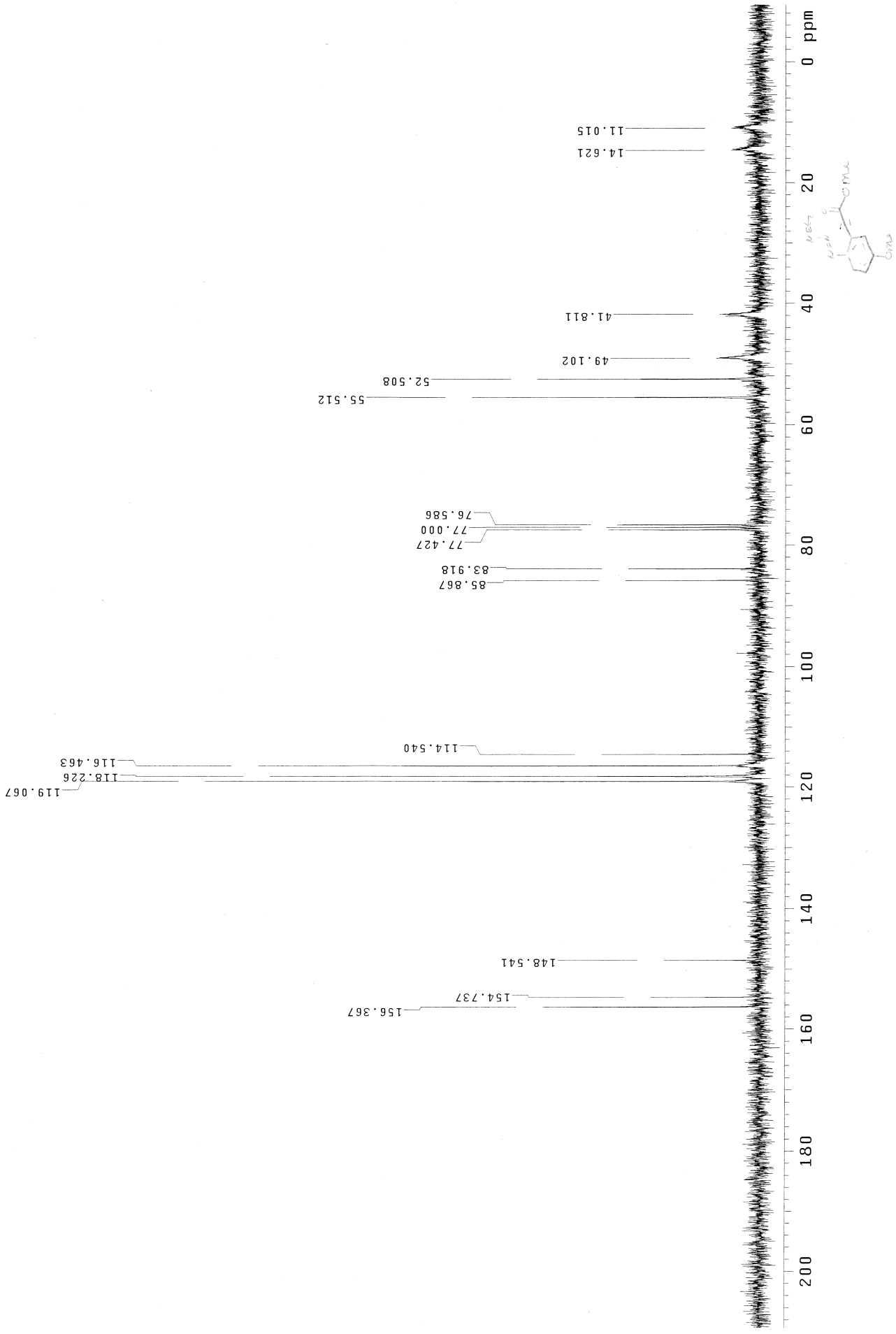
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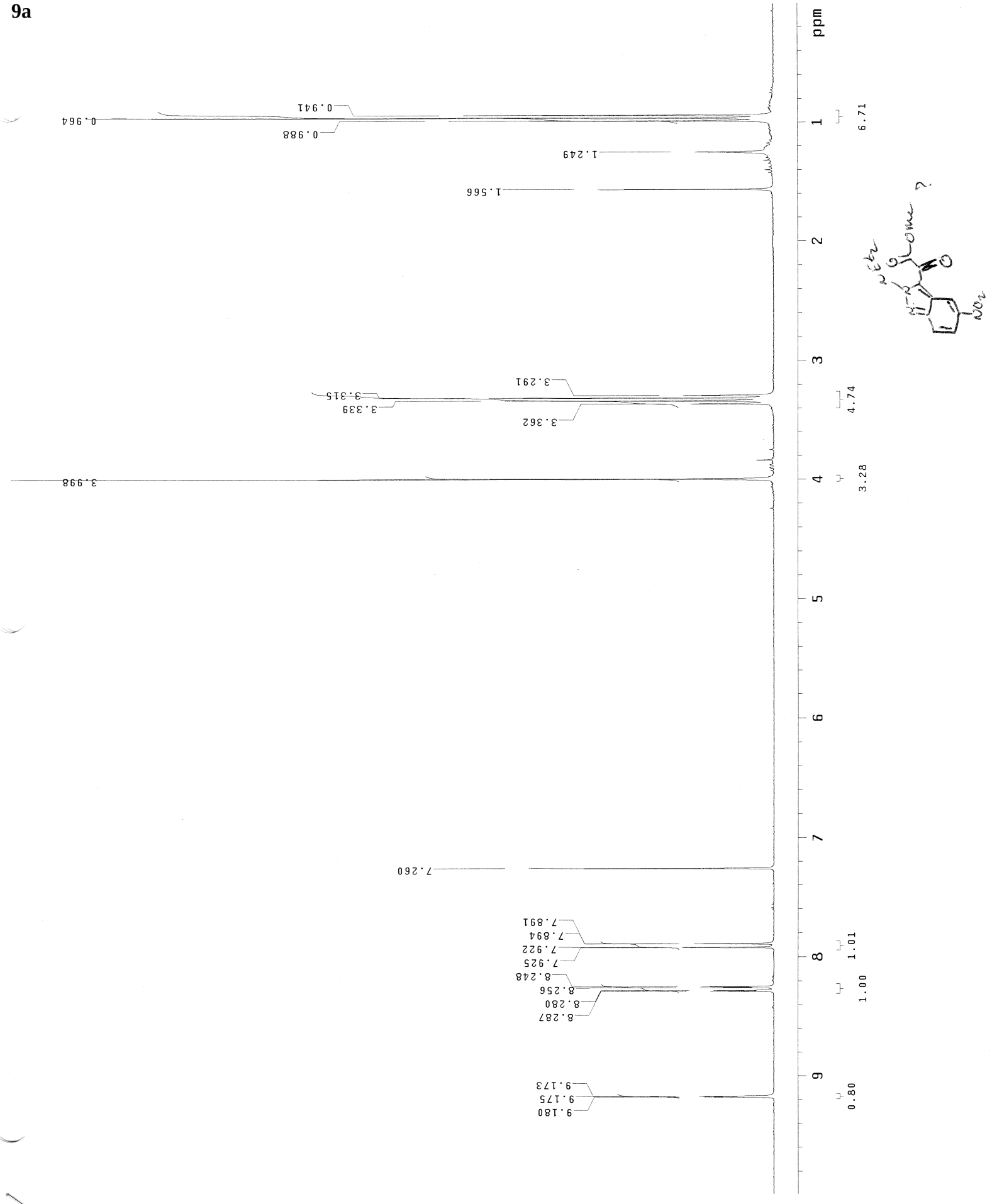
9a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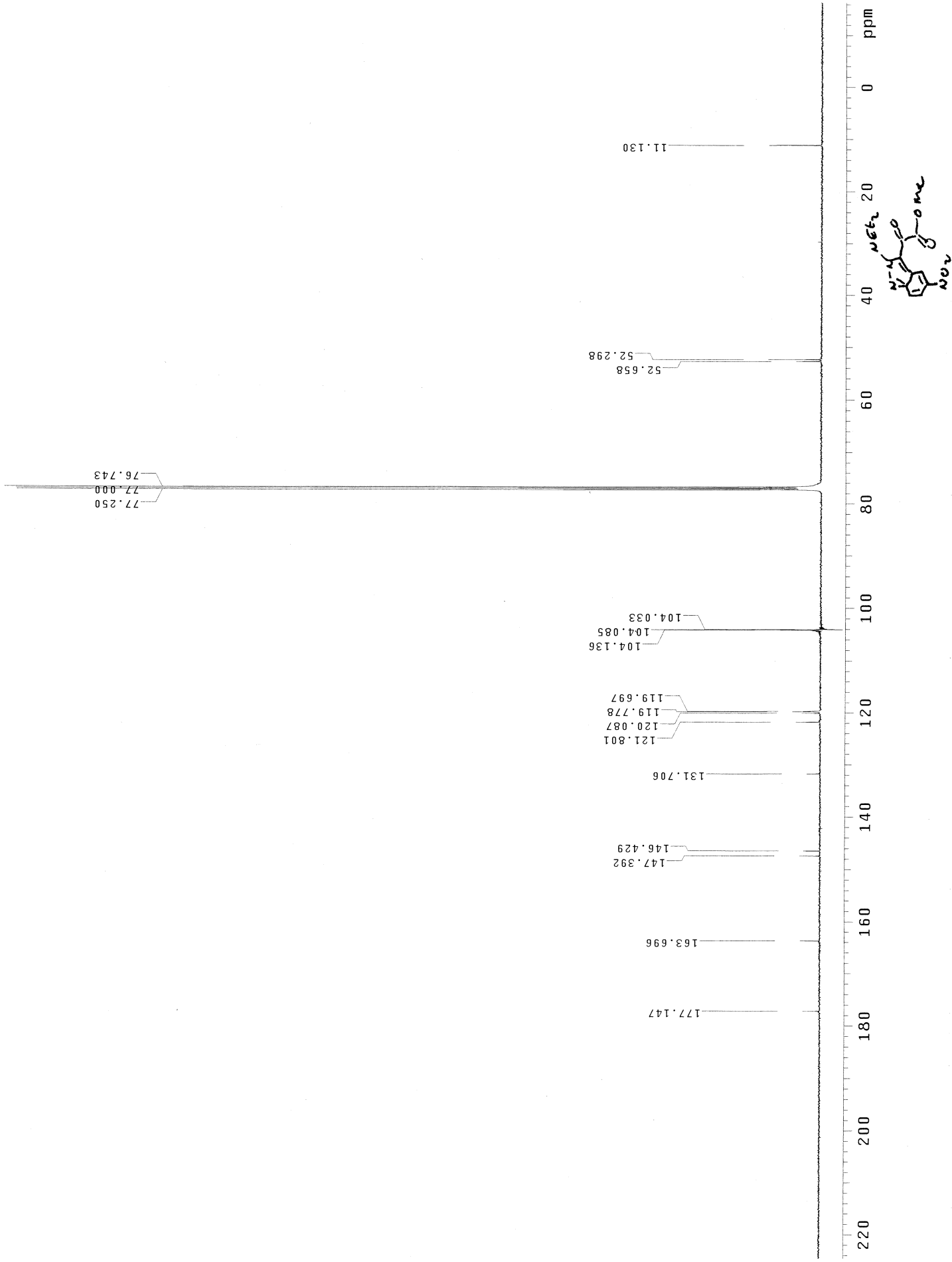
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ppm
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40
60
80
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140
160
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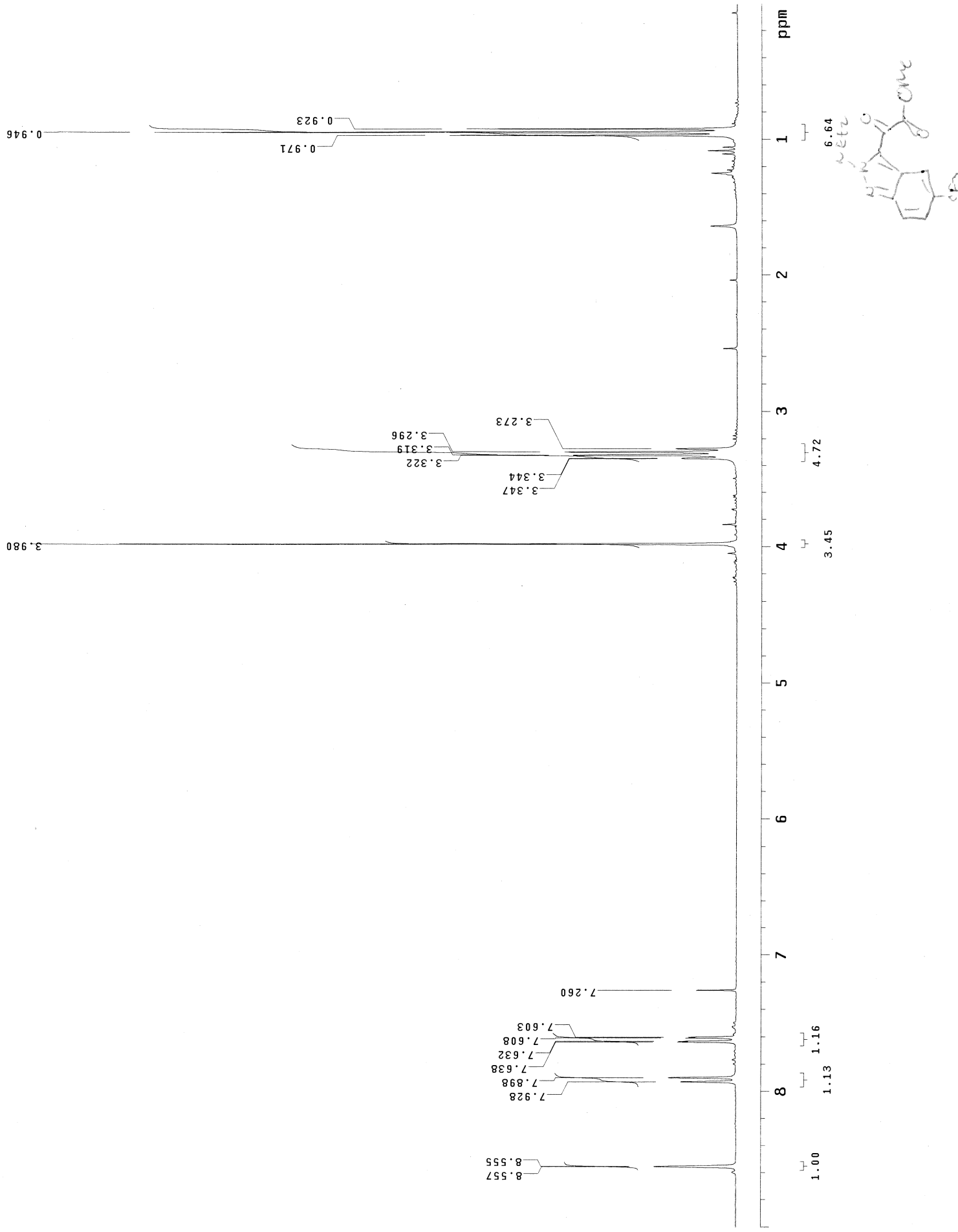
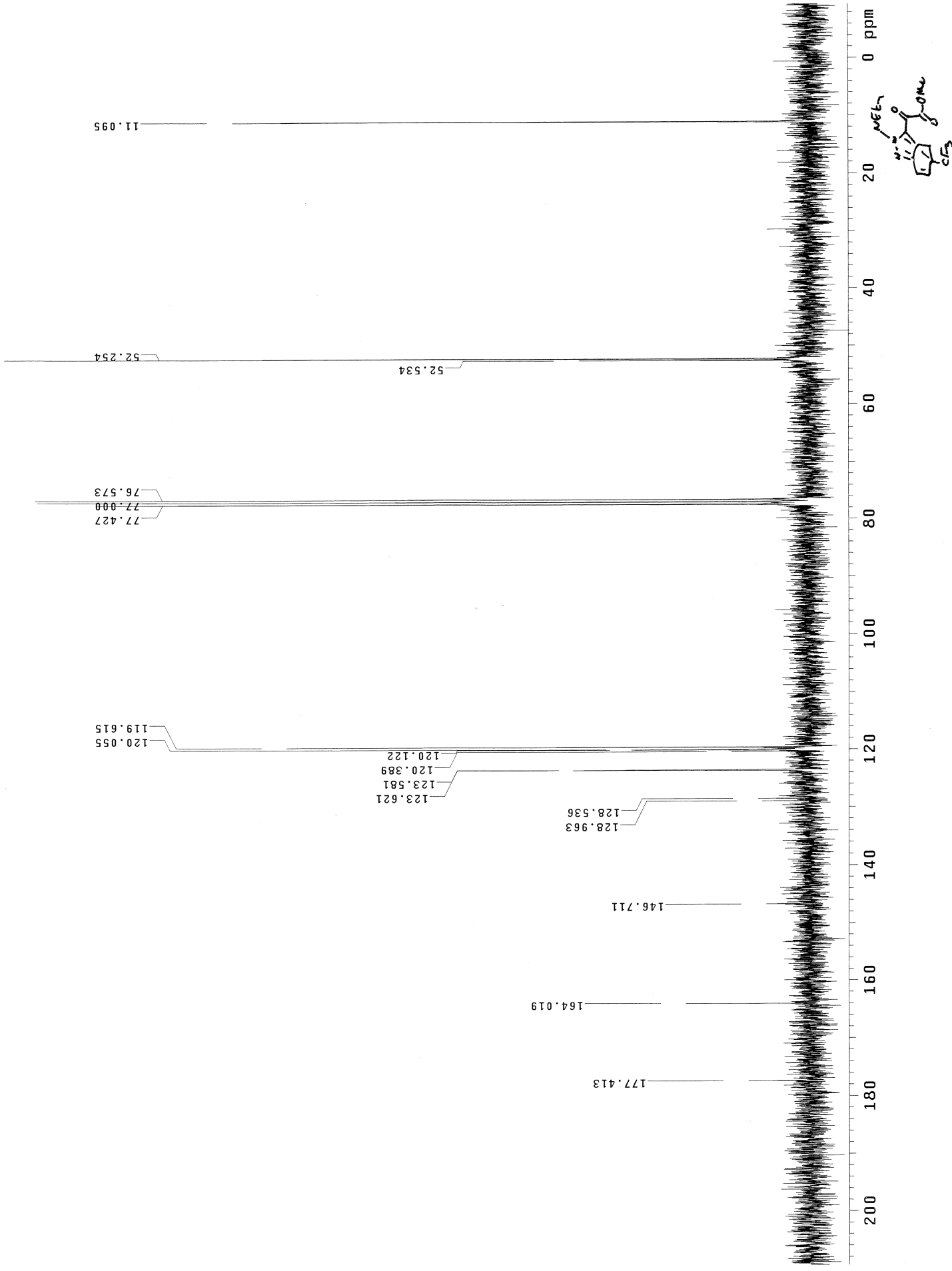
200
220

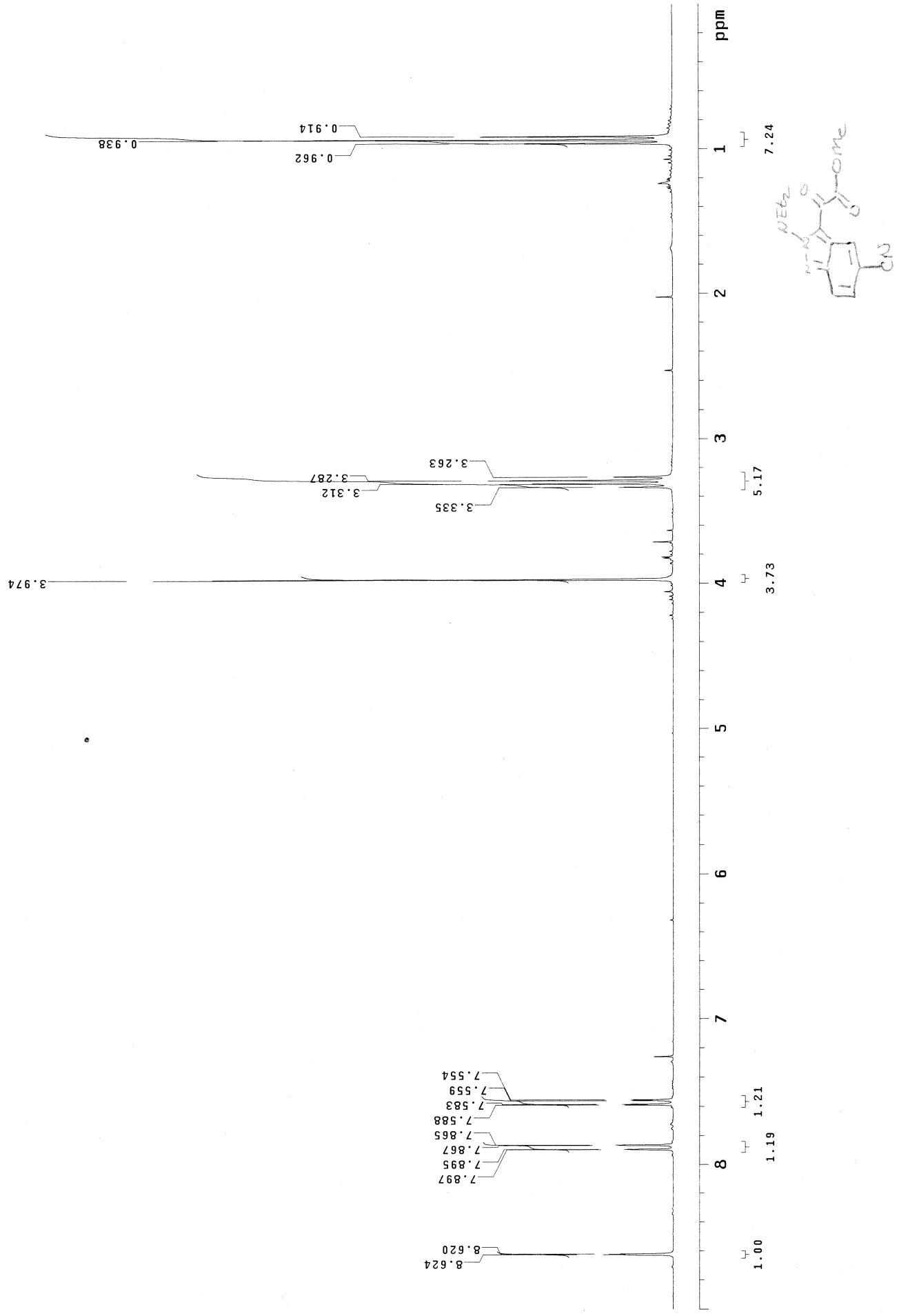
9b


ppm
8.557
8.555
7.928
7.898
7.638
7.632
7.608
7.603
7.260
3.980
3.347
3.344
3.322
3.319
3.296
3.273
0.971
0.923
0.946
1.00
1.13
1.16
3.45
4.72
6.64

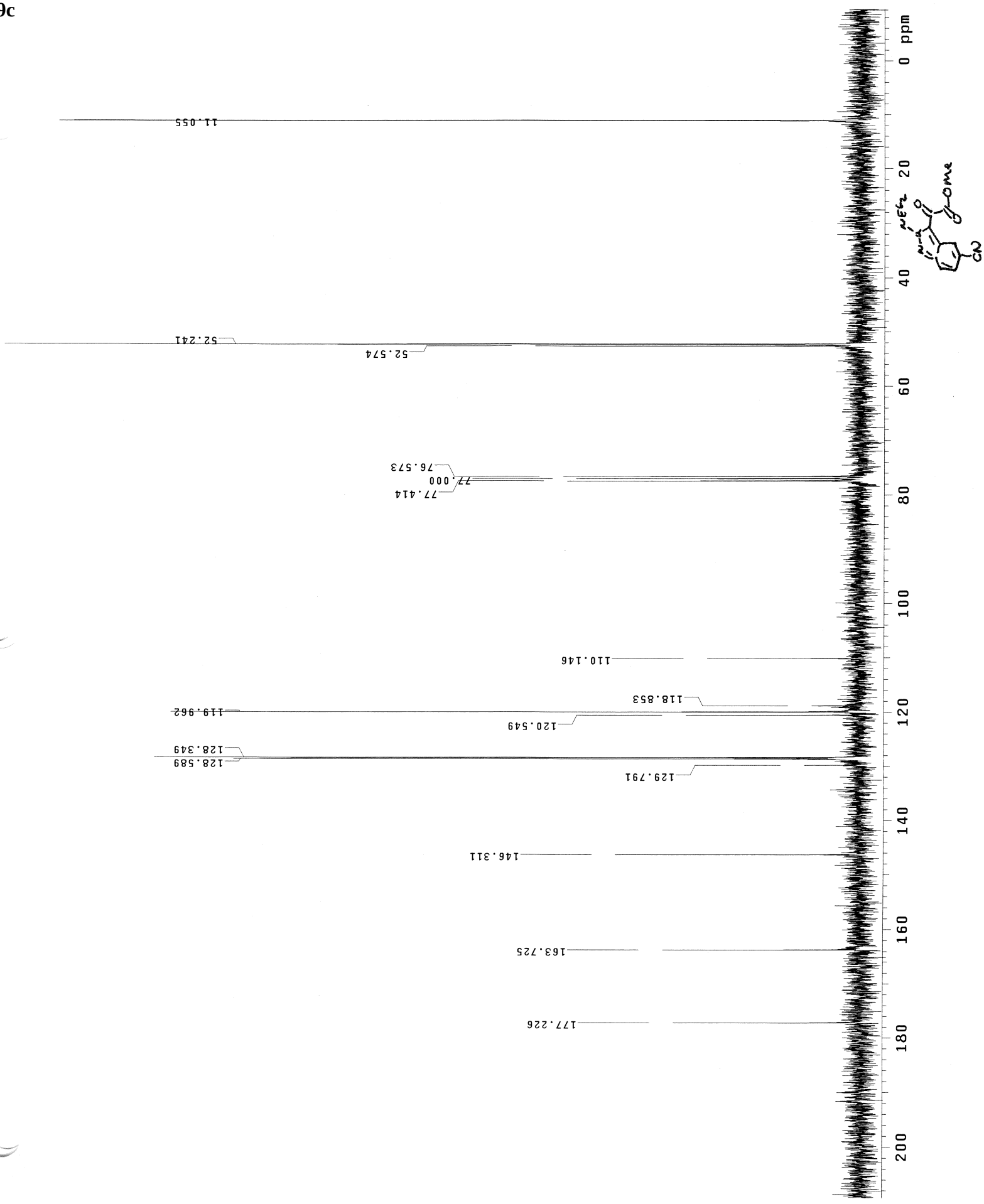
9b


177.413
164.019
146.711
128.963
128.536
123.621
123.581
120.389
120.122
120.055
119.615
77.427
77.000
76.573
52.534
52.254
11.095
0 ppm
20
40
60
80
100
120
140
160
180
200

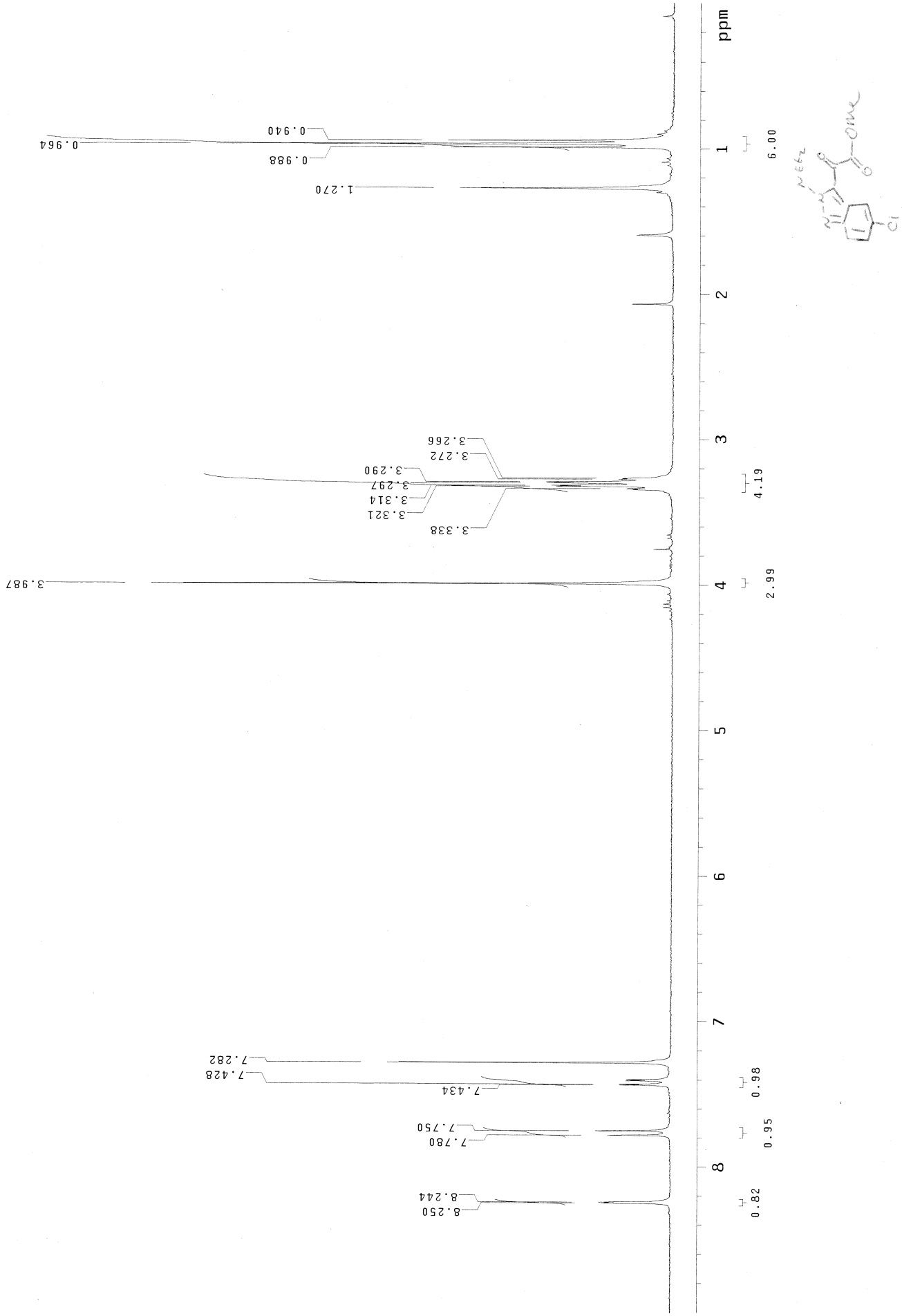
9c


ppm
1
2
3
4
5
6
7
8
7.24
5.17
3.73
1.21
1.19
1.00
0.914
0.938
0.962
3.263
3.287
3.312
3.335
3.974
7.554
7.559
7.583
7.588
7.865
7.867
7.895
7.897
8.620
8.624

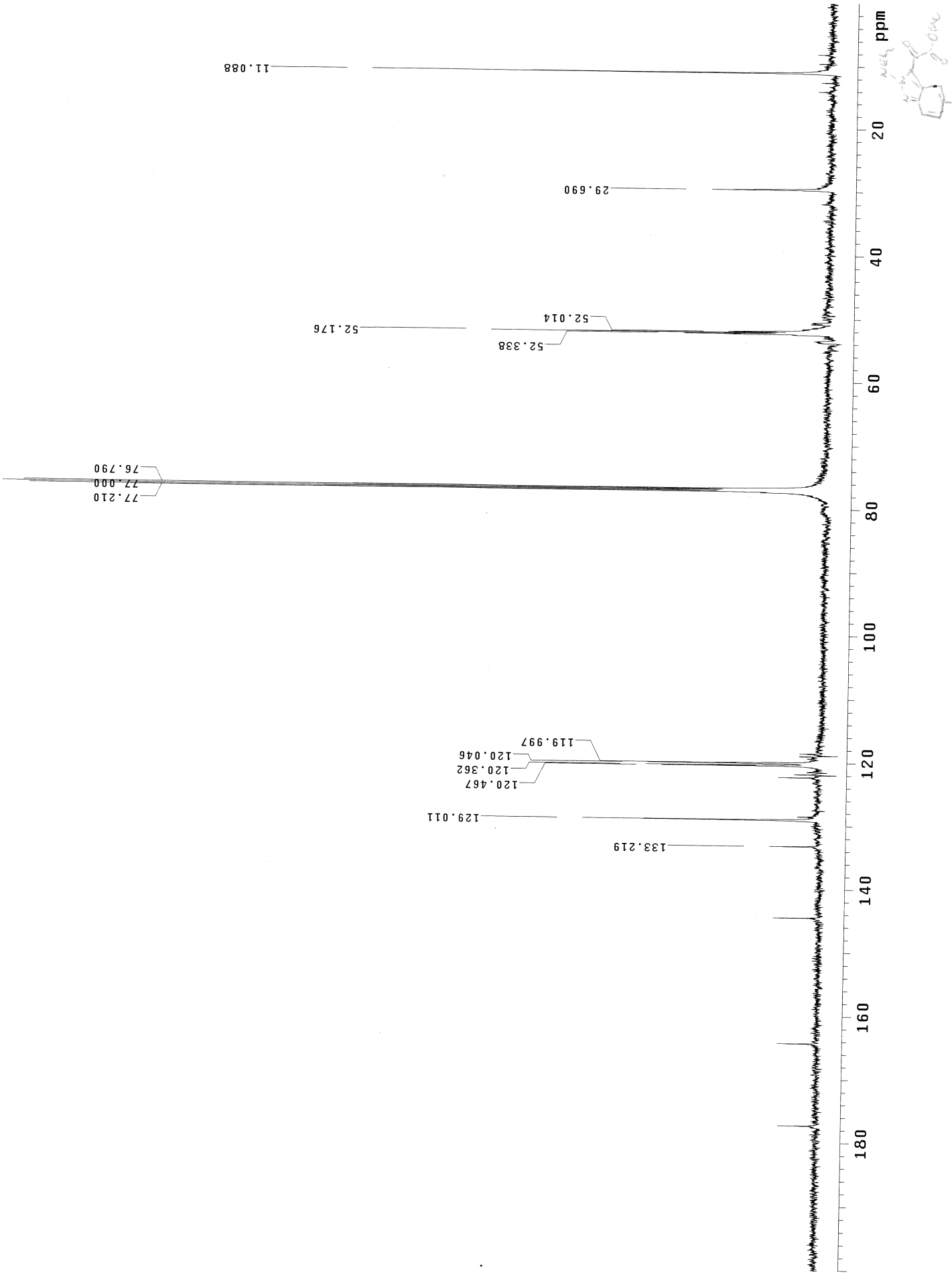
9c


177.226
163.725
146.311
129.791
128.589
128.349
120.549
119.962
118.853
110.146
77.414
77.000
76.573
52.574
52.241
11.055
0 ppm
20
40
60
80
100
120
140
160
180
200
OMe
Me
CN

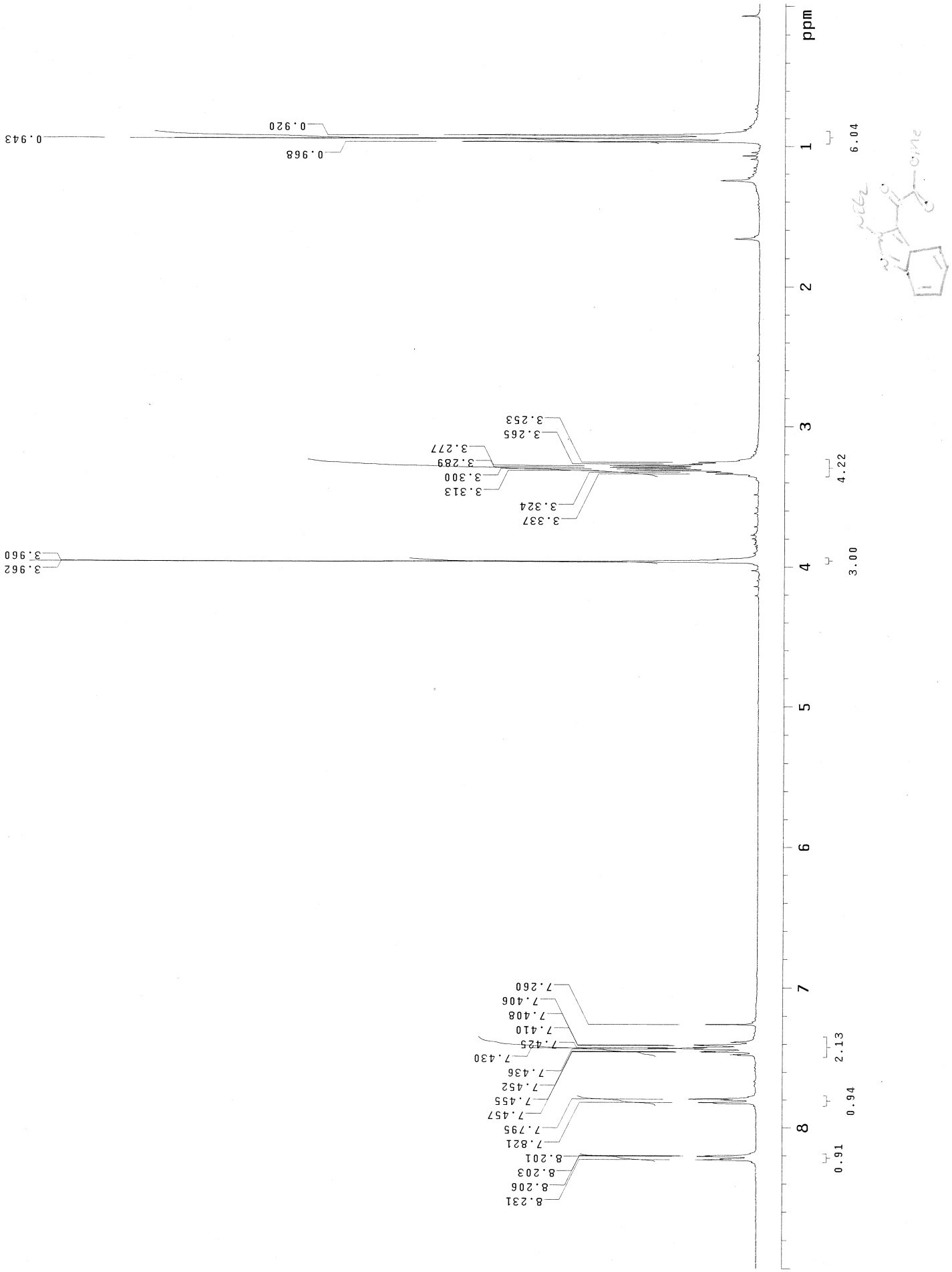
9d


8.250
8.244
7.780
7.750
7.434
7.428
7.282
3.987
3.338
3.321
3.314
3.297
3.290
3.272
3.266
1.270
0.988
0.940
0.964
ppm
0.82
0.95
0.98
2.99
4.19
6.00

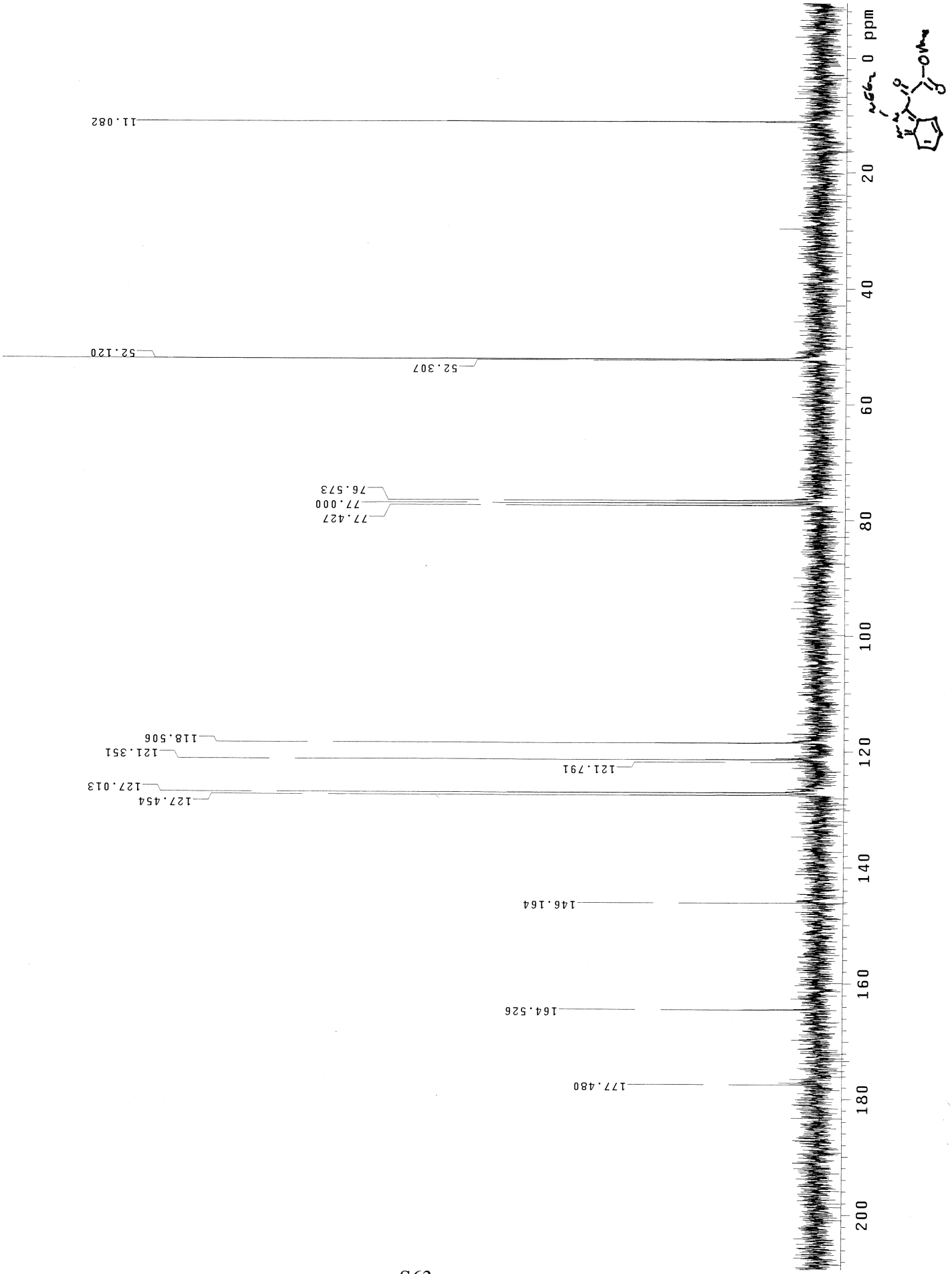
9d


11.088
29.690
52.014
52.176
52.338
76.790
77.000
77.210
119.997
120.046
120.362
120.467
129.011
133.219
ppm
20
40
60
80
100
120
140
160
180

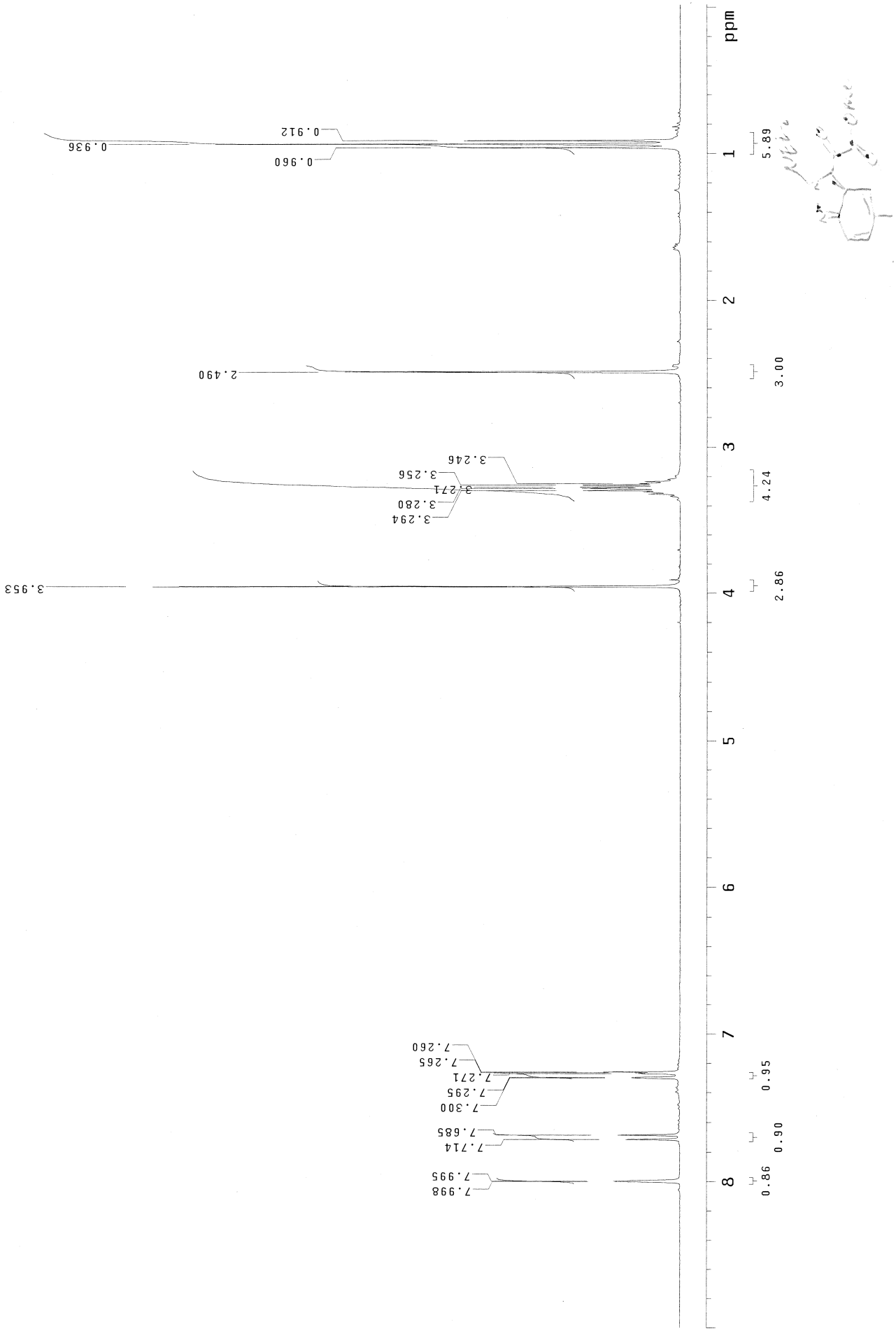
9e


0.943
0.920
0.968
3.962
3.960
3.337
3.324
3.313
3.300
3.289
3.277
3.265
3.253
8.231
8.206
8.203
8.201
7.821
7.795
7.457
7.455
7.452
7.436
7.430
7.425
7.410
7.408
7.406
7.260
ppm
6.04
4.22
3.00
2.13
0.94
0.91

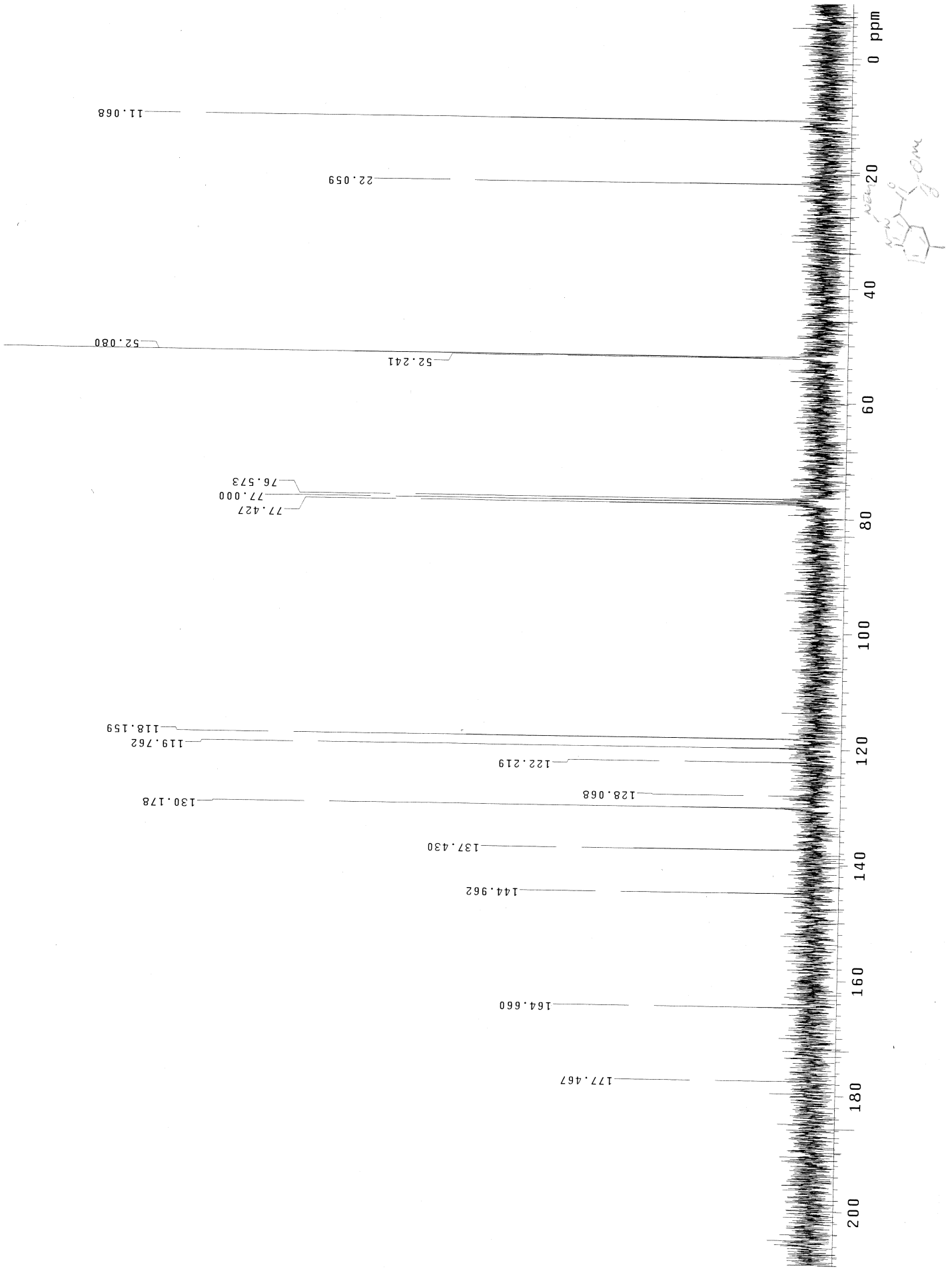
9e


177.480
164.526
146.164
127.454
127.013
121.791
121.351
118.506
77.427
77.000
76.573
52.307
52.120
11.082
0 ppm

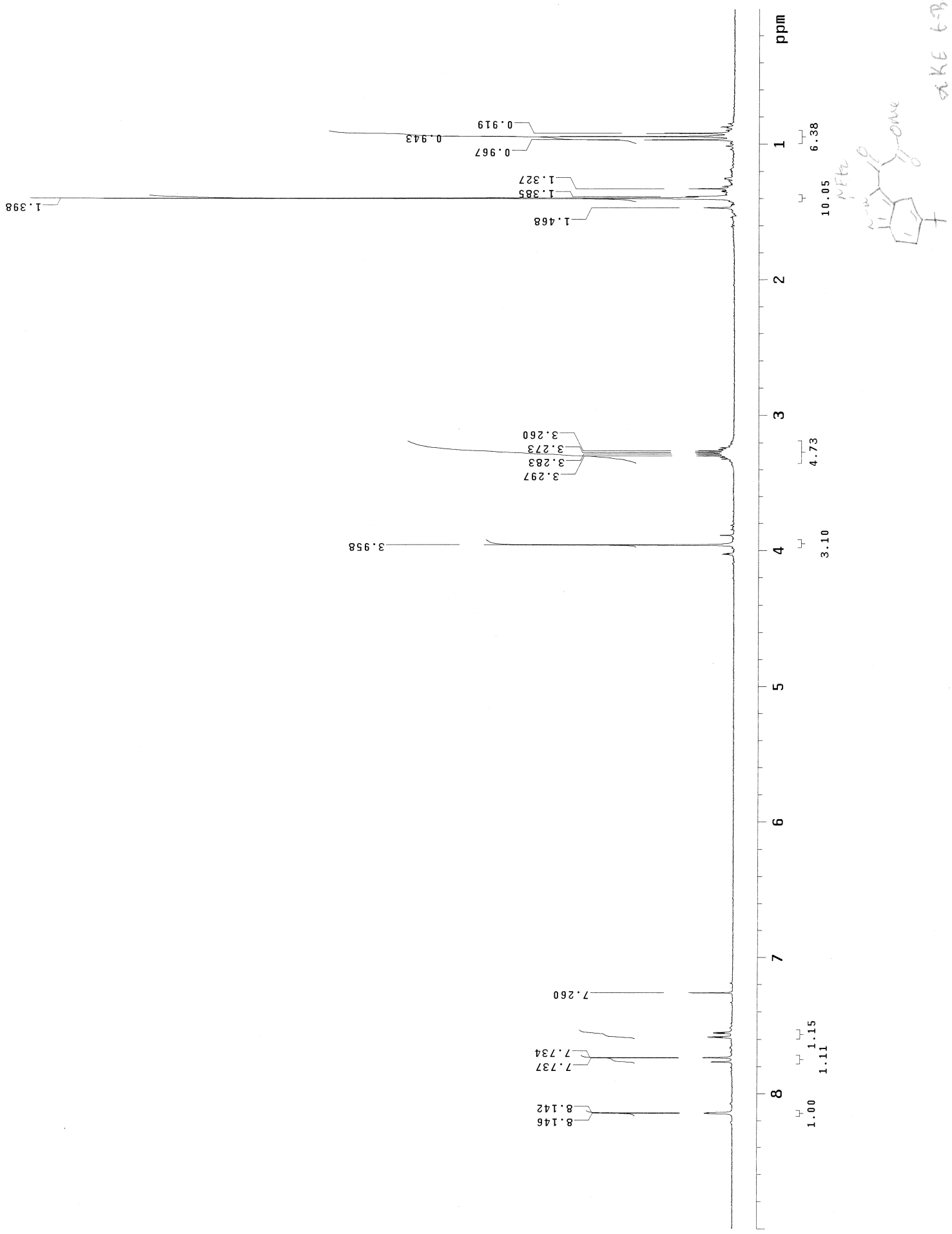
9f


ppm
1
2
3
4
5
6
7
8
5.89
3.00
4.24
2.86
0.95
0.90
0.86
0.912
0.936
0.960
2.490
3.246
3.256
3.271
3.280
3.294
3.953
7.260
7.265
7.271
7.295
7.300
7.685
7.714
7.995
7.998

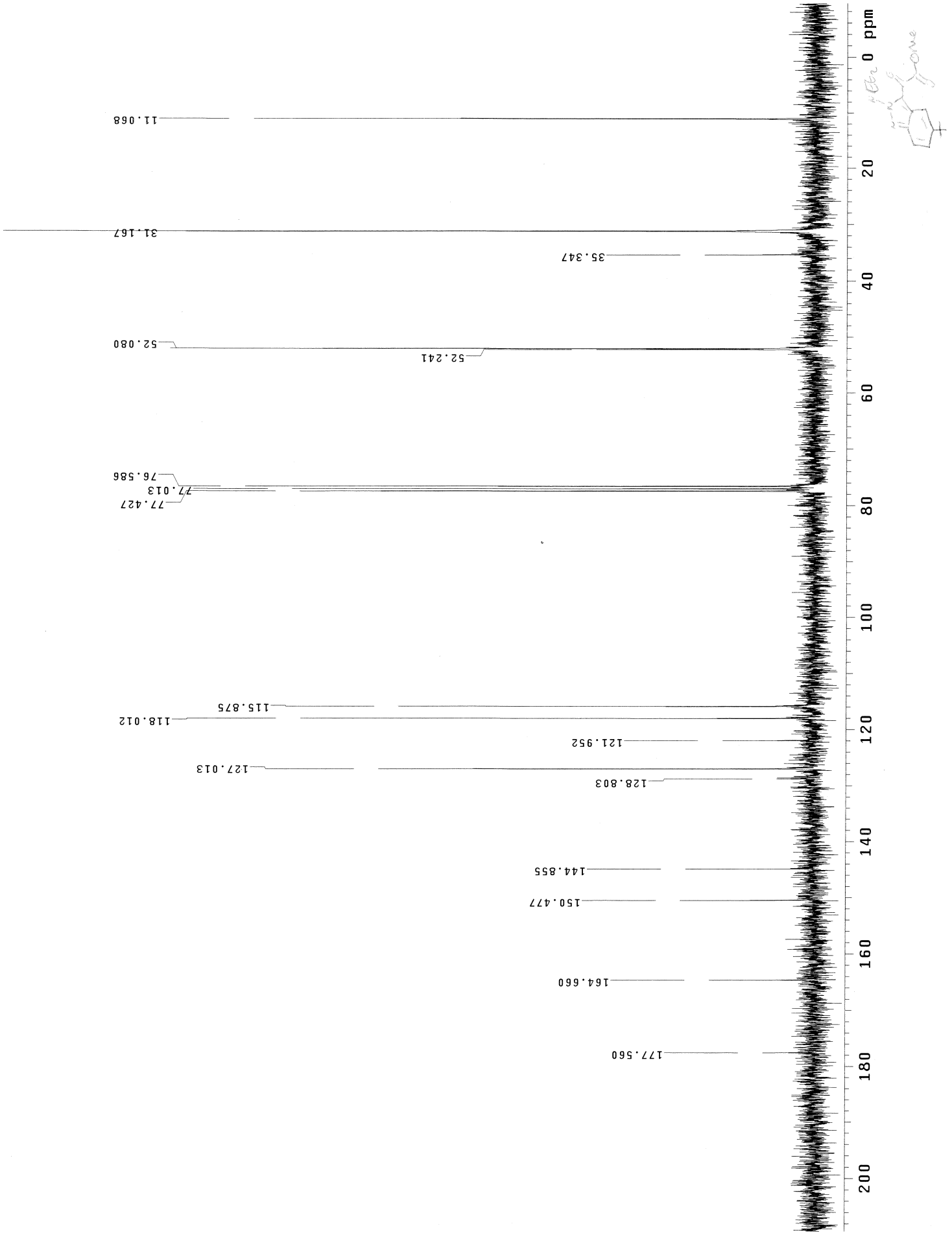
9f


177.467
164.660
144.962
137.430
130.178
128.068
122.219
119.762
118.159
77.427
77.000
76.573
52.241
52.080
22.059
11.068
0 ppm
20
40
60
80
100
120
140
160
180
200

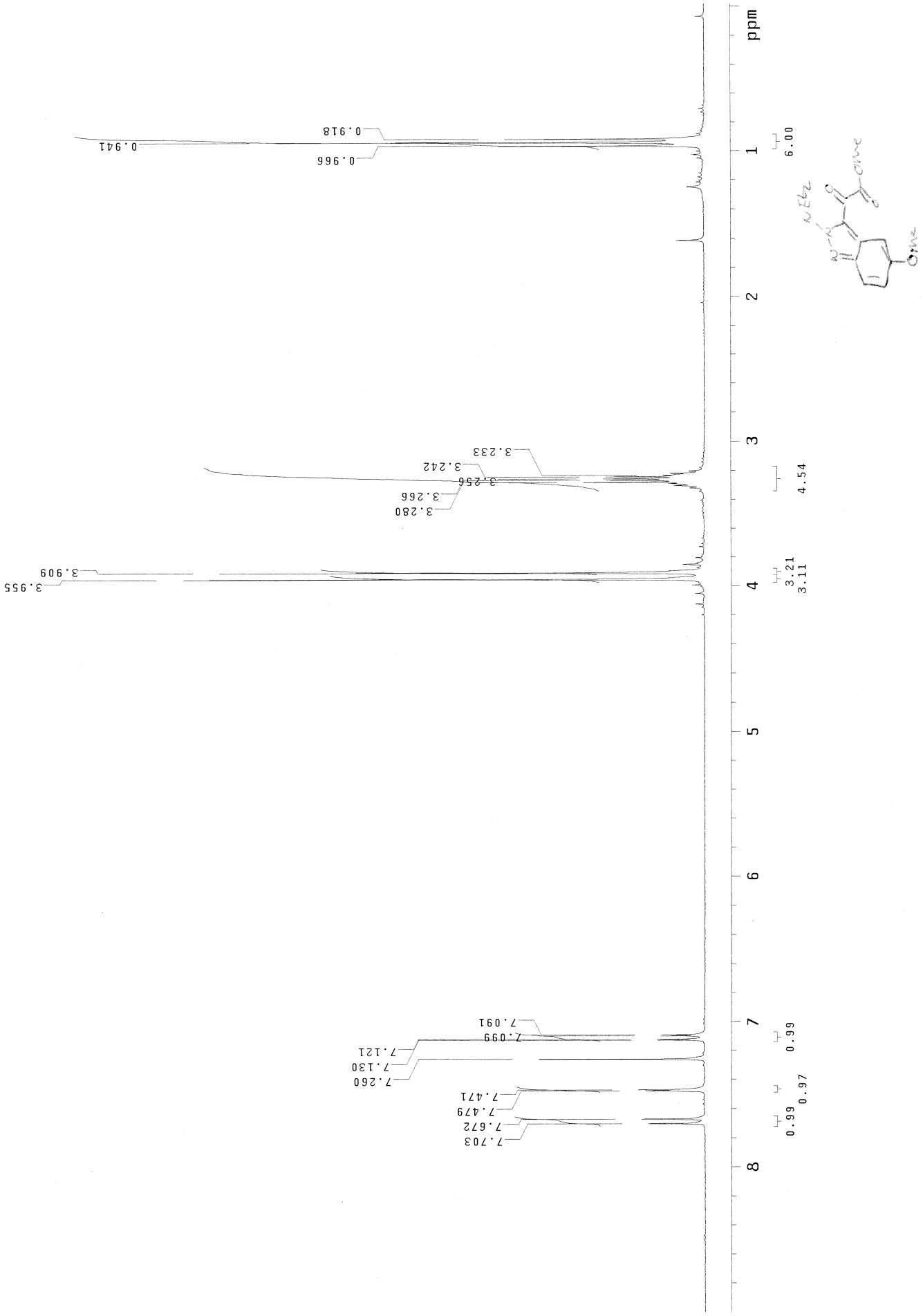
9g


ppm
1
2
3
4
5
6
7
8
6.38
10.05
4.73
3.10
1.15
1.11
1.00
0.919
0.943
0.967
1.327
1.385
1.398
1.468
3.260
3.273
3.283
3.297
3.958
7.260
7.734
7.737
8.142
8.146

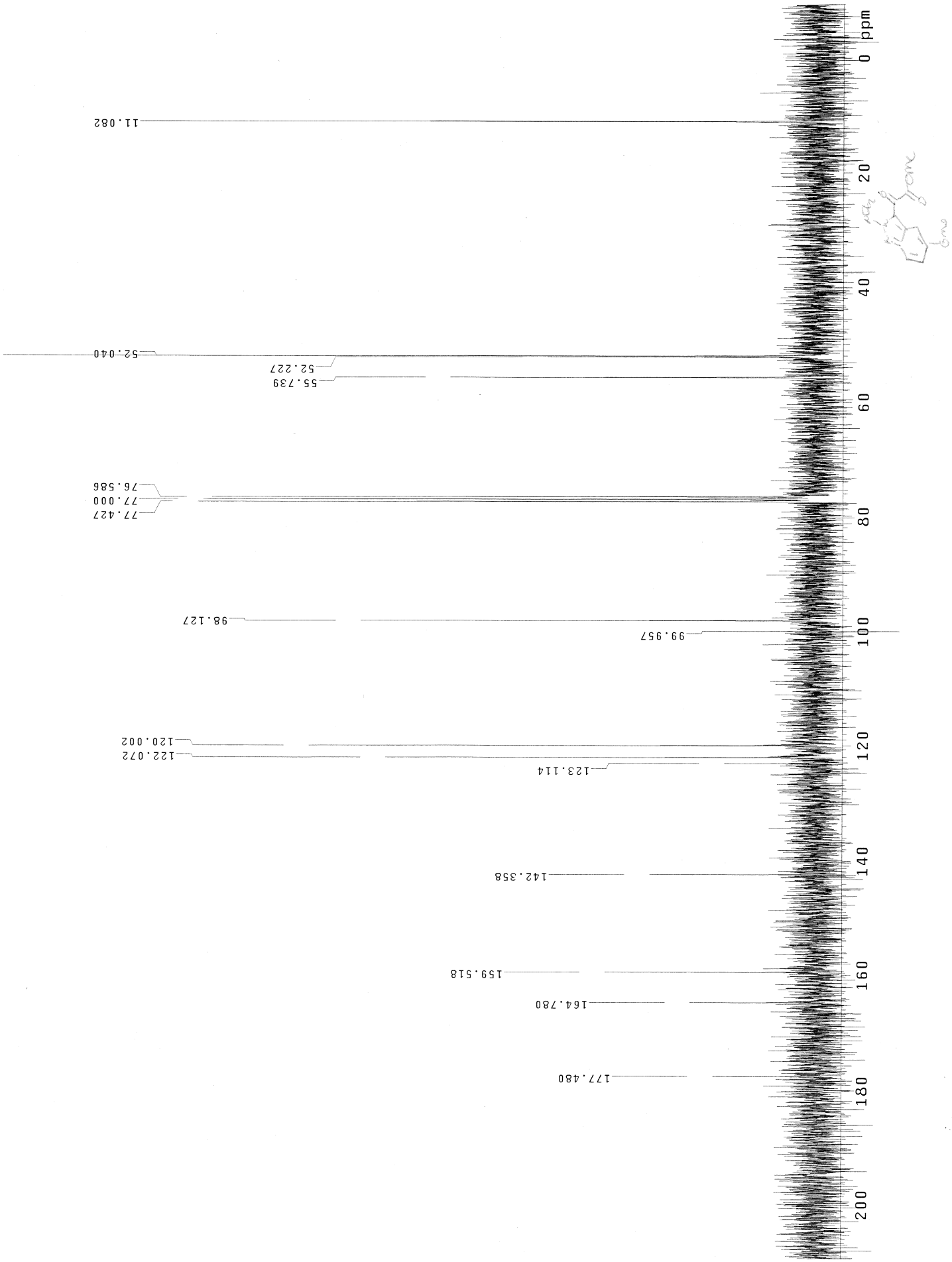
9g


177.560
164.660
150.477
144.855
128.803
127.013
121.952
118.012
115.875
77.427
77.013
76.586
52.241
52.080
35.347
31.167
11.068
0 ppm
20
40
60
80
100
120
140
160
180
200

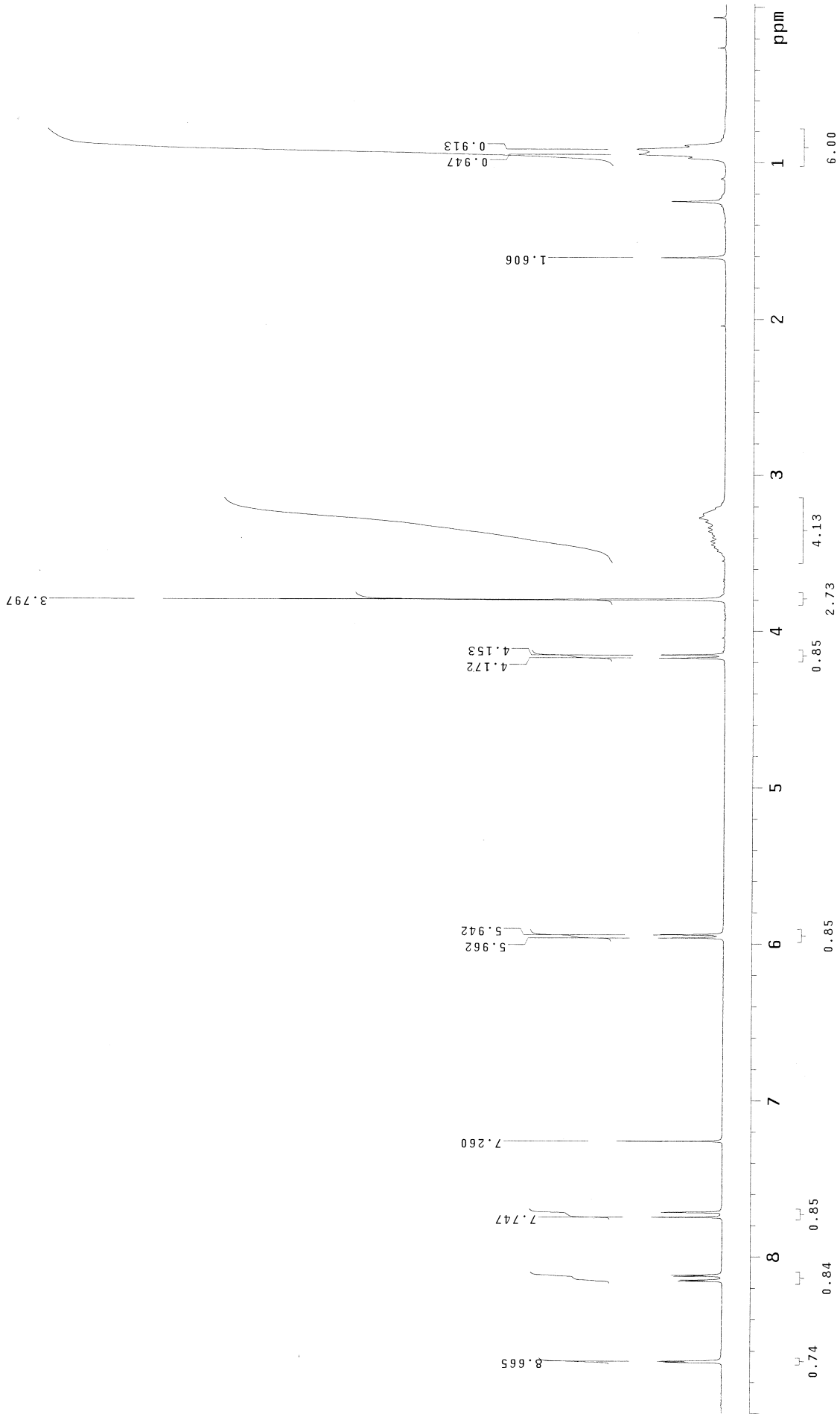
9h


0.918
0.941
0.966
3.233
3.242
3.256
3.266
3.280
3.909
3.955
7.091
7.099
7.121
7.130
7.260
7.471
7.479
7.672
7.703
ppm
1
2
3
4
5
6
7
8
6.00
4.54
3.21
3.11
0.99
0.97
0.99

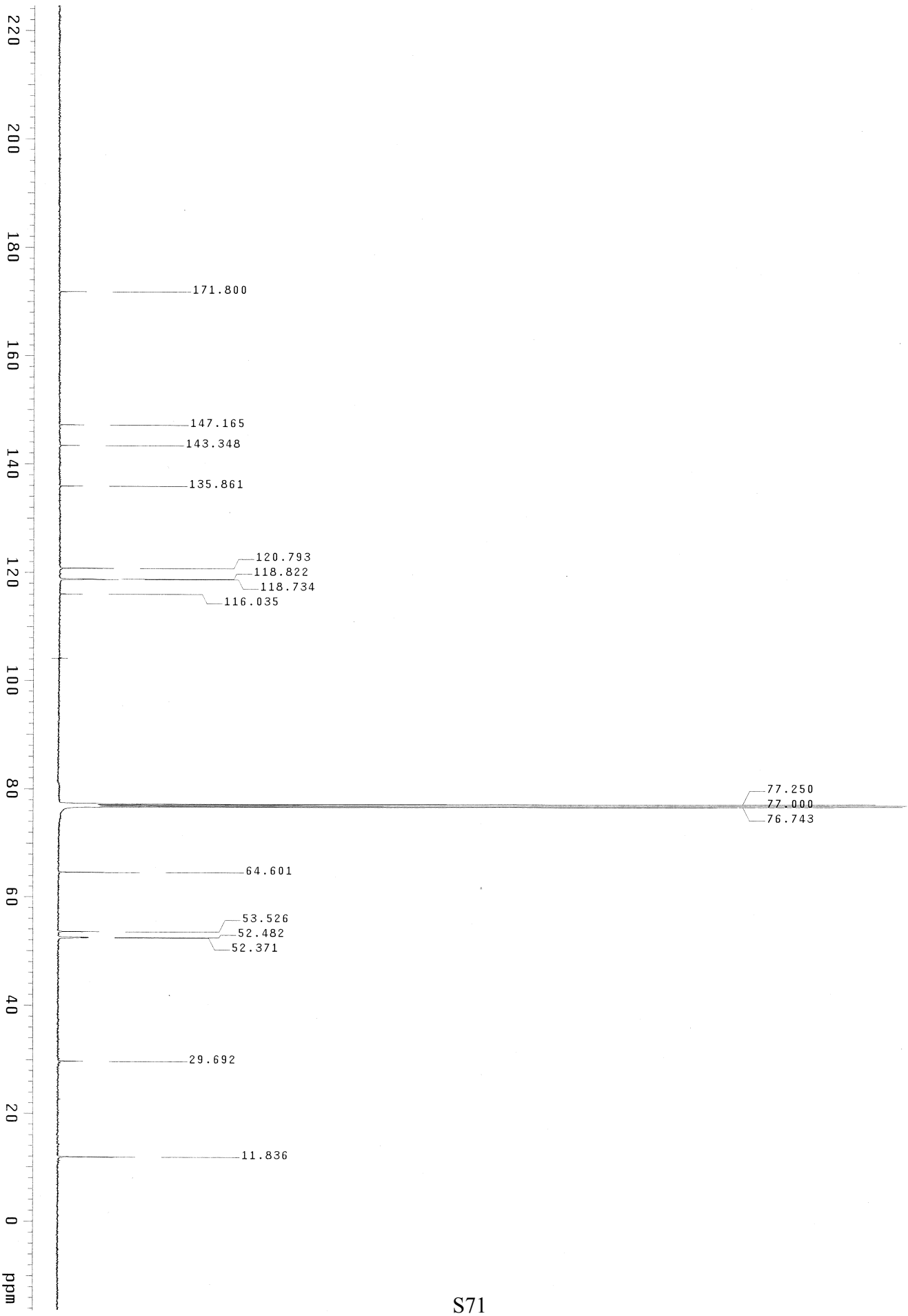
9h


11.082
52.040
52.227
55.739
76.586
77.000
77.427
98.127
99.957
120.002
122.072
123.114
142.358
159.518
164.780
177.480
ppm

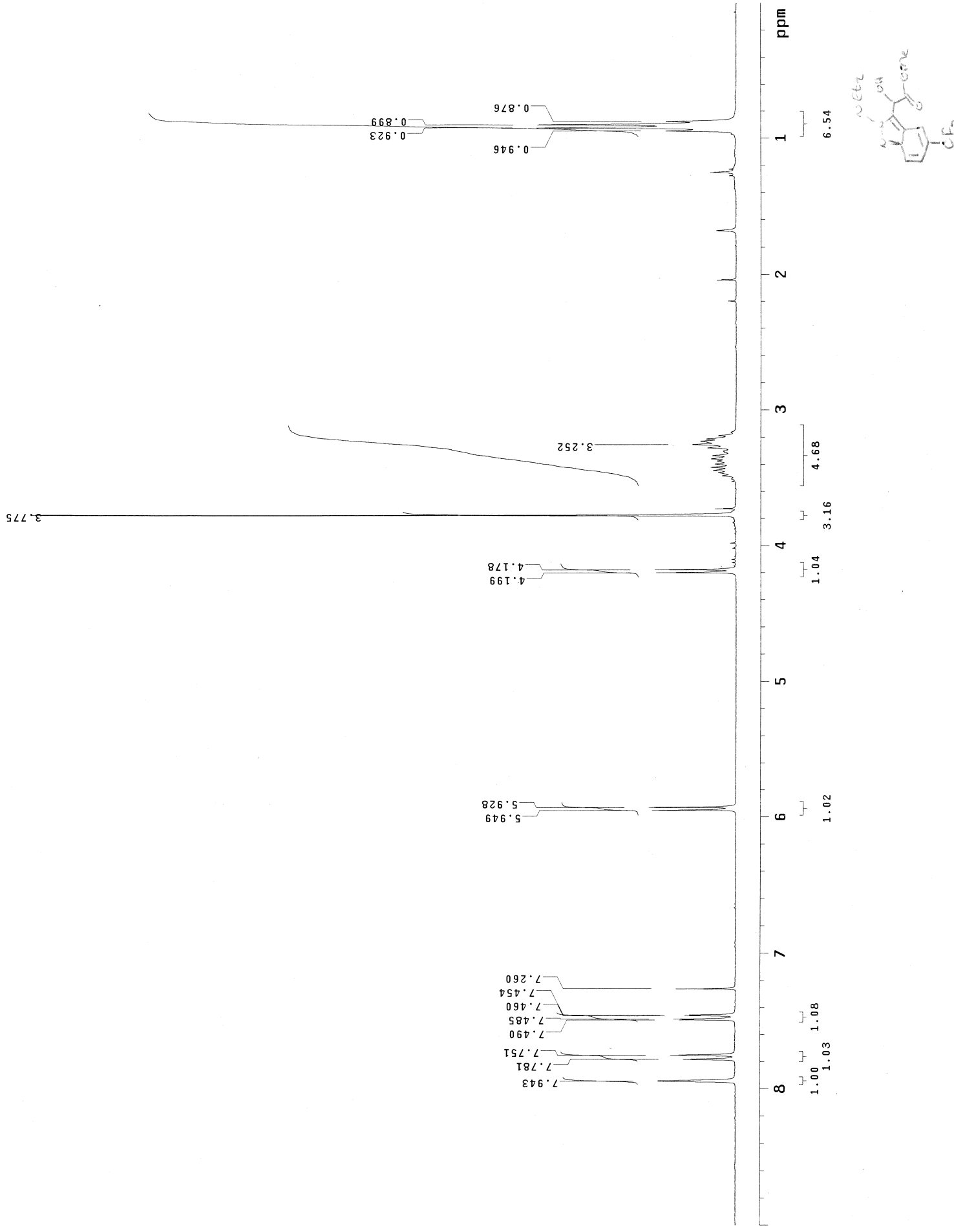
10a


ppm
1
2
3
4
5
6
7
8
0.913
0.947
1.606
3.797
4.153
4.172
5.942
5.962
7.260
7.747
8.665
6.00
4.13
2.73
0.85
0.85
0.85
0.84
0.74

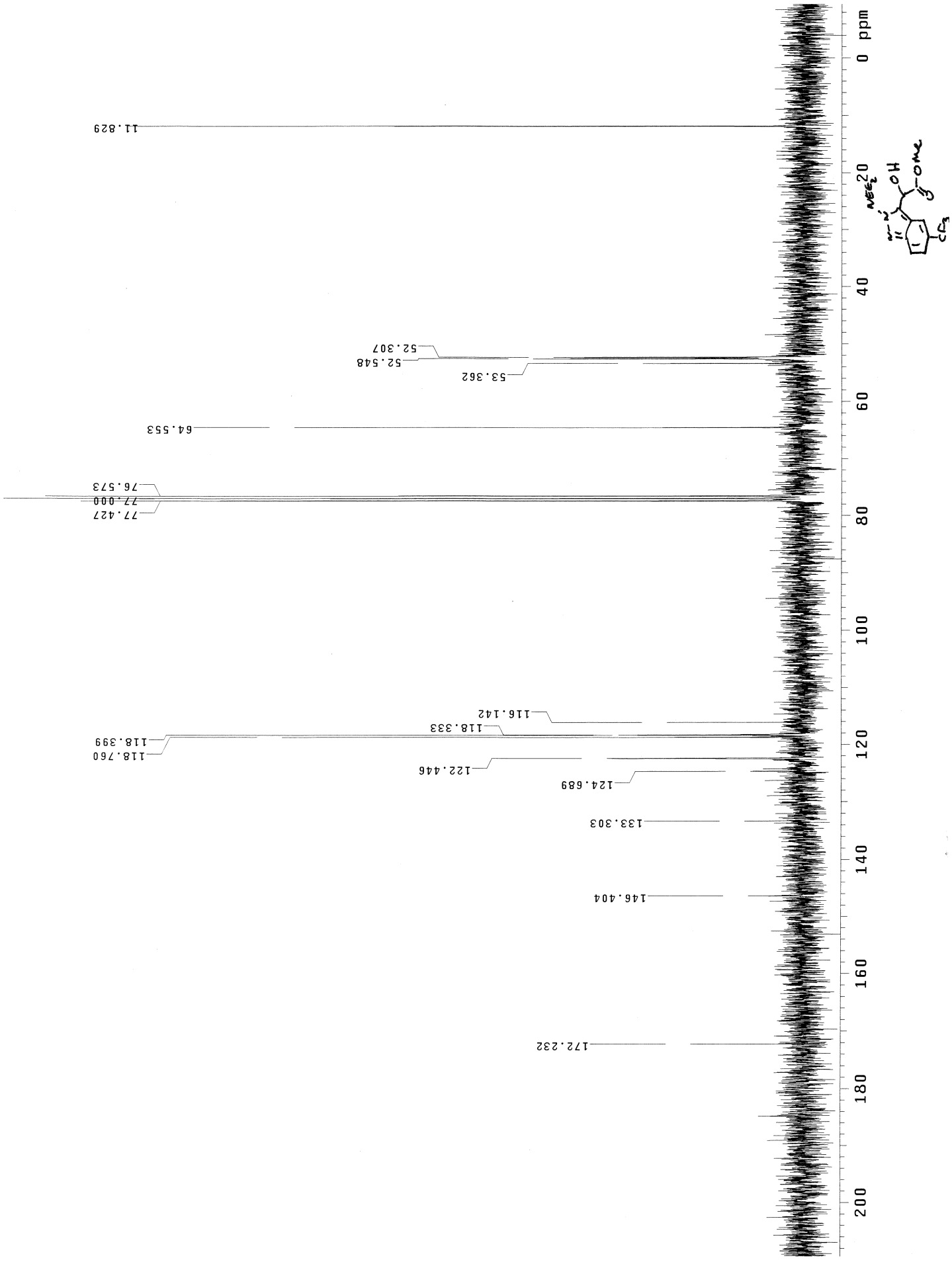
10a


220
200
180
160
140
120
100
80
60
40
20
0
ppm
171.800
147.165
143.348
135.861
120.793
118.822
118.734
116.035
77.250
77.000
76.743
64.601
53.526
52.482
52.371
29.692
11.836

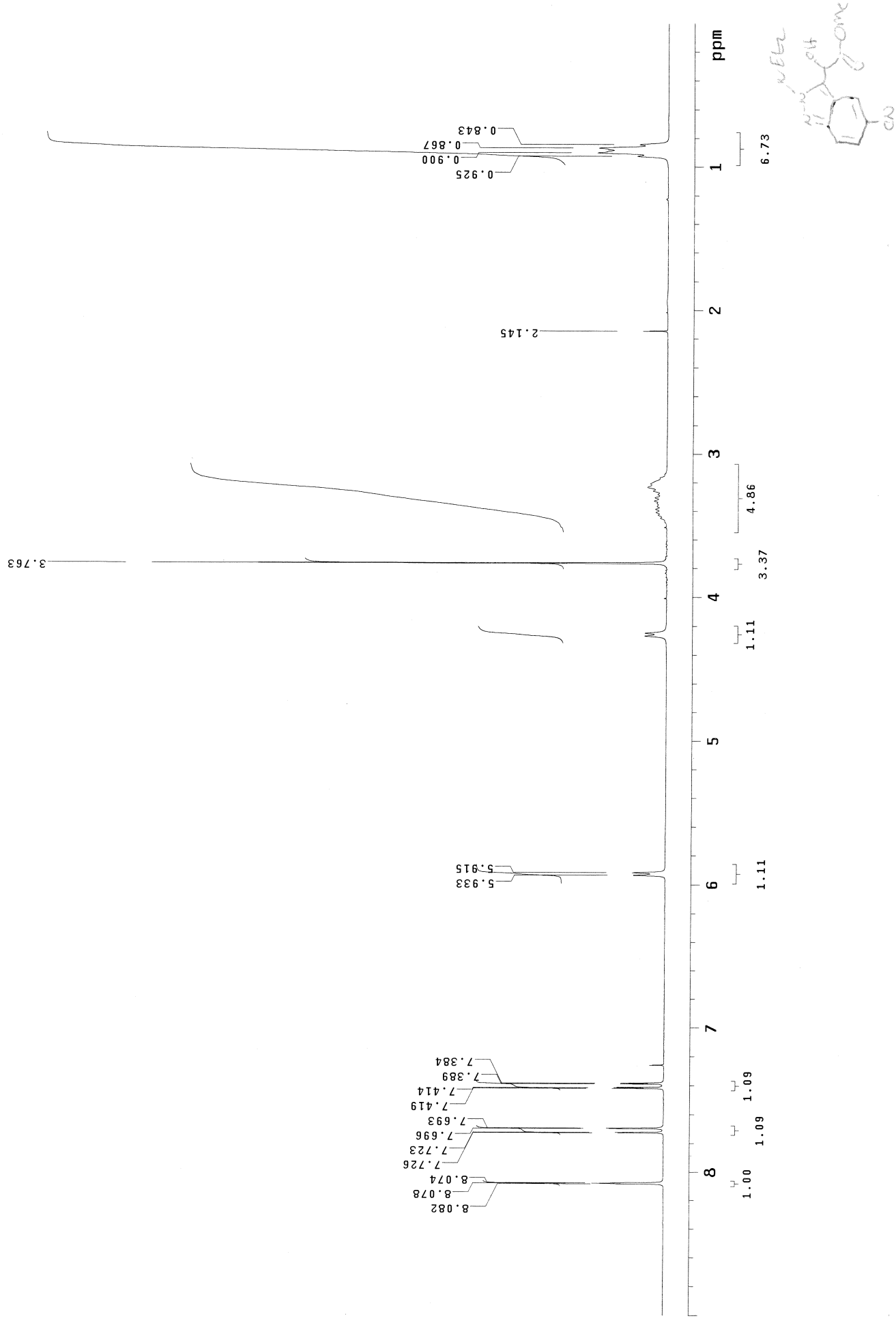
10b


ppm
1
2
3
4
5
6
7
8
6.54
4.68
3.16
1.04
1.02
1.08
1.03
1.00
0.876
0.923
0.899
0.946
3.252
3.775
4.178
4.199
5.928
5.949
7.260
7.454
7.460
7.485
7.490
7.751
7.781
7.943

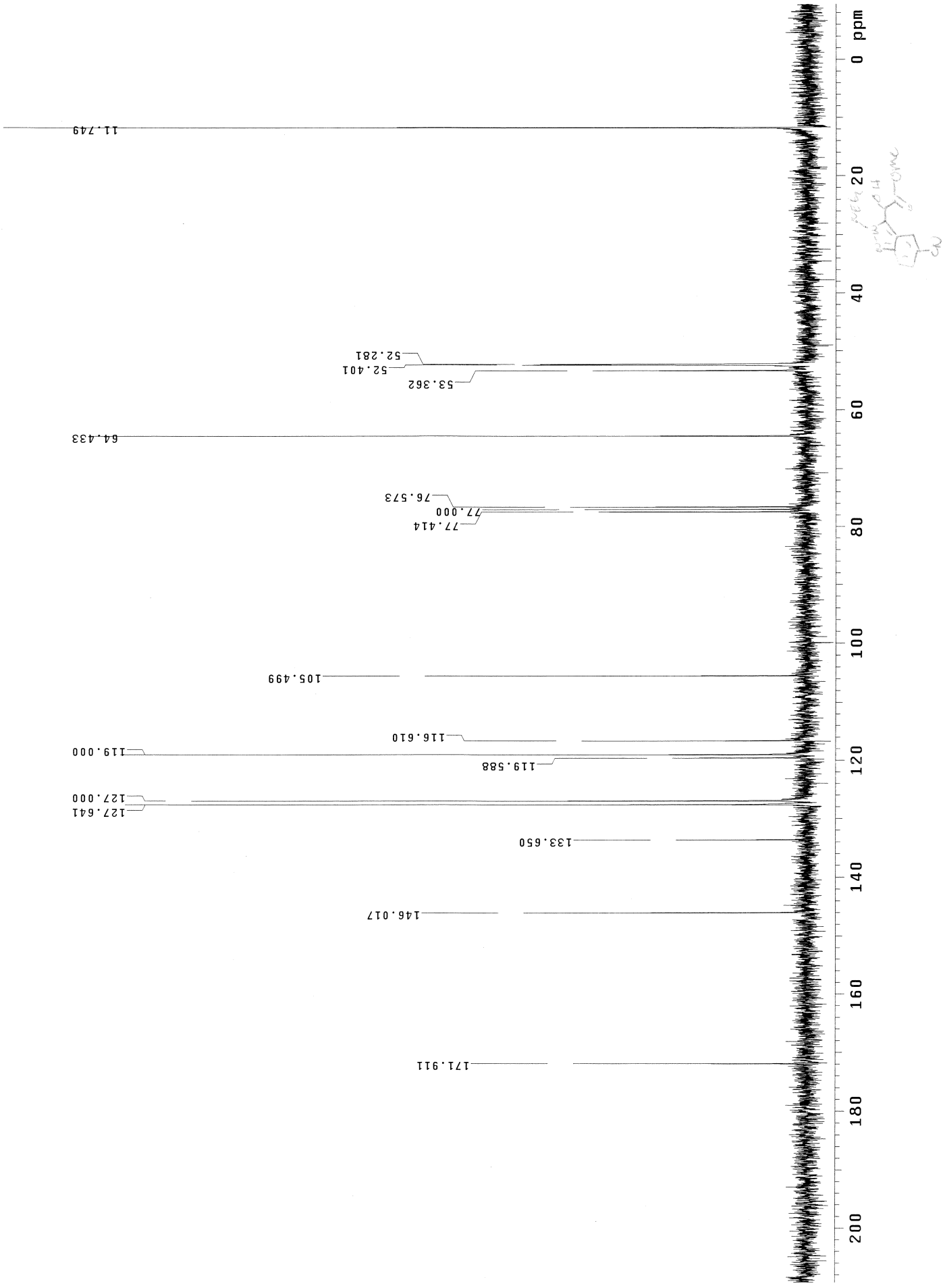
10b


11.829
52.307
52.548
53.362
64.553
76.573
77.000
77.427
116.142
118.333
118.399
118.760
122.446
124.689
133.303
146.404
172.232
0 ppm
20
40
60
80
100
120
140
160
180
200

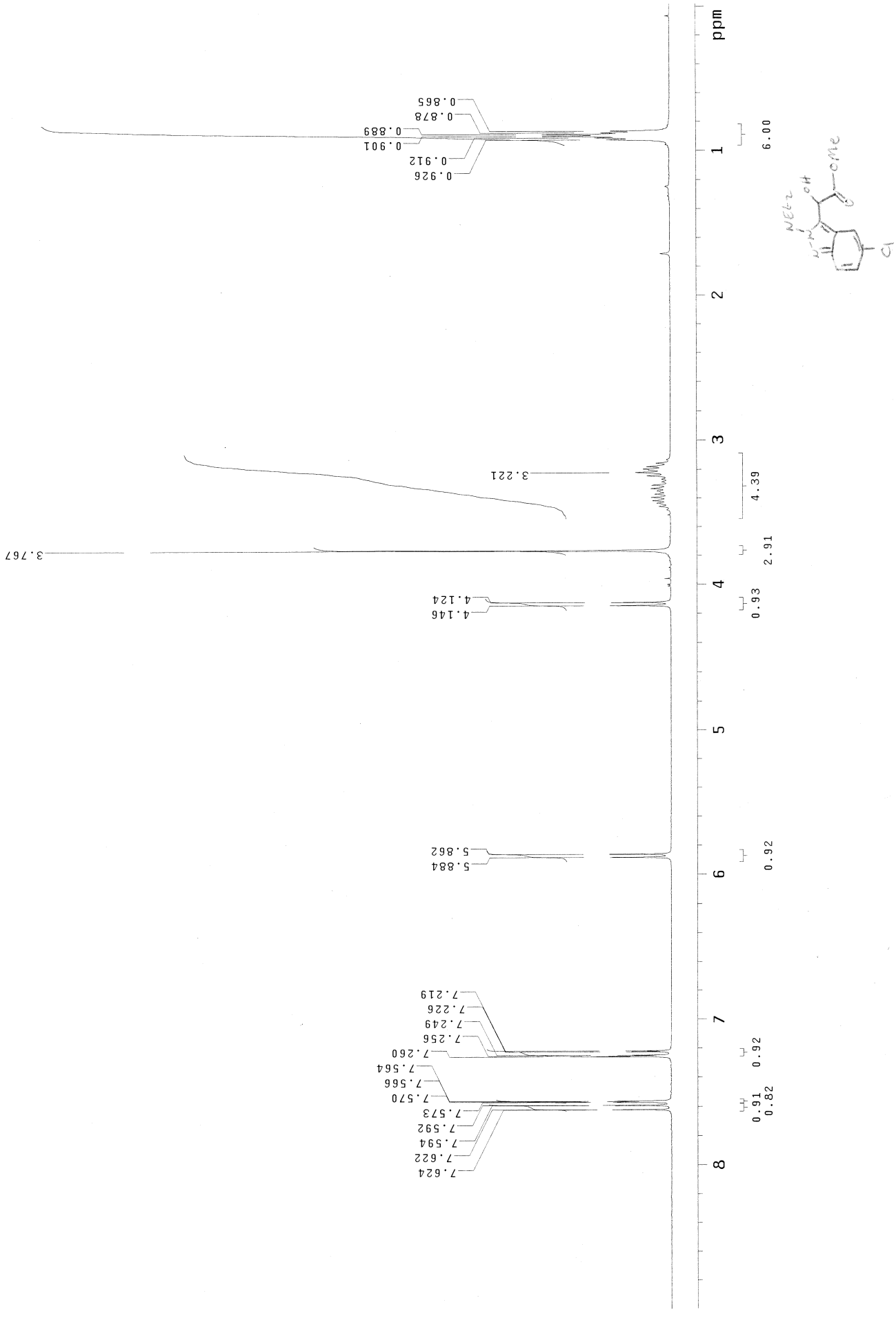
10c


0.843
0.867
0.900
0.925
2.145
3.763
5.915
5.933
7.384
7.389
7.414
7.419
7.693
7.696
7.723
7.726
8.074
8.078
8.082
ppm
1
2
3
4
5
6
7
8
6.73
4.86
3.37
1.11
1.11
1.09
1.09
1.00

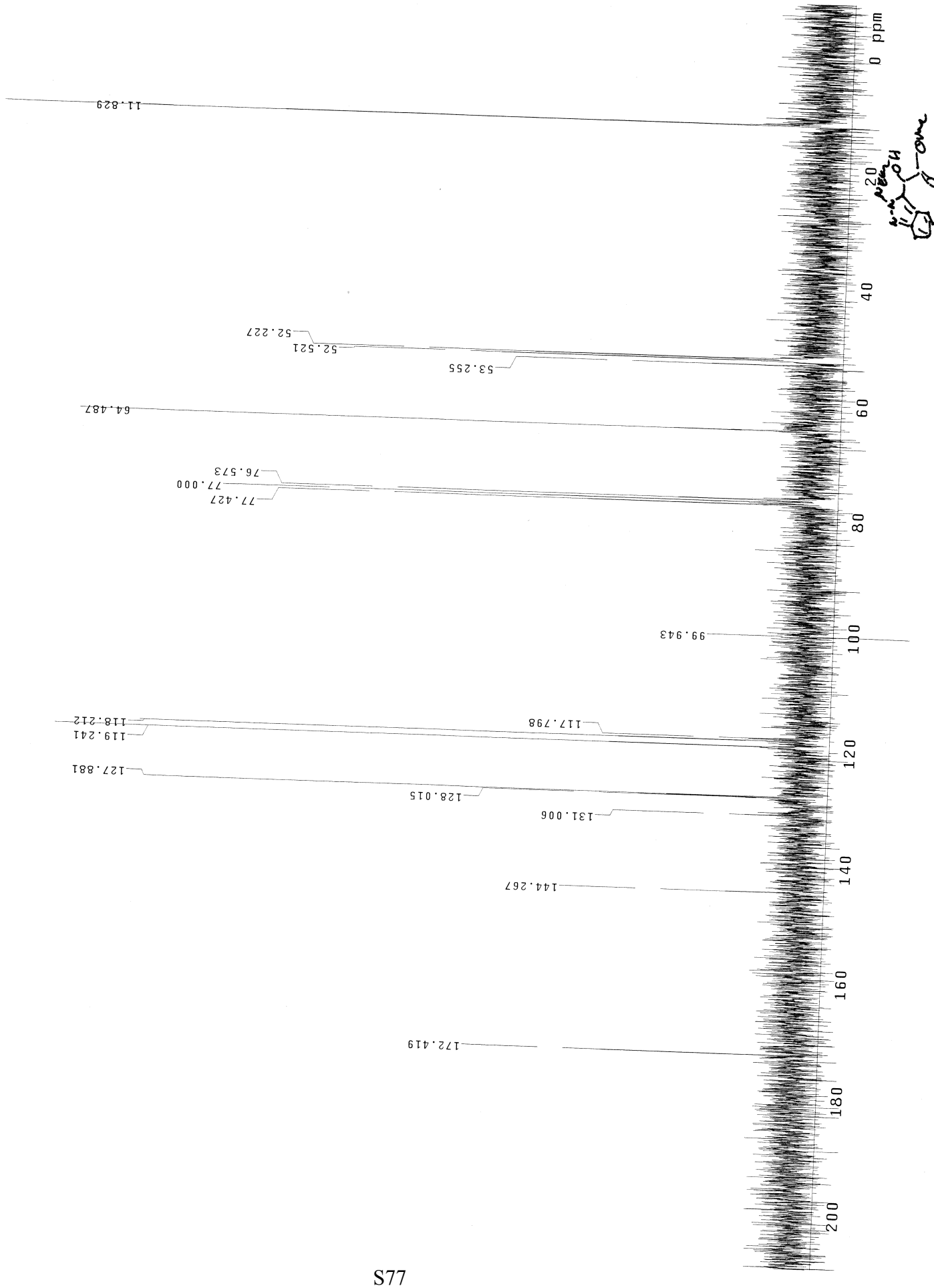
10c


11.749
52.281
52.401
53.362
64.433
76.573
77.000
77.414
105.499
116.610
119.000
119.588
127.000
127.641
133.650
146.017
171.911
0 ppm
20
40
60
80
100
120
140
160
180
200

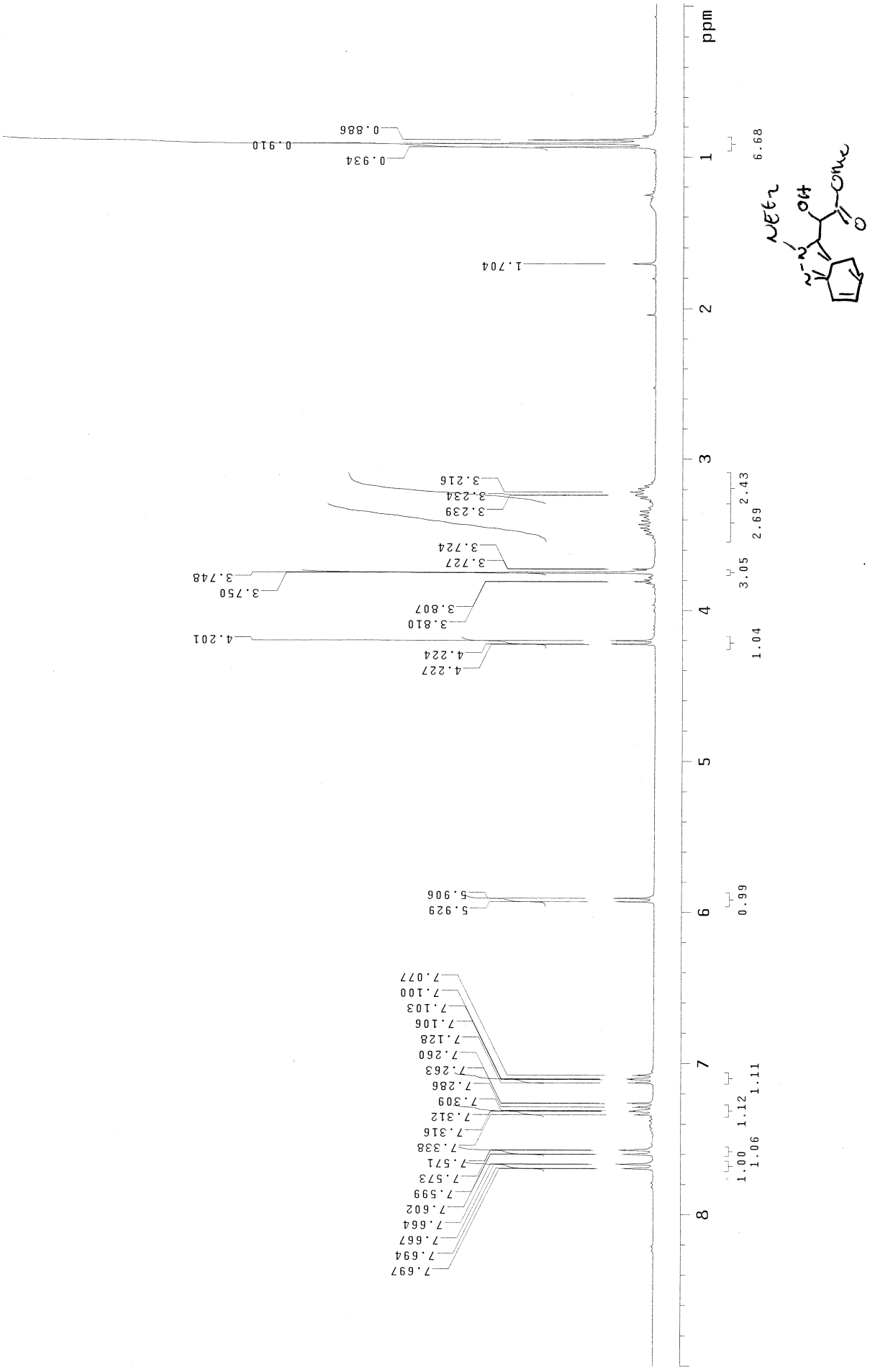
10d


ppm
0.865
0.878
0.889
0.901
0.912
0.926
3.221
3.767
4.124
4.146
5.862
5.884
7.219
7.226
7.249
7.256
7.260
7.564
7.566
7.570
7.573
7.592
7.594
7.622
7.624
6.00
4.39
2.91
0.93
0.92
0.92
0.91
0.82

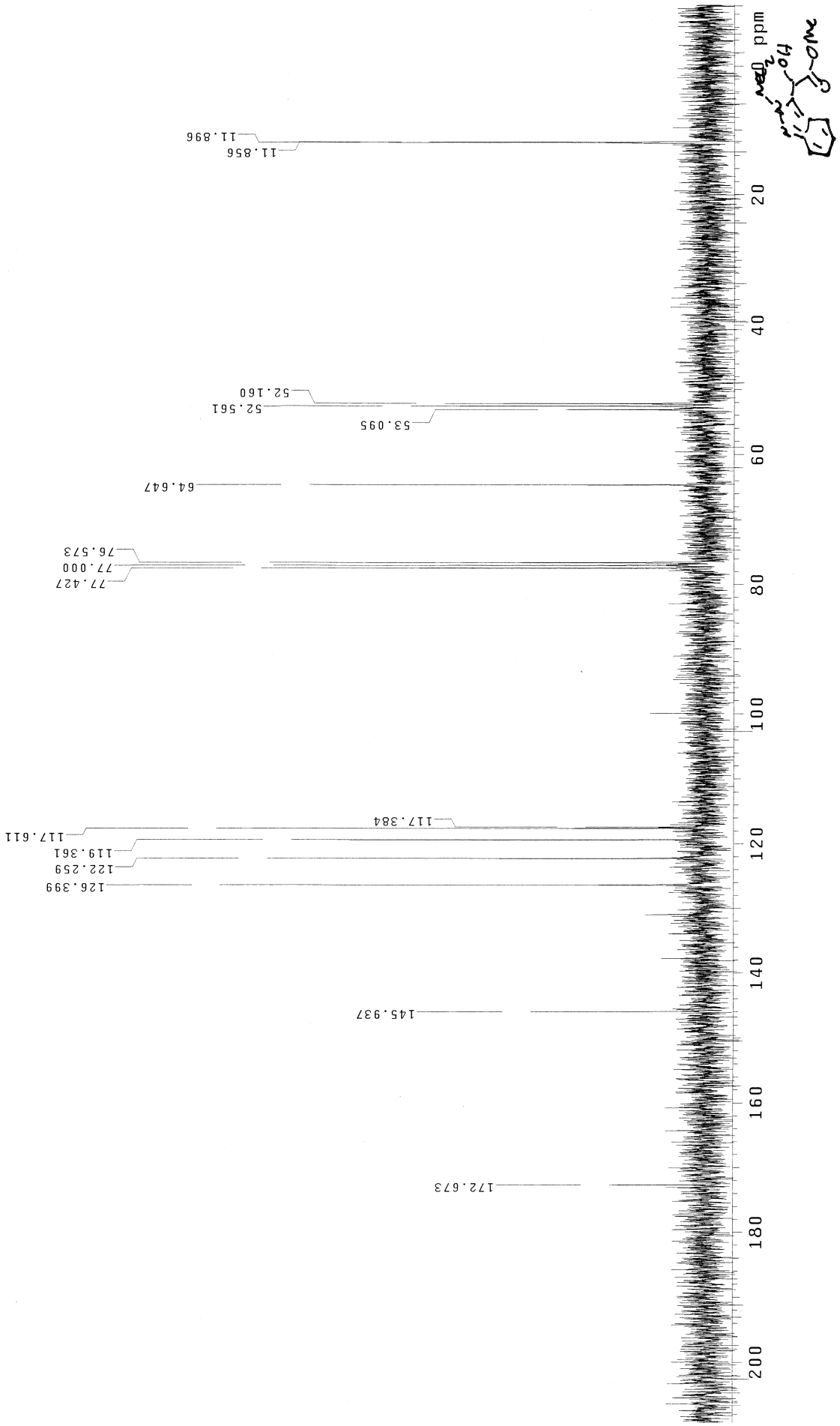
10d


11.829
52.227
52.521
53.255
64.487
76.573
77.000
77.427
99.943
117.798
118.212
119.241
127.881
128.015
131.006
144.267
172.419
0 ppm
20
40
60
80
100
120
140
160
180
200

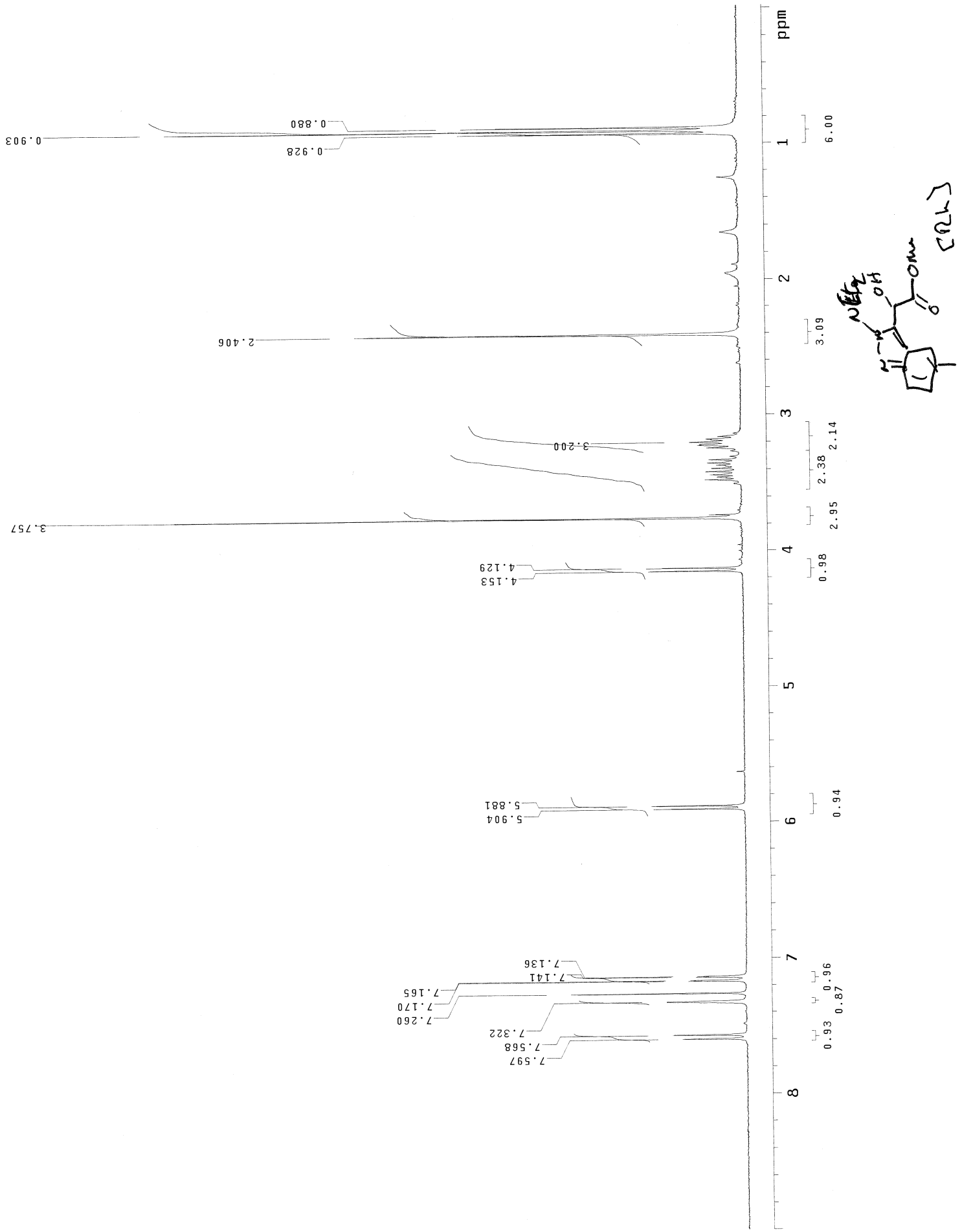
10e


0.886
0.910
0.934
1.704
3.216
3.234
3.239
3.724
3.727
3.748
3.750
3.807
3.810
4.201
4.224
4.227
5.906
5.929
7.077
7.100
7.103
7.106
7.128
7.260
7.263
7.286
7.309
7.312
7.316
7.338
7.571
7.573
7.599
7.602
7.664
7.667
7.694
7.697
ppm
1
2
3
4
5
6
7
8
6.68
2.43
2.69
3.05
1.04
0.99
1.00
1.06
1.12
1.11

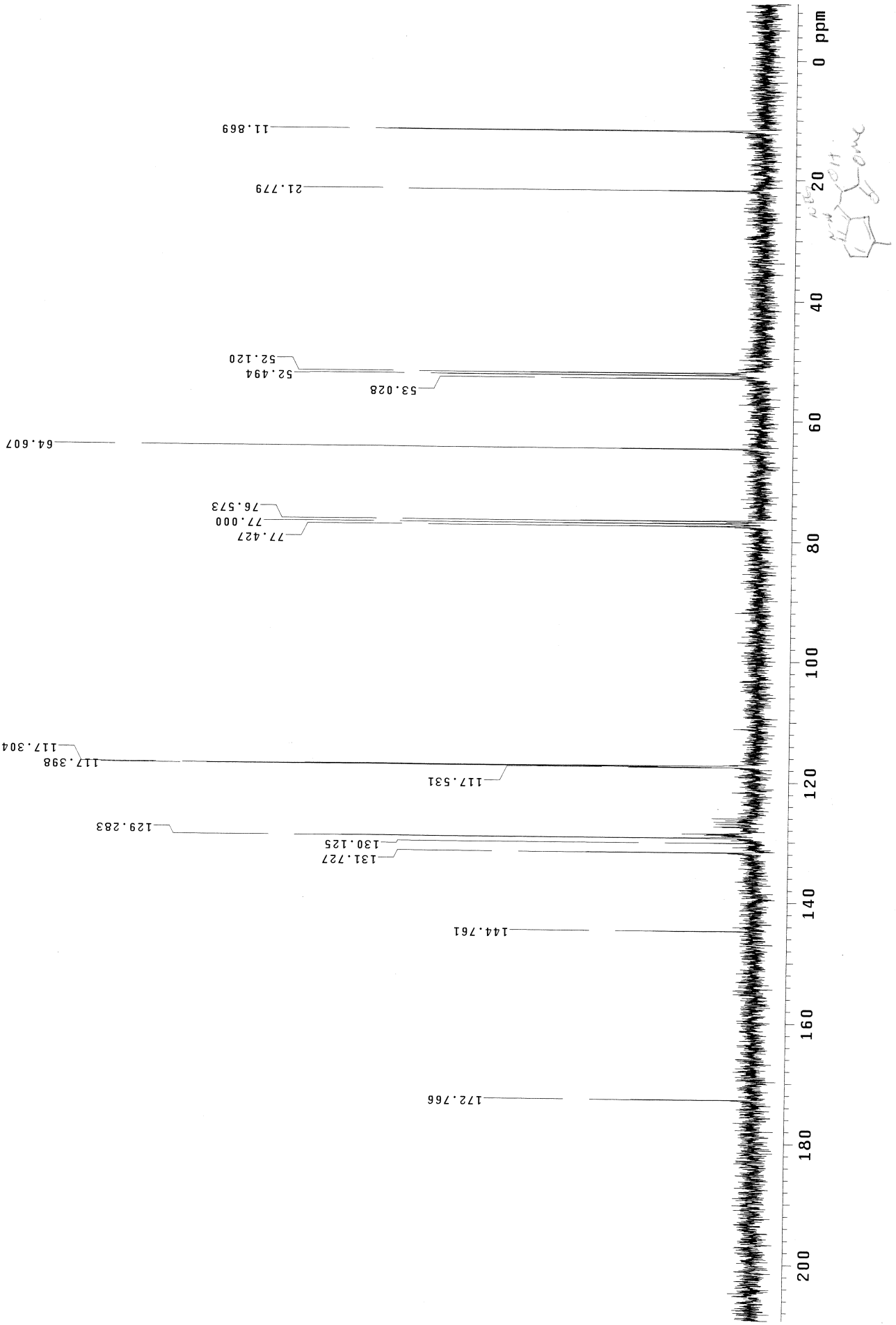
10e


11.896
11.856
52.160
52.561
53.095
64.647
76.573
77.000
77.427
117.384
117.611
119.361
122.259
126.399
145.937
172.673
ppm
20
40
60
80
100
120
140
160
180
200

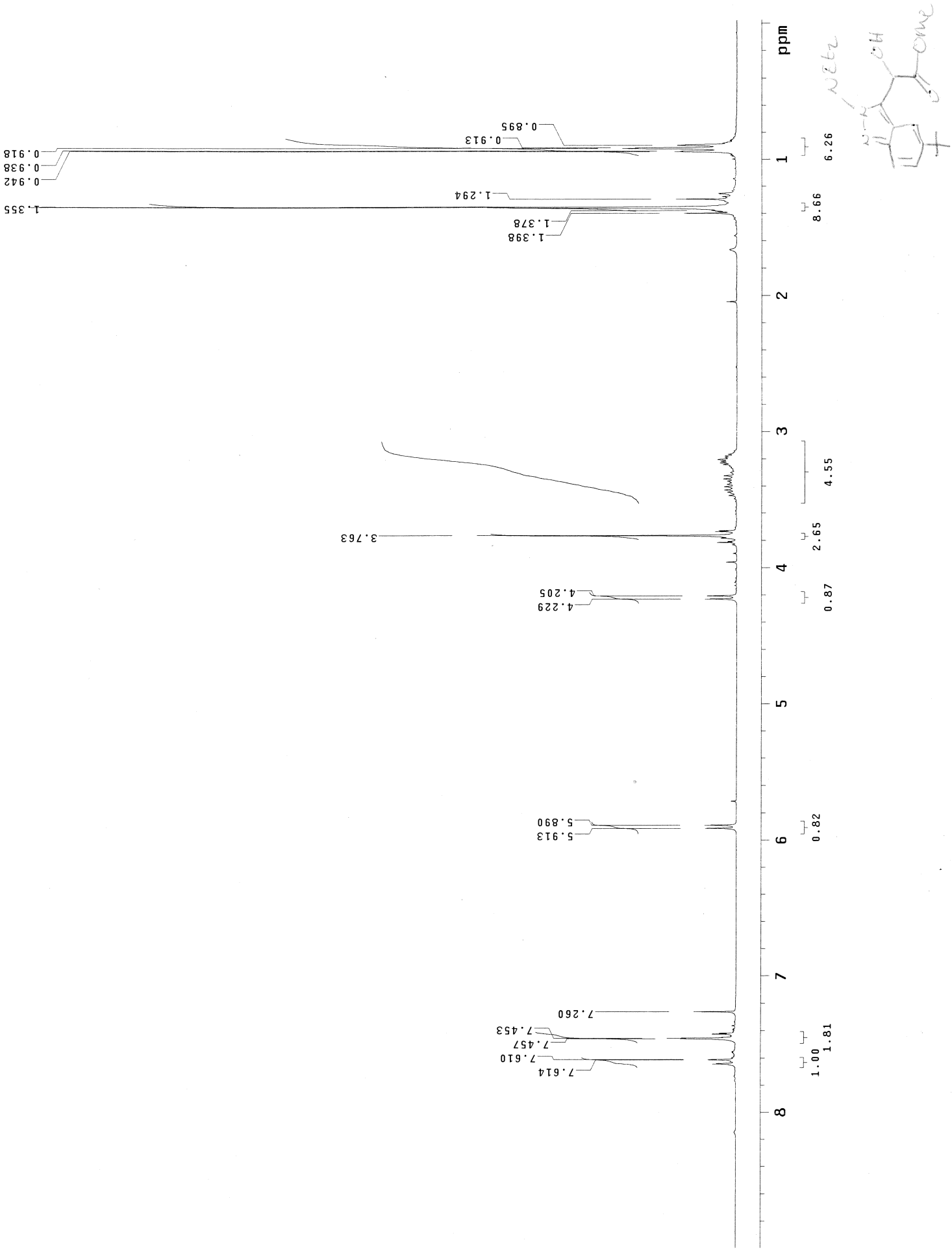
10f


ppm
1
2
3
4
5
6
7
8
6.00
3.09
2.14
2.38
2.95
0.98
0.94
0.96
0.87
0.93
0.903
0.928
0.880
2.406
3.200
3.757
4.153
4.129
5.904
5.881
7.597
7.568
7.322
7.260
7.170
7.165
7.141
7.136

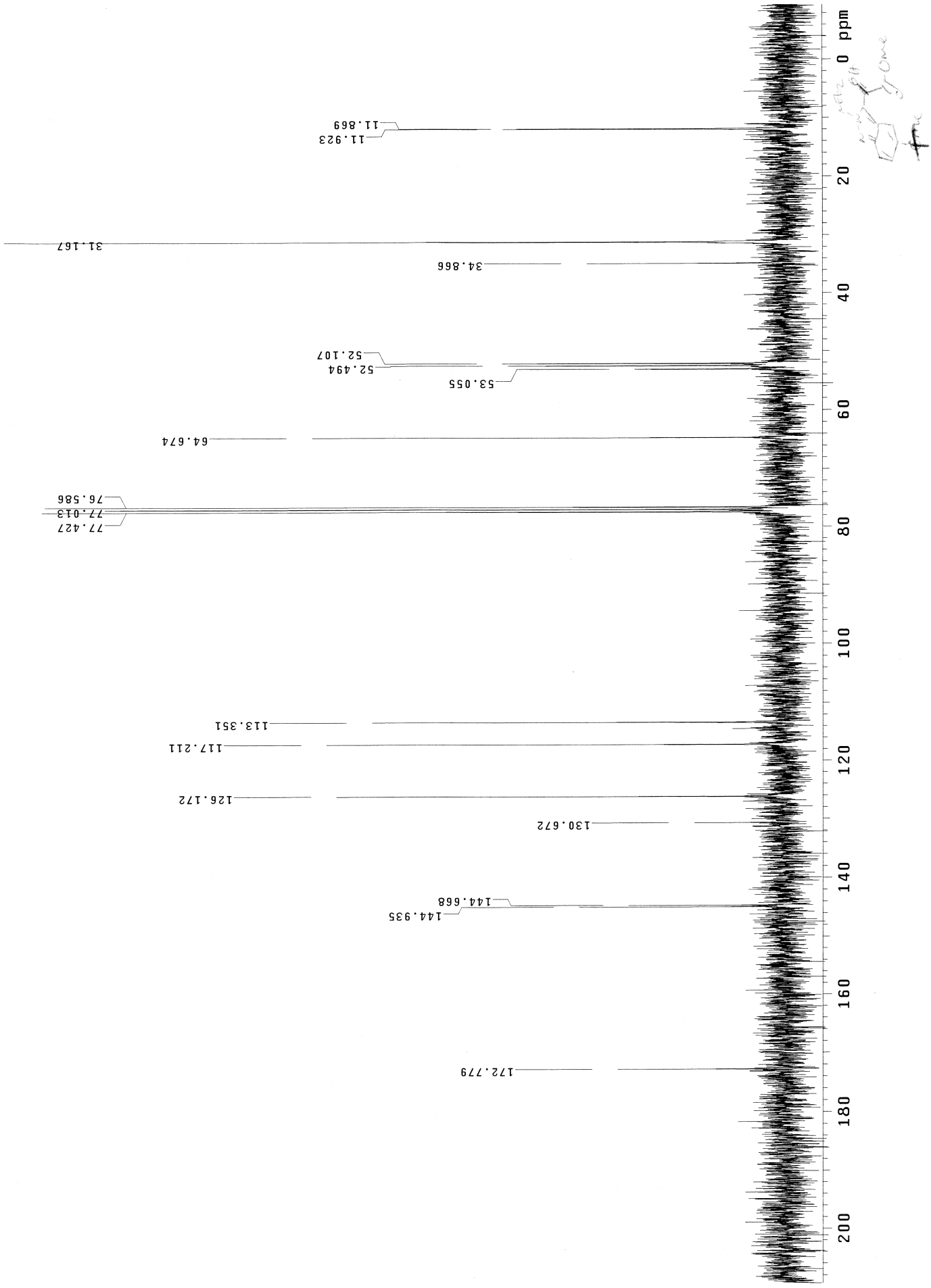
10f


172.766
144.761
131.727
130.125
129.283
117.531
117.398
117.304
64.607
77.427
77.000
76.573
53.028
52.494
52.120
21.779
11.869
0 ppm

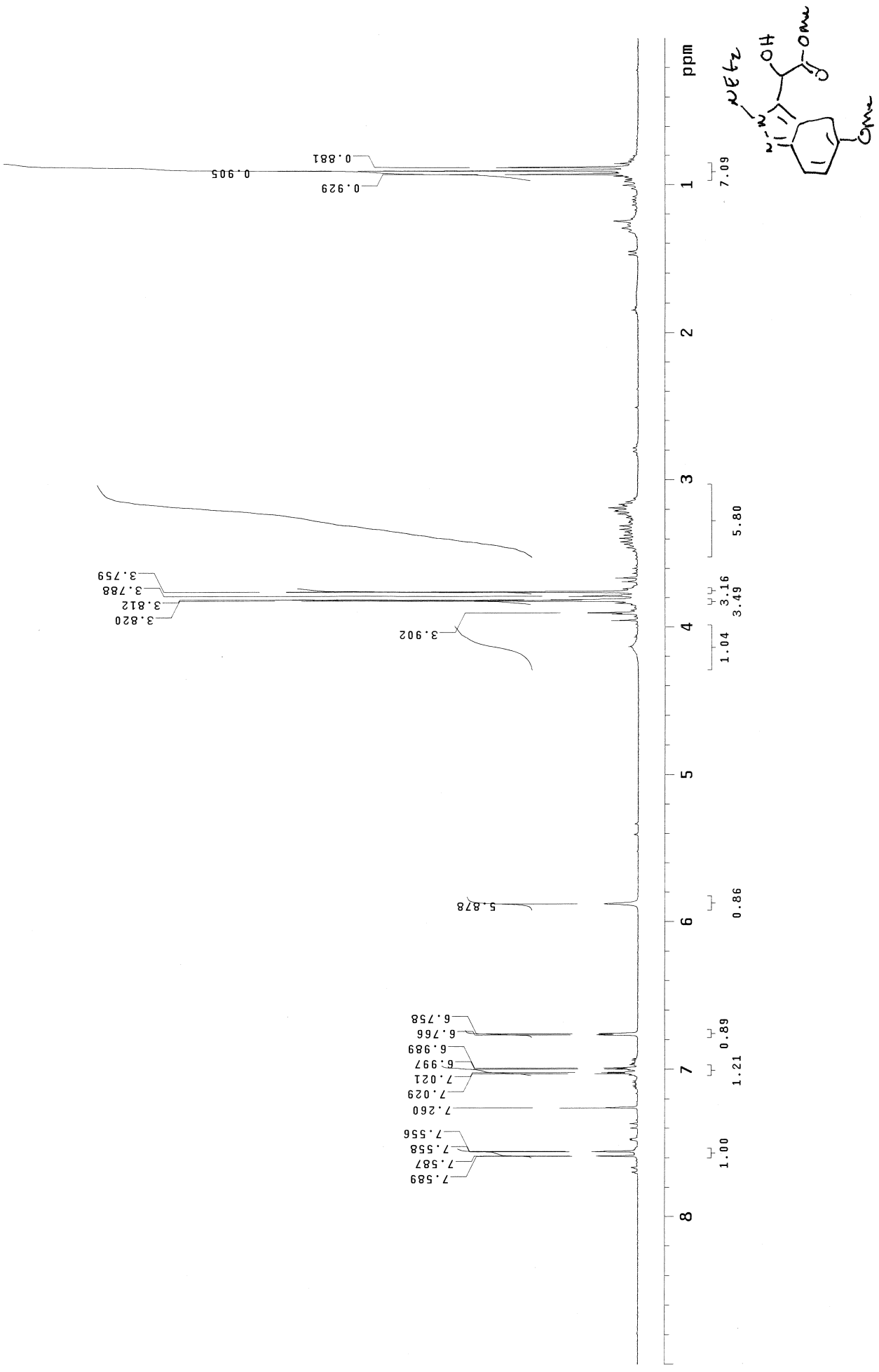
10g


ppm
0.895
0.913
0.918
0.938
0.942
1.294
1.355
1.378
1.398
3.763
4.205
4.229
5.890
5.913
7.260
7.453
7.457
7.610
7.614
6.26
8.66
4.55
2.65
0.87
0.82
1.81
1.00

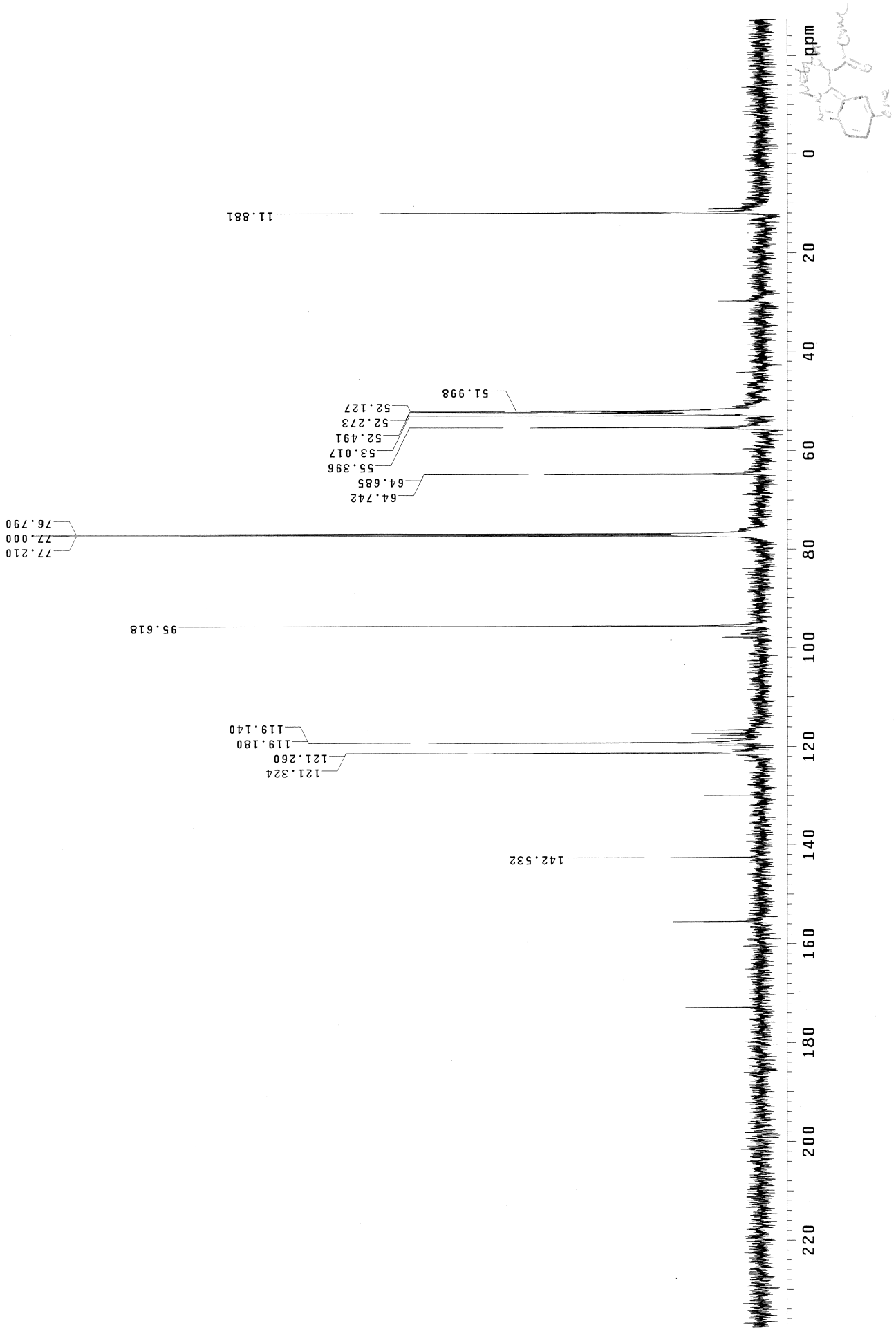
10g


172.779
144.935
144.668
130.672
126.172
117.211
113.351
77.427
77.013
76.586
64.674
53.055
52.494
52.107
34.866
31.167
11.923
11.869
ppm

10h


0.881
0.905
0.929
3.759
3.788
3.812
3.820
3.902
5.878
6.758
6.766
6.989
6.997
7.021
7.029
7.260
7.556
7.558
7.587
7.589
ppm
1
2
3
4
5
6
7
8
7.09
5.80
3.16
3.49
1.04
0.86
0.89
1.21
1.00

10h


11.881
51.998
52.127
52.273
52.491
53.017
55.396
64.685
64.742
76.790
77.000
77.210
95.618
119.140
119.180
121.260
121.324
142.532
ppm
0
20
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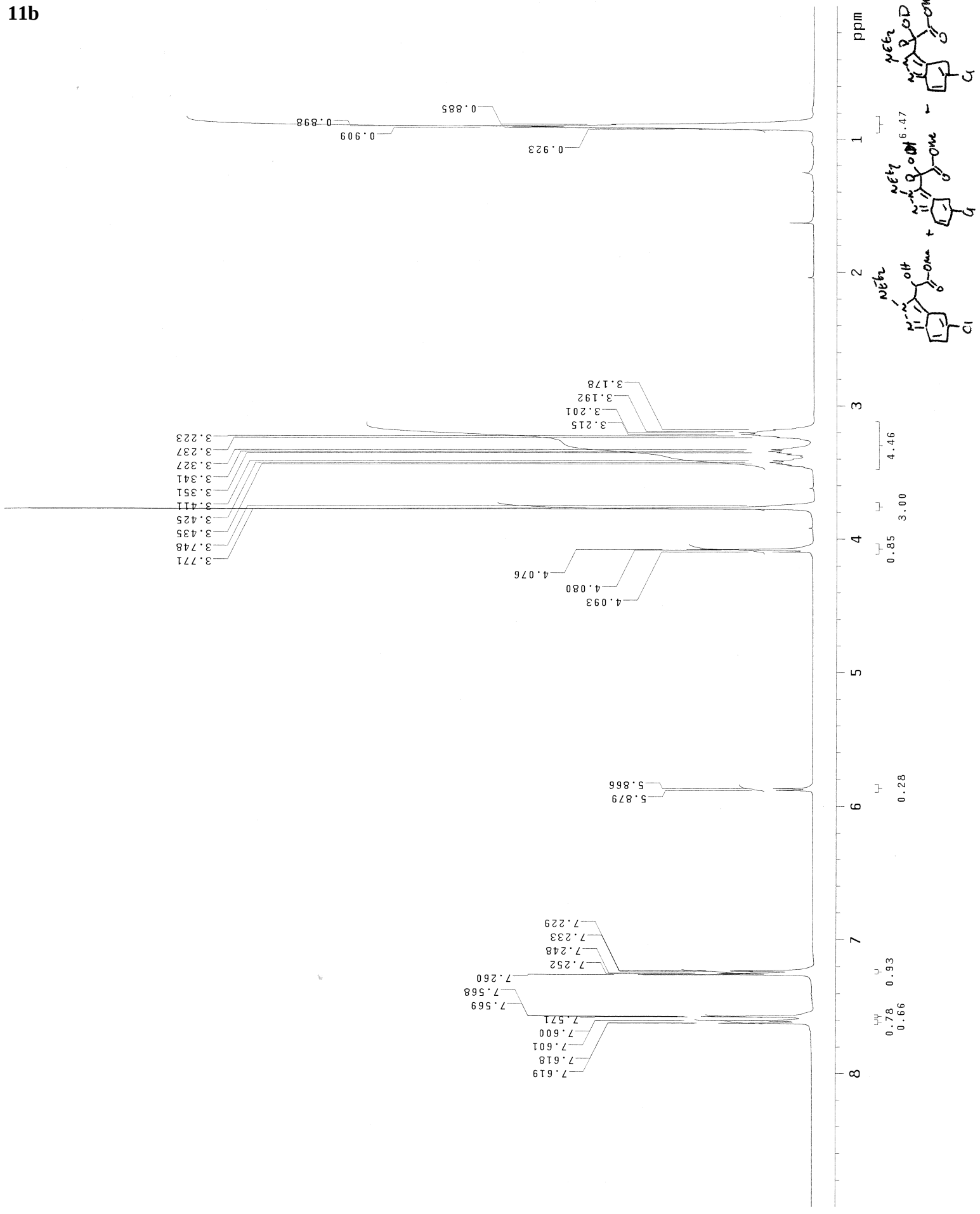
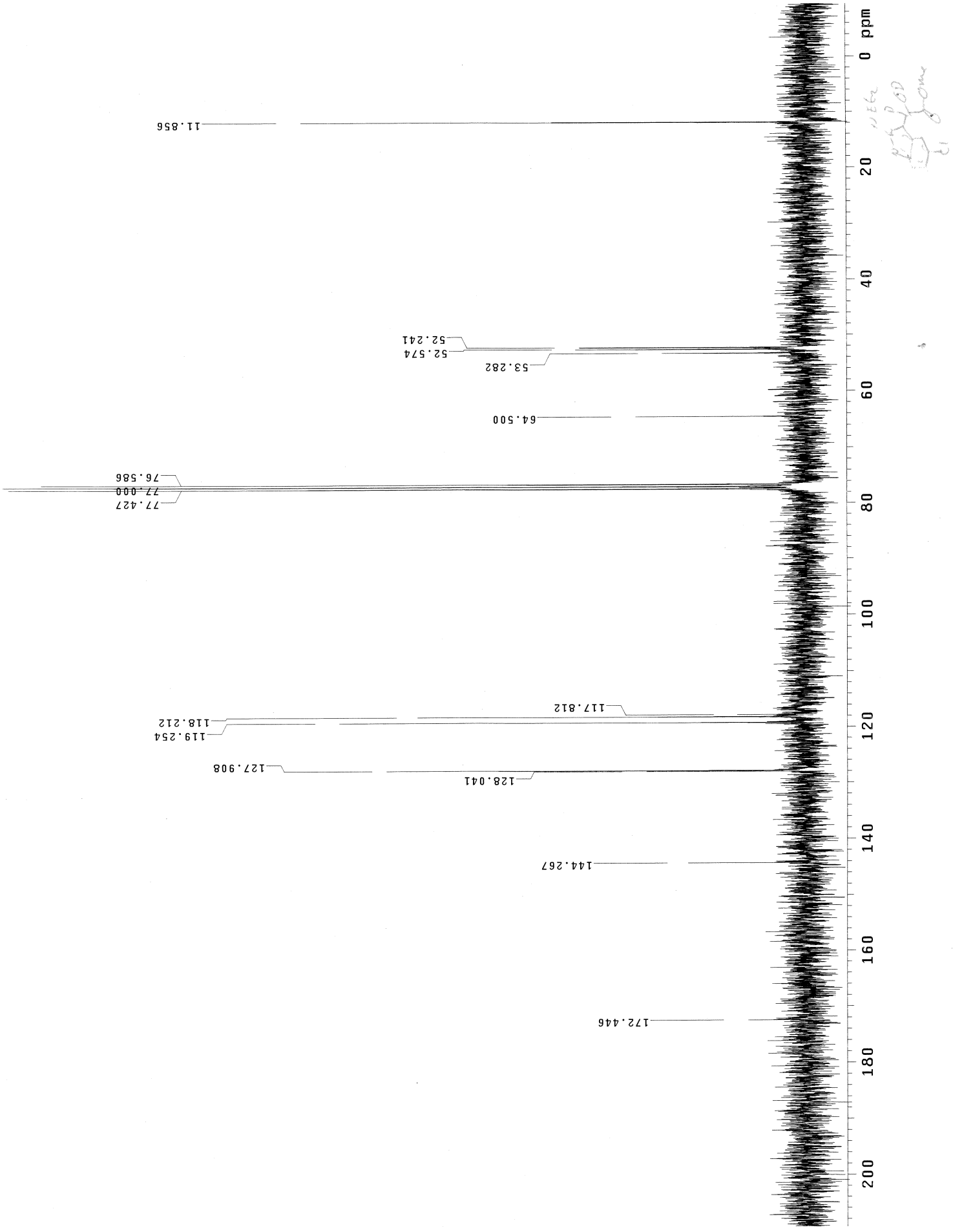
60
80
100
120
140
160
180
200
220

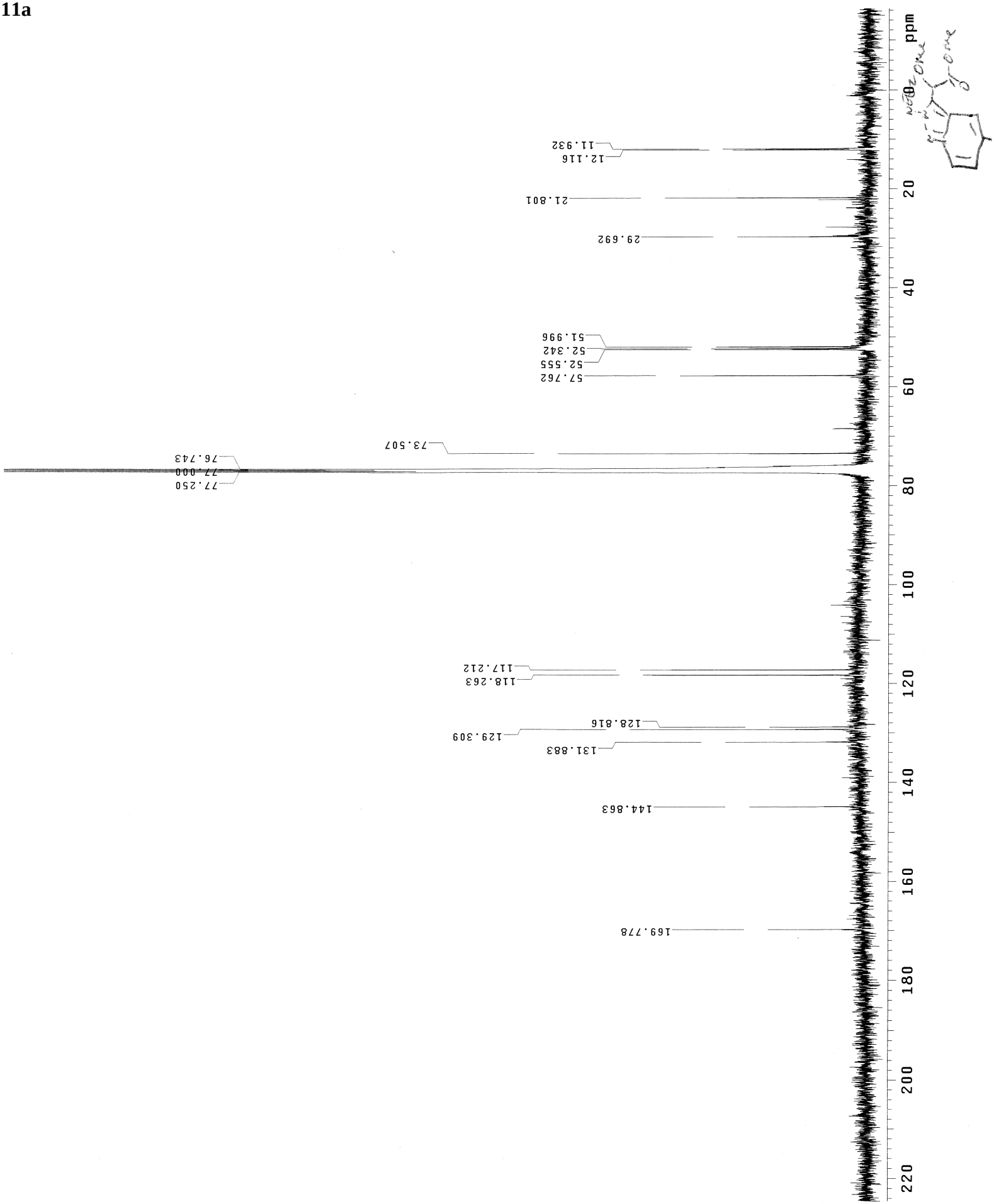
11b


ppm
1
2
3
4
5
6
7
8
0.885
0.898
0.909
0.923
3.178
3.192
3.201
3.215
3.223
3.237
3.327
3.341
3.351
3.411
3.425
3.435
3.748
3.771
4.076
4.080
4.093
5.866
5.879
7.229
7.233
7.248
7.252
7.260
7.568
7.569
7.571
7.600
7.601
7.618
7.619
4.46
3.00
0.85
0.28
0.93
0.78
0.66
6.47

11b


11.856
52.241
52.574
53.282
64.500
76.586
77.000
77.427
117.812
118.212
119.254
127.908
128.041
144.267
172.446
0 ppm
20
40
60
80
100
120
140
160
180
200

11a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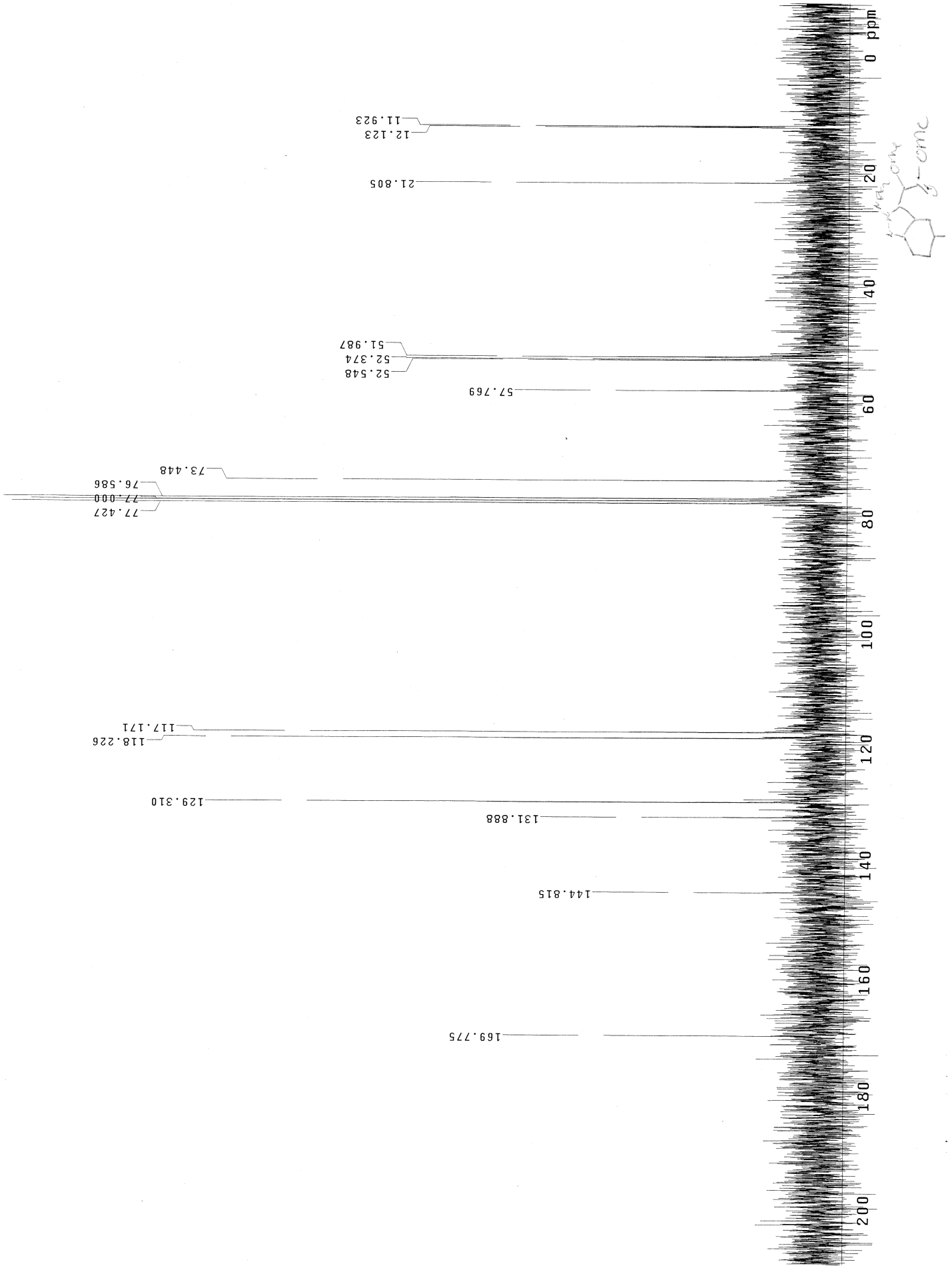
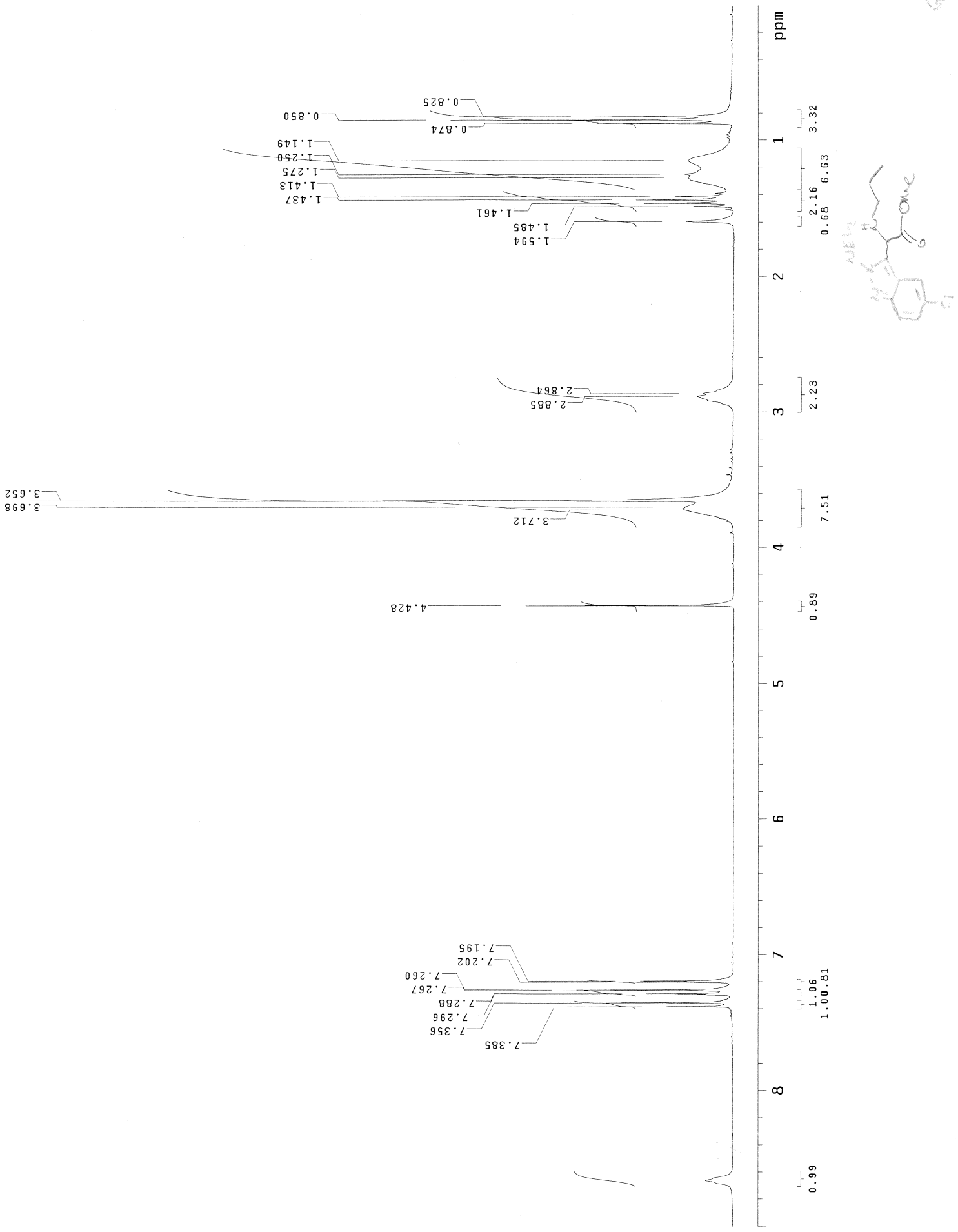
12.116
21.801
29.692
51.996
52.342
52.555
57.762
73.507
76.743
77.000
77.250
117.212
118.263
128.816
129.309
131.883
144.863
169.778
ppm

11a


11.923
12.123
21.805
51.987
52.374
52.548
57.769
73.448
76.586
77.000
77.427
117.171
118.226
129.310
131.888
144.815
169.775
0 ppm
20
40
60
80
100
120
140
160
180
200

11c


ppm
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2
3
4
5
6
7
8
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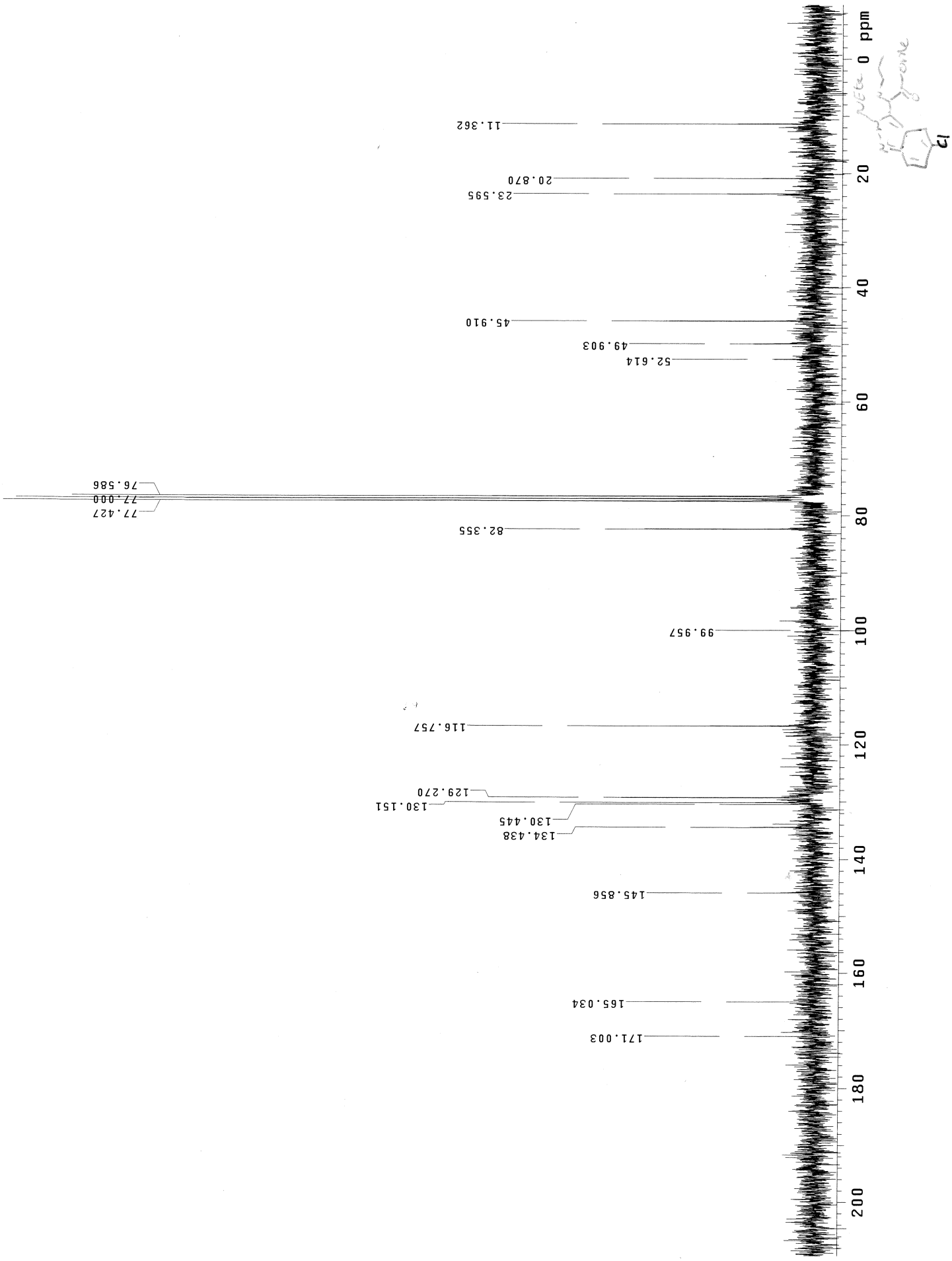
1.06
1.00
0.81
0.89
7.51
2.23
2.16
0.68
6.63
3.32
7.385
7.356
7.296
7.288
7.267
7.260
7.202
7.195
4.428
3.712
3.698
3.652
2.864
2.885
1.594
1.485
1.461
1.437
1.413
1.275
1.250
1.149
0.874
0.850
0.825

11c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23.595
45.910
49.903
52.614
76.586
77.000
77.427
82.355
99.957
116.757
129.270
130.151
130.445
134.438
145.856
165.034
171.003
0
20
40
60
80
100
120
140
160
180
200
ppm