Synthesis of Substituted Carbazoles, Indoles and Dibenzofurans by Vinylic to Aryl Palladium Migration

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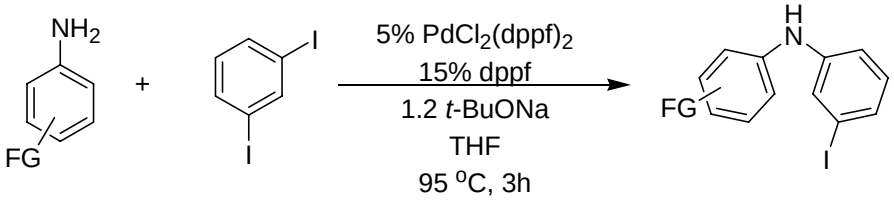
I. General Procedures. All ^{1}H and ^{13}C spectra were collected in $CDCl_3$ unless noted otherwise. Thin-layer chromatography was performed using 60-mesh silica gel plates, and visualization was effected with short wavelength UV light (254 nm) and a basic $KMnO_4$ solution. High resolution mass spectra were recorded using EI.

All reagents were used directly as obtained commercially unless otherwise noted. Anhydrous forms of acetonitrile, DMF, diethyl ether, ethyl acetate, hexanes, and 4,4-dimethyl-2-pentyne were purchased from Lancaster Synthesis, Inc. 3-Iodoaniline, 2-(trimethylsilyl)phenyl trifluoromethanesulfonate, cesium fluoride, 1,3-diiodobenzene, 1,1'-bis(diphenylphosphino)ferrocene (dppf), sodium *tert*-butoxide, *p*-toluidine, *p*-anisidine, *p*-chloroaniline, *o*-methoxyaniline, methyl 4-aminobenzoate, 1-naphthylamine, 5,6,7,8-tetrahydronaphthalen-1-ylamine, 1-phenyl-1-butyne, 1-phenyl-1-propyne, 4-octyne, diphenylacetylene, 3,5-dimethoxyaniline, sodium thiomethoxide, and trifluoroacetic acid-*d* were purchased from Aldrich Chemical Co., Inc. Cesium pivalate was prepared according to the procedure of Campo and Larock.[1] The substituted alkynes were prepared by the Sonogashira coupling of aryl iodides with 1-butyne using 5 mol % of $PdCl_2(PPh_3)_2$, 2 mol % of CuI in Et_3N solvent at room temperature.[2]

II. Noncommercial compounds.

***N*-Phenyl-3-iodoaniline**. This compound was prepared according to the reported procedure:[3] ^{1}H NMR ($CDCl_3$) δ 5.67 (s, 1H), 6.94-7.10 (m, 5H), 7.23-7.41 (m, 4H); ^{13}C NMR ($CDCl_3$) 95.2, 116.5, 119.1, 122.3, 125.9, 129.7, 129.8, 131.1, 142.2, 145.1; IR ($CDCl_3$) 3427, 3061, 3034, 1584 cm^{-1}; HRMS m/z 294.9858 (calcd for $C_{12}H_{10}NI$, 294.9863).

Other aniline starting materials were prepared through the following palladium-catalyzed amination reaction.[4] The typical yield is ~30%.



***N*-*p*-Tolyl-3-iodoaniline**. ^{1}H NMR ($CDCl_3$) δ 2.34 (s, 3H), 5.58 (s, 1H), 6.93-7.26 (m, 7H), 7.34 (s, 1H); ^{13}C NMR ($CDCl_3$) 21.1, 95.3, 115.7, 120.2, 124.9, 129.0, 130.3, 131.0, 132.3, 139.3, 145.9; IR ($CDCl_3$) 3427, 3028, 2922, 1587 cm^{-1}; HRMS m/z 309.0018 (calcd for $C_{13}H_9IN$, 309.0015).

***N*-(2-Methoxyphenyl)-3-iodoaniline**. ^{1}H NMR ($CDCl_3$) δ 3.89 (s, 3H), 6.15 (s, 1H), 6.92-7.01 (m, 4H), 7.09-7.12 (m, 1H), 7.26-7.35 (m, 2 H), 7.51 (t, *J* = 1.7 Hz, 1H); ^{13}C NMR ($CDCl_3$) 55.9, 95.2, 111.0, 116.2, 117.2, 121.1, 121.3, 126.5, 129.9, 131.0, 131.9, 144.7, 149.0; IR ($CDCl_3$) 3418, 3060, 2962, 1244; HRMS m/z 324.9969 (calcd for $C_{13}H_9INO$, 324.9964).

***N*-(4-Methoxyphenyl)-3-iodoaniline**. ^{1}H NMR ($CDCl_3$) δ 3.83 (s, 3H), 5.51 (s, 1H), 6.82-7.23 (m, 8H); ^{13}C NMR ($CDCl_3$) 55.9, 95.5, 114.7, 115.1, 123.5, 123.9, 128.3, 131.1, 134.7, 147.1, 156.1; IR ($CDCl_3$) 3425, 3006, 2957, 1245 cm^{-1}; HRMS m/z 324.9967 (calcd for $C_{13}H_9INO$, 324.9964).

Methyl *N*-(3-iodophenyl)benzoate. ^{1}H NMR ($CDCl_3$) δ 3.88 (s, 3H), 6.10 (s, 1H), 6.98-7.13 (m, 4H), 7.35 (d, *J* = 7.8 Hz, 1H), 7.50 (s, 1H), 7.92 (d, *J* = 8.7 Hz, 1H); ^{13}C NMR ($CDCl_3$) 52.1, 95.0, 115.6, 119.1, 122.2, 128.6, 131.1, 131.8, 131.9, 142.7, 147.3, 167.1; IR ($CDCl_3$) 3340, 2945, 1694, 1580 cm^{-1}; HRMS m/z 352.9913 (calcd for $C_{14}H_{12}INO_2$, 352.9918).

***N*-(4-Chlorophenyl)-3-iodoaniline**. ^{1}H NMR ($CDCl_3$) δ 5.64 (s, 1H), 6.96-7.00 (m, 4H), 7.23-7.28 (m, 3H), 7.36 (s, 1H); ^{13}C NMR ($CDCl_3$) 95.3, 116.8, 120.1, 126.1, 126.8, 129.7, 130.2, 131.2, 140.9, 144.6; IR ($CDCl_3$) 3427, 3061, 3034, 1583 cm^{-1}; HRMS m/z 328.9473 (calcd for $C_{12}H_9ClIN$, 328.9468).

***N*-(3-Iodophenyl)naphthalen-1-amine**. ^{1}H NMR ($CDCl_3$) δ 5.83 (s, 1H), 6.85-6.97 (m, 2H), 7.21 (dt, *J* = 7.6, 1.3 Hz, 1H), 7.30 (t, *J* = 1.9 Hz, 1H), 7.37-7.56 (m, 4H), 7.65 (d, *J* = 7.8 Hz, 1H), 7.88-8.00 (m, 2H); ^{13}C NMR ($CDCl_3$) 95.2, 115.9, 118.2, 122.1, 124.5, 125.3, 126.2, 126.6, 128.6, 128.8, 129.1, 131.0, 134.9, 137.7, 146.9; IR ($CDCl_3$) 3415, 3060, 1574 cm^{-1}; HRMS m/z 345.0018 (calcd for $C_{18}H_{12}IN$, 345.0015).

***N*-(3-Iodophenyl)-5,6,7,8-tetrahydronaphthalen-1-amine**. ^{1}H NMR ($CDCl_3$) δ 1.79-1.90 (m, 4H), 2.60 (t, *J* = 6.1 Hz, 2H), 2.84 (t, *J* = 6.1 Hz, 2H), 5.31 (s, 1H), 6.87-6.90 (m, 2H), 6.96 (t, *J* = 7.7 Hz, 1H), 7.11 (d, *J* = 4.3 Hz, 2H), 7.20-7.22 (dd, *J* = 7.6, 0.9 Hz, 1H), 7.30 (s, 1H); ^{13}C NMR ($CDCl_3$) 23.0, 23.3, 25.0, 30.2, 95.3, 116.1, 117.6, 124.4, 125.5, 126.1, 128.9, 129.0, 131.0, 139.1, 140.0, 146.1; IR ($CDCl_3$) 3396, 3054, 2927, 1578 cm^{-1}; HRMS m/z 349.0331 (calcd for $C_{16}H_{16}IN$, 349.0328).

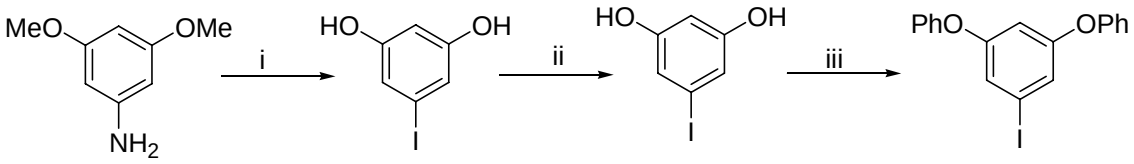
***N*-Allyl-3-iodoaniline**. This compound was prepared according to the reported procedure:[5] ^{1}H NMR ($CDCl_3$) δ 3.74 (d, *J* = 5.1 Hz, 2H), 3.81 (s, 1H), 5.19-5.33 (m, 2H), 5.87-5.99 (m, 1H), 6.57 (dd, *J* = 8.1, 2.4 Hz, 1H), 6.89 (t, *J* = 8.1 Hz, 1H), 6.97 (t, *J* = 1.6 Hz, 1H), 7.05 (d, *J* = 7.8 Hz, 1H); ^{13}C NMR ($CDCl_3$) 46.5, 95.6, 112.5, 116.9, 121.7, 126.6, 130.9, 135.0, 149.5; IR ($CDCl_3$) 3417, 3076, 2847, 1590 cm^{-1}; HRMS m/z 258.9862 (calcd for $C_9H_{10}NI$, 258.9858).

3-(3-Iodophenylamino)cyclohex-2-enone. 3-Iodoaniline (2 mmol) and cyclohexane-1,3-dione (2 mmol) were dissolved in 10 mL toluene and then the mixture was heated at 100 ^{o}C in the presence of 8 mmol anhydrous $MgSO_4$ and a catalytic amount of TsOH. After 12 h, the reaction mixture was filtered, and the toluene was removed from the filtrate. The residue obtained was purified by flash chromatography to afford a 90% yield of the imine product: ^{1}H NMR ($CDCl_3$) δ 1.96-2.02 (m, 2H), 2.32 (t, *J* = 6.2 Hz, 2H), 2.50 (t, *J* = 6.2 Hz, 2H), 5.51 (s, 1H), 7.00 (t, *J* = 8.0 Hz, 1H), 7.10 (dd, *J* = 8.0, 0.9 Hz, 1H), 7.40-7.48 (m, 3H); ^{13}C NMR ($CDCl_3$) 22.0, 29.8, 36.7, 123.3, 130.9, 132.8, 134.6, 139.8,

162.8, 198.9; IR ($CDCl_3$) 3247, 3056, 2945, 1566 cm^{-1}; HRMS m/z 312.9968 (calcd for $C_{12}H_{12}INO$, 312.9964).

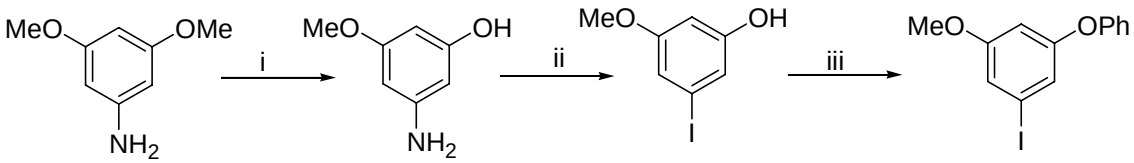
1-Iodo-3-phenoxybenzene. This compound was prepared by the reported procedure:[6] ^1H NMR ($CDCl_3$) δ 6.96-7.07 (m, 4H), 7.16 (t, *J* = 7.4 Hz, 1H), 7.35-7.44 (m, 4H); ^{13}C NMR ($CDCl_3$) 94.5, 118.2, 119.5, 124.2, 127.8, 130.2, 131.3, 132.4, 156.6, 158.3; IR ($CDCl_3$) 3075, 2965, 1582 cm^{-1}; HRMS m/z 295.9702 (calcd for $C_{12}H_9IO$, 295.9698).

1-Iodo-3,5-diphenoxybenzene. This compound was prepared by the strategy shown below: ^1H NMR ($CDCl_3$) δ 6.63 (t, *J* = 2.2 Hz, 1H), 7.02-7.04 (m, 6H), 7.13-7.17 (m, 2H), 7.35-7.39 (m, 4H); ^{13}C NMR ($CDCl_3$) 94.1, 108.7, 119.8, 122.0, 124.5, 130.2, 156.1, 159.4; IR ($CDCl_3$) 3073, 3039, 1575 cm^{-1}; HRMS m/z 387.9964 (calcd for $C_{18}H_{13}IO_2$, 387.9960).



(i) (a) $NaNO_2$, HCl (b) KI; (ii) BBr_3; (iii) 6 CsF, 2.2 2-(trimethylsilyl)phenyl trifluoromethanesulfonate, MeCN.

1-Iodo-3-methoxy-5-phenoxybenzene. This compound was prepared by the strategy shown below:[7] ^1H NMR ($CDCl_3$) δ 3.76 (s, 3H), 6.57 (t, *J* = 2.2 Hz, 1H), 6.97 (t, *J* = 1.5 Hz, 1H), 7.03-7.09 (m, 3H), 7.18 (t, *J* = 7.3 Hz, 1H), 7.36-7.42 (m, 2H); ^{13}C NMR ($CDCl_3$) 55.9, 94.4, 104.9, 118.3, 119.8, 120.2, 124.3, 130.2, 156.4, 159.3, 161.5; IR ($CDCl_3$) 3074, 2960, 1586 cm^{-1}; HRMS m/z 325.9808 (calcd for $C_{13}H_{11}IO_2$, 325.9804).



(i) NaSMe, DMA, 140 ^oC; (ii) (a) $NaNO_2$, HCl; (b) KI; (iii) 4 CsF, 1.1 2-(trimethylsilyl)phenyl trifluoromethanesulfonate, MeCN.

Compound **29-d**: ^1H NMR ($CDCl_3$) δ 3.76 (s, 3H), 6.52 (s, 0.08H), 6.92 (s, 0.11H), 6.99-7.04 (m, 2H), 7.15 (t, *J* = 7.32 Hz, 1H), 7.34-7.39 (m, 2H).

III. Experimental Procedures. The aryl halide (0.25 mmol), alkyne (0.25 mmol), $Pd(OAc)_2$ (2.8 mg, 0.0125 mmol), *bis*(diphenylphosphino)methane (dppm) (4.8 mg, 0.0125 mmol) and CsO_2CCMe_3 (CsPiv) (0.117 g, 0.5 mmol) in 4 mL of DMF were stirred under Ar at 100 ^oC for 6 h. The reaction mixture was allowed to cool to room temperature, diluted with diethyl ether (25 mL) and washed with 5% Na_2CO_3 (25 mL). The aqueous layer was re-extracted with diethyl ether (25 mL) twice. The organic layers were combined, dried ($MgSO_4$), filtered, and the solvent was removed under reduced pressure. The residue was purified by flash chromatography on silica gel.

For the products reported in entries 1, 5, 9, 13, 15 and 16 of Table 2; entry 1 in Table 3; and entries 2-4, 8, and 9 in Table 3, GC-mass spectral analysis shows two regioisomers, which cannot be separated by flash chromatography. The ratio of these isomers was determined by ^1H NMR spectroscopy.

(*E*)-4-(1-Phenylbut-1-enyl)-9*H*-carbazole (1a). ^1H NMR ($CDCl_3$) δ 1.11 (t, *J* = 7.4 Hz, 3H), 2.94 (q, *J* = 7.4 Hz, 2H), 6.74 (s, 1H), 7.11-7.20 (m, 2H), 7.35-7.53 (m, 9H), 8.05 (s, 1H), 8.20 (d, *J* = 7.9 Hz, 1H); ^{13}C NMR ($CDCl_3$) 13.4, 25.9, 109.4, 110.7, 119.6, 120.2, 120.9, 123.0, 123.3, 125.7, 125.8, 126.9, 128.7, 128.9, 129.0, 138.2, 139.9, 139.9, 140.1, 144.6; IR ($CDCl_3$) 3471, 3056, 2968, 2934, 1599 cm^{-1}; HRMS m/z 297.1522 (calcd for $C_{22}H_{19}N$, 297.1518).

(*E*)-4-(4,4-Dimethylpent-2-en-2-yl)-9*H*-carbazole (2). ^1H NMR ($CDCl_3$) δ 1.34 (s, 9H), 2.28 (d, *J* = 1.3 Hz, 3H), 5.67 (d, *J* = 1.4 Hz, 1H), 6.96 (dd, *J* = 6.9, 1.2 Hz, 1H), 7.19-7.42 (m, 5H), 8.06 (s, 1H), 8.14 (d, *J* = 7.8 Hz, 1H); ^{13}C NMR ($CDCl_3$) 19.2, 31.2, 33.1, 108.8, 110.6, 119.4, 119.7, 120.2, 123.0, 123.2, 125.6, 125.9, 134.8, 139.6, 139.8, 139.9, 143.3; IR ($CDCl_3$) 3473, 2960, 2867, 1600 cm^{-1}; HRMS m/z 263.1679 (calcd for $C_{19}H_{21}N$, 263.1674).

4-[1-(2,2-Dimethylpropylidene)pentyl]-9*H*-carbazole (4a). ^1H NMR ($CDCl_3$) δ 0.81 (t, *J* = 7.2 Hz, 3H), 1.22-1.40 (m, 13H), 2.71-2.78 (m, 2H), 5.62 (s, 1H), 6.97 (dd, *J* = 7.1, 1.1 Hz, 1H), 7.19-7.42 (m, 5H), 8.01 (s, 1H), 8.20 (d, *J* = 8.1 Hz, 1H); ^{13}C NMR ($CDCl_3$) 14.2, 23.4, 31.4, 31.7, 32.4, 33.2, 108.7, 110.6, 119.3, 120.5, 120.7, 123.2, 123.4, 125.5, 139.3, 139.8, 139.9, 140.1, 141.9; IR ($CDCl_3$) 3410, 2957, 2866, 1599 cm^{-1}; HRMS m/z 305.2148 (calcd for $C_{22}H_{27}N$, 305.2144).

(*E*)-4-(1-Phenylprop-1-enyl)-9*H*-carbazole (5a). ^{1}H NMR ($CDCl_3$) δ 2.47 (s, 3H), 6.78 (s, 1H), 7.12-7.20 (m, 2H), 7.33-7.54 (m, 9H), 8.10 (s, 1H), 8.14 (d, *J* = 7.8 Hz, 1H); ^{13}C NMR ($CDCl_3$) 19.9, 109.4, 110.7, 119.4, 119.6, 120.2, 122.9, 123.1, 125.8, 125.9, 126.8, 128.6, 129.3, 129.4, 138.3 (2C), 139.9, 140.1, 141.4; IR ($CDCl_3$) 3471, 3060, 3026, 1601, 1456 cm^{-1}; HRMS m/z 283.1367 (calcd for $C_{18}H_{19}N$, 283.1361).

(*E*)-4-(1,2-Diphenylvinyl)-9*H*-carbazole (6). ^{1}H NMR ($CDCl_3$) δ 7.03-7.14 (m, 3H), 7.23-7.42 (m, 14H), 8.03 (s, 1H), 8.37 (d, *J* = 8.1 Hz, 1H); ^{13}C NMR ($CDCl_3$) 109.8, 110.8, 119.6, 121.3, 121.7, 123.0, 123.39, 125.7, 125.9, 127.3, 127.7, 128.5, 128.7, 129.8, 130.2, 131.1, 137.6, 140.0, 140.3, 140.4, 140.7, 141.3; IR ($CDCl_3$) 3414, 3054, 1599, 1455 cm^{-1}; HRMS m/z 345.1522 (calcd for $C_{26}H_{19}N$, 345.1518).

(*E*)-Ethyl 4-[1-(9*H*-carbazol-4-yl)but-1-enyl]benzoate (7a). ^{1}H NMR ($CDCl_3$) δ 1.90 (t, *J* = 7.5 Hz, 3H), 1.44 (t, *J* = 7.2 Hz, 3H), 1.91 (q, *J* = 7.5 Hz, 2H), 4.43 (q, *J* = 7.2 Hz, 2H), 6.73 (s, 1H), 7.10 (dd, *J* = 6.7, 1.7 Hz, 1H), 7.15 (td, *J* = 6.8, 1.5 Hz, 1H), 7.37-7.46 (m, 4H), 7.53 (d, *J* = 8.1 Hz, 2H), 8.10-8.20 (m, 4H); ^{13}C NMR ($CDCl_3$) 13.3, 14.6, 26.0, 6.19, 109.6, 110. 8, 119.6, 119.9, 120.8, 122.8, 123.1, 125.6, 125.8, 128.2, 128.8, 128.9, 130.0, 139.4, 139.9, 140.1, 142.8, 146.7, 166.8; IR ($CDCl_3$) 3472, 2968, 2873, 1710 cm^{-1}; HRMS m/z 369.1736 (calcd for $C_{25}H_{23}NO_2$, 369.1729).

(*E*)-4-[1-(2-Methoxyphenyl)but-1-enyl]-9*H*-carbazole (8a). ^{1}H NMR ($CDCl_3$) δ 1.00 (t, *J* = 7.5 Hz, 3H), 2.80 (q, *J* = 7.5 Hz, 2H), 3.84 (s, 3H), 6.77 (s, 1H), 6.95 (d, *J* = 8.0 Hz, 1H), 6.97-7.17 (m, 3H), 7.29-7.53 (m, 6H), 8.11 (s, 1H), 8.36 (d, *J* = 7.8 Hz, 1H); ^{13}C NMR ($CDCl_3$) 13.3, 26.1, 55.5, 109.1, 110.5, 110.8, 118.3, 119.3, 120.2, 120.4, 121.2, 123.5, 124.7, 125.5, 125.6, 127.3, 128.3, 130.1, 139.9, 140.1, 144.0, 157.8; IR ($CDCl_3$) 3472, 2966, 2934, 1245 cm^{-1}; HRMS m/z 327.1628 (calcd for $C_{23}H_{21}NO$, 327.1623).

(*E*)-5-(1,2-Diphenylvinyl)-3-methyl-9*H*-carbazole (9). ^{1}H NMR ($CDCl_3$) δ 2.36 (s, 3H), 7.02-7.05 (m, 2H), 7.20-7.40 (m, 14H), 7.95 (s, 1H), 8.10 (s, 1H); ^{13}C NMR ($CDCl_3$) 21.8, 109.8, 110.4, 121.3, 121.6, 123.1, 123.5, 125.5, 127.2, 127.2, 127.6, 128.5, 128.5, 128.6, 129.7, 130.3, 131.1, 137.8, 138.2, 140.2, 140.5, 140.7, 141.4; IR ($CDCl_3$) 3413, 3053, 3022, 1599, 1491 cm^{-1}; HRMS m/z 359.1678 (calcd for $C_{27}H_{21}N$, 359.1674).

(*E*)-5-(1,2-Diphenylvinyl)-3-methoxy-9*H*-carbazole (10). ^{1}H NMR ($CDCl_3$) δ 3.58 (s, 3H), 7.02-7.07 (m, 3H), 7.22-7.42 (m, 13H), 7.81 (d, *J* = 2.5 Hz, 1H), 7.98 (s, 1H); ^{13}C NMR ($CDCl_3$) 55.8, 105.2, 110.1, 111.5, 115.8, 121.5, 121.6, 123.6, 125.6, 127.3, 127.8, 128.7, 129.7, 130.3, 131.3, 134.8, 137.7, 140.1, 140.5, 141.1 (2C), 153.5; IR ($CDCl_3$) 3415, 3054, 2949, 1582, 1478 cm^{-1}; HRMS m/z 375.1629 (calcd for $C_{27}H_{21}NO$, 375.1623).

5-(1-Benzylidenepropyl)-1-methoxy-9*H*-carbazole (11a). ^{1}H NMR ($CDCl_3$) δ 1.08 (t, *J* = 7.5 Hz, 3H), 2.91 (q, *J* = 7.5 Hz, 2H), 4.0 (s, 3H), 6.7 (s, 1H), 6.89 (d, *J* = 7.6 Hz, 1H), 7.06-7.10 (m, 2H), 7.30-7.50 (m, 7H), 7.77 (d, *J* = 8.0 Hz, 1H), 8.37 (s, 1H); ^{13}C NMR ($CDCl_3$) 13.4, 25.9, 55.8, 105.8, 109.7, 115.6, 119.7, 120.0, 124.2, 125.5, 126.8, 128.6, 128.9, 129.0, 130.3, 138.2, 139.8, 139.9, 144.5, 145.8; IR ($CDCl_3$) 3421, 2964, 2932, 1598 cm^{-1}; HRMS m/z 327.1625 (calcd for $C_{23}H_{21}NO$, 327.1623).

Methyl 5-(1,2-diphenylvinyl)-9*H*-carbazole-3-carboxylate (12). ^{1}H NMR ($CDCl_3$) δ 3.72 (s, 3H), 7.03 (s, 1H), 7.09 (t, *J* = 4.2 Hz, 1H), 7.20-7.42 (m, 13H), 8.07 (dd, *J* = 8.5, 1.4 Hz, 1H), 8.41 (s, 1H), 9.00 (d, *J* = 1.4 Hz, 1H); ^{13}C NMR ($CDCl_3$) 51.9, 110.1, 110.2, 121.4, 121.6, 122.6, 122.9, 125.6, 126.4, 127.2, 127.5, 127.7, 128.3, 128.5, 129.8, 130.4, 131.5, 137.5, 140.0, 140.5, 140.7, 140.9, 142.7, 167.9; IR ($CDCl_3$) 3323, 3021, 2947, 1691 cm^{-1}; HRMS m/z 403.1578 (calcd for $C_{28}H_{21}NO_2$, 403.1572)

(*E*)-3-Chloro-5-(1-phenylbut-1-enyl)-9*H*-carbazole (13a). ^{1}H NMR ($CDCl_3$) δ 1.09 (t, *J* = 7.5 Hz, 3H), 2.91 (q, *J* = 7.5 Hz, 2H), 6.73 (s, 1H), 7.14 (d, *J* = 7.2 Hz, 1H), 7.29-7.52 (m, 10H), 8.08 (s, 1H), 8.19 (d, *J* = 1.5 Hz, 1H); ^{13}C NMR ($CDCl_3$) 13.4, 25.7, 109.6, 111.7, 120.5, 122.6, 124.5, 124.9, 125.9, 126.4, 127.1, 128.8, 129.2, 129.7, 137.9, 138.2, 140.0, 140.6, 144.0; IR ($CDCl_3$) 3471, 2944, 2833 cm^{-1}; HRMS m/z 331.1132 (calcd for $C_{22}H_{18}NCl$, 331.1128).

(*E*)-7-(1-Phenylbut-1-enyl)-11*H*-benzo[*a*]carbazole (14a). ^{1}H NMR ($CDCl_3$) δ 1.10 (t, *J* = 7.6 Hz, 3H), 2.95 (q, *J* = 7.6 Hz, 2H), 6.75 (s, 1H), 7.16 (dd, *J* = 7.3, 1.2 Hz, 1H), 7.26-7.60 (m, 10H), 7.98 (d, *J* = 7.5 Hz, 1H), 8.14 (d, *J* = 8.1 Hz, 1H), 8.23 (d, *J* = 8.1 Hz, 1H), 8.87 (s, 1H); ^{13}C NMR ($CDCl_3$) 13.3, 26.1, 109.8, 118.5, 120.1, 120.6 (2C), 121.1, 121.8, 121.9, 124.7, 125.5, 125.7, 126.9, 128.7, 129.0, 129.1 (2C), 132.3, 135.3, 138.2, 139.1, 139.3, 144.5; IR ($CDCl_3$) 3472, 3060, 2969, 1572 cm^{-1}; HRMS m/z 347.1682 (calcd for $C_{26}H_{21}N$, 347.1674).

7-(1,2-Diphenylvinyl)-2,3,4,11-tetrahydro-1*H*-benzo[*a*]carbazole (15). ^{1}H NMR ($CDCl_3$) δ 1.91-2.03 (m, 4H), 2.93 (m, 4H), 6.86 (d, *J* = 8.2 Hz, 1H), 6.99 (dd, *J* = 7.2, 0.8 Hz, 1H), 7.07 (s, 1H), 7.23-7.40 (m, 12H), 8.01 (s, 1H), 8.09 (d, *J* = 8.2 Hz, 1H); ^{13}C NMR ($CDCl_3$) 23.1, 13.6, 24.6, 29.9, 109.8, 119.1, 120.0, 120.4, 121.2, 121.6, 122.0, 124.9, 127.2, 127.6, 128.4, 128.6, 129.8, 130.2, 131.0, 134.9, 137.7, 139.1, 139.9, 140.2, 140.8, 141.3; IR ($CDCl_3$) 3434, 3053, 2929, 1601 cm^{-1}; HRMS m/z 399.1993 (calcd for $C_{30}H_{25}N$, 399.1987).

(*E*)-3-Methyl-4-(1-phenylbut-1-en-2-yl)-*1H*-indole (16a). ^{1}H NMR ($CDCl_3$) δ 1.09 (t, *J* = 7.2 Hz, 3H), 2.36 (s, 3H), 2.77 (q, *J* = 7.2 Hz, 2H), 6.47 (s, 1H), 6.96-6.99 (m, 2H), 7.18 (t, *J* = 7.8 Hz, 1H), 7.27-7.32 (m, 2H), 7.41 (d, *J* = 4.1 Hz, 4H), 7.93 (s, 1H); ^{13}C NMR ($CDCl_3$) 13.2, 13.4, 27.1, 110.0, 112.5, 119.7, 121.7, 122.9, 125.6, 126.6, 128.5, 128.9, 129.0, 137.3, 137.9, 138.4, 144.4; IR ($CDCl_3$) 3418, 3021, 2964, 1598 cm^{-1}; HRMS m/z 261.1518 (calcd for $C_{19}H_{19}N$, 261.1521).

4-(1,2-Diphenylvinyl)-3-methyl-1*H*-indole (17). ^{1}H NMR ($CDCl_3$) δ 2.24 (d, *J* = 0.8 Hz, 3H), 6.68 (s, 1H), 6.89 (dd, *J* = 7.2, 0.8 Hz, 1H), 6.99 (d, *J* = 1.0 Hz, 1H), 7.11-7.32 (m, 12H), 7.99 (s, 1H); ^{13}C NMR ($CDCl_3$) 13.7, 110.4, 112.8, 121.7, 121.8, 123.2, 126.8, 127.3, 128.3 (2C), 128.4, 129.6, 130.5, 137.6, 137.9, 138.1, 141.3, 141.4; IR ($CDCl_3$) 3422, 3053, 3021, 1695 cm^{-1}; HRMS m/z 309.1522 (calcd for $C_{23}H_{19}N$, 309.1518).

3-Methyl-4-(1-methyl-2-phenylvinyl)-1*H*-indole (18a). ^{1}H NMR ($CDCl_3$) δ 2.34-2.35 (m, 6H), 6.51 (d, *J* = 1.0 Hz, 1H), 6.96-6.99 (m, 2H), 7.18 (t, *J* = 8.0 Hz, 1H), 7.26-7.31 (m, 3H), 7.39-7.43 (m, 4H), 7.96 (s, 1H); ^{13}C NMR ($CDCl_3$) 12.8, 21.8, 110.1, 112.4, 119.1, 121.9, 122.8, 126.5, 128.4, 129.2, 129.4, 137.3, 138.5 (2C), 139.8; IR ($CDCl_3$) 3416, 3051, 2919, 1597 cm^{-1}; HRMS m/z 247.1365 (calcd for $C_{18}H_{17}N$, 247.1361).

5-(1,2-Diphenylvinyl)-1,2,3,9-tetrahydro-carbazol-4-one (19). ^{1}H NMR ($CDCl_3$) δ 2.05-2.12 (m, 2H), 2.48 (t, *J* = 6.1 Hz, 2H), 2.80 (t, *J* = 6.2 Hz, 2H), 6.51 (s, 1H), 7.02-7.34 (m, 13H), 9.72 (s, 1H); NMR ($CDCl_3$) 23.4, 23.8, 38.8, 110.8, 113.9, 123.9, 124.4, 125.4, 126.2, 126.8, 127.2, 127.3, 127.9, 128.0, 129.5, 134.0, 137.0, 138.5, 143.4, 144.2, 191.9; IR ($CDCl_3$) 3168, 3052, 2952, 1621 cm^{-1}; HRMS m/z 363.1631 (calcd for $C_{26}H_{21}NO$, 363.1623).

1-(1-Benzylidenepropyl)-3-phenoxydibenzofuran (21a). ^{1}H NMR ($CDCl_3$) δ 1.11 (t, *J* = 7.5 Hz, 3H), 7.87 (q, *J* = 7.5 Hz, 2 H), 6.76 (s, 1H), 7.05 (d, *J* = 2.2 Hz, 1H), 7.04-7.58 (m, 14H), 8.01 (dd, *J* = 7.7, 0.6 Hz, 1H); ^{13}C NMR ($CDCl_3$) 13.3, 25.6, 100.9, 111.7, 114.5, 117.8, 119.3, 122.2, 123.0, 123.9, 124.2, 126.4, 127.3, 128.4, 128.8, 129.8, 130.2, 137.6, 140.9, 142.5, 156.9, 157.4, 157.5; IR ($CDCl_3$) 3023, 2966, 1628 cm^{-1}; HRMS m/z 390.1624 (calcd for $C_{28}H_{22}O_2$, 390.1620).

1-(1-Benzylidenepropyl)-3-methoxydibenzofuran (22a). ^{1}H NMR ($CDCl_3$) δ 1.11 (t, *J* = 7.6 Hz, 3H), 2.88 (q, *J* = 7.6 Hz, 2H), 3.94 (s, 3H), 6.73 (s, 1H), 6.87 (s, 1H), 7.05 (s, 1H), 7.21-7.57 (m, 8H), 7.82 (d, *J* = 7.2 Hz, 1H); ^{13}C NMR ($CDCl_3$) 13.2, 25.6, 56.0, 95.2, 111.0, 111.5, 115.5, 121.9, 122.8, 124.6, 125.7, 127.2, 128.7, 129.5, 137.7, 140.6, 142.9, 156.7, 158.0, 159.7; IR ($CDCl_3$) 3056, 3022, 2964, 1627 cm^{-1}; HRMS m/z 328.1468 (calcd for $C_{23}H_{20}O_2$, 328.1463).

3-Methoxy-1-(1-methyl-2-phenylvinyl)dibenzofuran (23a). ^{1}H NMR ($CDCl_3$) δ 2.45 (d, *J* = 1.3 Hz, 3H), 3.9 (s, 3H), 6.81 (s, 1H), 6.88 (d, *J* = 2.2 Hz, 1H), 7.07 (d, *J* = 2.2 Hz, 1H), 7.25-7.57 (m, 8H), 7.93 (d, *J* = 7.2 Hz, 1H); ^{13}C NMR ($CDCl_3$) 19.6, 56.0, 95.2, 110.6, 111.5, 114.7, 121.9, 122.8, 124.4, 125.8, 127.1, 128.7, 129.3, 130.2, 130.2, 136.5, 137.8, 142.2, 156.7, 158.0, 159.9; IR ($CDCl_3$) 3054, 2938, 2835, 1627 cm^{-1}; HRMS m/z 314.1311 (calcd for $C_{22}H_{18}O_2$, 314.1307).

3-Methoxy-1-(1,3,3-trimethylbut-1-enyl)dibenzofuran (24a). ^{1}H NMR ($CDCl_3$) δ 1.31 (s, 9H), 2.23 (d, *J* = 1.0 Hz, 1H), 3.90 (s, 1H), 5.68 (d, *J* = 1.0 Hz, 1H), 6.69 (d, *J* = 1.7 Hz, 1H), 6.97 (d, *J* = 1.7 Hz, 1H), 7.25-7.38 (m, 3H), 7.51 (d, *J* = 6.1 Hz, 1H), 7.88 (d, *J* = 6.0 Hz, 1H); ^{13}C NMR ($CDCl_3$) 18.9, 31.2, 56.0, 94.5, 110.7, 111.4, 121.8, 122.6, 124.5, 125.5, 130.1, 133.2, 140.5, 143.8, 156.5, 157.8, 159.8; IR ($CDCl_3$) 2956, 2865, 1628 cm^{-1}; HRMS m/z 294.1624 (calcd for $C_{20}H_{22}O_2$, 294.1620).

3-Methoxy-1-(1-propylpent-1-enyl)dibenzofuran (25). ^{1}H NMR ($CDCl_3$) δ 0.89 (t, *J* = 7.3 Hz, 3H), 1.02 (t, *J* = 7.4 Hz, 3H), 1.32-1.45 (m, 2H), 1.48-1.60 (m, 2H), 2.31 (q, *J* = 7.3 Hz, 2H), 2.58 (t, *J* = 7.4 Hz, 2H), 3.90 (s, 3H), 5.67 (t, *J* = 7.2 Hz, 1H), 6.71 (d, *J* = 2.2 Hz, 1H), 6.99 (d, *J* = 2.2 Hz, 1H), 7.22-7.38 (m, 2H), 7.52 (d, *J* = 8.2 Hz, 1H), 7.88 (d, *J* = 7.8 Hz, 1H); ^{13}C NMR ($CDCl_3$) 14.3, 14.4, 22.0, 23.2, 30.6, 33.6, 55.9, 94.5, 111.3, 111.4, 115.2, 121.9, 122.6, 124.7, 125.5, 130.9, 138.8, 141.4, 156.6, 157.8, 159.6; IR ($CDCl_3$) 2957, 2930, 2869 cm^{-1}; HRMS m/z 308.1781 (calcd for $C_{21}H_{24}O_2$, 308.1776).

(*E*)-1-(1,2-Diphenylvinyl)-3-methoxydibenzofuran (26). ^{1}H NMR ($CDCl_3$) δ 3.86 (s, 3H), 6.72 (s, 1H), 7.06-7.37 (m, 14H), 7.54 (d, *J* = 8.1 Hz, 1H), 7.92 (d, *J* = 8.1 Hz, 1H); ^{13}C NMR ($CDCl_3$) 56.0, 95.7, 111.5, 112.8, 115.8, 122.0, 122.8, 124.5, 125.9, 127.5, 127.9, 128.5, 128.8, 129.8, 130.3, 131.6, 137.1, 140.0, 140.1, 140.9, 156.8, 158.2, 159.6; IR ($CDCl_3$) 3054, 3022, 2958, 1629 cm^{-1}; HRMS m/z 376.1470 (calcd for $C_{27}H_{20}O_2$, 376.1463).

(*E*)-1-(2-Deutero-1,2-diphenylvinyl)-2,4-dideutero-3-methoxydibenzofuran (26-d). This compound contains 70% deuterium in the vinylic position: ^{1}H NMR ($CDCl_3$) δ 3.86 (s, 3H), 6.72 (s, 0.30H), 7.09-7.37 (m, 12H), 7.54 (d, *J* = 8.1 Hz, 1H), 7.92 (d, *J* = 8.1 Hz, 1H). Compound **26-d** obtained from the reaction conducted in the presence of 10 equiv of D_2O: ^{1}H NMR ($CDCl_3$) δ 3.86 (s, 3H), 6.72 (s, 0.13H), 7.37-7.37 (m, 12H), 7.54 (d, *J* = 8.1 Hz, 1H), 7.92 (d, *J* = 8.1 Hz, 1H).

Ethyl 4-[2-(3-methoxydibenzofuran-1-yl)but-1-enyl]benzoate (27a). ^{1}H NMR ($CDCl_3$) δ 1.09 (t, *J* = 7.4 Hz, 3H), 1.43 (t, *J* = 7.1 Hz, 3H), 2.86 (q, *J* = 7.4 Hz, 2H), 3.93 (s, 3H), 4.42 (q, *J* = 7.1 Hz, 2H), 6.72 (s, 1H), 6.83 (d, *J* = 2.2 Hz, 1H), 7.06 (d, *J* = 2.1 Hz, 1H), 7.22 (t, *J* = 7.7 Hz, 1H), 7.33-7.55 (m, 4 H), 7.87 (d, *J* = 7.7 Hz, 1H), 8.12 (d, *J* = 8.3 Hz, 2H); ^{13}C NMR ($CDCl_3$) 13.2, 14.6, 25.7, 56.0, 61.2, 95.4, 111.0, 111.6, 115.3, 121.7, 122.8, 124.4, 125.8, 128.8, 128.8, 129.1, 129.9, 140.0, 142.2, 145.0, 156.7, 158.0, 159.7, 166.7; IR ($CDCl_3$) 2969, 2935, 2873, 1716 cm^{-1}; HRMS m/z 400.1679 (calcd for $C_{26}H_{24}O_4$, 400.1675).

3-Methoxy-1-[1-(2-methoxybenzylidene)propyl]dibenzofuran (28a). ^{1}H NMR ($CDCl_3$) δ 1.01 (t, *J* = 7.6 Hz, 3H), 2.77 (q, 7.5 Hz, 2H), 3.84 (s, 3H), 3.93 (s, 3H), 6.79 (s, 1H), 6.87 (d, *J* = 2.2 Hz, 1H), 6.95 (d, *J* = 8.2 Hz, 1H), 7.03-7.08 (m, 2H), 7.19-7.25 (m, 1H), 7.30-7.38 (m, 2H), 7.47-7.54 (m, 2H), 8.14 (d, *J* = 7.2 Hz, 1H); ^{13}C NMR ($CDCl_3$) 13.3, 25.8, 55.5, 56.0, 95.0, 110.8, 110.9, 111.3, 115.7, 120.5, 122.4, 122.6, 124.7, 125.6, 126.8, 128.6, 130.0, 140.5, 142.3, 156.6, 157.7, 157.9, 159.6; IR ($CDCl_3$) 2962, 2933, 2834, 1627 cm^{-1}; HRMS m/z 358.1573 (calcd for $C_{24}H_{22}O_3$, 358.1569).

References

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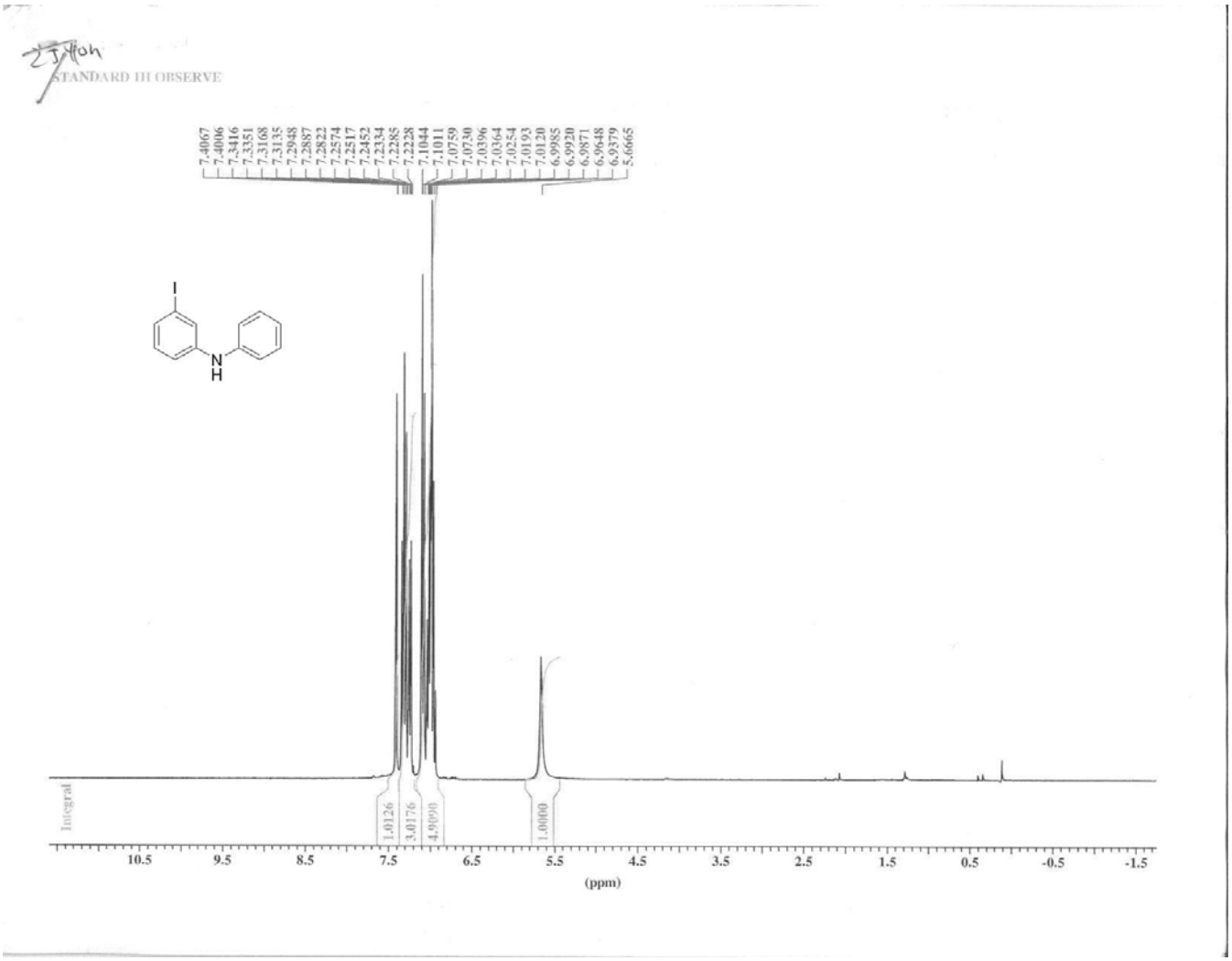
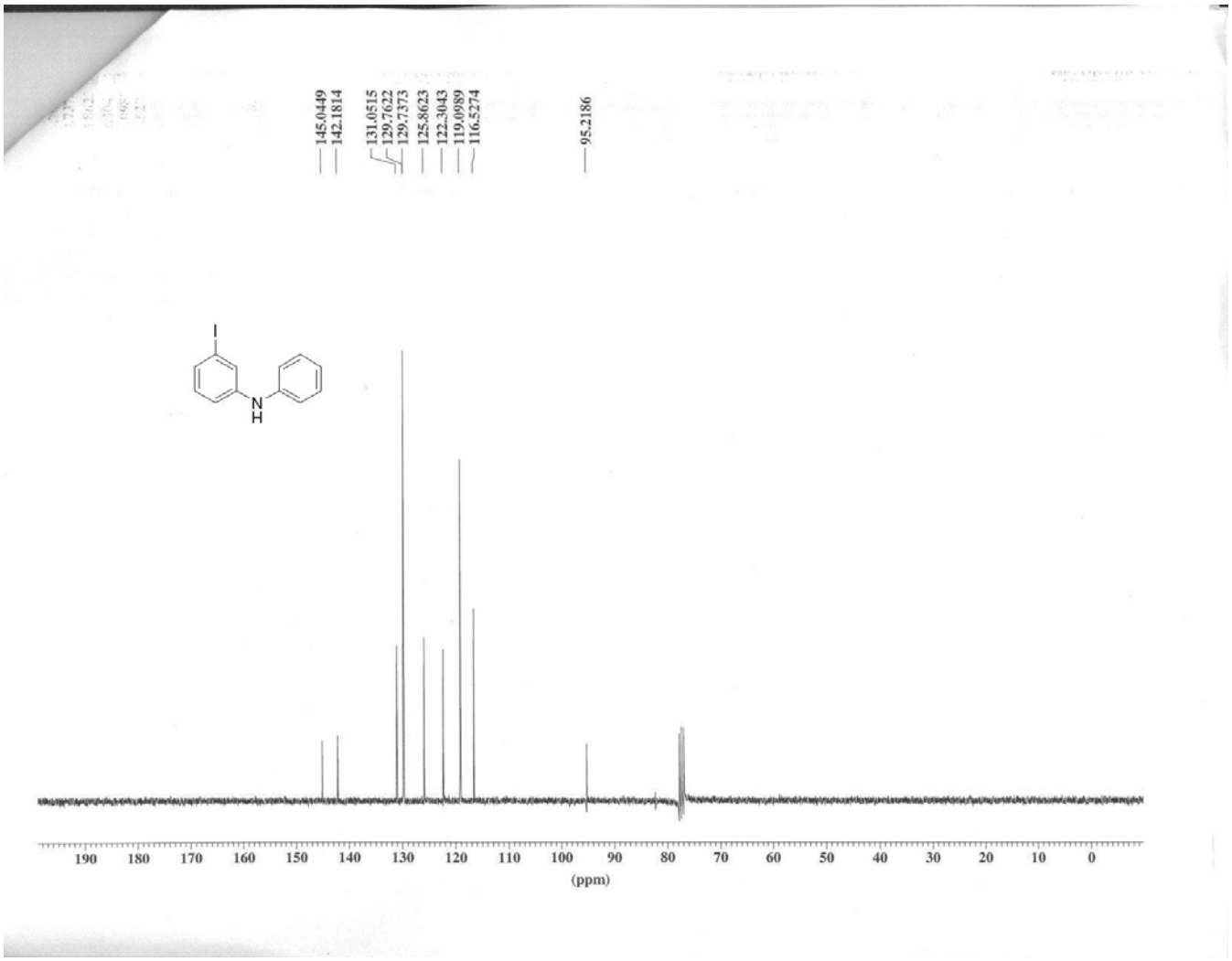
IV. Characterization Data for Selected Compounds.

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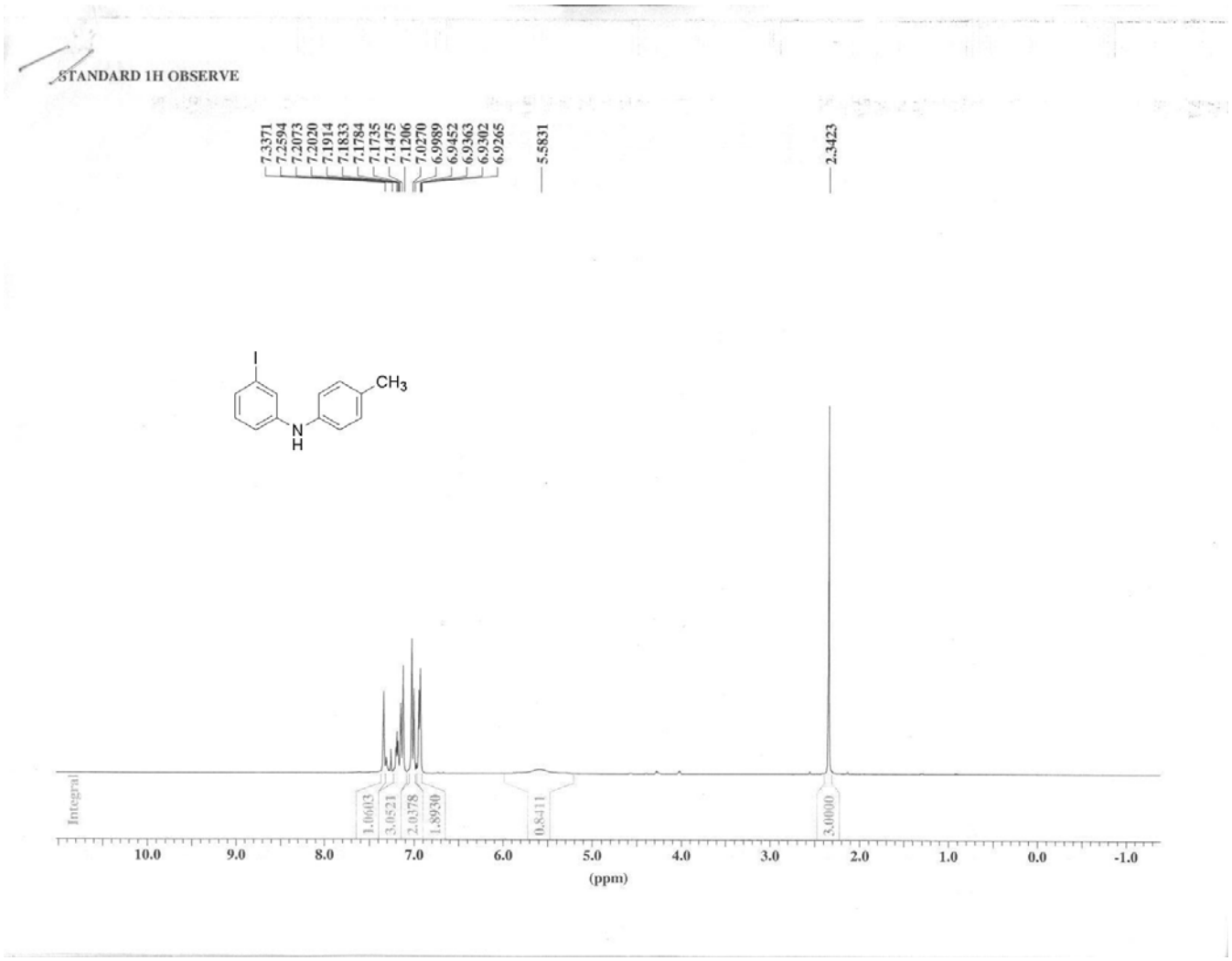
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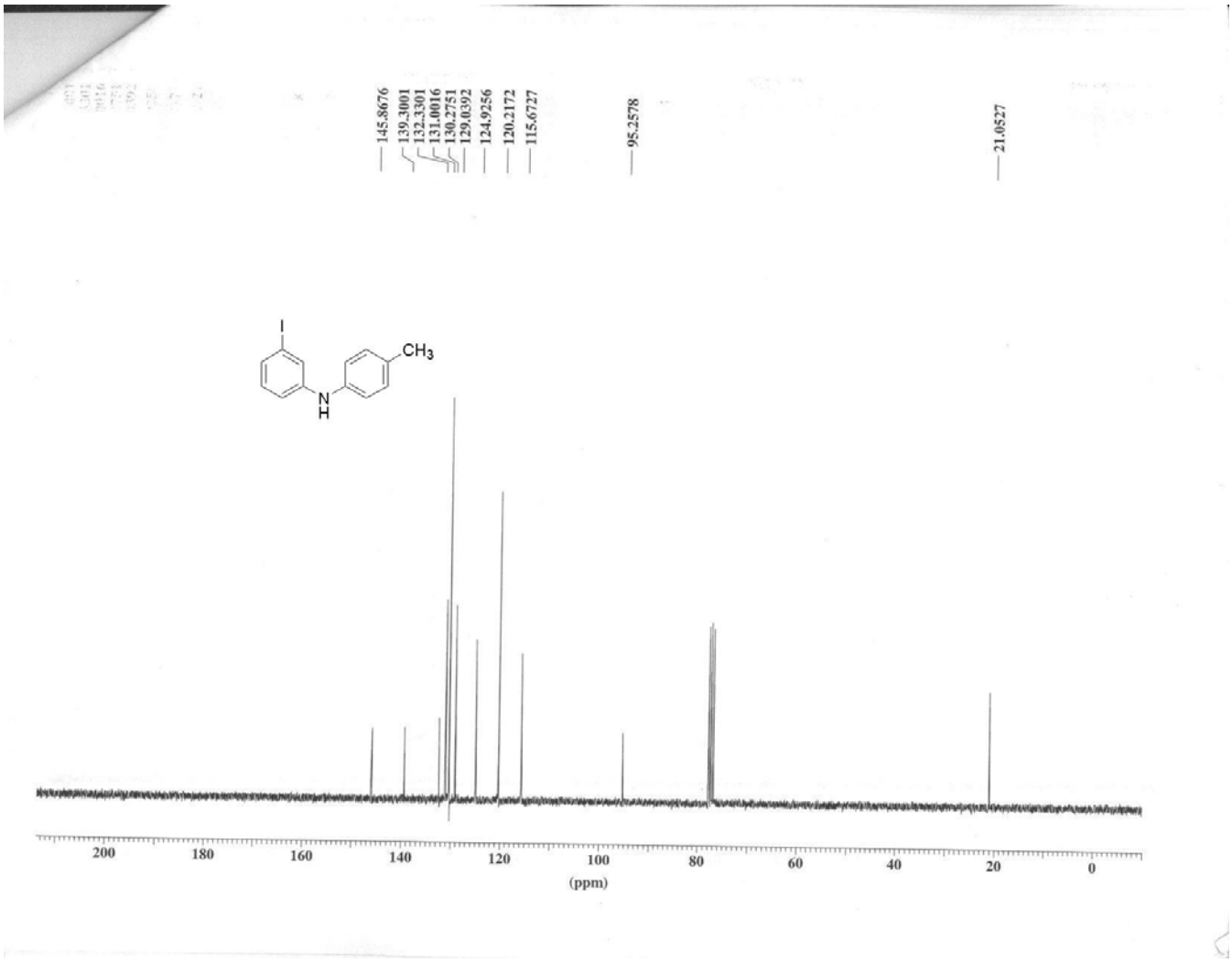
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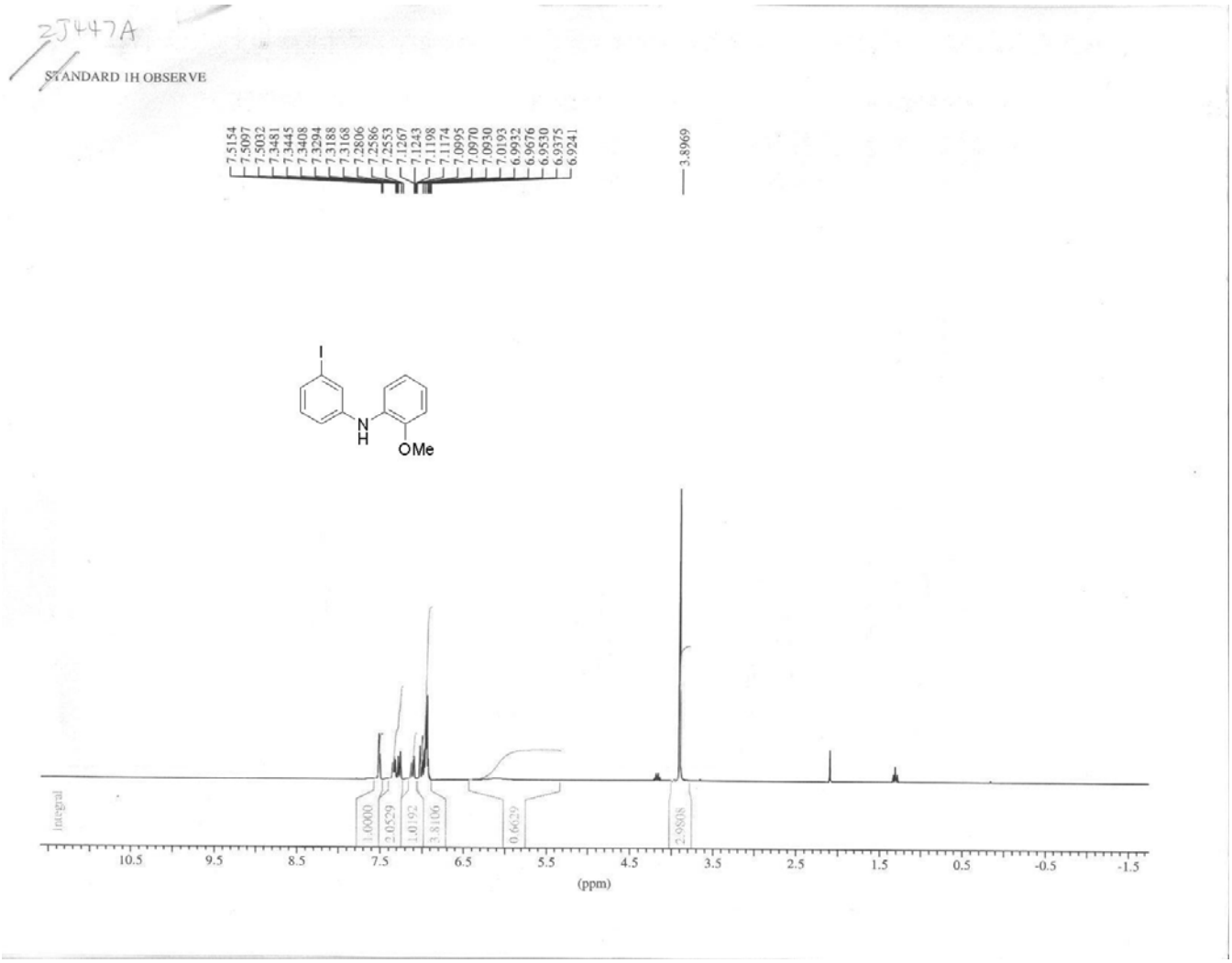
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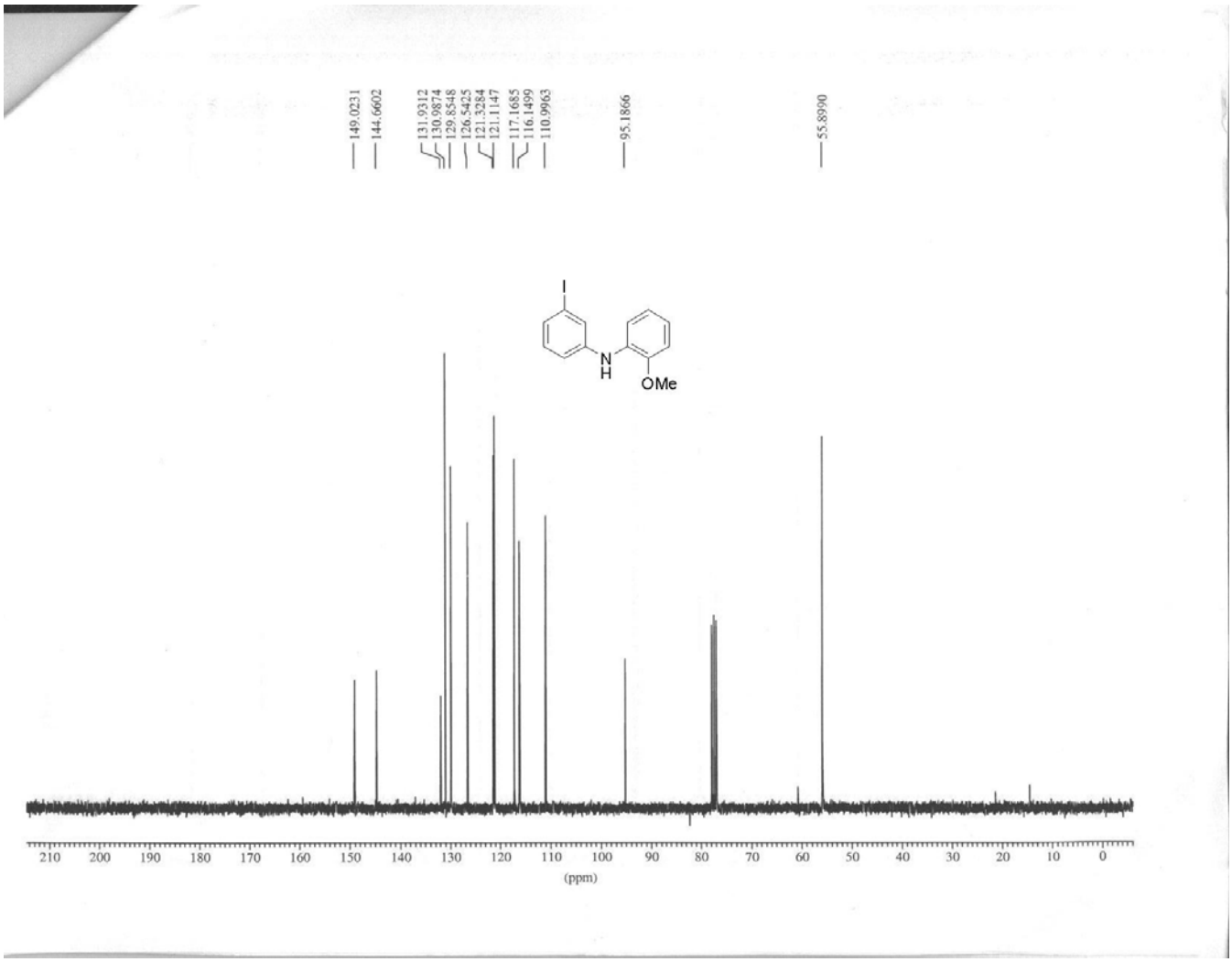
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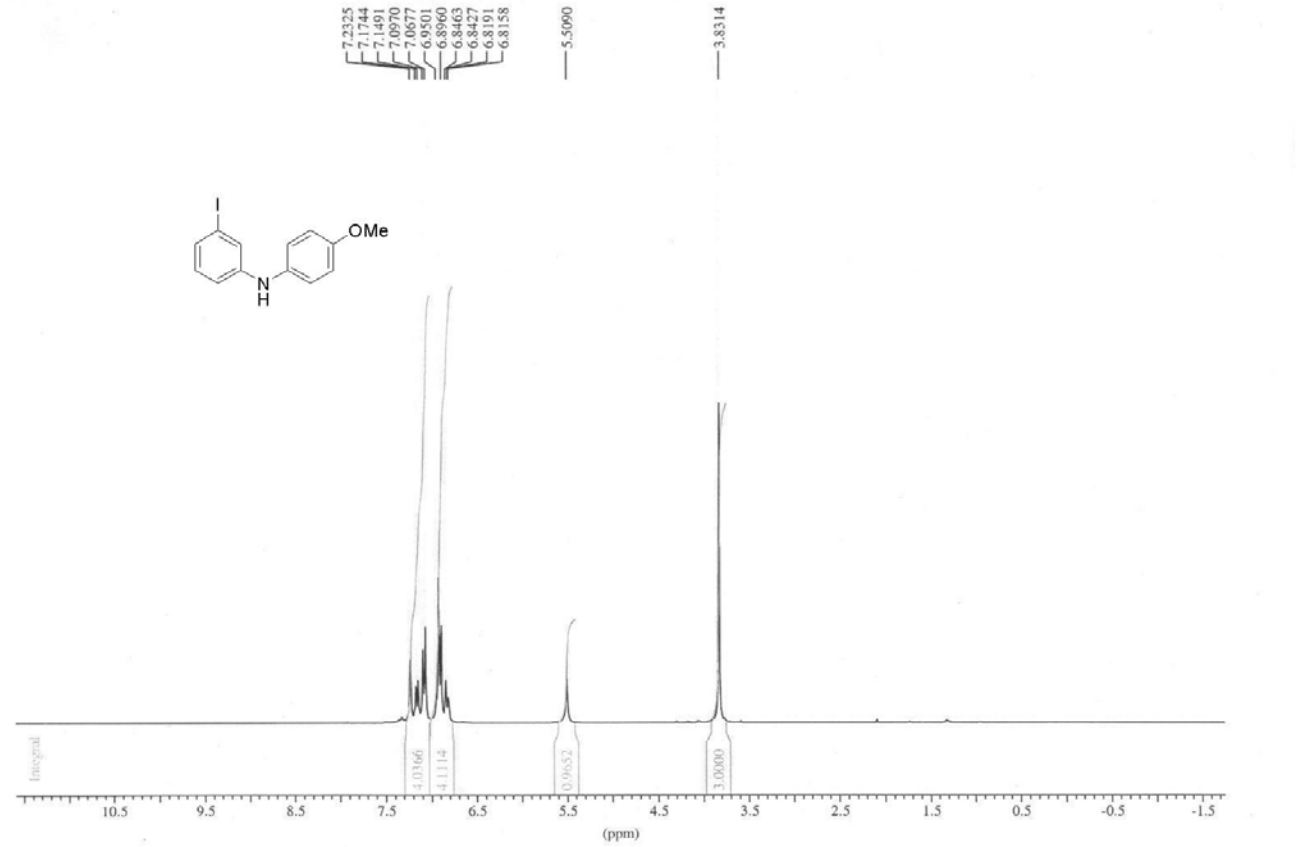

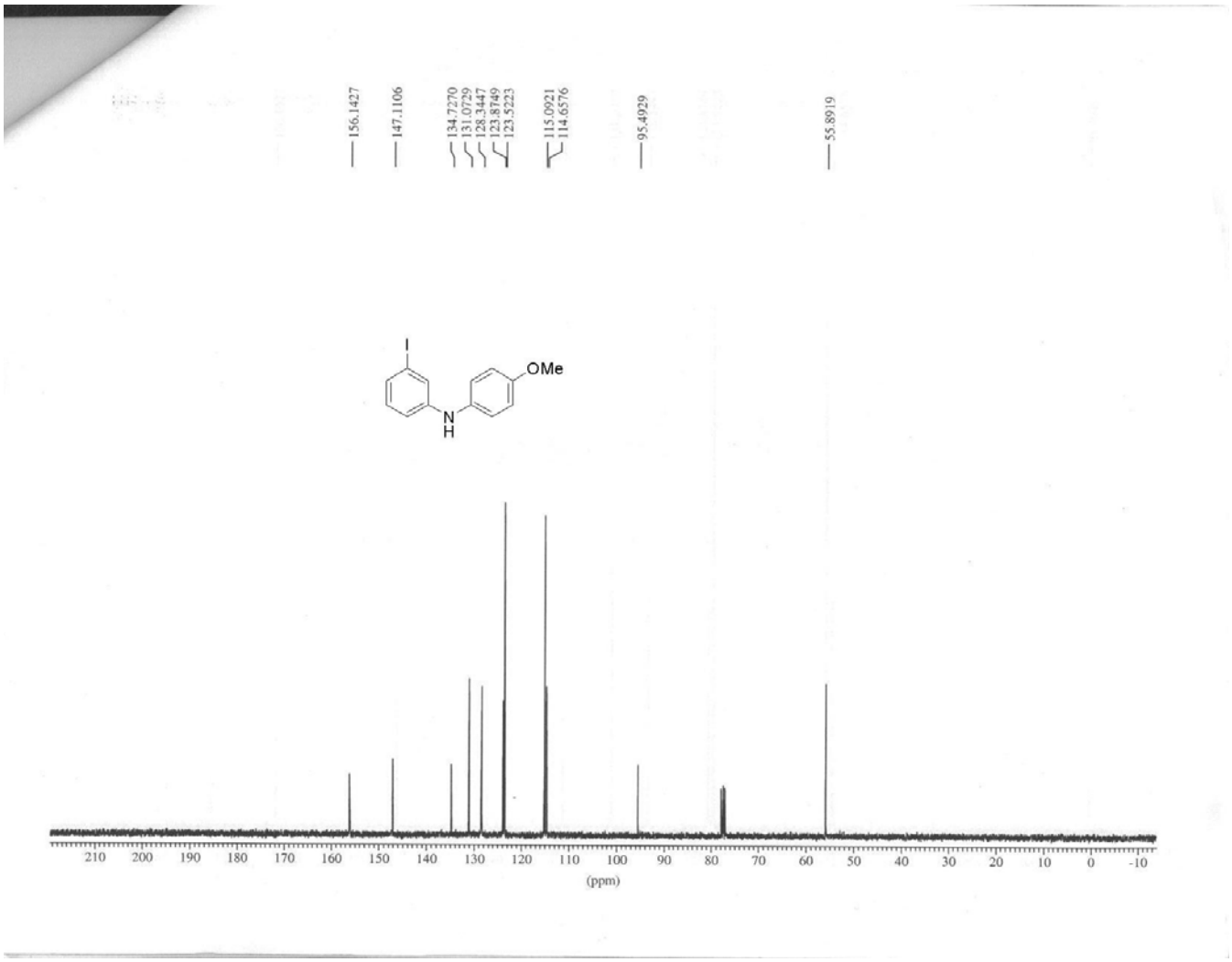
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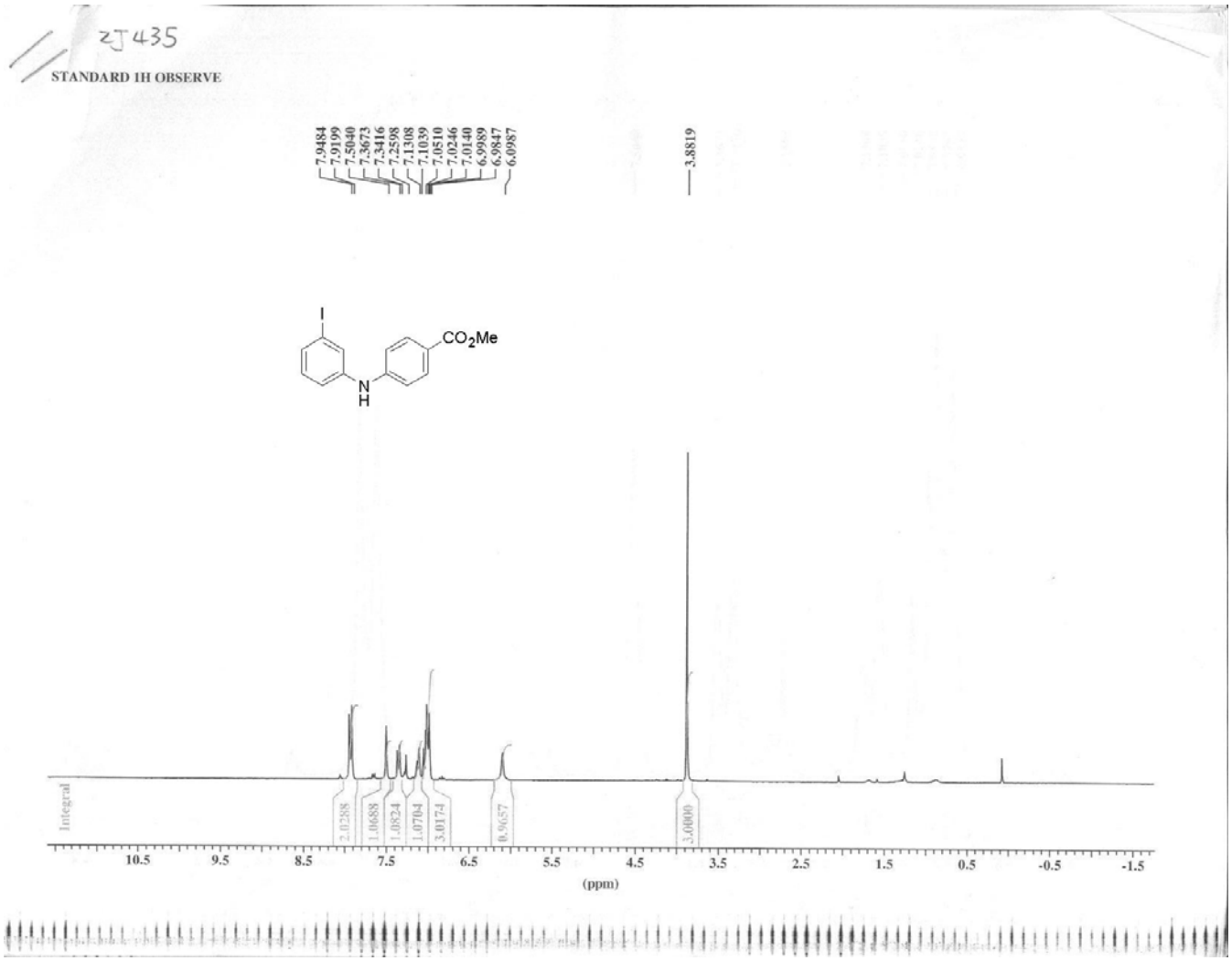
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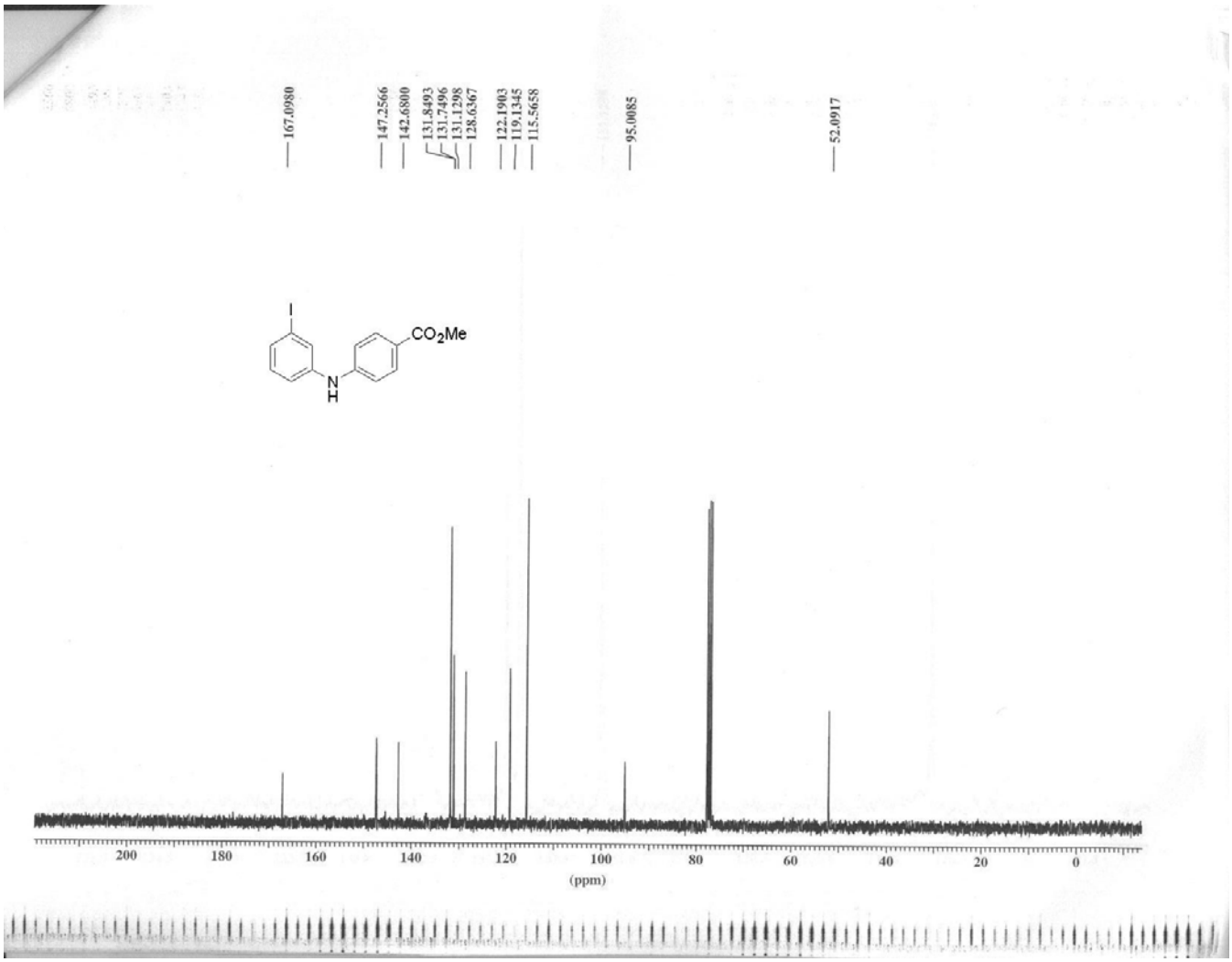
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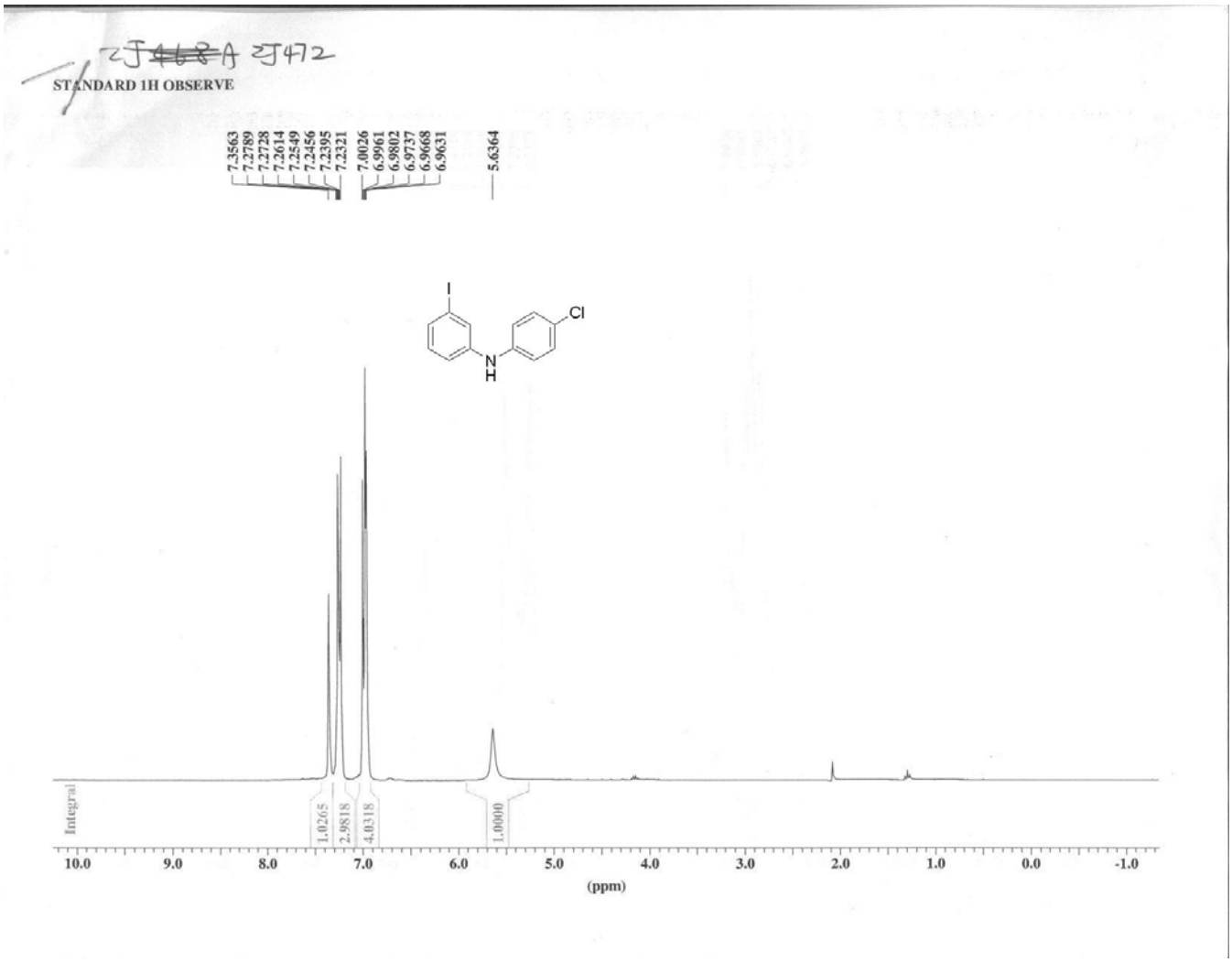
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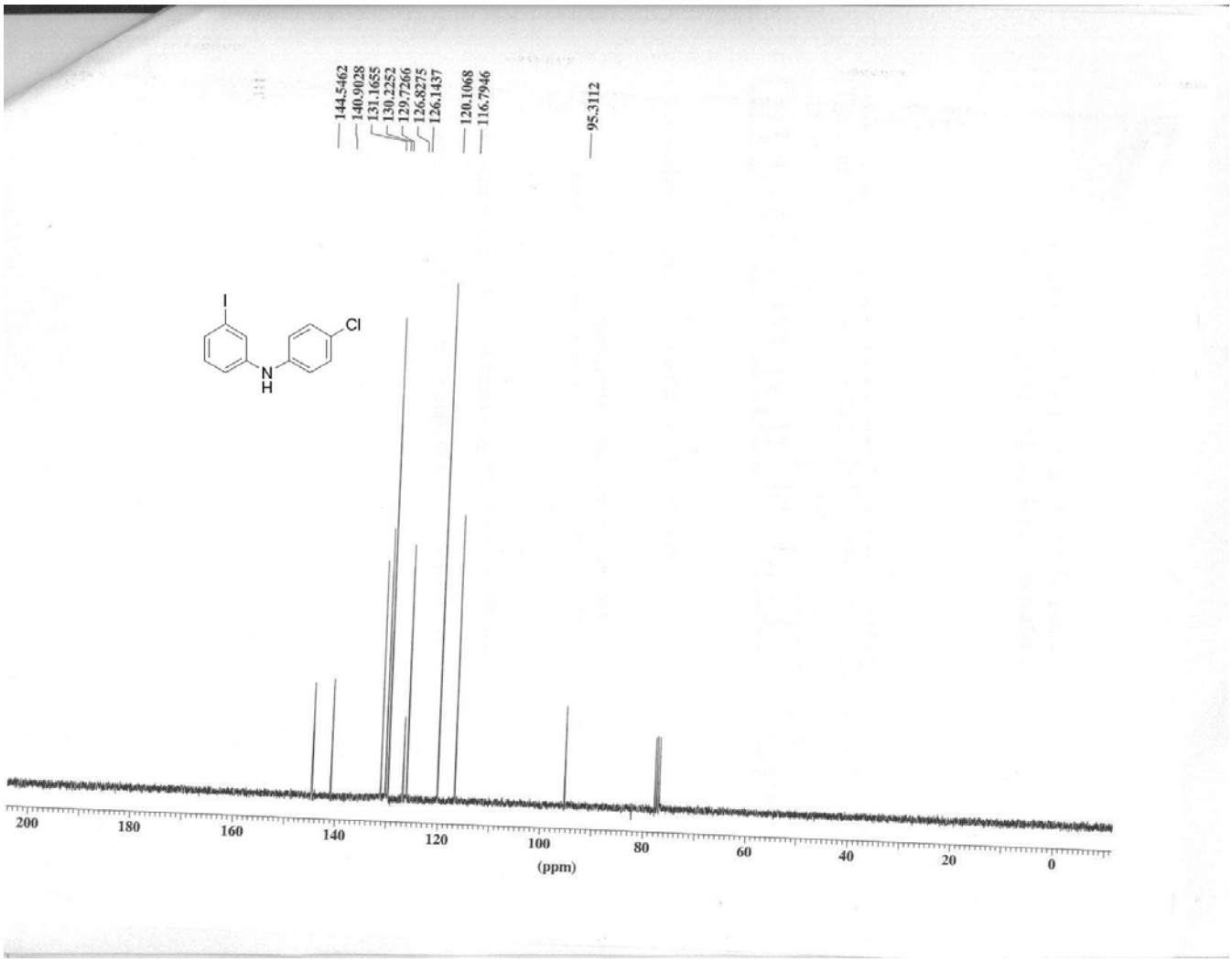
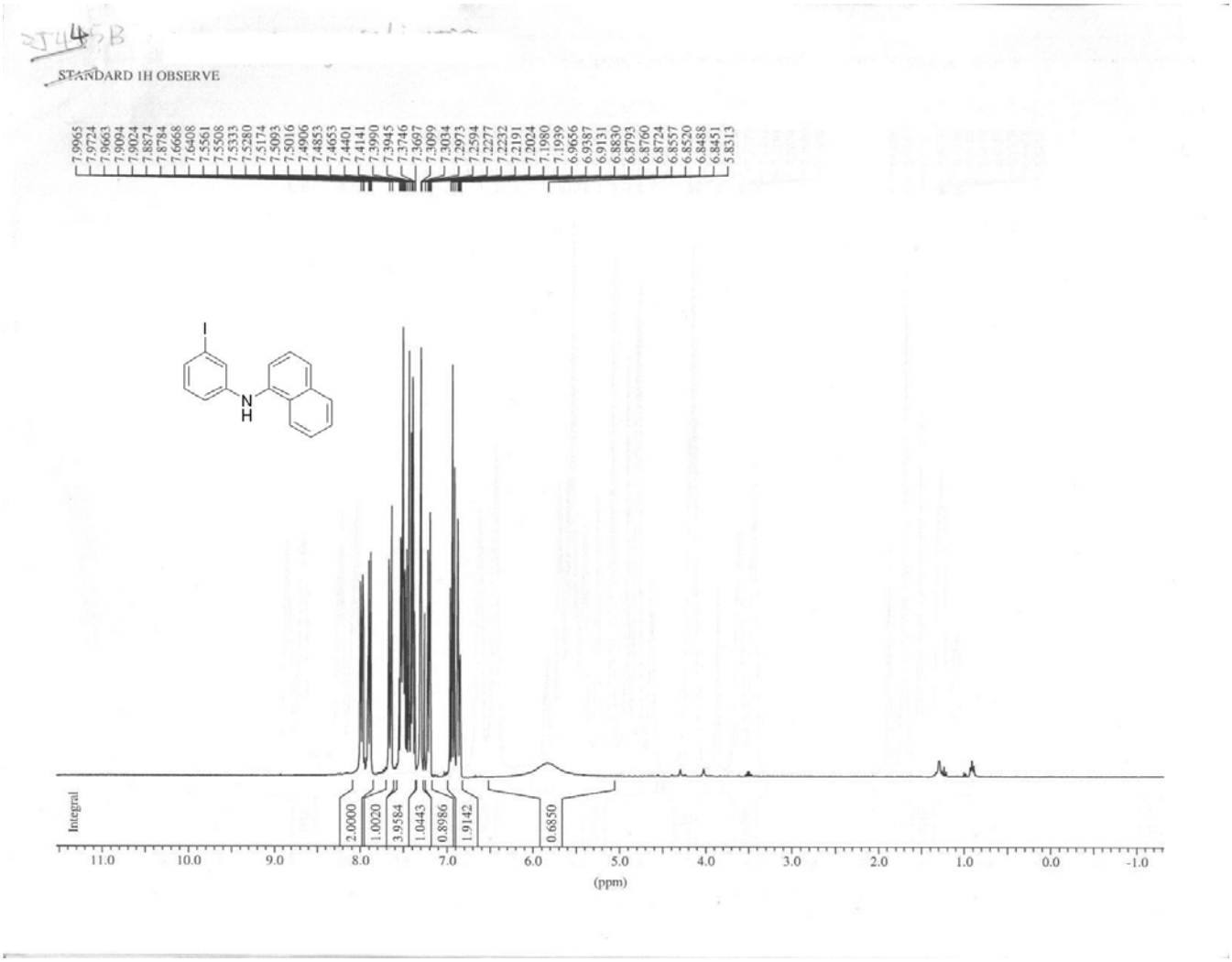
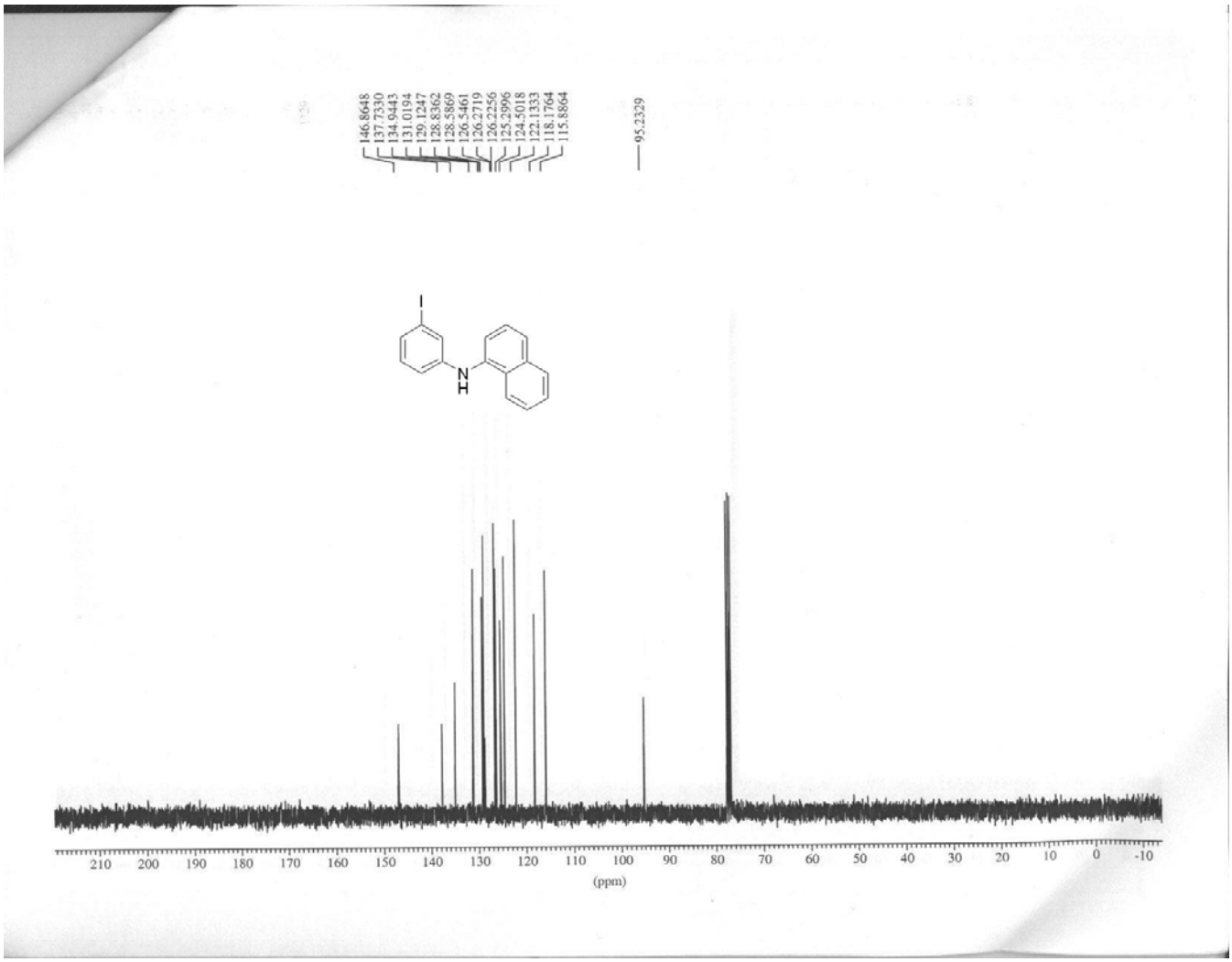
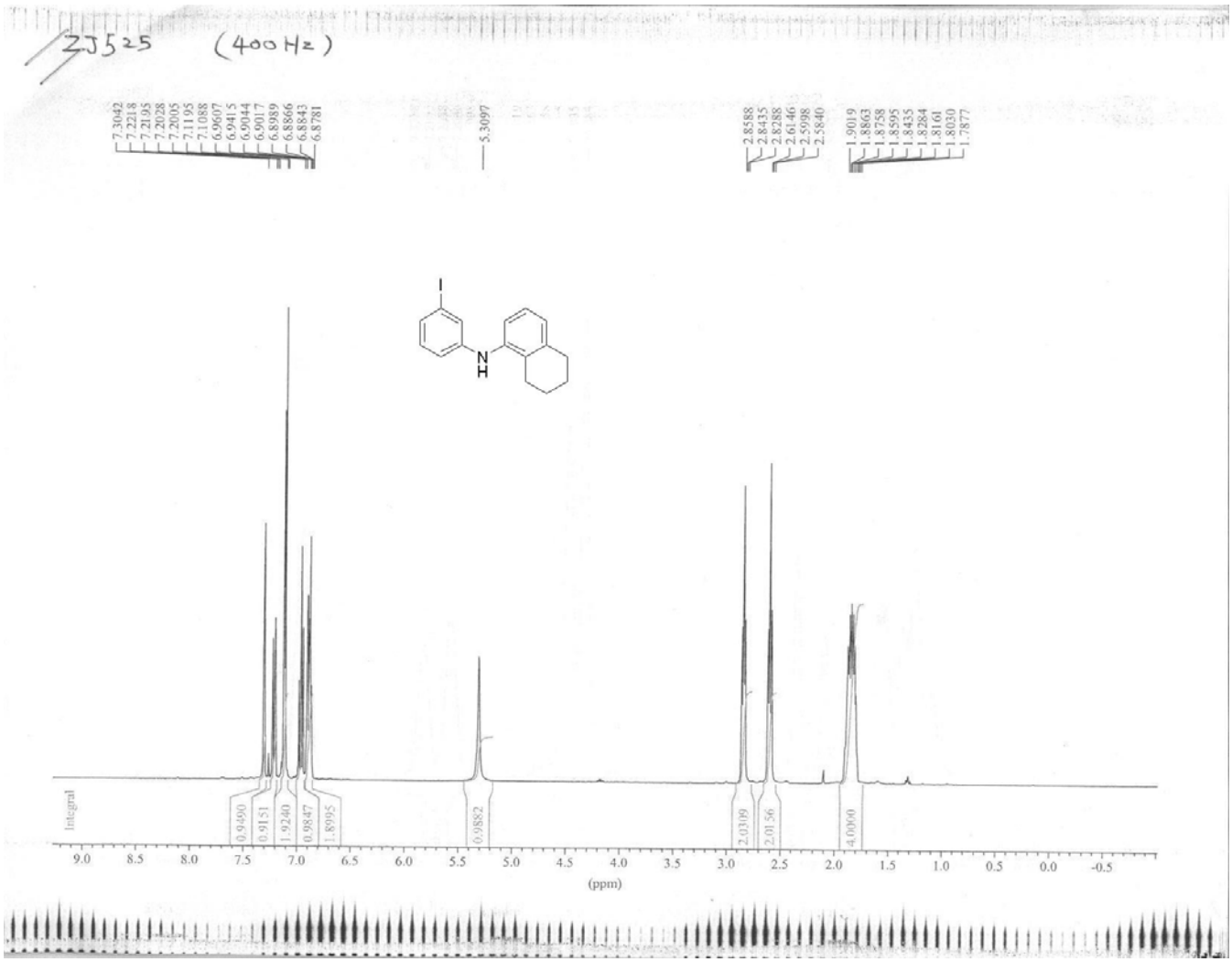
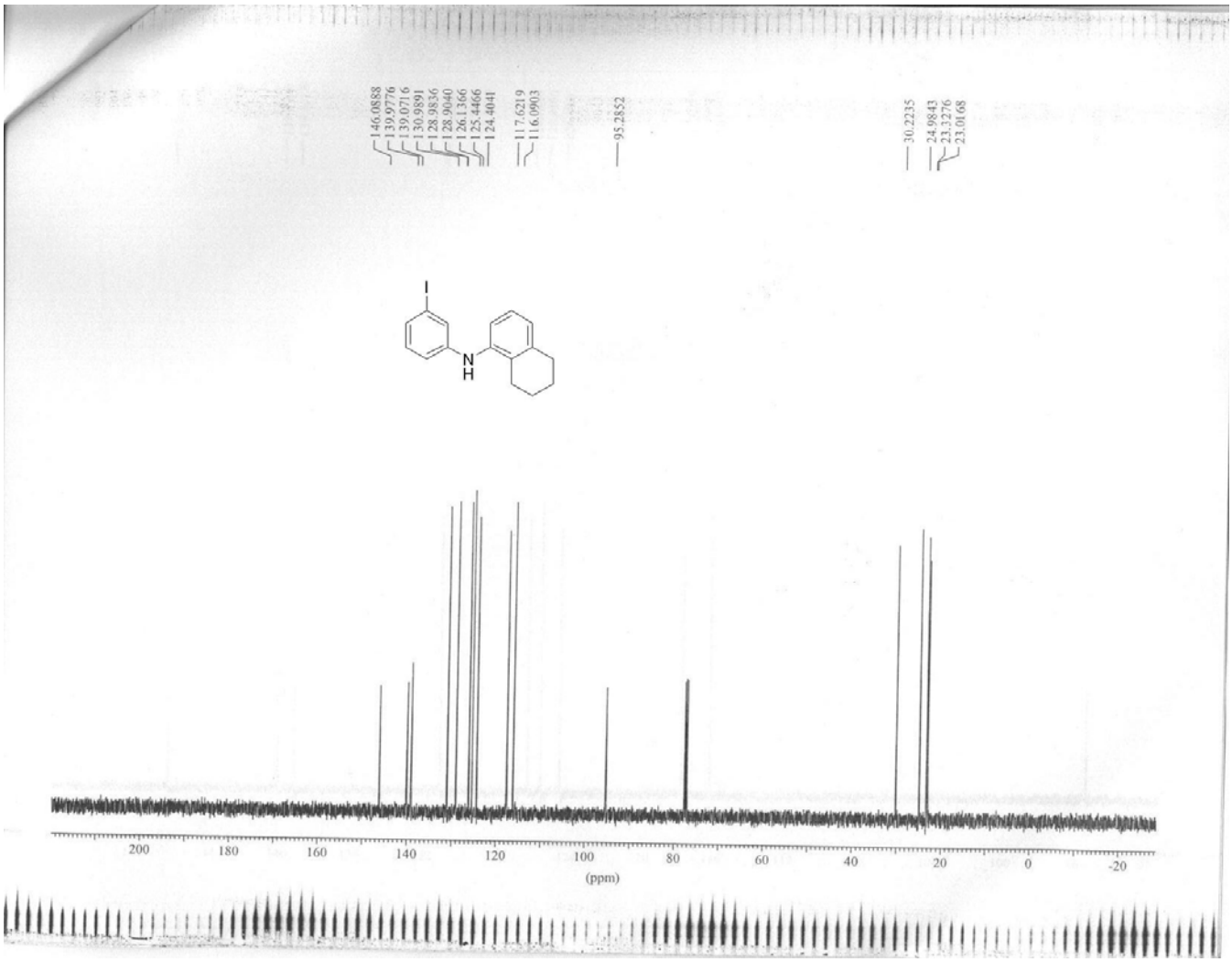
7.2321
7.0026
6.9961
6.9802
6.9737
6.9668
6.9631
5.6364
I
Cl
N
H
Integral
1.0265
2.9818
4.0318
1.0000
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
(ppm)

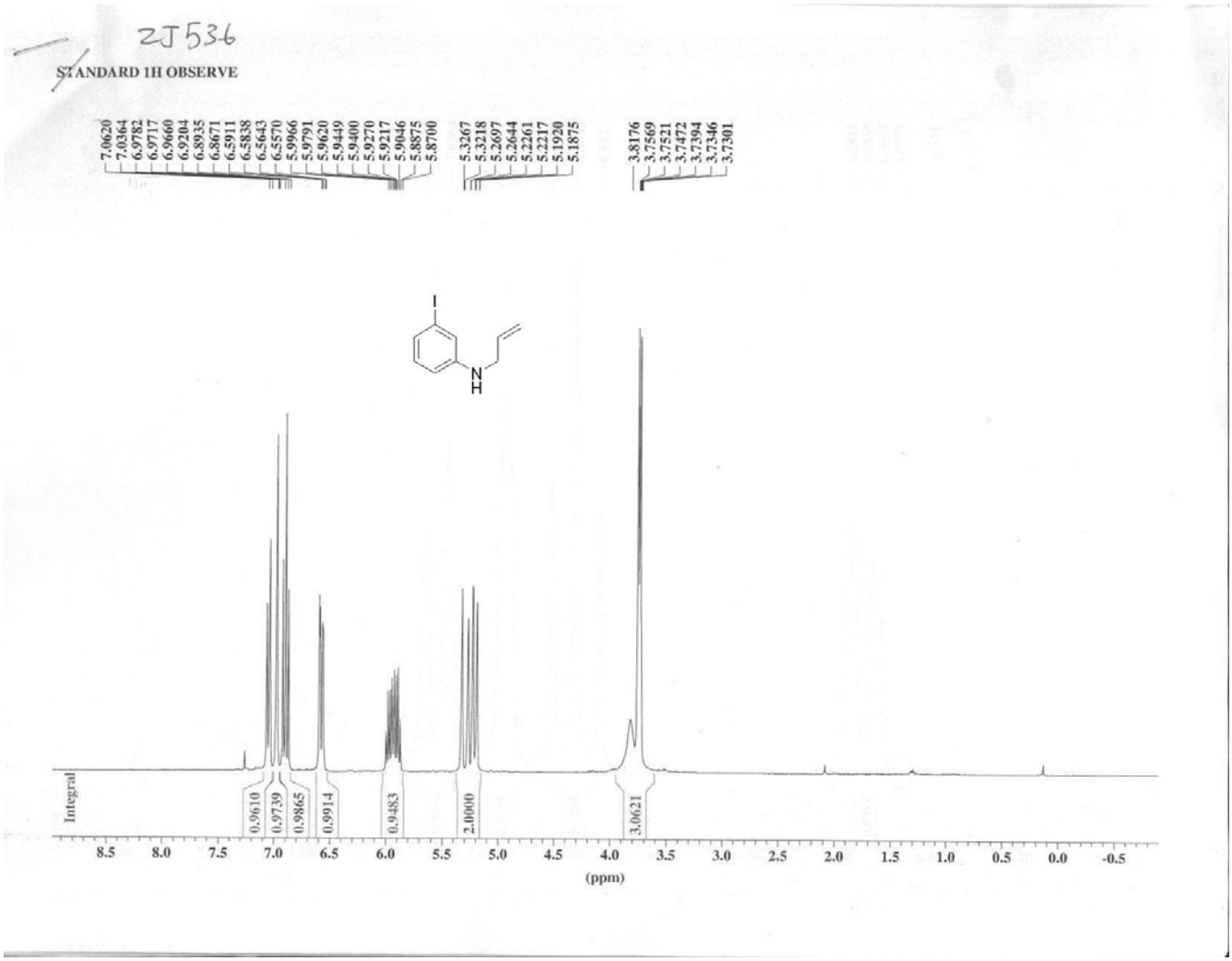

144.5462
140.9028
131.1655
130.2252
129.7266
126.8275
126.1437
120.1068
116.7946
95.3112
I
Cl
N
H
200
180
160
140
120
100
80
60
40
20
0
(ppm)

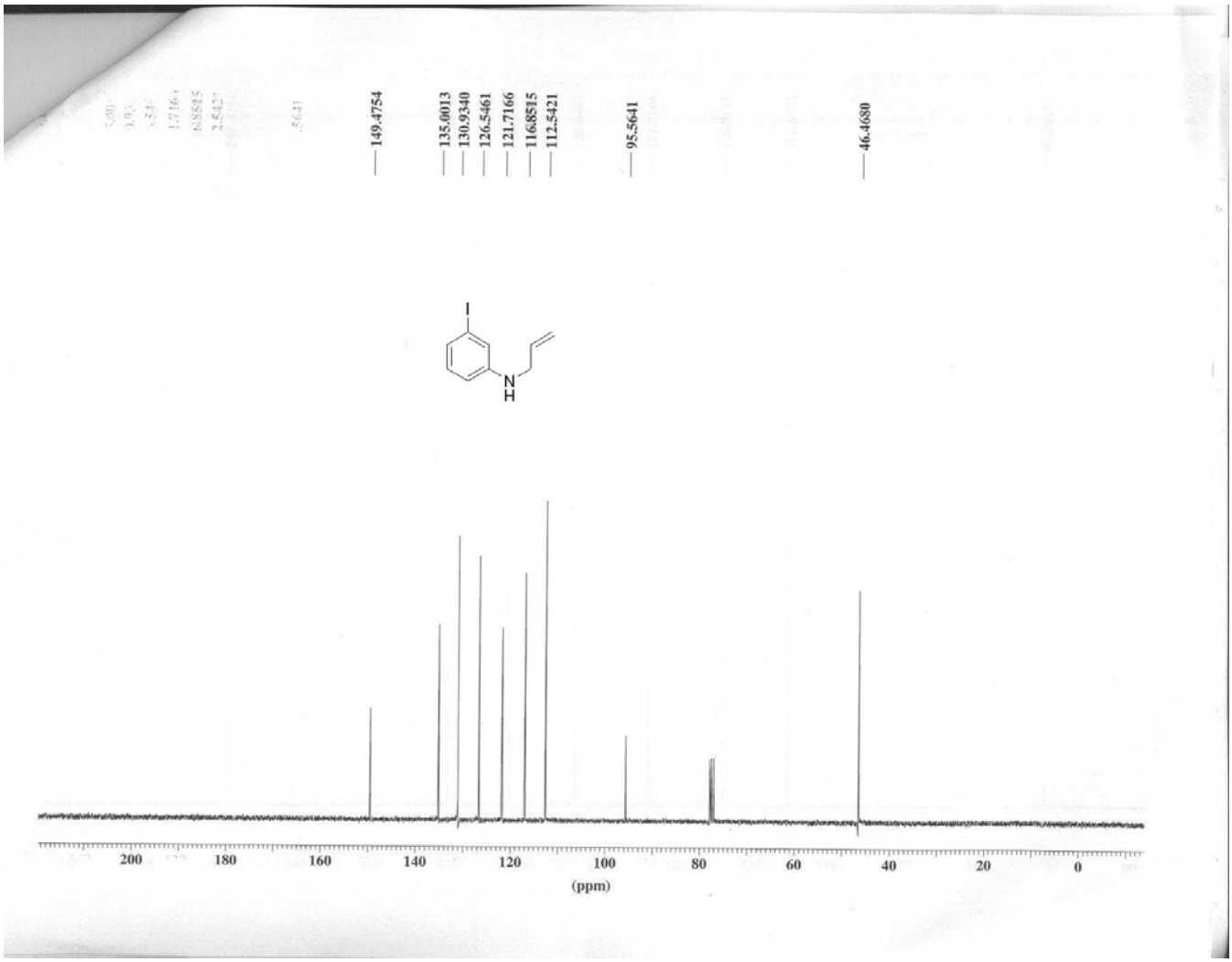

STANDARD 1H OBSERVE
7.9965
7.9724
7.9663
7.9094
7.9024
7.8874
7.8784
7.6668
7.6408
7.5561
7.5508
7.5333
7.5280
7.5174
7.5093
7.5016
7.4906
7.4853
7.4653
7.4401
7.4141
7.3990
7.3945
7.3746
7.3697
7.3099
7.3034
7.2973
7.2594
7.2277
7.2232
7.2191
7.2024
7.1980
7.1939
6.9656
6.9387
6.9131
6.8830
6.8793
6.8760
6.8724
6.8557
6.8520
6.8488
6.8451
5.8313
I
N
H
Integral
2.0000
1.0020
3.9584
1.0443
0.8986
1.9142
0.6850
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
(ppm)

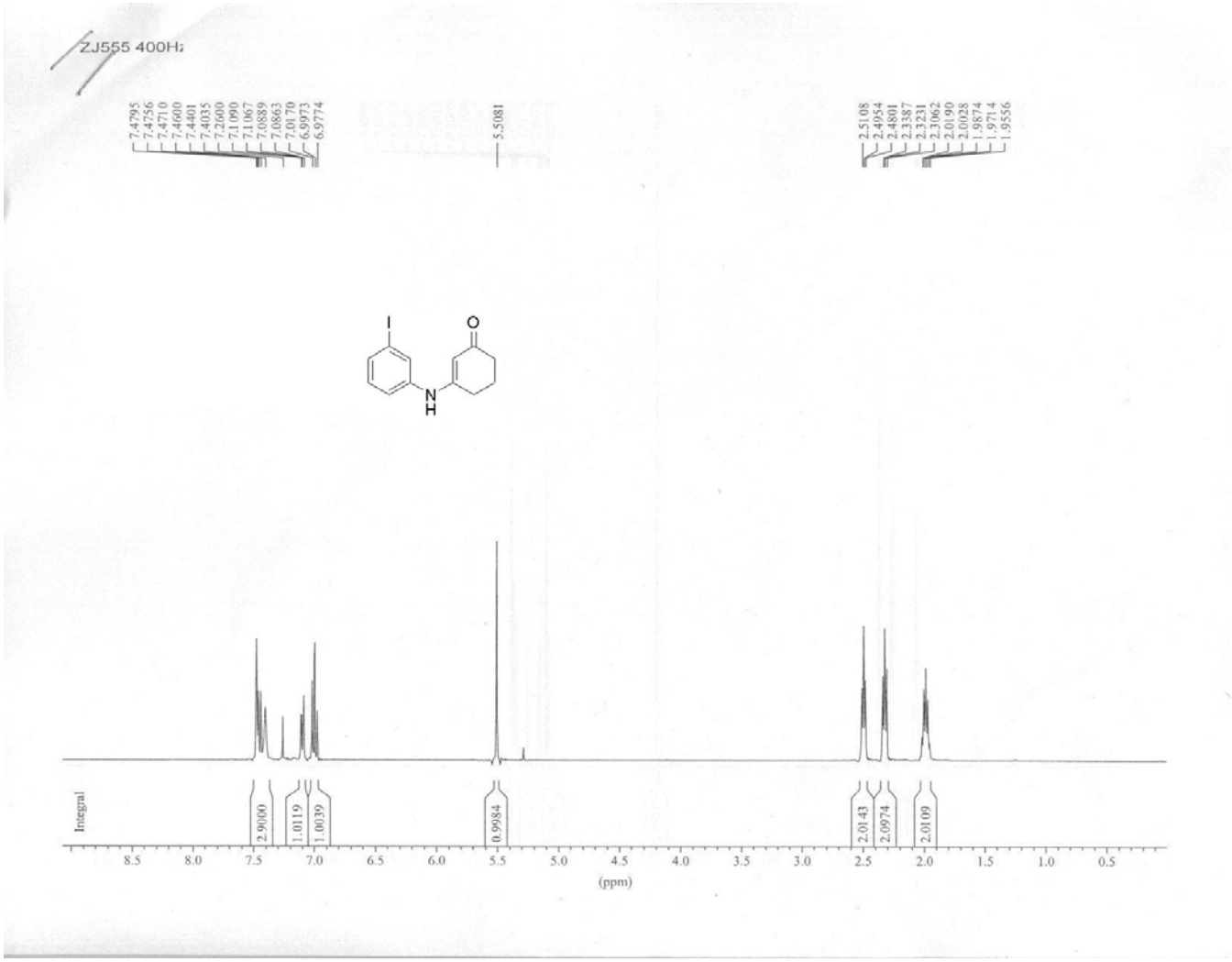

146.8648
137.7330
134.9443
131.0194
129.1247
128.8362
128.5869
126.5461
126.2719
126.2256
125.2996
124.5018
122.1333
118.1764
115.8864
95.2329
I
N
H
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
(ppm)

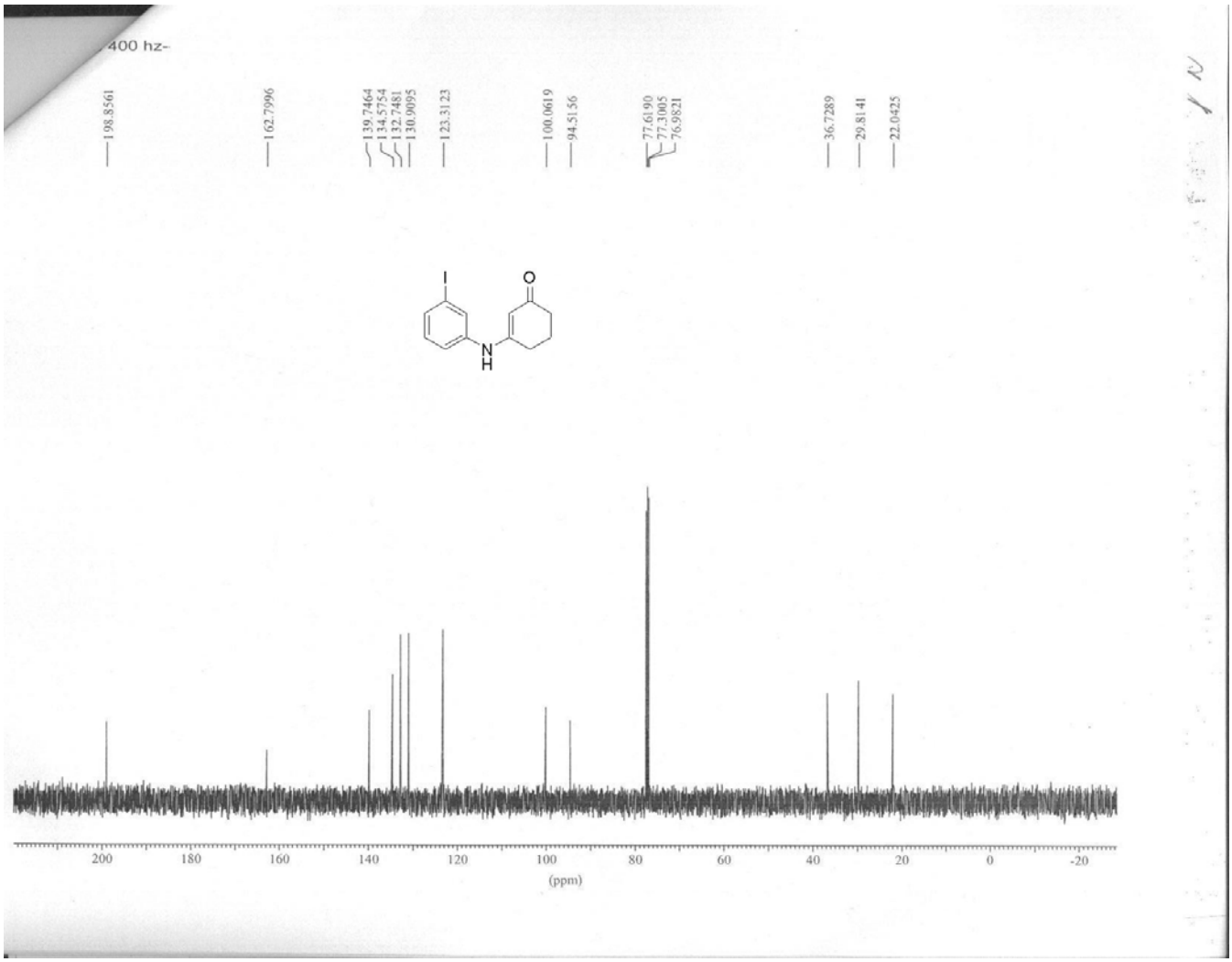

ZJ525 (400 Hz)
7.3042
7.2218
7.2195
7.2028
7.2005
7.1195
7.1088
6.9607
6.9415
6.9044
6.9017
6.8989
6.8866
6.8843
6.8781
5.3097
2.8588
2.8435
2.8288
2.6146
2.5998
2.5840
1.9019
1.8863
1.8758
1.8595
1.8435
1.8284
1.8161
1.8030
1.7877
I
NH
Integral
0.9490
0.9151
1.9240
0.9847
1.8995
0.9882
2.0389
2.0156
4.0000
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 -0.5
(ppm)

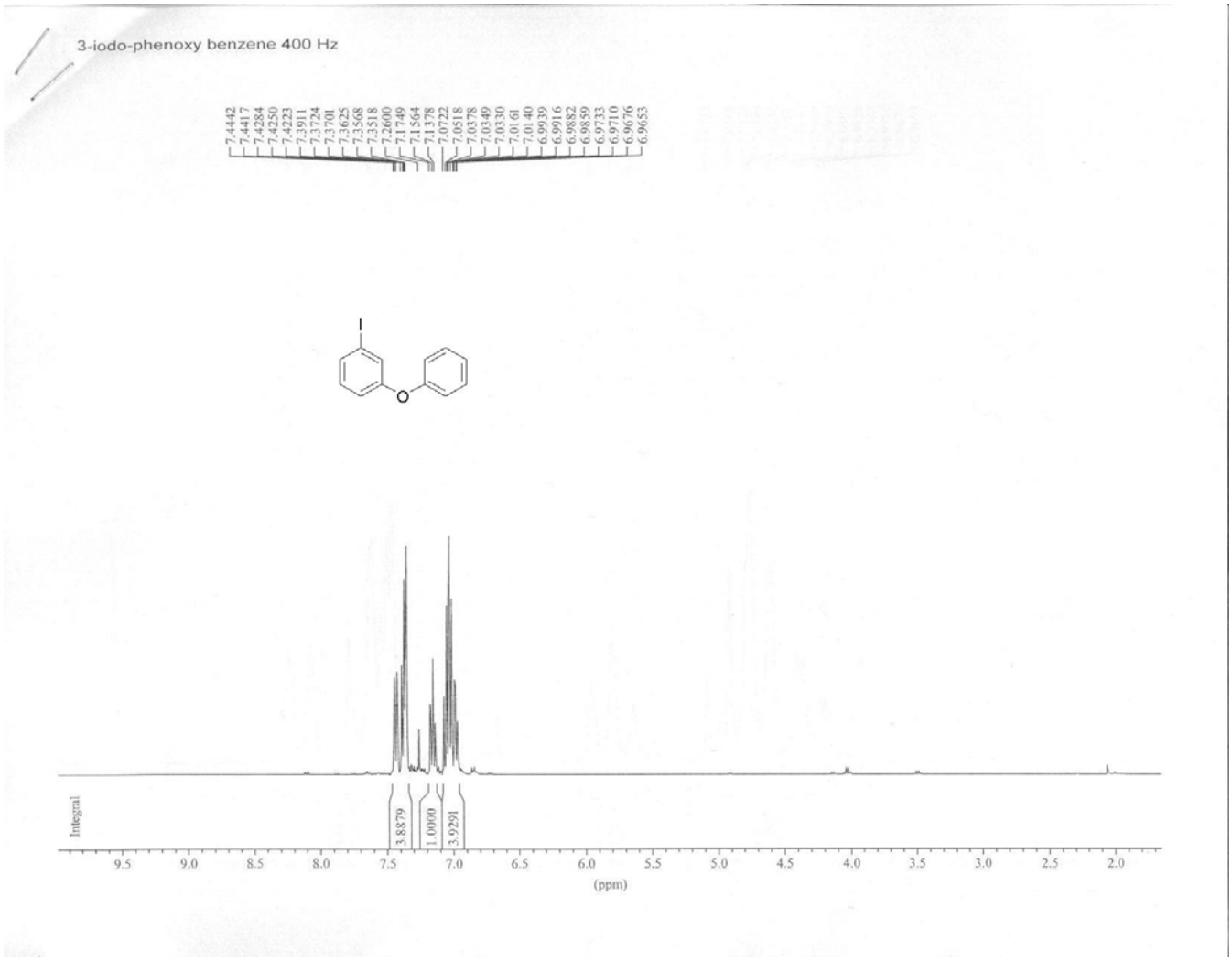

146.0888
139.9776
139.0716
130.9891
128.9836
128.9040
126.1366
125.4466
124.4041
117.6219
116.0903
95.2852
30.2235
24.9843
23.3276
23.0168
I
N
H
200
180
160
140
120
100
80
60
40
20
0
-20
(ppm)

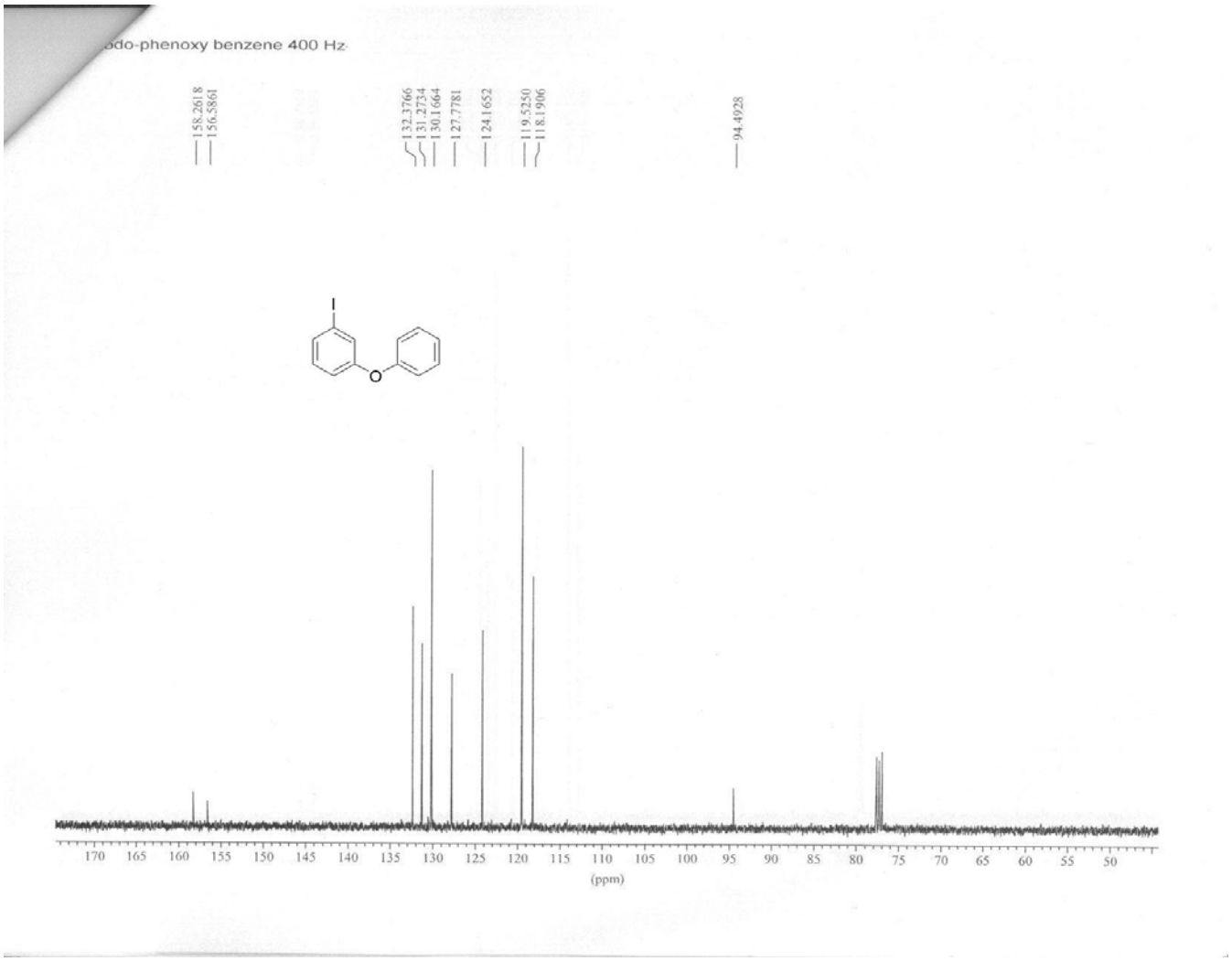

ZJ536
STANDARD 1H OBSERVE
7.0620
7.0364
6.9782
6.9717
6.9660
6.9204
6.8935
6.8671
6.5911
6.5838
6.5643
6.5570
5.9966
5.9791
5.9620
5.9449
5.9400
5.9270
5.9217
5.9046
5.8875
5.8700
5.3267
5.3218
5.2697
5.2644
5.2261
5.2217
5.1920
5.1875
3.8176
3.7569
3.7521
3.7472
3.7394
3.7346
3.7301
I
N
H
Integral
0.9610
0.9739
0.9865
0.9914
0.9483
2.0000
3.0621
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
-0.5
(ppm)

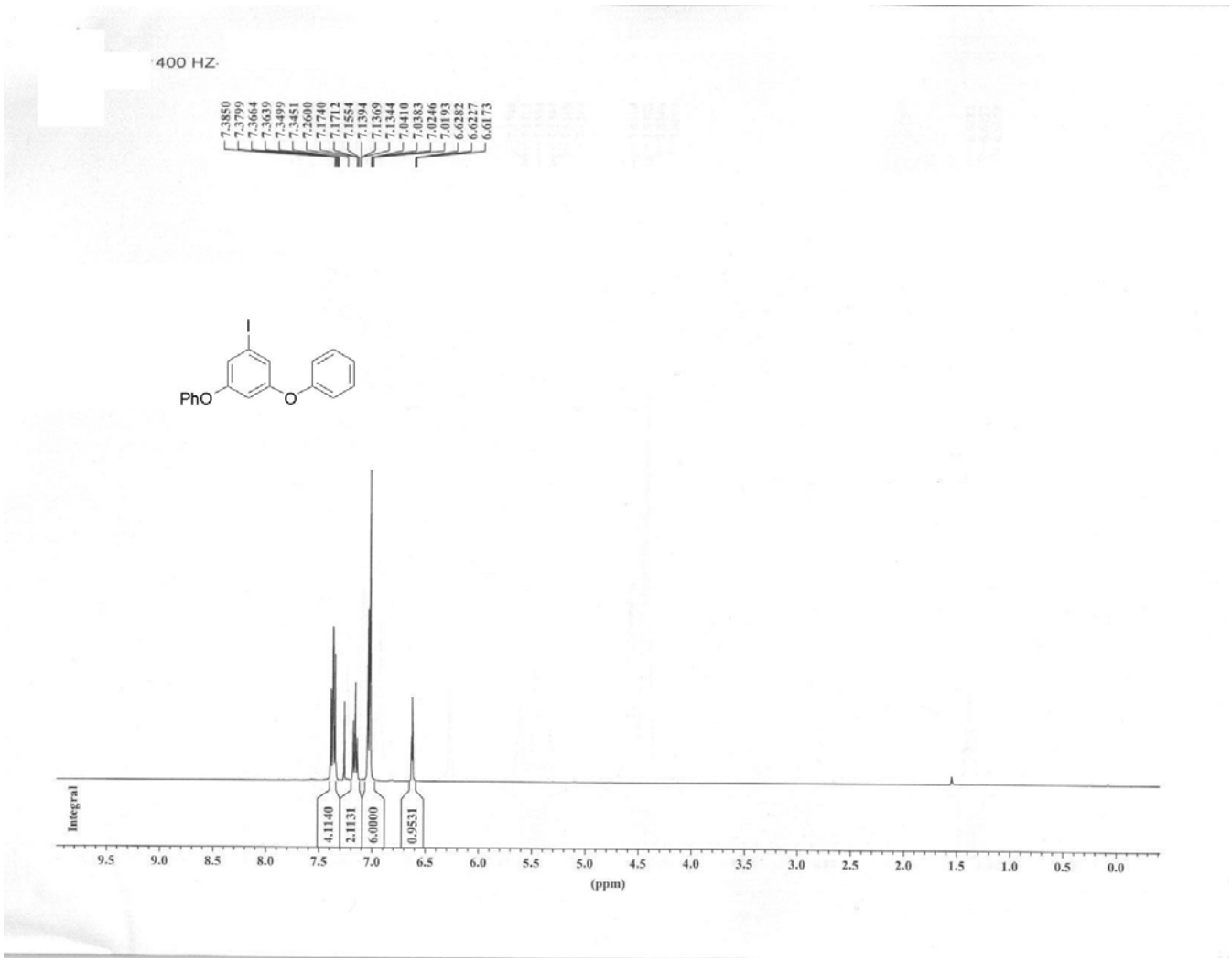

149.4754
135.6013
130.9340
126.5461
121.7166
116.8515
112.5421
95.5641
46.4680
I
N
H
200
180
160
140
120
100
80
60
40
20
0
(ppm)

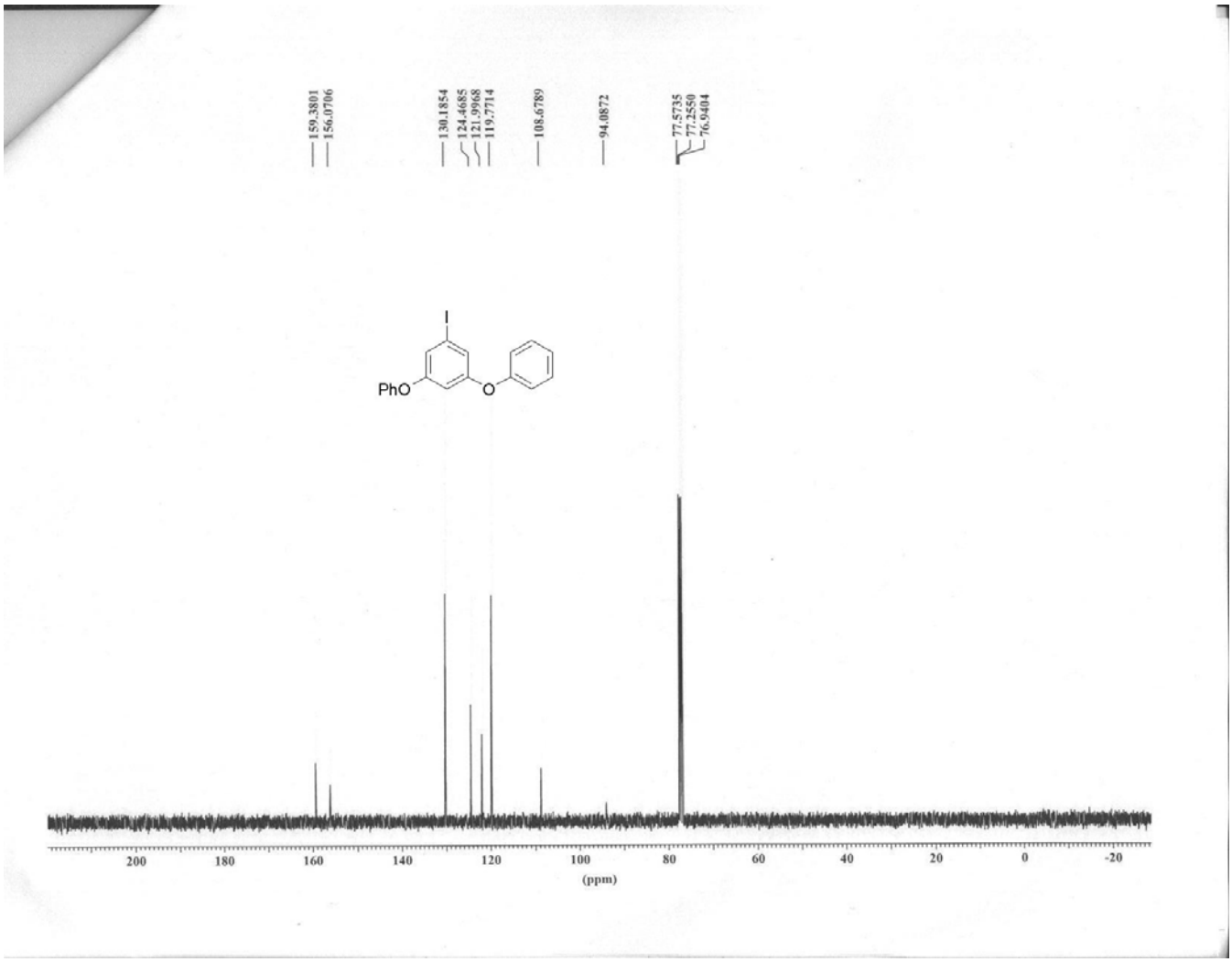

ZJ555 400Hz
7.4795
7.4756
7.4710
7.4600
7.4401
7.4035
7.2600
7.1090
7.1067
7.0889
7.0863
7.0170
6.9973
6.9774
5.5081
2.5108
2.4954
2.4801
2.3387
2.3231
2.3062
2.0190
2.0028
1.9874
1.9714
1.9556
I
O
N
H
Integral
2.9000
1.0119
1.0039
0.9984
2.0143
2.0974
2.0109
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
(ppm)

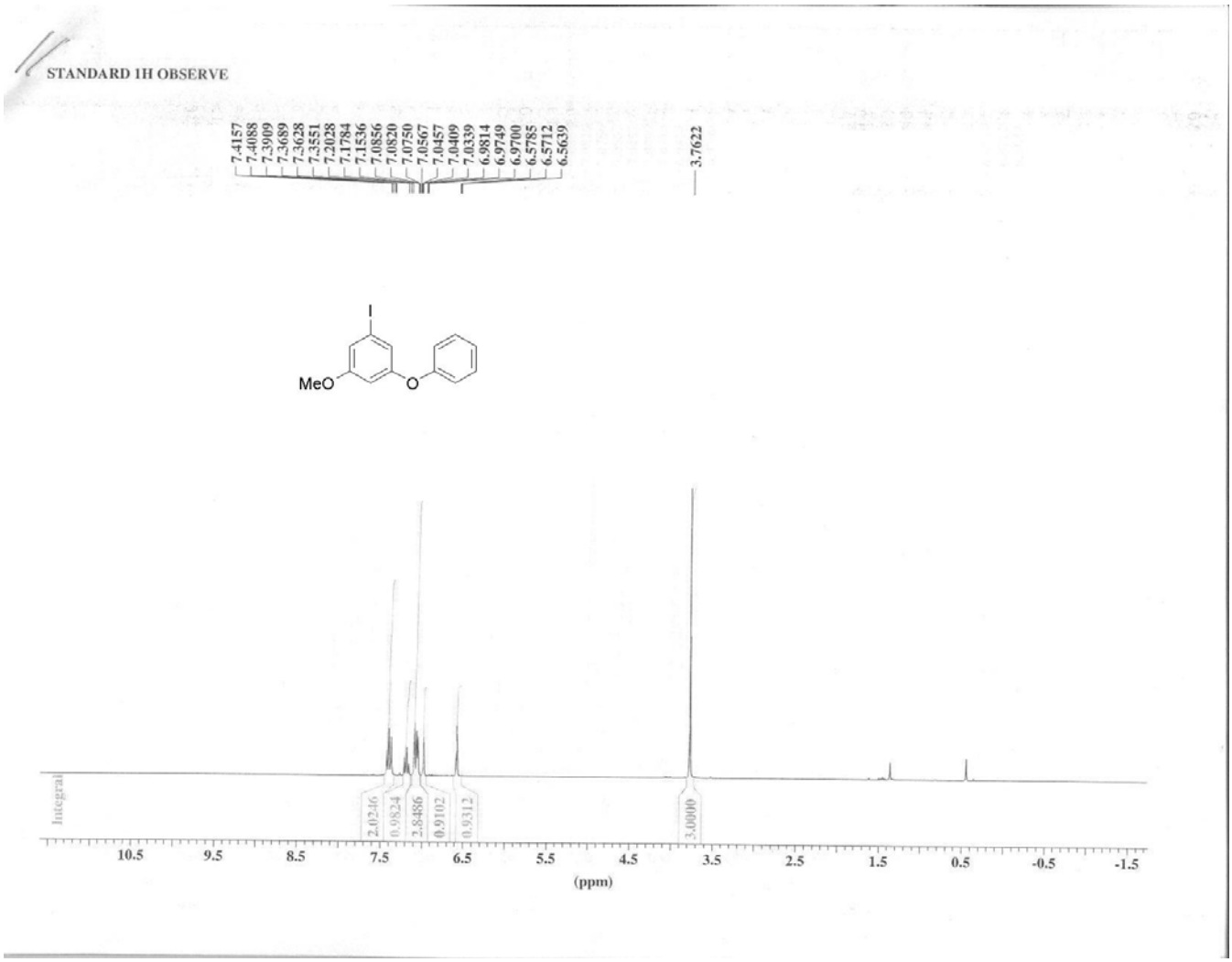

400 hz-
198.8561
162.7996
139.7464
134.5754
132.7481
130.9095
123.3123
100.0619
94.5156
77.6190
77.3005
76.9821
36.7289
29.8141
22.0425
I
O
N
H
200
180
160
140
120
100
80
60
40
20
0
-20
(ppm)

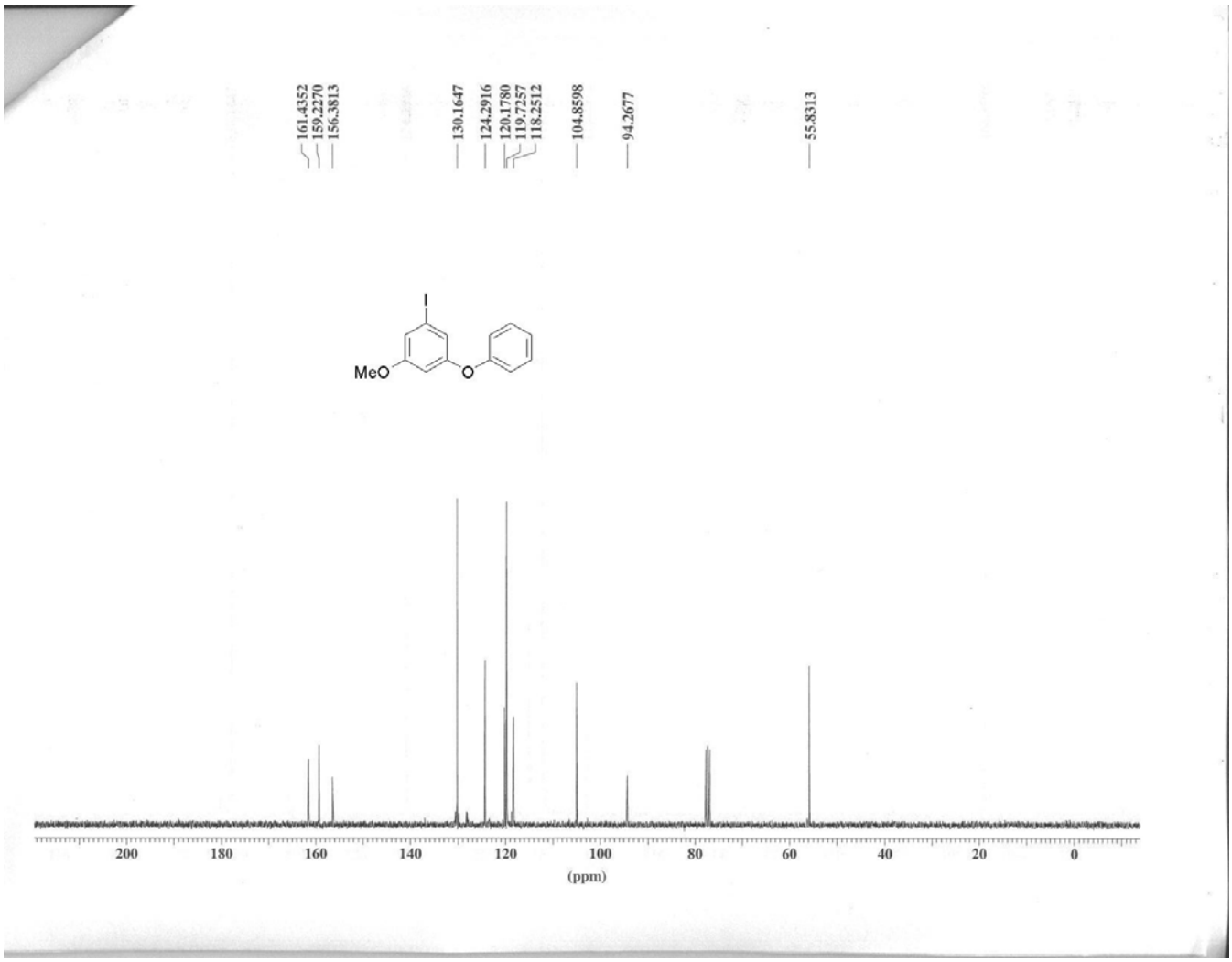

3-iodo-phenoxy benzene 400 Hz
7.4442
7.4417
7.4284
7.4250
7.4223
7.3911
7.3724
7.3701
7.3625
7.3568
7.3518
7.2600
7.1749
7.1564
7.1378
7.0722
7.0518
7.0378
7.0349
7.0330
7.0161
7.0140
6.9939
6.9916
6.9882
6.9859
6.9733
6.9710
6.9676
6.9653
I
O
Integral
3.8879
1.0000
3.9291
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
(ppm)

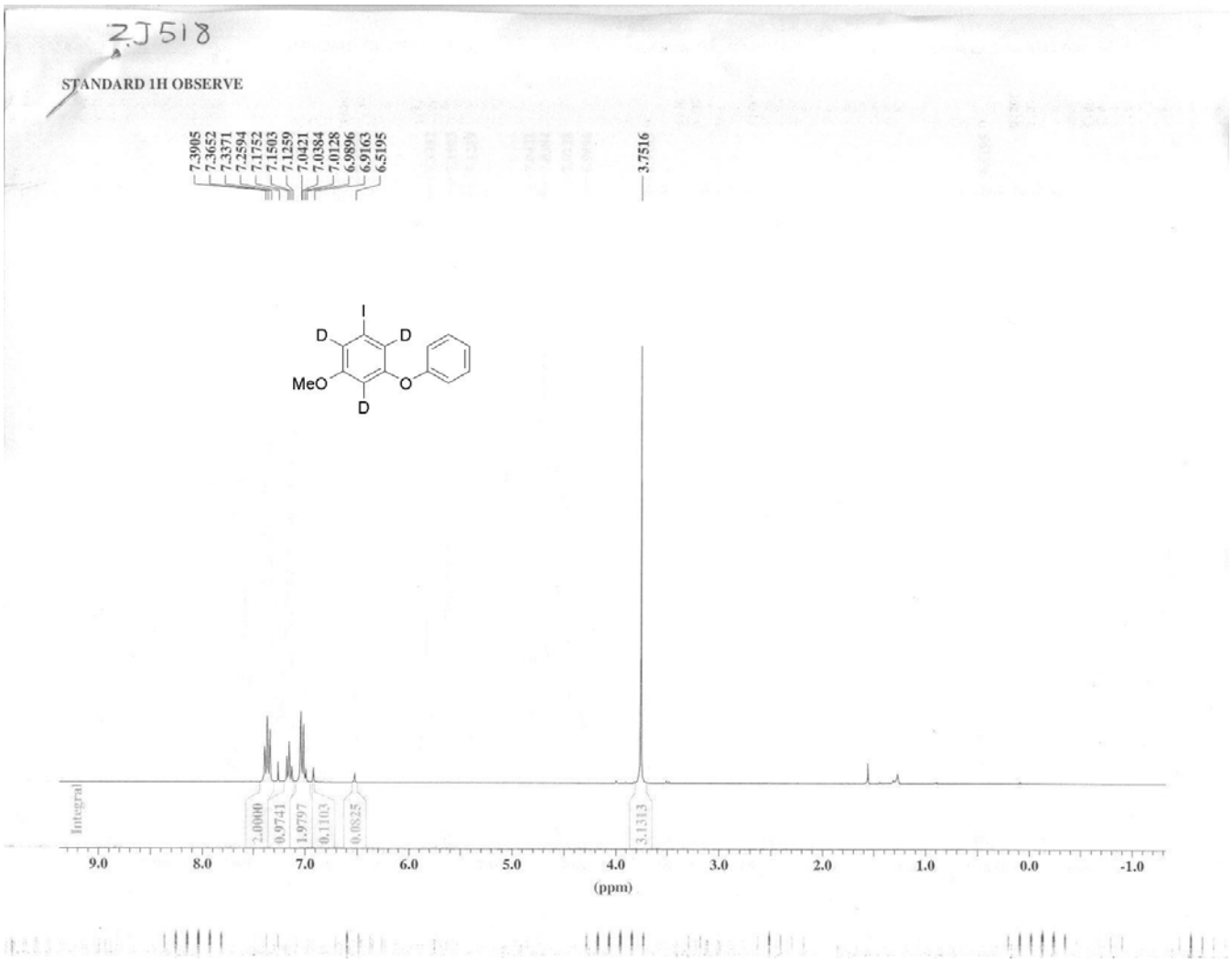

odo-phenoxy benzene 400 Hz
158.2618
156.5861
132.3766
131.2734
130.1664
127.7781
124.1652
119.5250
118.1906
94.4928
I
O
170 165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50
(ppm)

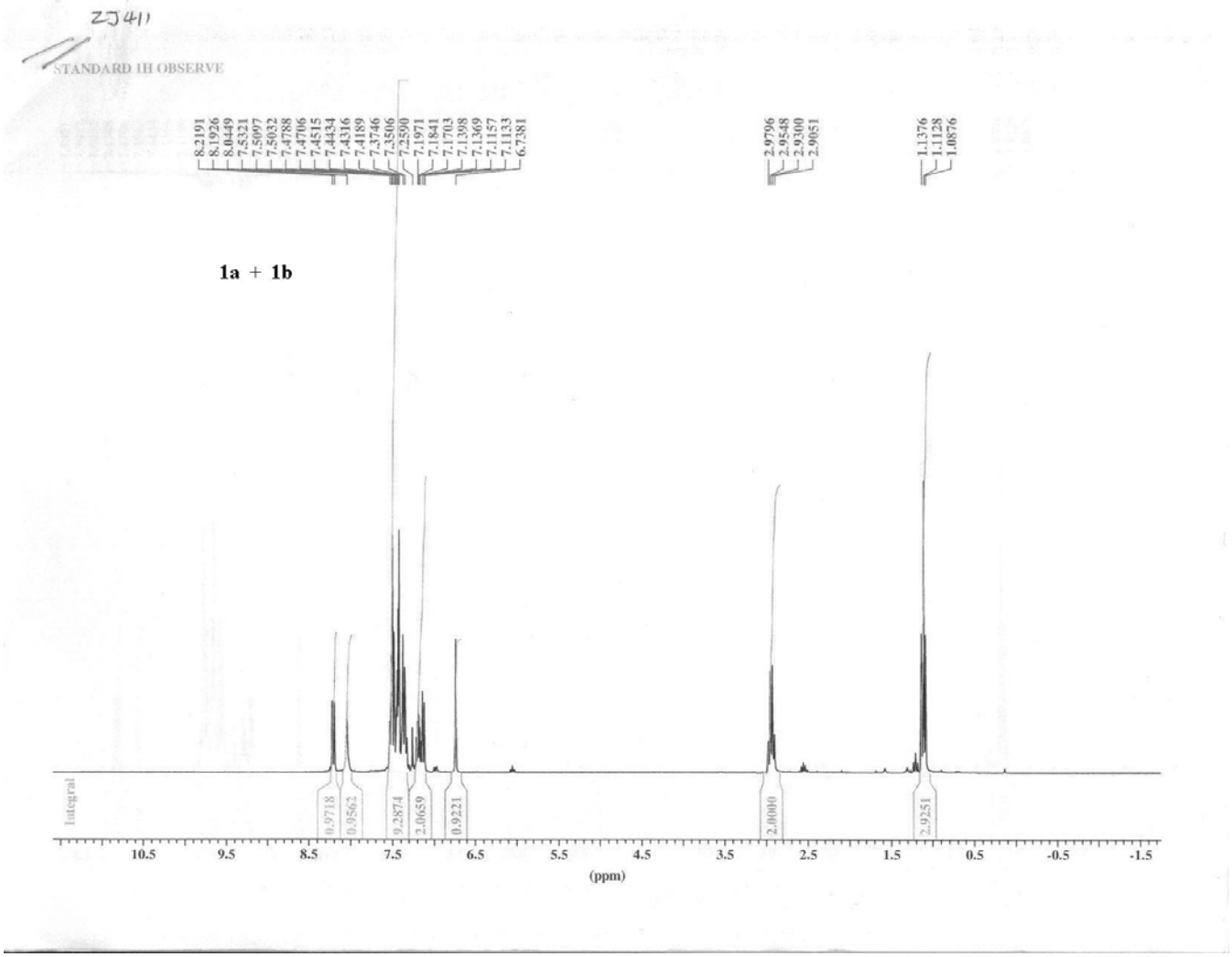

400 HZ
7.3850
7.3799
7.3664
7.3639
7.3499
7.3451
7.2600
7.1740
7.1712
7.1554
7.1394
7.1369
7.1344
7.0410
7.0383
7.0246
7.0193
6.6282
6.6227
6.6173
I
PhO
O
Integral
4.1140
2.1131
6.0000
0.9531
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
(ppm)


159.3801
156.0706
130.1854
124.4685
121.9968
119.7714
108.6789
94.0872
77.5735
77.2550
76.9404
I
PhO
O
200
180
160
140
120
100
80
60
40
20
0
-20
(ppm)


STANDARD 1H OBSERVE
7.4157
7.4088
7.3909
7.3689
7.3628
7.3551
7.2028
7.1784
7.1536
7.0856
7.0820
7.0750
7.0567
7.0457
7.0409
7.0339
6.9814
6.9749
6.9700
6.5785
6.5712
6.5639
3.7622
I
MeO
O
Integral
2.0246
0.9824
3.8486
0.9102
0.9312
3.0000
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
-1.5
(ppm)


161.4352
159.2270
156.3813
130.1647
124.2916
120.1780
119.7257
118.2512
104.8598
94.2677
55.8313
I
MeO
O
200
180
160
140
120
100
80
60
40
20
0
(ppm)


ZJ518
STANDARD 1H OBSERVE
7.3905
7.3652
7.3371
7.2594
7.1752
7.1503
7.1259
7.0421
7.0384
7.0128
6.9896
6.9163
6.5195
3.7516
I
D
D
MeO
O
D
Integral
2.0000
0.9741
1.9797
0.1103
0.0825
3.1313
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
(ppm)

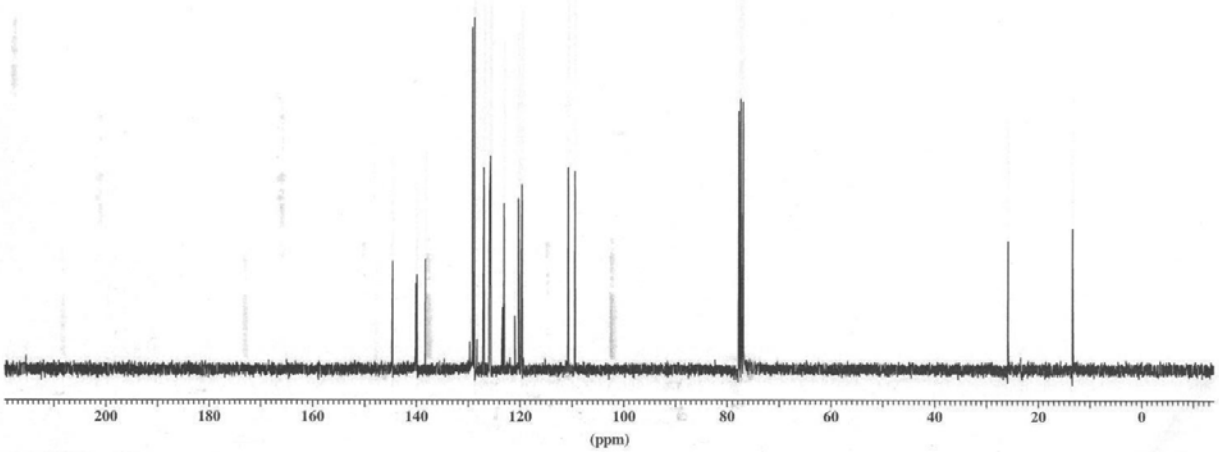

ZJ41
STANDARD 1H OBSERVE
8.2191
8.1926
8.0449
7.5321
7.5097
7.5032
7.4788
7.4706
7.4515
7.4434
7.4316
7.4189
7.3746
7.3506
7.2590
7.1971
7.1841
7.1703
7.1398
7.1369
7.1157
7.1133
6.7381
2.9796
2.9548
2.9300
2.9051
1.1376
1.1128
1.0876
1a + 1b
Integral
0.9718
0.9562
9.2874
2.0659
0.9221
2.0000
2.9251
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
-1.5
(ppm)

144.5676
140.0729
139.9340
139.8948
138.2138
129.0356
128.8967
128.6795
126.9165
125.7590
125.6557
123.2802
123.0309
120.9260
120.1602
119.5904
110.7150
109.3901

25.8465

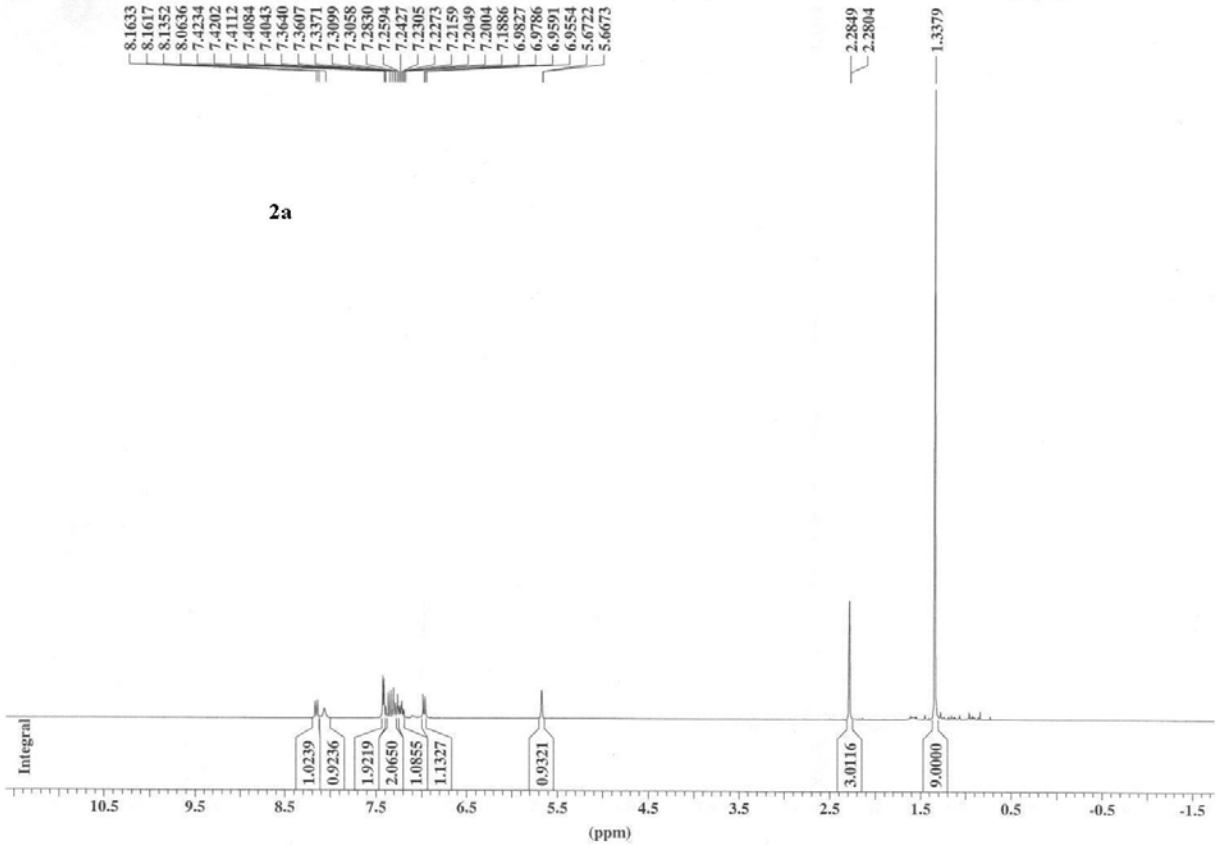
13.3704

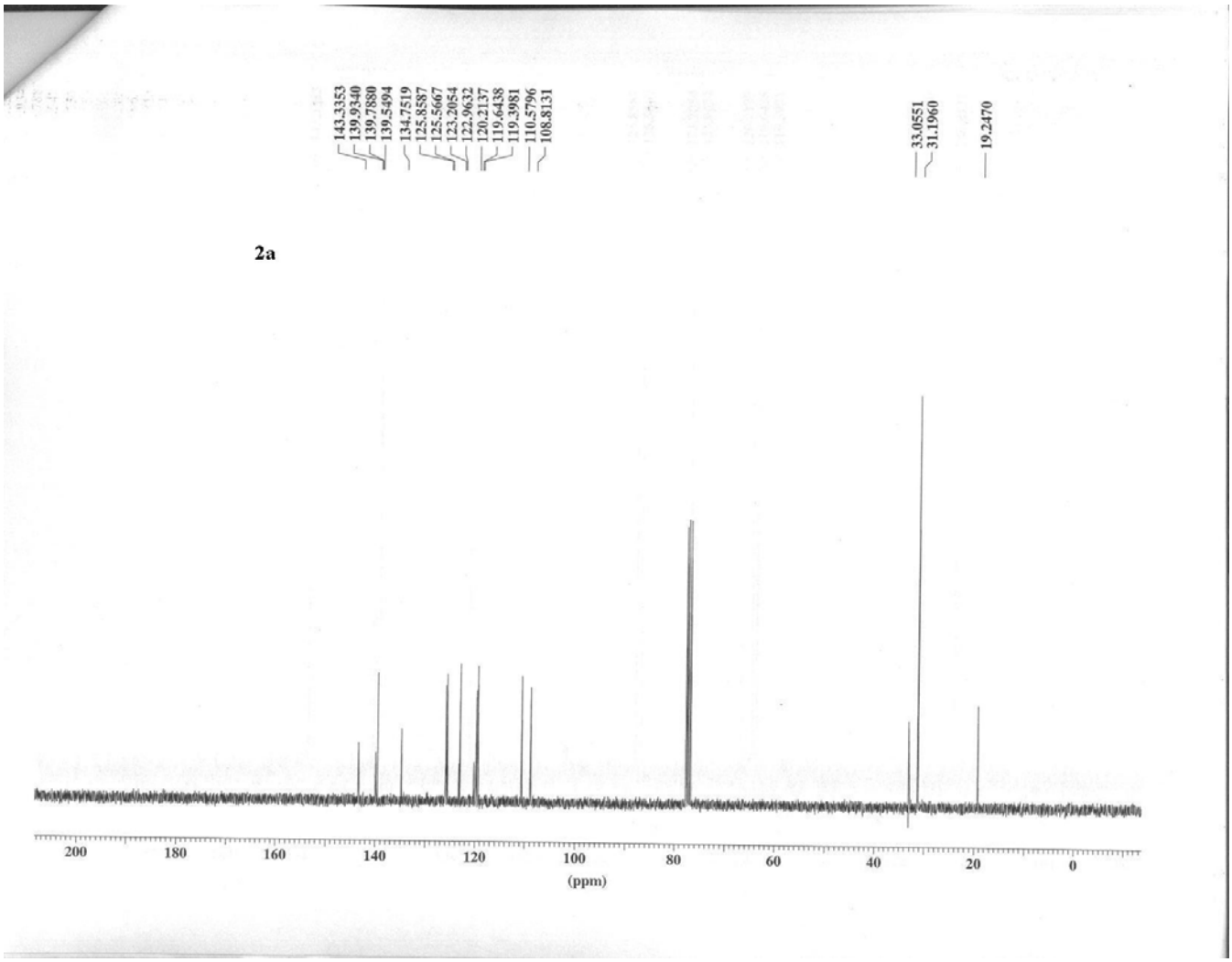
1a + 1b

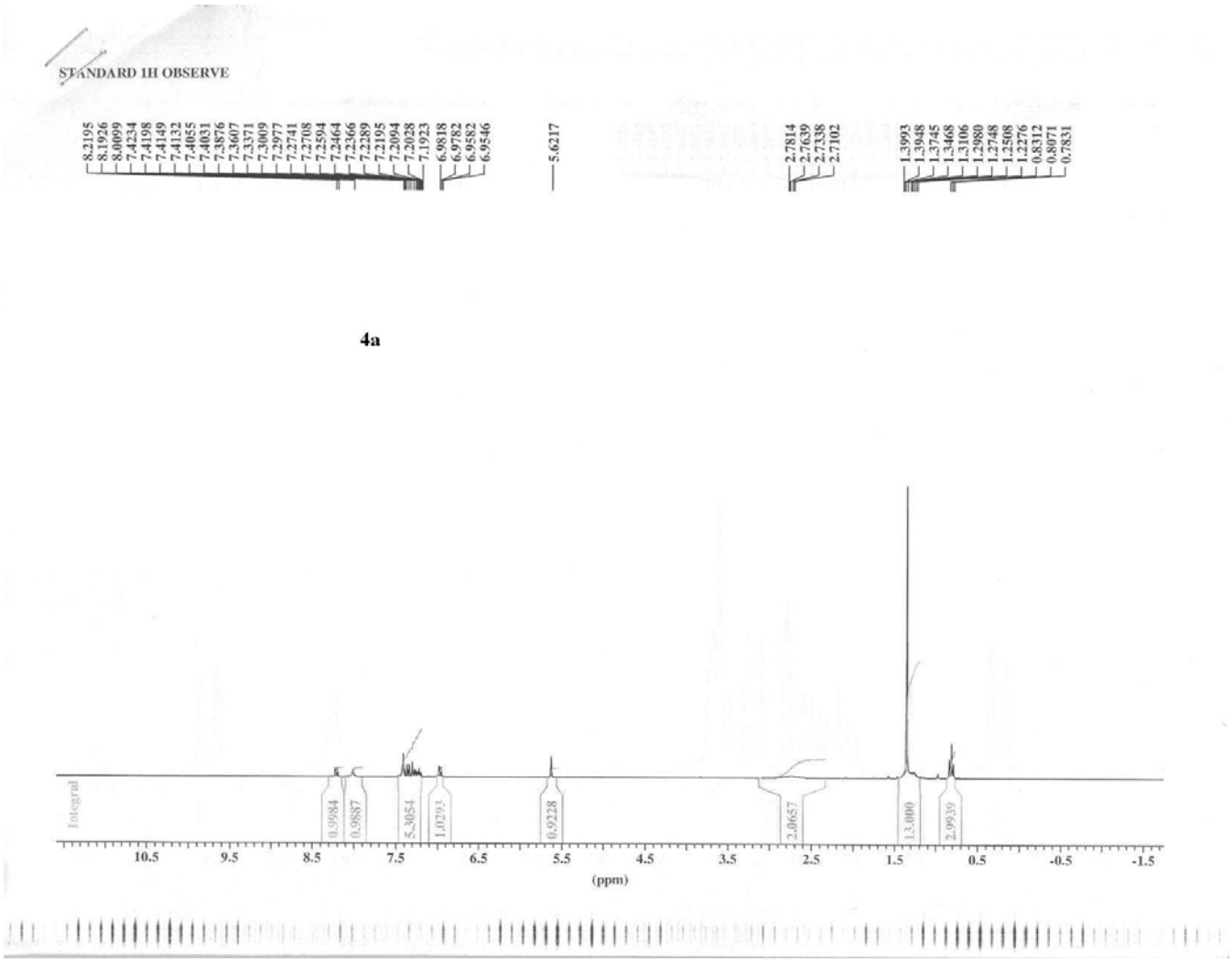


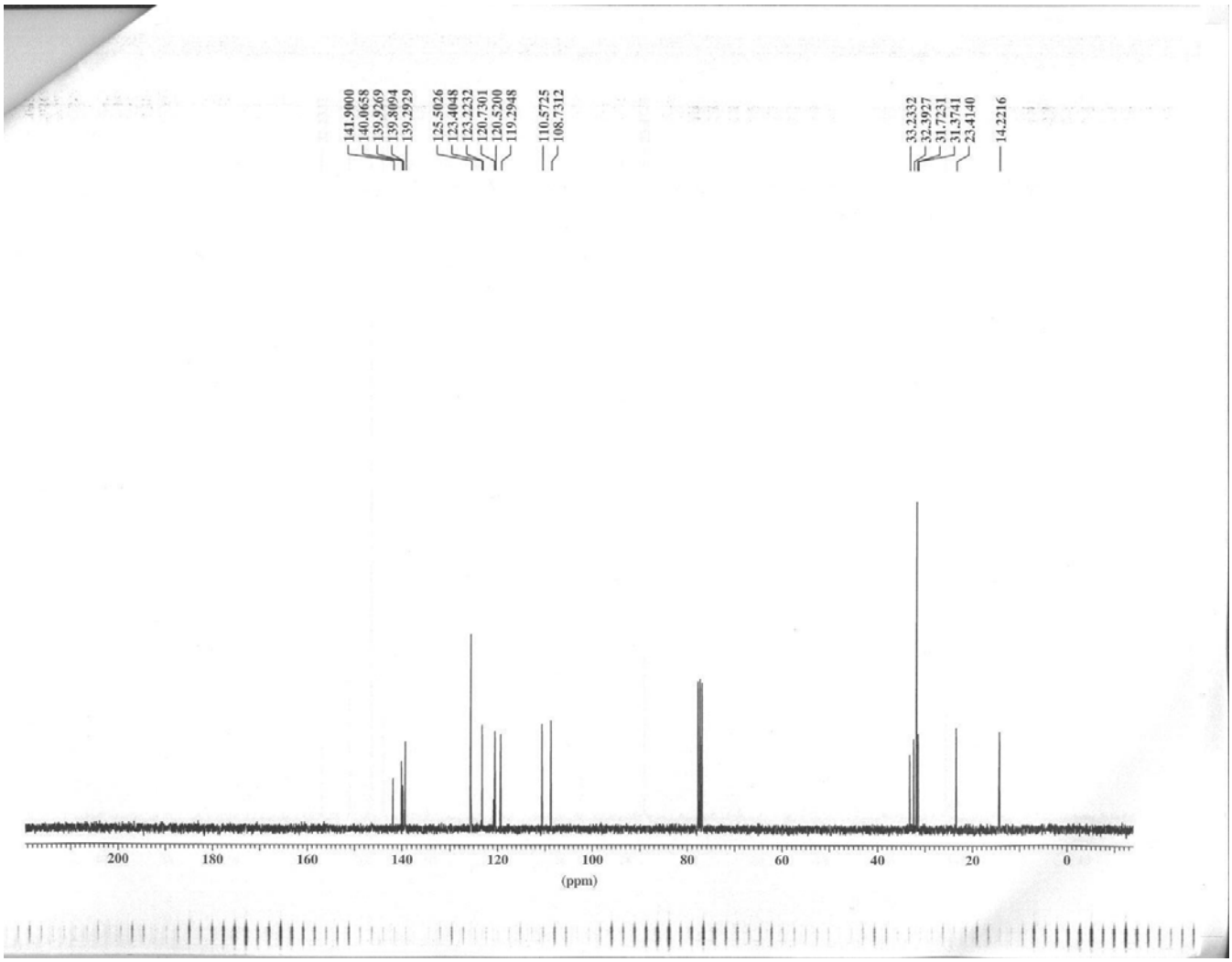
ZJ464A

STANDARD 1H OBSERVE




143.3353
139.9340
139.7880
139.5494
134.7519
125.8587
125.5667
123.2054
122.9632
120.2137
119.6438
119.3981
110.5796
108.8131
33.0551
31.1960
19.2470
2a
200
180
160
140
120
100
80
60
40
20
0
(ppm)


STANDARD 1H OBSERVE
8.2195
8.1926
8.0099
7.4234
7.4198
7.4149
7.4132
7.4055
7.4031
7.3876
7.3607
7.3371
7.3009
7.2977
7.2741
7.2708
7.2594
7.2464
7.2366
7.2289
7.2195
7.2094
7.2028
7.1923
6.9818
6.9782
6.9582
6.9546
5.6217
2.7814
2.7639
2.7338
2.7102
1.3993
1.3948
1.3745
1.3468
1.3106
1.2980
1.2748
1.2508
1.2276
0.8312
0.8071
0.7831
4a
Integral
0.9984
0.9887
5.3054
1.0293
0.9228
2.0657
13.000
2.9939
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
-1.5
(ppm)

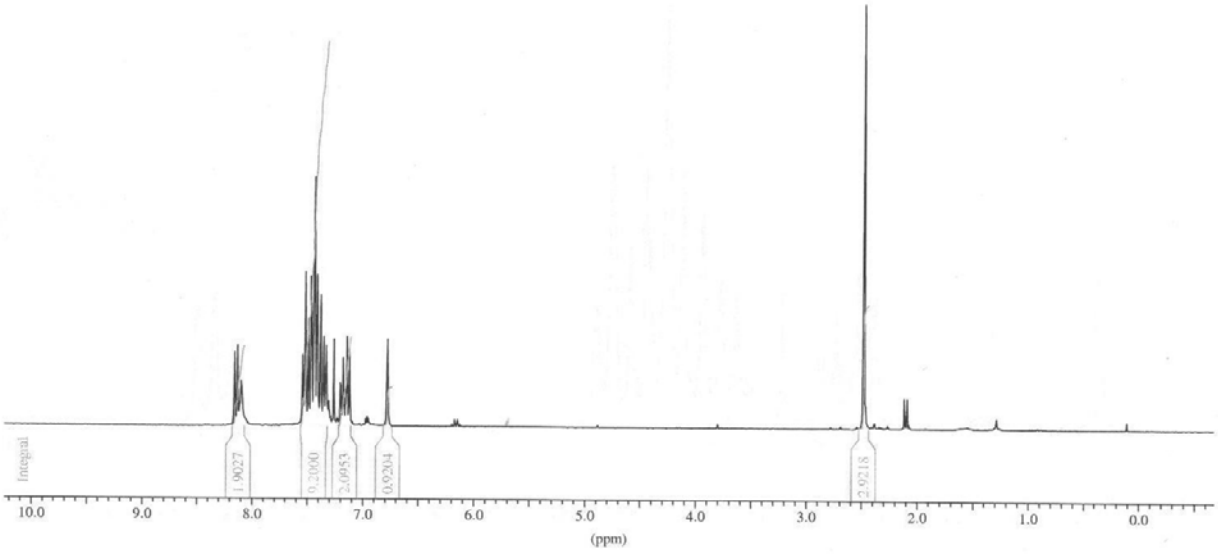

141.9000
140.0658
139.9269
139.8094
139.2929
125.5026
123.4048
123.2232
120.7301
120.5200
119.2948
110.5725
108.7312
33.2332
32.3927
31.7231
31.3741
23.4140
14.2216
200
180
160
140
120
100
80
60
40
20
0
(ppm)

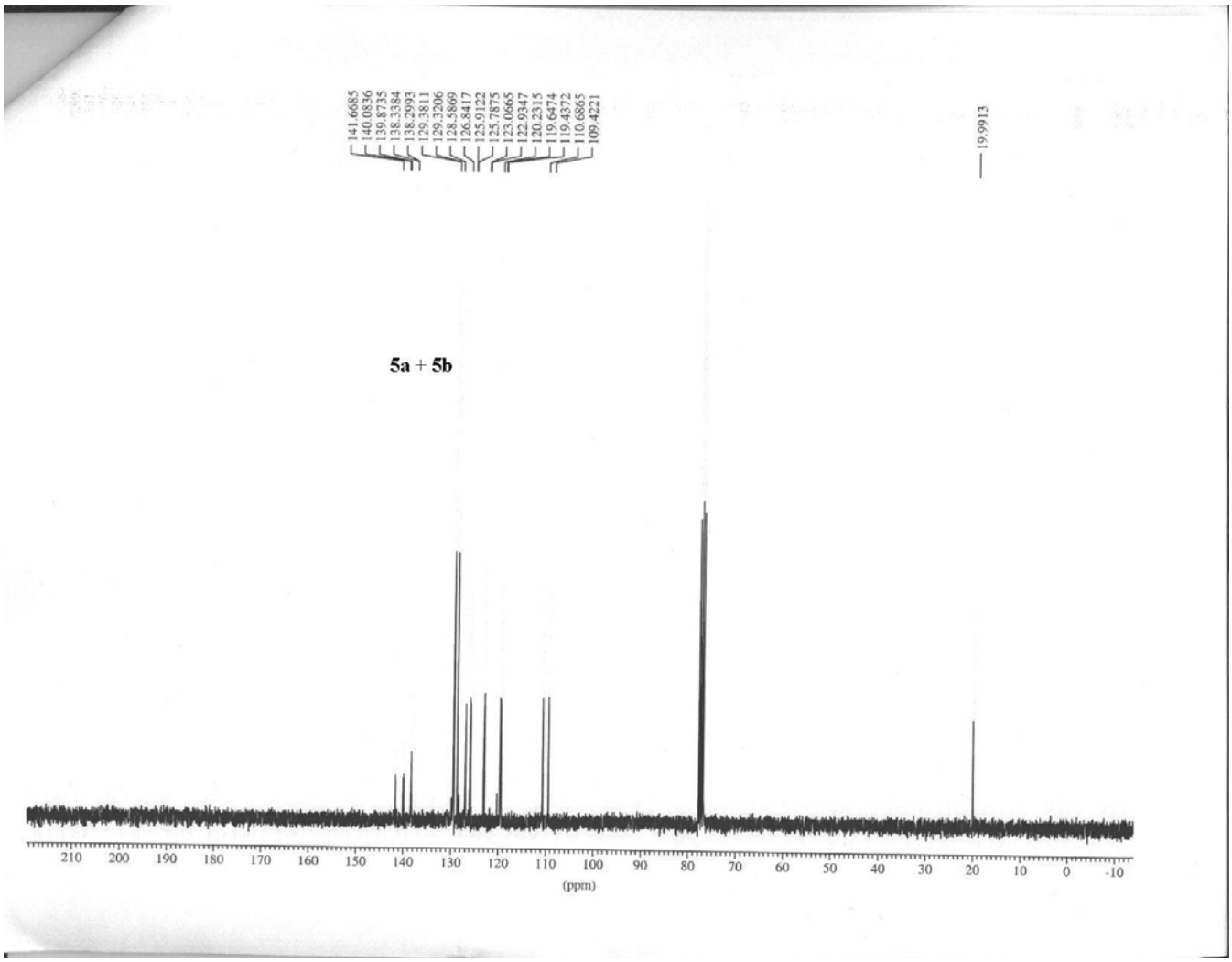
STANDARD 1H OBSERVE zJ422r

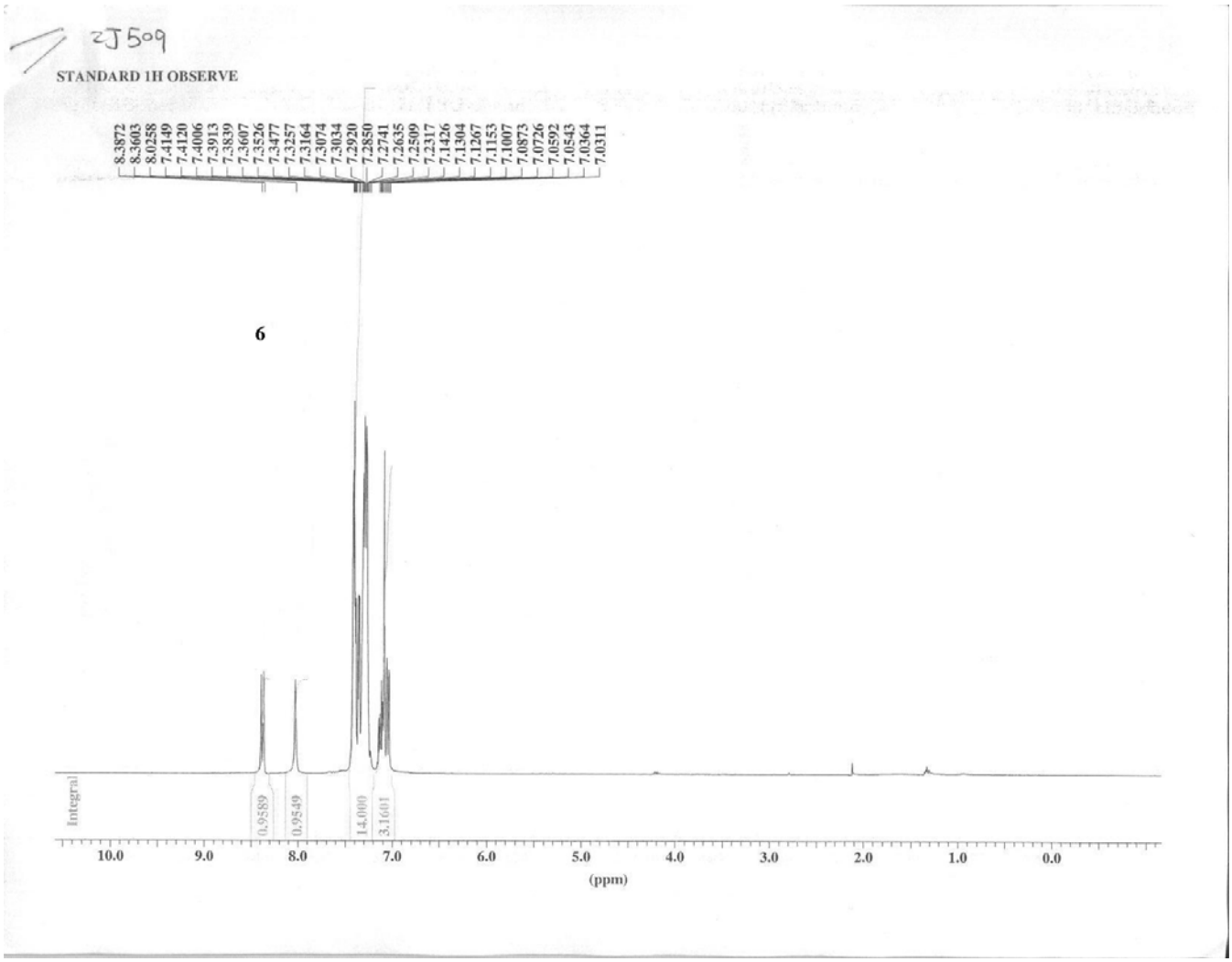
8.1531
8.1271
8.0958
7.5419
7.5182
7.4910
7.4666
7.4609
7.4340
7.4153
7.4104
7.3827
7.3787
7.3555
7.3518
7.3294
7.2594
7.2041
7.1963
7.1841
7.1768
7.1703
7.1573
7.1499
7.1430
7.1394
7.1198
7.1157
6.7763

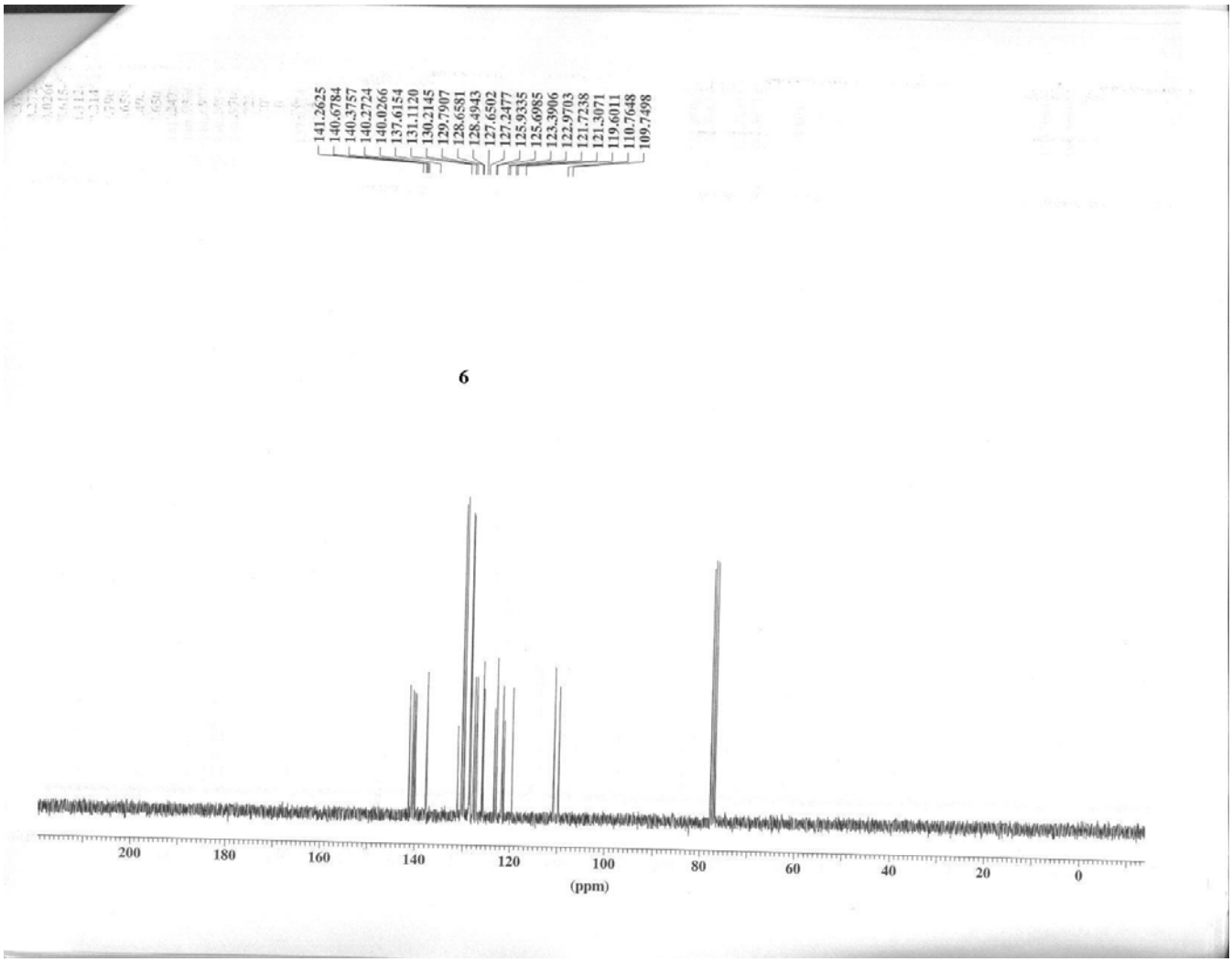
2.4770

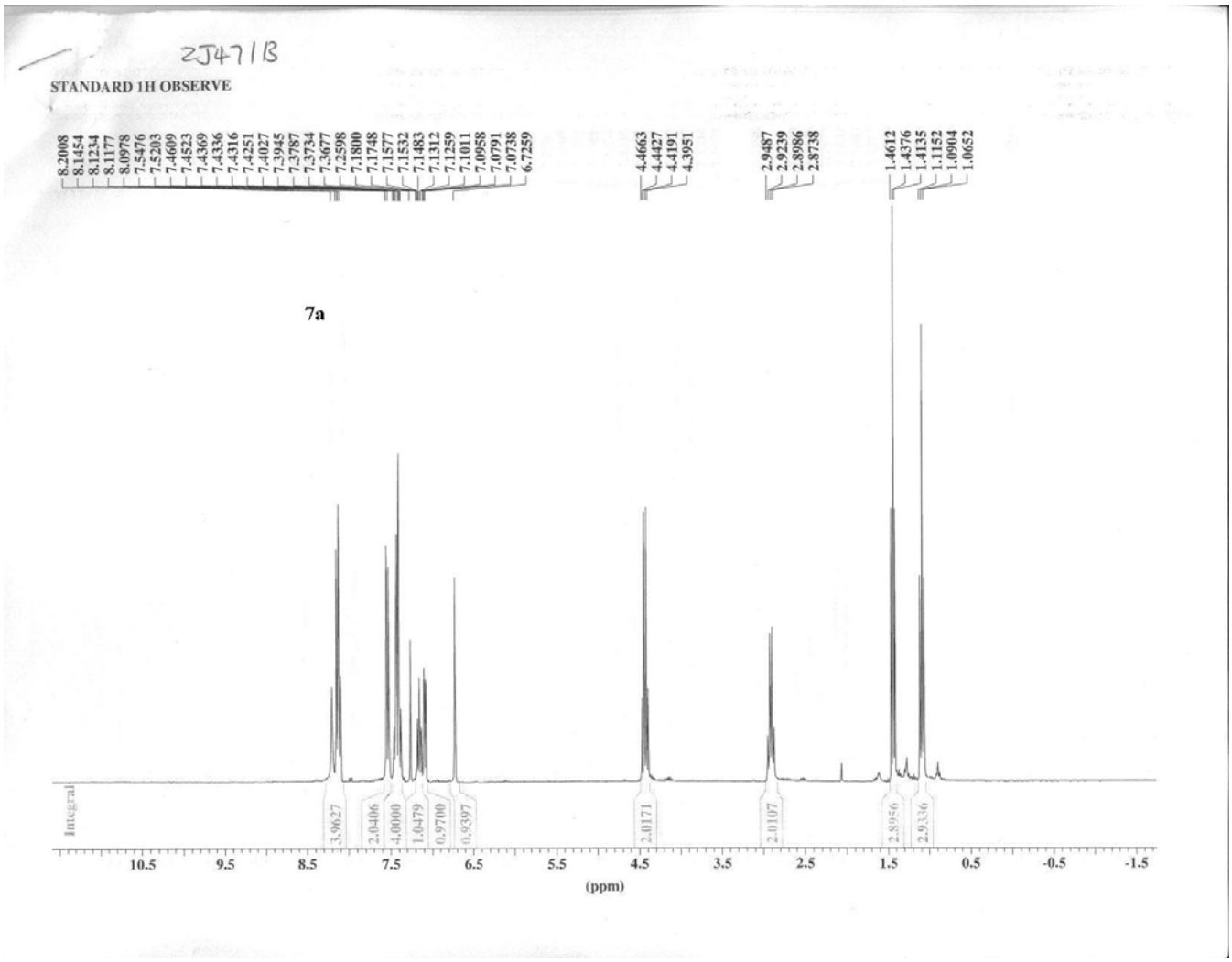
5a + 5b

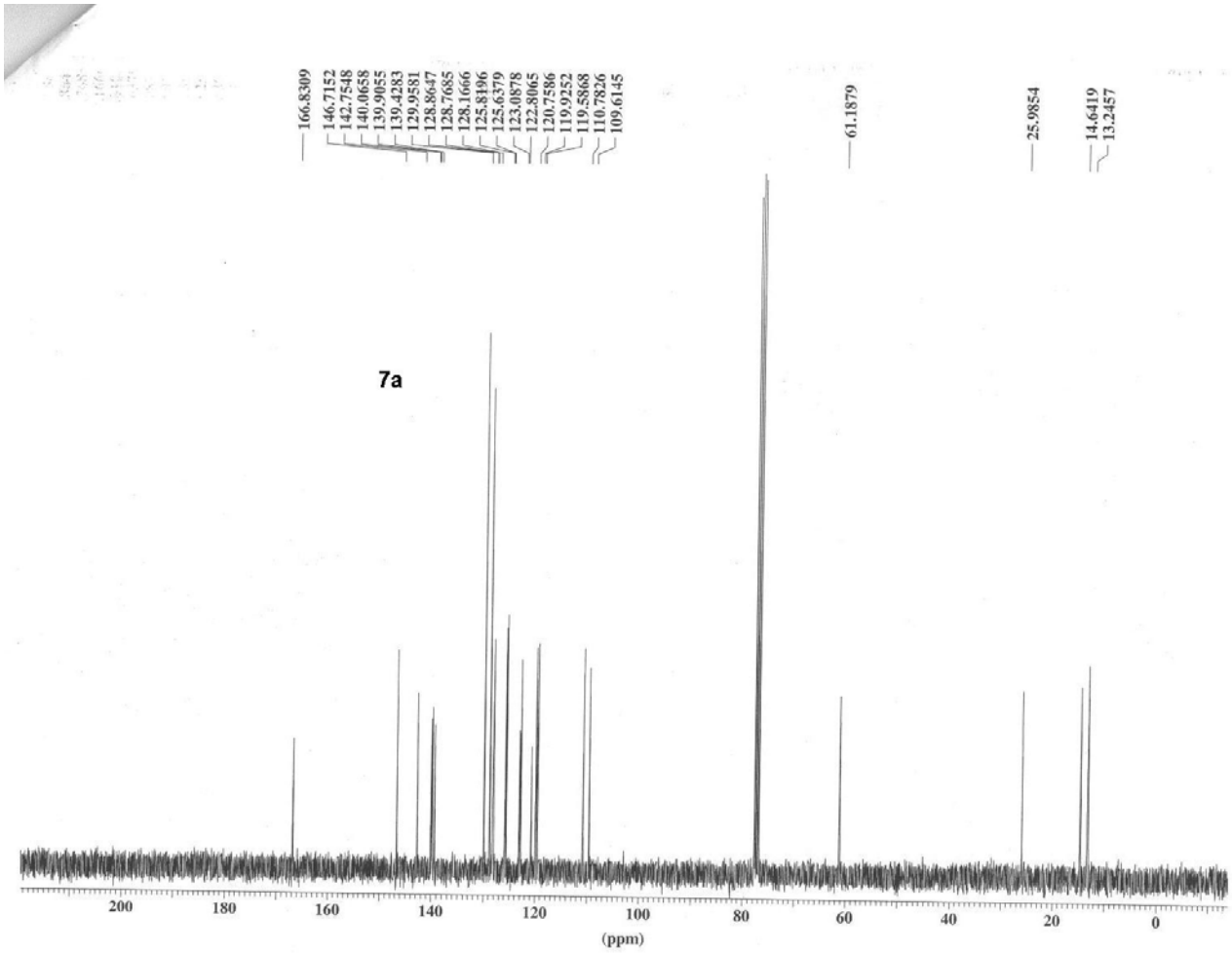



141.6685
140.0836
139.8735
138.3384
138.2993
129.3811
129.3206
128.5869
126.8417
125.9122
125.7875
123.0665
122.9347
120.2315
119.6474
119.4372
110.6865
109.4221
19.9913
5a + 5b
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
(ppm)


ZJ509
STANDARD 1H OBSERVE
8.3872
8.3603
8.0258
7.4149
7.4120
7.4006
7.3913
7.3839
7.3607
7.3526
7.3477
7.3257
7.3164
7.3074
7.3034
7.2920
7.2850
7.2741
7.2635
7.2509
7.2317
7.1426
7.1304
7.1267
7.1153
7.1007
7.0873
7.0726
7.0592
7.0543
7.0364
7.0311
6
Integral
0.9589
0.9549
1.4.000
3.1601
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
(ppm)


141.2625
140.6784
140.3757
140.2724
140.0266
137.6154
131.1120
130.2145
129.7907
128.6581
128.4943
127.6502
127.2477
125.9335
125.6985
123.3906
122.9703
121.7238
121.3071
119.6011
110.7648
109.7498
6
200
180
160
140
120
100
80
60
40
20
0
(ppm)


ZJ471B
STANDARD 1H OBSERVE
8.2008
8.1454
8.1234
8.1177
8.0978
7.5476
7.5203
7.4609
7.4523
7.4369
7.4336
7.4316
7.4251
7.4027
7.3945
7.3787
7.3734
7.3677
7.2598
7.1800
7.1748
7.1577
7.1532
7.1483
7.1312
7.1259
7.1011
7.0958
7.0791
7.0738
6.7259
4.4663
4.4427
4.4191
4.3951
2.9487
2.9239
2.8986
2.8738
1.4612
1.4376
1.4135
1.1152
1.0904
1.0652
7a
Integral
3.9627
2.0406
4.0000
1.0479
0.9700
0.9397
2.0171
2.0107
2.8956
2.9336
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
-1.5
(ppm)


166.8309
146.7152
142.7548
140.0658
139.9055
139.4283
129.9581
128.8647
128.7685
128.1666
125.8196
125.6379
123.0878
122.8065
120.7586
119.9252
119.5868
110.7826
109.6145
61.1879
25.9854
14.6419
13.2457
7a
200
180
160
140
120
100
80
60
40
20
0
(ppm)

ZJ489B

STANDARD 1H OBSERVE

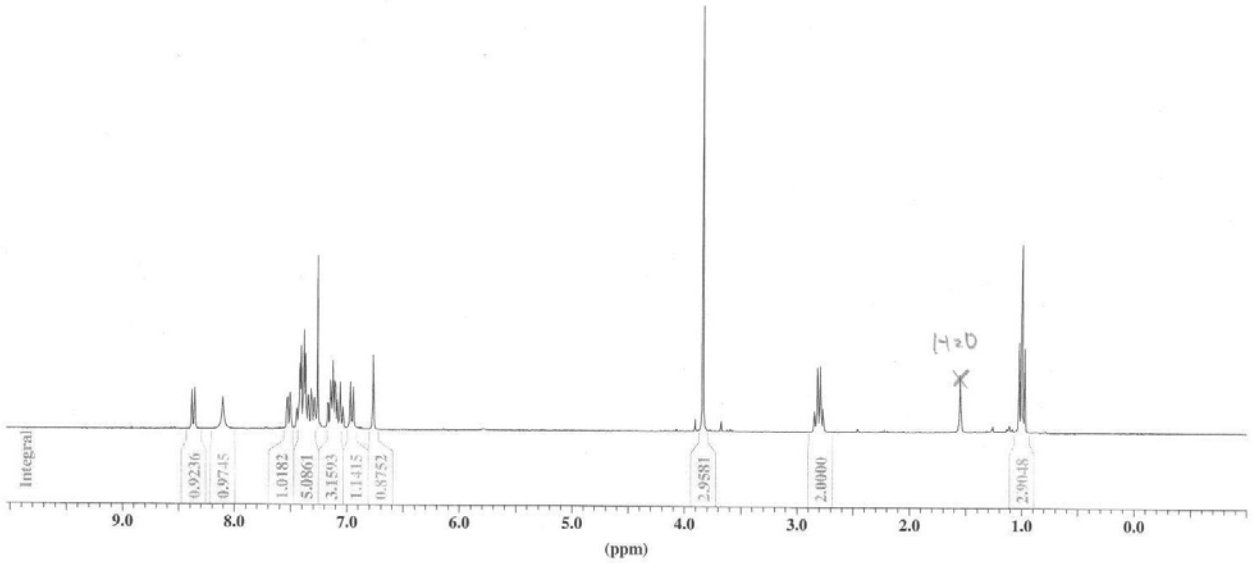
7.4320
7.4206
7.4185
7.4096
7.4059
7.3876
7.3827
7.3734
7.3685
7.3612
7.3571
7.3461
7.3428
7.3172
7.2912
7.2863
7.2594
7.1715
7.1666
7.1491
7.1446
7.1402
7.1280
7.1227
7.1052
7.1003
7.0836
7.0588
7.0360
6.9688
6.9416
6.7662

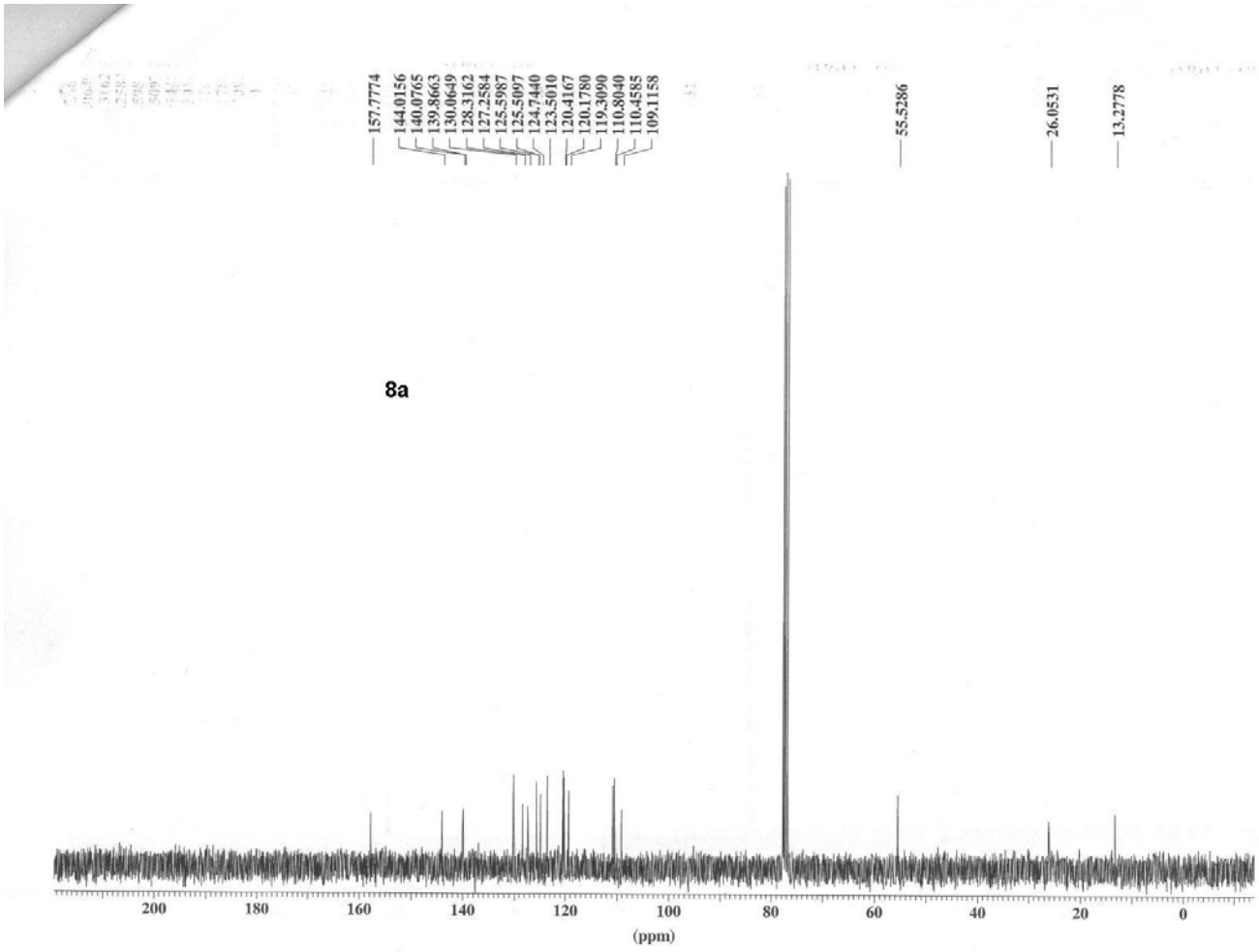
3.8351

2.8416
2.8168
2.7920
2.7672

1.0208
0.9960
0.9712

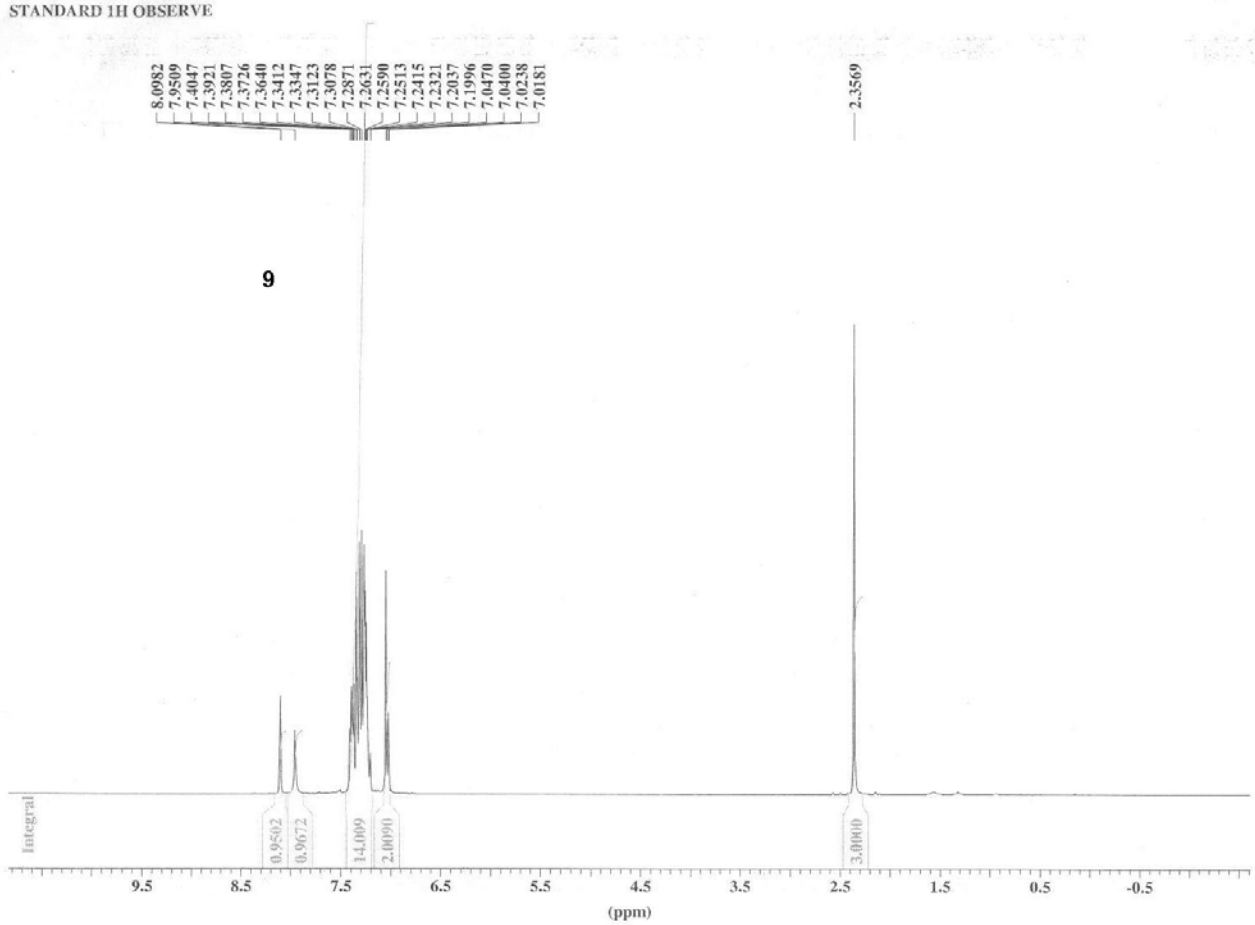
8a

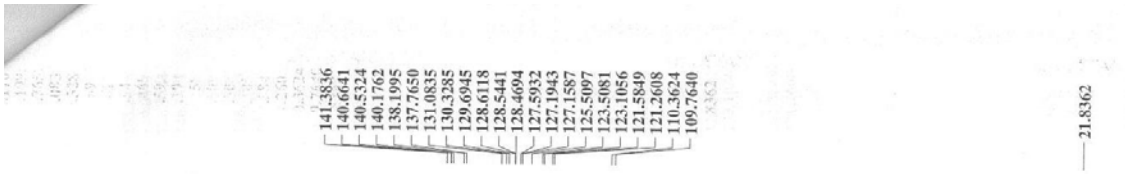



157.7774
144.0156
140.0765
139.8663
130.0649
128.3162
127.2584
125.5987
125.5097
124.7440
123.5010
120.4167
120.1780
119.3090
110.8040
110.4585
109.1158
55.5286
26.0531
13.2778
8a
200
180
160
140
120
100
80
60
40
20
0
(ppm)

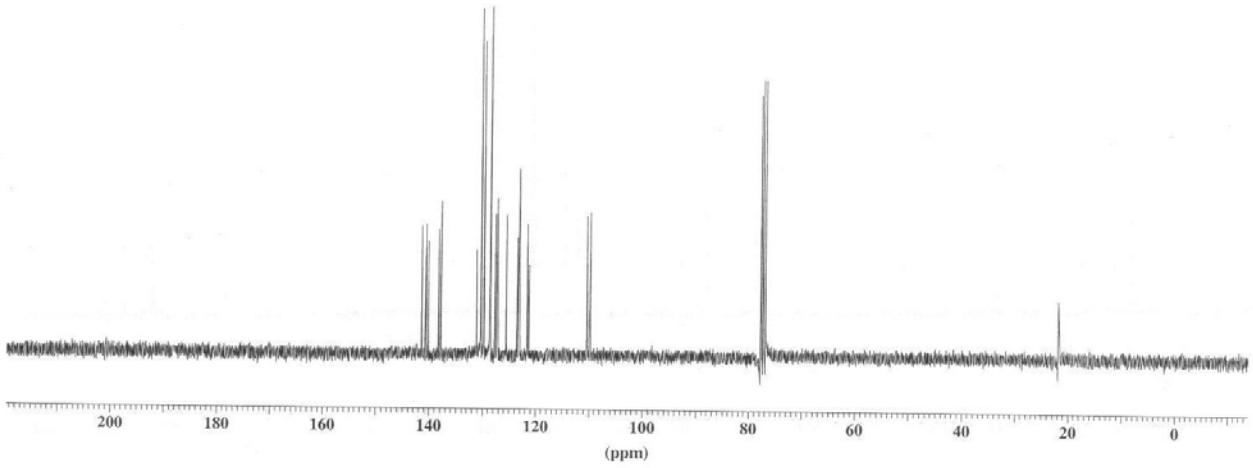
ZJ510

STANDARD 1H OBSERVE



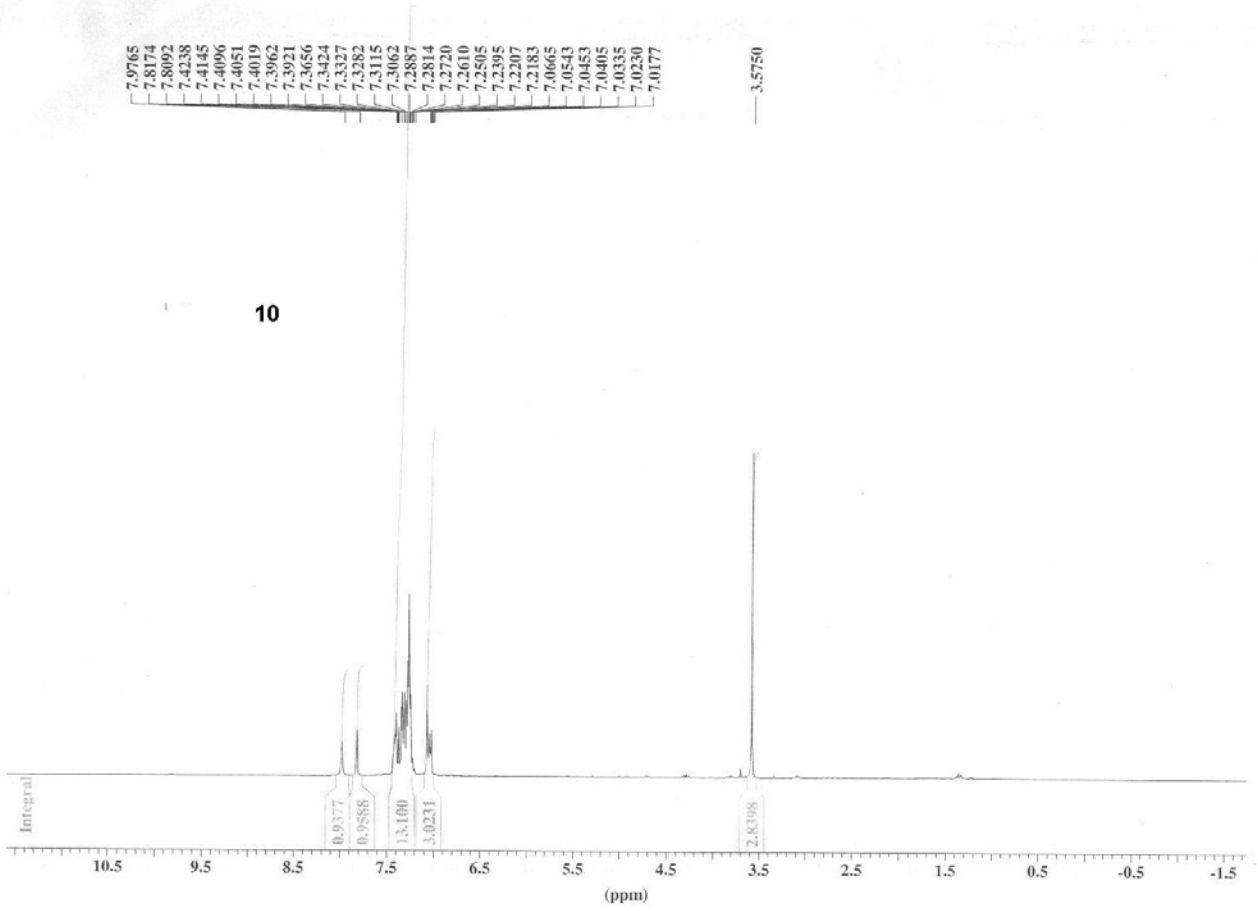

141.3836
140.6641
140.5324
140.1762
138.1995
137.7650
131.0835
130.3285
129.6945
128.6118
128.5441
128.4694
127.5932
127.1943
127.1587
125.5097
123.5081
123.1056
121.5849
121.2608
110.3624
109.7640
21.8362

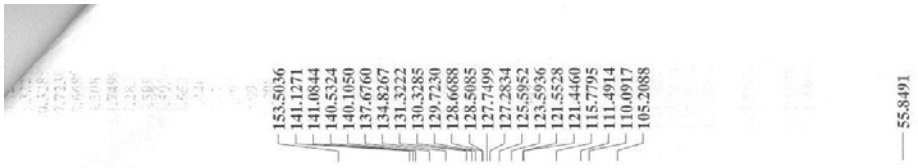
9


200
180
160
140
120
100
80
60
40
20
0
(ppm)

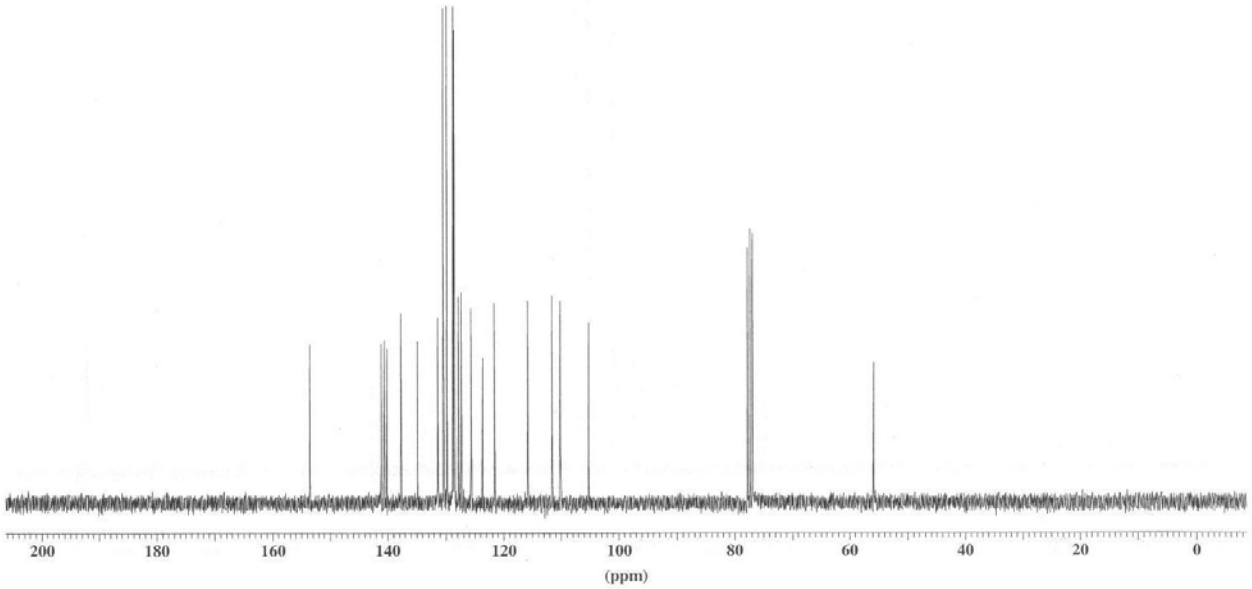
ZJ511

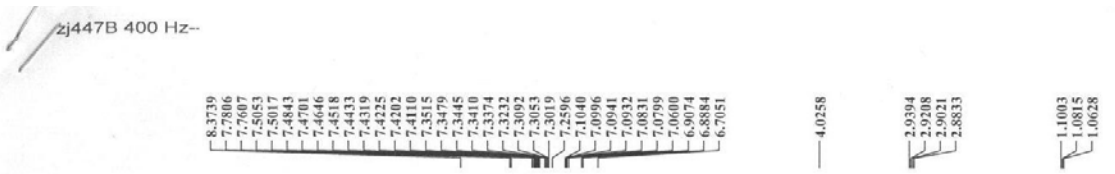
STANDARD 1H OBSERVE



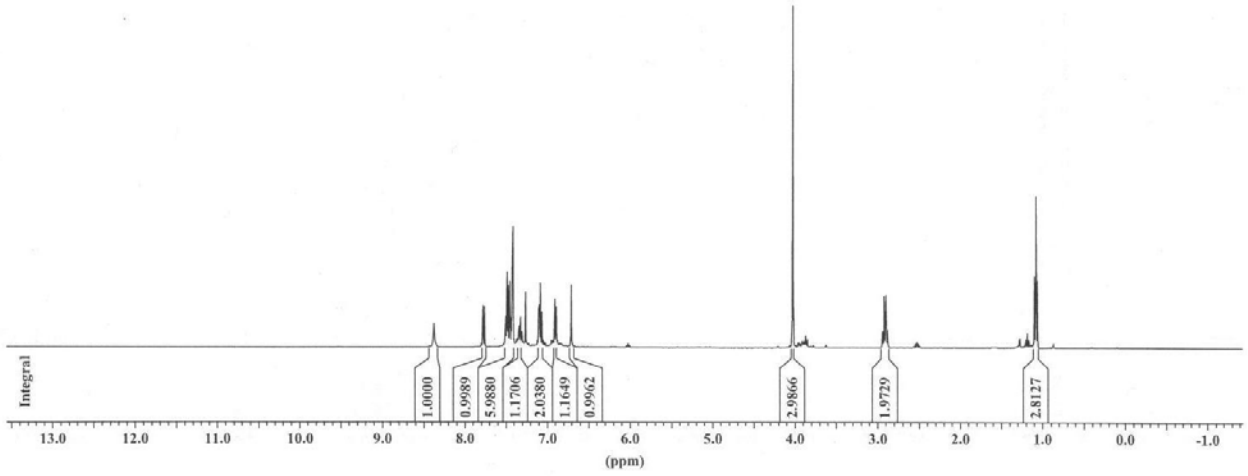

153.5036
141.1271
141.0844
140.5324
140.1050
137.6760
134.8267
131.3222
130.3285
129.7230
128.6688
128.5085
127.7499
127.2834
125.5952
123.5936
121.5528
121.4460
115.7795
111.4914
110.0917
105.2088
55.8491

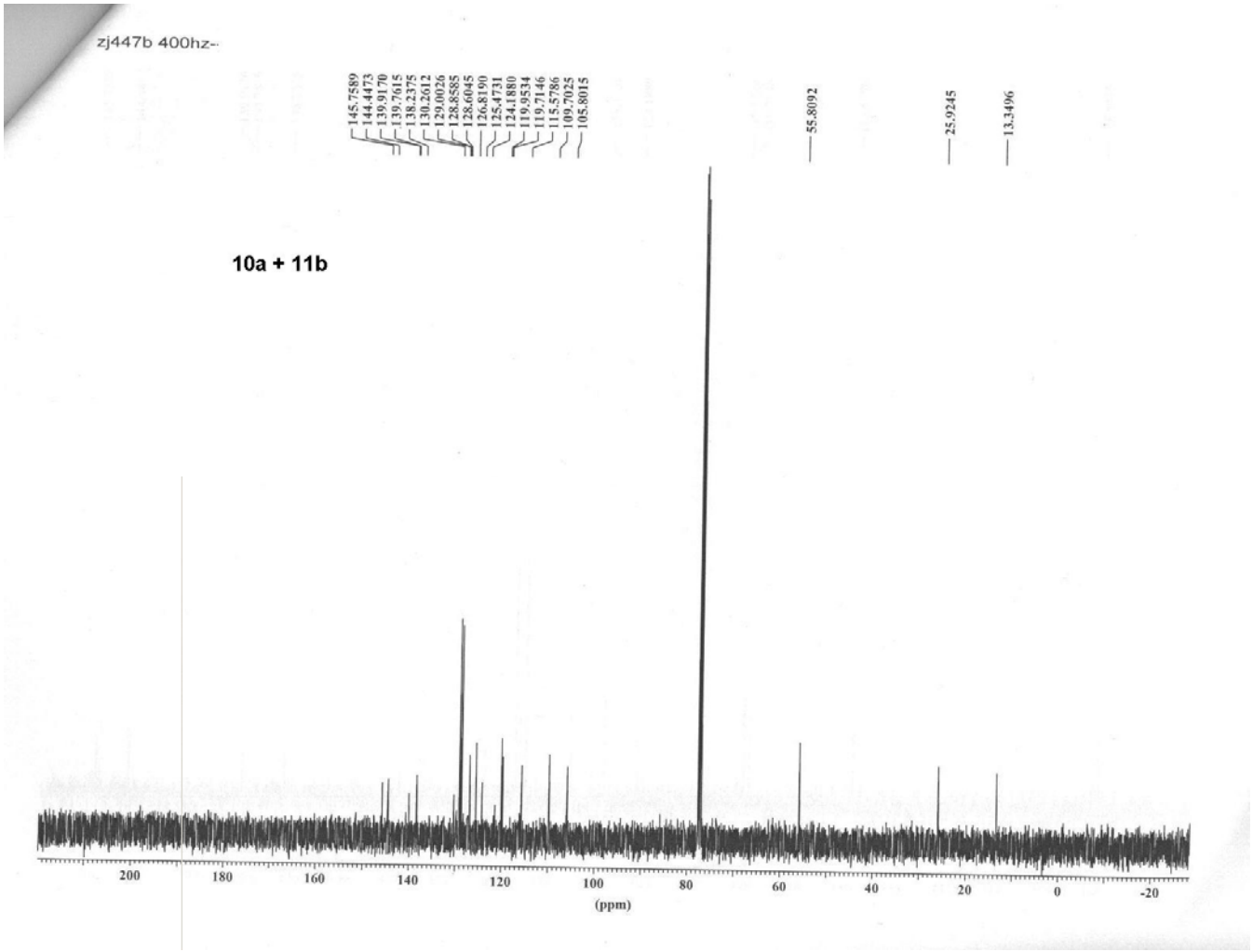
10

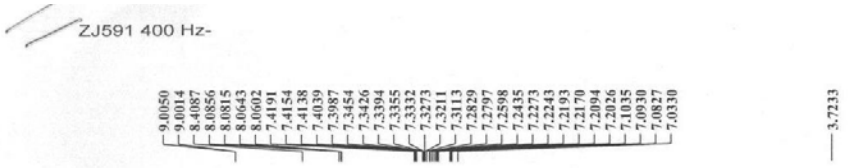

200
180
160
140
120
100
80
60
40
20
0
(ppm)


zj447B 400 Hz--
8.3739
7.7806
7.7607
7.6053
7.5017
7.4843
7.4701
7.4646
7.4518
7.4433
7.4319
7.4225
7.4202
7.4110
7.3515
7.3479
7.3445
7.3410
7.3374
7.3232
7.3092
7.3053
7.3019
7.2596
7.1040
7.0996
7.0941
7.0932
7.0831
7.0799
7.0600
6.9074
6.8884
6.7051
4.0258
2.9394
2.9208
1.9021
2.8833
1.1003
1.0815
1.0628

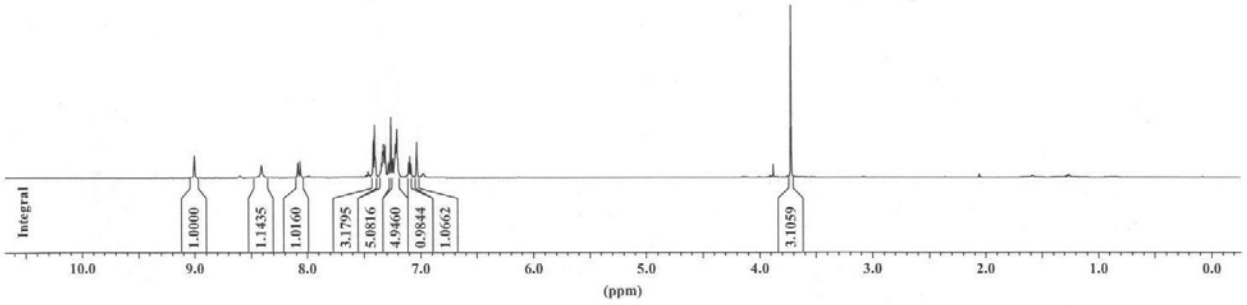
10a + 11b

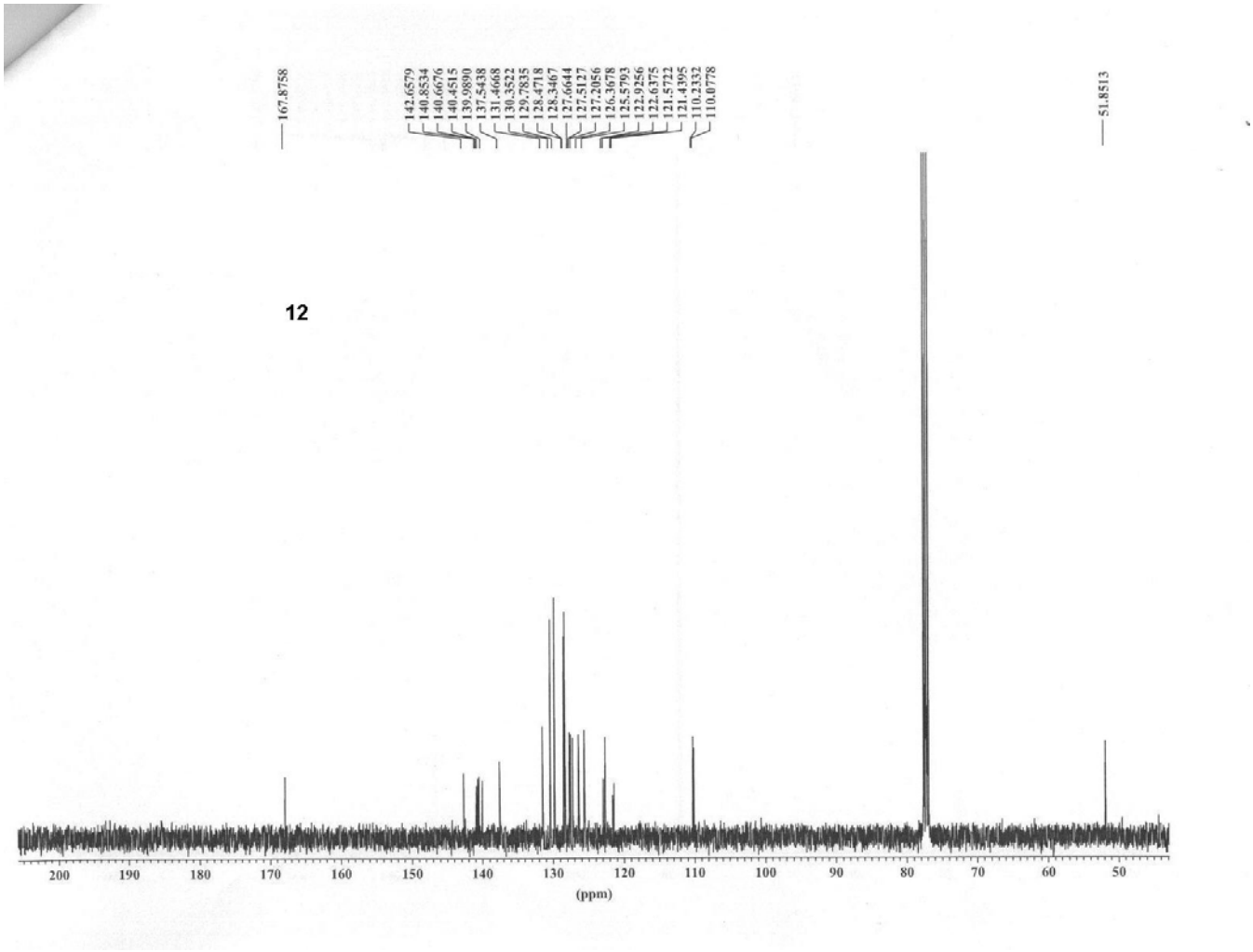

Integral
1.0000
0.9989
5.9880
1.1706
2.0380
1.1649
0.9962
2.9866
1.9729
2.8127
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
(ppm)


zj447b 400hz-
145.7589
144.4473
139.9170
139.7615
138.2375
130.2612
129.0026
128.8585
128.6045
126.8190
125.4731
124.1880
119.9534
119.7146
115.5786
109.7025
105.8015
55.8092
25.9245
13.3496
10a + 11b
200
180
160
140
120
100
80
60
40
20
0
-20
(ppm)


ZJ591 400 Hz-
9.0050
9.0014
8.4087
8.0856
8.0815
8.0643
8.0602
7.4191
7.4154
7.4138
7.4039
7.3987
7.3454
7.3426
7.3394
7.3355
7.3332
7.3273
7.3211
7.3113
7.2829
7.2797
7.2598
7.2435
7.2273
7.2243
7.2193
7.2170
7.2094
7.2026
7.1035
7.0930
7.0827
7.0330
3.7233

12


Integral
1.0000
1.1435
1.0160
3.1795
5.0816
4.9460
0.9844
1.0662
3.1059
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
(ppm)


167.8758
142.6579
140.8534
140.6676
140.4515
139.9890
137.5438
131.4668
130.3522
129.7835
128.4718
128.3467
127.6644
127.5127
127.2056
126.3678
125.5793
122.9256
122.6375
121.5722
121.4395
110.2332
110.0778
51.8513
12
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
(ppm)

2J486B

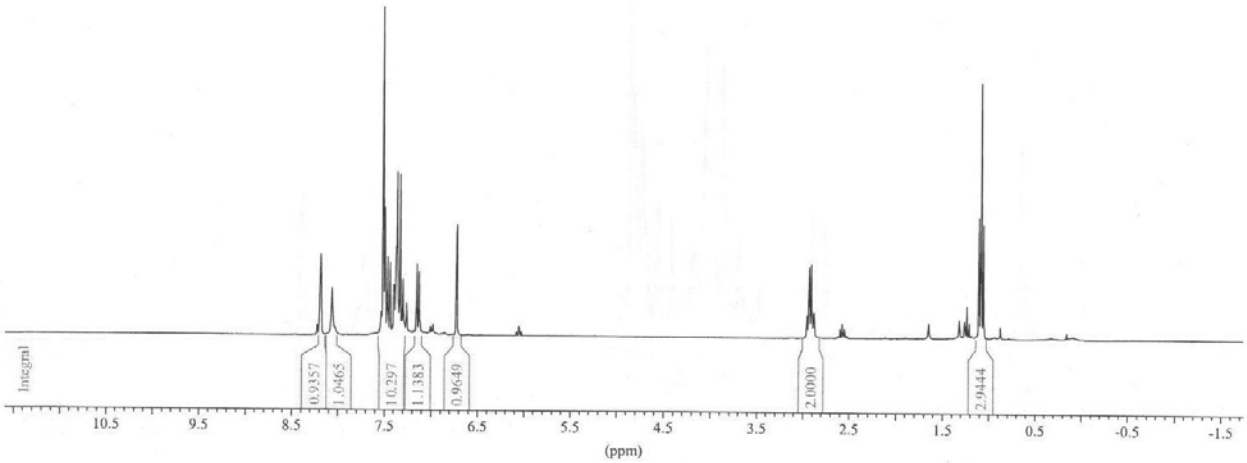
STANDARD 1H OBSERVE

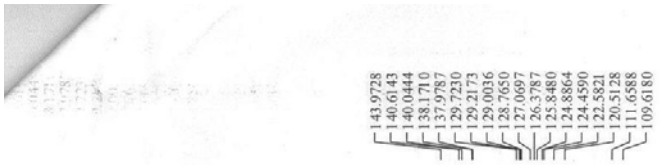
8.1914
8.1849
8.0620
7.5154
7.5081
7.4938
7.4881
7.4637
7.4613
7.4369
7.3974
7.3909
7.3689
7.3616
7.3579
7.3502
7.3457
7.3294
7.2997
7.2594
7.1491
7.1463
7.1251
7.1219
6.7210

2.9536
2.9287
2.9035
2.8791

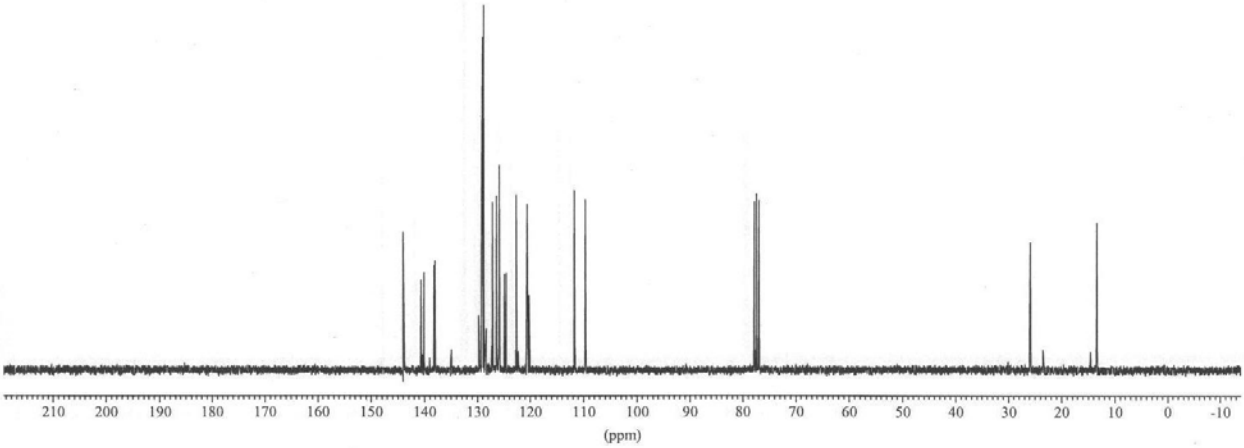
1.1075
1.0827
1.0574

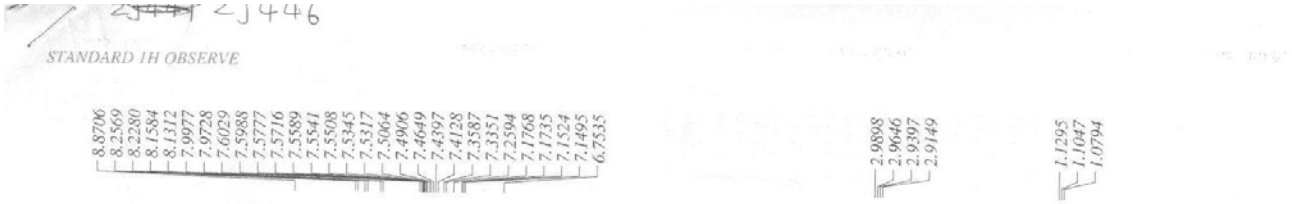
13a + 13b



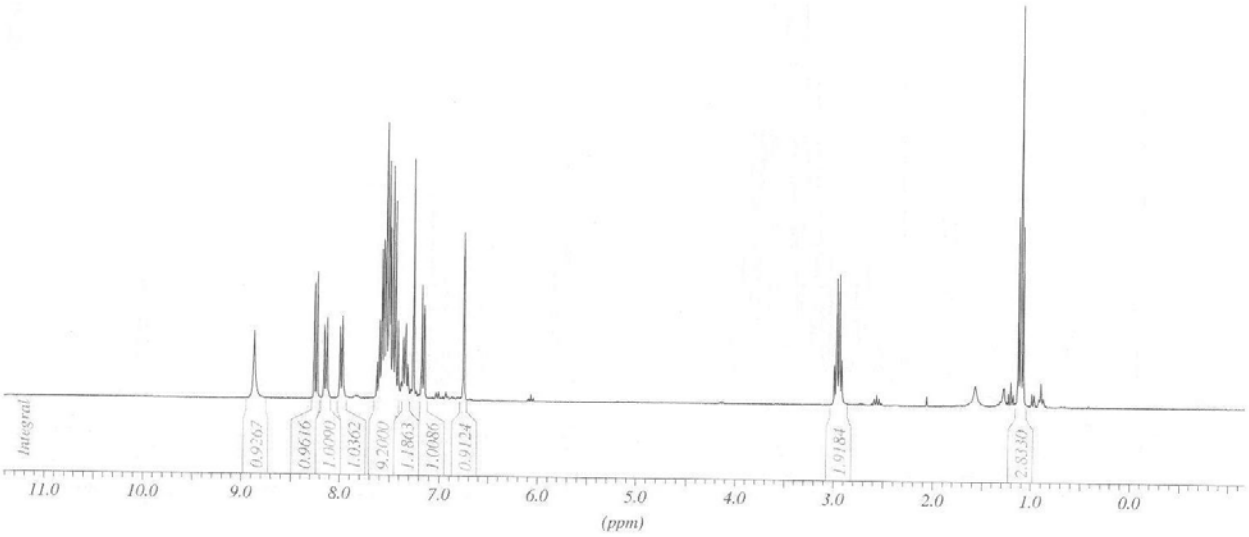

143.9728
140.6143
140.0444
138.1710
137.9787
129.7230
129.2173
129.0036
128.7650
127.0697
126.3787
125.8480
124.8864
124.4590
122.5821
120.5128
111.6588
109.6180
25.7575
13.3490

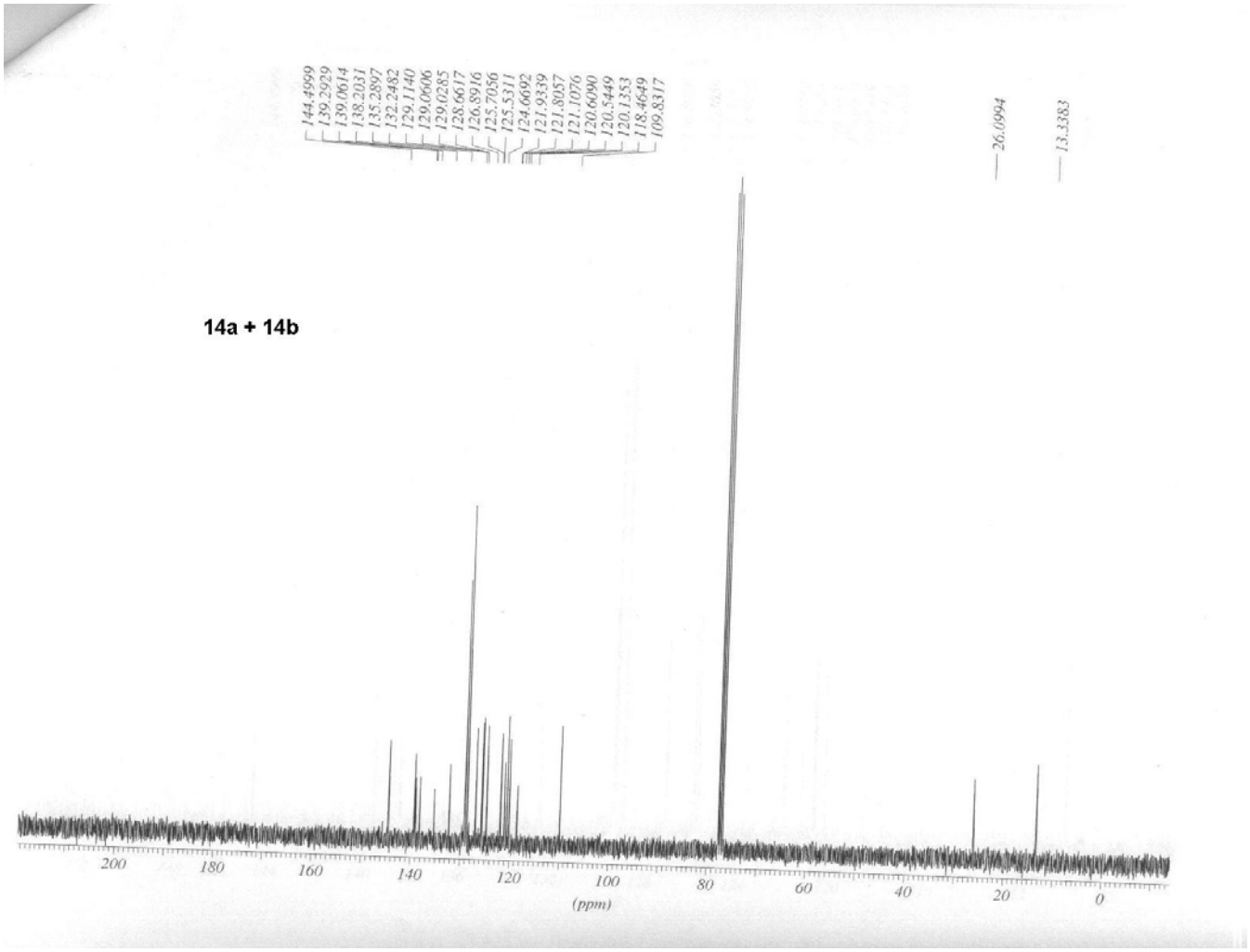
13a + 13b

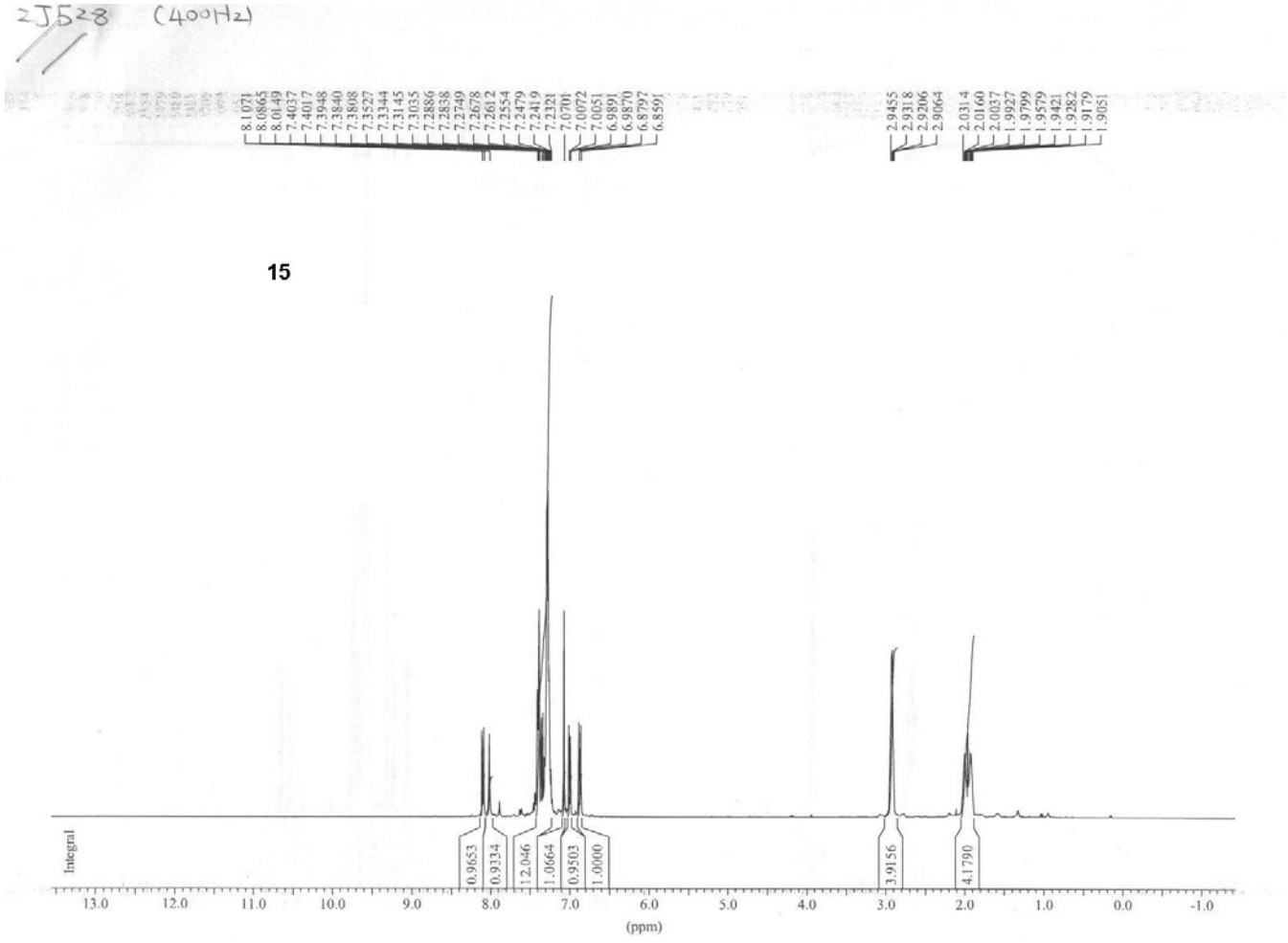

210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
(ppm)

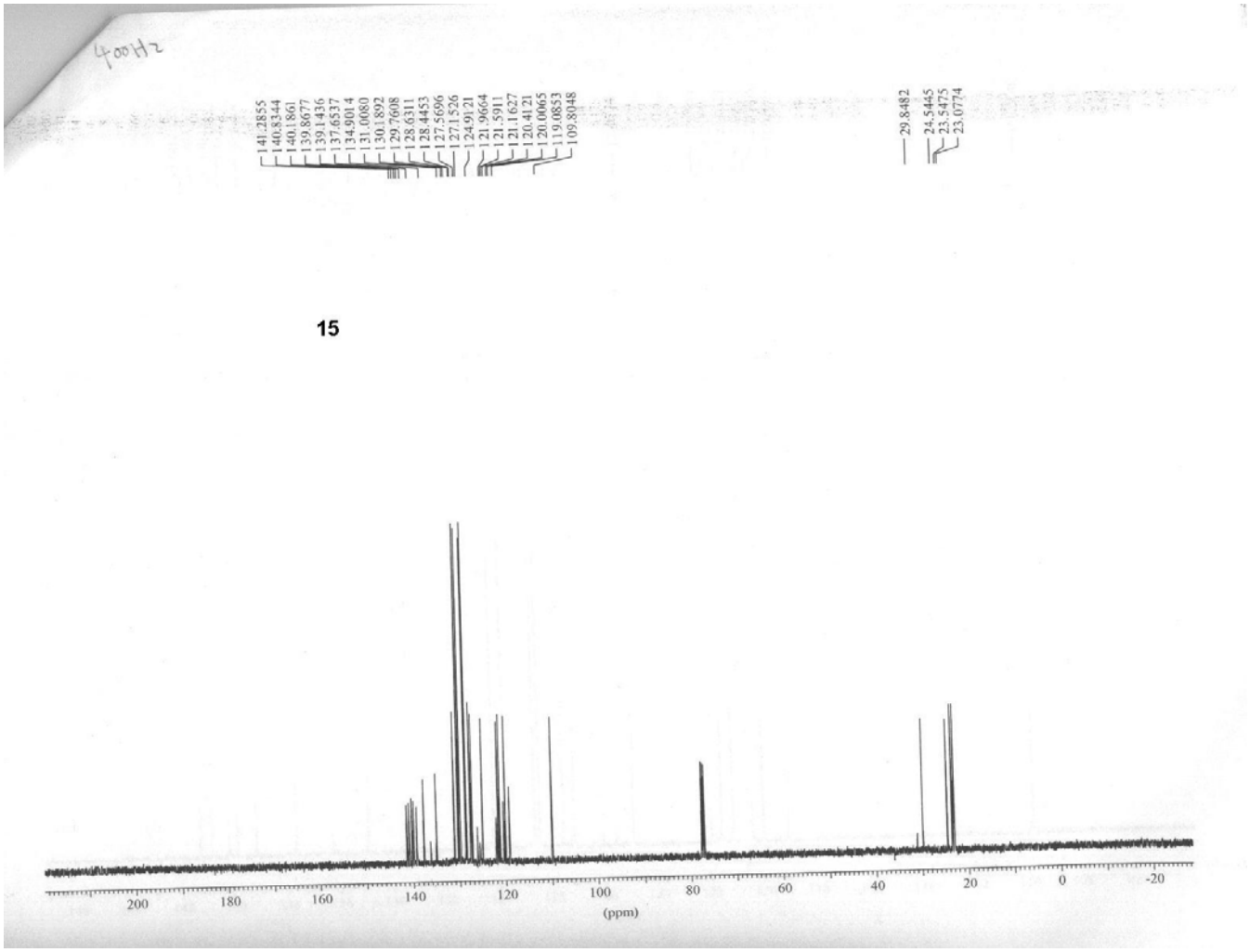

2J446
STANDARD IH OBSERVE
8.8706
8.2569
8.2280
8.1584
8.1312
7.9977
7.9728
7.6029
7.5988
7.5777
7.5716
7.5589
7.5541
7.5508
7.5345
7.5317
7.5064
7.4906
7.4649
7.4397
7.4128
7.3587
7.3351
7.2594
7.1768
7.1735
7.1524
7.1495
6.7535
2.9898
2.9646
2.9397
2.9149
1.1295
1.1047
1.0794

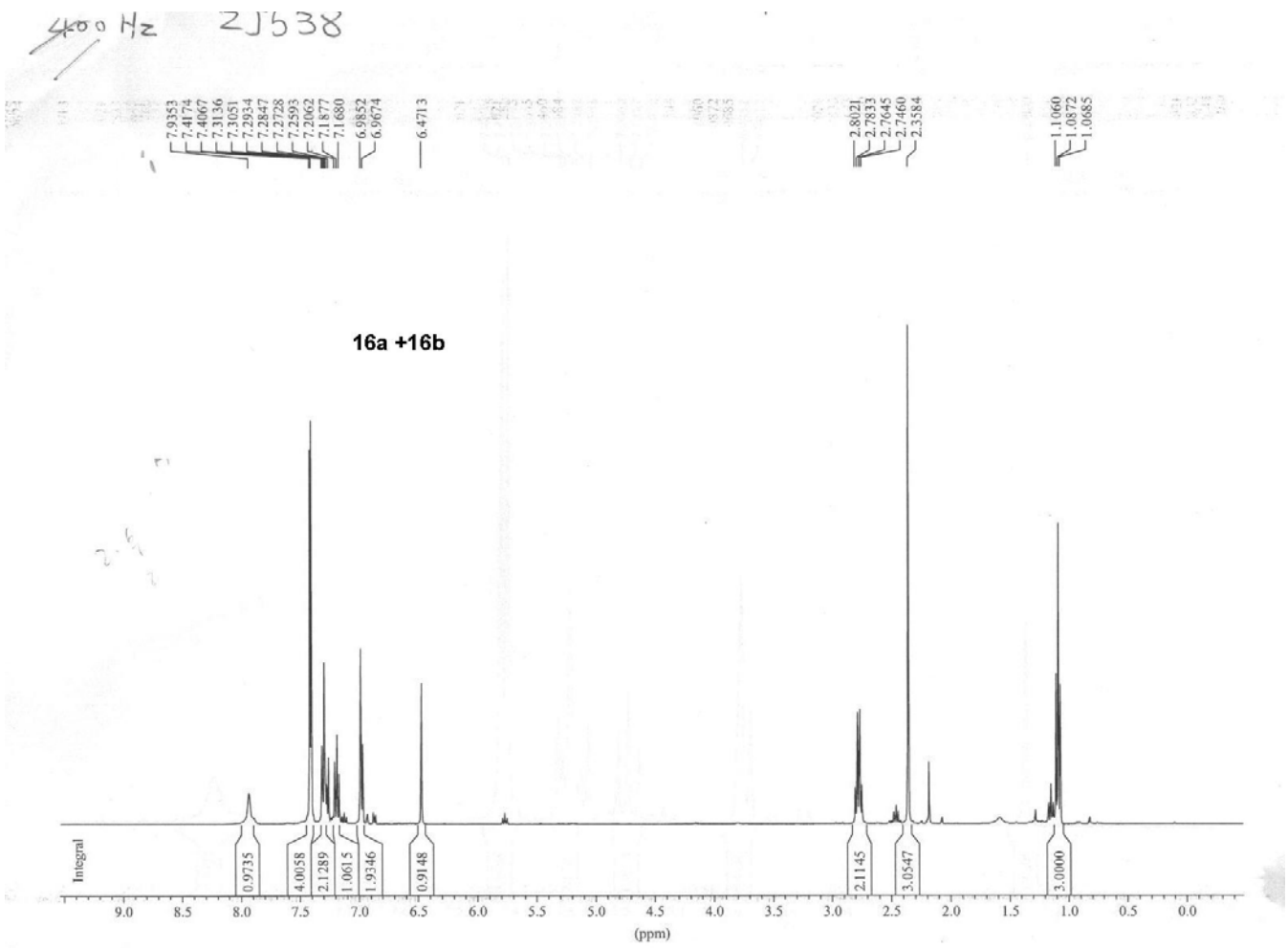
14a + 14b

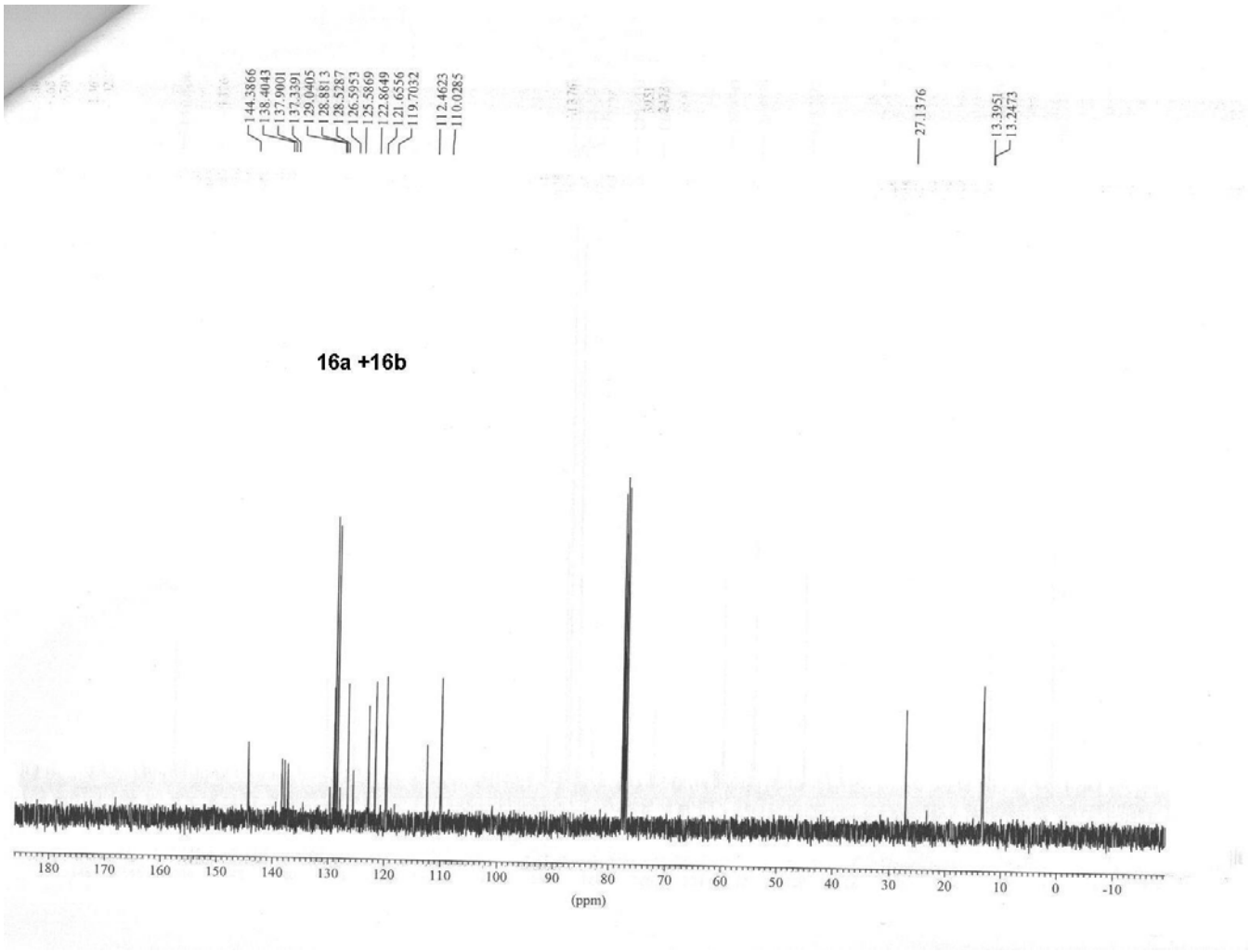

Integral
0.9267
0.9616
1.0090
1.0362
9.2000
1.1863
1.0086
0.9124
1.9184
2.8330
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
(ppm)

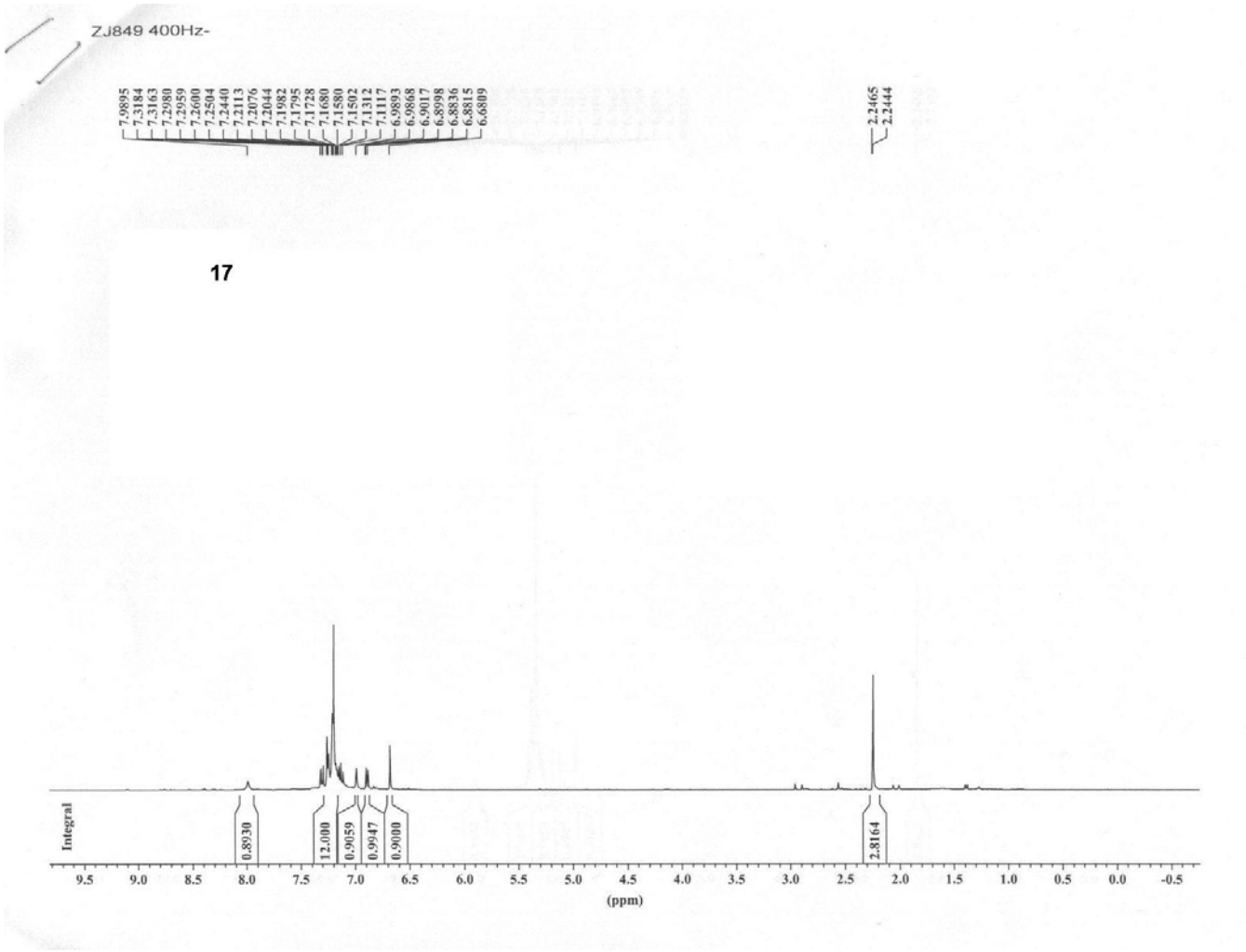

144.4999
139.2929
139.0614
138.2031
135.2897
132.2482
129.1140
129.0606
129.0285
128.6617
126.8916
125.7056
125.5311
124.6692
121.9339
121.8057
121.1076
120.6090
120.5449
120.1353
118.4649
109.8317
26.0994
13.3383
14a + 14b
200
180
160
140
120
100
80
60
40
20
0
(ppm)

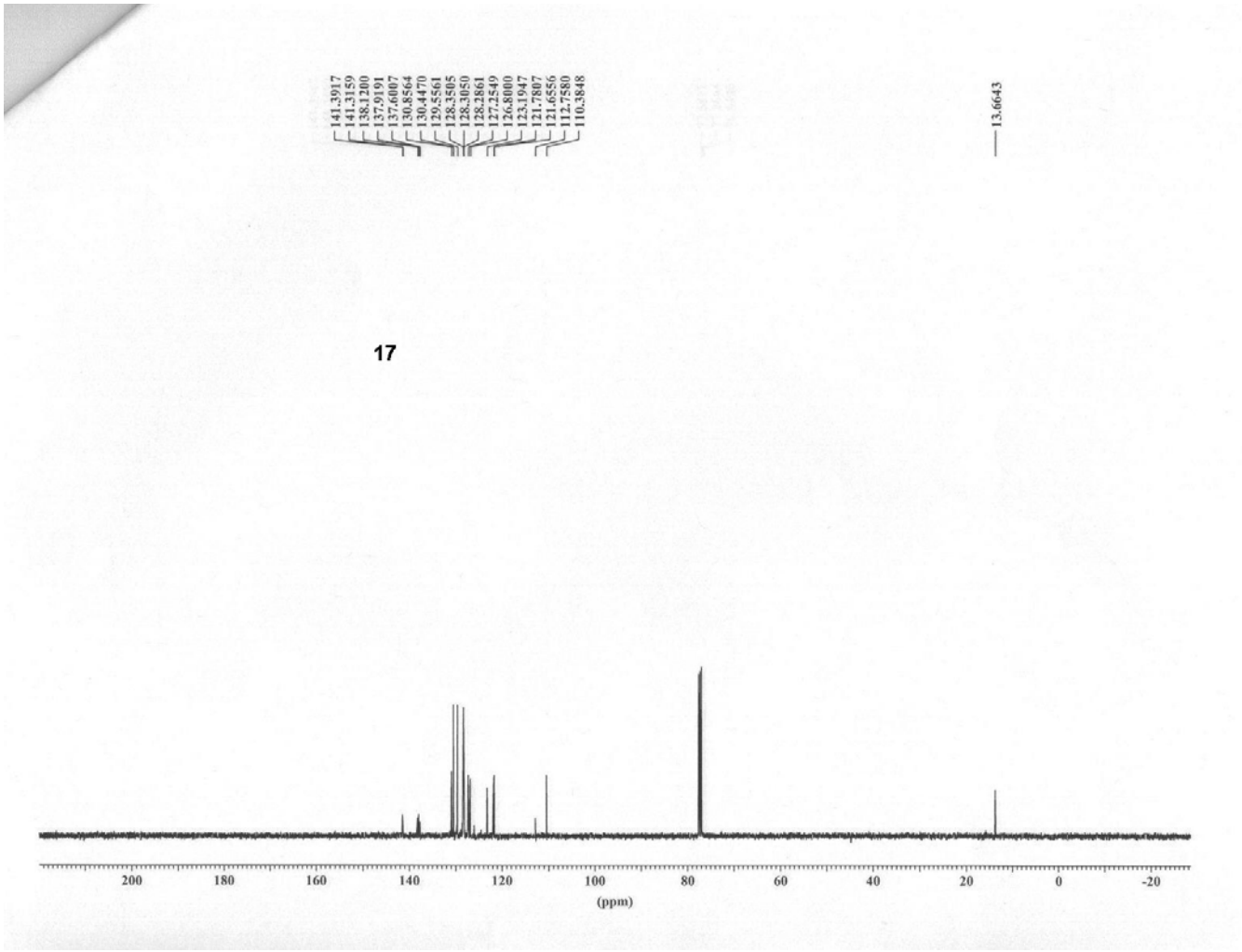

2J528 (400Hz)
8.1071
8.0865
8.0149
7.4637
7.4017
7.3948
7.3840
7.3808
7.3527
7.3344
7.3145
7.3035
7.2886
7.2838
7.2749
7.2678
7.2612
7.2554
7.2479
7.2419
7.2321
7.0701
7.0072
7.0051
6.9891
6.9870
6.8797
6.8591
2.9455
2.9318
2.9206
2.9064
2.0314
2.0160
2.0037
1.9927
1.9799
1.9579
1.9421
1.9282
1.9179
1.9051
15
Integral
0.9653
0.9334
12.046
1.0664
0.9503
1.0000
3.9156
4.1790
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
(ppm)


400Hz
141.2855
140.8344
140.1861
139.8677
139.1436
137.6537
134.9014
131.0080
130.1892
129.7608
128.6311
128.4453
127.5696
127.1526
124.9121
121.9664
121.5911
121.1627
120.4121
120.0065
119.0853
109.8048
29.8482
24.5445
23.5475
23.0774
15
200
180
160
140
120
100
80
60
40
20
0
-20
(ppm)


400 Hz
2J538
7.9353
7.4174
7.4067
7.3136
7.3051
7.2934
7.2847
7.2728
7.2593
7.2062
7.1877
7.1680
6.9852
6.9674
6.4713
2.8021
2.7833
2.7645
2.7460
2.3584
1.1060
1.0872
1.0685
16a +16b
Integral
0.9735
4.0058
2.1289
1.0615
1.9346
0.9148
2.1145
3.0547
3.0000
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
(ppm)

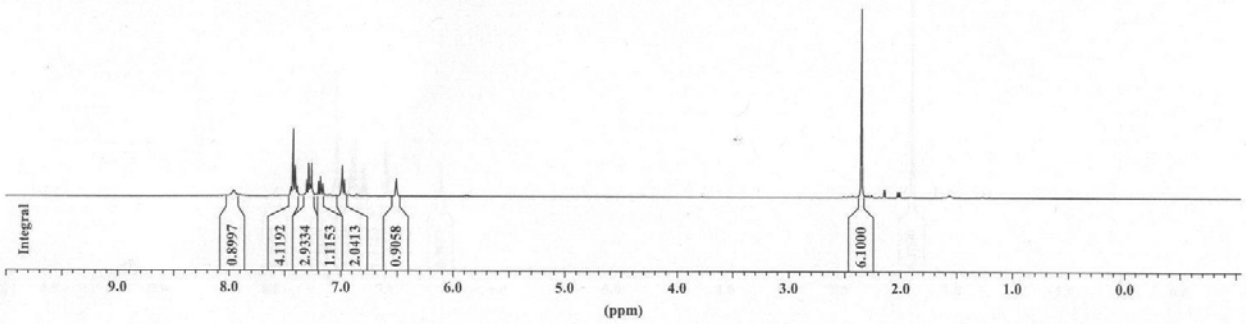

144.3866
138.4043
137.9001
137.3391
129.0405
128.8813
128.5287
126.5953
125.5869
122.8649
121.6556
119.7032
112.4623
110.0285
27.1376
13.3951
13.2473
16a +16b
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
(ppm)

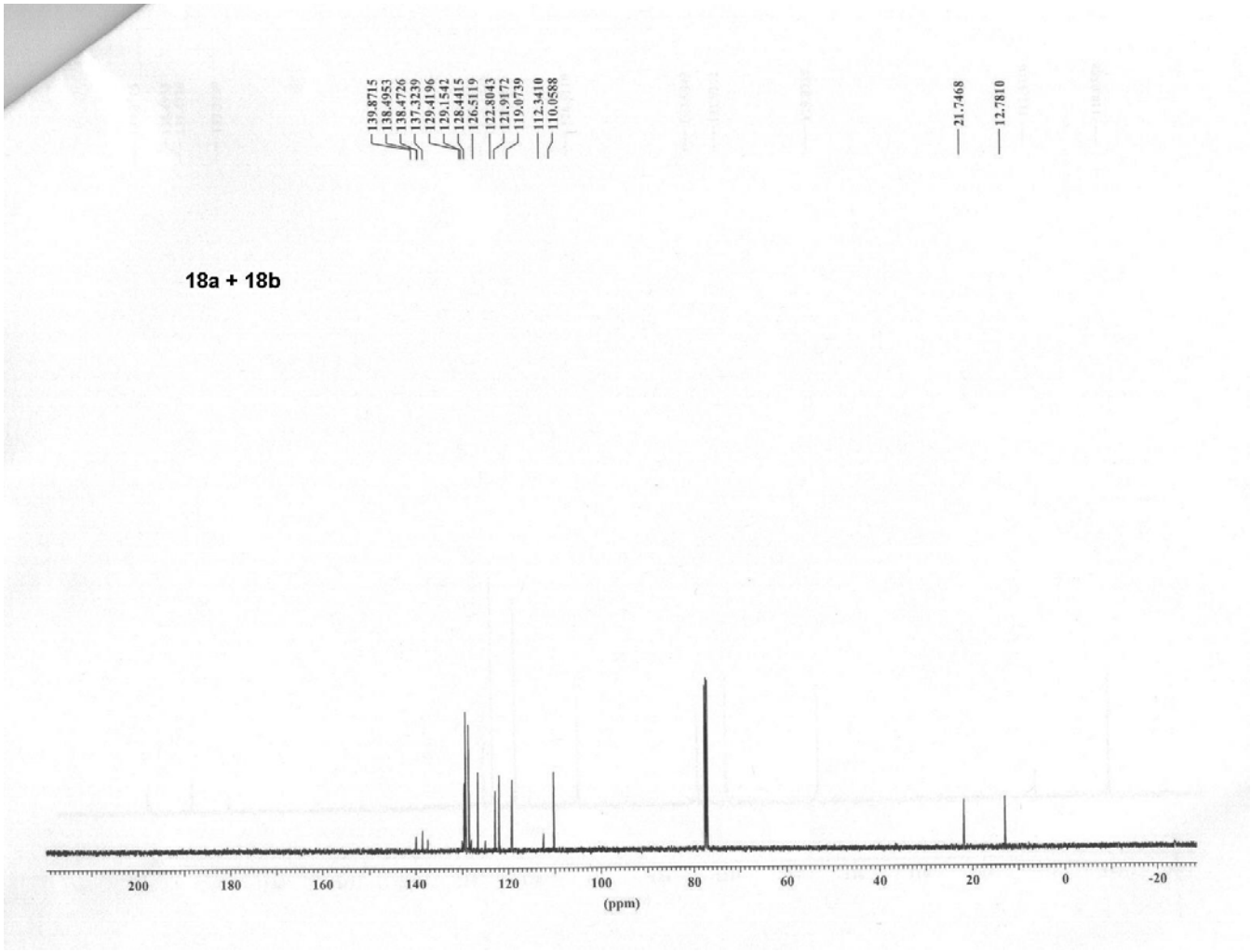

ZJ849 400Hz-
7.9895
7.3184
7.3163
7.2980
7.2959
7.2600
7.2504
7.2440
7.2113
7.2076
7.2044
7.1982
7.1795
7.1728
7.1680
7.1580
7.1502
7.1312
7.1117
6.9893
6.9868
6.9017
6.8998
6.8836
6.8815
6.6809
2.2465
2.2444
17
Integral
0.8930
12.000
0.9059
0.9947
0.9000
2.8164
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
(ppm)


141.3917
141.3159
138.1200
137.9191
137.6007
130.8564
130.4470
129.5561
128.3505
128.3050
128.2861
127.2549
126.8000
123.1947
121.7807
121.6556
112.7580
110.3848
13.6643
17
200
180
160
140
120
100
80
60
40
20
0
-20
(ppm)

ZJ850 400Hz-

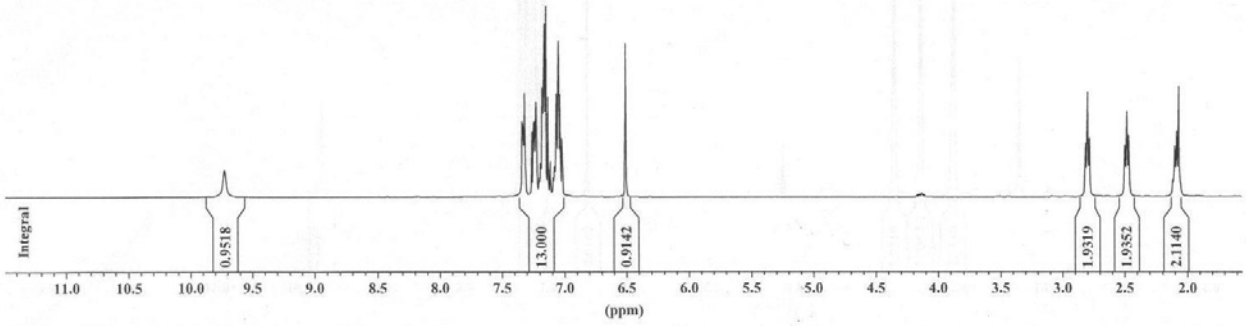
18a + 18b

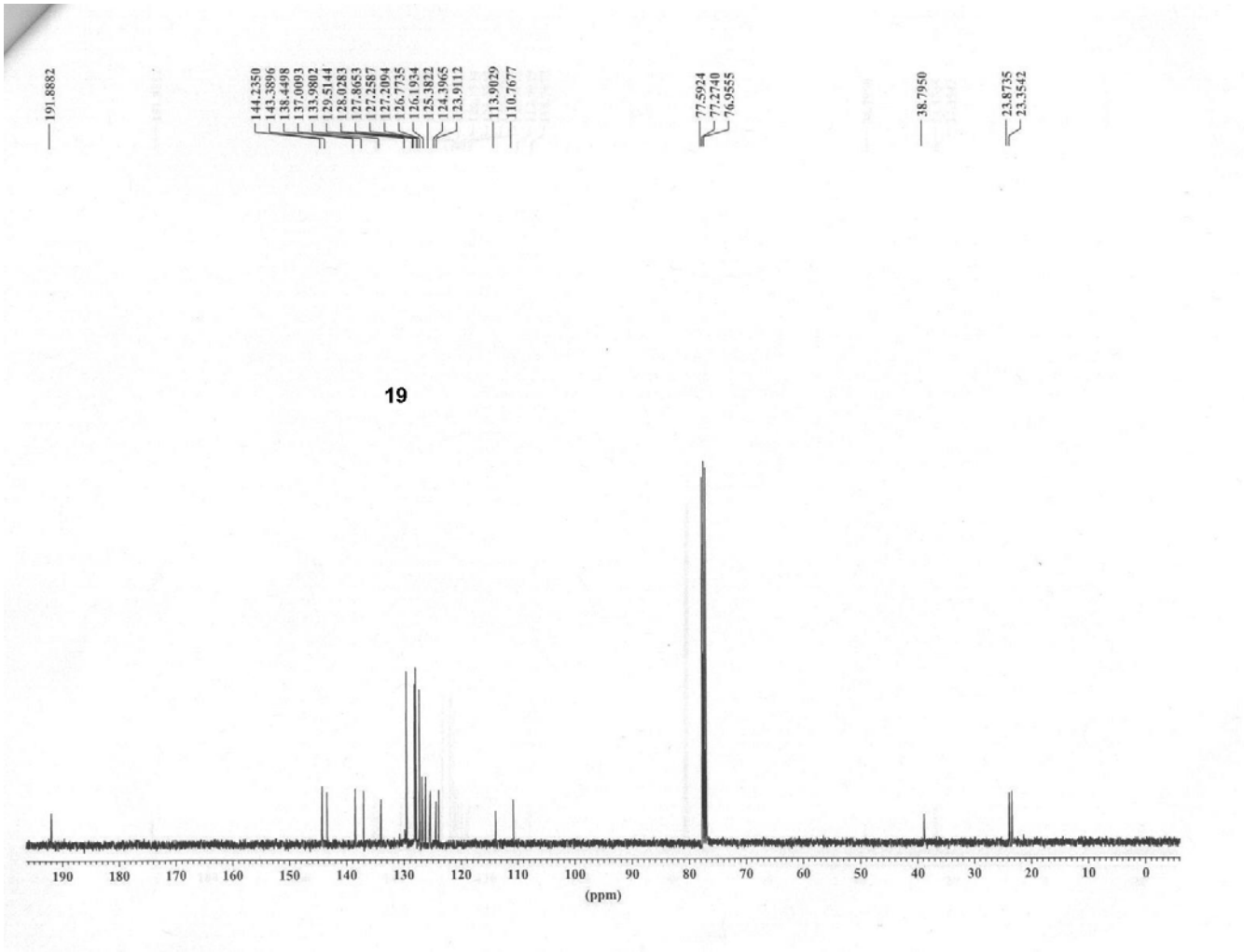


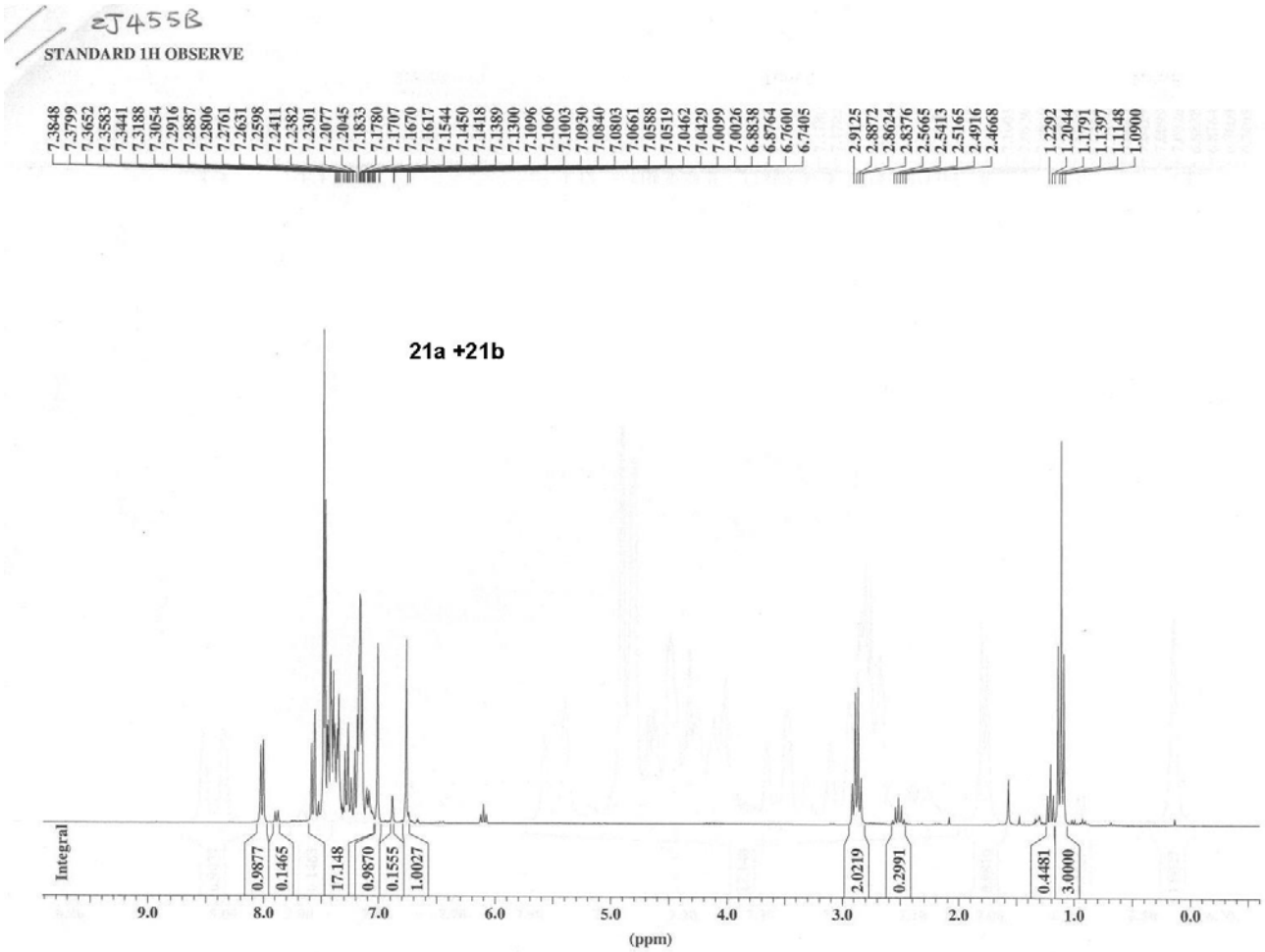

139.8715
138.4953
138.4726
137.3239
129.4196
129.1542
128.4415
126.5119
122.8043
121.9172
119.0739
112.3410
110.0588
21.7468
12.7810
18a + 18b
200
180
160
140
120
100
80
60
40
20
0
-20
(ppm)

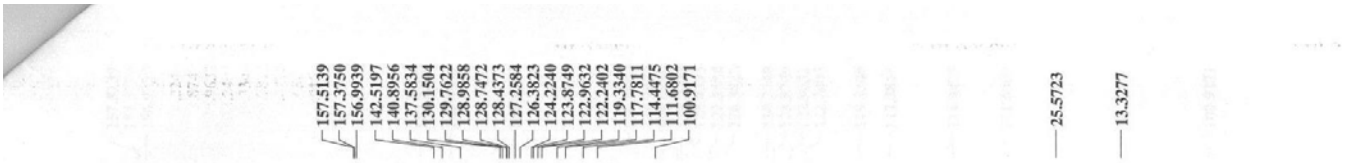
ZJ847H 400Hz-

19

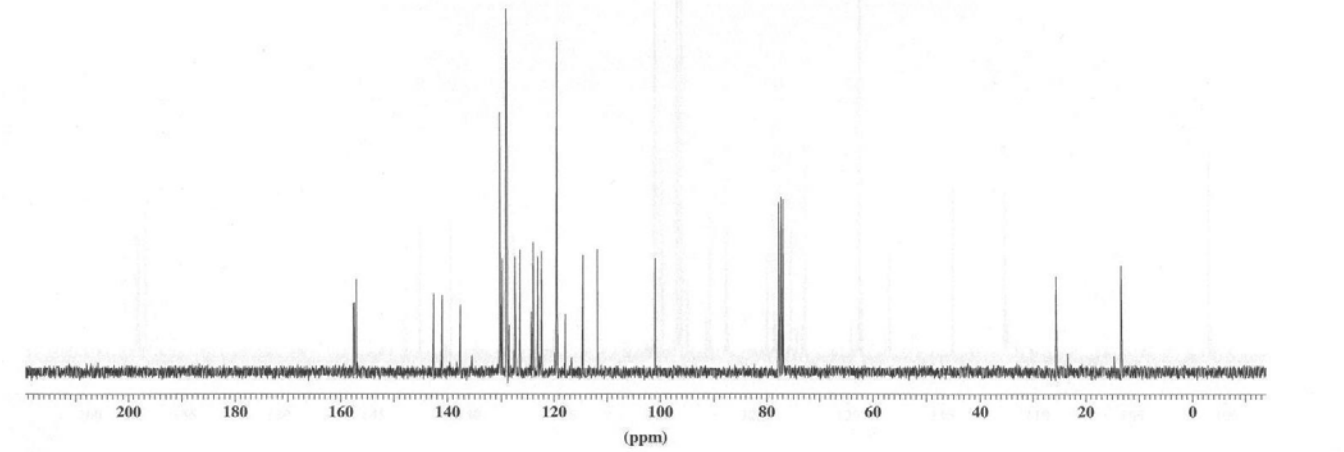



191.8882
144.2350
143.3896
138.4498
137.0093
133.9802
129.5144
128.0283
127.8653
127.2587
127.2094
126.7735
126.1934
125.3822
124.3965
123.9112
113.9029
110.7677
77.5924
77.2740
76.9555
38.7950
23.8735
23.3542
19
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
(ppm)


EJ455B
STANDARD 1H OBSERVE
7.3848
7.3799
7.3652
7.3583
7.3441
7.3188
7.3054
7.2916
7.2887
7.2806
7.2761
7.2631
7.2598
7.2411
7.2382
7.2301
7.2077
7.2045
7.1833
7.1780
7.1707
7.1670
7.1617
7.1544
7.1450
7.1418
7.1389
7.1300
7.1096
7.1060
7.1003
7.0930
7.0840
7.0803
7.0661
7.0588
7.0519
7.0462
7.0429
7.0099
7.0026
6.8838
6.8764
6.7600
6.7405
2.9125
2.8872
2.8624
2.8376
2.5665
2.5413
2.5165
2.4916
2.4668
1.2292
1.2044
1.1791
1.1397
1.1148
1.0900
21a +21b
Integral
0.9877
0.1465
17.148
0.9870
0.1555
1.0027
2.0219
0.2991
0.4481
3.0000
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
(ppm)


157.5139
157.3750
156.9939
142.5197
140.8956
137.5834
130.1504
129.7622
128.9858
128.7472
128.4373
127.2584
126.3823
124.2240
123.8749
122.9632
122.2402
119.3340
117.7811
114.4475
111.6802
100.9171
25.5723
13.3277

21a +21b


200
180
160
140
120
100
80
60
40
20
0
(ppm)

STANDARD 1H OBSERVE

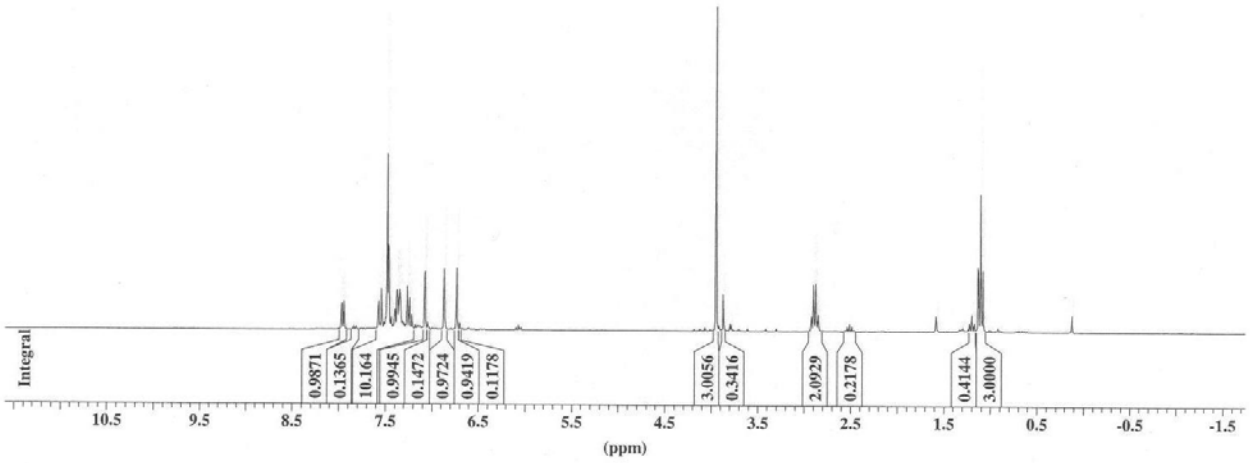
7.8381
7.8141
7.8117
7.5671
7.5402
7.4771
7.4662
7.4596
7.4312
7.3957
7.3913
7.3709
7.3673
7.3644
7.3489
7.3441
7.3400
7.3339
7.2594
7.2362
7.2338
7.2118
7.2085
7.0742
7.0669
7.0400
7.0323
6.8650
6.8573
6.7287
6.7014
6.6937

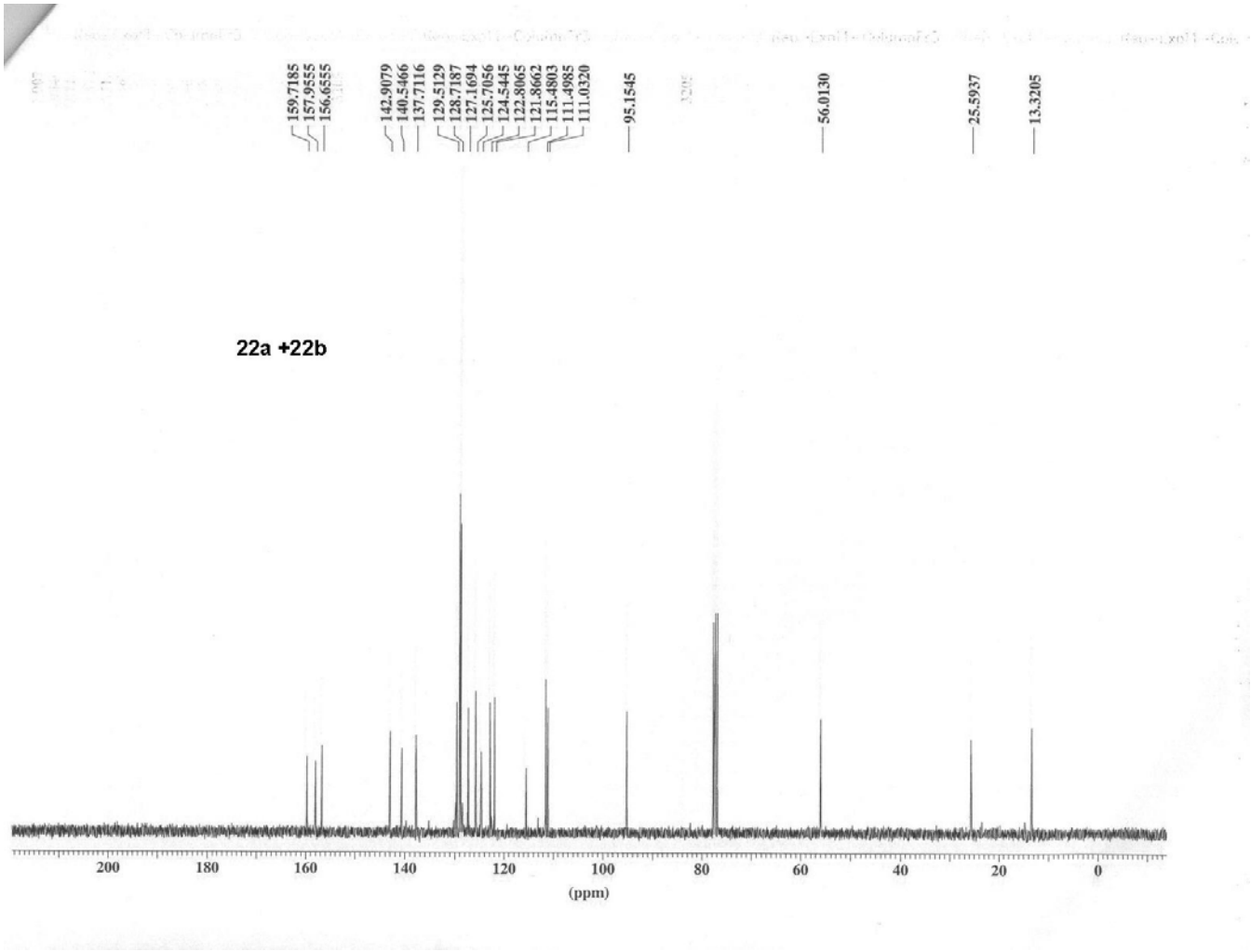
3.9446
3.8685

2.9206
2.8954
2.8705
2.8461
2.5584
2.5336
2.5087
2.4839
2.4591

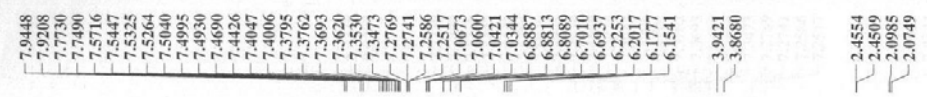
1.2215
1.1966
1.1714
1.1299
1.1051
1.0798

22a +22b

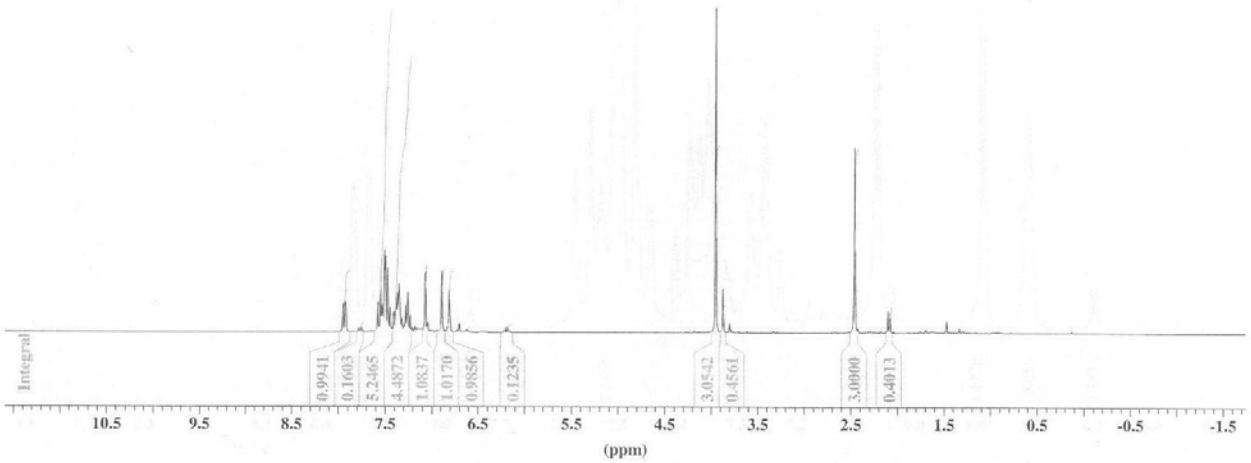



159.7185
157.9555
156.6555
142.9079
140.5466
137.7116
129.5129
128.7187
127.1694
125.7056
124.5445
122.8065
121.3662
115.4803
111.4985
111.0320
95.1545
56.0130
25.5937
13.3205
22a +22b
200
180
160
140
120
100
80
60
40
20
0
(ppm)

STANDARD 1H OBSERVE

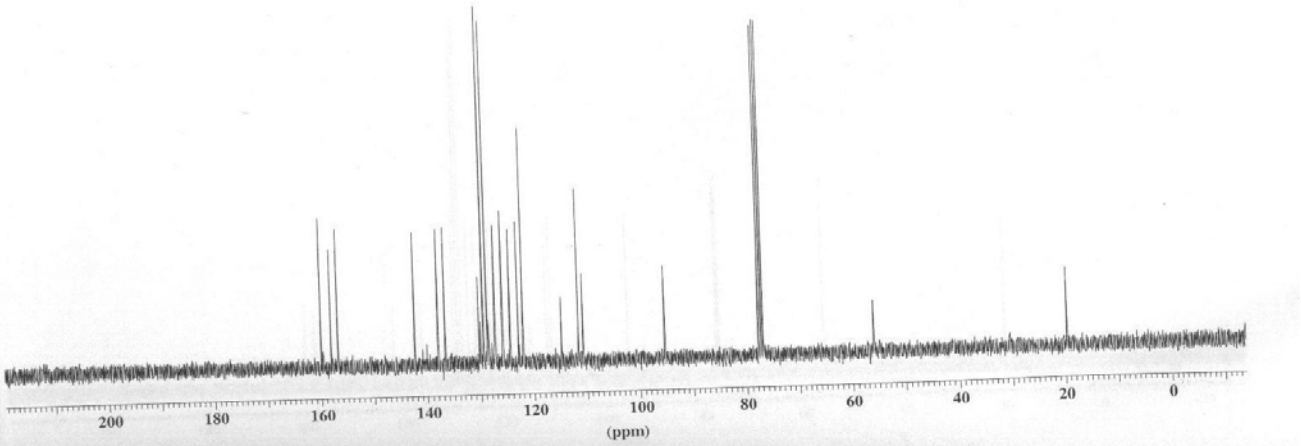


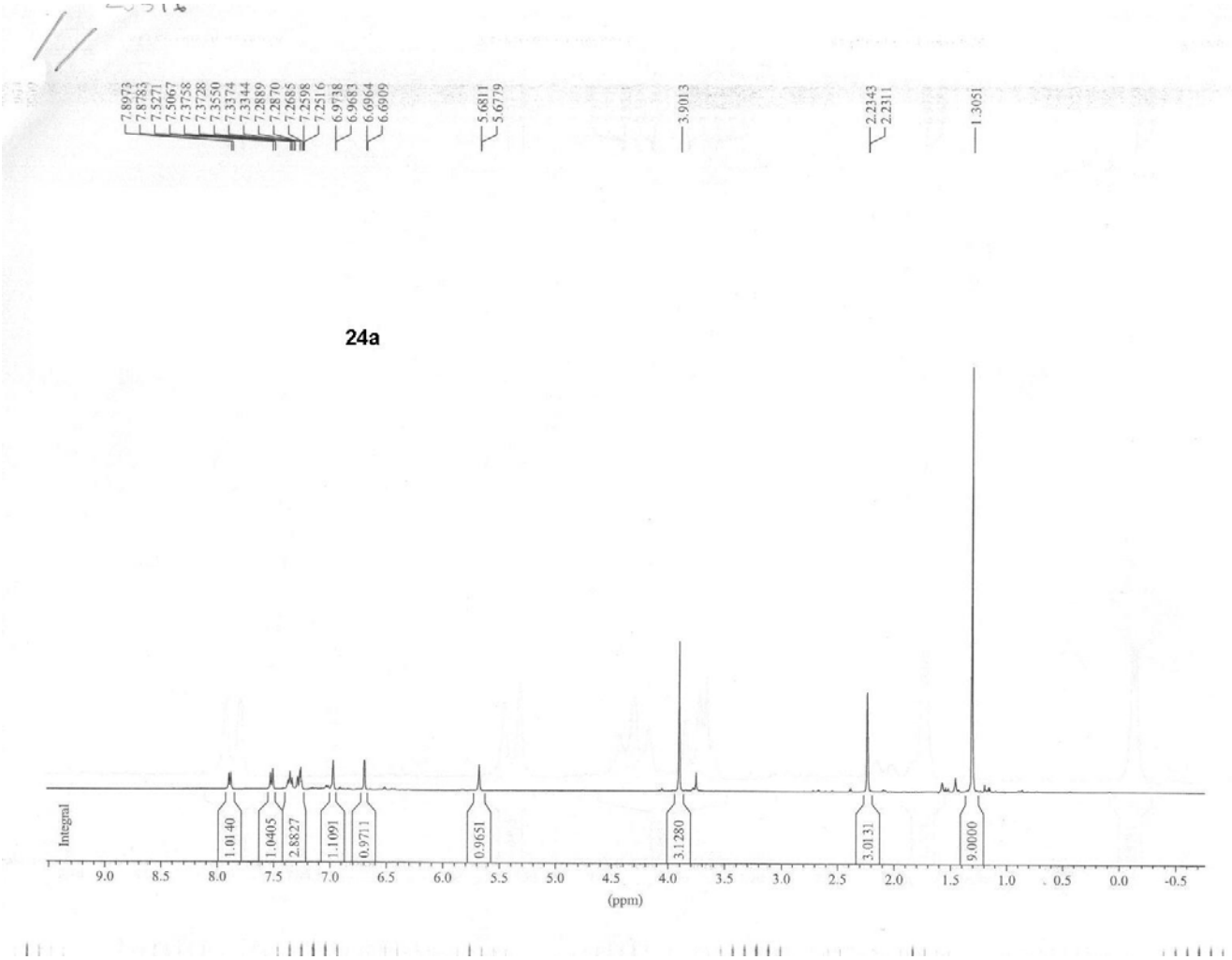
23a +23b

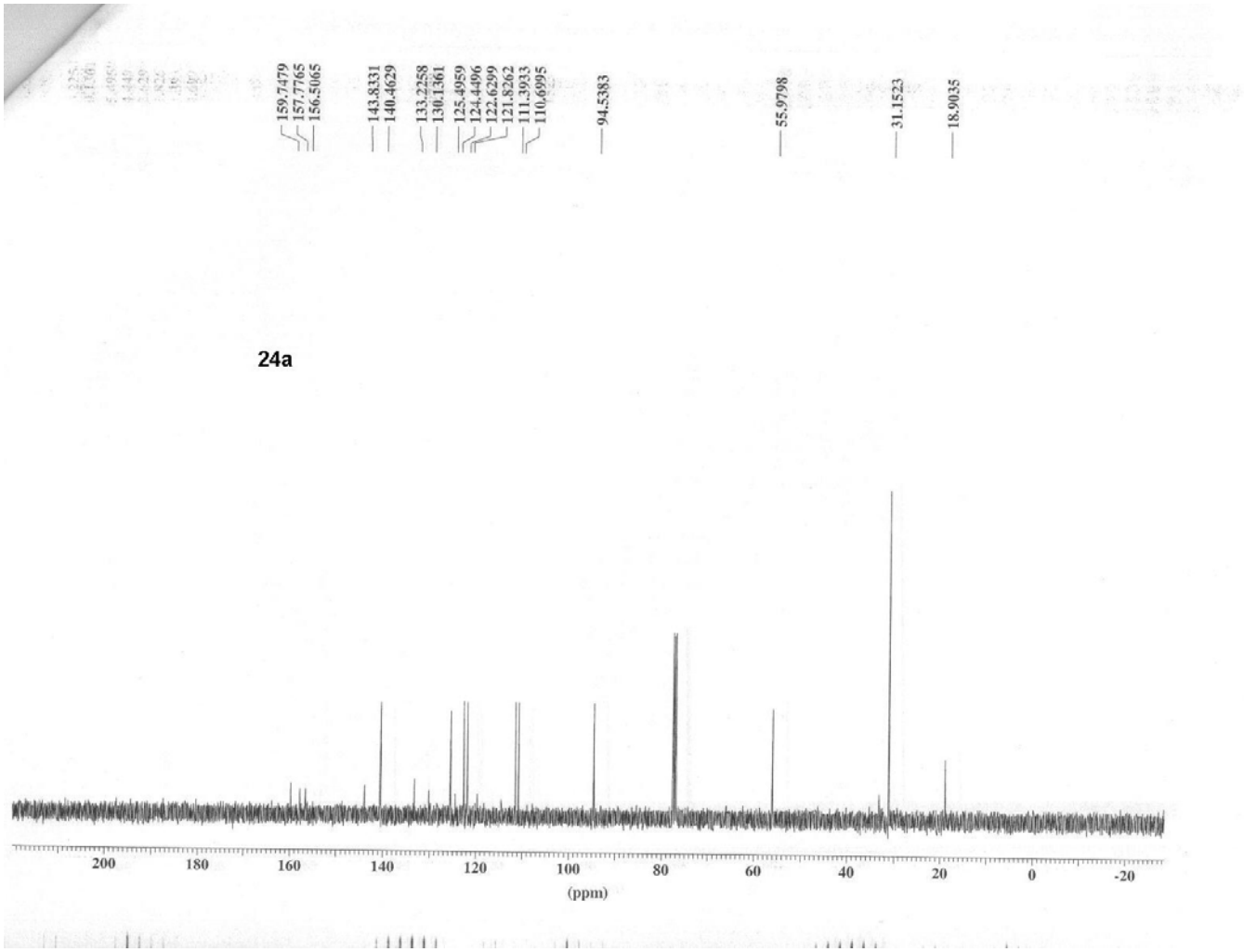


159.8716
158.0196
156.6627
142.1956
137.8113
136.5398
130.1718
130.1504
129.3170
126.6617
127.1373
125.7519
124.3522
122.8278
121.8983
114.6790
111.5056
110.5868
95.2293
56.0486
56.0130
19.6174
19.6031

23a +23b




7.8973
7.8783
7.5271
7.5067
7.3758
7.3728
7.3550
7.3374
7.3344
7.2889
7.2870
7.2685
7.2598
7.2516
6.9738
6.9683
6.6964
6.6909
5.6811
5.6779
3.9013
2.2343
2.2311
1.3051
24a
Integral
1.0140
1.0405
2.8827
1.1091
0.9711
0.9651
3.1280
3.0131
9.0000
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
-0.5
(ppm)

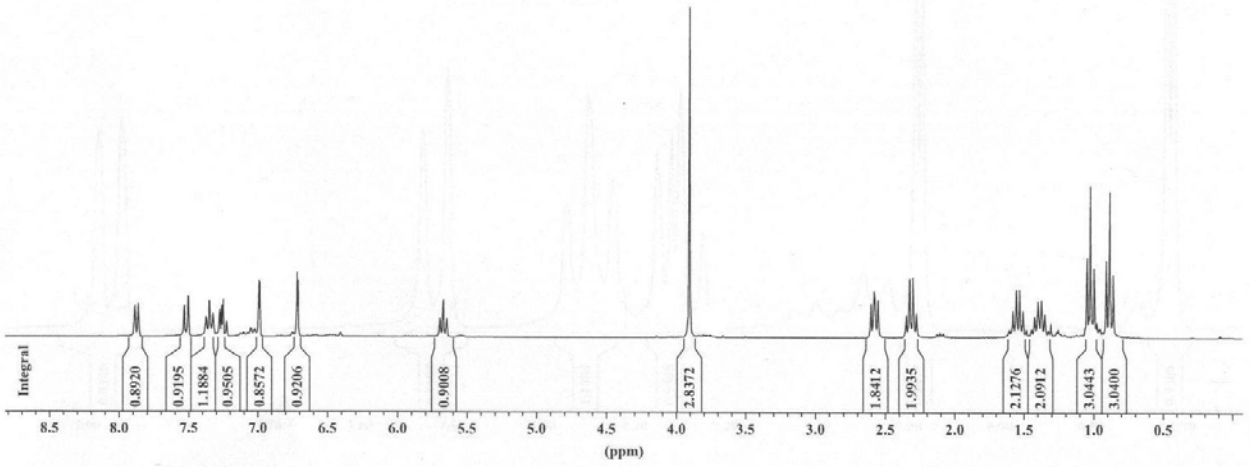

159.7479
157.7765
156.5065
143.8331
140.4629
133.2258
130.1361
125.4959
124.4496
122.6299
121.8262
111.3933
110.6995
94.5383
55.9798
31.1523
18.9035
24a
200
180
160
140
120
100
80
60
40
20
0
-20
(ppm)

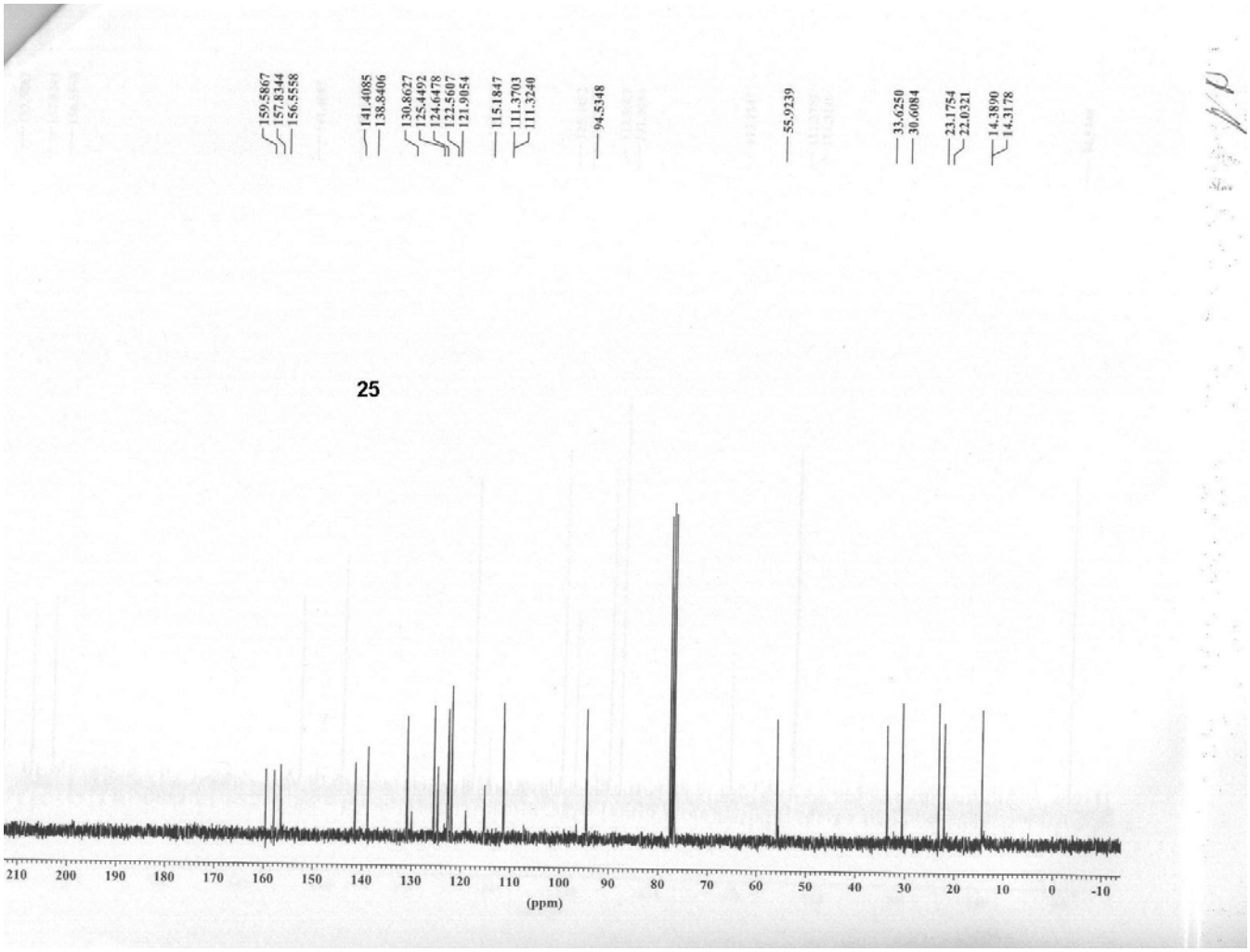
ZJ511

STANDARD 1H OBSERVE

7.8866
7.8609
7.5305
7.5232
7.3750
7.3586
7.3481
7.3237
7.3192
7.2741
7.2586
7.2488
7.2240
6.9908
6.9835
6.7153
6.7080
5.6938
5.6697
5.6453
3.9022
2.6019
2.5771
2.5507
2.3480
2.3236
2.2987
2.2739
1.6040
1.5796
1.5548
1.5304
1.5055
1.4811
1.4465
1.4237
1.3989
1.3733
1.3484
1.3240
1.0477
1.0233
0.9988
0.9089
0.8845
0.8601

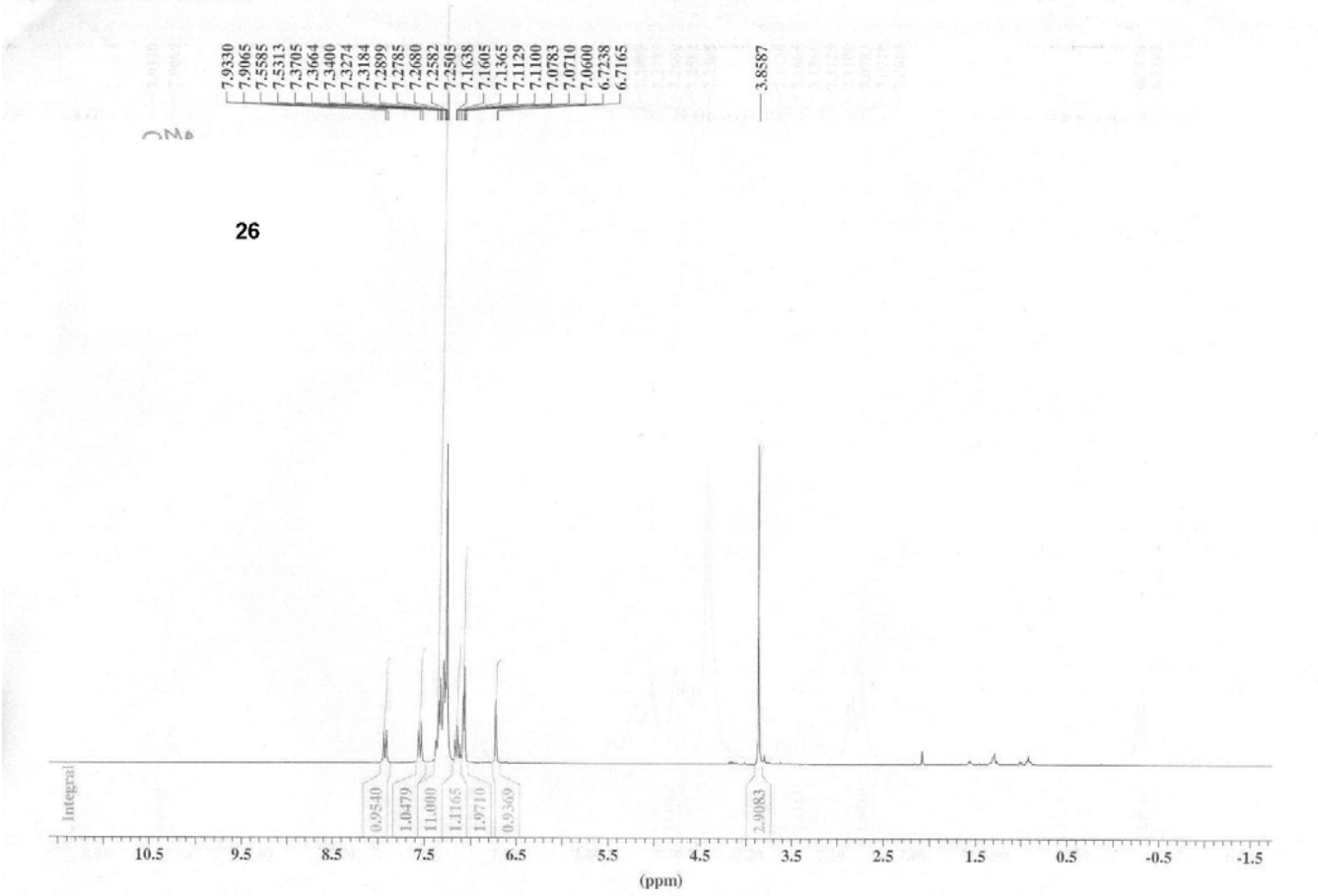
25



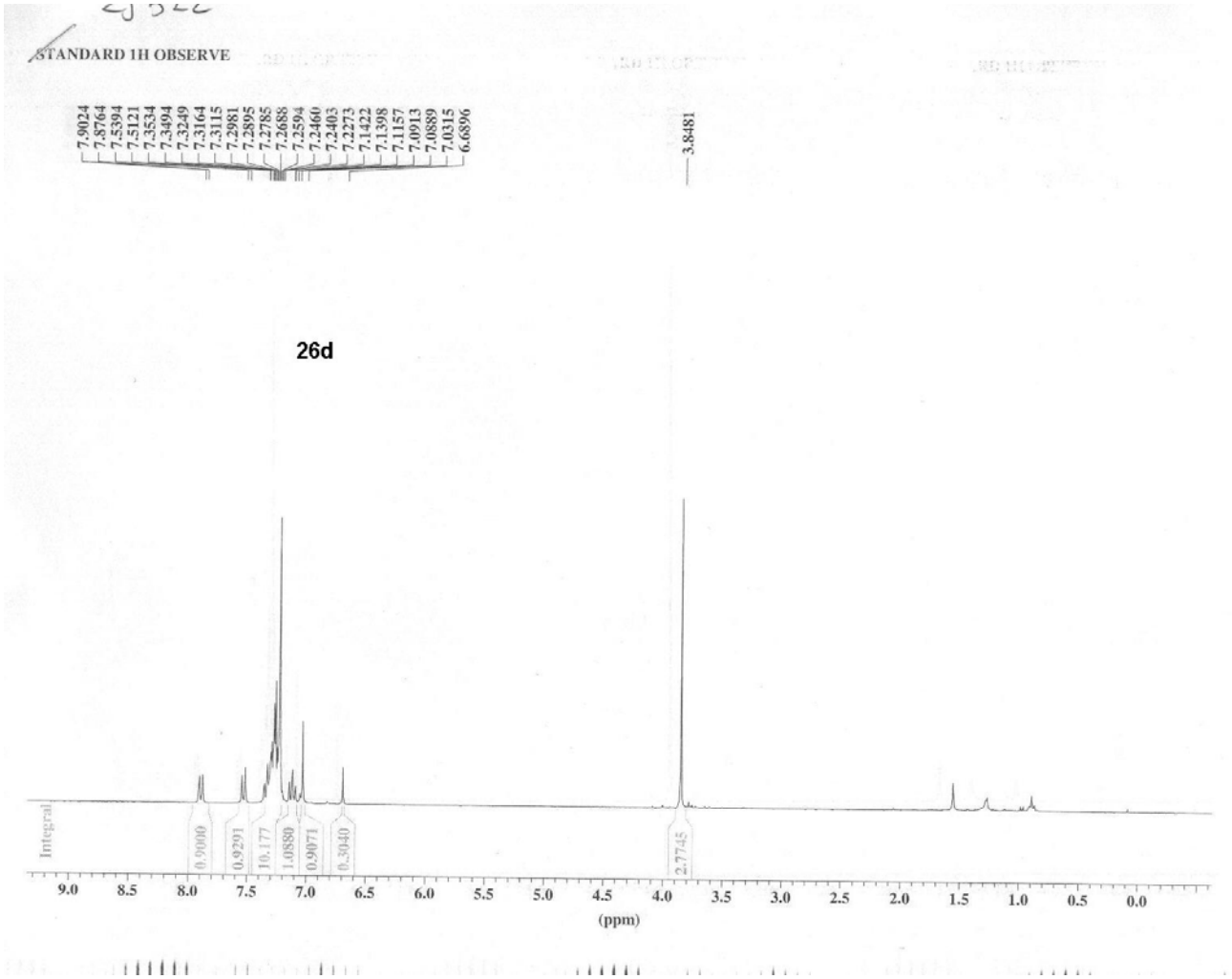

159.5867
157.8344
156.5558
141.4085
138.8406
130.8627
125.4492
124.6478
122.5607
121.9054
115.1847
111.3703
111.3240
94.5348
55.9239
33.6250
30.6084
23.1754
22.0321
14.3890
14.3178
25
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
(ppm)

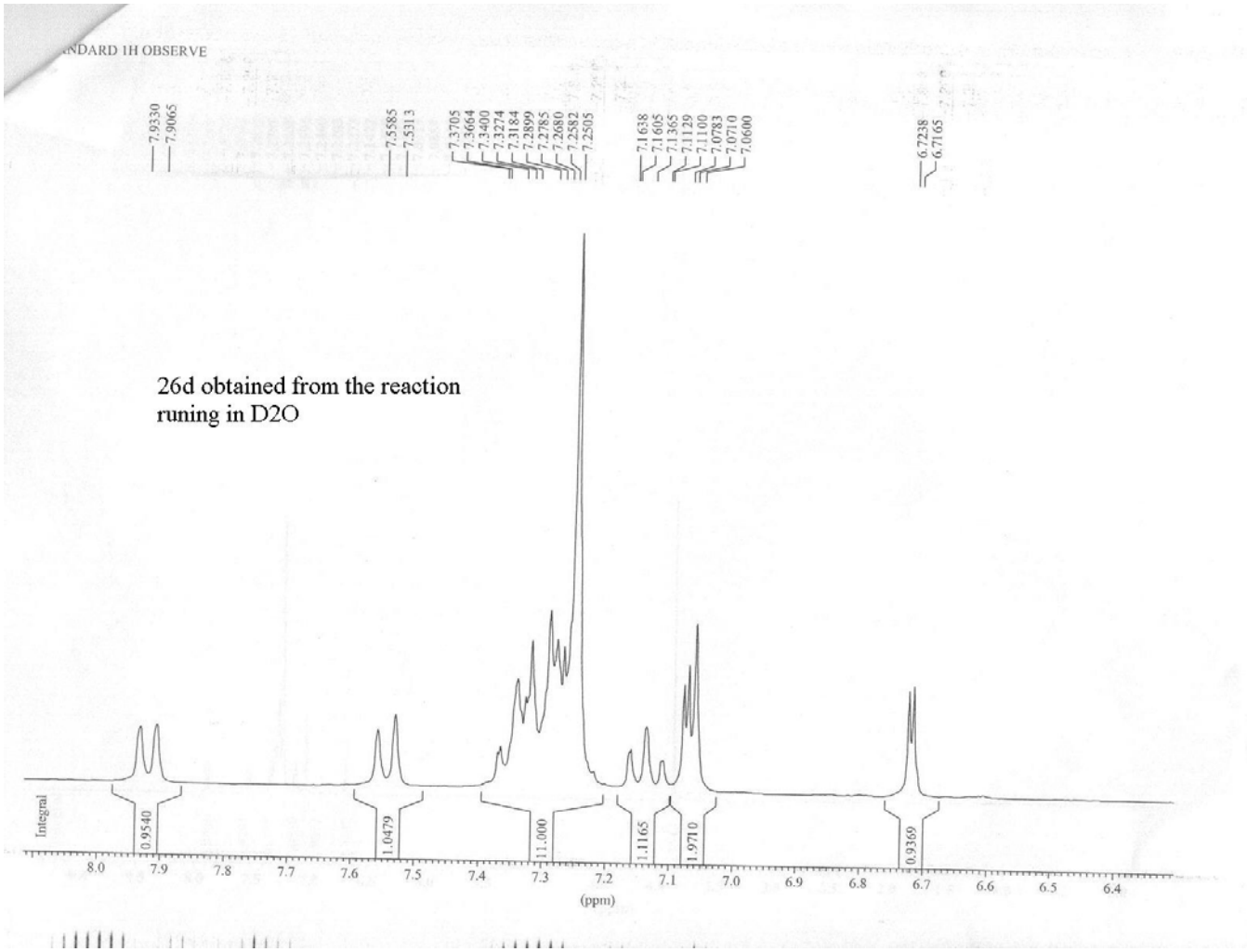
ZJ514

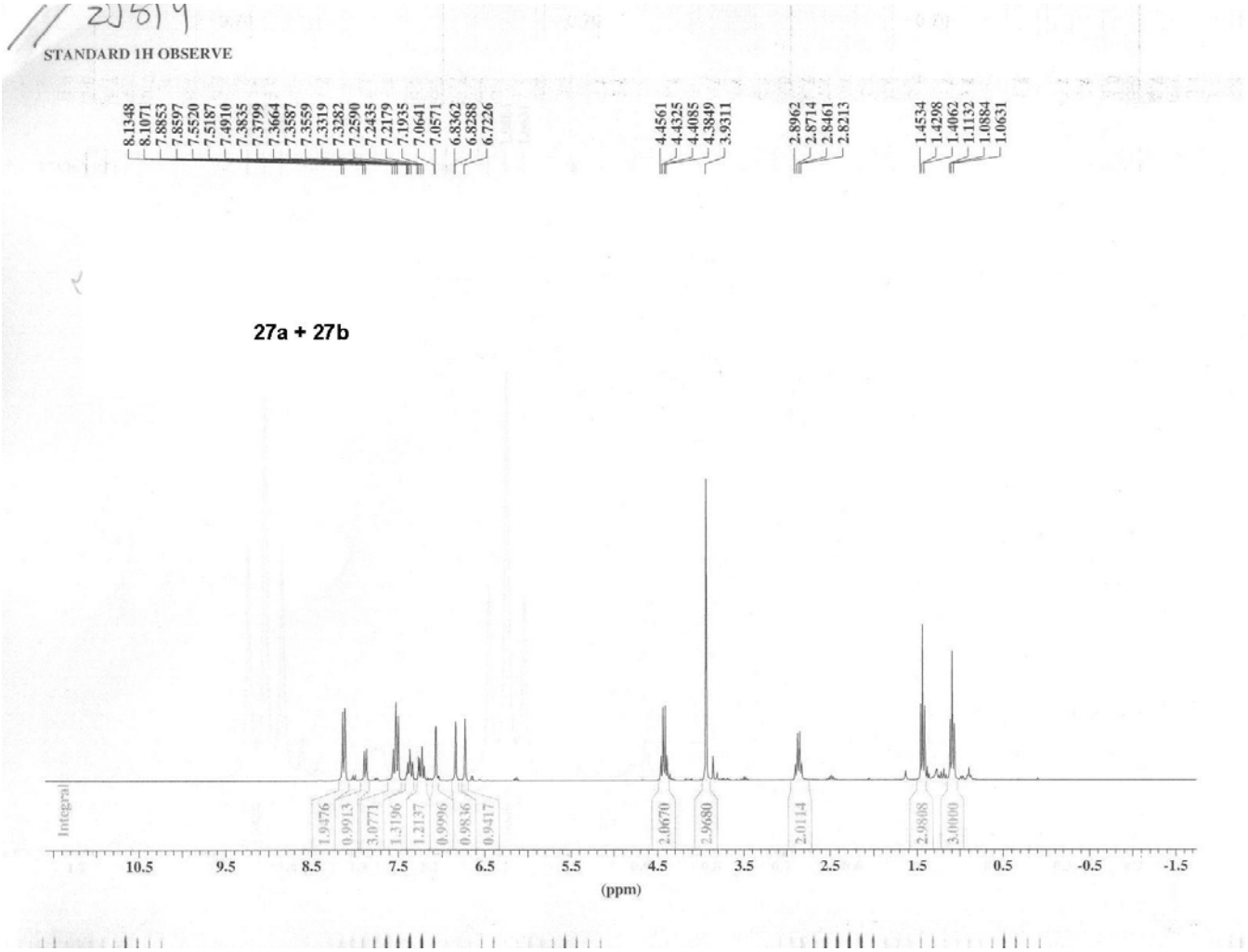
STANDARD 1H OBSERVE

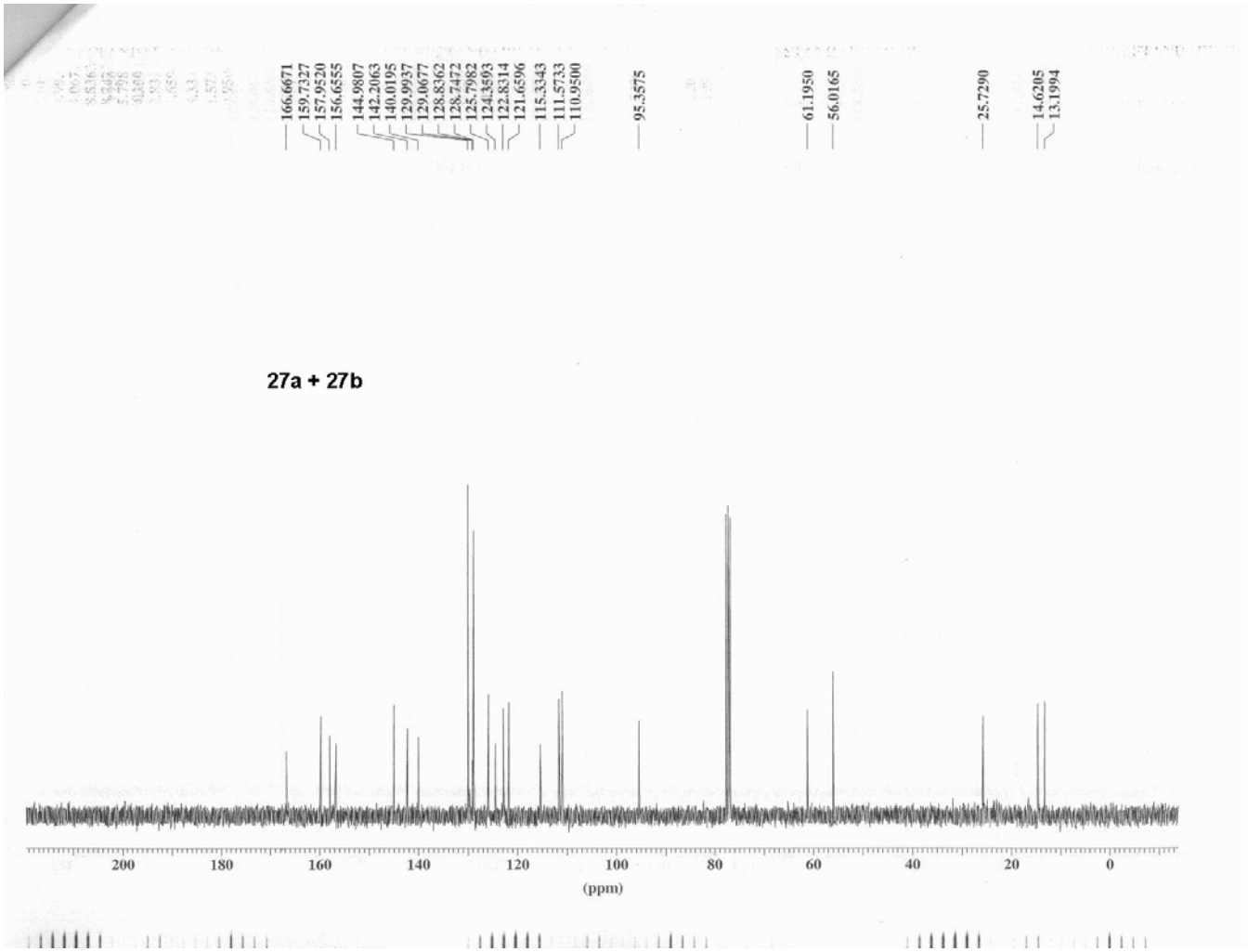


26


STANDARD 1H OBSERVE
7.9024
7.8764
7.5394
7.5121
7.3534
7.3494
7.3249
7.3164
7.3115
7.2981
7.2895
7.2785
7.2688
7.2594
7.2460
7.2403
7.2273
7.1422
7.1398
7.1157
7.0913
7.0889
7.0315
6.6896
3.8481
26d
Integral
0.9000
0.9291
10.177
1.0880
0.9071
0.3040
2.7745
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
(ppm)


NDARD 1H OBSERVE
7.9330
7.9065
7.5585
7.5313
7.3705
7.3664
7.3400
7.3274
7.3184
7.2899
7.2785
7.2680
7.2582
7.2505
7.1638
7.1605
7.1365
7.1129
7.1100
7.0783
7.0710
7.0600
6.7238
6.7165
26d obtained from the reaction
runing in D2O
Integral
0.9540
1.0479
11.000
1.1165
1.9710
0.9369
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
6.8
6.7
6.6
6.5
6.4
(ppm)


STANDARD 1H OBSERVE
8.1348
8.1071
7.8853
7.8597
7.5520
7.5187
7.4910
7.3835
7.3799
7.3664
7.3587
7.3559
7.3319
7.3282
7.2590
7.2435
7.2179
7.1935
7.0641
7.0571
6.8362
6.8288
6.7226
4.4561
4.4325
4.4085
4.3849
3.9311
2.8962
2.8714
2.8461
2.8213
1.4534
1.4298
1.4062
1.1132
1.0884
1.0631
27a + 27b
Integral
1.9476
0.9913
3.0771
1.3196
1.2137
0.9996
0.9836
0.9417
2.0670
2.9680
2.0114
2.9868
3.0000
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
-1.5
(ppm)


166.6671
159.7327
157.9520
156.6555
144.9807
142.2063
140.0195
129.9937
129.0677
128.8362
128.7472
125.7982
124.3593
122.8314
121.6596
115.3343
111.5733
110.9500
95.3575
61.1950
56.0165
25.7290
14.6205
13.1994
27a + 27b
200
180
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120
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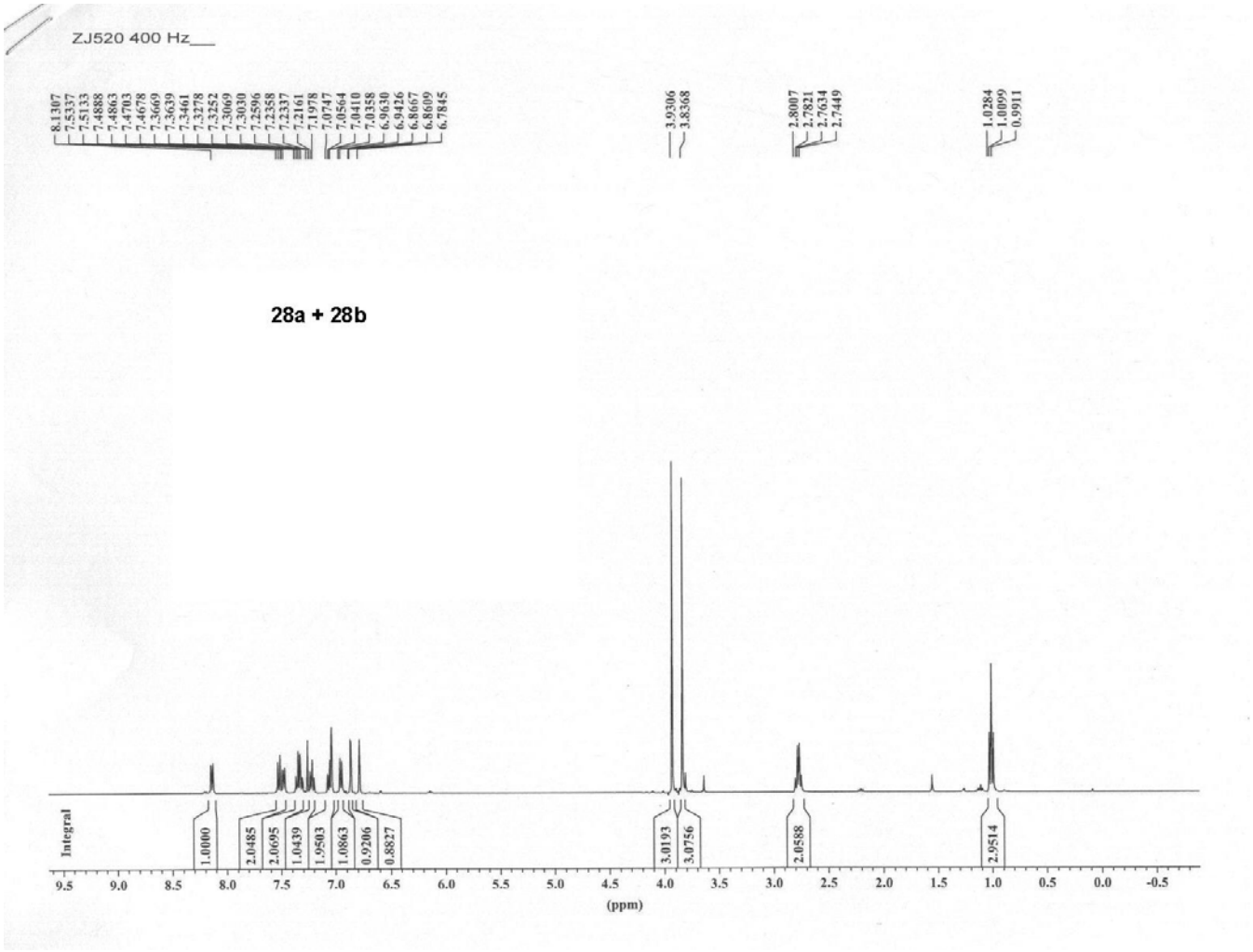
80
60
40
20
0
(ppm)


ZJ520 400 Hz___
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7.4863
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7.4678
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7.3639
7.3461
7.3278
7.3252
7.3069
7.3030
7.2596
7.2358
7.2337
7.2161
7.1978
7.0747
7.0564
7.0410
7.0358
6.9630
6.9426
6.8667
6.8609
6.7845
3.9306
3.8368
2.8007
2.7821
2.7634
2.7449
1.0284
1.0099
0.9911
28a + 28b
Integral
1.0000
2.0485
2.0695
1.0439
1.9503
1.0863
0.9206
0.8827
3.0193
3.0756
2.0588
2.9514
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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3.0
2.5
2.0
1.5
1.0
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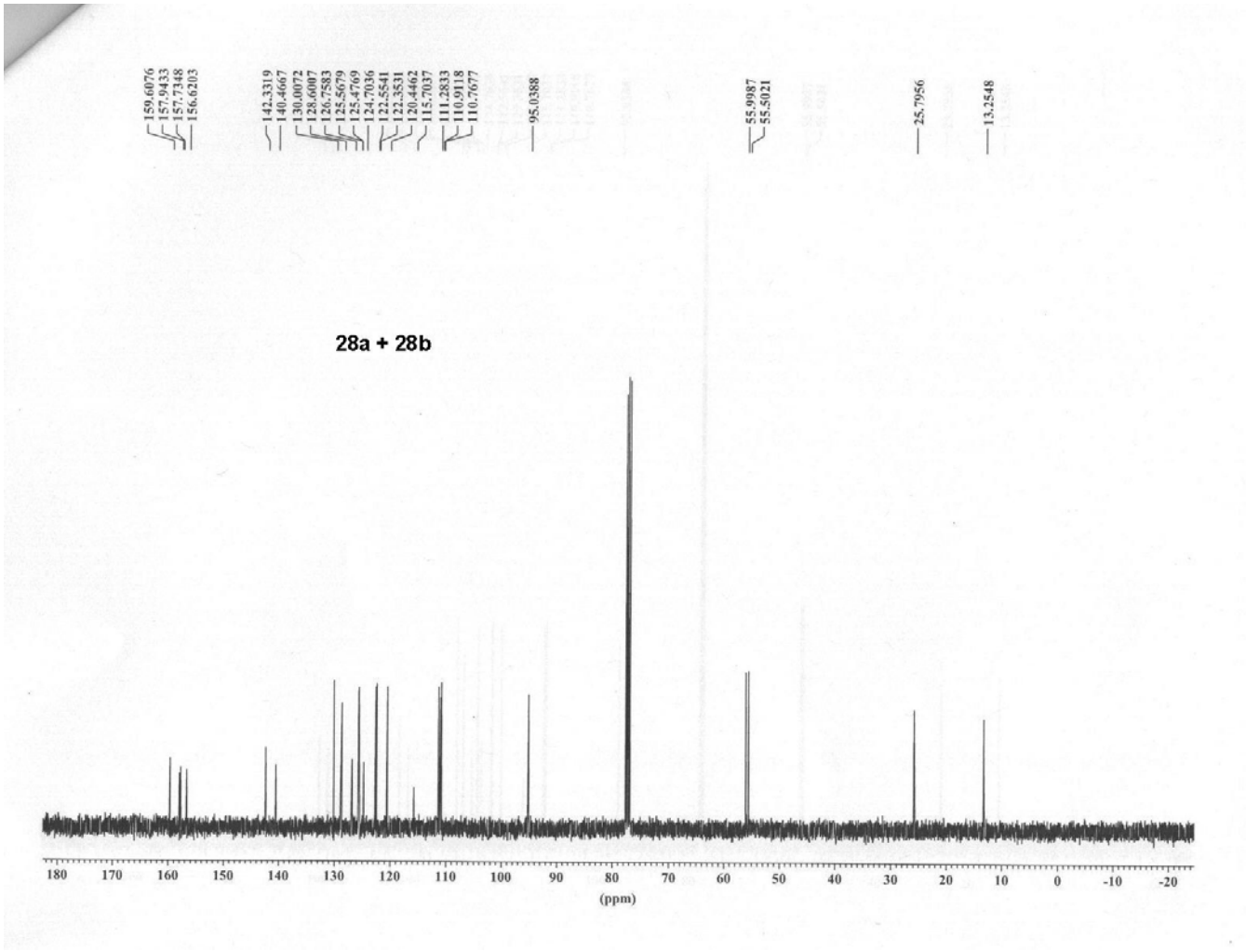
-0.5
(ppm)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157.9433
157.7348
156.6203
142.3319
140.4667
130.0072
128.6007
126.7583
125.5679
125.4769
124.7036
122.5541
122.3531
120.4462
115.7037
111.2833
110.9118
110.7677
95.0388
55.9987
55.5021
25.7956
13.2548
28a + 28b
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20
(ppm)