SUPPLEMENTARY INFORMATION

Scandium Triflate Catalyzed Cycloaddition of Imines with 1,1-Cyclopropanediesters: Efficient and Diastereoselective Synthesis of Multisubstituted Pyrrolidines

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Part 1. Spectral data (^{1}H NMR, ^{13}C NMR, IR, LRMS, HRMS and E.A.).

(*cis*, E)-Dimethyl 1-benzyl-2-phenyl-5-styrylpyrrolidine-3,3-dicarboxylate (3b): colorless oil (91% yield). ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.44 (d, J = 6.9 Hz, 1H), 7.31-7.07 (m, 13H), 6.55 (d, J = 16.2 Hz, 1H), 6.16 (dd, J = 11.4, 15.9 Hz, 1H), 4.67 (s, 1H), 3.83 (d, J = 14.1 Hz, 1H), 3.70 (s, 3H), 3.64 (d, J = 14.1 Hz, 1H), 3.42-3.34 (m, 1H), 3.06 (s, 3H), 2.81 (dd, J_{AB} = 13.5 Hz, J_{AX} = 10.8 Hz, 1H), 2.25 (dd, J_{AB} = 13.5 Hz, J_{BX} = 6.6 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 171.96, 169.55, 139.24, 136.87, 136.51, 131.98, 131.66, 129.82, 128.84, 128.41, 127.75, 127.70, 127.54, 127.44, 126.73, 126.34, 70.54, 63.95, 63.92, 54.07, 52.77, 51.96, 39.23; LRMS-ESI: 456.1 $(M + H)^+$; IR (thin film, cm^{-1}): 3027, 2951, 2830, 1733, 967, 755, 699; HRMS-ESI: Exact mass calcd for $C_{29}H_{30}NO_4$ $[M + H]^+$, 456.2169. Found 456.2167.

(*cis*, E)-Dimethyl 1-benzyl-2-(4-fluorophenyl)-5-styryl pyrrolidine-3,3-dicarboxylate (3c): colorless oil (94% yield). ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.41-7.21 (m, 7H), 7.17-7.04 (m, 5H), 6.94 (t, J = 8.7 Hz, 2H), 6.60 (d, J = 15.9 Hz, 1H), 6.16 (dd, J = 8.4, 15.9 Hz, 1H), 4.65 (s, 1H), 3.78 (d, J = 13.8 Hz, 1H), 3.71 (s, 3H), 3.66 (d, J = 13.8 Hz, 1H), 3.42-3.34 (m, 1H), 3.12 (s, 3H), 2.79 (dd, J_{AB} = 13.2 Hz, J_{AX} = 10.8 Hz, 1H), 2.17 (dd, J_{AB} = 13.2 Hz, J_{BX} = 6.0 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 171.86, 169.41, 162.15 (d, $^1J_{CF}$ = 241.90 Hz), 136.79, 136.50, 135.11, 135.07, 132.20, 131.41, 130.37 (d, $^3J_{CF}$ = 8.1 Hz), 129.74, 128.44, 127.62 (d, $^4J_{CF}$ = 2.9 Hz), 126.80, 126.36, 114.51 (d, $^2J_{CF}$ = 20.62 Hz), 69.95, 64.04, 63.88, 54.30, 52.81, 52.03, 39.09; LRMS-ESI: 474.0 [$(M + H)^+$, 100]; IR (thin film, cm^{-1}): 2951, 1734, 1508, 1271, 1222, 751, 696; HRMS-ESI: Exact mass calcd for $C_{29}H_{29}ClNO_4$ $[M + H]^+$, 474.2075. Found 474.2076.

(cis)-Dimethyl 1-benzyl-2-(4-chlorophenyl)-5-styryl pyrrolidine-3,3-dicarboxylate (3d): white solid (92% yield). ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.37-7.03 (m, 14H), 6.57 (d, J = 15.6 Hz, 1H), 6.16 (dd, J = 8.1, 15.9 Hz, 1H), 4.64 (s, 1H), 3.77 (d, J = 13.5 Hz, 1H), 3.71 (s, 3H), 3.65 (d, J = 13.5 Hz, 1H), 3.38 (ddd, J = 6.3, 8.1, 12.9 Hz, 1H), 2.78 (dd, J_{AB} =13.5 Hz, J_{AX} = 10.2 Hz, 1H), 2.27 (dd, J_{AB} =13.5 Hz, J_{BX} = 6.3 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 171.77, 169.32, 137.97, 136.75, 136.31, 133.13, 132.26, 131.30, 130.18, 129.76, 128.45, 127.85, 127.77, 127.53, 126.85, 126.37, 69.87, 63.99, 63.86, 54.22, 52.86, 52.09, 39.07; LRMS-EI: 490 [$(M + H)^+$, 2.27], 91 (100); IR (thin film, cm^{-1}): 3467, 3028, 2950, 2815, 1732, 1489, 1088, 967, 699; Anal. Calcd. for $C_{29}H_{28}ClNO_4$: C, 71.09; H, 5.76; N, 2.86. Found: C, 71.20; H, 5.83; N, 2.61.

(cis, E)-Dimethyl 1-benzyl-2-(4-bromophenyl)-5-styryl pyrrolidine-3,3-dicarboxylate (3e): colorless oil (71% yield). ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.40-7.03 (m, 14H), 6.56 (d, J = 15.9 Hz, 1H), 6.16 (dd, J = 8.1, 15.9 Hz, 1H), 4.62 (s, 1H), 3.77 (d, J = 14.1 Hz, 1H), 3.72 (s, 3H), 3.65 (d, J = 14.1 Hz, 1H), 3.38 (ddd, J = 6.3, 8.4, 10.5 Hz, 1H), 3.13 (s, 3H), 2.77 (dd, J_{AB} = 13.5 Hz, J_{AX} = 10.5 Hz, 1H), 2.27 (dd, J_{AB} = 13.5 Hz, J_{BX} = 6.6 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 171.77, 169.32, 138.53, 136.77, 136.30, 132.28, 131.31, 130.82, 130.57, 129.78, 128.47, 127.80, 127.54, 126.88, 126.38, 121.36, 69.96, 64.00, 63.86, 54.23, 52.87, 52.12, 39.10; LRMS-ESI: 534.0 [$(M + H)^+$, 100]; IR (thin film, cm^{-1}): 3030, 2948, 1737, 1270; HRMS-ESI: Exact mass calcd for $C_{29}H_{29}BrNO_4$ $[M + H]^+$, 534.1274. Found 534.1273.

(cis, E)-Dimethyl 1-benzyl-2-(4-(methoxycarbonyl)phenyl) -5-styrylpyrrolidine-3,3-dicarboxylate (3f): Reaction was performed at refuxed CH_2Cl_2: colorless oil (52% yield). ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.93 (d, J = 8.4 Hz, 2H), 7.48 (d, J = 8.1 Hz, 2H), 7.37-7.22 (m, 5H), 7.17-7.03 (m, 5H), 6.59 (d, J = 15.9 Hz, 1H), 6.20 (dd, J = 8.4, 15.9 Hz, 1H), 4.73 (s, 1H), 3.91 (s, 3H), 3.78 (d, J = 13.5 Hz, 1H), 3.74 (s, 3H), 3.68 (d, J = 13.5 Hz, 1H), 3.43 (ddd, J = 6.3, 7.8, 10.5 Hz, 1H), 3.07 (s, 1H), 2.81 (dd, J_{AB} = 13.5 Hz, J_{AX} = 10.8 Hz, 1H), 2.30 (dd, J_{AB} = 13.5

Hz, J_{BX} = 6.0 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 171.74, 169.13, 167.02, 145.11, 136.77, 136.37, 132.38, 131.22, 129.77, 129.23, 128.98, 128.88, 128.49, 127.79, 127.57, 126.90, 126.41, 70.31, 64.22, 64.12, 54.58, 52.94, 52.07, 52.02, 39.20; LRMS-ESI: 514.0 [$(M + H)^+$, 100]; IR (thin film, cm^{-1}): 3430, 2952, 1733, 1435, 766, 750, 705; HRMS-ESI: Exact mass calcd for $C_{31}H_{32}NO_6$ [$M + H]^+$, 514.2224. Found 514.2225.

(cis, E)-Dimethyl 1-benzyl-5-styryl-2-p-tolylpyrrolidine-3, 3-dicarboxylate (3g): colorless oil (86% yield). ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.35-7.08 (m, 14H), 6.54 (d, *J* = 15.9 Hz, 1H), 6.18 (dd, *J* = 7.8, 15.9 Hz, 1H), 4.62 (s, 1H), 3.84 (d, *J* = 14.3 Hz, 1H), 3.70 (s, 3H), 3.60 (d, *J* = 14.3 Hz, 1H), 3.36 (ddd, *J* = 6.3, 8.1, 10.4 Hz, 1H), 3.10 (s, 1H), 2.78 (dd, J_{AB} = 12.9 Hz, J_{AX} = 10.5 Hz, 1H), 2.31(s, 3), 2.24 (dd, J_{AB} = 12.9 Hz, J_{BX} = 6.0 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 172.01, 169.71, 137.13, 136.94, 136.53, 136.02, 131.86, 131.84, 129.86, 128.76, 128.50, 128.41, 127.72, 127.39, 126.71, 126.35, 70.29, 63.81, 63.79, 53.84, 52.71, 51.98, 39.22, 21.12; LRMS-ESI: 470.1 [$(M + H)^+$, 100]; IR (thin film, cm^{-1}): 3472, 3060, 3027, 1734, 1270, 750, 696; HRMS-ESI: Exact mass calcd for $C_{30}H_{32}NO_4$ [$M + H]^+$, 470.2326. Found 470.2328.

(cis, E)-Dimethyl 1-benzyl-2-(4-methoxyphenyl)-5-styryl pyrrolidine-3,3-dicarboxylate (3h): white solid (86% yield). ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.38-7.07 (m, 12H), 6.82 (d, *J* = 8.7 Hz, 2H), 6.54 (d, *J* = 15.9 Hz, 1H), 6.15 (dd, *J* = 8.1, 15.9 Hz, 1H), 4.60 (s, 1H), 3.82 (d, *J* = 14.3 Hz, 1H), 3.79 (s, 3H), 3.70 (s, 3H), 3.61 (d, *J* = 14.3 Hz, 1H), 3.35 (ddd, *J* = 6.3, 8.1, 9.0 Hz, 1H), 2.78 (dd, J_{AB} =13.5 Hz, J_{AX} = 10.5 Hz, 1H), 2.24 (dd, J_{AB} =13.5 Hz, J_{BX} = 6.4 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 172.02, 169.72, 158.90, 136.88, 136.48, 131.87, 131.76, 131.05, 129.90, 129.80, 128.39, 127.70, 127.39, 126.69, 126.32, 113.14, 69.98, 63.75, 63.70, 55.16, 53.79, 52.71, 52.08, 39.11; LRMS-EI: 486 [$(M + H)^+$, 3.80], 91 (100); IR (thin film, cm^{-1}): 3026, 3001, 2950, 2837, 1731; Anal. Calcd. for $C_{30}H_{31}NO_5$: C, 74.21`; H, 6.43; N, 2.88. Found: C, 74.11; H, 6.64; N, 2.71.

(cis, E)-dimethyl 1-benzyl-2-(2-methoxyphenyl)-5-styryl pyrrolidine-3,3-dicarboxylate (3i): colorless oil (59% yield). ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.59 (d, *J* = 6.9 Hz, 1H), 7.29 (d, *J* = 4.5 Hz, 4H), 7.25-7.18 (m, 1H), 7.14-7.02 (m, 6H), 6.89 (t, *J* = 7.5 Hz, 1H), 6.79 (d, *J* = 8.4 Hz, 1H), 6.56 (d, *J* = 15.9 Hz, 1H), 6.10 (dd, *J* = 8.1, 15.9 Hz, 1H), 5.36 (s, 1H), 3.78-3.66 (m, 8H), 3.42 (ddd, *J* = 5.1, 8.1, 11.4 Hz, 1H), 3.04 (s, 3H), 2.85 (dd, J_{AB} = 12.9 Hz, J_{AX} = 12.9 Hz, 1H), 2.21 (dd, J_{AB} = 12.9 Hz, J_{BX} = 5.1 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 172.01, 169.52, 157.61, 137.63, 136.96, 131.85, 131.81, 129.68, 129.57, 128.87, 128.39, 128.16, 127.40, 127.35, 126.44, 126.31, 120.02, 109.82, 64.45, 63.65, 62.83, 55.67, 55.54, 52.77, 51.77, 40.34; LRMS-ESI: 486.1 [$(M + H)^+$, 100]; IR (thin film, cm^{-1}): 3030, 2950, 2830, 1732, 966, 751, 697; HRMS-ESI: Exact mass calcd for $C_{30}H_{32}NO_5$ [$M + H]^+$, 486.2275. Found 486.2274.

(cis, E)-Dimethyl 1-benzyl-2-(2,4-dichlorophenyl)-5-styryl pyrrolidine-3,3- dicarboxylate (3j): colorless oil (59% yield). ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.56 (d, *J* = 8.4 Hz, 1H), 7.39-7.24 (m, 5H), 7.13-7.07 (m, 7H), 6.64 (d, *J* = 15.9 Hz, 1H), 6.15 (dd, *J* = 8.1, 15.9 Hz, 1H), 5.34 (s, 1H), 3.80 (d, *J* = 13.2 Hz, 1H), 3.75 (s, 3H), 3.65 (d, *J* = 13.2 Hz, 1H), 3.48 (ddd, *J* = 4.8, 8.1, 11.7 Hz, 1H), 3.13 (s, 3H), 2.82 (dd, J_{AB} = 13.2 Hz, J_{AX} = 10.2 Hz, 1H), 2.27 (dd, J_{AB} = 13.2 Hz, J_{BX} = 4.8 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 172.42, 168.75, 137.09, 136.83, 136.64, 134.82, 133.15, 132.83, 131.84, 130.78, 129.61, 128.52, 128.02 (3C), 127.66, 126.80 (3C), 126.39, 65.77, 64.41, 63.75, 55.91, 53.11, 51.93, 39.94; LRMS-EI: 524 [$(M + H)^+$, 0.12], 84 (100), 91 (7.86); IR (thin film, cm^{-1}): 3022, 2807, 1736, 967, 914, 750, 697; HRMS-ESI: Exact mass calcd for $C_{29}H_{28}Cl_2NO_4$ [$M + H]^+$, 524.1390. Found 524.1389.

(cis, E)-Dimethyl 2-(benzo[d][1,3]dioxol-5-yl)-1-benzyl-5-styryl pyrrolidine-3,3-dicarboxylate (3k): white solid (94% yield). ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.31-7.08 (m, 10H), 6.99 (d, *J* = 1.2 Hz, 1H), 6.90 (dd, *J* = 1.8, 8.7 Hz, 1H), 6.72 (d, *J* = 7.8 Hz, 1H), 6.54 (d, *J* = 16.2 Hz, 1H), 6.14 (dd, *J* = 7.8, 16.2 Hz, 1H), 5.90 (s, 2H), 4.58 (s, 1H), 3.81 (d, *J* = 14.1 Hz, 1H), 3.69 (s, 3H), 3.64 (d, *J* = 14.1 Hz, 1H), 3.34 (ddd, *J* = 6.9, 9.0, 10.8 Hz, 1H), 3.21 (s, 3H), 2.77 (dd, J_{AB} =12.9 Hz, J_{AX} = 10.5 Hz, 1H), 2.24 (dd, J_{AB} = 2.9 Hz, J_{BX} = 6.3 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 171.87, 169.50, 147.15, 146.78, 136.81, 136.45, 133.12, 131.98, 131.58, 129.79, 128.39, 127.70, 127.41, 126.73, 126.32, 122.26, 109.10, 107.52, 100.77, 70.19, 63.74, 63.70, 53.93, 52.71, 52.11, 39.04; LRMS-EI: 500 [$(M + H)^+$, 3.99], 91 (100); IR (thin film, cm^{-1}): 3027, 2874, 1733, 802, 751, 697, 625; Anal. Calcd. for $C_{30}H_{29}NO_6$: C, 72.13; H, 5.85; N, 2.80. Found: C, 72.11; H, 5.93; N, 2.77.

(cis)-Diethyl 1-benzyl-2-(4-chlorophenyl)-5-vinyl pyrrolidine-3,3-dicarboxylate (3l): colorless oil (92% yield). ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.31-7.25 (m, 2H), 7.18-7.13 (m, 5H), 7.04-7.01 (m, 2H), 5.84 (ddd, *J* = 8.1, 9.9, 17.4 Hz, 1H), 5.27 (d, *J* = 17.1 Hz, 1H), 5.16 (d, *J* = 9.9 Hz, 1H), 4.60 (s, 1H), 4.27-4.06 (m, 2H), 3.76-3.60 (m, 3H), 3.45-3.32 (m, 1H), 3.25-3.17 (m, 1H), 2.69 (dd, J_{AB} = 13.5 Hz, J_{AX} = 10.8 Hz, 1H), 2.21 (dd, J_{AB} = 13.5 Hz, J_{BX} = 6.3 Hz, 1H), 1.20 (t, J = 7.2 Hz, 3H), 0.81 (t, J = 7.2 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 171.26, 168.80, 139.66, 138.34, 136.37, 132.91, 130.27, 129.73, 127.63, 126.74 (3C), 117.26, 69.52, 64.36, 63.83, 61.56, 61.16, 54.08, 38.91, 13.87, 13.82; LRMS-EI: 442 [$(M + H)^+$, 0.12], 91 (100); IR (thin film, cm^{-1}): 2982, 2815, 1731, 924, 701; HRMS-ESI: Exact mass calcd for $C_{25}H_{29}ClNO_4$ [$M + H]^+$, 442.1780. Found 442.1777.

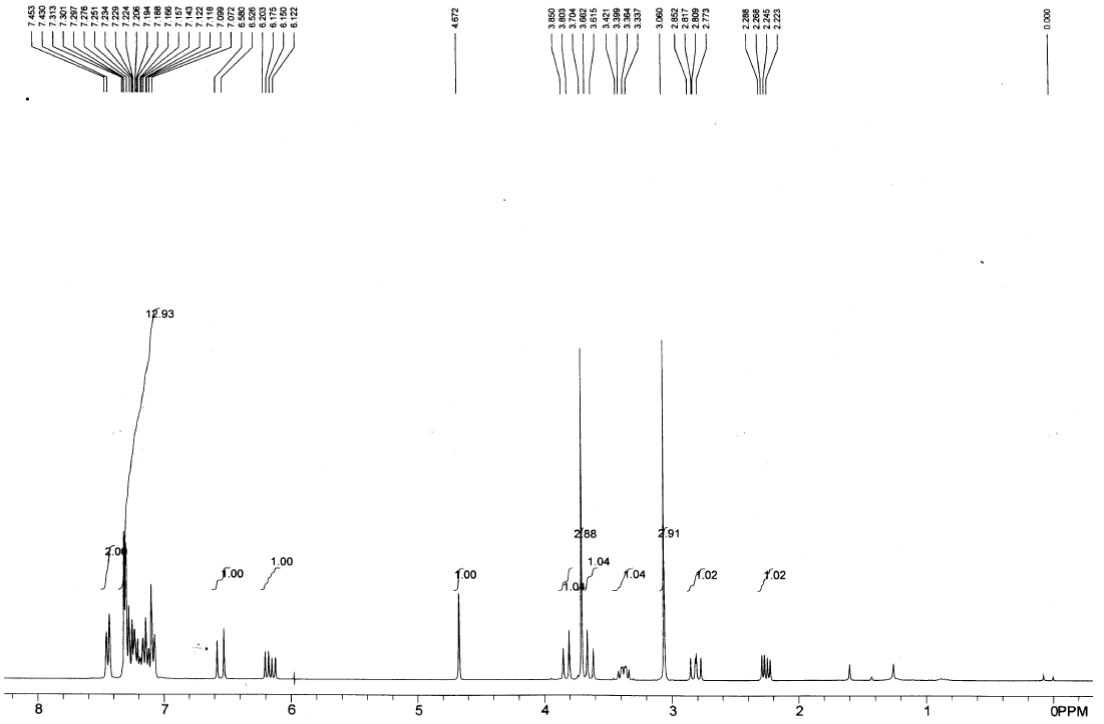
(*cis*)-Diethyl 1-benzyl-2-(4-chlorophenyl)-5-phenylpyrroli-dine-3,3-dicarboxylate (3m): colorless oil (85% yield). ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.62-7.59 (m, 2H), 7.45-7.38 (m, 4H), 7.33-7.22 (m, 3H), 7.14-7.12 (m, 3H), 6.89-6.86 (m, 2H), 4.70 (s, 1H), 4.27-4.06 (m, 2H), 3.77-3.66 (m, 2H), 3.62 (d, *J* = 14.0 Hz, 1H), 3.54 (d, *J* = 14.0 Hz, 1H), 3.44-3.34 (m, 1H), 2.85 (dd, J_{AB} =13.5 Hz, J_{AX} = 11.1 Hz, 1H), 2.42 (dd, J_{AB} =13.5 Hz, J_{BX} = 6.6 Hz, 1H), 1.18 (t, *J* = 7.2 Hz, 3H), 0.80 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 171.28, 169.02, 141.45, 138.14, 134.78, 133.00, 130.44, 130.06, 128.56, 127.86, 127.78, 127.61, 127.57, 126.88, 68.69, 64.24, 63.72, 61.51, 61.20,

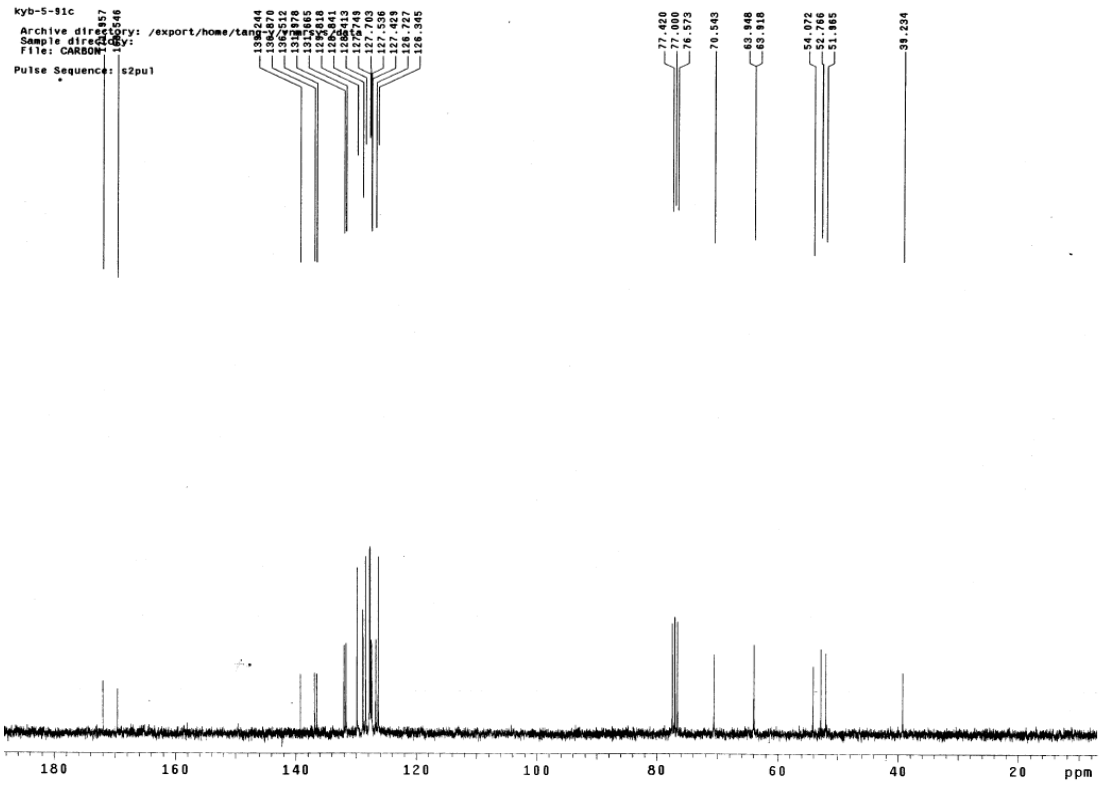
52.69, 42.09, 13.86, 13.31; LRMS-EI: 492 $(M + H)^+$, 91 (100); IR (thin film, cm^{-1}): 2981, 1732, 1489, 1260, 702; HRMS-ESI: Exact mass calcd for $C_{29}H_{31}ClNO_4$ $[M + H]^+$, 492.1936. Found 492.1936.

(*cis*)-Dimethyl 1-benzyl-2-(4-chlorophenyl)-5-phenylpyrroli dine-3,3-dicarboxylate (3o): Reaction was performed at refuxed CH_2Cl_2: colorless oil (98% yield). ^1H NMR (300 MHz, $CDCl_3$): δ 7.60 (d, J = 6.6 Hz, 2H), 7.42 (dd, J = 8.1, 8.7 Hz, 4H), 7.34-7.24 (m, 3H), 7.15-7.13 (m, 3H), 6.88-6.85 (m, 2H), 4.69 (s, 1H), 3.76-3.68 (m, 1H), 3.69 (s, 3H), 3.62 (d, J = 14.4 Hz, 1H), 3.53 (d, J = 14.4 Hz, 1H), 3.11 (s, 3H), 2.84 (dd, J_{AB} = 13.5 Hz, J_{AX} = 10.5 Hz, 1H), 2.41 (dd, J_{AB} = 13.5 Hz, J_{BX} = 6.3 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 171.80, 169.48, 141.37, 137.91, 134.64, 133.14, 130.33, 130.13, 128.64, 127.92, 127.91, 127.70, 127.66, 126.97, 68.86, 64.20, 63.79, 52.80, 52.53, 52.07, 41.96; LRMS-EI: 464 [$(M + H)^+$, 0.93], 91 (100); IR (thin film, cm^{-1}): 3028, 2951, 2830, 1735, 1489, 1267, 1199, 760, 515; HRMS-ESI: Exact mass calcd for $C_{27}H_{27}ClNO_4$ $[M + H]^+$, 464.1623. Found 464.1625.

Part 2. ^{1}H NMR and ^{13}C NMR spectra for all new compounds

3b





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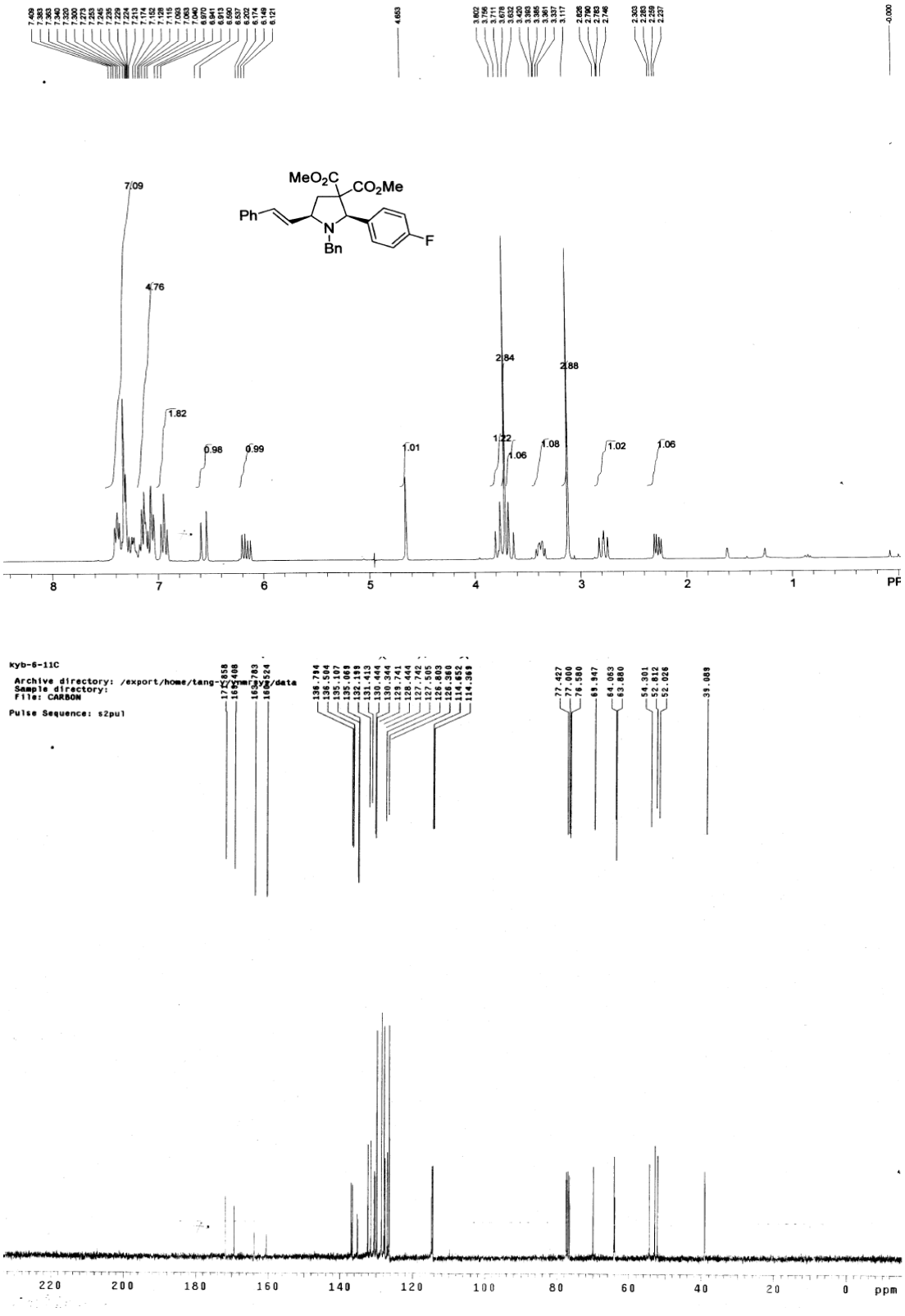
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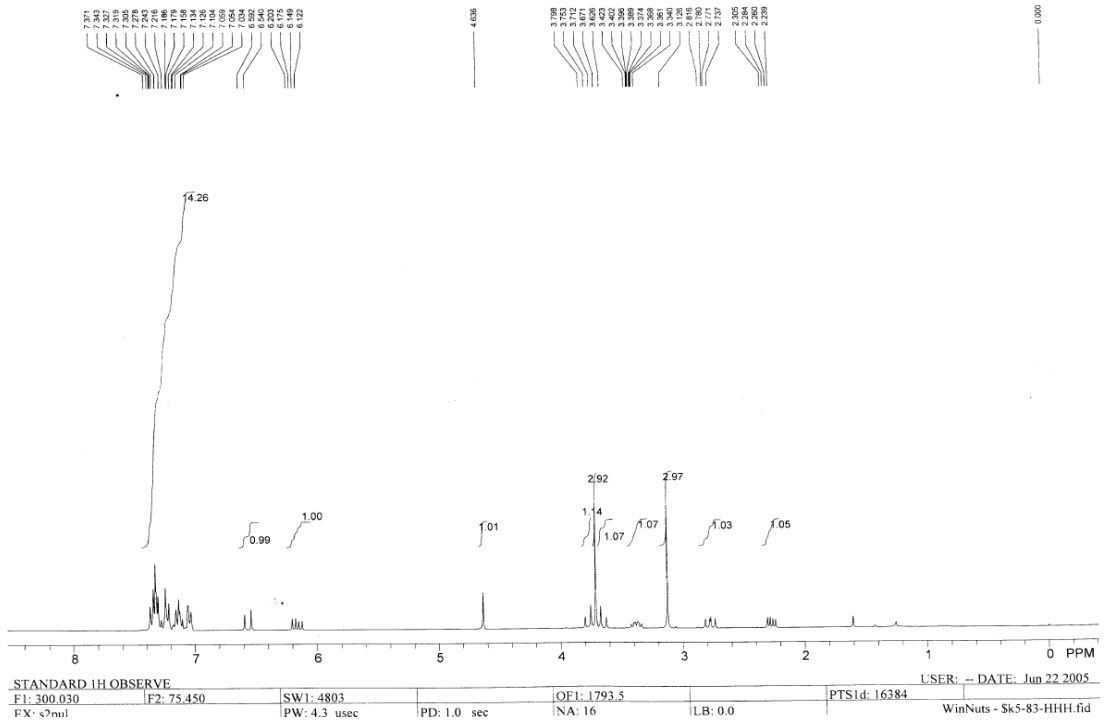
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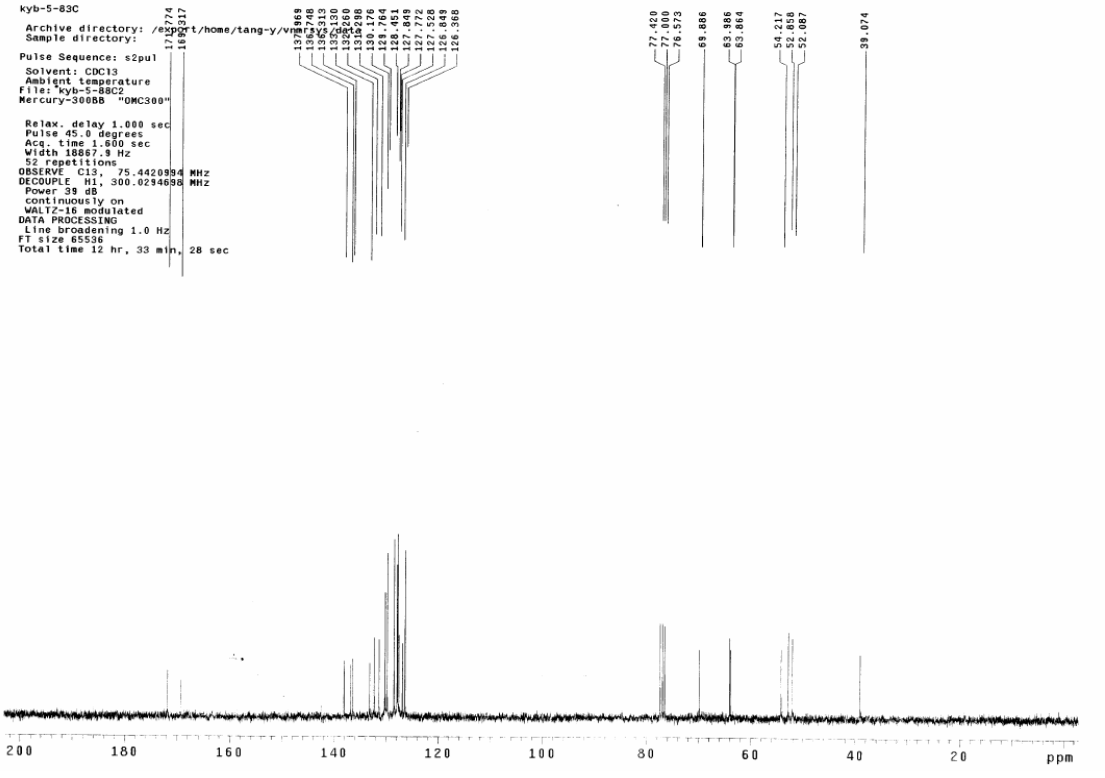
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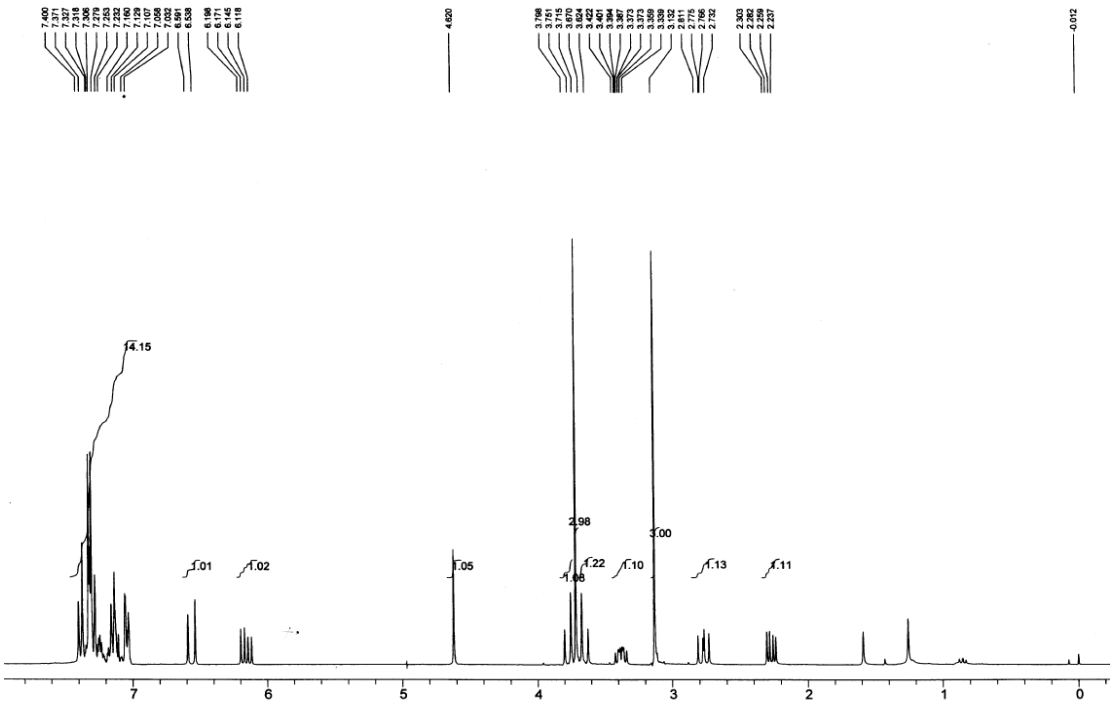
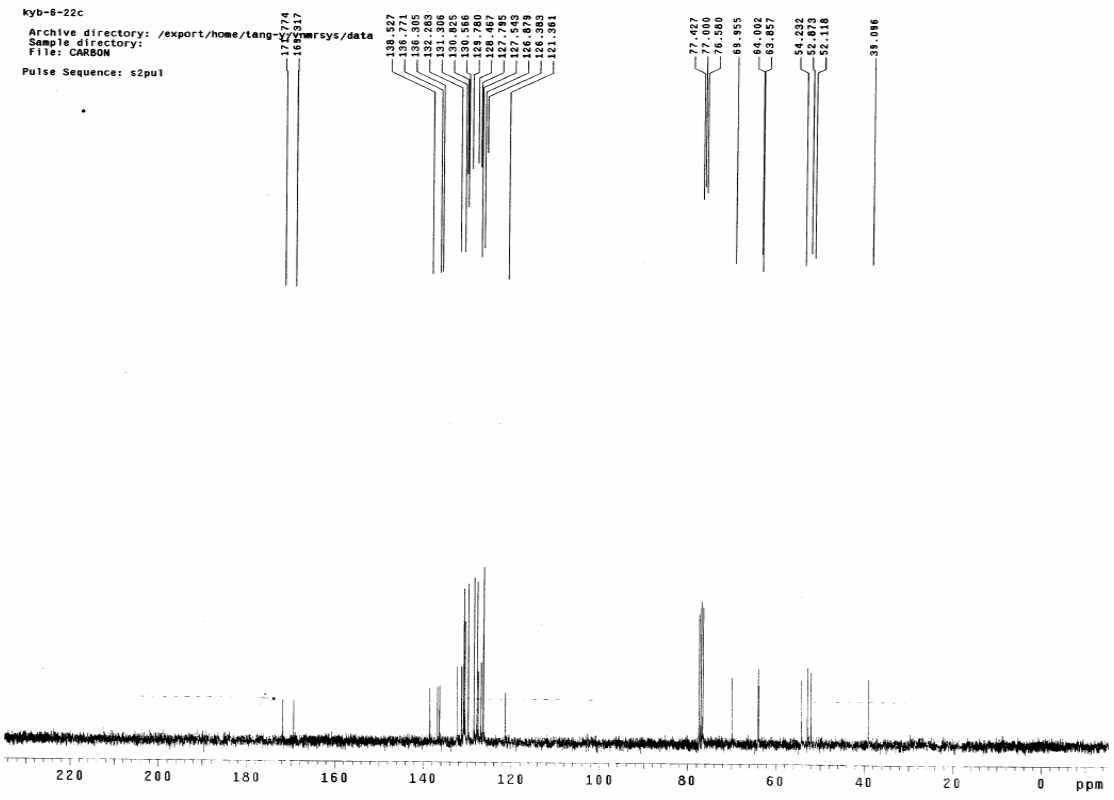
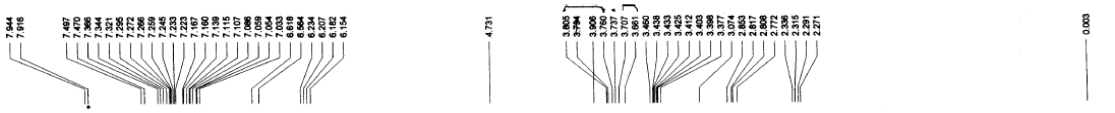
ppm

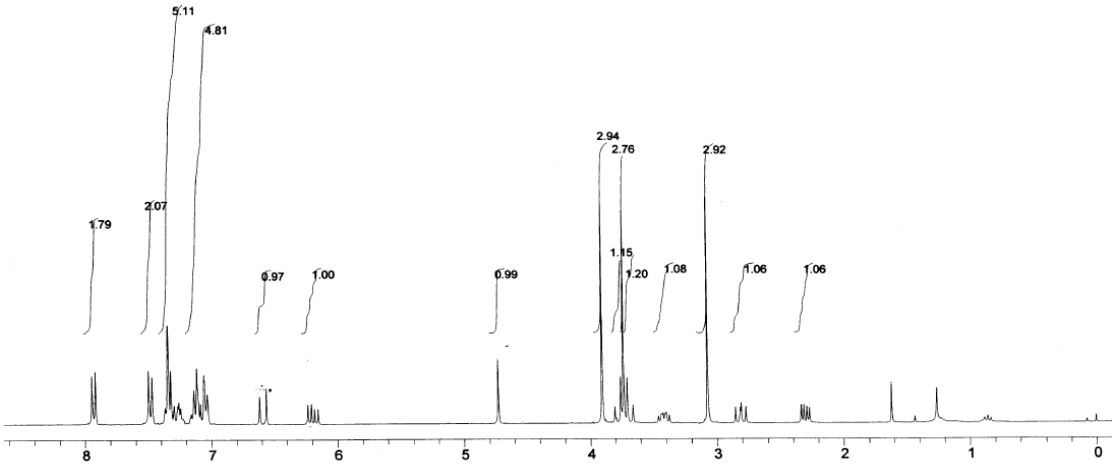
3e

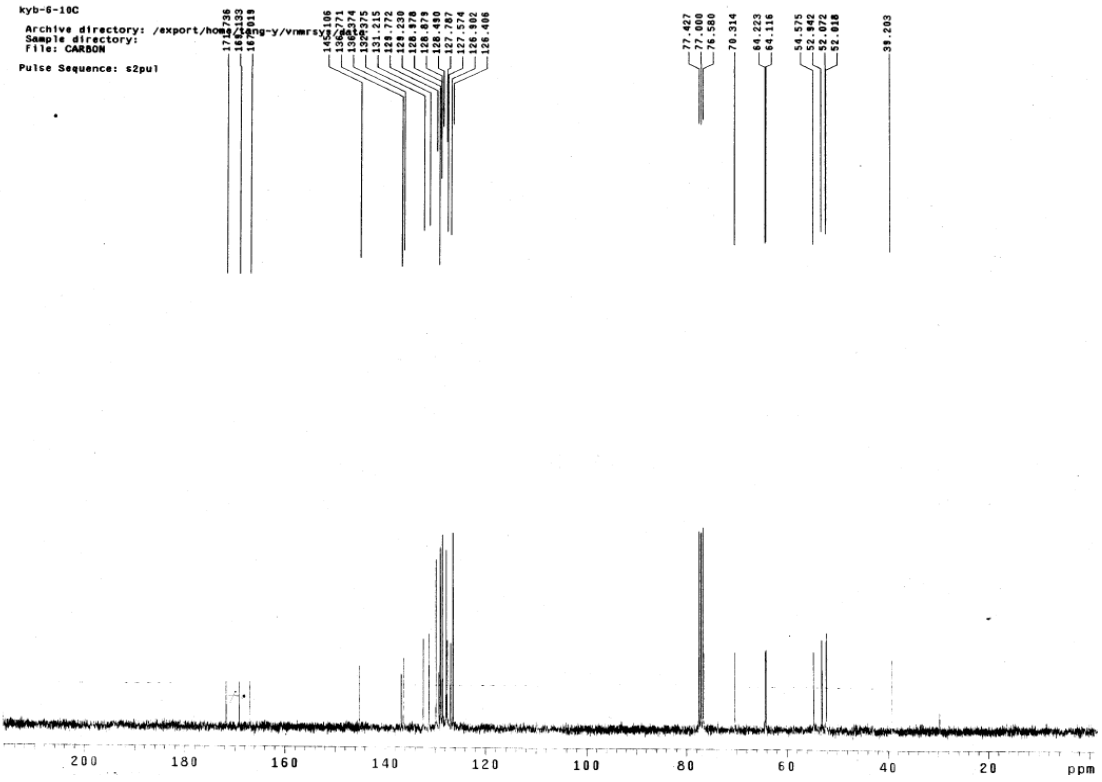




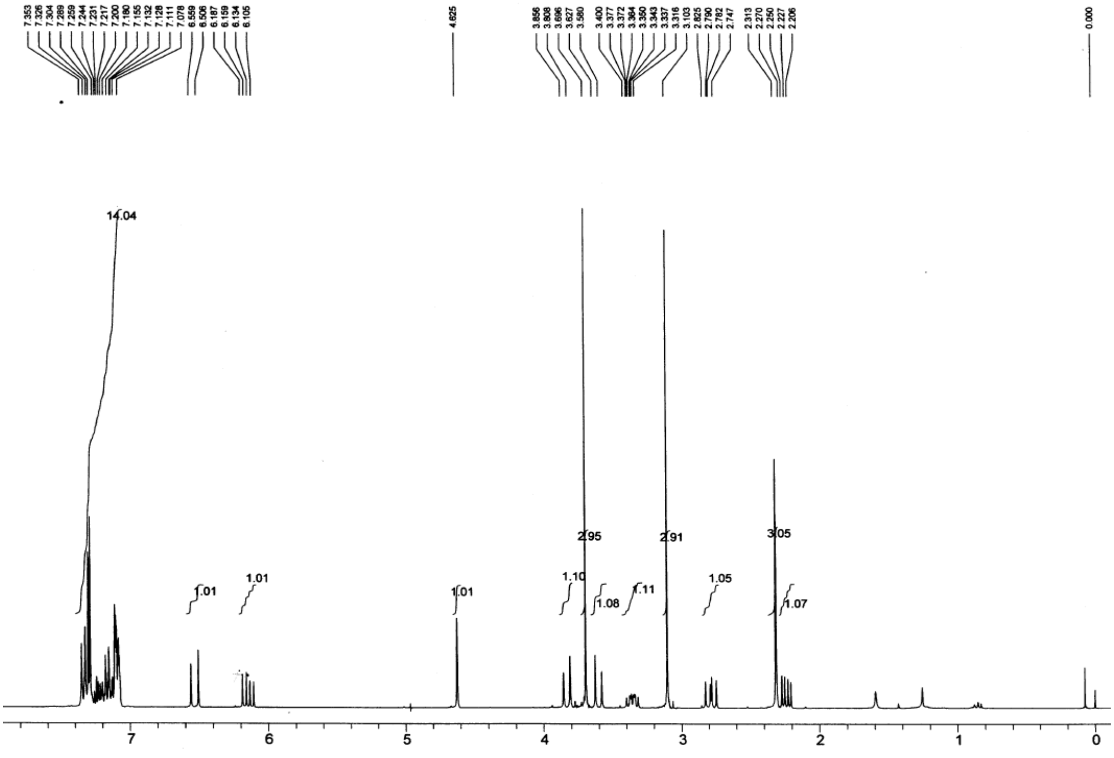
3f

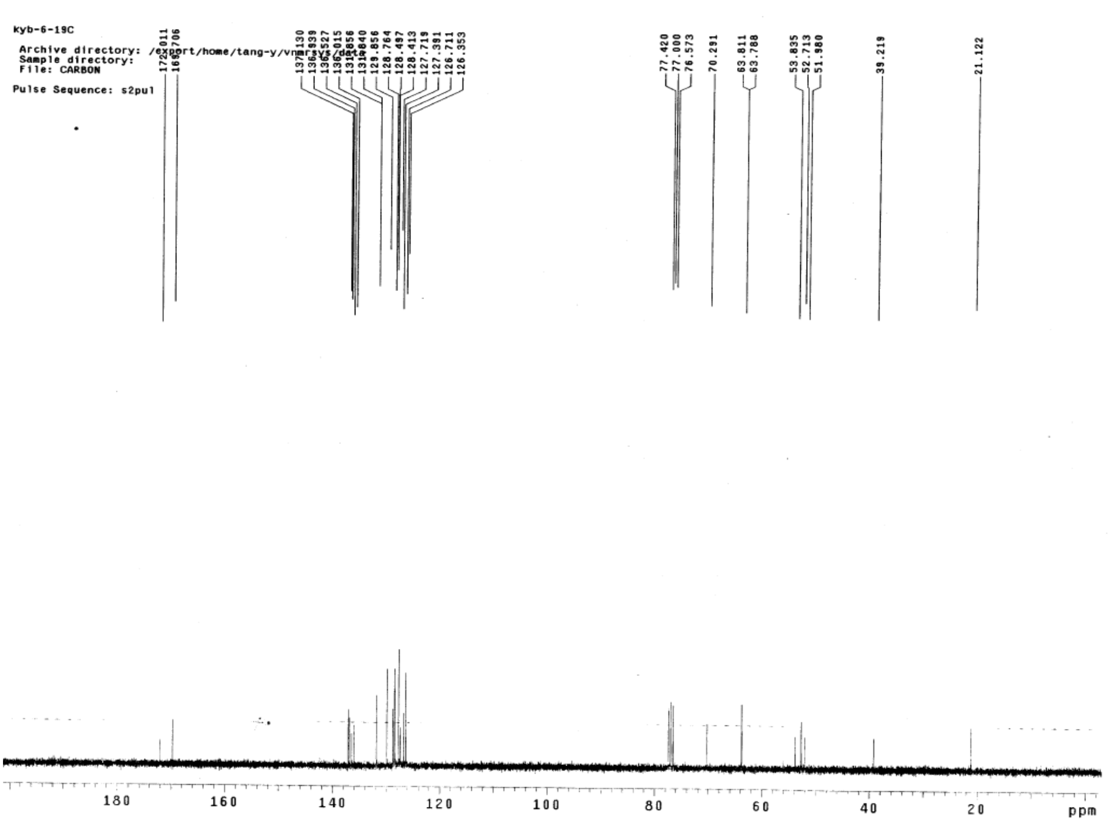



5.11
4.81
2.94
2.76
2.92
2.07
1.79
1.15
1.20
1.08
1.06
1.06
0.97
1.00
0.99
8
7
6
5
4
3
2
1
0

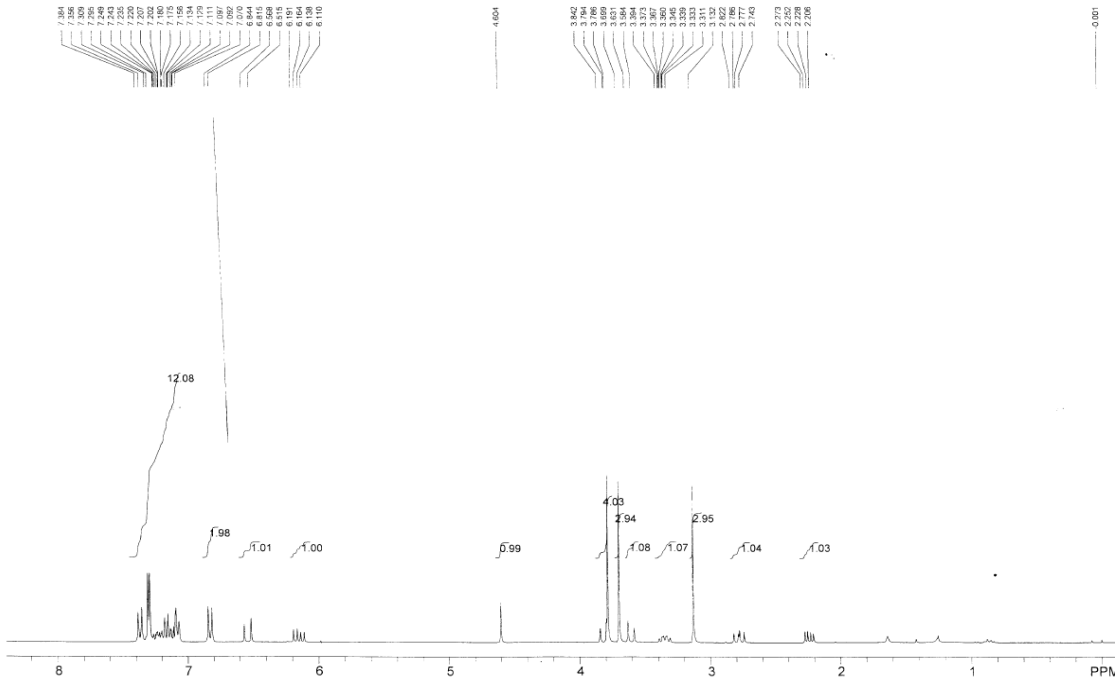

kyb-6-10C
Archive directory: /export/home/zeng-y/vnmrsys/data
Sample directory:
File: CARBON
Pulse Sequence: s2pul
77.427
77.000
76.580
70.314
64.223
64.116
54.575
52.842
52.072
52.018
39.203
200
180
160
140
120
100
80
60
40
20
ppm

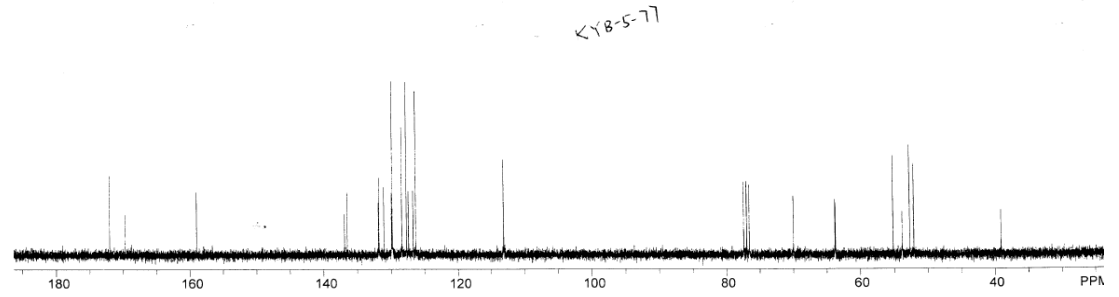
3g



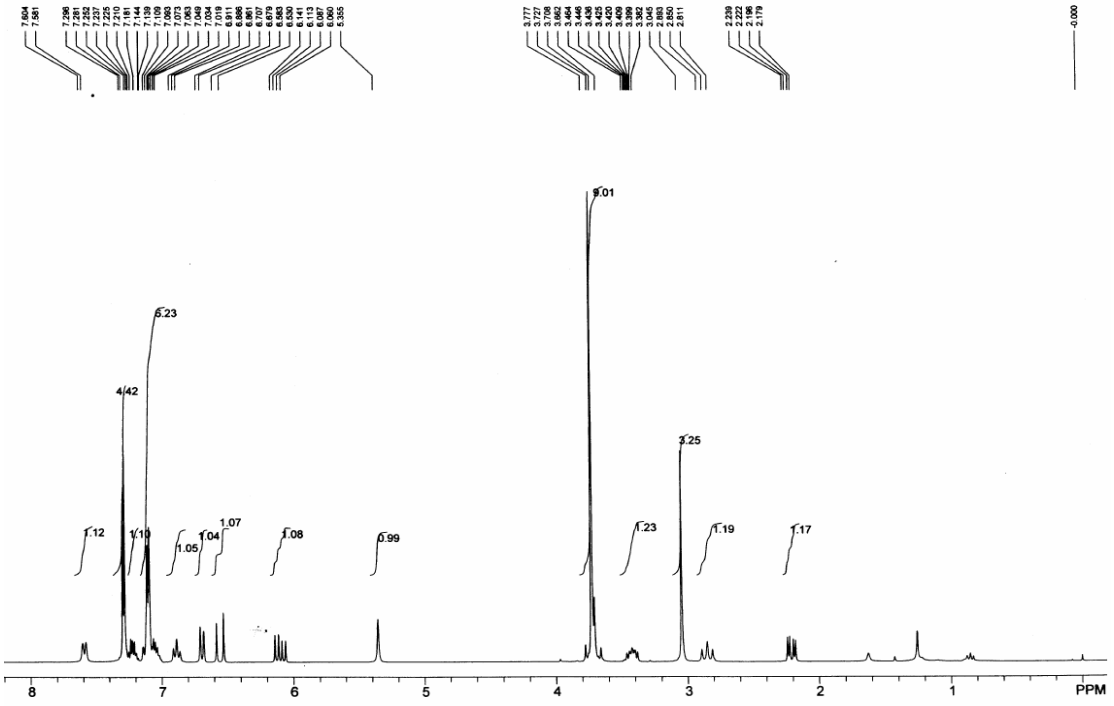

kyb-6-19C
Archive directory: /export/home/tang-y/vnmrsys/data
Sample directory:
File: CARBON
Pulse Sequence: s2pul

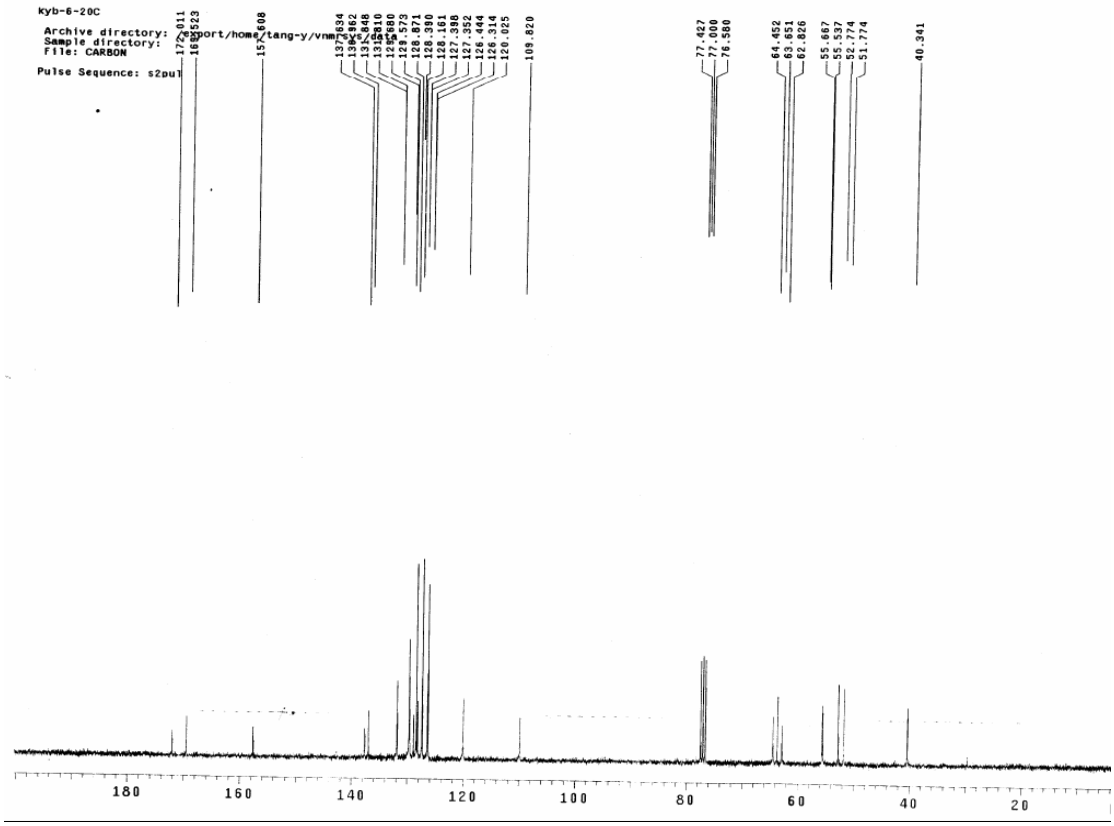
3h



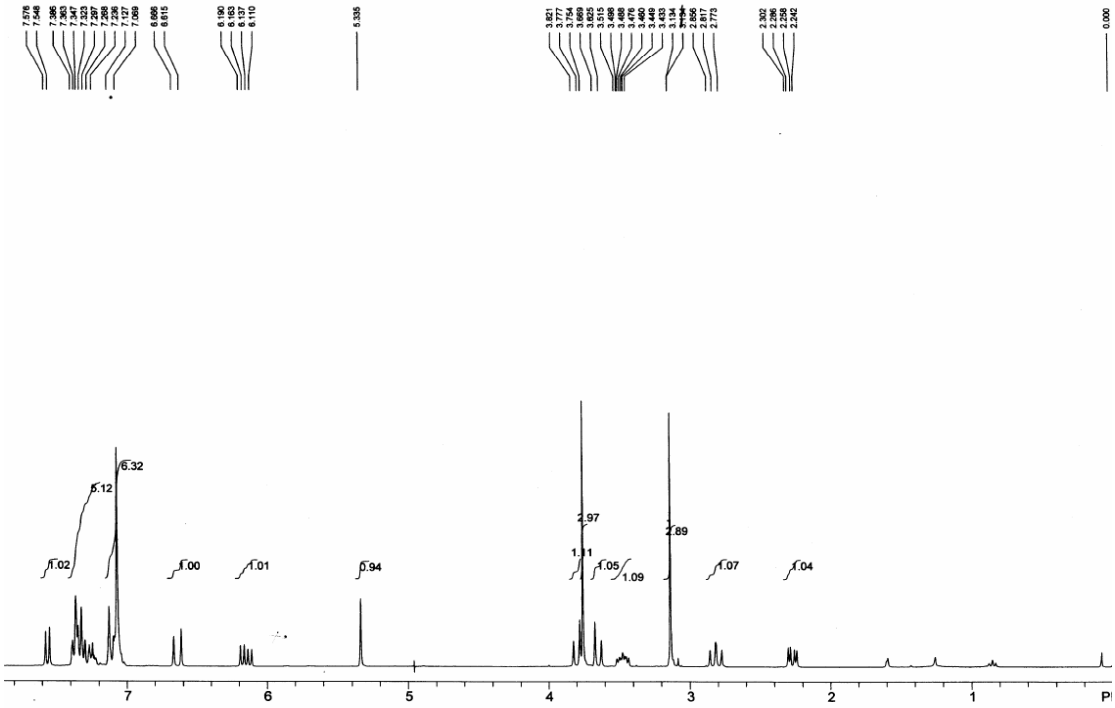


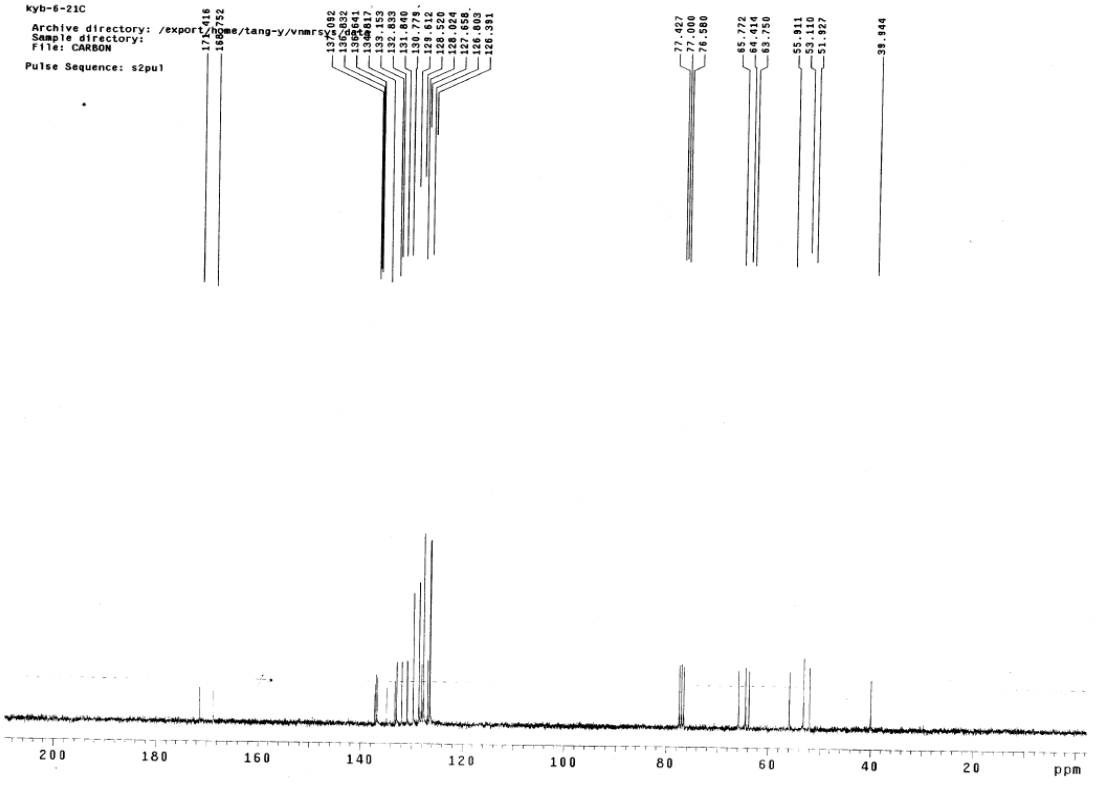
3i


9.01
6.23
4.42
3.25
1.12
1.10
1.05
1.04
1.07
1.08
0.99
1.23
1.19
1.17
PPM

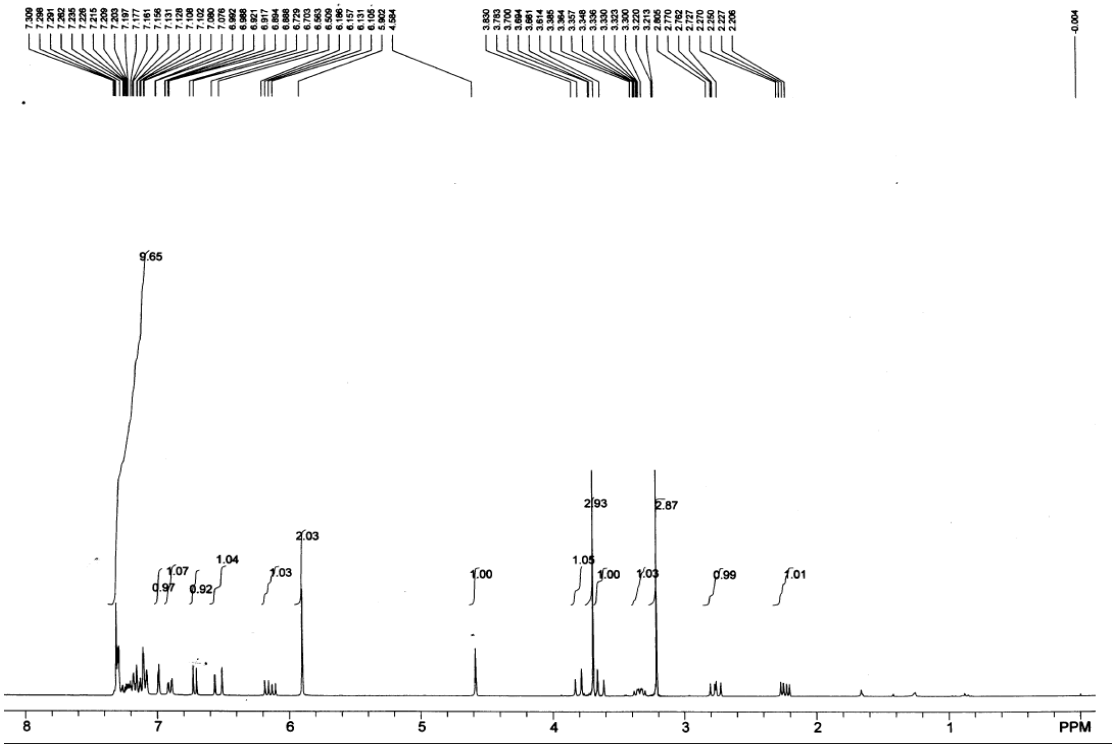

kyb-6-20C
Archive directory: /export/home/tang-y/vnmrsys/data
Sample directory:
File: CARBON
Pulse Sequence: s2pul

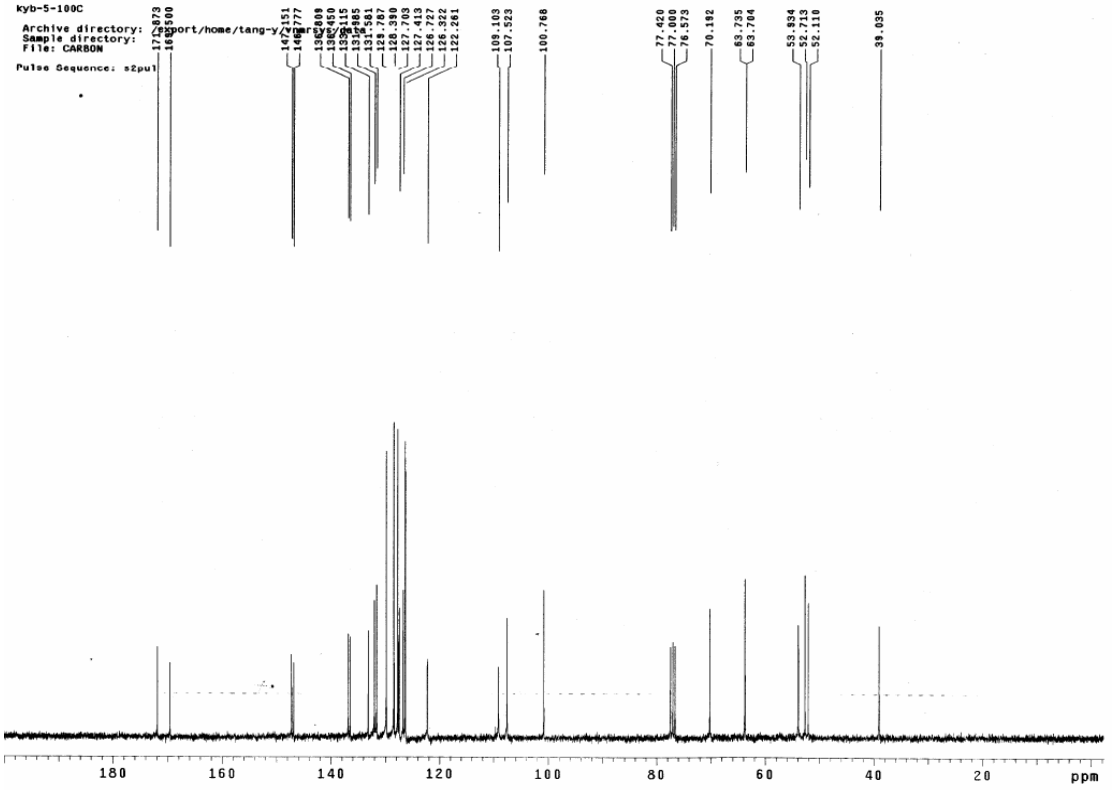
3j


6.32
5.12
2.97
2.89
1.11
1.02
1.00
1.01
0.94
1.05
1.09
1.07
1.04

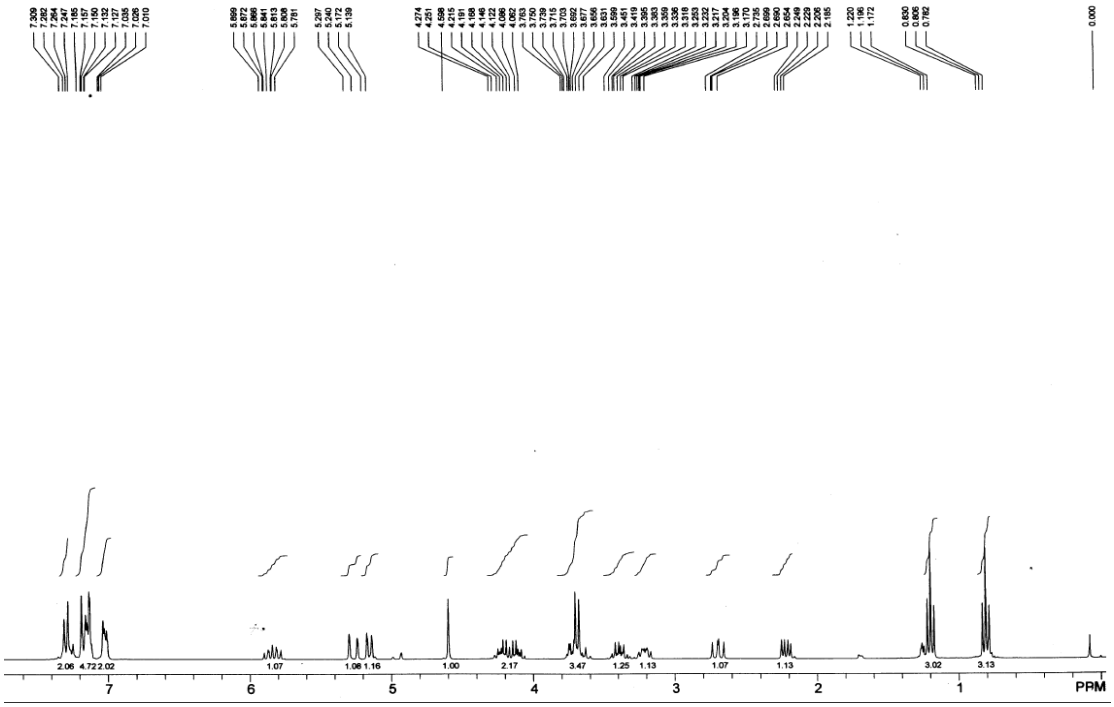

kyb-6-21C
Archive directory: /export/home/tang-y/vnmrsys
Sample directory:
File: CARBON
Pulse Sequence: s2pul
77.427
77.000
76.580
65.772
64.414
63.750
55.911
53.110
51.927
39.844
ppm

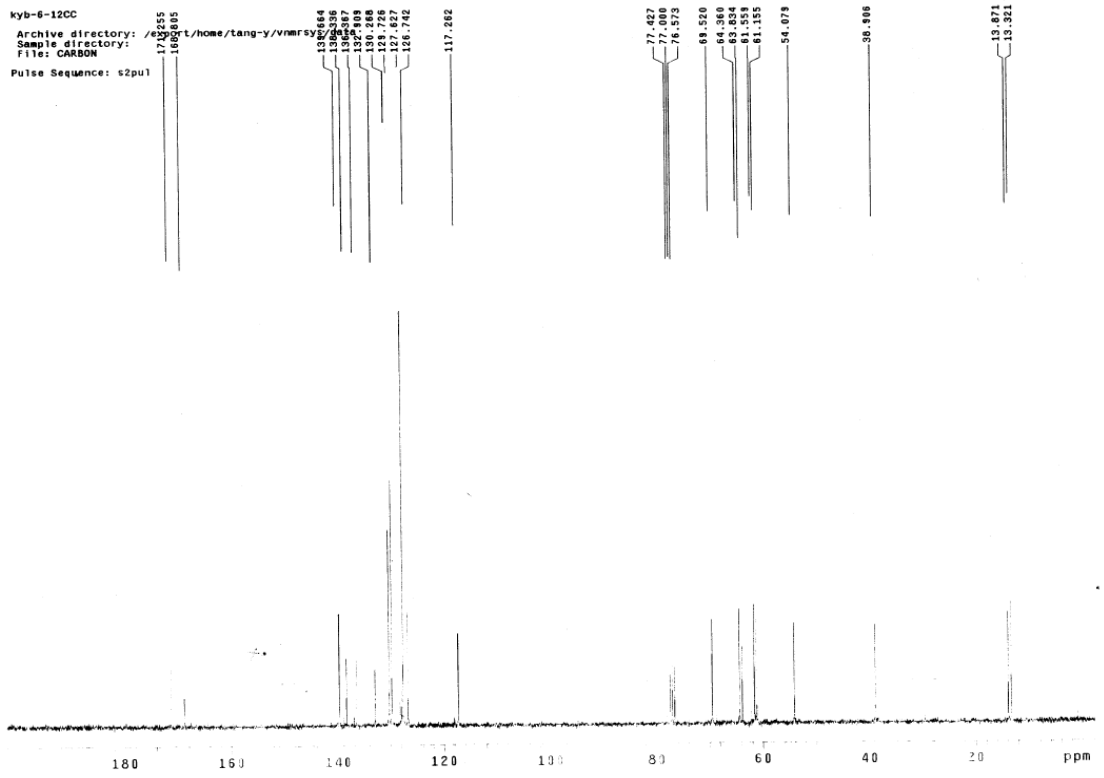
3k


9.65
2.93
2.87
2.03
1.07
1.04
1.03
1.00
1.05
1.00
1.03
0.99
1.01
0.97
0.92
8
7
6
5
4
3
2
1
PPM

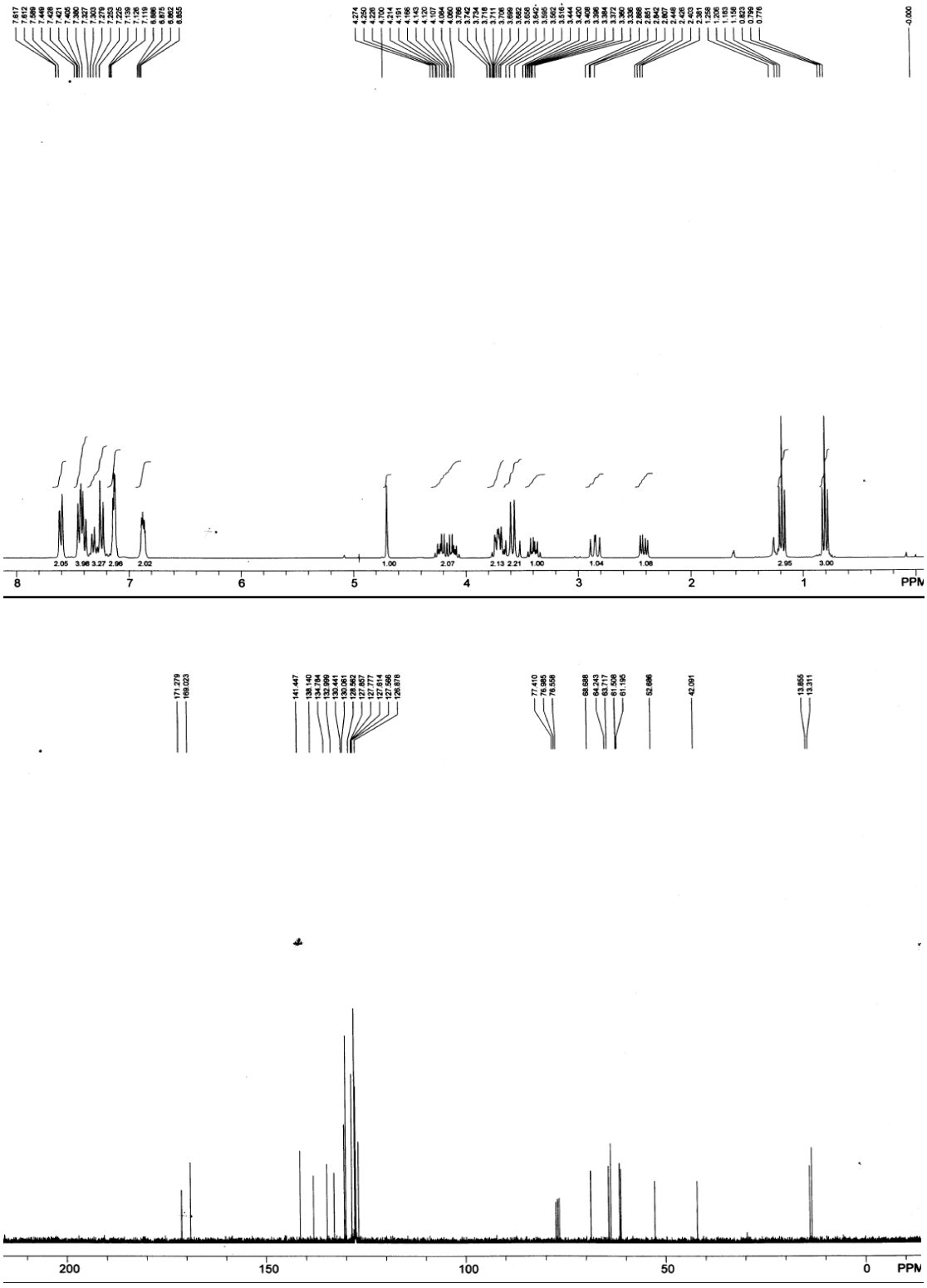

kyb-5-100C
Archive directory: /export/home/tang-y
Sample directory:
File: CARBON
Pulse Sequence: s2pul
77.420
77.000
76.573
70.182
63.735
63.704
53.934
52.713
52.110
39.035
109.103
107.523
100.768
180
160
140
120
100
80
60
40
20
ppm

3l

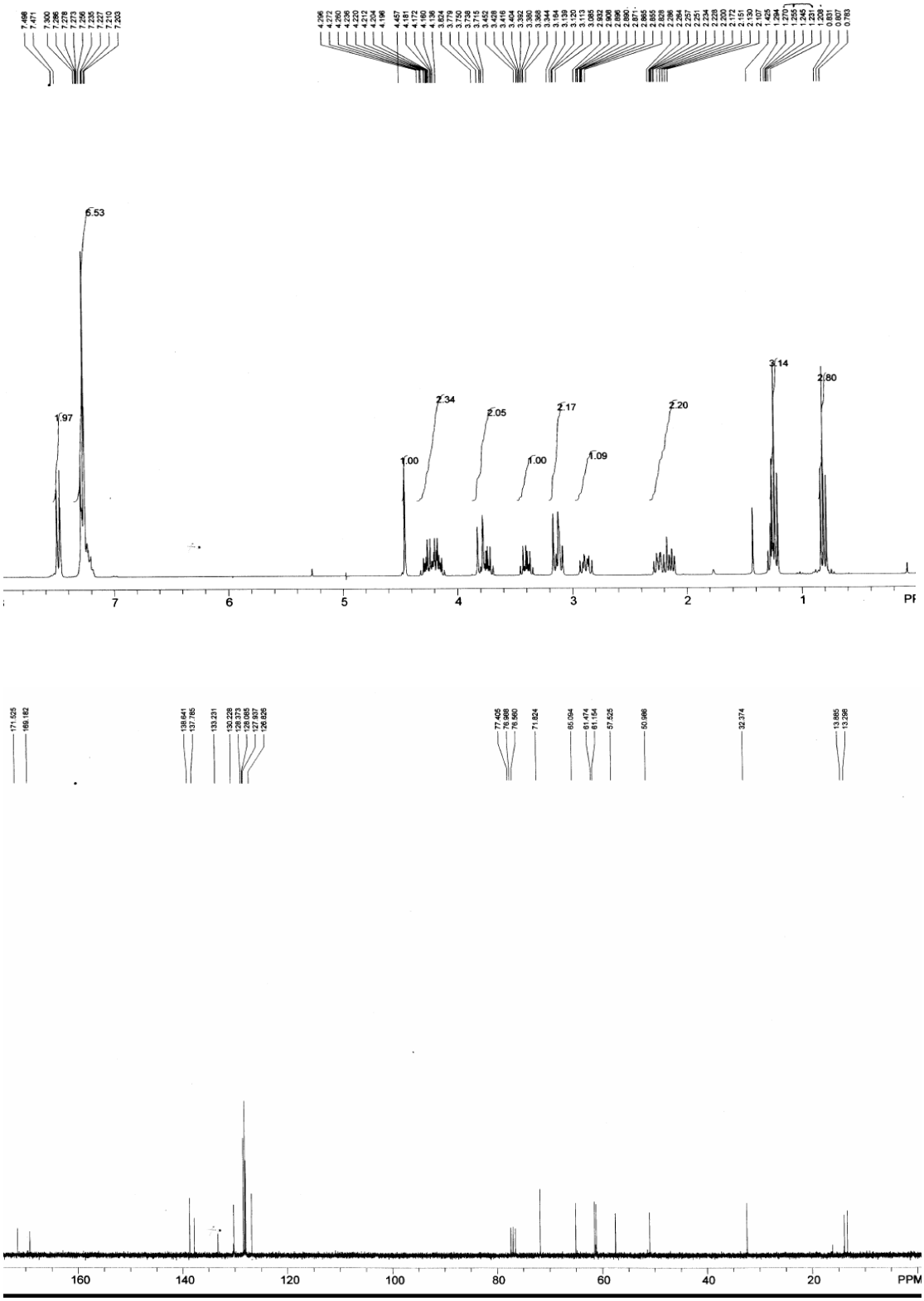

2.06 4.72 2.02
1.07
1.08 1.16
1.00
2.17
3.47
1.25 1.13
1.07
1.13
3.02
3.13
7
6
5
4
3
2
1
PPM


kyb-6-12CC
Archive directory: /export/home/tang-y/vnmrsys/data
Sample directory:
File: CARBON
Pulse Sequence: s2pul
77.427
77.000
76.573
69.520
64.360
63.834
61.559
61.155
54.079
38.906
13.871
13.321
180
160
140
120
100
80
60
40
20
ppm

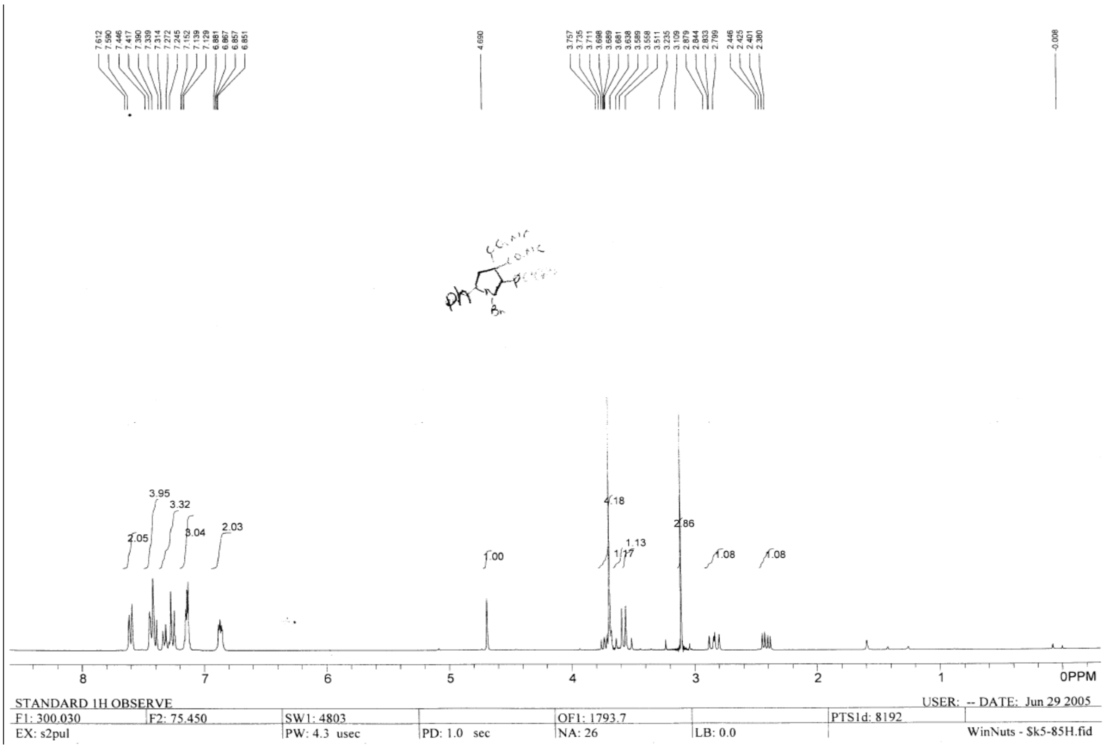
3m

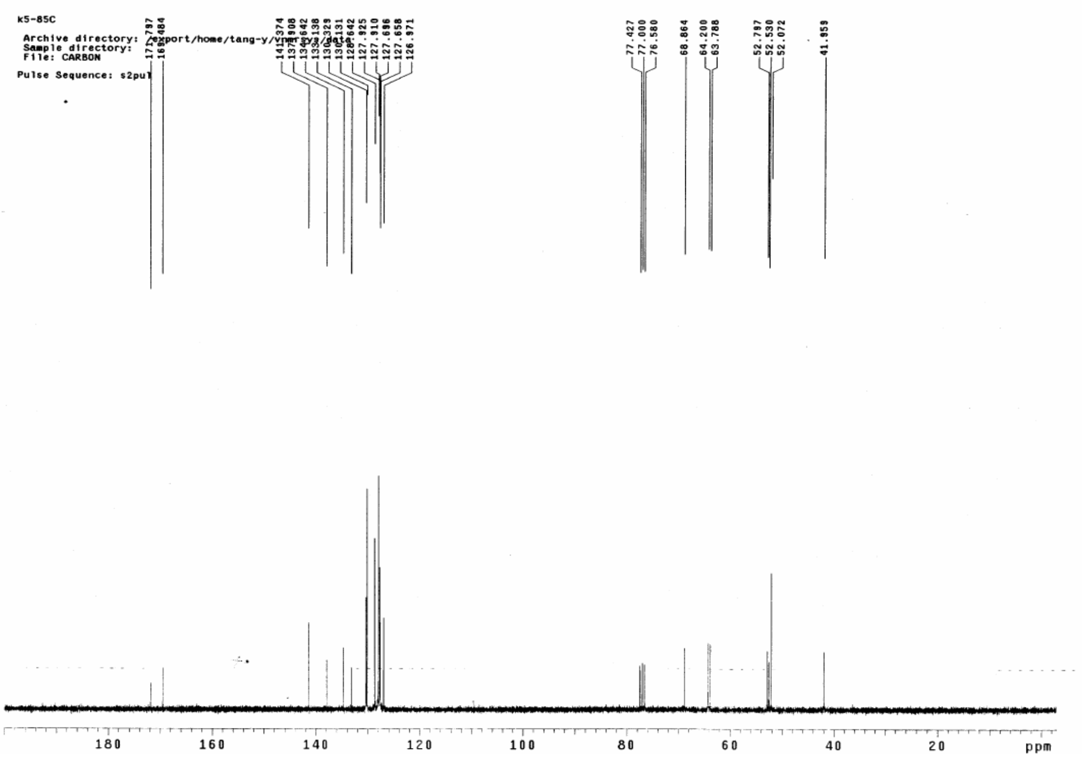


3n

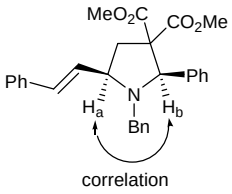
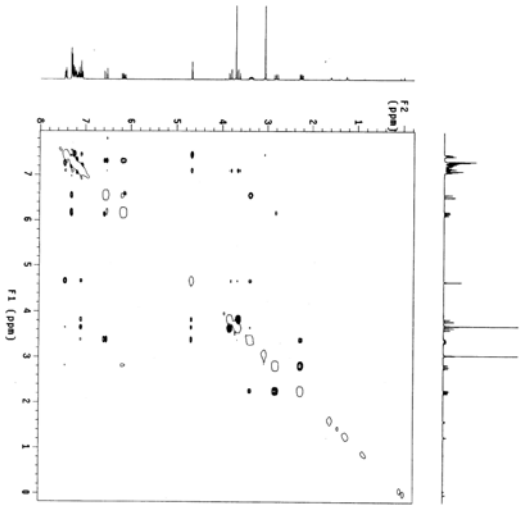
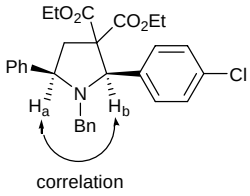
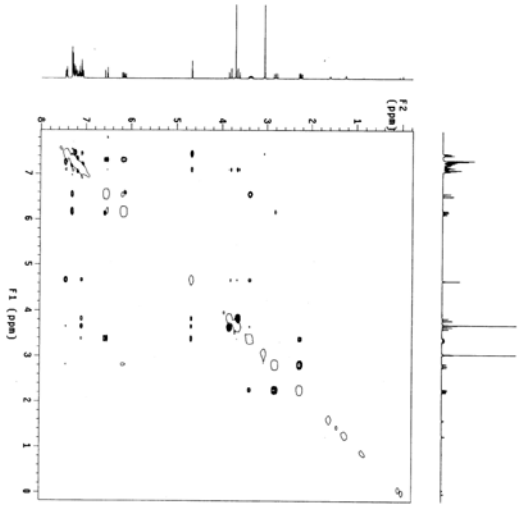

6.53
1.97
2.34
2.05
2.17
2.20
1.00
1.00
1.09
3.14
2.80
7
6
5
4
3
2
1
PPM
160
140
120
100
80
60
40
20
PPM

3o


STANDARD 1H OBSERVE
USER: -- DATE: Jun 29 2005
F1: 300.030
F2: 75.450
SW1: 4803
OF1: 1793.7
PTS1d: 8192
EX: s2pul
PW: 4.3 usec
PD: 1.0 sec
NA: 26
LB: 0.0
WinNuts - $k5-85H.fid
0PPM


k5-85C
Archive directory:
Sample directory:
File: CARBON
Pulse Sequence: s2pul
ppm

Part 3. Stereochemical assignment

^{1}H-^{1}H NOESY  	
^{1}H-^{1}H NOESY  	
^{1}H-^{1}H COSY