Supplementary Material (ESI) for Chemical Communications

Supporting Information

An efficient preparation of indolizines through a tandem palladium-catalyzed cross-coupling reaction and cycloisomerization

Hyunseok Kim,[†] Kwangmoo Lee,[†] Sunggak Kim, [*,‡] and Phil Ho Lee[*,†]

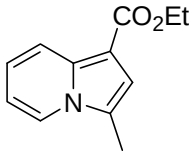
[†]*Department of Chemistry, Kangwon National University, Chuncheon 200-701, Republic of Korea.*
[‡] *Division of Chemistry and Biological Chemistry, School of Physical & Mathematical Sciences, Nanyang Technological University, Singapore 637371*

phlee@kangwon.ac.kr

Table of Contents

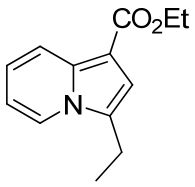
Experimental Section

General: Reactions were carried out in oven-dried glassware under nitrogen atmosphere. All commercial reagents were used without purification. Toluene was dried with CaH_2. All reaction mixtures were stirred magnetically and were monitored by thin-layer chromatography using silica gel percolated glass plates, which were visualized with UV light and then developed using either iodine or a solution of anisaldehyde. Flash column chromatography was carried out using silica gel (230-400 mesh). ^{1}H NMR (300 MHz or 400 MHz) and ^{13}C NMR (100 MHz) spectra were recorded on NMR spectrometer. Deuterated chloroform was used as the solvent, and chemical shift values (δ) are reported in parts per million relative to the residual signals of this solvent (δ 7.24 for ^{1}H and δ 77.0 for ^{13}C). Infrared spectra were recorded on FT-IR spectrometer as either a thin film pressed between two sodium chloride plates or as a solid suspended in a potassium bromide disk. Mass spectra were obtained from the KBSI on high resolution mass spectrometer.

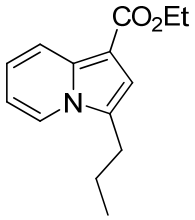


1-Ethoxycarbonyl-3-methylindolizine (3a)[1]: To a suspension of $Pd(OAc)_2$ (5.4 mg, 0.024 mmol, 8 mol %) and Xantphos (28.0 mg, 0.048 mmol, 16 mol %) in THF (0.4 mL) was added 2-pyridinyl trifluoromethanesulfonate (46.0 μL, 0.3 mmol) at room temperature under nitrogen atmosphere. After being stirred for 30 min, organoindium reagent generated in situ from indium (69.0 mg, 0.6 mmol), sodium iodide (135.0 mg,

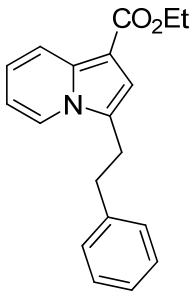
0.9 mmol) and ethyl 4-bromo-2-pentynoate (185.0 mg, 0.9 mmol) in THF (0.8 mL) was added and the mixture was stirred at 90 ^{o}C for 1h 30min. The reaction mixture was quenched with saturated $NaHCO_3$. The aqueous layer was extracted with CH_2Cl_2 (3 x 20 mL) and the combined organic layers were washed with brine, dried over $MgSO_4$, filtered and concentrated under reduced pressure. The residue was purified by silica gel column chromatograghy (EtOAc/hexane = 1/10) give 1-ethoxycarbonyl-3-methylindolizine (45.0 mg, 75%). Deep blue liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.19 (d, J = 9.0 Hz, 1H), 7.79 (d, J = 7.0 Hz, 1H), 7.04 (t, J = 7.8 Hz, 1H), 7.04 (s, 1H), 6.77 (t, J = 6.8 Hz, 1H), 4.36 (q, J = 7.1 Hz, 2H), 2.45 (s, 3H), 1.40 (t, J = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.6, 136.0, 123.1, 121.4, 121.3, 120.3, 115.1, 112.6, 103.2, 59.8, 15.1, 11.9; IR (film) 2979, 1686, 1525, 1509, 1424, 1384, 1309, 1222, 1122, 1107, 1042 cm^{-1}; HRMS (EI) calcd for $C_{12}H_{13}NO_2$ 203.0946, found 203.0945.



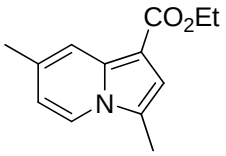
1-Ethoxycarbonyl-3-ethylindolizine (3b)[2]: Deep blue liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.20 (dt, J = 9.0, 1.2, 1.0 Hz, 1H), 7.82 (d, J = 7.0 Hz, 1H), 7.10-7.01 (m, 2H), 6.75 (td, J = 7.0, 1.1 Hz, 1H), 4.37 (q, J = 7.1 Hz, 2H), 2.78 (q, J = 7.5 Hz, 2H), 1.41 (t, J = 7.3 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.2, 134.7, 126.0, 121.6, 120.2, 118.9, 111.8, 111.1, 101.7, 58.4, 17.9, 13.7, 10.3; IR (film) 2973, 1685, 1509, 1425, 1218, 1078, 1051, 775, 738 cm^{-1}; HRMS (EI) calcd for $C_{13}H_{15}NO_2$ 217.1103, found 217.1103.



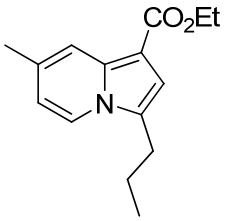
1-Ethoxycarbonyl-3-propylindolizine (3c): Deep blue solid. m.p. 32 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.19 (dt, *J* = 9.0, 1.2 Hz, 1H), 7.84 (d, *J* = 7.0 Hz, 1H), 7.05-7.00 (m, 2H), 6.73 (td, *J* = 6.7, 1.3 Hz, 1H), 4.36 (q, *J* = 7.1 Hz, 2H), 2.75 (t, *J* = 7.5 Hz, 2H), 1.80 (q, *J* = 7.5 Hz, 2H), 1.41 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.6, 136.0, 125.9, 123.1, 121.5, 120.4, 114.1, 112.5, 103.2, 59.8, 28.2, 20.6, 15.1, 14.4; IR (film) 2961, 2872, 1687, 1509, 1425, 1215, 1094, 1055, 776, 737 cm^{-1}; HRMS (EI) calcd for $C_{14}H_{17}NO_2$ 231.1259, found 231.1259.



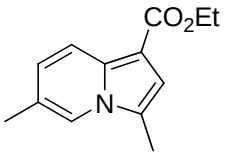
1-Ethoxycarbonyl-3-phenethylindolizine (3d): Deep blue liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.20 (d, *J* = 9.0 Hz, 1H), 7.77 (d, *J* = 7.1 Hz, 1H), 7.31 (t, *J* = 7.1 Hz, 3H), 7.25-7.22 (m, 3H), 7.03 (dd, *J* = 9.0, 6.6 Hz, 2H), 6.71 (t, *J* = 6.6 Hz, 1H), 4.37 (q, *J* = 7.1 Hz, 2H), 3.09 (s, 4H), 1.41 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.6, 141.4, 136.1, 129.0, 128.7, 126.8, 125.3, 123.0, 121.7, 120.4, 114.2, 112.6, 103.4, 59.8, 34.0, 28.3, 15.1; IR (film) 2978, 1685, 1509, 1425, 1218, 1065, 1041, 775, 738, 699 cm^{-1}; HRMS (EI) calcd for $C_{19}H_{19}NO_2$ 293.1416, found 293.1416.



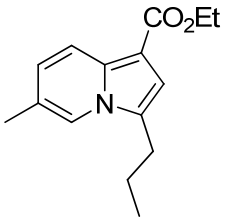
1-Ethoxycarbonyl-3,7-dimethylindolizine (3e): Red brown liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 (s, 1H), 7.69 (d, *J* = 7.0 Hz, 1H), 6.95 (s, 1H), 6.61 (dd, *J* = 7.0, 1.7 Hz, 1H), 4.35 (q, *J* = 7.1 Hz, 2H), 2.42 (s, 3H), 2.39 (s, 3H), 1.40 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.3, 136.2, 132.0, 122.2, 120.2, 118.3, 114.8, 114.3, 101.1, 59.2, 21.3, 14.7, 11.4; IR (film) 2978, 1683, 1513, 1418, 1231, 1182, 1075, 1040, 774 cm^{-1}; HRMS (EI) calcd for $C_{13}H_{15}NO_2$ 217.1103, found 217.1103.



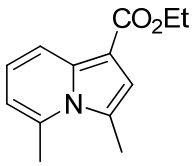
1-Ethoxycarbonyl-7-methyl-3-propylindolizine (3f): Brown solid. m.p. 56 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 (s, 1H), 7.74 (d, *J* = 7.1 Hz, 1H), 6.94 (s, 1H), 6.58 (dd, *J* = 7.1, 1.6 Hz, 1H), 4.35 (q, *J* = 7.1 Hz, 2H), 2.73 (t, *J* = 7.5 Hz, 2H), 2.38 (s, 3H), 1.83-1.74 (m, 2H), 1.43 (t, *J* = 7.1 Hz, 3H), 1.04 (t, *J* = 7.5 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.8, 136.7, 132.5, 125.3, 122.7, 118.8, 115.1, 113.7, 101.6, 59.6, 28.2, 21.7, 20.7, 15.1, 14.5; IR (film) 2961, 2872, 1685, 1514, 1229, 1181, 1053, 774 cm^{-1}; HRMS (EI) calcd for $C_{15}H_{19}NO_2$ 245.1416, found 245.1416.



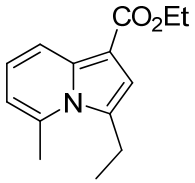
1-Ethoxycarbonyl-3,6-dimethylindolizine (3g): Red brown liquid ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.09 (d, *J* = 9.1 Hz, 1H), 7.57 (s, 1H), 6.67 (s, 1H), 6.90 (dd, *J* = 9.1, 1.2 Hz, 1H), 4.34 (q, *J* = 7.1 Hz, 2H), 2.42 (s, 3H), 2.33 (s, 3H), 1.39 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.6, 134.8, 124.7, 122.1, 120.9, 120.9, 119.6, 114.8, 102.7, 59.7, 18.9, 15.1, 11.9; IR (film) 2978, 1686, 1525, 1427, 1293, 1226, 1086, 1056, 784 cm^{-1}; HRMS (EI) calcd for $C_{13}H_{15}NO_2$ 217.1103, found 217.1103.



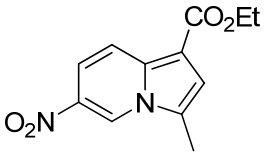
1-Ethoxycarbonyl-5-methyl-3-propylindolizine (3h): Blue green solid. m.p. 52 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.09 (d, *J* = 9.4 Hz, 1H), 7.61 (s, 1H), 6.98 (s, 1H), 6.88 (dd, *J* = 9.0, 1.3 Hz, 1H), 4.35 (q, *J* = 7.1 Hz, 2H), 2.72 (t, *J* = 7.5 Hz, 2H), 2.31 (s, 3H), 1.87-1.75(m, 2H), 1.40 (t, *J* = 7.1 Hz, 3H), 1.05 (t, *J* = 7.5 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.7, 134.9, 125.6, 124.7, 122.0, 120.9, 119.7, 113.8, 102.8, 59.7, 28.2, 20.6, 18.9, 15.1, 14.5; IR (film) 2960, 2872, 1686, 1510, 1438, 1214, 1054, 800 cm^{-1}; HRMS (EI) calcd for $C_{15}H_{19}NO_2$ 245.1416, found 245.1416.



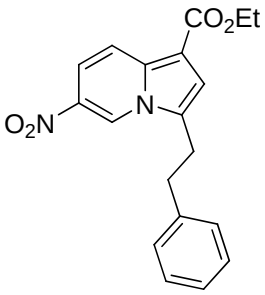
1-Ethoxycarbonyl-3,5-dimethylindolizine (3i): Red brown solid. m.p. 58 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 (d, J = 9.0 Hz, 1H), 6.92 (s, 1H), 6.82 (dd, J = 9.0, 6.7 Hz, 1H), 6.34 (d, J = 6.7 Hz, 1H), 4.33 (q, J = 7.1 Hz, 2H), 2.83 (s, 3H), 2.79 (s, 3H), 1.38 (t, J = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.4, 138.8, 136.3, 123.7, 122.1, 118.5, 117.8, 114.2, 102.7, 59.7, 21.9, 17.4, 15.1; IR (film) 2978, 1687, 1525, 1427, 1293, 1226, 1086, 1056, 784 cm^{-1}; HRMS (EI) calcd for $C_{13}H_{15}NO_2$ 217.1103, found 217.1103.



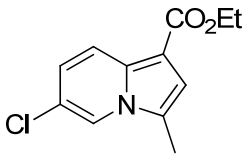
1-Ethoxycarbonyl-3-ethyl-5-methylindolizine (3j): Deep blue solid. m.p. 60 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14 (d, J = 9.0 Hz, 1H), 7.03 (s, 1H), 6.68 (dd, J = 9.0, 6.7 Hz, 1H), 6.39 (d, J = 6.7 Hz, 1H), 4.35 (q, J = 7.1 Hz, 2H), 3.26 (q, J = 7.3 Hz, 2H), 2.86 (s, 3H), 1.42-1.25 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.0, 137.5, 134.9, 129.1, 120.6, 117.1, 114.0, 113.1, 101.5, 58.3, 22.2, 20.9, 13.7, 13.4; IR (film) 2775, 1685, 1525, 1428, 1222, 1086, 1044, 783 cm^{-1}; HRMS (EI) calcd for $C_{14}H_{17}NO_2$ 231.1259, found 231.1259.



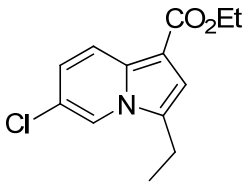
1-Ethoxycarbonyl-3methyl-6-nitroindolizine (3k): Orange solid. m.p. 102 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.96 (d, *J* = 1.7 Hz, 1H), 8.25 (d, *J* = 10.0 Hz, 1H), 7.74 (dd, *J* = 10.0, 2.0 Hz, 1H), 7.21 (d, *J* = 0.7 Hz, 1H), 4.39 (q, *J* = 7.1 Hz, 2H), 2.58 (s, 3H), 1.42 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.1, 137.1, 134.9, 124.2, 123.4, 119.6, 118.3, 114.2, 106.6, 60.1, 14.5, 11.5; IR (film) 2980, 1695, 1537, 1434, 1348, 1321, 1236, 1057, 803 cm^{-1}; HRMS (EI) calcd for $C_{12}H_{12}N_2O_4$ 248.0797, found 248.0797.



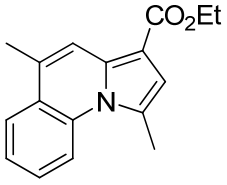
1-Ethoxycarbonyl-6-nitro-3-phenethylindolizine (3l): Orange solid. m.p. 105 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.77 (d, *J* = 1.8 Hz, 1H), 8.22 (d, *J* = 10.0 Hz, 1H), 7.69 (dd, *J* = 10.0, 1.8 Hz, 1H), 7.30-7.17 (m, 6H), 4.39 (q, *J* = 7.1 Hz, 2H), 3.22-3.10 (m, 4H), 1.42 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.6, 140.5, 137.4, 135.3, 129.2, 128.6, 127.1, 123.7, 120.0, 117.9, 114.7, 107.1, 66.3, 60.6, 34.5, 28.1,15.0; IR (film) 2980, 1693, 1533, 1499, 1350, 1219, 1050, 819 cm^{-1}; HRMS (EI) calcd for $C_{19}H_{18}N_2O_4$ 338.1267, found 338.1267.



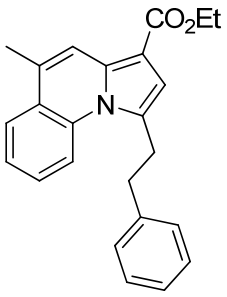
6-Chloro-1-ethoxycarbonyl-3-methylindolizine (3m): Apicot solid. m.p. 60 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14 (d, J = 9.6 Hz, 1H), 7.82 (s, 1H), 7.04 (s, 1H), 6.98 (dd, J = 9.6, 1.7 Hz 1H), 4.35 (q, J = 7.1 Hz, 2H), 2.44 (s, 3H), 1.40 (t, J = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.7, 132.5, 121.0, 120.4, 120.0, 119.5, 119.3, 114.5, 103.1, 58.6, 13.6, 10.4; IR (film) 2928, 1691, 1523, 1503, 1433, 1224, 1055, 797 cm^{-1}; HRMS (EI) calcd for $C_{12}H_{12}ClNO_2$ 237.0557, found 237.0557.



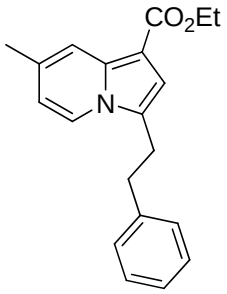
6-Chloro-1-ethoxycarbonyl-3-ethylindolizine (3n): Gray solid. m.p. 69 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14 (d, J = 9.5 Hz, 1H), 7.84 (s, 1H), 7.05 (s, 1H), 6.97 (dd, J = 9.5, 1.7 Hz, 1H), 4.36 (q, J = 7.1 Hz, 2H), 2.76 (q, J = 7.4 Hz, 2H), 1.41 (t, J = 7.3 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.2, 134.0, 127.9, 122.5, 120.9, 120.8, 114.0, 104.6, 60.0, 19.4, 15.0, 11.6; IR (film) 2974, 1690, 1521, 1503, 1221, 1047, 800 cm^{-1}; HRMS (EI) calcd for $C_{13}H_{14}ClNO_2$ 251.0713, found 251.0713.



3-Ethoxycarbonyl-1,5-dimethylpyrrolo[1,2-*a*]quinoline (3o): Red brown solid. m.p. 63 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.40 (d, J = 8.5 Hz, 1H), 8.09 (s, 1H), 7.84 (dd, J = 8.1, 1.5 Hz, 1H), 7.55-7.51 (m, 1H), 7.45-7.41 (m, 1H), 6.89 (s, 1H), 4.37 (q, J = 7.1 Hz, 2H), 2.92 (s, 3H), 2.55 (s, 3H), 1.41 (t, J = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.6, 135.8, 135.7, 129.6, 127.8, 126.5, 126.1, 125.6, 124.3, 118.7, 116.9, 115.9, 104.8, 59.9, 19.8, 19.2, 15.0; IR (film) 2975, 1689, 1447, 1419, 1251, 1205, 1085, 749 cm^{-1}; HRMS (EI) calcd for $C_{17}H_{17}NO_2$ 267.1259, found 267.1259.



3-Ethoxycarbonyl-5-methyl-1-phenethylpyrrolo[1,2-*a*]quinoline (3p): Red brown. solid. m.p. 93 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.35 (d, J = 8.6 Hz, 1H), 8.14 (s, 1H), 7.87 (dd, J = 8.0, 1.4 Hz, 1H), 7.53 (t, J = 7.5 Hz, 1H), 7.45 (t, J = 7.5 Hz, 1H), 7.39-7.27 (m, 5H), 7.04 (s, 1H), 4.39 (q, J = 7.1 Hz, 2H), 3.57 (t, J = 8.5, 8.0 Hz, 2H), 3.18 (t, J = 8.5, 8.0 Hz, 2H), 2.58 (s, 3H), 1.43 (t, J = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.6, 141.6, 136.0, 135.5, 130.9, 130.0, 129.1, 128.9, 128.0, 126.8, 126.3, 125.7, 124.4, 118.8, 117.4, 114.4, 105.0, 60.0, 35.4, 34.5, 19.8, 15.1; IR (film) 2927, 1689, 1556, 1449, 1421, 1251, 1206, 1088, 748, 698 cm^{-1}; HRMS (EI) calcd for $C_{24}H_{23}NO_2$ 357.1729, found 357.1729.

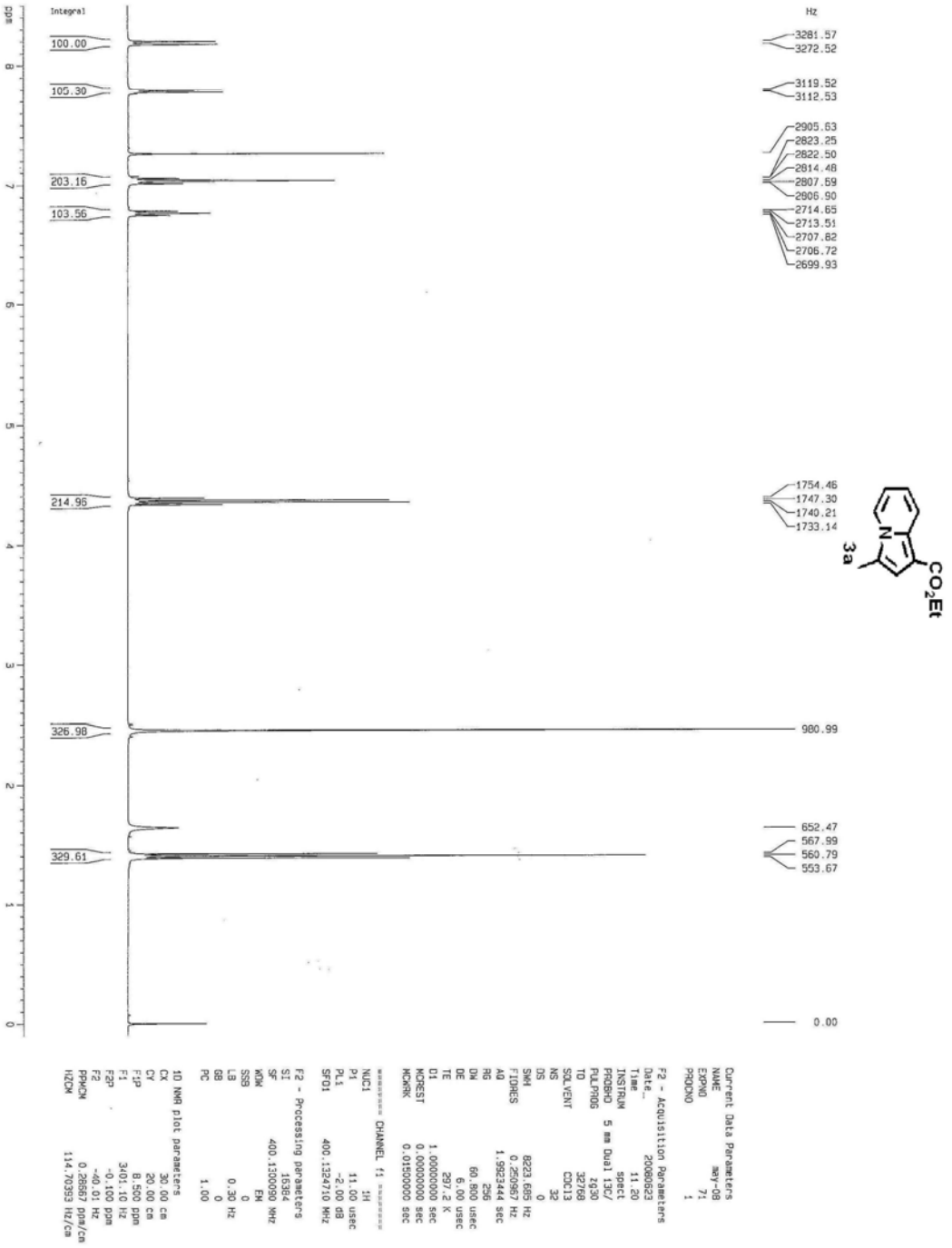


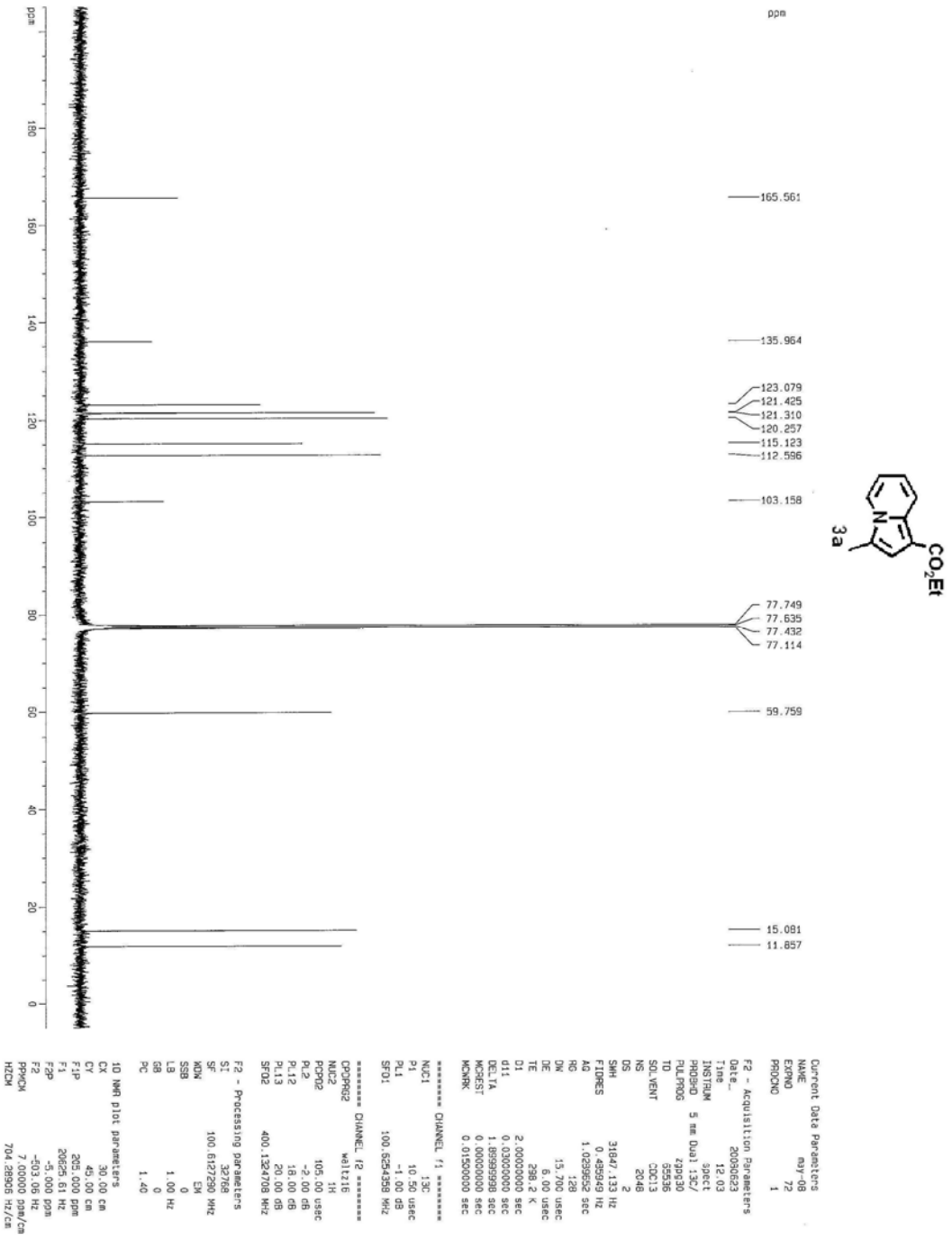
1-Ethoxycarbonyl-7-methyl-3-phenethylindolizine (3q): Red brown liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 (s, 1H), 7.68 (d, *J* = 7.1 Hz, 1H), 7.31 (t, *J* = 7.1 Hz, 2H), 7.25-7.21 (m, 3H), 7.03 (s, 1H), 6.56 (dd, *J* = 7.1, 1.7 Hz, 1H), 4.36 (q, *J* = 7.1 Hz, 2H), 3.09-3.05 (m, 4H), 2.38 (s, 3H), 1.41 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.3, 140.1, 135.3, 131.2, 127.6, 127.3, 125.3, 123.2, 121.1, 117.4, 113.8, 112.4, 101.3, 58.3, 32.6, 26.9, 20.2, 13.7; IR (film) 2930, 1684, 1513, 1227, 1183, 1063, 1041, 774, 700 cm^{-1}; HRMS (EI) calcd for $C_{20}H_{21}NO_2$ 307.1572, found 307.1572.

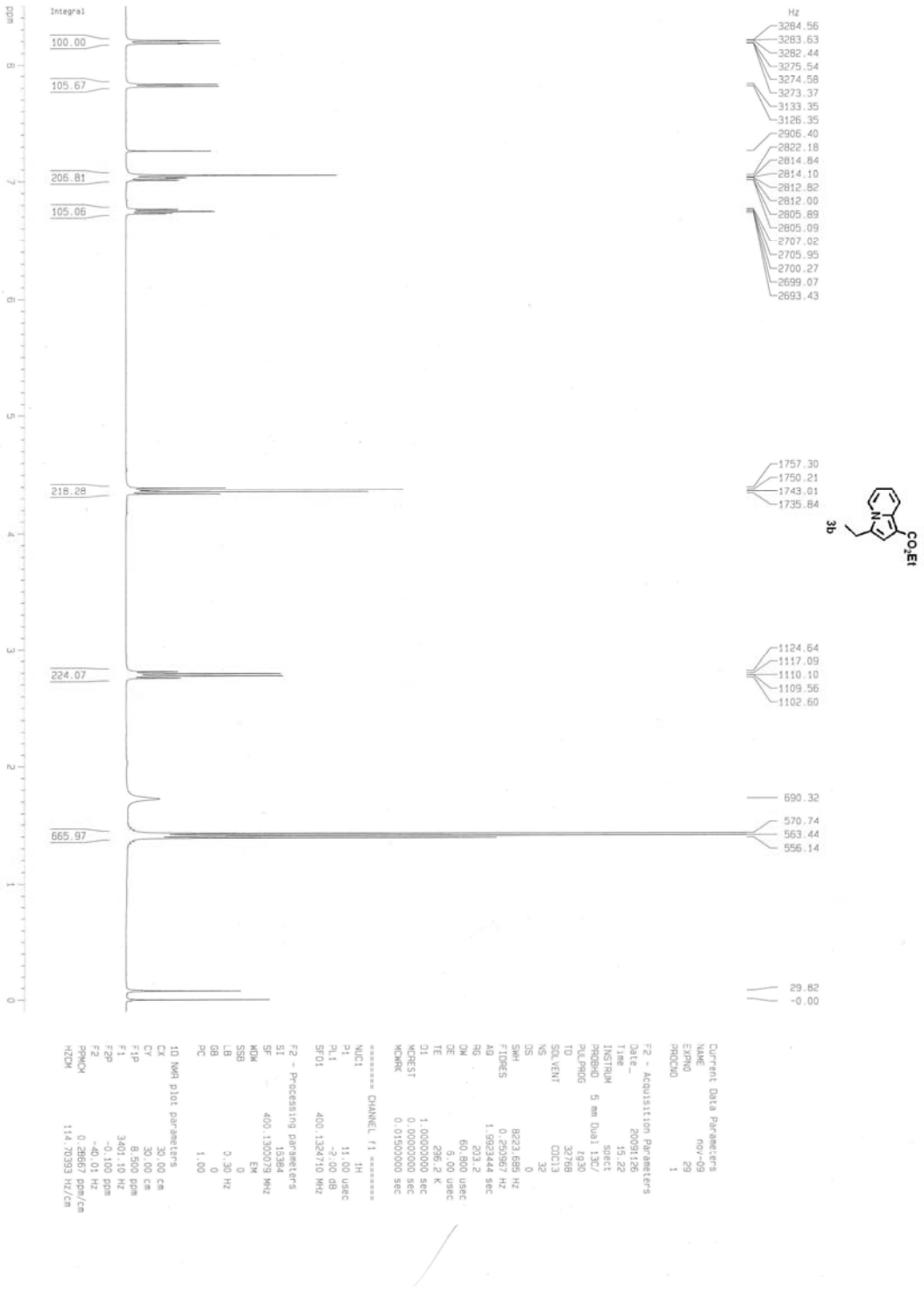
References

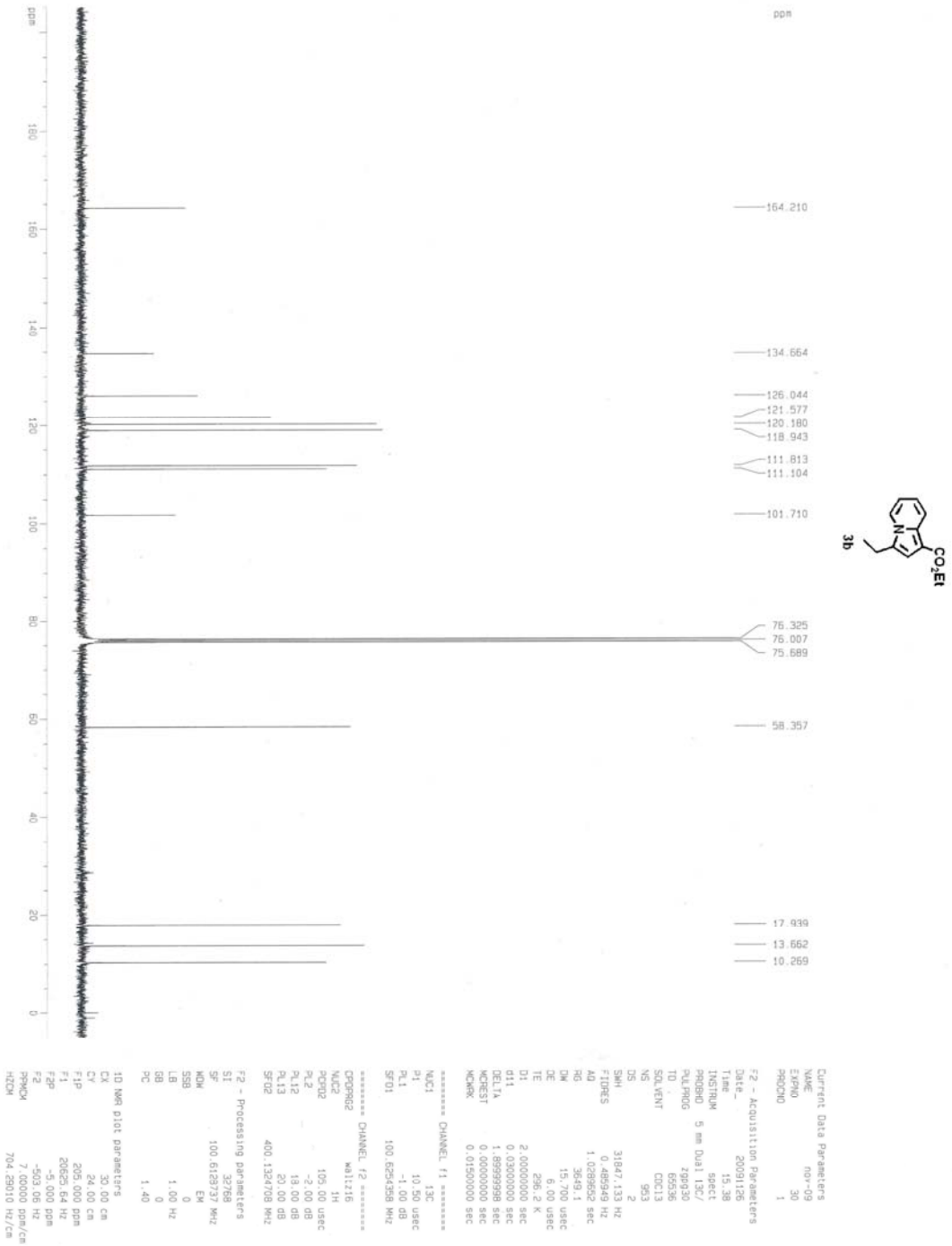
1. (a) T. Tamura, Y. Sumida, Y. Ikeda, *Chem. Pharm. Bull.*, 1972, **20**, 1058; (b) D. R. Bragg, D. G. Wibberley, *J. Chem. Soc*. 1963, 3277.

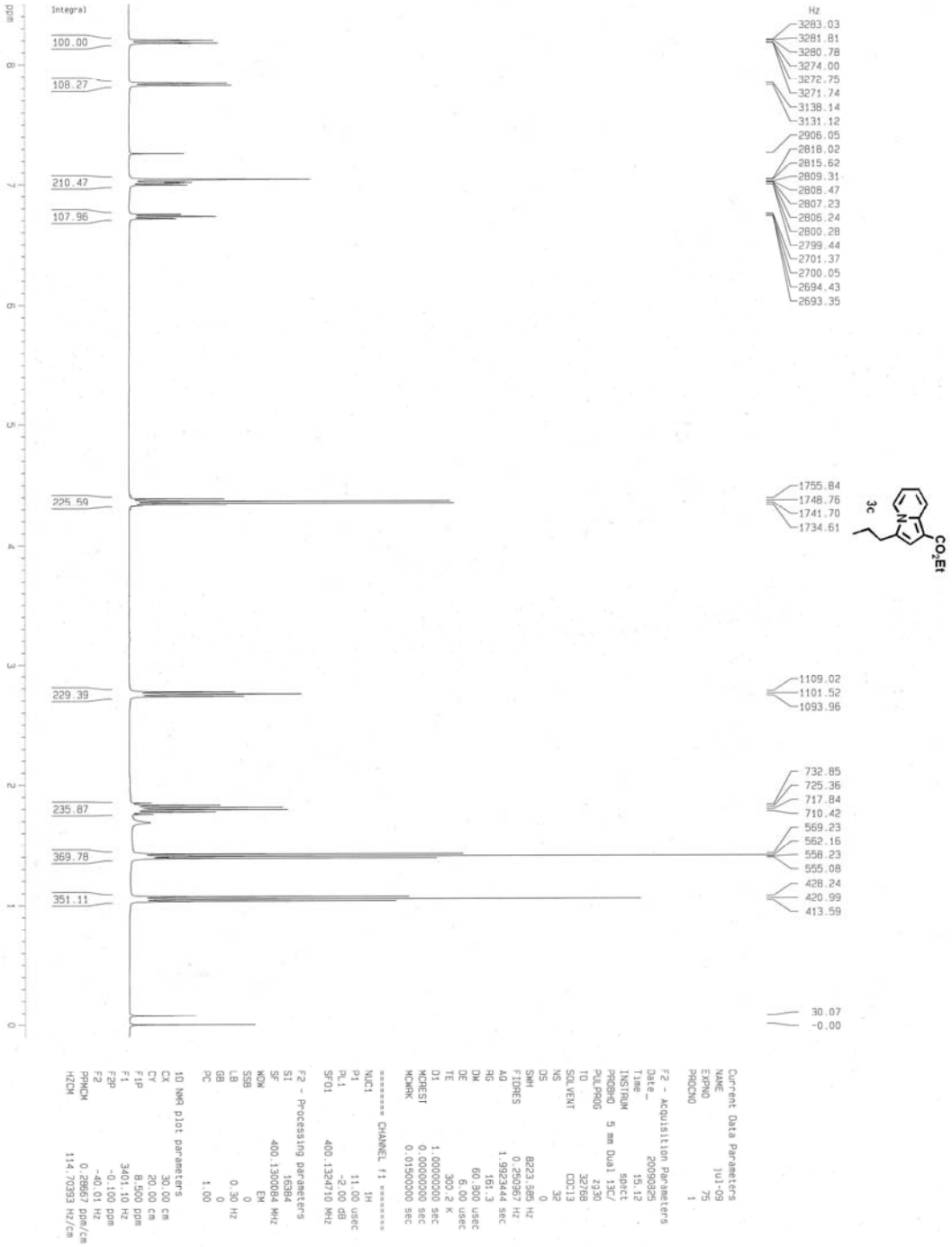
2. A. R. Katritzky, G. Oiu, B. Yang, H. Y. He, *J. Org. Chem.*, 1999, **64**, 7618.

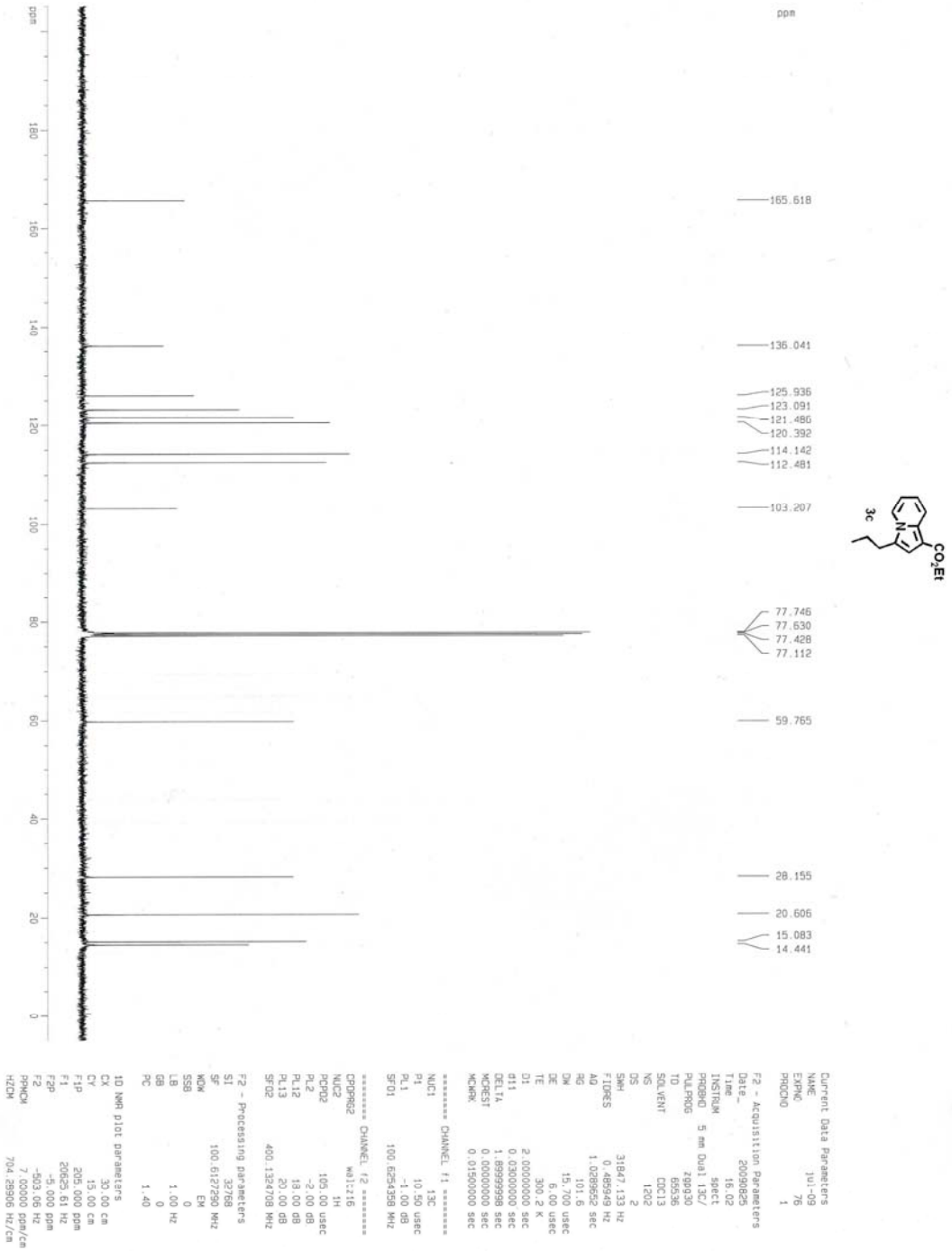

ppm
Integral
100.00
105.30
203.16
103.56
214.96
326.98
329.61
Hz
3281.57
3272.52
3119.52
3112.53
2905.63
2823.25
2822.50
2814.48
2807.59
2806.90
2714.65
2713.51
2707.82
2706.72
2699.93
1754.46
1747.30
1740.21
1733.14
900.99
652.47
567.99
560.79
553.67
0.00
3a
CO2Et
Current Data Parameters
NAME may-08
EXPNO 71
PROCNO 1
F2 - Acquisition Parameters
Date_ 20080823
Time 11.20
INSTRUM spect
PROBHD 5 mm Dual 13C/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9923444 sec
RG 256
DW 60.800 usec
DE 6.00 usec
TE 297.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
CHANNEL f1
NUC1 1H
P1 11.00 usec
PL1 -2.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 16384
SF 400.1300090 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 30.00 cm
CY 20.00 cm
F1P 8.500 ppm
F2P -0.100 ppm
F1 3401.10 Hz
F2 -40.01 Hz
PPMCM 0.28567 ppm/cm
HZCM 114.70393 Hz/cm

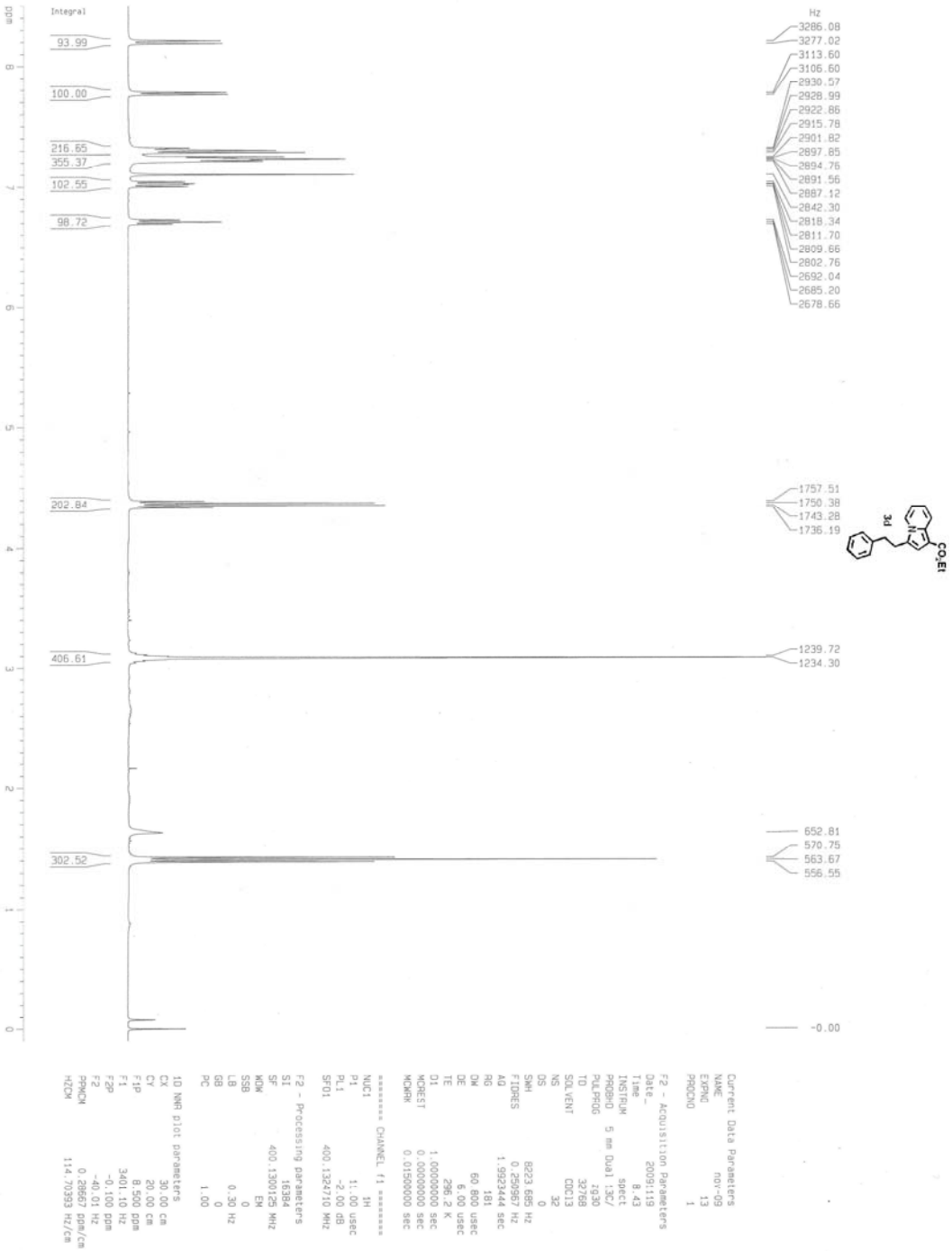

ppm
165.561
135.964
123.079
121.425
121.310
120.257
115.123
112.596
103.158
77.749
77.635
77.432
77.114
59.759
15.081
11.857
3a
CO2Et
Current Data Parameters
NAME
EXPNO 72
PROCNO 1
F2 - Acquisition Parameters
Date_ 20030623
Time 12.03
INSTRUM spect
PROBHD 5 mm Dual 13C/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 2
SWH 31847.133 Hz
FIDRES 0.485949 Hz
AQ 1.0239652 sec
RG 128
DW 15.700 usec
DE 6.00 usec
TE 298.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 -1.00 dB
SFO1 100.6254358 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 105.00 usec
PL2 -2.00 dB
PL12 18.00 dB
PL13 20.00 dB
SFO2 400.1324708 MHz
F2 - Processing parameters
SI 32768
SF 100.6127290 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 30.00 cm
CY 45.00 cm
F1P 205.000 ppm
F1 20625.61 Hz
F2P -5.000 ppm
F2 -503.06 Hz
PPMCM 7.00000 ppm/cm
HZCM 704.28906 Hz/cm

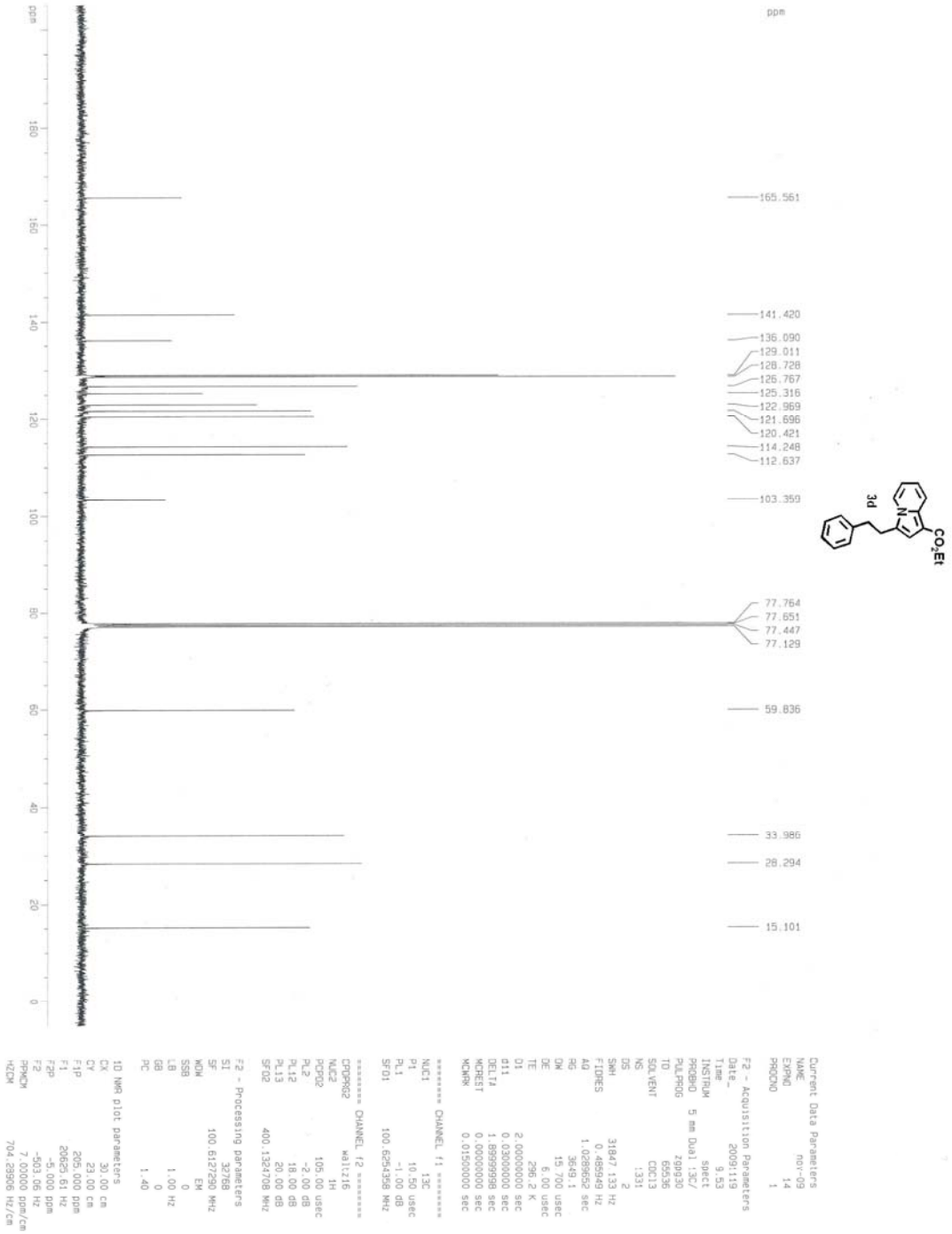

Integral
100.00
105.67
206.81
105.06
218.28
224.07
665.97
29.82
-0.00
Hz
3284.56
3283.63
3282.44
3275.54
3274.58
3273.37
3133.35
3126.35
2906.40
2822.18
2814.84
2814.10
2812.82
2812.00
2805.89
2805.09
2707.02
2705.95
2700.27
2699.07
2693.43
1757.30
1750.21
1743.01
1735.84
1124.64
1117.09
1110.10
1109.56
1102.60
690.32
570.74
563.44
556.14
3b
CO2Et
Current Data Parameters
NAME moy-09
EXPNO 29
PROCNO 1
F2 - Acquisition Parameters
Date_ 20091126
Time 15.22
INSTRUM spect
PROBHD 5 mm Dual 13C/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 8223.685 Hz
FIDRES 0.250867 Hz
AQ 1.9923444 sec
RG 203.2
DW 60.800 usec
DE 6.00 usec
TE 296.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 11.00 usec
PL1 -2.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 16384
SF 400.1300079 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 30.00 cm
CY 30.00 cm
F1P 8.500 ppm
F1 3401.10 Hz
F2P -0.100 ppm
F2 -40.01 Hz
PPMCM 0.28667 ppm/cm
HZCM 114.70393 Hz/cm

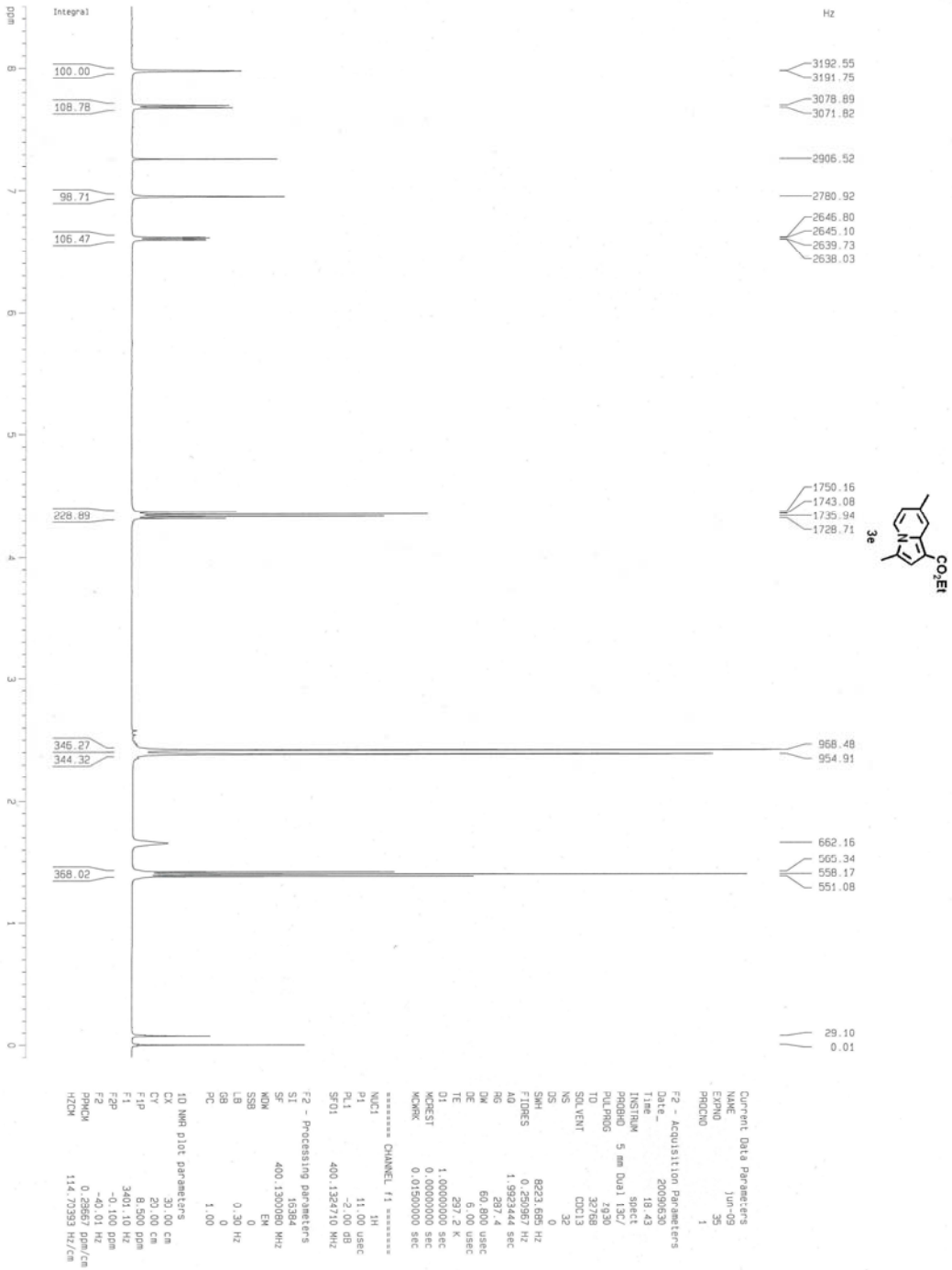

ppm
164.210
134.664
126.044
121.577
120.180
118.943
111.813
111.104
101.710
76.325
76.007
75.689
58.357
17.939
13.662
10.269
3b
CO2Et
N
Current Data Parameters
NAME nov-09
EXPNO 30
PROCNO 1
F2 - Acquisition Parameters
Date_ 20091126
Time_ 15.38
INSTRUM spect
PROBHD 5 mm Dual 13C/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 993
DS 2
SWH 31847.133 Hz
FIDRES 0.485949 Hz
AQ 1.0289602 sec
RG 3649.1
DW 15.700 usec
DE 6.00 usec
TE 296.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 -1.00 dB
SFO1 100.6254358 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 105.00 usec
PL2 -2.00 dB
PL12 18.00 dB
PL13 20.00 dB
SF02 400.1324708 MHz
F2 - Processing parameters
SI 32768
SF 100.6129737 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 30.00 cm
CY 24.00 cm
F1P 205.000 ppm
F1 20625.64 Hz
F2P -5.000 ppm
F2 -503.06 Hz
PPMCM 7.00000 ppm/cm
HZCM 704.29010 Hz/cm

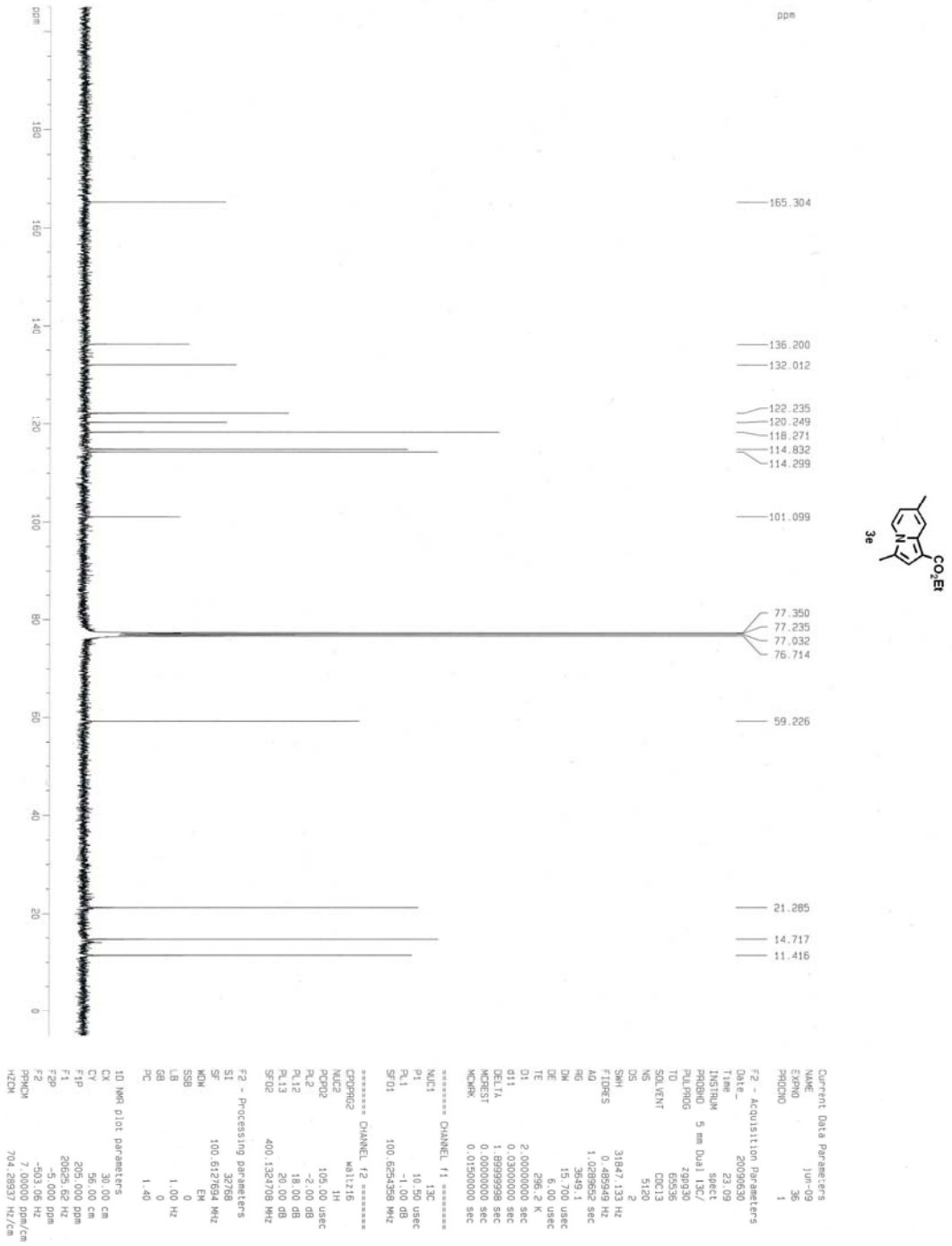

Integral
100.00
108.27
210.47
107.96
225.59
229.39
235.87
369.78
351.11
Hz
3283.03
3281.81
3280.78
3274.00
3272.75
3271.74
3138.14
3131.12
2906.05
2818.02
2815.62
2809.31
2808.47
2807.23
2806.24
2800.28
2799.44
2701.37
2700.05
2694.43
2693.35
1755.84
1748.76
1741.70
1734.61
1109.02
1101.52
1093.96
732.85
725.36
717.84
710.42
569.23
562.16
558.23
555.08
428.24
420.99
413.59
30.07
-0.00
3c
CO2Et
Current Data Parameters
NAME
EXPNO
PROCNO
F2 - Acquisition Parameters
Date_
Time
INSTRUM
PROBHD 5 mm Dual 13C/
PULPROG
TD
SOLVENT
NS
DS
SWH
FIDRES
AQ
RG
DW
DE
TE
D1
MCREST
MCWRK
======== CHANNEL f1 ========
NUC1
P1
PL1
SF01
F2 - Processing parameters
SI
SF
WDW
SSB
LB
GB
PC
1D NMR plot parameters
CX
CY
F1P
F1
F2P
F2
PPMCM
HZCM

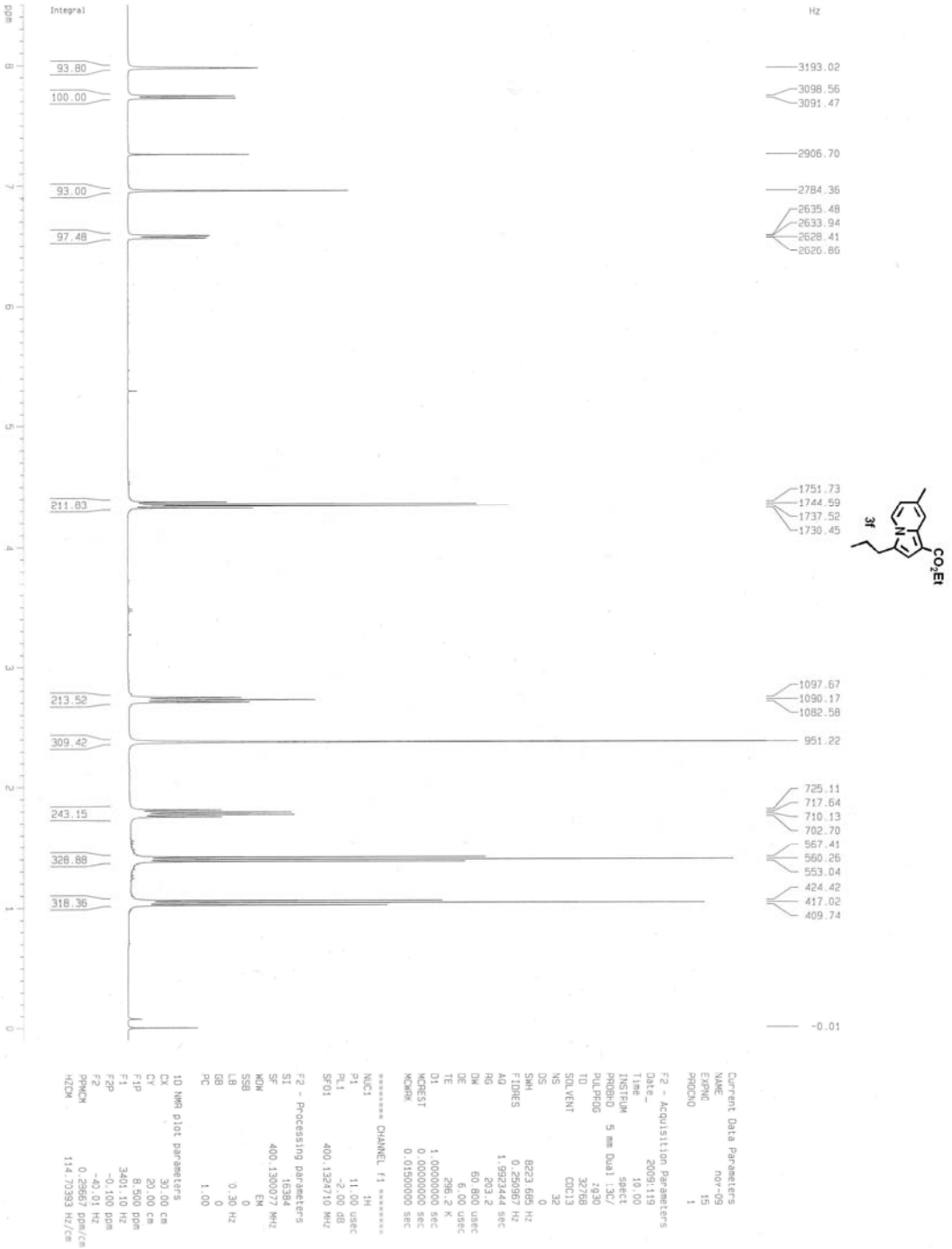

ppm
165.618
136.041
125.936
123.091
121.486
120.392
114.142
112.481
103.207
77.746
77.630
77.428
77.112
59.765
28.155
20.606
15.083
14.441
3c
CO2Et
Current Data Parameters
NAME
EXPNO
PROCNO
F2 - Acquisition Parameters
Date_
Time
INSTRUM
PROBHD 5 mm Dual 13C/
PULPROG
TD
SOLVENT
NS
DS
SWH
FIDRES
AQ
RG
DW
DE
TE
D1
d11
DELTA
MCREST
MCWRK
======== CHANNEL f1 ========
NUC1
P1
PL1
SFO1
======== CHANNEL f2 ========
CPDPRG2
NUC2
PCPD2
PL2
PL12
PL13
SFO2
F2 - Processing parameters
SI
SF
WDW
SSB
LB
GB
PC
1D NMR plot parameters
CX
CY
F1P
F1
F2P
F2
PPMCM
HZCM

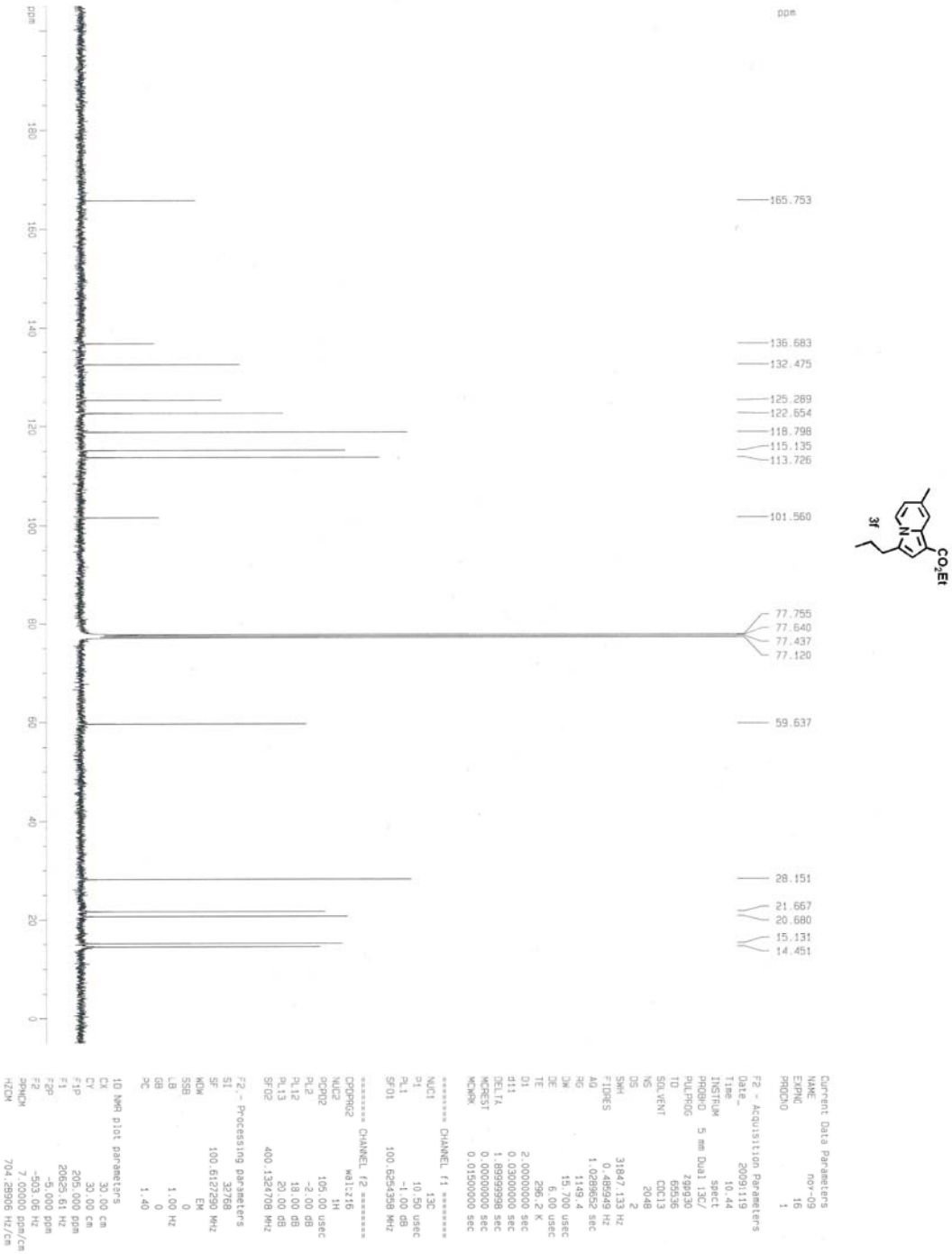

Integral
93.99
100.00
216.65
355.37
102.55
98.72
202.84
406.61
302.52
Hz
3286.08
3277.02
3113.60
3106.60
2930.57
2928.99
2922.86
2915.78
2901.82
2897.85
2894.76
2891.56
2887.12
2842.30
2818.34
2811.70
2809.66
2802.76
2692.04
2685.20
2678.66
1757.51
1750.38
1743.28
1736.19
1239.72
1234.30
652.81
570.75
563.67
556.55
-0.00
3d
CO2Et
Current Data Parameters
NAME
EXPNO 13
PROCNO 1
F2 - Acquisition Parameters
Date_ 20091119
Time 8.43
INSTRUM spect
PROBHD 5 mm Dual 13C/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 8223.685 Hz
FIDRES 0.250957 Hz
AQ 1.9923444 sec
RG 181
DW 60.800 usec
DE 6.00 usec
TE 296.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 11.00 usec
PL1 -2.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 16384
SF 400.1300125 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 30.00 cm
CY 20.00 cm
F1P 8.500 ppm
F1 3401.10 Hz
F2P -0.100 ppm
F2 -40.01 Hz
PPMCM 0.28667 ppm/cm
HZCM 114.70393 Hz/cm

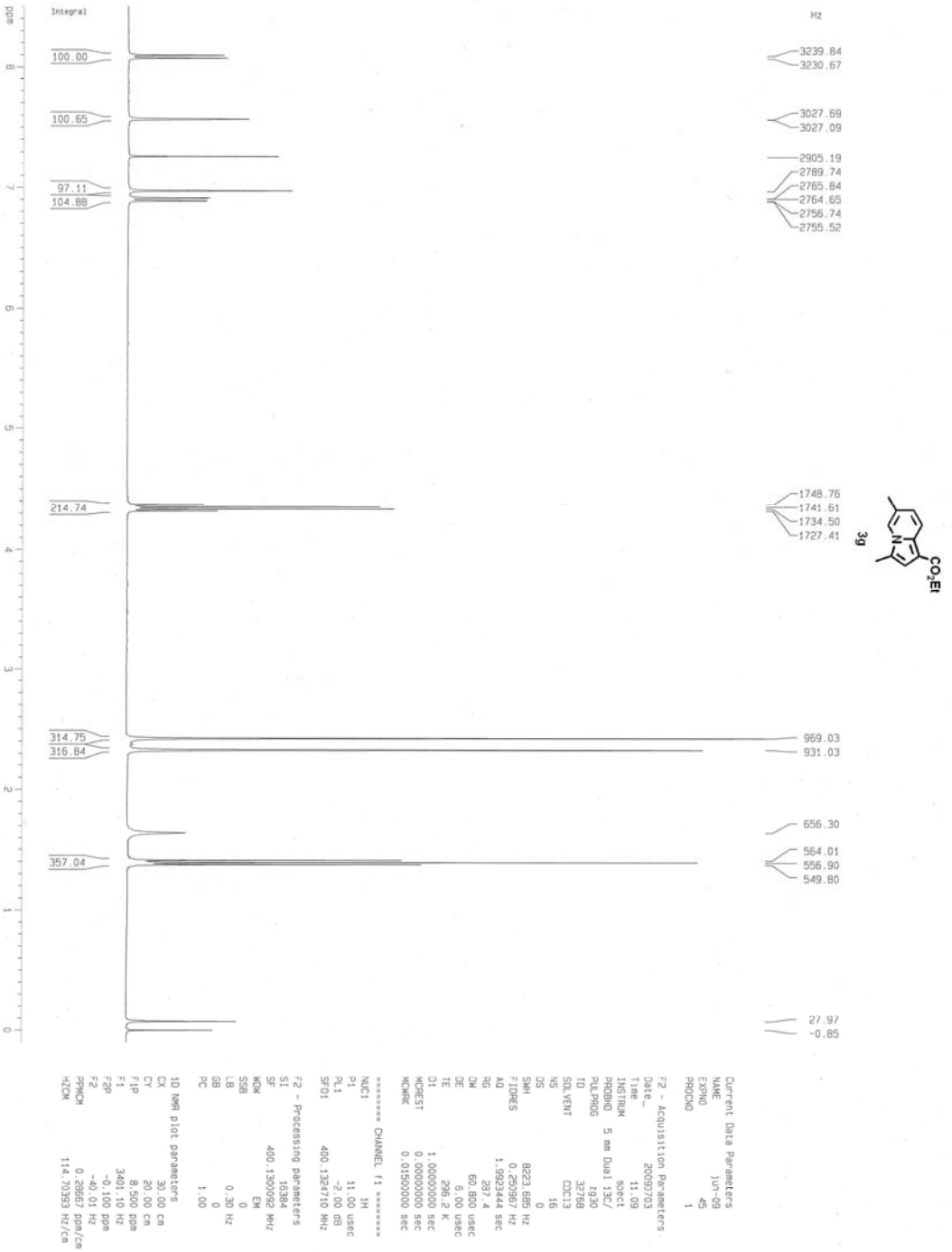

ppm
165.561
141.420
136.090
129.011
128.728
126.767
125.316
122.969
121.696
120.421
114.248
112.637
103.359
77.764
77.651
77.447
77.129
59.836
33.986
28.294
15.101
3d
N
CO2Et
Current Data Parameters
NAME nov-09
EXPNO 14
PROCNO 1
F2 - Acquisition Parameters
Date_ 20091119
Time_ 9.53
INSTRUM spect
PROBHD 5 mm Dual 13C/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1331
DS 2
SWH 31847.133 Hz
FIDRES 0.485949 Hz
AQ 1.0286652 sec
RG 3649.1
DW 15.700 usec
DE 6.00 usec
TE 296.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 -1.00 dB
SFO1 100.6254358 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 105.00 usec
PL2 -2.00 dB
PL12 18.00 dB
PL13 20.00 dB
SFO2 400.1324708 MHz
F2 - Processing parameters
SI 32768
SF 100.6127290 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 30.00 cm
CY 23.00 cm
F1P 205.000 ppm
F1 20625.61 Hz
F2P -5.000 ppm
F2 -503.06 Hz
PPMCM 7.03000 ppm/cm
HZCM 704.29906 Hz/cm

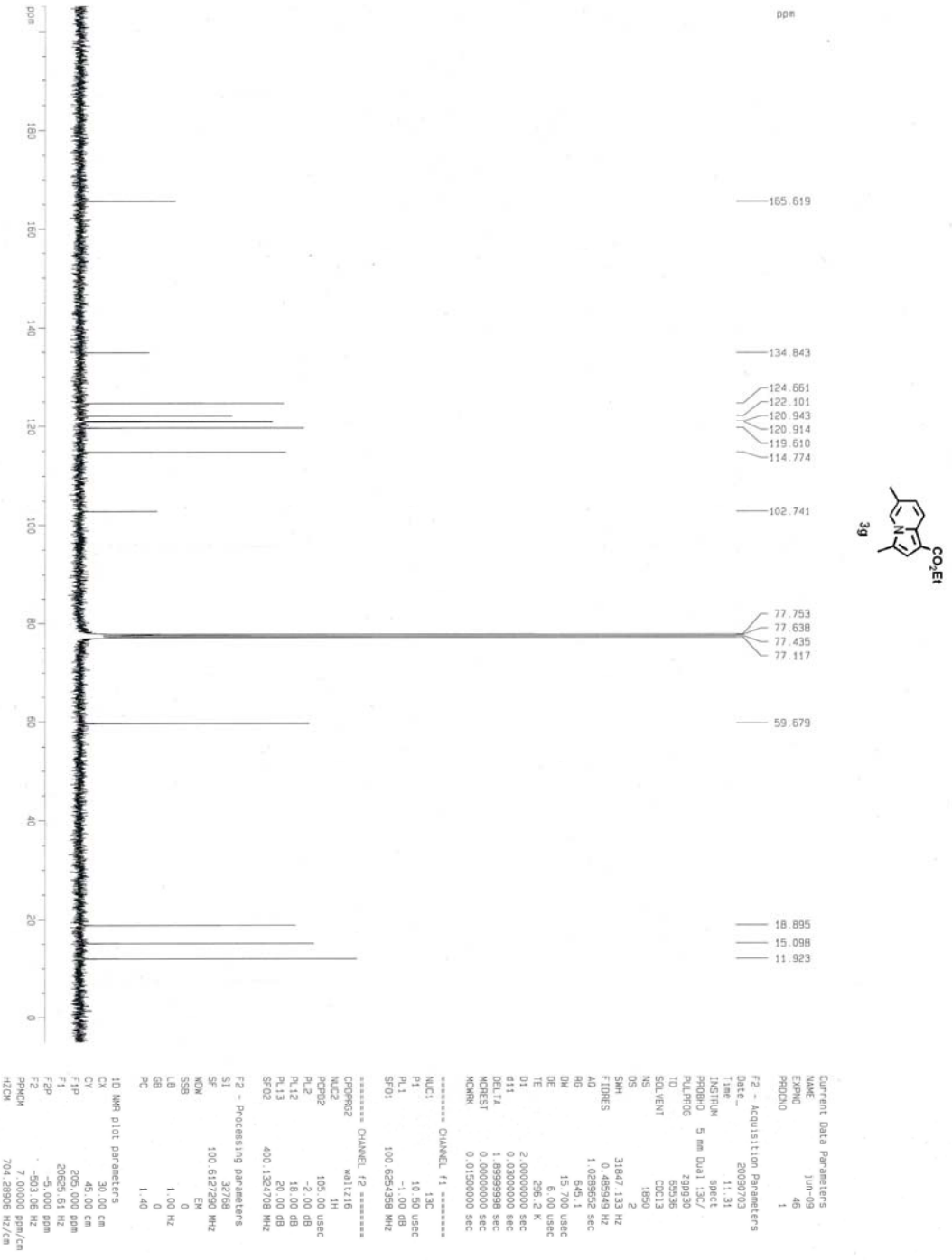

Integral
100.00
108.78
98.71
106.47
228.89
345.27
344.32
368.02
Hz
3192.55
3191.75
3078.89
3071.82
2906.52
2780.92
2646.80
2645.10
2639.73
2638.03
1750.16
1743.08
1735.94
1728.71
968.48
954.91
662.16
565.34
558.17
551.08
29.10
0.01
3e
CO2Et
Current Data Parameters
NAME jun-09
EXPNO 35
PROCNO 1
F2 - Acquisition Parameters
Date_ 20090630
Time 18.43
INSTRUM spect
PROBHD 5 mm Dual 13C/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 8223.685 Hz
FIDRES 0.250987 Hz
AQ 1.9923444 sec
RG 287.4
DW 60.800 usec
DE 6.00 usec
TE 297.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 11.00 usec
PL1 -2.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 16384
SF 400.1300080 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 30.00 cm
CY 20.00 cm
F1P 8.500 ppm
F1 3401.10 Hz
F2P -0.100 ppm
F2 -40.01 Hz
PPMCM 0.29667 ppm/cm
HZCM 114.70393 Hz/cm

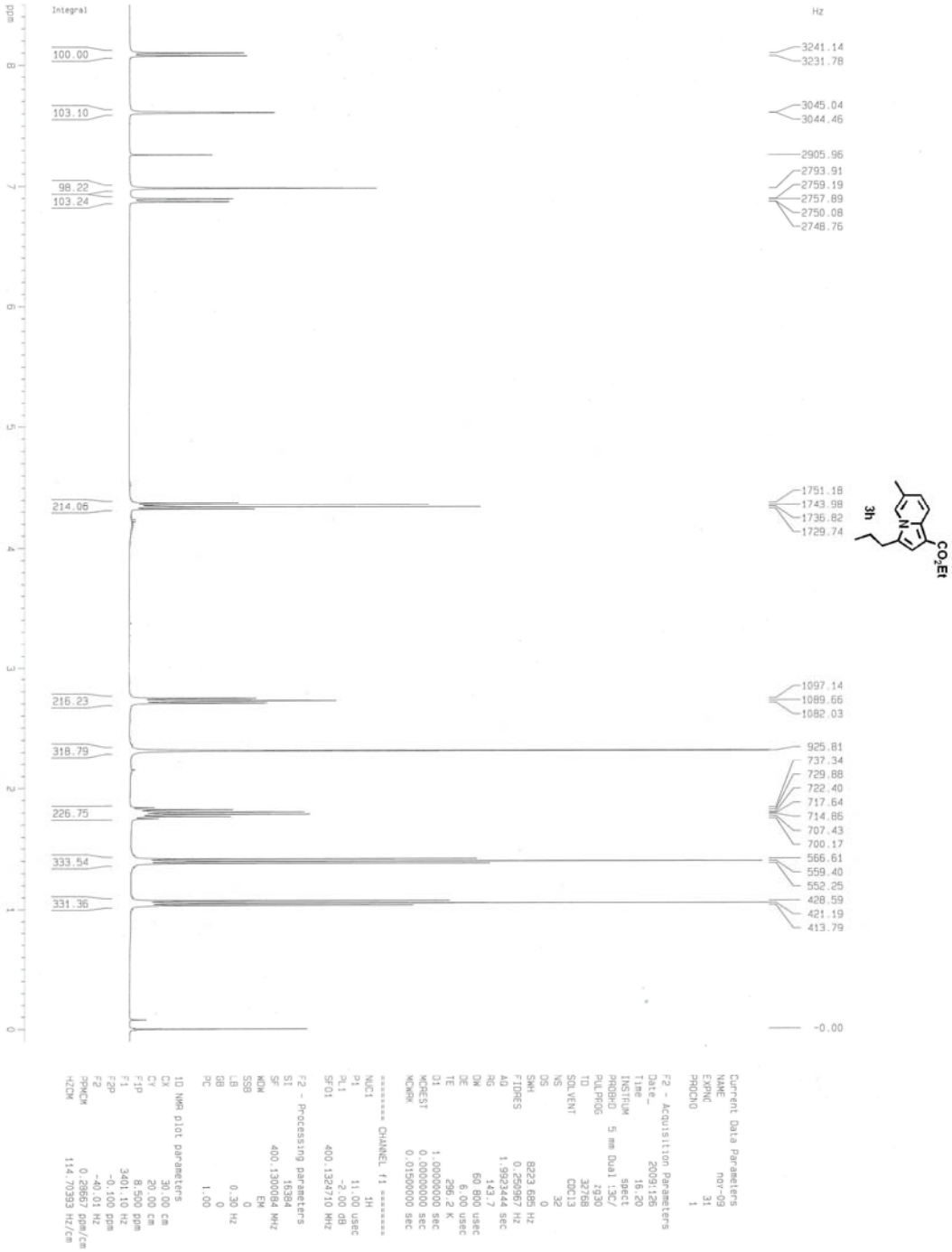

ppm
165.304
136.200
132.012
122.235
120.249
118.271
114.832
114.299
101.099
77.350
77.235
77.032
76.714
59.226
21.285
14.717
11.416
3e
CO2Et
Current Data Parameters
NAME jun-09
EXPNO 36
PROCNO 1
F2 - Acquisition Parameters
Date_ 20090630
Time 23.09
INSTRUM spect
PROBHD 5 mm Dual 13C/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 5120
DS 2
SWH 31847.133 Hz
FIDRES 0.485949 Hz
AQ 1.0289682 sec
RG 3649.1
DW 15.700 usec
DE 6.00 usec
TE 296.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 -1.00 dB
SFO1 100.6254358 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 105.00 usec
PL2 -2.00 dB
PL12 18.00 dB
PL13 20.00 dB
SFO2 400.1324708 MHz
F2 - Processing parameters
SI 32768
SF 100.6127684 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 30.00 cm
CY 56.00 cm
F1P 205.000 ppm
F1 20625.62 Hz
F2P -5.000 ppm
F2 -503.06 Hz
PPMCM 7.00000 ppm/cm
HZCM 704.28937 Hz/cm

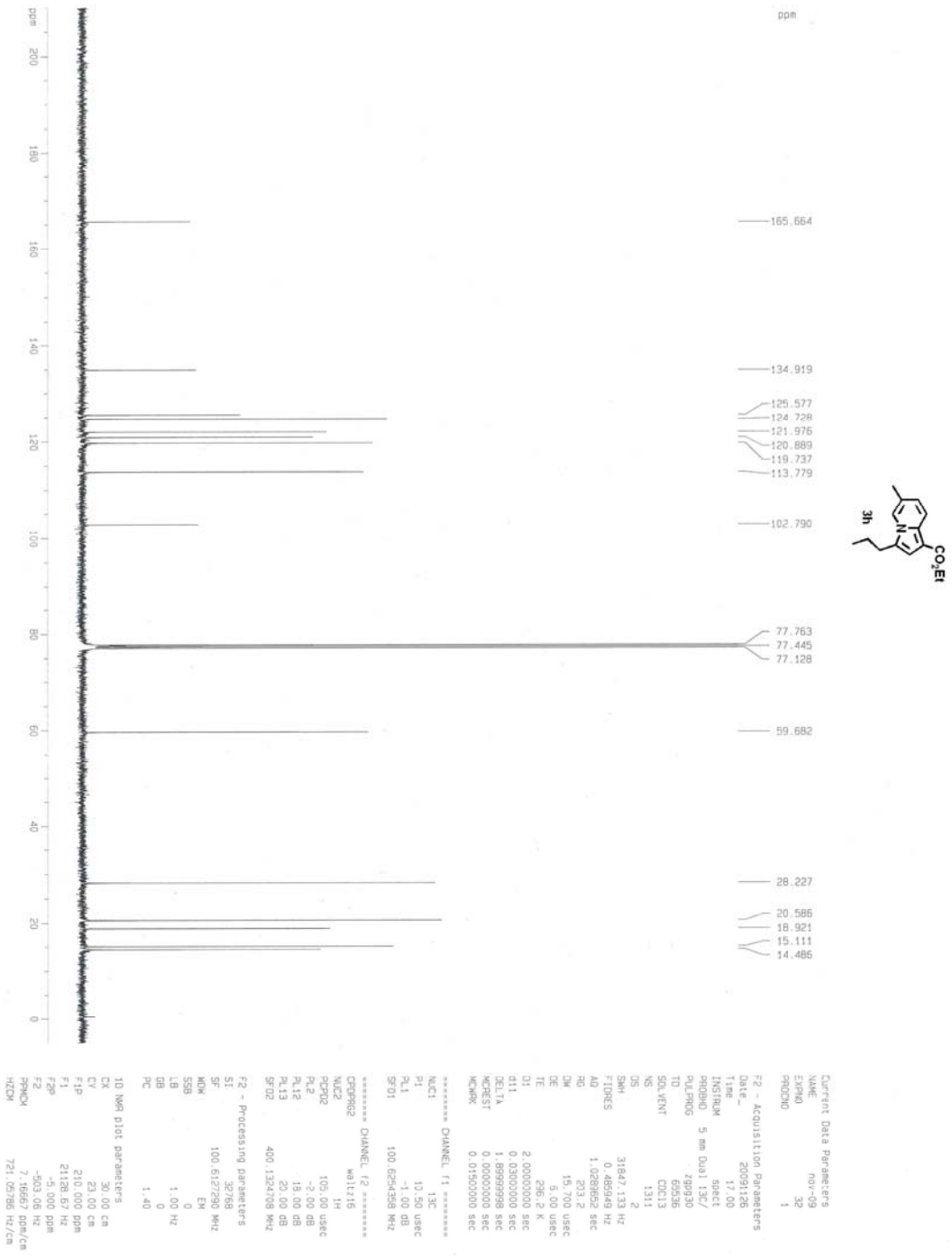

Integral
93.80
100.00
93.00
97.48
211.83
213.52
309.42
243.15
328.88
318.36
Hz
3193.02
3098.56
3091.47
2906.70
2784.36
2635.48
2633.94
2628.41
2626.86
1751.73
1744.59
1737.52
1730.45
1097.67
1090.17
1082.58
951.22
725.11
717.64
710.13
702.70
567.41
560.26
553.04
424.42
417.02
409.74
-0.01
3f
CO2Et
Current Data Parameters
NAME nov-09
EXPNO 15
PROCNO 1
F2 - Acquisition Parameters
Date_ 20091119
Time 10.00
INSTRUM spect
PROBHD 5 mm Dual 13C/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9923444 sec
RG 203.2
DW 60.800 usec
DE 6.00 usec
TE 296.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 11.00 usec
PL1 -2.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 16384
SF 400.1300077 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 30.00 cm
CY 20.00 cm
F1P 8.500 ppm
F1 3401.10 Hz
F2P -0.100 ppm
F2 -40.01 Hz
PPMCM 0.29667 ppm/cm
HZCM 114.70393 Hz/cm

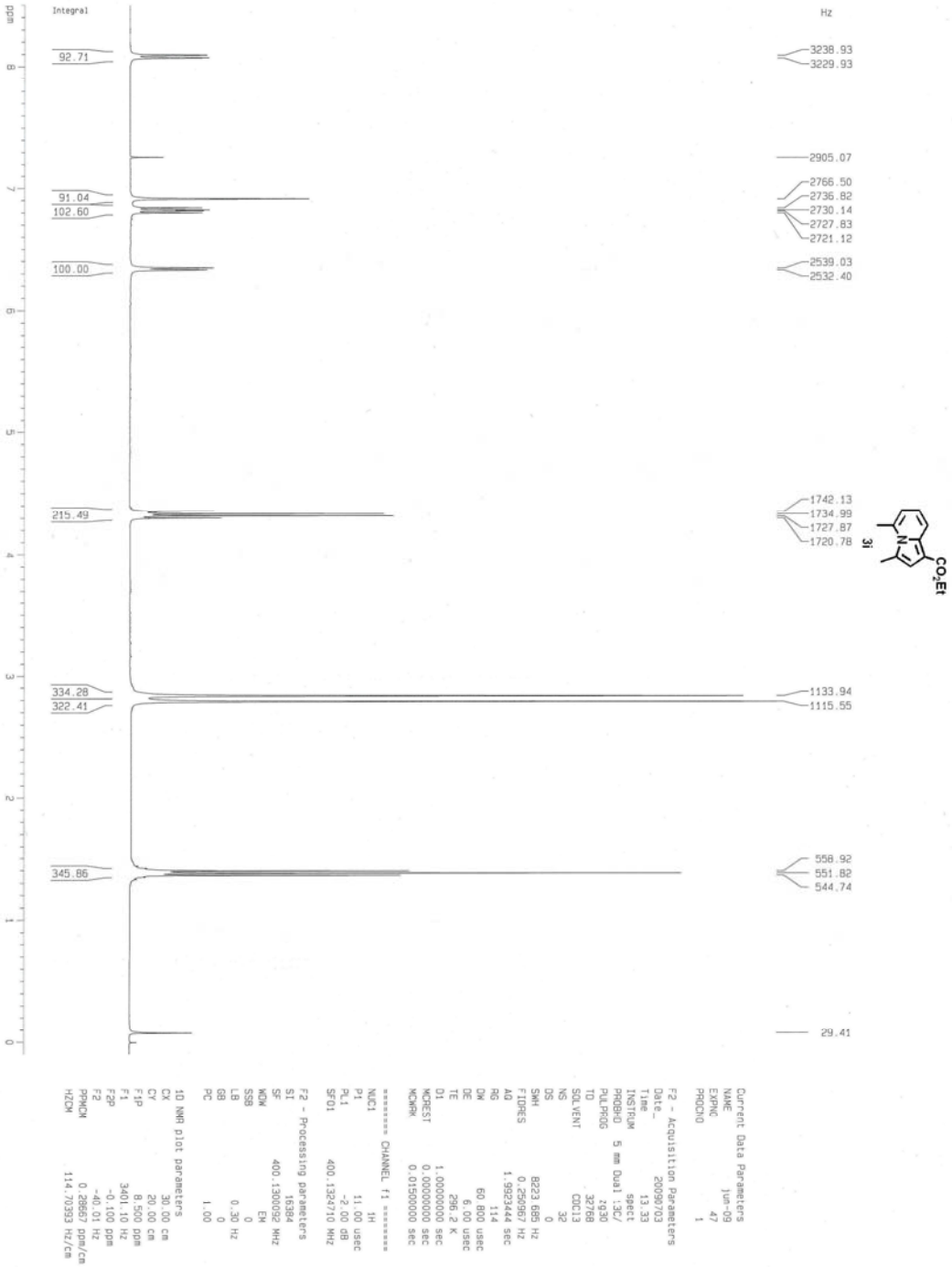

ppm
165.753
136.683
132.475
125.289
122.654
118.798
115.135
113.726
101.560
77.755
77.640
77.437
77.120
59.637
28.151
21.667
20.680
15.131
14.451
3f
CO2Et
Current Data Parameters
NAME nov-09
EXPNO 16
PROCNO 1
F2 - Acquisition Parameters
Date_ 20091119
Time_ 10.44
INSTRUM spect
PROBHD 5 mm Dual 13C/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 2
SWH 31847.133 Hz
FIDRES 0.485949 Hz
AQ 1.0286652 sec
RG 1149.4
DW 15.700 usec
DE 6.00 usec
TE 296.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 -1.00 dB
SFO1 100.6254358 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 105.00 usec
PL2 -2.00 dB
PL12 18.00 dB
PL13 20.00 dB
SFO2 400.1324708 MHz
F2 - Processing parameters
SI 32768
SF 100.6127290 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 30.00 cm
CY 30.00 cm
F1P 205.000 ppm
F1 20625.61 Hz
F2P -5.000 ppm
F2 -503.06 Hz
PPMCM 7.00000 ppm/cm
HZCM 704.28906 Hz/cm

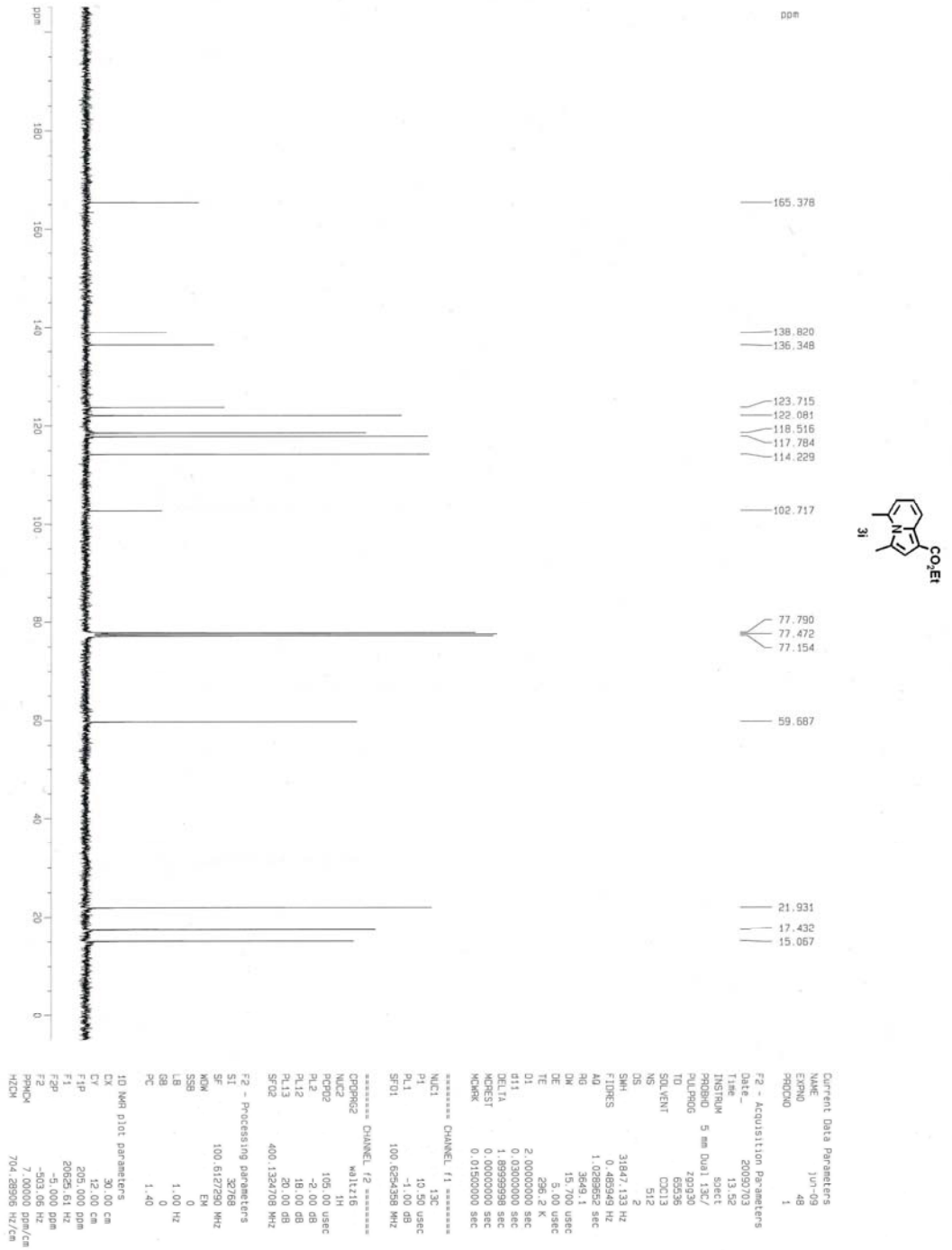

ppm
Integral
100.00
100.65
97.11
104.88
214.74
314.75
316.84
357.04
Hz
3239.84
3230.67
3027.69
3027.09
2905.19
2789.74
2765.84
2764.65
2756.74
2755.52
1748.76
1741.61
1734.50
1727.41
969.03
931.03
656.30
564.01
556.90
549.80
27.97
-0.85
3g
CO2Et
Current Data Parameters
NAME jun-09
EXPNO 45
PROCNO 1
F2 - Acquisition Parameters
Date_ 20090703
Time 11.09
INSTRUM spect
PROBHD 5 mm Dual 13C/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9923444 sec
RG 287.4
DW 60.800 usec
DE 6.00 usec
TE 296.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 11.00 usec
PL1 -2.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 16384
SF 400.1300092 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 30.00 cm
CY 20.00 cm
F1P 8.500 ppm
F1 3401.10 Hz
F2P -0.100 ppm
F2 -40.01 Hz
PPMCM 0.29667 ppm/cm
HZCM 114.70393 Hz/cm

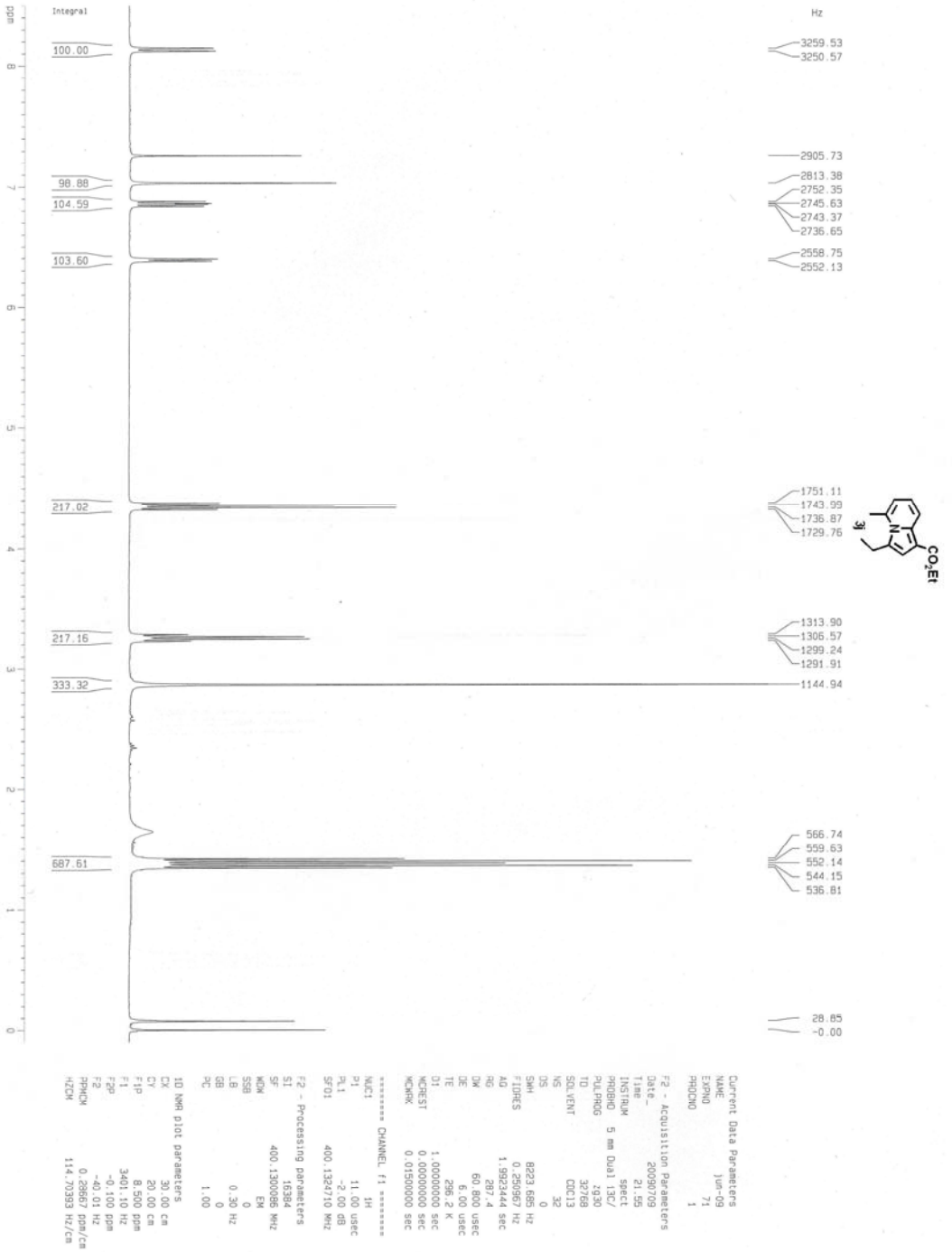

ppm
165.619
134.843
124.661
122.101
120.943
120.914
119.610
114.774
102.741
77.753
77.638
77.435
77.117
59.679
18.895
15.098
11.923
3g
CO2Et
N
Current Data Parameters
NAME jun-09
EXPNO 46
PROCNO 1
F2 - Acquisition Parameters
Date_ 20090703
Time 11.31
INSTRUM spect
PROBHD 5 mm Dual 13C/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1850
DS 2
SWH 31847.133 Hz
FIDRES 0.485949 Hz
AQ 1.0289632 sec
RG 645.1
DW 15.700 usec
DE 6.00 usec
TE 296.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 -1.00 dB
SFO1 100.6254358 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 105.00 usec
PL2 -2.00 dB
PL12 18.00 dB
PL13 20.00 dB
SFO2 400.1324708 MHz
F2 - Processing parameters
SI 32768
SF 100.6127290 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 30.00 cm
CY 45.00 cm
F1P 205.000 ppm
F1 20625.61 Hz
F2P -5.000 ppm
F2 -503.06 Hz
PPMCM 7.00000 ppm/cm
HZCM 704.28906 Hz/cm

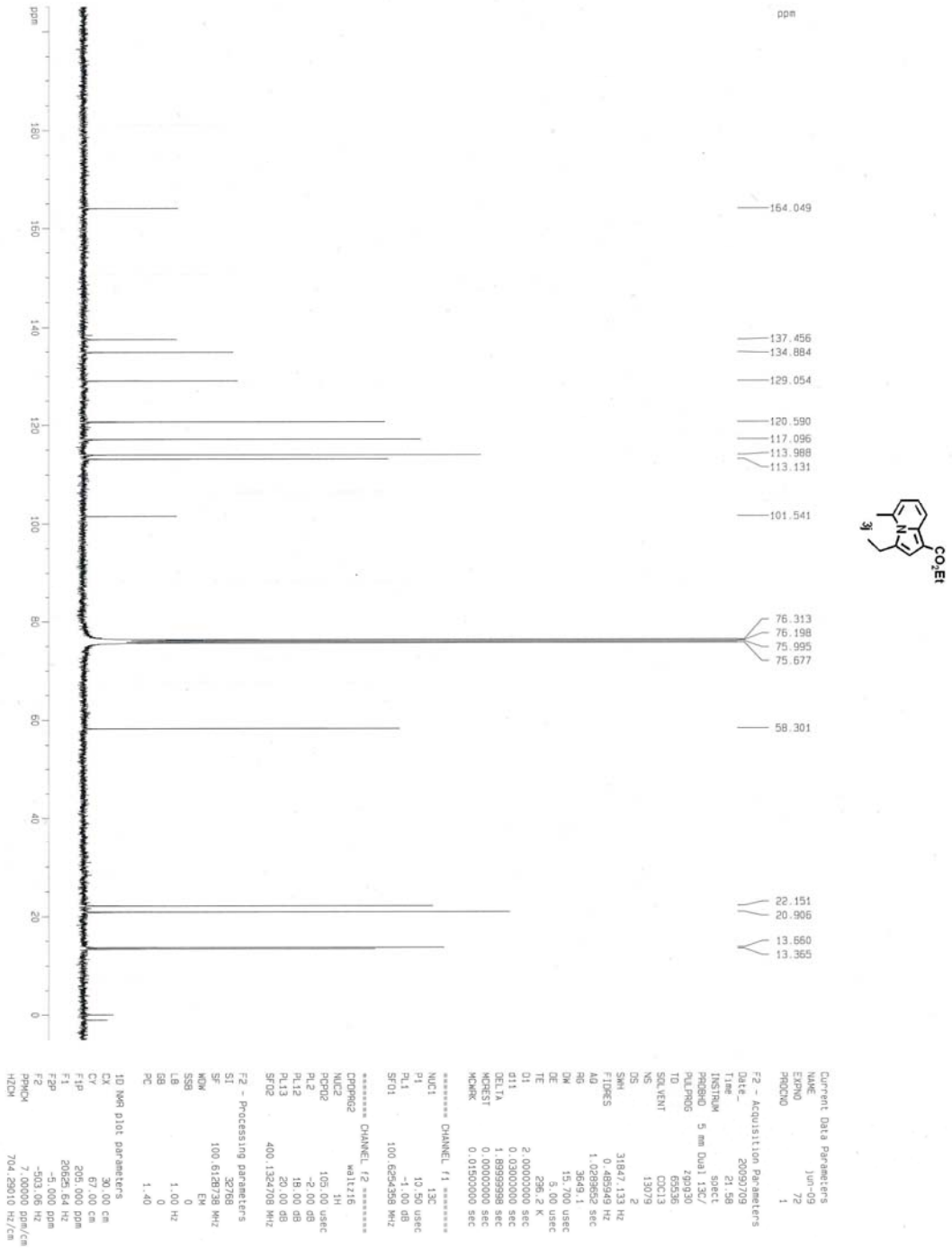

ppm
Integral
100.00
103.10
98.22
103.24
214.06
216.23
318.79
226.75
333.54
331.36
Hz
3241.14
3231.78
3045.04
3044.46
2905.96
2793.91
2759.19
2757.89
2750.08
2748.76
1751.18
1743.98
1736.82
1729.74
1097.14
1089.66
1082.03
925.81
737.34
729.88
722.40
717.64
714.86
707.43
700.17
566.61
559.40
552.25
428.59
421.19
413.79
-0.00
3h
CO2Et
Current Data Parameters
NAME nov-09
EXPNO 31
PROCNO 1
F2 - Acquisition Parameters
Date_ 2009126
Time 16.20
INSTRUM spect
PROBHD 5 mm Dual 13C/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 8223.685 Hz
FIDRES 0.250987 Hz
AQ 1.9923444 sec
RG 143.7
DW 60.800 usec
DE 6.00 usec
TE 296.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 11.00 usec
PL1 -2.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 16384
SF 400.1300084 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 30.00 cm
CY 20.00 cm
F1P 8.500 ppm
F1 3401.10 Hz
F2P -0.100 ppm
F2 -40.01 Hz
PPMCM 0.29667 ppm/cm
HZCM 114.70393 Hz/cm

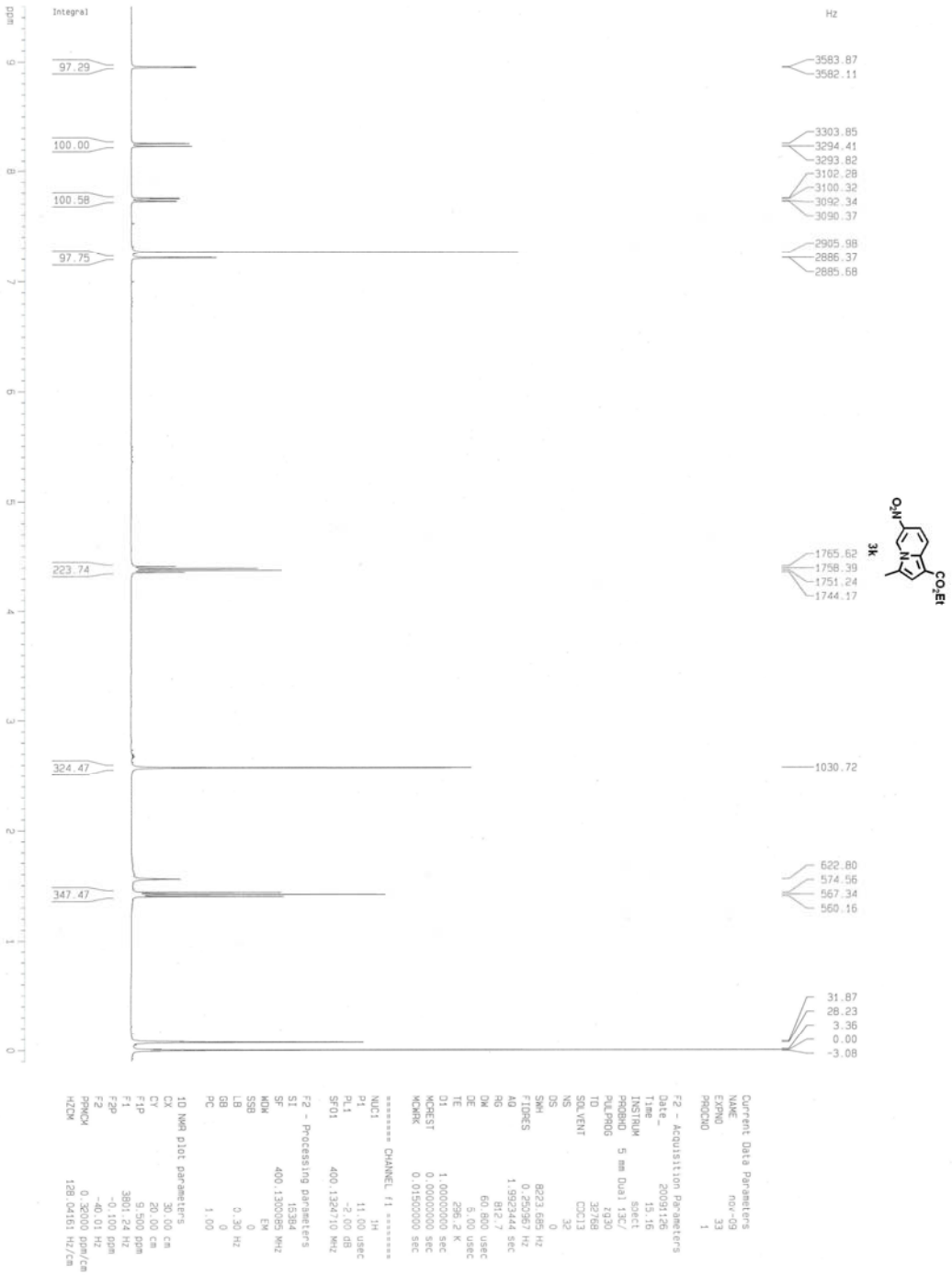

ppm
165.664
134.919
125.577
124.728
121.976
120.889
119.737
113.779
102.790
77.763
77.445
77.128
59.682
28.227
20.586
18.921
15.111
14.486
3h
CO2Et

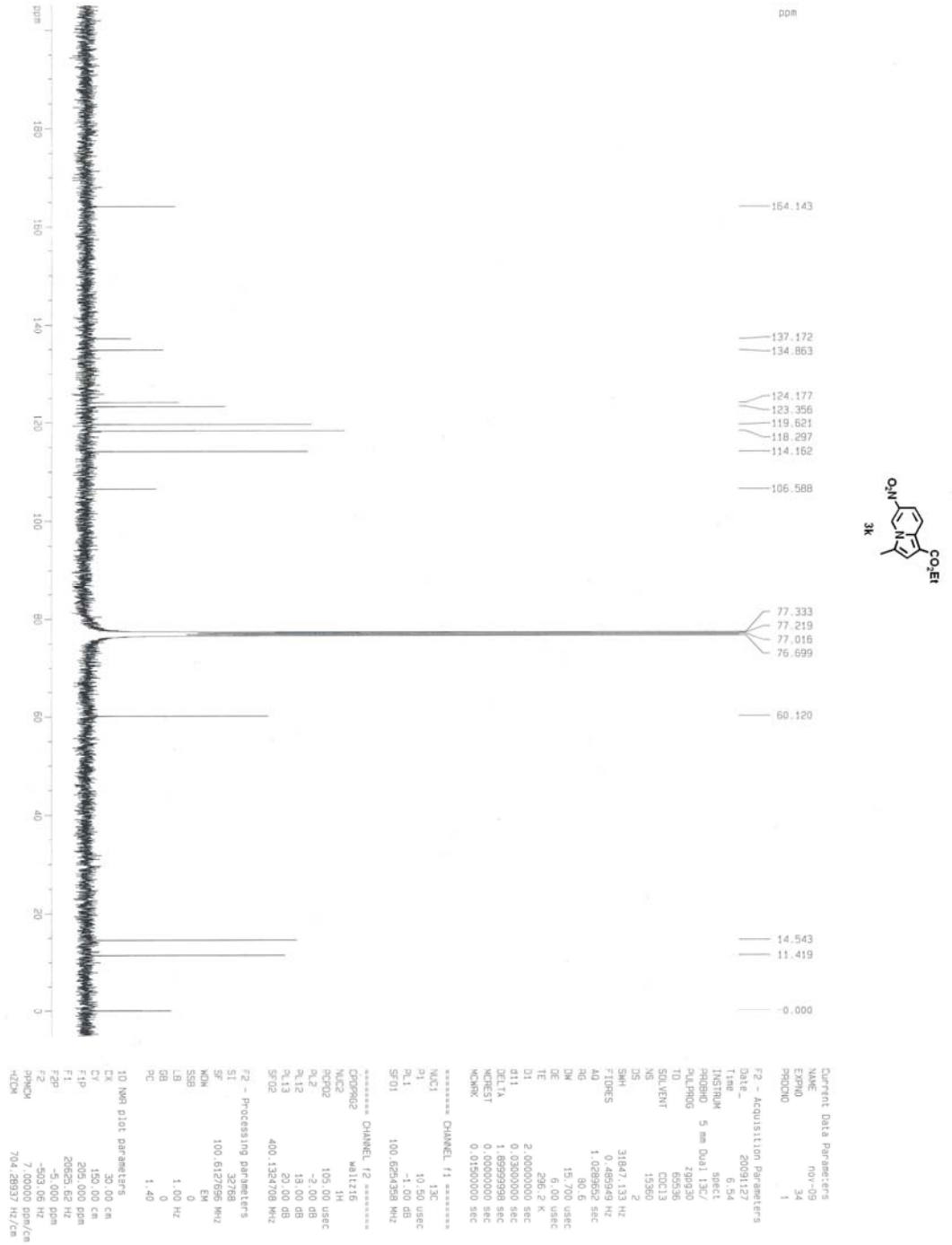

Integral
92.71
91.04
102.60
100.00
215.49
334.28
322.41
345.86
Hz
3238.93
3229.93
2905.07
2766.50
2736.82
2730.14
2727.83
2721.12
2539.03
2532.40
1742.13
1734.99
1727.87
1720.78
1133.94
1115.55
558.92
551.82
544.74
29.41
31
CO2Et
Current Data Parameters
NAME
EXPNO
PROCNO
F2 - Acquisition Parameters
Date_
Time
INSTRUM
PROBHD 5 mm Dual 13C/
PULPROG
TD
SOLVENT
NS
DS
SWH
FIDRES
AQ
RG
DW
DE
TE
D1
MCREST
MCWRK
======== CHANNEL f1 ========
NUC1
P1
PL1
SFO1
F2 - Processing parameters
SI
SF
WDW
SSB
LB
GB
PC
1D NMR plot parameters
CX
CY
F1P
F1
F2P
F2
PPMCM
HZCM

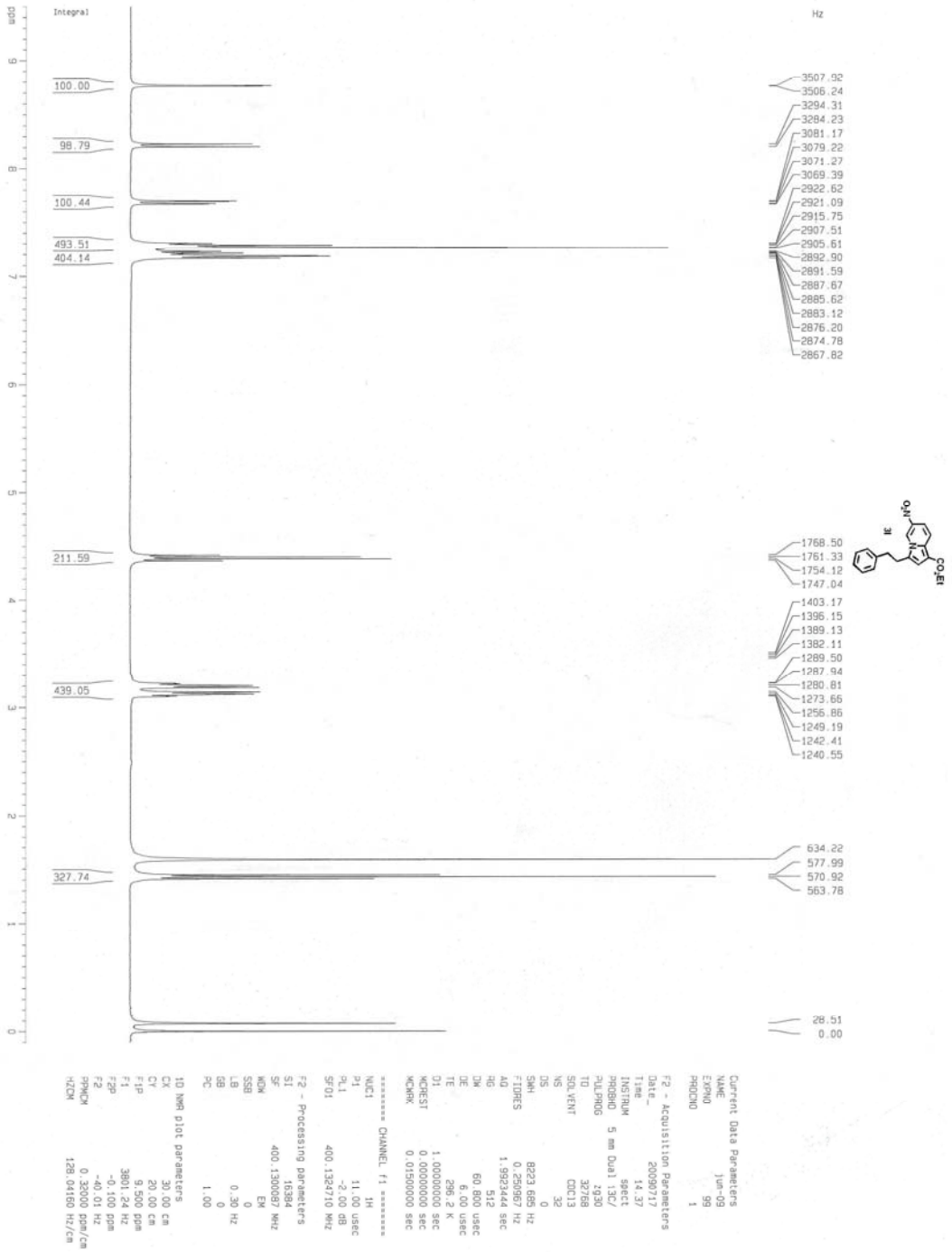

ppm
165.378
138.820
136.348
123.715
122.081
118.516
117.784
114.229
102.717
77.790
77.472
77.154
59.587
21.931
17.432
15.067
3i
CO2Et
Current Data Parameters
NAME jun-09
EXPNO 48
PROCNO 1
F2 - Acquisition Parameters
Date_ 20090703
Time 13.52
INSTRUM spect
PROBHD 5 mm Dual 13C/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 512
DS 2
SWH 31847.133 Hz
FIDRES 0.485949 Hz
AQ 1.0289652 sec
RG 3649.1
DW 15.700 usec
DE 5.00 usec
TE 296.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 -1.00 dB
SFO1 100.6254358 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 105.00 usec
PL2 -2.00 dB
PL12 18.00 dB
PL13 20.00 dB
SFO2 400.1324708 MHz
F2 - Processing parameters
SI 32768
SF 100.6127290 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 30.00 cm
CY 12.00 cm
F1P 205.000 ppm
F1 20625.61 Hz
F2P -5.000 ppm
F2 -503.06 Hz
PPMCM 7.00000 ppm/cm
HZCM 704.28906 Hz/cm

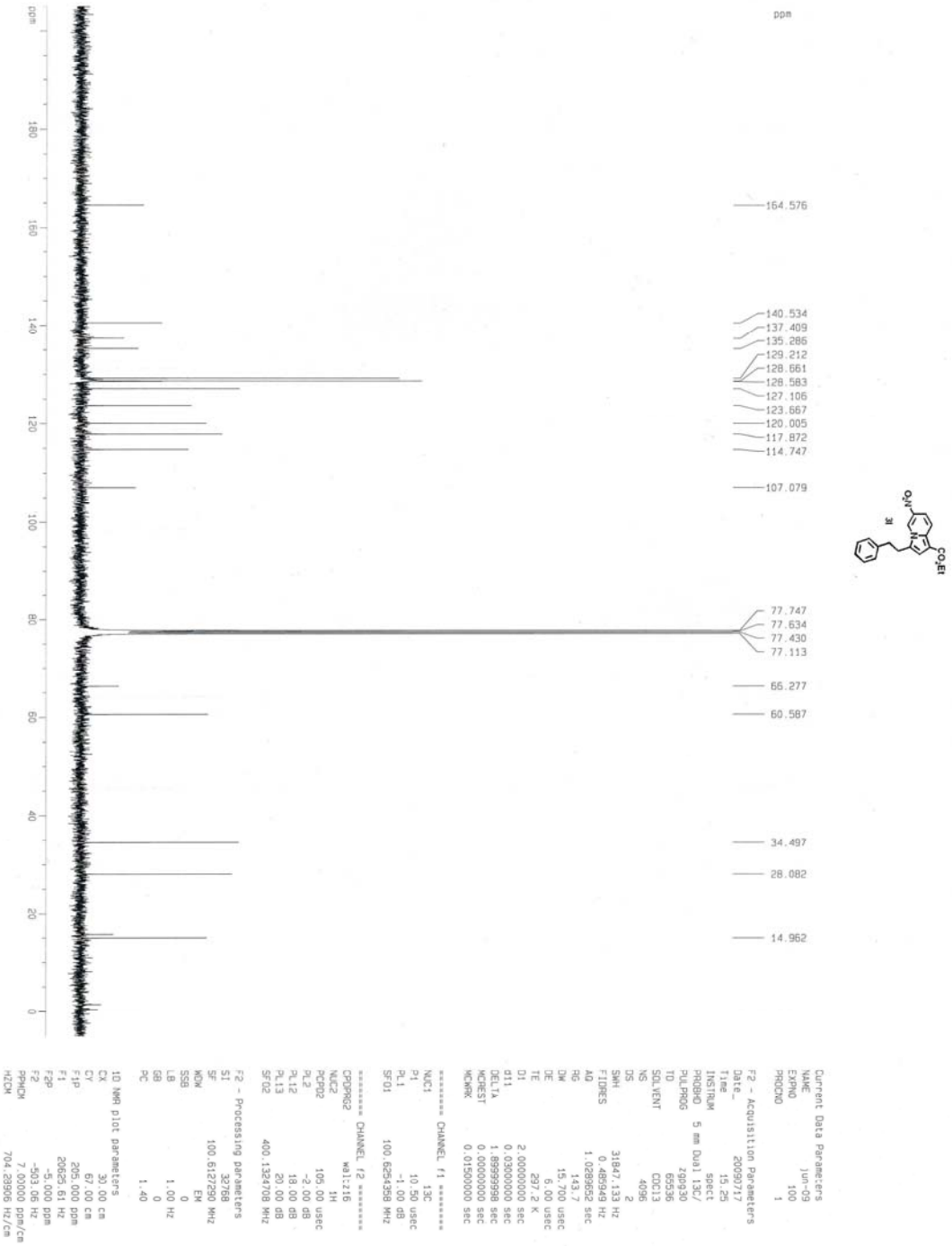

Integral
100.00
98.88
104.59
103.60
217.02
217.16
333.32
687.61
28.85
-0.00
Hz
3259.53
3250.57
2905.73
2813.38
2752.35
2745.63
2743.37
2736.65
2558.75
2552.13
1751.11
1743.99
1736.87
1729.76
1313.90
1306.57
1299.24
1291.91
1144.94
566.74
559.63
552.14
544.15
536.81
ppm
8
7
6
5
4
3
2
1
0
CO2Et
Current Data Parameters
NAME jun-09
EXPNO 71
PROCNO 1
F2 - Acquisition Parameters
Date_ 20090709
Time 21.55
INSTRUM spect
PROBHD 5 mm Dual 13C/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9923444 sec
RG 287.4
DW 60.800 usec
DE 6.00 usec
TE 296.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 11.00 usec
PL1 -2.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 16384
SF 400.1300086 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 30.00 cm
CY 20.00 cm
F1P 8.500 ppm
F1 3401.10 Hz
F2P -0.100 ppm
F2 -40.01 Hz
PPMCM 0.29667 ppm/cm
HZCM 114.70393 Hz/cm

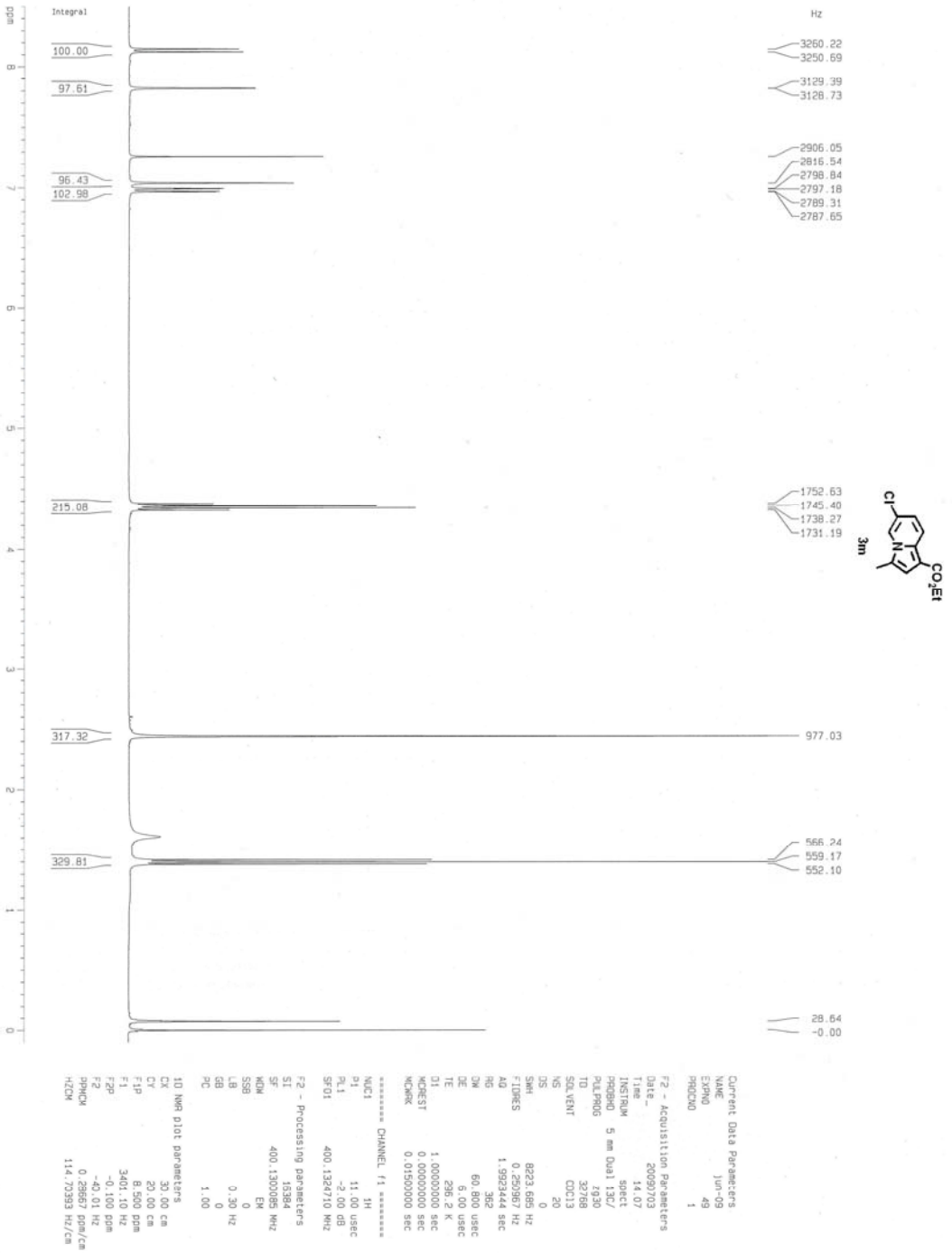

ppm
164.049
137.456
134.884
129.054
120.590
117.096
113.988
113.131
101.541
76.313
76.198
75.995
75.677
58.301
22.151
20.906
13.660
13.365
3j
CO2Et
Current Data Parameters
NAME jun-09
EXPNO 72
PROCNO 1
F2 - Acquisition Parameters
Date_ 20090709
Time 21.58
INSTRUM spect
PROBHD 5 mm Dual 13C/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 13079
DS 2
SWH 31847.133 Hz
FIDRES 0.485949 Hz
AQ 1.0289652 sec
RG 3649.1
DW 15.700 usec
DE 5.00 usec
TE 296.2 K
D1 2.00000000 sec
D11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 -1.00 dB
SFO1 100.6254358 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 105.00 usec
PL2 -2.00 dB
PL12 18.00 dB
PL13 20.00 dB
SFO2 400.1324708 MHz
F2 - Processing parameters
SI 32768
SF 100.6128736 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 30.00 cm
CY 67.00 cm
F1P 205.000 ppm
F1 20525.64 Hz
F2P -5.000 ppm
F2 -503.06 Hz
PPMCM 7.00000 ppm/cm
HZCM 704.29010 Hz/cm

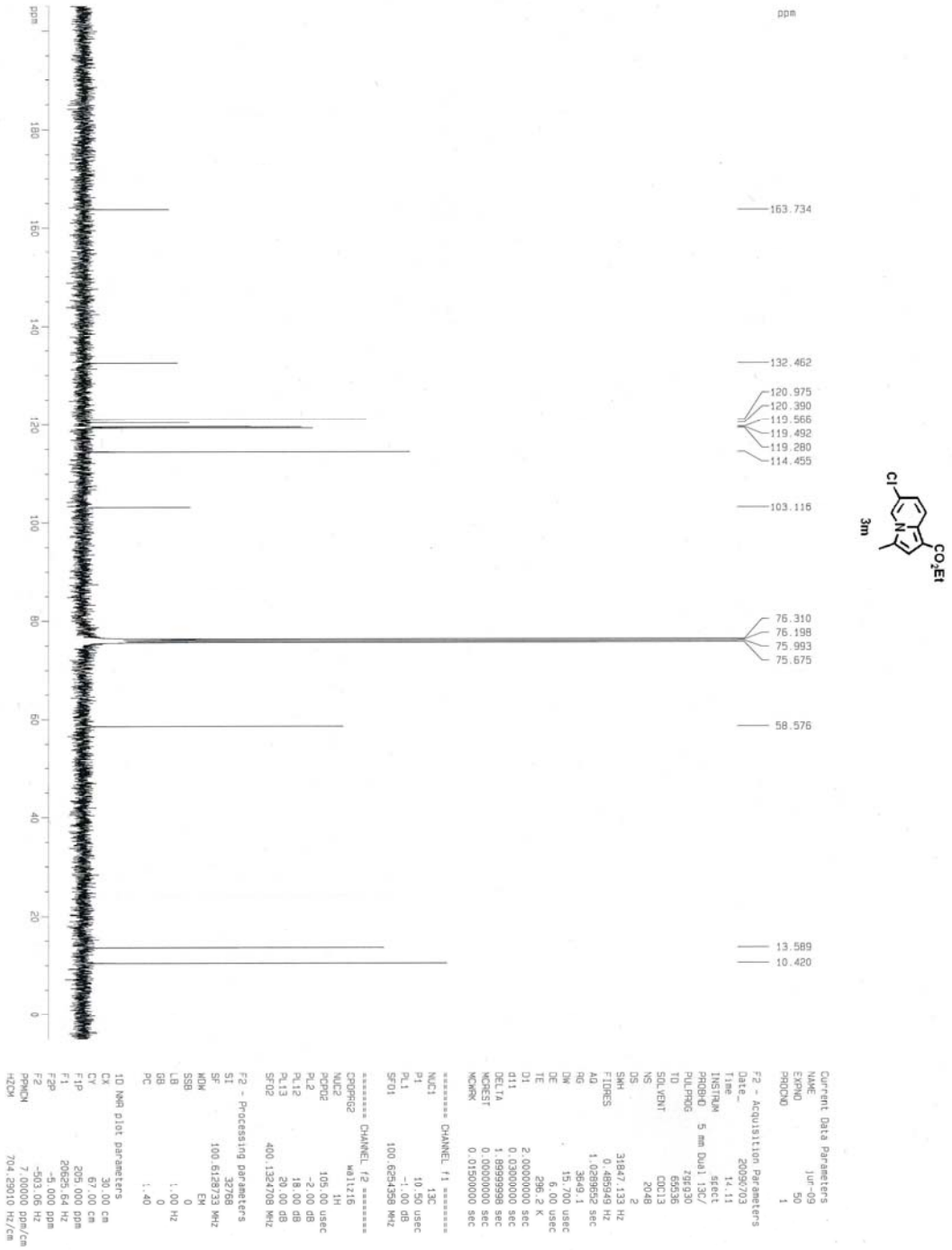

ppm
Integral
97.29
100.00
100.58
97.75
223.74
324.47
347.47
Hz
3583.87
3582.11
3303.85
3294.41
3293.82
3102.28
3100.32
3092.34
3090.37
2905.98
2886.37
2885.68
1765.62
1758.39
1751.24
1744.17
1030.72
622.80
574.56
567.34
560.16
31.87
28.23
3.36
0.00
-3.08
O2N
CO2Et
3k
Current Data Parameters
NAME mor-59
EXPNO 33
PROCNO 1
F2 - Acquisition Parameters
Date_ 20091126
Time 15.16
INSTRUM spect
PROBHD 5 mm Dual 13C/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9923444 sec
RG 812.7
DW 60.800 usec
DE 5.00 usec
TE 296.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 11.00 usec
PL1 -2.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 16384
SF 400.1300085 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 30.00 cm
CY 20.00 cm
F1P 9.500 ppm
F1 3801.24 Hz
F2P -0.100 ppm
F2 -40.01 Hz
PPMCM 0.32000 ppm/cm
HZCM 128.04161 Hz/cm

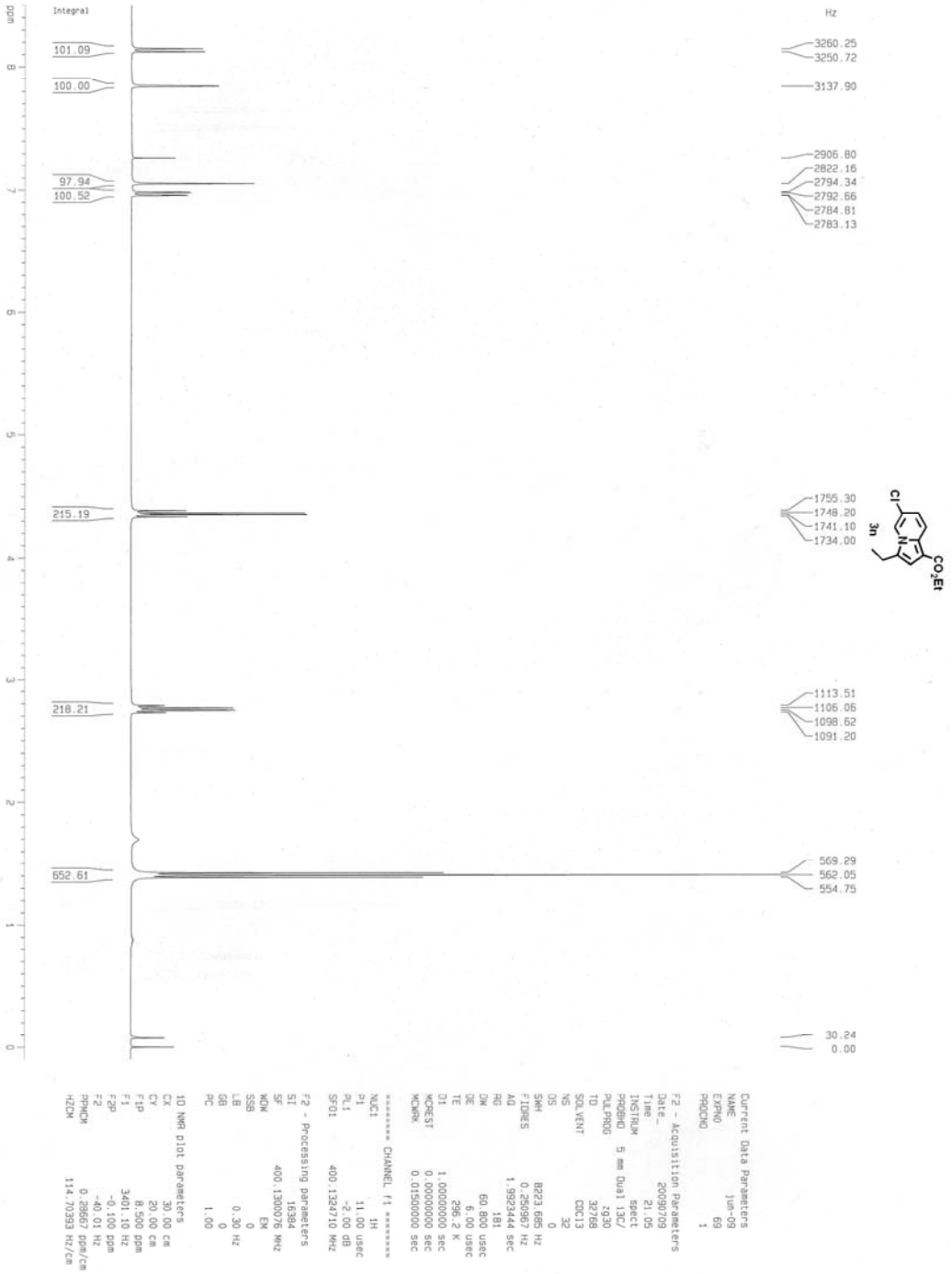

ppm
164.143
137.172
134.863
124.177
123.356
119.621
118.297
114.162
106.588
77.333
77.219
77.016
76.699
60.120
14.543
11.419
0.000
3k
O2N
CO2Et
Current Data Parameters
NAME nov-09
EXPNO 34
PROCNO 1
F2 - Acquisition Parameters
Date_ 20091127
Time_ 6.54
INSTRUM spect
PROBHD 5 mm Dual 13C/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 15360
DS 2
SWH 31847.133 Hz
FIDRES 0.485949 Hz
AQ 1.0289652 sec
RG 80.6
DW 15.700 usec
DE 6.00 usec
TE 296.2 K
D1 2.00000000 sec
D11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 -1.00 dB
SFO1 100.6254358 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 105.00 usec
PL2 -2.00 dB
PL12 13.00 dB
PL13 20.00 dB
SF02 400.1324708 MHz
F2 - Processing parameters
SI 32768
SF 100.6127696 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 30.00 cm
CY 150.00 cm
F1P 205.000 ppm
F1 20625.62 Hz
F2P -5.000 ppm
F2 -503.06 Hz
PPMCM 7.00000 ppm/cm
HZCM 704.28937 Hz/cm

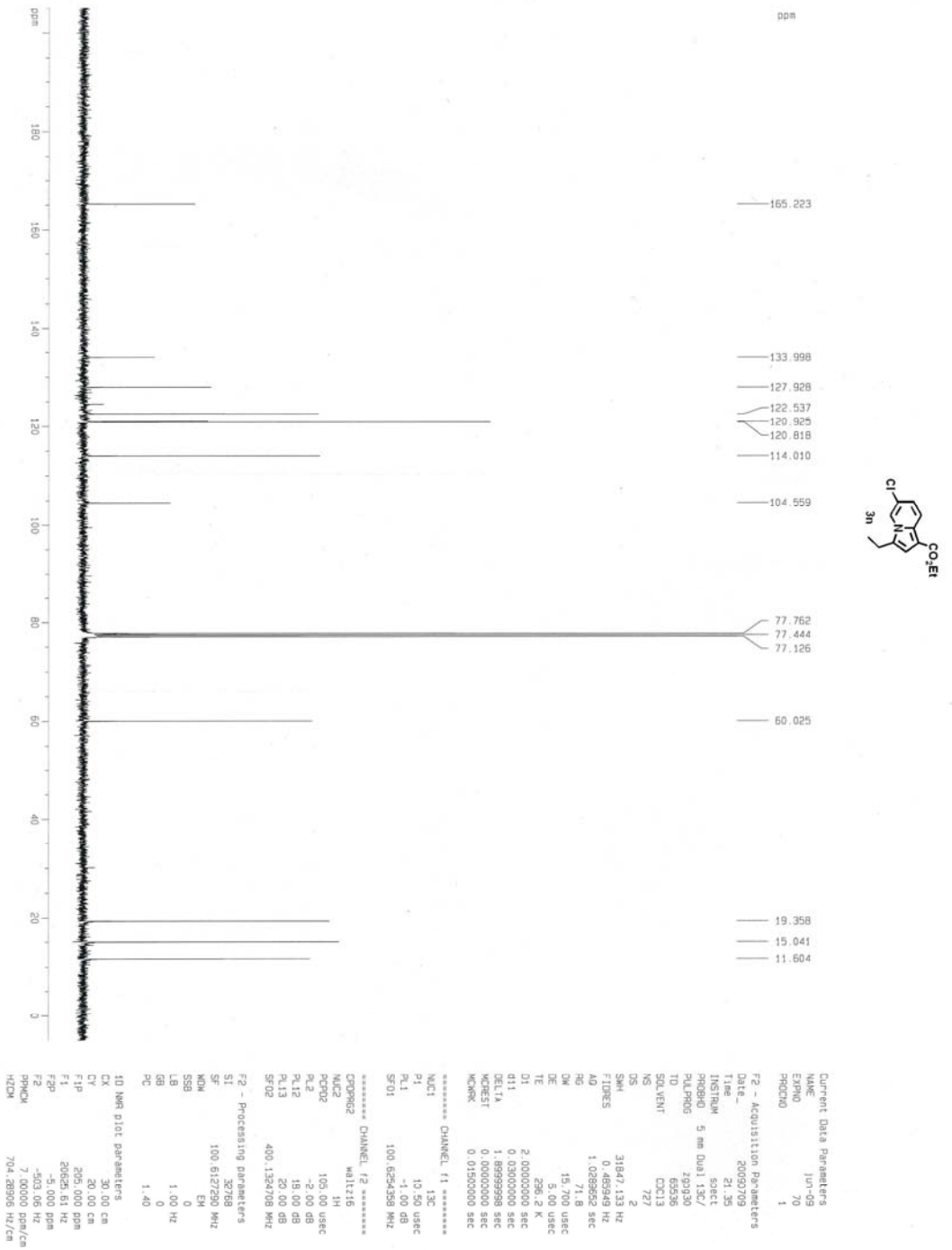

ppm
Integral
100.00
98.79
100.44
493.51
404.14
211.59
439.05
327.74
Hz
3507.92
3506.24
3294.31
3284.23
3081.17
3079.22
3071.27
3069.39
2922.62
2921.09
2915.75
2907.51
2905.61
2892.90
2891.59
2887.67
2885.62
2883.12
2876.20
2874.78
2867.82
1768.50
1761.33
1754.12
1747.04
1403.17
1396.15
1389.13
1382.11
1289.50
1287.94
1280.81
1273.65
1256.86
1249.19
1242.41
1240.55
634.22
577.99
570.92
563.78
28.51
0.00
Current Data Parameters
NAME
EXPNO
PROCNO
F2 - Acquisition Parameters
Date_
Time
INSTRUM
PROBHD 5 mm Dual 13C/
PULPROG
TD
SOLVENT
NS
DS
SWH
FIDRES
AQ
RG
DW
DE
TE
D1
MCREST
MCWRK
======== CHANNEL f1 ========
NUC1
P1
PL1
SFO1
F2 - Processing parameters
SI
SF
WDW
SSB
LB
GB
PC
1D NMR plot parameters
CX
CY
F1P
F1
F2P
F2
PPMCM
HZCM

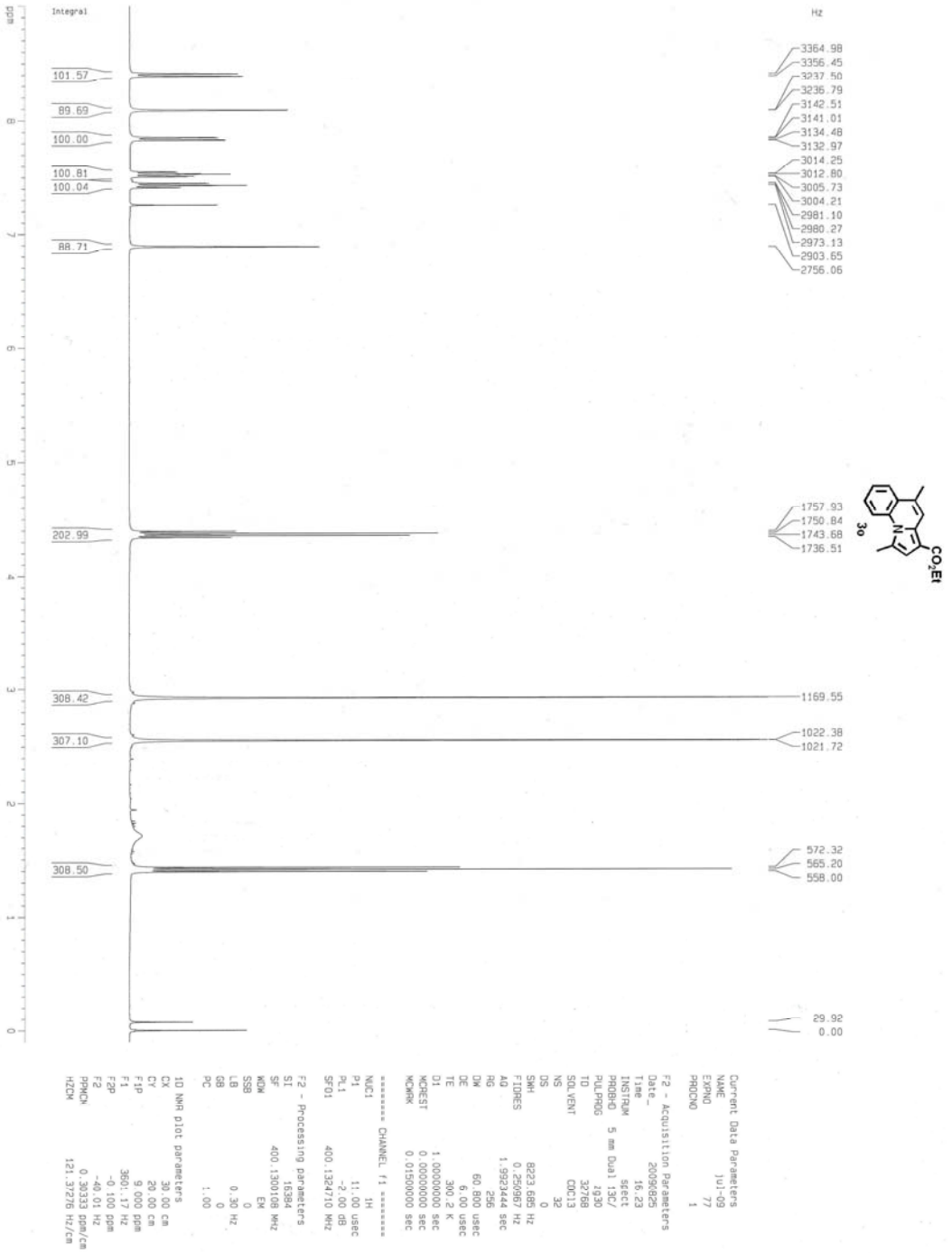

ppm
164.576
140.534
137.409
135.286
129.212
128.661
128.583
127.106
123.667
120.005
117.872
114.747
107.079
77.747
77.634
77.430
77.113
66.277
60.587
34.497
28.082
14.962
NO2
N
CO2Et
Current Data Parameters
NAME jun-09
EXPNO 100
PROCNO 1
F2 - Acquisition Parameters
Date_ 20090717
Time 15.23
INSTRUM spect
PROBHD 5 mm Dual 13C/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 4096
DS 2
SWH 31847.133 Hz
FIDRES 0.485949 Hz
AQ 1.0289652 sec
RG 143.7
DW 15.700 usec
DE 6.00 usec
TE 297.2 K
D1 2.00000000 sec
D11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 -1.00 dB
SFO1 100.6254358 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 105.00 usec
PL2 -2.00 dB
PL12 18.00 dB
PL13 20.00 dB
SFO2 400.1324708 MHz
F2 - Processing parameters
SI 32768
SF 100.6127290 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 30.00 cm
CY 67.00 cm
F1P 205.000 ppm
F1 20625.61 Hz
F2P -5.000 ppm
F2 -503.06 Hz
PPHCM 7.00000 ppm/cm
HZCM 704.28906 Hz/cm

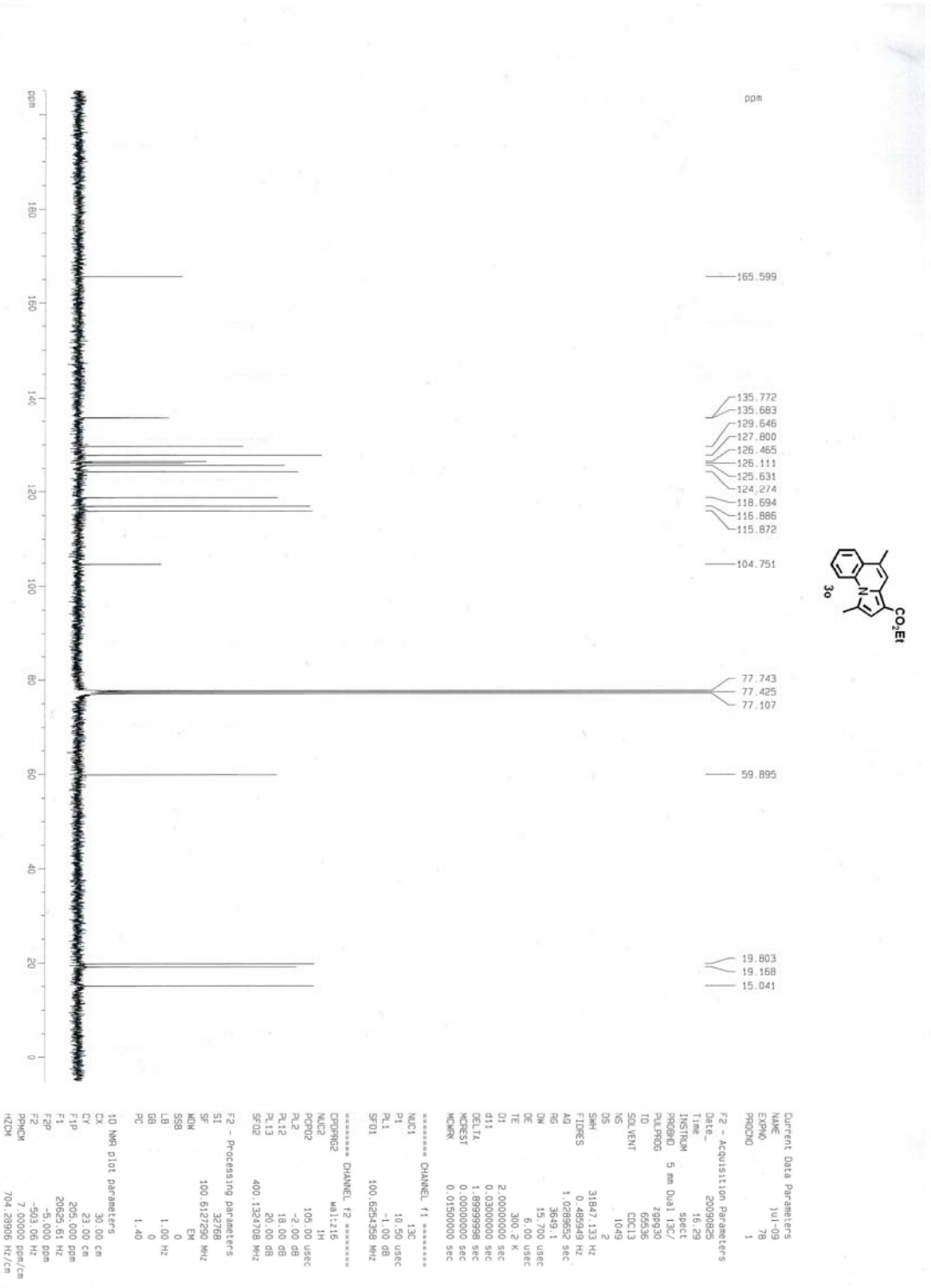

Integral
Hz
100.00
97.61
96.43
102.98
215.08
317.32
329.81
3260.22
3250.69
3129.39
3128.73
2906.05
2816.54
2798.84
2797.18
2789.31
2787.65
1752.63
1745.40
1738.27
1731.19
977.03
566.24
559.17
552.10
28.64
-0.00
3m
Cl
N
CO2Et
Current Data Parameters
NAME jun-09
EXPNO 49
PROCNO 1
F2 - Acquisition Parameters
Date_ 20090703
Time 14.07
INSTRUM spect
PROBHD 5 mm Dual 13C/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 20
DS 0
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9923444 sec
RG 362
DW 60.800 usec
DE 6.00 usec
TE 296.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 11.00 usec
PL1 -2.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 16384
SF 400.1300085 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 30.00 cm
CY 20.00 cm
F1P 8.500 ppm
F1 3401.10 Hz
F2P -0.100 ppm
F2 -40.01 Hz
PPMCM 0.29667 ppm/cm
HZCM 114.70393 Hz/cm

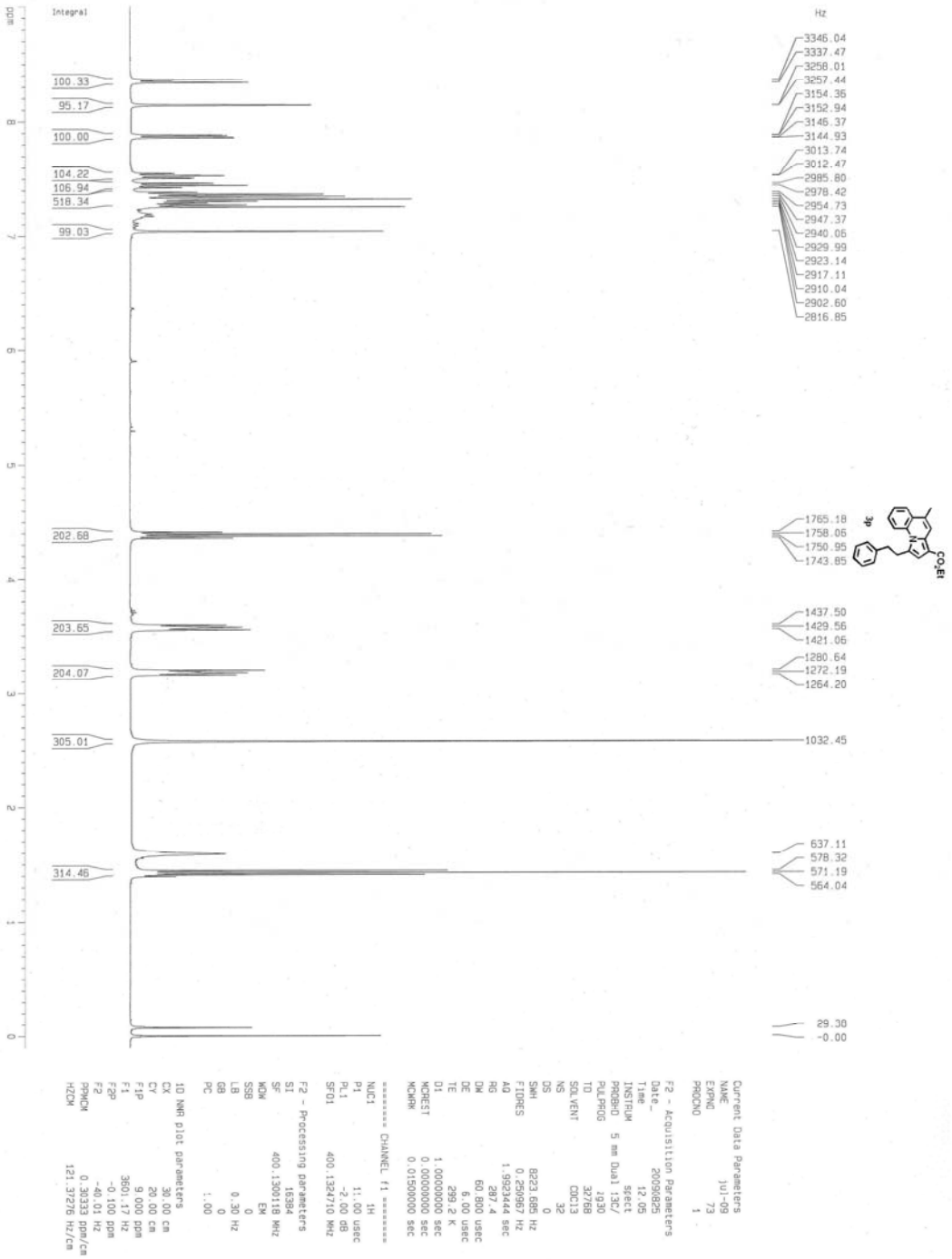

ppm
163.734
132.462
120.975
120.390
119.566
119.492
119.280
114.455
103.116
76.310
76.198
75.993
75.675
58.576
13.589
10.420
Cl
N
CO2Et
3m
Current Data Parameters
NAME jur-09
EXPNO 50
PROCNO 1
F2 - Acquisition Parameters
Date_ 20090703
Time 14.11
INSTRUM spect
PROBHD 5 mm Dual 13C/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 2
SWH 31847.133 Hz
FIDRES 0.485949 Hz
AQ 1.0289692 sec
RG 3649.1
DW 15.700 usec
DE 6.00 usec
TE 296.2 K
D1 2.00000000 sec
D11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 -1.00 dB
SF01 100.6254358 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 105.00 usec
PL2 -2.00 dB
PL12 18.00 dB
PL13 20.00 dB
SFO2 400.1324708 MHz
F2 - Processing parameters
SI 32768
SF 100.6128733 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 30.00 cm
CY 67.00 cm
F1P 205.000 ppm
F1 20625.64 Hz
F2P -5.000 ppm
F2 -503.06 Hz
PPMCM 7.00000 ppm/cm
HZCM 704.23010 Hz/cm

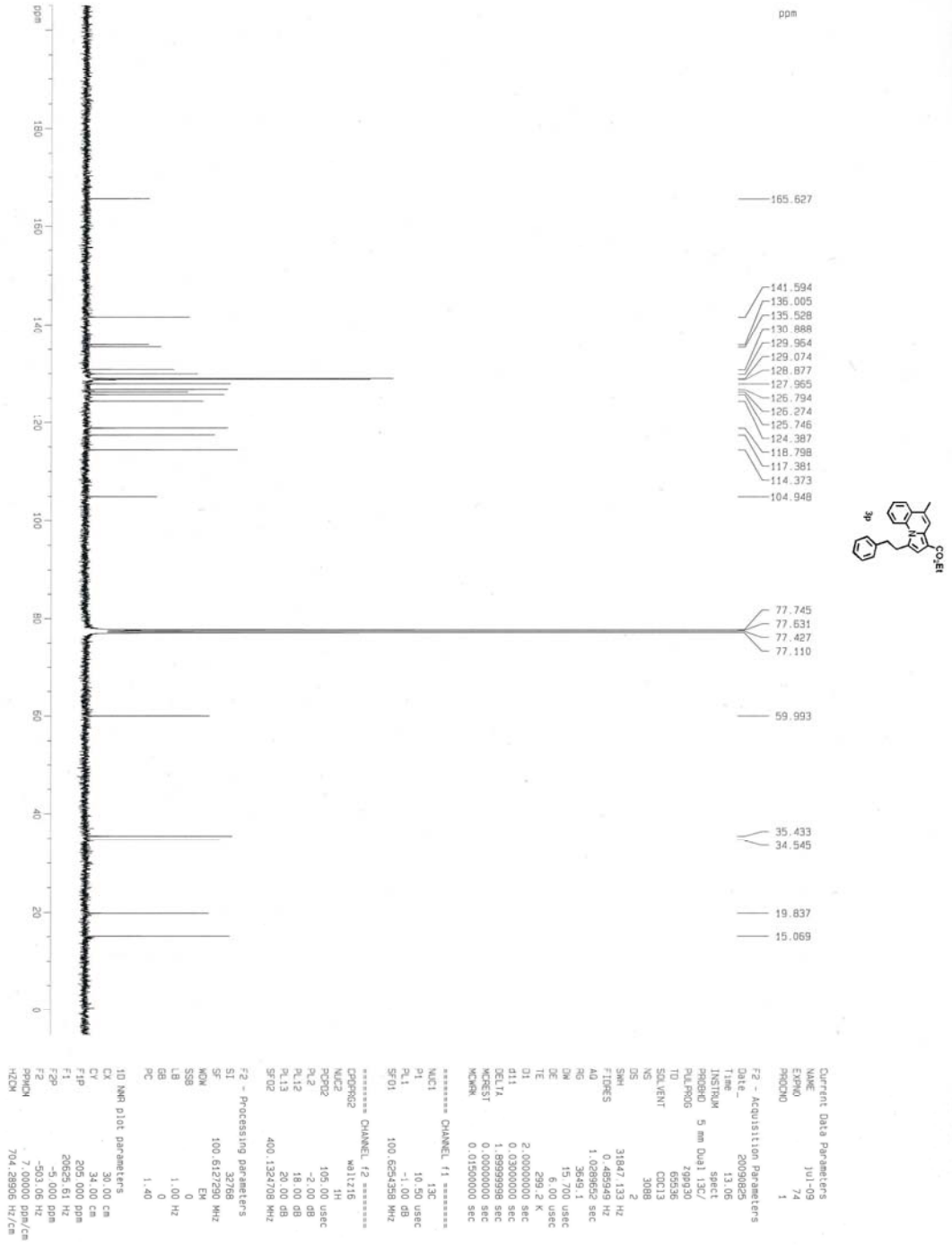

Integral
101.09
100.00
97.94
100.52
215.19
218.21
652.61
Hz
3260.25
3250.72
3137.90
2906.80
2822.16
2794.34
2792.66
2784.81
2783.13
1755.30
1748.20
1741.10
1734.00
1113.51
1106.06
1098.62
1091.20
569.29
562.05
554.75
30.24
0.00
3n
Cl
N
CO2Et
Current Data Parameters
NAME
EXPNO
PROCNO
F2 - Acquisition Parameters
Date_
Time
INSTRUM
PROBHD 5 mm Dual 13C/
PULPROG
TD
SOLVENT
NS
DS
SWH
FIDRES
AQ
RG
DW
DE
TE
D1
MCREST
MCWRK
======== CHANNEL f1 ========
NUC1
P1
PL1
SFO1
F2 - Processing parameters
SI
SF
WDW
SSB
LB
GB
PC
1D NMR plot parameters
CX
CY
F1P
F1
F2P
F2
PPMCM
HZCM

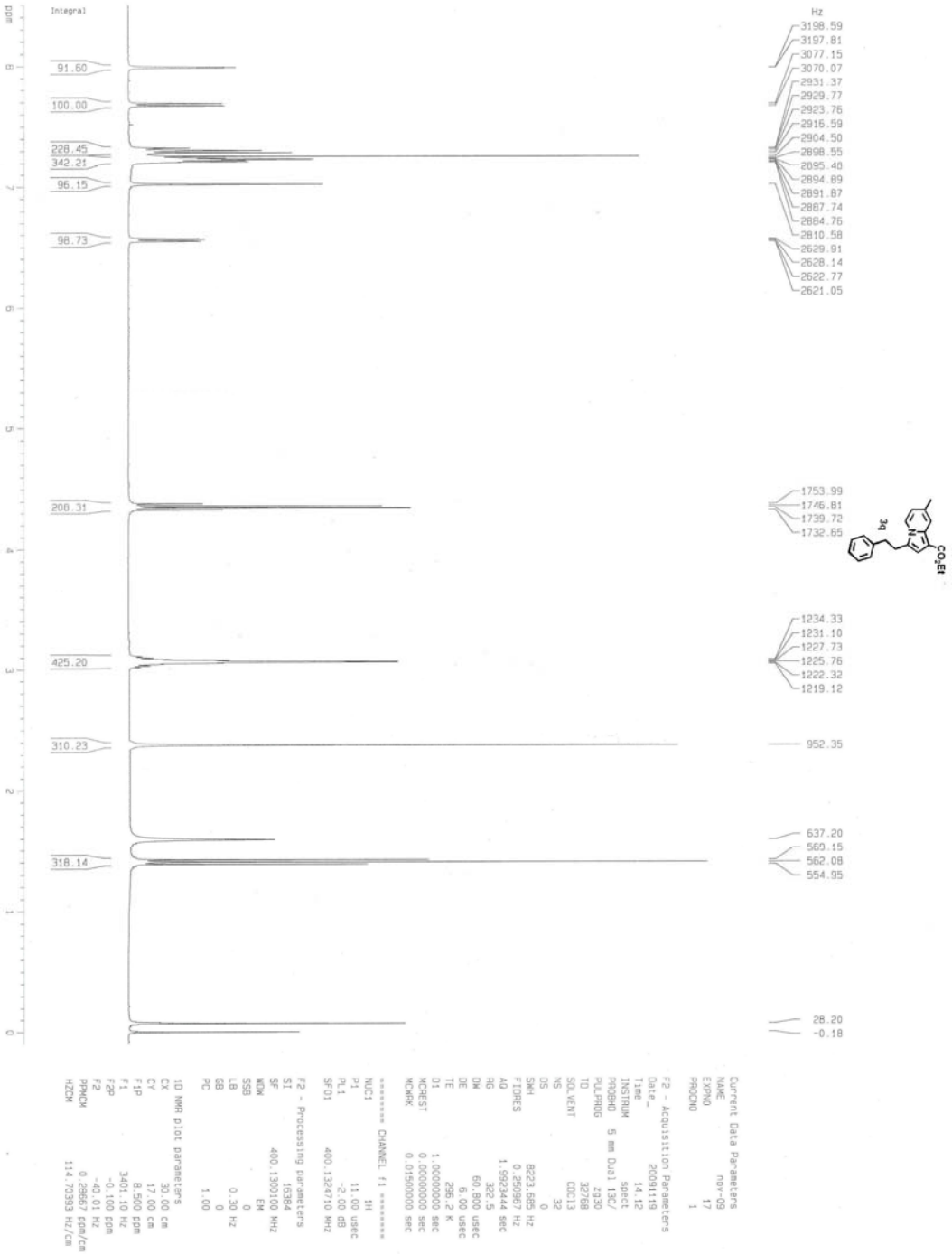

ppm
165.223
133.998
127.928
122.537
120.925
120.818
114.010
104.559
77.762
77.444
77.126
60.025
19.358
15.041
11.604
3n
Cl
CO2Et
Current Data Parameters
NAME jun-09
EXPNO 70
PROCNO 1
F2 - Acquisition Parameters
Date_ 20090709
Time 21.35
INSTRUM spect
PROBHD 5 mm Dual 13C/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 727
DS 2
SWH 31847.133 Hz
FIDRES 0.485949 Hz
AQ 1.0289652 sec
RG 71.8
DW 15.700 usec
DE 5.00 usec
TE 296.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 -1.00 dB
SFO1 100.6254358 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 105.00 usec
PL2 -2.00 dB
PL12 18.00 dB
PL13 20.00 dB
SFO2 400.1324708 MHz
F2 - Processing parameters
SI 32768
SF 100.6127290 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 30.00 cm
CY 20.00 cm
F1P 205.000 ppm
F1 20625.61 Hz
F2P -5.000 ppm
F2 -503.06 Hz
PPMCM 7.00000 ppm/cm
HZCM 704.28906 Hz/cm

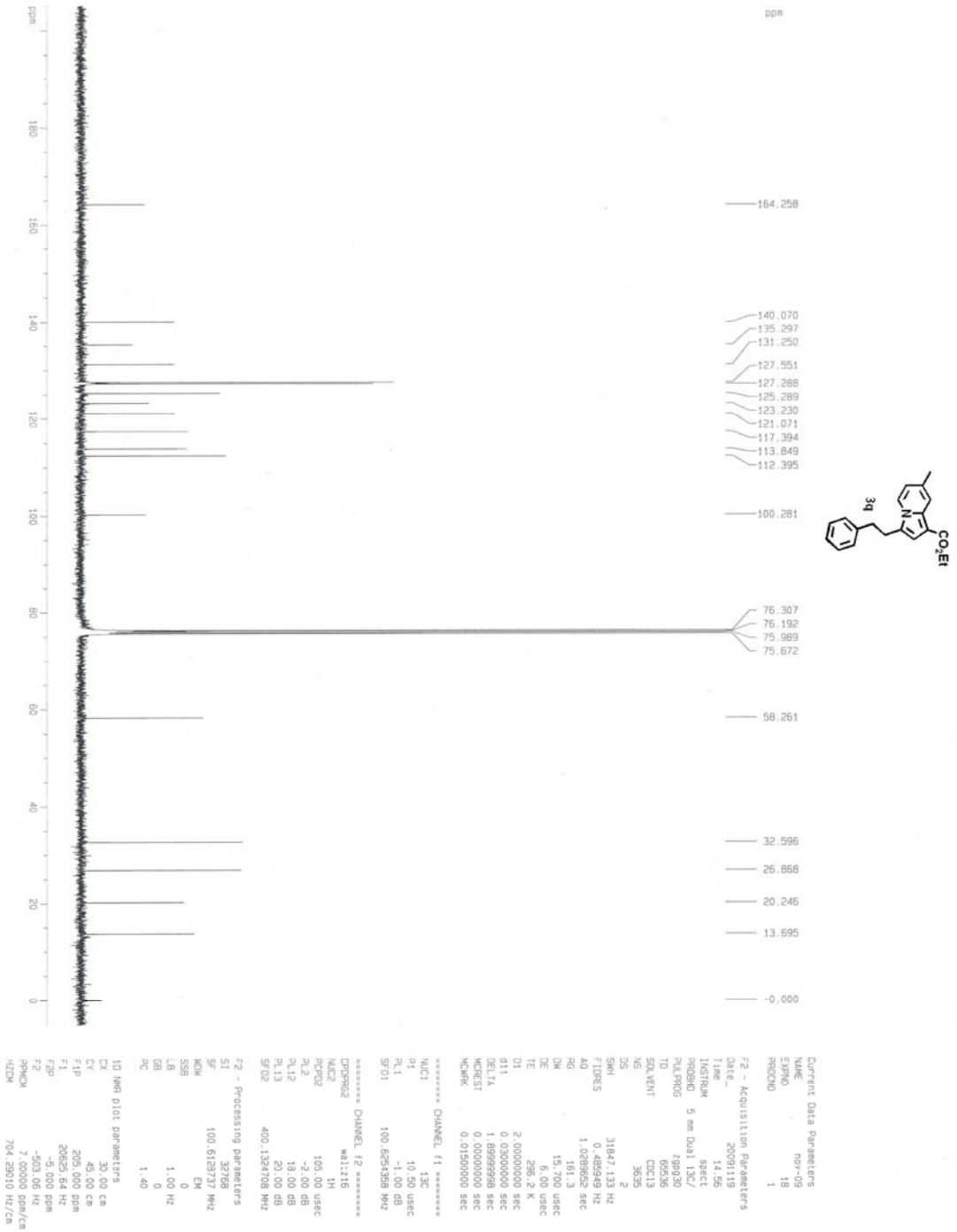

ppm
Integral
101.57
89.69
100.00
100.81
100.04
88.71
202.99
308.42
307.10
308.50
Hz
3364.98
3356.45
3237.50
3236.79
3142.51
3141.01
3134.48
3132.97
3014.25
3012.80
3005.73
3004.21
2981.10
2980.27
2973.13
2903.65
2756.06
1757.93
1750.84
1743.68
1736.51
1169.55
1022.38
1021.72
572.32
565.20
558.00
29.92
0.00
3o
CO2Et
Current Data Parameters
NAME
EXPNO
PROCNO
F2 - Acquisition Parameters
Date_
Time
INSTRUM
PROBHD 5 mm Dual 13C/
PULPROG
TD
SOLVENT
NS
DS
SWH
FIDRES
AQ
RG
DW
DE
TE
D1
MCREST
MCWRK
======== CHANNEL f1 ========
NUC1
P1
PL1
SFO1
F2 - Processing parameters
SI
SF
WDW
SSB
LB
GB
PC
1D NMR plot parameters
CX
CY
F1P
F1
F2P
F2
PPMCM
HZCM


ppm
165.599
135.772
135.683
129.646
127.800
126.465
126.111
125.631
124.274
118.694
116.886
115.872
104.751
77.743
77.425
77.107
59.895
19.803
19.168
15.041
3o
CO2Et
Current Data Parameters
NAME jul-09
EXPNO 78
PROCNO 1
F2 - Acquisition Parameters
Date_ 20090825
Time 16.29
INSTRUM spect
PROBHD 5 mm Dual 13C/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1049
DS 2
SWH 31847.133 Hz
FIDRES 0.485949 Hz
AQ 1.0289652 sec
RG 3649.1
DW 15.700 usec
DE 6.00 usec
TE 300.2 K
D1 2.00000000 sec
D11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 -1.00 dB
SFO1 100.6254358 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 105.00 usec
PL2 -2.00 dB
PL12 18.00 dB
PL13 20.00 dB
SFO2 400.1324708 MHz
F2 - Processing parameters
SI 32768
SF 100.6127290 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 30.00 cm
CY 23.00 cm
F1P 205.000 ppm
F1 20625.61 Hz
F2P -5.000 ppm
F2 -503.06 Hz
PPMCM 7.00000 ppm/cm
HZCM 704.28906 Hz/cm


Integral
100.33
95.17
100.00
104.22
106.94
518.34
99.03
202.68
203.65
204.07
305.01
314.46
Hz
3346.04
3337.47
3258.01
3257.44
3154.36
3152.94
3146.37
3144.93
3013.74
3012.47
2985.80
2978.42
2954.73
2947.37
2940.06
2929.99
2923.14
2917.11
2910.04
2902.60
2816.85
1765.18
1758.06
1750.95
1743.85
1437.50
1429.56
1421.06
1280.64
1272.19
1264.20
1032.45
637.11
578.32
571.19
564.04
29.30
-0.00
3p
CO2Et
Current Data Parameters
NAME
EXPNO 73
PROCNO 1
F2 - Acquisition Parameters
Date_ 20090825
Time 12.05
INSTRUM spect
PROBHD 5 mm Dual 13C/
PULPROG z930
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9923444 sec
RG 287.4
DW 60.800 usec
DE 6.00 usec
TE 299.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 11.00 usec
PL1 -2.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 16384
SF 400.1300118 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 30.00 cm
CY 20.00 cm
F1P 9.000 ppm
F1 3601.17 Hz
F2P -0.100 ppm
F2 -40.01 Hz
PPMCM 0.30333 ppm/cm
HZCM 121.37276 Hz/cm


ppm
165.627
141.594
136.005
135.528
130.888
129.964
129.074
128.877
127.965
126.794
126.274
125.746
124.387
118.798
117.381
114.373
104.948
77.745
77.631
77.427
77.110
59.993
35.433
34.545
19.837
15.069
3p
CO2Et
Current Data Parameters
NAME jul-09
EXPNO 74
PROCNO 1
F2 - Acquisition Parameters
Date_ 20090825
Time 13.06
INSTRUM spect
PROBHD 5 mm Dual 13C/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 3088
DS 2
SWH 31847.133 Hz
FIDRES 0.485949 Hz
AQ 1.0289682 sec
RG 3649.1
DW 15.700 usec
DE 6.00 usec
TE 299.2 K
D1 2.00000000 sec
D11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 -1.00 dB
SFO1 100.6254358 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 105.00 usec
PL2 -2.00 dB
PL12 18.00 dB
PL13 20.00 dB
SFO2 400.1324708 MHz
F2 - Processing parameters
SI 32768
SF 100.6127290 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 30.00 cm
CY 34.00 cm
F1P 205.000 ppm
F1 20625.61 Hz
F2P -5.000 ppm
F2 -503.06 Hz
PPMCM 7.00000 ppm/cm
HZCM 704.28906 Hz/cm


Integral
91.60
100.00
228.45
342.21
96.15
98.73
200.31
425.20
310.23
318.14
Hz
3198.59
3197.81
3077.15
3070.07
2931.37
2929.77
2923.76
2916.59
2904.50
2898.55
2895.40
2894.89
2891.87
2887.74
2884.76
2810.58
2629.91
2628.14
2622.77
2621.05
1753.99
1746.81
1739.72
1732.65
1234.33
1231.10
1227.73
1225.76
1222.32
1219.12
952.35
637.20
569.15
562.08
554.95
28.20
-0.18
3q
CO2Et
Current Data Parameters
NAME nov-09
EXPNO 17
PROCNO 1
F2 - Acquisition Parameters
Date_ 20091119
Time 14.12
INSTRUM spect
PROBHD 5 mm Dual 13C/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 8223.685 Hz
FIDRES 0.250987 Hz
AQ 1.9923444 sec
RG 322.5
DW 60.800 usec
DE 6.00 usec
TE 296.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 11.00 usec
PL1 -2.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 16384
SF 400.1300100 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 30.00 cm
CY 17.00 cm
F1P 8.500 ppm
F1 3401.10 Hz
F2P -0.100 ppm
F2 -40.01 Hz
PPMCM 0.29667 ppm/cm
HZCM 114.70393 Hz/cm


ppm
164.258
140.070
135.297
131.250
127.551
127.288
125.289
123.230
121.071
117.394
113.849
112.395
100.281
76.307
76.192
75.989
75.672
58.261
32.596
26.868
20.246
13.695
-0.000
3q
N
CO2Et
Current Data Parameters
NAME nov-09
EXPNO 18
PROCNO 1
F2 - Acquisition Parameters
Date_ 20091119
Time 14.56
INSTRUM spect
PROBHD 5 mm Dual 13C/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 3635
DS 2
SWH 31847.133 Hz
FIDRES 0.485949 Hz
AQ 1.0289652 sec
RG 161.3
DW 15.700 usec
DE 6.00 usec
TE 296.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 -1.00 dB
SFO1 100.6254358 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 105.00 usec
PL2 -2.00 dB
PL12 18.00 dB
PL13 20.00 dB
SFO2 400.1324708 MHz
F2 - Processing parameters
SI 32768
SF 100.6123737 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 30.00 cm
CY 45.00 cm
F1P 205.000 ppm
F1 20625.64 Hz
F2P -5.000 ppm
F2 -503.06 Hz
PPMCM 7.00000 ppm/cm
HZCM 704.29010 Hz/cm