Electronic Supplementary Material (ESI) for RSC Advances

Supporting information

Synthesis of polysubstituted quinolines *via* copper(II)-catalyzed annulation of 2-aminoaryl ketones with alkynoates

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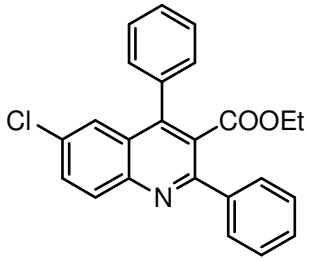
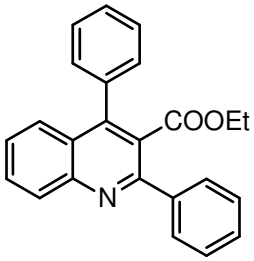
General. ^{1}H NMR spectra was determined on a Bruker 400 (400 MHz) spectrometer as solutions in $CDCl_3$. Chemical shifts are expressed in parts per million (δ) and are referenced to tetramethylsilane (TMS) as internal standard and the signals were reported as s (singlet), d (doublet), t (triplet), m (multiplet) and coupling constants *J* were given in Hz. ^{13}C NMR spectra was recorded at 100 MHz in $CDCl_3$ solution. Elemental analyses were done by a Perkin-Elmer autoanalyzer. TLC was done on silica gel coated glass slide (Merck, Silica gel G for TLC). Silica gel (60-120 mesh, SRL, India) was used for column chromatography. Petroleum ether refers to the fraction boiling in the range of 60-80 ^{o}C unless otherwise mentioned. All solvents were dried and distilled before use. Commercially available substrates were freshly distilled before the reaction. All reactions were executed using oven dried glassware.

Typical procedure for the synthesis of 6-chloro-2,4-diphenylquinoline-3-carboxylic acid ethyl ester (Table 2, 3aa).[1]



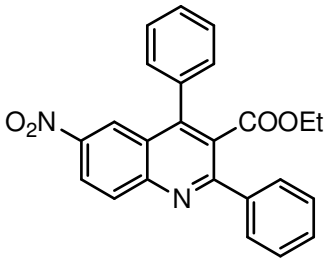
2-Amino-5-chlorobenzophenone (231 mg, 1 mmol) and ethyl phenylpropiolate (174 mg, 1 mmol) was mixed in a sealed tube and stirred at room temperature for 10 min. Then copper triflate (36 mg, 0.1 mmol) was added to the reaction mixture and heated at 110 ^{o}C. After completion (TLC), the reaction mixture was extracted with dichloromethane (10 mL x 2). Solvent was evaporated to furnish the crude product which was subjected to column chromatography on silica gel using petroleum ether/ethyl acetate as an eluent to obtain the analytically pure product (348 mg, 90 %). Yellow oil. IR (KBr): 1722 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.00 (d, *J* = 9.2 Hz, 1H), 7.64-7.62 (m, 2H), 7.61-7.48 (m, 1H), 7.44 (s, 1H), 7.34-7.23 (m, 8H), 3.74 (q, *J* = 7.2 Hz, 2H), 0.65 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.5, 155.9, 146.0,

145.9, 139.6, 134.6, 132.8, 131.2, 131.1, 129.1, 128.8, 128.6, 128.3, 128.2, 128.2, 127.7, 126.0, 124.9, 61.1, 13.1.



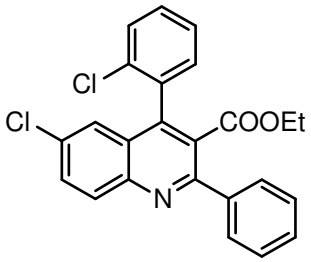
2,4-Diphenylquinoline-3-carboxylic acid ethyl ester (3ba).[1]

Yellow solid (324 mg, 92%); Mp 86-88 ^{o}C; IR (KBr): 1722 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.15 (d, *J* = 9.2 Hz, 1H), 7.70-7.66 (m, 3H), 7.54 (d, *J* = 8.4 Hz, 1H), 7.44-7.32 (m, 9H), 3.79 (q, *J* = 7.2 Hz, 2H), 0.74 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 168.1, 155.9, 147.8, 147.1, 140.2, 135.5, 130.4, 129.7, 129.3, 128.8, 128.5, 128.4, 128.3, 128.2, 127.1, 127.0, 126.5, 125.5, 61.2, 13.3.



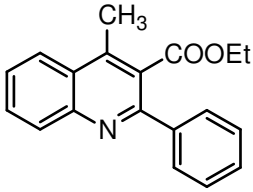
6-Nitro-2,4-diphenylquinoline-3-carboxylic acid ethyl ester (3ca).[1]

Yellow solid (318 mg, 80%); Mp 124-126 ^{o}C; IR (KBr): 1722 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.60 (s, 1H), 8.53 (dd, J_1 = 9.2 Hz, J_2 = 2.4 Hz, 1H), 8.36 (d, *J* = 9.2 Hz, 1H), 7.81-7.79 (m, 2H), 7.59-7.56 (m, 3H), 7.53-7.50 (m, 3H), 7.46-7.43 (m, 2H), 3.94 (q, *J* = 7.2 Hz, 2H), 0.86 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.2, 159.3, 149.7, 149.0, 145.8, 139.2, 133.9, 131.5, 129.6, 129.3, 129.2, 128.8, 128.6, 128.5, 124.8, 123.8, 123.5, 61.6, 13.3.



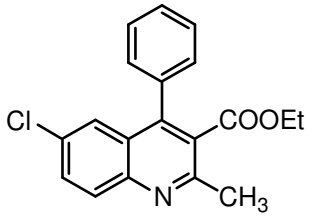
6-Chloro-4-(2-chloro-phenyl)-2-phenylquinoline-3-carboxylic acid ethyl ester (3da).

Yellow gummy mass (345 mg, 82%); IR (KBr)**:** 1722 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.17 (m, 1H), 7.77-7.31 (m, 11H), 3.88 (m, 2H), 0.80 (m, 3H) ; ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.2, 156.4, 145.9, 143.9, 139.6, 133.8, 133.5, 133.2, 131.5, 131.4, 130.8, 130.3, 129.5, 129.0, 128.4, 128.3, 127.7, 126.6, 125.7, 124.7, 61.3, 13.2. Anal. Calcd for $C_{24}H_{17}Cl_2NO_2$: C, 68.26; H, 4.06; N, 3.32. Found: C, 68.17; H, 4.01; N 3.23.



4-Methyl-2-phenylquinoline-3-carboxylic acid ethyl ester (3ea).[1]

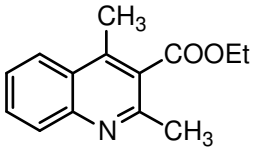
Yellow oil (265 mg, 91%); IR (KBr): 1717 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.98 (d, J = 8.4 Hz, 1H), 7.77 (d, J = 8.4 Hz, 1H), 7.56-7.48 (m, 3H), 7.33-7.21 (m, 4H), 3.97 (q, J = 7.2 Hz, 2H), 2.52 (s, 3H), 0.81 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 168.6, 155.7, 146.8, 142.3, 140.3, 129.9, 129.8, 128.3, 128.0, 127.9, 127.0, 126.5, 125.6, 123.6, 61.1, 15.2, 13.2.



6-Chloro-2-methyl-4-phenylquinoline-3-carboxylic acid ethyl ester (3ab).

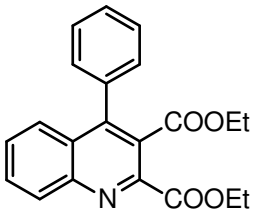
Yellow gummy mass (286 mg, 88%); IR (KBr): 1714 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.87 (d, J = 9.2 Hz, 1H), 7.50 (dd, J_1 = 8.8 Hz, J_2 = 2.4 Hz, 1H), 7.42 (d, J = 2.4 Hz, 1H), 7.38-7.35 (m, 3H), 7.24-7.21 (m,

2H), 3.95 (q, *J* = 7.2 Hz, 2H), 2.65 (s, 3H), 0.82 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.8, 154.7, 145.8, 145.1, 134.8, 132.1, 130.9, 130.3, 129.1, 128.5, 128.2, 127.9, 125.7, 124.9, 61.2, 23.5, 13.4. Anal. Calcd for $C_{19}H_{16}ClNO_2$: C, 70.05; H, 4.95; N, 4.30. Found: C, 70.01; H, 4.87; N 4.19.



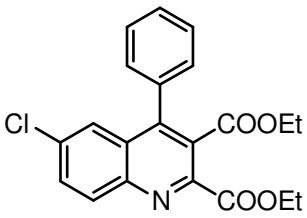
2,4-Dimethylquinoline-3-carboxylic acid ethyl ester (3eb).

Yellow oil (204 mg, 89%); IR (KBr): 1714 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.88 (d, *J* = 8.0 Hz, 1H), 7.79 (d, *J* = 8.4 Hz, 1H), 757-7.52 (m, 1H), 7.37-7.33 (m, 1H), 4.35 (q, *J* = 7.2 Hz, 2H), 2.58 (s, 3H), 2.48 (s, 3H), 1.29 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 168.8, 154.0, 146.7, 141.1, 129.7, 128.9, 127.7, 126.0, 125.4, 123.7, 61.4, 23.5, 15.4, 13.9. Anal. Calcd for $C_{14}H_{15}NO_2$: C, 73.34; H, 6.59; N, 6.11. Found: C, 73.24; H, 6.48; N, 6.05.



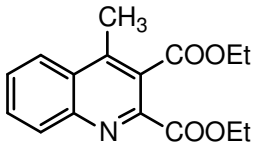
4-Phenylquinoline-2,3-dicarboxylic acid diethyl ester (3bc).[2]

Pale yellow solid (304 mg, 87%); Mp 94-96 ^{o}C; IR (KBr): 1740 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.23 (d, *J* = 8.4 Hz, 1H), 7.71 (t, *J* = 7.2 Hz, 1H), 7.53 (d, *J* = 8.4 Hz, 1H), 7.48 (d, *J* = 7.2 Hz, 1H), 7.41-7.28 (m, 3H), 7.27-7.26 (m, 2H), 4.45 (q, *J* = 7.2 Hz, 2H), 4.01 (q, *J* = 7.2 Hz, 2H), 1.37 (t, *J* = 7.2 Hz, 3H), 0.90 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.0, 165.1, 147.8, 147.0, 145.7, 134.6, 130.8, 130.5, 129.3, 128.9, 128.6, 128.1, 127.4, 126.9, 126.5, 62.5, 61.4, 14.1, 13.5.



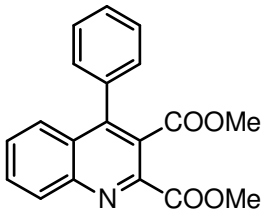
6-Chloro-4-phenylquinoline-2,3-dicarboxylic acid diethyl ester (3ac).[2]

White solid (321 mg, 84%); Mp 154-156 ^{o}C; IR (KBr): 1738 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.28 (s, 1H), 7.76 (s, 1H), 7.64-7.48 (m, 4H), 7.36-7.38 (m, 2H), 4.70-4.40 (m, 2H), 4.30-4.00 (m, 2H), 1.47 (m, 3H), 1.01-0.98 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 166.7, 165.0, 147.1, 145.9, 145.3, 135.3, 134.0, 132.1, 131.9, 129.2, 129.0, 128.4, 125.3, 62.7, 61.6, 14.1, 13.5.



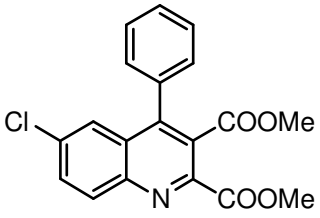
4-Methylquinoline-2,3-dicarboxylic acid diethyl ester (3ec).[2]

Brown oil (250 mg, 87%); IR (KBr): 1740 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.17 (d, *J* = 8.8 Hz, 1H), 7.99 (d, *J* = 8.4 Hz, 1H), 7.71 (t, *J* = 7.2 Hz, 1H), 7.62-7.59 (m, 1H), 4.46-4.36 (m, 4H), 2.67 (s, 3H), 1.39-1.31 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.6, 165.2, 146.0, 145.6, 143.6, 130.7, 130.4, 128.6, 127.6, 126.8, 123.8, 62.2, 61.6, 15.2, 13.9, 13.8.



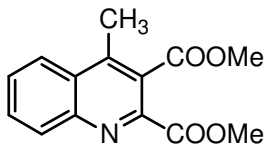
4-Phenylquinoline-2,3-dicarboxylic acid dimethyl ester (3bd).[2]

Brown solid (273 mg, 85%); Mp 124-126 ^{o}C; IR (KBr): 1730 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.24 (d, *J* = 8.4 Hz, 1H), 7.75-7.70 (m, 1H), 7.56-7.47 (m, 2H), 7.42-7.40 (m, 3H), 7.28-7.26 (m, 2H), 3.98 (s, 3H), 3.55 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.5, 165.4, 147.9, 146.9, 144.7, 134.4, 130.9, 130.5, 129.2, 129.1, 128.7, 128.2, 127.5, 127.1, 126.5, 53.3, 52.3.



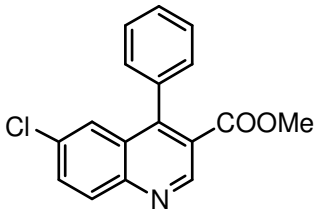
6-Chloro-4-phenylquinoline-2,3-dicarboxylic acid dimethyl ester (3ad).[2]

Pale yellow solid (295 mg, 83%); Mp 164-165 ^{o}C; IR (KBr): 1730 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.17 (d, *J* = 8.8 Hz, 1H), 7.67-7.64 (m, 1H), 7.50 (d, *J* = 2.0 Hz, 1H), 7.44-7.42 (m, 3H), 7.27-7.25 (m, 2H), 3.98 (s, 3H), 3.55 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.1, 165.1, 147.1, 145.3, 144.8, 135.5, 133.6, 132.0, 129.1, 129.0, 128.4, 128.3, 127.9, 125.3, 53.4, 52.4.



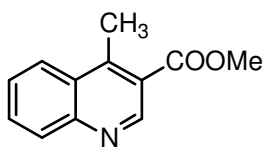
4-Methylquinoline-2,3-dicarboxylic acid dimethyl ester (3ed).

Brown oil (218 mg, 84%); IR (KBr): 1730 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.12 (d, *J* = 8.4 Hz, 1H), 7.92 (d, *J* = 8.8 Hz, 1H), 7.69-7.65 (m, 1H), 7.56-7.52 (m, 1H), 3.94 (s, 3H), 3.90 (s, 3H), 2.59 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 168.1, 165.5, 146.1, 144.7, 143.6, 130.7, 130.6, 128.8, 127.7, 126.9, 123.8, 53.1, 52.6, 15.3. Anal. Calcd for $C_{14}H_{13}NO_4$: C, 64.86; H, 5.05; N, 5.40. Found: C, 64.78; H, 5.01; N, 5.34.



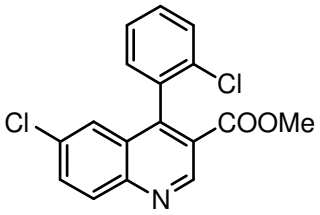
6-Chloro-4-phenylquinoline-3-carboxylic acid methyl ester (3be).

Yellow gummy mass (196 mg, 66%); IR (KBr): 1718 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.31 (s, 1H), 8.22-8.10 (m, 1H), 7.72-7.69 (m, 1H), 7.53-7.49 (m, 1H), 7.44-7.42 (m, 3H), 7.23-7.21 (m, 2H), 3.61 (s, 3H) ; ^{13}C NMR (100 MHz, $CDCl_3$): δ 166.7, 150.1, 149.9, 136.3, 131.0, 129.5, 128.7, 128.3, 128.1, 128.0, 127.5, 127.2, 52.1. Anal. Calcd for $C_{17}H_{12}ClNO_2$: C, 68.58; H, 4.06; N, 4.70. Found: C, 68.52; H, 4.01; N, 4.62.



4-Methylquinoline-3-carboxylic acid methyl ester (3ee).

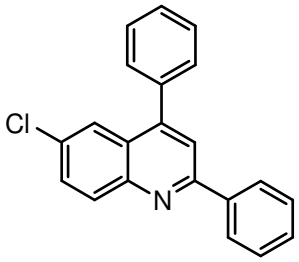
Yellow gummy mass (137 mg, 68%); IR (KBr): 1722 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 9.24 (s, 1H), 8.17 (d, *J* = 8.4 Hz, 1H), 8,12 (d, *J* = 8.4 Hz, 1H), 7.79 (t, *J* = 6.8 Hz, 1H), 7.62 (t, *J* = 6.8 Hz, 1H), 4.00 (s, 3H), 2.99 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.1, 150.2, 148.4, 147.8, 130.8, 130.0, 127.6, 127.1, 124.9, 122.9, 52.3, 15.3. Anal. Calcd for $C_{12}H_{11}NO_2$: C, 71.63; H, 5.51; N, 6.96. Found: C, 71.54; H, 5.43; N, 6.87.



6-Chloro-4-(2-chloro-phenyl)-quinoline-3-carboxylic acid methyl ester (3de).

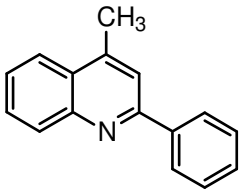
Brown gummy mass (199 mg, 60%); IR (KBr): 1720 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 9.47 (s, 1H), 8.17 (d, *J* = 9.2 Hz, 1H), 7.76 (dd, J_1 = 8.8 Hz, J_2 = 2.4 Hz, 1H), 7.60 (d, *J* = 8.0 Hz, 1H), 7.50-7.45 (m, 2H), 7.39 (d, *J* = 2.2 Hz, 1H), 7.22-7.20 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 165.4, 150.5, 147.8, 146.9, 134.8, 133.7, 132.7, 132.3, 131.3, 130.0, 130.0, 129.5, 127.4, 126.7, 125.6, 123.0, 52.4. Anal. Calcd for $C_{17}H_{11}C_{l2}NO_2$: C, 61.47; H, 3.34; N, 4.22. Found: C, 61.41; H, 3.24; N, 4.15.

Typical procedure for the synthesis of 6-chloro-2,4-diphenylquinoline (5af).[2]



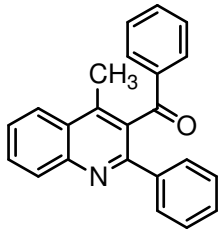
2-Amino-5-chlorobenzophenone (231 mg, 1 mmol) and phenylpropioloic acid (146 mg, 1 mmol) was mixed in a sealed tube and stirred at room temperature for 10 min. Then copper triflate (36 mg, 0.1 mmol) was added to the reaction mixture and heated at 110 ^oC. After completion (TLC), the reaction mixture was extracted with dichloromethane (10 mL x 2). Solvent was evaporated to furnished the crude product which

was subjected to column chromatography on silica gel to obtain the analytically pure product using petroleum ether/ethyl acetate as an eluent (white solid, 277 mg, 88%); Mp 124-125 ^{o}C; IR (KBr): 1620 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.08-8.05 (m, 3H), 7.76 (d, J = 2.4 Hz, 1H), 7.71 (s, 1H), 7.54 (dd, J_1 = 9.2 Hz, J_2 = 2.4 Hz, 1H), 7.47-7.33 (m, 8H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 157.0, 148.3, 147.1, 139.1, 137.6, 132.1, 131.6,130.3, 129.5, 129.3, 128.8, 128.7, 128.6, 127.4, 126.4, 124.4, 119.9.



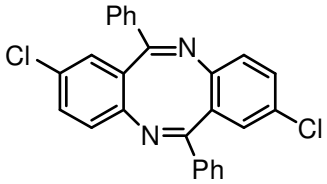
4-Methyl-2-phenylquinoline (5ef).[2]

White oil (184 mg, 84%); IR (KBr): 1640 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.08-8.02 (m, 3H), 7.86-7.82 (m, 1H), 7.61-7.75 (m, 2H), 7.43-7.32 (m, 4H), 2.61 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 157.1, 148.1, 144.9, 139.8, 130.3, 129.4, 129.2, 128.8, 127.6, 127.3, 126.1, 123.7, 119.8, 19.0.



(4-Methyl-2-phenyl-quinolin-3-yl)-phenyl-methanone (7eg).[3]

Yellow oil (281 mg, 87%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.13 (d, J = 8.4 Hz, 1H), 7.97 (d, J = 8.0 Hz, 1H), 7.67 (t, J = 8.0 Hz, 1H), 7.5-7.48 (m, 3H), 7.43 (dd, J_1 = 1.6 Hz, J_2 = 7.6 Hz, 2H), 7.29 (t, J = 7.6 Hz, 1H), 7.17-7.08 (m, 5H), 2.49 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 198.4, 156.1, 147.3, 142.5, 140.0, 137.5, 133.5, 132.5, 130.3, 130.2, 129.3, 129.2, 128.6, 128.5, 128.2, 127.0, 126.3, 124.0, 15.8.



2,8-Dichloro-6,12-diphenyldibenzo[*b*,*f*][1,5]diazocine (8).[2]

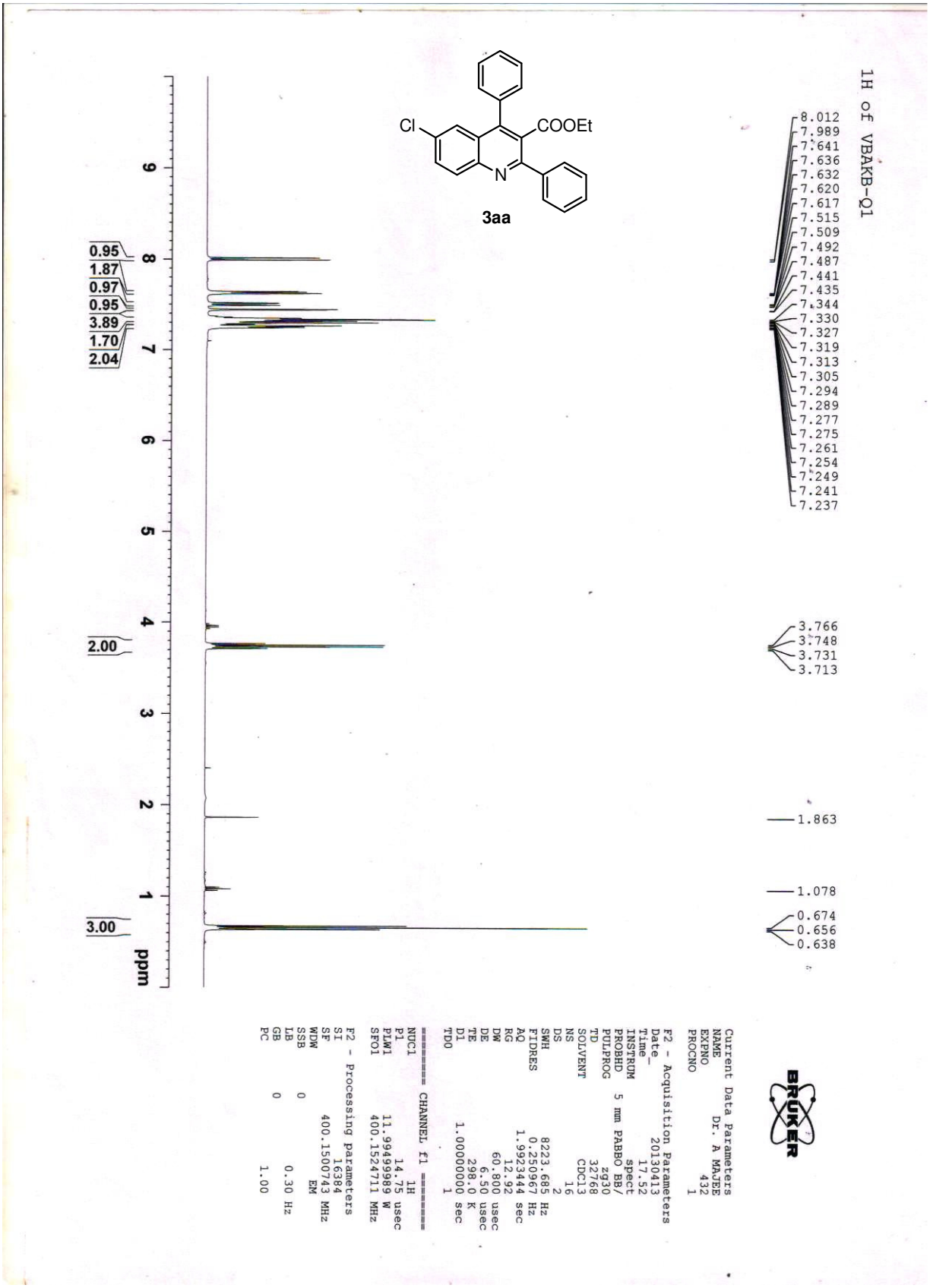
Yellow solid, 230 mg, 54%; Mp 210-212 ^{o}C; IR (KBr): 1586 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.54 (d, *J* = 7.2 Hz, 4H), 7.45-7.24 (m, 8H), 6.91-6.87 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 168.9, 150.2, 13.2, 131.7, 130.2, 129.5, 129.2, 128.9, 128.2, 127.3, 122.6.

References:

1 S. Cai, J. Zeng, Y. Bai and X. –W. Liu, *J. Org. Chem.*, 2012, **77**, 801.

2 T. Chanda, R. K. Verma and M. S. Singh, *Chem. Asian J.,* 2012, **7**, 728.

3 B.V. S. Reddy, A. Venkateswarlu, G. N. Reddy and Y.V. R. Reddy, *Tetrahedron Lett.,* 2013, **54**, 5767.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3aa
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7.632
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7.617
7.515
7.509
7.492
7.487
7.441
7.435
7.344
7.330
7.327
7.319
7.313
7.305
7.294
7.289
7.277
7.275
7.261
7.254
7.249
7.241
7.237
3.766
3.748
3.731
3.713
1.863
1.078
0.674
0.656
0.638
0.95
1.87
0.97
0.95
3.89
1.70
2.04
2.00
3.00
ppm
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EXPNO 432
PROCNO 1
F2 - Acquisition Parameters
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Time 17.52
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PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.992344 sec
RG 12.92
DW 60.800 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
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P1 14.75 usec
PLW1 11.99499989 W
SFO1 400.1524711 MHz
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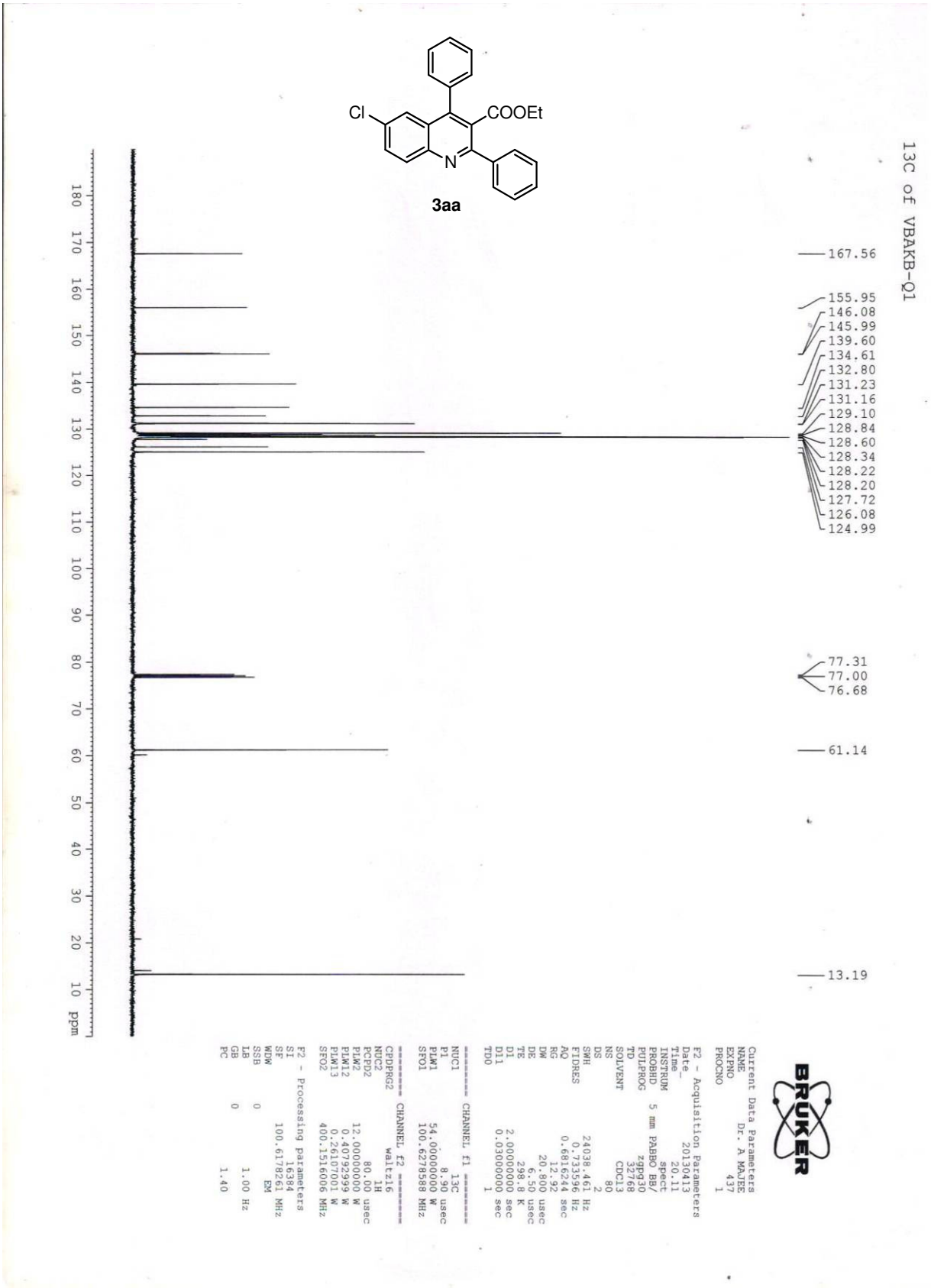
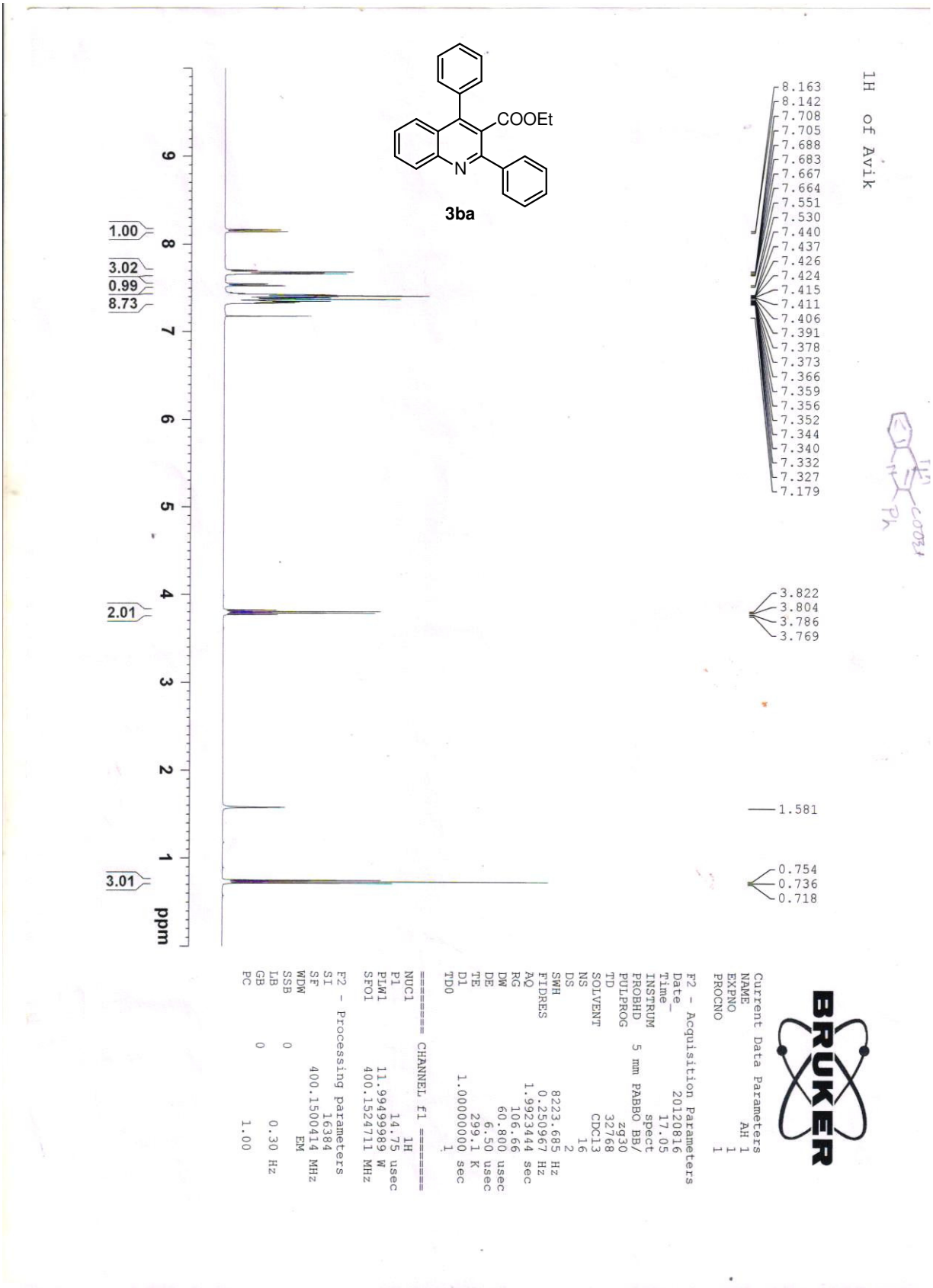
LB 0.30 Hz
GB 0
PC 1.00
BRUKER

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8.142
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7.705
7.688
7.683
7.667
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7.551
7.530
7.440
7.437
7.426
7.424
7.415
7.411
7.406
7.391
7.378
7.373
7.366
7.359
7.356
7.352
7.344
7.340
7.332
7.327
7.179
3.822
3.804
3.786
3.769
1.581
0.754
0.736
0.718
COOEt
N
3ba
1.00
3.02
0.99
8.73
2.01
3.01
ppm
Current Data Parameters
NAME AH 1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120816
Time_ 17.05
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PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9923444 sec
RG 106.66
DW 60.800 usec
DE 6.50 usec
TE 299.1 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
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P1 14.75 usec
PLW1 11.99499989 W
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F2 - Processing parameters
SI 16384
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SSB 0
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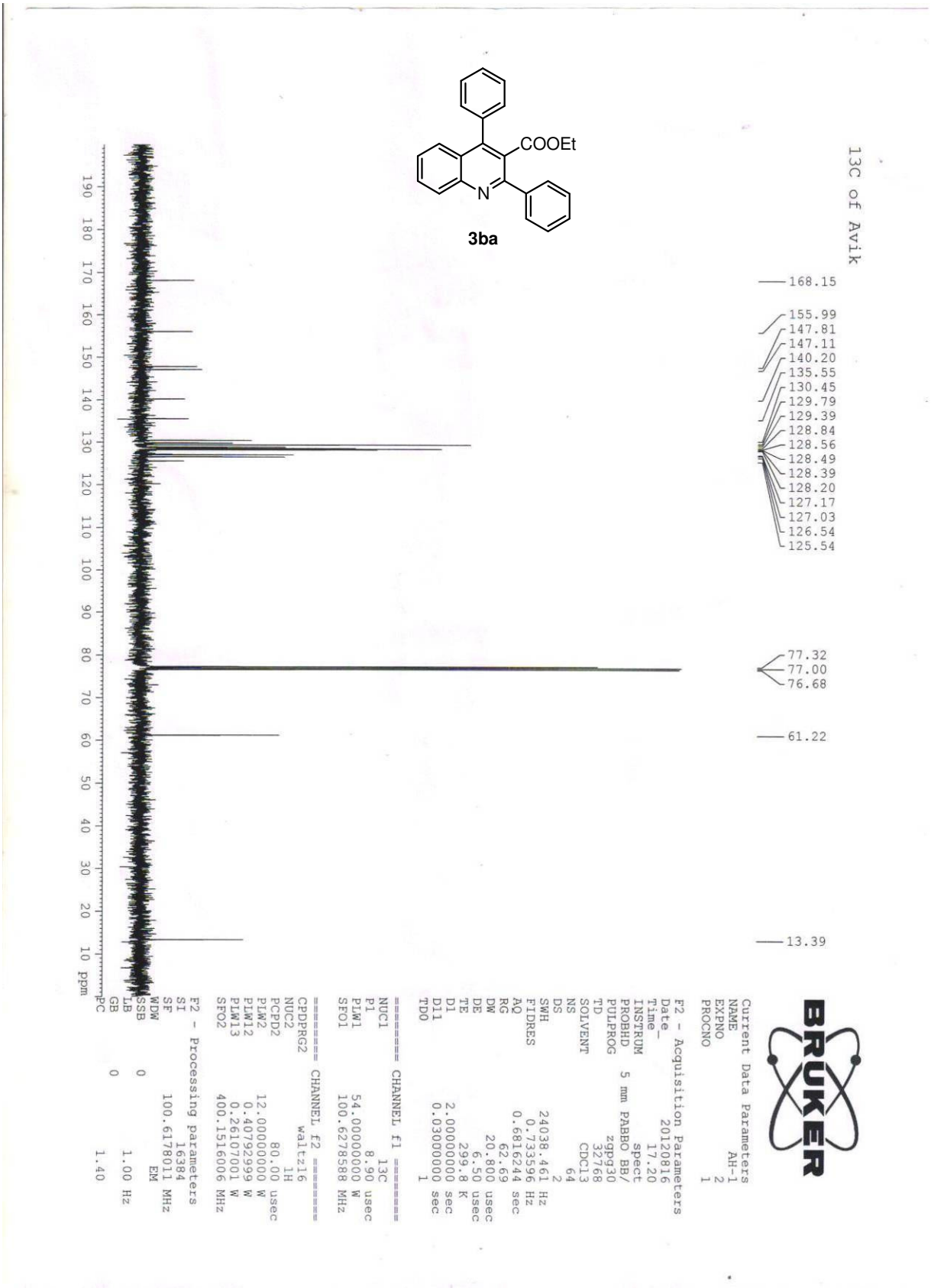
GB 0
PC 1.00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N
3ba
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147.81
147.11
140.20
135.55
130.45
129.79
129.39
128.84
128.56
128.49
128.39
128.20
127.17
127.03
126.54
125.54
77.32
77.00
76.68
61.22
13.39
ppm
Current Data Parameters
NAME AH-1
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120816
Time 17.20
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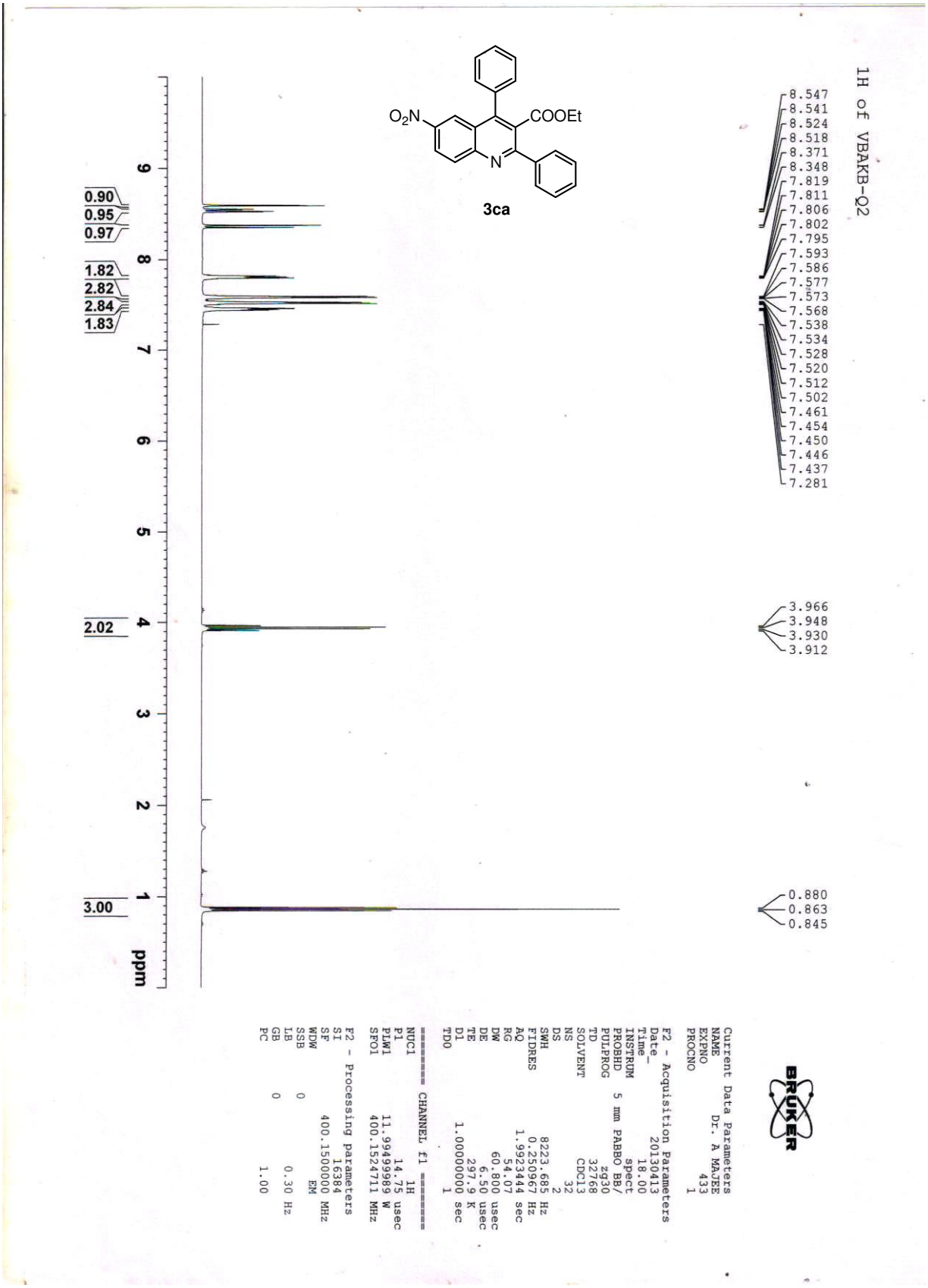
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 64
DS 2
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.681244 sec
RG 62.69
DW 20.800 usec
DE 6.50 usec
TE 299.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 8.90 usec
PLW1 54.00000000 W
SFO1 100.6278588 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PLW2 12.00000000 W
PLW12 0.40792999 W
PLW13 0.26107001 W
SFO2 400.1516006 MHz
F2 - Processing parameters
SI 16384
SF 100.6178011 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40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O2N
COOEt
N
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8.541
8.524
8.518
8.371
8.348
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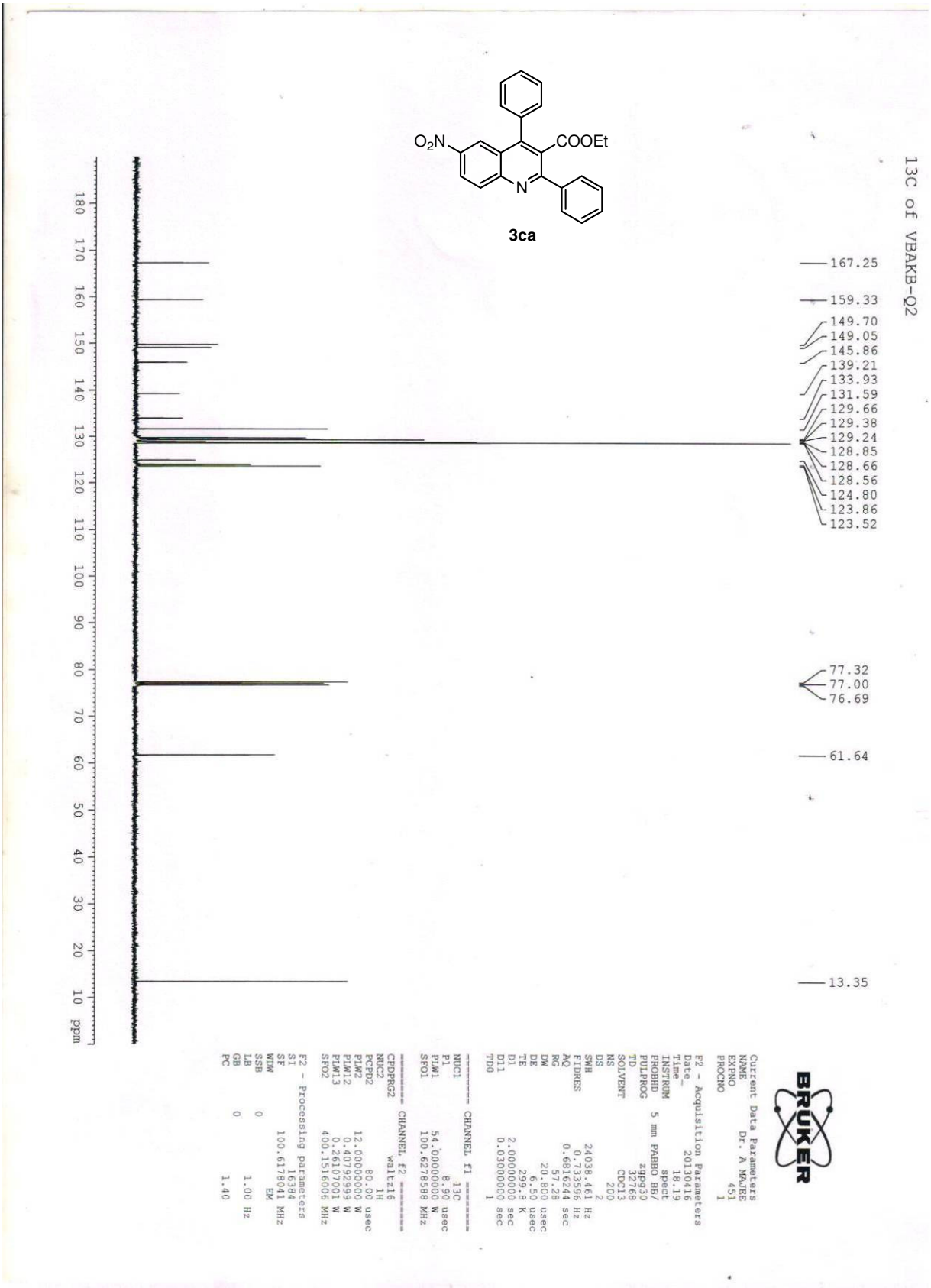
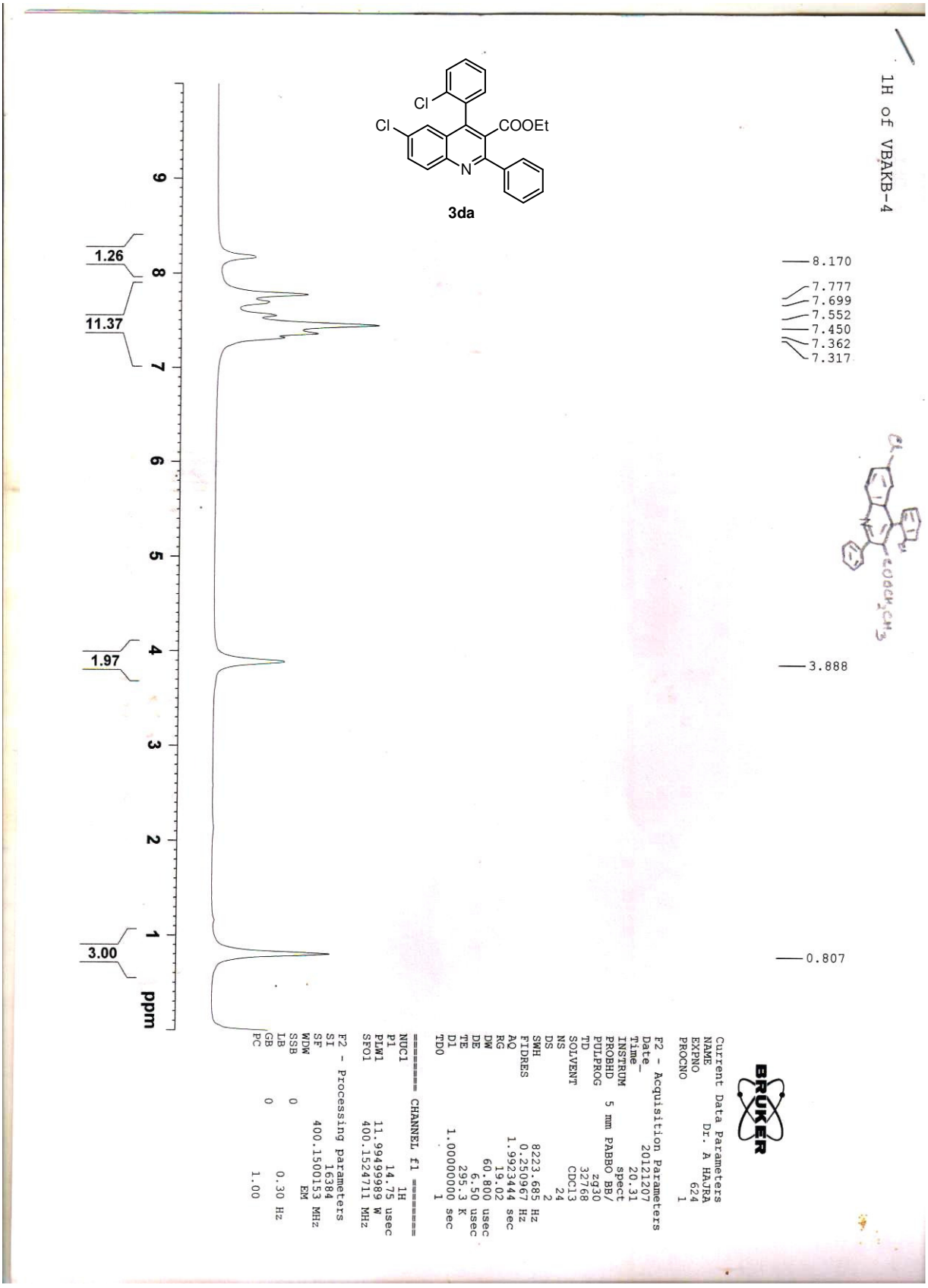
7.811
7.806
7.802
7.795
7.593
7.586
7.577
7.573
7.568
7.538
7.534
7.528
7.520
7.512
7.502
7.461
7.454
7.450
7.446
7.437
7.281
3.966
3.948
3.930
3.912
0.880
0.863
0.845
0.90
0.95
0.97
1.82
2.82
2.84
1.83
2.02
3.00
ppm
Current Data Parameters
NAME Dr. A MAJEE
EXPNO 433
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130413
Time_ 18.00
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 2
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.992344 sec
RG 54.07
DW 60.800 usec
DE 6.50 usec
TE 297.9 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.75 usec
PLW1 11.99499969 W
SFO1 400.1524711 MHz
F2 - Processing parameters
SI 16384
SF 400.1500000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
BRUKER


13C of VBAKB-Q2
3ca
167.25
159.33
149.70
149.05
145.86
139.21
133.93
131.59
129.66
129.38
129.24
128.85
128.66
128.56
124.80
123.86
123.52
77.32
77.00
76.69
61.64
13.35
ppm
Current Data Parameters
NAME
EXPNO
PROCNO
F2 - Acquisition Parameters
Date_
Time
INSTRUM
PROBHD
PULPROG
TD
SOLVENT
NS
DS
SWH
FIDRES
AQ
RG
DW
DE
TE
D1
D11
TD0
CHANNEL f1
NUC1
P1
PLW1
SFO1
CHANNEL f2
CPDPRG2
NUC2
PCPD2
PLW2
PLW12
PLW13
SFO2
F2 - Processing parameters
SI
SF
WDW
SSB
LB
GB
PC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Cl
Cl
COOEt
N
3da
8.170
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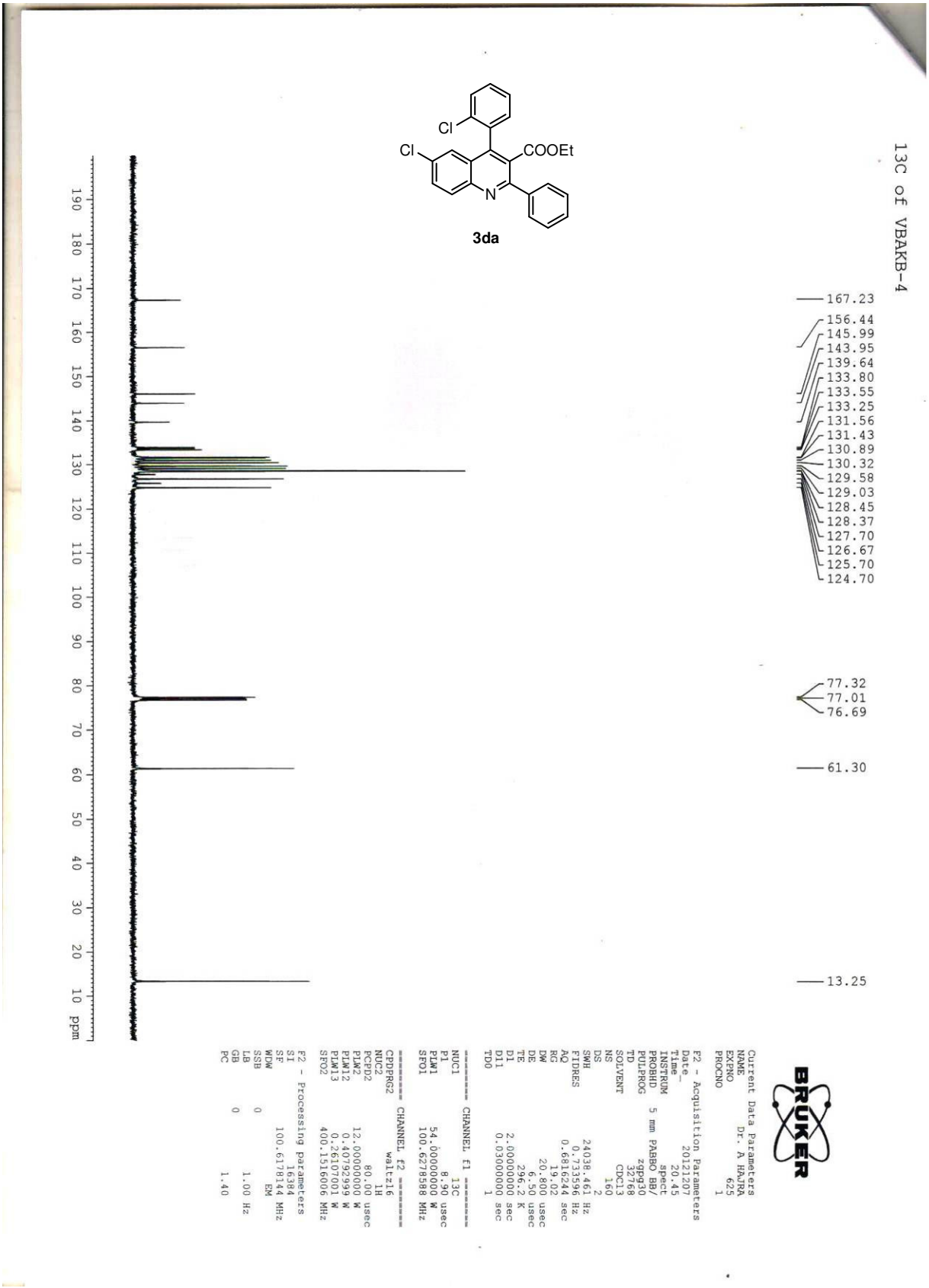
7.699
7.552
7.450
7.362
7.317
3.888
0.807
1.26
11.37
1.97
3.00
ppm
Current Data Parameters
NAME Dr. A HAJRA
EXPNO 624
PROCNO 1
F2 - Acquisition Parameters
Date_ 20121207
Time_ 20.31
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG z930
TD 32768
SOLVENT CDCl3
NS 24
DS 2
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9923444 sec
RG 19.02
DW 60.800 usec
DE 6.50 usec
TE 295.3 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.75 usec
PLW1 11.99499989 W
SFO1 400.1524711 MHz
F2 - Processing parameters
SI 16384
SF 400.1500153 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
BRUKER


13C of VBAKB-4
Cl
Cl
COOEt
N
3da
167.23
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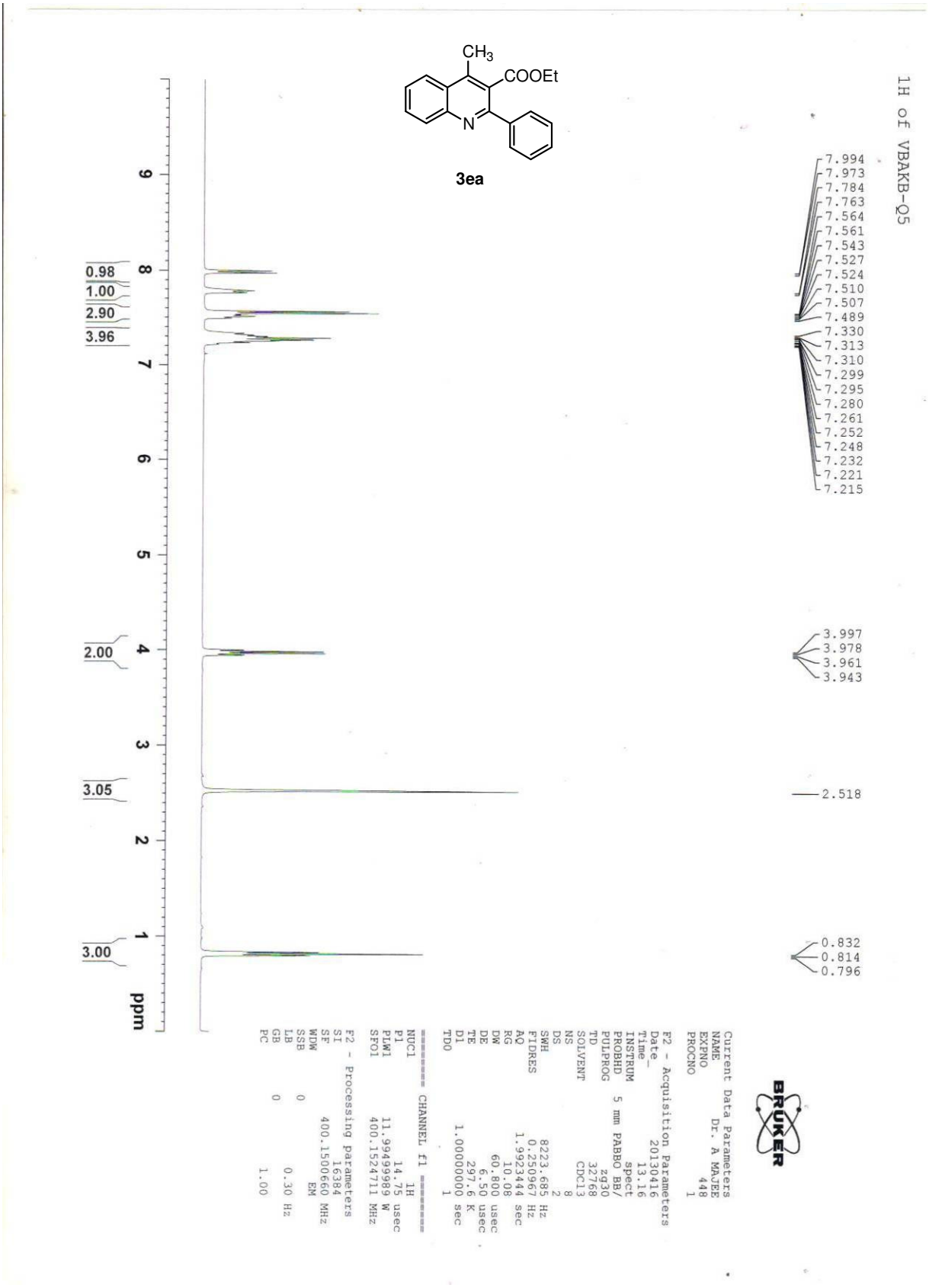
145.99
143.95
139.64
133.80
133.55
133.25
131.56
131.43
130.89
130.32
129.58
129.03
128.45
128.37
127.70
126.67
125.70
124.70
77.32
77.01
76.69
61.30
13.25
ppm
Current Data Parameters
NAME Dr. A HAJRA
EXPNO 625
PROCNO 1
F2 - Acquisition Parameters
Date_ 20121207
Time_ 20.45
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 160
DS 2
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6816244 sec
RG 19.02
DW 20.800 usec
DE 6.50 usec
TE 296.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 8.90 usec
PLW1 54.00000000 W
SFO1 100.6278588 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PLW2 12.00000000 W
PLW12 0.40792999 W
PLW13 0.26107001 W
SFO2 400.1516006 MHz
F2 - Processing parameters
SI 16384
SF 100.6178144 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


1H of VBAKB-Q5
3ea
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7.973
7.784
7.763
7.564
7.561
7.543
7.527
7.524
7.510
7.507
7.489
7.330
7.313
7.310
7.299
7.295
7.280
7.261
7.252
7.248
7.232
7.221
7.215
3.997
3.978
3.961
3.943
2.518
0.832
0.814
0.796
0.98
1.00
2.90
3.96
2.00
3.05
3.00
ppm
Current Data Parameters
NAME Dr. A MAJEE
EXPNO 448
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130416
Time 13.16
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 2
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.992344 sec
RG 10.08
DW 60.800 usec
DE 6.50 usec
TE 297.6 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.75 usec
PLW1 11.99499989 W
SFO1 400.1524711 MHz
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WDW EM
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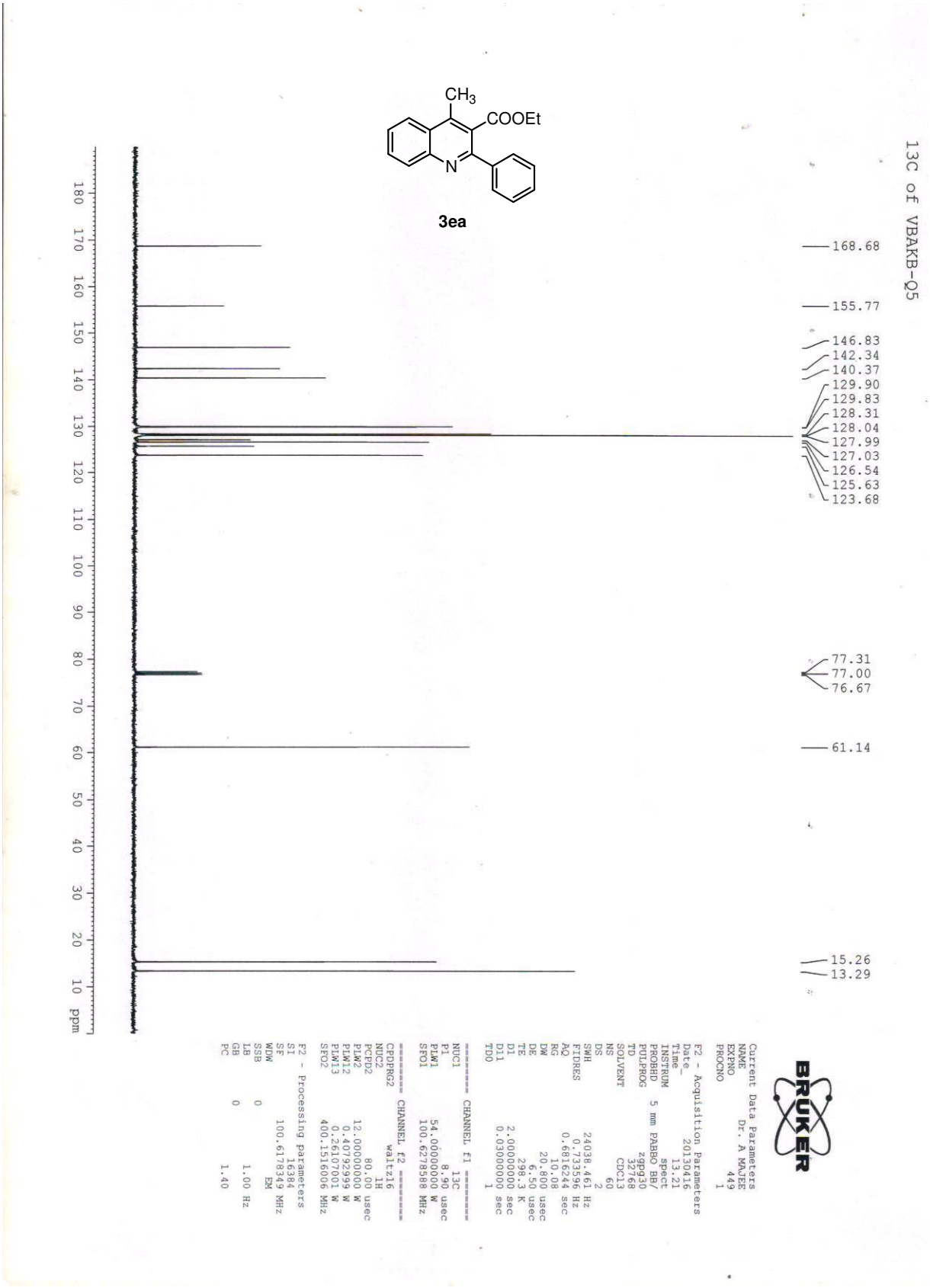
GB 0
PC 1.00
BRUKER


13C of VBAKB-Q5
CH3
COOEt
N
3ea
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146.83
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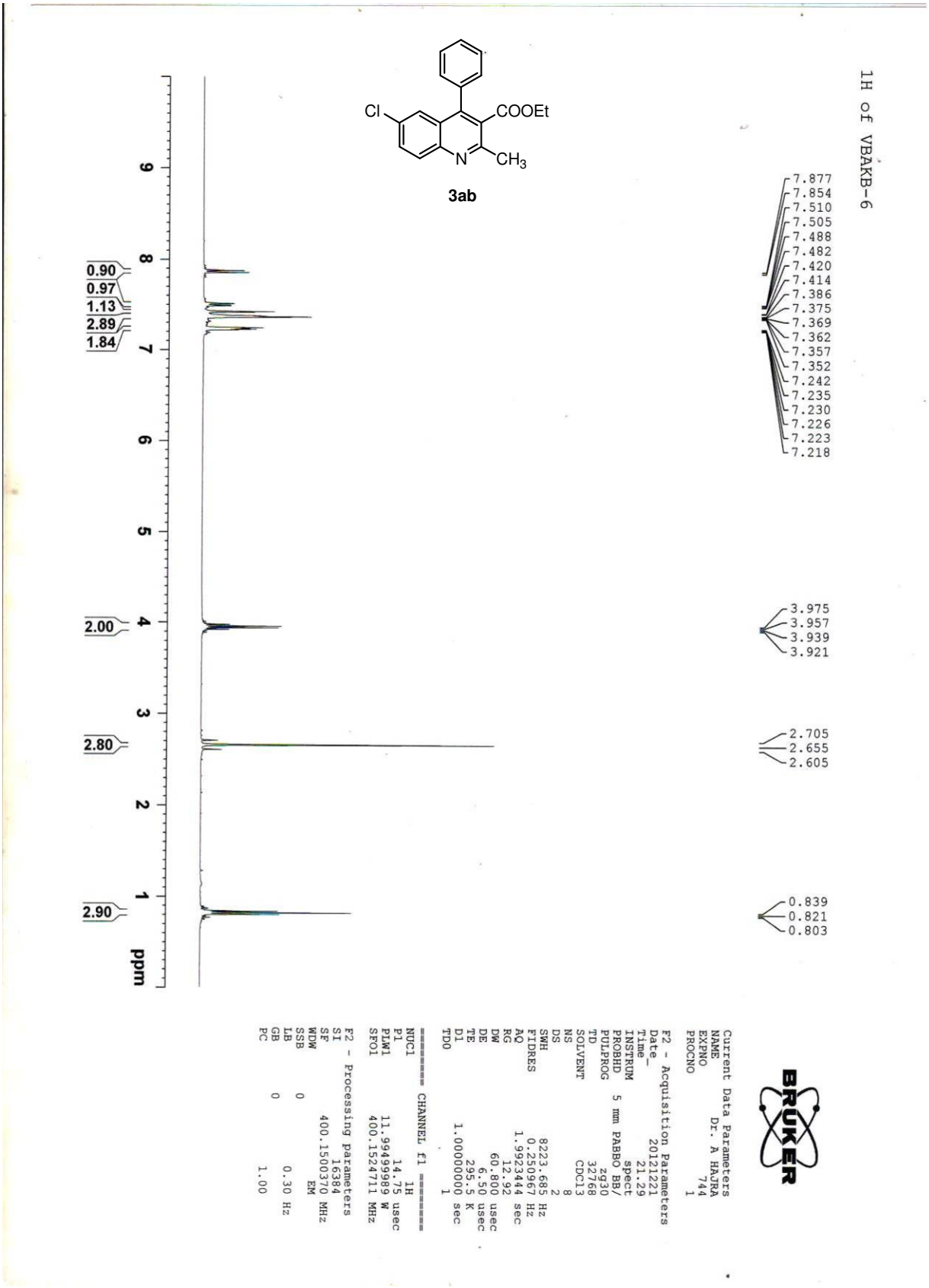
140.37
129.90
129.83
128.31
128.04
127.99
127.03
126.54
125.63
123.68
77.31
77.00
76.67
61.14
15.26
13.29
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm
Current Data Parameters
NAME Dr. A MAJEE
EXPNO 449
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130416
Time 13.21
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 60
DS 2
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6816244 sec
RG 10.08
DW 20.800 usec
DE 6.50 usec
TE 298.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 8.90 usec
PLW1 54.00000000 W
SFO1 100.6278588 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PLW2 12.00000000 W
PLW12 0.40792999 W
PLW13 0.26107001 W
SFO2 400.1516006 MHz
F2 - Processing parameters
SI 16384
SF 100.6178349 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40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7.226
7.223
7.218
3.975
3.957
3.939
3.921
2.705
2.655
2.605
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0.821
0.803
0.90
0.97
1.13
2.89
1.84
2.00
2.80
2.90
ppm
Current Data Parameters
NAME Dr. A HAJRA
EXPNO 744
PROCNO 1
F2 - Acquisition Parameters
Date_ 20121221
Time_ 21.29
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PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 2
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9923444 sec
RG 12.92
DW 60.800 usec
DE 6.50 usec
TE 295.5 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.75 usec
PLW1 11.99499989 W
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F2 - Processing parameters
SI 16384
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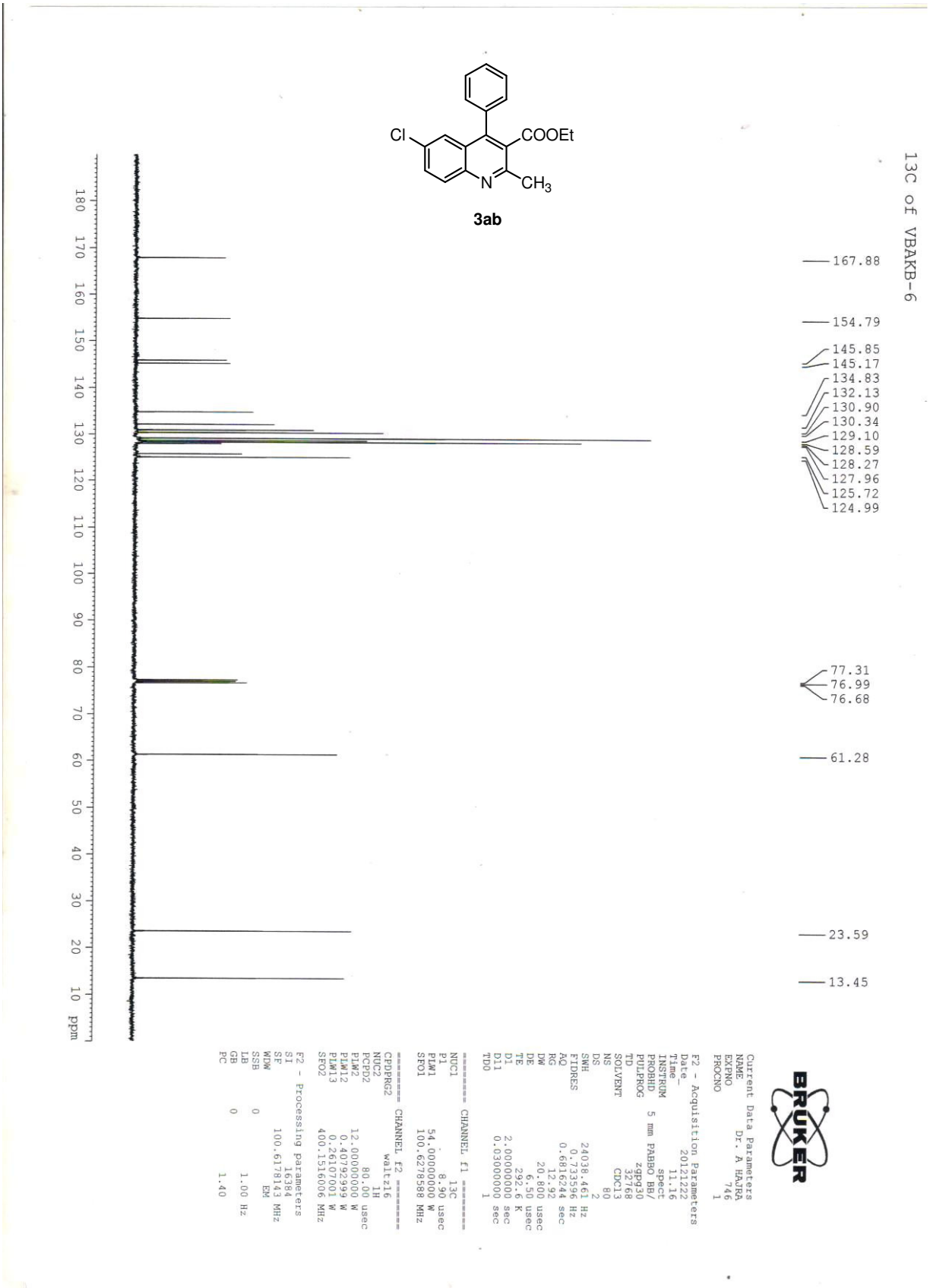
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
BRUKER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COOEt
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CH3
3ab
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145.85
145.17
134.83
132.13
130.90
130.34
129.10
128.59
128.27
127.96
125.72
124.99
77.31
76.99
76.68
61.28
23.59
13.45
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm
Current Data Parameters
NAME Dr. A HAJRA
EXPNO 746
PROCNO 1
F2 - Acquisition Parameters
Date_ 20121222
Time 11.16
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 80
DS 2
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6816244 sec
RG 12.92
DW 20.800 usec
DE 6.50 usec
TE 292.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
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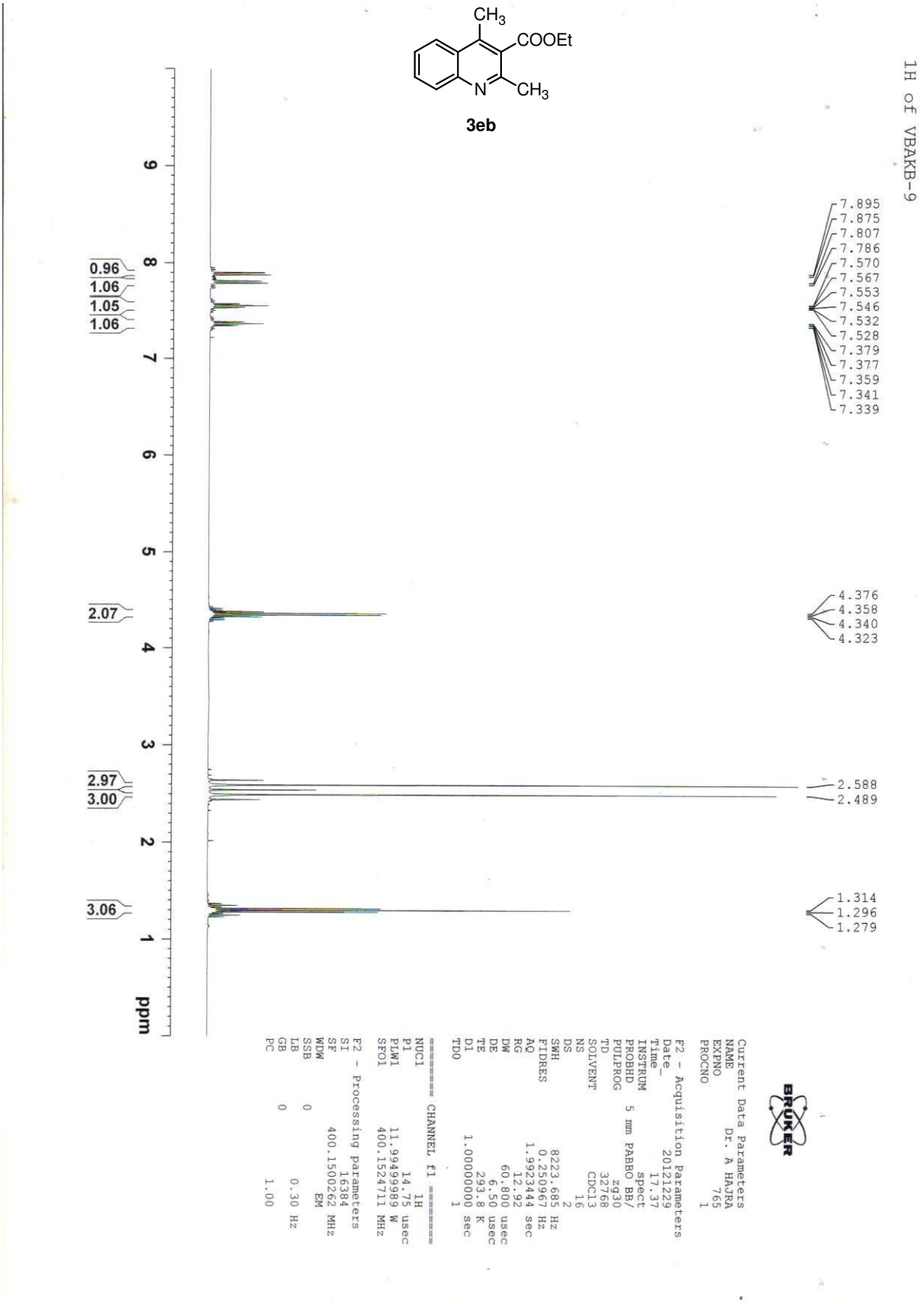
NUC1 13C
P1 8.90 usec
PLW1 54.00000000 W
SFO1 100.6278588 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PLW2 12.00000000 W
PLW12 0.40792999 W
PLW13 0.26107001 W
SFO2 400.1516006 MHz
F2 - Processing parameters
SI 16384
SF 100.6178143 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40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COOEt
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CH3
3eb
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7.786
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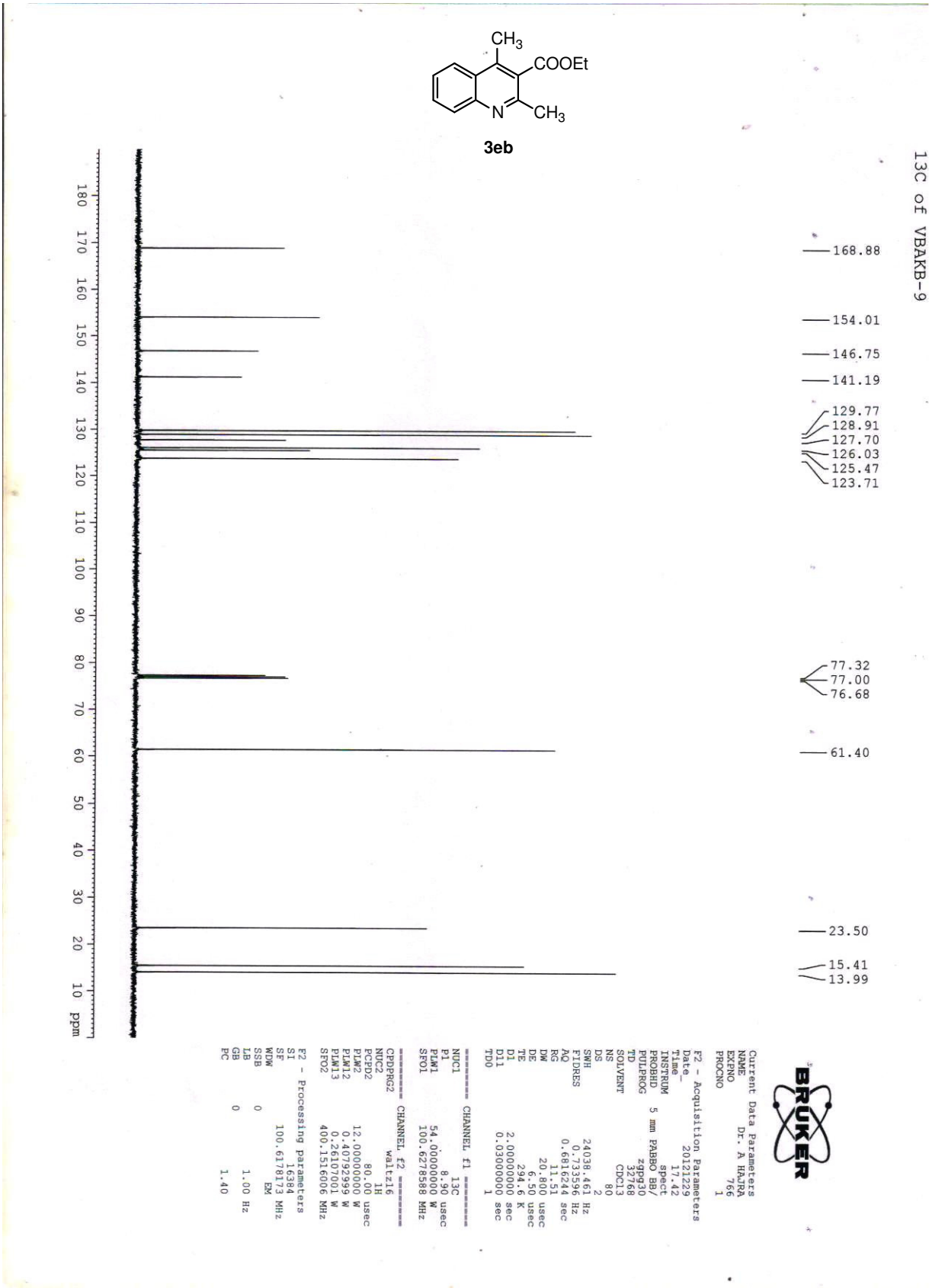
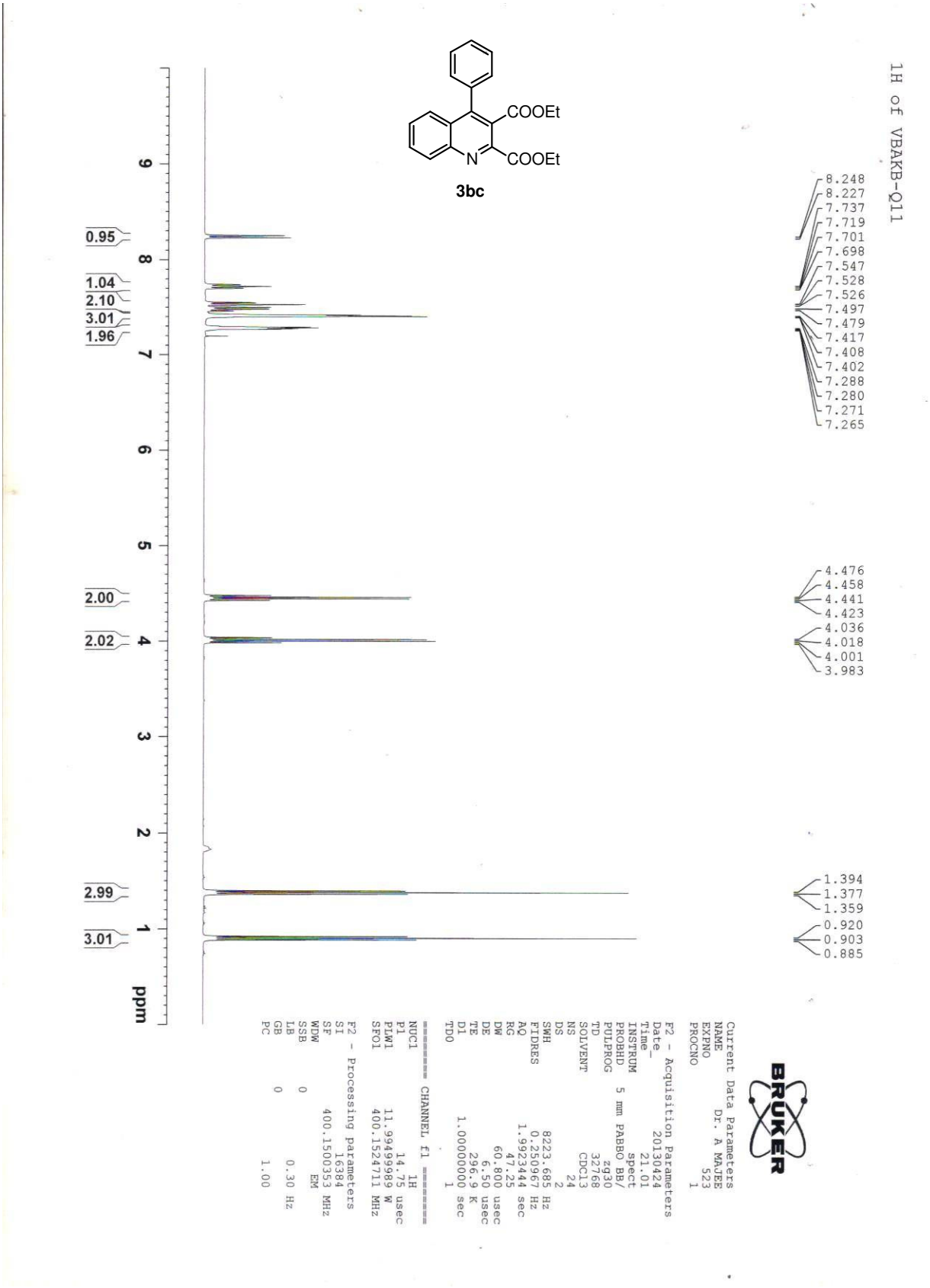
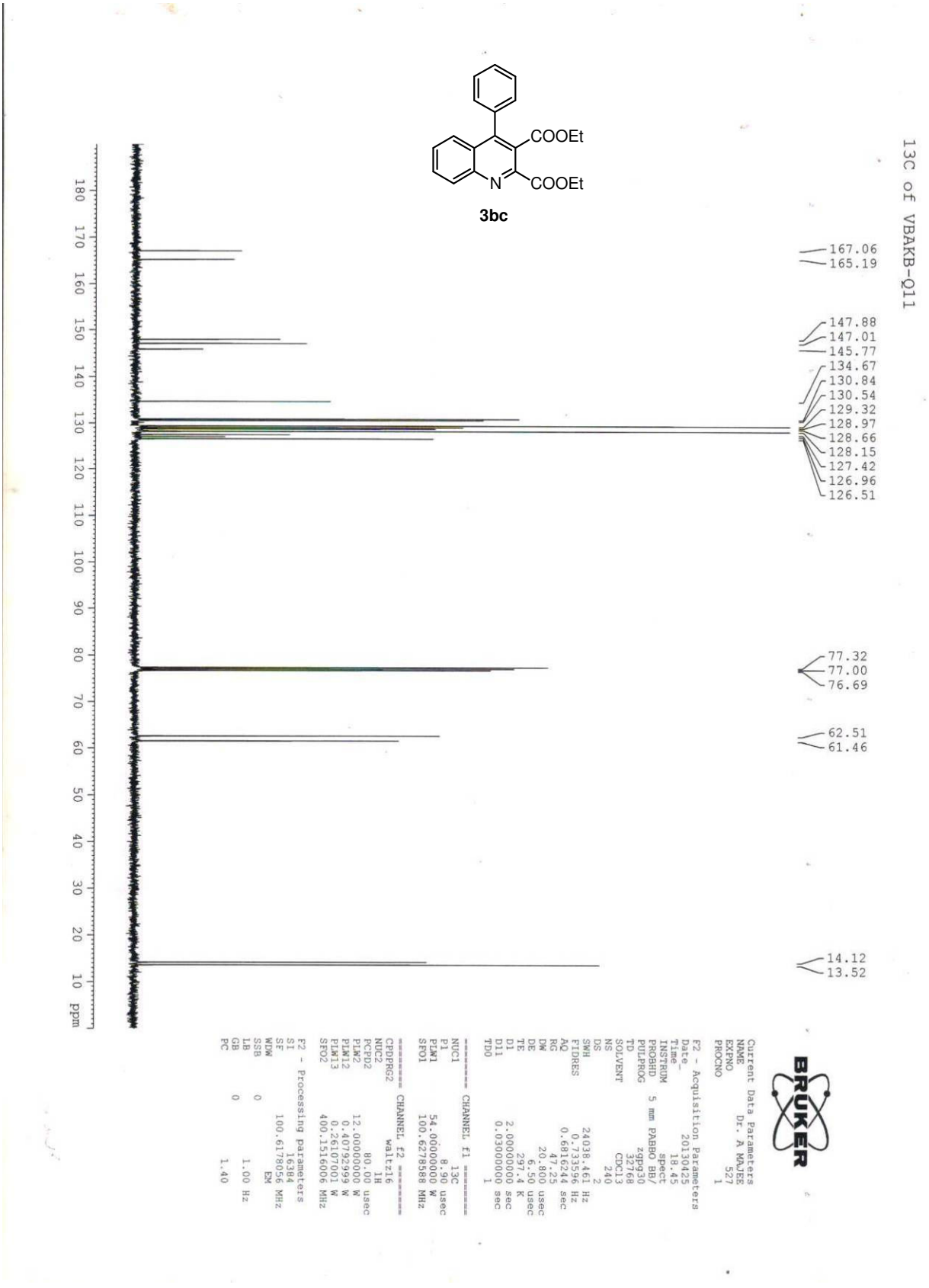
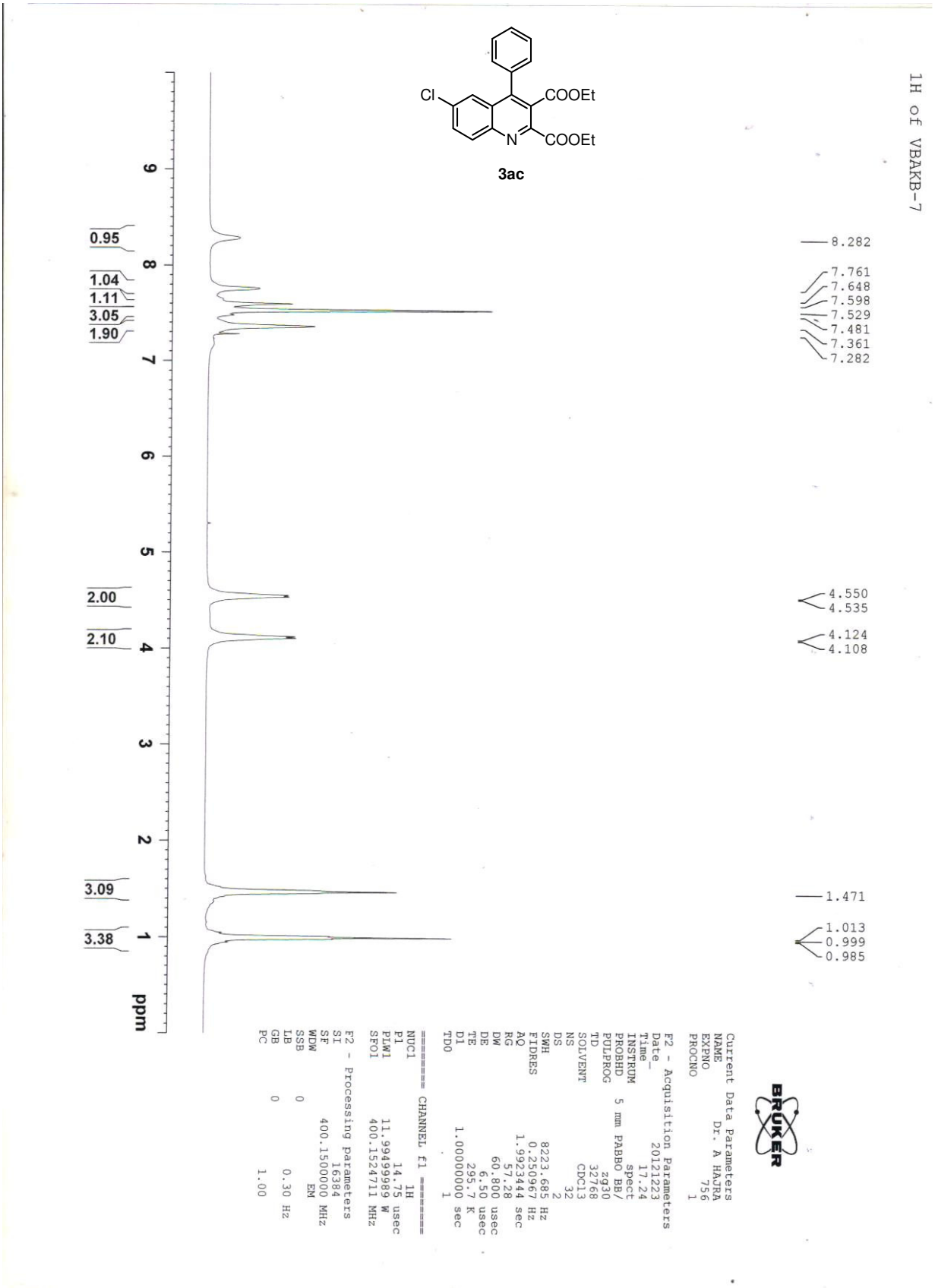
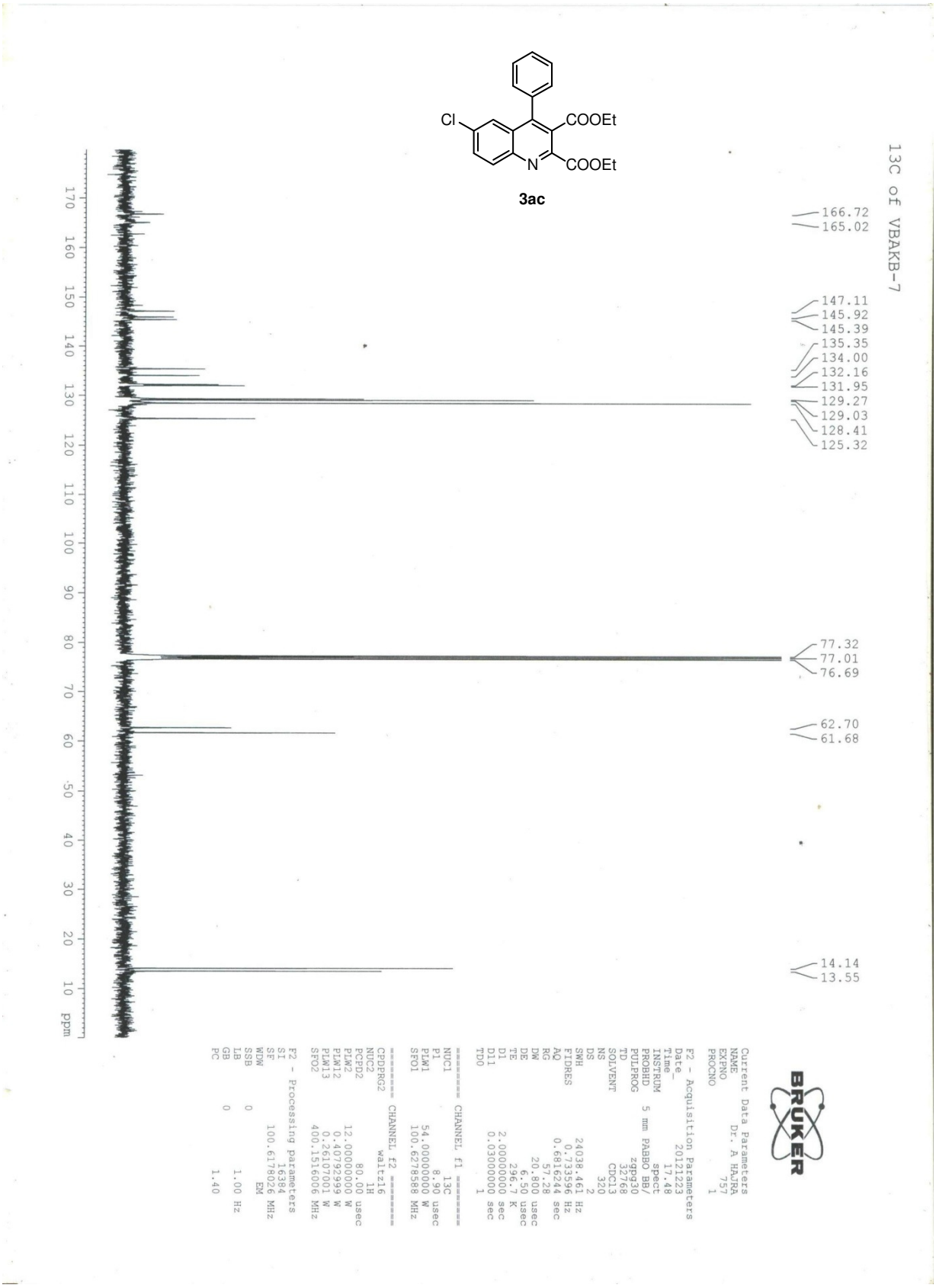
7.567
7.553
7.546
7.532
7.528
7.379
7.377
7.359
7.341
7.339
4.376
4.358
4.340
4.323
2.588
2.489
1.314
1.296
1.279
0.96
1.06
1.05
1.06
2.07
2.97
3.00
3.06
ppm
Current Data Parameters
NAME Dr. A HAJRA
EXPNO 765
PROCNO 1
F2 - Acquisition Parameters
Date_ 20121229
Time_ 17.37
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.992344 sec
RG 12.92
DW 60.800 usec
DE 6.50 usec
TE 293.8 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.75 usec
PLW1 11.99499989 W
SFO1 400.1524711 MHz
F2 - Processing parameters
SI 16384
SF 400.1500262 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
BRUKER

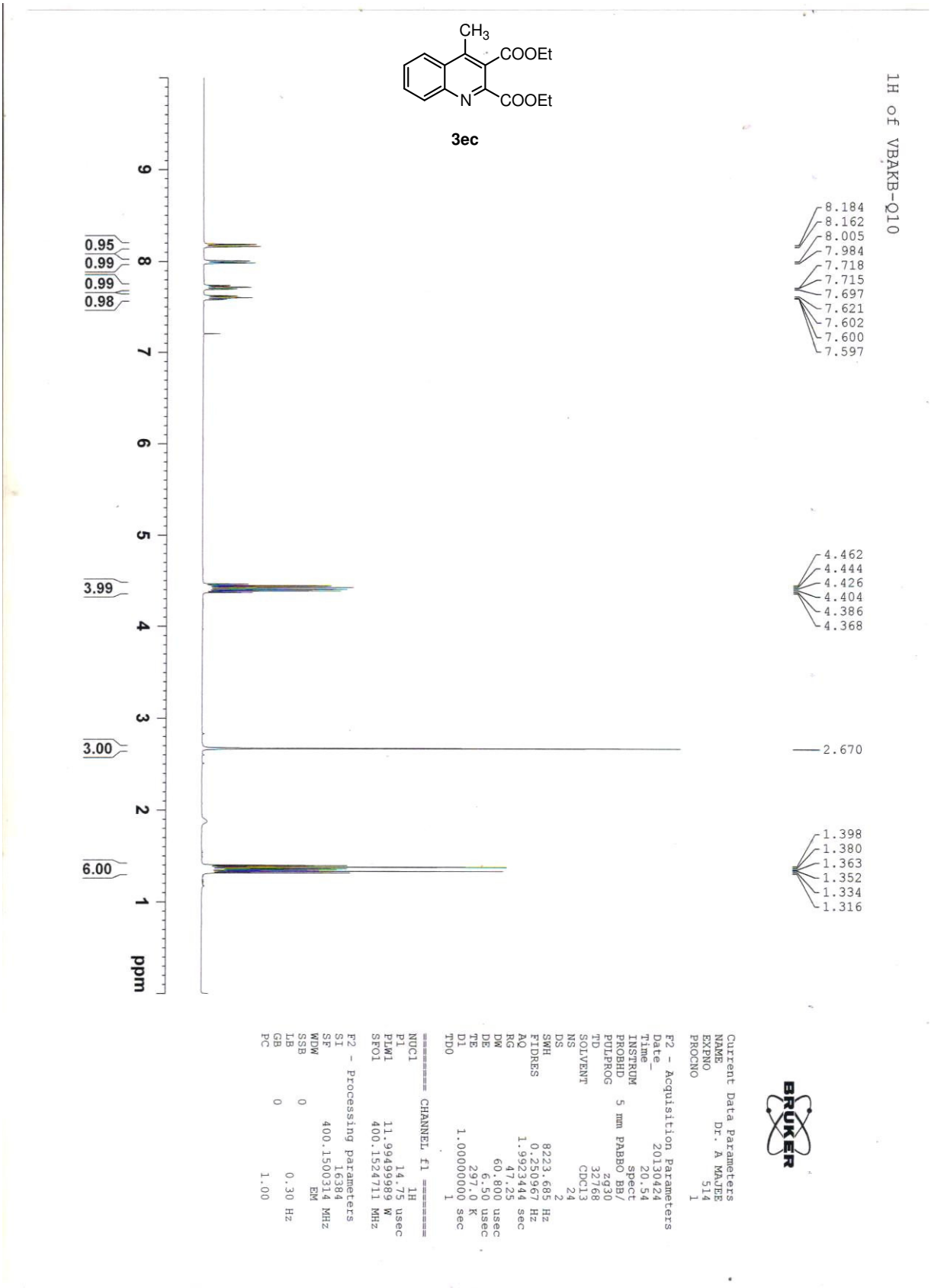

CH3
COOEt
N
CH3
3eb
13C of VBAKB-9
168.88
154.01
146.75
141.19
129.77
128.91
127.70
126.03
125.47
123.71
77.32
77.00
76.68
61.40
23.50
15.41
13.99
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm
Current Data Parameters
NAME Dr. A HAJRA
EXPNO 766
PROCNO 1
F2 - Acquisition Parameters
Date_ 20121229
Time_ 17.42
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 80
DS 2
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6816244 sec
RG 11.51
DW 20.800 usec
DE 6.50 usec
TE 294.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 8.90 usec
PLW1 54.00000000 W
SFO1 100.6278588 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PLW2 12.00000000 W
PLW12 0.40792999 W
PLW13 0.26107001 W
SFO2 400.1516006 MHz
F2 - Processing parameters
SI 16384
SF 100.6178173 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
BRUKER


1H of VBAKB-Q11
COOEt
COOEt
N
3bc
8.248
8.227
7.737
7.719
7.701
7.698
7.547
7.528
7.526
7.497
7.479
7.417
7.408
7.402
7.288
7.280
7.271
7.265
4.476
4.458
4.441
4.423
4.036
4.018
4.001
3.983
1.394
1.377
1.359
0.920
0.903
0.885
0.95
1.04
2.10
3.01
1.96
2.00
2.02
2.99
3.01
ppm
Current Data Parameters
NAME Dr. A MAJEE
EXPNO 523
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130424
Time_ 21.01
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 24
DS 2
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9923444 sec
RG 47.25
DW 60.800 usec
DE 6.50 usec
TE 296.9 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.75 usec
PLW1 11.99499989 W
SFO1 400.1524711 MHz
F2 - Processing parameters
SI 16384
SF 400.1500353 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
BRUKER

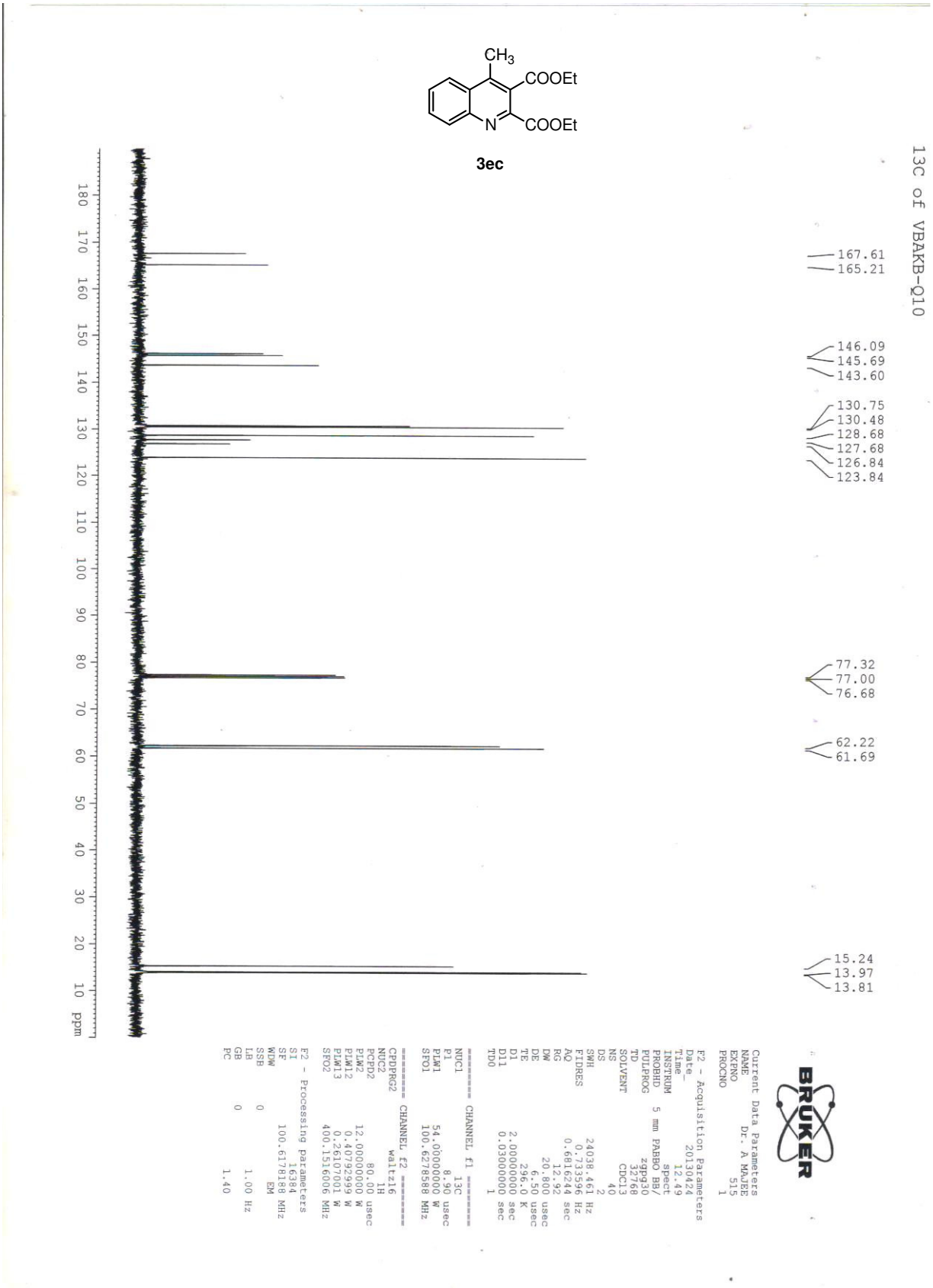

13C of VBAKB-Q11
COOEt
COOEt
N
3bc
167.06
165.19
147.88
147.01
145.77
134.67
130.84
130.54
129.32
128.97
128.66
128.15
127.42
126.96
126.51
77.32
77.00
76.69
62.51
61.46
14.12
13.52
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm
Current Data Parameters
NAME Dr. A MAJEE
EXPNO 527
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130425
Time 18.45
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 240
DS 2
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6816244 sec
RG 47.25
DW 20.800 usec
DE 6.50 usec
TE 297.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 8.90 usec
PLW1 54.00000000 W
SFO1 100.6278588 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PLW2 12.00000000 W
PLW12 0.40729299 W
PLW13 0.22617001 W
SFO2 400.1516006 MHz
F2 - Processing parameters
SI 16384
SF 100.6178056 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
BRUKER

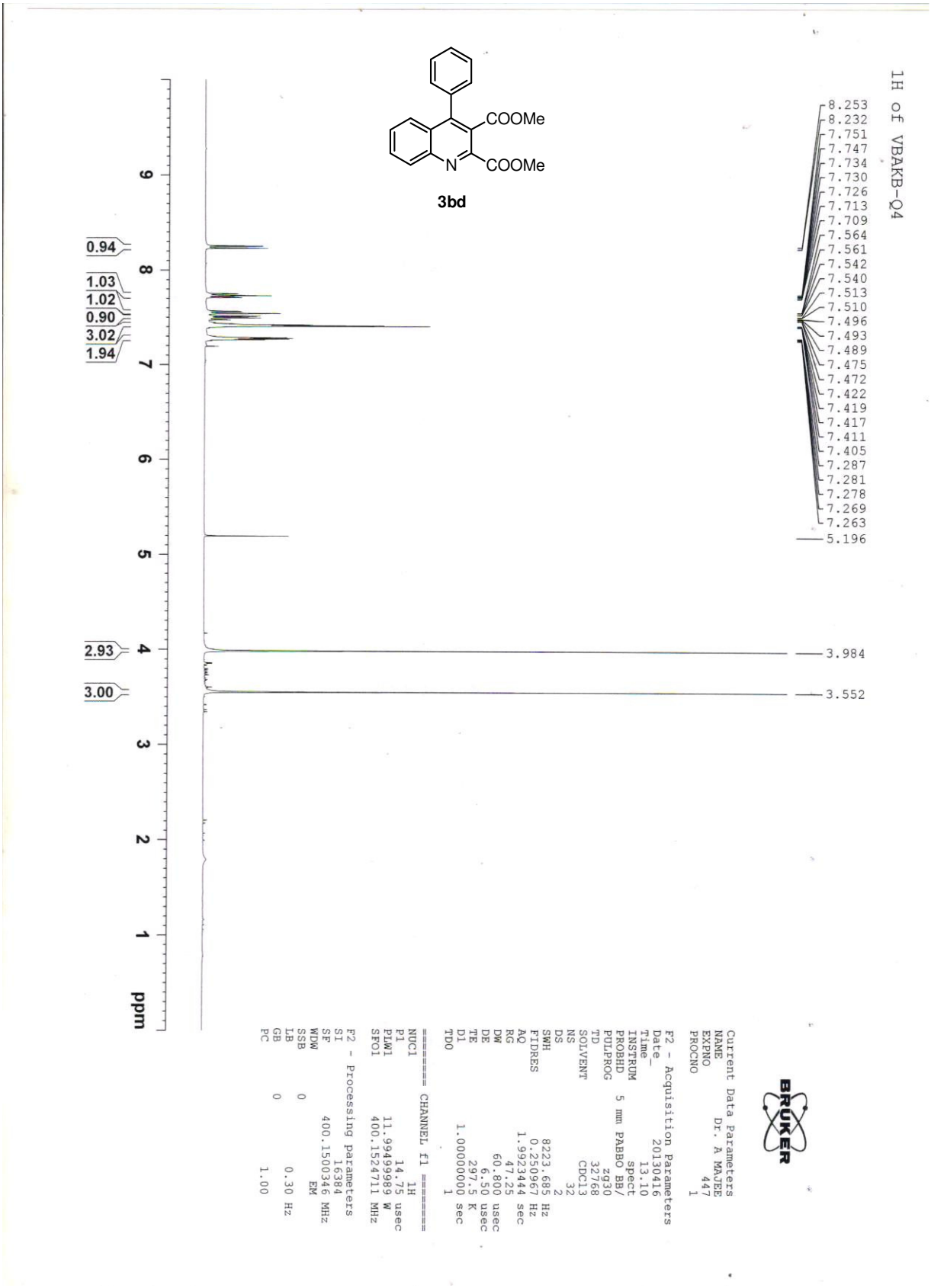

1H of VBAKB-7
Cl
COOEt
N
COOEt
3ac
0.95
1.04
1.11
3.05
1.90
2.00
2.10
3.09
3.38
ppm
8.282
7.761
7.648
7.598
7.529
7.481
7.361
7.282
4.550
4.535
4.124
4.108
1.471
1.013
0.999
0.985
Current Data Parameters
NAME Dr. A HAJRA
EXPNO 756
PROCNO 1
F2 - Acquisition Parameters
Date_ 20121223
Time 17.24
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 2
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.992444 sec
RG 57.28
DW 60.800 usec
DE 6.50 usec
TE 295.7 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.75 usec
PLW1 11.99499989 W
SFO1 400.1524711 MHz
F2 - Processing parameters
SI 16384
SF 400.1500000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
BRUKER

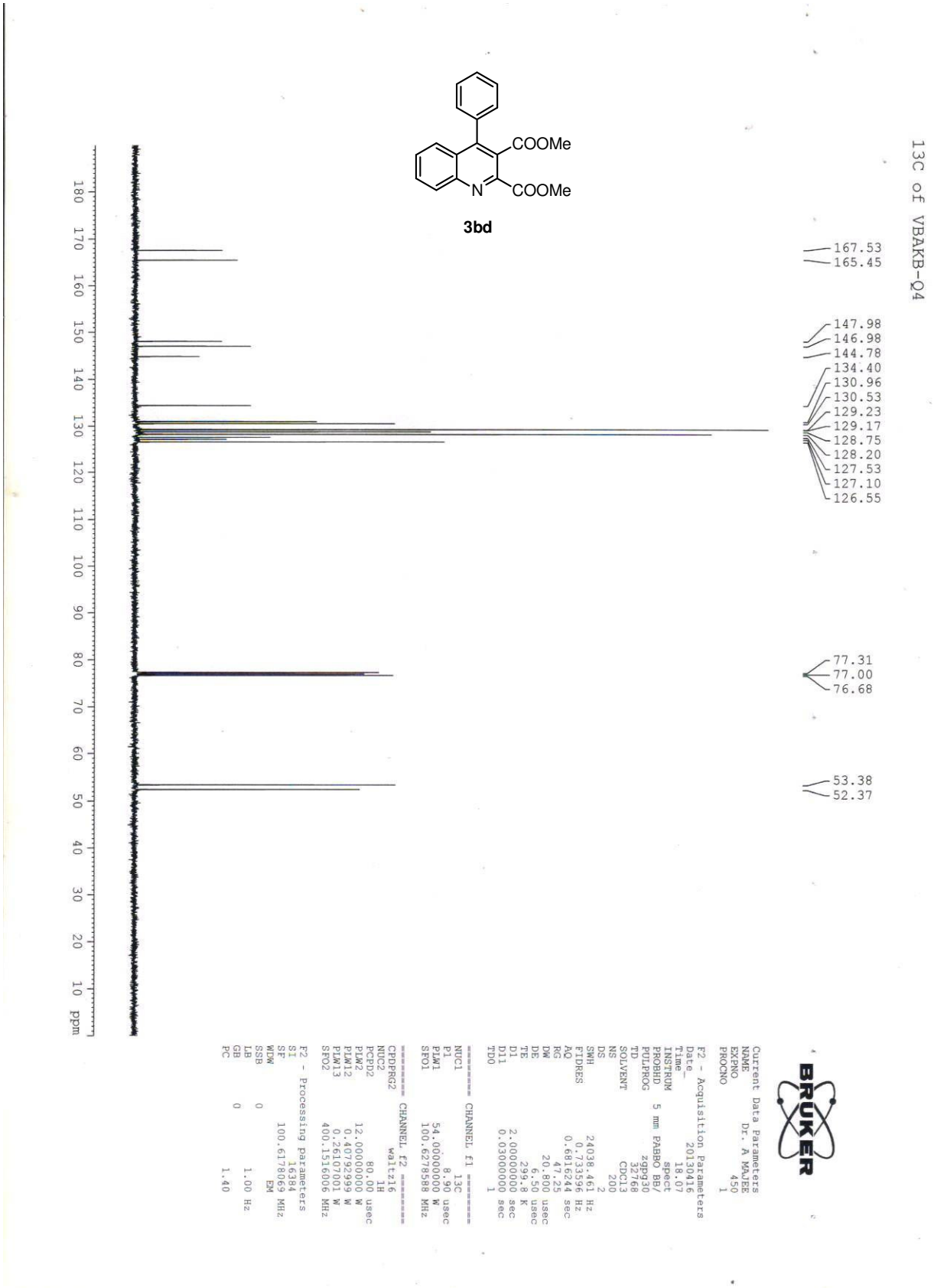

13C of VBAKB-7
Cl
COOEt
N
COOEt
3ac
166.72
165.02
147.11
145.92
145.39
135.35
134.00
132.16
131.95
129.27
129.03
128.41
125.32
77.32
77.01
76.69
62.70
61.68
14.14
13.55
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm
BRUKER
Current Data Parameters
NAME Dr. A HAJRA
EXPNO 757
PROCNO 1
F2 - Acquisition Parameters
Date_ 20121223
Time_ 17.48
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 320
DS 2
SWH 24038.461 Hz
FIDRES 0.733594 Hz
AQ 0.6816244 sec
RG 57.28
DW 20.800 usec
DE 6.50 usec
TE 296.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 8.90 usec
PLW1 54.00000000 W
SFO1 100.6278588 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PLW2 12.00000000 W
PLW12 0.40792999 W
PLW13 0.26107001 W
SFO2 400.1516006 MHz
F2 - Processing parameters
SI 16384
SF 100.6178026 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

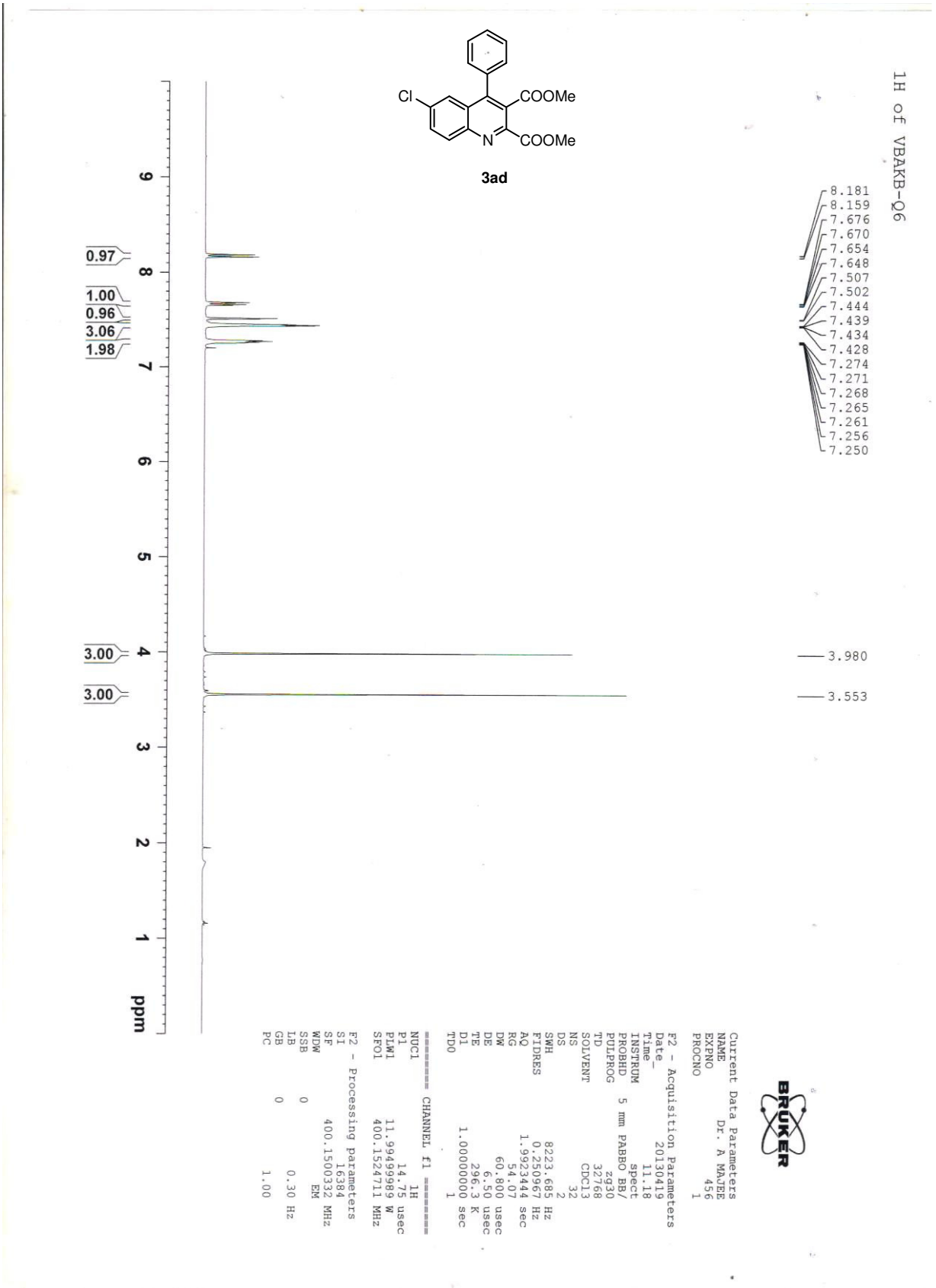

1H of VBAKB-Q10
CH3
COOEt
N
COOEt
3ec
8.184
8.162
8.005
7.984
7.718
7.715
7.697
7.621
7.602
7.600
7.597
4.462
4.444
4.426
4.404
4.386
4.368
2.670
1.398
1.380
1.363
1.352
1.334
1.316
0.95
0.99
0.99
0.98
3.99
3.00
6.00
ppm
Current Data Parameters
NAME Dr. A MAJEE
EXPNO 514
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130424
Time_ 20.54
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 24
DS 2
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9923444 sec
RG 47.25
DW 60.800 usec
DE 6.50 usec
TE 297.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.75 usec
PLW1 11.99499989 W
SFO1 400.1524711 MHz
F2 - Processing parameters
SI 16384
SF 400.1500314 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
BRUKER

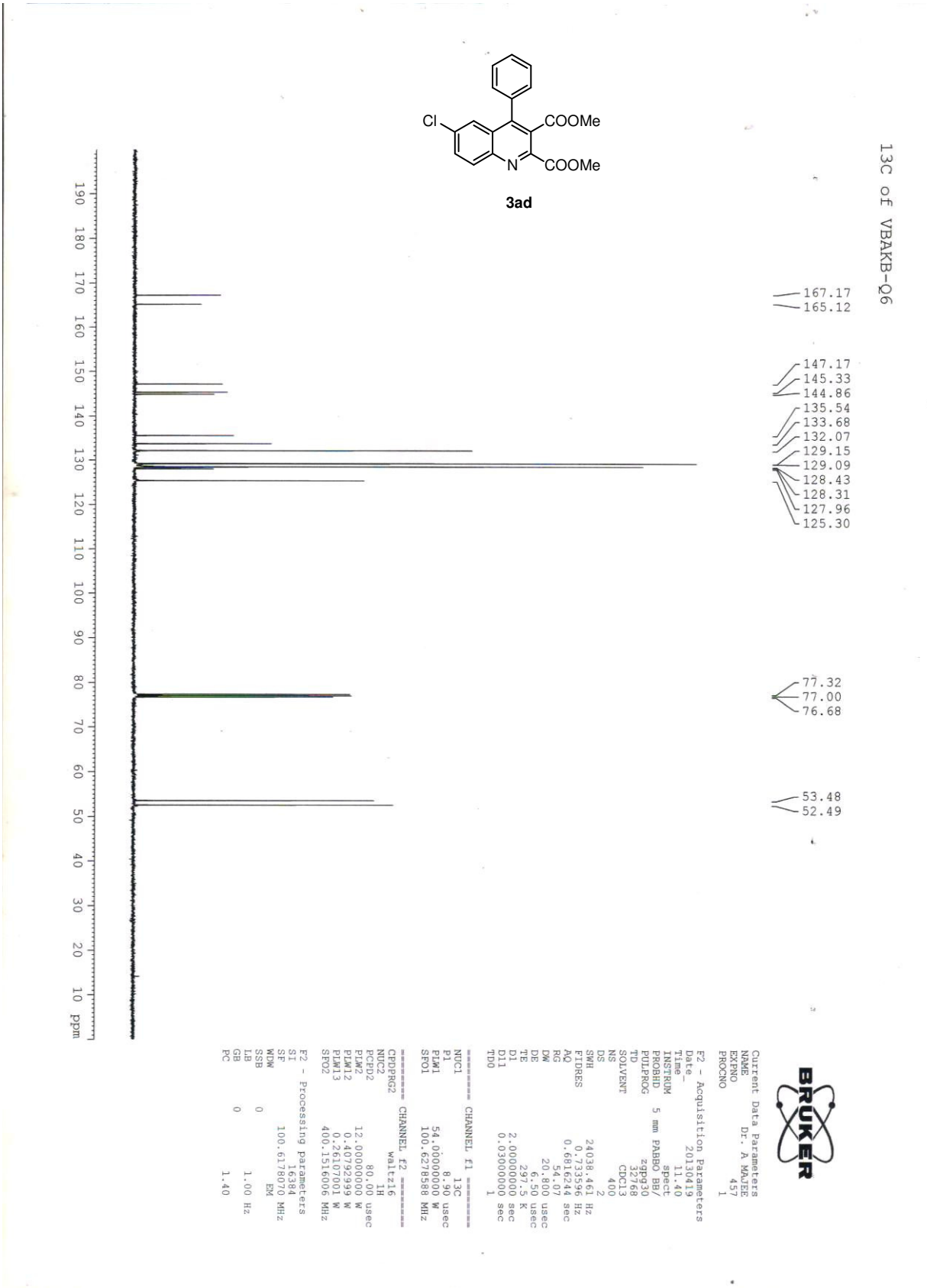
3ec

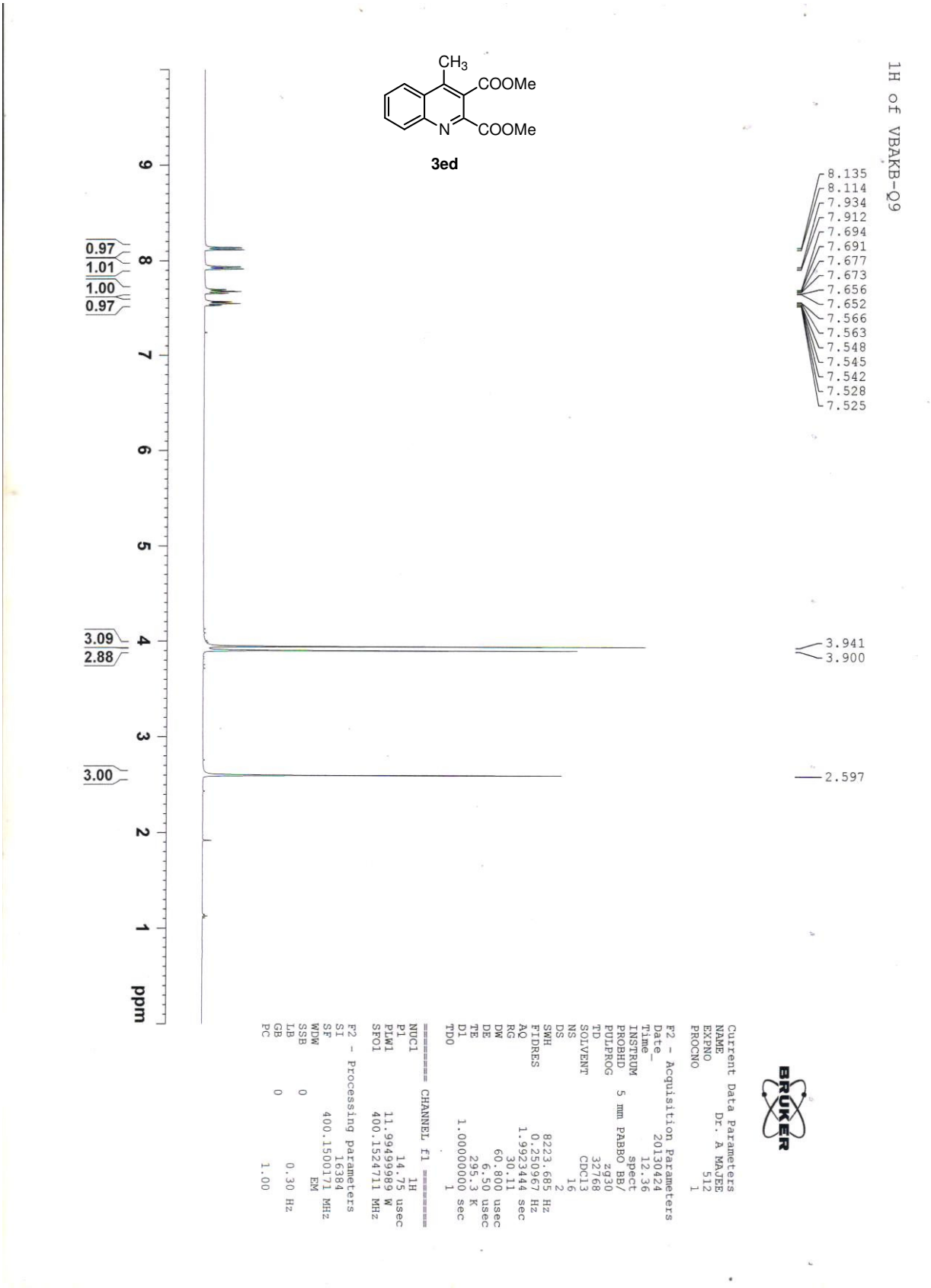

CH3
COOEt
N
COOEt
3ec
13C of VBAKB-Q10
167.61
165.21
146.09
145.69
143.60
130.75
130.48
128.68
127.68
126.84
123.84
77.32
77.00
76.68
62.22
61.69
15.24
13.97
13.81
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm
Current Data Parameters
NAME Dr. A MAJEE
EXPNO 515
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130424
Time_ 12.49
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 40
DS 2
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6816244 sec
RG 12.92
DW 20.800 usec
DE 6.50 usec
TE 296.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 8.90 usec
PLW1 54.00000000 W
SFO1 100.6278588 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PLW2 12.00000000 W
PLW12 0.40792999 W
PLW13 0.26107001 W
SFO2 400.1516006 MHz
F2 - Processing parameters
SI 16384
SF 100.6178188 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


1H of VBAKB-Q4
COOMe
COOMe
N
3bd
8.253
8.232
7.751
7.747
7.734
7.730
7.726
7.713
7.709
7.564
7.561
7.542
7.540
7.513
7.510
7.496
7.493
7.489
7.475
7.472
7.422
7.419
7.417
7.411
7.405
7.287
7.281
7.278
7.269
7.263
5.196
3.984
3.552
0.94
1.03
1.02
0.90
3.02
1.94
2.93
3.00
ppm
Current Data Parameters
NAME Dr. A MAJEE
EXPNO 447
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130416
Time_ 13.10
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 2
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9923444 sec
RG 47.25
DW 60.800 usec
DE 6.50 usec
TE 297.5 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.75 usec
PLW1 11.99499989 W
SFO1 400.1524711 MHz
F2 - Processing parameters
SI 16384
SF 400.1500346 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00


13C of VBAKB-Q4
COOMe
COOMe
N
3bd
167.53
165.45
147.98
146.98
144.78
134.40
130.96
130.53
129.23
129.17
128.75
128.20
127.53
127.10
126.55
77.31
77.00
76.68
53.38
52.37
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm
BRUKER
Current Data Parameters
NAME Dr. A MAJEE
EXPNO 450
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130415
Time 18.07
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 200
DS 2
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6816244 sec
RG 47.25
DW 20.800 usec
DE 6.50 usec
TE 299.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 8.90 usec
PLW1 54.00000000 W
SFO1 100.6278588 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PLW2 12.00000000 W
PLW12 0.40792999 W
PLW13 0.26107001 W
SFO2 400.1516006 MHz
F2 - Processing parameters
SI 16384
SF 100.6178069 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

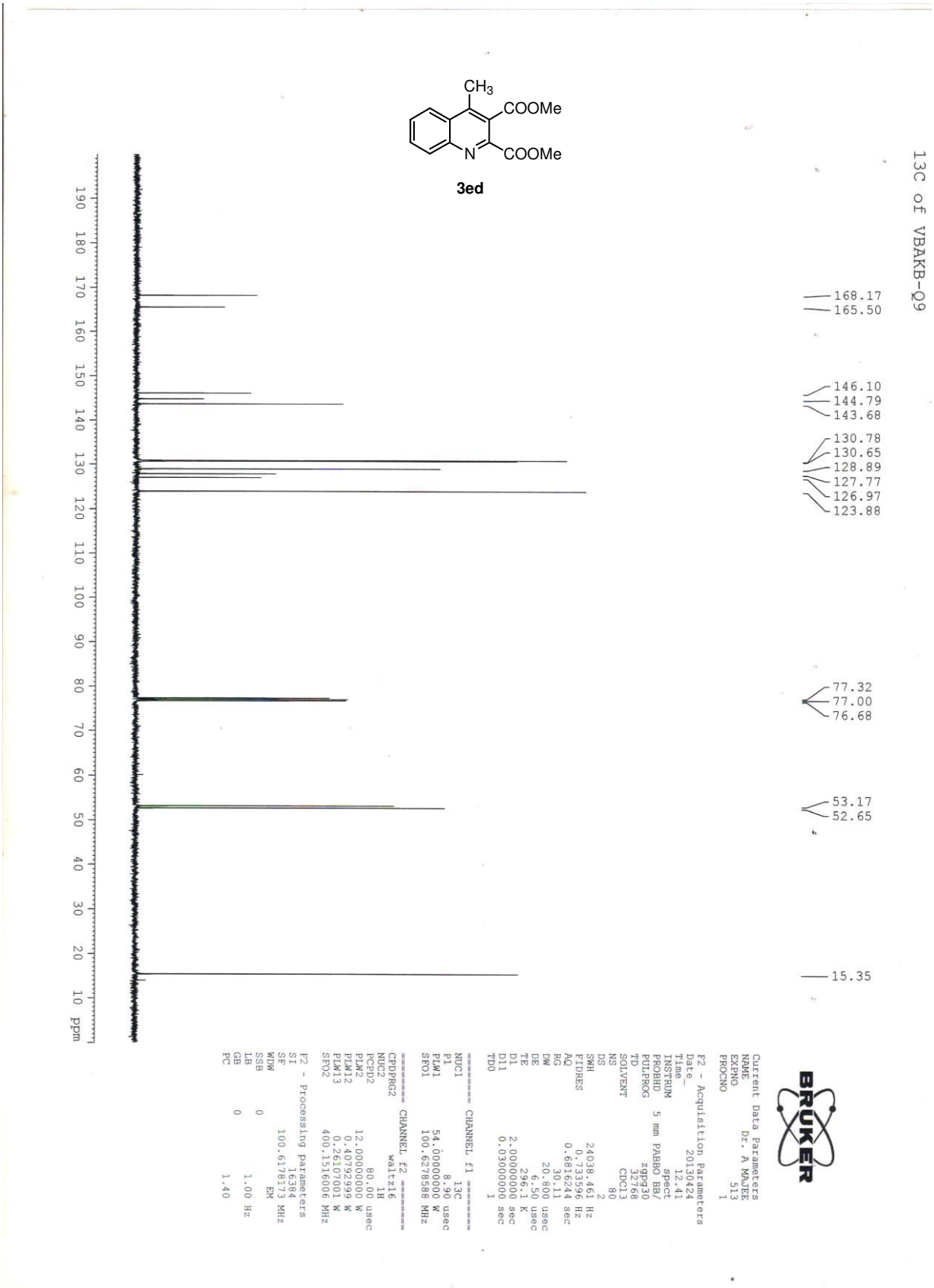

1H of VBAKB-Q6
Cl
COOMe
COOMe
N
3ad
8.181
8.159
7.676
7.670
7.654
7.648
7.507
7.502
7.444
7.439
7.434
7.428
7.274
7.271
7.268
7.265
7.261
7.256
7.250
3.980
3.553
0.97
1.00
0.96
3.06
1.98
3.00
3.00
ppm
Current Data Parameters
NAME Dr. A MAJEE
EXPNO 456
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130419
Time_ 11.18
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 2
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.992344 sec
RG 54.07
DW 60.800 usec
DE 6.50 usec
TE 296.3 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.75 usec
PLW1 11.99499989 W
SFO1 400.1524711 MHz
F2 - Processing parameters
SI 16384
SF 400.1500332 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

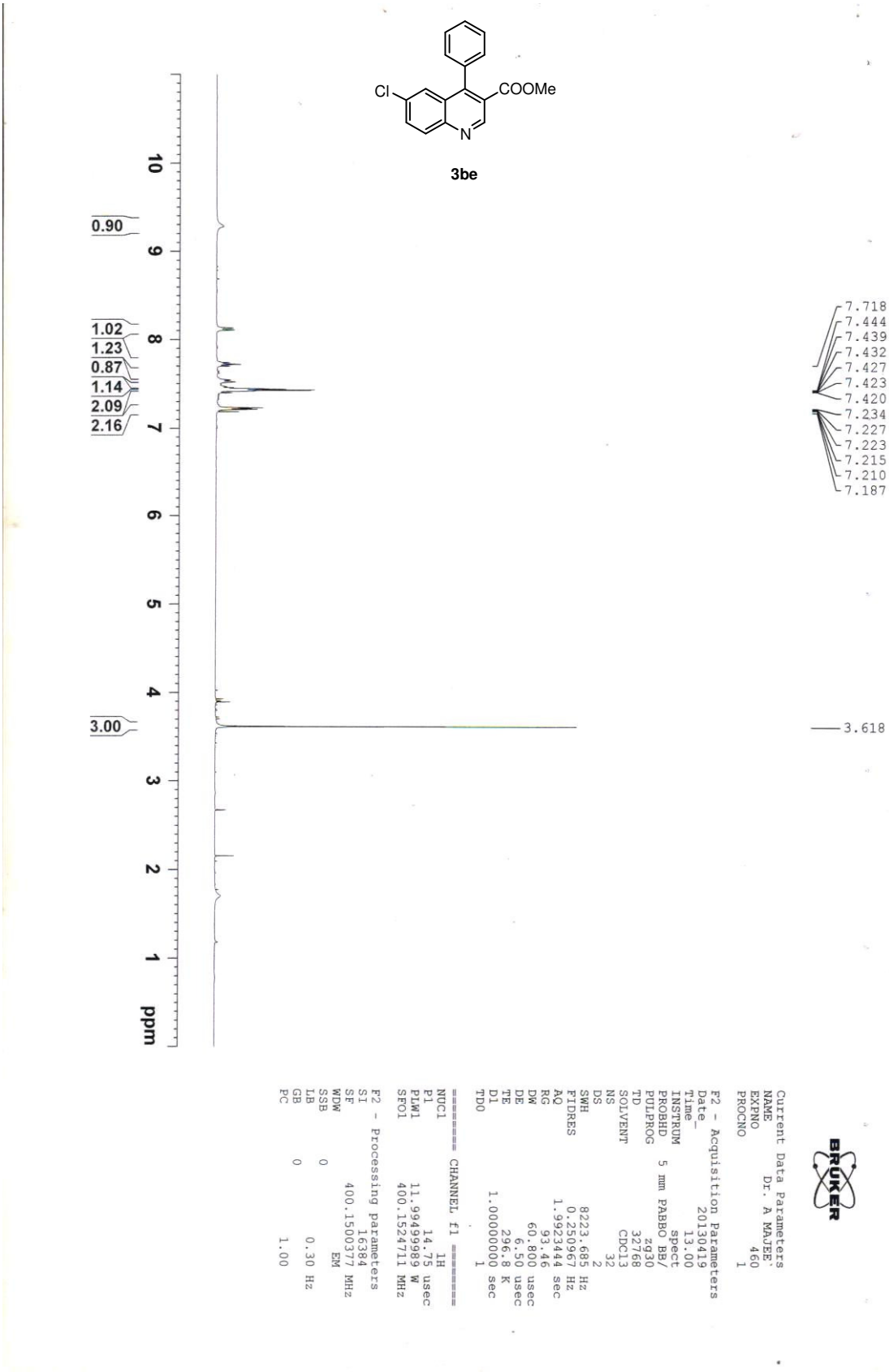

13C of VBAKB-Q6
Cl
COOMe
N
COOMe
3ad
167.17
165.12
147.17
145.33
144.86
135.54
133.68
132.07
129.15
129.09
128.43
128.31
127.96
125.30
77.32
77.00
76.68
53.48
52.49
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm
Current Data Parameters
NAME Dr. A MAJEE
EXPNO 457
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130419
Time_ 11.40
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 400
DS 2
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.681244 sec
RG 54.07
DW 20.800 usec
DE 6.50 usec
TE 297.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 8.90 usec
PLW1 54.00000000 W
SFO1 100.6278588 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PLW2 12.00000000 W
PLW12 0.47079299 W
PLW13 0.26107001 W
SFO2 400.1516006 MHz
F2 - Processing parameters
SI 16384
SF 100.6178070 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

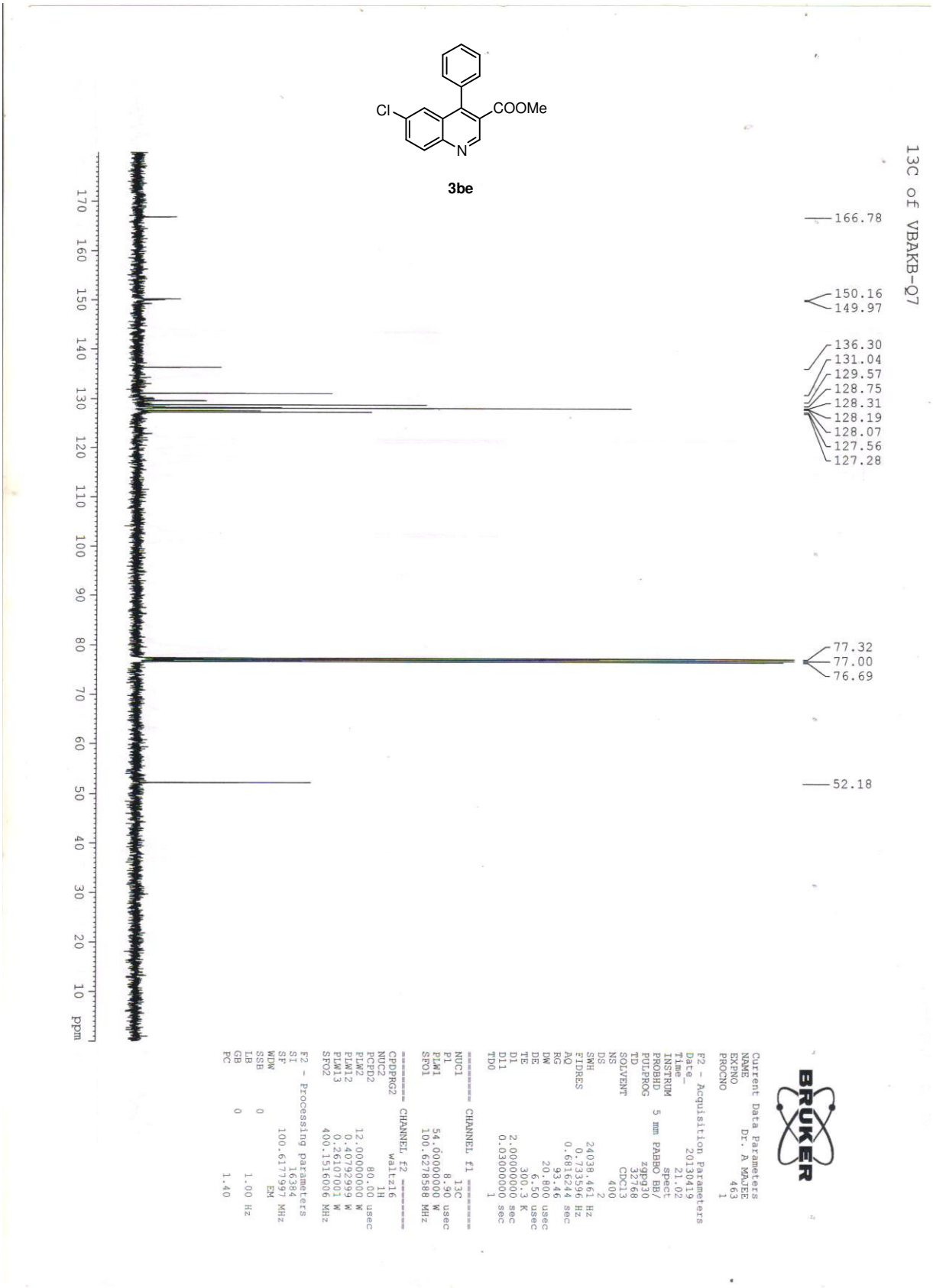

1H of VBAKB-Q9
8.135
8.114
7.934
7.912
7.694
7.691
7.677
7.673
7.656
7.652
7.566
7.563
7.548
7.545
7.542
7.528
7.525
3.941
3.900
2.597
0.97
1.01
1.00
0.97
3.09
2.88
3.00
ppm
Current Data Parameters
NAME Dr. A MAJEE
EXPNO 512
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130424
Time_ 12.36
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9923444 sec
RG 30.11
DW 60.800 usec
DE 6.50 usec
TE 295.3 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.75 usec
PL1 11.99499969 W
SFO1 400.1524711 MHz
F2 - Processing parameters
SI 16384
SF 400.1500171 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
BRUKER

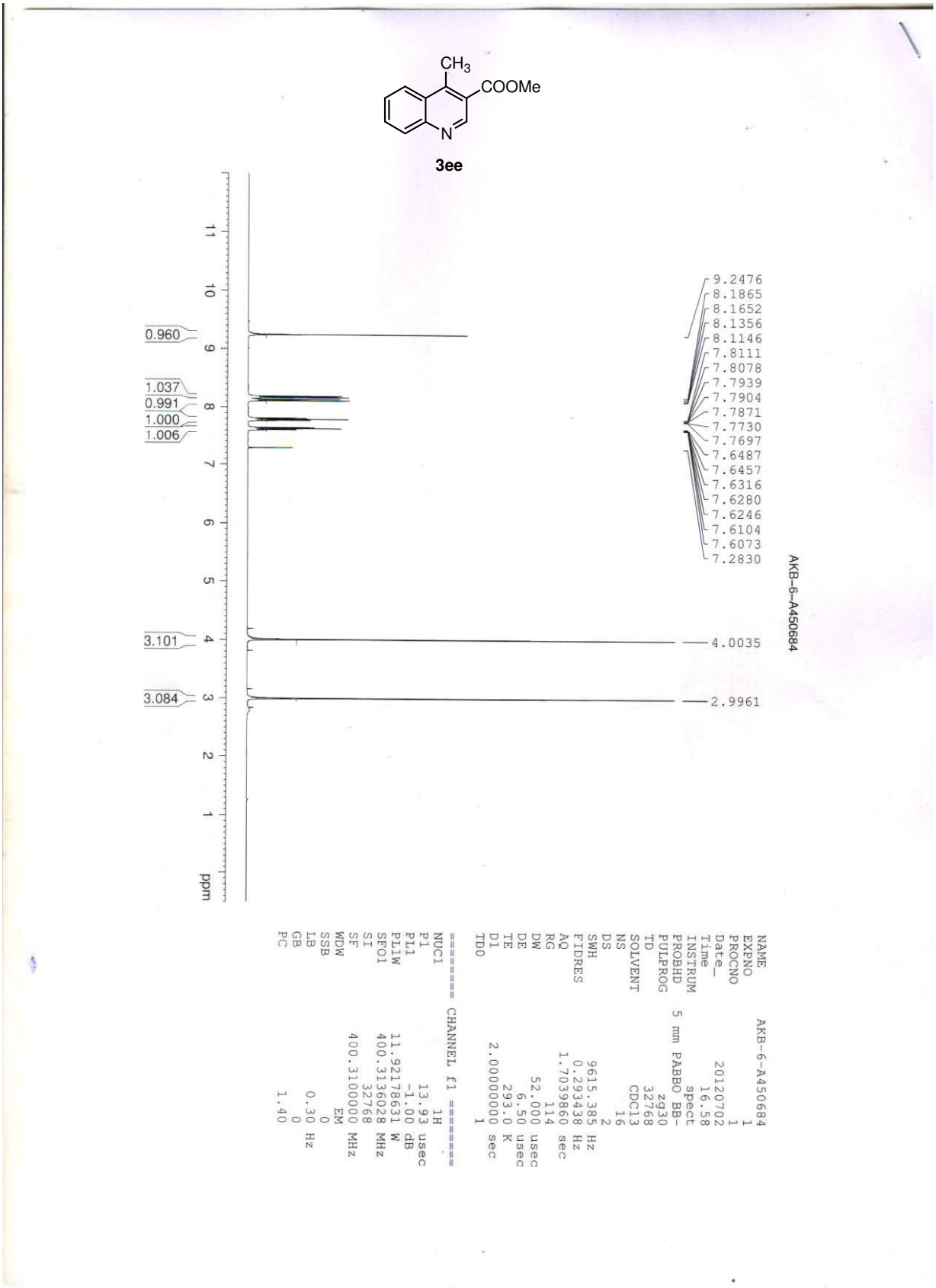
CH3
COOMe
COOMe
N

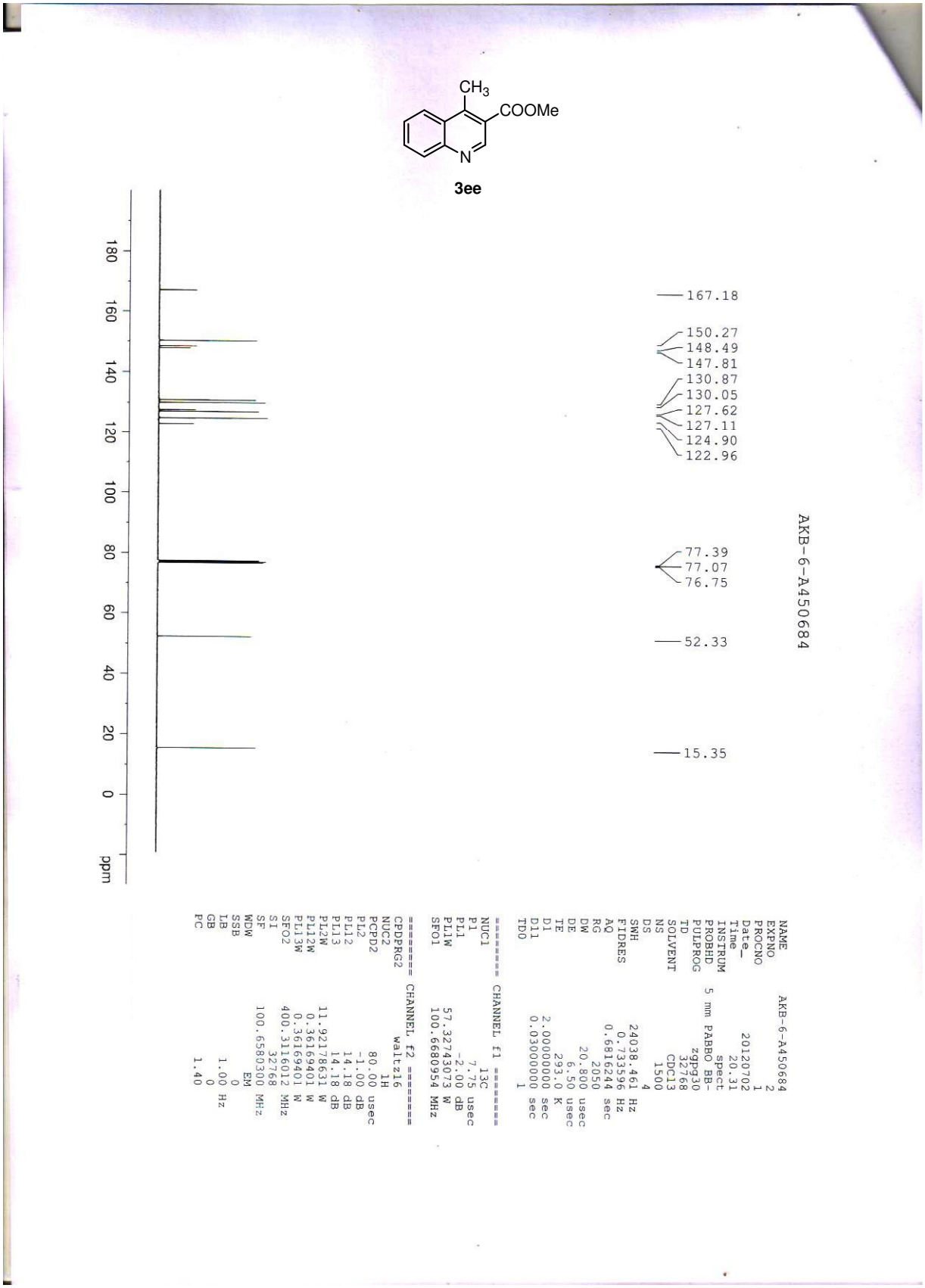
3ed

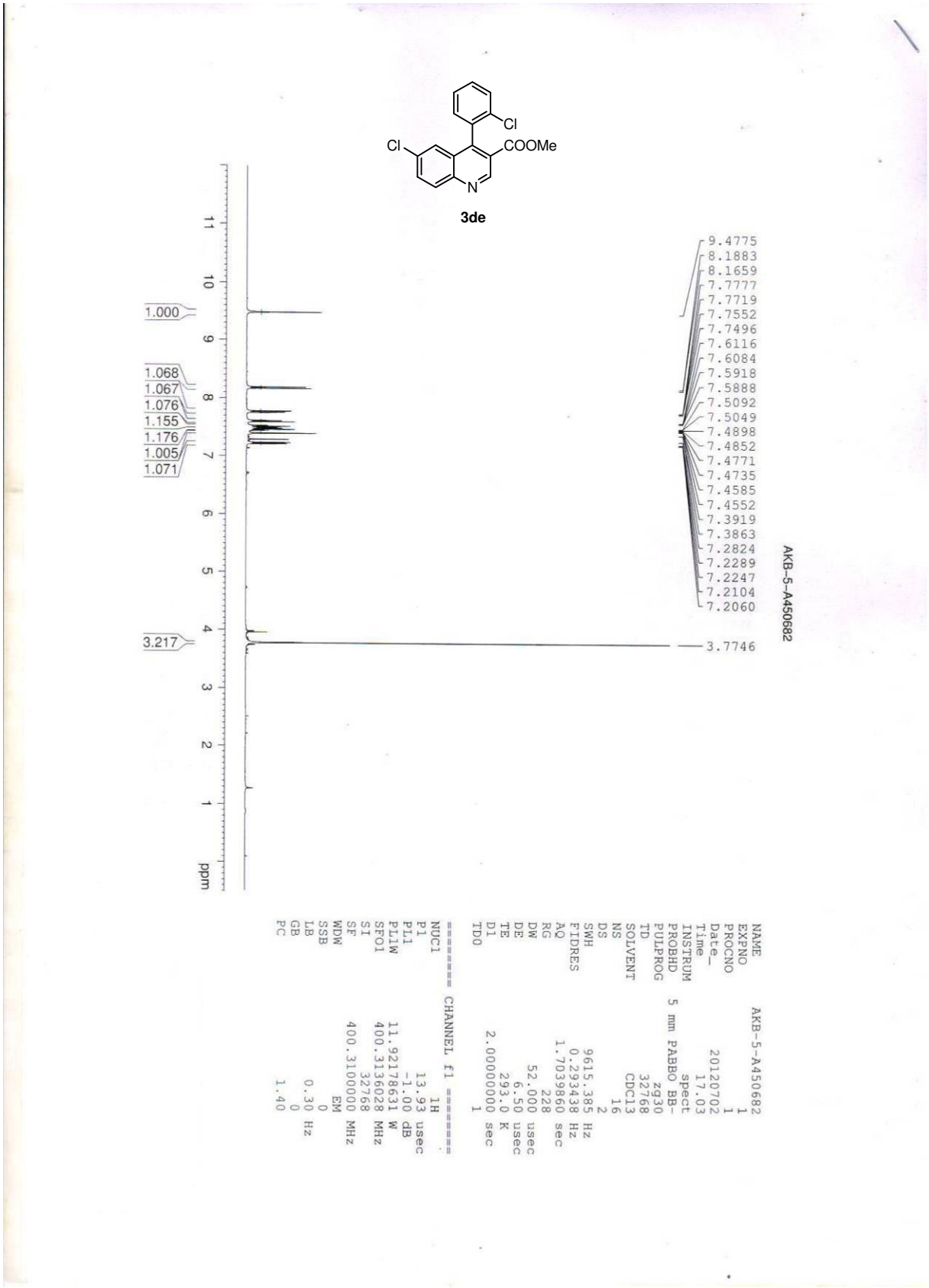

13C of VBAKB-Q9
CH3
COOMe
COOMe
N
3ed
168.17
165.50
146.10
144.79
143.68
130.78
130.65
128.89
127.77
126.97
123.88
77.32
77.00
76.68
53.17
52.65
15.35
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm
BRUKER
Current Data Parameters
NAME
EXPNO
PROCNO
F2 - Acquisition Parameters
Date_
Time
INSTRUM
PROBHD
PULPROG
TD
SOLVENT
NS
DS
SWH
FIDRES
AQ
RG
DW
DE
TE
D1
D11
TD0
======== CHANNEL f1 ========
NUC1
P1
PLW1
SFO1
======== CHANNEL f2 ========
CPDPRG2
NUC2
PCPD2
PLW2
PLW12
PLW13
SFO2
F2 - Processing parameters
SI
SF
WDW
SSB
LB
GB
PC

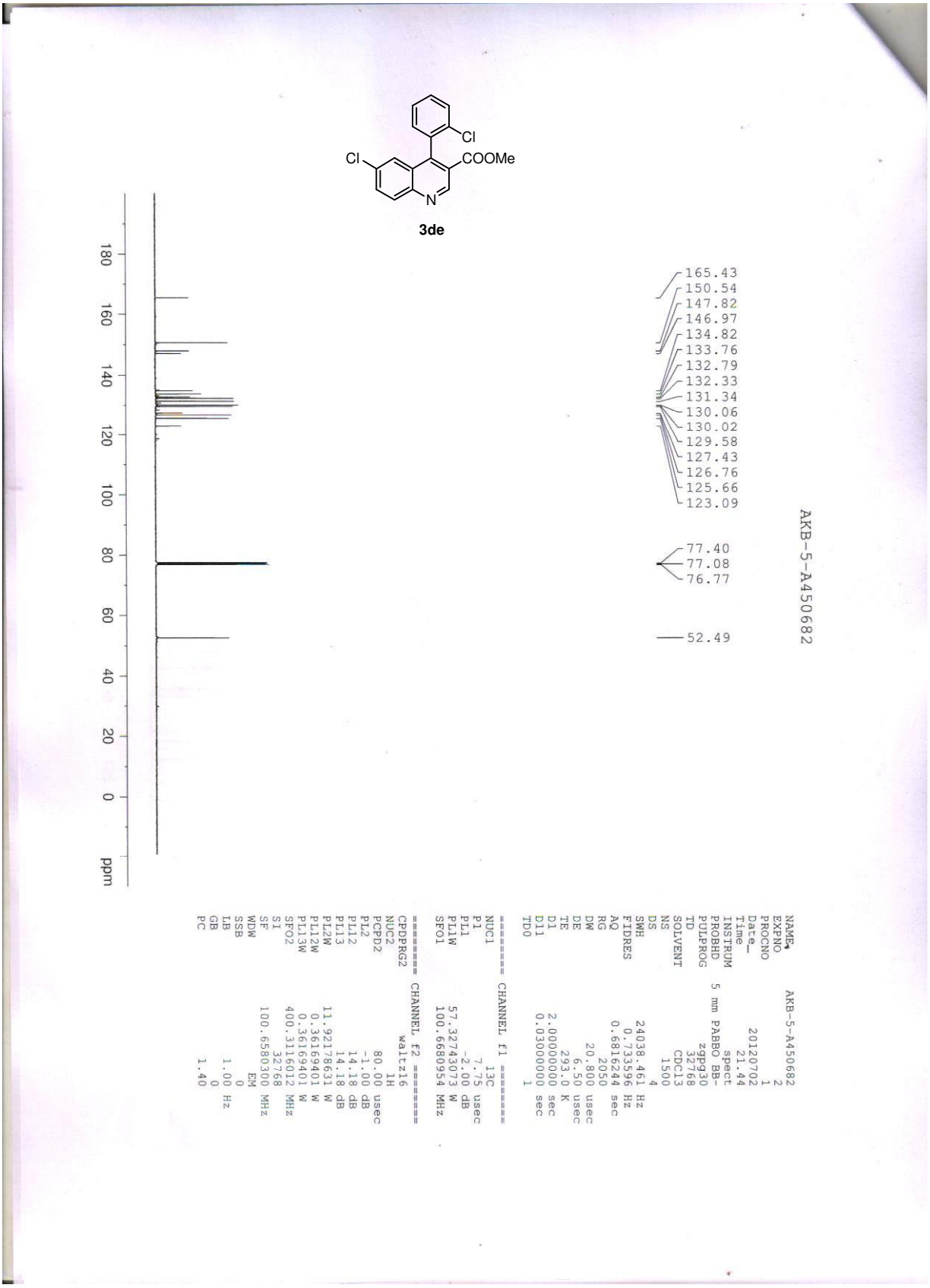

1H of VBAKB-Q7
Cl
COOMe
N
3be
0.90
1.02
1.23
0.87
1.14
2.09
2.16
3.00
10
9
8
7
6
5
4
3
2
1
ppm
7.718
7.444
7.439
7.432
7.427
7.423
7.420
7.234
7.227
7.223
7.215
7.210
7.187
3.618
Current Data Parameters
NAME Dr. A MAJEE'
EXPNO 460
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130419
Time_ 13.00
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 2
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9923444 sec
RG 93.46
DW 60.800 usec
DE 6.50 usec
TE 296.8 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.75 usec
PLW1 11.99499989 W
SFO1 400.1524711 MHz
F2 - Processing parameters
SI 16384
SF 400.1500377 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

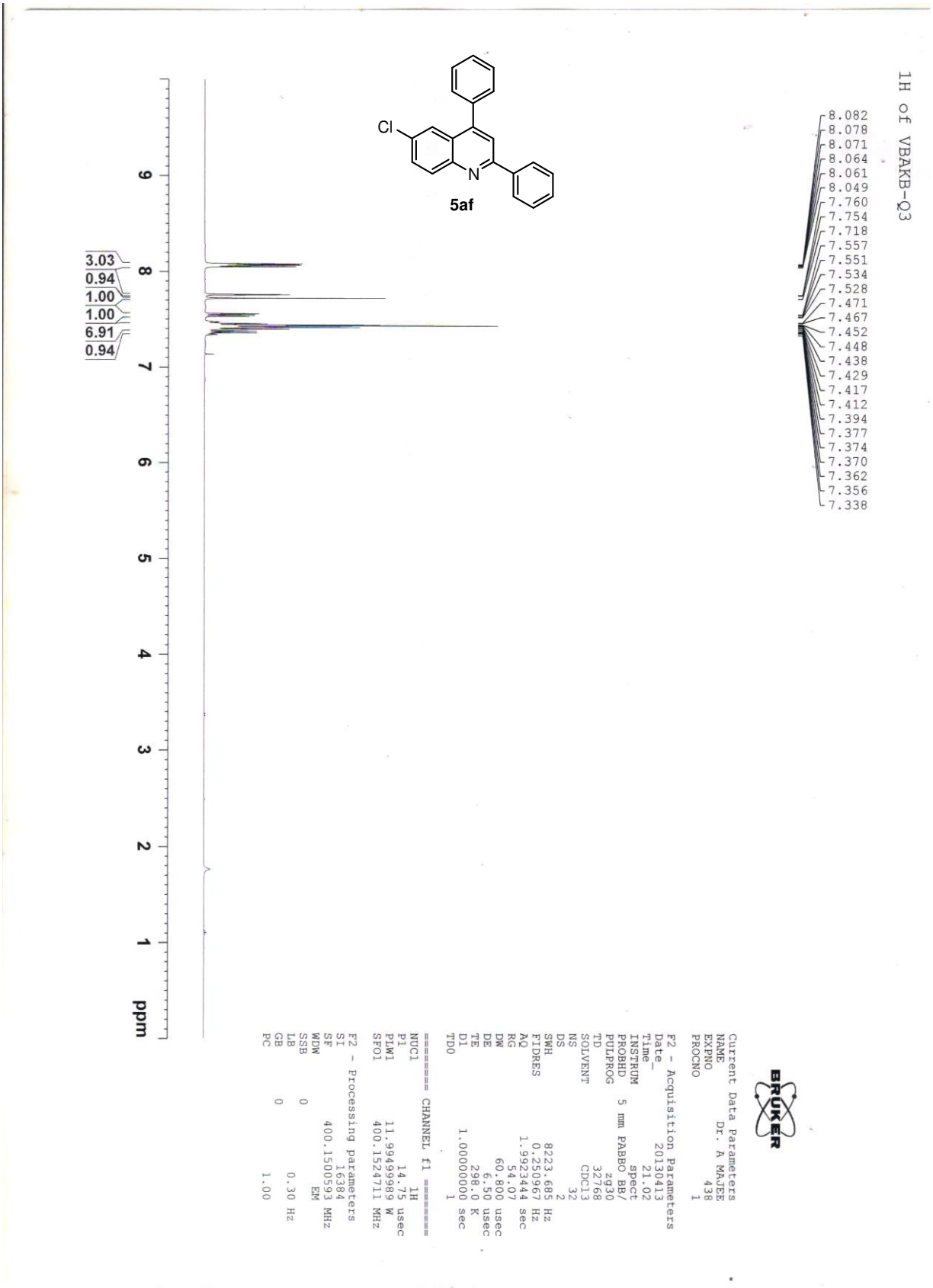

13C of VBAKB-Q7
Cl
COOMe
N
3be
166.78
150.16
149.97
136.30
131.04
129.57
128.75
128.31
128.19
128.07
127.56
127.28
77.32
77.00
76.69
52.18
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm
Current Data Parameters
NAME Dr. A MAJEE
EXPNO 463
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130419
Time_ 21.02
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 400
DS 2
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6816244 sec
RG 93.46
DW 20.800 usec
DE 6.50 usec
TE 300.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 8.90 usec
PLW1 54.00000000 W
SFO1 100.6278588 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PLW2 12.00000000 W
PLW12 0.40729999 W
PLW13 0.26107001 W
SFO2 400.1516006 MHz
F2 - Processing parameters
SI 16384
SF 100.6177997 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

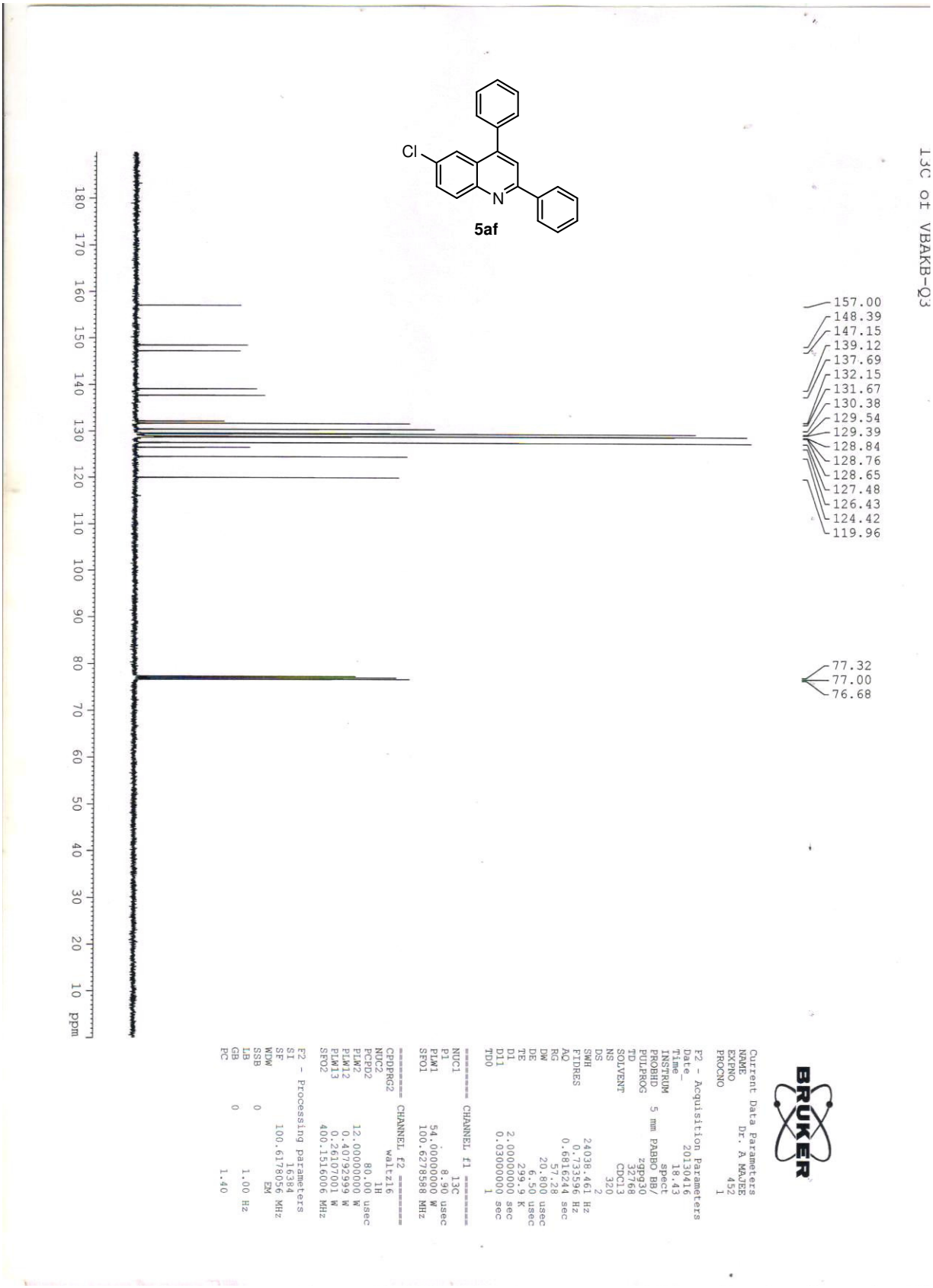

CH3
COOMe
N
3ee
9.2476
8.1865
8.1652
8.1356
8.1146
7.8111
7.8078
7.7939
7.7904
7.7871
7.7730
7.7697
7.6487
7.6457
7.6316
7.6280
7.6246
7.6104
7.6073
7.2830
0.960
1.037
0.991
1.000
1.006
3.101
3.084
4.0035
2.9961
ppm
AKB-6-A450684
NAME AKB-6-A450684
EXPNO 1
PROCNO 1
Date_ 20120702
Time 16.58
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 9615.385 Hz
FIDRES 0.293438 Hz
AQ 1.7039860 sec
RG 114
DW 52.000 usec
DE 6.50 usec
TE 293.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 13.93 usec
PL1 -1.00 dB
PL1W 11.92178631 W
SFO1 400.3136028 MHz
SI 32768
SF 400.3100000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40

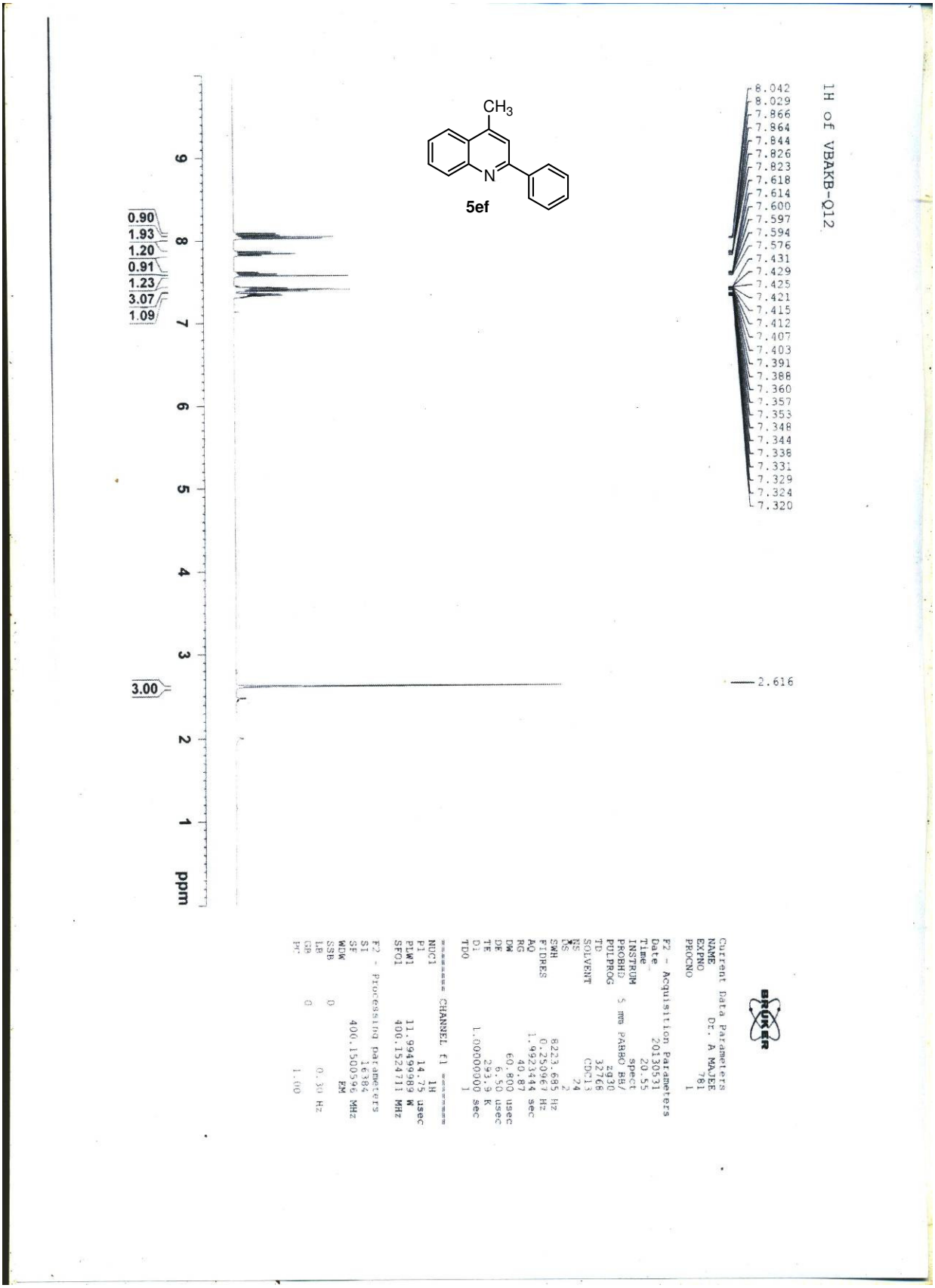

CH3
COOMe
N
3ee
AKB-6-A450684
167.18
150.27
148.49
147.81
130.87
130.05
127.62
127.11
124.90
122.96
77.39
77.07
76.75
52.33
15.35
180
160
140
120
100
80
60
40
20
0
ppm
NAME AKB-6-A450684
EXPNO 2
PROCNO 1
Date_ 20120702
Time 20.31
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 1500
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6816244 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 293.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 7.75 usec
PL1 -2.00 dB
PL1W 57.32743073 W
SFO1 100.6680954 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -1.00 dB
PL12 14.18 dB
PL13 14.18 dB
PL2W 11.92178631 W
PL12W 0.36169401 W
PL13W 0.36169401 W
SFO2 400.3116012 MHz
SI 32768
SF 100.6580300 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

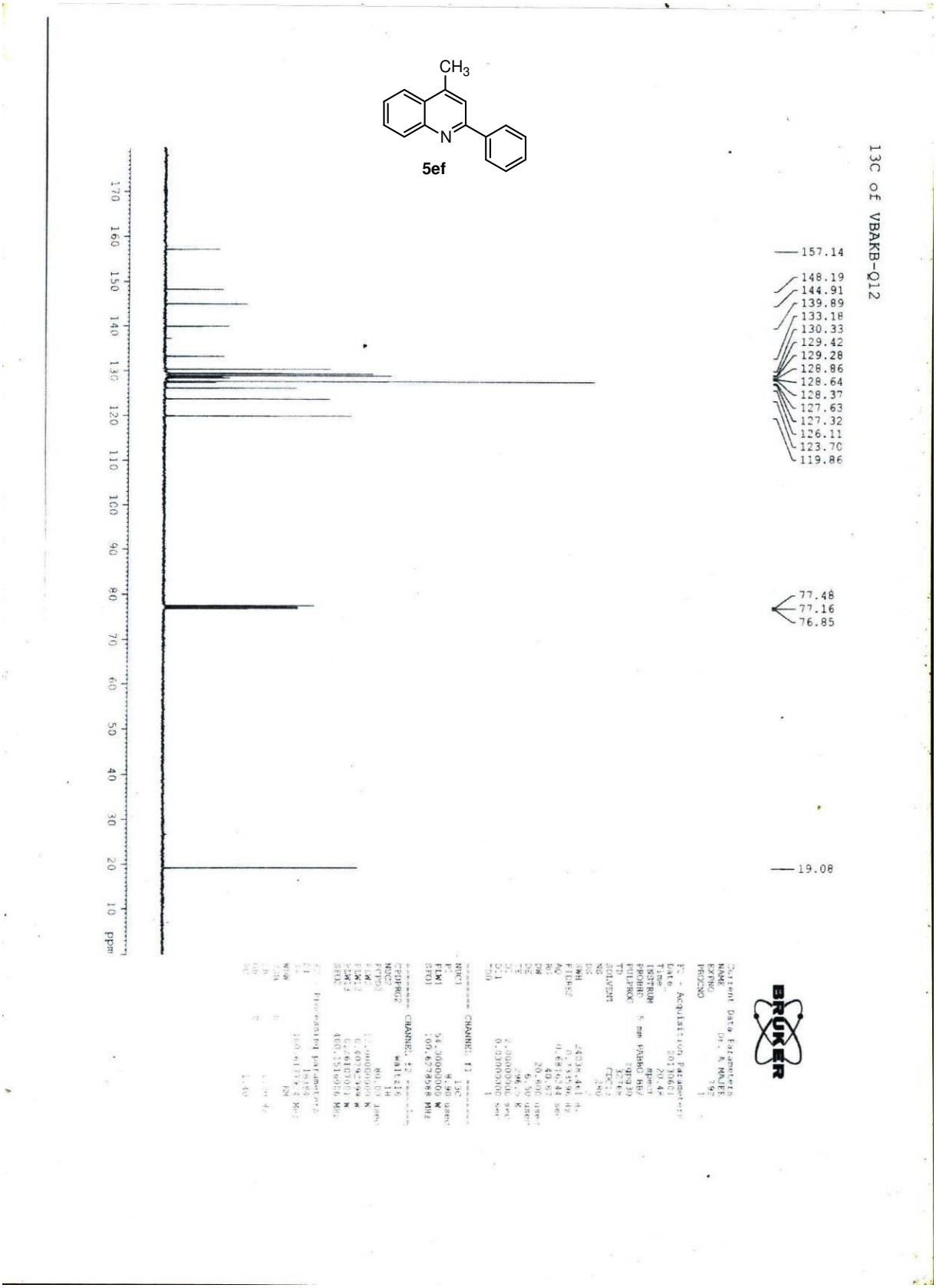

Cl
Cl
COOMe
N
3de
AKB-5-A450682
9.4775
8.1883
8.1659
7.7777
7.7719
7.7552
7.7496
7.6116
7.6084
7.5918
7.5888
7.5092
7.5049
7.4898
7.4852
7.4771
7.4735
7.4585
7.4552
7.3919
7.3863
7.2824
7.2289
7.2247
7.2104
7.2060
3.7746
1.000
1.068
1.067
1.076
1.155
1.176
1.005
1.071
3.217
ppm
NAME AKB-5-A450682
EXPNO 1
PROCNO 1
Date_ 20120702
Time 17.03
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 9615.385 Hz
FIDRES 0.293438 Hz
AQ 1.7039860 sec
RG 228
DW 52.000 usec
DE 6.50 usec
TE 293.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 13.93 usec
PL1 -1.00 dB
PL1W 11.92178631 W
SFO1 400.3136028 MHz
SI 32768
SF 400.3100000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40

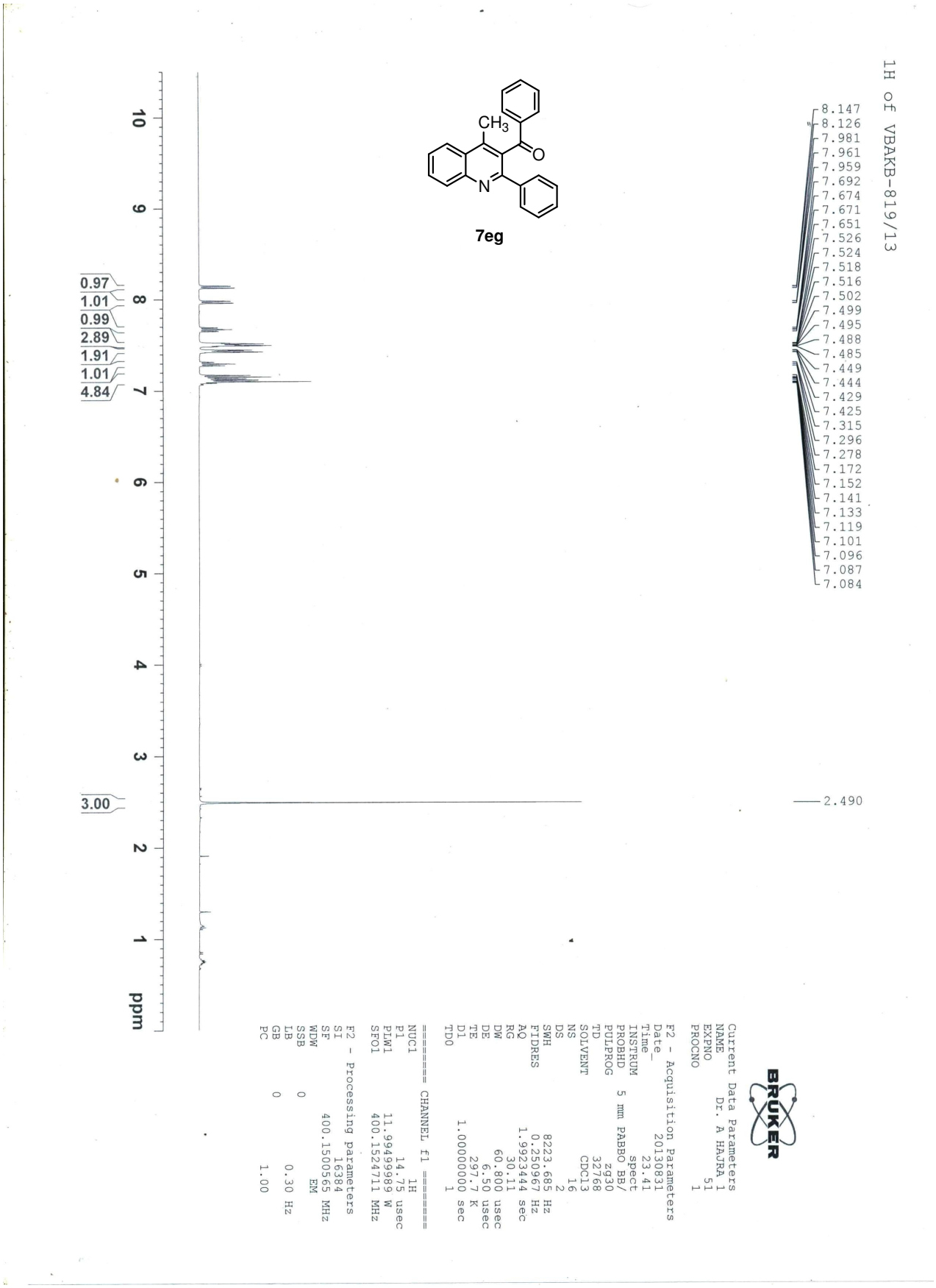

Cl
Cl
COOMe
N
3de
AKB-5-A450682
165.43
150.54
147.82
146.97
134.82
133.76
132.79
132.33
131.34
130.06
130.02
129.58
127.43
126.76
125.66
123.09
77.40
77.08
76.77
52.49
180
160
140
120
100
80
60
40
20
0
ppm
NAME AKB-5-A450682
EXPNO 2
PROCNO 1
Date_ 20120702
Time_ 21.44
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 1500
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6816244 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 293.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 7.75 usec
PL1 -2.00 dB
PL1W 57.32743073 W
SFO1 100.6680954 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -1.00 dB
PL12 14.18 dB
PL13 14.18 dB
PL2W 11.92178631 W
PL12W 0.36169401 W
PL13W 0.36169401 W
SFO2 400.3116012 MHz
SI 32768
SF 100.6580300 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

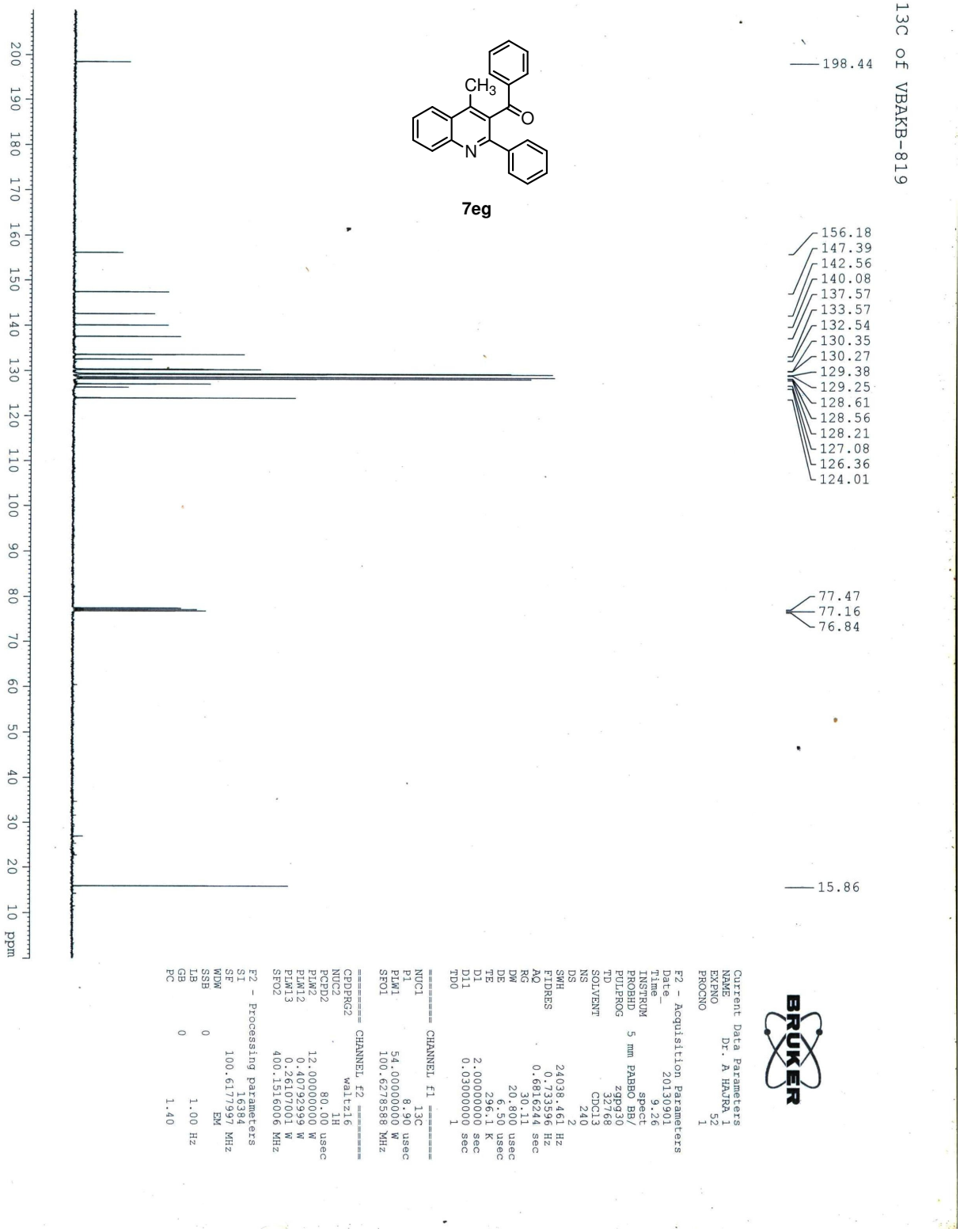

1H of VBAKB-Q3
8.082
8.078
8.071
8.064
8.061
8.049
7.760
7.754
7.718
7.557
7.551
7.534
7.528
7.471
7.467
7.452
7.448
7.438
7.429
7.417
7.412
7.394
7.377
7.374
7.370
7.362
7.356
7.338
Cl
N
5af
3.03
0.94
1.00
1.00
6.91
0.94
9
8
7
6
5
4
3
2
1
ppm
BRUKER
Current Data Parameters
NAME Dr. A MAJEE
EXPNO 438
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130413
Time_ 21.02
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 2
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9923444 sec
RG 54.07
DW 60.800 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.75 usec
PLW1 11.99499989 W
SFO1 400.1527711 MHz
F2 - Processing parameters
SI 16384
SF 400.1500593 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00


13C of VBAKB-Q3
Cl
N
5af
157.00
148.39
147.15
139.12
137.69
132.15
131.67
130.38
129.54
129.39
128.84
128.76
128.65
127.48
126.43
124.42
119.96
77.32
77.00
76.68
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm
BRUKER
Current Data Parameters
NAME Dr. A MAJEE
EXPNO 452
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130416
Time_ 18.43
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 320
DS 2
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6816244 sec
RG 57.28
DW 20.800 usec
DE 6.50 usec
TE 299.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 8.90 usec
PLW1 54.00000000 W
SFO1 100.6278588 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PLW2 12.00000000 W
PLW12 0.40792999 W
PLW13 0.26107001 W
SFO2 400.1516006 MHz
F2 - Processing parameters
SI 16384
SF 100.6178056 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


1H of VBAKB-Q12
8.042
8.029
7.866
7.864
7.844
7.826
7.823
7.618
7.614
7.600
7.597
7.594
7.576
7.431
7.429
7.425
7.421
7.415
7.412
7.407
7.403
7.391
7.388
7.360
7.357
7.353
7.348
7.344
7.338
7.331
7.329
7.324
7.320
2.616
CH3
N
5ef
0.90
1.93
1.20
0.91
1.23
3.07
1.09
3.00
ppm
Current Data Parameters
NAME Dr. A MAJEE
EXPNO 781
PROCNO 1
F2 - Acquisition Parameters
Date 20130531
Time 20.55
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 24
DS 2
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.992344 sec
RG 40.87
DW 60.800 usec
DE 6.50 usec
TE 293.9 K
D1 1.00000000 sec
TD0 1
CHANNEL f1
NUC1 1H
P1 14.75 usec
PLW1 11.99499989 W
SFO1 400.1524711 MHz
F2 - Processing parameters
SI 16384
SF 400.1500596 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00


13C of VBAKB-Q12
CH3
N
5ef
157.14
148.19
144.91
139.89
133.18
130.33
129.42
129.28
128.86
128.64
128.37
127.63
127.32
126.11
123.70
119.86
77.48
77.16
76.85
19.08
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm
BRUKER


1H of VBAKB-819/13
8.147
8.126
7.981
7.961
7.959
7.692
7.674
7.671
7.651
7.526
7.524
7.518
7.516
7.502
7.499
7.495
7.488
7.485
7.449
7.444
7.429
7.425
7.315
7.296
7.278
7.172
7.152
7.141
7.133
7.119
7.101
7.096
7.087
7.084
2.490
CH3
O
N
7eg
0.97
1.01
0.99
2.89
1.91
1.01
4.84
3.00
10
9
8
7
6
5
4
3
2
1
ppm
BRUKER
Current Data Parameters
NAME Dr. A HAJRA 1
EXPNO 51
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130831
Time 23.41
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9923444 sec
RG 30.11
DW 60.800 usec
DE 6.50 usec
TE 297.7 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.75 usec
PLW1 11.99499989 W
SFO1 400.1524711 MHz
F2 - Processing parameters
SI 16384
SF 400.1500565 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00


13C of VBAKB-819
198.44
156.18
147.39
142.56
140.08
137.57
133.57
132.54
130.35
130.27
129.38
129.25
128.61
128.56
128.21
127.08
126.36
124.01
77.47
77.16
76.84
15.86
CH3
O
N
7eg
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm
Current Data Parameters
NAME Dr. A HAJRA 1
EXPNO 52
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130901
Time_ 9.26
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 240
DS 2
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6816244 sec
RG 30.11
DW 20.800 usec
DE 6.50 usec
TE 296.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 8.90 usec
PLW1 54.00000000 W
SFO1 100.6278588 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PLW2 12.00000000 W
PLW12 0.40792999 W
PLW13 0.26107001 W
SFO2 400.1516006 MHz
F2 - Processing parameters
SI 16384
SF 100.6177997 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40