Ruthenium(II)-catalyzed remote C-H addition of 8 aminoquinoline amide to activated aldehyde

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Table of Contents

Content	Page no.
1. General Information……..	S2
2. Typical experimental procedure for the compound **3a**…….	S2
3. Characterization data for the synthesized compounds (**3a**-**3s** and **5a**, **5b)** ….	S3-S13
4. References…….	S13
5. Structure Determination (X-ray crystallographic data for **3d**):	S13-S14
6. NMR spectra for the synthesized products…….	S15-S57

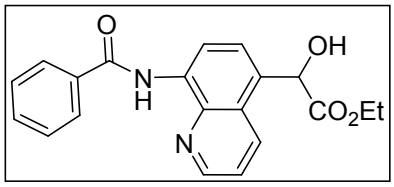
1. General Information:

All reagents were purchased from commercial sources and used without further purification. ^{1}H NMR spectra were determined on 400 MHz spectrometer as solutions in $CDCl_3$. Chemical shifts were expressed in parts per million (δ) and the signals were reported as s (singlet), br s (broad singlet), d (doublet), dd (doublet of doublet), t (triplet), q (quartet), m (multiplet), and coupling constants (J) were given in Hz. $^{13}C\{^1H\}$ NMR spectra were recorded at 100 MHz in $CDCl_3$ solution. Chemical shifts as internal standard were referenced to $CDCl_3$ (δ = 7.26 for ^{1}H and δ = 77.16 for $^{13}C\{^1H\}$ NMR) as internal standard. TLC was done on silica gel coated glass slide. All solvents were dried and distilled before use. Commercially available solvents were freshly distilled before the reaction. All reactions involving moisture sensitive reactants were executed using oven dried glassware. All the 8-aminoquinoline amides were prepared by the reported method.[1]

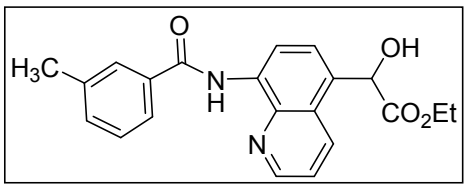
2. Typical experimental procedure for the compound ethyl 2-(8-benzamidoquinolin-5-yl)-2-hydroxyacetate (3a):

N-(Quinolin-8-yl)benzamide (**1a**) (0.2 mmol, 49.6 mg), ethyl glyoxalate solution (**2a**) (2 equiv., 40.8 mg), [Ru(*p*-Cy)Cl_2]$_2$ (5 mol%, 3.06 mg), $AgSbF_6$ (10mol%, 6.86 mg), and NaOAc (2 equiv., 32.8 mg) was taken in a reaction tube with cap. Then 1,2-DCE (2 mL) was added to it and stirred at 100°C for 8 h. After completion of the reaction (TLC), the reaction mixture was quenched with water (2 mL). The reaction mixture was then extracted with ethyl acetate. The organic phase was dried over anhydrous Na_2SO_4 and concentrated under reduced pressure to get the crude residue which was purified by column chromatography on silica gel (60-120 mesh) using petroleum ether:ethyl acetate = 4:1 as an eluent to afford the pure product (**3a**) (51.8 mg, 74%) as a light yellow gummy mass.

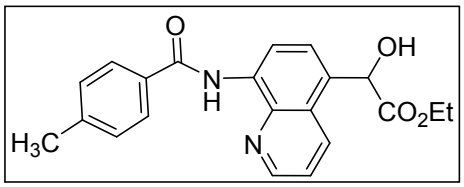
3. Characterization data for the synthesized compounds (**3a-3s** and **5a**, **5b**):



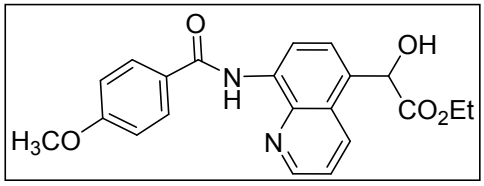
Ethyl 2-(8-benzamidoquinolin-5-yl)-2-hydroxyacetate (3a): Light yellow gummy mass (74%, 51.8 mg); R_f = 0.45 (PE:EA = 80:20); ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.82 (s, 1H), 8.89-8.85 (m, 2H), 8.57 (dd, J = 8.8 Hz, 1.6 Hz, 1H), 8.08-8.06 (m, 2H), 7.60-7.50 (m, 5H), 5.68 (s, 1H), 4.28-4.17 (m, 2H), 3.67 (br s, 1H), 1.14 (t, J = 7.2 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 173.9, 165.6, 148.2, 139.1, 135.3, 135.0, 133.1, 132.0, 128.9, 128.2, 127.6, 127.4, 126.2, 121.9, 115.7, 71.5, 62.6, 14.1; Anal. Calcd for $C_{20}H_{18}N_2O_4$: C, 68.56; H, 5.18; N, 8.00%; Found: C, 68.80; H, 5.11; N, 8.12%.



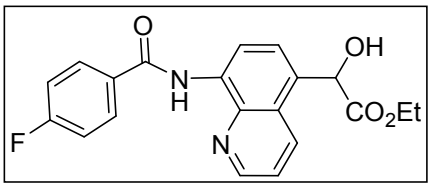
Ethyl 2-hydroxy-2-(8-(3-methylbenzamido)quinolin-5-yl)acetate (3b): Light yellow gummy mass (76%, 55.4 mg); R_f = 0.55 (PE:EA = 75:25); ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.77 (s, 1H), 8.88-8.85 (m, 2H), 8.56 (dd, J = 8.4 Hz, 1.6 Hz, 1H), 7.87-7.84 (m, 2H), 7.58 (d, J = 8.0 Hz, 1H), 7.52-7.49 (m, 1H), 7.44-7.38 (m, 2H), 5.68 (s, 1H), 4.29-4.12 (m, 2H), 3.69 (br s,1H), 2.47 (s, 3H), 1.14 (t, J = 7.2 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 173.8, 165.9, 148.2, 139.1, 138.8, 135.4, 135.1, 133.1, 132.8, 128.8, 128.2, 127.6, 126.2, 124.3, 121.9, 115.8, 71.5, 62.5, 21.6, 14.1; Anal. Calcd for $C_{21}H_{20}N_2O_4$: C, 69.22; H, 5.53; N, 7.69%; Found: C, 69.40; H, 5.58; N, 7.77%.



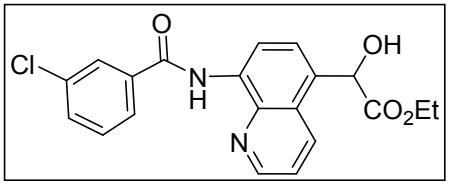
Ethyl 2-hydroxy-2-(8-(4-methylbenzamido)quinolin-5-yl)acetate (**3c**): White solid (82%, 59.7 mg); R_f = 0.45 (PE:EA = 80:20); M.p. 89-90 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.79 (s, 1H), 8.89-8.86 (m, 2H), 8.56 (dd, J = 8.4 Hz, 1.6 Hz, 1H), 7.98-7.96 (m, 2H), 7.59 (d, J = 8.0 Hz, 1H), 7.53-7.50 (m, 1H), 7.34 (d, J = 8.0 Hz, 2H), 5.68 (s, 1H), 4.28-4.14 (m, 2H), 3.60 (br s, 1H), 2.45 (s, 3H), 1.14 (t, J = 7.2 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 173.9, 165.6, 148.2, 142.6, 139.2, 135.5, 133.1, 132.3, 129.6, 128.0, 127.7, 127.4, 126.2, 121.9, 115.7, 71.5, 62.6, 21.6, 14.1; Anal. Calcd for $C_{21}H_{20}N_2O_4$: C, 69.22; H, 5.53; N, 7.69%; Found: C, 69.01; H, 5.61; N, 7.60%.



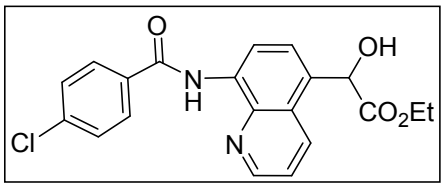
Ethyl 2-hydroxy-2-(8-(4-methoxybenzamido)quinolin-5-yl)acetate (3d): White solid (78%, 59.4 mg); R_f = 0.50 (PE:EA = 70:30); M.p. 85-86 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.70 (s, 1H), 8.83-8.78 (m, 2H), 8.55 (dd, J = 8.8 Hz, 1.2 Hz, 1H), 8.03-7.99 (m, 2H), 7.54 (d, J = 8.0 Hz, 1H), 7.49-7.45 (m, 1H), 7.02-6.99 (m, 2H), 5.66 (s, 1H), 4.27-4.10 (m, 2H), 3.87 (s, 4H), 1.12 (t, J = 7.2 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 173.7, 165.1, 162.6, 148.1, 139.0, 135.4, 133.2, 129.2. 128.0, 127.5, 127.2, 126.1, 121.8, 115.5, 114.1, 71.5, 62.4, 55.5, 14.0; HRMS (ESI-TOF) *m/z*: $[M + H]^+$Calcd for $C_{21}H_{20}N_2O_5$: 381.1445; found: 381.1449.



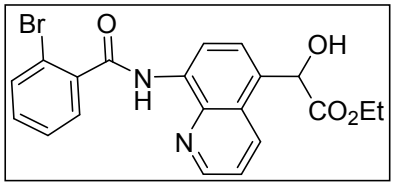
Ethyl 2-(8-(4-fluorobenzamido)quinolin-5-yl)-2-hydroxyacetate (**3e**): White solid (68%, 50.0 mg); R_f = 0.55 (PE:EA = 75:25); M.p 102-103 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.77 (s, 1H), 8.87-8.84 (m, 2H), 8.57 (dd, J = 8.4 Hz, 1.6 Hz, 1H), 8.10-8.06 (m, 2H), 7.60 (d, J = 8.0 Hz, 1H), 7.54-7.51 (m, 1H), 7.24-7.20 (m, 2H), 5.64 (s, 1H), 4.26-4.16 (m, 2H), 3.64 (br s, 1H), 1.14 (t, J = 7.2 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 173.9, 164.5, 148.2, 139.1, 134.2 ($J_{C\text{-}F}$ = 200.0 Hz), 131.3 ($J_{C\text{-}F}$ = 4.0 Hz), 129.89, 129.81, 128.3, 127.6, 126.2, 122.0, 116.1, 115.9, 115.8, 71.5, 62.6, 14.1; Anal. Calcd for $C_{20}H_{17}FN_2O_4$: C, 65.21; H, 4.65; N, 7.60%; Found: C, 65.05; H, 4.59; N, 7.51%.



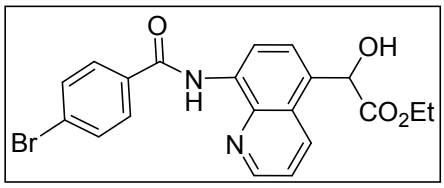
Ethyl 2-(8-(3-chlorobenzamido)quinolin-5-yl)-2-hydroxyacetate (**3f**): White solid (72%, 55.3 mg); R_f = 0.55 (PE:EA = 80:20); M.p. 94-95 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.76 (s, 1H), 8.87 (dd, J = 4.4 Hz, 1.6 Hz, 1H), 8.83 (d, J = 8.0 Hz, 1H), 8.57 (dd, J = 8.8 Hz, 1.6 Hz, 1H), 8.04 (t, J = 2.0 Hz, 1H), 7.94-7.91 (m, 1H), 7.60-7.46 (m, 4H), 5.68 (d, J = 3.2 Hz, 1H), 4.27-4.14 (m, 2H), 3.70 (d, J = 4.0 Hz, 1H), 1.14 (t, J = 7.2 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 173.8, 164.1, 148.3, 139.0, 136.8, 135.1, 135.0, 133.2, 132.1, 130.2, 128.6, 127.8, 127.5, 126.2, 125.4, 122.0, 115.9, 71.4, 62.6, 14.1; Anal. Calcd for $C_{20}H_{17}ClN_2O_4$: C, 62.42; H, 4.45; N, 7.28%; Found: C, 62.25; H, 4.55; N, 7.39%.



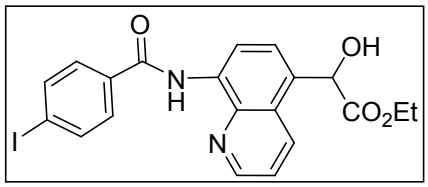
Ethyl 2-(8-(4-chlorobenzamido)quinolin-5-yl)-2-hydroxyacetate (**3g):** White solid (76%, 58.4 mg); R_f= 0.50 (PE:EA = 75:25); M.p. 131-132 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.77 (s, 1H), 8.86-8.82 (m, 2H), 8.57 (dd, J = 8.8 Hz, 1.6 Hz, 1H), 8.01-7.98 (m, 2H), 7.58 (d, J = 8.0 Hz, 1H), 7.53-7.49 (m, 3H), 5.67 (d, J = 3.6 Hz, 1H), 4.27-4.14 (m, 2H), 3.69 (d, J = 4.4 Hz, 1H), 1.14 (t, J = 7.2 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 173.8, 164.5, 148.2, 139.0, 138.3, 135.1, 133.4, 133.2, 129.2, 128.8, 128.5, 127.5, 126.2, 122.0, 115.8, 71.5, 62.6, 14.1; Anal. Calcd for $C_{20}H_{17}ClN_2O_4$: C, 62.42; H, 4.45; N, 7.28%; Found: C, 62.60; H, 4.49; N, 7.19%.



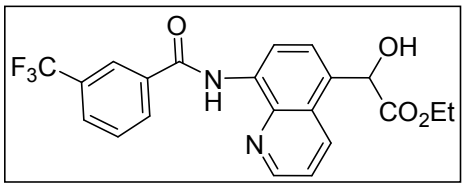
Ethyl 2-(8-(2-bromobenzamido)quinolin-5-yl)-2-hydroxyacetate (3h): Yellow gummy mass (65%, 55.8 mg); R_f = 0.45 (PE:EA = 80:20); ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.86 (s, 1H), 8.93 (d, J = 8.0 Hz, 1H), 8.89 (dd, J = 4.4 Hz, 1.6 Hz, 1H), 8.64 (dd, J = 8.8 Hz, 1.6 Hz, 1H), 8.09-8.07 (m, 2H), 7.72 (d, J = 8.4 Hz, 1H), 7.60-7.56 (m, 3H), 6.52 (s, 1H), 4.26-4.11 (m, 2H), 1.15 (t, J = 7.2 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 170.4, 169.0, 165.7, 148.4, 139.0, 136.0, 135.0, 134.4, 133.3, 132.1, 129.2, 129.0, 127.4, 126.3, 124.1, 122.3, 115.8, 72.6, 62.1, 14.1; Anal. Calcd for $C_{20}H_{17}BrN_2O_4$: C, 55.96; H, 3.99; N, 6.53%; Found: C, 55.81; H, 3.93; N, 6.63%.



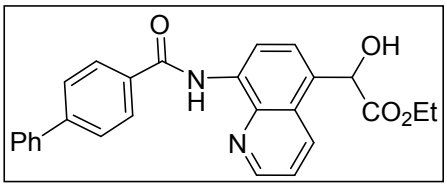
Ethyl 2-(8-(4-bromobenzamido)quinolin-5-yl)-2-hydroxyacetate (3i): Yellow solid (70%, 60.1 mg); R_f = 0.50 (PE:EA = 80:20); M.p. 134-135 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.79 (s, 1H), 8.87-8.84 (m, 2H), 8.57 (dd, J = 8.8 Hz, 1.6 Hz, 1H), 7.95-7.92 (m, 2H), 7.70-7.67 (m, 2H), 7.60 (d, J = 8.0 Hz, 1H), 7.55-7.51 (m, 1H), 5.68 (d, J = 3.6 Hz, 1H), 4.30-4.13 (m, 2H), 3.60 (d, J = 4.0 Hz, 1H), 1.14 (t, J = 7.2 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 173.8, 164.6, 148.3, 139.1, 135.1, 133.9, 133.2, 132.2, 129.0, 128.5, 127.6, 126.8, 126.2, 122.0, 115.9, 71.5, 62.6, 14.1; Anal. Calcd for $C_{20}H_{17}BrN_2O_4$: C, 55.96; H, 3.99; N, 6.53%; Found: C, 56.14; H, 4.06; N, 6.41%.



Ethyl 2-hydroxy-2-(8-(4-iodobenzamido)quinolin-5-yl)acetate (3j): White solid (72%, 68.7 mg); R_f = 0.50 (PE:EA = 70:30); M.p. 155-156 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.77 (s, 1H), 8.85-8.81 (m, 2H), 8.56 (d, J = 8.4 Hz, 1H), 7.88 (dd, J = 8.4 Hz, 1.6 Hz, 2H), 7.77 (dd, J = 8.4 Hz, 2.0 Hz, 2H), 7.58 (dd, J = 8.0 Hz, 2.8 Hz, 1H), 7.53-7.49 (m, 1H), 5.67 (s, 1H), 4.27-4.12 (m, 2H), 3.70 (d, J = 11.6 Hz, 1H), 1.13 (t, J = 7.2 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 173.8, 164.8, 148.2, 139.0, 138.1, 135.0, 134.4, 133.2, 128.9, 128.5, 127.5, 126.2, 122.0, 115.8, 99.2, 71.4, 62.5, 14.0; HRMS (ESI-TOF) *m/z*: $[M + H]^+$ Calcd for $C_{20}H_{17}IN_2O_4$: 477.0306; found: 477.0302.

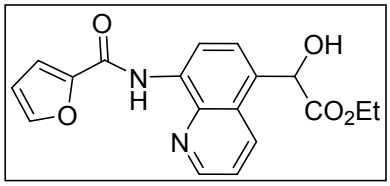


Ethyl 2-hydroxy-2-(8-(3-(trifluoromethyl)benzamido)quinolin-5-yl)acetate (3k): White solid (61%, 51.0 mg); R_f = 0.55 (PE:EA = 80:20); M.p. 102-103 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.85 (s, 1H), 8.88-8.85 (m, 2H), 8.58 (dd, J = 8.8 Hz, 1.6 Hz, 1H), 8.33 (s, 1H), 8.23 (d, J = 7.6 Hz, 1H), 7.84 (d, J = 8.0 Hz, 1H), 7.69 (t, J = 8.0 Hz, 1H), 7.61 (d, J = 8.4 Hz, 1H), 7.55-7.52 (m, 1H), 5.69 (s, 1H), 4.30-4.13 (m, 2H), 3.66 (br s, 1H), 1.14 (t, J = 7.2 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 173.8, 164.1, 148.4, 139.1, 135.9, 134.9, 133.3, 131.7, 131.4, 130.4, 129.5, 128.7, 128.6 ($J_{C\text{-}F}$ = 8.0 Hz, 5.0 Hz), 127.5, 126.2, 124.7 ($J_{C\text{-}F}$ = 8.0 Hz, 5.0 Hz), 122.1, 116.0, 71.4, 62.6, 14.1; Anal. Calcd for $C_{21}H_{17}F_3N_2O_4$: C, 60.29; H, 4.10; N, 6.70%; Found: C, 60.48; H, 4.18; N, 6.61%.

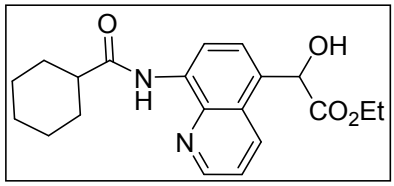


Ethyl 2-(8-([1,1'-biphenyl]-4-carboxamido)quinolin-5-yl)-2-hydroxyacetate (3l): White solid (77%, 65.6 mg); R_f = 0.45 (PE:EA = 75:25); M.p. 92-93 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.87 (s, 1H), 8.91-8.88 (m, 2H), 8.58 (dd, J = 8.8 Hz, 1.6 Hz, 1H), 8.16-8.14 (m, 2H), 7.79-7.76 (m, 2H), 7.67-7.65 (m, 2H), 7.61 (d, J = 8.0 Hz, 1H), 7.55-7.47 (m, 3H), 7.43-7.39 (m, 1H), 5.69 (s, 1H), 4.29-4.15 (m, 2H), 3.65 (br s, 1H), 1.15 (t, J = 7.2 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 173.9, 165.3, 148.2, 144.8, 140.1, 139.1, 135.4, 133.7, 133.2, 129.1, 128.2, 127.9,

127.7, 127.6, 127.3, 126.2, 122.0, 115.8, 71.5, 62.6, 14.1; Anal. Calcd for $C_{26}H_{22}N_2O_4$: C, 73.23; H, 5.20; N, 6.57%; Found: C, 73.39; H, 5.13; N, 6.46%.

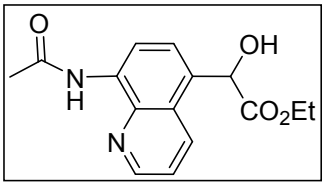


Ethyl 2-(8-(furan-2-carboxamido)quinolin-5-yl)-2-hydroxyacetate (3m): White solid (79%, 53.7 mg); R_f = 0.45 (PE:EA = 80:20); M.p. 112-113 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.84 (s, 1H), 8.90 (dd, J = 4.0 Hz, 1.6 Hz, 1H), 8.82 (d, J = 8.0 Hz, 1H), 8.56 (dd, J = 8.8 Hz, 1.6 Hz, 1H), 7.63 (t, J = 1.2 Hz, 1H), 7.58 (d, J = 8.0 Hz, 1H), 7.54-7.51 (m, 1H), 7.30 (d, J = 3.6 Hz, 1H), 6.59 (dd, J = 3.6 Hz, 1.6 Hz, 1H), 5.68 (d, J = 3.2 Hz, 1H), 4.28-7.14 (m, 2H), 3.60 (d, J = 4.0 Hz, 1H), 1.14 (t, J = 7.2 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 173.9, 156.5, 148.3, 144.7, 139.0, 135.0, 133.1, 128.3, 127.5, 126.2, 122.0, 115.9, 115.4, 112.6, 71.5, 62.6, 14.1; Anal. Calcd for $C_{18}H_{16}N_2O_5$: C, 63.53; H, 4.74; N, 8.23%; Found: C, 63.32; H, 4.79; N, 8.31%.

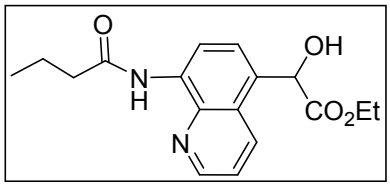


Ethyl 2-(8-(cyclohexanecarboxamido)quinolin-5-yl)-2-hydroxyacetate (3n): White solid (72%, 51.3 mg); R_f = 0.55 (PE:EA = 80:20); M.p. 153-154 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.96 (s, 1H), 8.81 (dd, J = 4.0 Hz, 1.6 Hz, 1H), 8.73 (d, J = 8.0 Hz, 1H), 8.53 (dd, J = 8.4 Hz, 1.6 Hz, 2H), 7.53-7.47 (m, 2H), 5.64 (s, 1H), 4.25-4.12 (m, 1H), 3.66 (br s, 1H), 2.49-2.42 (m, 1H), 2.08-2.04 (m, 2H), 1.88-1.84 (m, 2H), 1.74-1.70 (m, 1H), 1.66-1.56 (m, 2H), 1.42-1.26 (m, 3H), 1.12 (t, J = 7.2 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): 175.1, 173.9, 148.0, 138.8, 135.4,

133.1, 127.8, 127.6, 126.1, 121.8, 115.6, 71.5, 62.5, 47.0, 29.8, 25.8, 14.0; Anal. Calcd for $C_{20}H_{24}N_2O_4$: C, 67.40; H, 6.79; N, 7.86%; Found: C, 67.63; H, 6.87; N, 7.72%.

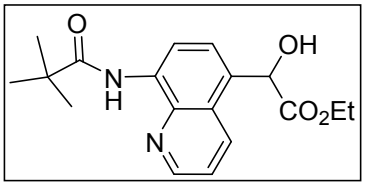


Ethyl 2-(8-acetamidoquinolin-5-yl)-2-hydroxyacetate (3o): White solid (74%, 42.6 mg); R_f = 0.45 (PE:EA = 75:25); M.p. 191-192 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.86 (s, 1H), 8.81 (dd, J = 4.0 Hz, 1.6 Hz, 1H), 8.71 (d, J = 8.0 Hz, 1H), 8.54 (dd, J = 8.8 Hz, 1.6 Hz, 1H), 7.54-7.48 (m, 2H), 5.65 (s, 1H), 4.26-4.11 (m, 2H), 2.34 (s, 3H), 3.58 (br s, 1H), 1.13 (t, J = 7.2 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 173.8, 168.9, 147.9, 138.5, 135.2, 133.0, 127.8, 127.5, 126.0, 121.7, 115.5, 71.3, 62.4, 25.1, 13.9; Anal. Calcd for $C_{15}H_{16}N_2O_4$: C, 62.49; H, 5.59; N, 9.72%; Found: C, 62.30; H, 5.63; N, 9.81%.

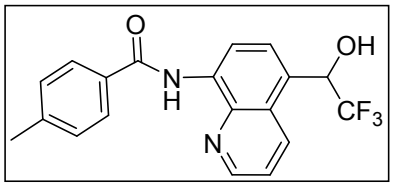


Ethyl 2-(8-butyramidoquinolin-5-yl)-2-hydroxyacetate (3p): Yellow gummy mass (79%, 49.9 mg); R_f = 0.55 (PE:EA = 70:30); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.89 (s, 1H), 8.81 (dd, J = 4.0 Hz, 1.6 Hz, 1H), 8.74 (d, J = 8.4 Hz, 1H), 8.53 (dd, J = 8.8 Hz, 1.6 Hz, 1H), 7.54 (d, J = 8.0 Hz, 1H), 7.51-7.48 (m, 1H), 5.65 (s, 1H), 4.26-4.13 (m, 2H), 3.55 (br s, 1H), 2.54 (t, J = 7.6 Hz, 2H), 1.89-1.80 (m, 2H), 1.13 (t, J = 7.2 Hz, 3H), 1.05 (t, J = 7.6 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 173.9, 172.0, 148.0, 138.7, 135.4, 133.1, 127.8, 127.7, 126.1, 121.8, 115.6, 71.5, 62.6,

40.3, 19.2, 14.1, 13.9; Anal. Calcd for $C_{17}H_{20}N_2O_4$: C, 64.54; H, 6.37; N, 8.86%; Found: C, 64.36; H, 6.43; N, 8.75%.

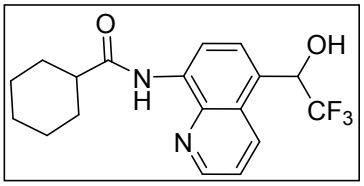


Ethyl 2-hydroxy-2-(8-pivalamidoquinolin-5-yl)acetate (3q): Yellow gummy mass (80%, 52.8 mg); R_f = 0.50 (PE:EA = 75:25); ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.35 (s, 1H), 8.82 (dd, J = 4.4 Hz, 1.6 Hz, 1H), 8.74 (d, J = 8.0 Hz, 1H), 8.53 (dd, J = 8.8 Hz, 1.6 Hz, 1H), 7.54 (d, J = 8.0 Hz, 1H), 7.50-7.47 (m, 1H), 5.64 (s, 1H), 4.25-4.14 (m, 2H), 3.55 (br s, 1H), 1.41 (s, 9H), 1.12 (t, J = 7.2 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 177.5, 173.9, 148.1, 139.1, 135.5, 133.0, 127.74, 127.70, 126.1, 121.8, 115.4, 71.5, 62.5, 40.5, 27.8, 14.0; Anal. Calcd for $C_{18}H_{22}N_2O_4$: C, 65.44; H, 6.71; N, 8.48%; Found: C, 65.59; H, 6.67; N, 8.40%.

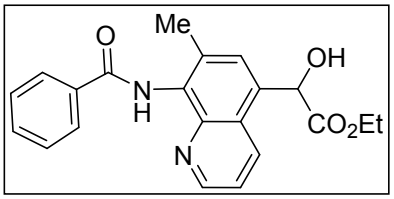


4-Methyl-*N*-(5-(2,2,2-trifluoro-1-hydroxyethyl)quinolin-8-yl)benzamide (3r): White solid (61%, 43.9 mg); R_f = 0.50 (PE:EA = 80:20); M.p. 178-179 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.71 (s, 1H), 8.82 (dd, J = 4.4 Hz, 1.6 Hz, 1H), 8.75 (d, J = 8.0 Hz, 1H), 8.50 (d, J = 8.4 Hz, 1H), 7.91 (d, J = 8.0 Hz, 2H), 7.75 (d, J = 8.0 Hz, 1H), 7.48-7.44 (m, 1H), 7.34 (d, J = 8.0 Hz, 2H), 5.63 (q, J = 6.8, 1H), 3.82 (br s, 1H), 2.46 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 165.8, 148.2, 142.9, 138.6, 135.7, 132.9, 131.9, 129.7, 128.2, 127.4, 126.2 ($J_{C\text{-}F}$ = 22.0 Hz),

124.1, 123.3, 122.0, 115.6, 70.4 ($J_{C\text{-}F}$ = 66.0 Hz, 33.0 Hz), 21.7 ; Anal. Calcd for $C_{19}H_{15}F_3N_2O_2$: C, 63.33; H, 4.20; N, 7.77%; Found: C, 63.54; H, 4.26; N, 7.89%.

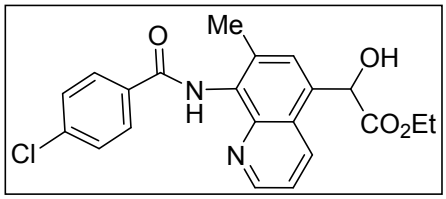


***N*-(5-(2,2,2-trifluoro-1-hydroxyethyl)quinolin-8-yl)cyclohexanecarboxamide (3s):** White solid (69%, 48.6 mg); R_f = 0.55 (PE:EA = 80:20); M.p. 142-1432 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.98 (s, 1H), 8.81 (dd, J = 4.4 Hz, 1.6 Hz, 1H), 8.68 (d, J = 8.0 Hz, 1H), 8.55 (d, J = 8.4 Hz, 1H), 7.73 (d, J = 8.0 Hz, 1H), 7.52-7.49 (m, 1H), 5.64 (q, J = 6.8 Hz, 1H), 3.72 (br s, 1H), 2.48-2.40 (m, 1H), 2.06-2.02 (m, 2H), 1.88-1.84 (m, 2H), 1.74-1.72 (m, 1H), 1.63-1.54 (m, 2H), 1.41-1.29 (m, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 175.4, 148.1, 138.4, 135.8, 132.9, 128.2, 126.2 ($J_{C\text{-}F}$ = 19.0 Hz), 123.8, 123.3, 121.9, 115.6, 70.4 ($J_{C\text{-}F}$ = 65.0 Hz, 33.0 Hz), 47.0, 29.8, 29.7, 25.8; Anal. Calcd for $C_{18}H_{19}F_3N_2O_2$: C, 61.36; H, 5.44; N, 7.95%; Found: C, 61.50; H, 5.49; N, 8.02%.



Ethyl 2-(8-benzamido-7-methylquinolin-5-yl)-2-hydroxyacetate (5a): Yellow gummy mass (81%, 59.0 mg); R_f = 0.50 (PE:EA = 80:20); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.57 (s, 1H), 8.79 (dd, J = 4.4 Hz, 1.6 Hz, 1H), 8.50 (dd, J = 8.8 Hz, 1.6 Hz, 1H), 8.09-8.07 (m, 2H), 7.60-7.56 (m, 1H), 7.54-7.50 (m, 3H), 7.43-7.40 (m, 1H), 5.70 (s, 1H), 4.32-4.09 (m, 2H), 3.74 (br s, 1H), 2.52 (s, 3H), 1.16 (t, J = 7.2 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 173.7, 166.0, 148.7, 142.6,

134.6, 133.1, 132.4, 132.1, 130.8, 130.5, 128.8, 128.0, 124.7, 120.9, 71.0, 62.7, 20.6, 14.1; Anal. Calcd for $C_{21}H_{20}N_2O_4$: C, 69.22; H, 5.53; N, 7.69%; Found: C, 69.01; H, 5.63; N, 7.57%.



Ethyl 2-(8-(4-chlorobenzamido)-7-methylquinolin-5-yl)-2-hydroxyacetate (5b): White solid (75%, 59.7 mg); R_f = 0.50 (PE:EA = 80:20); M.p. 162-163 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.62 (s, 1H), 8.77 (dd, J = 4.4 Hz, 1.6 Hz, 1H), 8.48 (dd, J = 8.4 Hz, 1.6 Hz, 1H), 8.02-7.99 (m, 2H), 7.52 (s, 1H), 7.49-7.45 (m, 2H), 7.42-7.39 (m, 1H), 5.68 (s, 1H), 4.29-4.10 (m, 2H), 3.70 (br s, 1H), 2.50 (s, 3H), 1.15 (t, J = 7.2 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 173.7, 164.9, 148.9, 142.8, 138.3, 133.1, 132.8, 132.3, 131.0, 130.4, 129.4, 129.0, 128.7, 124.6, 121.0, 71.0, 62.7, 20.6, 14.1; Anal. Calcd for $C_{21}H_{19}ClN_2O_4$: C, 63.24; H, 4.80; N, 7.02%; Found: C, 63.09; H, 4.71; N, 7.15%.

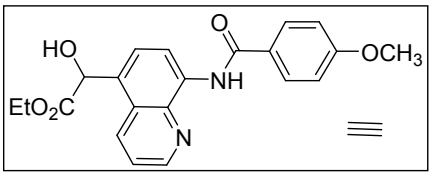
4. References:

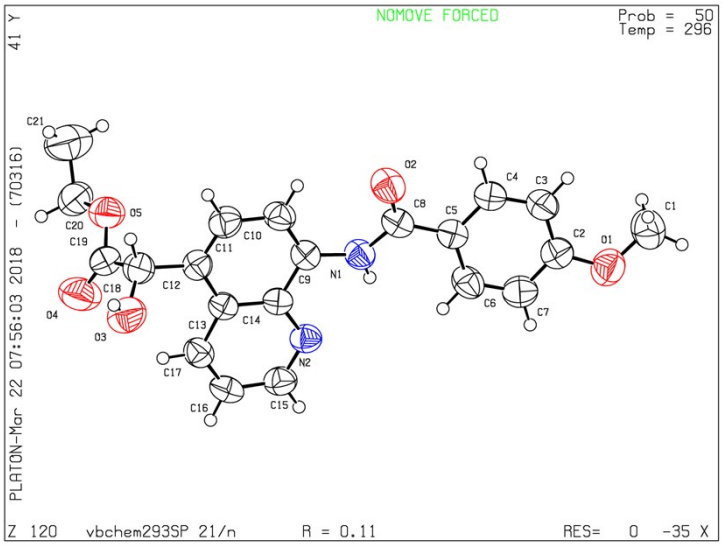
[1] a) C. J. Whiteoak, O. Planas, A. Company, X. Ribas, *Adv. Synth. Catal*. **2016**, *358*, 1679;

b) Y. He, N. Zhao, L. Qiu, X. Zhang, X. Fan, *Org. Lett*. **2016**, *18*, 6054.

5. Structure Determination (X-ray crystallographic data for 3d):

The white crystals of **3d** was obtained by crystallization from a solution in dichloromethane/petroleum ether after purification by column chromatography. Chemical Formula**:** $C_{21}H_{20}N_2O_5$.





ORTEP (with 50% probability) diagram for the structure ethyl 2-hydroxy-2-(8-(4-methoxybenzamido)quinolin-5-yl)acetate (**3d**).

Wavelength	0.71073 Å	
Formula	C21 H20 N2 O5	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 8.809(11) Å	α = 90°
	b = 12.652(16) Å	β = 91.413(13)°
	c = 16.37(2) Å	γ = 90°
Volume	1824(4) Å^3	
Z	4	
R-factor (%)	11.41	

The crystallographic data have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication with a CCDC reference number CCDC **1831821**.

6. NMR spectra for the synthesized products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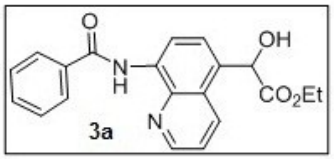
1.126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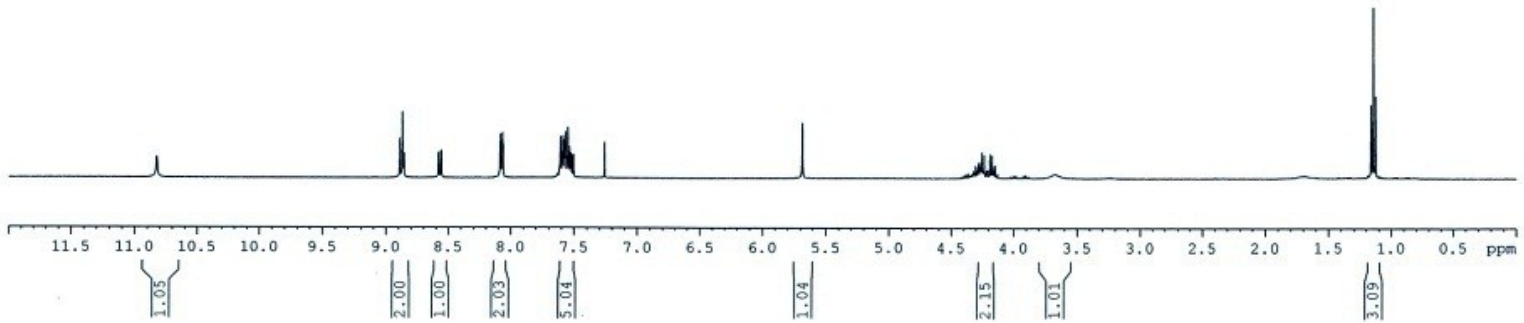
N
H
OH
CO2Et
N

3a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5.04
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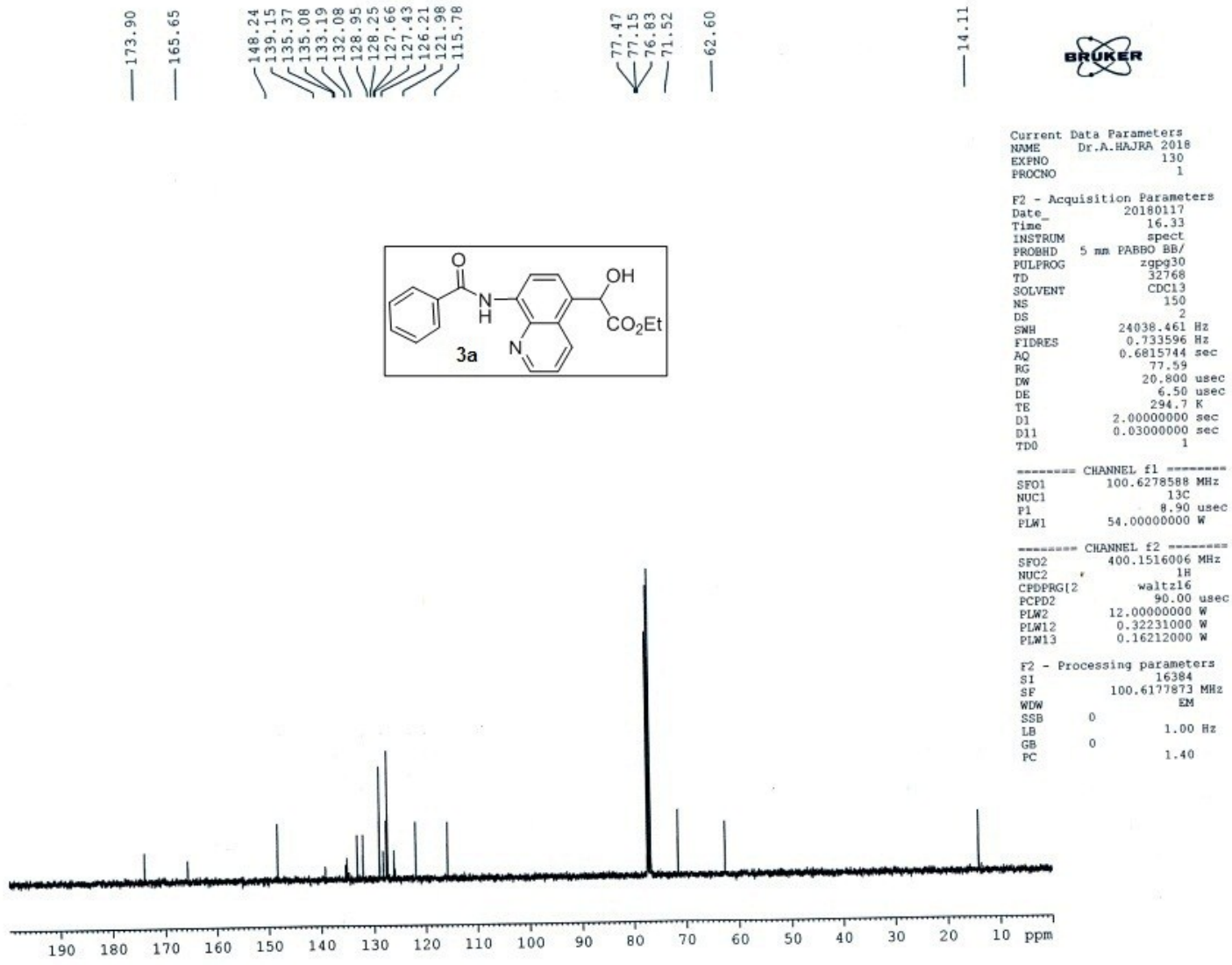
3.09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PROCNO 1
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Time 16.33
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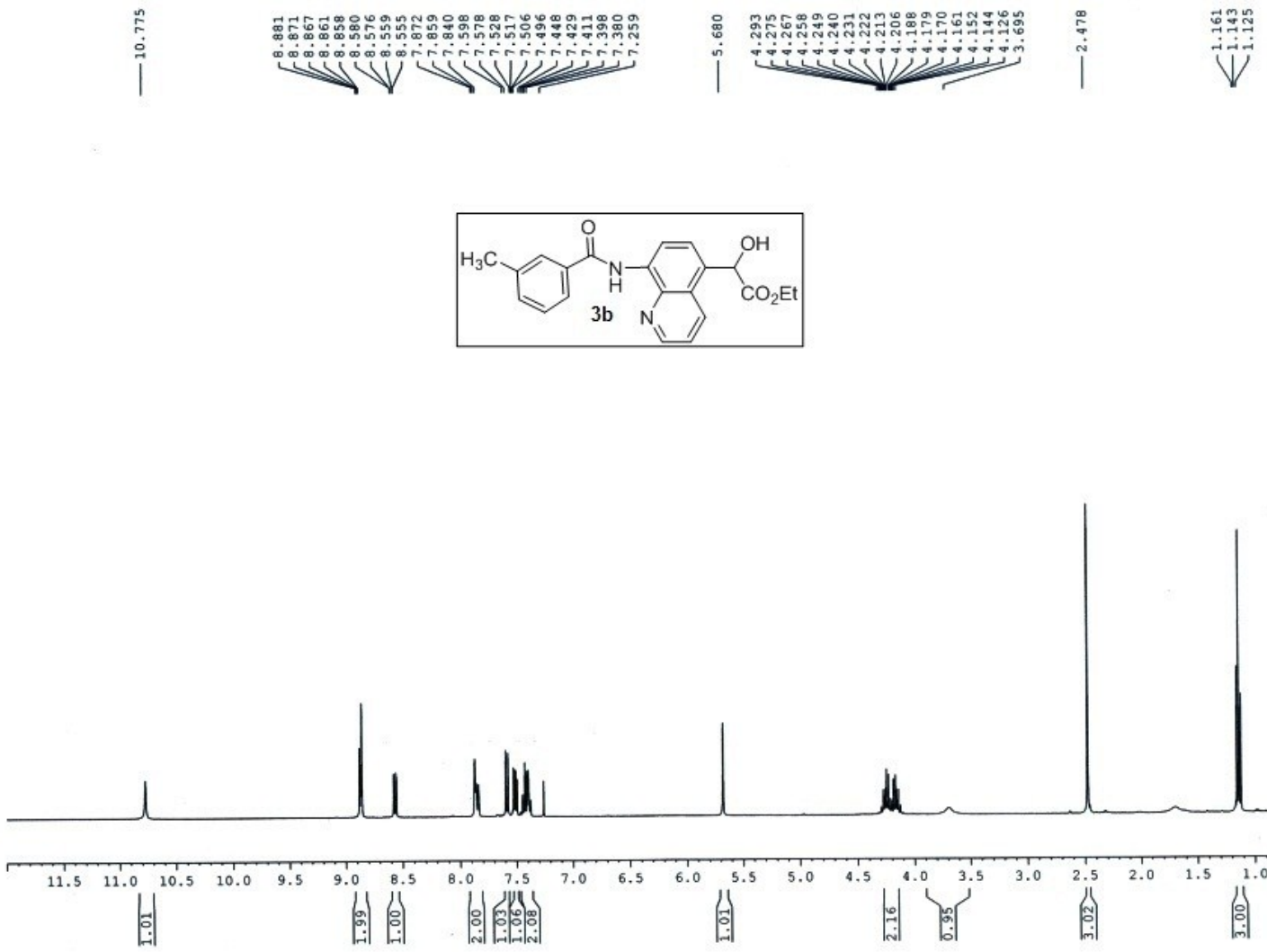
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N
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2.08
1.01
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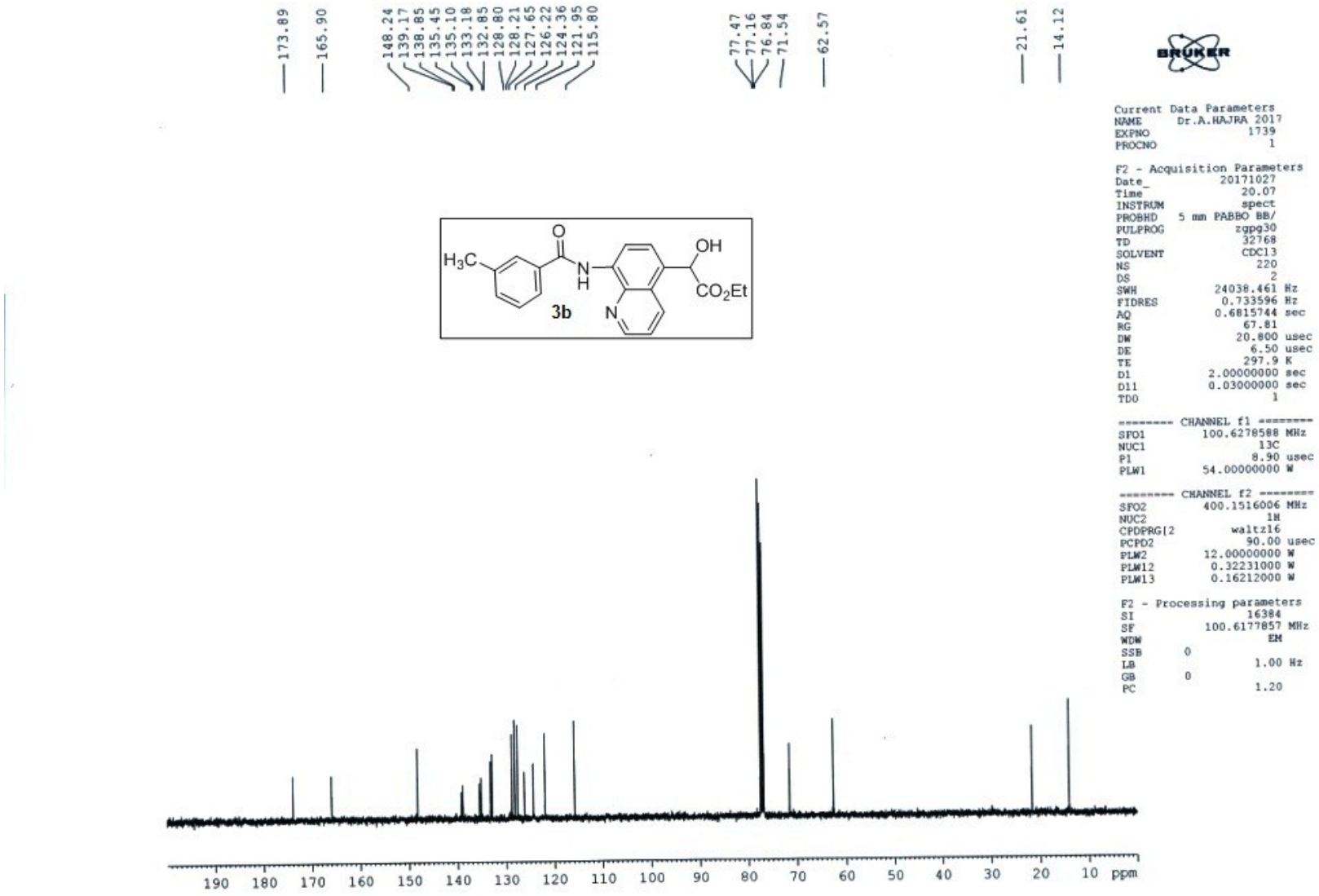
3.00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3b
Current Data Parameters
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Time 20.07
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7.504
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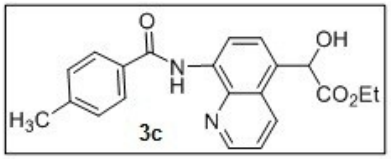
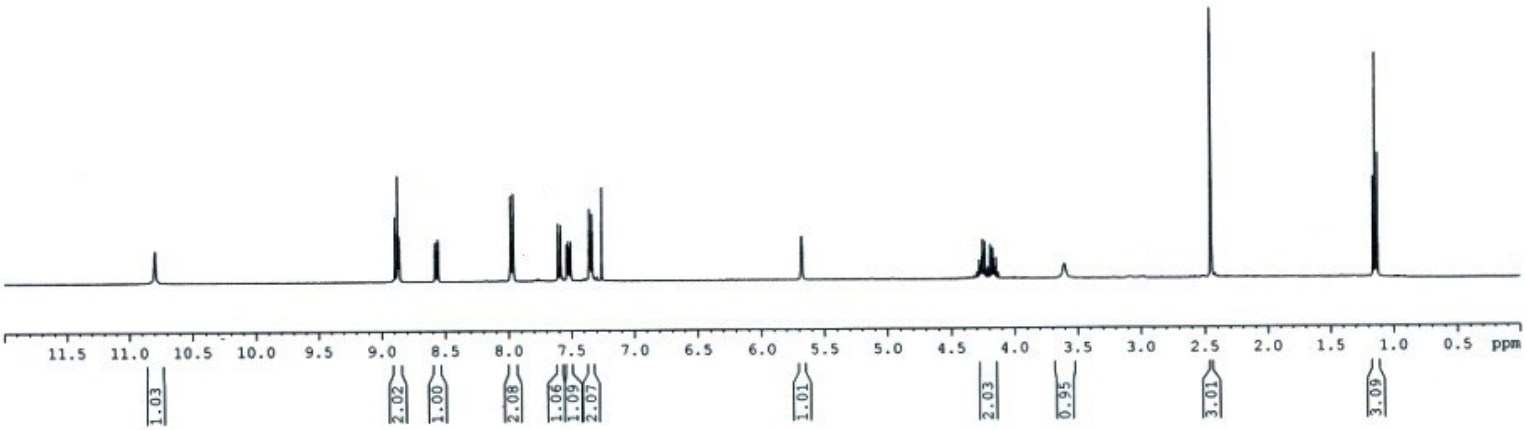
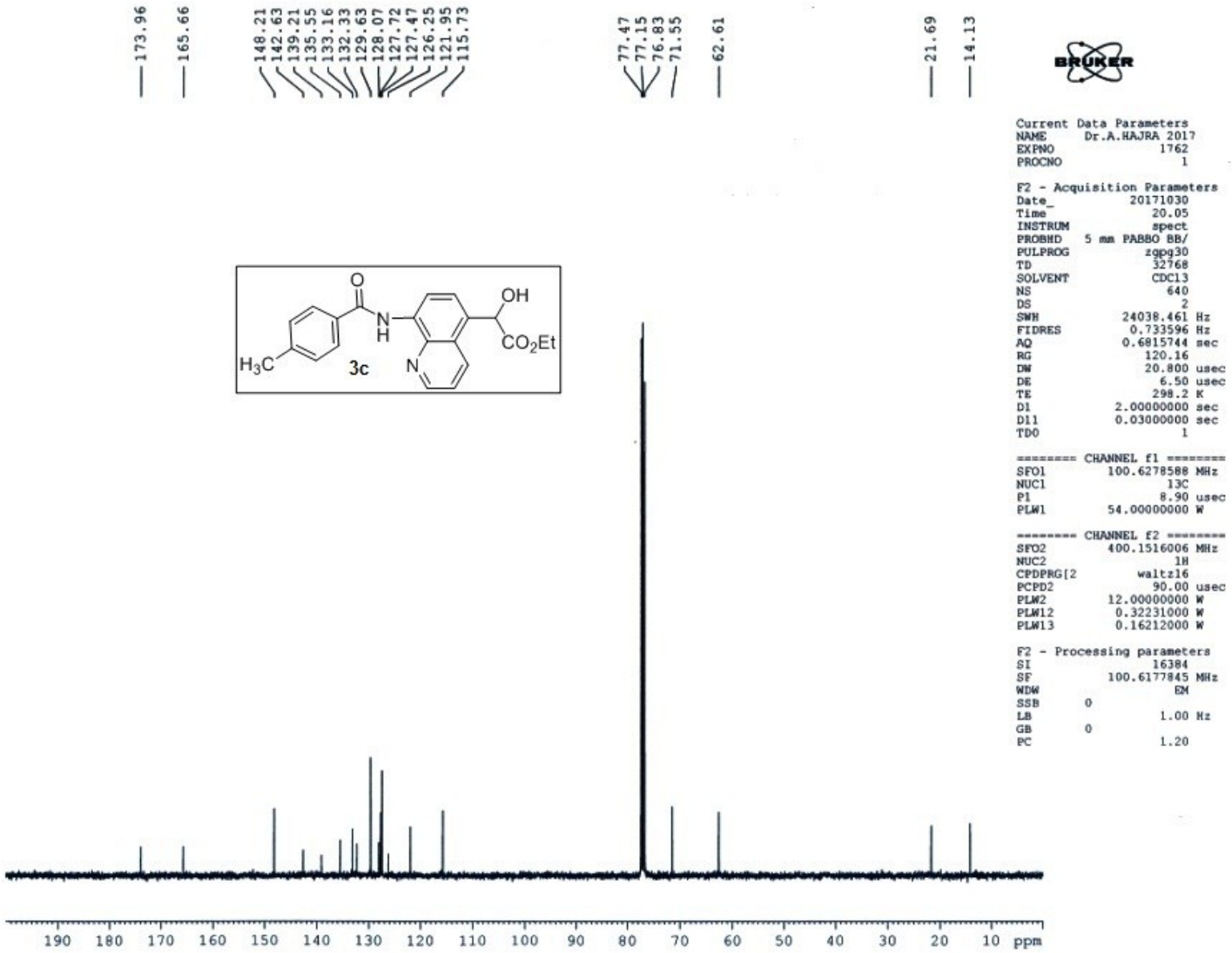
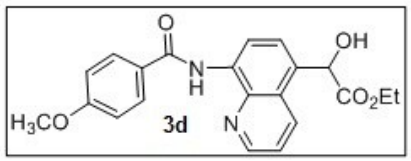
1.146
1.128


O
N
H
OH
CO2Et
H3C
N
3c

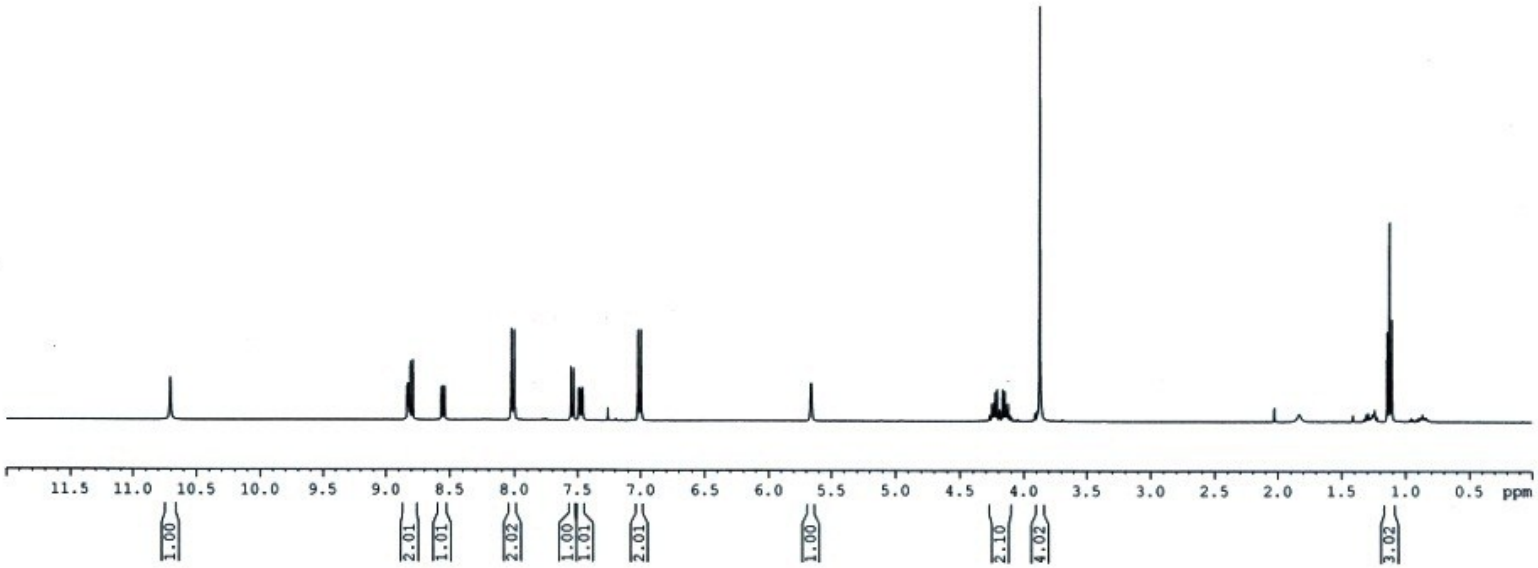

11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
1.03
2.02
1.00
2.08
1.06
1.09
2.07
1.01
2.03
0.95
3.01
3.09

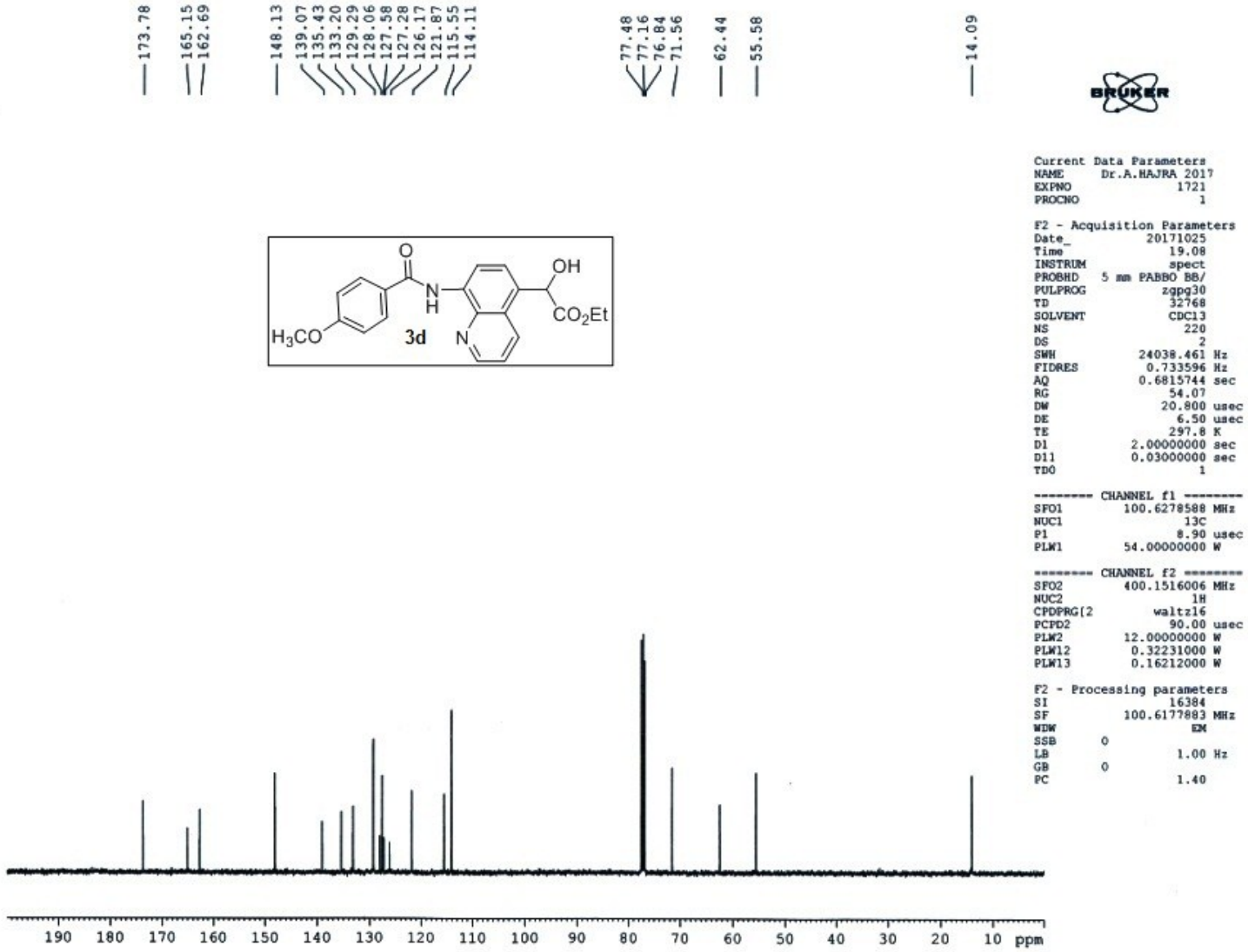

173.96
165.66
148.21
142.63
139.21
135.55
133.16
132.33
129.63
128.07
127.72
127.47
126.25
121.95
115.73
77.47
77.15
76.83
71.55
62.61
21.69
14.13
BRUKER
Current Data Parameters
NAME Dr.A.HAJRA 2017
EXPNO 1762
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171030
Time 20.05
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 640
DS 2
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 120.16
DW 20.800 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6278588 MHz
NUC1 13C
P1 8.90 usec
PLW1 54.00000000 W
======== CHANNEL f2 ========
SFO2 400.1516006 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 12.00000000 W
PLW12 0.32231000 W
PLW13 0.16212000 W
F2 - Processing parameters
SI 16384
SF 100.6177845 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.20
O
N
H
OH
CO2Et
H3C
3c
N
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


10.705
8.834
8.831
8.824
8.820
8.809
8.789
8.566
8.563
8.544
8.541
8.034
8.026
8.021
8.009
8.004
7.997
7.554
7.534
7.491
7.480
7.470
7.459
7.259
7.028
7.020
7.016
7.005
6.998
6.992
5.663
4.273
4.255
4.246
4.237
4.228
4.220
4.210
4.192
4.187
4.170
4.160
4.152
4.143
4.134
4.125
4.107
3.874
1.145
1.127
1.109

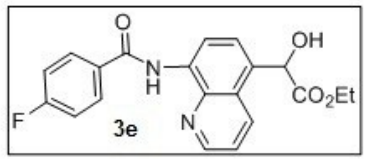

O
N
H
OH
CO2Et
H3CO
N

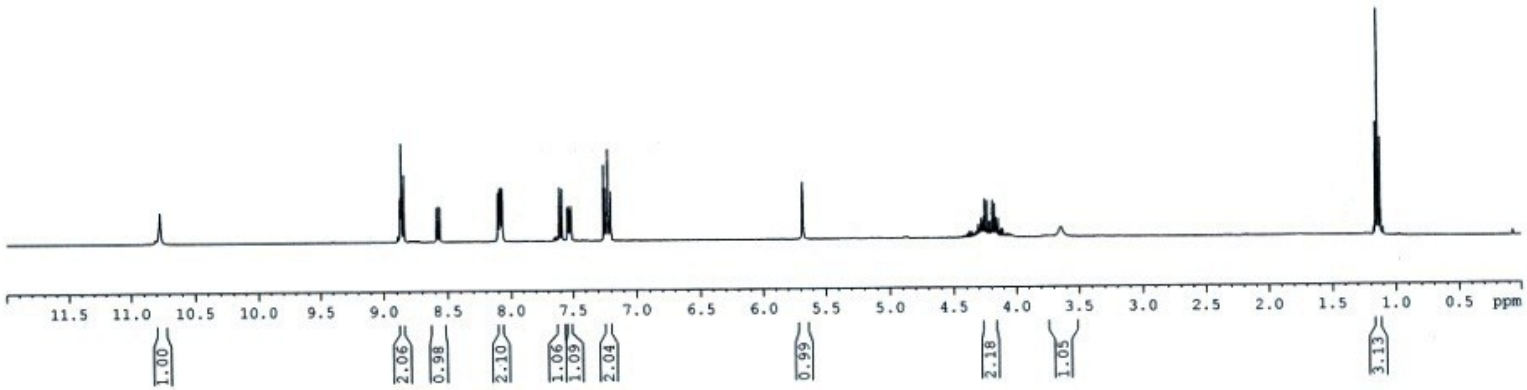
3d

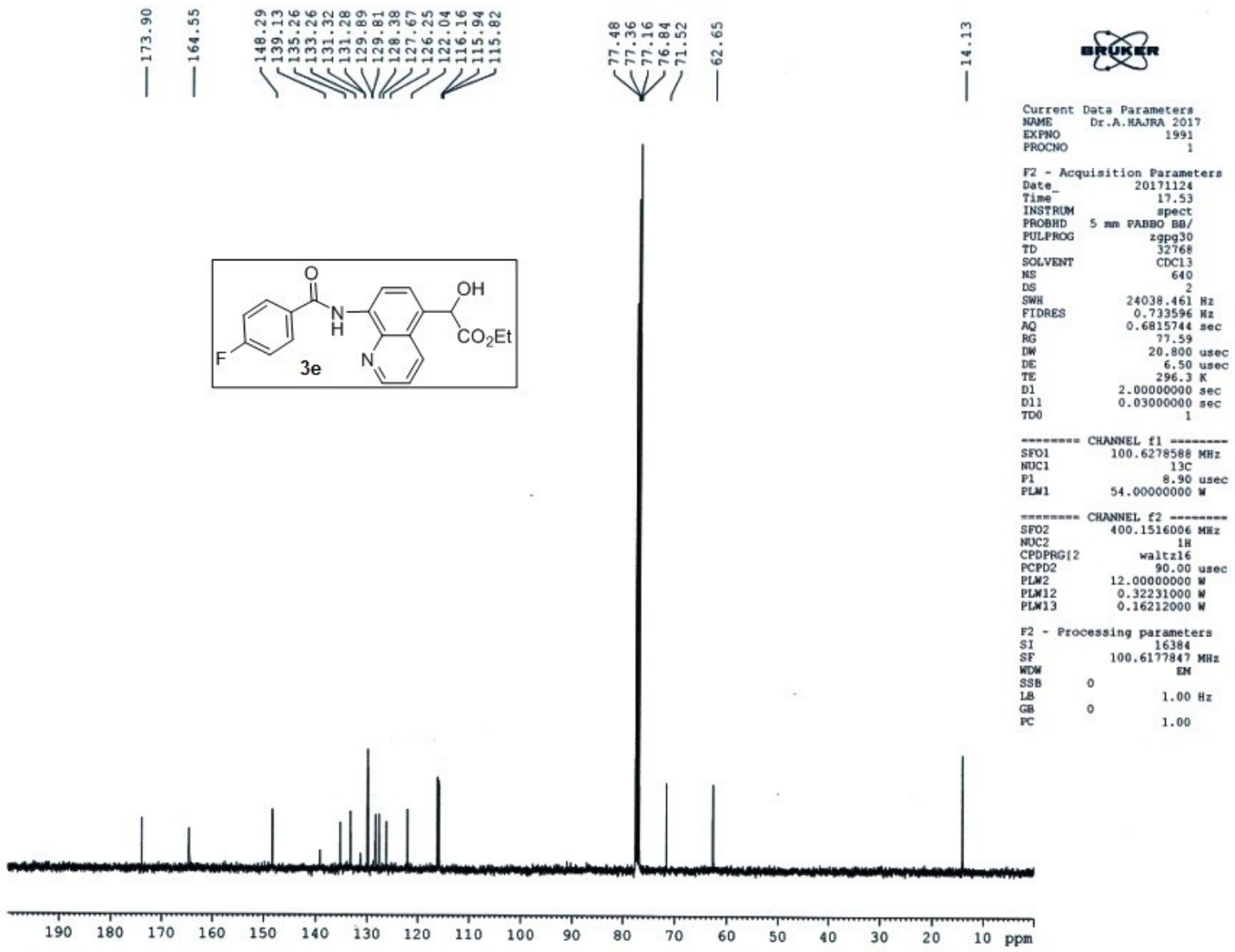

11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
1.00
2.01
1.01
2.02
1.00
1.01
2.01
1.00
2.10
4.02
3.02


173.78
165.15
162.69
148.13
139.07
135.43
133.20
129.29
128.06
127.58
127.28
126.17
121.87
115.55
114.11
77.48
77.16
76.84
71.56
62.44
55.58
14.09
BRUKER
O
N
H
OH
CO2Et
H3CO
3d
N
Current Data Parameters
NAME Dr.A.HAJRA 2017
EXPNO 1721
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171025
Time 19.08
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 220
DS 2
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 54.07
DW 20.800 usec
DE 6.50 usec
TE 297.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
CHANNEL f1
SFO1 100.6278588 MHz
NUC1 13C
P1 8.90 usec
PLW1 54.00000000 W
CHANNEL f2
SFO2 400.1516006 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 12.00000000 W
PLW12 0.32231000 W
PLW13 0.16212000 W
F2 - Processing parameters
SI 16384
SF 100.6177883 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


10.774
8.872
8.868
8.862
8.858
8.842
8.587
8.583
8.566
8.562
8.104
8.099
8.091
8.086
8.083
8.074
8.069
7.610
7.590
7.546
7.535
7.524
7.514
7.259
7.245
7.240
7.224
7.207
7.202
5.684
4.263
4.255
4.246
4.237
4.219
4.210
4.192
4.184
4.174
4.165
3.642
1.163
1.145
1.127

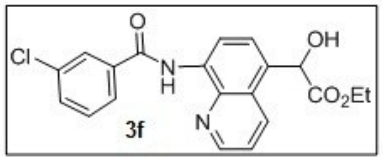

O
N
H
OH
CO2Et
F
N
3e

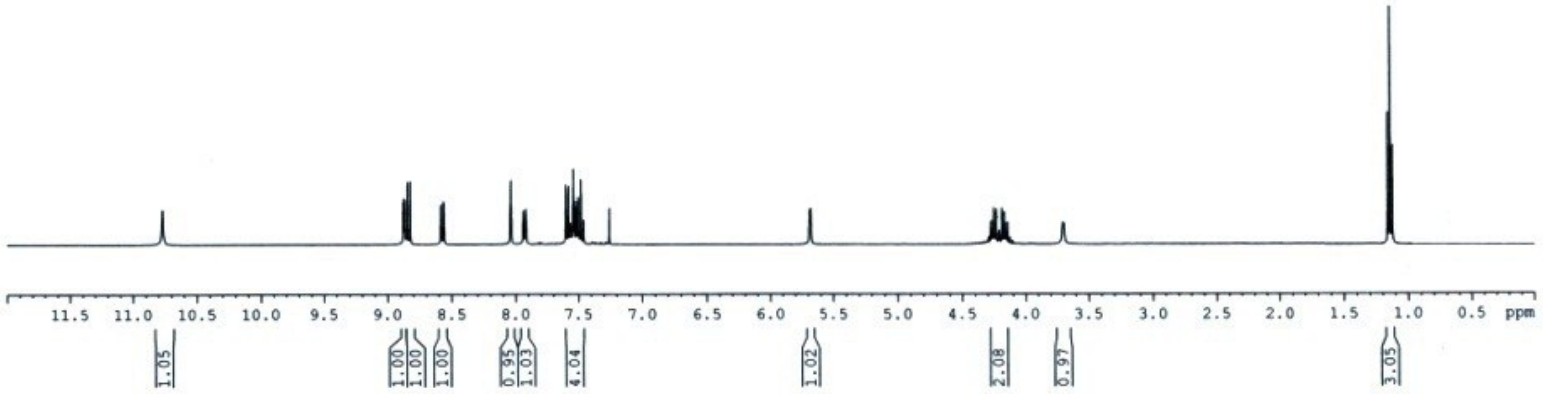

11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
1.00
2.06
0.98
2.10
1.06
1.09
2.04
0.99
2.18
1.05
3.13

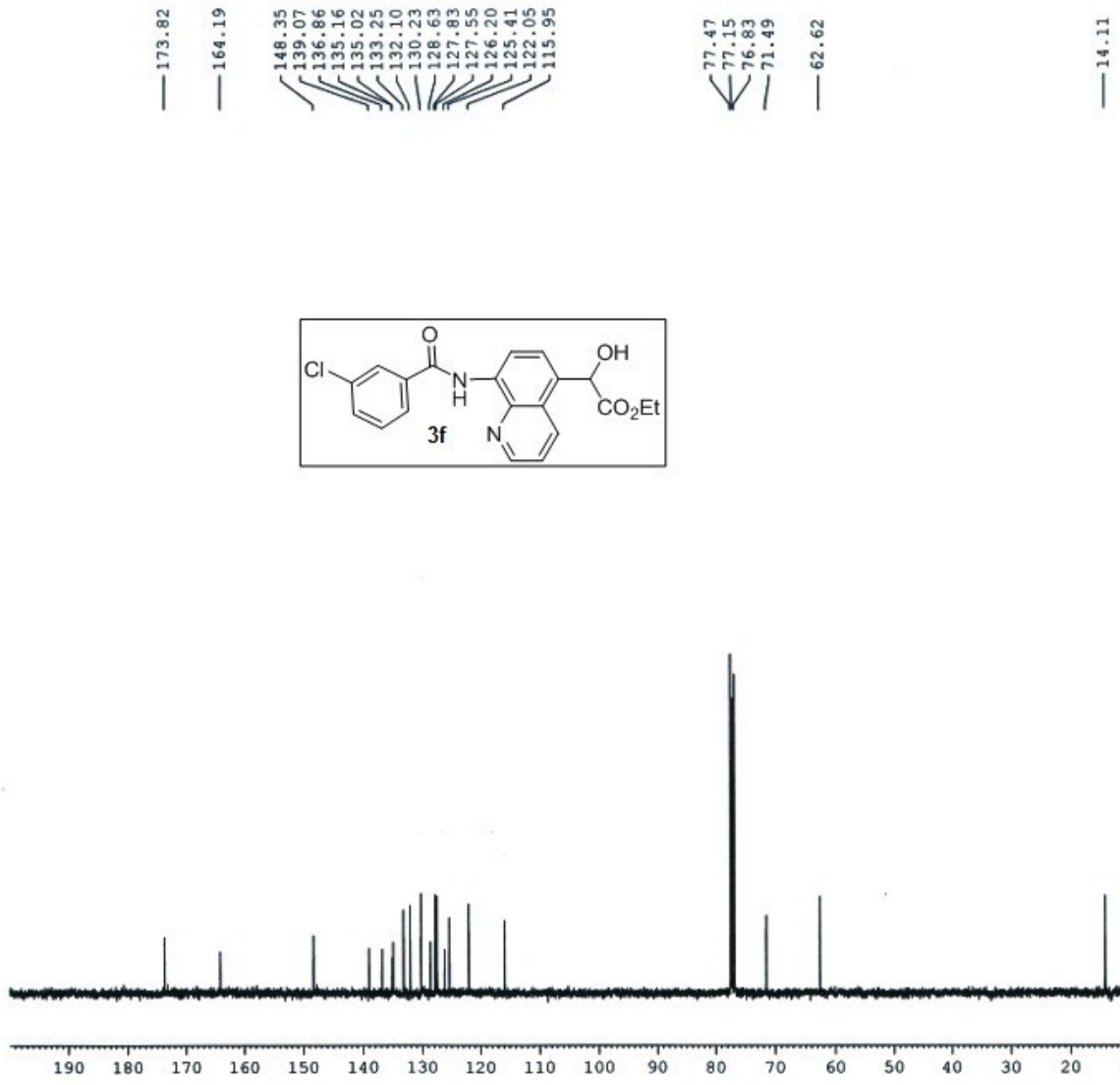



```
Current Data Parameters
NAME      Dr.A.HAJRA 2017
EXPNO             1991
PROCNO               1

F2 - Acquisition Parameters
Date_         20171124
Time             17.53
INSTRUM          spect
PROBHD   5 mm PABBO BB/
PULPROG        zgpg30
TD              32768
SOLVENT          CDCl3
NS                 640
DS                   2
SWH          24038.461 Hz
FIDRES        0.733596 Hz
AQ            0.6815744 sec
RG                77.59
DW               20.800 usec
DE                6.50 usec
TE               296.3 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1       100.6278588 MHz
NUC1               13C
P1                8.90 usec
PLW1       54.00000000 W

======== CHANNEL f2 ========
SFO2       400.1516006 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2            90.00 usec
PLW2       12.00000000 W
PLW12       0.32231000 W
PLW13       0.16212000 W

F2 - Processing parameters
SI                16384
SF         100.6177847 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.00
```


10.769
8.878
8.874
8.867
8.864
8.845
8.825
8.585
8.582
8.564
8.560
8.046
8.041
8.037
7.943
7.940
7.937
7.924
7.921
7.917
7.602
7.582
7.568
7.565
7.563
7.560
7.548
7.543
7.532
7.521
7.510
7.501
7.482
7.462
7.259
5.687
5.679
4.278
4.269
4.260
4.251
4.242
4.233
4.215
4.206
4.189
4.171
4.161
4.153
4.144
3.706
3.696
1.161
1.143
1.125


Cl
O
N
H
OH
CO2Et
N
3f


11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
1.05
1.00
1.00
1.00
0.95
1.03
4.04
1.02
2.08
0.97
3.05



BRUKER

Current Data Parameters
NAME Dr.A.HAJRA 2017
EXPNO 1862
PROCNO 1

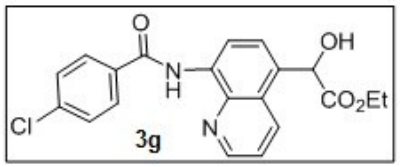
F2 - Acquisition Parameters
Date_ 20171108
Time 12.55
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 150
DS 2
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 77.59
DW 20.800 usec
DE 6.50 usec
TE 296.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6278588 MHz
NUC1 13C
P1 8.90 usec
PLW1 54.00000000 W

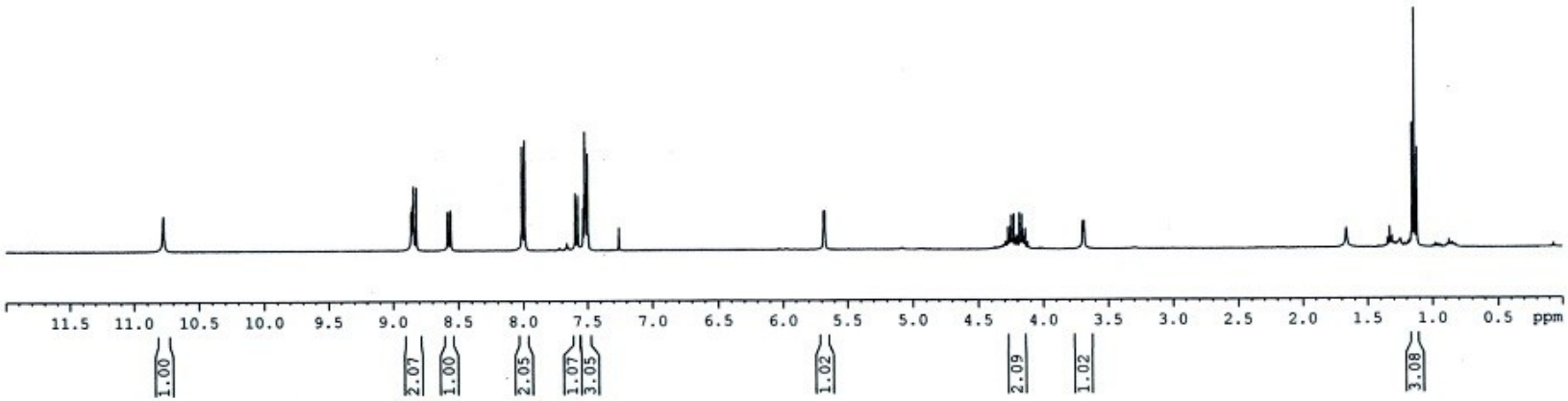
======== CHANNEL f2 ========
SFO2 400.1516006 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 12.00000000 W
PLW12 0.32231000 W
PLW13 0.16212000 W

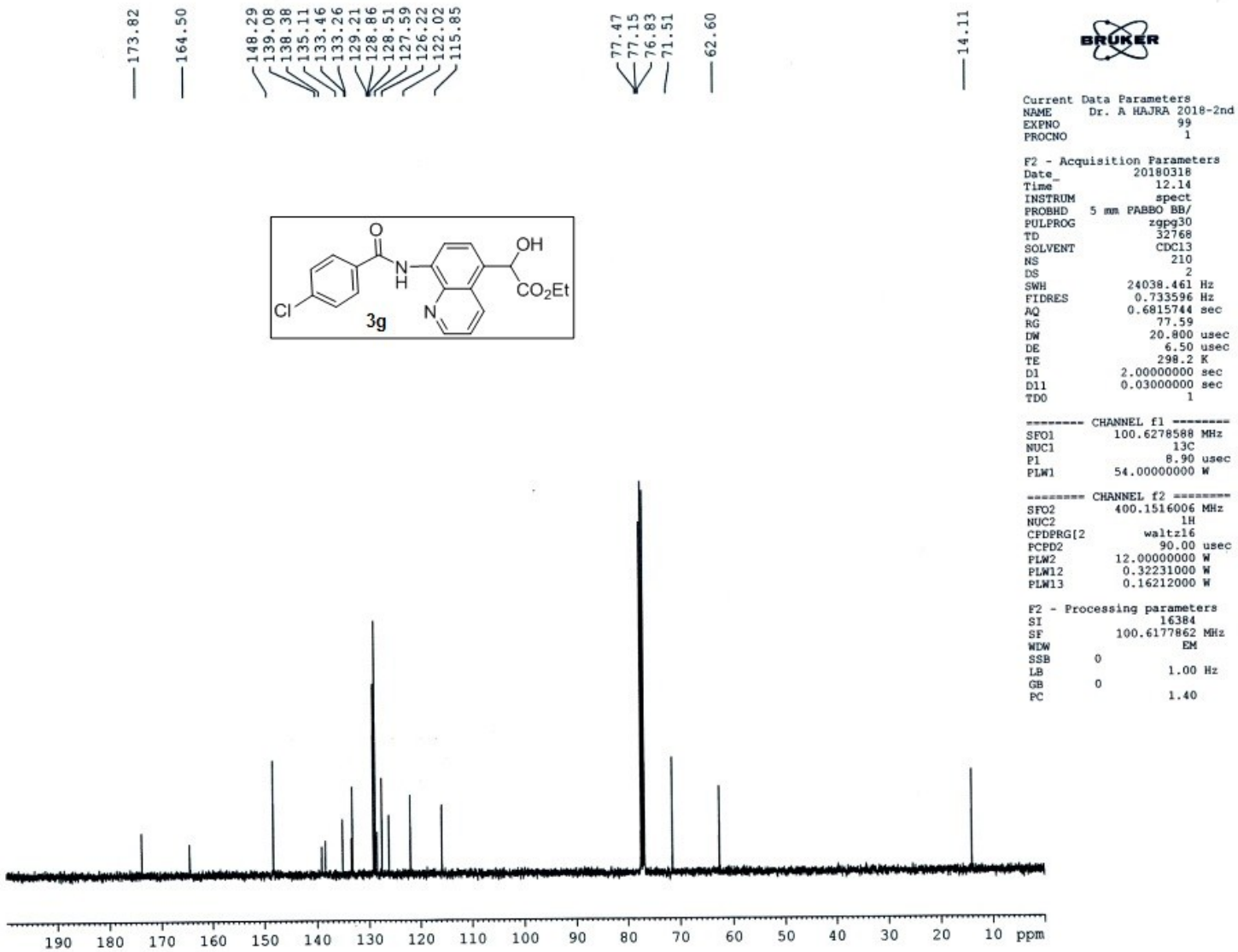
F2 - Processing parameters
SI 16384
SF 100.6177868 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.20


10.775
8.863
8.859
8.852
8.848
8.842
8.822
8.583
8.580
8.562
8.558
8.017
8.011
8.007
7.995
7.990
7.984
7.596
7.576
7.535
7.524
7.521
7.516
7.514
7.503
7.500
7.494
7.258
5.683
5.674
4.275
4.266
4.257
4.248
4.230
4.212
4.204
4.187
4.169
4.160
4.151
4.142
3.696
3.685
1.158
1.140
1.122

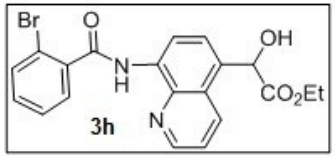

O
N
H
OH
CO2Et
Cl
N

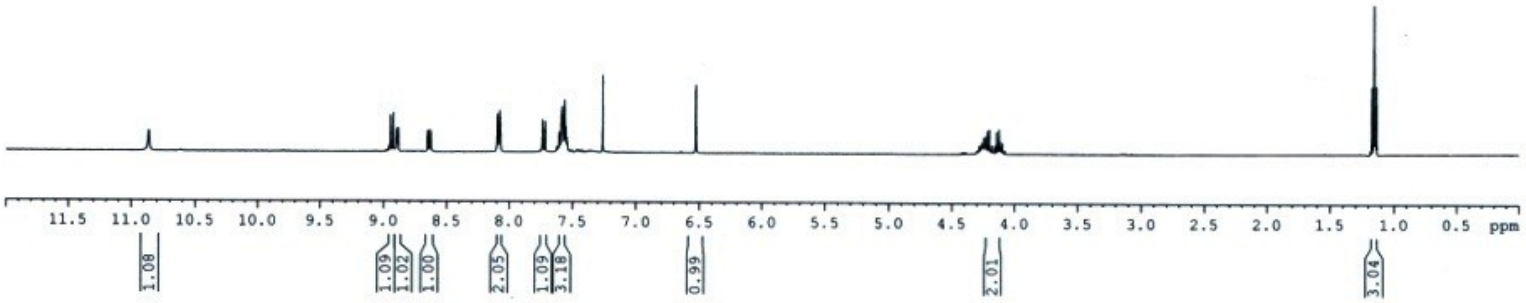
3g

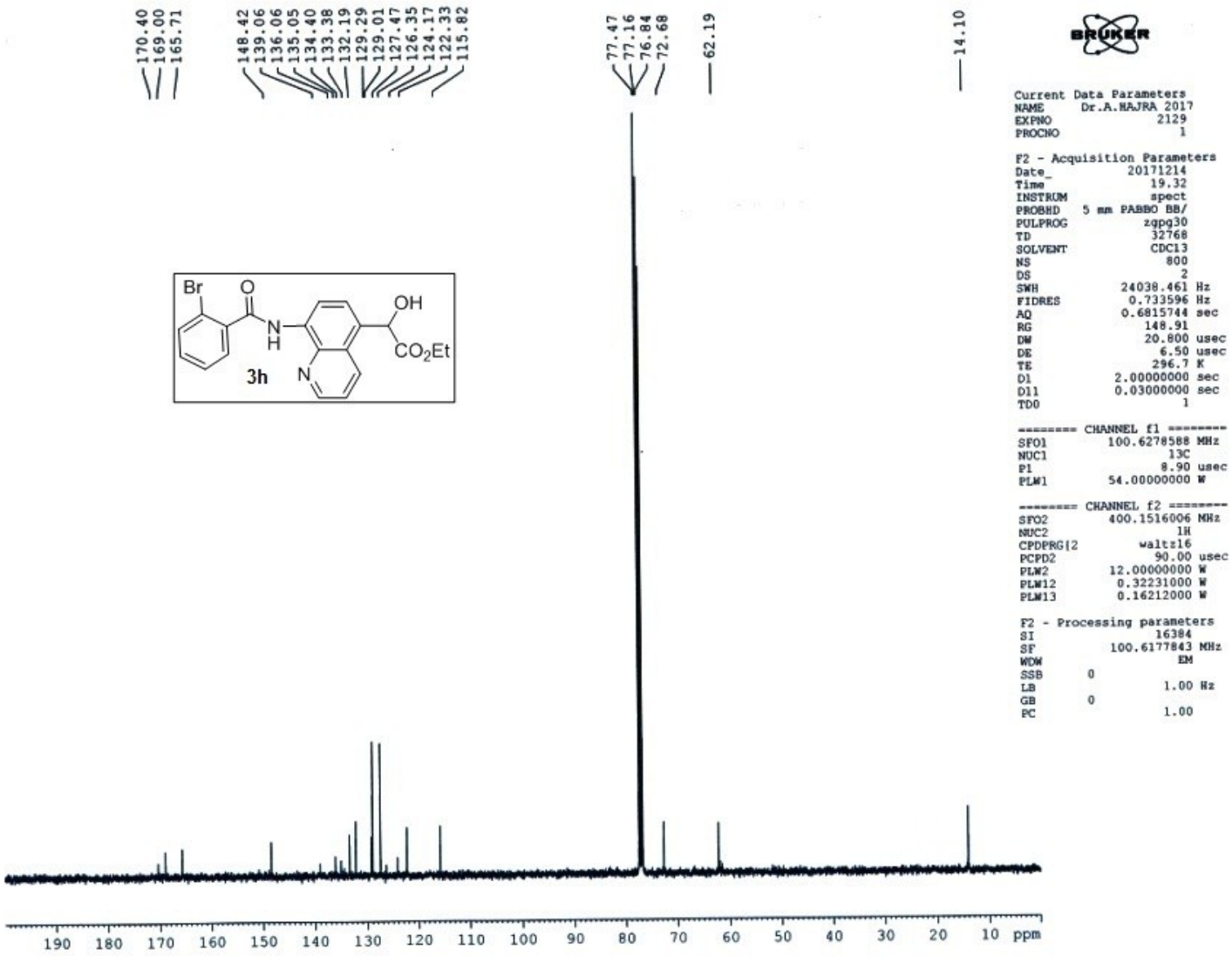

11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
1.00
2.07
1.00
2.05
1.07
3.05
1.02
2.09
1.02
3.08


173.82
164.50
148.29
139.08
138.38
135.11
133.46
133.26
129.21
128.86
128.51
127.59
126.22
122.02
115.85
77.47
77.15
76.83
71.51
62.60
14.11
3g
Cl
O
N
H
OH
CO2Et
N
BRUKER
Current Data Parameters
NAME Dr. A HAJRA 2018-2nd
EXPNO 99
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180318
Time 12.14
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 210
DS 2
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 77.59
DW 20.800 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
CHANNEL f1
SFO1 100.6278588 MHz
NUC1 13C
P1 8.90 usec
PLW1 54.00000000 W
CHANNEL f2
SFO2 400.1516006 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 12.00000000 W
PLW12 0.32231000 W
PLW13 0.16212000 W
F2 - Processing parameters
SI 16384
SF 100.6177862 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

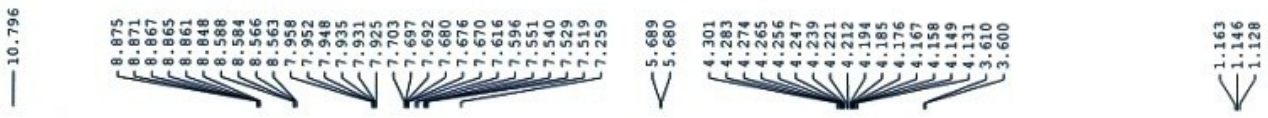

10.864
8.944
8.924
8.898
8.894
8.887
8.884
8.653
8.649
8.631
8.627
8.096
8.092
8.089
8.076
8.072
7.736
7.715
7.604
7.590
7.586
7.584
7.578
7.574
7.561
7.259
6.527
4.264
4.245
4.236
4.226
4.218
4.209
4.200
4.142
4.125
4.116
1.172
1.154
1.137


Br
O
N
H
OH
CO2Et
N
3h


11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
1.08
1.09
1.02
1.00
2.05
1.09
3.18
0.99
2.01
3.04




```
Current Data Parameters
NAME      Dr.A.HAJRA 2017
EXPNO             2129
PROCNO               1

F2 - Acquisition Parameters
Date_         20171214
Time             19.32
INSTRUM          spect
PROBHD   5 mm PABBO BB/
PULPROG       zgpg30
TD             32768
SOLVENT        CDCl3
NS               800
DS                 2
SWH        24038.461 Hz
FIDRES         0.733596 Hz
AQ             0.6815744 sec
RG               148.91
DW              20.800 usec
DE               6.50 usec
TE              296.7 K
D1          2.00000000 sec
D11         0.03000000 sec
TD0                1

======== CHANNEL f1 ========
SFO1       100.6278588 MHz
NUC1              13C
P1               8.90 usec
PLW1       54.00000000 W

======== CHANNEL f2 ========
SFO2       400.1516006 MHz
NUC2              1H
CPDPRG[2        waltz16
PCPD2            90.00 usec
PLW2       12.00000000 W
PLW12       0.32231000 W
PLW13       0.16212000 W

F2 - Processing parameters
SI               16384
SF         100.6177843 MHz
WDW                EM
SSB        0
LB               1.00 Hz
GB         0
PC               1.00
```


10.796
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8.861
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8.588
8.584
8.566
8.563
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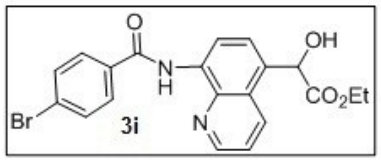
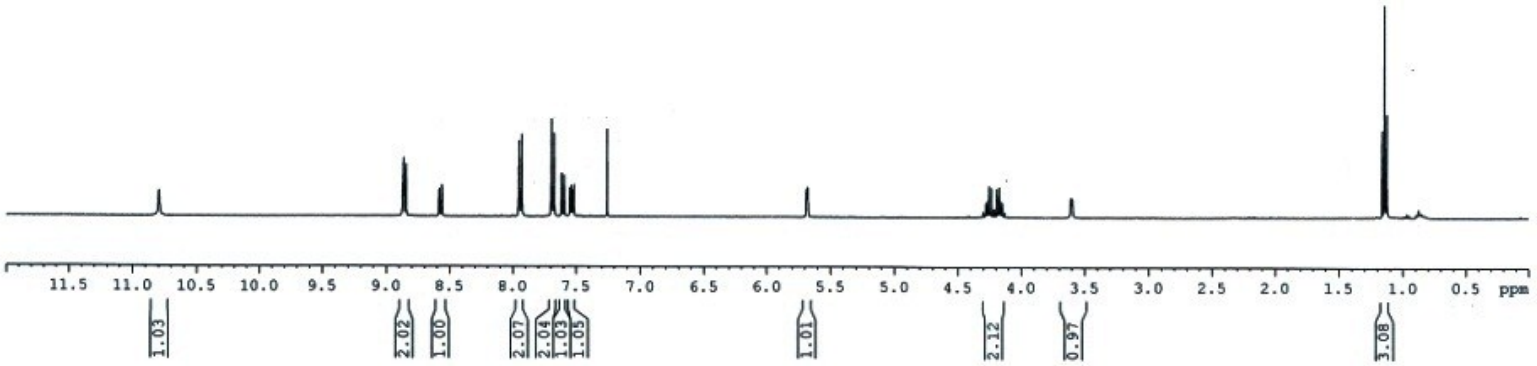
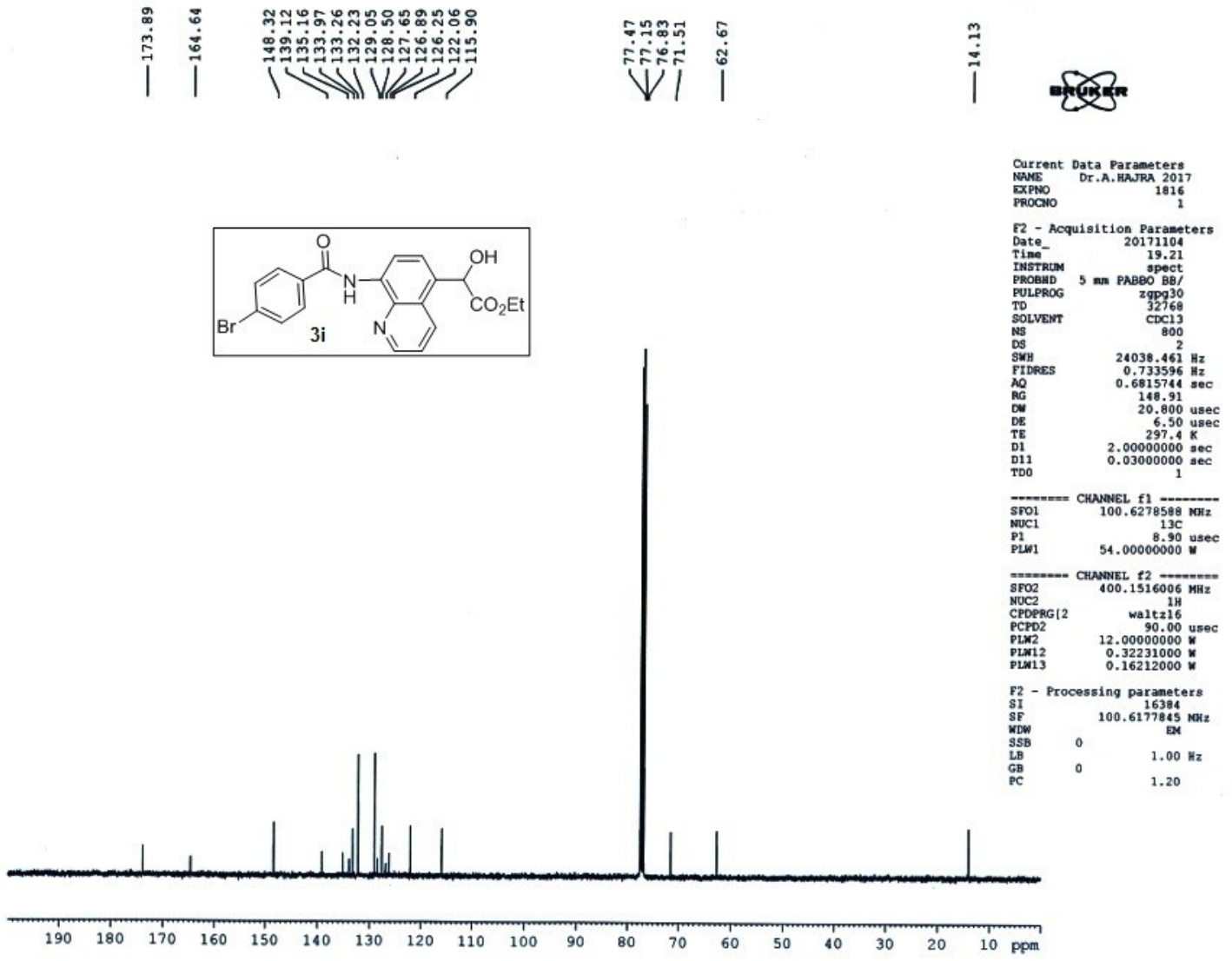
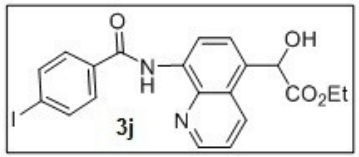
7.952
7.948
7.935
7.931
7.925
7.703
7.697
7.692
7.680
7.676
7.670
7.616
7.596
7.551
7.540
7.529
7.519
7.259
5.689
5.680
4.301
4.283
4.274
4.265
4.256
4.247
4.239
4.221
4.212
4.194
4.185
4.176
4.167
4.158
4.149
4.131
3.610
3.600
1.163
1.146
1.128


O
N
H
OH
CO2Et
Br
N
3i

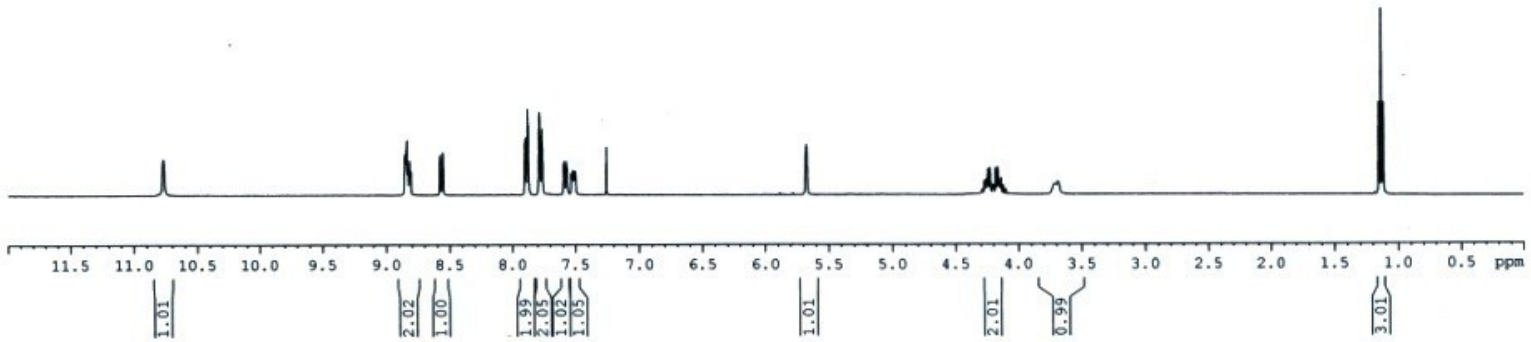

11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
1.03
2.02
1.00
2.07
2.04
1.03
1.05
1.01
2.12
0.97
3.08

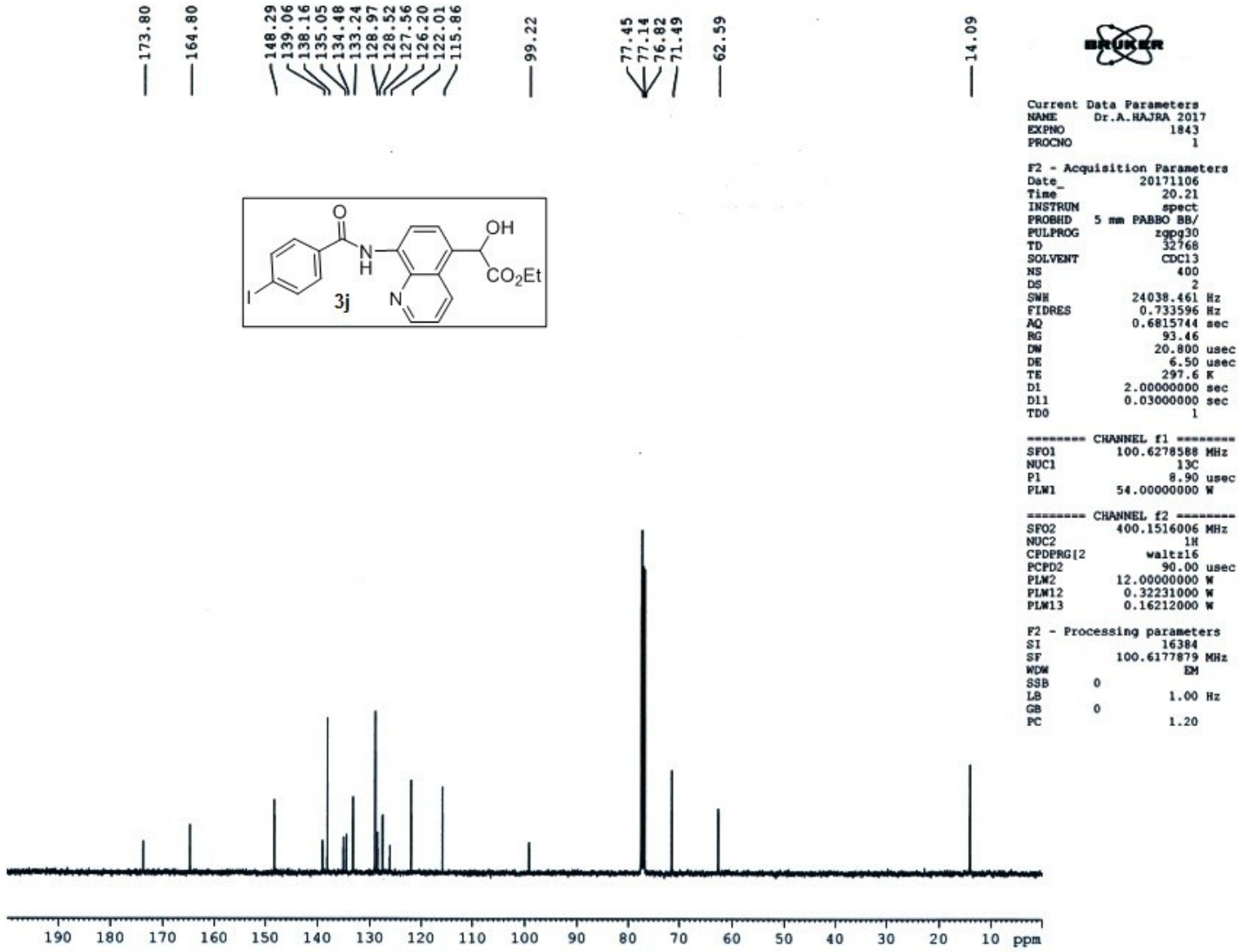

173.89
164.64
148.32
139.12
135.16
133.97
133.26
132.23
129.05
128.50
127.65
126.89
126.25
122.06
115.90
77.47
77.15
76.83
71.51
62.67
14.13
BRUKER
O
N
H
OH
CO2Et
Br
N
3i
Current Data Parameters
NAME Dr.A.HAJRA 2017
EXPNO 1816
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171104
Time 19.21
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 800
DS 2
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 148.91
DW 20.800 usec
DE 6.50 usec
TE 297.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6278588 MHz
NUC1 13C
P1 8.90 usec
PLW1 54.00000000 W
======== CHANNEL f2 ========
SFO2 400.1516006 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 12.00000000 W
PLW12 0.32231000 W
PLW13 0.16212000 W
F2 - Processing parameters
SI 16384
SF 100.6177845 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.20
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


10.773
8.856
8.850
8.845
8.841
8.830
8.821
8.810
8.578
8.557
7.901
7.897
7.880
7.876
7.789
7.784
7.768
7.763
7.595
7.588
7.575
7.568
7.535
7.529
7.525
7.519
7.514
7.508
7.503
7.498
7.259
5.674
4.273
4.271
4.264
4.255
4.253
4.247
4.238
4.228
4.210
4.202
4.184
4.166
4.158
4.149
4.140
4.122
3.718
3.689
1.155
1.137
1.119

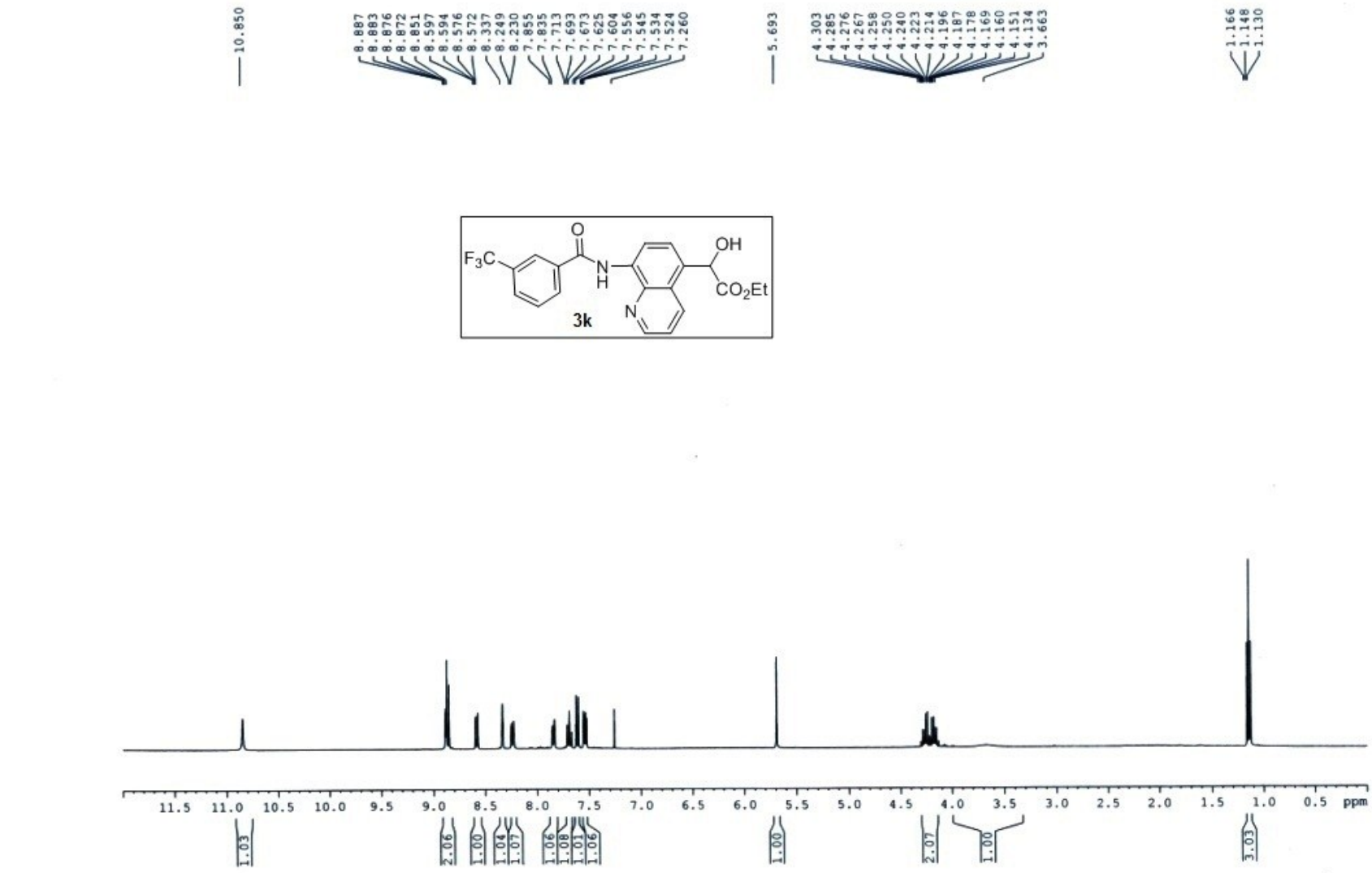

O
N
H
OH
CO2Et
I
N

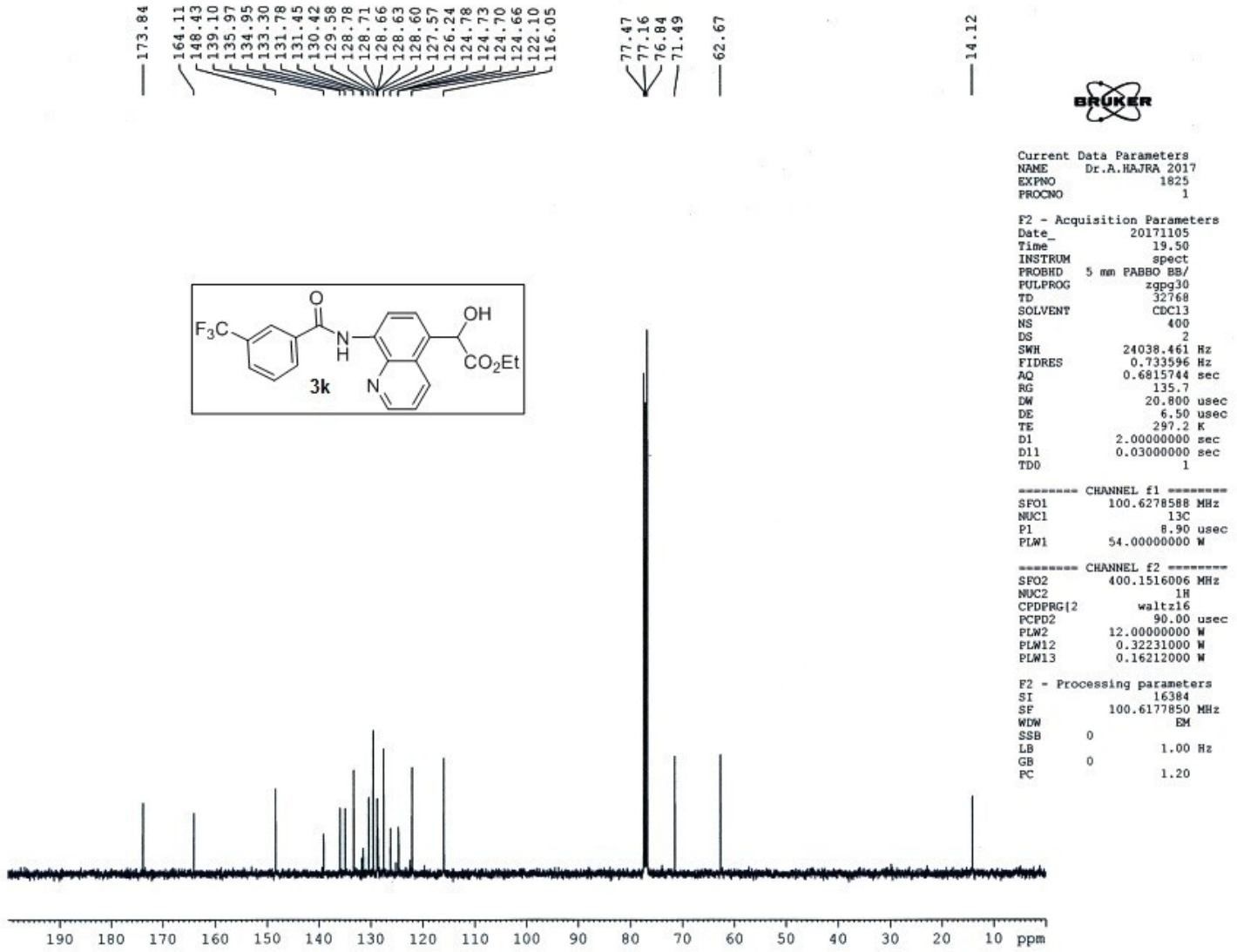
3j


11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
1.01
2.02
1.00
1.99
2.05
1.02
1.05
1.01
2.01
0.99
3.01



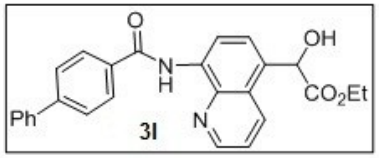

```
Current Data Parameters
NAME      Dr.A.HAJRA 2017
EXPNO             1843
PROCNO               1

F2 - Acquisition Parameters
Date_         20171106
Time             20.21
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            0.6815744 sec
RG               93.46
DW               20.800 usec
DE                6.50 usec
TE               297.6 K
D1          2.00000000 sec
D11         0.03000000 sec
TD0                1

======== CHANNEL f1 ========
SFO1       100.6278588 MHz
NUC1              13C
P1                8.90 usec
PLW1      54.00000000 W

======== CHANNEL f2 ========
SFO2       400.1516006 MHz
NUC2              1H
CPDPRG[2       waltz16
PCPD2            90.00 usec
PLW2      12.00000000 W
PLW12      0.32231000 W
PLW13      0.16212000 W

F2 - Processing parameters
SI               16384
SF         100.6177879 MHz
WDW                EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.20
```


10.850
8.887
8.883
8.876
8.872
8.851
8.597
8.594
8.576
8.572
8.337
8.249
8.230
7.855
7.835
7.713
7.693
7.673
7.625
7.604
7.556
7.545
7.534
7.524
7.260
5.693
4.303
4.285
4.276
4.267
4.258
4.250
4.240
4.223
4.214
4.196
4.187
4.178
4.169
4.160
4.151
4.134
3.663
1.166
1.148
1.130
F3C
O
N
H
OH
CO2Et
N
3k
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
1.03
2.06
1.00
1.04
1.07
1.06
1.08
1.01
1.06
1.00
2.07
1.00
3.03

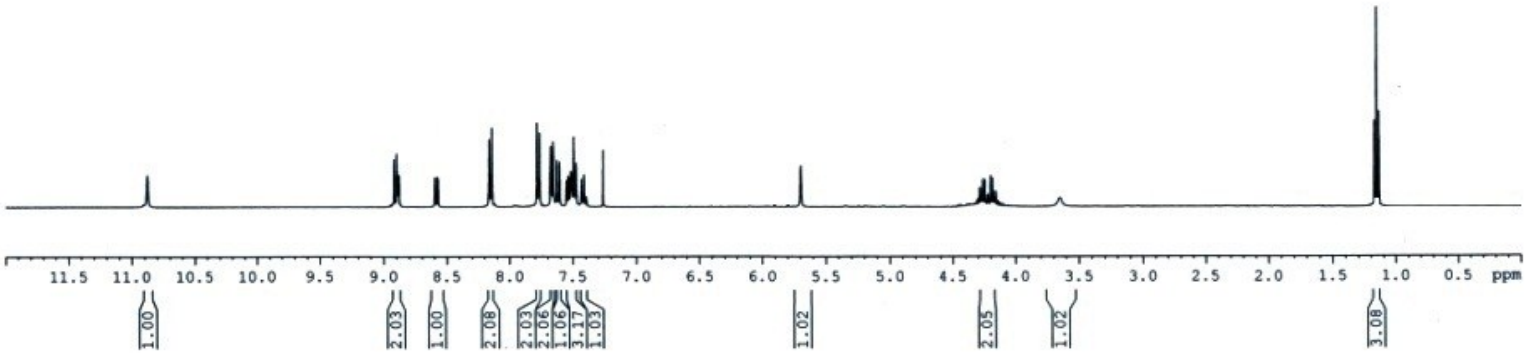


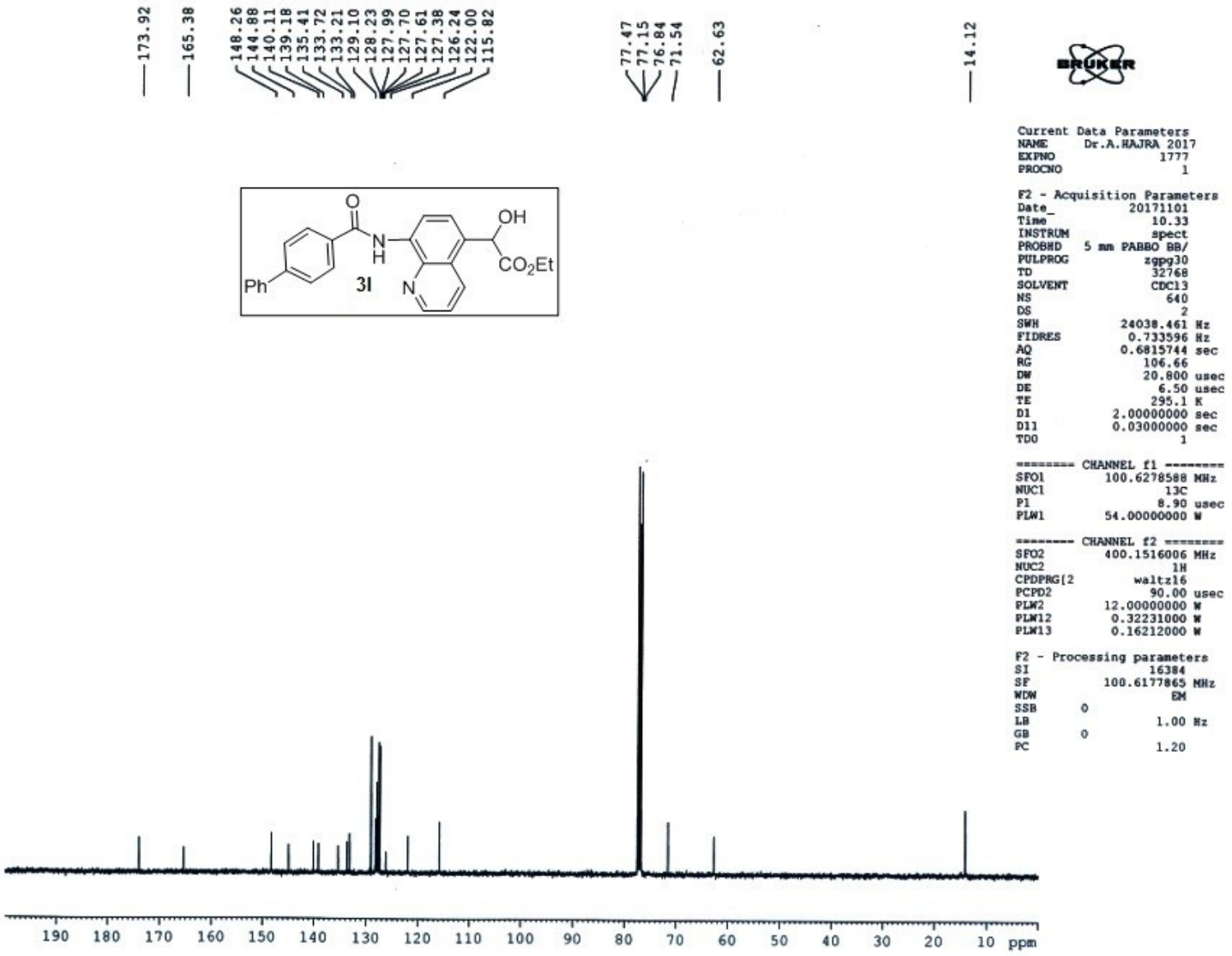

```
Current Data Parameters
NAME      Dr.A.HAJRA 2017
EXPNO             1825
PROCNO               1

F2 - Acquisition Parameters
Date_         20171105
Time             19.50
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          0.6815744 sec
RG              135.7
DW             20.800 usec
DE              6.50 usec
TE             297.2 K
D1          2.00000000 sec
D11         0.03000000 sec
TD0                1

======== CHANNEL f1 ========
SFO1       100.6278588 MHz
NUC1             13C
P1              8.90 usec
PLW1       54.00000000 W

======== CHANNEL f2 ========
SFO2       400.1516006 MHz
NUC2             1H
CPDPRG[2       waltz16
PCPD2          90.00 usec
PLW2       12.00000000 W
PLW12       0.32231000 W
PLW13       0.16212000 W

F2 - Processing parameters
SI              16384
SF         100.6177850 MHz
WDW                EM
SSB      0
LB              1.00 Hz
GB       0
PC              1.20
```

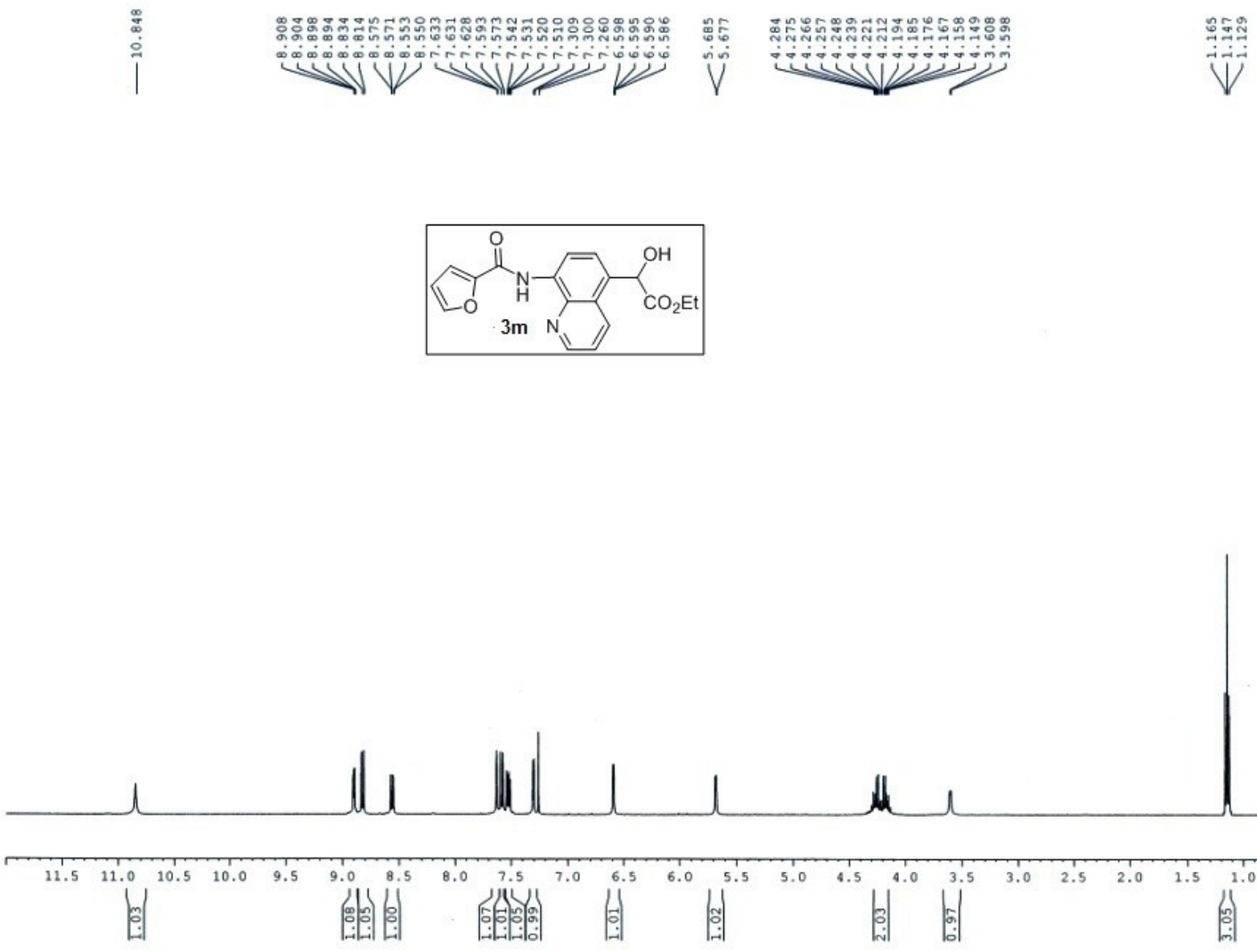

10.878
8.918
8.898
8.894
8.890
8.883
8.880
8.597
8.593
8.575
8.572
8.164
8.159
8.146
8.143
7.790
7.785
7.781
7.769
7.764
7.679
7.675
7.670
7.657
7.626
7.606
7.550
7.540
7.529
7.518
7.512
7.507
7.493
7.474
7.430
7.427
7.417
7.412
7.407
7.398
7.394
7.391
7.260
5.696
4.290
4.281
4.272
4.263
4.245
4.227
4.219
4.202
4.184
4.175
4.166
4.157
3.651
1.173
1.155
1.137

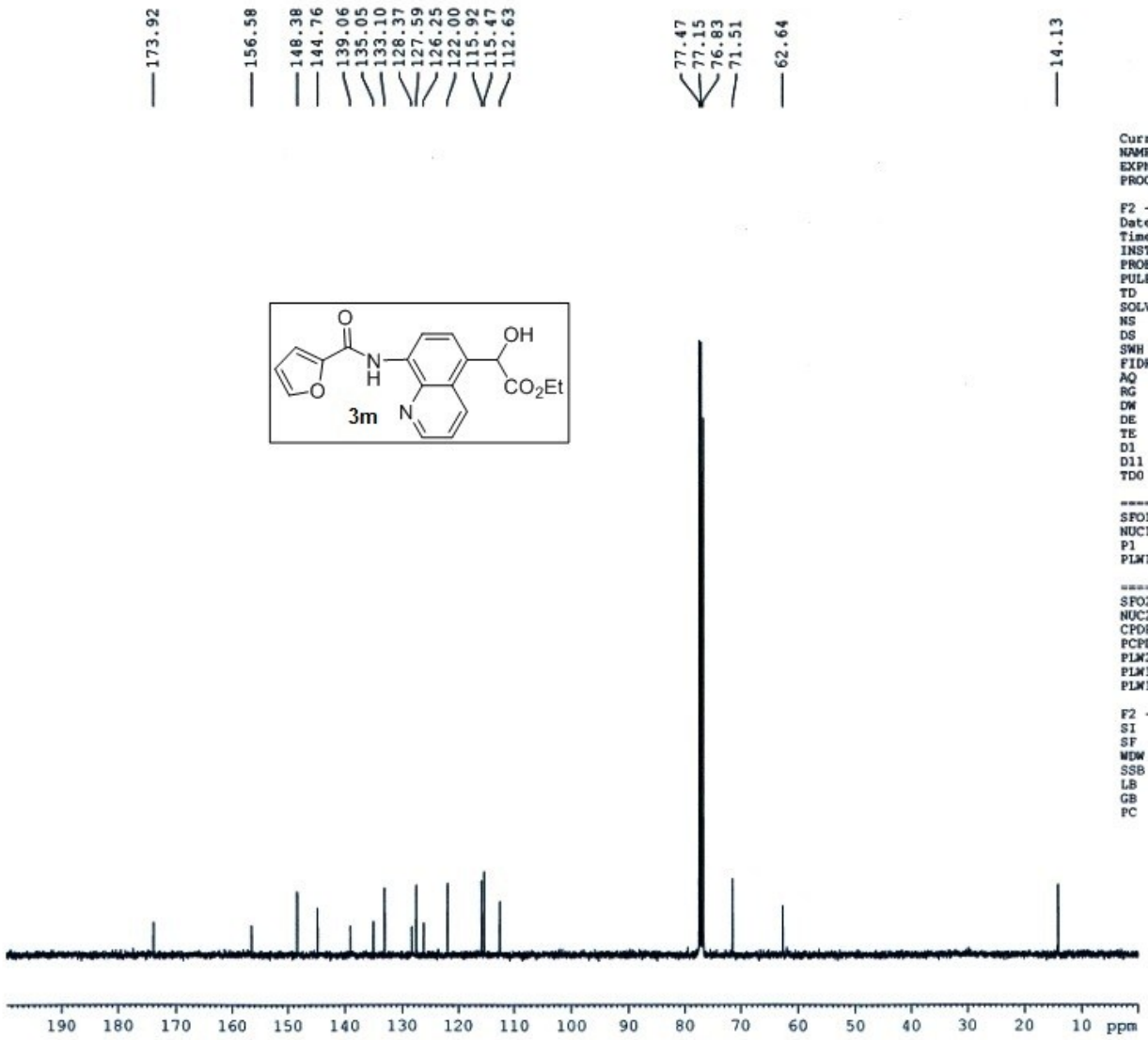

O
N
H
OH
CO2Et
Ph
N

3l


11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
1.00
2.03
1.00
2.08
2.03
2.06
1.06
3.17
1.03
1.02
2.05
1.02
3.08

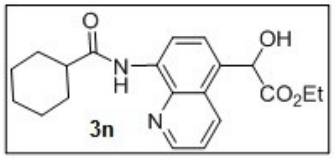

173.92
165.38
148.26
144.88
140.11
139.18
135.41
133.72
133.21
129.10
128.23
127.99
127.70
127.61
127.38
126.24
122.00
115.82
77.47
77.15
76.84
71.54
62.63
14.12
BRUKER
Current Data Parameters
NAME Dr.A.HAJRA 2017
EXPNO 1777
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171101
Time 10.33
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 640
DS 2
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 106.66
DW 20.800 usec
DE 6.50 usec
TE 295.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6278588 MHz
NUC1 13C
P1 8.90 usec
PLW1 54.00000000 W
======== CHANNEL f2 ========
SFO2 400.1516006 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 12.00000000 W
PLW12 0.32231000 W
PLW13 0.16212000 W
F2 - Processing parameters
SI 16384
SF 100.6177865 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.20
O
N
H
OH
CO2Et
Ph
N
3l
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

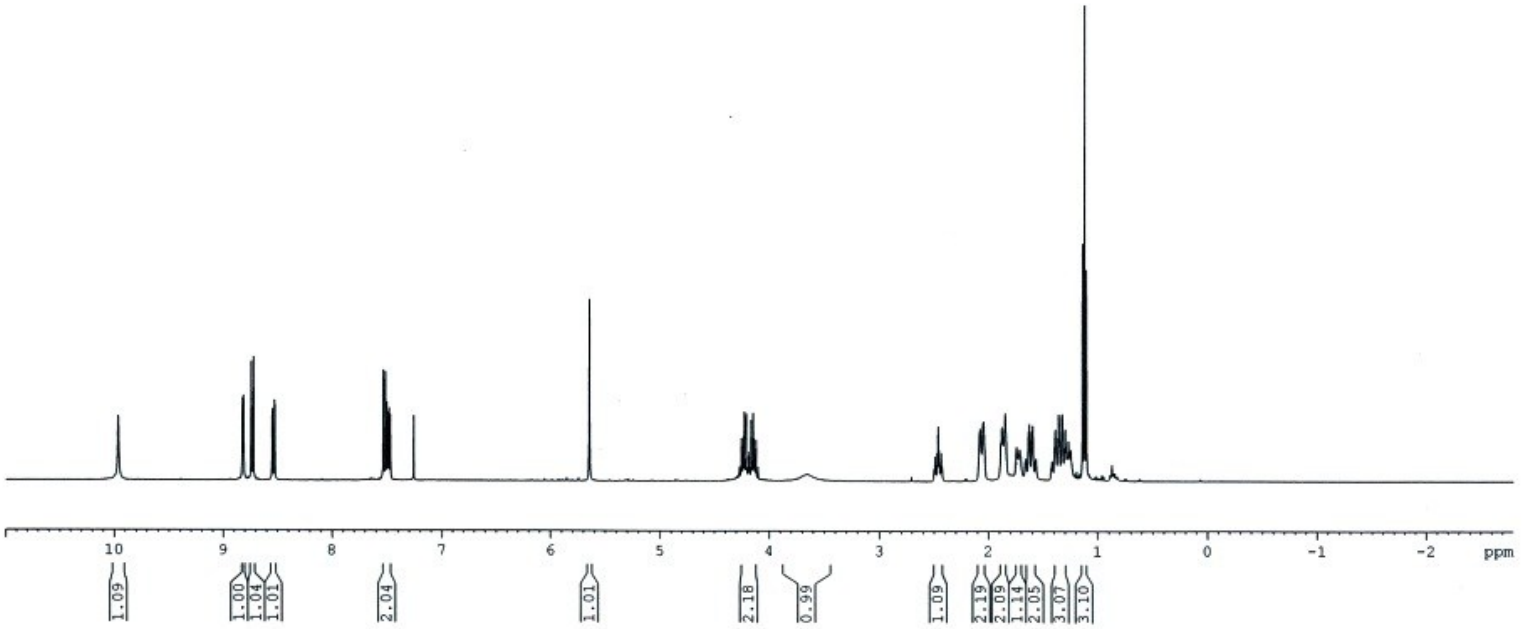

10.848
8.908
8.904
8.898
8.894
8.834
8.814
8.575
8.571
8.553
8.550
7.633
7.631
7.628
7.593
7.573
7.542
7.531
7.520
7.510
7.309
7.300
7.260
6.598
6.595
6.590
6.586
5.685
5.677
4.284
4.275
4.266
4.257
4.248
4.239
4.221
4.212
4.194
4.185
4.176
4.167
4.158
4.149
3.608
3.598
1.165
1.147
1.129
O
N
H
O
OH
CO2Et
3m
N
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
1.03
1.08
1.05
1.00
1.07
1.01
1.05
0.99
1.01
1.02
2.03
0.97
3.05

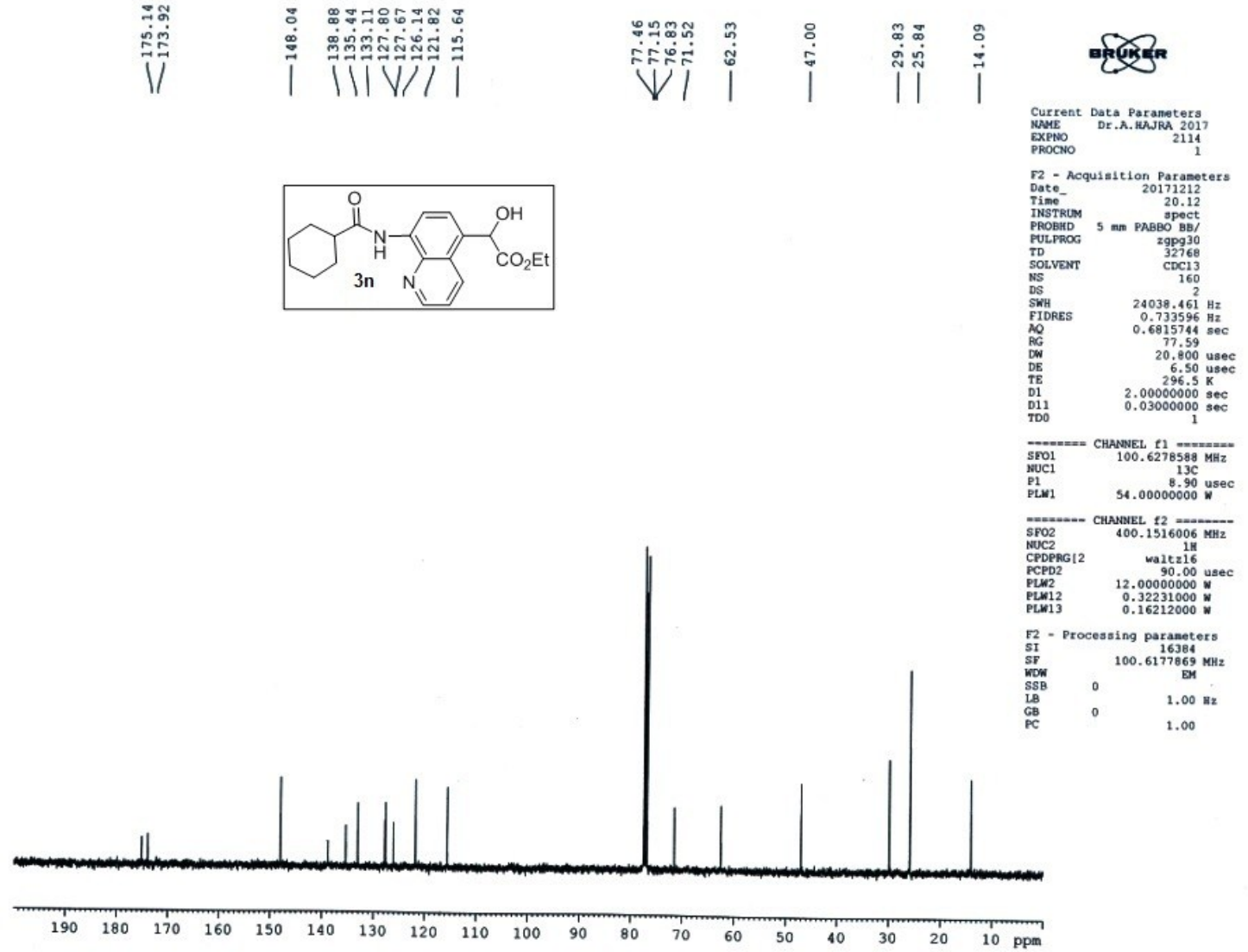


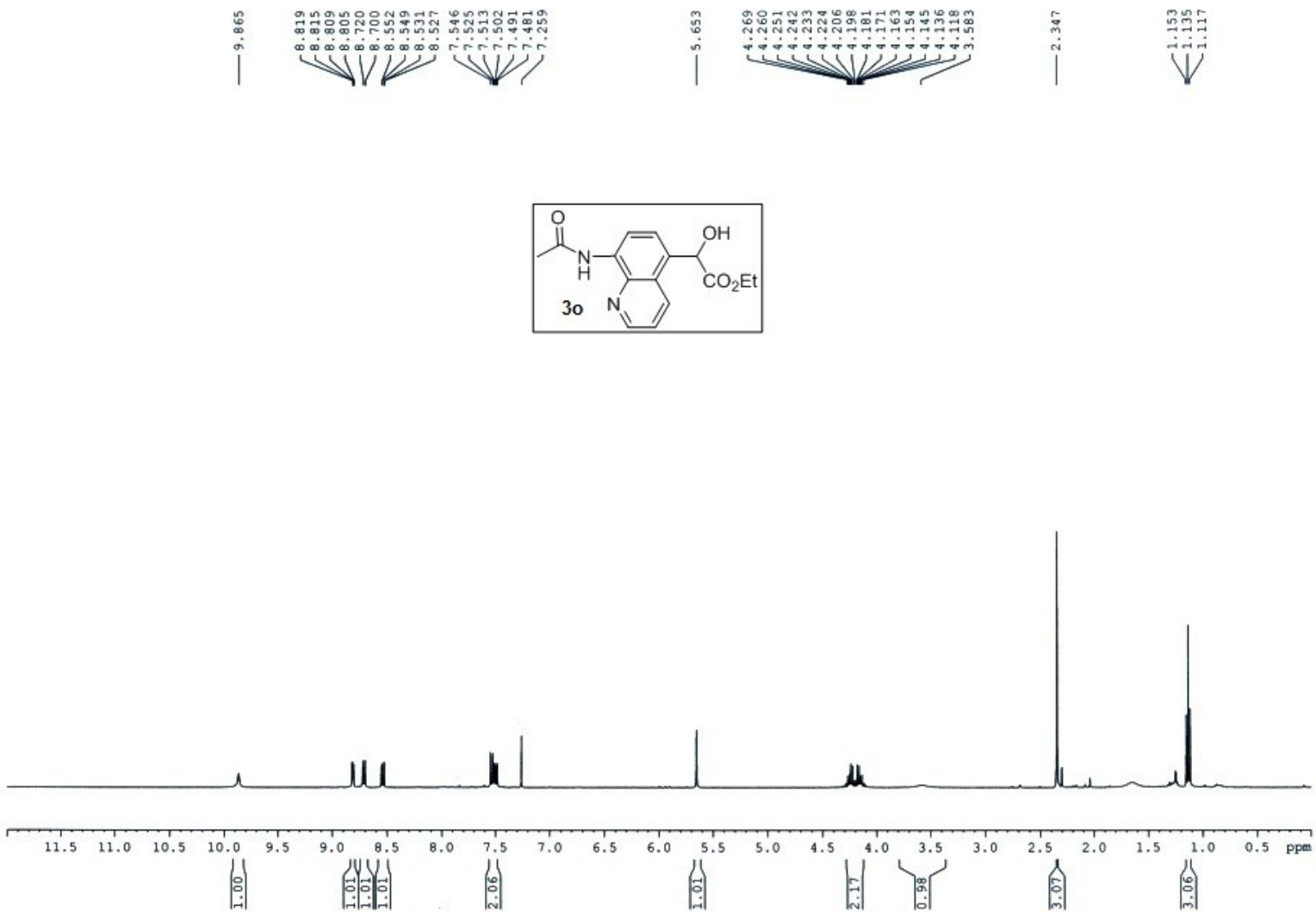

```
Current Data Parameters
NAME      Dr.A.HAJRA 2017
EXPNO             1789
PROCNO               1

F2 - Acquisition Parameters
Date_          20171102
Time              17.29
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD              32768
SOLVENT          CDCl3
NS                 800
DS                   2
SWH          24038.461 Hz
FIDRES        0.733596 Hz
AQ            0.6815744 sec
RG                135.7
DW               20.800 usec
DE                6.50 usec
TE               297.6 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1        100.6278588 MHz
NUC1                13C
P1                 8.90 usec
PLW1        54.00000000 W

======== CHANNEL f2 ========
SFO2        400.1516006 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2        12.00000000 W
PLW12        0.32231000 W
PLW13        0.16212000 W

F2 - Processing parameters
SI                 16384
SF          100.6177845 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.20
```

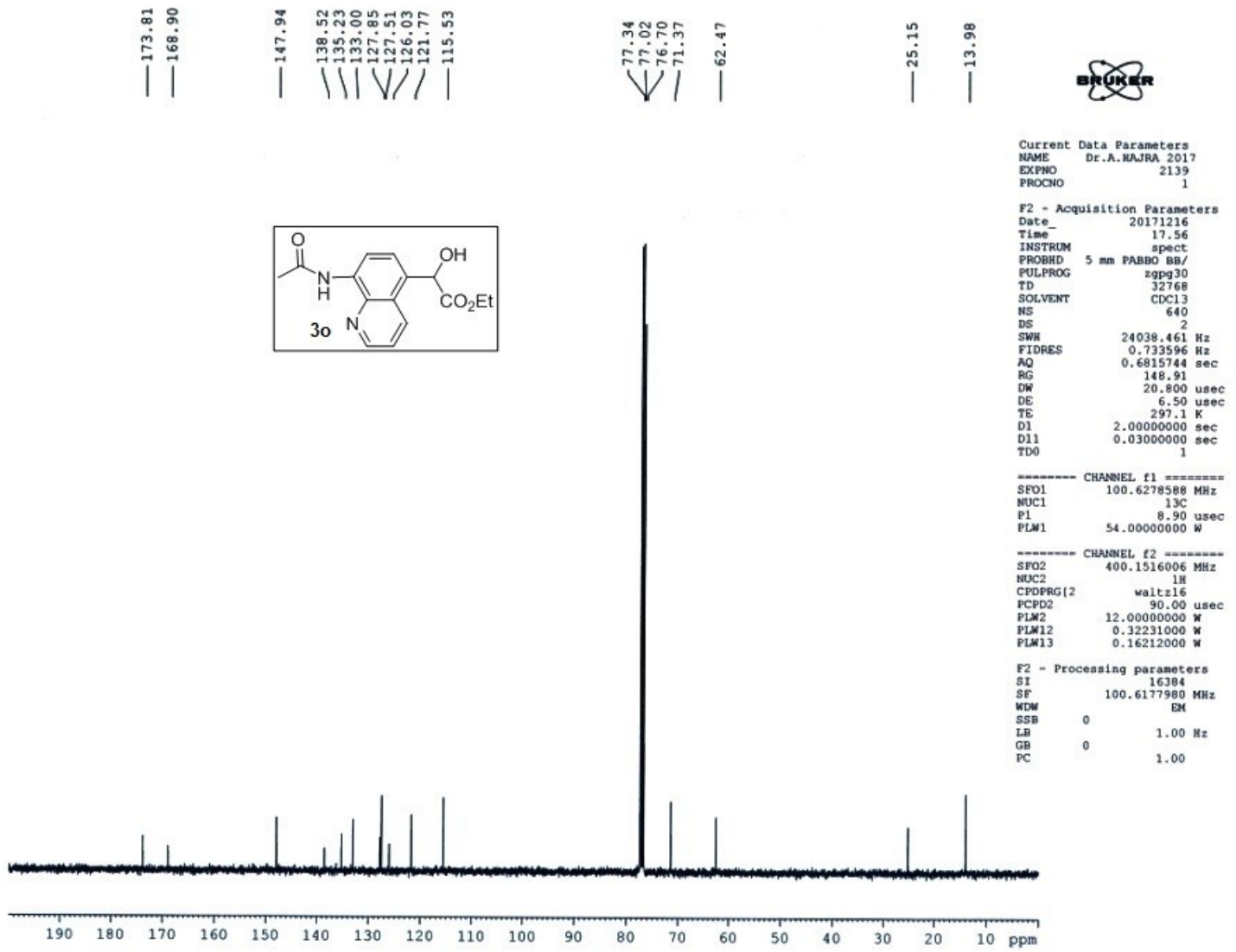

9.962
8.824
8.820
8.814
8.810
8.740
8.720
8.548
8.544
8.527
8.523
7.536
7.516
7.502
7.491
7.480
7.470
7.260
5.645
4.253
4.244
4.235
4.226
4.218
4.208
4.190
4.182
4.165
4.155
4.147
4.138
4.129
4.120
3.664
2.493
2.485
2.473
2.464
2.455
2.444
2.435
2.426
2.084
2.079
2.049
2.045
1.889
1.881
1.873
1.856
1.849
1.744
1.736
1.716
1.709
1.706
1.666
1.658
1.635
1.628
1.604
1.597
1.574
1.566
1.429
1.398
1.390
1.366
1.359
1.353
1.328
1.308
1.301
1.293
1.284
1.277
1.270
1.267
1.263
1.141
1.123
1.105


O
OH
N
H
CO2Et
N
3n

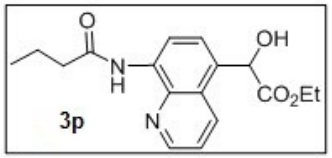

10
9
8
7
6
5
4
3
2
1
0
-1
-2
ppm
1.09
1.00
1.04
1.01
2.04
1.01
2.18
0.99
1.09
2.19
2.09
1.14
2.05
3.07
3.10


175.14
173.92
148.04
138.88
135.44
133.11
127.80
127.67
126.14
121.82
115.64
77.46
77.15
76.83
71.52
62.53
47.00
29.83
25.84
14.09
O
N
H
OH
CO2Et
N
3n
BRUKER
Current Data Parameters
NAME Dr.A.HAJRA 2017
EXPNO 2114
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171212
Time 20.12
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 0.6815744 sec
RG 77.59
DW 20.800 usec
DE 6.50 usec
TE 296.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6278588 MHz
NUC1 13C
P1 8.90 usec
PLW1 54.00000000 W
======== CHANNEL f2 ========
SFO2 400.1516006 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 12.00000000 W
PLW12 0.32231000 W
PLW13 0.16212000 W
F2 - Processing parameters
SI 16384
SF 100.6177869 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

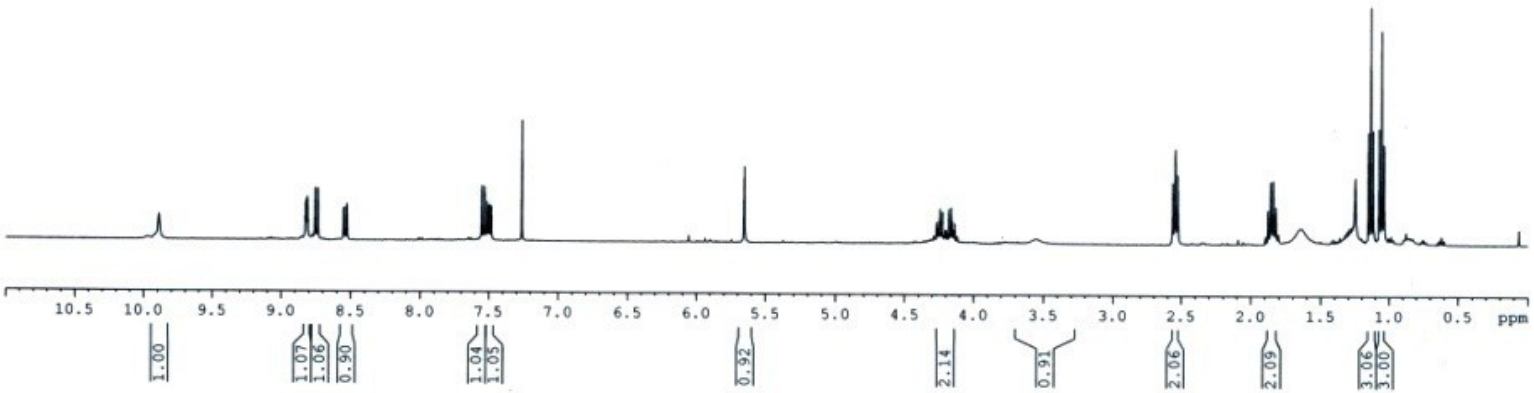

9.865
8.819
8.815
8.809
8.805
8.720
8.700
8.552
8.549
8.531
8.527
7.546
7.525
7.513
7.502
7.491
7.481
7.259
5.653
4.269
4.260
4.251
4.242
4.233
4.224
4.206
4.198
4.181
4.171
4.163
4.154
4.145
4.136
4.118
3.583
2.347
1.153
1.135
1.117
O
N
H
OH
CO2Et
N
3o
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
1.00
1.01
1.01
1.01
2.06
1.01
2.17
0.98
3.07
3.06

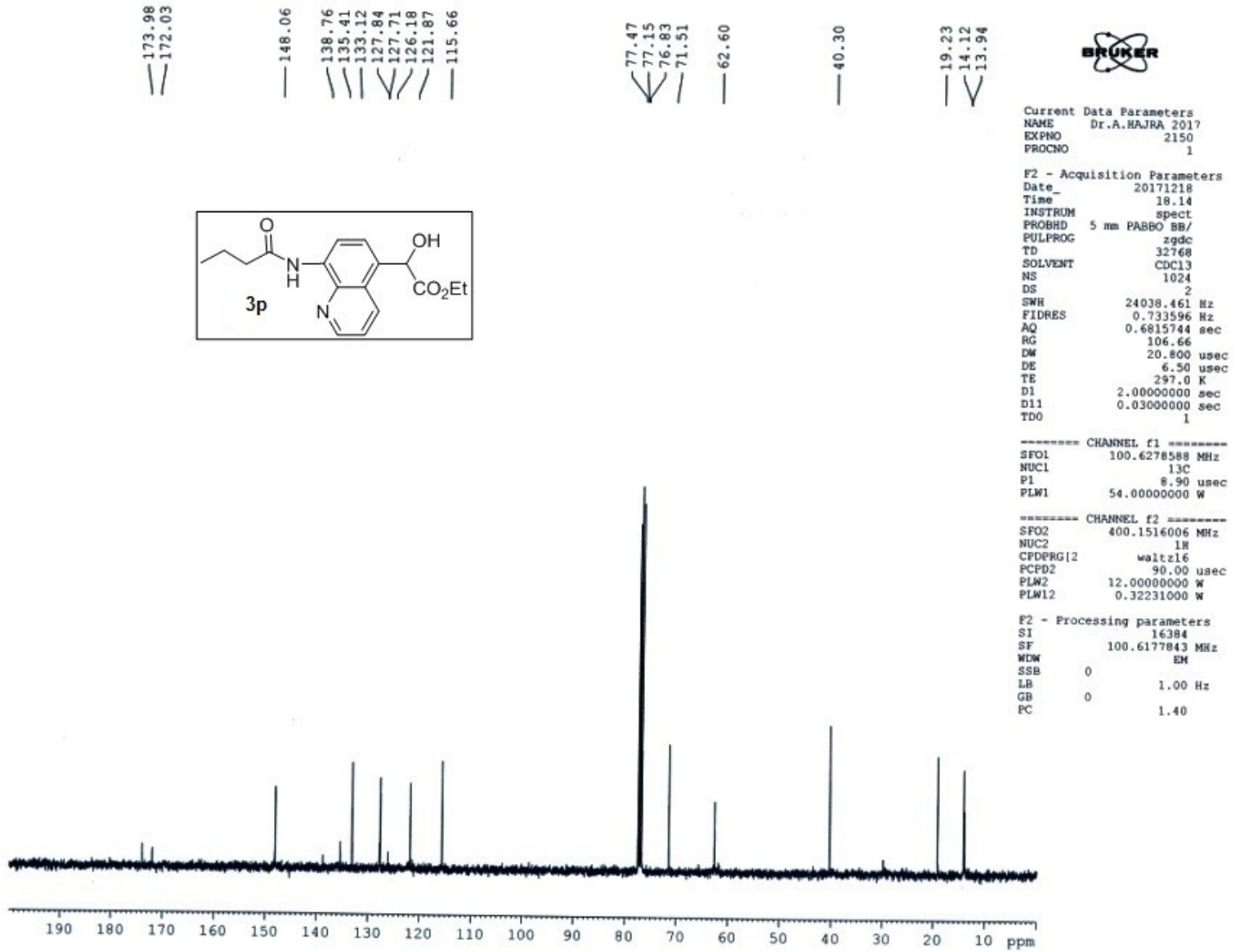

173.81
168.90
147.94
138.52
135.23
133.00
127.85
127.51
126.03
121.77
115.53
77.34
77.02
76.70
71.37
62.47
25.15
13.98
BRUKER
O
N
H
OH
CO2Et
N
3o
Current Data Parameters
NAME Dr.A.HAJRA 2017
EXPNO 2139
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171216
Time 17.56
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 640
DS 2
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 148.91
DW 20.800 usec
DE 6.50 usec
TE 297.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6278588 MHz
NUC1 13C
P1 8.90 usec
PLW1 54.00000000 W
======== CHANNEL f2 ========
SFO2 400.1516006 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 12.00000000 W
PLW12 0.32231000 W
PLW13 0.16212000 W
F2 - Processing parameters
SI 16384
SF 100.6177980 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

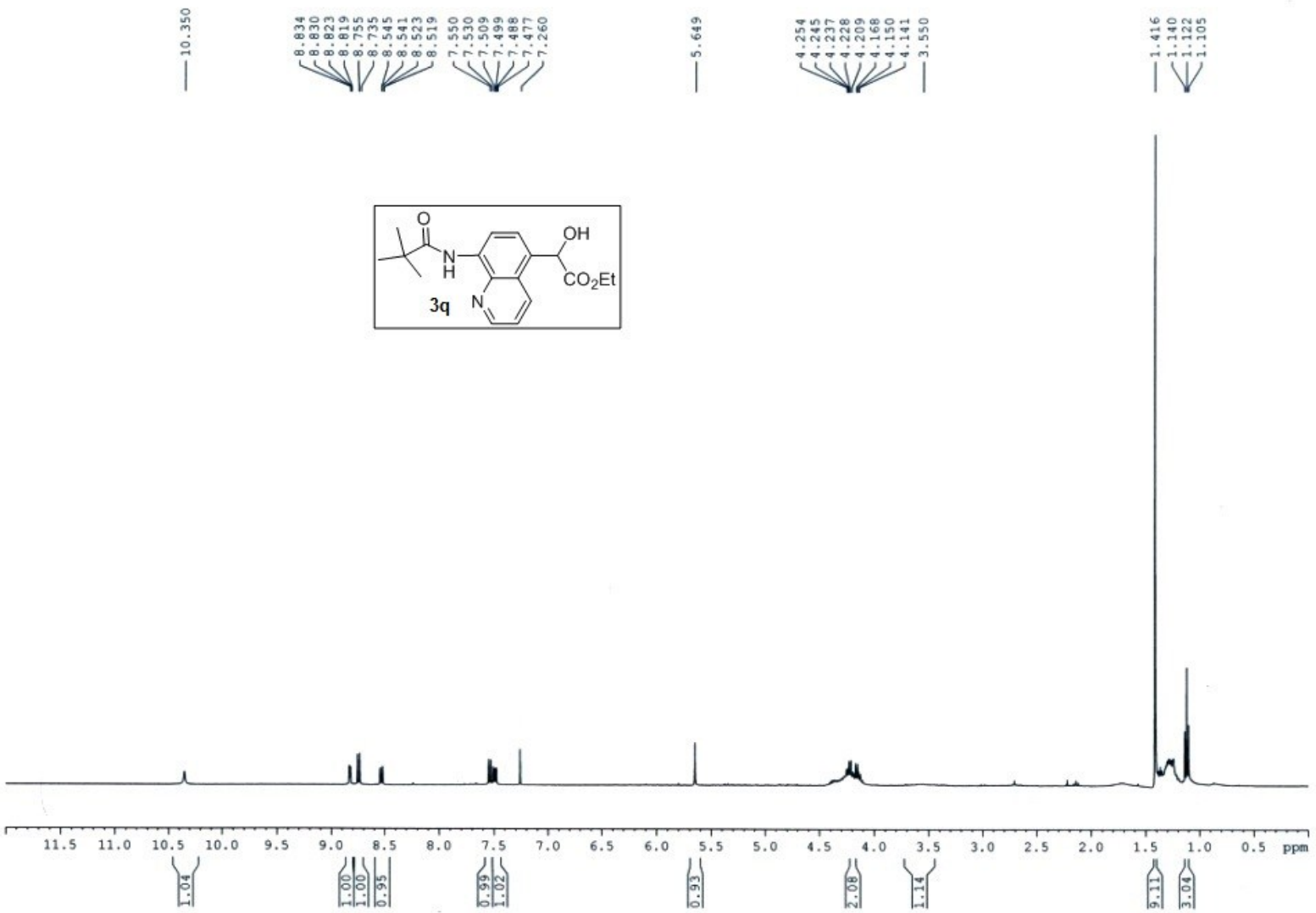

9.892
8.824
8.820
8.814
8.810
8.757
8.736
8.551
8.547
8.529
8.525
7.552
7.532
7.514
7.503
7.492
7.482
7.260
5.653
4.269
4.260
4.251
4.242
4.234
4.224
4.207
4.197
4.179
4.161
4.152
4.144
4.134
3.550
2.563
2.545
2.526
1.895
1.877
1.859
1.840
1.822
1.804
1.153
1.136
1.118
1.074
1.056
1.037

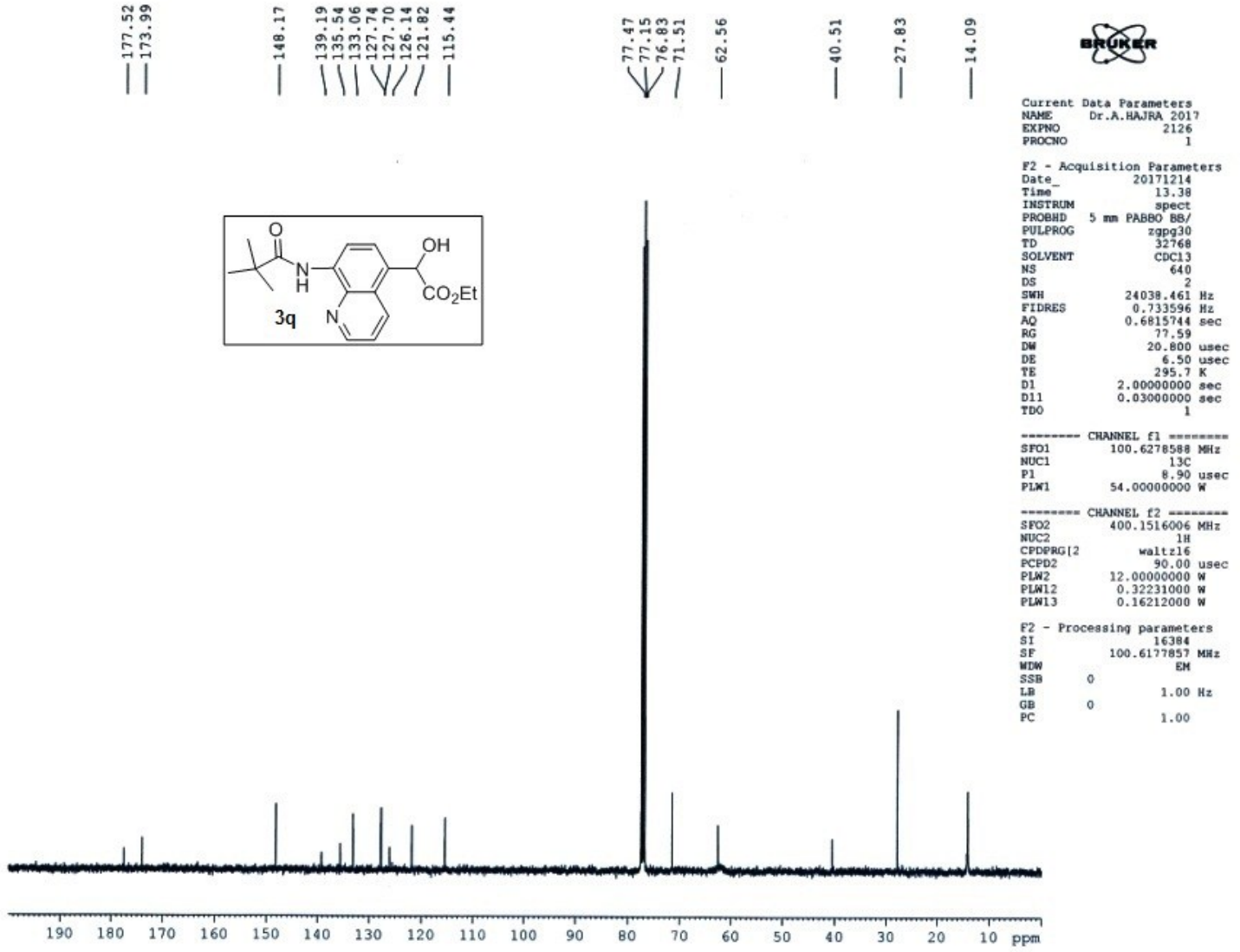

O
N
H
OH
CO2Et
N

3p

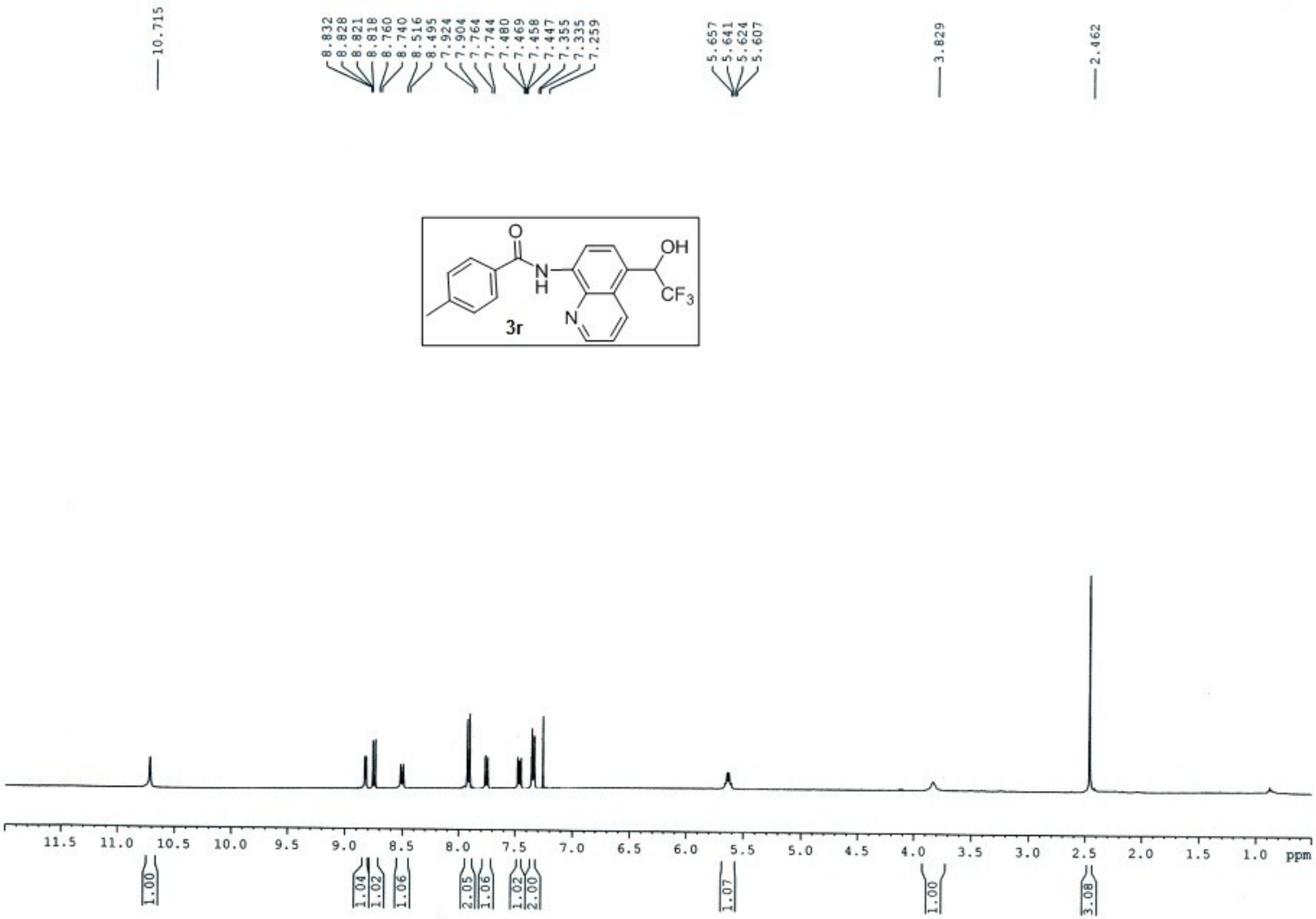

10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
1.00
1.07
1.06
0.90
1.04
1.05
0.92
2.14
0.91
2.06
2.09
3.06
3.00

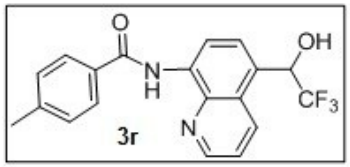

173.98
172.03
148.06
138.76
135.41
133.12
127.84
127.71
126.18
121.87
115.66
77.47
77.15
76.83
71.51
62.60
40.30
19.23
14.12
13.94
3p
OH
CO2Et
Current Data Parameters
NAME Dr.A.HAJRA 2017
EXPNO 2150
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171218
Time 18.14
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgdc
TD 32768
SOLVENT CDCl3
NS 1024
DS 2
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 106.66
DW 20.800 usec
DE 6.50 usec
TE 297.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
CHANNEL f1
SFO1 100.6278588 MHz
NUC1 13C
P1 8.90 usec
PLW1 54.00000000 W
CHANNEL f2
SFO2 400.1516006 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 12.00000000 W
PLW12 0.32231000 W
F2 - Processing parameters
SI 16384
SF 100.6177843 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

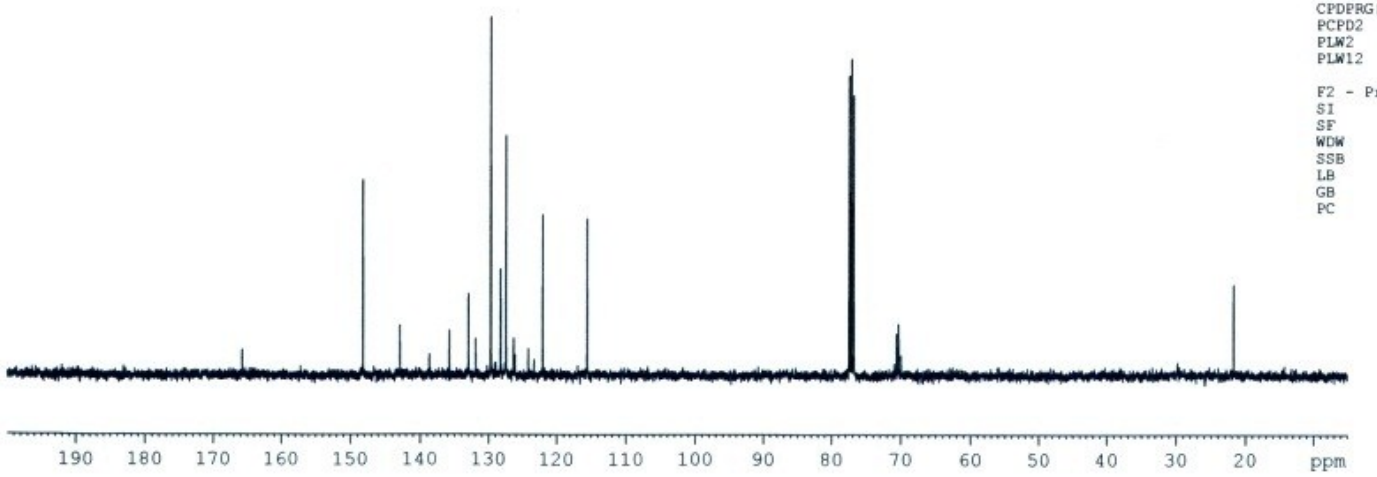

10.350
8.834
8.830
8.823
8.819
8.755
8.735
8.545
8.541
8.523
8.519
7.550
7.530
7.509
7.499
7.488
7.477
7.260
5.649
4.254
4.245
4.237
4.228
4.209
4.168
4.150
4.141
3.550
1.416
1.140
1.122
1.105
O
N
H
OH
CO2Et
N
3q
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
1.04
1.00
1.00
0.95
0.99
1.02
0.93
2.08
1.14
9.11
3.04



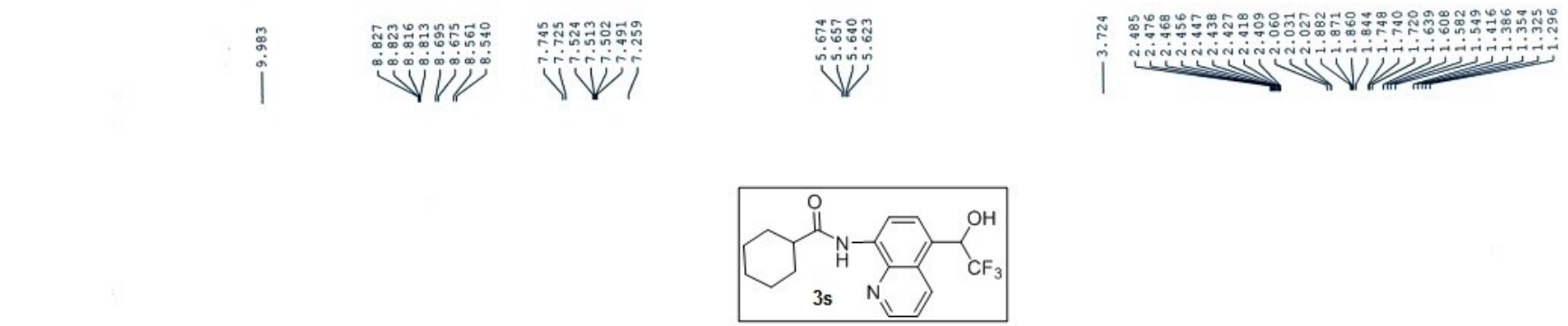

```
Current Data Parameters
NAME      Dr.A.HAJRA 2017
EXPNO             2126
PROCNO               1

F2 - Acquisition Parameters
Date_         20171214
Time             13.38
INSTRUM          spect
PROBHD   5 mm PABBO BB/
PULPROG        zgpg30
TD              32768
SOLVENT         CDCl3
NS                640
DS                  2
SWH         24038.461 Hz
FIDRES       0.733596 Hz
AQ           0.6815744 sec
RG               77.59
DW              20.800 usec
DE               6.50 usec
TE              295.7 K
D1          2.00000000 sec
D11         0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1       100.6278588 MHz
NUC1              13C
P1               8.90 usec
PLW1      54.00000000 W

======== CHANNEL f2 ========
SFO2       400.1516006 MHz
NUC2              1H
CPDPRG[2       waltz16
PCPD2           90.00 usec
PLW2      12.00000000 W
PLW12      0.32231000 W
PLW13      0.16212000 W

F2 - Processing parameters
SI               16384
SF         100.6177857 MHz
WDW                EM
SSB       0
LB               1.00 Hz
GB        0
PC               1.00
```

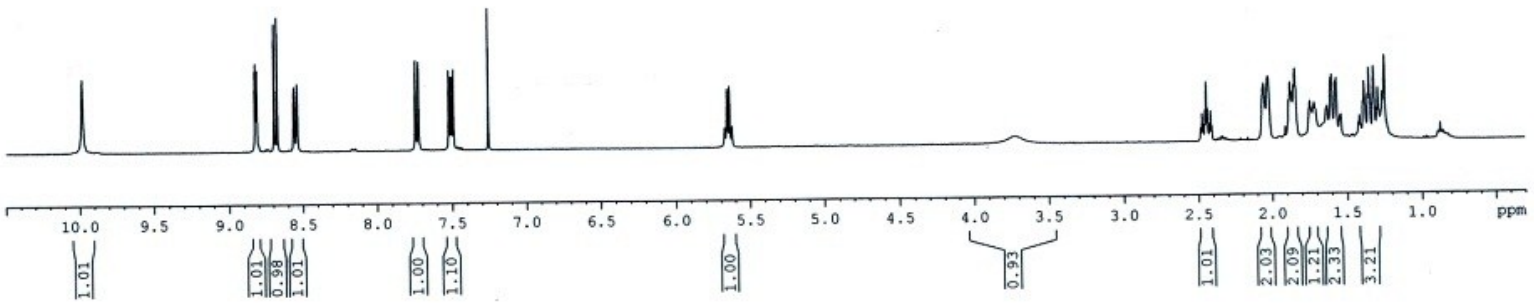

10.715
8.832
8.828
8.821
8.818
8.760
8.740
8.516
8.495
7.924
7.904
7.764
7.744
7.480
7.469
7.458
7.447
7.355
7.335
7.259
5.657
5.641
5.624
5.607
3.829
2.462
O
N
H
OH
CF3
N
3r
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
1.00
1.04
1.02
1.06
2.05
1.06
1.02
2.00
1.07
1.00
3.08

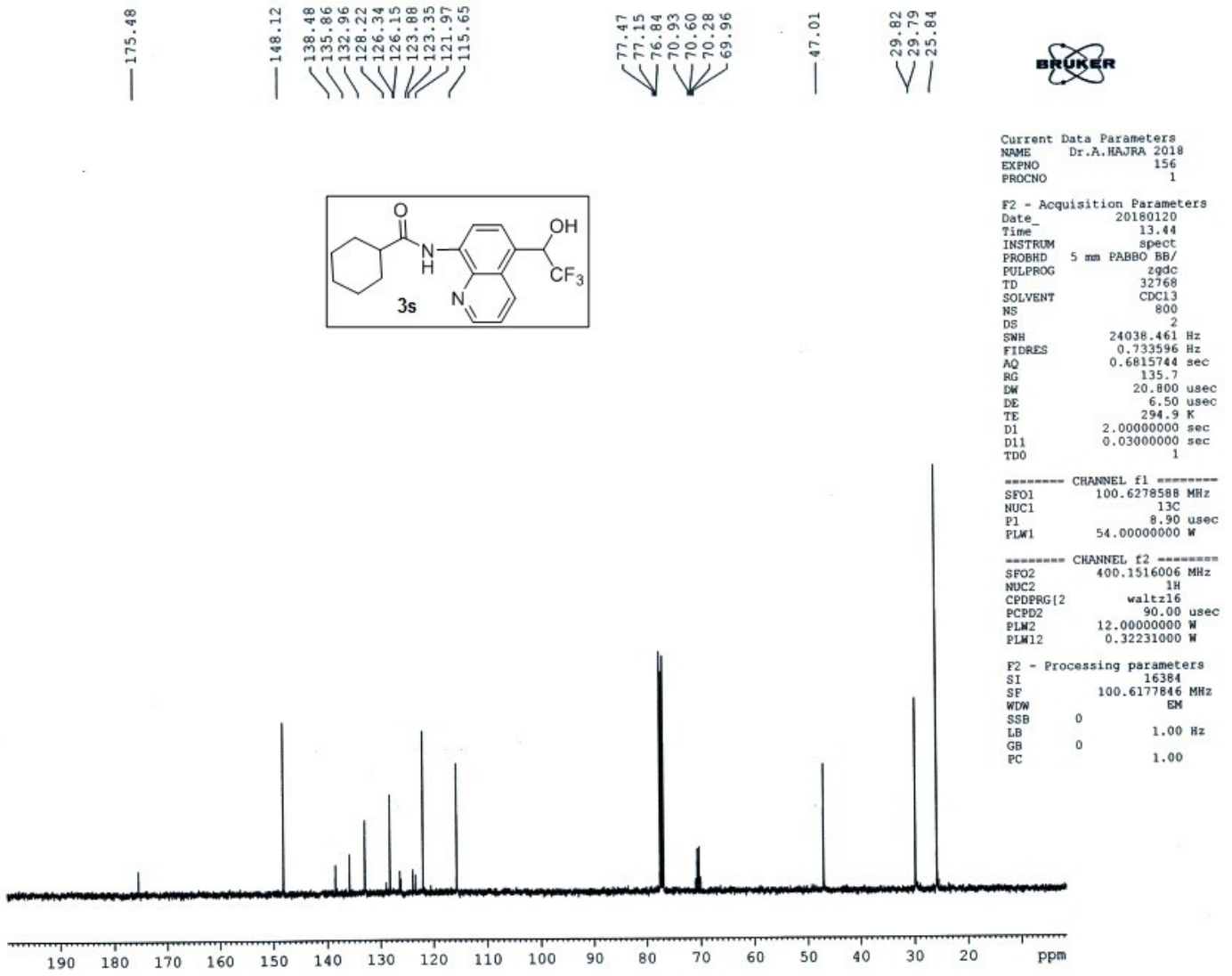




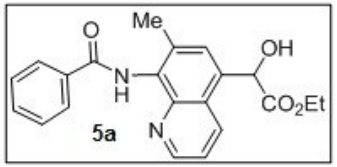

```
Current Data Parameters
NAME      Dr.A.HAJRA 2018
EXPNO                145
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180119
Time              13.24
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG           zgdc
TD               32768
SOLVENT          CDCl3
NS                 800
DS                   2
SWH          24038.461 Hz
FIDRES        0.733596 Hz
AQ            0.6815744 sec
RG               148.91
DW              20.800 usec
DE               6.50 usec
TE               294.2 K
D1          2.00000000 sec
D11         0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1       100.6278588 MHz
NUC1               13C
P1              8.90 usec
PLW1       54.00000000 W

======== CHANNEL f2 ========
SFO2       400.1516006 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2           90.00 usec
PLW2       12.00000000 W
PLW12       0.32231000 W

F2 - Processing parameters
SI                16384
SF         100.6177836 MHz
WDW                EM
SSB       0
LB              1.00 Hz
GB        0
PC              1.00
```

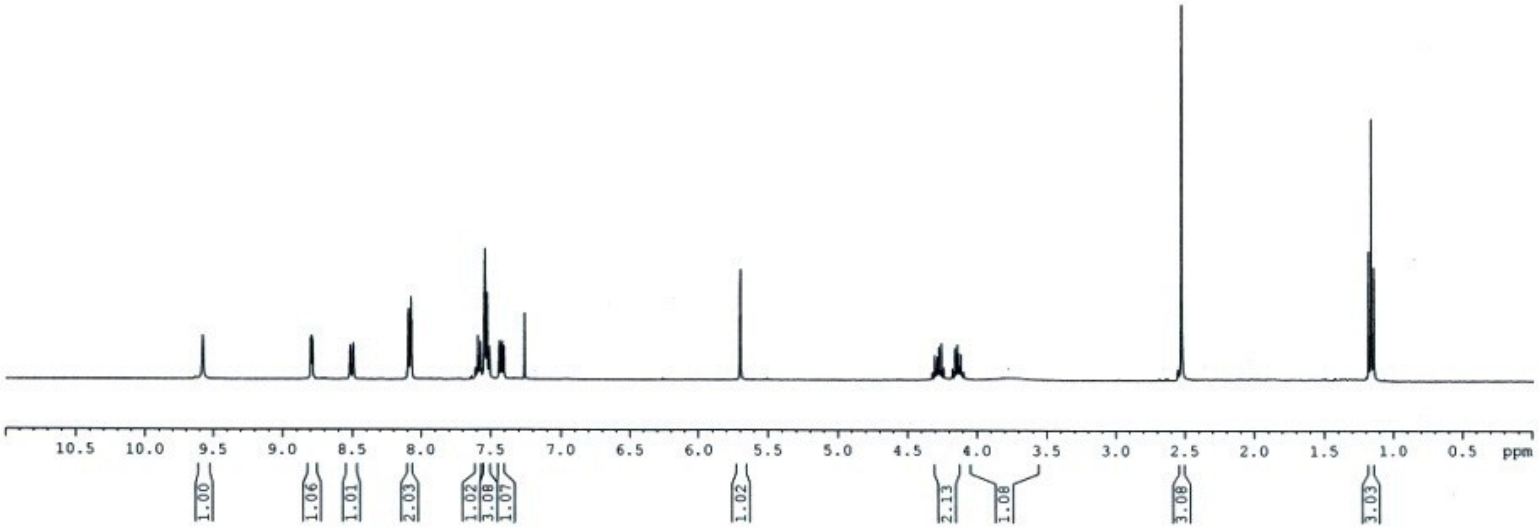

9.983
8.827
8.823
8.816
8.813
8.695
8.675
8.561
8.540
7.745
7.725
7.524
7.513
7.502
7.491
7.259
5.674
5.657
5.640
5.623
3.724
2.485
2.476
2.468
2.456
2.447
2.438
2.427
2.418
2.409
2.060
2.031
2.027
1.882
1.871
1.860
1.844
1.748
1.740
1.720
1.639
1.608
1.582
1.549
1.416
1.386
1.354
1.325
1.296
O
N
H
OH
CF3
N
3s

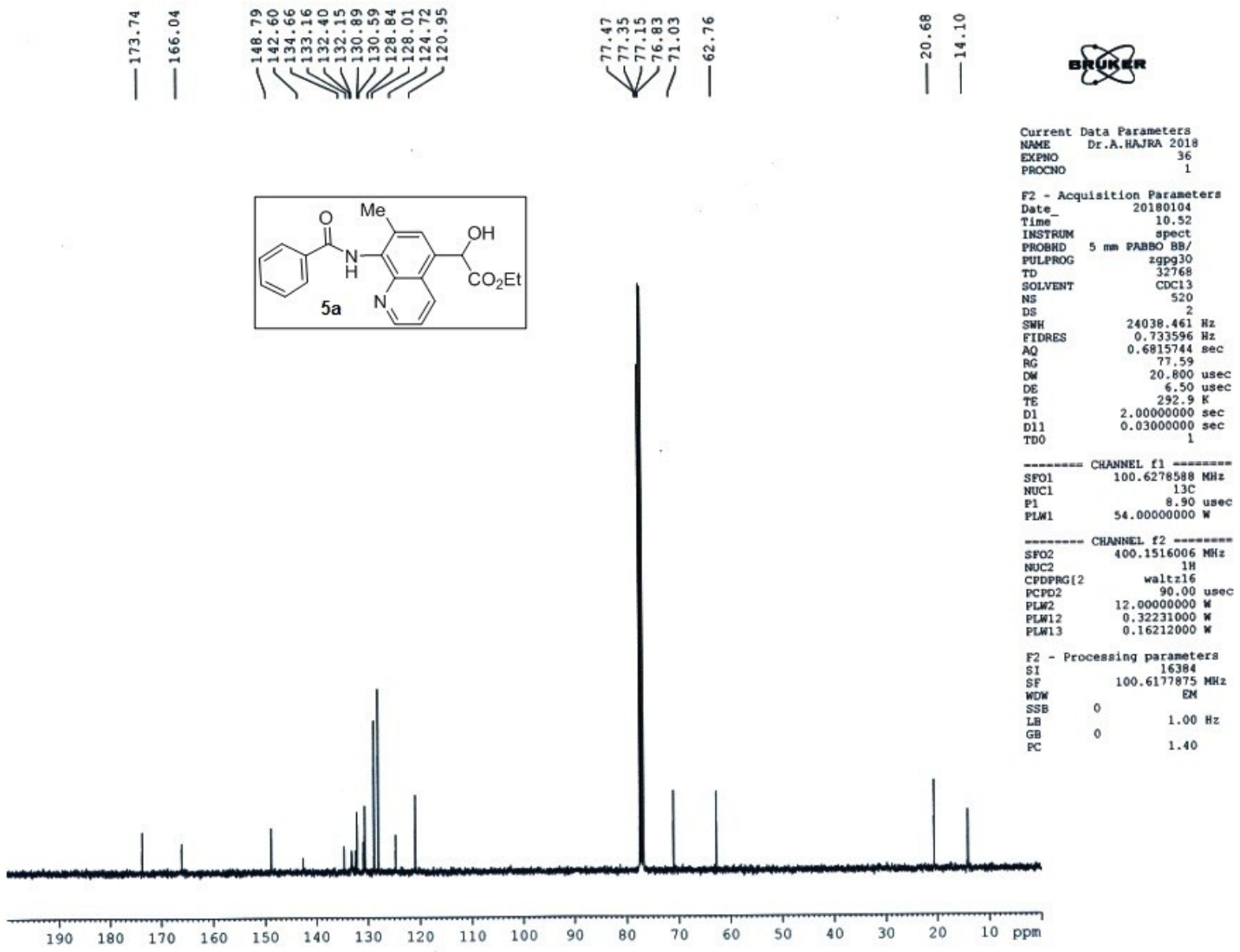

10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
1.01
1.01
0.98
1.01
1.00
1.10
1.00
0.93
1.01
2.03
2.09
1.21
2.33
3.21


175.48
148.12
138.48
135.86
132.96
128.22
126.34
126.15
123.88
123.35
121.97
115.65
77.47
77.15
76.84
70.93
70.60
70.28
69.96
47.01
29.82
29.79
25.84
BRUKER
O
N
H
OH
CF3
N
3s
Current Data Parameters
NAME Dr.A.HAJRA 2018
EXPNO 156
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180120
Time 13.44
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgdc
TD 32768
SOLVENT CDCl3
NS 800
DS 2
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 135.7
DW 20.800 usec
DE 6.50 usec
TE 294.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6278588 MHz
NUC1 13C
P1 8.90 usec
PLW1 54.00000000 W
======== CHANNEL f2 ========
SFO2 400.1516006 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 12.00000000 W
PLW12 0.32231000 W
F2 - Processing parameters
SI 16384
SF 100.6177846 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


9.577
8.799
8.796
8.789
8.785
8.517
8.513
8.495
8.492
8.092
8.074
8.070
7.609
7.606
7.597
7.590
7.584
7.575
7.572
7.569
7.542
7.530
7.526
7.513
7.509
7.505
7.439
7.428
7.417
7.407
7.260
5.701
4.320
4.302
4.293
4.285
4.275
4.266
4.258
4.240
4.178
4.160
4.151
4.142
4.133
4.125
4.115
4.109
4.098
3.749
2.528
1.182
1.164
1.146


Me
O
N
H
OH
CO2Et
N
5a


10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
1.00
1.06
1.01
2.03
1.02
3.08
1.07
1.02
2.13
1.08
3.08
3.03



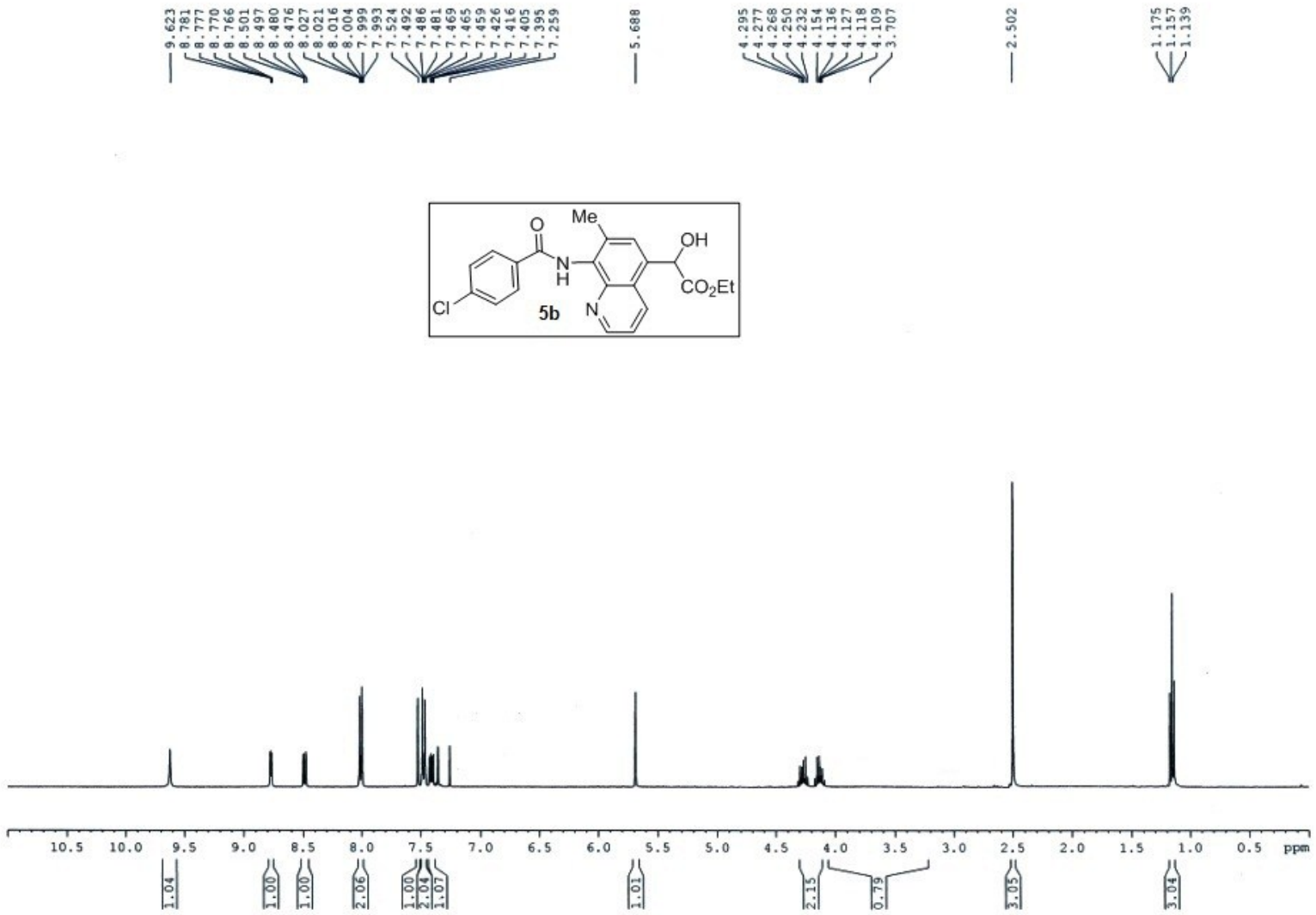
Current Data Parameters
NAME Dr.A.HAJRA 2018
EXPNO 36
PROCNO 1

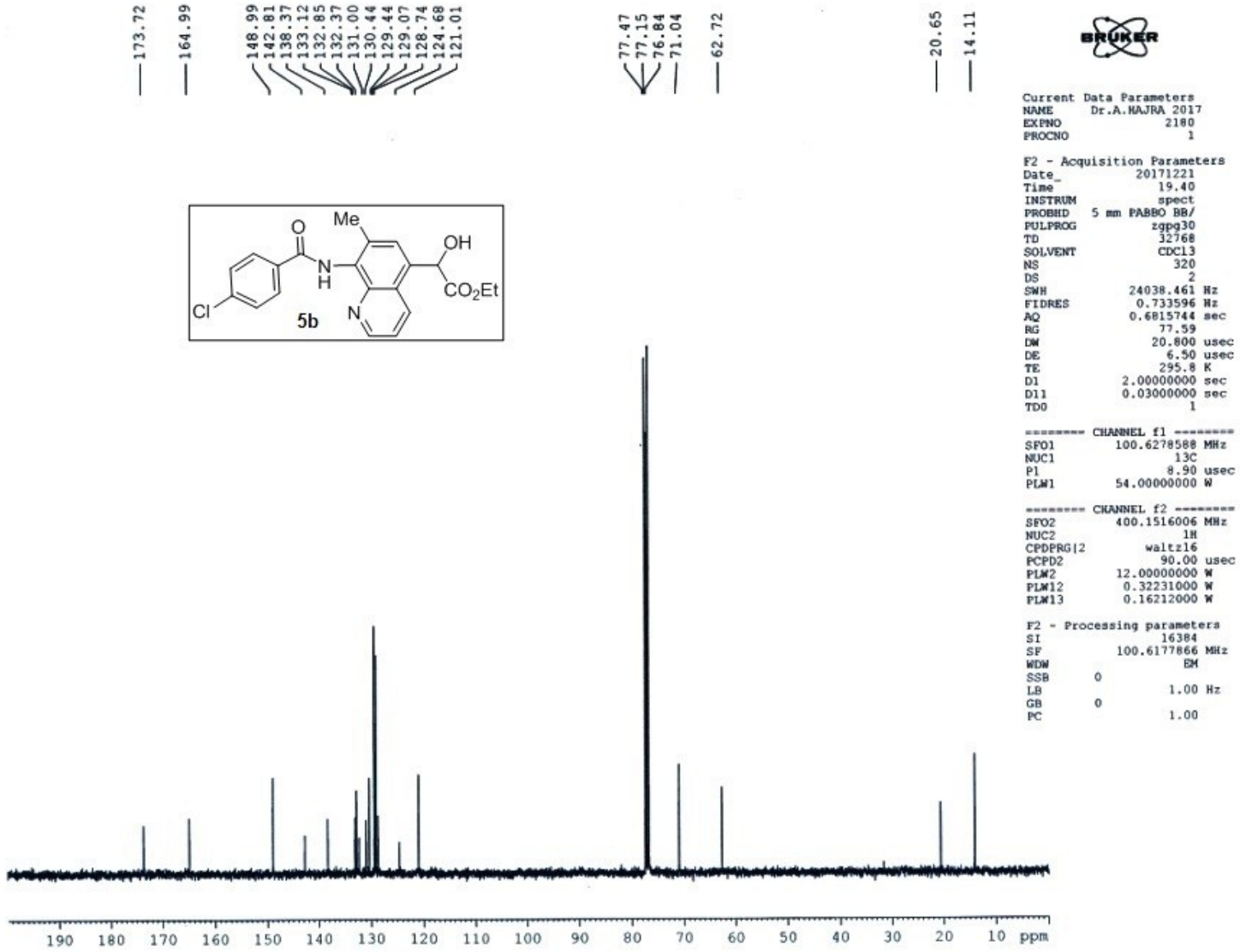
F2 - Acquisition Parameters
Date_ 20180104
Time 10.52
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 520
DS 2
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 77.59
DW 20.800 usec
DE 6.50 usec
TE 292.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6278588 MHz
NUC1 13C
P1 8.90 usec
PLW1 54.00000000 W

======== CHANNEL f2 ========
SFO2 400.1516006 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 12.00000000 W
PLW12 0.32231000 W
PLW13 0.16212000 W

F2 - Processing parameters
SI 16384
SF 100.6177875 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


9.623
8.781
8.777
8.770
8.766
8.501
8.497
8.480
8.476
8.027
8.021
8.016
8.004
7.999
7.993
7.524
7.492
7.486
7.481
7.469
7.465
7.459
7.426
7.416
7.405
7.395
7.259
5.688
4.295
4.277
4.268
4.250
4.232
4.154
4.136
4.127
4.118
4.109
3.707
2.502
1.175
1.157
1.139
Me
OH
O
N
H
CO2Et
Cl
N
5b
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
1.04
1.00
1.00
2.06
1.00
2.04
1.07
1.01
2.15
0.79
3.05
3.04


173.72
164.99
148.99
142.81
138.37
133.12
132.85
132.37
131.00
130.44
129.44
129.07
128.74
124.68
121.01
77.47
77.15
76.84
71.04
62.72
20.65
14.11
Me
O
OH
N
H
CO2Et
Cl
N
5b
BRUKER
Current Data Parameters
NAME Dr.A.HAJRA 2017
EXPNO 2180
PROCNO 1
F2 - Acquisition Parameters
Date_ 20171221
Time 19.40
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 0.6815744 sec
RG 77.59
DW 20.800 usec
DE 6.50 usec
TE 295.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6278588 MHz
NUC1 13C
P1 8.90 usec
PLW1 54.00000000 W
======== CHANNEL f2 ========
SFO2 400.1516006 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 12.00000000 W
PLW12 0.32231000 W
PLW13 0.16212000 W
F2 - Processing parameters
SI 16384
SF 100.6177866 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm