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Simple and Efficient one-pot multi-step strategy for synthesis of 2-substituted (1,2,5-triarylpyrrolo[3,2-*c*] pyridin-3-yl)-*N*- arylacetamide derivatives in water

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Electronic Supplementary Information (ESI)

Supplementary Information Available: complete product characterization data, analytical details.

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General information

All reagents were purchased from commercial suppliers and were used without further purification. The reactions were monitored by thin-layer chromatography (TLC) analysis using silica gel (GF254) plates. ^{1}H NMR spectra were recorded on a 400 MHz instrument (Bruker Avance 400 Spectrometer). Chemical shifts (δ) are given in ppm relative to TMS as the internal reference, with coupling constants (J) in Hz. ^{13}C NMR spectra were recorded at 100 MHz. Chemical shift were reported in ppm with the internal chloroform signal at 77.7 ppm and dimethyl sulphoxide signal at 39.9 ppm as a standard. HRMS (ESI) was measured with a Waters XEVO G2-XS QTOF/H-CLASS instrument. Single-crystal X-ray diffraction measurement was carried out on a Rigaku Saturn CCD diffractometer at 100(2) K using graphite monochromated Mo Kα radiation (λ = 0.71073 Å). The structure was solved by direct methods and refined by full-matrix least squares on F^2 using the SHELXTL-97 program package.

X-ray Crystallography

Single-crystal X-ray diffraction measurement was carried out on a Rigaku Saturn CCD diffractometer at 100.00(10) K using graphite monochromated CuKα radiation (λ = 1.54184). An empirical absorption correction was applied using the SADABS program. The structure was solved by direct methods and refined by full-matrix least squares on F^2 using the SHELXTL-97 program package.

General procedure for the synthesis of products 5.

Typically, 6-methyl-1-aryl-4-(phenylamino)pyridin-2(1*H*)-one **1** (0.4 mmol), 2,2-dihydroxy-1-phenylethan-1-one **2** (0.4 mmol), and Meldrum acid **3** (0.4 mmol) were introduced in a 10-mL reaction vial with acetic acid (0.04 mmol) and water (3 mL). Subsequently, the reaction vial was stirred and heated at 80 °C. The reaction was monitored by TLC until conversion of the substrates was complete about 2 hours. The mixture was cooled to room temperature. The resulted precipitate was filtered and the crude products were further purified by recrystallization from the mixture of hot 95% ethanol and *N*,*N*-dimethylformamide to give the pure products **5**.

General procedure for the synthesis of products 7.

Similarly, 6-methyl-1-aryl-4-(phenylamino)pyridin-2(1*H*)-one **1** (0.4 mmol), 2,2-dihydroxy-1-phenylethan-1-one **2** (0.4 mmol), and Meldrum acid **3** (0.4 mmol) were introduced in a 10-mL reaction vial with acetic acid (0.04 mmol) and water (3 mL). Subsequently, the reaction vial was stirred and heated 80 ^{o}C for about 2 hours. Then, alcohol **6** (0.8 mmol) was added the mixture and stirred for another 2 hours. The mixture was cooled and the precipitate was filtered. The crude products were further purified by recrystallization from hot 95% ethanol to give the pure products **7**.

General procedure for the synthesis of products 9.

Similarly, 6-methyl-1-aryl-4-(phenylamino)pyridin-2(1*H*)-one **1** (0.4 mmol), 2,2-dihydroxy-1-phenylethan-1-one **2** (0.4 mmol), and Meldrum acid **3** (0.4 mmol) were introduced in a 10-mL reaction vial with acetic acid (0.04 mmol) and water (3 mL). Subsequently, the reaction vial was stirred and heated 80 ^{o}C for about 2 hours. Then, alcohol **6** (0.8 mmol) was added the mixture and stirred for another 2 hours. Lastly, amine **8** (0.4 mmol) was added above mixture for about 4 hours indicated by TLC. The crude products were further purified by recrystallization from the mixture of hot 95% ethanol and *N*,*N*-dimethylformamide to give the pure desired products **9**.

Spectral data of the compounds

2-(2-(4-bromophenyl)-6-methyl-4-oxo-1,5-diphenyl-4,5-dihydro-1H-pyrrolo[3,2-c]pyridin-3-yl)acetic acid (5a)

Pale yellow solid; Mp: >300 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 7.54-7.62 (m, 3H, ArH), 7.45 (t, J = 8.0 Hz, 5H, ArH), 7.29-7.30 (m, 2H, ArH), 7.17-7.22 (m, 4H, ArH), 6.39 (s, 1H, CH), 3.78 (s, 2H, CH_2), 2.05 (s, 3H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 172.3, 162.8, 141.0, 140.5, 138.2, 136.5, 136.1, 132.3, 131.6, 129.9, 129.8, 129.2, 128.6, 128.2, 128.0, 127.6, 122.6, 112.5, 112.0, 96.6, 33.9, 22.1; HRMS (ESI) m/z calcd for $C_{28}H_{22}BrN_2O_3$ $[M + H]^+$: 513.0808, found: 513.0811.

2-(2-(4-bromophenyl)-6-methyl-4-oxo-1,5-di-p-tolyl-4,5-dihydro-1H-pyrrolo[3,2-c]pyridin-3-yl)acetic acid (5b)

White powder; Mp: >300 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 13.90 (s, 1H, OH),

7.34-7.41 (m, 4H, ArH), 7.13-7.19 (m, 6H, ArH), 7.01 (s, 2H, ArH), 6.31 (s, 1H, CH), 3.72 (s, 2H, CH_2), 2.43 (s, 3H, CH_3), 2.39 (s, 3H, CH_3), 2.01 (s, 3H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 172.2, 162.5, 141.2, 141.3, 140.5, 140.4, 140.3, 138.2, 136.5, 136.1, 132.3, 131.6, 129.2, 128.6, 128.1, 128.0, 127.6, 96.6, 33.9, 22.6, 22.1; HRMS (ESI) m/z calcd for $C_{30}H_{26}BrN_2O_3$ $[M + H]^+$: 541.1121, found: 541.1116.

2-(1,5-bis(4-fluorophenyl)-6-methyl-4-oxo-2-phenyl-4,5-dihydro-1H-pyrrolo[3,2-c]pyridin-3-yl)acetic acid (5c)

Pale yellow solid; Mp: >300 °C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 7.28-7.39 (m, 8H, ArH), 7.11-7.18 (m, 8H, ArH), 6.35 (s, 1H, CH), 3.79 (s, 2H, CH), 2.07 (s, 3H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 172.2, 162.9, 162.6 ($^1J_{CF}$ = 247.8 Hz), 162.0 ($^{1'}J_{CF}$ = 248.0 Hz), 140.8, 140.2, 137.6, 134.1 ($^4J_{CF}$ = 2.8 Hz), 132.7 ($^{4'}J_{CF}$ = 2.8 Hz), 130.9, 130.1 ($^3J_{CF}$ = 8.6 Hz), 129.3 ($^{3'}J_{CF}$ = 8.7 Hz), 128.8, 128.5, 128.3, 127.9, 116.9 ($^2J_{CF}$ = 22.9 Hz), 116.6 ($^{2'}J_{CF}$ = 22.9 Hz), 112.4, 111.7, 96.5, 33.8, 22.1; HRMS (ESI) m/z calcd for $C_{28}H_{21}F_2N_2O_3$ $[M + H]^+$: 471.1515, found: 471.1511.

2-(1,5-dibenzyl-2-(4-bromophenyl)-6-methyl-4-oxo-4,5-dihydro-1H-pyrrolo[3,2-c]pyridin-3-yl)acetic acid (5d)

Pale yellow solid; Mp: 230-232 °C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 7.59 (d, J = 8.4 Hz, 2H, ArH), 7.28-7.37 (m, 8H, ArH), 7.17 (d, J = 6.8 Hz, 2H, ArH), 6.93 (d, J = 7.6 Hz, 2H, ArH), 5.51 (s, 2H, CH_2), 5.18 (s, 2H, CH_2), 3.74 (s, 2H, CH_2), 2.37 (s, 3H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 172.4, 168.4, 140.2, 140.1, 136.6, 136.5, 136.4, 132.5, 132.0, 129.1, 128.9, 127.9, 127.5, 126.3, 125.7, 123.5, 112.2, 111.3, 97.0, 48.0, 47.2, 34.0, 21.3; HRMS (ESI) m/z calcd for $C_{30}H_{26}BrN_2O_3$ $[M + H]^+$: 541.1121, found: 541.1129.

2-(2-(4-bromophenyl)-1,5-dibutyl-6-methyl-4-oxo-4,5-dihydro-1H-pyrrolo[3,2-c]pyridin-3-yl)acetic acid (5e)

Gray powder; Mp: >300 °C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 7.62 (d, J = 8.4 Hz, 2H, ArH), 7.28 (d, J = 8.4 Hz, 2H, ArH), 6.37 (s, CH, ArH), 4.12 (t, J = 7.6 Hz, 2H, CH_2), 3.88 (d, J = 7.2 Hz, 2H, CH_2), 3.58 (s, 2H, CH_2), 2.51 (s, 3H, CH_3), 1.66-1.70 (m, 2H, CH_2), 1.40-1.47 (m, 4H, CH_2), 1.04-1.10 (m, 2H, CH_2), 0.96 (t, J = 7.2 Hz, 3H, CH_3), 0.75 (t, J = 7.2 Hz, 2H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 172.6, 162.0, 139.3, 138.8, 135.8, 132.5, 132.0, 128.5, 123.2, 112.2, 110.8, 96.6, 44.4, 44.1, 32.8, 32.3, 31.2, 21.1, 20.3, 19.8, 13.8, 13.5; HRMS (ESI) m/z calcd for $C_{24}H_{30}BrN_2O_3$ $[M + H]^+$:

473.1434, found: 473.1433.

2-(6-methyl-4-oxo-1,2,5-triphenyl-4,5-dihydro-1H-pyrrolo[3,2-c]pyridin-3-yl)acetic acid (5f)

White solid; Mp: 285-286 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 7.49-7.61 (m, 5H, ArH), 7.40-7.46 (m, 4H, ArH), 7.31-7.34 (m, 9H, ArH), 7.24-7.28 (m, 2H, ArH), 7.19 (d, J = 7.6 Hz, 2H, ArH), 6.40 (s, 1H, CH), 3.81 (s, 2H, CH), 2.06 (s, 3H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 172.5, 162.9 140.9, 140.1, 138.4, 137.5, 136.9, 131.0, 129.9, 129.6, 129.5, 129.4, 129.1, 129.0, 128.8, 128.4, 128.1, 127.8, 127.6, 127.5, 112.6, 111.7, 96.7, 33.9, 22.2; HRMS (ESI) m/z calcd for $C_{28}H_{23}N_2O_3$ $[M + H]^+$: 435.1703, found: 435.1698.

2-(2-(4-fluorophenyl)-6-methyl-4-oxo-1,5-diphenyl-4,5-dihydro-1H-pyrrolo[3,2-c]pyridin-3-yl)acetic acid (5g)

Pale yellow solid; Mp: >300 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 7.54-7.62 (m, 3H, ArH), 7.42-7.46 (m, 3H, ArH), 7.29-7.33 (m, 5H, ArH), 7.18 (d, J = 6.8 Hz, 2H, ArH), 7.03 (t, J = 8.8 Hz, 2H, ArH), 6.39 (s, 1H, CH), 3.78 (s, 2H, CH), 2.05 (s, 3H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 172.4, 162.8 ($^{1}J_{CF}$ = 247.4 Hz), 140.8, 140.3, 138.3, 136.6, 136.3, 132.7 ($^{3}J_{CF}$ = 8.2 Hz), 129.9, 129.6, 129.2, 128.5, 128.3, 127.6, 125.2, 125.1, 115.5 ($^{2}J_{CF}$ = 22.0 Hz), 115.4, 112.4, 111.7, 96.6, 33.9, 22.1; HRMS (ESI) m/z calcd for $C_{28}H_{22}FN_2O_3$ $[M + H]^+$: 453.1609, found: 453.1605.

ethyl 2-(2-(4-bromophenyl)-6-methyl-4-oxo-1,5-diphenyl-4,5-dihydro-1H-pyrrolo[3,2-c]pyridin-3-yl)acetate (7a)

Brown powder; Mp: 246-248 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 7.52 (t, J = 7.2 Hz, 2H, ArH), 7.38-7.46 (m, 7H, ArH), 7.28 (t, J = 5.6 Hz, 2H, ArH), 7.19 (d, J = 7.2 Hz, 2H, ArH), 7.05 (d, J = 8.0 Hz, 2H, ArH), 6.16 (s, 1H, CH), 4.12-4.18 (m, 2H, CH_2), 3.98 (s, 2H, CH_2), 1.95 (s, 3H, CH_3), 1.22 (m, J = 6.8 Hz, 3H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 172.5, 161.1, 140.0, 139.3, 137.0, 134.4, 131.8, 131.5, 129.7, 129.5, 129.4, 128.8, 128.3, 127.9, 127.7, 122.0, 113.6, 112.8, 94.5, 60.7, 30.8, 22.3, 14.2; HRMS (ESI) m/z calcd for $C_{30}H_{26}BrN_2O_3$ $[M + H]^+$: 541.1121, found: 541.1123.

methyl 2-(2-(4-bromophenyl)-6-methyl-4-oxo-1,5-diphenyl-4,5-dihydro-1H-pyrrolo[3,2-c]pyridin-3-yl)acetate (7b)

Yellow powder; Mp: 238-240 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 7.53 (t, J = 8.0

Hz, 2H, ArH), 7.45 (t, J = 7.2 Hz, 1H, ArH), 7.35-7.42 (m, 3H, ArH), 7.26-7.29 (m, 5H, ArH), 7.17-7.22 (m, 4H, ArH), 6.19 (s, 1H, CH), 4.01 (s, 2H, CH_2), 3.69 (s, 3H, OCH_3), 1.96 (s, 3H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 173.1, 161.2, 139.8, 139.7, 139.4, 137.2, 135.8, 130.6, 130.4, 129.5, 129.2, 128.9, 128.3, 128.2, 127.7, 113.0, 112.7, 94.6, 52.0, 30.8, 22.2; HRMS (ESI) m/z calcd for $C_{29}H_{24}BrN_2O_3$ $[M + H]^+$: 527.0965, found: 527.0966.

isopropyl 2-(2-(4-bromophenyl)-6-methyl-4-oxo-1,5-diphenyl-4,5-dihydro-1H-pyrrolo[3,2-c]pyridin-3-yl)acetate (7c)

Yellow powder; Mp: 228-230 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 7.52 (t, J = 7.6 Hz, 2H, ArH), 7.33-7.46 (m, 4H, ArH), 7.25-7.29 (m, 5H, ArH), 7.16-7.21 (m, 4H, ArH), 6.19 (s, 1H, CH), 5.00-5.03 (m, 1H, CH), 4.00 (s, 2H, CH_2), 1.96 (s, 3H, CH_3), 1.21 (t, J = 6.0 Hz, 6H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 172.1, 161.2, 139.7, 139.5, 139.4, 137.3, 135.7, 130.8, 130.4, 129.5, 129.2, 128.9, 128.3, 128.1, 127.7, 127.6, 113.3, 112.8, 94.6, 67.8, 31.1, 25.3, 22.2, 21.8; HRMS (ESI) m/z calcd for $C_{31}H_{28}BrN_2O_3$ $[M + H]^+$: 555.1278, found: 555.1283.

tert-butyl 2-(2-(4-bromophenyl)-6-methyl-4-oxo-1,5-diphenyl-4,5-dihydro-1H-pyrrolo[3,2-c]pyridin-3-yl)acetate (7d)

Pale yellow solid; Mp: 289-290 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 7.51 (t, J = 7.6 Hz, 2H, ArH), 7.37-7.46 (m, 6H, ArH), 7.25-7.29 (m, 2H, ArH), 7.19 (d, J = 6.8 Hz, 2H, ArH), 7.06 (d, J = 6.8 Hz, 2H, ArH), 6.15 (s, 1H, CH), 3.95 (s, 2H, CH_2), 1.95 (s, 3H, CH_3), 1.42 (s, 9H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 171.8, 139.9, 139.8, 139.4, 137.1, 131.8, 131.3, 130.0, 129.4, 128.9, 128.2, 127.8, 127.7, 121.8, 114.3, 112.7, 94.4, 80.4, 31.7, 28.0, 22.2; HRMS (ESI) m/z calcd for $C_{32}H_{30}BrN_2O_3$ $[M + H]^+$: 569.1434, found: 569.1434.

ethyl 2-(2-(4-bromophenyl)-6-methyl-4-oxo-1,5-di-p-tolyl-4,5-dihydro-1H-pyrrolo[3,2-c]pyridin-3-yl)acetate (7e)

Pale yellow crystal; Mp: 258-260 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 7.39 (d, J = 8.0 Hz, 2H, ArH), 7.30 (t, J = 8.0 Hz, 3H, ArH), 7.20 (d, J = 8.0 Hz, 2H, ArH), 7.13 (d, J = 8.0 Hz, 2H, ArH), 7.06 (t, J = 4.4 Hz, 2H, ArH), 6.13 (s, 1H, CH), 4.12-4.16 (m, 2H, CH_2), 3.97 (s, 1H, CH), 2.41 (d, J = 10.0 Hz, 6H, CH_3), 1.95 (s, 3H, CH_3), 1.22 (t, J = 7.2 Hz, 3H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 172.5, 161.2, 140.0, 138.1, 137.8,

136.7,134.4, 131.9, 131.4, 130.2, 130.0, 129.8, 128.5, 127.9, 127.4, 121.8, 113.3, 112.6, 94.4, 60.7, 30.8, 22.2, 21.2, 14.2; HRMS (ESI) m/z calcd for $C_{32}H_{30}BrN_2O_3$ $[M + H]^+$: 569.1434, found: 569.1429.

ethyl 2-(2-(4-bromophenyl)-6-methyl-4-oxo-1,5-di-o-tolyl-4,5-dihydro-1H-pyrrolo[3,2-c]pyridin-3-yl)acetate (7f)

Brown solid; Mp: 170-172 °C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 7.26-7.38 (m, 7H, ArH), 7.18-7.23 (m, 3H,ArH), 7.05-7.08 (m, 2H, ArH), 5.87 (s, 1H, CH), 4.12-4.18 (m, 2H, CH_2), 3.94-4.06 (m, 2H, CH_2), 2.13 (d, J = 4.4 Hz, 3H, CH_3), 1.96 (d, J = 4.0 Hz, 3H, CH_3), 1.86 (s, 3H, CH_3), 1.20-1.25 (m, 3H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 172.4, 160.4, 140.1, 139.6, 138.5, 136.6, 136.5, 136.1, 136.0, 134.7, 131.4, 131.2, 131.0, 129.8, 129.7, 129.2, 129.0, 128.7, 128.6, 127.1, 126.8, 121.9, 115.3, 113.2, 112.7, 94.4, 60.7, 30.9, 21.7, 17.7, 17.6, 14.2; HRMS (ESI) m/z calcd for $C_{32}H_{30}BrN_2O_3$ $[M + H]^+$: 569.1434, found: 569.1432.

ethyl 2-(2-(4-bromophenyl)-1,5-bis(2,4-dimethylphenyl)-6-methyl-4-oxo-4,5-dihydro-1H-pyrrolo[3,2-c]pyridin-3-yl)acetate (7g)

Yellow solid; Mp: 222-224 °C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 7.37 (d, J = 8.4 Hz, 2H, ArH), 7.03-7.18 (m, 8H, ArH), 5.86 (s, 1H, CH), 4.12-4.15 (m, 2H, CH_2), 3.99 (s, 2H, CH_2), 2.38 (d, J = 2.4 Hz, 6H, CH_3), 2.08 (d, J = 4.0 Hz, 3H, CH_3), 1.87-1.92 (s, 6H, CH_3), 1.19-1.24 (m, 3H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 172.5, 172.4, 160.6, 140.2, 139.7, 138.8, 138.3, 136.0, 135.8, 135.6, 134.7, 133.4, 132.0, 131.8, 131.5, 131.3, 129.9 128.9, 128.4, 127.8, 127.5, 121.8, 113.0, 112.6, 94.4, 60.6, 30.9, 21.7, 21.2, 17.6, 17.5, 14.2; HRMS (ESI) m/z calcd for $C_{34}H_{34}BrN_2O_3$ $[M + H]^+$: 597.1747, found: 597.1754.

ethyl 2-(2-(4-bromophenyl)-1,5-bis(4-fluorophenyl)-6-methyl-4-oxo-4,5-dihydro-1H-pyrrolo[3,2-c]pyridin-3-yl)acetate (7h)

Yellow powder; Mp: >300 °C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 7.41 (d, J = 8.4 Hz, 2H, ArH), 7.11-7.23 (m, 8H, ArH), 7.04 (d, J = 8.4 Hz, 2H, ArH), 6.11 (s, 1H, CH), 4.12-4.18 (m, 2H, CH_2), 3.94 (s, 2H, CH_2), 1.96 (s, 3H, CH_3), 1.23 (t, J = 8.0 Hz, 3H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 172.4, 162.3 ($^1J_{CF}$ = 242.3 Hz), 162.2 ($^{1'}J_{CF}$ = 242.5 Hz), 140.0, 135.1 ($^4J_{CF}$ = 3.0 Hz), 134.6 ($^{4'}J_{CF}$ = 3.0 Hz), 132.9, 131.9, 131.6, 130.6, 130.5 ($^3J_{CF}$ = 9.0 Hz), 129.4 ($^{3'}J_{CF}$ = 8.9 Hz), 122.2, 116.5 ($^2J_{CF}$ = 22.8 Hz), 116.4 ($^{2'}J_{CF}$ =

22.7 Hz), 113.6, 112.7, 94.5, 60.8, 30.8, 22.3, 14.2; HRMS (ESI) m/z calcd for $C_{30}H_{24}BrF_2N_2O_3$ $[M + H]^+$: 577.0933, found: 577.0929.

ethyl 2-(2-(4-bromophenyl)-1,5-bis(2-fluorophenyl)-6-methyl-4-oxo-4,5-dihydro-1H-pyrrolo[3,2-c]pyridin-3-yl)acetate (7i)

Yellow solid; Mp: 245-246 °C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 7.39-7.48 (m, 5H, ArH), 7.19-7.36 (m, 7H, ArH), 7.08 (d, J = 8.4 Hz, 2H, ArH), 6.03 (s, 1H, CH), 4.12-4.17 (m, 2H,CH_2), 3.80-4.02 (m, 1H, CH_2), 7.75-3.80 (m, 1H, CH_2), 1.99 (s, 3H, CH_3), 1.22 (t, J = 4.0 Hz, 3H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 172.2, 172.1, 160.4 ($^1J_{CF}$ = 242.5 Hz), 160.2 ($^{1'}J_{CF}$ = 242.4 Hz), 140.6, 140.5 ($^4J_{CF}$ = 2.1 Hz), 140.1 ($^{4'}J_{CF}$ = 2.7 Hz), 134.9, 131.5, 130.9 ($^3J_{CF}$ = 7.5 Hz), 130.5, 130.4, 130.3, 130.2 ($^{3'}J_{CF}$ = 6.6 Hz), 129.3, 124.9, 122.3, 117.0 ($^2J_{CF}$ = 22.5 Hz), 116.8 ($^{2'}J_{CF}$ = 22.4 Hz), 113.8, 112.8, 94.7, 94.6, 60.7, 30.8, 21.5, 14.1; HRMS (ESI) m/z calcd for $C_{30}H_{24}BrF_2N_2O_3$ $[M + H]^+$: 577.0933, found: 577.0932.

ethyl 2-(2-(4-bromophenyl)-1,5-bis(3-chlorophenyl)-6-methyl-4-oxo-4,5-dihydro-1H-pyrrolo[3,2-c]pyridin-3-yl)acetate (7j)

Yellow crystal; Mp: 275-276 °C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 7.42-7.49 (m, 4H, ArH), 7.27-7.38 (m, 2H, ArH), 7.28 (d, J = 6.8 Hz, 3H, ArH), 7.17 (d, J = 6.8 Hz, 1H, ArH), 7.01-7.06 (m, 3H, ArH), 6.15 (s, 1H, CH), 4.13-4.19 (m, 2H, CH_2), 3.93 (s, 2H, CH_2), 1.99 (s, 3H, CH_3), 1.23 (m, J = 6.8 Hz, 3H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 172.3, 160.8, 140.3, 139.9, 138.0, 135.1, 135.0, 134.5, 131.8, 131.7, 130.5, 129.3, 129.1, 128.8, 128.3, 127.7, 127.3, 126.1, 122.3, 114.1, 112.8, 94.5, 60.8, 30.8, 22.2, 14.2; HRMS (ESI) m/z calcd for $C_{30}H_{24}BrCl_2N_2O_3$ $[M + H]^+$: 609.0342, found: 609.0344.

ethyl 2-(6-methyl-4-oxo-1,2,5-triphenyl-4,5-dihydro-1H-pyrrolo[3,2-c]pyridin-3-yl)acetate (7k).

Brown solid; Mp: 261-262 °C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 7.49-7.53 (m, 2H, ArH), 7.31-7.44 (m, 6H, ArH), 7.23-7.25 (m, 5H, ArH), 7.15-7.20 (m, 4H, ArH), 6.16 (s, 1H, CH), 4.10-4.15 (m, 2H, CH_2), 3.98 (s, 2H, CH_2), 1.94 (m, 3H, CH_3), 1.20 (t, J = 3.2 Hz, 3H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 172.6, 139.6, 139.4, 137.3, 130.7, 130.4, 129.5, 129.2, 128.9, 128.3, 128.1, 127.7, 127.6, 113.1, 94.6, 60.6, 30.9, 22.2, 14.1; HRMS (ESI) m/z calcd for $C_{30}H_{27}N_2O_3$ $[M + H]^+$: 463.2016, found: 463.2011.

ethyl 2-(2-(4-fluorophenyl)-6-methyl-4-oxo-1,5-diphenyl-4,5-dihydro-1H-

pyrrolo[3,2-c]pyridin-3-yl)acetate (7l).

Pale yellow crystal; Mp: 256-258 °C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 7.46-7.51 (m, 2H, ArH), 7.36-7.44 (m, 4H, ArH), 7.26-7.29 (m, 3H, ArH), 7.14-7.20 (m, 4H, ArH), 6.96 (d, J = 8.4 Hz, 2H, ArH), 6.17 (s, 1H, CH), 4.12-4.17 (m, 2H, CH_2), 3.97 (s, 2H, CH_2), 1.95 (s, 3H, CH_3), 1.22 (m, J = 6.8 Hz, 3H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 172.5, 161.1 ($^1J_{CF}$ = 247.2 Hz), 139.7 ($^4J_{CF}$ = 2.0 Hz), 139.4, 137.1, 134.7, 132.1 ($^3J_{CF}$ = 8.0 Hz), 129.9, 129.6, 129.5, 129.3, 128.9, 128.3, 127.8, 127.7, 126.8, 115.3 ($^2J_{CF}$ = 22.0 Hz), 113.2, 112.6, 94.6, 60.7, 30.8, 22.2, 14.2; HRMS (ESI) m/z calcd for $C_{30}H_{26}FN_2O_3$ $[M + H]^+$: 481.1922, found: 481.1933.

2-(2-(4-bromophenyl)-6-methyl-4-oxo-1,5-diphenyl-4,5-dihydro-1H-pyrrolo[3,2-c]pyridin-3-yl)-N-phenylacetamide (9a).

White powder; Mp: >300 °C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 11.23 (s, 1H, NH), 7.58-7.67 (m, 5H, ArH), 7.44-7.48 (m, 7H, ArH), 7.28-7.34 (m, 4H, ArH), 7.18-7.19 (m, 2H, ArH), 7.04-7.06 (m, 1H, ArH), 6.29 (s, 1H, CH), 3.81 (s, 2H, CH_2), 2.02 (s, 3H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 170.2, 162.2, 140.8, 140.1, 139.6, 139.2, 136.9, 135.4, 132.7, 131.3, 129.9, 129.6, 128.9, 128.7, 128.5, 128.4, 128.2 127.7, 123.1, 122.3, 119.4, 114.4, 112.2, 95.6, 34.9, 22.1; HRMS (ESI) m/z calcd for $C_{34}H_{27}BrN_3O_2$ $[M + H]^+$: 588.1281, found: 588.1277.

2-(2-(4-bromophenyl)-6-methyl-4-oxo-1,5-diphenyl-4,5-dihydro-1H-pyrrolo[3,2-c]pyridin-3-yl)-N-(p-tolyl)acetamide (9b).

White powder; Mp: >300 °C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 11.10 (s, 1H, NH), 7.55-7.63 (m, 3H,ArH), 7.42-7.48 (m, 9H, ArH), 7.27-7.31 (m, 3H, ArH), 7.07-7.17 (m, 4H, ArH), 6.26 (s, 1H, CH), 3.78 (s, 2H, CH_2), 2.29 (s, 3H, CH_3), 2.00 (s, 3H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 170.0, 162.2, 140.8, 140.1, 139.2, 137.0, 136.9, 135.4, 132.7, 132.5, 131.3, 129.8, 129.6, 129.2, 128.9, 128.5, 128.4, 128.2, 127.7, 122.2, 119.3, 114.6, 112.2, 95.6, 34.8, 22.1, 20.9; HRMS (ESI) m/z calcd for $C_{35}H_{29}BrN_3O_2$ $[M + H]^+$: 602.1438, found: 602.1447.

2-(2-(4-bromophenyl)-6-methyl-4-oxo-1,5-diphenyl-4,5-dihydro-1H-pyrrolo[3,2-c]pyridin-3-yl)-N-(4-methoxyphenyl)acetamide (9c).

White solid; Mp: 286-288 °C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 11.9 (s, 1H, NH), 7.65 (t, J = 7.6 Hz, 2H, ArH), 7.18 (d, J = 7.2 Hz, 1H, ArH), 7.53 (d, J = 8.4 Hz, 2H,

ArH), 7.31 (d, J = 7.6 Hz, 2H, ArH), 7.18 (d, J = 6.8 Hz, 2H, ArH), 6.29 (s, 1H, CH), 3.80 (s, 5H, OMe + CH_2), 2.02 (s, 3H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 169.8, 162.2, 155.5, 140.8, 140.1, 139.2, 136.9, 135.4, 133.0, 132.7, 131.3, 129.9, 129.6, 128.9, 128.5, 128.4, 128.2, 127.7, 122.2, 120.8, 114.6, 113.9, 112.3, 95.6, 55.5, 34.8, 22.2; HRMS (ESI) m/z calcd for $C_{35}H_{29}BrN_3O_3$ $[M + H]^+$: 618.1387, found: 618.1391.

2-(2-(4-bromophenyl)-6-methyl-4-oxo-1,5-diphenyl-4,5-dihydro-1H-pyrrolo[3,2-c]pyridin-3-yl)-N-(4-fluorophenyl)acetamide (9d).

White powder; Mp: 293-294 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 11.28 (s, 1H, NH), 7.63-7.67 (m, 2H, ArH), 7.54-7.60 (m, 3H, ArH), 7.39-7.48 (m, 7H, ArH), 7.29-7.32 (m, 3H, ArH), 7.18 (d, J = 6.8 Hz, 2H, ArH), 6.97 (t, J = 8.8 Hz, 2H, ArH), 6.30 (s, 1H, CH), 3.79 (s, 2H, CH_2), 2.02 (s, 3H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 170.1, 161.2 ($^1J_{CF}$ = 245.2 Hz), 157.4, 140.8, 140.2, 139.2, 136.8, 135.7, 135.5 ($^4J_{CF}$ = 2.0 Hz), 132.6, 131.3, 129.9, 129.6, 129.0, 128.4 ($^3J_{CF}$ = 8.2 Hz), 127.7, 122.3, 120.9, 120.8, 161.1 ($^2J_{CF}$ = 22.2 Hz), 114.3, 112.2, 95.7, 34.8, 22.1; HRMS (ESI) m/z calcd for $C_{34}H_{26}BrFN_3O_2$ $[M + H]^+$: 606.1187, found: 606.1196.

2-(2-(4-bromophenyl)-6-methyl-4-oxo-1,5-diphenyl-4,5-dihydro-1H-pyrrolo[3,2-c]pyridin-3-yl)-N-(4-chlorophenyl)acetamide (9e).

Pale yellow powder; Mp: 261-262 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 11.36 (s, 1H, NH), 7.63-7.67 (m, 2H, ArH), 7.59 (d, J = 7.6 Hz, 1H, ArH), 7.54 (d, J = 8.8 Hz, 2H, ArH), 7.38-7.48 (m, 7H, ArH), 7.38-7.48 (m, 4H, ArH), 7.29-7.31 (m, 4H, ArH), 7.24 (d, J = 8.4 Hz, 2H, ArH), 7.18 (d, J = 6.8 Hz, 2H, ArH), 6.30 (s, 1H, CH), 3.78 (s, 2H, CH_2), 2.02 (s, 3H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 170.2, 162.2, 140.9, 140.2, 139.1, 138.2, 136.8, 135.6, 132.6, 131.4, 129.9, 129.6, 129.0, 128.6, 128.3, 127.8, 127.7, 122.4, 120.6, 114.1, 112.2, 95.7, 34.9, 22.1; HRMS (ESI) m/z calcd for $C_{34}H_{26}BrClN_3O_2$ $[M + H]^+$: 622.0891, found: 622.0898.

N-(4-bromophenyl)-2-(2-(4-bromophenyl)-6-methyl-4-oxo-1,5-diphenyl-4,5-dihydro-1H-pyrrolo[3,2-c]pyridin-3-yl)acetamide (9f).

White powder; Mp: >300 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 11.40 (s, 1H, NH), 7.64 (d, J = 6.8 Hz, 2H, ArH), 7.59 (d, J = 6.0 Hz, 1H, ArH), 7.19-7.51 (m, 11H, ArH), 7.30 (d, J = 7.2 Hz, 2H, ArH), 7.19 (s, 2H, ArH), 6.30 (s, 1H, CH), 3.78 (s, 1H, CH_2), 2.02 (s, 3H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 170.3, 162.2, 140.9, 140.2,

139.1, 138.7, 136.8, 135.6, 132.6, 131.6, 131.4, 129.9, 129.6, 129.0, 128.4, 128.3, 127.7, 122.4, 121.0, 115.4, 114.1, 112.2, 95.7, 35.0, 22.1; HRMS (ESI) m/z calcd for $C_{34}H_{26}Br_2N_3O_2$ $[M + H]^+$: 666.0386, found: 666.0396.

2-(2-(4-bromophenyl)-6-methyl-4-oxo-1,5-diphenyl-4,5-dihydro-1H-pyrrolo[3,2-c]pyridin-3-yl)-N-(4-(trifluoromethyl)phenyl)acetamide (9g).

Pale yellow crystal; Mp: 282-284 ^oC; ^1H NMR (400 MHz, $CDCl_3$, TMS): δ 11.62 (s, 1H, NH), 7.59-7.71 (m, 4H, ArH), 7.60 (d, J = 7.6 Hz, 1H, ArH), 7.29-7.54 (m, 8H, ArH), 7.17-7.19 (m, 4H, ArH), 7.18 (d, J = 6.4 Hz, 1H, ArH), 6.31 (s, 1H, CH)，3.81 (s, 2H, CH_2), 2.03 (s, 3H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 170.6, 162.3, 142.7, 140.9, 140.3, 139.1, 136.8, 135.7, 132.6, 132.3, 131.6, 131.4, 129.9, 129.7, 129.6, 129.1, 128.3, 127.6, 125.9, 122.4, 119.0, 113.8, 112.1, 95.7, 35.1, 22.1; HRMS (ESI) m/z calcd for $C_{35}H_{26}BrF_3N_3O_2$ $[M + H]^+$: 656.1155, found: 656.1156.

2-(2-(4-bromophenyl)-6-methyl-4-oxo-1,5-diphenyl-4,5-dihydro-1H-pyrrolo[3,2-c]pyridin-3-yl)-N-(3-chlorophenyl)acetamide (9h).

Yellow solid; Mp: 286-288 ^oC; ^1H NMR (400 MHz, $CDCl_3$, TMS): δ 11.47 (s, 1H, NH), 7.65-7.69 (m, 2H, ArH), 7.54-7.59 (m, 3H, ArH), 7.29-7.48 (m, 10H, ArH), 7.18-7.22 (m, 3H, ArH), 7.00 (d, J = 7.6 Hz, 1H, ArH), 6.30 (s, 1H, CH)，3.79 (s, 2H, CH_2), 2.03 (s, 3H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 170.4, 162.2, 140.9, 140.8, 140.3, 139.1, 136.8, 135.6, 134.2, 132.6, 132.4, 131.6, 131.4, 130.0, 129.8, 129.6, 129.0, 128.3, 127.7, 123.1, 122.4, 119.4, 117.4, 114.1, 112.1, 95.7, 35.0, 22.1; HRMS (ESI) m/z calcd for $C_{34}H_{26}BrClN_3O_2$ $[M + H]^+$: 622.0891, found: 622.0885.

2-(2-(4-bromophenyl)-6-methyl-4-oxo-1,5-diphenyl-4,5-dihydro-1H-pyrrolo[3,2-c]pyridin-3-yl)-N-(2,4-dichlorophenyl)acetamide (9i).

Yellow crystal; Mp: 283-284 ^oC; ^1H NMR (400 MHz, $CDCl_3$, TMS): δ 10.55 (s, 1H, NH), 8.19 (d, J = 8.4 Hz, 1H, ArH), 7.57-7.61 (m, 2H, ArH), 7.53 (d, J = 7.2 Hz, 1H, ArH), 7.52-7.54 (m, 5H, ArH), 7.29-7.44 (m, 6H, ArH), 7.21 (s, 3H, ArH), 6.29 (s, 1H, CH)，3.94 (s, 2H, CH_2)，2.03 (s, 3H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 171.0, 161.8, 140.4, 140.2, 138.8, 136.9, 135.2, 134.6, 132.5, 131.3, 129.7, 129.6, 129.0, 128.8, 128.6, 128.5, 128.2, 127.6, 127.1, 125.5, 124.8, 122.3, 114.0, 112.4, 95.3, 34.6, 22.2; HRMS (ESI) m/z calcd for $C_{34}H_{25}BrCl_2N_3O_2$ $[M + H]^+$: 656.0502, found: 656.0509.

2-(2-(4-bromophenyl)-6-methyl-4-oxo-1,5-diphenyl-4,5-dihydro-1H-pyrrolo[3,2-

c]pyridin-3-yl)-N-(2,4-dimethylphenyl)acetamide (9j).

White crystal; Mp: 248-250 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 10.19 (s, 1H, NH), 7.76 (d, J = 8.0 Hz, 1H, ArH), 7.56-7.60 (m, 2H, ArH), 7.53 (d, J = 6.8 Hz, 1H, ArH), 7.41-7.45 (m, 8H, ArH), 7.20-7.29 (m, 5H, ArH), 6.99 (d, J = 8.0 Hz, 1H, ArH), 6.96 (s, 1H, ArH), 6.30 (s, 1H, CH), 3.88 (s, 2H, CH_2), 2.29 (s, 3H, CH_3), 2.16 (s, 3H, CH_3), 2.03 (s, 3H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 170.6, 161.9, 140.5 140.1, 139.0, 137.0, 135.3, 134.3, 133.8, 132.7, 131.3, 131.0, 129.7, 129.6, 128.8, 128.5, 128.1, 127.7, 126.6, 123.4, 122.2, 114.9, 112.4, 95.4, 34.4, 22.2, 20.9, 18.3; HRMS (ESI) m/z calcd for $C_{36}H_{31}BrN_3O_2$ $[M + H]^+$: 616.1594, found: 616.1597.

2-(2-(4-bromophenyl)-6-methyl-4-oxo-1,5-diphenyl-4,5-dihydro-1H-pyrrolo[3,2-c]pyridin-3-yl)-N-(2,6-dimethylphenyl)acetamide (9k).

Yellow solid; Mp: 228-230 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 10.29 (s, 1H, NH), 7.93 (d, J = 8.0 Hz, 1H, ArH), 7.52-7.61 (m, 4H, ArH), 7.41-7.44 (m, 8H, ArH), 7.27-7.31 (m, 3H, ArH), 7.13-7.22 (m, 5H, ArH), 7.02 (d, J = 7.2 Hz, 1H, ArH), 6.31 (s, 1H, CH), 3.90 (s, 2H, CH_2), 2.21 (s, 3H, CH_3), 2.02 (s, 6H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 170.7, 161.9, 140.6, 140.1, 138.9, 137.0, 136.9, 135.3, 132.7, 132.4, 131.6, 131.3, 130.3, 129.9, 129.8, 129.7, 129.6, 128.8, 128.5, 128.3, 128.2, 127.6, 126.1, 124.3, 123.2, 122.2, 114.7, 112.4, 95.5, 34.5, 22.2, 18.5; HRMS (ESI) m/z calcd for $C_{36}H_{31}BrN_3O_2$ $[M + H]^+$: 616.1594, found: 616.1593.

2-(2-(4-bromophenyl)-6-methyl-4-oxo-1,5-di-p-tolyl-4,5-dihydro-1H-pyrrolo[3,2-c]pyridin-3-yl)-N-(p-tolyl)acetamide (9l).

White crystal; Mp:263-264 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 11.14 (s, 1H, NH), 7.42-7.50 (m, 8H, ArH), 7.17-7.29 (m, 4H, ArH), 7.04-7.10 (m, 4H, ArH), 6.25 (s, 1H, CH), 3.78 (s, 2H, CH_2), 2.51 (s, 3H, CH_3), 2.41 (s, 3H, CH_3), 2.31 (s, 3H, CH_3), 2.01 (s, 3H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 170.1, 162.3, 140.8, 140.1, 138.8, 138.1, 137.1, 136.5, 135.4, 134.3, 132.7, 132.5, 131.3, 130.5, 130.2, 129.1, 128.7, 128.1, 127.4, 122.1, 119.4, 114.3, 112.1, 95.5, 34.9, 22.1, 21.3, 21.2, 20.9; HRMS (ESI) m/z calcd for $C_{37}H_{33}BrN_3O_2$ $[M + H]^+$: 630.1751, found: 630.1755.

2-(2-(4-bromophenyl)-1,5-bis(4-methoxyphenyl)-6-methyl-4-oxo-4,5-dihydro-1H-pyrrolo[3,2-c]pyridin-3-yl)-N-(p-tolyl)acetamide (9m).

Pale yellow crystal; Mp: 237-238 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 11.14 (s, 1H,

NH), 7.42-7.50 (m, 6H, ArH), 7.20-7.29 (m, 2H, ArH), 7.08-7.7.14 (m, 6H, ArH), 6.93 (d, J = 8.4 Hz, 2H, ArH), 6.22 (s, 1H, CH), 3.94 (s, 3H, OMe), 3.85 (s, 3H, OMe), 3.78 (s, 2H, CH_2), 2.31 (s, 3H, CH_3), 2.02 (s, 3H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 170.1, 162.5, 159.6, 159.1, 141.0, 140.4, 137.1, 135.5, 132.7, 132.5, 131.8, 131.3, 129.6, 129.3, 129.2, 128.8, 128.6, 122.1, 119.4, 115.0, 114.7, 114.2, 112.0, 95.5, 55.6, 55.5, 34.9, 22.2, 20.9; HRMS (ESI) m/z calcd for $C_{37}H_{33}BrN_3O_4$ $[M + H]^+$: 662.1649, found: 662.1655.

2-(2-(4-bromophenyl)-1,5-bis(4-fluorophenyl)-6-methyl-4-oxo-4,5-dihydro-1H-pyrrolo[3,2-c]pyridin-3-yl)-N-(p-tolyl)acetamide (9n).

White crystal; Mp: 260-262 ^{o}C; ^{1}H NMR (400 MHz, DMSO-d_6, TMS): δ 10.66 (s, 1H, NH), 7.55 (d, J = 8.0 Hz, 2H, ArH), 7.30-7.43 (m, 12H, ArH), 7.08 (d, J = 8.0 Hz, 2H, ArH), 6.31 (s, 1H, CH), 3.67 (s, 2H, CH), 2.24 (s, 3H, CH_3), 1.95 (s, 3H, CH_3); ^{13}C NMR (100 MHz, DMSO-d_6, TMS): δ 169.3, 163.0, 161.8 ($^1J_{CF}$ = 243.2 Hz), 161.3 ($^{1'}J_{CF}$ = 243.2 Hz), 141.3, 140.9, 137.3, 135.6, 135.1, 133.1, 133.0, 132.5, 132.3, 131.8, 131.6, 131.3 ($^3J_{CF}$ = 9.0 Hz), 130.5 ($^{3'}J_{CF}$ = 8.0 Hz), 129.6, 129.3, 122.1, 119.2, 117.1, 116.7 ($^2J_{CF}$ = 22.2 Hz), 116.5 ($^{2'}J_{CF}$ = 22.2 Hz), 114.0, 111.8, 95.0, 34.4, 22.0, 20.8; HRMS (ESI) m/z calcd for $C_{35}H_{27}BrF_2N_3O_2$ $[M + H]^+$: 638.1249, found: 638.1248.

2-(1,5-dibenzyl-2-(4-bromophenyl)-6-methyl-4-oxo-4,5-dihydro-1H-pyrrolo[3,2-c]pyridin-3-yl)-N-(p-tolyl)acetamide (9o).

Pale yellow solid; Mp: 261-262 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 11.16 (s, 1H, NH), 7.59 (d, J = 8.0 Hz, 2H, ArH), 7.60 (d, J = 8.0 Hz, 2H, ArH), 7.29-7.38 (m, 8H, ArH), 7.19 (s, 2H, ArH), 6.99 (d, J = 8.0 Hz, 3H, ArH), 6.20 (s,1H, CH), 5.55 (s, 2H, CH_2), 5.15 (s, 2H, CH_2), 3.75 (s, 2H, CH_2), 2.36 (s, 3H, CH_3), 2.29 (s, 3H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 170.0, 161.8, 139.9, 139.8, 137.1, 137.0, 136.9, 135.9, 132.8, 132.4, 131.7, 129.1, 129.0, 128.9, 128.4, 127.7, 127.3, 126.1, 125.8, 123.2, 119.4, 113.5, 112.0, 95.9, 47.9, 47.0, 35.1, 21.4, 20.9; HRMS (ESI) m/z calcd for $C_{37}H_{33}BrN_3O_2$ $[M + H]^+$: 630.1751, found: 630.1751.

2-(2-(4-fluorophenyl)-6-methyl-4-oxo-1,5-diphenyl-4,5-dihydro-1H-pyrrolo[3,2-c]pyridin-3-yl)-N-(p-tolyl)acetamide (9p).

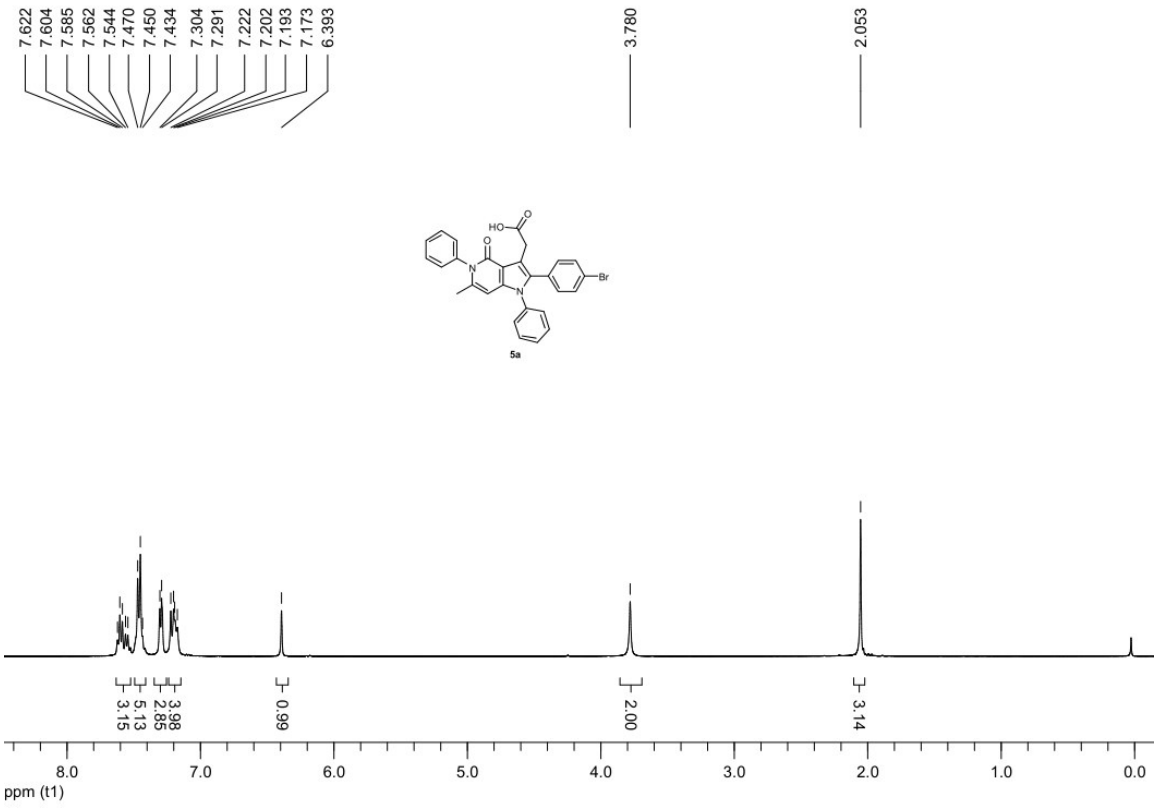
Gray powder; Mp: >300 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$, TMS): δ 11.15 (s, 1H, NH), 7.64 (d, J = 7.6 Hz, 2H, ArH), 7.41-7.65 (m, 10H, ArH), 6.29 (s, 1H, CH), 3.80 (s, 2H,

CH_2), 2.32 (s, 3H, CH_3), 2.02 (s, 3H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 170.2, 162.2 ($^1J_{CF}$ = 242.2 Hz), 140.6, 139.9, 139.2, 137.1, 137.0, 135.6, 133.1, 133.0, 132.5, 129.9, 129.5, 129.2, 129.0, 128.9, 128.5, 128.3, 128.1, 127.7, 126.2, 125.7, 121.1, 119.3, 115.2 ($^2J_{CF}$ = 21.2 Hz), 114.1, 112.2, 95.6, 34.9, 22.1, 20.9; HRMS (ESI) m/z calcd for $C_{35}H_{29}FN_3O_2$ $[M + H]^+$: 542.2238, found: 542.2247.

2-(2-(4-methoxyphenyl)-6-methyl-4-oxo-1,5-diphenyl-4,5-dihydro-1H-pyrrolo[3,2-c]pyridin-3-yl)-N-(p-tolyl)acetamide (9q).

White powder; Mp: >300 ^oC; ^1H NMR (400 MHz, $CDCl_3$, TMS): δ 11.20 (s, 1H, NH), 7.51-7.67 (m, 7H, ArH), 7.29-7.47 (m, 6H, ArH), 7.19 (d, J = 8.0 Hz, 2H, ArH), 7.10 (d, J = 8.0 Hz, 2H, ArH), 6.88 (d, J = 8.0 Hz, 2H, ArH), 6.29 (s, 1H, CH), 3.82 (s, 5H, OMe + CH_2), 2.32 (s, 3H, CH_3), 2.01 (s, 3H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$, TMS): δ 170.4, 162.2, 159.1, 140.3, 139.5, 139.3, 137.2, 136.6, 132.5, 132.3, 129.9, 129.8, 129.5, 129.4, 129.2, 129.1, 128.8, 128.5, 128.3, 127.9, 127.8, 125.7, 121.9, 121.1, 119.3, 113.5, 112.2, 95.7, 55.2, 35.0, 22.1, 20.9; HRMS (ESI) m/z calcd for $C_{36}H_{32}N_3O_3$ $[M + H]^+$: 554.2438, found: 554.2440.

^1H and ^{13}C NMR Spectra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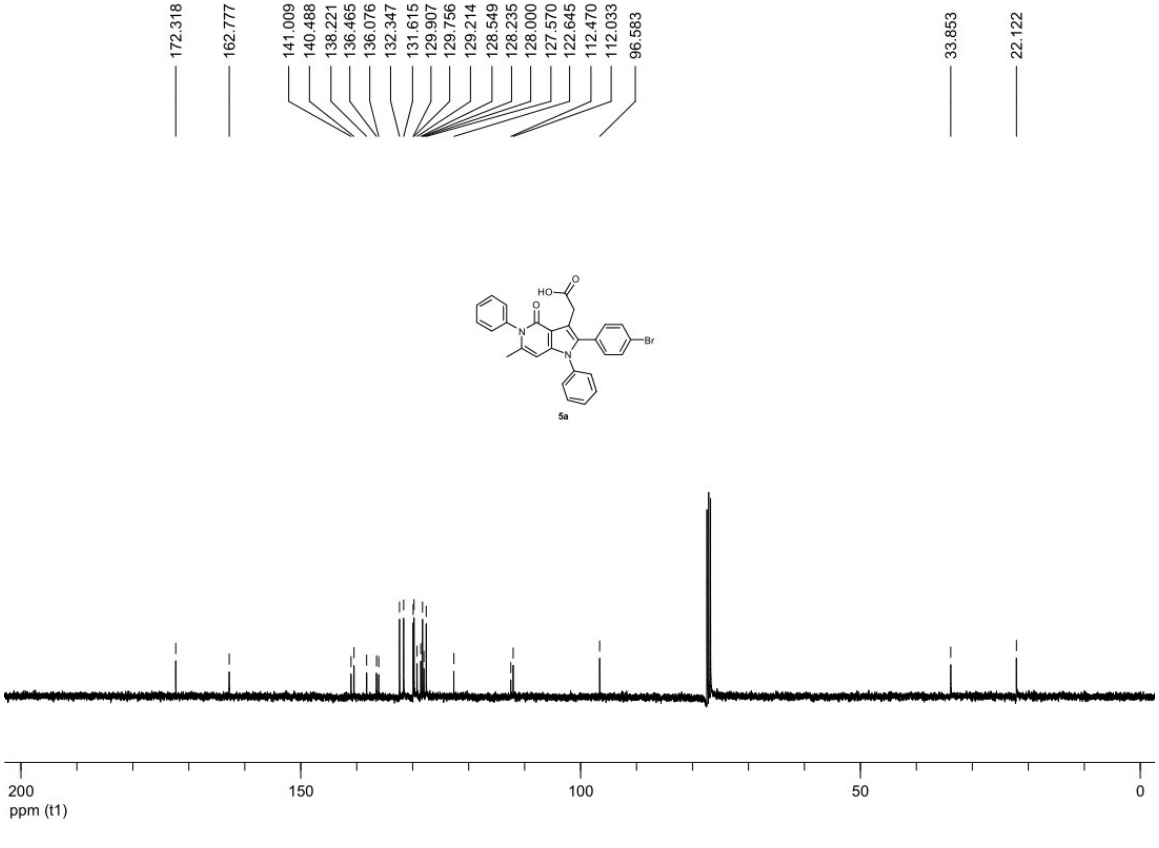
7.450
7.434
7.304
7.291
7.222
7.202
7.193
7.173
6.393
3.780
2.053
HO
O
N
Br
5a
3.15
5.13
2.85
3.98
0.99
2.00
3.14
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)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129.756
129.214
128.549
128.235
128.000
127.570
122.645
112.470
112.033
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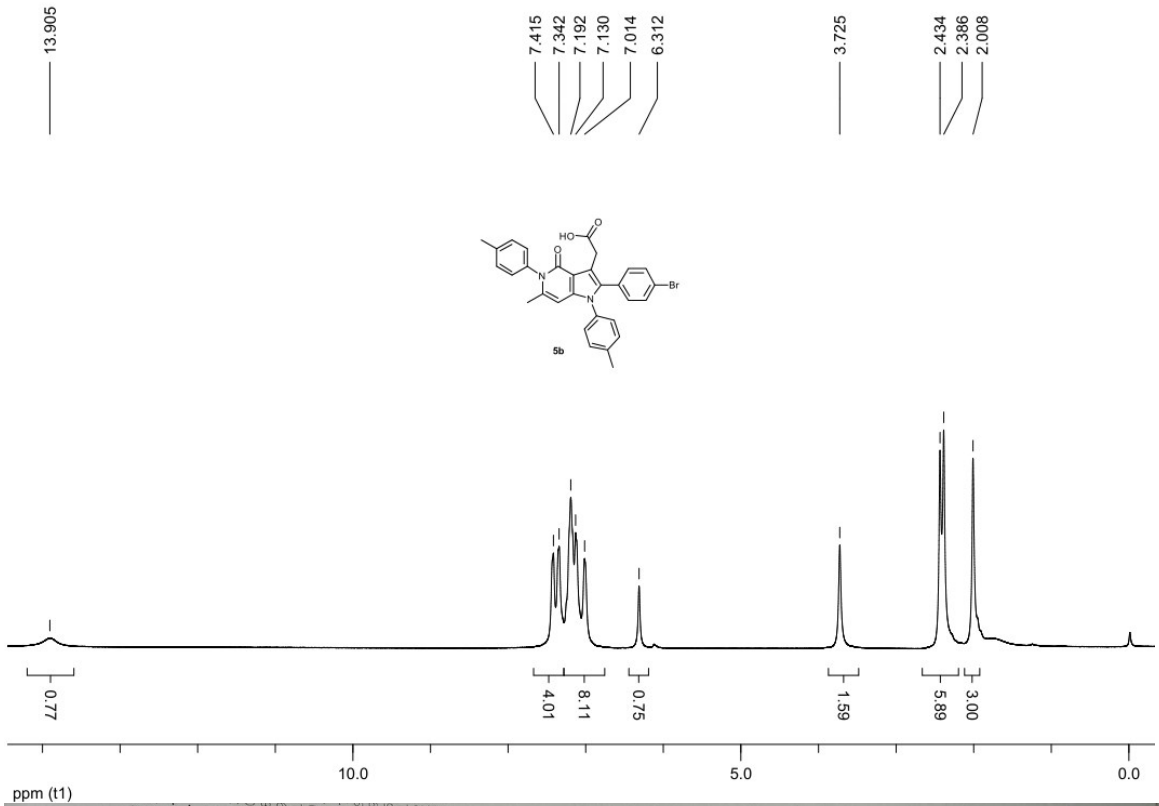
33.853
22.122
HO
O
N
Br
5a
200
150
100
50
0
ppm (t1)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7.342
7.192
7.130
7.014
6.312
3.725
2.434
2.386
2.008
HO
O
N
Br
5b
0.77
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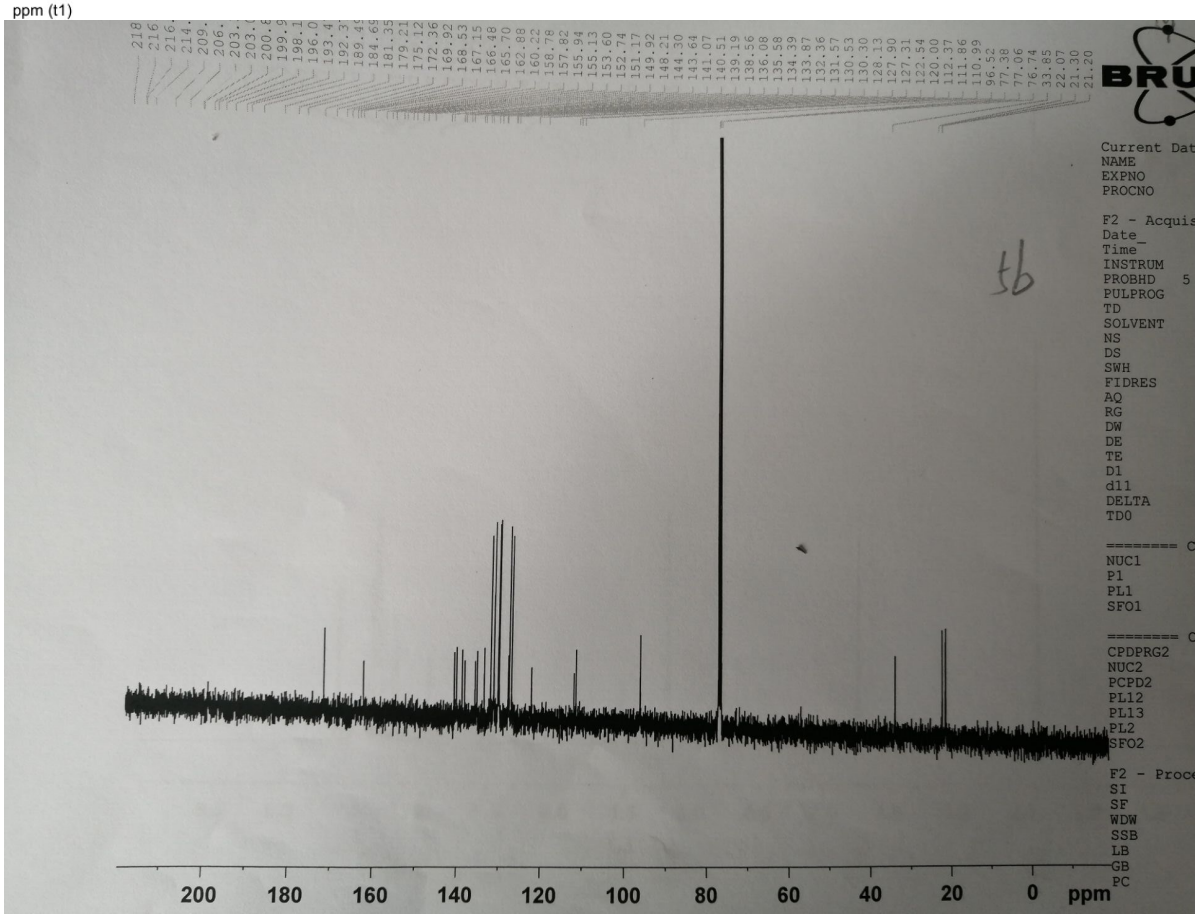
8.11
0.75
1.59
5.89
3.00
10.0
5.0
0.0
ppm (t1)


5b
Current Dat
NAME
EXPNO
PROCNO
F2 - Acquis
Date_
Time
INSTRUM
PROBHD 5
PULPROG
TD
SOLVENT
NS
DS
SWH
FIDRES
AQ
RG
DW
DE
TE
D1
d11
DELTA
TD0
NUC1
P1
PL1
SFO1
CPDPRG2
NUC2
PCPD2
PL12
PL13
PL2
SFO2
F2 - Proc
SI
SF
WDW
SSB
LB
GB
PC
200
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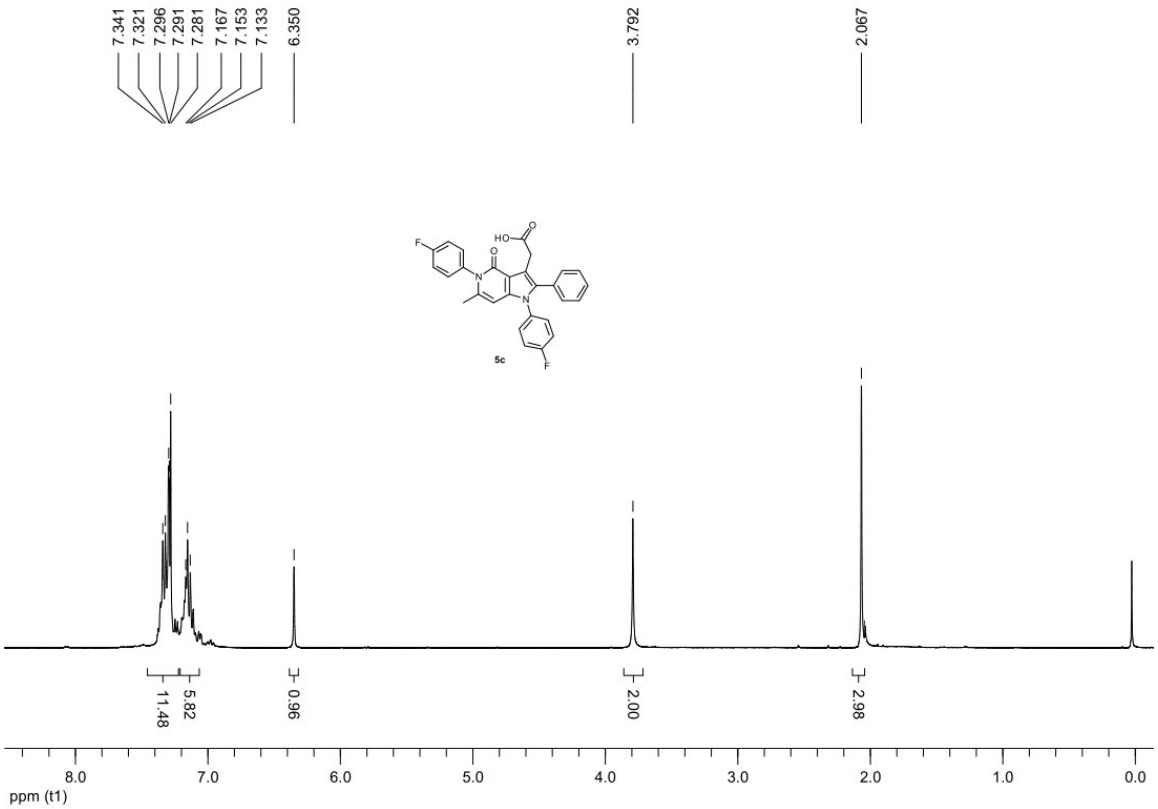
160
140
120
100
80
60
40
20
0
ppm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7.296
7.291
7.281
7.167
7.153
7.133
6.350
3.792
2.067
5c
11.48
5.82
0.96
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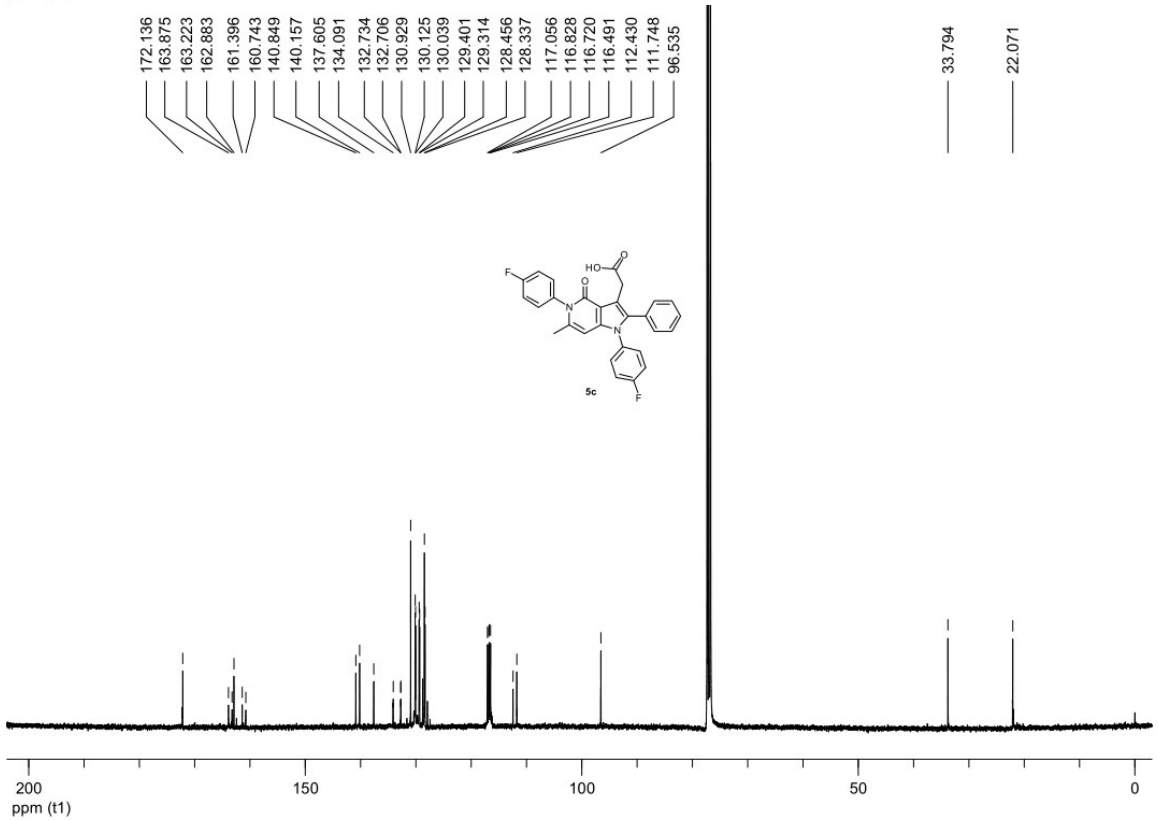
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)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140.849
140.157
137.605
134.091
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132.706
130.929
130.125
130.039
129.401
129.314
128.456
128.337
117.056
116.828
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22.071
5c
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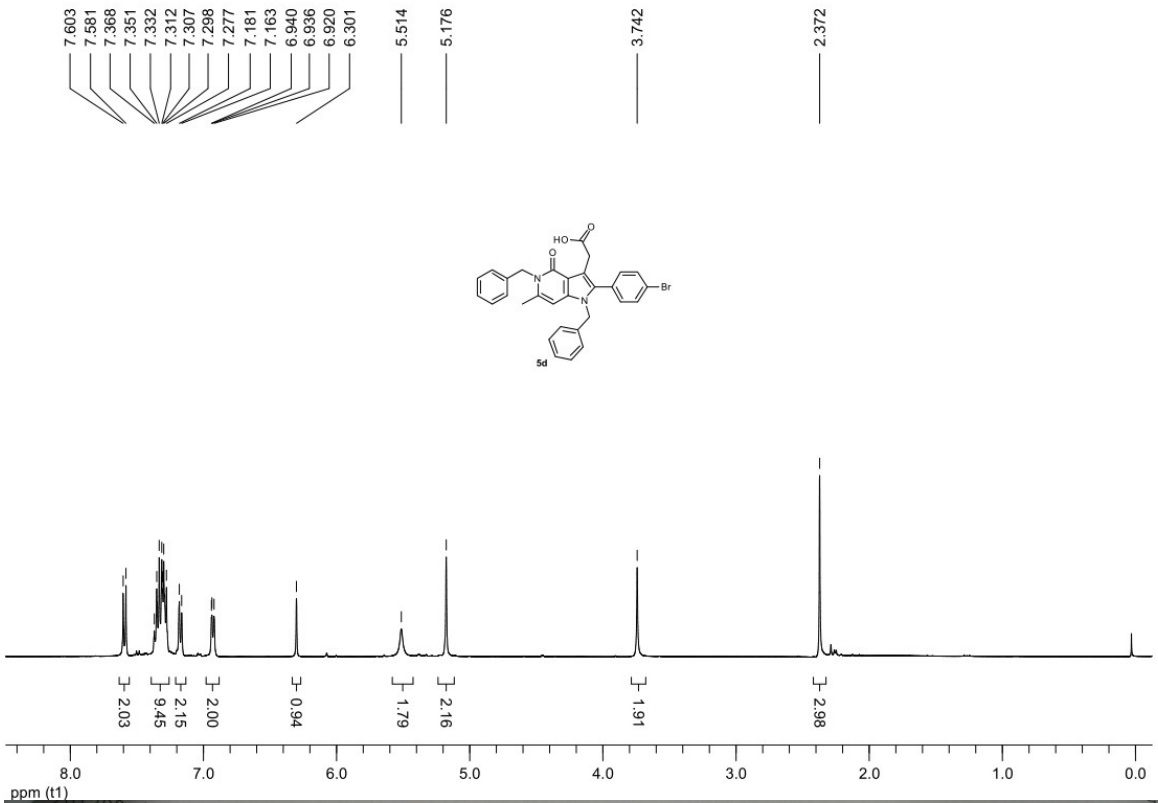
150
100
50
0
ppm (t1)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7.298
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7.163
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6.936
6.920
6.301
5.514
5.176
3.742
2.372
HO
O
O
N
Br
N
5d
2.03
9.45
2.15
2.00
0.94
1.79
2.16
1.91
2.98
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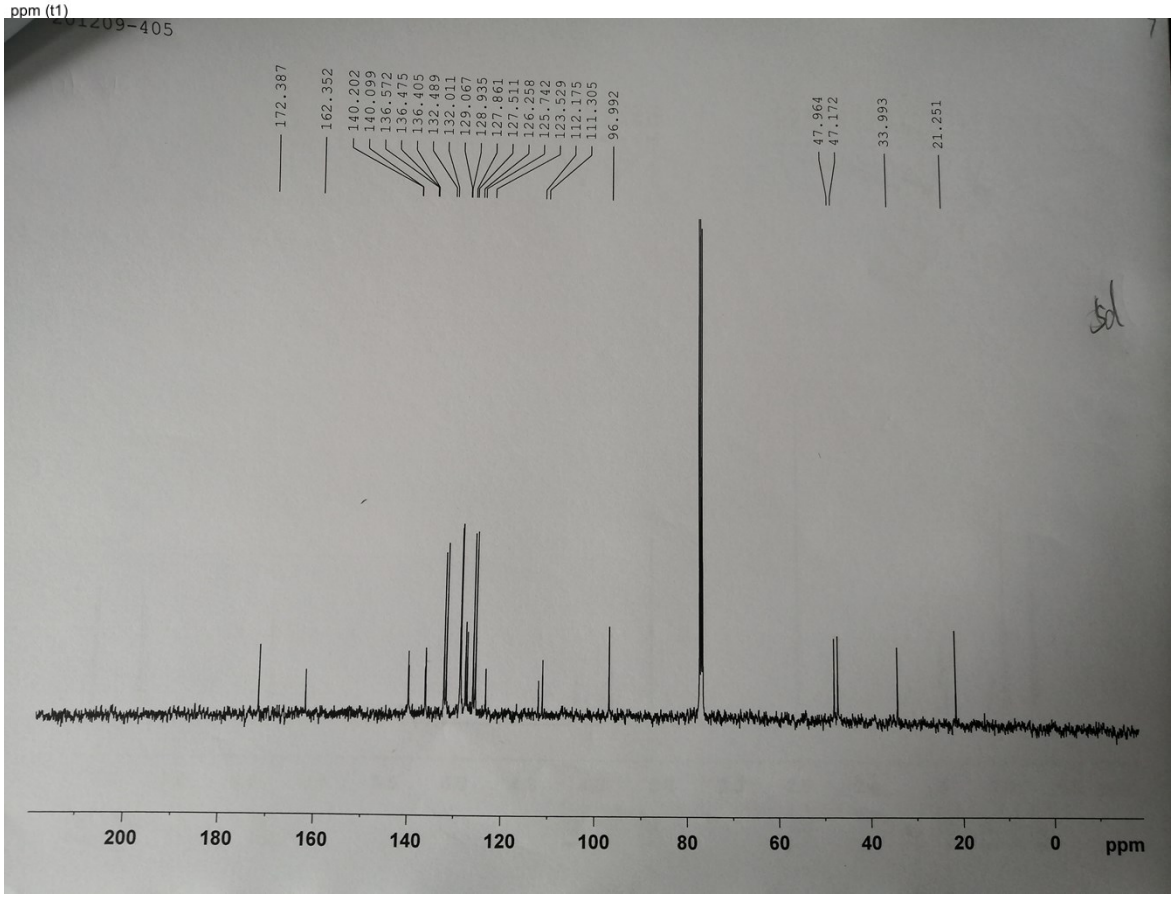
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)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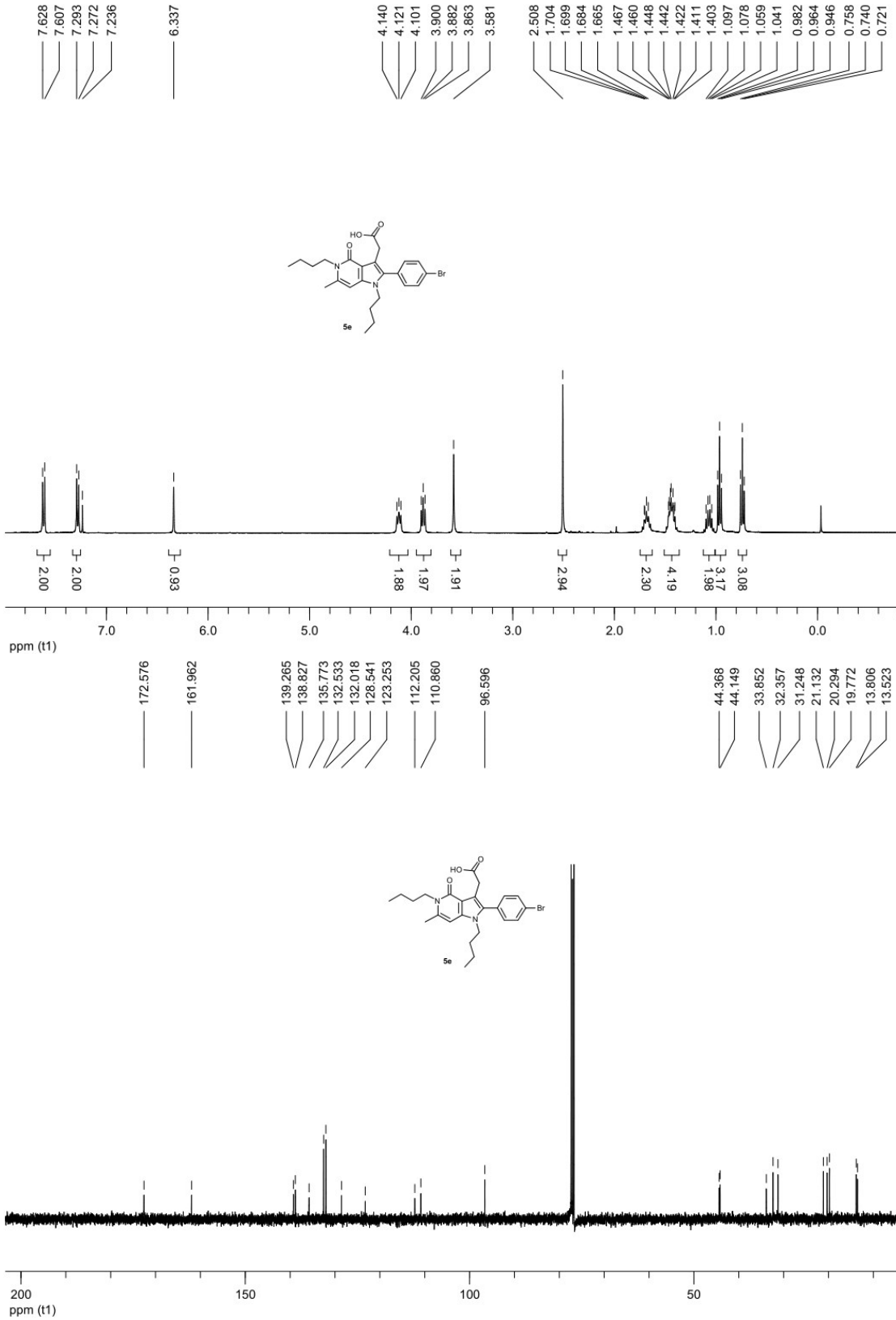
127.511
126.258
125.742
123.529
122.175
111.305
96.992
47.964
47.172
33.993
21.251
5d
200
180
160
140
120
100
80
60
40
20
0
ppm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4.101
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3.882
3.863
3.581
2.508
1.704
1.699
1.684
1.665
1.467
1.460
1.448
1.442
1.422
1.411
1.403
1.097
1.078
1.059
1.041
0.982
0.964
0.946
0.758
0.740
0.721
HO
O
N
Br
5e
2.00
2.00
0.93
1.88
1.97
1.91
2.94
2.30
4.19
1.98
3.17
3.08
7.0
6.0
5.0
4.0
3.0
2.0
1.0
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-1.0
ppm (t1)
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161.962
139.265
138.827
135.773
132.533
132.018
128.541
123.253
112.205
110.860
96.596
44.368
44.149
33.852
32.357
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21.132
20.294
19.772
13.806
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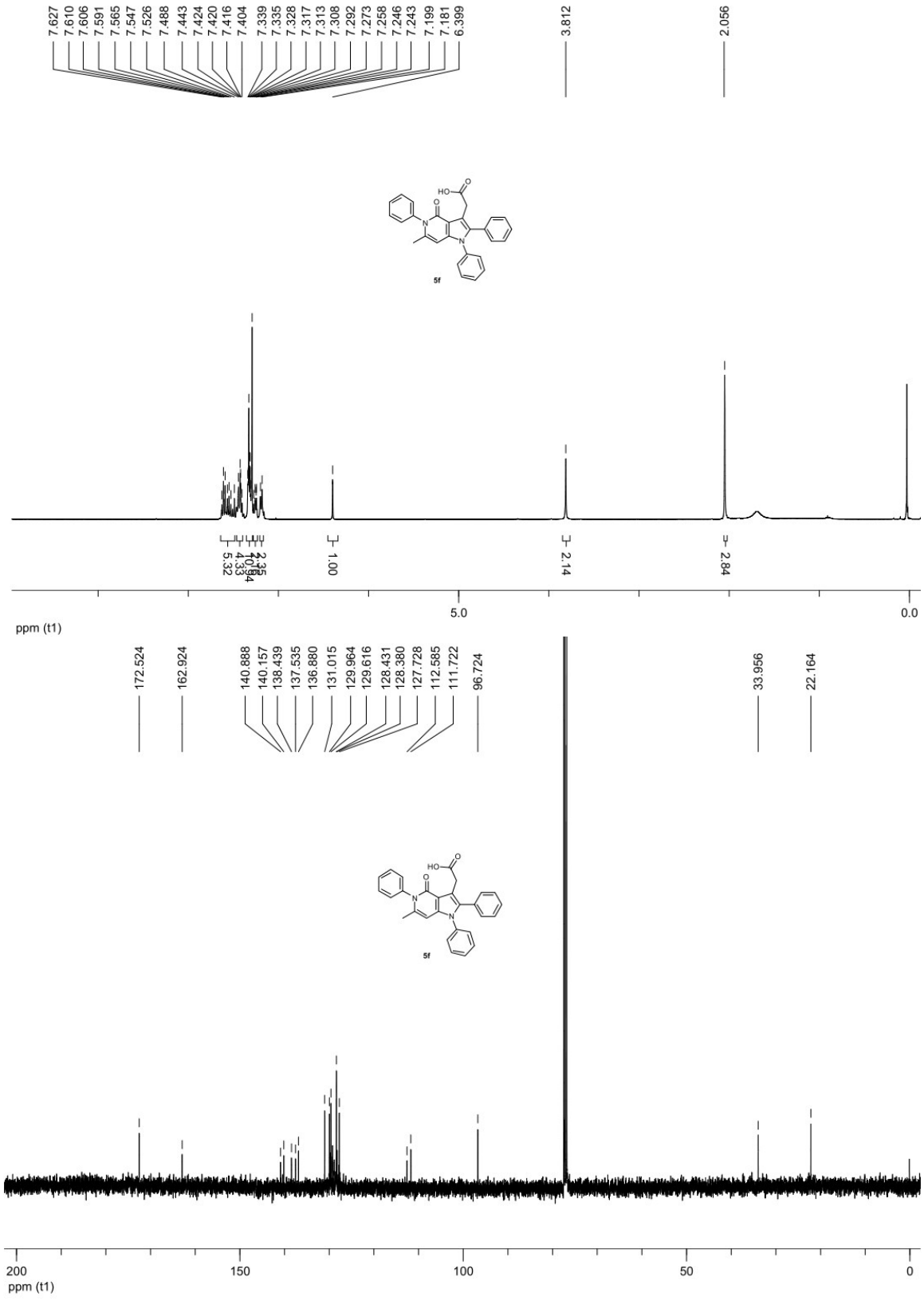
50
0
ppm (t1)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7.420
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7.404
7.339
7.335
7.328
7.317
7.313
7.308
7.292
7.273
7.258
7.246
7.243
7.199
7.181
6.399
3.812
2.056
5f
5.32
4.33
2.14
1.00
2.84
5.0
0.0
ppm (t1)
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162.924
140.888
140.157
138.439
137.535
136.880
131.015
129.964
129.616
128.431
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111.722
96.724
33.956
22.164
5f
200
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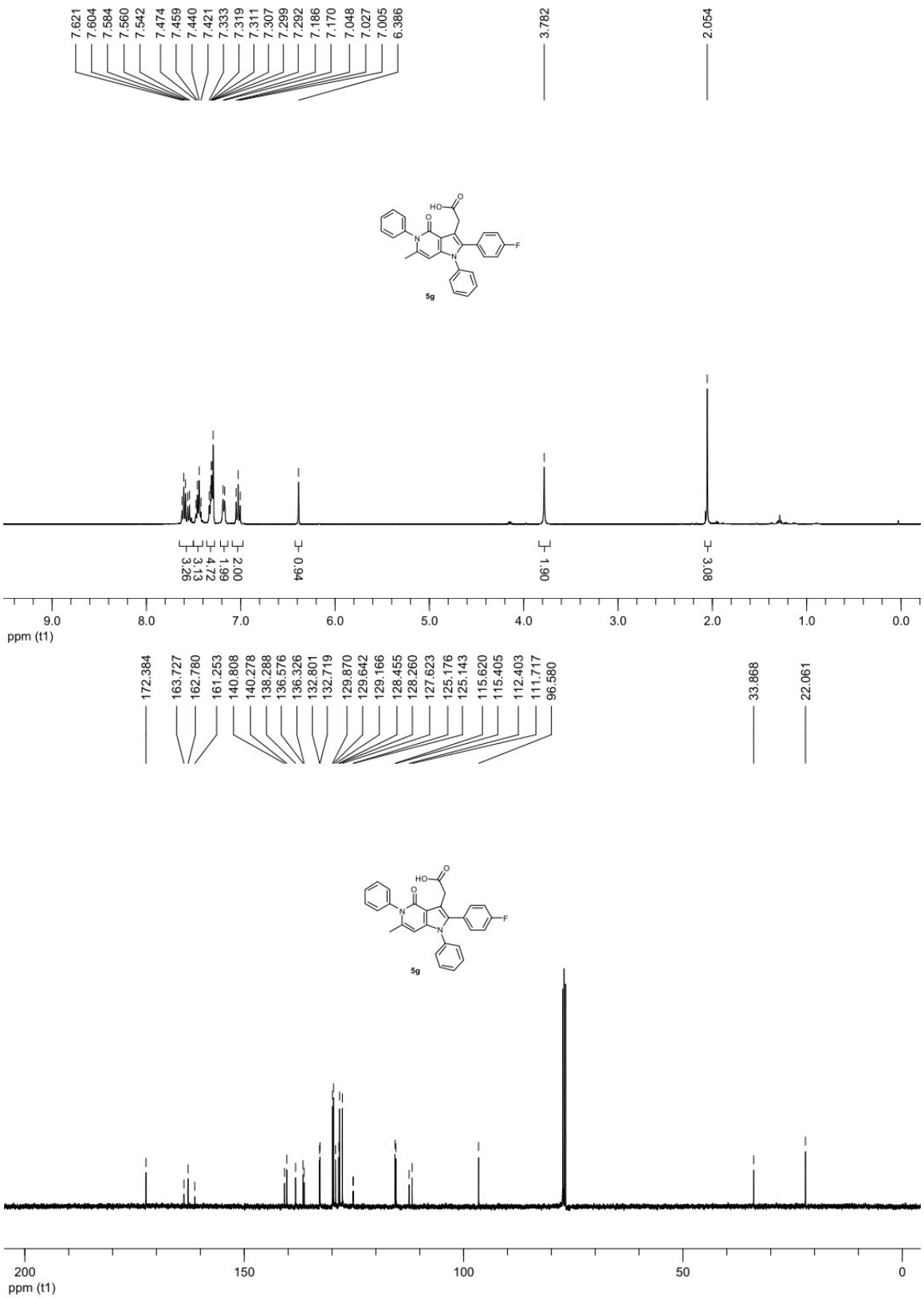
100
50
0
ppm (t1)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7.307
7.299
7.292
7.186
7.170
7.048
7.027
7.005
6.386
3.782
2.054
HO
O
N
F
5g
3.26
3.13
4.72
1.99
2.00
0.94
1.90
3.08
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)
172.384
163.727
162.780
161.253
140.808
140.278
138.288
136.576
136.326
132.801
132.719
129.870
129.642
129.166
128.455
128.260
127.623
125.176
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100
50
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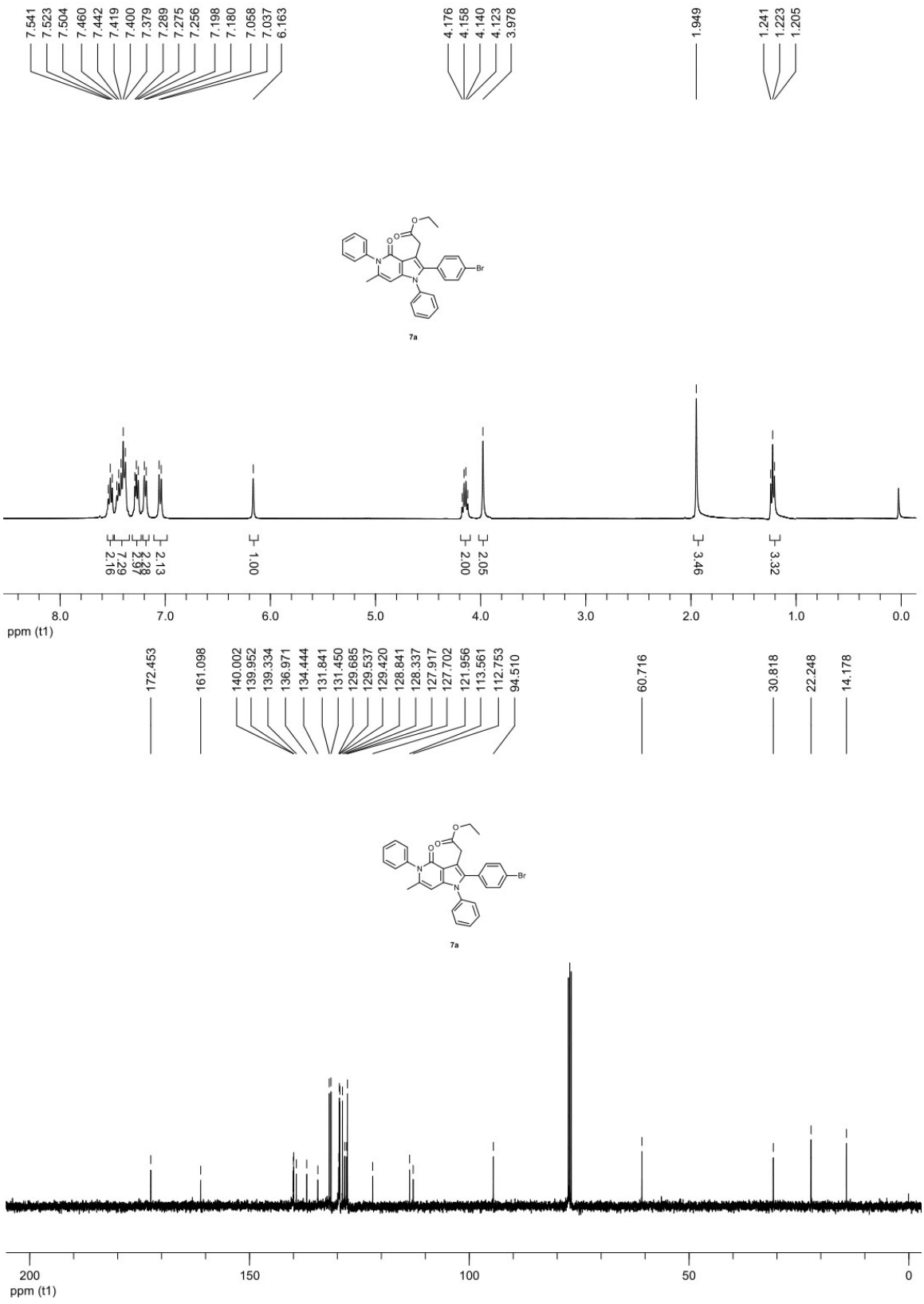
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7.037
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4.176
4.158
4.140
4.123
3.978
1.949
1.241
1.223
1.205
7a
2.16
7.29
2.28
2.13
1.00
2.00
2.05
3.46
3.32
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)
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140.002
139.952
139.334
136.971
134.444
131.841
131.450
129.685
129.537
129.420
128.841
128.337
127.917
127.702
121.956
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60.716
30.818
22.248
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100
50
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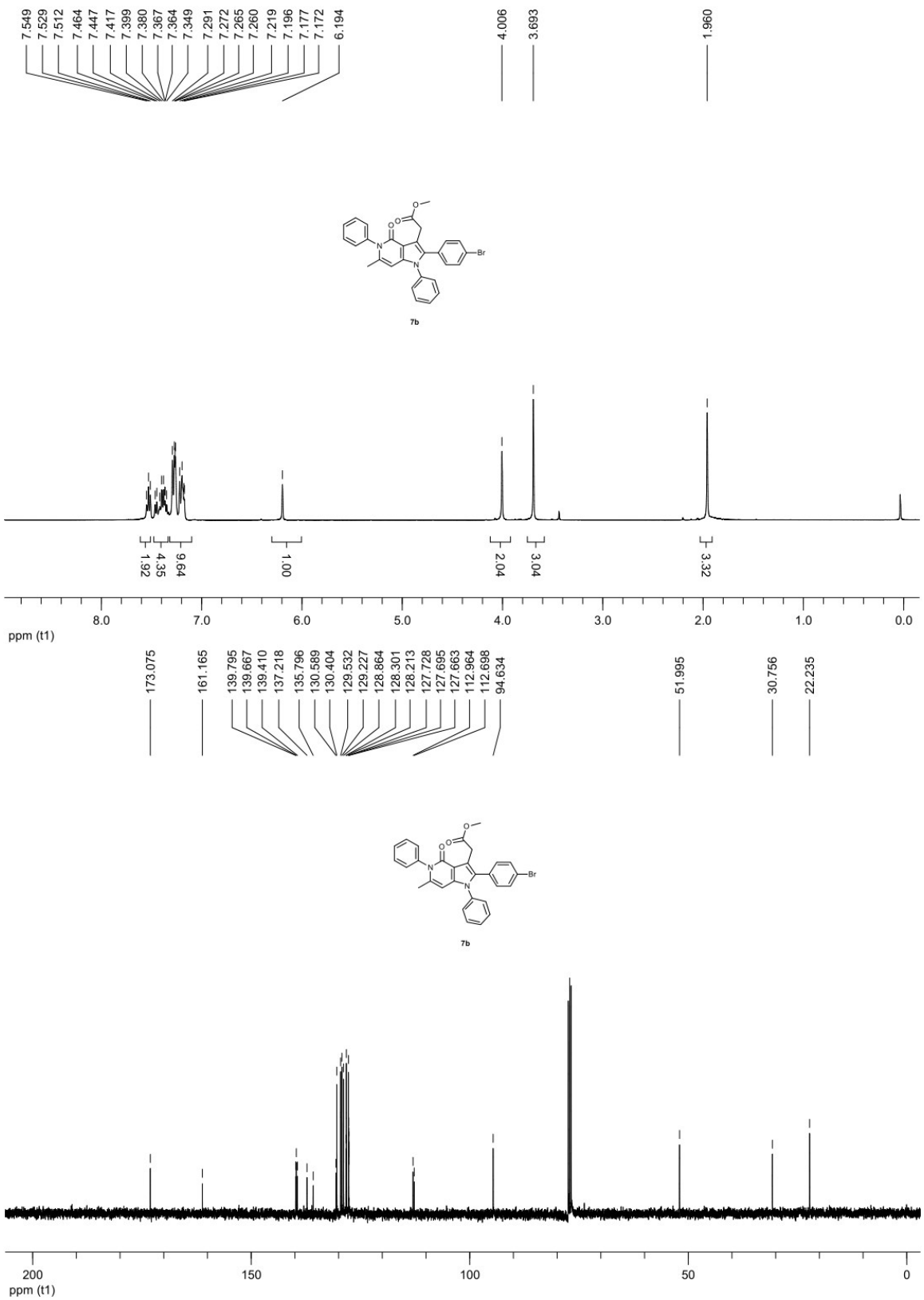
ppm (t1)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7.265
7.260
7.219
7.196
7.177
7.172
6.194
4.006
3.693
1.960
7b
1.92
3.54
9.64
1.00
2.04
3.04
3.32
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)
173.075
161.165
139.795
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139.410
137.218
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130.589
130.404
129.532
129.227
128.864
128.301
128.213
127.728
127.695
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30.756
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7b
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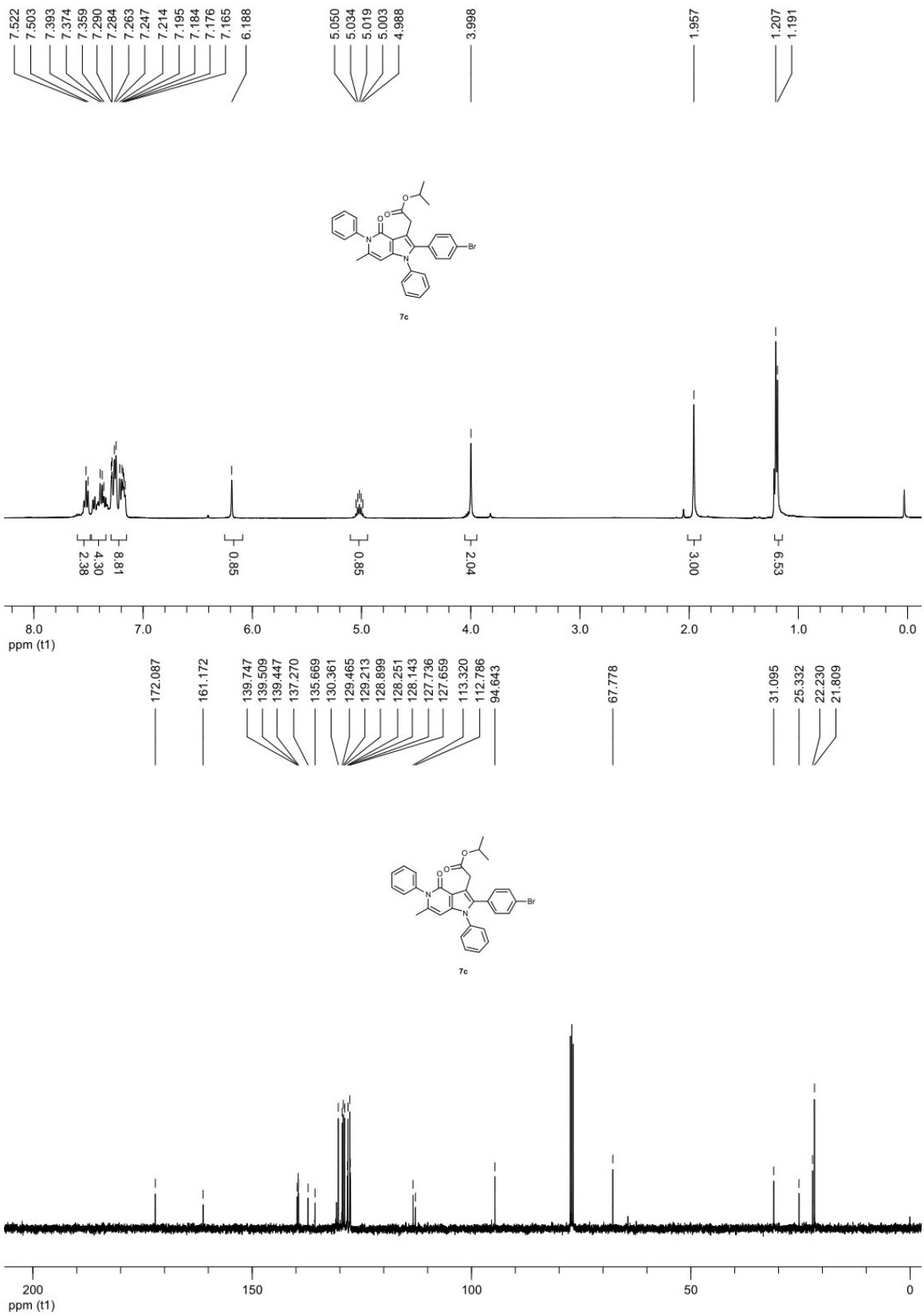
100
50
0
ppm (t1)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7.176
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6.188
5.050
5.034
5.019
5.003
4.988
3.998
1.957
1.207
1.191
7c
2.38
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0.85
0.85
2.04
3.00
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8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)
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139.447
137.270
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129.213
128.899
128.251
128.143
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127.659
113.320
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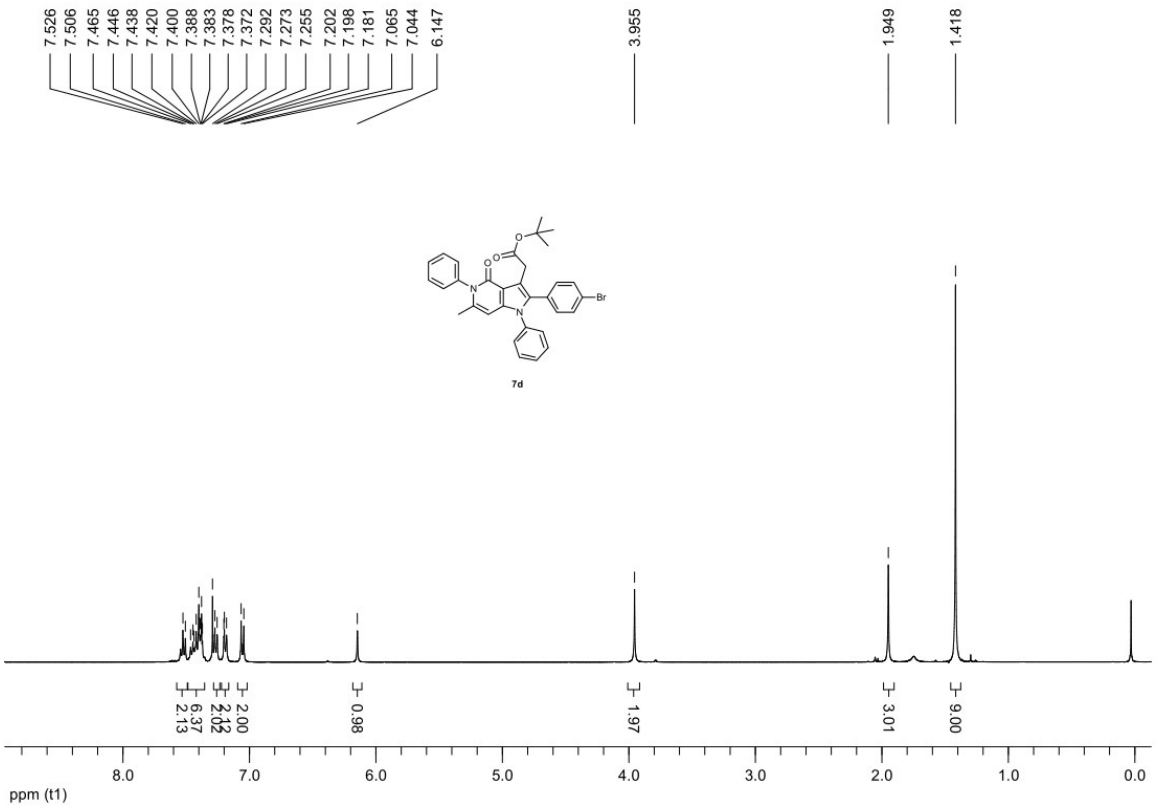
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7.255
7.202
7.198
7.181
7.065
7.044
6.147
3.955
1.949
1.418
7d
2.13
6.37
2.12
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1.97
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5.0
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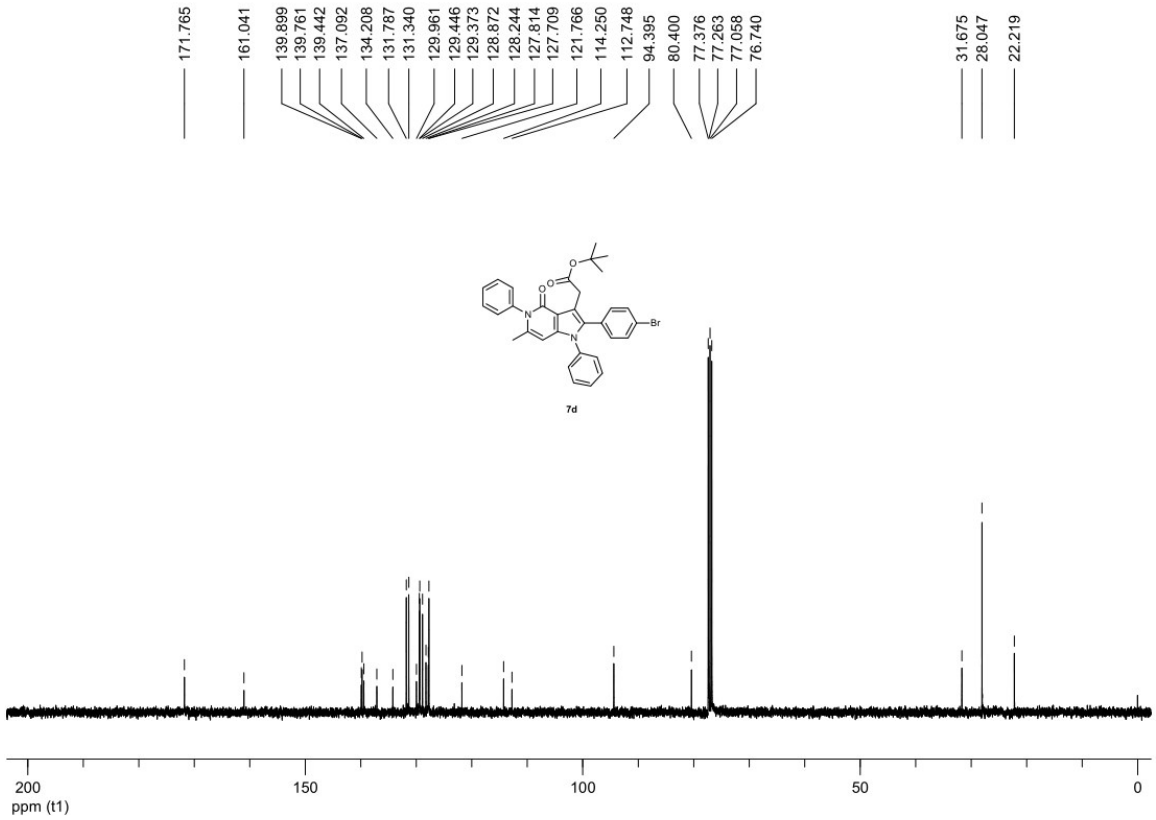
ppm (t1)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128.872
128.244
127.814
127.709
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114.250
112.748
94.395
80.400
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76.740
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7d
200
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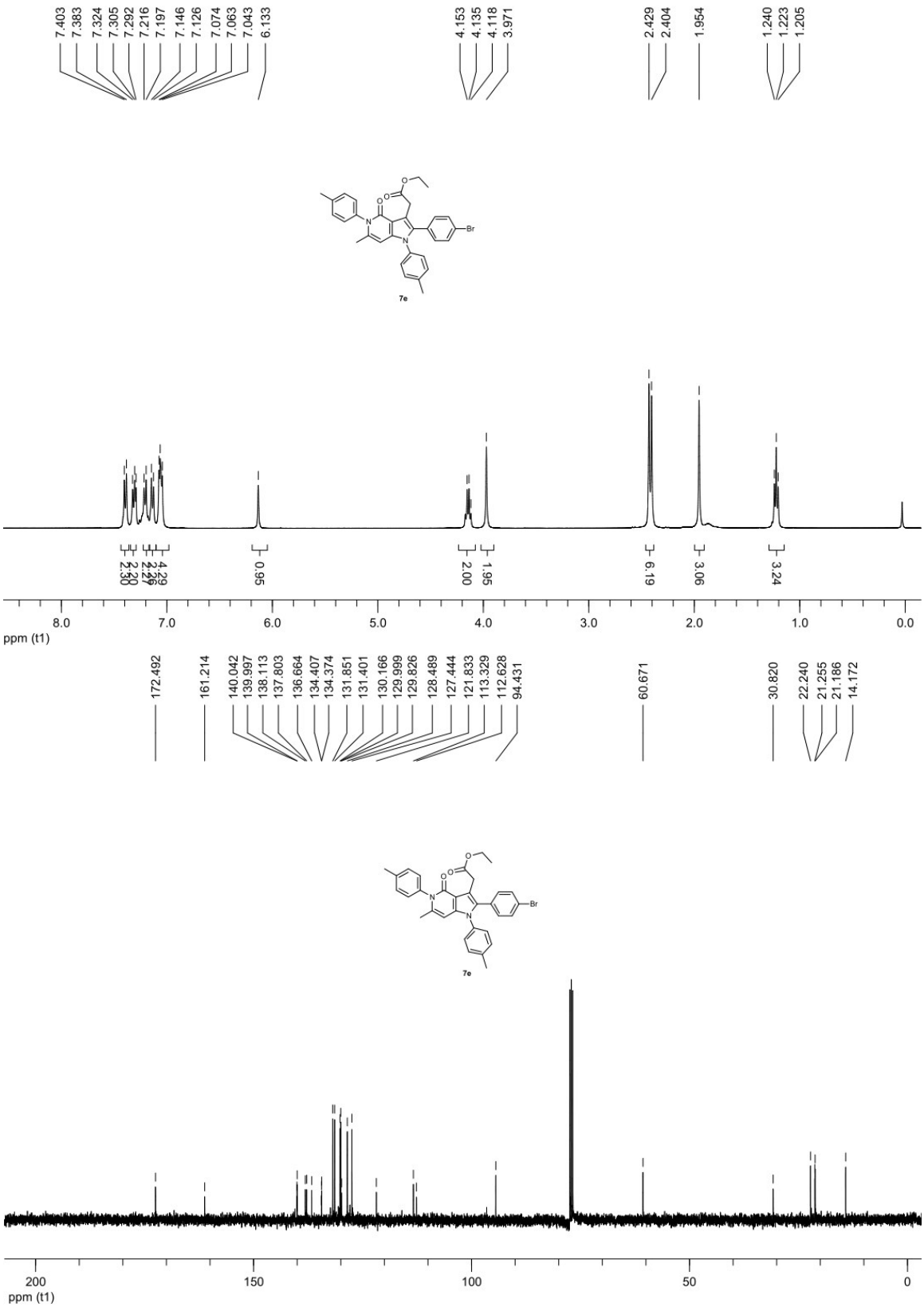
ppm (t1)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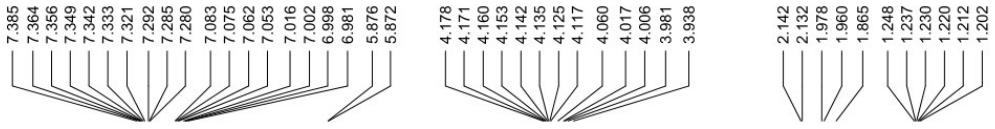
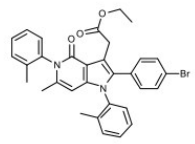
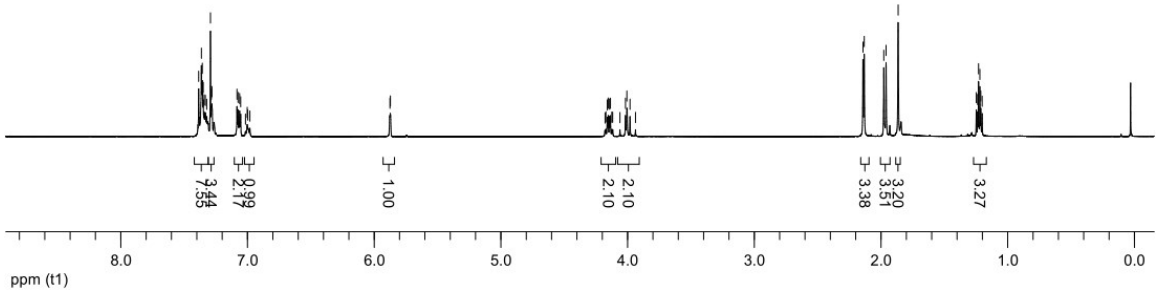
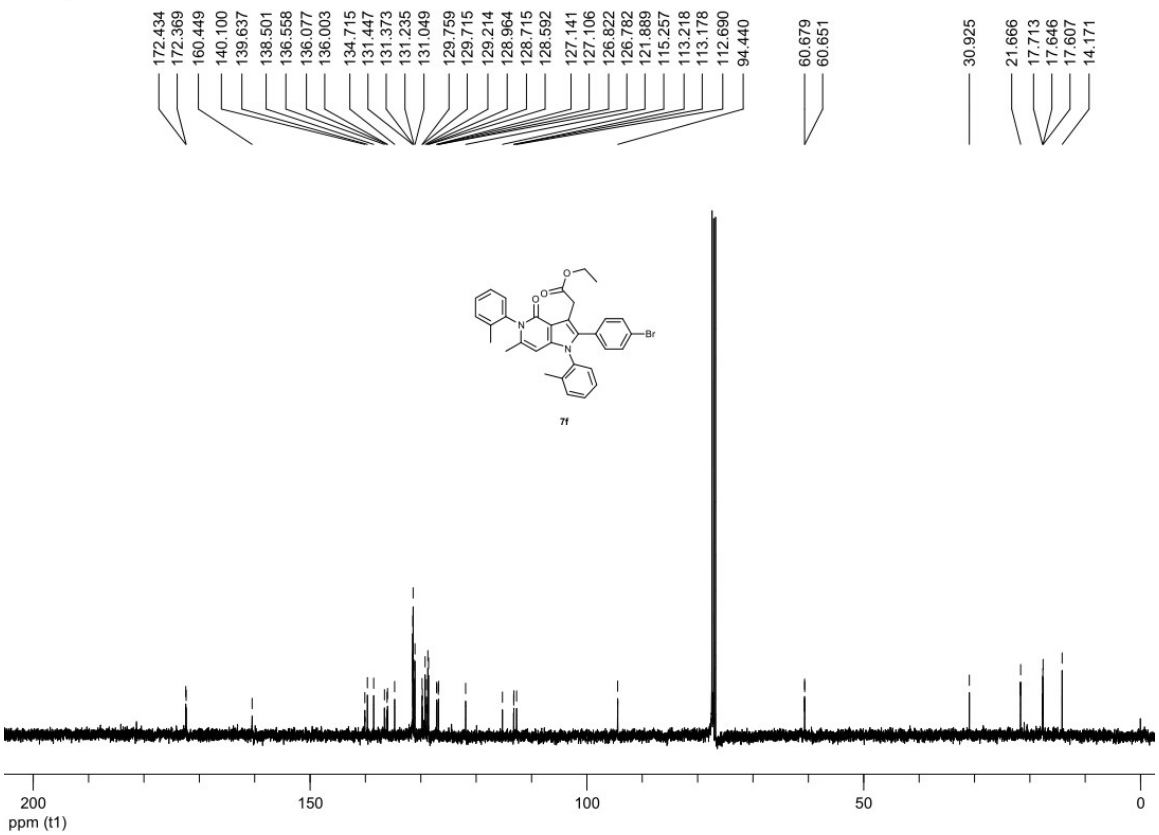
6.133
4.153
4.135
4.118
3.971
2.429
2.404
1.954
1.240
1.223
1.205
Br
7e
2.30
2.27
2.26
4.29
0.95
2.00
1.95
6.19
3.06
3.24
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)
172.492
161.214
140.042
139.997
138.113
137.803
136.664
134.407
134.374
131.851
131.401
130.166
129.999
129.826
128.489
127.444
121.833
113.329
112.628
94.431
60.671
30.820
22.240
21.255
21.186
14.172
Br
7e
200
150
100
50
0
ppm (t1)


7.385
7.364
7.356
7.349
7.342
7.333
7.321
7.292
7.285
7.280
7.083
7.075
7.062
7.053
7.016
7.002
6.998
6.981
5.876
5.872
4.178
4.171
4.160
4.153
4.142
4.135
4.125
4.117
4.060
4.017
4.006
3.981
3.938
2.142
2.132
1.978
1.960
1.865
1.248
1.237
1.230
1.220
1.212
1.202

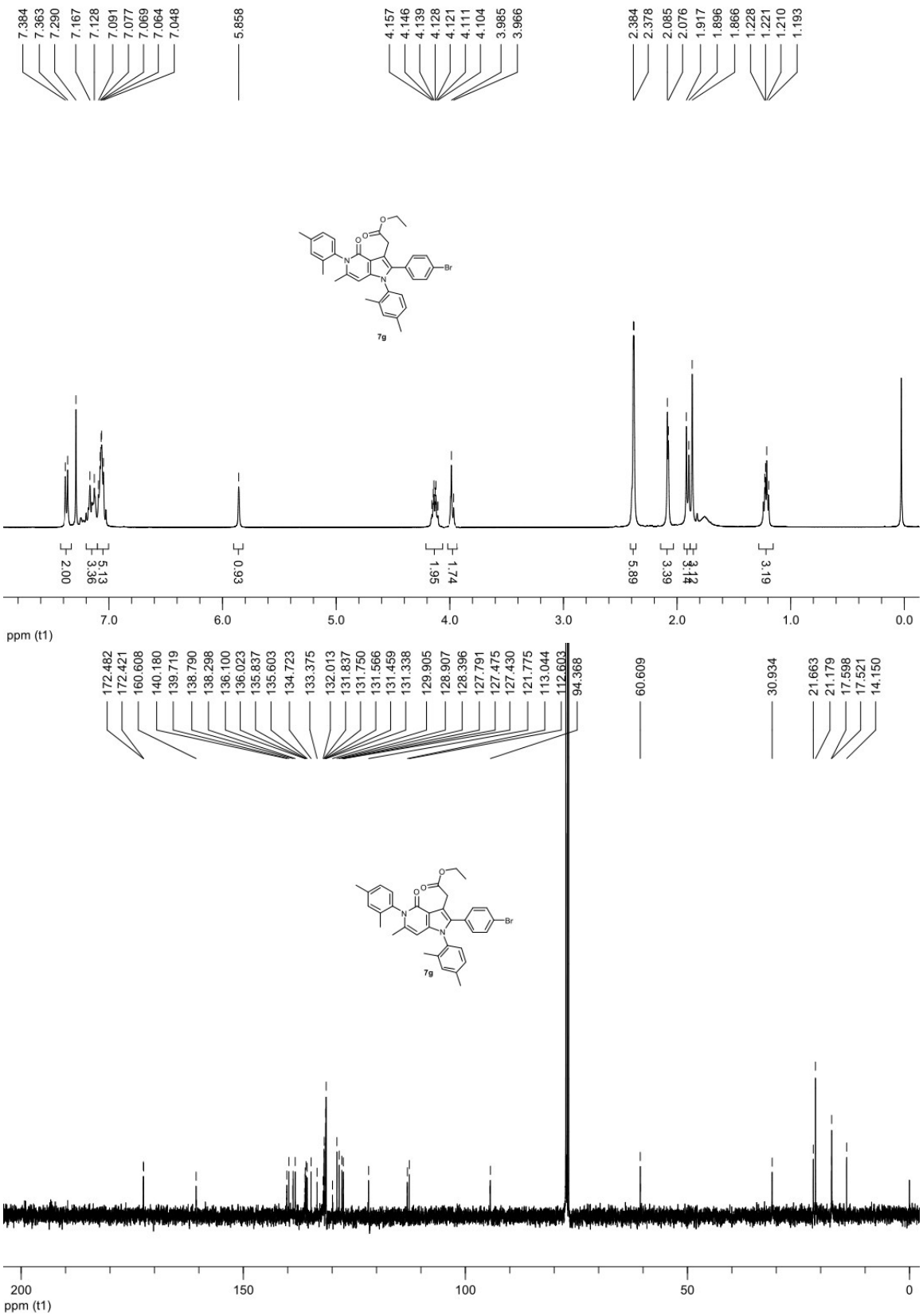

O
O
O
N
N
Br

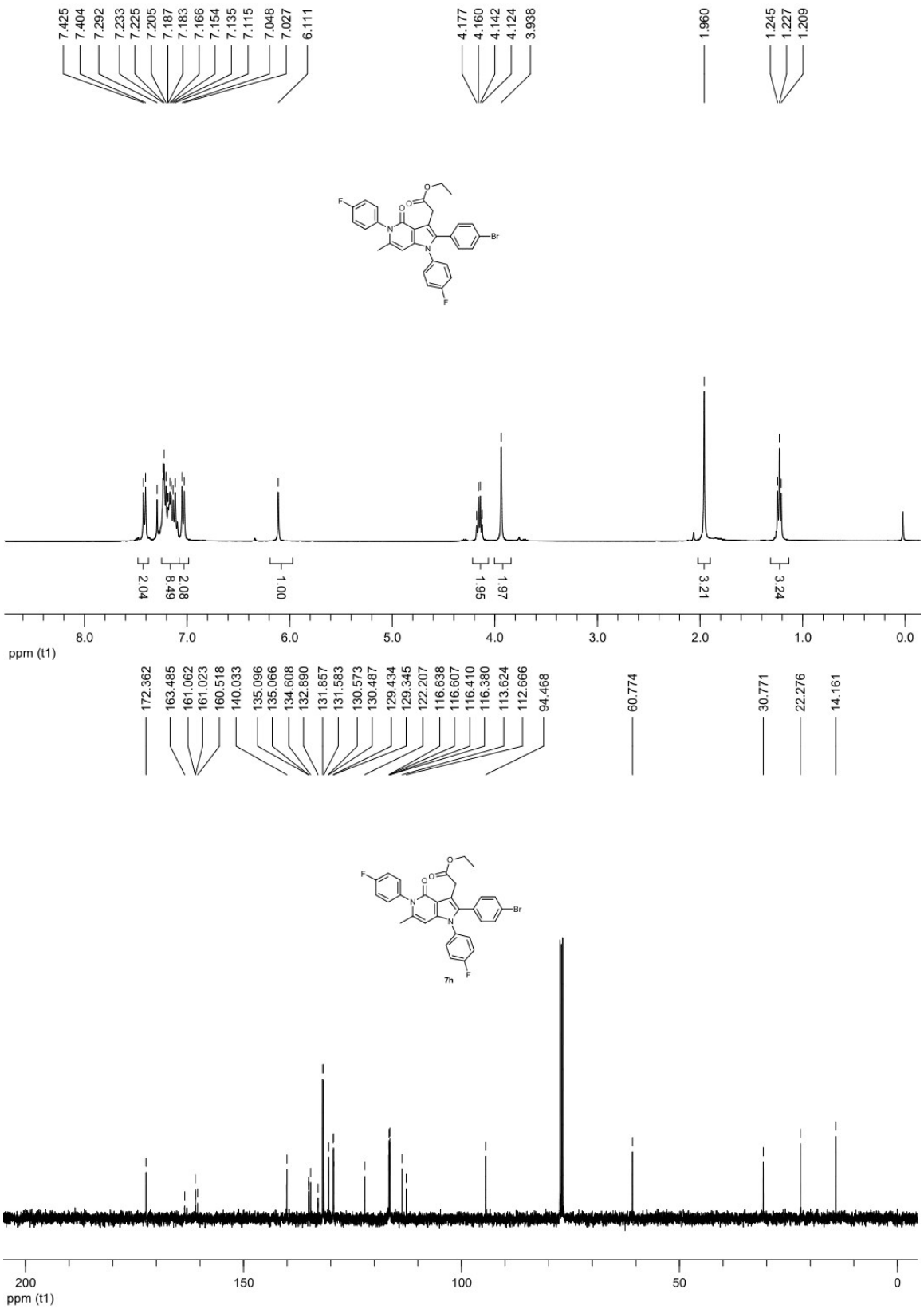
7f

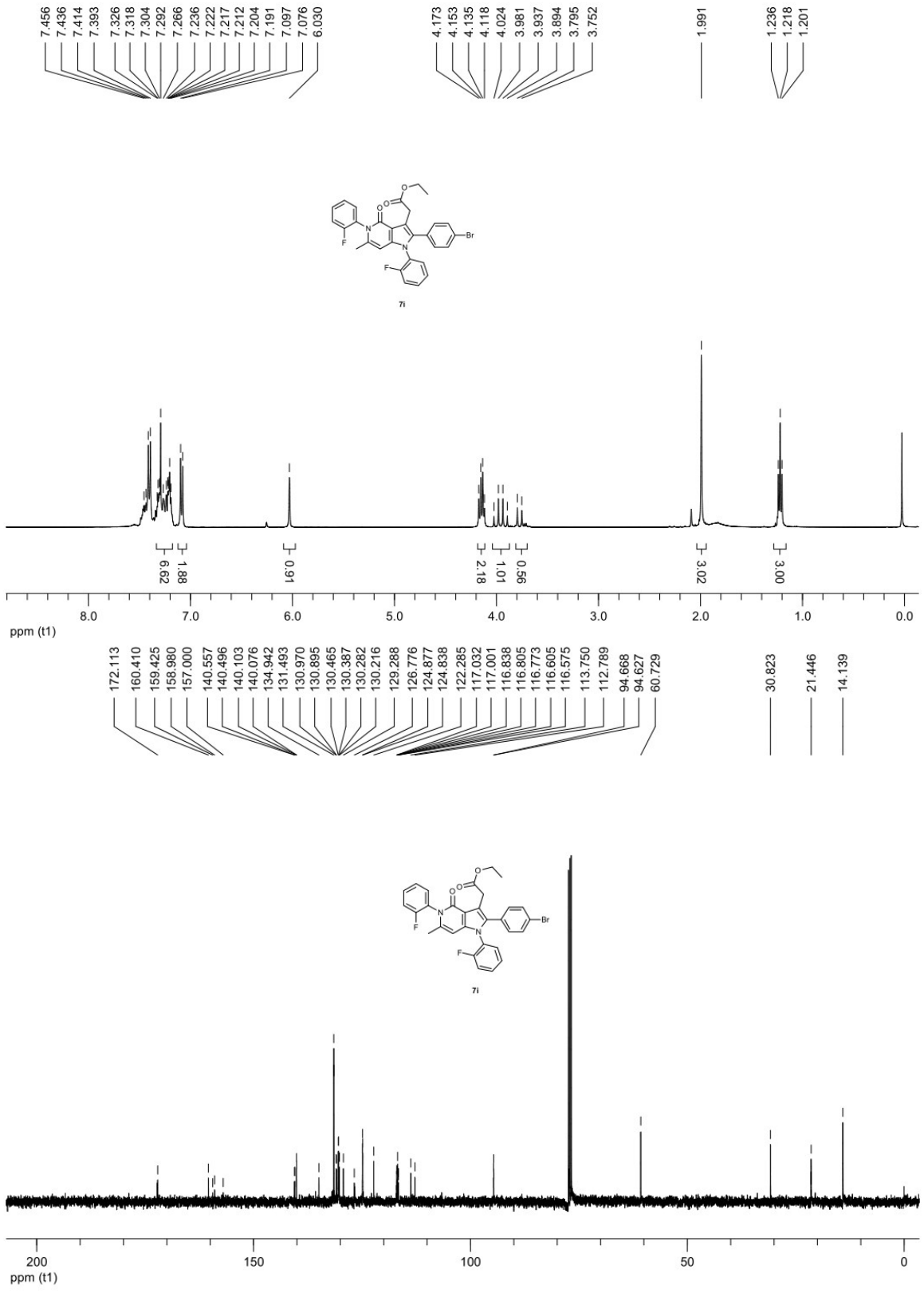

7.44
7.55
2.17
0.99
1.00
2.10
2.10
3.38
3.51
3.20
3.27
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)

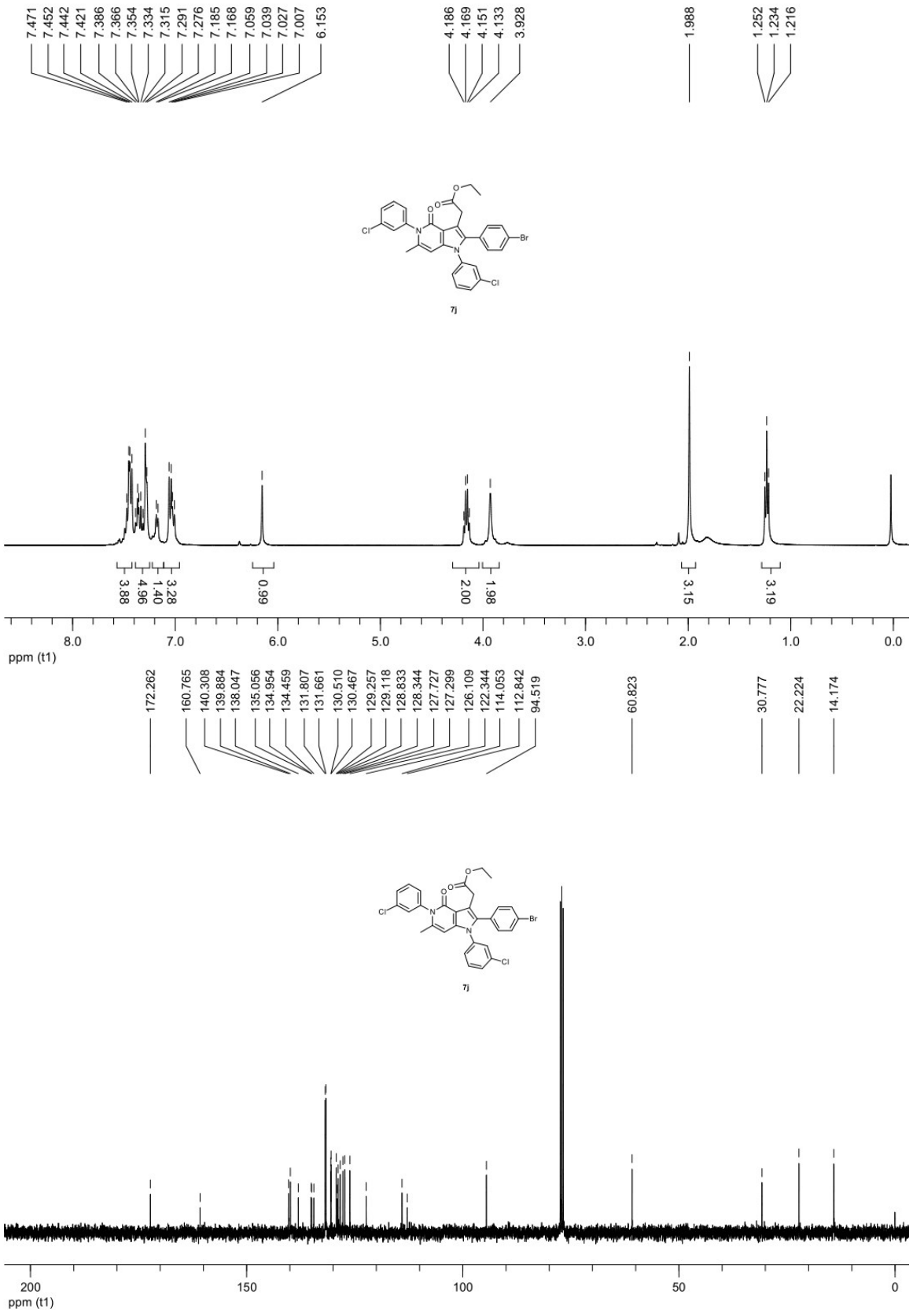

172.434
172.369
160.449
140.100
139.637
138.501
136.558
136.077
136.003
134.715
131.447
131.373
131.235
131.049
129.759
129.715
129.214
128.964
128.715
128.592
127.141
127.106
126.822
126.782
121.889
115.257
113.218
113.178
112.690
94.440
60.679
60.651
30.925
21.666
17.713
17.646
17.607
14.171
O
O
O
N
N
Br
200
150
100
50
0
ppm (t1)

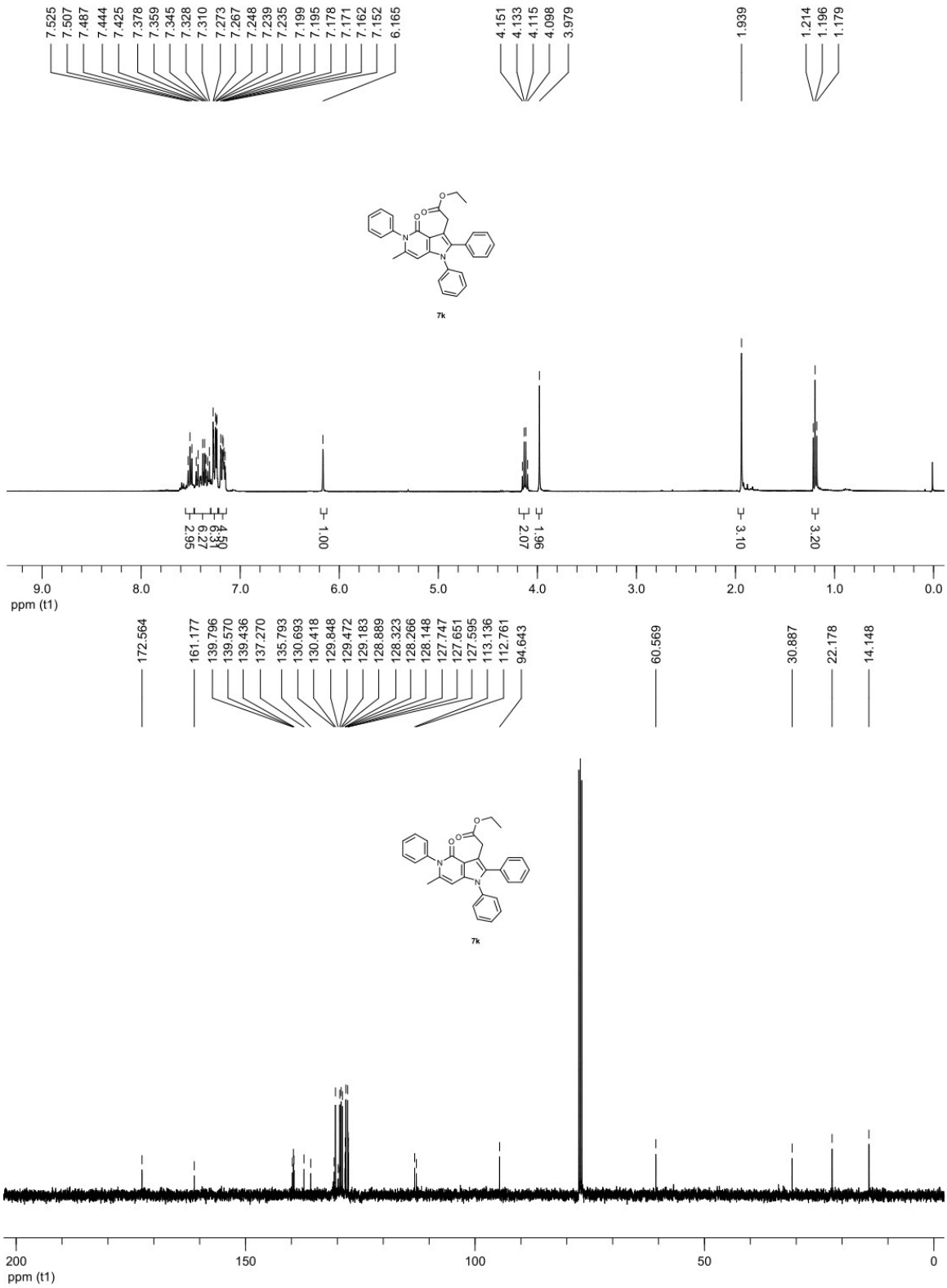
7f

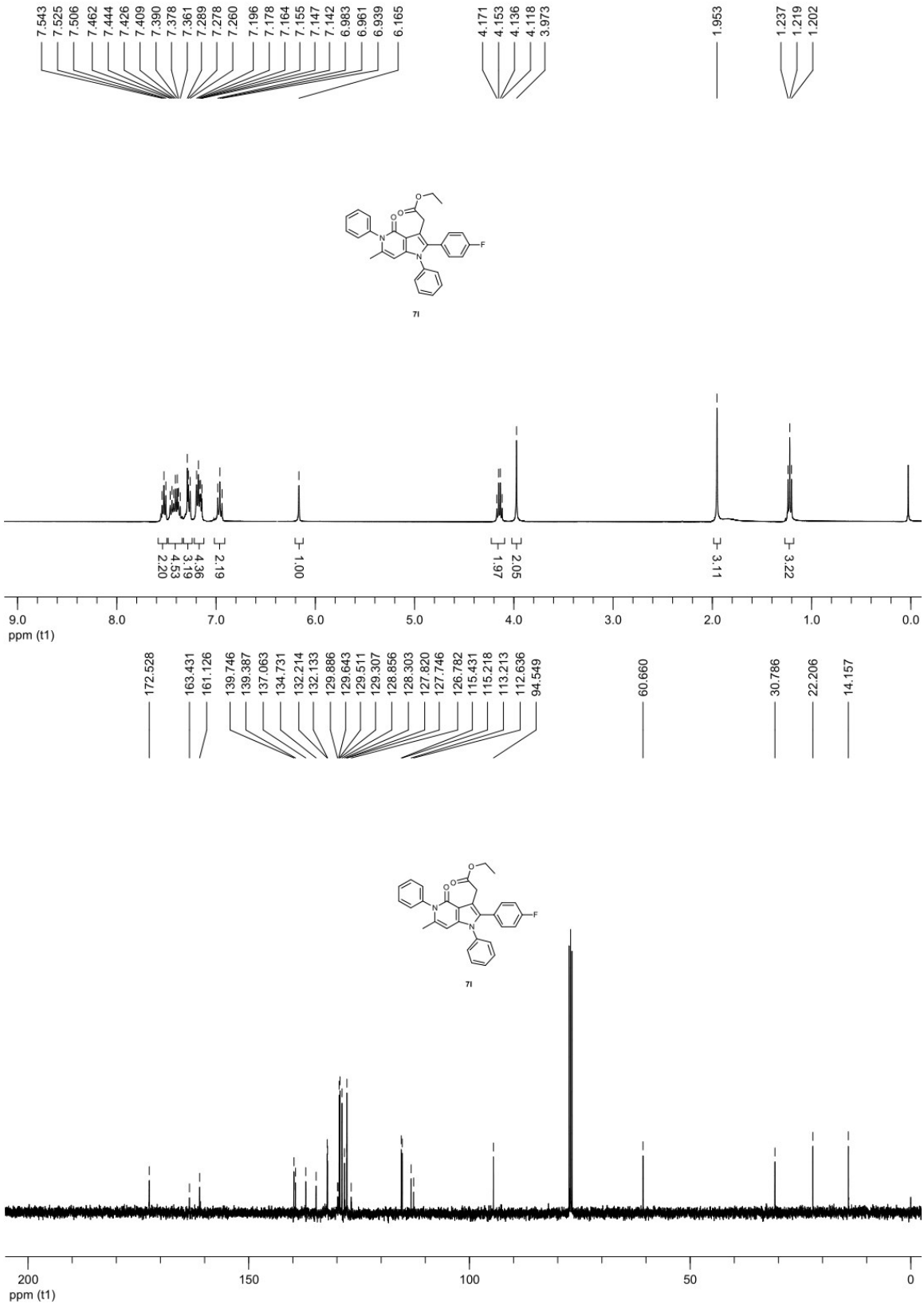

7.384
7.363
7.290
7.167
7.128
7.091
7.077
7.069
7.064
7.048
5.858
4.157
4.146
4.139
4.128
4.121
4.111
4.104
3.985
3.966
2.384
2.378
2.085
2.076
1.917
1.896
1.866
1.228
1.221
1.210
1.193
7g
2.00
5.13
3.36
0.93
1.95
1.74
5.89
3.39
3.12
3.14
3.19
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)
172.482
172.421
160.608
140.180
139.719
138.790
138.298
136.100
136.023
135.837
135.603
134.723
133.375
132.013
131.837
131.750
131.566
131.459
131.338
129.905
128.907
128.396
127.791
127.475
127.430
121.775
113.044
112.603
94.368
60.609
30.934
21.663
21.179
17.598
17.521
14.150
7g
200
150
100
50
0
ppm (t1)

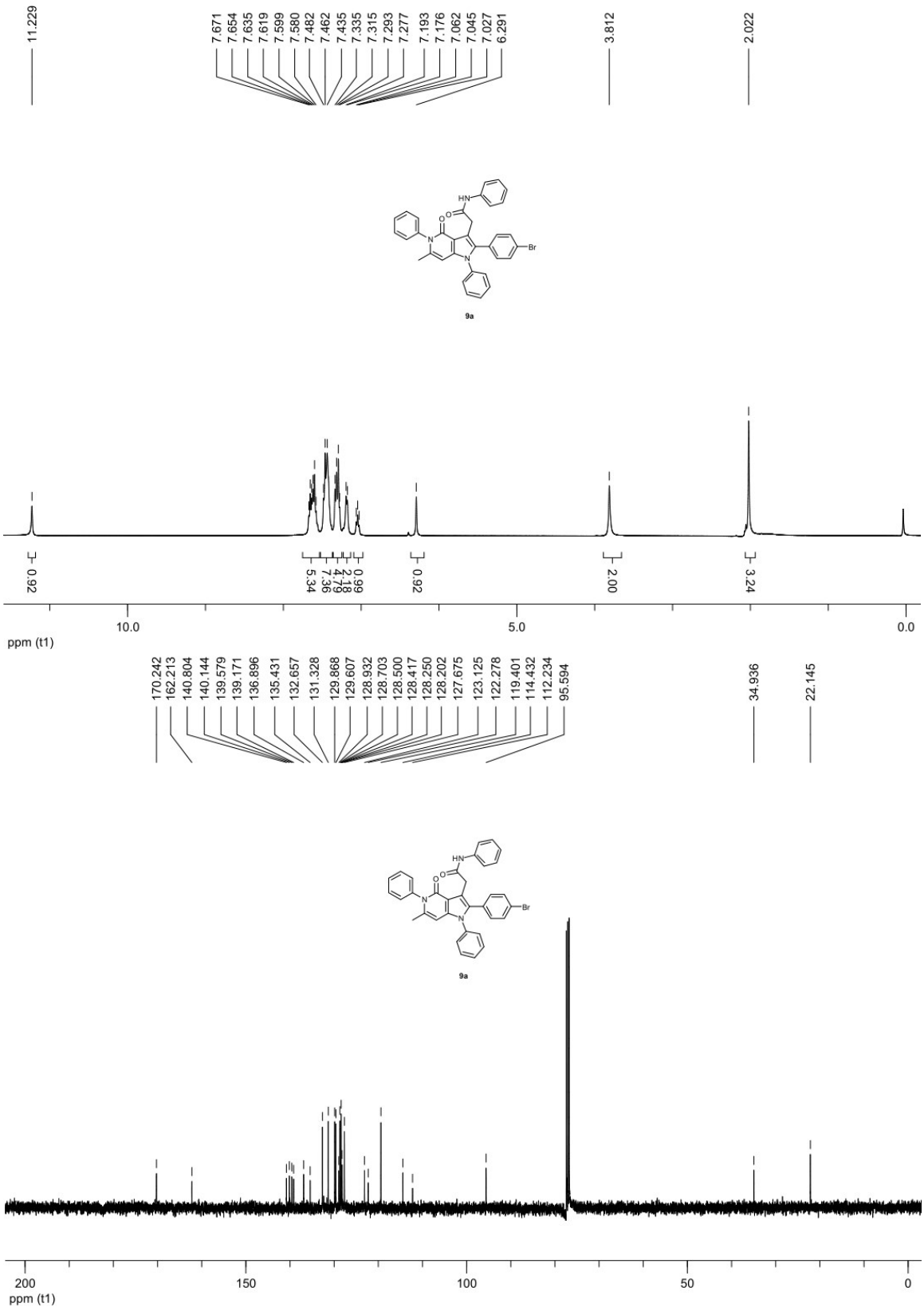

7.425
7.404
7.292
7.233
7.225
7.205
7.187
7.183
7.166
7.154
7.135
7.115
7.048
7.027
6.111
4.177
4.160
4.142
4.124
3.938
1.960
1.245
1.227
1.209
F
O
O
N
Br
N
F
2.04
8.49
2.08
1.00
1.95
1.97
3.21
3.24
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)
172.362
163.485
161.062
161.023
160.518
140.033
135.096
135.066
134.608
132.890
131.857
131.583
130.573
130.487
129.434
129.345
122.207
116.638
116.607
116.410
116.380
113.624
112.666
94.468
60.774
30.771
22.276
14.161
7h
200
150
100
50
0
ppm (t1)

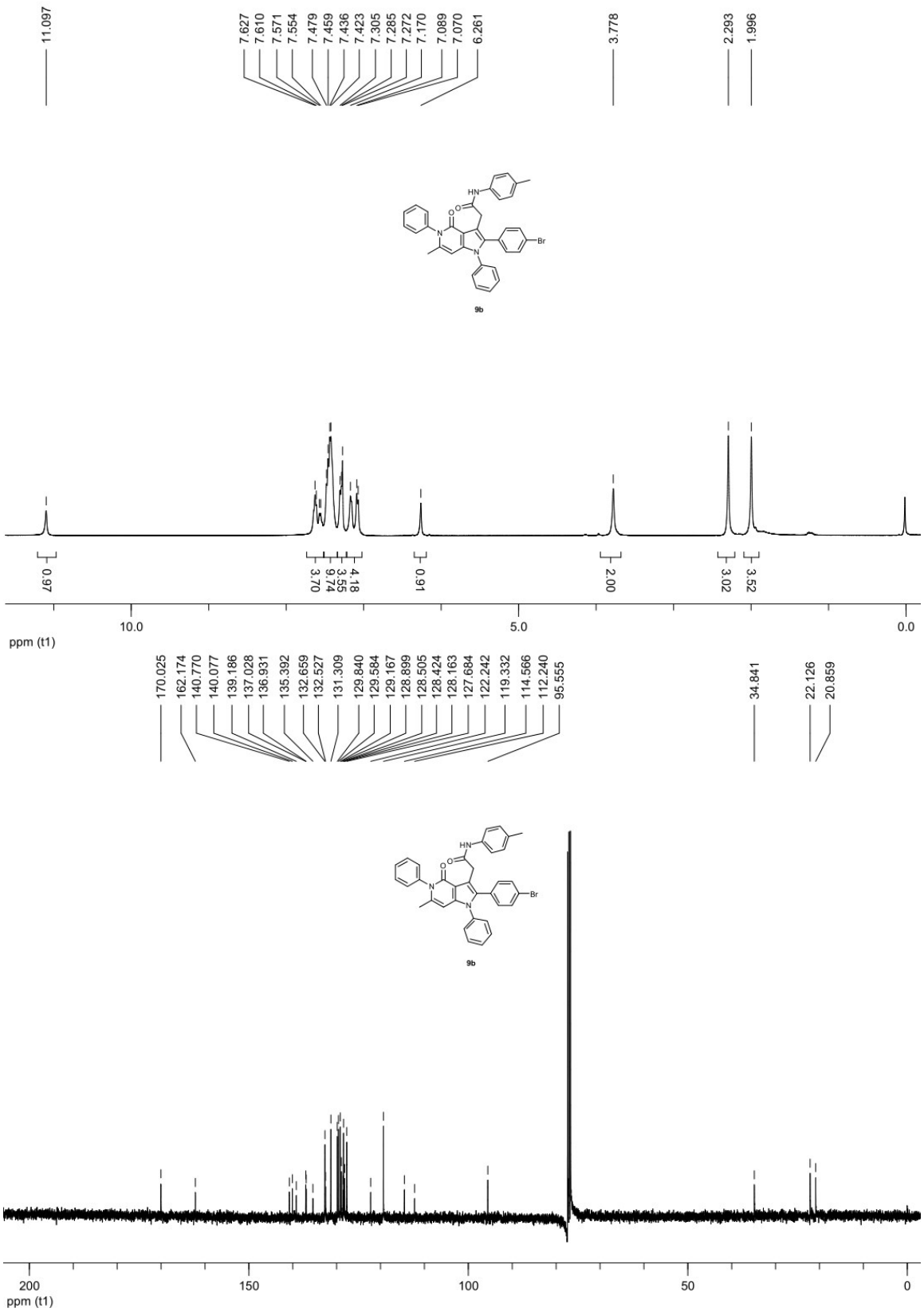

7.456
7.436
7.414
7.393
7.326
7.318
7.304
7.292
7.266
7.236
7.222
7.217
7.212
7.204
7.191
7.097
7.076
6.030
4.173
4.153
4.135
4.118
4.024
3.981
3.937
3.894
3.795
3.752
1.991
1.236
1.218
1.201
7i
6.62
1.88
0.91
2.18
1.01
0.56
3.02
3.00
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)
172.113
160.410
159.425
158.980
157.000
140.557
140.496
140.103
140.076
134.942
131.493
130.970
130.895
130.465
130.387
130.282
130.216
129.288
126.776
124.877
124.838
122.285
117.032
117.001
116.838
116.805
116.773
116.605
116.575
113.750
112.789
94.668
94.627
60.729
30.823
21.446
14.139
7i
200
150
100
50
0
ppm (t1)

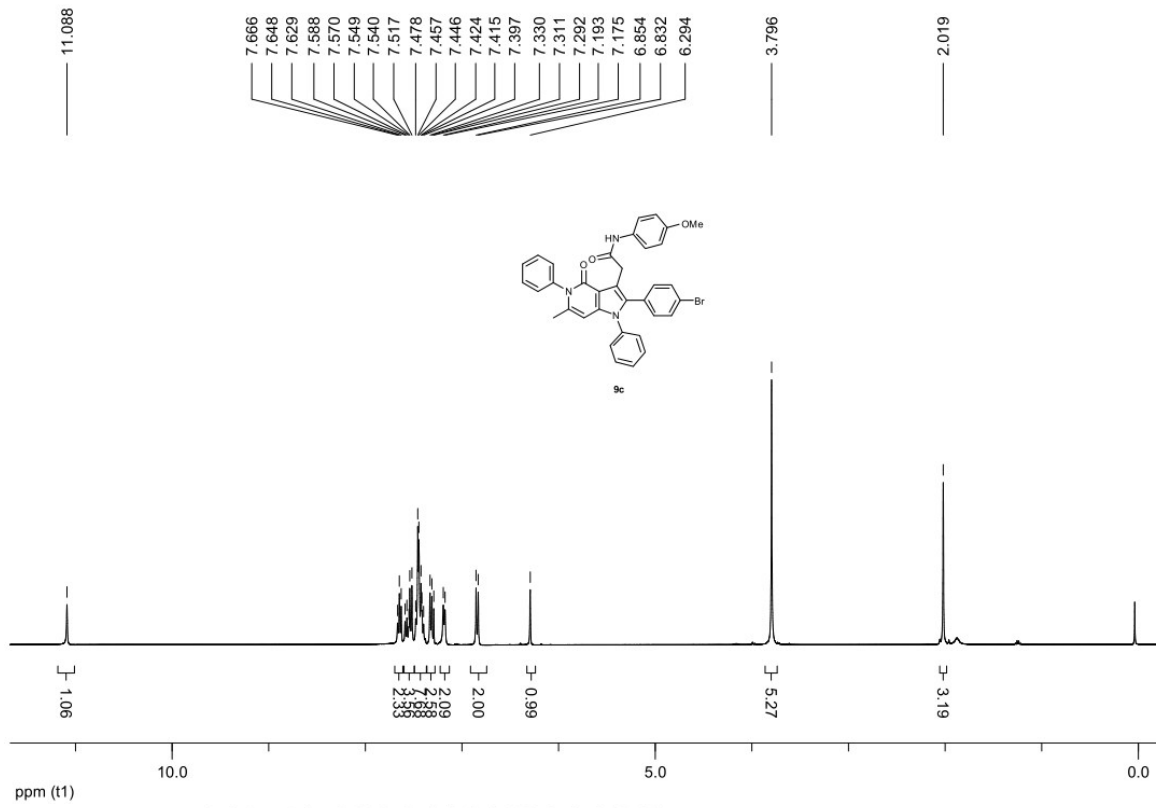

7.471
7.452
7.442
7.421
7.386
7.366
7.354
7.334
7.315
7.291
7.276
7.185
7.168
7.059
7.039
7.027
7.007
6.153
4.186
4.169
4.151
4.133
3.928
1.988
1.252
1.234
1.216
7j
3.88
4.96
1.40
3.82
6.99
2.00
1.98
3.15
3.19
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)
172.262
160.765
140.308
139.884
138.047
135.056
134.954
134.459
131.807
131.661
130.510
130.467
129.257
129.118
128.833
128.344
127.727
127.299
126.109
122.344
114.053
112.842
94.519
60.823
30.777
22.224
14.174
7j
200
150
100
50
0
ppm (t1)

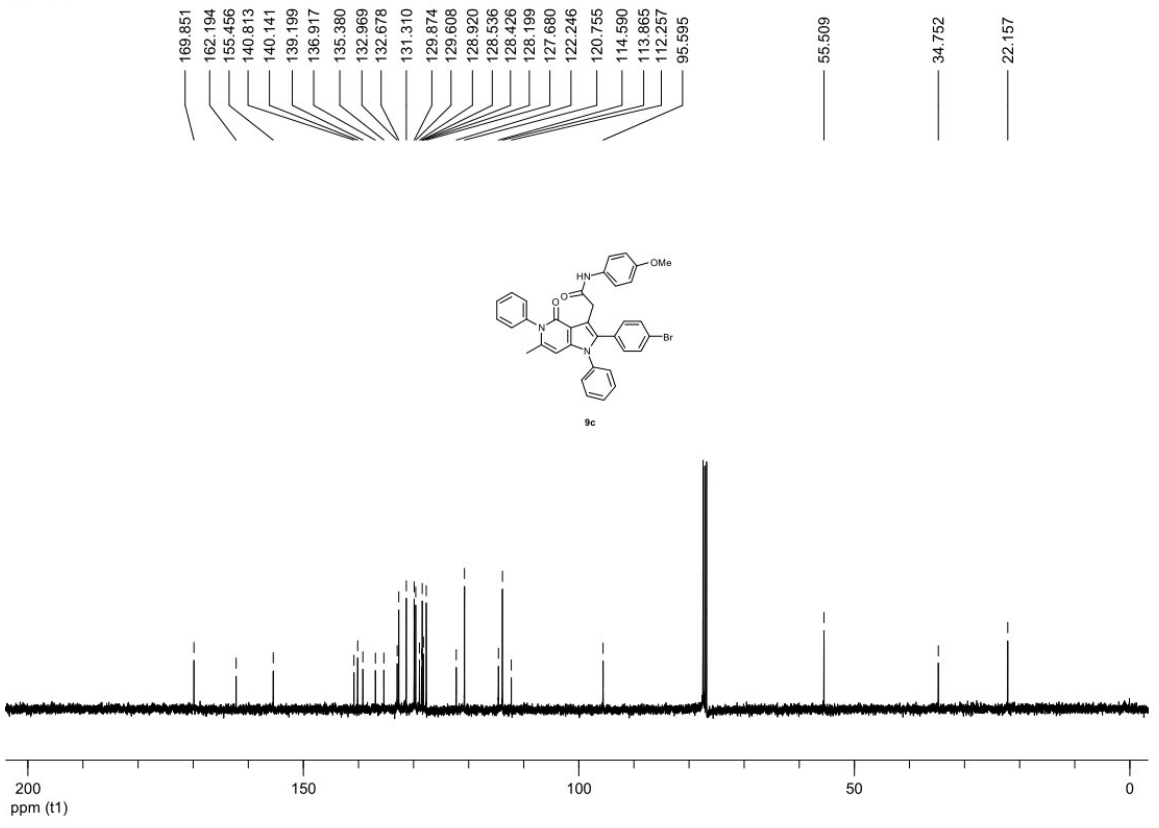

7.525
7.507
7.487
7.444
7.425
7.378
7.359
7.345
7.328
7.310
7.273
7.267
7.248
7.239
7.235
7.199
7.195
7.178
7.171
7.162
7.152
6.165
4.151
4.133
4.115
4.098
3.979
1.939
1.214
1.196
1.179
7k
2.95
6.27
6.31
4.50
1.00
2.07
1.96
3.10
3.20
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)
172.564
161.177
139.796
139.570
139.436
137.270
135.793
130.693
130.418
129.848
129.472
129.183
128.889
128.323
128.266
128.148
127.747
127.651
127.595
113.136
112.761
94.643
60.569
30.887
22.178
14.148
7k
200
150
100
50
0
ppm (t1)

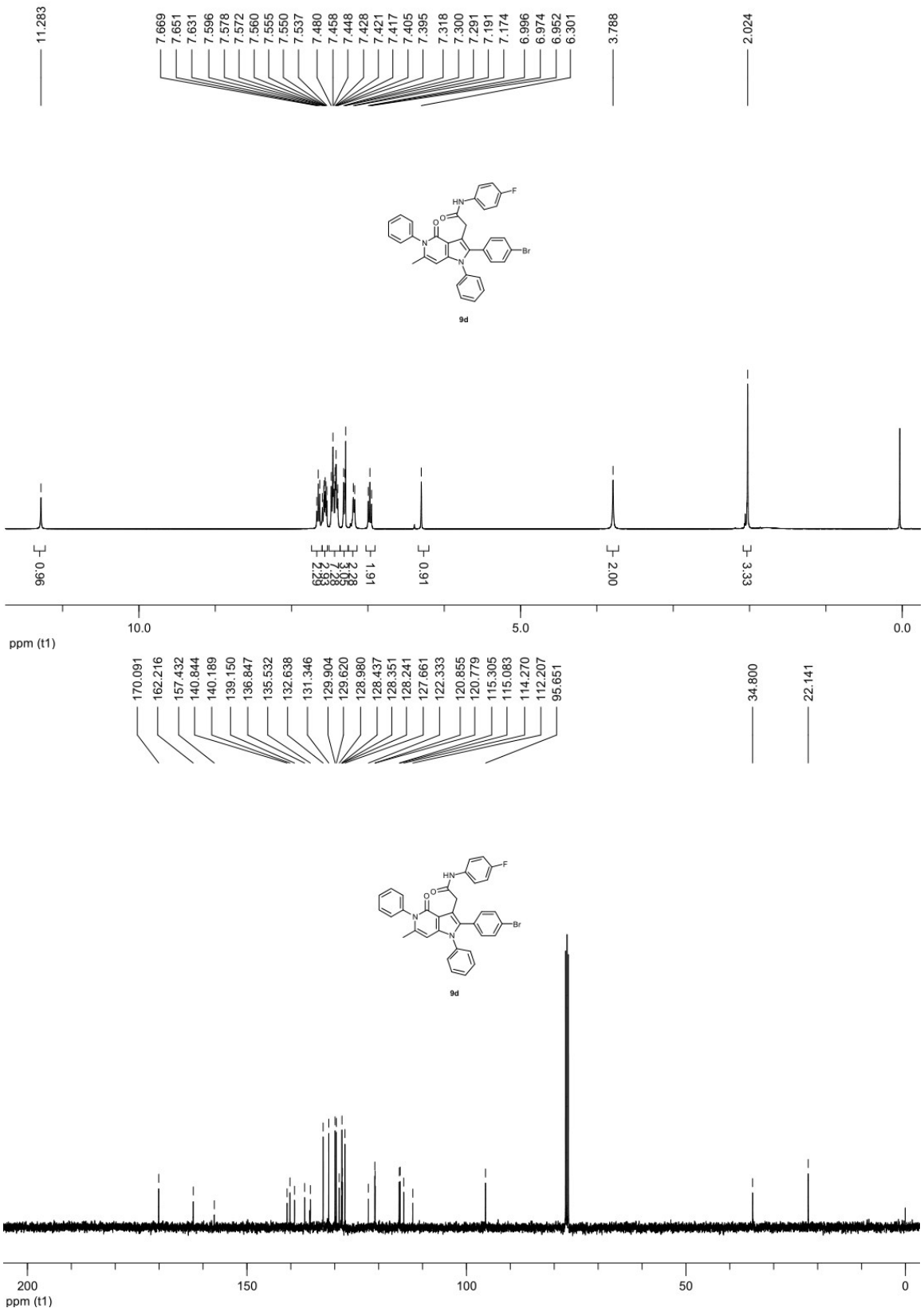

7.543
7.525
7.506
7.462
7.444
7.426
7.409
7.390
7.378
7.361
7.289
7.278
7.260
7.196
7.178
7.164
7.155
7.147
7.142
6.983
6.961
6.939
6.165
4.171
4.153
4.136
4.118
3.973
1.953
1.237
1.219
1.202
7l
2.20
4.53
3.19
4.36
2.19
1.00
1.97
2.05
3.11
3.22
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)
172.528
163.431
161.126
139.746
139.387
137.063
134.731
132.214
132.133
129.886
129.643
129.511
129.307
128.856
128.303
127.820
127.746
126.782
115.431
115.218
113.213
112.636
94.549
60.660
30.786
22.206
14.157
7l
200
150
100
50
0
ppm (t1)

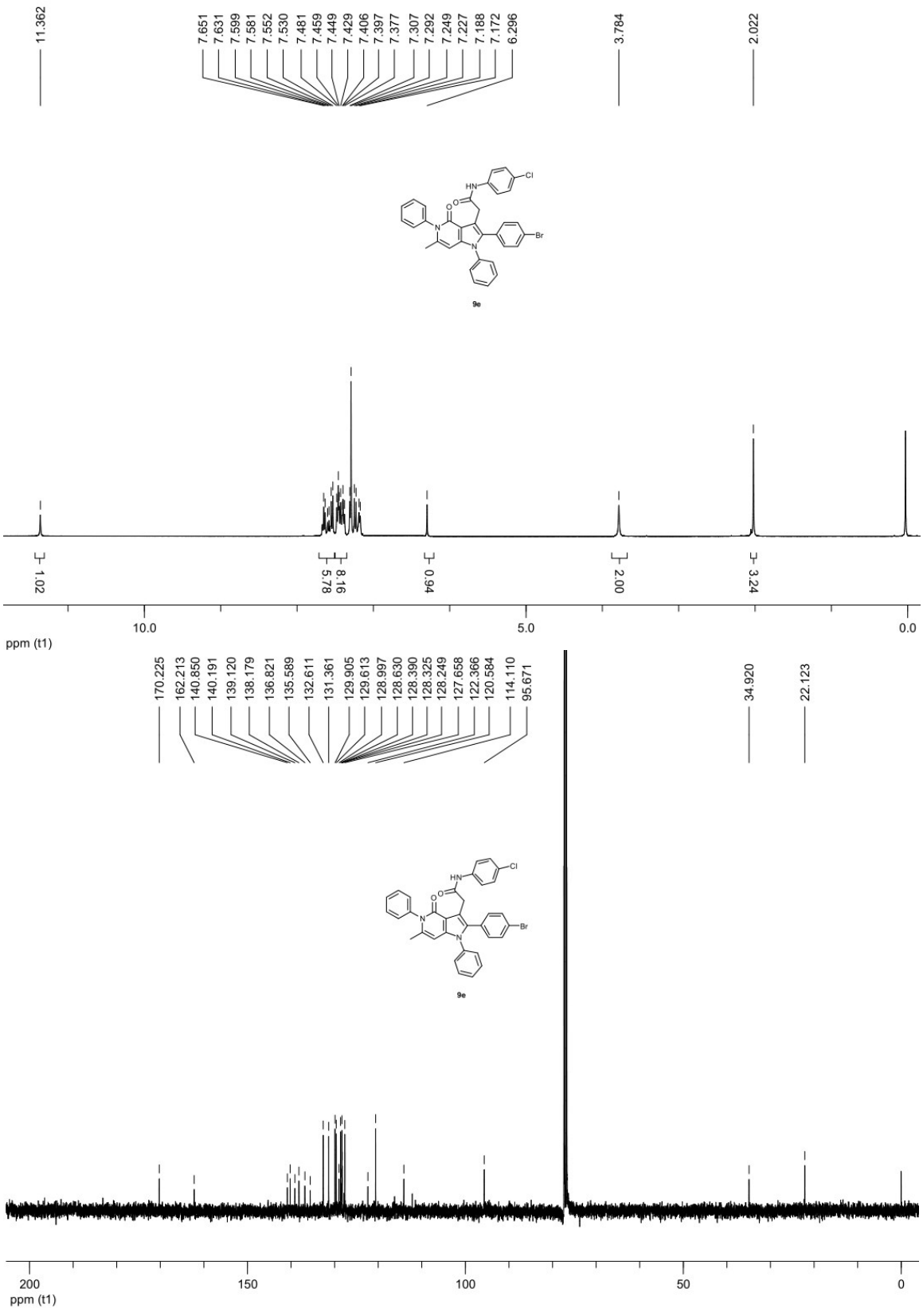

11.229
7.671
7.654
7.635
7.619
7.599
7.580
7.482
7.462
7.435
7.335
7.315
7.293
7.277
7.193
7.176
7.062
7.045
7.027
6.291
3.812
2.022
HN
O
N
Br
9a
0.92
5.34
7.36
4.78
2.18
0.99
0.92
2.00
3.24
10.0
5.0
0.0
ppm (t1)
170.242
162.213
140.804
140.144
139.579
139.171
136.896
135.431
132.657
131.328
129.868
129.607
128.932
128.703
128.500
128.417
128.250
128.202
127.675
123.125
122.278
119.401
114.432
112.234
95.594
34.936
22.145
200
150
100
50
0
ppm (t1)

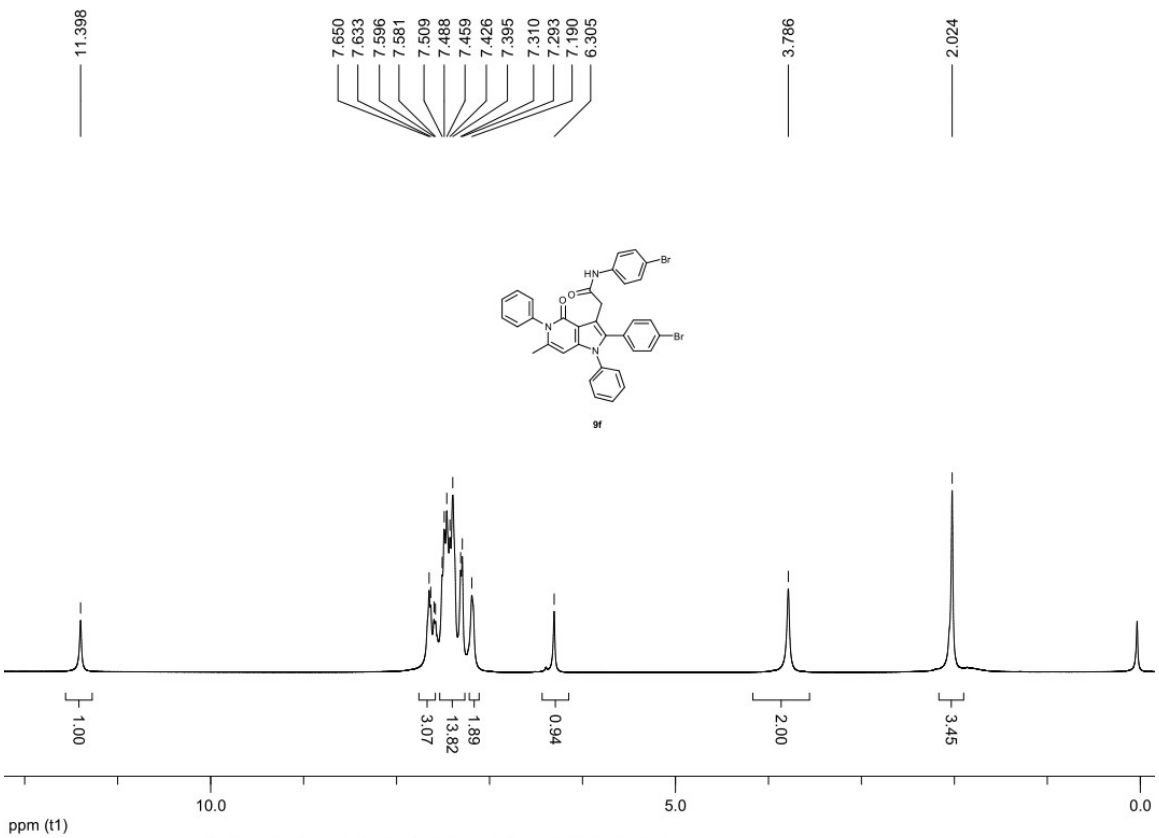

11.097
7.627
7.610
7.571
7.554
7.479
7.459
7.436
7.423
7.305
7.285
7.272
7.170
7.089
7.070
6.261
3.778
2.293
1.996
9b
0.97
3.70
9.74
3.55
4.18
0.91
2.00
3.02
3.52
10.0
5.0
0.0
ppm (t1)
170.025
162.174
140.770
140.077
139.186
137.028
136.931
135.392
132.659
132.527
131.309
129.840
129.584
129.167
128.899
128.505
128.424
128.163
127.684
122.242
119.332
114.566
112.240
95.555
34.841
22.126
20.859
9b
200
150
100
50
0
ppm (t1)

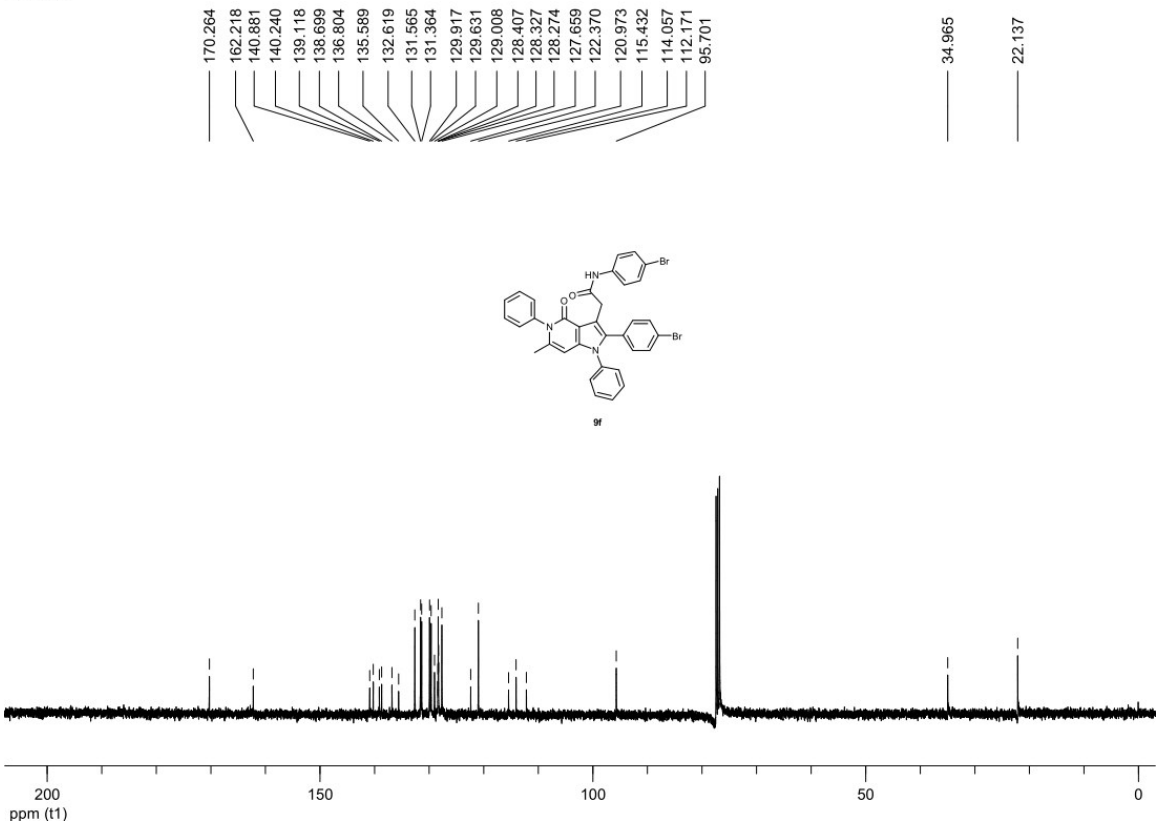

11.088
7.666
7.648
7.629
7.588
7.570
7.549
7.540
7.517
7.478
7.457
7.446
7.424
7.415
7.397
7.330
7.311
7.292
7.193
7.175
6.854
6.832
6.294
3.796
2.019
9c
1.06
2.09
2.00
0.99
5.27
3.19
10.0
5.0
0.0
ppm (t1)

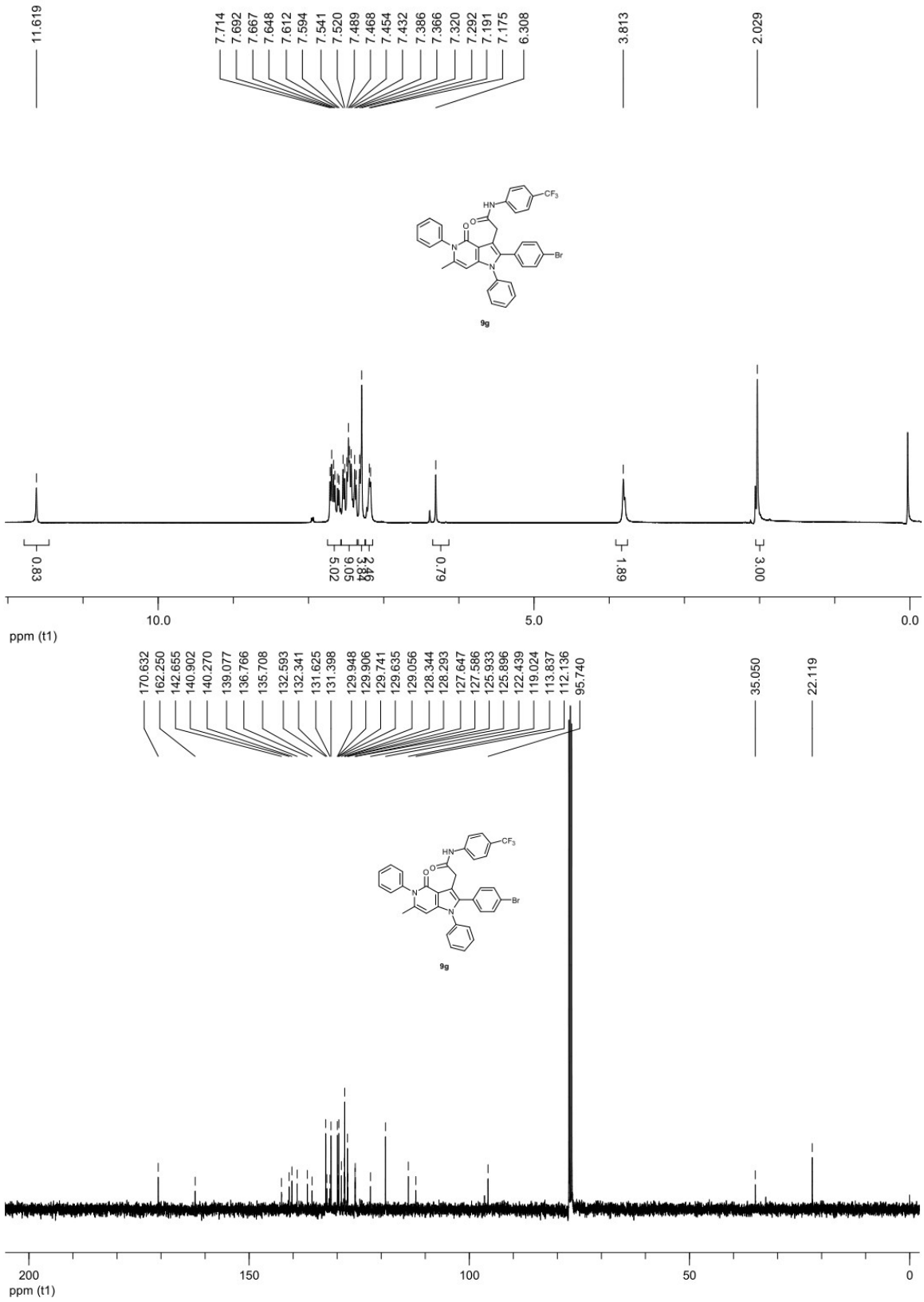

169.851
162.194
155.456
140.813
140.141
139.199
136.917
135.380
132.969
132.678
131.310
129.874
129.608
128.920
128.536
128.426
128.199
127.680
122.246
120.755
114.590
113.865
112.257
95.595
55.509
34.752
22.157
9c
200
150
100
50
0
ppm (t1)

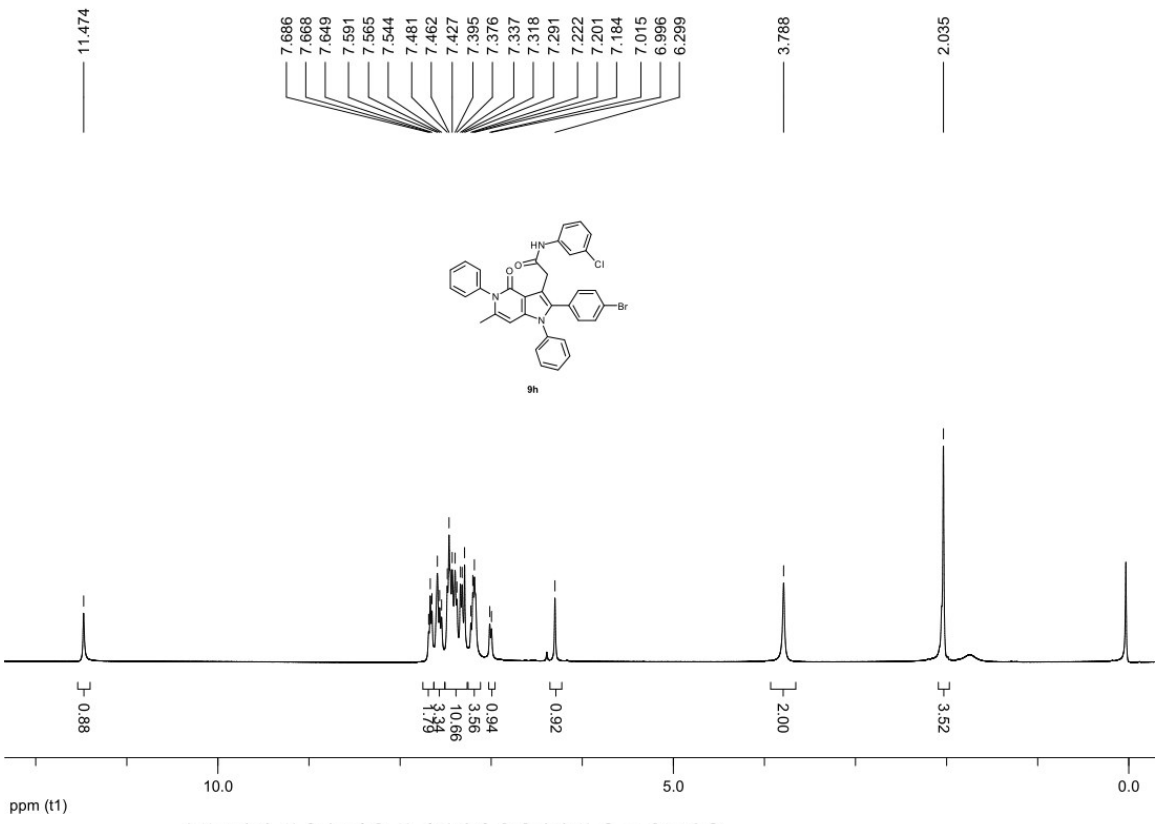

11.283
7.669
7.651
7.631
7.596
7.578
7.572
7.560
7.555
7.550
7.537
7.480
7.458
7.448
7.428
7.421
7.417
7.405
7.395
7.318
7.300
7.291
7.191
7.174
6.996
6.974
6.952
6.301
3.788
2.024
HN
F
O
N
Br
9d
0.96
1.91
0.91
2.00
3.33
10.0
5.0
0.0
ppm (t1)
170.091
162.216
157.432
140.844
140.189
139.150
136.847
135.532
132.638
131.346
129.904
129.620
128.980
128.437
128.351
128.241
127.661
122.333
120.855
120.779
115.305
115.083
114.270
112.207
95.651
34.800
22.141
200
150
100
50
0
ppm (t1)

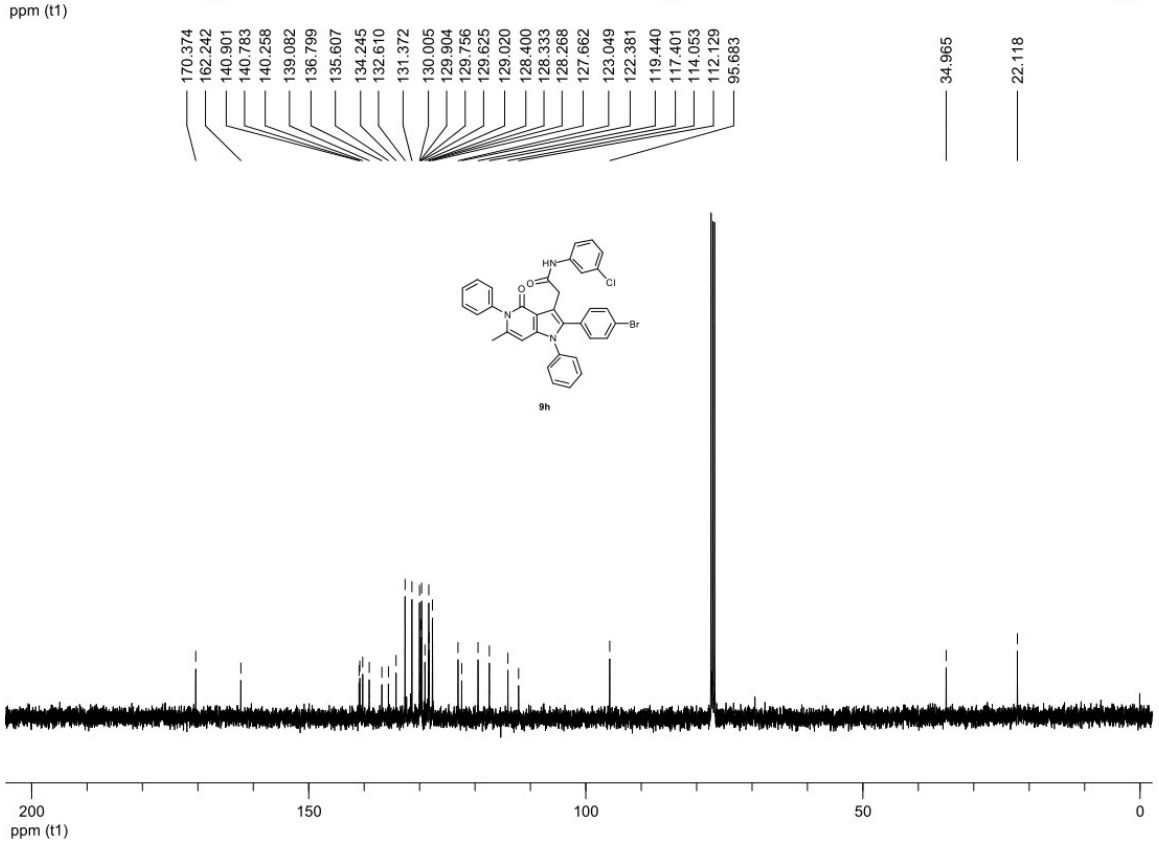

11.362
7.651
7.631
7.599
7.581
7.552
7.530
7.481
7.459
7.449
7.429
7.406
7.397
7.377
7.307
7.292
7.249
7.227
7.188
7.172
6.296
3.784
2.022
HN
Cl
O
N
Br
9e
1.02
5.78
8.19
0.94
2.00
3.24
10.0
5.0
0.0
ppm (t1)
170.225
162.213
140.850
140.191
139.120
138.179
136.821
135.589
132.611
131.361
129.905
129.613
128.997
128.630
128.390
128.325
128.249
127.658
122.366
120.584
114.110
95.671
34.920
22.123
200
150
100
50
0
ppm (t1)

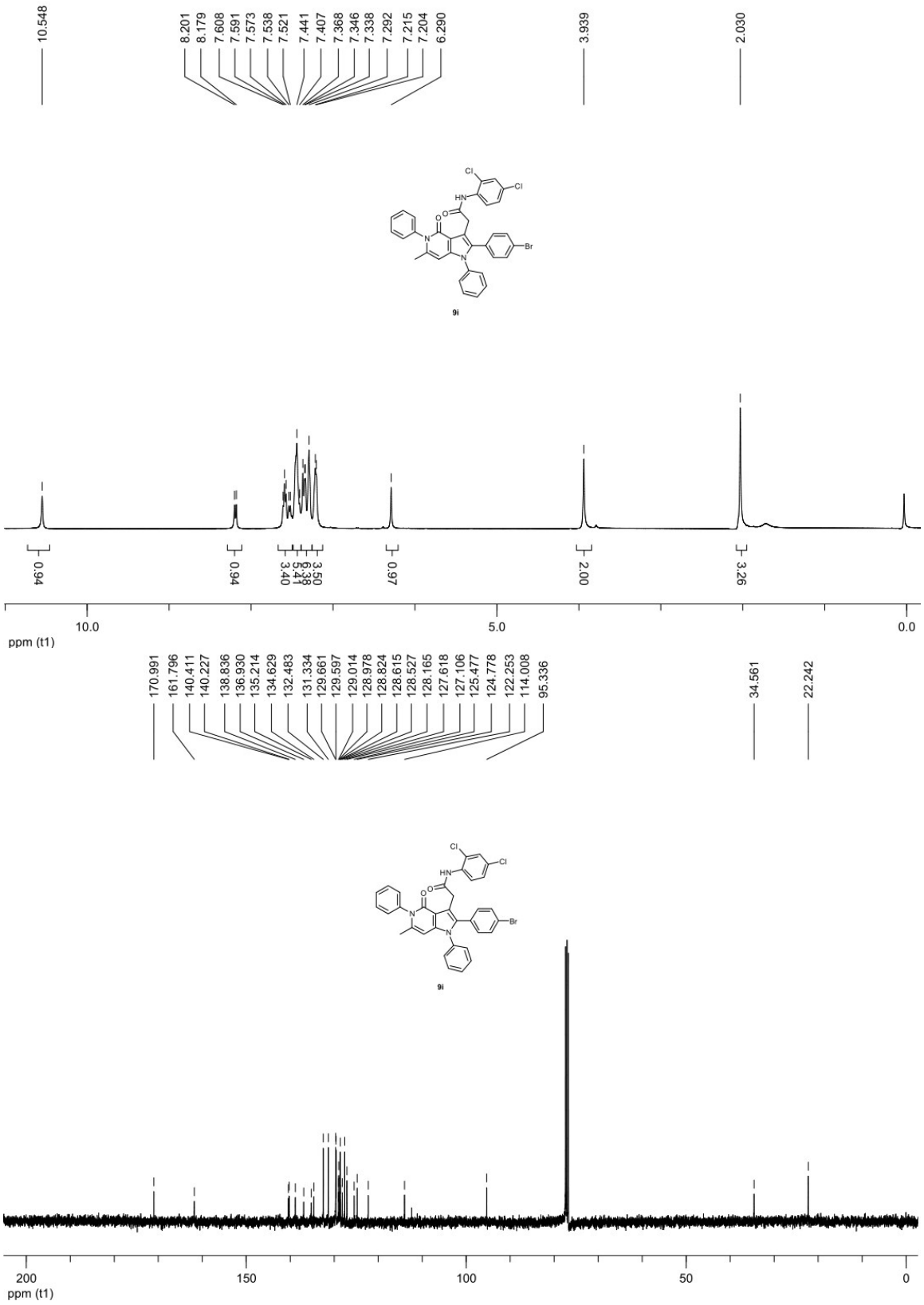

11.398
7.650
7.633
7.596
7.581
7.509
7.488
7.459
7.426
7.395
7.310
7.293
7.190
6.305
3.786
2.024
9f
1.00
3.07
13.82
1.89
0.94
2.00
3.45
10.0
5.0
0.0
ppm (t1)

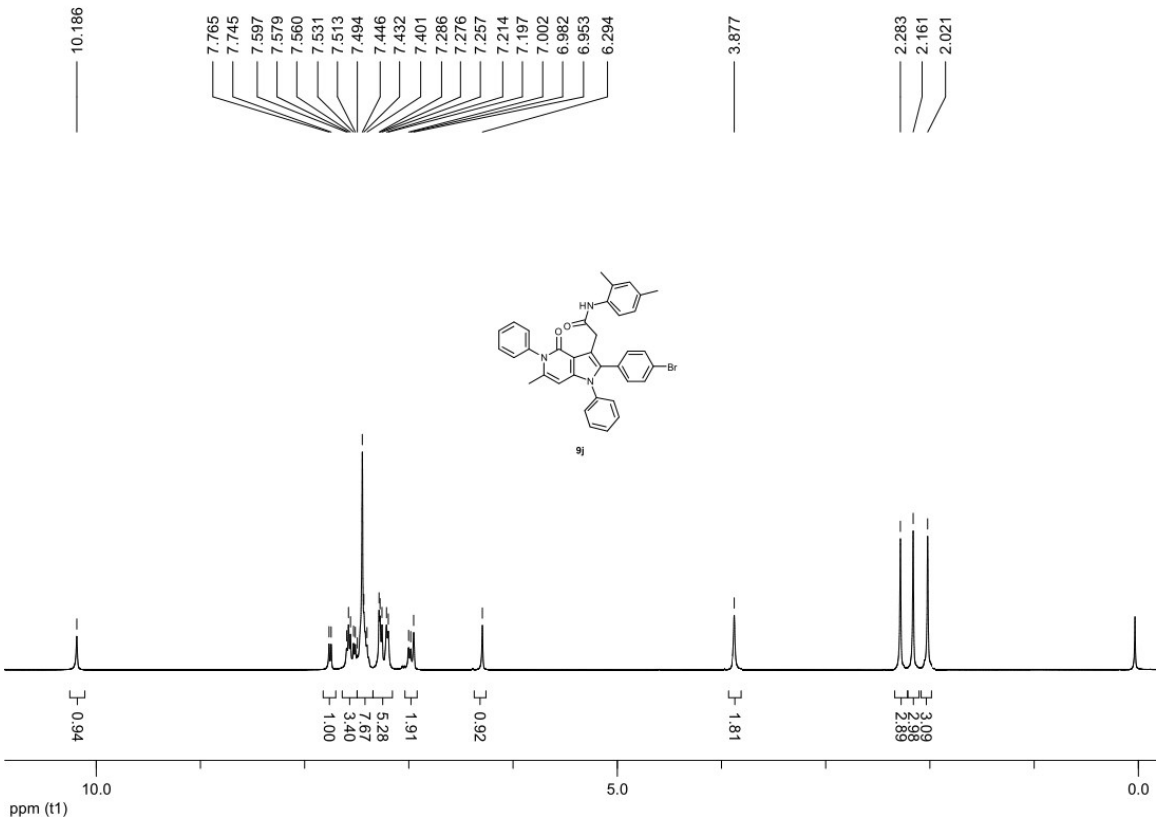

170.264
162.218
140.881
140.240
139.118
138.699
136.804
135.589
132.619
131.565
131.364
129.917
129.631
129.008
128.407
128.327
128.274
127.659
122.370
120.973
115.432
114.057
112.171
95.701
34.965
22.137
9f
200
150
100
50
0
ppm (t1)

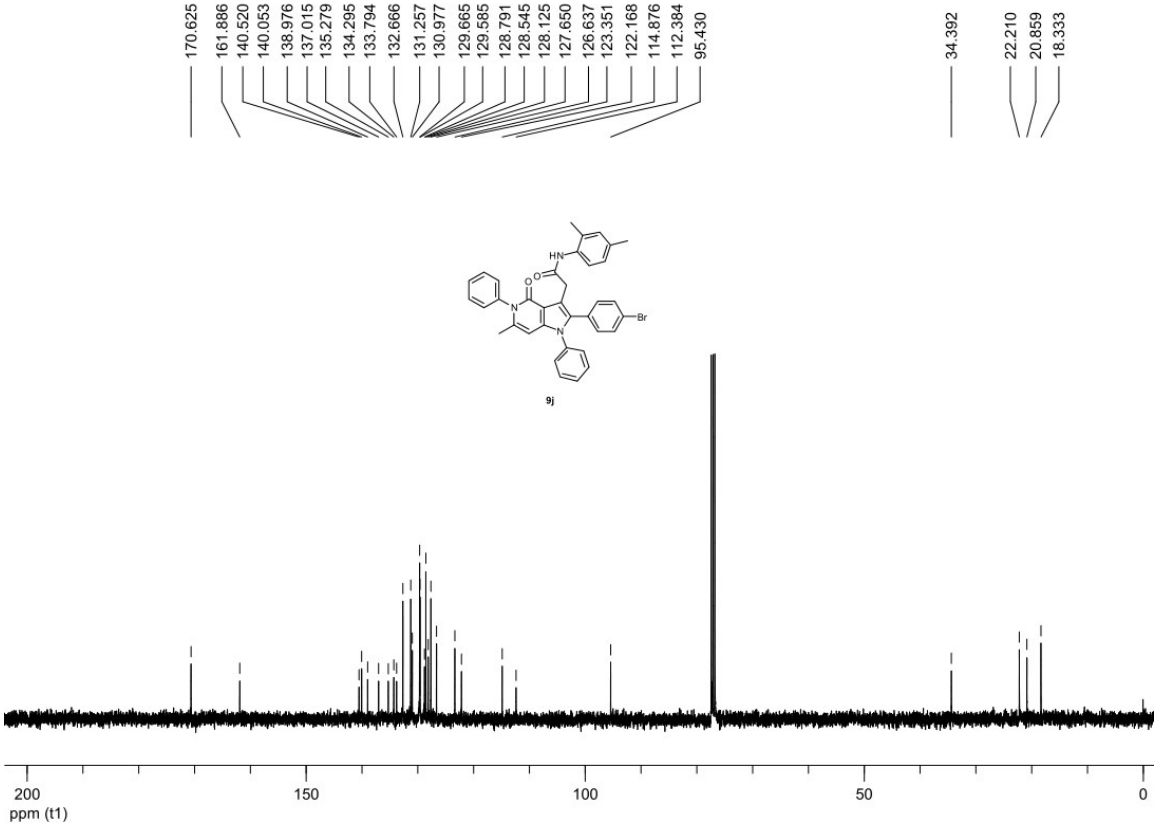

11.619
7.714
7.692
7.667
7.648
7.612
7.594
7.541
7.520
7.489
7.468
7.454
7.432
7.386
7.366
7.320
7.292
7.191
7.175
6.308
3.813
2.029
9g
0.83
5.02
0.79
1.89
3.00
10.0
5.0
0.0
ppm (t1)
170.632
162.250
142.655
140.902
140.270
139.077
136.766
135.708
132.593
132.341
131.625
131.398
129.948
129.906
129.741
129.635
129.056
128.344
128.293
127.647
127.586
125.933
125.896
122.439
119.024
113.837
112.136
95.740
35.050
22.119
9g
200
150
100
50
0
ppm (t1)

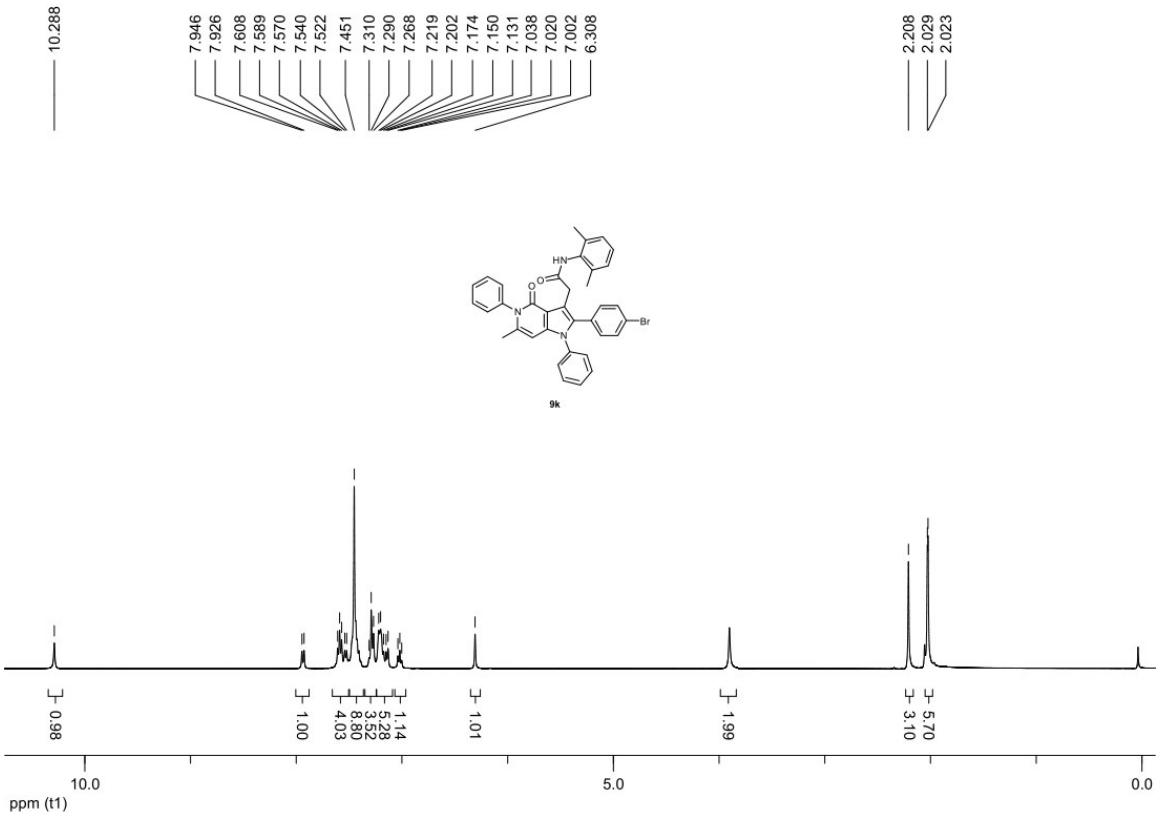

11.474
7.686
7.668
7.649
7.591
7.565
7.544
7.481
7.462
7.427
7.395
7.376
7.337
7.318
7.291
7.222
7.201
7.184
7.015
6.996
6.299
3.788
2.035
HN
Cl
O
N
Br
9h
0.88
3.79
3.34
10.66
3.56
0.94
0.92
2.00
3.52
10.0
5.0
0.0
ppm (t1)

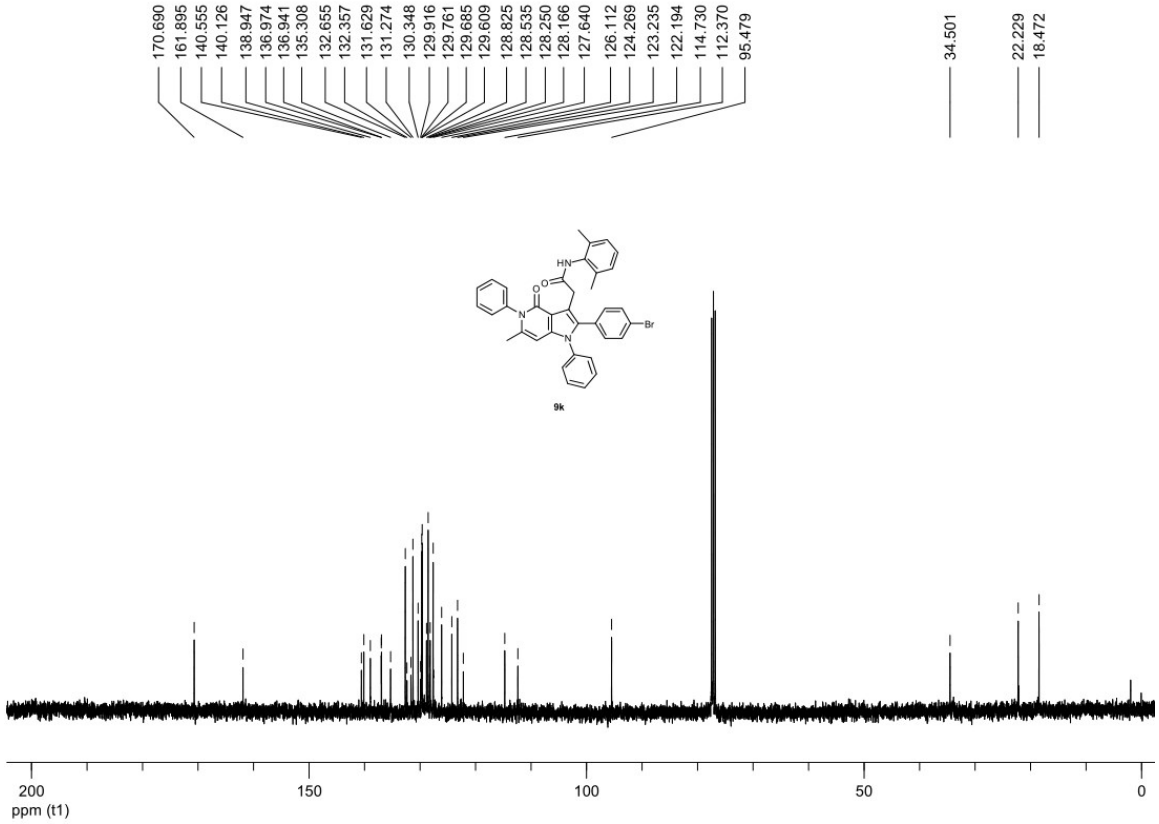

170.374
162.242
140.901
140.783
140.258
139.082
136.799
135.607
134.245
132.610
131.372
130.005
129.904
129.756
129.625
129.020
128.400
128.333
128.268
127.662
123.049
122.381
119.440
117.401
114.053
112.129
95.683
34.965
22.118
HN
Cl
O
N
Br
9h
200
150
100
50
0
ppm (t1)

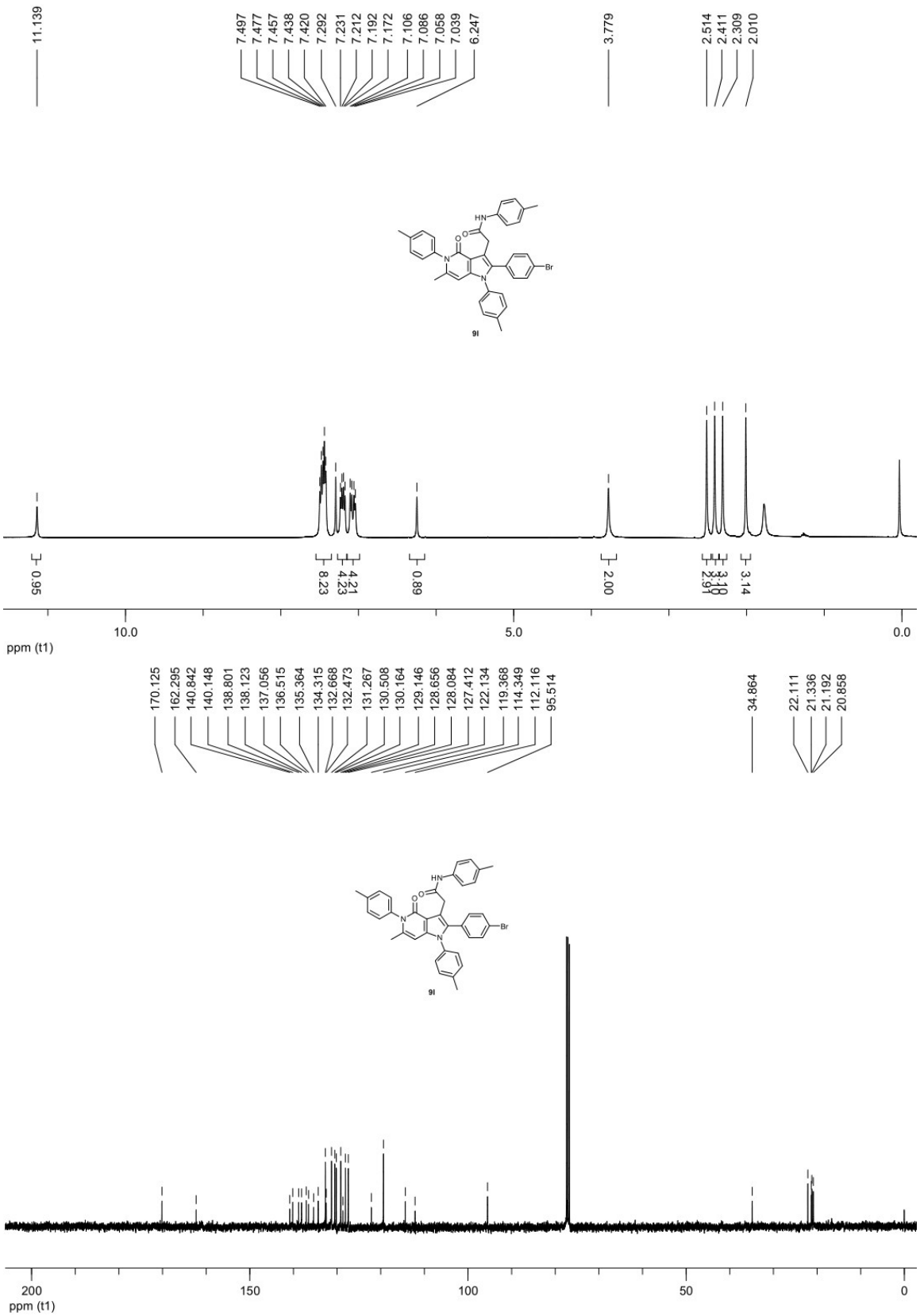

10.548
8.201
8.179
7.608
7.591
7.573
7.538
7.521
7.441
7.407
7.368
7.346
7.338
7.292
7.215
7.204
6.290
3.939
2.030
9i
0.94
0.94
3.40
5.41
6.38
3.50
0.97
2.00
3.26
10.0
5.0
0.0
ppm (t1)
170.991
161.796
140.411
140.227
138.836
136.930
135.214
134.629
132.483
131.334
129.661
129.597
129.014
128.978
128.824
128.615
128.527
128.165
127.618
127.106
125.477
124.778
122.253
114.008
95.336
34.561
22.242
9i
200
150
100
50
0
ppm (t1)

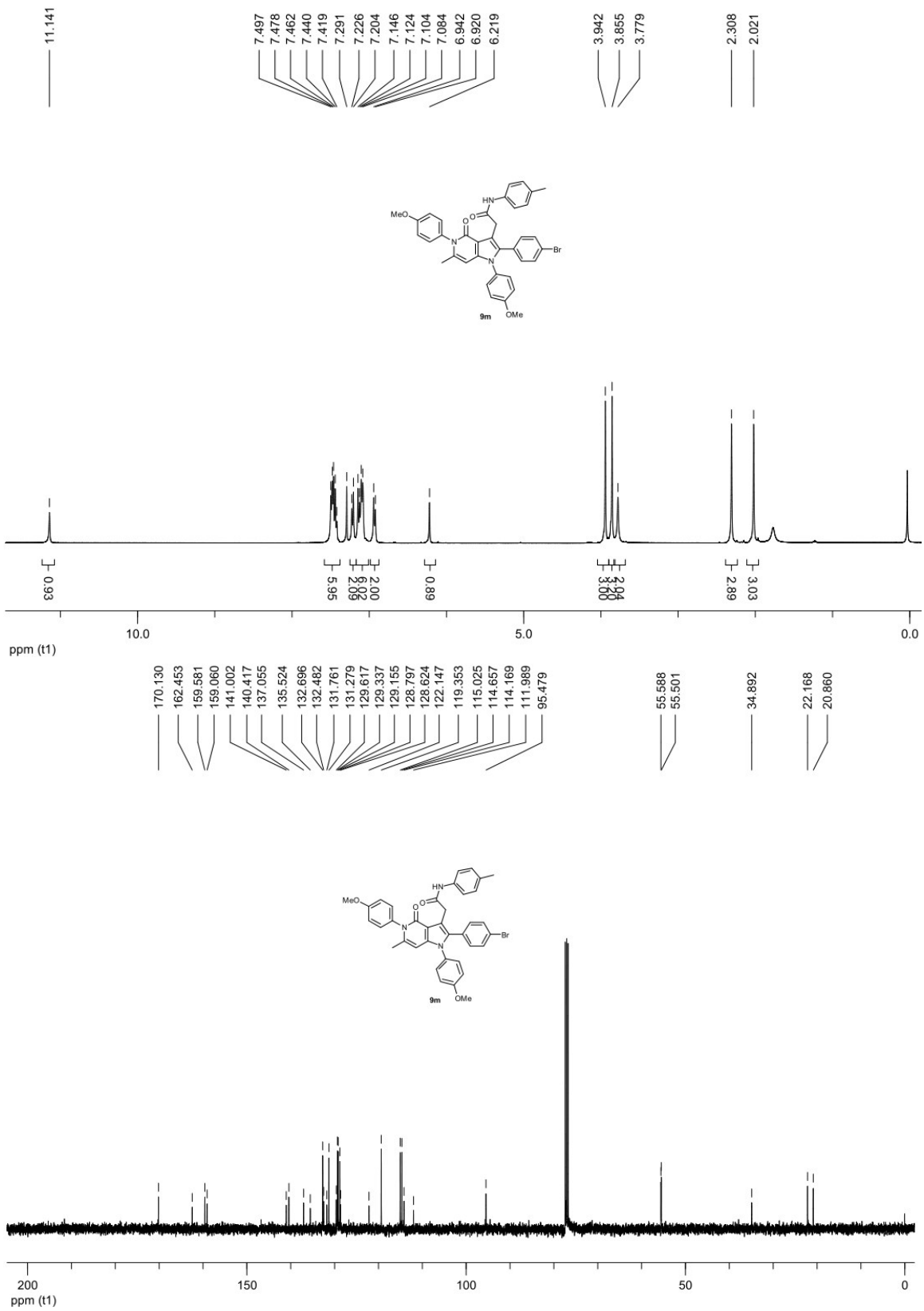

10.186
7.765
7.745
7.597
7.579
7.560
7.531
7.513
7.494
7.446
7.432
7.401
7.286
7.276
7.257
7.214
7.197
7.002
6.982
6.953
6.294
3.877
2.283
2.161
2.021
HN
O
N
Br
9j
0.94
1.00
3.40
7.67
5.28
1.91
0.92
1.81
2.89
2.98
3.09
10.0
5.0
0.0
ppm (t1)

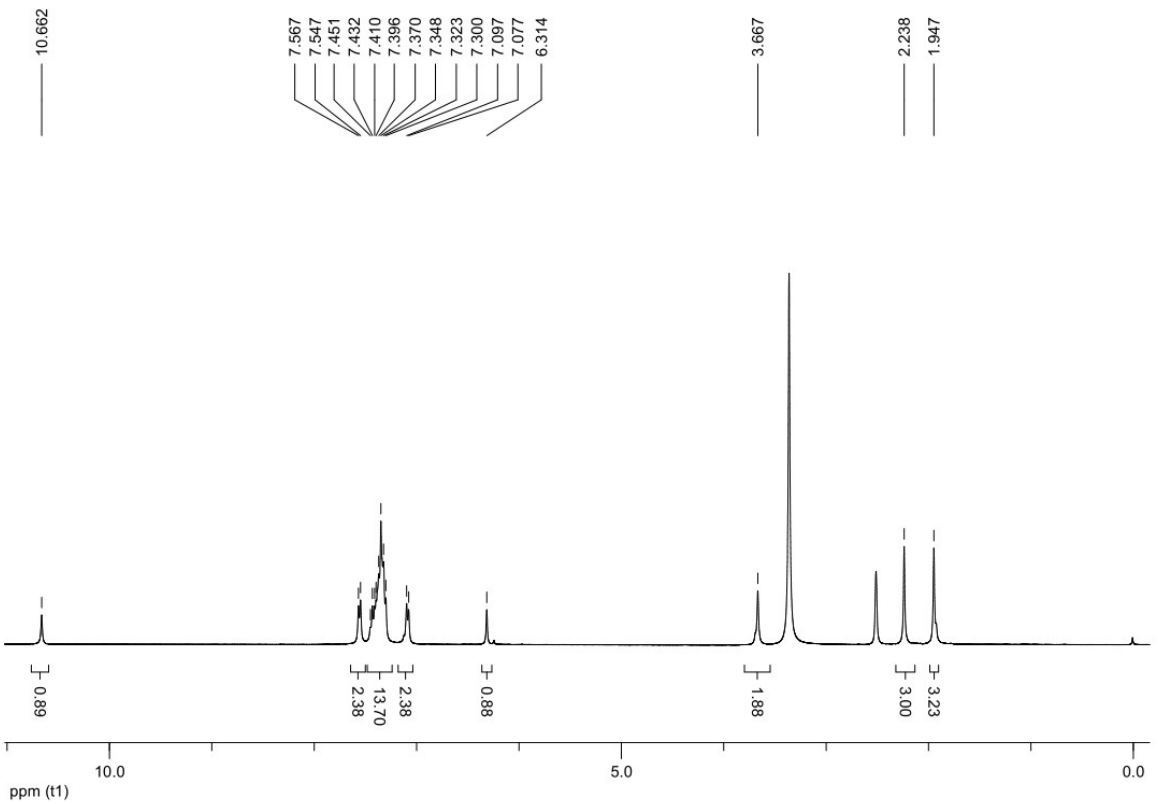

170.625
161.886
140.520
140.053
138.976
137.015
135.279
134.295
133.794
132.666
131.257
130.977
129.665
129.585
128.791
128.545
128.125
127.650
126.637
123.351
122.168
114.876
112.384
95.430
34.392
22.210
20.859
18.333
HN
O
N
Br
9j
200
150
100
50
0
ppm (t1)

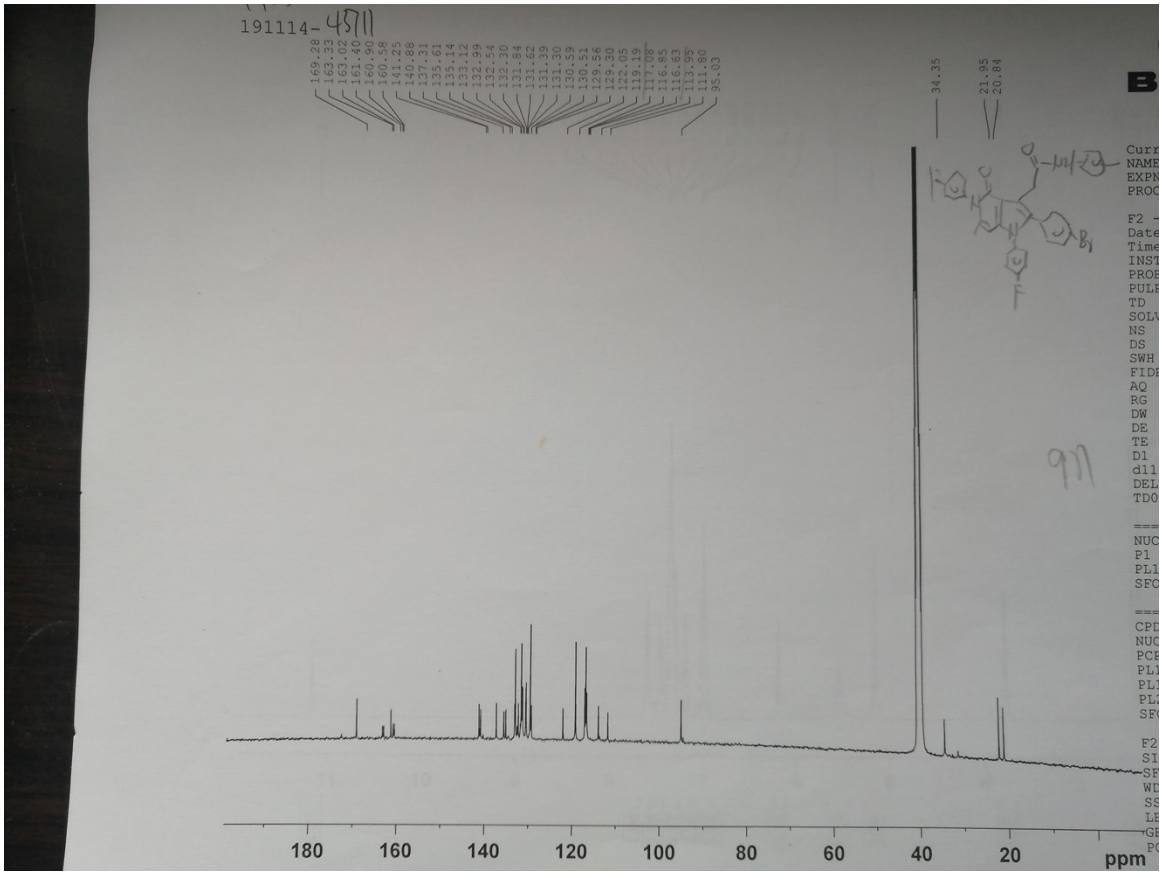

10.288
7.946
7.926
7.608
7.589
7.570
7.540
7.522
7.451
7.310
7.290
7.268
7.219
7.202
7.174
7.150
7.131
7.038
7.020
7.002
6.308
2.208
2.029
2.023
HN
O
N
Br
9k
0.98
1.00
4.03
8.80
3.52
5.28
1.14
1.01
1.99
3.10
5.70
10.0
5.0
0.0
ppm (t1)

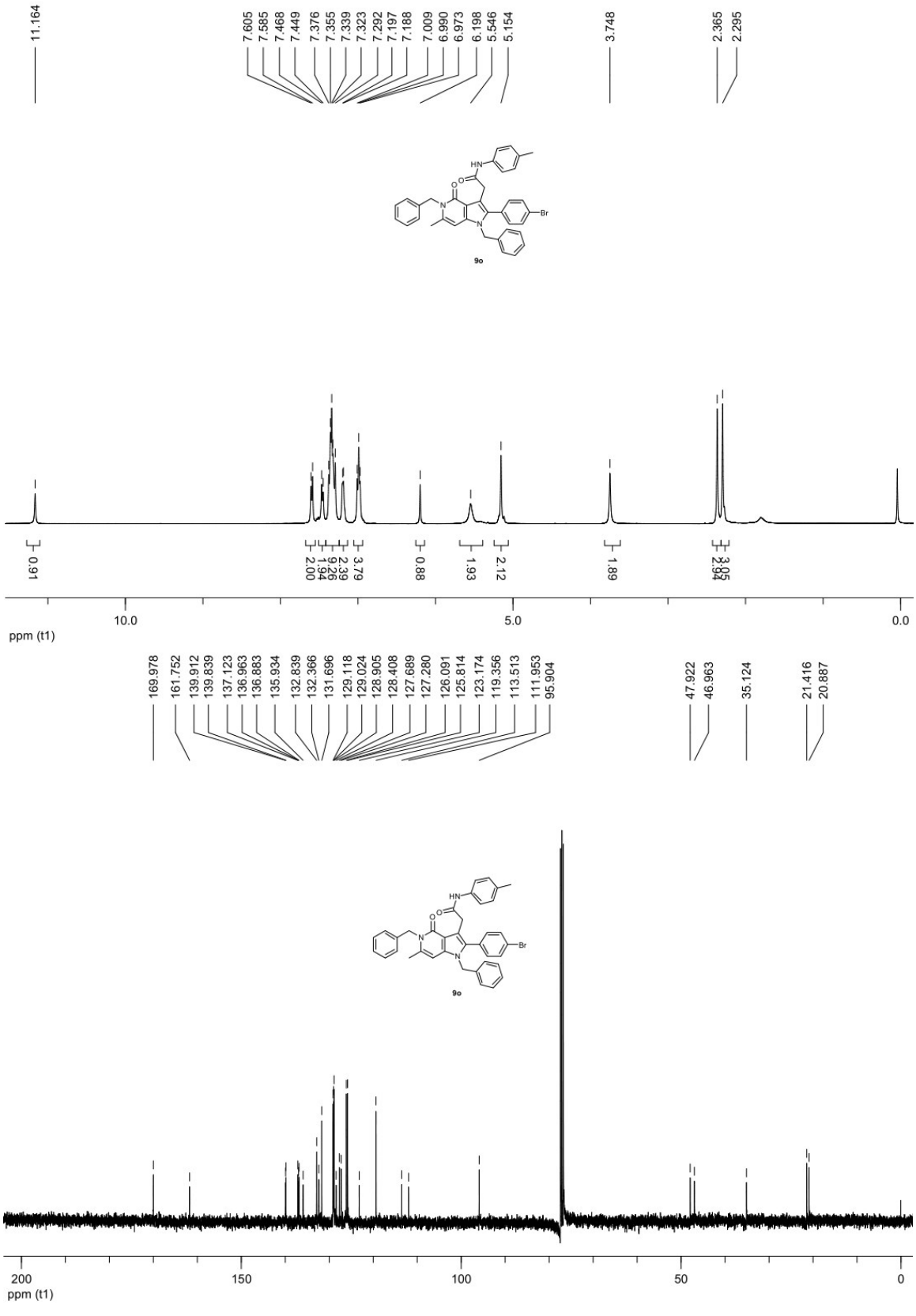

170.690
161.895
140.555
140.126
138.947
136.974
136.941
135.308
132.655
132.357
131.629
131.274
130.348
129.916
129.761
129.685
129.609
128.825
128.535
128.250
128.166
127.640
126.112
124.269
123.235
122.194
114.730
112.370
95.479
34.501
22.229
18.472
HN
O
N
Br
9k
200
150
100
50
0
ppm (t1)


11.139
7.497
7.477
7.457
7.438
7.420
7.292
7.231
7.212
7.192
7.172
7.106
7.086
7.058
7.039
6.247
3.779
2.514
2.411
2.309
2.010
HN
O
N
Br
9l
0.95
8.23
4.21
4.23
0.89
2.00
3.14
10.0
5.0
0.0
ppm (t1)
170.125
162.295
140.842
140.148
138.801
138.123
137.056
136.515
135.364
134.315
132.668
132.473
131.267
130.508
130.164
129.146
128.656
128.084
127.412
122.134
119.368
114.349
112.116
95.514
34.864
22.111
21.336
21.192
20.858
200
150
100
50
0
ppm (t1)


11.141
7.497
7.478
7.462
7.440
7.419
7.291
7.226
7.204
7.146
7.124
7.104
7.084
6.942
6.920
6.219
3.942
3.855
3.779
2.308
2.021
MeO
HN
O
N
Br
9m
OMe
0.93
6.96
2.09
2.09
2.00
0.89
3.00
3.00
2.04
2.89
3.03
10.0
5.0
0.0
ppm (t1)
170.130
162.453
159.581
159.060
141.002
140.417
137.055
135.524
132.696
132.482
131.761
131.279
129.617
129.337
129.155
128.797
128.624
122.147
119.353
115.025
114.657
114.169
111.989
95.479
55.588
55.501
34.892
22.168
20.860
200
150
100
50
0
ppm (t1)


10.662
7.567
7.547
7.451
7.432
7.410
7.396
7.370
7.348
7.323
7.300
7.097
7.077
6.314
3.667
2.238
1.947
0.89
2.38
13.70
2.38
0.88
1.88
3.00
3.23
10.0
5.0
0.0
ppm (t1)


191114-4511
169.28
163.33
163.02
161.40
160.90
160.58
141.25
140.88
137.31
135.61
135.44
133.42
132.89
132.54
132.30
131.84
131.62
131.39
131.30
130.59
130.51
129.56
129.30
122.05
119.19
117.08
116.85
116.63
113.95
111.80
95.03
34.35
21.35
20.84
180
160
140
120
100
80
60
40
20
ppm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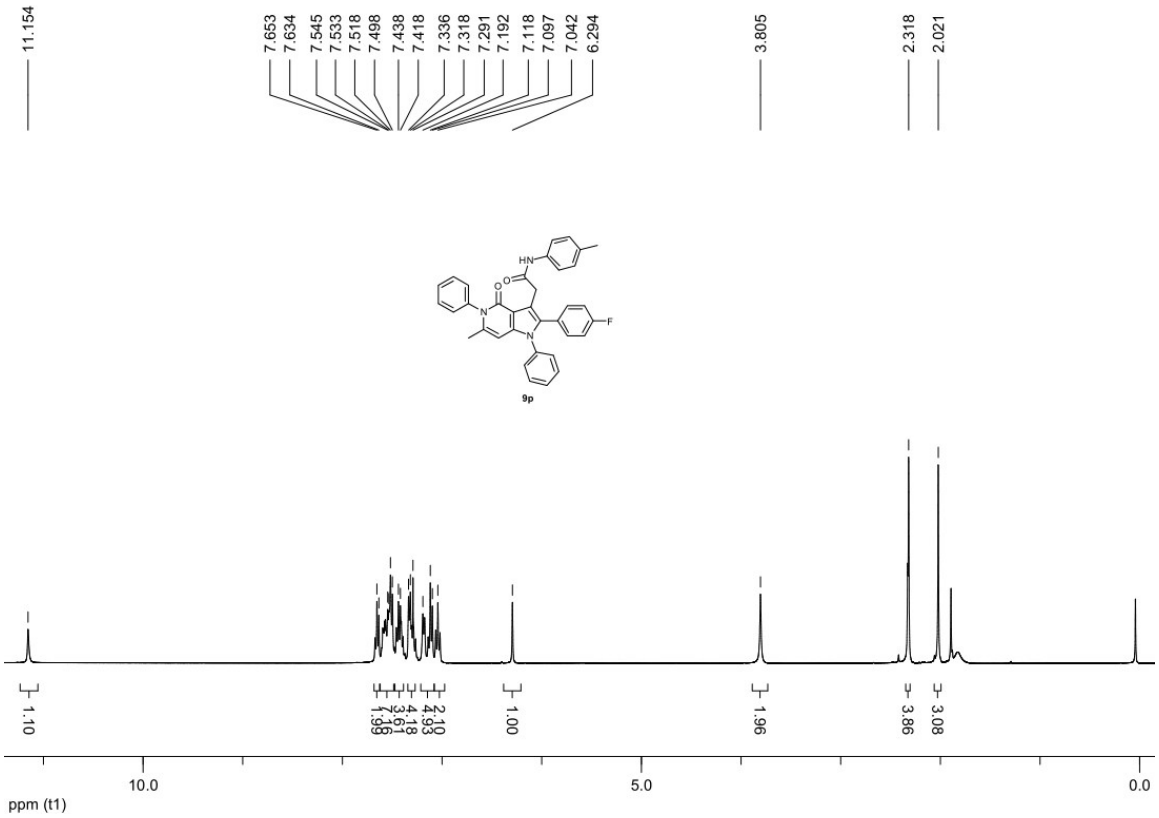
7.585
7.468
7.449
7.376
7.355
7.339
7.323
7.292
7.197
7.188
7.009
6.990
6.973
6.198
5.546
5.154
3.748
2.365
2.295
9o
0.91
2.00
1.94
1.96
2.39
3.79
0.88
1.93
2.12
1.89
2.95
2.95
10.0
5.0
0.0
ppm (t1)
169.978
161.752
139.912
139.839
137.123
136.963
136.883
135.934
132.839
132.366
131.696
129.118
129.024
128.905
128.408
127.689
127.280
126.091
125.814
123.174
119.356
113.513
111.953
95.904
47.922
46.963
35.124
21.416
20.887
9o
200
150
100
50
0
ppm (t1)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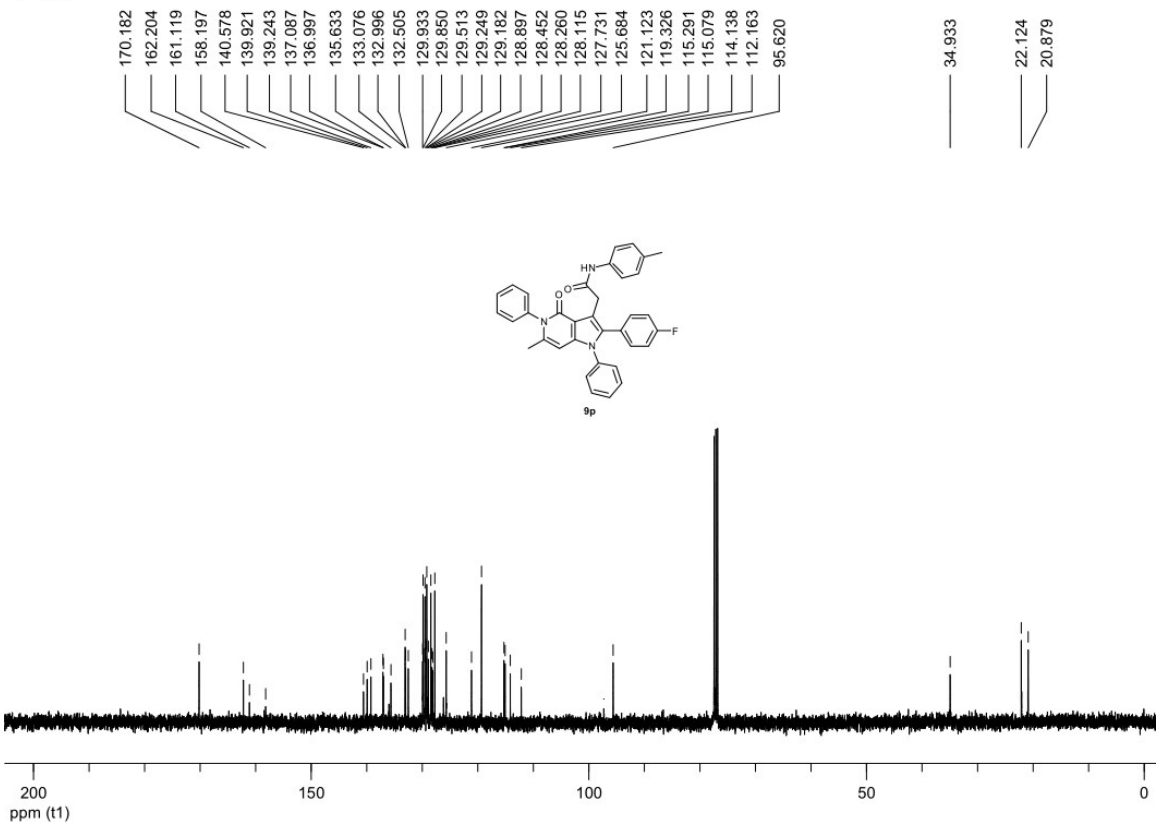
7.518
7.498
7.438
7.418
7.336
7.318
7.291
7.192
7.118
7.097
7.042
6.294
3.805
2.318
2.021
HN
O
O
N
F
N
9p
1.10
1.69
1.16
3.61
4.18
2.10
4.63
1.00
1.96
3.86
3.08
10.0
5.0
0.0
ppm (t1)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158.197
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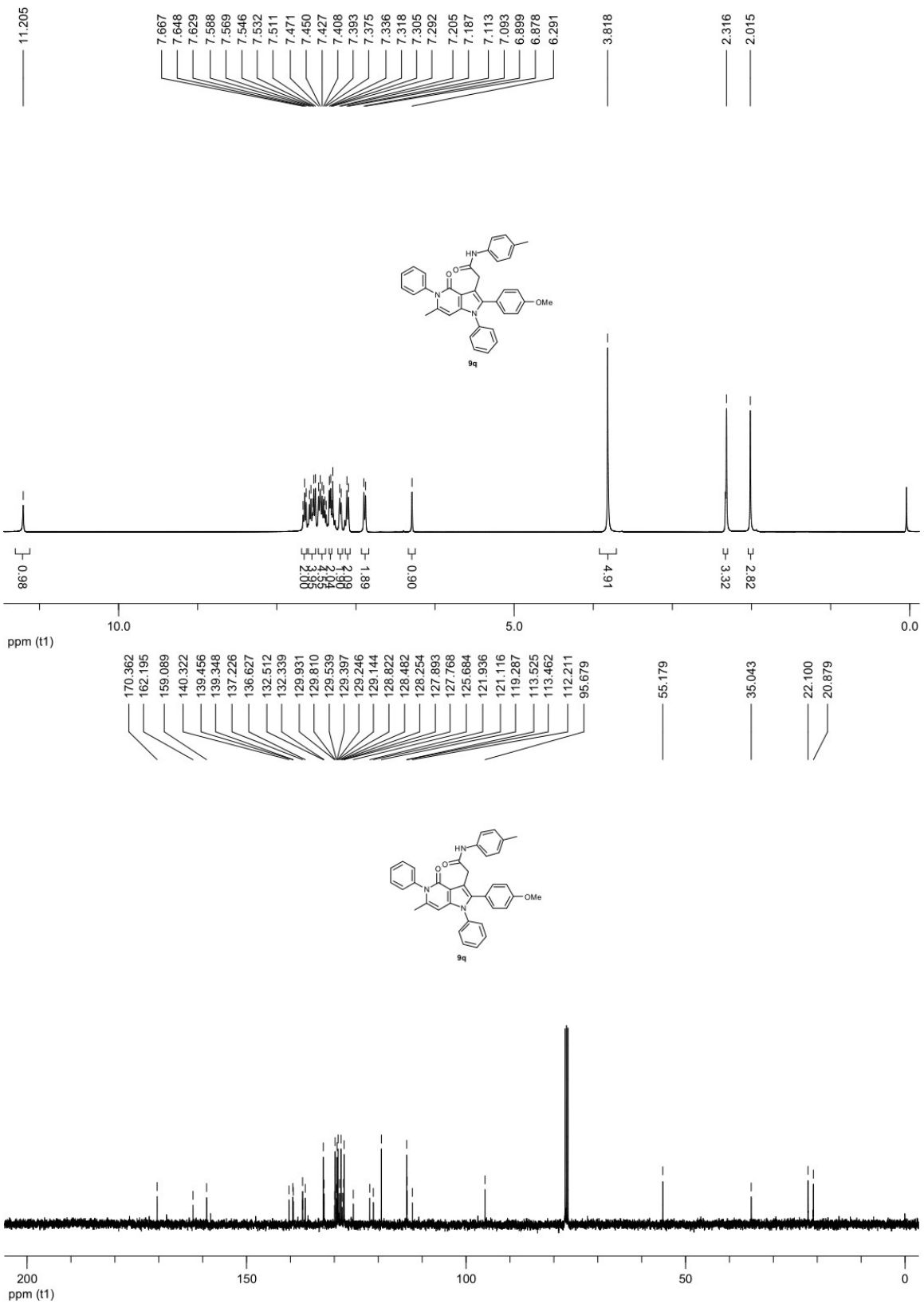
139.921
139.243
137.087
136.997
135.633
133.076
132.996
132.505
129.933
129.850
129.513
129.249
129.182
128.897
128.452
128.260
128.115
127.731
125.684
121.123
119.326
115.291
115.079
114.138
112.163
95.620
34.933
22.124
20.879
HN
O
O
N
F
N
9p
200
150
100
50
0
ppm (t1)


11.205
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7.629
7.588
7.569
7.546
7.532
7.511
7.471
7.450
7.427
7.408
7.393
7.375
7.336
7.318
7.305
7.292
7.205
7.187
7.113
7.093
6.899
6.878
6.291
3.818
2.316
2.015
HN
O
O
N
OMe
N
9q
0.98
1.89
0.90
4.91
3.32
2.82
10.0
5.0
0.0
ppm (t1)
170.362
162.195
159.089
140.322
139.456
139.348
137.226
136.627
132.512
132.339
129.931
129.810
129.539
129.397
129.246
129.144
128.822
128.482
128.254
127.893
127.768
125.684
121.936
121.116
119.287
113.525
113.462
112.211
95.679
55.179
35.043
22.100
20.879
HN
O
O
N
OMe
N
9q
200
150
100
50
0
ppm (t1)