Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Characterization of the compounds 5b and 5d-5j.

3-Iodo-6-bromo-4-phenyl-2-(trifluoromethyl)quinoline (5b)

Pale yellow solid: mp 128 – 129 ^{o}C; ^{1}H NMR (200 MHz, $CDCl_3$): δ 8.08 (d, 1H, J = 8.7 Hz), 7.86 (dd, 1H, J = 8.7, 2.2 Hz), 7.66-7.54 (m, 3H), 7.50 (d, 1H, J = 2.2 Hz), 7.25-7.16 (m, 2H). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ 156.2, 147.9 (q, J = 33.2), 143.7, 140.6, 134.5, 131.6, 129.7, 129.2, 129.0, 128.8, 124.1, 121.1 (q, J = 276.7 Hz), 91.0. ^{19}F NMR (376.3 MHz, $CDCl_3$) δ –65.57 (s, 3F). MS (ESI): m/z = 478 $[M+H]^+$. HRMS: m/z calcd for $C_{16}H_9BrF_3IN$ $[M+H]^+$ 477.8915, found 477.8910.

3-Iodo-4-phenyl-2-(trifluoromethyl)quinoline (5d)

White solid: mp 123 - 124 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.21 (d, 1H, J = 8.3 Hz), 7.81-7.74 (m, 1H), 7.60-7.46 (m, 4H), 7.39 (d, 1H, J = 8.3 Hz), 7.24-7.18 (m, 2H). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ 157.1, 147.4 (q, J = 33.0 Hz), 145.1, 141.3, 130.8, 130.0, 129.5, 128.90, 128.86, 128.76, 127.0, 121.3 (q, J = 276.0 Hz), 89.6, (one sp^2 carbon missing due to overlap). ^{19}F NMR (376.3 MHz, $CDCl_3$) δ –65.41 (s, 3F). MS (ESI): m/z = 422 $[M+Na]^+$. HRMS: m/z calcd for $C_{16}H_9F_3INNa$ $[M+Na]^+$ 421.9629, found 421.9612.

3-Iodo-4-phenyl-2-trifluoromethylbenzo[h]quinoline (5e)

Off white solid: mp 163 - 164 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$): δ 9.36 (dd, 1H, J = 7.5, 1.5 Hz), 7.87-7.68 (m, 4H), 7.62-7.50, (m, 3H), 7.28-7.21 (m, 3H). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ 156.2, 146.2 (q, J = 33.0 Hz), 143.8, 141.6, 133.3, 130.7, 130.68, 129.3, 129.0, 128.80, 128.75, 127.9, 127.7, 127.1, 124.9, 123.4, 121.6 (q, J = 273.6 Hz), 91.3. ^{19}F NMR (376.3 MHz, $CDCl_3$) δ –65.09 (s, 3F). MS (ESI): m/z = 450 $[M+H]^+$. HRMS: m/z calcd for $C_{20}H_{12}F_3IN$ $[M+H]^+$ 449.9966, found 449.9955.

3-Iodo-4-(4-methoxyphenyl)-2-trifluoromethylquinoline (5f)

Pale yellow solid: mp 150-151^{o}C; ^{1}H NMR (200 MHz, $CDCl_3$): δ 8.20 (d, 1H, J = 8.8 Hz), 7.84-7.73 (m, 1H), 7.54-7.45 (m, 2H), 7.19-7.01 (m, 4H), 3.92 (s, 3H). ^{13}C NMR (75.5 MHz, $CDCl_3$): 159.9, 157.0, 147.5 (q, J = 33.2 Hz), 145.2, 139.7, 133.6, 130.8, 130.3, 129.9, 129.4, 127.1, 121.3 (q, J = 276.9 Hz), 114.1, 90.5, 55.3. ^{19}F NMR

(376.3 MHz, $CDCl_3$) δ -65.42 (s, 3F). MS (ESI): m/z = 430 $[M+H]^+$. HRMS: m/z calcd for $C_{17}H_{12}F_3INO$ $[M+H]^+$ 429.9915, found 429.9910.

4-(4-tert-Butylphenyl)-3-iodo-2-trifluoromethylquinoline (5g)

White solid: mp 164 - 165°C; ^1H NMR (300 MHz, $CDCl_3$): δ 8.20 (d, 1H, J = 8.3 Hz), 7.82-7.73 (m, 1H), 7.58-7.40 (m, 4H), 7.13 (d, J = 8.3 Hz, 2H), 1.44 (s, 9H). ^{13}C NMR (75.5 MHz, $CDCl_3$): 157.3, 151.9, 147.4 (q, J = 33.1 Hz), 145.1, 138.2, 130.7, 130.0, 129.4, 129.1, 128.6, 127.2, 125.5, 121.3 (q, J = 276.5 Hz), 89.9, 34.8, 31.4. ^{19}F NMR (376.3 MHz, $CDCl_3$) δ –65.38 (s, 3F). MS (ESI): m/z = 456 $[M+H]^+$. HRMS: m/z calcd for $C_{20}H_{18}F_3IN$ $[M+H]^+$ 456.0436, found 456.0440.

3-Iodo-6-methyl-4-naphthalen-1-yl-2-trifluoromethylquinoline (5h)

Pale yellow solid: mp 154-155°C; ^1H NMR (300 MHz, $CDCl_3$): δ 8.15 (d, 1H, J = 8.7 Hz), 8.04 (d, 1H, J = 8.3 Hz), 7.97 (d, 1H, J = 8.3 Hz), 7.69-7.57 (m, 2H), 7.55-7.47 (m, 1H), 7.39-7.23 (m, 2H), 7.05 (d, 1H, J = 8.3 Hz), 6.91 (s, 1H), 2.33 (s, 3H). ^{13}C NMR (75.5 MHz, $CDCl_3$): 155.1, 146.7 (q, J = 33.1 Hz), 143.8, 140.3, 139.0, 133.6, 133.4, 130.7, 129.7, 129.5, 129.2, 128.6, 127.2, 126.9, 126.5, 125.6, 125.5, 125.0, 121.4 (q, J = 276.3 Hz), 90.9, 21.8. ^{19}F NMR (376.3 MHz, $CDCl_3$) δ – 65.11 (s, 3F). MS (ESI): m/z = 464 $[M+H]^+$. HRMS: m/z calcd for $C_{21}H_{14}F_3IN$ $[M+H]^+$ 464.0123, found 464.0128.

4-Cyclohex-1-enyl-3-iodo-2-trifluoromethylquinoline (5i) White solid: mp 104-105°C; ^1H NMR (300 MHz, $CDCl_3$): δ 8.18 (d, 1H, J = 8.3 Hz), 7.96 (d, 1H, J = 8.3 Hz), 7.84-7.75 (m, 1H), 7.66-7.58 (m, 1H), 5.75-5.68 (m, 1H), 2.50-2.31 (m, 3H), 2.22-2.08 (m, 1H), 2.03-1.78 (m, 4H). ^{13}C NMR (75.5 MHz, $CDCl_3$): 159.1, 147.5 (q, J = 33.1 Hz), 145.2, 139.0, 130.7, 130.1, 129.8, 129.3, 128.0, 126.4, 121.3 (q, J = 276.5 Hz), 88.6, 28.8, 25.2, 22.6, 21.8. ^{19}F NMR (376.3 MHz, $CDCl_3$) δ –65.34 (s, 3F). MS (ESI): m/z = 404 $[M+H]^+$. HRMS: m/z calcd for $C_{16}H_{14}F_3IN$ $[M+H]^+$ 456.0436, found 456.0440.

3-Iodo-2-nonafluorobutyl-4-phenyl-quinoline (5j)

White solid: mp 123 - 124 ^{o}C; ^{1}H NMR (200 MHz, $CDCl_3$): δ 8.18 (d, 1H, J = 8.8 Hz), 7.83-7.73 (m, 1H), 7.64-7.46 (m, 4H), 7.44-7.37 (m, 1H), 7.27-7.16 (m, 2H). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ 157.2, 147.2 (t, J = 26.1 Hz), 144.8, 141.5, 130.8, 129.9, 129.7, 129.0, 128.83, 128.77, 128.6, 127.0, 89.6. ^{19}F NMR (376.3 MHz, $CDCl_3$) δ -81.48 (t, 3F, J = 11.5 Hz), -104.27 (t, 2F, J = 11.5 Hz), -118.32--118.48 (m, 2F), -123.0--123.15 (m, 2F). MS (ESI): m/z = 550 $[M+H]^+$. HRMS: m/z calcd for $C_{19}H_{10}F_9IN$ $(M+H)^+$ 549.9714, found 549.9717.

Characterization of the compounds 4b-4e, 4k-4r and 4t

(4-Bromo-phenyl)-(3-phenyl-1-trifluoromethyl-prop-2-ynyl)-amine (4b)

The indicated compound was obtained in an 98 % yield as a pale brown solid: mp 51 - 52 °C; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.48-7.42 (m, 2H), 7.40-7.28 (m, 5H), 6.65 (d, 2H, J = 9.1 Hz), 4.90-4.78 (m, 1H), 4.01 (s, 1H). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ 143.9, 132.1, 131.9, 129.2, 128.3, 123.6 (q, J = 282.0 Hz), 121.1, 116.1, 112.1, 86.5, 79.9, 50.5 (q, J = 34.7 Hz). ^{19}F NMR (376.3 MHz, $CDCl_3$) δ –75.96 (d, 3F, J = 4.9 Hz).MS (ESI): m/z = 354 $[M+H]^+$. HRMS: m/z calcd for $C_{16}H_{12}F_3NBr$ $[M+H]^+$ 354.0105, found 354.0107.

(4-Fluoro-phenyl)-(3-phenyl-1-trifluoromethyl-prop-2-ynyl)-amine (4c)

The indicated compound was obtained in an 96 % yield as a pale brown oil. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.47-7.41 (m, 2H), 7.37-7.28 (m, 3H), 7.01-6.91 (m, 2H), 6.79-6.70 (m, 2H), 4.83-4.71 (m, 1H), 3.86 (d, 1H, J = 8.3 Hz). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ 157.4 (d, J = 239.3 Hz), 141.2, 131.9, 129.2, 128.4, 123.7, (q, J = 281.8 Hz), 121.2, 116.2 (d, J = 13.2 Hz), 116.0 (d, J = 28.5 Hz), 86.4, 80.3, 51.5 (q, J = 34.3 Hz). ^{19}F NMR (376.3 MHz, $CDCl_3$) δ –76.02 (d, 3F, J = 4.9 Hz), -123.82—123.91 (m, 1F). MS (ESI): m/z = 294 $[M+H]^+$. HRMS: m/z calcd for $C_{16}H_{12}F_4N$ $[M+H]^+$ 294.0905, found 294.0900.

Phenyl-(3-phenyl-1-trifluoromethyl-prop-2-ynyl)-amine(4d)

The indicated compound was obtained in an 96 % yield as a pale yellow oil. ^{1}H NMR

(300 MHz, $CDCl^3$): δ 7.45-7.37 (m, 2H), 7.36-7.16 (m, 5H), 6.88-6.79 (m 1H), 6.74 (d, 2H, J = 8.3 Hz), 4.93-4.80 (m, 1H), 3.94 (d, 1H, J = 8.3 Hz). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ 145.0, 131.9, 129.4, 129.1, 128.3, 123.7 (q, J = 281 Hz), 121.3, 120.2, 114.5, 86.2, 80.5, 50.6 (q, J = 35.1 Hz). ^{19}F NMR (376.3 MHz, CDCl3) δ –76.05 (d, 3F, J = 4.9 Hz). MS (ESI): m/z = 276 $[M+H]^+$. HRMS: m/z calcd for $C_{16}H_{13}F_3N$ $[M+H]^+$ 276.1000, found 276.0999.

Naphthalen-1-yl-(3-phenyl-1-trifluoromethyl-prop-2-ynyl)-amine (4e)

The indicated compound was obtained in an 96 % yield as a pale yellow solid: mp 76 - 77 ^oC; ^1H NMR (200 MHz, $CDCl_3$): δ 7.97-7.73 (m, 2H), 7.55-7.20 (m, 9H), 6.89 (d, 1H, J = 7.0 Hz), 5.15-4.95 (m, 1H), 4.57-4.42 (d, 1H, J =9.4 Hz). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ 140.2, 134.3, 131.9, 129.1, 128.7, 128.3, 126.1, 126.0, 125.6, 124.7, 123.8 (q, J = 281.0 Hz), 121.3, 121.0, 120.2, 108.6, 86.3, 80.6, 50.8 (q, J = 34.1 Hz). ^{19}F NMR (376.3 MHz, $CDCl_3$) δ –75.63 (d, 3F, J = 4.9 Hz). MS (ESI): m/z = 326 $[M+H]^+$. HRMS: m/z calcd for $C_{20}H_{15}F_3N$ $[M+H]^+$ 326.1156, found 326.1155.

(4-Methoxyphenyl)-(3-phenyl-1-trifluoromethyl-prop-2-ynyl)-amine (4k)

The indicated compound was obtained in an 97 % yield as a brown oil. ^1H NMR (300 MHz, $CDCl_3$): δ 7.43-7.37 (m, 2H), 7.34-7.22 (m, 3H), 6.80-6.22 (m, 4H), 4.75-4.64 (m, 1H), 3.73 (s, 3H), 3.65 (s, 1H). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ 154.1, 138.8, 131.9, 129.0, 128.3, 123.7 (q, J = 281.0 Hz), 121.4, 116.8, 114.8, 86.2, 80.8, 55.5, 52.0 (q, J = 35.1 Hz). ^{19}F NMR (376.3 MHz, $CDCl_3$) δ –76.08 (d, J = 6.1 Hz, 3F). MS (ESI): m/z = 306 $[M+H]^+$. HRMS: m/z calcd for $C_{17}H_{15}F_3NO$ $[M+H]^+$ 306.1105, found 306.1114.

(4-Methoxyphenyl)-[3-(4-methoxyphenyl)-1-trifluoromethyl-prop-2-ynyl]-amine (4l)

The indicated compound was obtained in an 95 % yield as a yellow oil. ^1H NMR (300 MHz, $CDCl_3$): δ 7.35-7.29 (m, 2H), 6.81-6.68 (m, 6H), 4.73-4.62 (m, 1H), 3.78 (s, 3H), 3.74 (s, 3H), 3.65 (d, 1H, J = 9.6 Hz). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ 160.3, 154.2, 139.0, 133.5, 123.9 (q, J = 282.0 Hz), 116.9, 114.9, 114.0, 113.5, 86.3, 79.6,

55.6, 55.3, 52.2 (q, J = 34.0 Hz). ^{19}F NMR (376.3 MHz, $CDCl_3$) δ –76.06 (d, 3F, J = 7.4 Hz). MS (ESI): = m/z 336 $[M+H]^+$. HRMS: m/z calcd for $C_{18}H_{16}F_3NO_2Na$ $[M+Na]^+$ 358.1030, found 358.1043.

(3-Methoxyphenyl)-(3-phenyl-1-trifluoromethyl-prop-2-ynyl)-amine (4m)

The indicated compound was obtained in an 98 % yield as a yellow oil. ^{1}H NMR (200 MHz, $CDCl_3$): δ 7.50-7.27 (m, 5H), 7.13 (m, 1H), 6.45-6.28 (m, 3H), 4.97-4.80 (m, 1H), 4.02 (d, 1H, J = 8.8 Hz), 3.79 (s, 3H). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ 160.8, 146.4, 131.9, 130.2, 129.1, 128.3, 123.7 (q, J = 281.0 Hz), 121.3, 107.1, 105.3, 100.7, 86.1, 80.4, 55.1, 50.4 (q, J = 35.1 Hz). ^{19}F NMR (376.3 MHz, $CDCl_3$) δ –76.03 (d, 3F, J = 7.4 Hz). MS (ESI): m/z = 306 $[M+H]^+$. HRMS: m/z calcd for $C_{17}H_{15}F_3NO$ $[M+H]^+$ 306.1105, found 306.1116.

(2-Methoxyphenyl)-(3-phenyl-1-trifluoromethyl-prop-2-ynyl)-amine (4n)

The indicated compound was obtained in an 95 % yield as a pale yellow solid: mp 70 - 71°C; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.52-7.45 (m, 2H), 7.40-7.28 (m, 3H), 6.96-6.88 (m, 1H), 6.86-6.76 (m, 3H), 4.99-4.88 (m, 1H), 4.73 (s, 1H), 3.93 (s, 3H). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ 147.5, 134.8, 131.9, 129.0, 128.3, 123.8 (q, J = 281.0 Hz), 121.4, 121.1, 119.4, 111.6, 110.2, 85.8, 80.7, 55.5, 50.1, (q, J = 35.1 Hz). ^{19}F NMR (376.3 MHz, $CDCl_3$) δ –75.96 (d, 3F, J = 7.4 Hz). MS (ESI): m/z = 306 $[M+H]^+$. HRMS: m/z calcd for $C_{17}H_{15}F_3NO$ $[M+H]^+$ 306.1105, found 306.1116.

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(4-Methoxyphenyl)-(1-pentafluoroethyl-3-phenyl-prop-2-ynyl)-amine (4o)

The indicated compound was obtained in an 97 % yield as a brown oil. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.46-7.39 (m, 2H), 7.38-7.29 (m, 3H), 6.85-6.75 (m, 4H), 4.91-4.76 (m, 1H), 3.79 (s, 3H), 3.59 (d, 1H, J = 10.5 Hz). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ 154.4, 138.8, 131.9, 129.1, 128.4, 121.5, 117.3, 114.9, 87.1, 80.4, 55.6, 51.0, (t, J = 26.3 Hz). ^{19}F NMR (376.3 MHz, $CDCl_3$) δ –81.06 (s, 3F), -120.13 (dd, 1F, J = 268.2 Hz, J = 9.8 Hz), -123.97 (dd, 1F, J = 268 Hz, J = 13 Hz). MS (ESI): m/z = 356 $[M+H]^+$. HRMS: m/z calcd for $C_{18}H_{15}F_5NO$ $[M+H]^+$ 356.1074, found 356.1093.

(4-Methoxyphenyl)-(1-nonafluorobutyl-3-phenyl-prop-2-ynyl)-amine (4p)

The indicated compound was obtained in an 97 % yield as a brown oil. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.45-7.40 (m, 2H), 7.38-7.28 (m, 3H), 6.86-6.75 (m, 4H), 4.99-4.86 (m, 1H), 3.79 (s, 3H), 3.61 (s, 1H). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ 154.3, 138.7, 131.9, 129.1, 128.3, 121.5, 117.2, 114.9, 87.1, 80.4, 55.5, 51.3 (t, J = 26.3 Hz). ^{19}F NMR (376.3 MHz, $CDCl_3$) δ –81.19 (t, 3F, J = 12 Hz), -116.68--117.63 (m, 1F), -119.15--120.13 (m, 1F), -121.58--121.90, (m, 2F), -126.36--126.62 (m, 2F). MS (ESI): m/z = 456 $[M+H]^+$. HRMS: m/z calcd for $C_{20}H_{15}F_9NO$ $[M+H]^+$ 456.1009, found 456.0992.

(4-Methoxyphenyl)-(3-p-tolyl-1-trifluoromethyl-prop-2-ynyl)-amine (4q)

The indicated compound was obtained in an 96 % yield as a pale brown oil. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.33 (d, 2H, J = 8.3 Hz), 7.12 (d, 2H, J = 8.3 Hz), 6.84-6.73 (m, 4H), 4.78-4.67 (m, 1H), 3.78 (s, 3H), 3.70 (d, 1H, J = 9.8 Hz), 2.39 (s, 3H). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ 154.0, 139.3, 138.9, 131.7, 129.0, 123.7 (q, J = 281.0 Hz), 118.3, 116.7, 114.7, 86.4, 80.1, 55.4, 52.0 (q, J = 32.9 Hz), 21.3. ^{19}F NMR (376.3 MHz, $CDCl_3$) δ –76.05 (d, 3F, J = 6.1 Hz). MS (ESI): m/z = 320 $[M+H]^+$. HRMS: m/z calcd for $C_{18}H_{17}F_3NO$ $[M+H]^+$ 320.1262, found 320.1266.

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(4-Methoxyphenyl)-(1-trifluoromethyl-non-2-ynyl)-amine (4r)

The indicated compound was obtained in an 94 % yield as a pale yellow oil. ^{1}H NMR (200 MHz, $CDCl_3$): δ 6.82-6.62 (m, 4H), 4.57-4.36 (m, 1H), 3.75 (s, 3H), 3.54 (d, 1H, J = 9.5 Hz), 2.20 (dt, 2H, J = 6.9, 2.6 Hz), 1.60-1.15 (m, 8H), 0.91 (t, 3H, J = 6.9 Hz). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ 154.0, 139.1, 123.9 (q, J = 281.0 Hz), 116.6, 114.7, 87.4, 72.1, 55.5, 51.5 (q, J = 32.9 Hz), 31.2, 28.3, 28.1, 22.4, 18.5, 13.9. ^{19}F NMR (376.3 MHz, $CDCl_3$) δ –76.49 (d, 3F, J = 6.1 Hz). MS (ESI): m/z = 314 $[M+H]^+$. HRMS: m/z calcd for $C_{17}H_{23}F_3NO$ $[M+H]^+$ 314.1731, found 314.1743.

(3-Cyclohex-1-enyl-1-trifluoromethyl-prop-2-ynyl)-(4-methoxyphenyl)-amine (4t)

The indicated compound was obtained in an 96 % yield as a brown solid: mp 43 - 44 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$): δ 6.80-6.63 (m, 4H), 6.15-6.08 (m, 1H), 4.65-4.48

(m, 1H), 3.73 (s, 3H), 3.56 (s, 1H), 2.15-2.02 (m 4H), 1.69-1.50 (m, 4H). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ 154.0, 139.0, 137.0, 123.8 (q, J = 281.5 Hz), 119.3, 116.7, 114.7, 88.0, 78.0, 55.5, 52.0 (q, J. = 33.9 Hz), 28.7, 25.5, 22.0, 21.2. ^{19}F NMR (376.3 MHz, $CDCl_3$) δ –76.27 (d, 3F, J = 4.9 Hz). MS (ESI): m/z = 310 $[M+H]^+$. HRMS: m/z calcd for $C_{17}H_{19}F_3NO$ $[M+H]^+$ 310.1418, found 310.1415.

Characterization of the compounds 5k-5t

3-Iodo-6-methoxy-4-phenyl-2-(trifluoromethyl)quinoline (5k)

Yellow solid: mp 146 - 147 ^oC; ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.08 (d, 1H, J = 9.4 Hz), 7.60-7.51 (m, 3H), 7.39 (dd, 1H, J = 9.4, 3.0 Hz), 7.24-7.19 (m, 2H), 6.54 (d, 1H, J = 3.0 Hz), 3.67 (s, 3H). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ 159.9, 155.2, 145.2 (q, J = 32.9 Hz), 141.6, 141.3, 131.5, 130.3, 128.89, 128.86, 128.83, 123.5, 121.5 (q, J = 276 Hz), 104.7, 90.3, 55.4. ^{19}F NMR (376.3 MHz, $CDCl_3$) δ –64.95 (s, 3F). MS (ESI): m/z = 430 $[M+H]^+$. HRMS: m/z calcd for $C_{17}H_{12}F_3INO$ $[M+H]^+$ 429.9915, found 429.9915.

3-Iodo-6-methoxy-4-(p-methoxyphenyl)-2-(trifluoromethyl)quinoline (5l)

Pale yellow solid: mp 154 - 155 ^oC; ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.10 (d, 1H, J = 9.2 Hz), 7.41 (dd, 1H, J = 9.2, 2.8 Hz), 7.18-7.06 (m, 4H), 6.65 (d, 1H, J = 2.8 Hz), 3.95 (s, 3H), 3.73 (s, 3H). ^{13}C NMR (50.3 MHz, $CDCl_3$): δ 159.8, 159.7, 155.1, 144.9 (q, J = 33.6 Hz), 141.3, 133.9, 131.4, 130.6, 130.1, 123.5, 121.5 (q, J = 274.7 Hz), 114.2, 104.7, 91.3, 55.4, 55.3. ^{19}F NMR (376.3 MHz, $CDCl_3$) δ –65.98 (s, 3F). MS (ESI): m/z 460 $[M+H]^+$. HRMS: m/z calcd for $C_{18}H_{14}F_3INO_2$ $(M+H)^+$ 460.0021, found 460.0018.

3,6-Diiodo-7-methoxy-4-phenyl-2-(trifluoromethyl)quinoline (5m)

Pale yellow solid: mp 179 – 180 ^oC; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.84 (s, 1H), 7.65-7.56 (m, 3H), 7.45 (s, 1H), 7.25-7.20 (m, 2H), 4.10 (s, 3H). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ 159.3, 155.6, 147.9 (q, J = 32.9 Hz), 146.8, 140.7, 137.9, 129.1,

128.9, 128.7, 121.2 (q, J = 276.6 Hz), 125.3, 107.3, 93.5, 87.4, 57.0. ^{19}F NMR (376.3 MHz, $CDCl_3$) δ –65.50 (s, 3F). MS (ESI): m/z 556 $[M+H]^+$. HRMS: m/z calcd for $C_{17}H_{11}F_3I_2NO$ $[M+H]^+$ 555.8883, found 555.8864.

3-Iodo-8-methoxy-4-phenyl-2-(trifluoromethyl)quinoline (5n)

Pale yellow solid: mp 199 - 200 °C; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.59-7.50, (m, 3H), 7.39 (t, 1H, J = 8.3 Hz), 7.23-7.18 (m, 2H), 7.08 (d, 1H, J = 7.5 Hz), 6.92 (d, 1H, J = 7.5 Hz), 4.11 (s, 3H). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ 156.9, 155.8, 146.1 (q, J = 32.8 Hz), 141.6, 137.2, 130.2, 129.94, 128.84, 128.76, 128.67, 121.3 (q, J = 276.3 Hz), 118.6, 109.0, 90.81, 56.5. ^{19}F NMR (376.3 MHz, $CDCl_3$) δ –65.10 (s, 3F). MS (ESI): m/z 430 $[M+H]^+$. HRMS: m/z calcd for $C_{17}H_{12}F_3INO$ $[M+H]^+$ 429.9915, found 429.9927.

3-Iodo-6-methoxy-2-(pentafluoroethyl)-4-phenyl-quinoline (5o)

White solid: mp 129 – 130 °C; ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.05 (d, 1H, J = 9.1 Hz), 7.61-7.50 (m, 3H), 7.37 (dd, 1H, J = 9.1, 3.0 Hz), 7.22-7.18 (m, 2H), 6.52 (d, 1H, J.=3.0 Hz), 3.67 (s, 3H). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ 160.1, 155.2, 144.4 (t, J = 26.5 Hz), 141.7, 141.0, 131.6, 130.1, 128.89, 128.85, 128.81, 123.5, 104.7, 90.2, 55.4. ^{19}F NMR (376.3 MHz, $CDCl_3$) δ –79.88 (s, 3F), -106.92 (s, 2F). MS (ESI): m/z = 480 $[M+H]^+$. HRMS: m/z calcd for $C_{18}H_{12}F_5INO$ $[M+H]^+$ 479.9883, found 479.9867.

3-Iodo-6-methoxy-2-(nonafluorobutyl)-4-phenyl-quinoline (5p)

White solid: mp 90 – 91 °C; ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.05 (d, 1H, J = 9.1 Hz), 7.61-7.50 (m, 3H), 7.38 (dd, 1H, J = 9.1, 3.0 Hz), 7.22-7.18 (m, 2H), 6.52 (d, 1H, J = 3.0 Hz), 3.67 (s, 3H). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ 160.2, 155.3, 144.5 (t, J = 27.2 Hz), 141.9, 141.1, 131.4, 130.1, 128.94, 128.89, 128.80, 123.6, 104.7, 90.4, 55.4. ^{19}F NMR (376.3 MHz, $CDCl_3$) δ –81.52 (t, 3F, J = 12.0 Hz), -104.08 (t, 2F, J = 12.0 Hz), -118.51--118.68 (m, 2F), -123.28--123.45 (m, 2F). MS (ESI): m/z = 580 $[M+H]^+$. HRMS: m/z calcd for $C_{20}H_{12}F_9INO$ $[M+H]^+$ 579.9819, found 579.9791.

3-Iodo-6-methoxy-4-p-tolyl-2-(trifluoromethyl)quinoline (5q)

White solid: mp 188 - 189 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.10 (d, 1H, J = 9.1 Hz), 7.44-7.36 (m, 3H), 7.12 (d, 2H, J = 7.5 Hz), 6.61 (d, 1H, J = 2.23 Hz), 3.27 (s, 3H), 2.54 (s, 3H). ^{13}C NMR (100.6 MHz, $CDCl_3$): δ 159.9, 155.4, 145.0 (q, J = 33.5 Hz), 141.3, 138.69, 138.65, 131.4, 130.5, 129.5, 128.7, 123.5, 121.5 (q, J = 276.0 Hz), 104.8, 90.7, 55.5, 21.5. ^{19}F NMR (376.3 MHz, $CDCl_3$) δ –64.95 (s, 3F). MS (ESI): m/z 444 $[M+H]^+$. HRMS: m/z calcd for $C_{18}H_{14}F_3INO$ $[M+H]^+$ 444.0072, found 444.0052.

4-Hexyl-3-iodo-6-methoxy-2-(trifluoromethyl)quinoline (5r)

White solid: mp 70 - 71 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.05 (d, 1H, J = 9.0 Hz), 7.40 (dd, 1H, J = 9.0, 2.6 Hz), 7.22 (d, 1H, J = 2.6 Hz), 4.0 (s, 3H), 3.35-3.27 (m, 2H), 1.72-1.53 (m, 4H), 1.49-1.32 (m, 5H), 0.94 (t, 3H, J = 6.8 Hz). ^{13}C NMR (75.5 MHz, $CDCl_3$): δ 160.0, 153.4, 145.1 (q, J = 32.9 Hz), 141.1, 132.2, 129.2, 122.9, 121.4 (q, J = 276.6 Hz), 102.4, 90.9, 55.6, 38.4, 31.4, 29.5, 28.4, 22.5, 13.9. ^{19}F NMR (376.3 MHz, $CDCl_3$) δ –64.87 (s, 3F). MS (ESI): m/z = 438 $[M+H]^+$. HRMS: m/z calcd for $C_{17}H_{20}F_3INO$ $[M+H]^+$ 438.0541, found 438.0539.

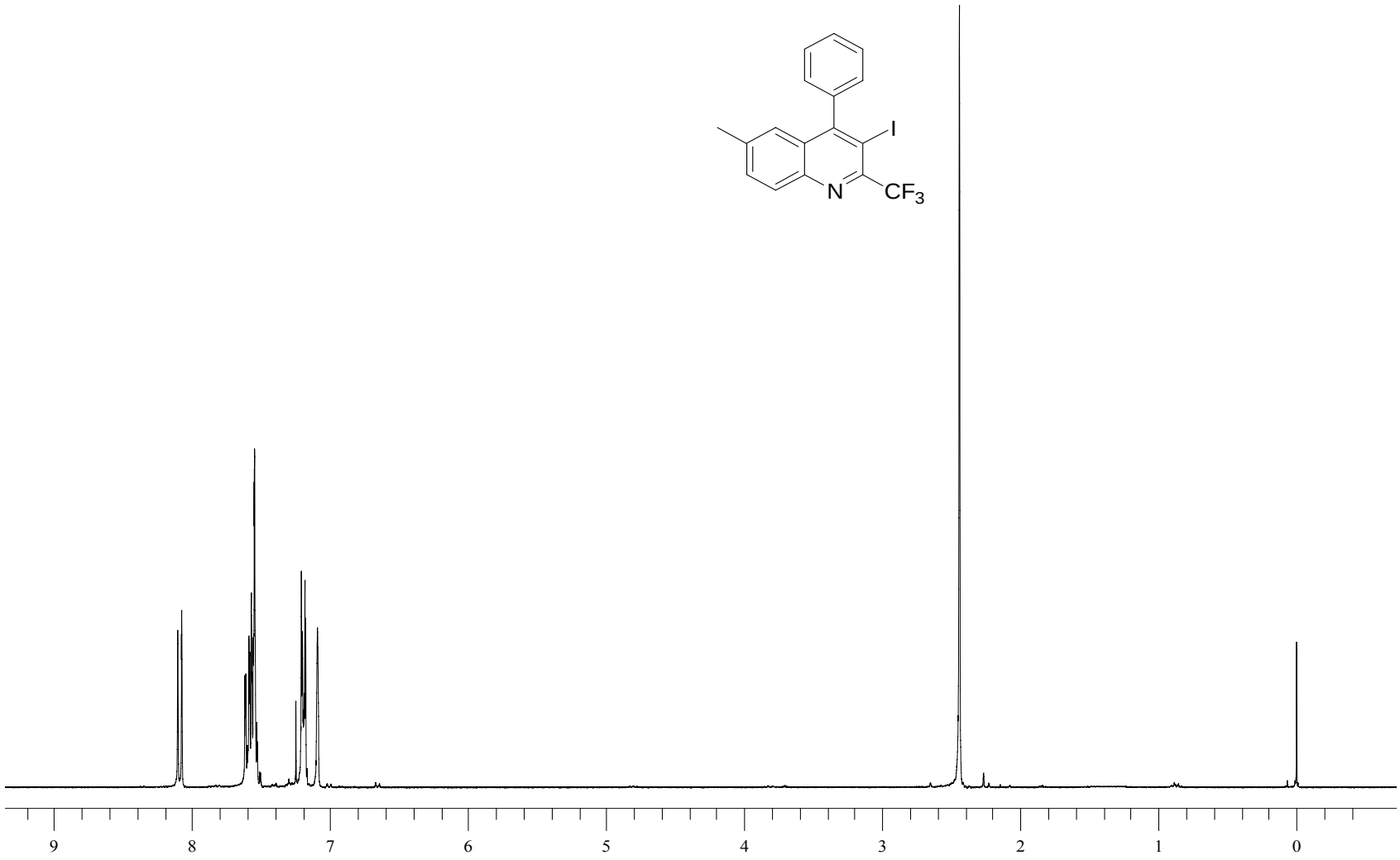
(3-Iodo-6-methoxy-2-trifluoromethyl quinolin-4-yl)-methanol (5s)

The reaction mixture was chromatographed using 10:2 hexane/EtOAc. Pale brown solid: mp 163 - 164 °C; ^{1}H NMR (200 MHz, DMSO D6): δ 8.00 (d, 1H, J = 9.0 Hz), 7.64 (d, 1H, J = 2.6 Hz), 7.42 (dd, 1H, J = 9.0, 2.6 Hz), 5.41 (s, 1H), 5.25 (s, 2H), 4.0 (s, 3H). ^{13}C NMR (75.5 MHz, DMSO D6): δ 159.6, 150.8, 143.8 (q, J = 32.2 Hz), 140.7, 131.3, 129.4, 123.6, 121.6 (q, J = 276.0 Hz), 103.4, 91.7, 65.3, 55.8. ^{19}F NMR (376.3 MHz, $CDCl_3$) δ –64.83 (s, 3F). MS (ESI): m/z = 384 $[M+H]^+$. HRMS: m/z calcd for $C_{12}H_{10}F_3INO_2$ $[M+H]^+$ 383.9708, found 383.9694.

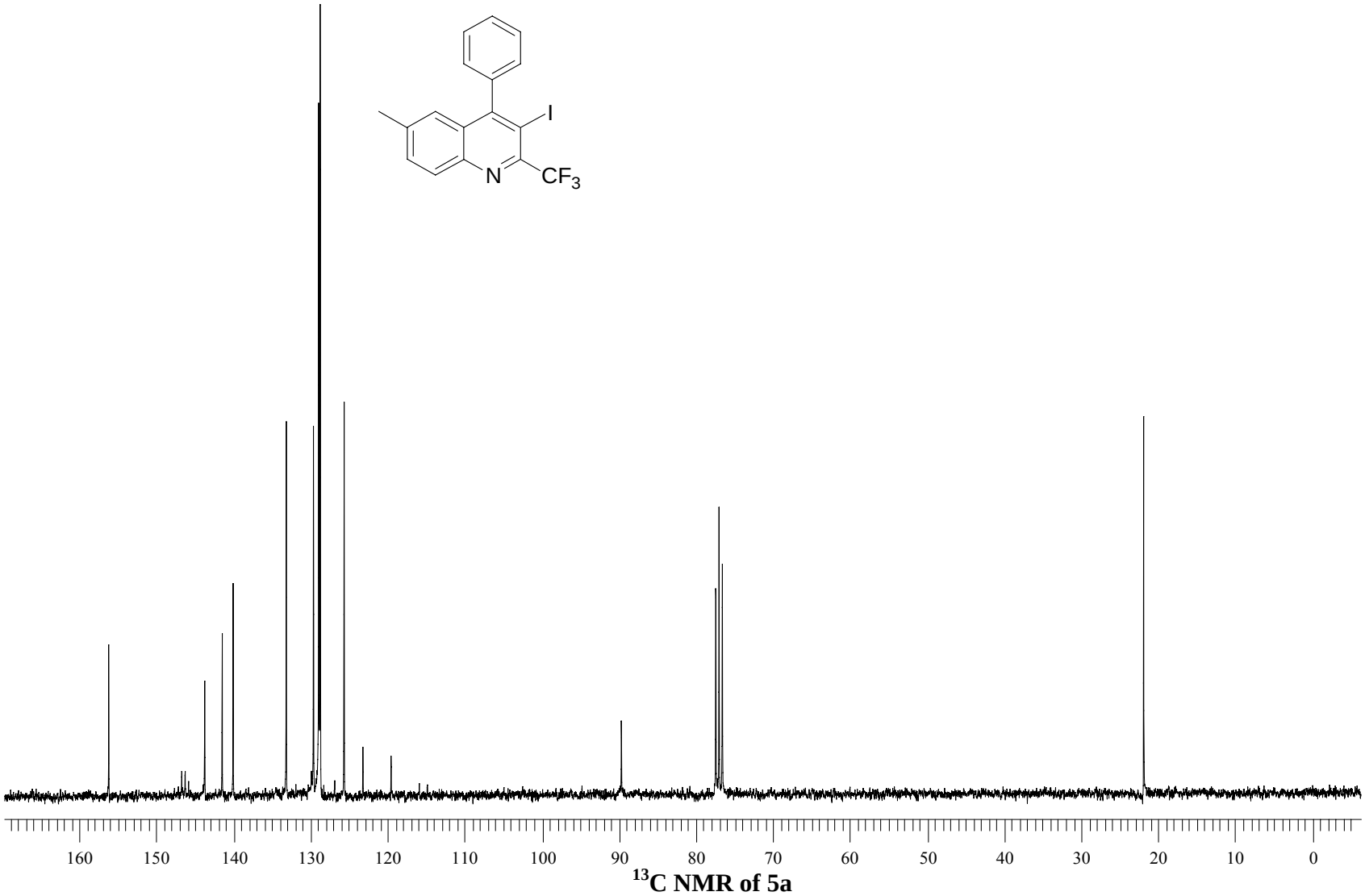
4-Cyclohex-1-enyl-3-iodo-6-methoxy-2-(trifluoromethyl)quinoline (5t)

Pale yellow solid: mp 144 – 145 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.06 (d, 1H, J = 9.4 Hz), 7.41 (dd, 1H, J = 9.4, 2.3 Hz), 7.16 (d, 1H, J = 2.3 Hz), 5.74-5.69 (m, 1H), 3.94 (s, 3H), 2.48-2.30 (m, 3H), 2.24-2.06 (m, 1H), 2.05-1.77 (m, 4H). ^{13}C NMR

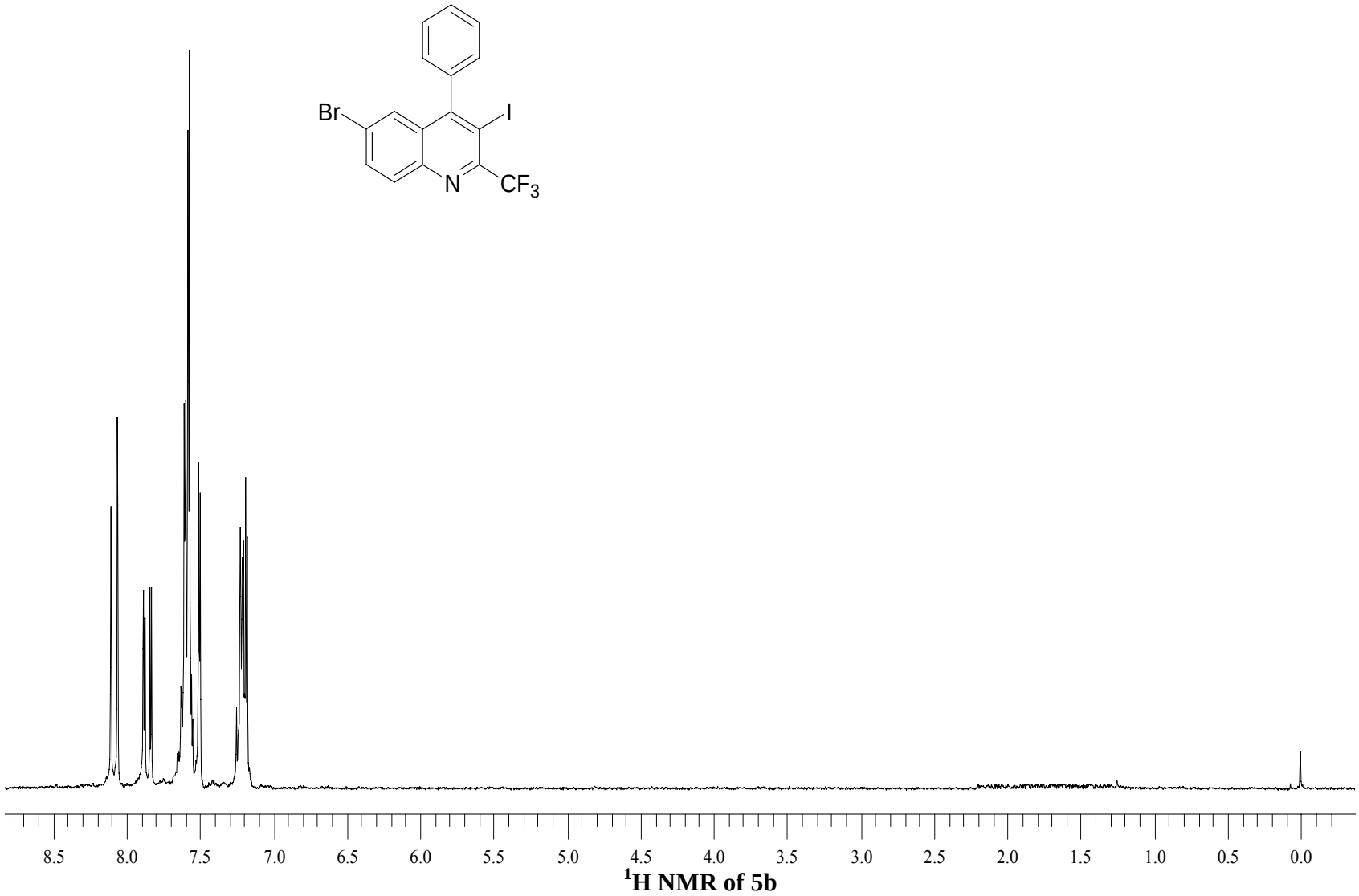
(75.5 MHz, $CDCl_3$): δ 159.8, 157.1, 145.0 (q, J = 32.9 Hz), 141.3, 139.2, 131.5, 129.6, 129.3, 121.4 (q, J = 276.6), 123.1, 104.1, 89.2, 55.4, 28.3, 25.2, 22.7, 21.8. ^{19}F NMR (376.3 MHz, $CDCl_3$) δ -64.90(s,3F). MS (ESI): m/z = 434 $[M+H]^+$. HRMS: m/z calcd for $C_{17}H_{16}F_3INO$ $[M+H]^+$ 434.0228, found 434.0225.



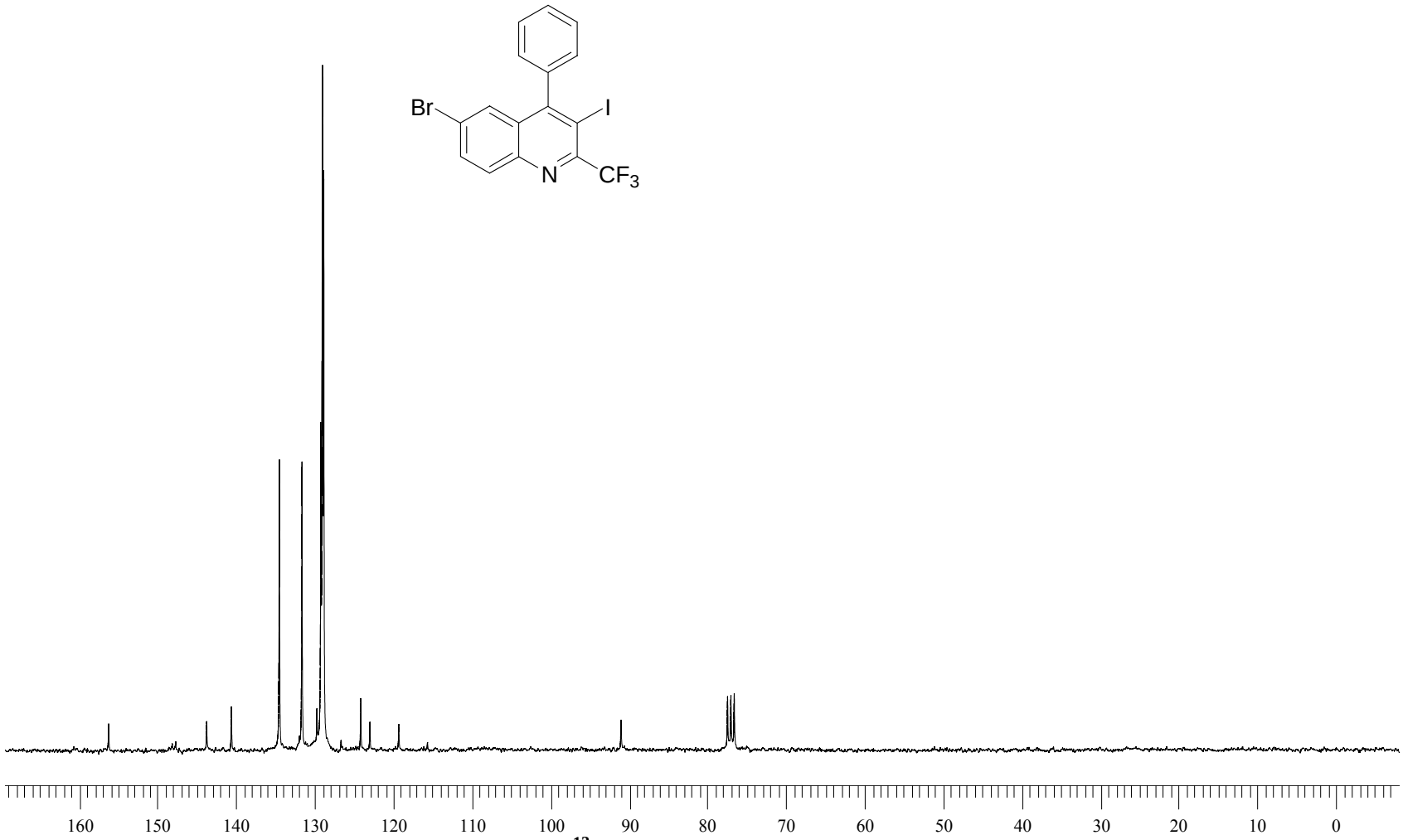
^{1}H NMR of 5a



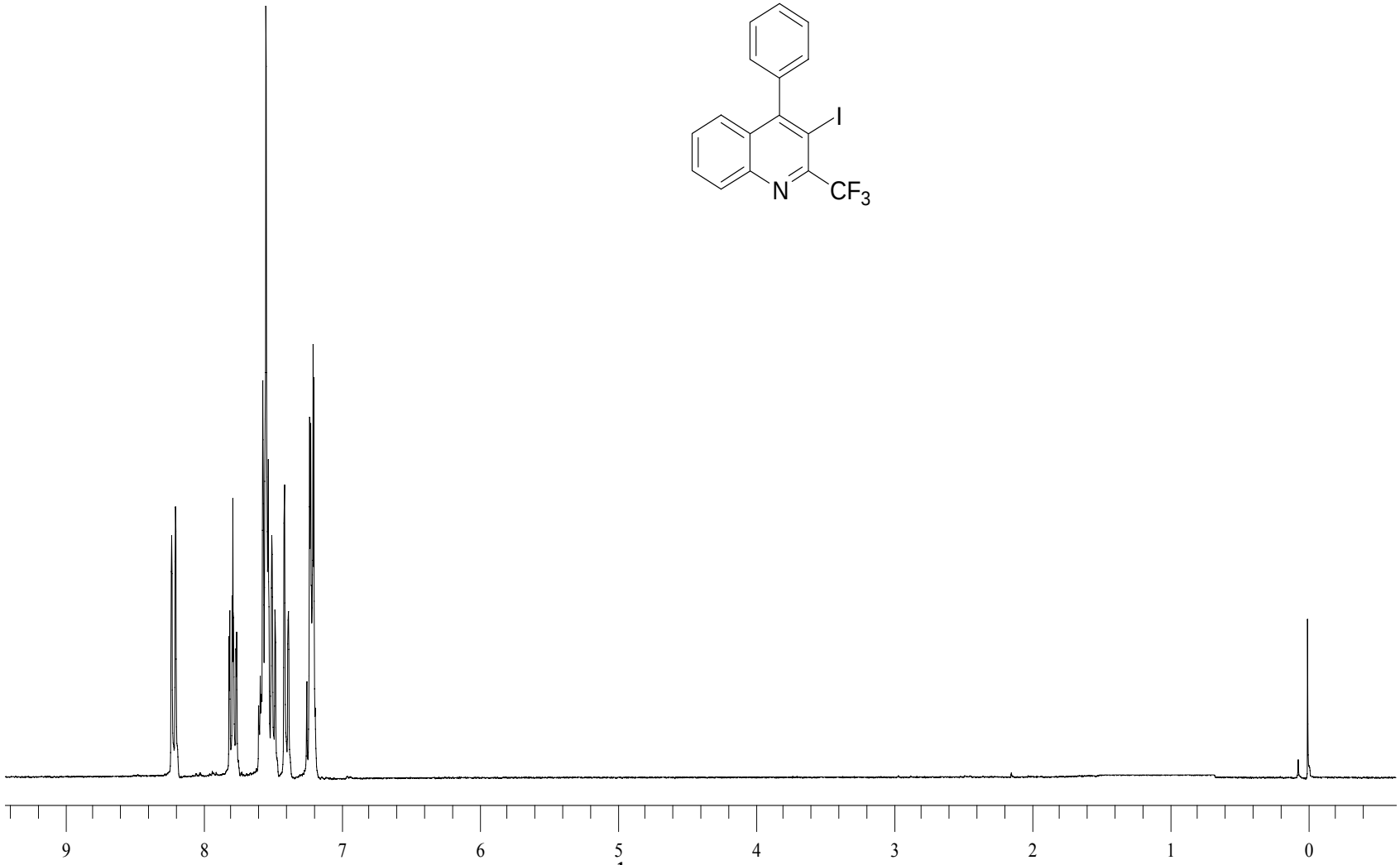
^{13}C NMR of 5a



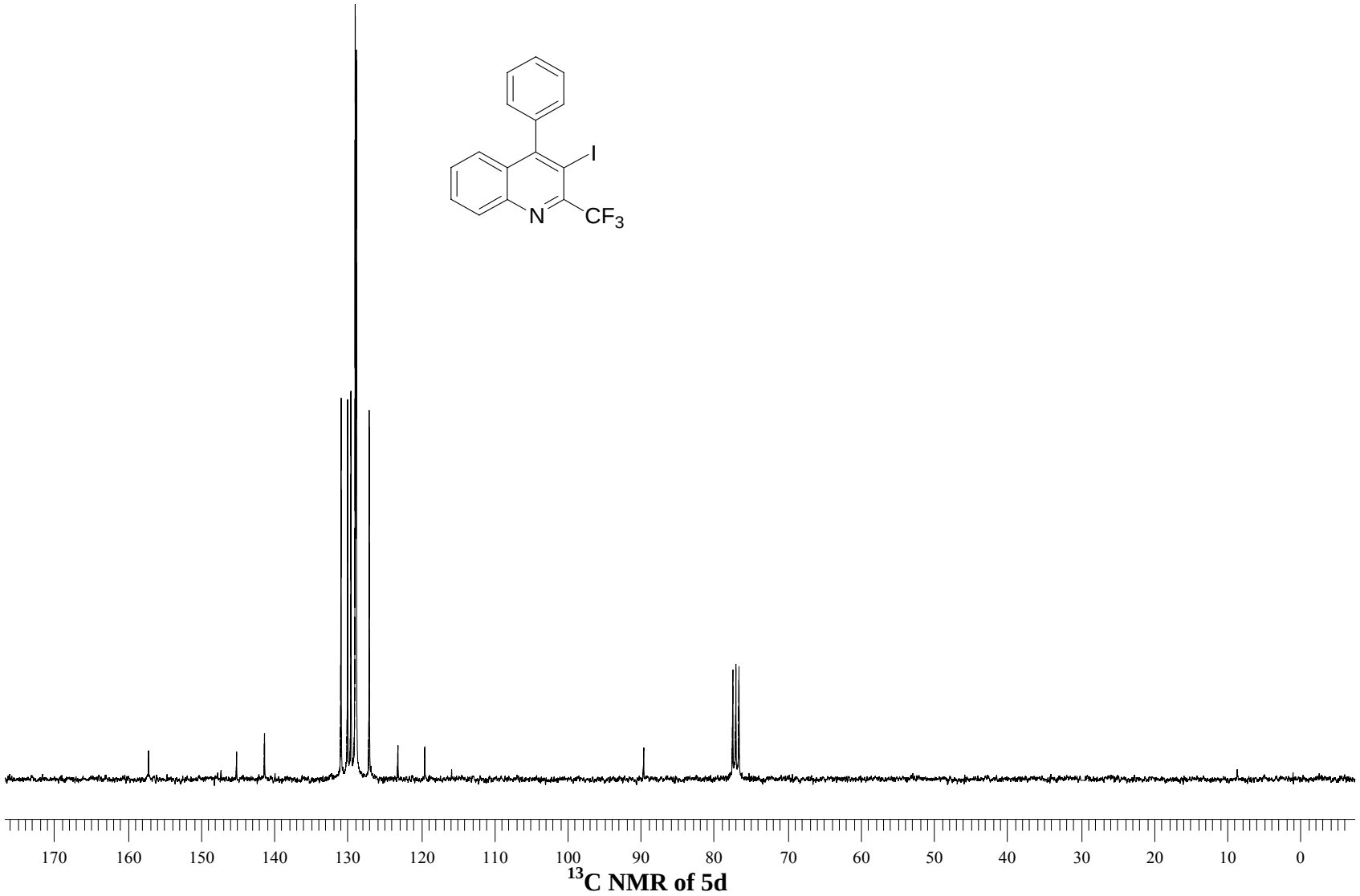
^{1}H NMR of 5b



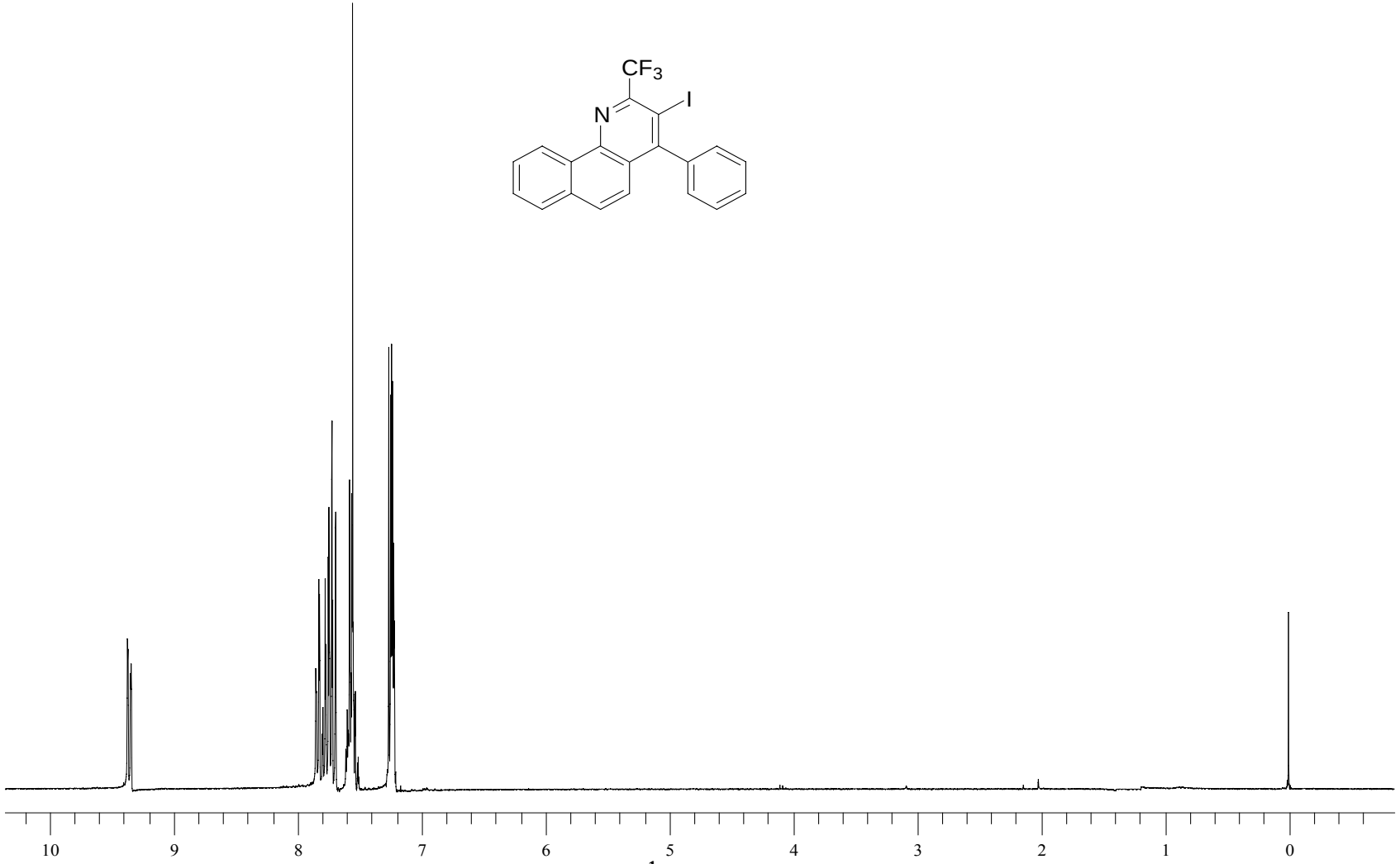
^{13}C NMR of 5b



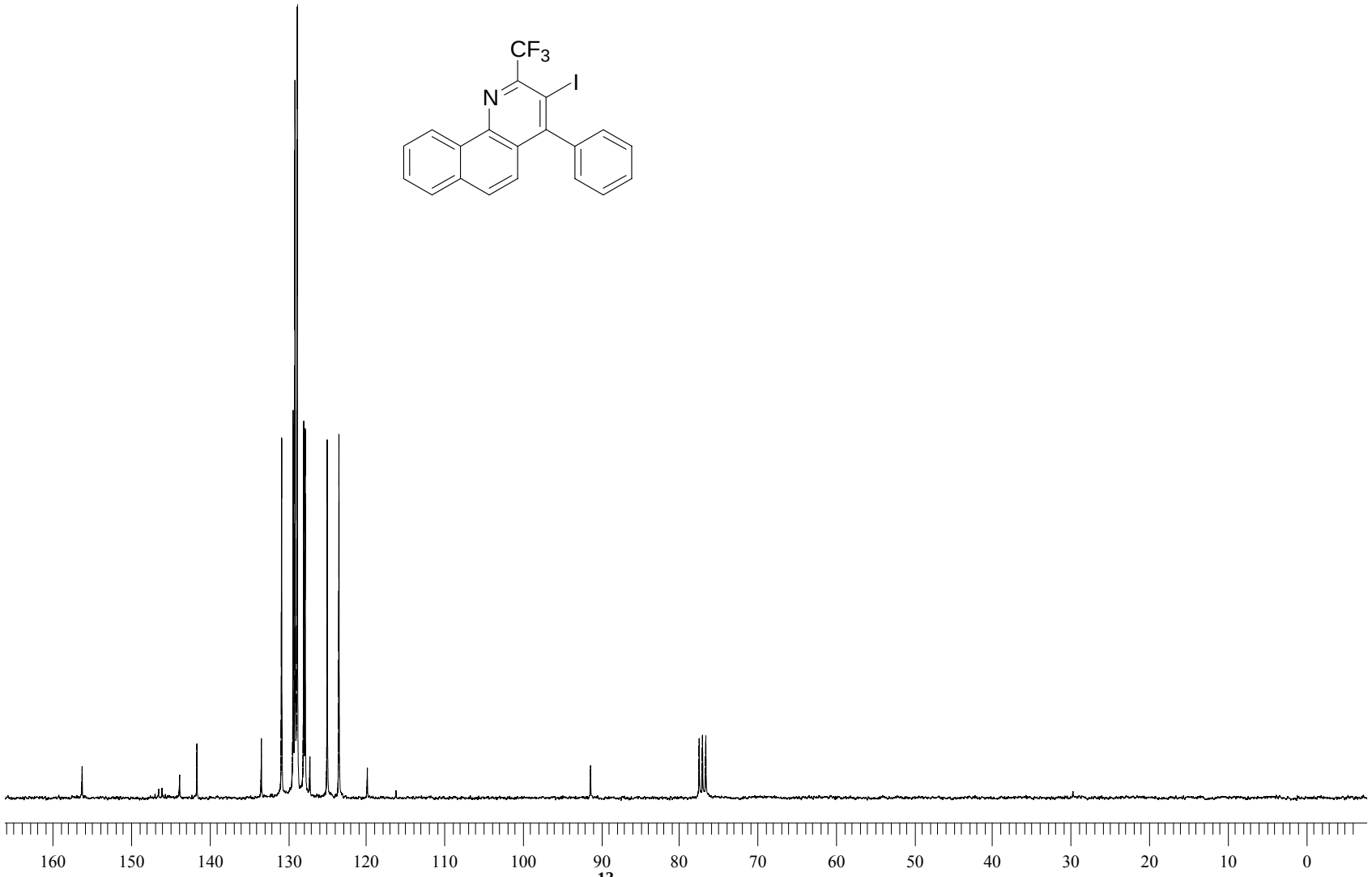
^{1}H NMR of 5d



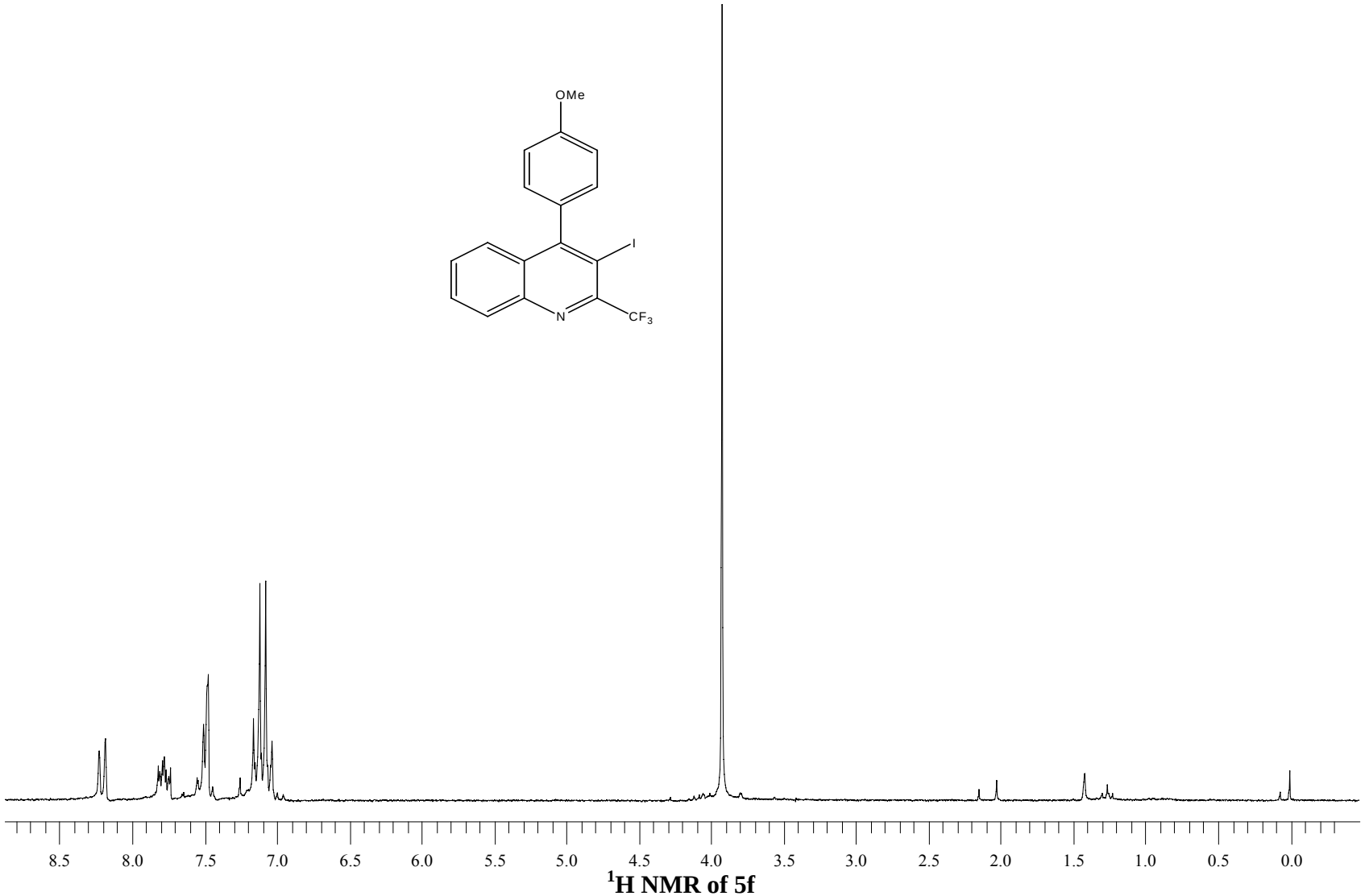
^{13}C NMR of 5d



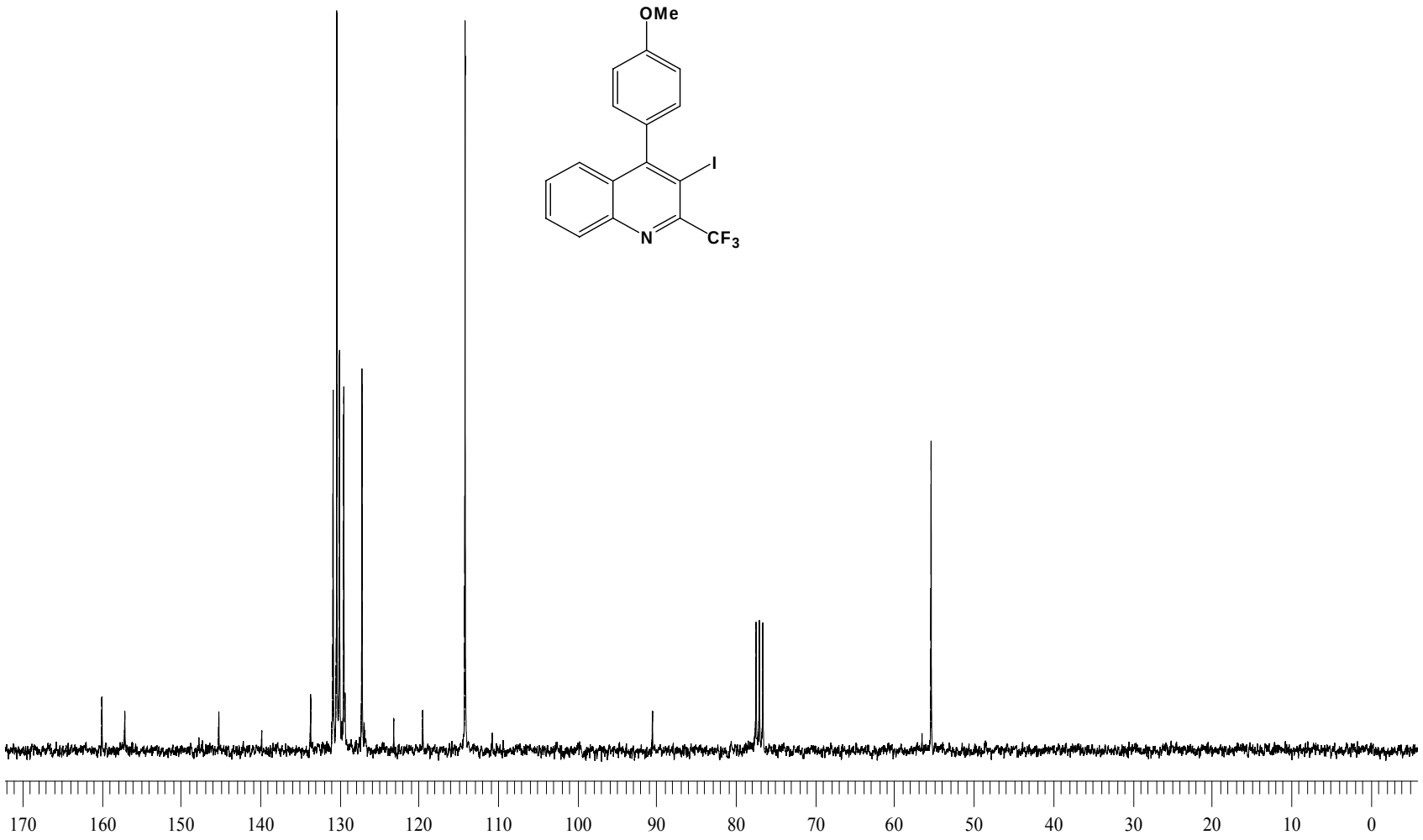
^{1}H NMR of 5e



^{13}C NMR of 5e



^{1}H NMR of 5f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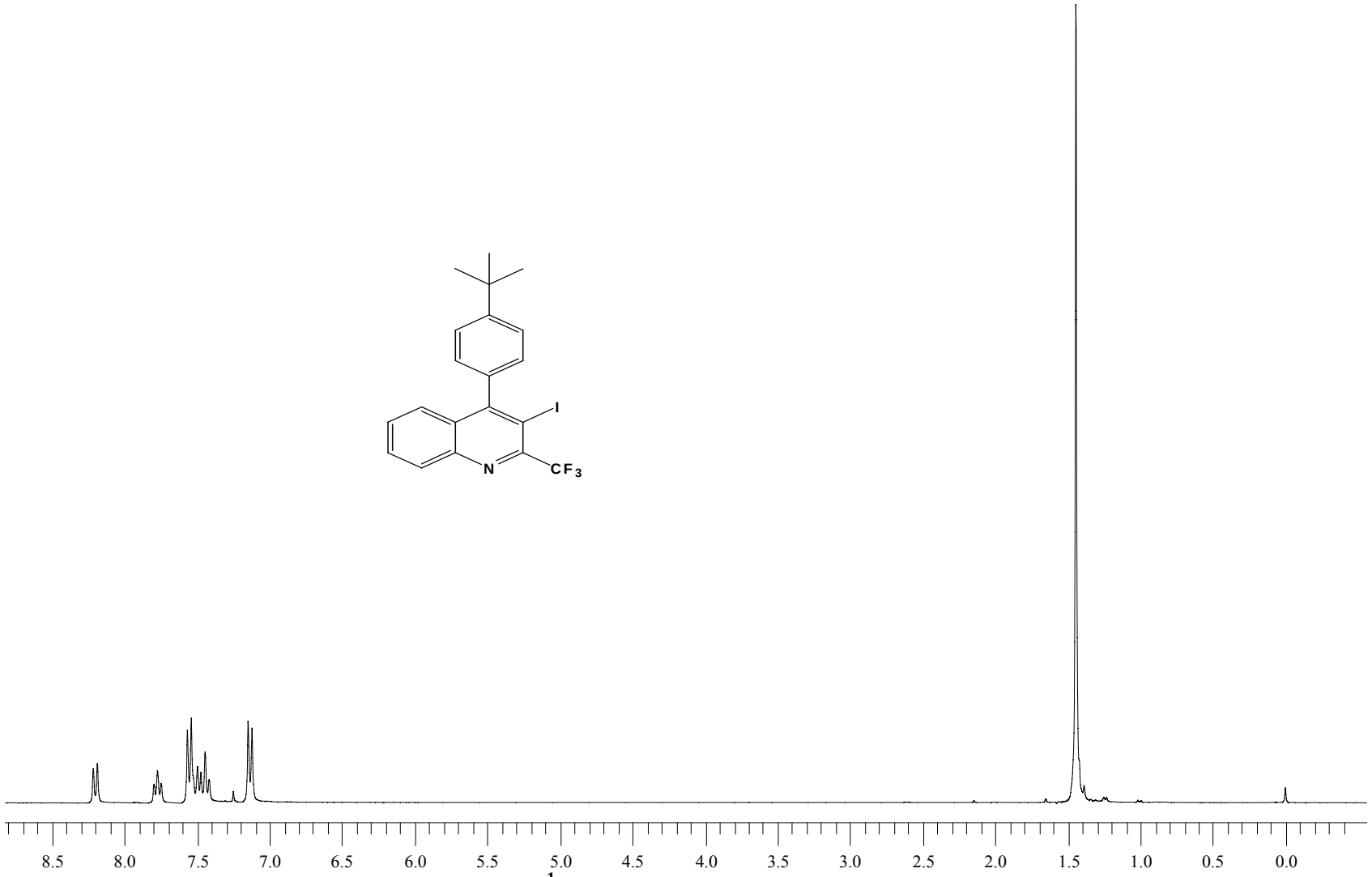
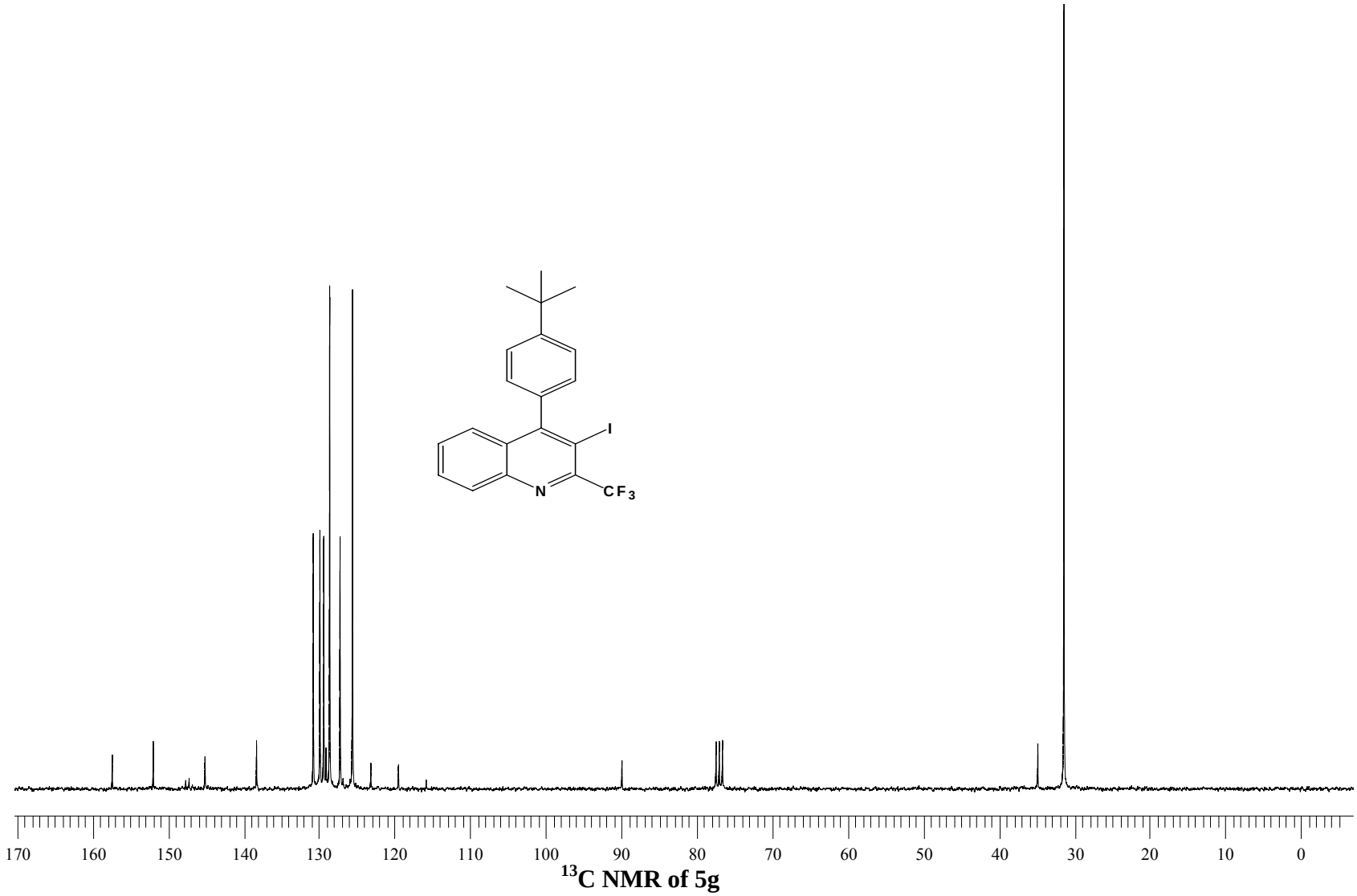
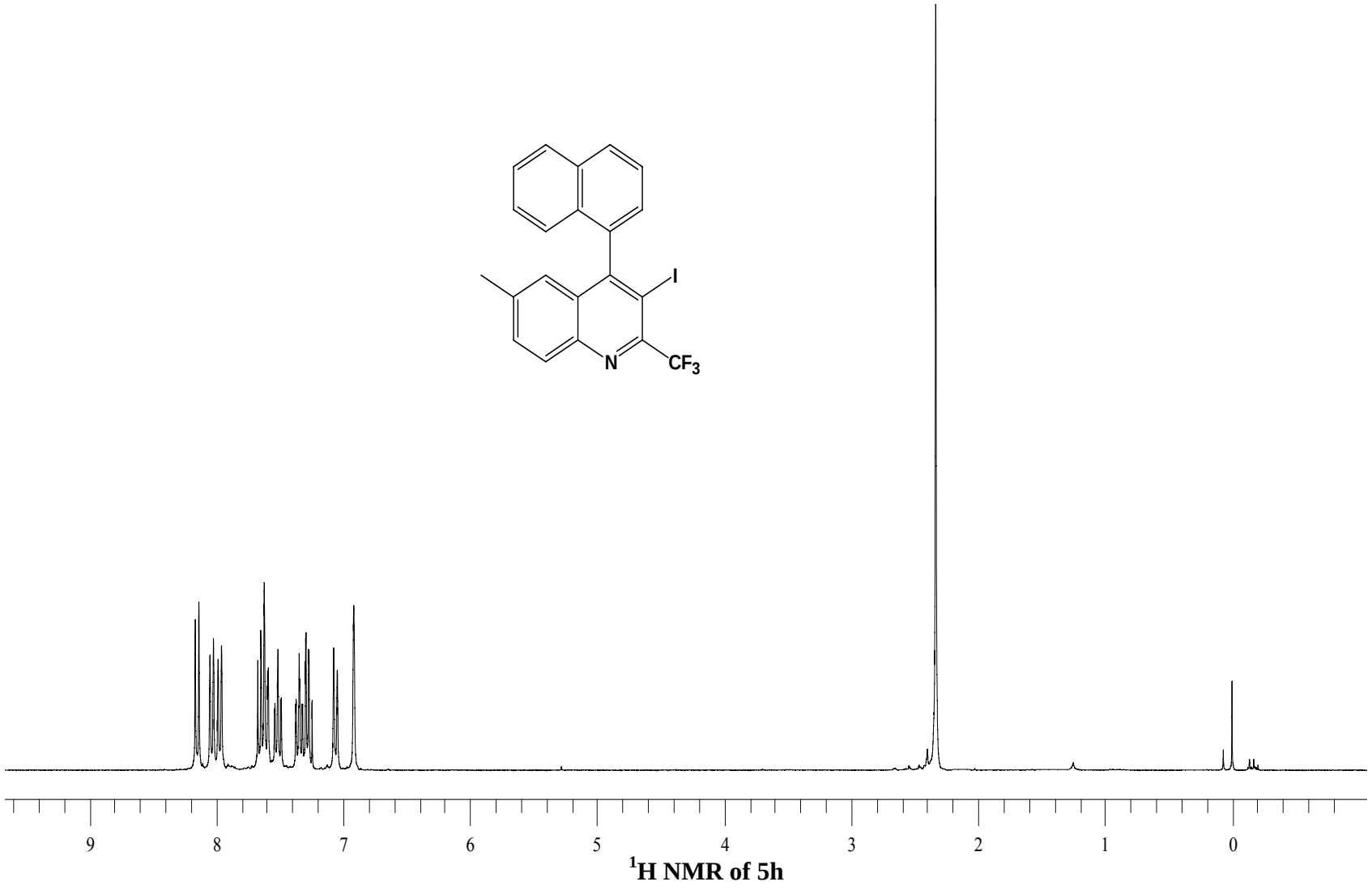
^{13}C NMR of 5f



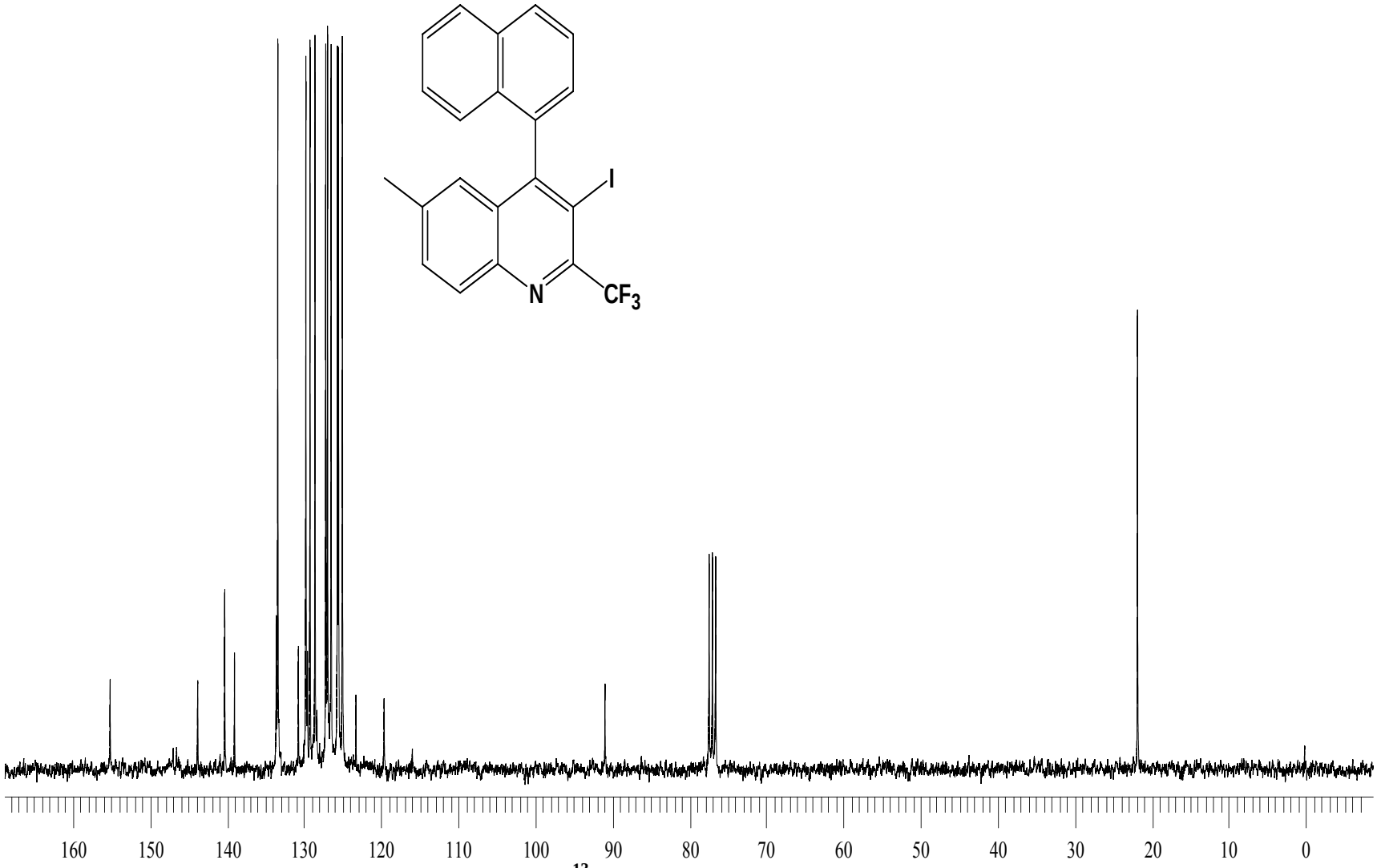
^{1}H NMR of 5g



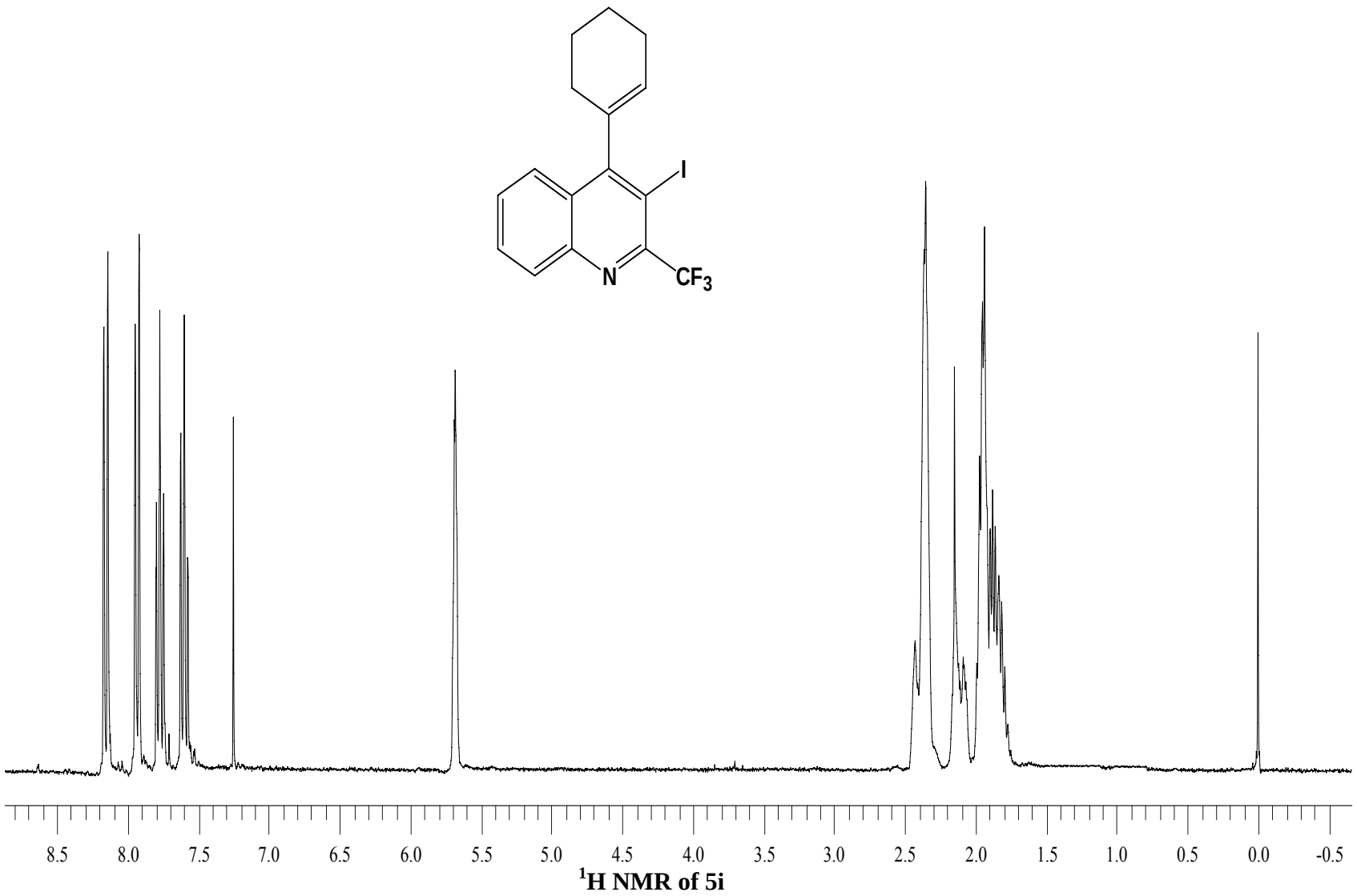
^{13}C NMR of 5g



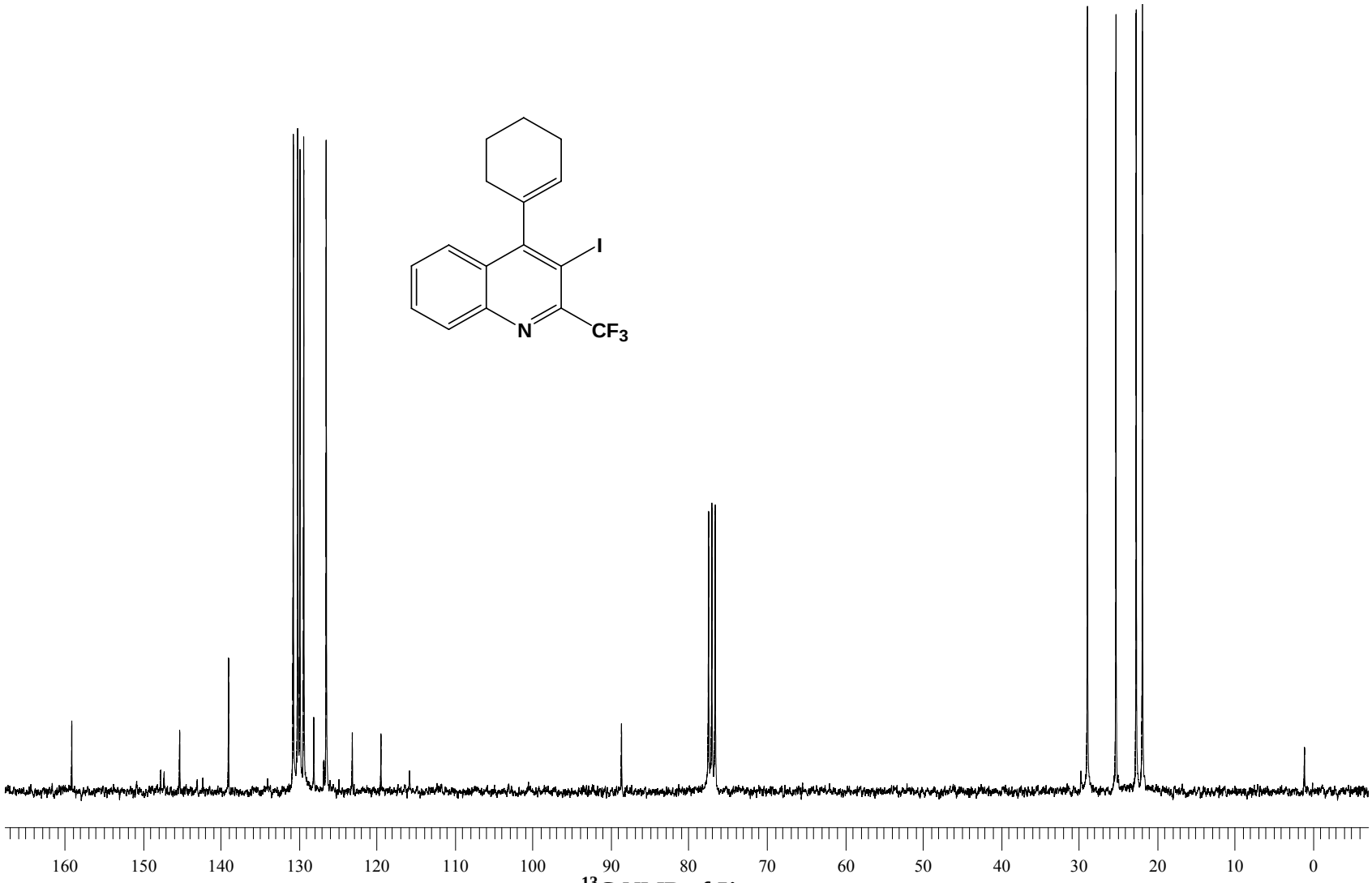
^{1}H NMR of 5h



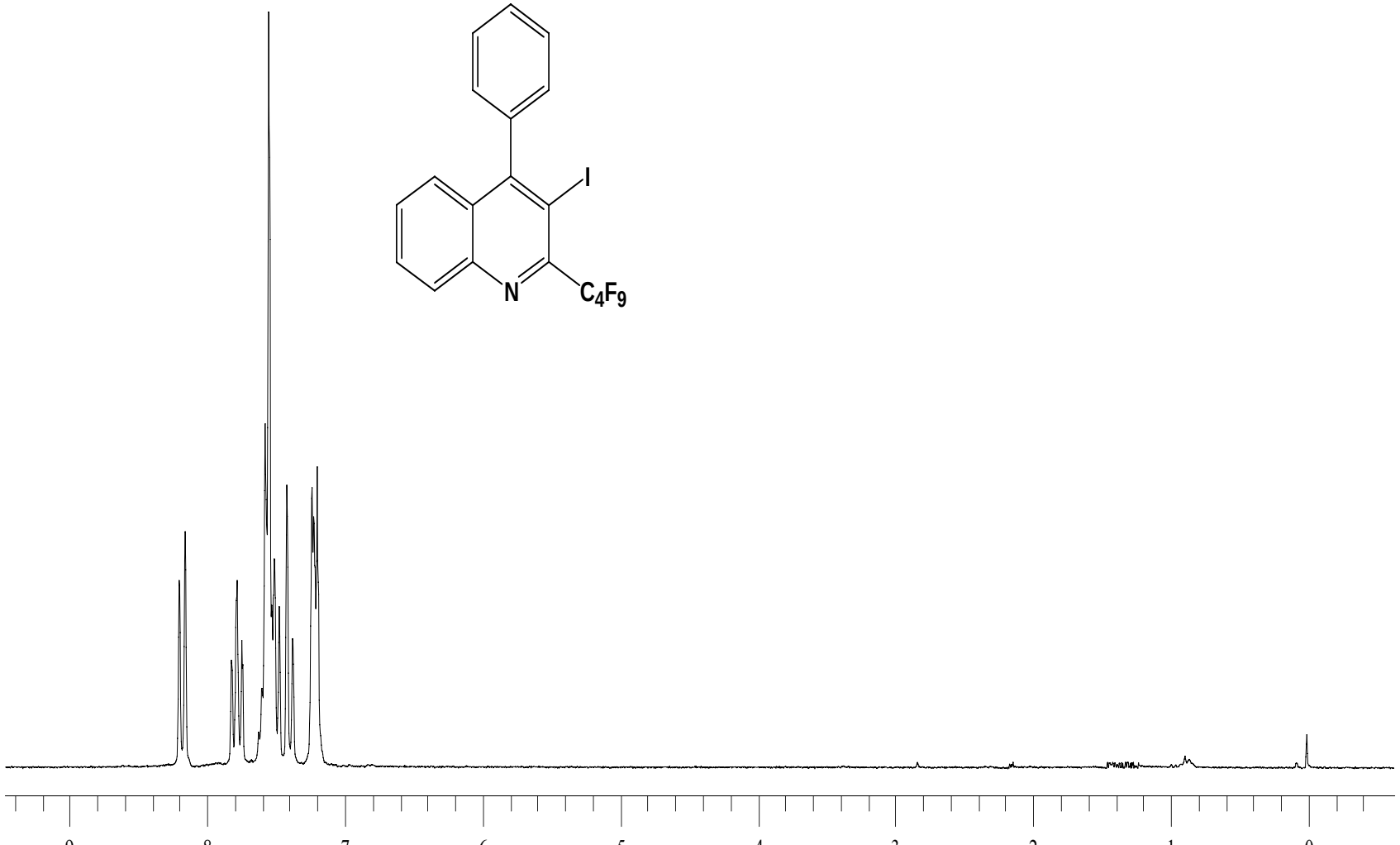
^{13}C NMR of 5h



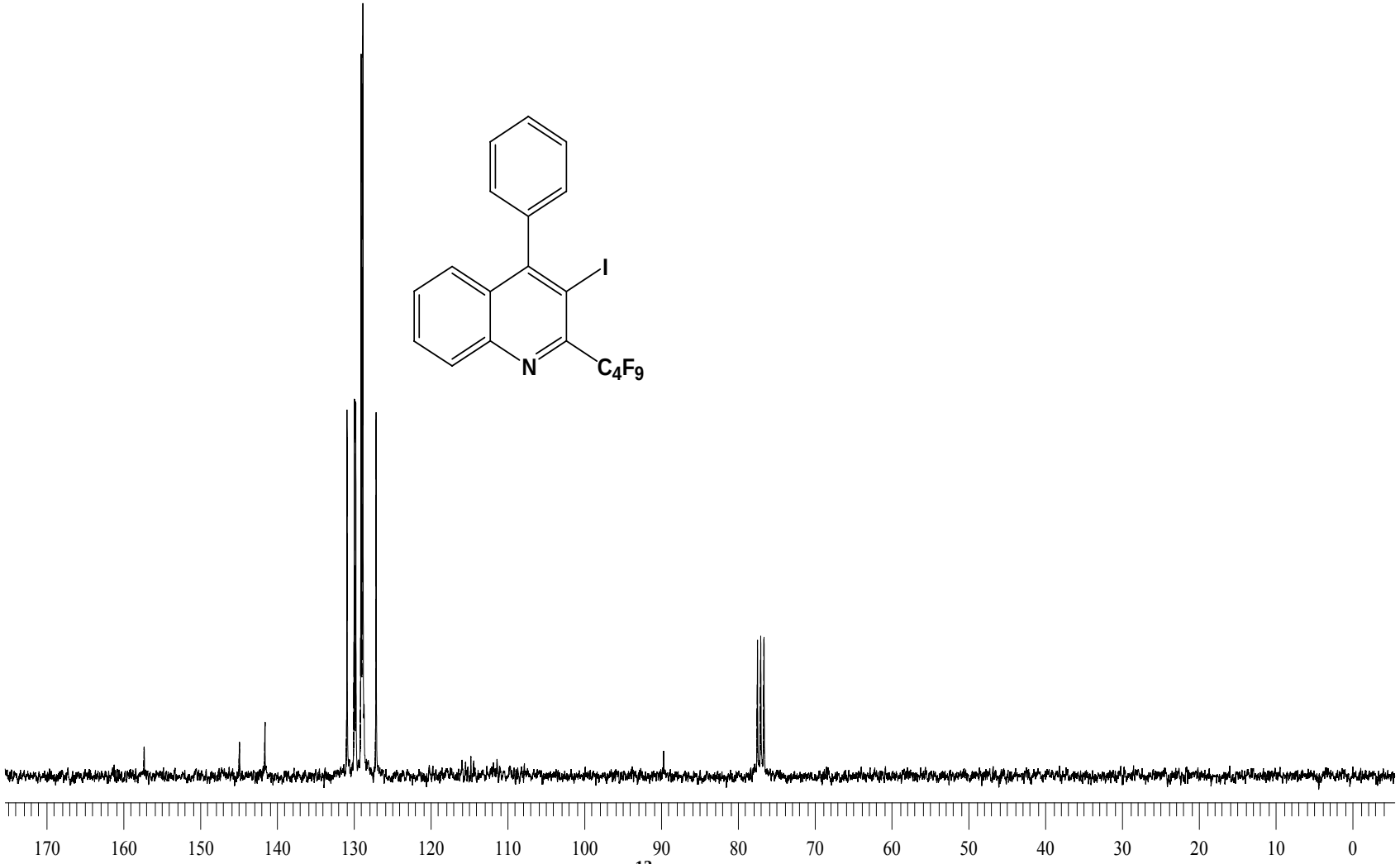
^{1}H NMR of 5i



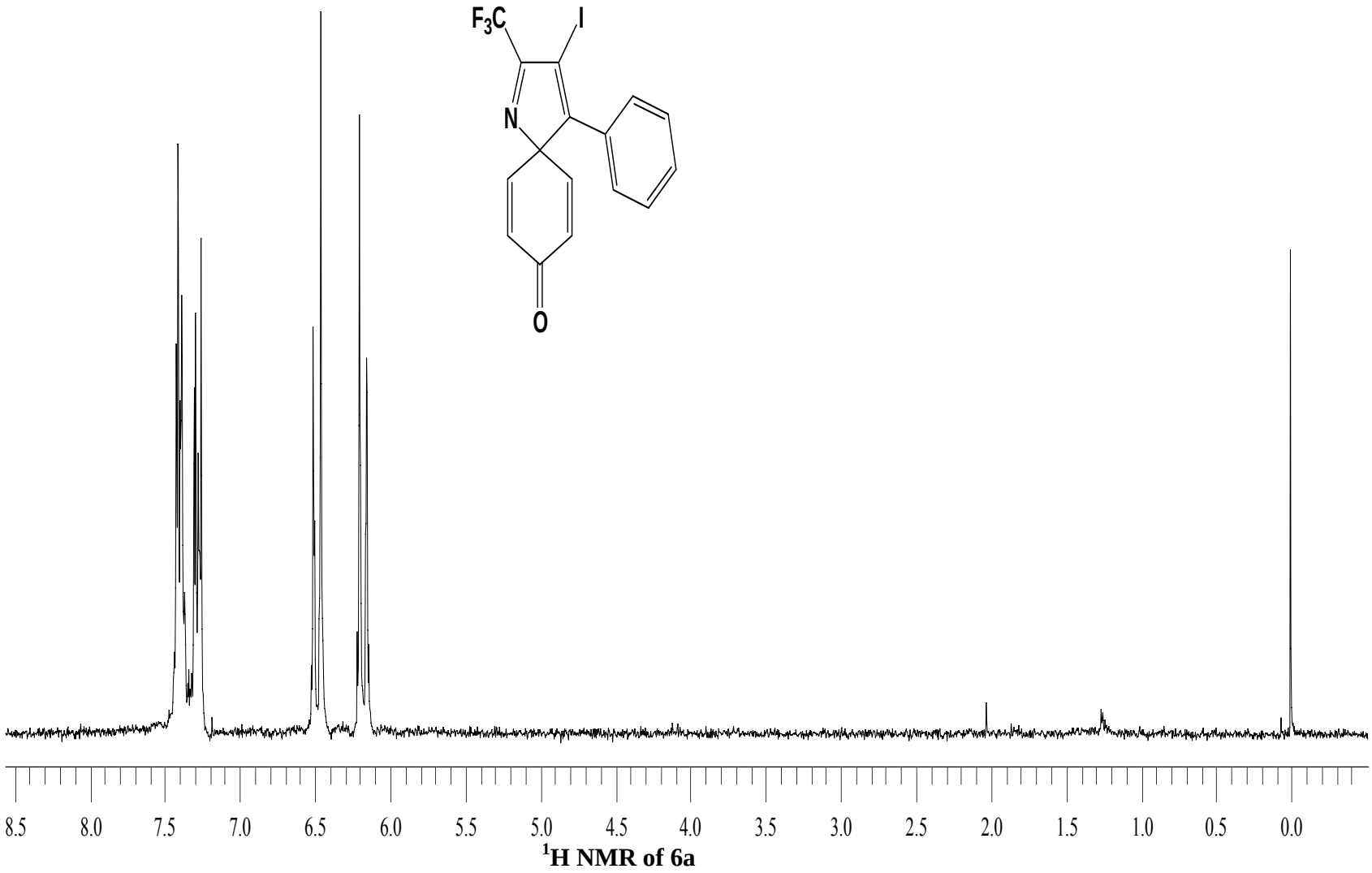
^{13}C NMR of 5i



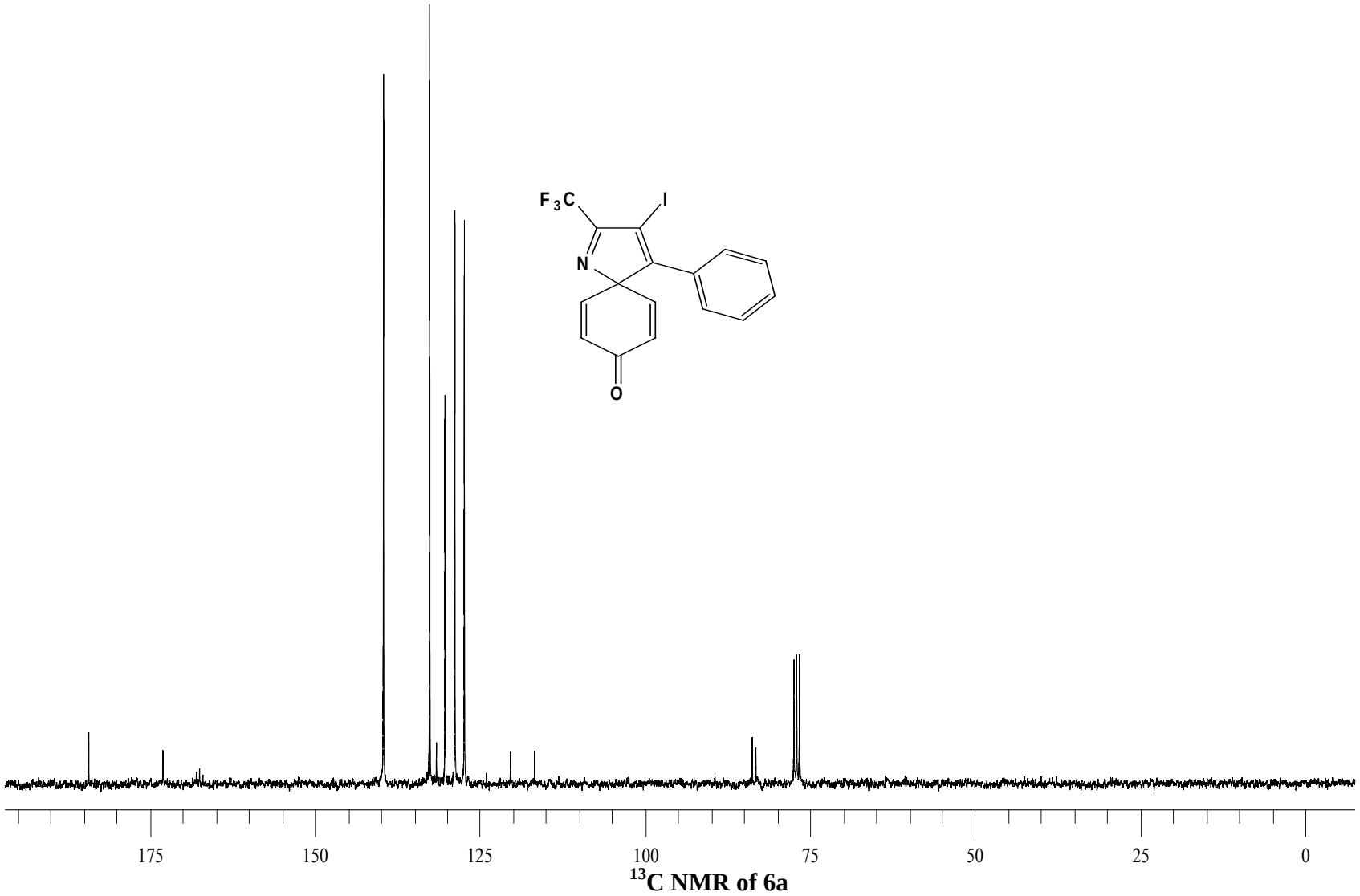
^{1}H NMR of 5j



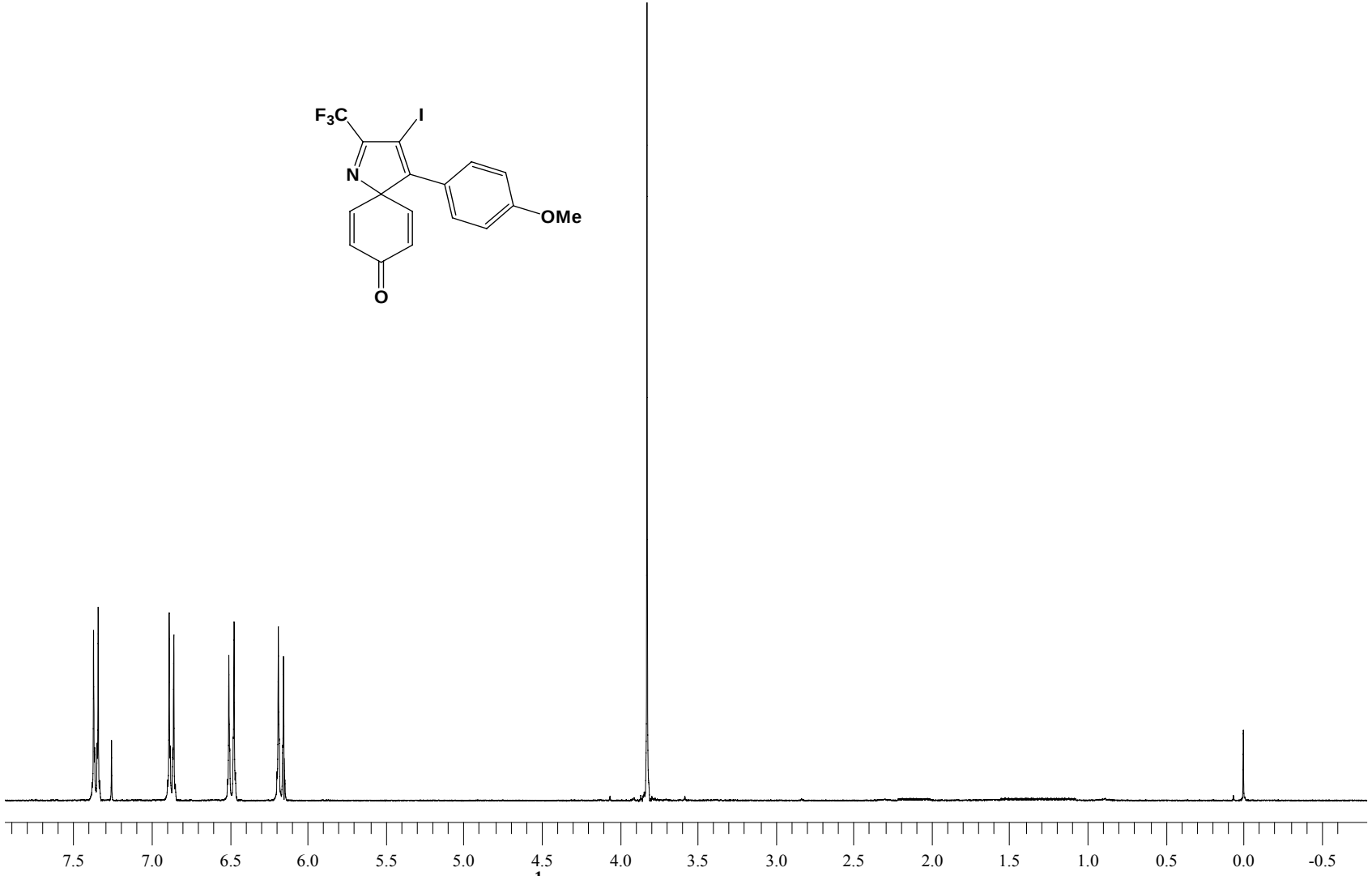
^{13}C NMR of 5j



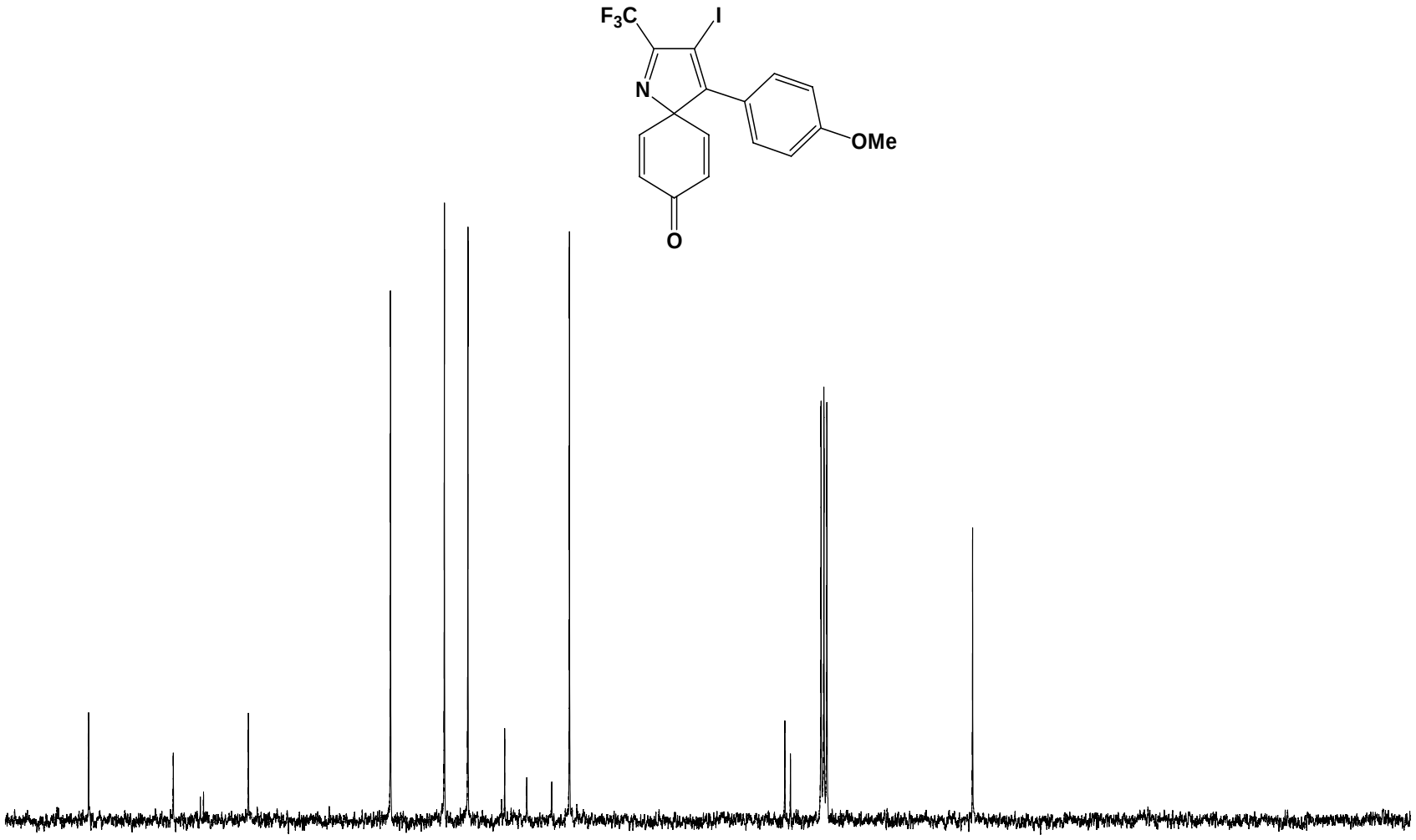
^{1}H NMR of 6a



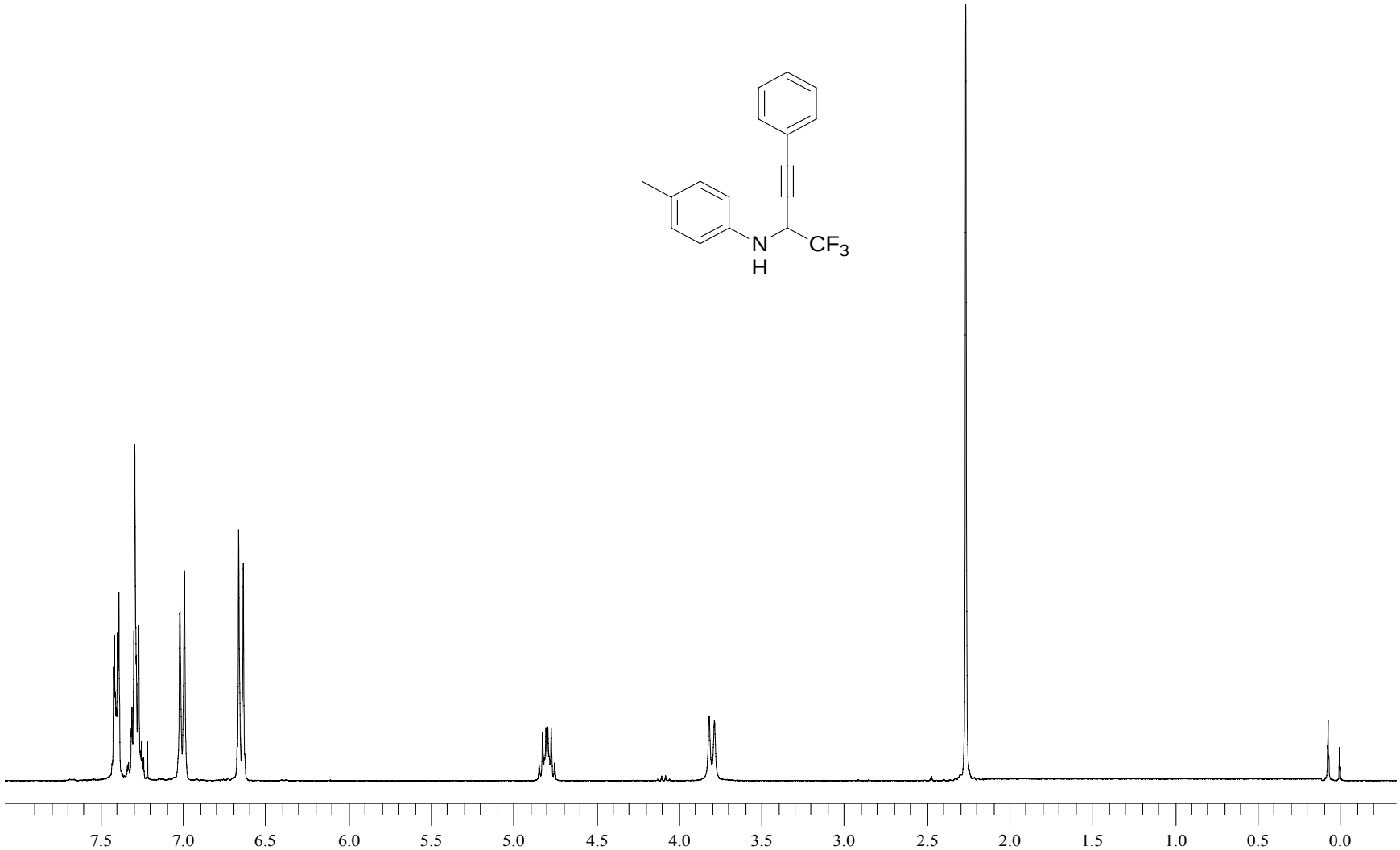
^{13}C NMR of 6a



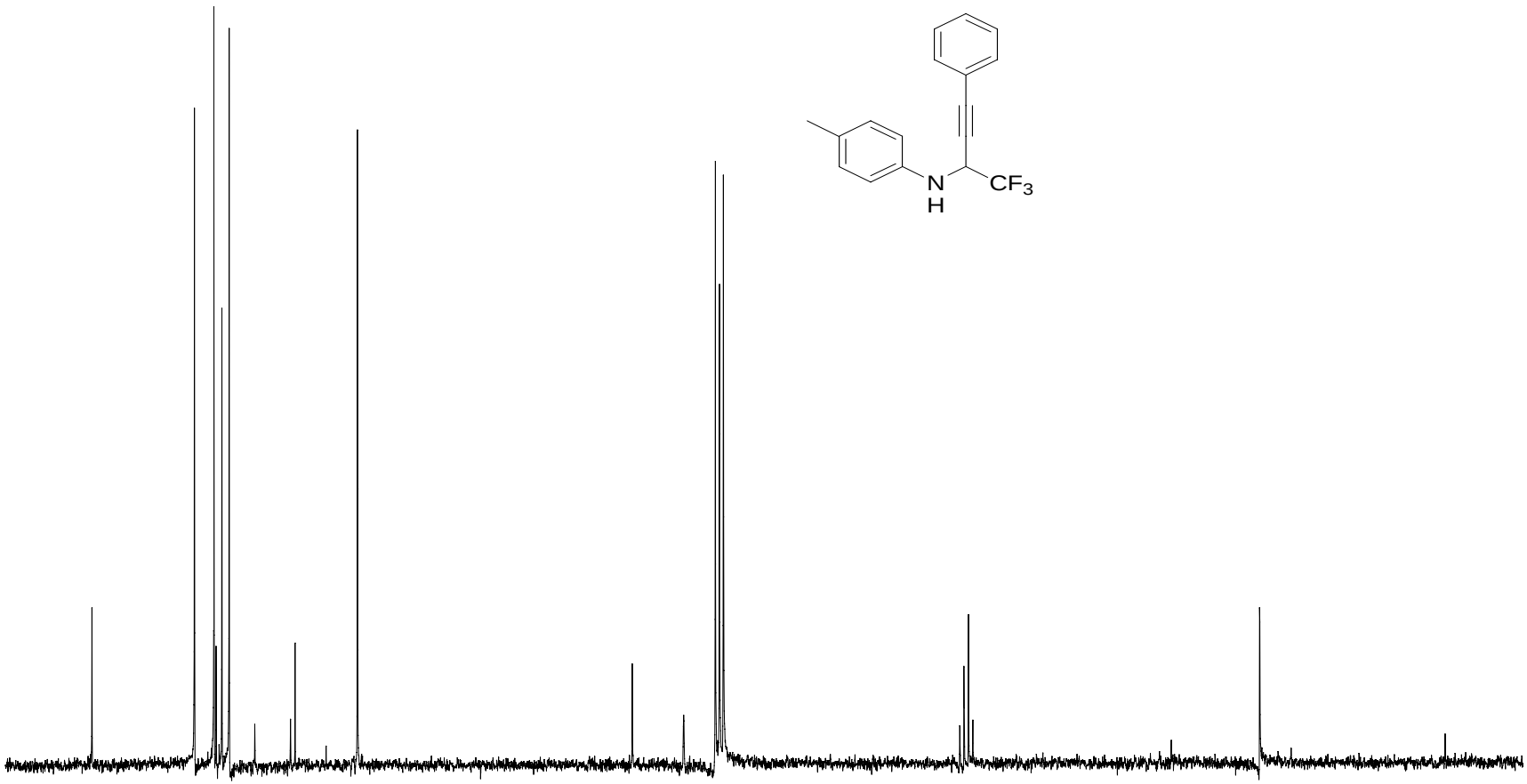
^{1}H NMR of 6b



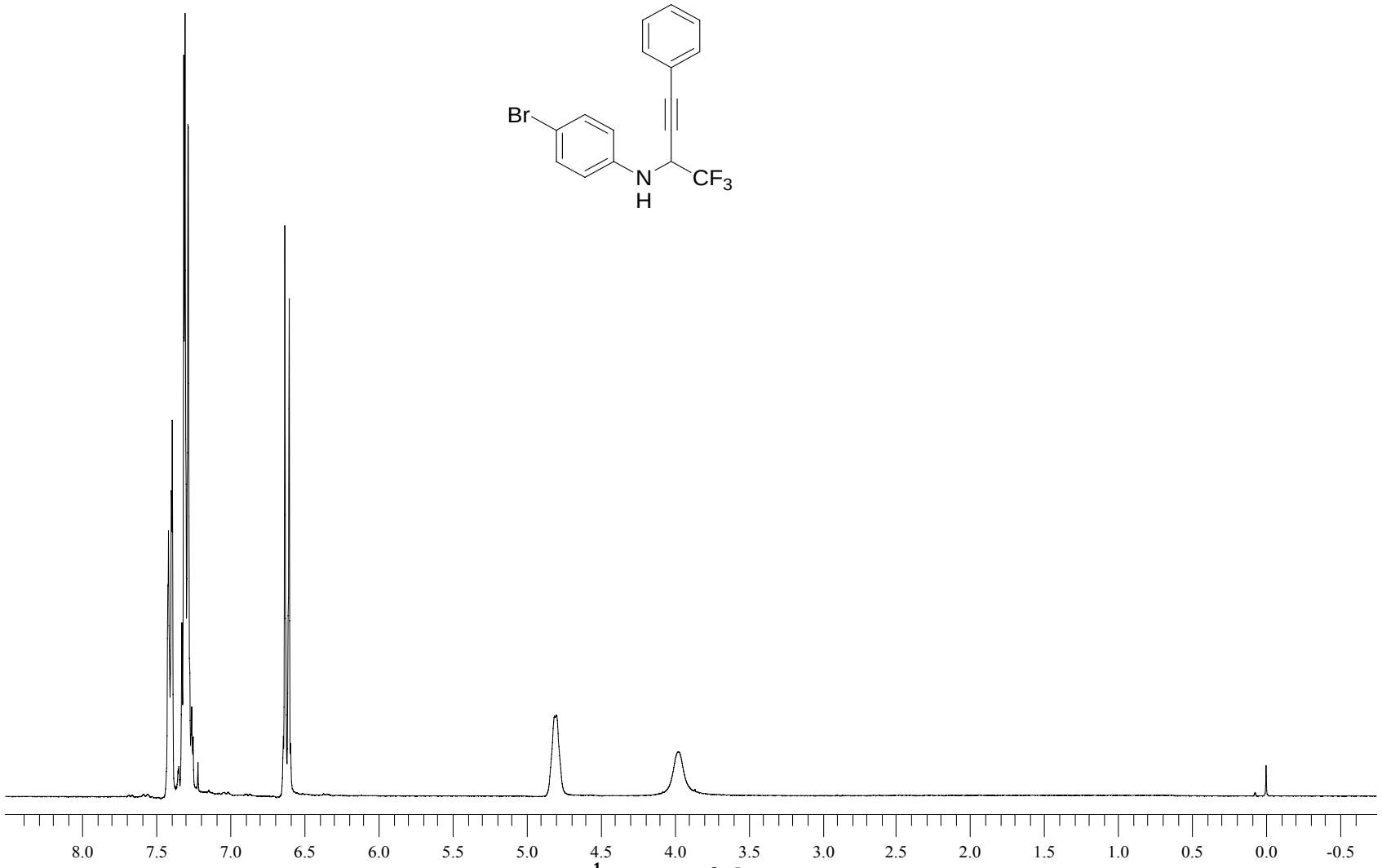
^{13}C NMR of 6b



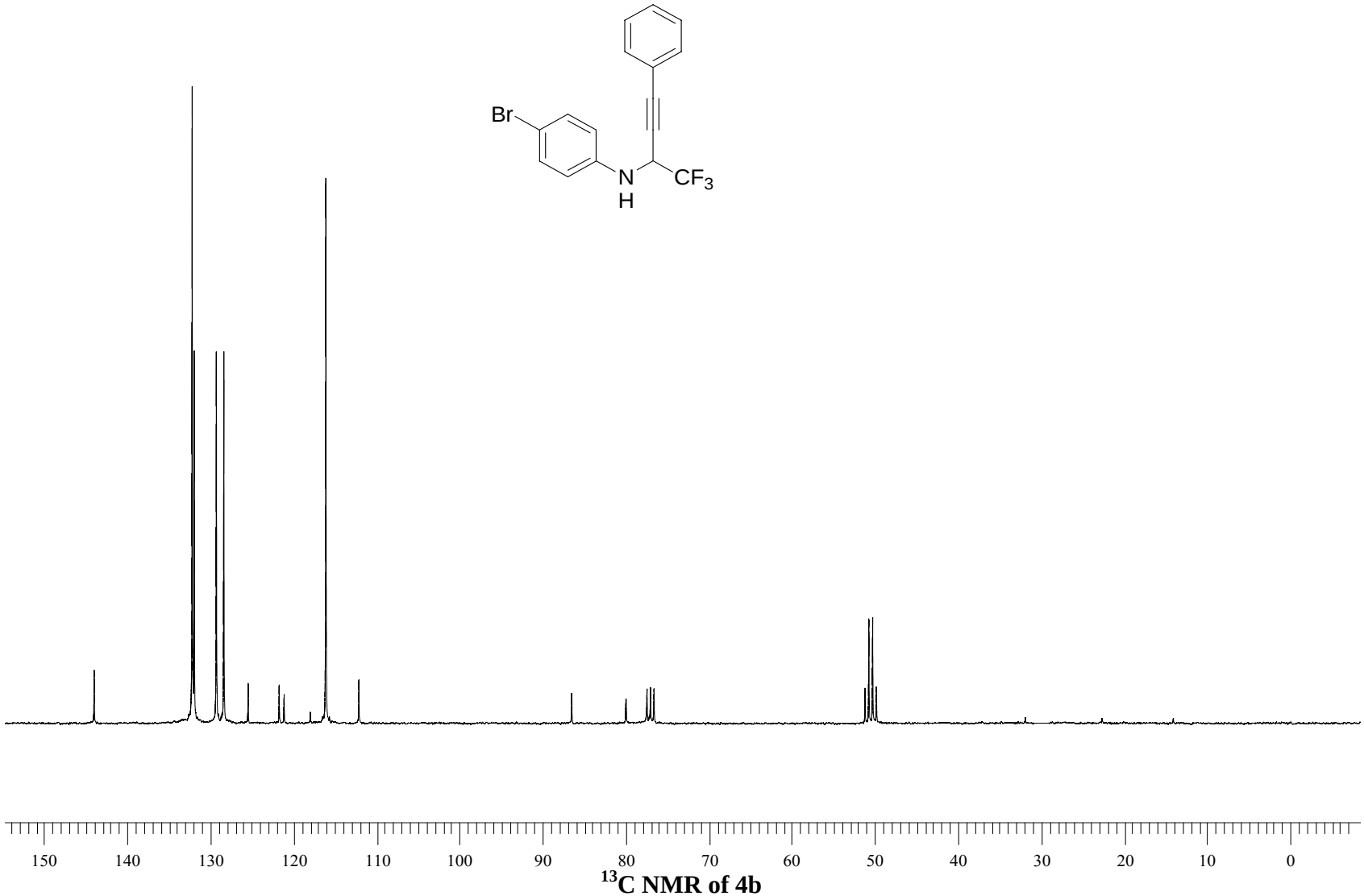
^{1}H NMR of 4a



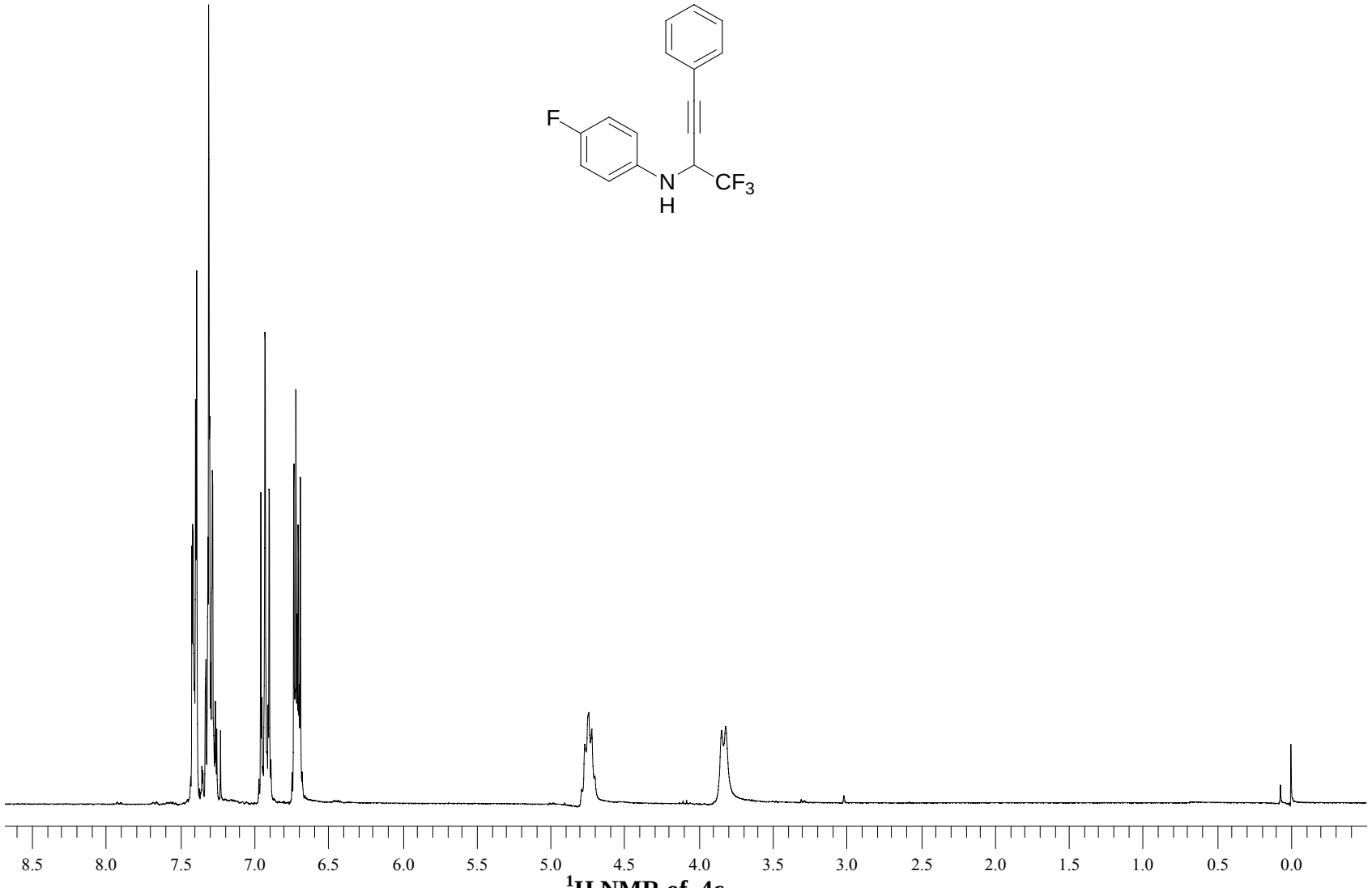
^{13}C NMR of 4a



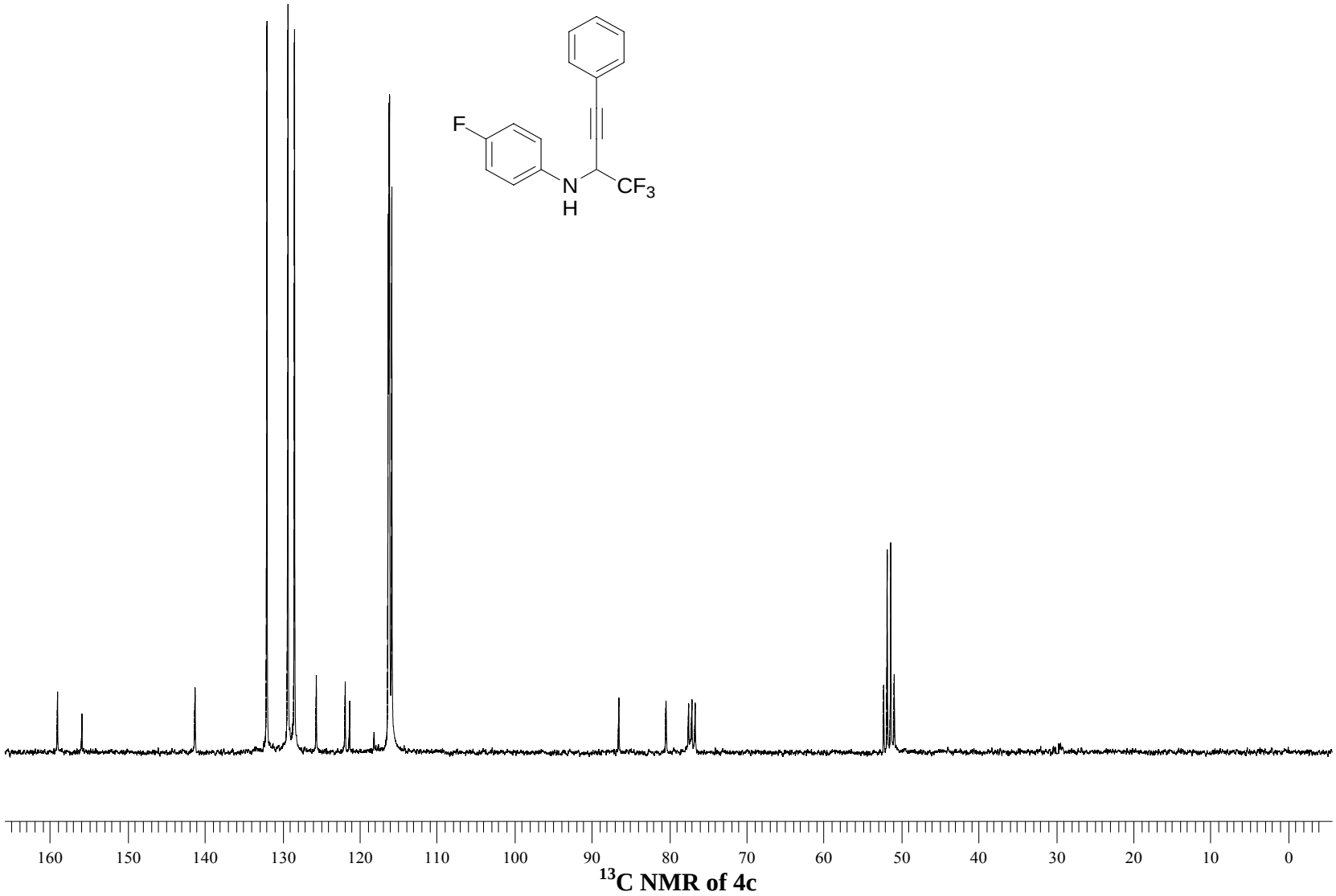
^{1}H NMR of 4b



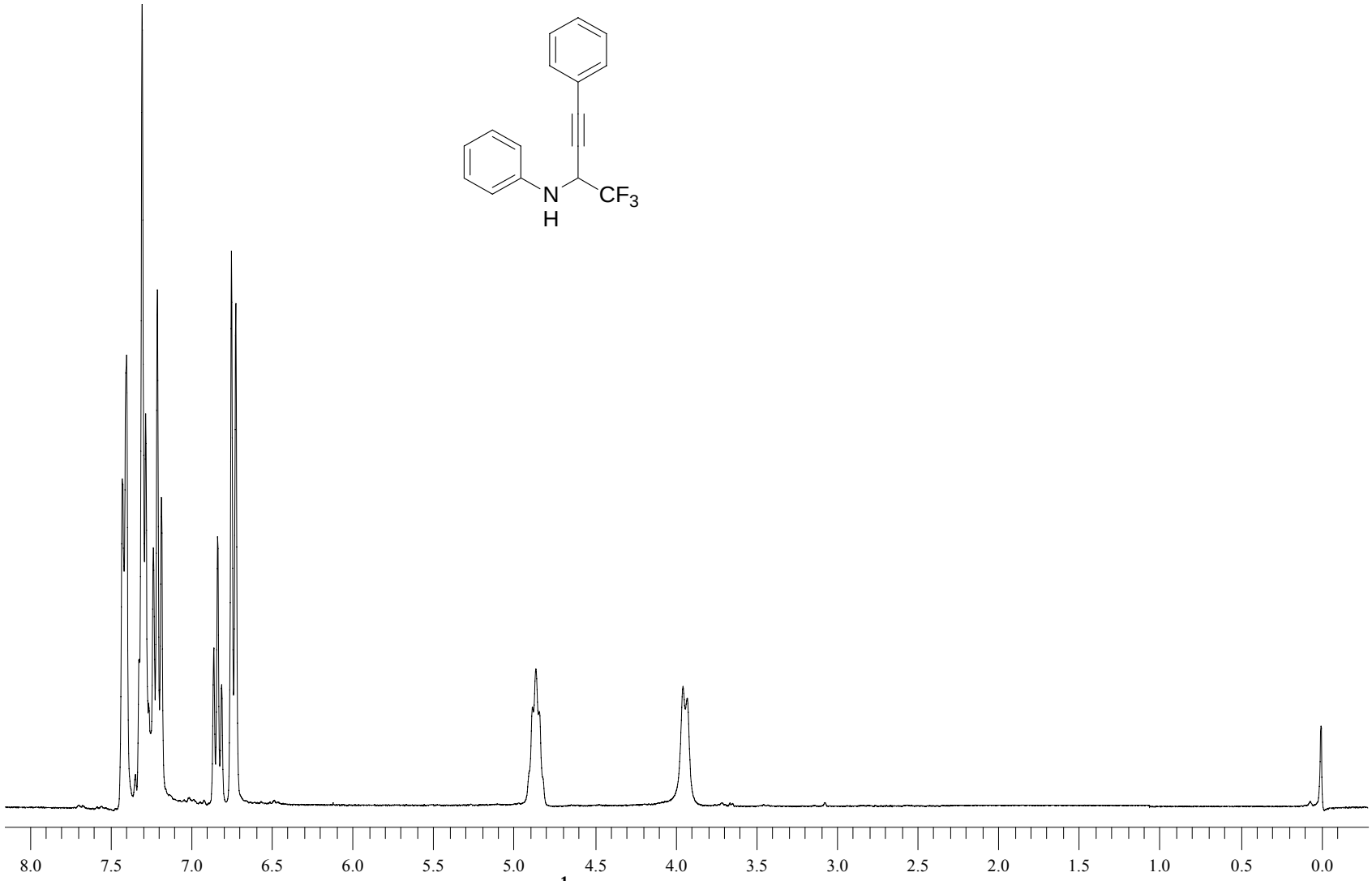
^{13}C NMR of 4b



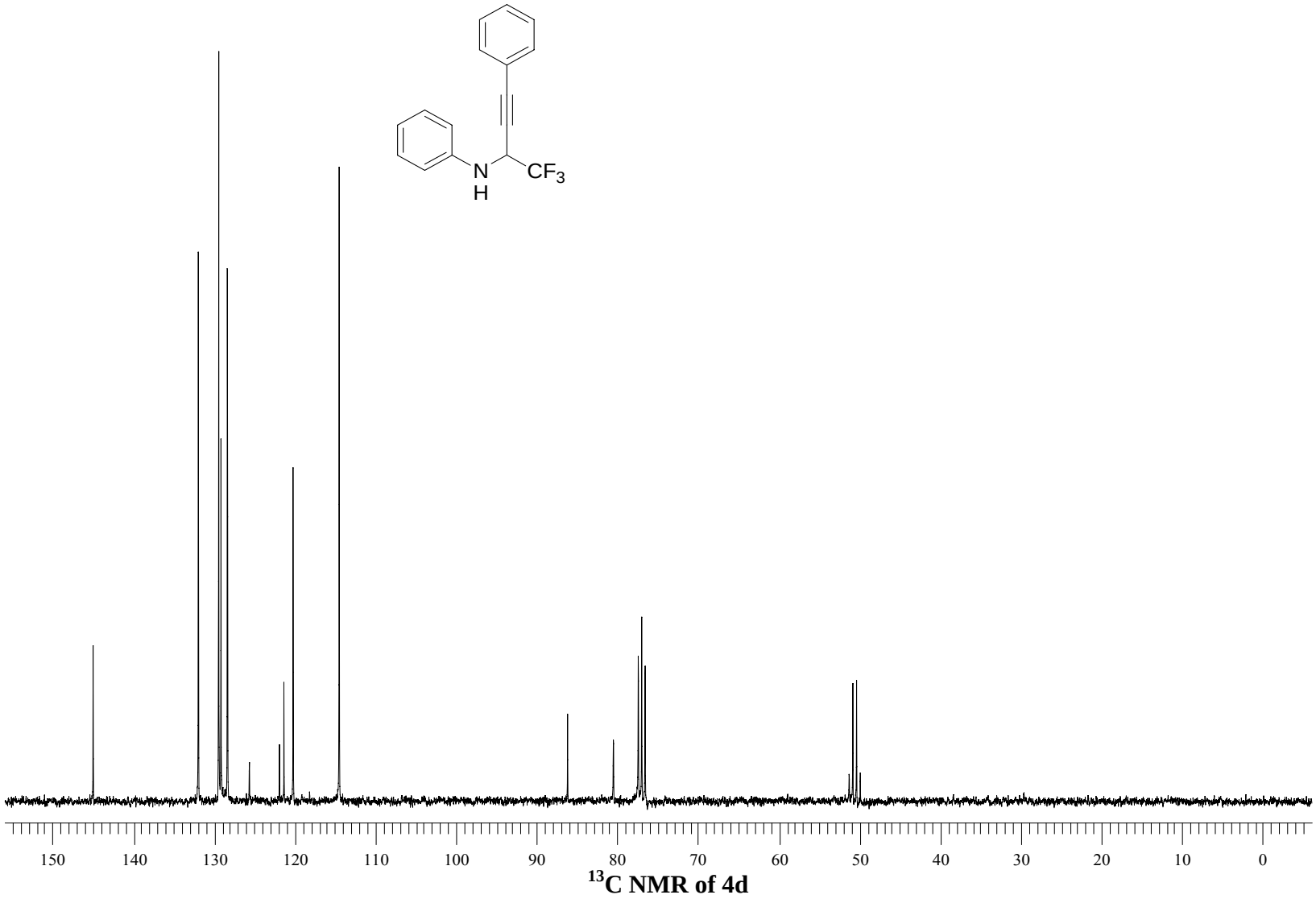
^{1}H NMR of 4c



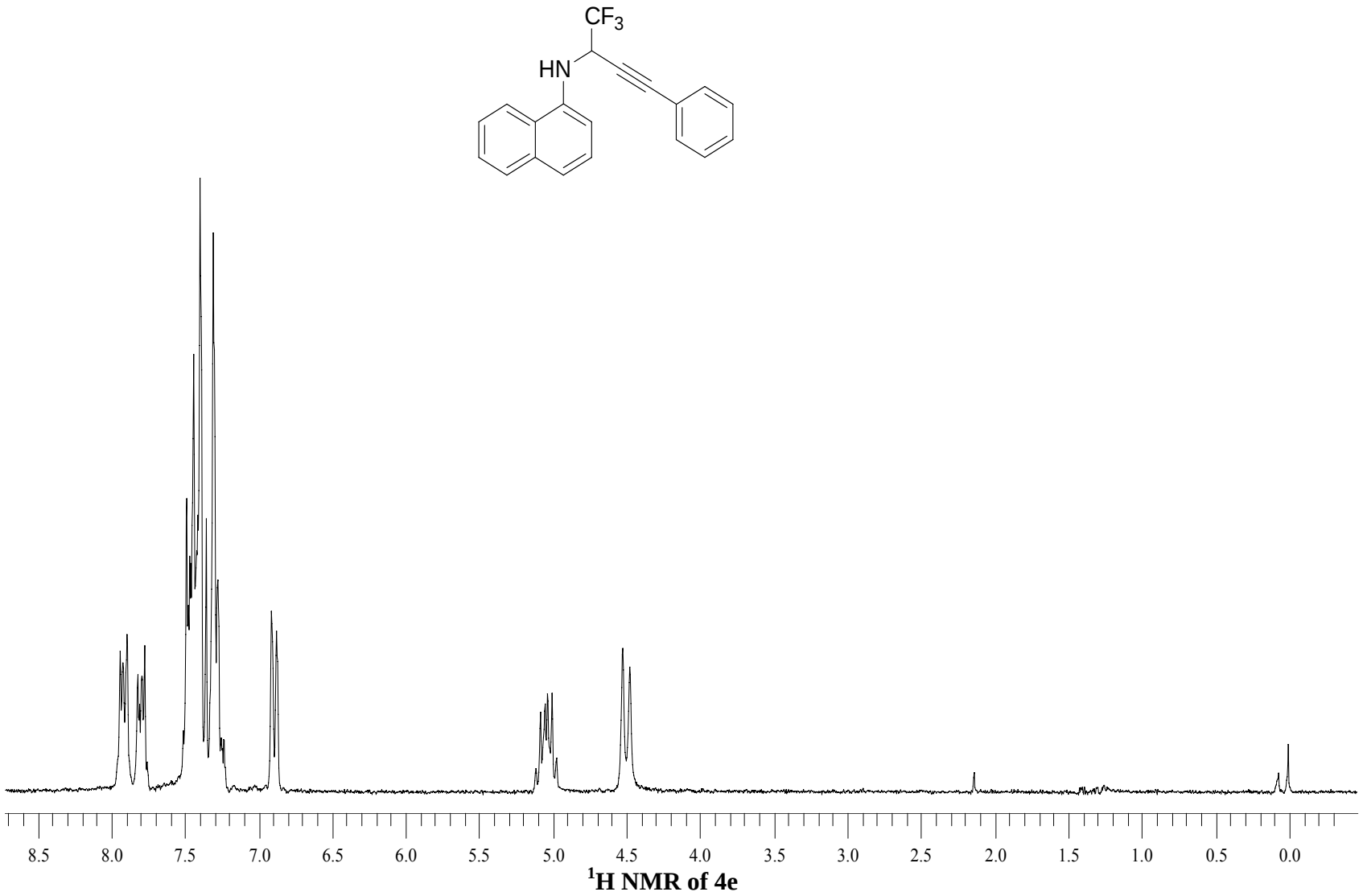
^{13}C NMR of 4c



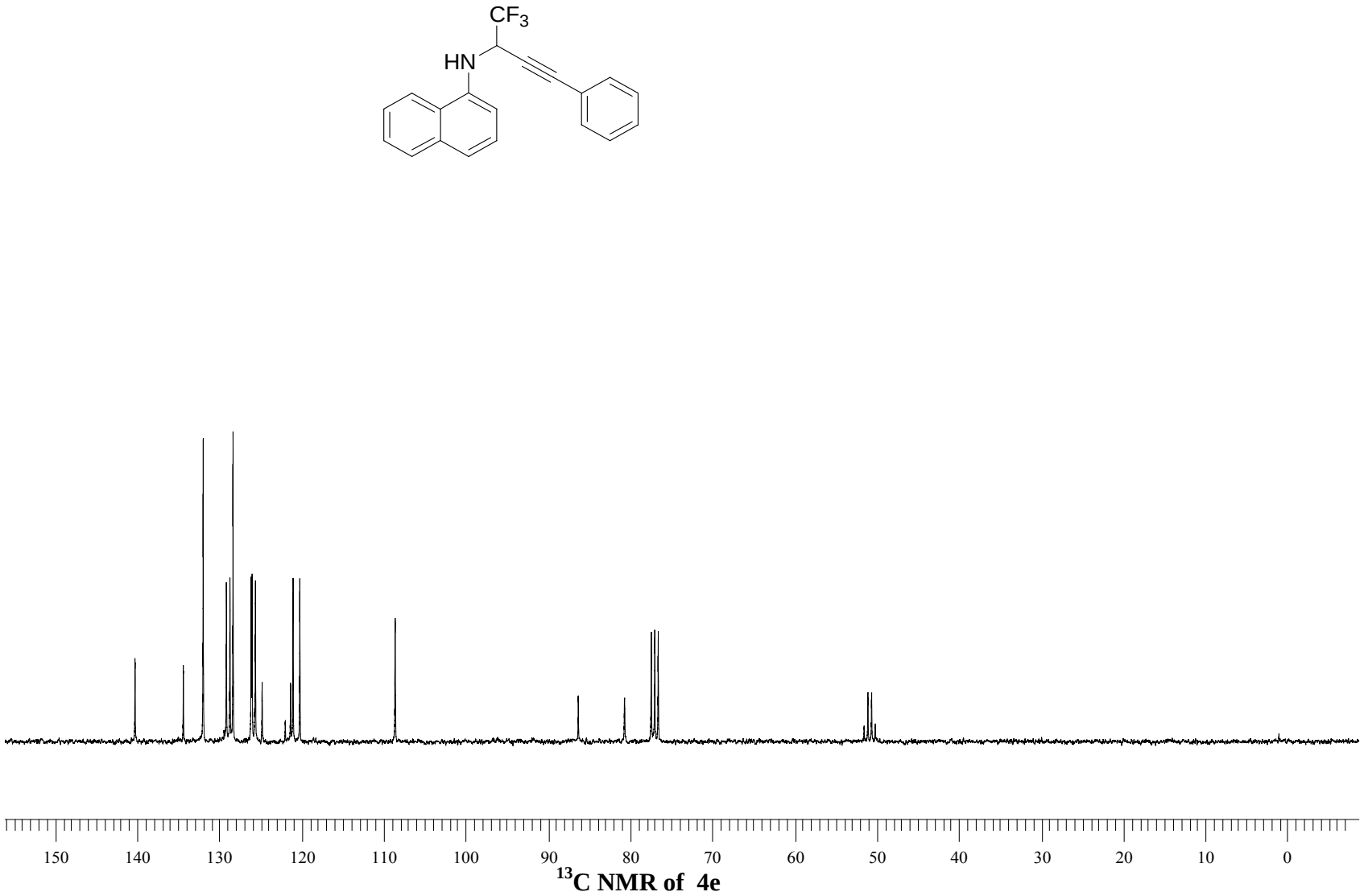
^{1}H NMR of 4d



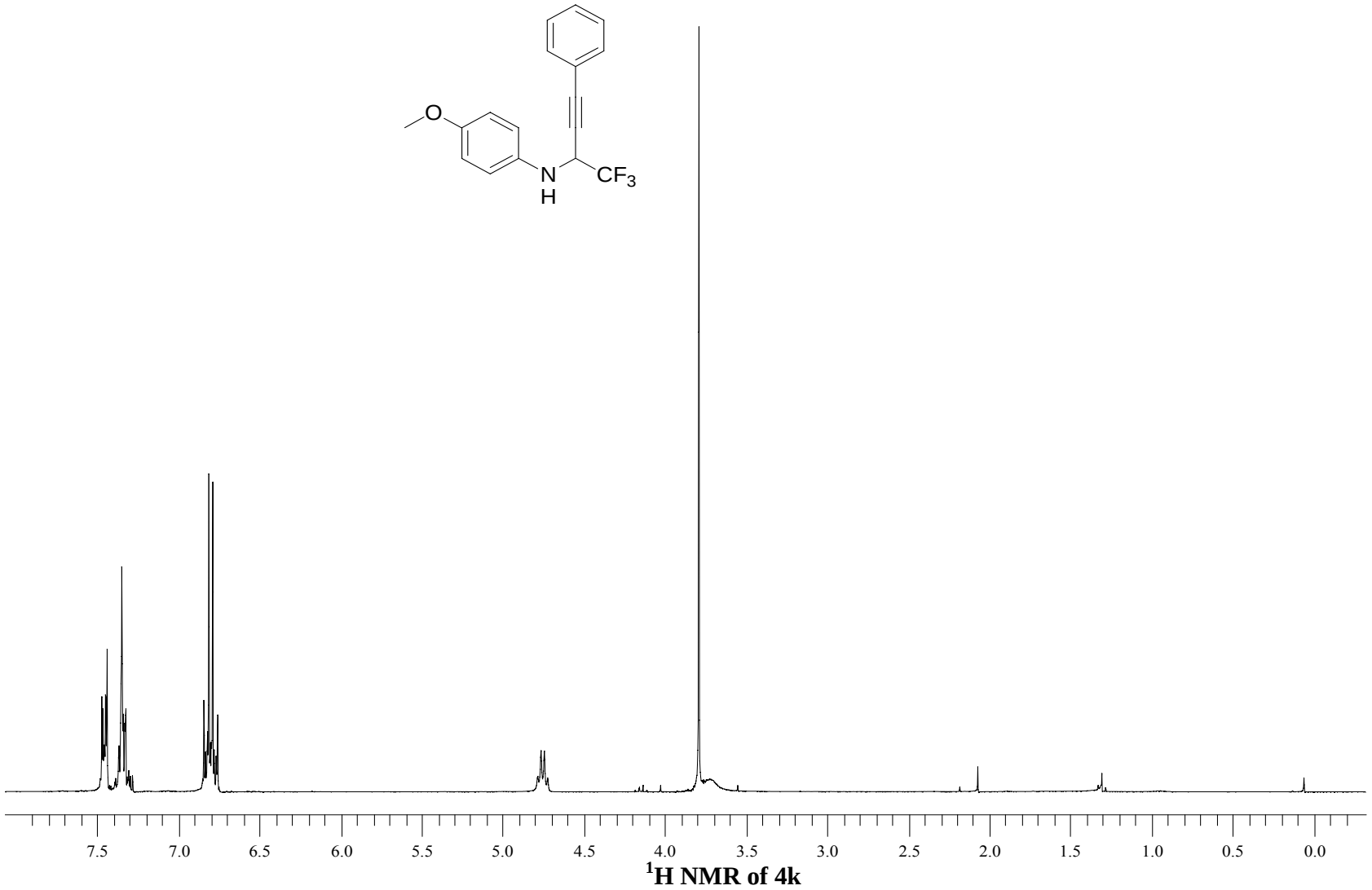
^{13}C NMR of 4d



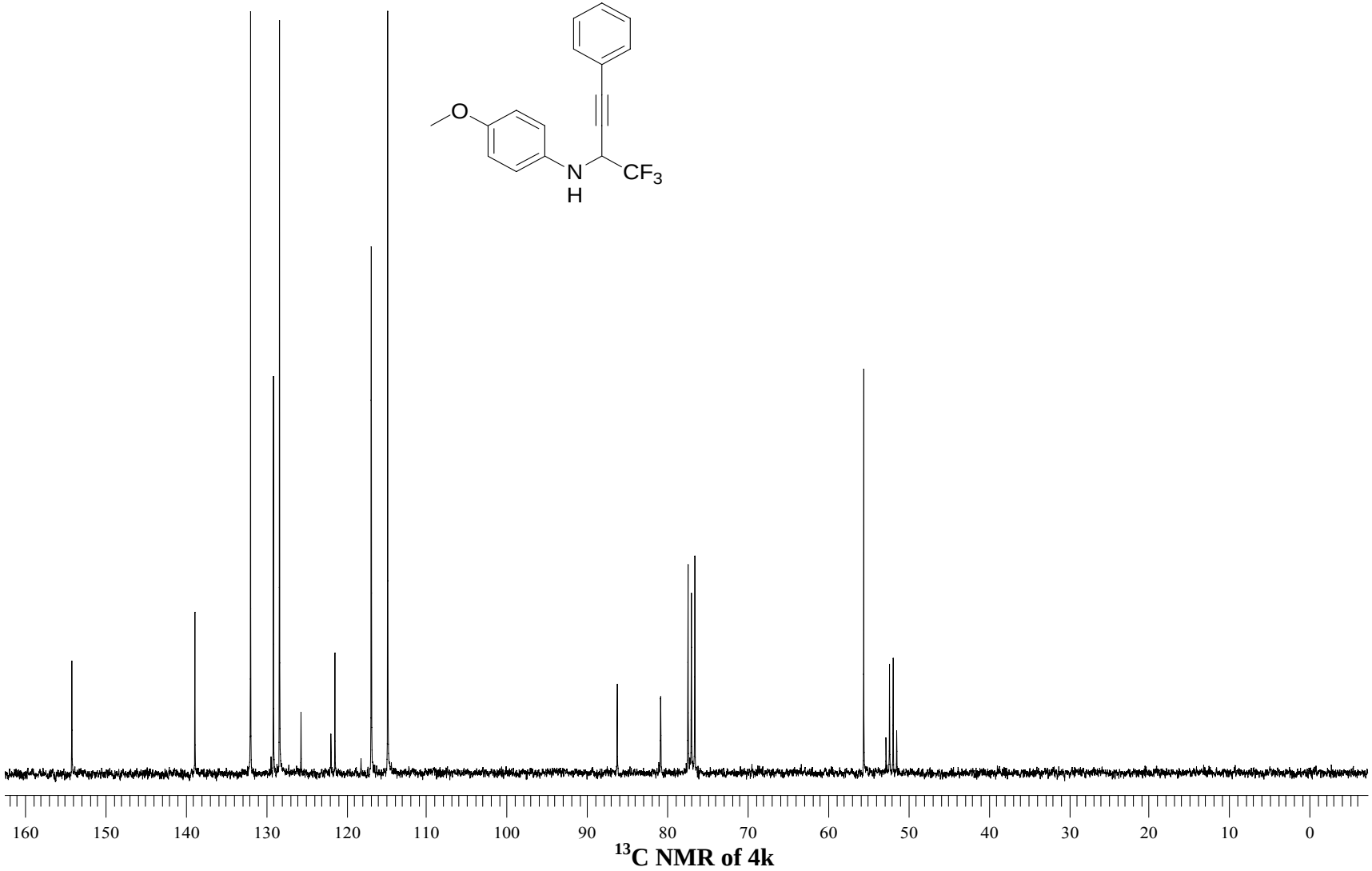
^{1}H NMR of 4e



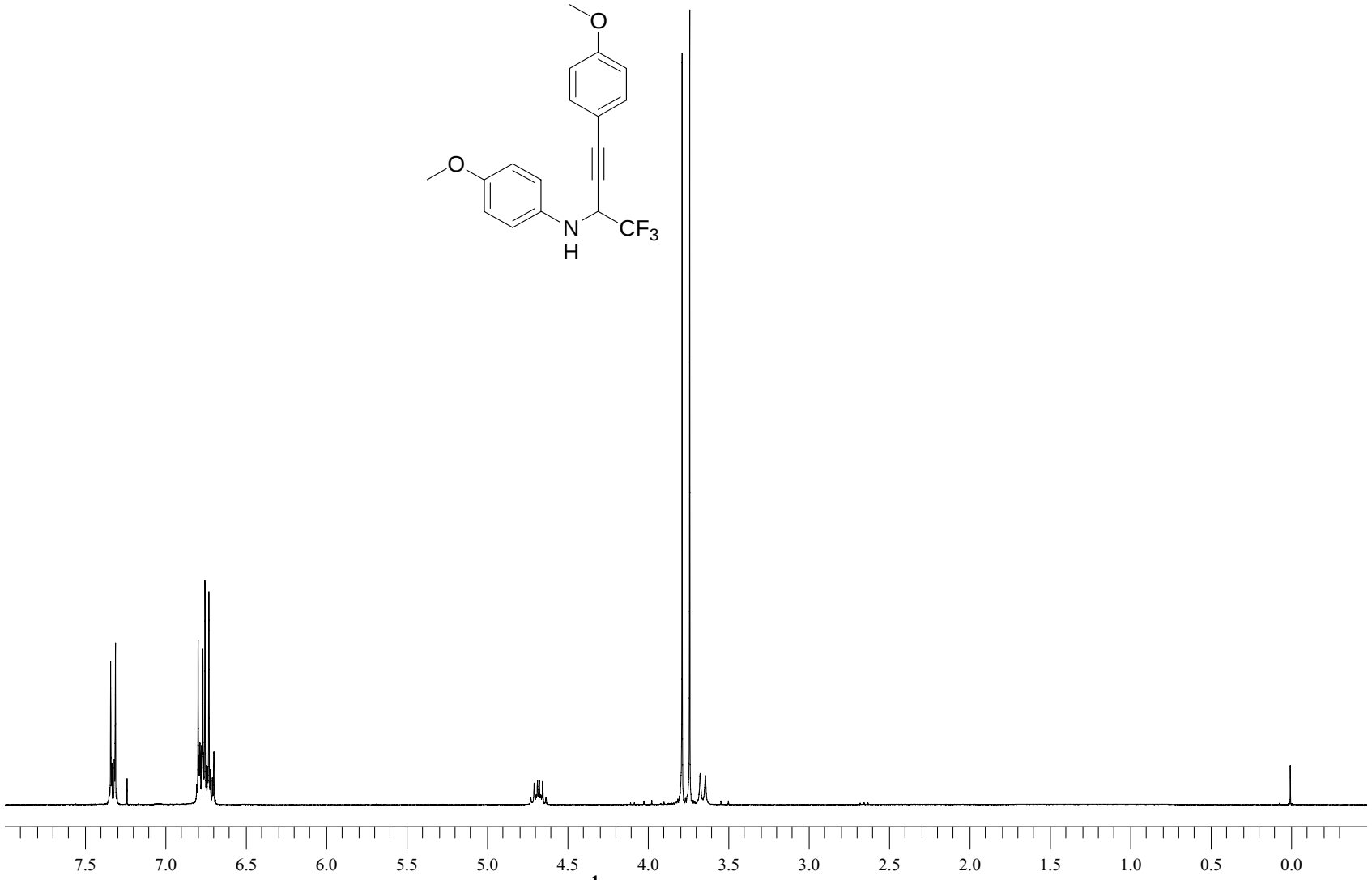
^{13}C NMR of 4e



^{1}H NMR of 4k



^{13}C NMR of 4k



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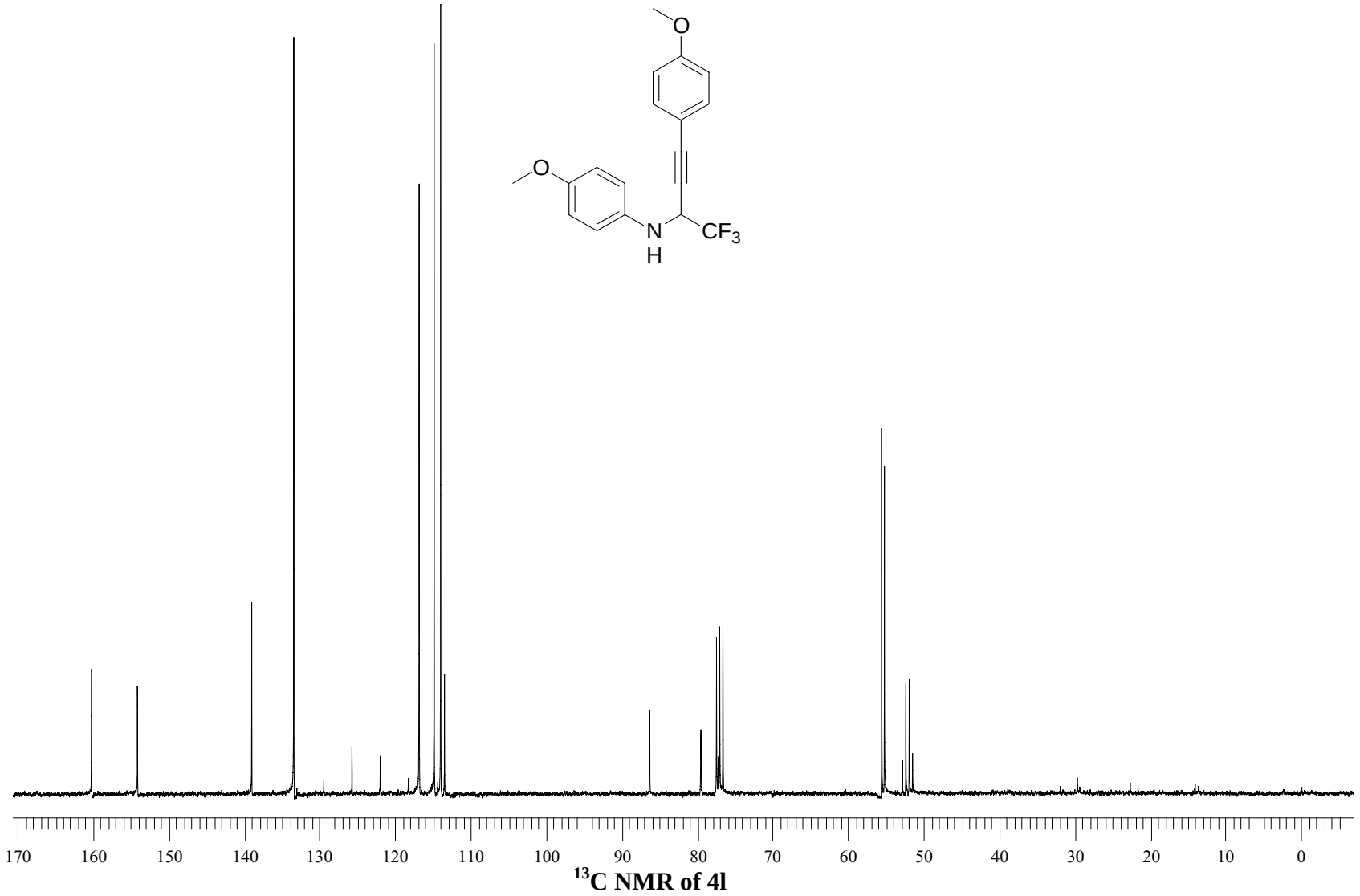
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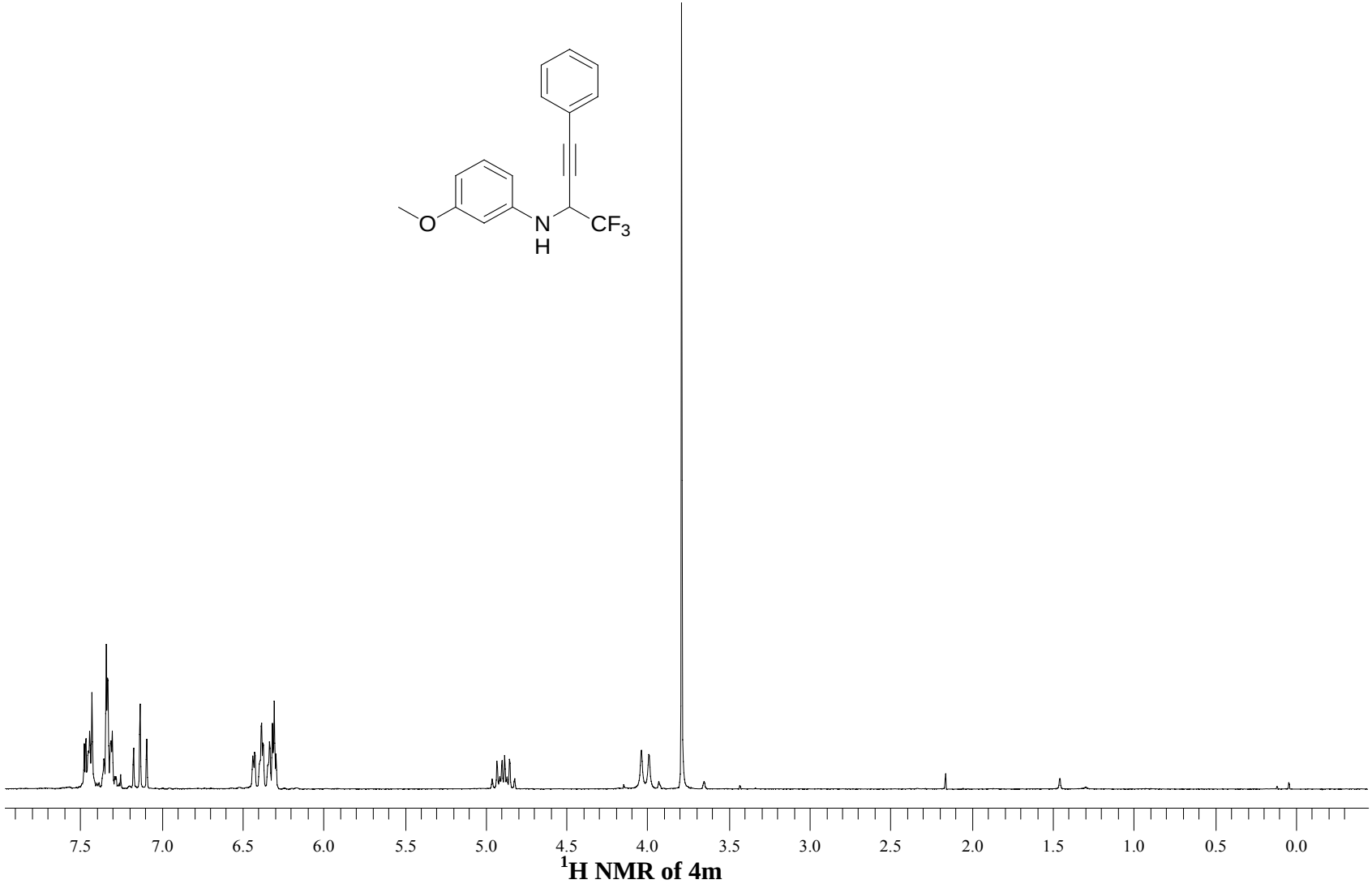
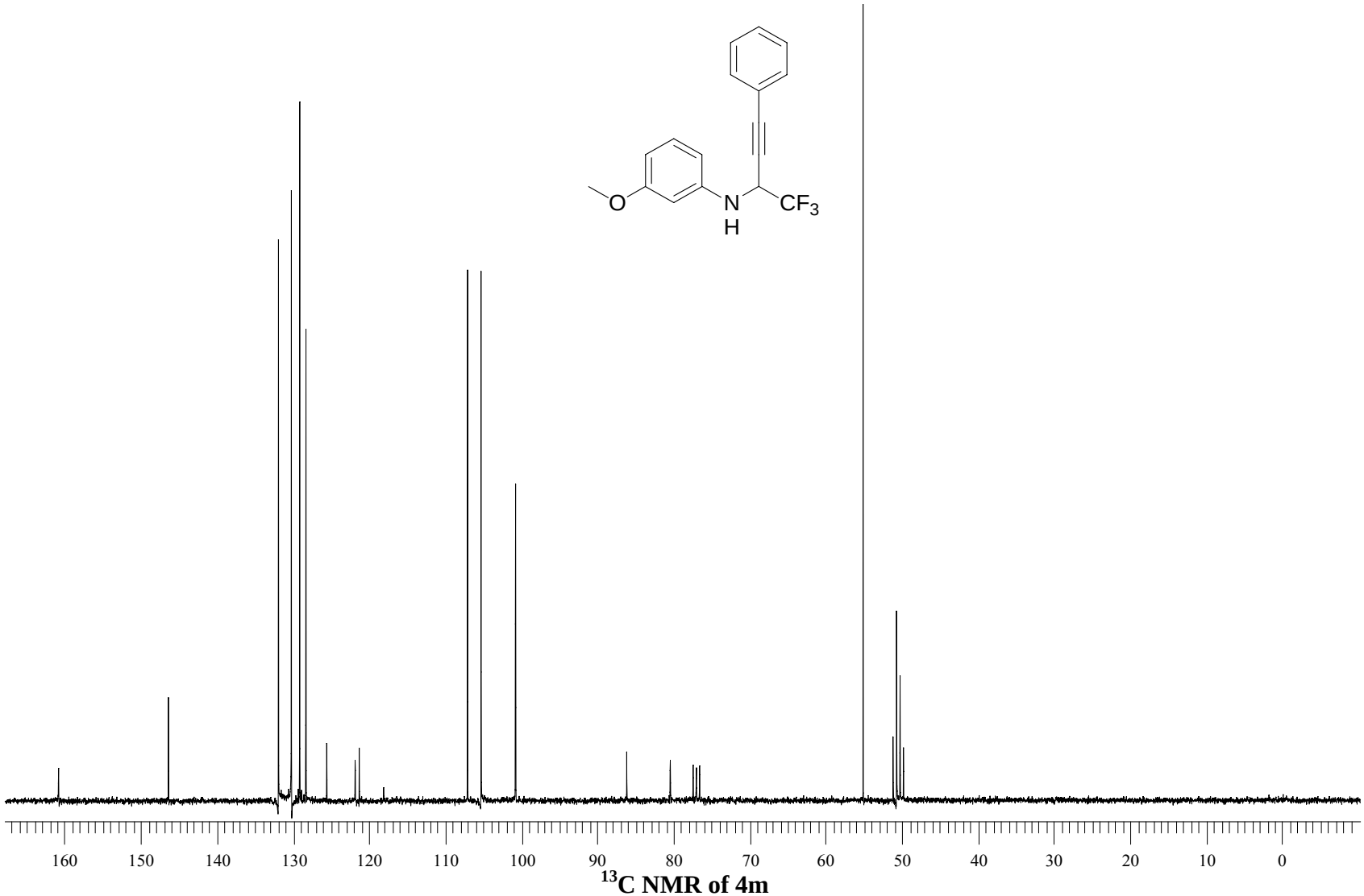
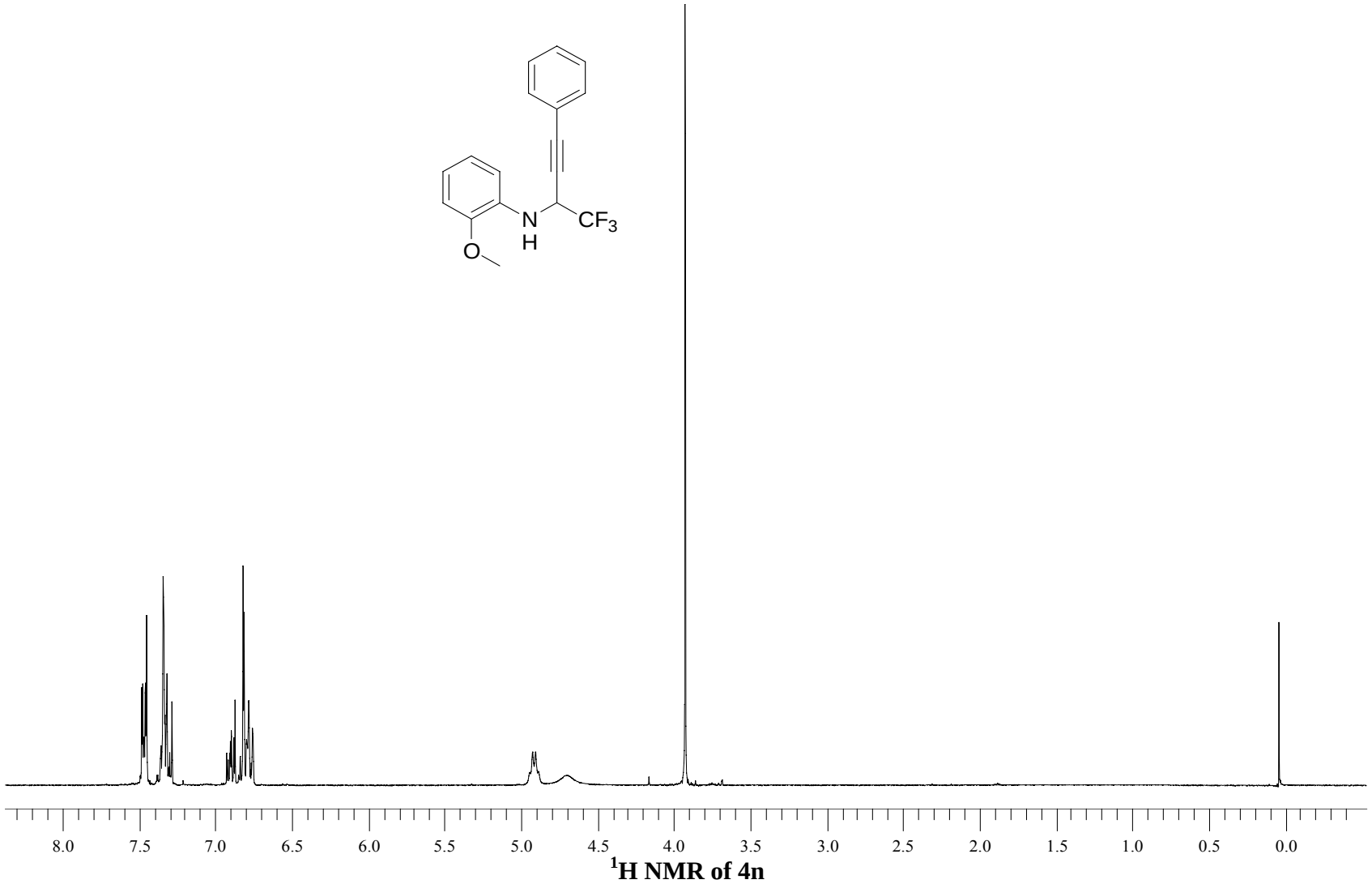
^{13}C NMR of 4l



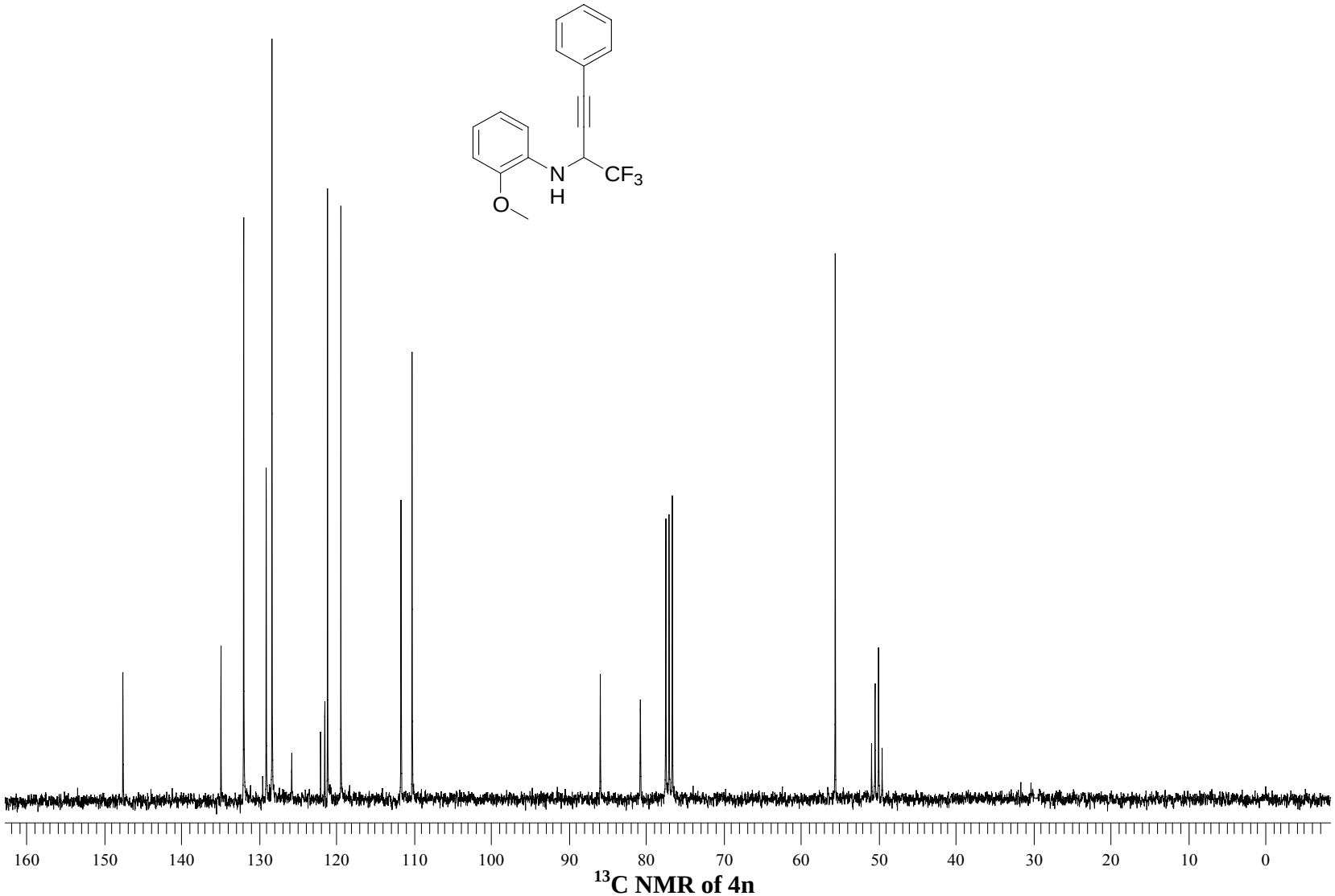
^{1}H NMR of 4m



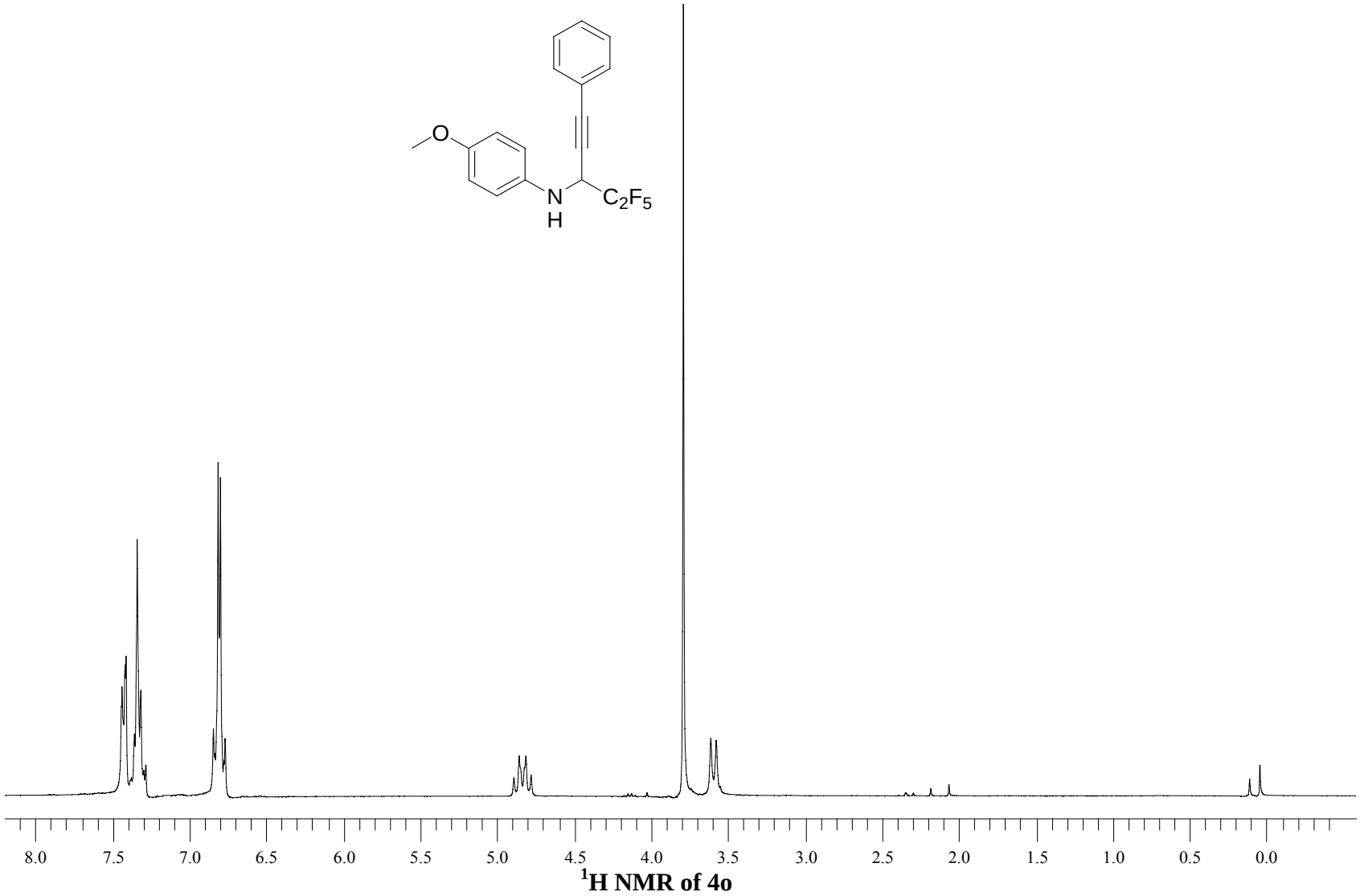
^{13}C NMR of 4m



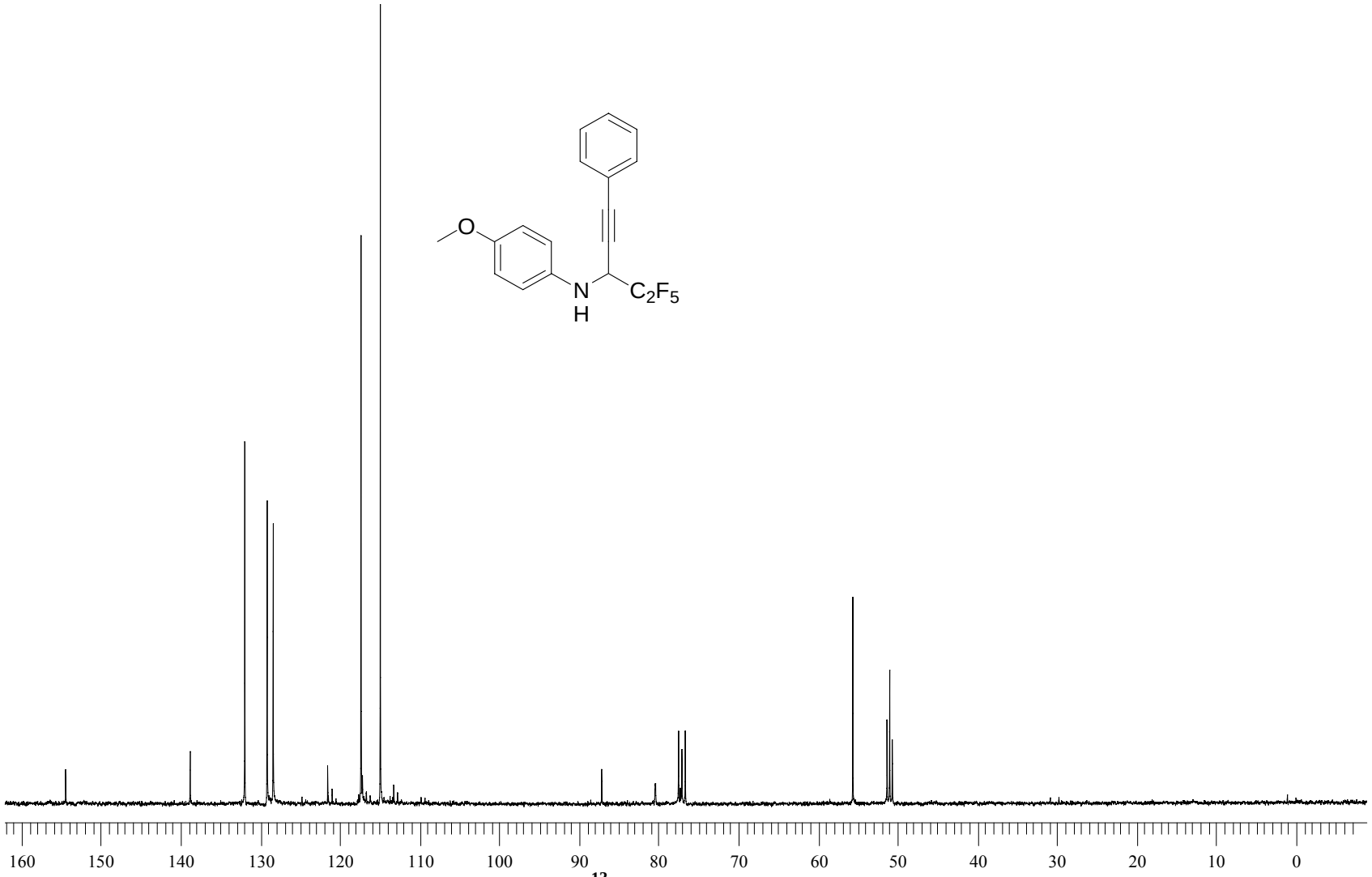
^{1}H NMR of 4n



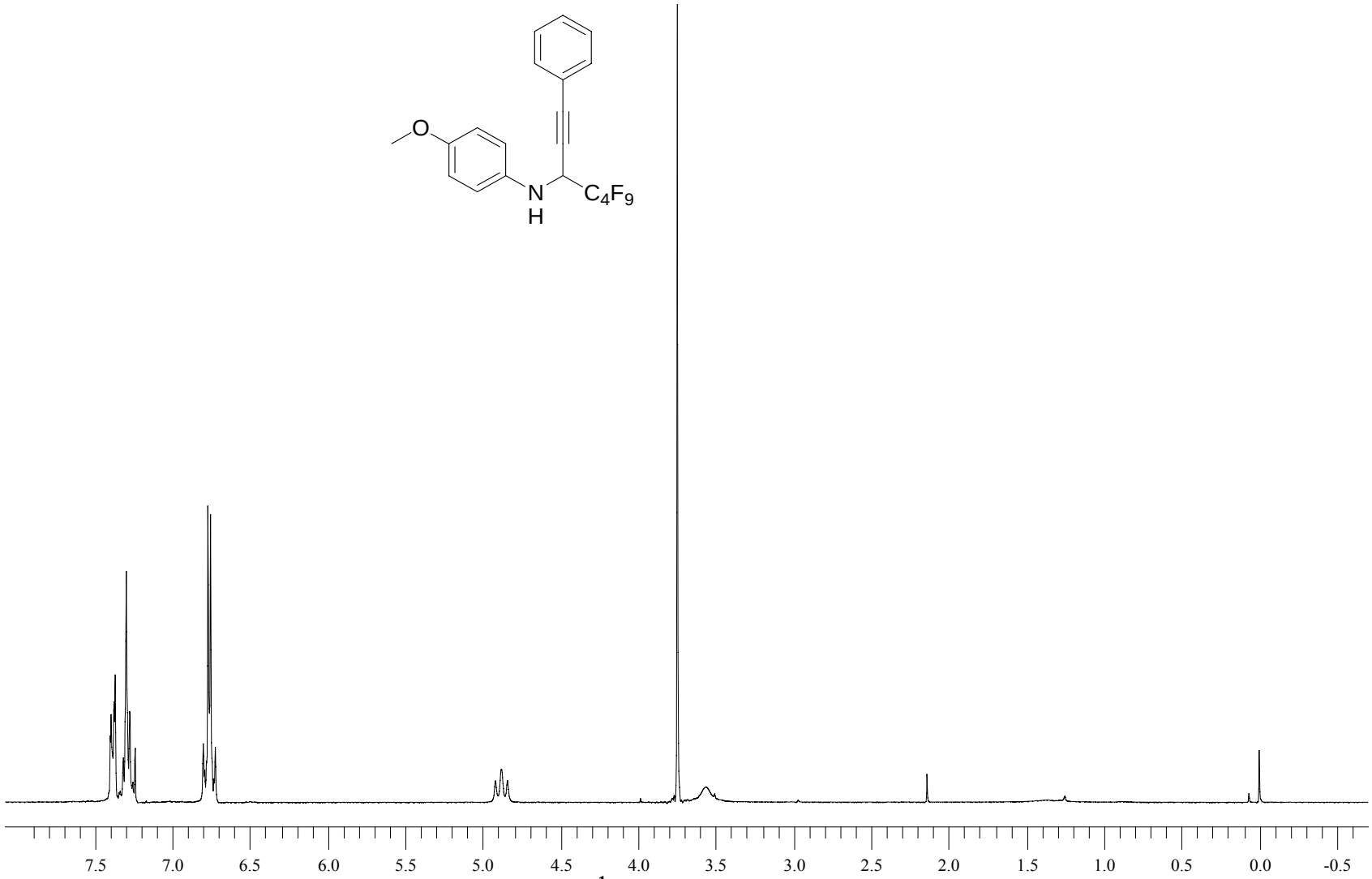
^{13}C NMR of 4n



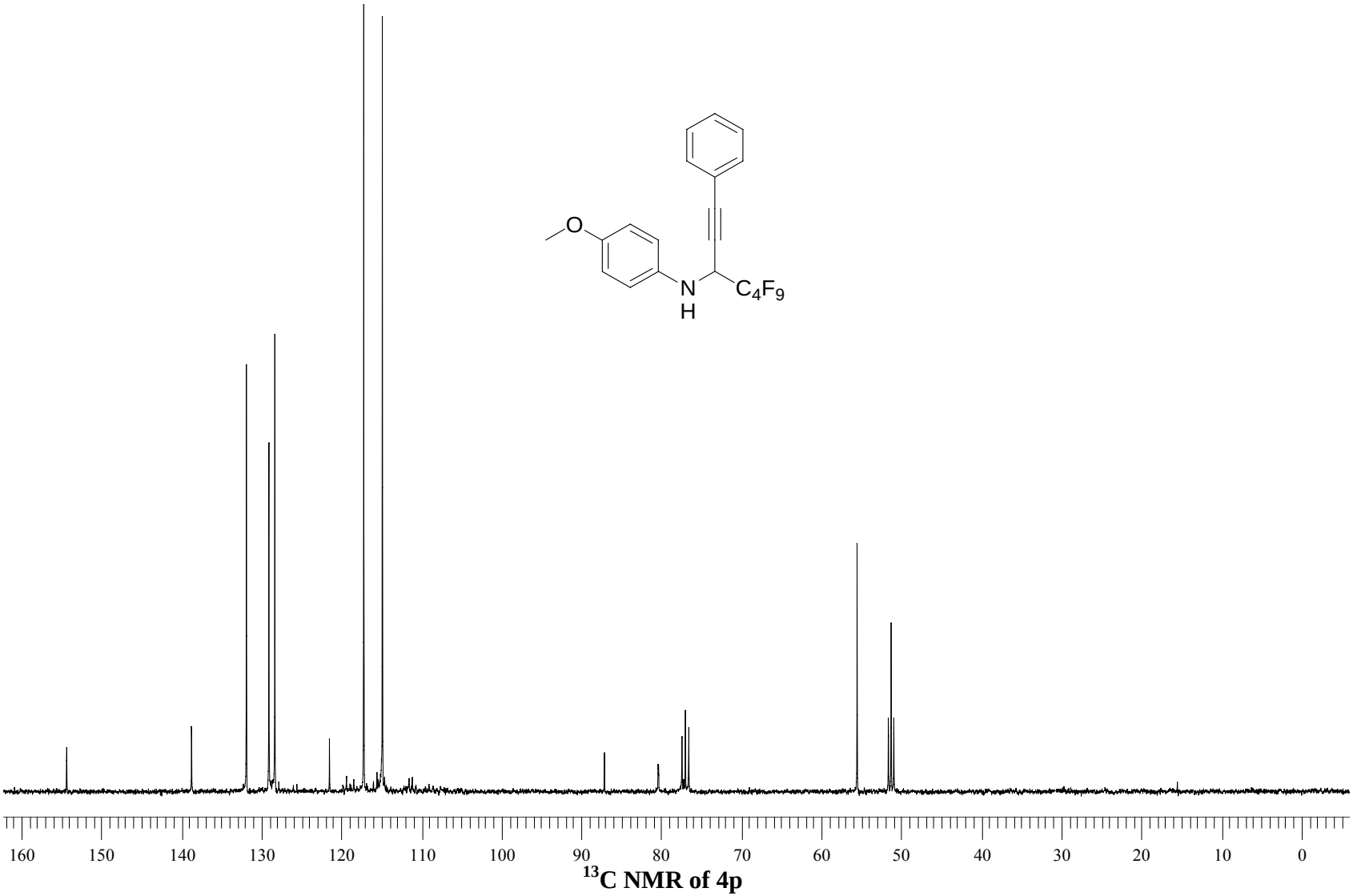
^{1}H NMR of 4o



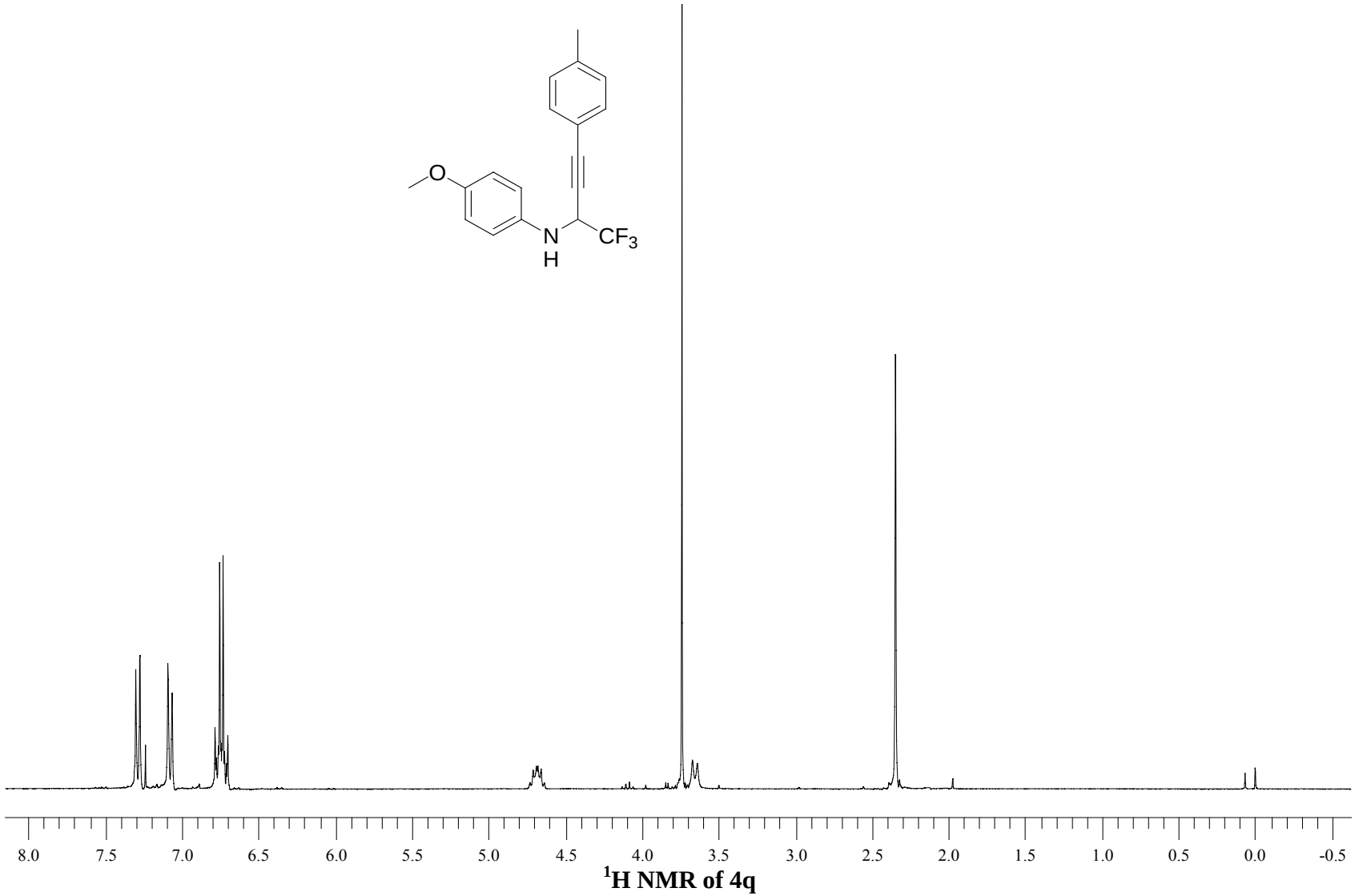
^{13}C NMR of 4o



^{1}H NMR of 4p



^{13}C NMR of 4p



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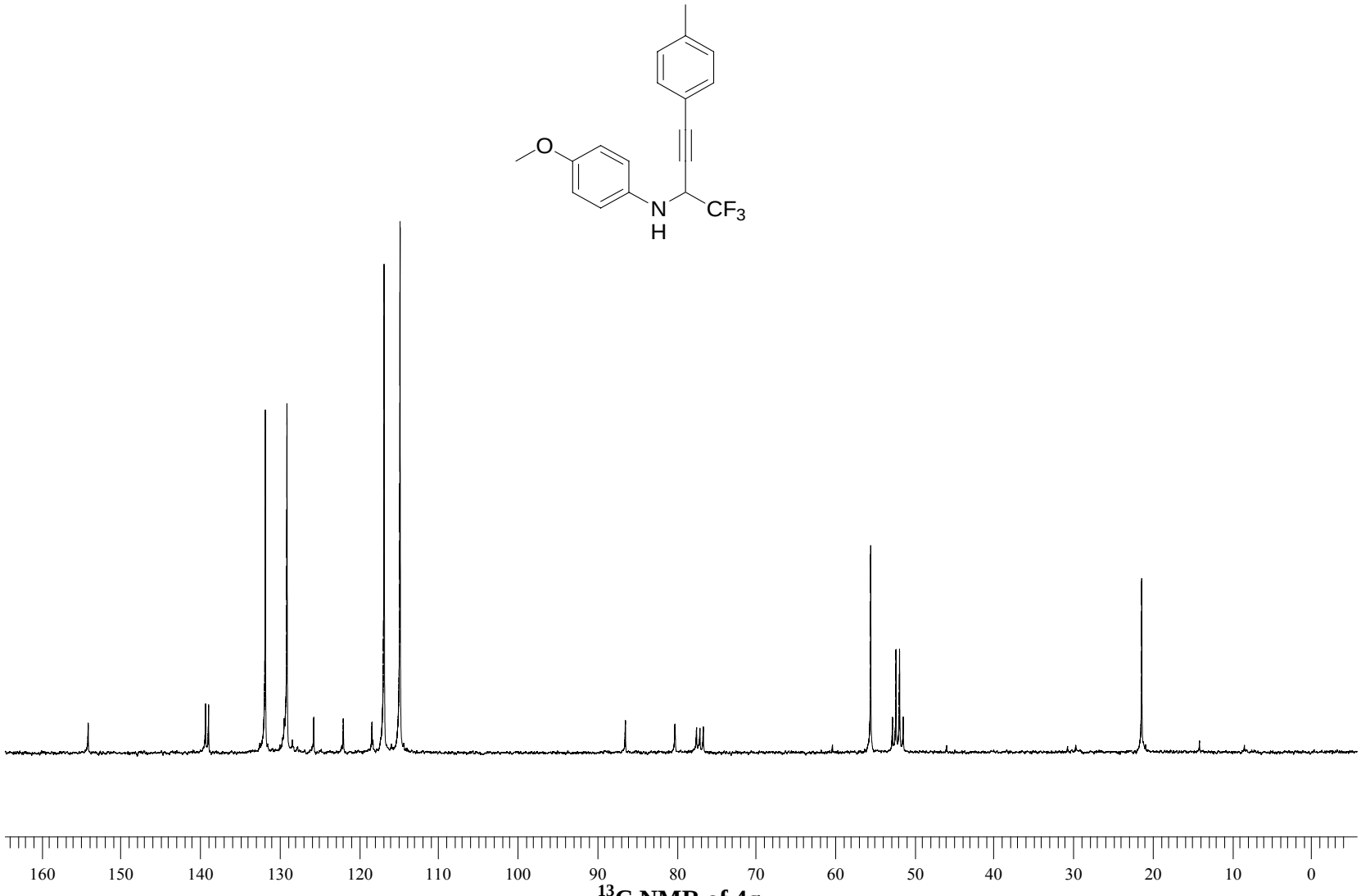
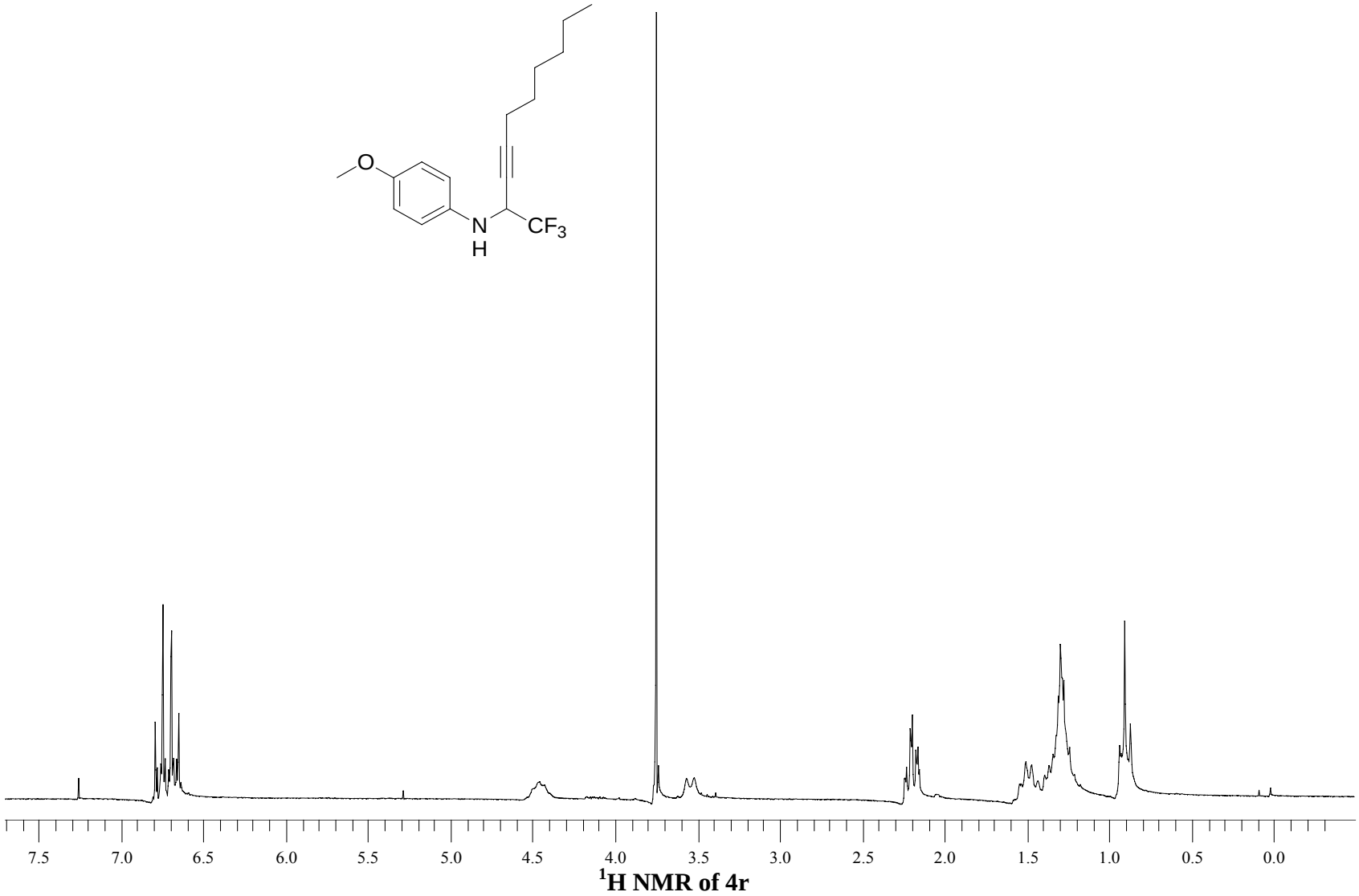


^{13}C NMR of 4q



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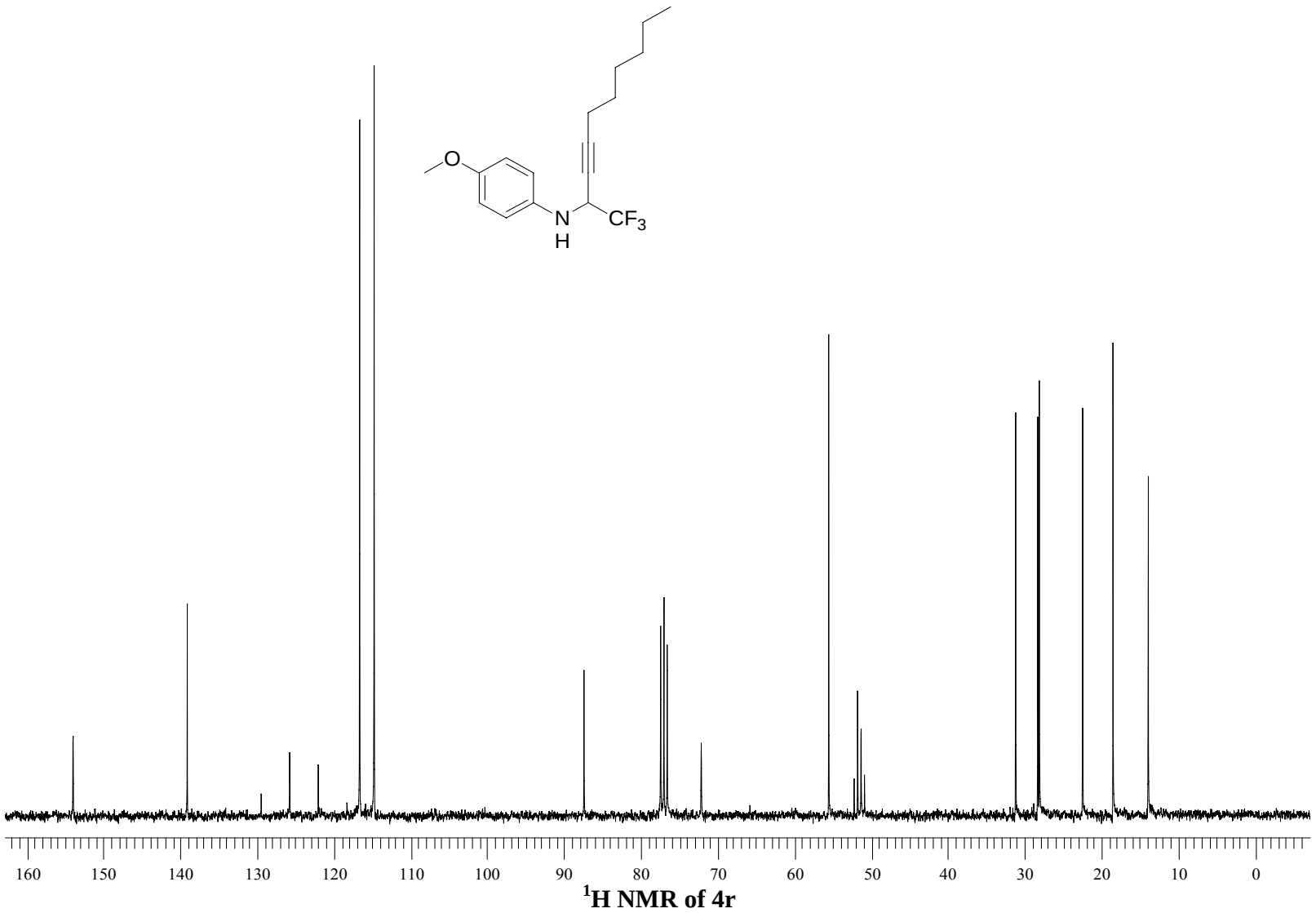

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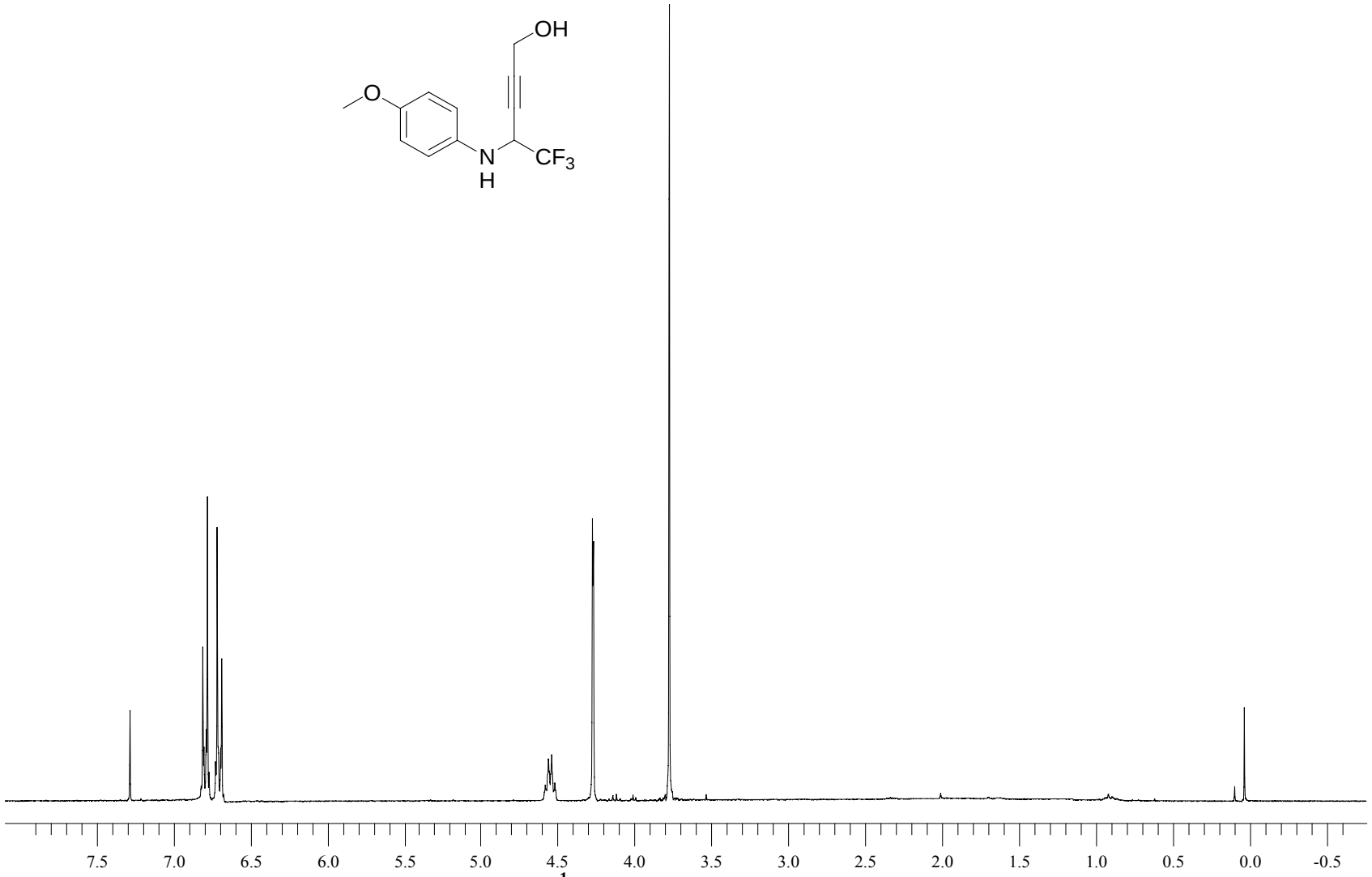
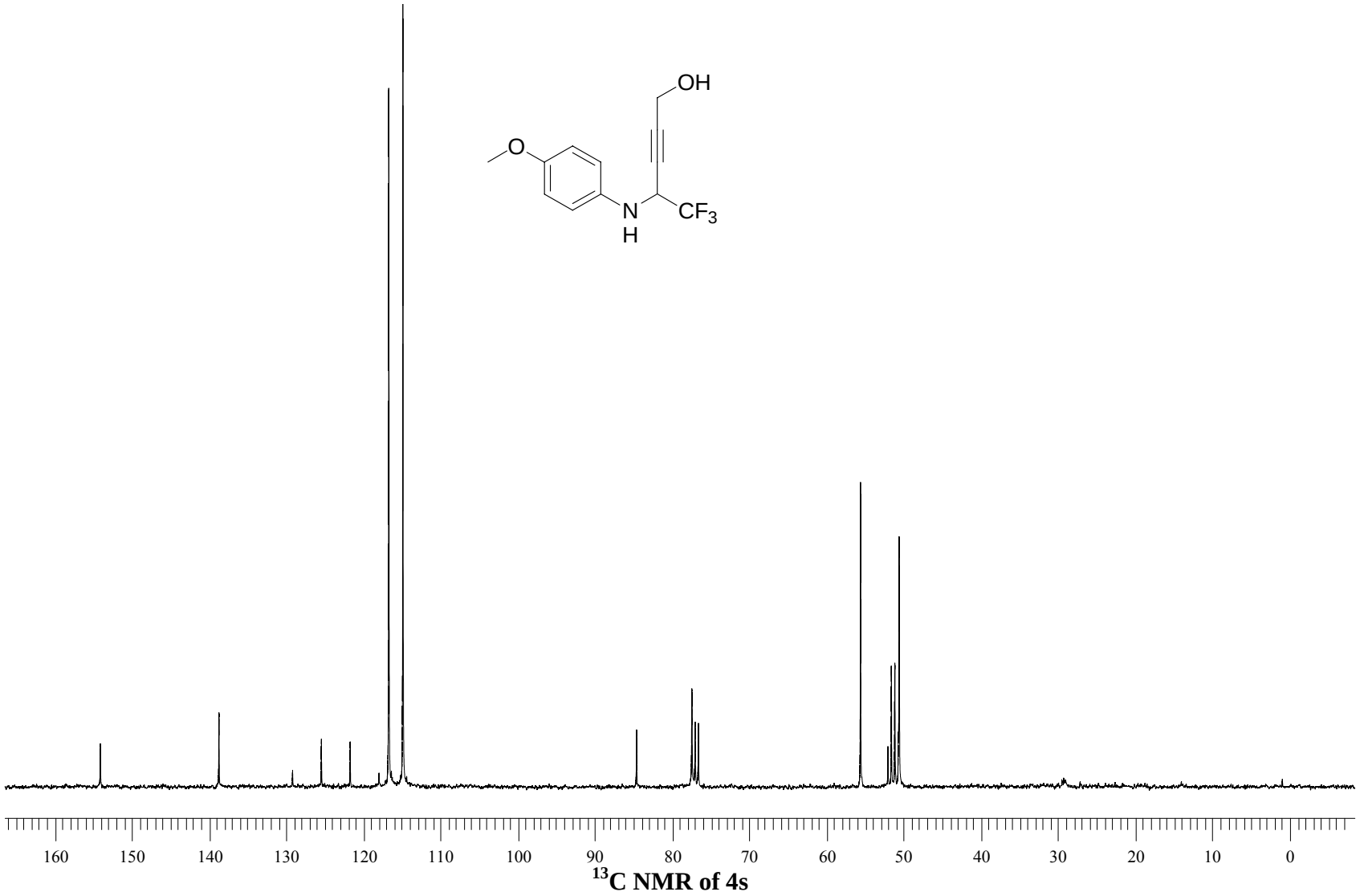
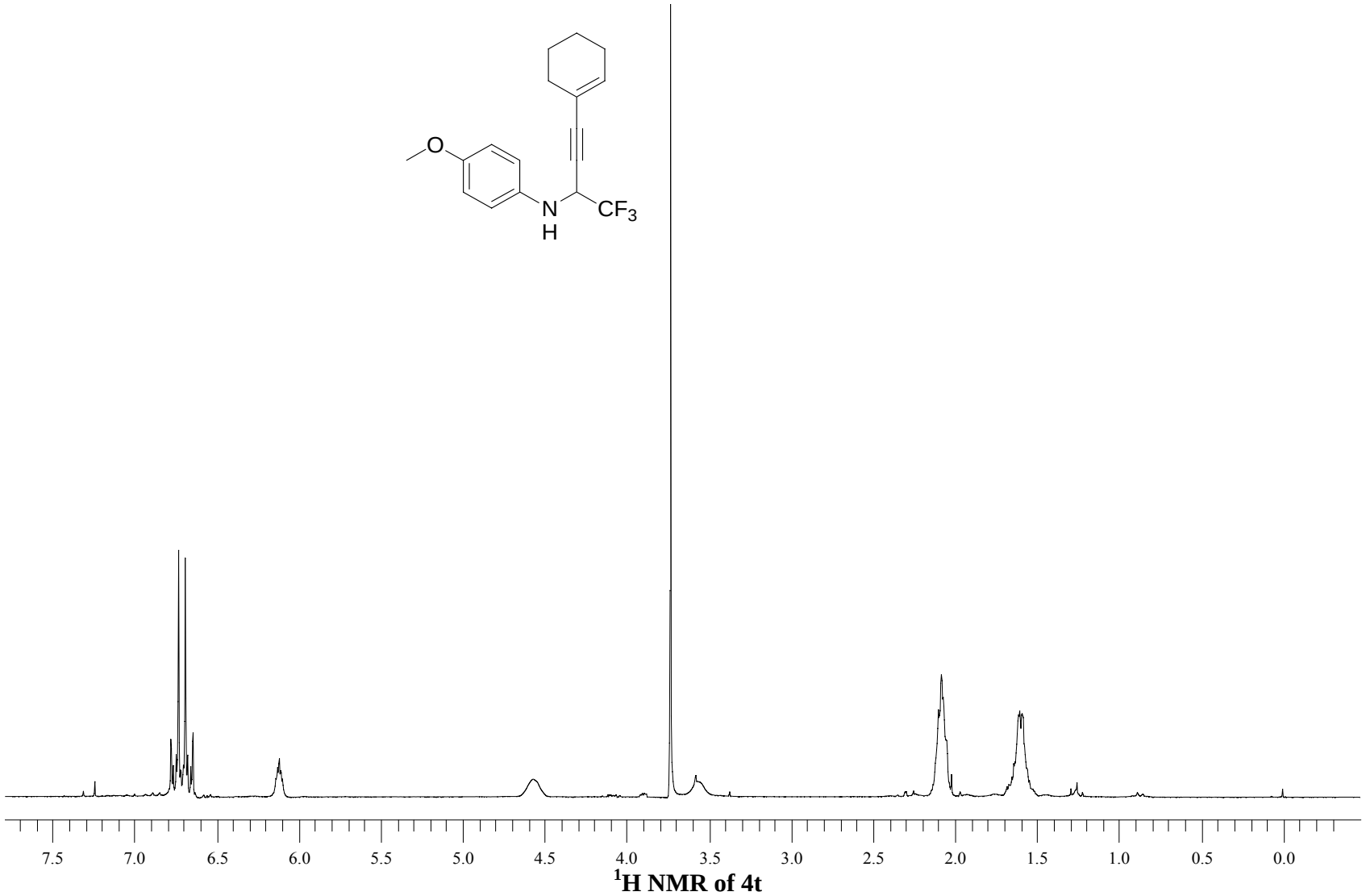


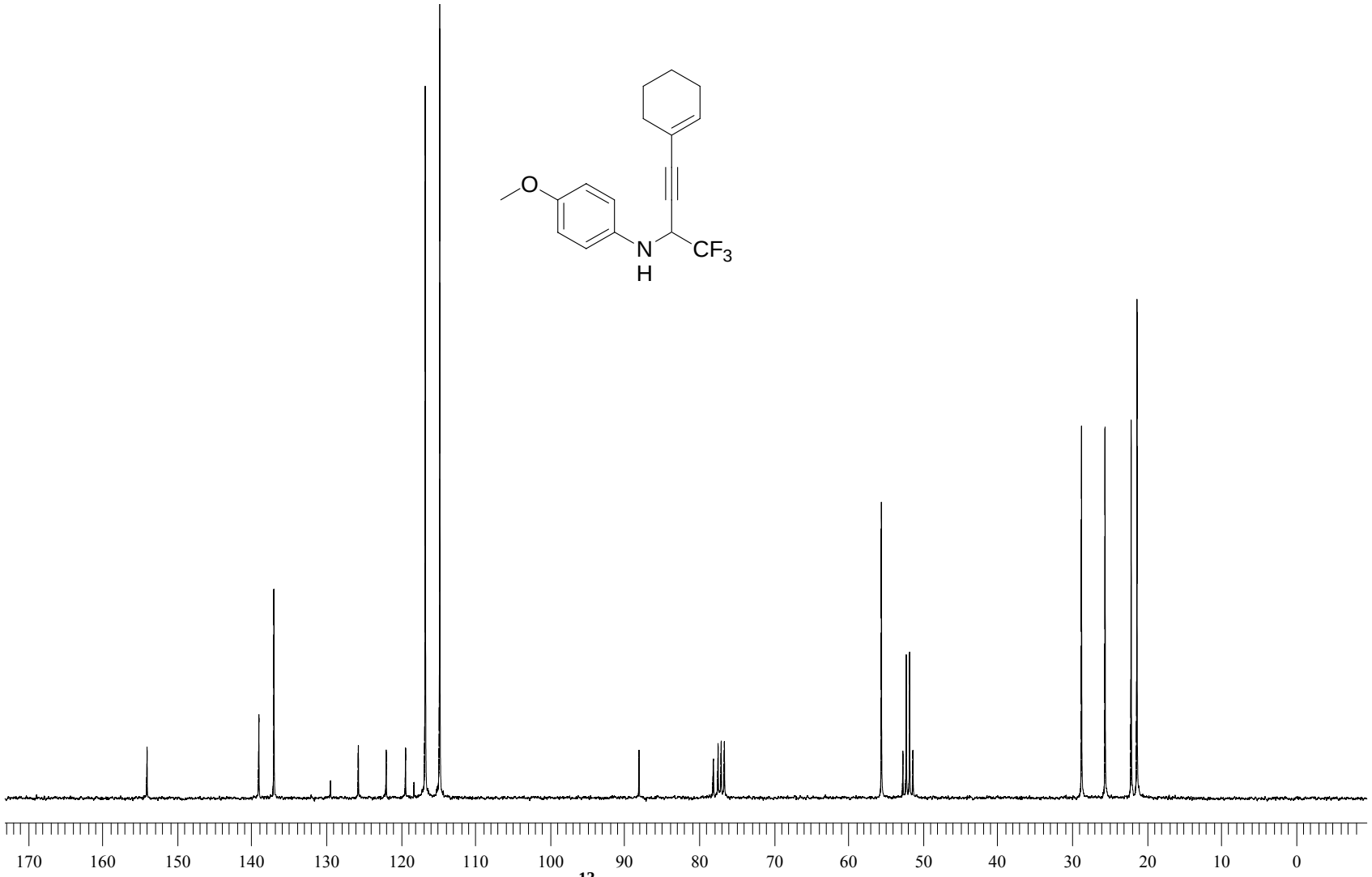
^{1}H NMR of 4s



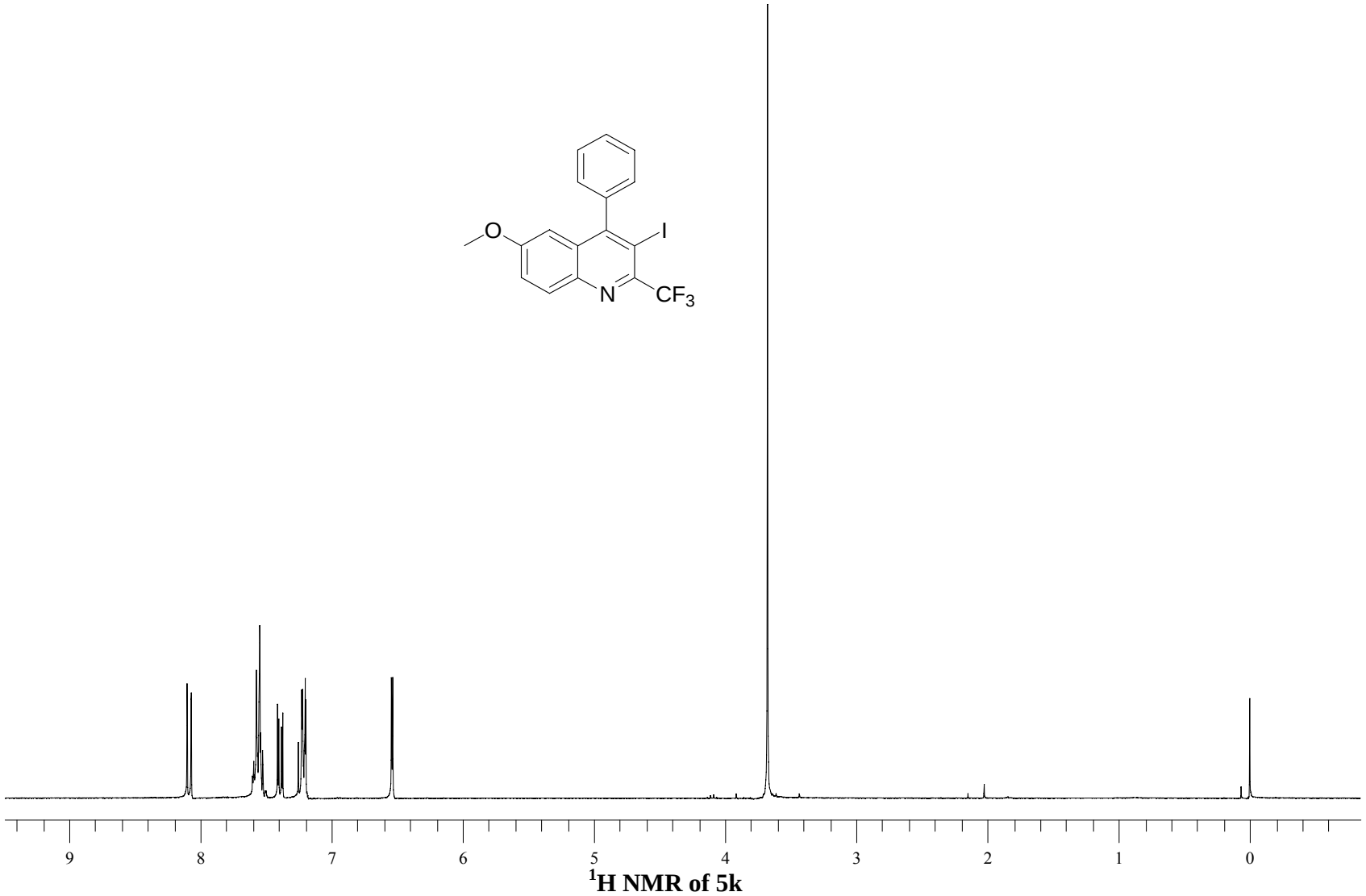
^{13}C NMR of 4s



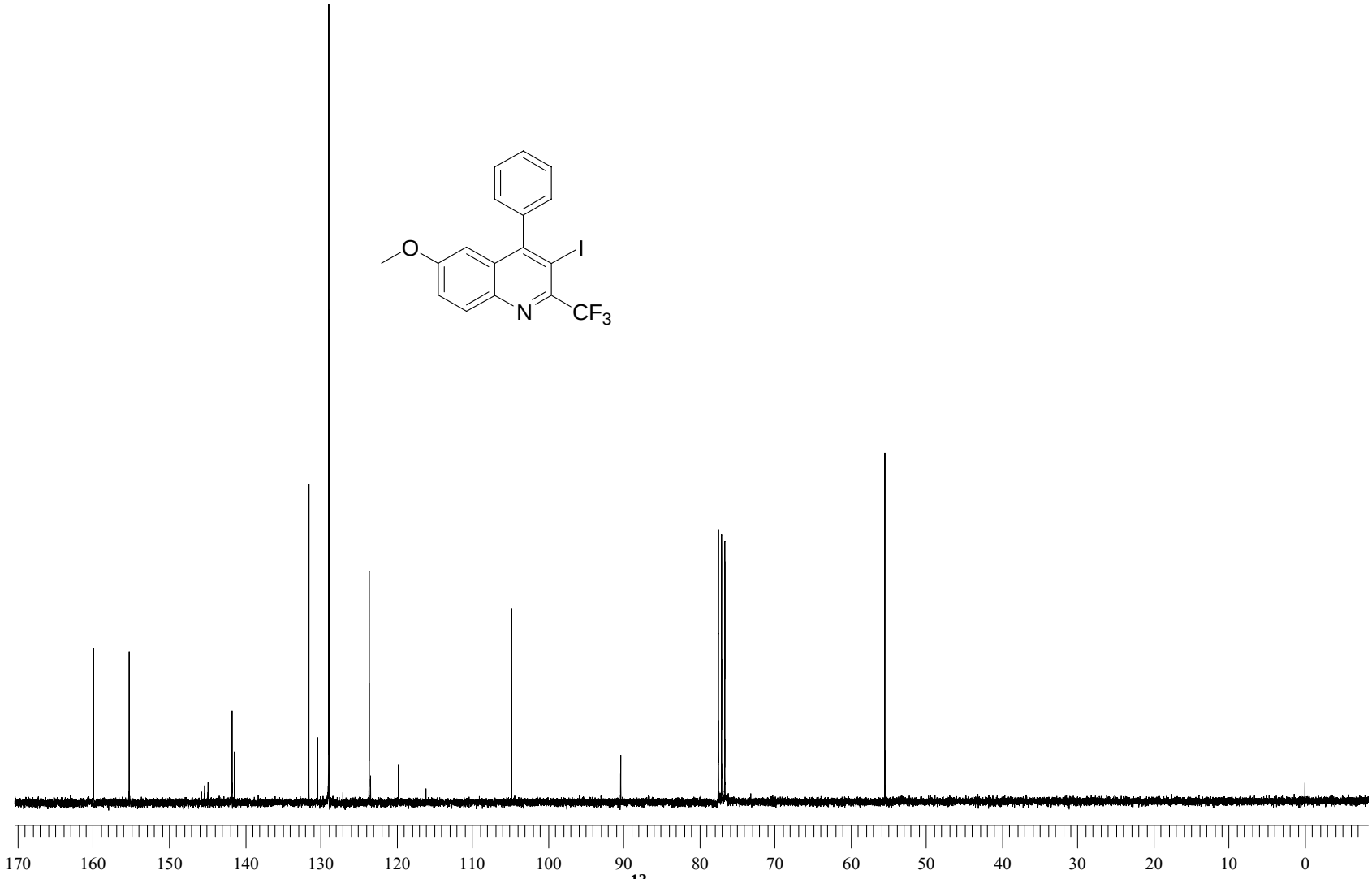
^{1}H NMR of 4t



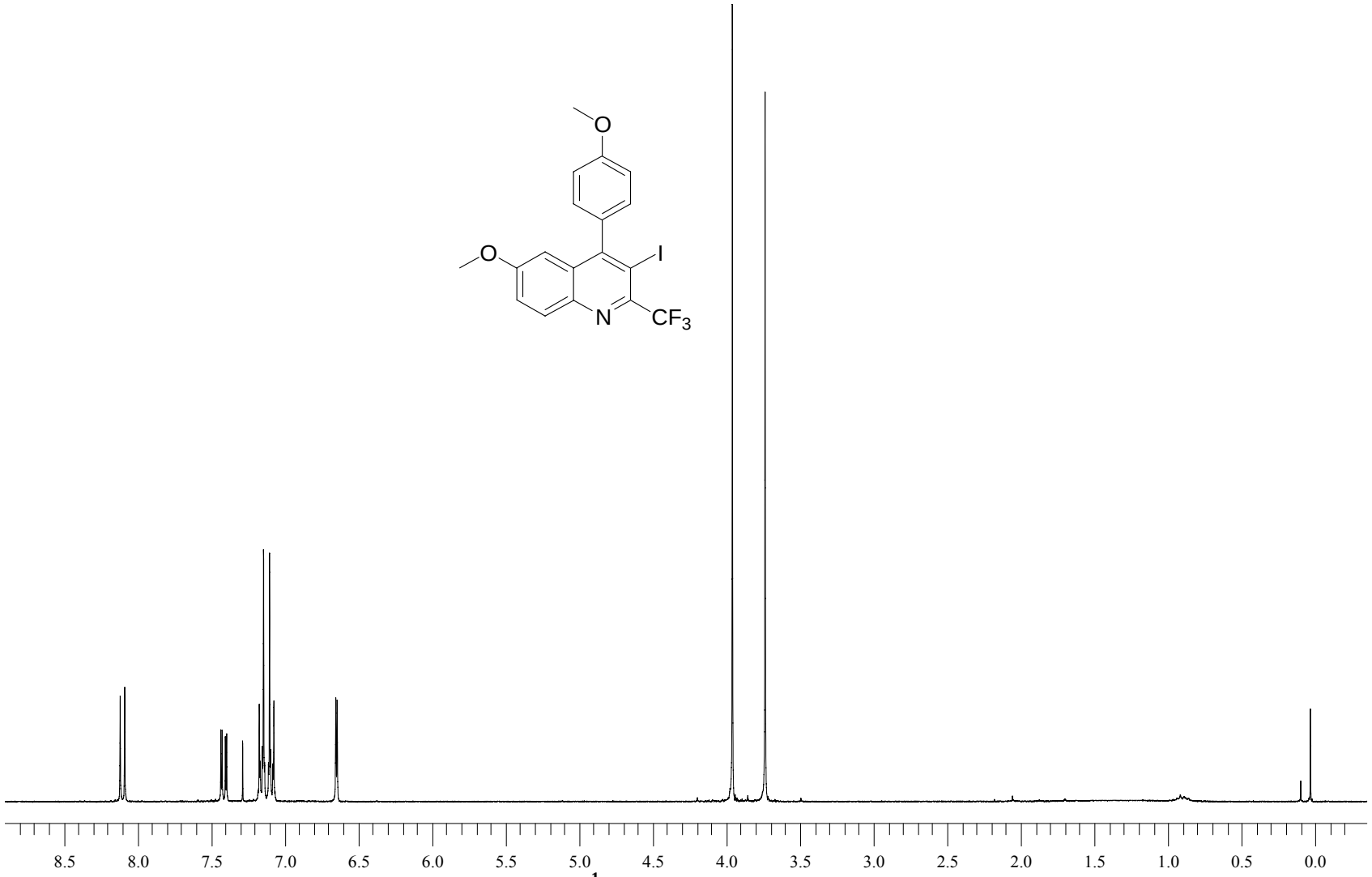
^{13}C NMR of 4t



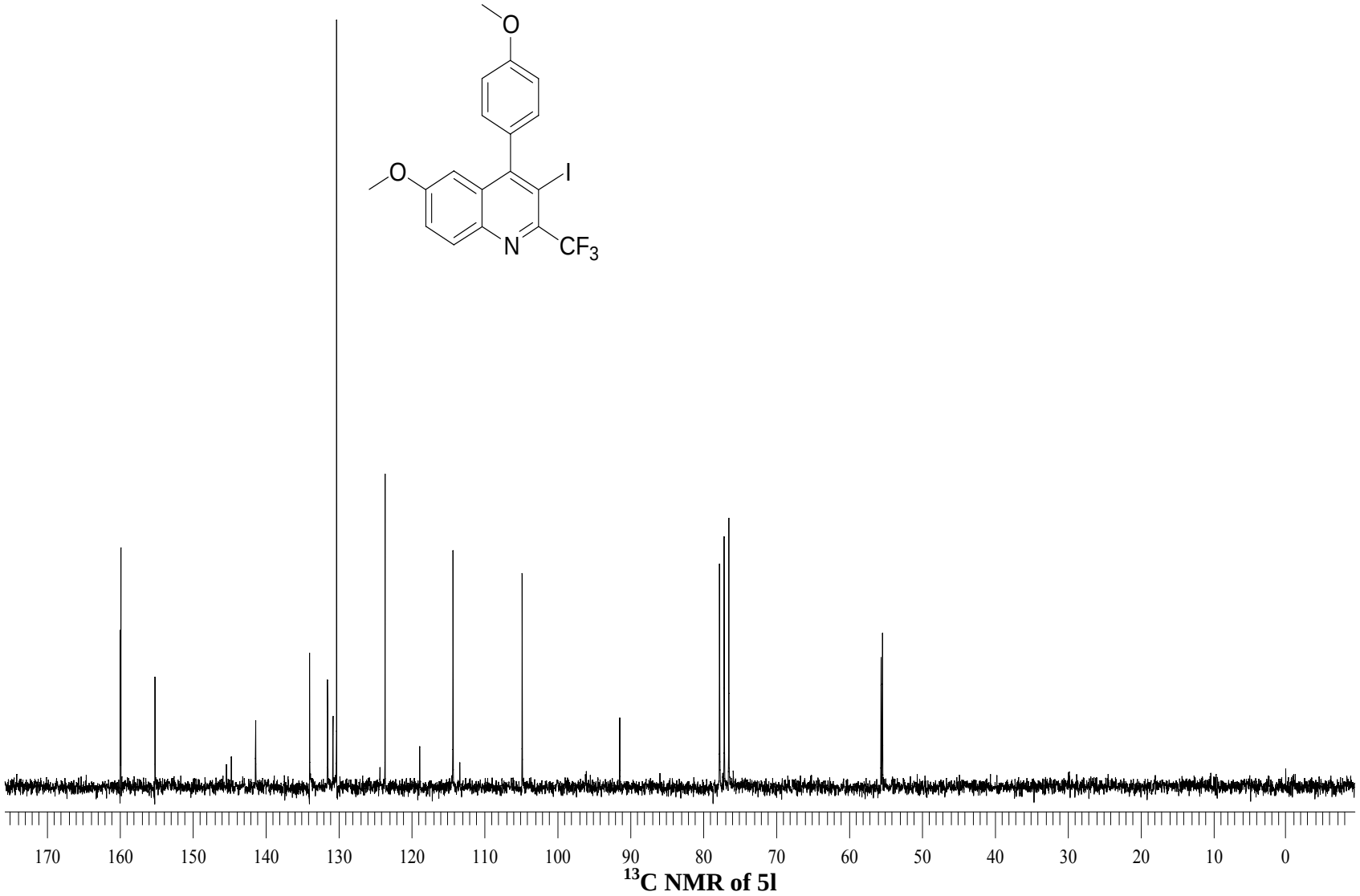
^{1}H NMR of 5k



^{13}C NMR of 5k



^{1}H NMR of 5l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CF3
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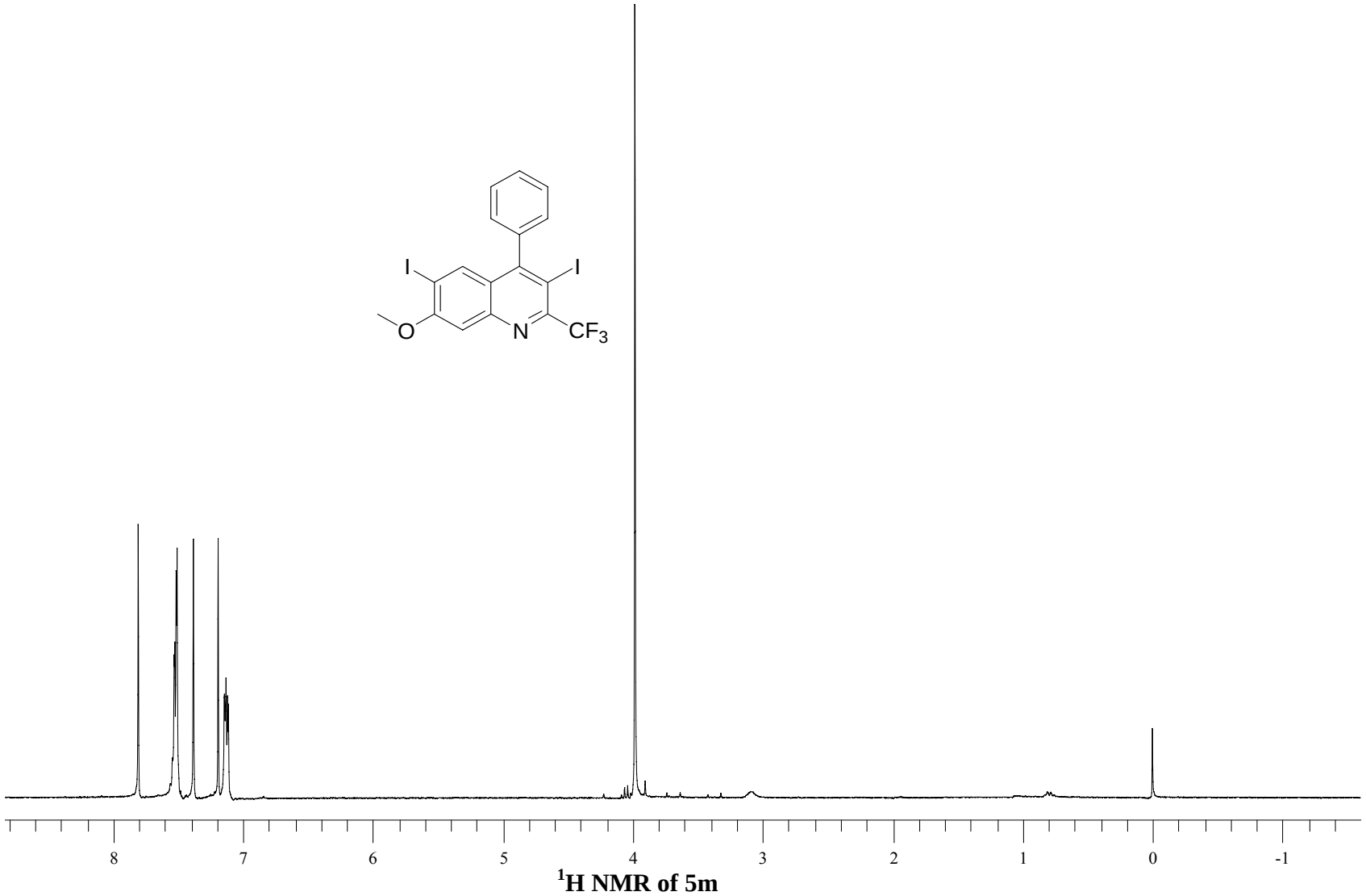
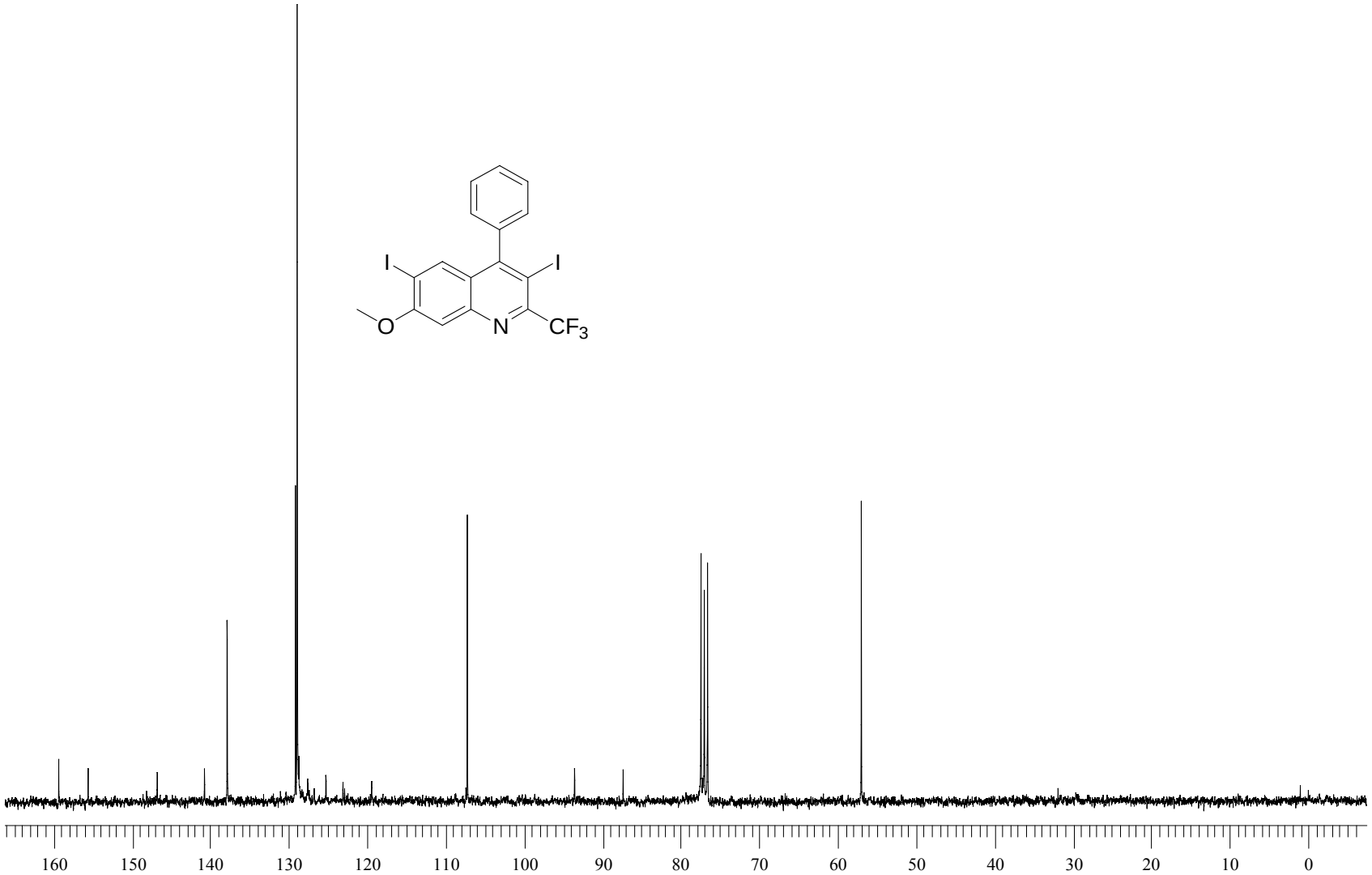
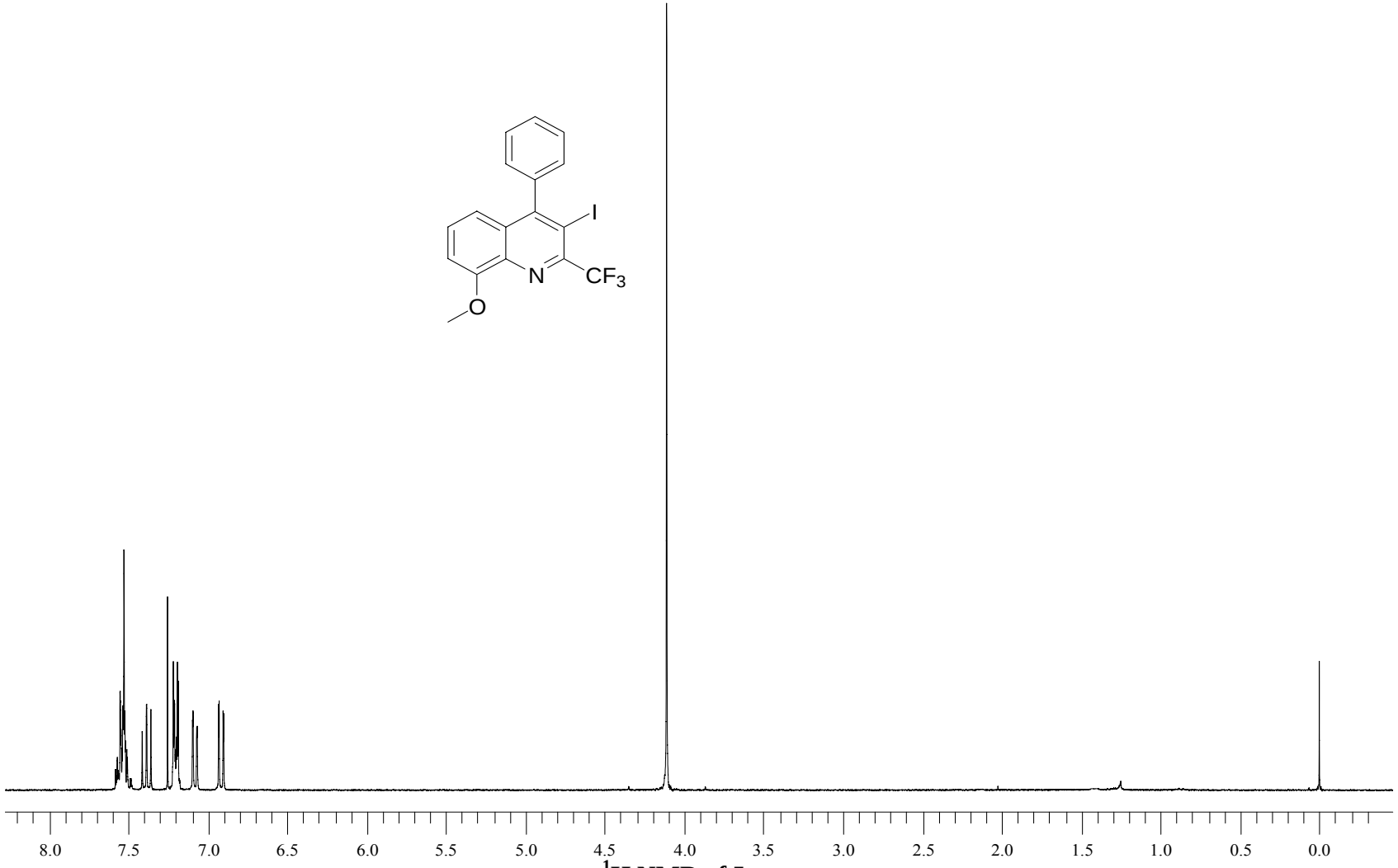
^{13}C NMR of 5l



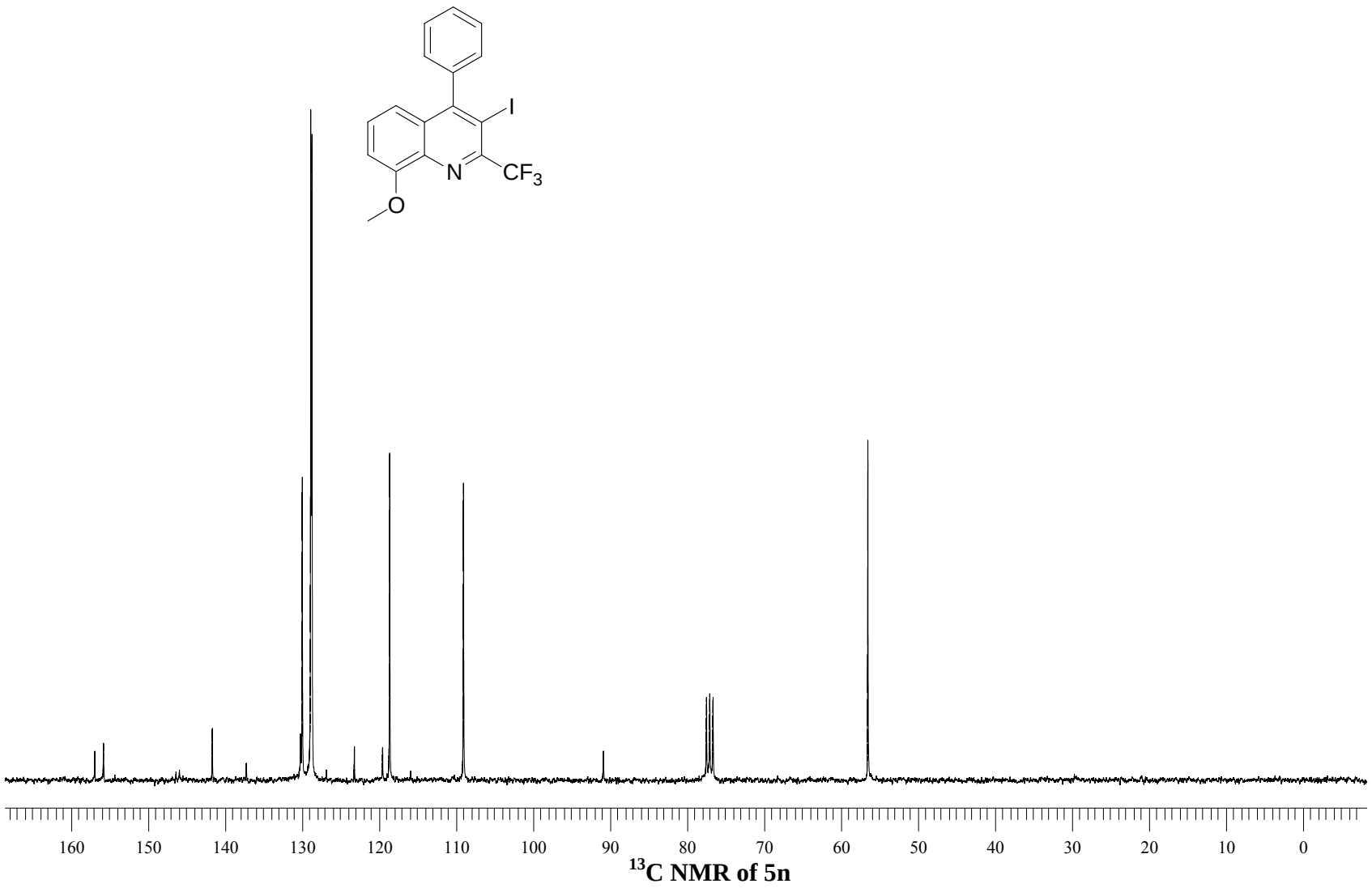
^{1}H NMR of 5m



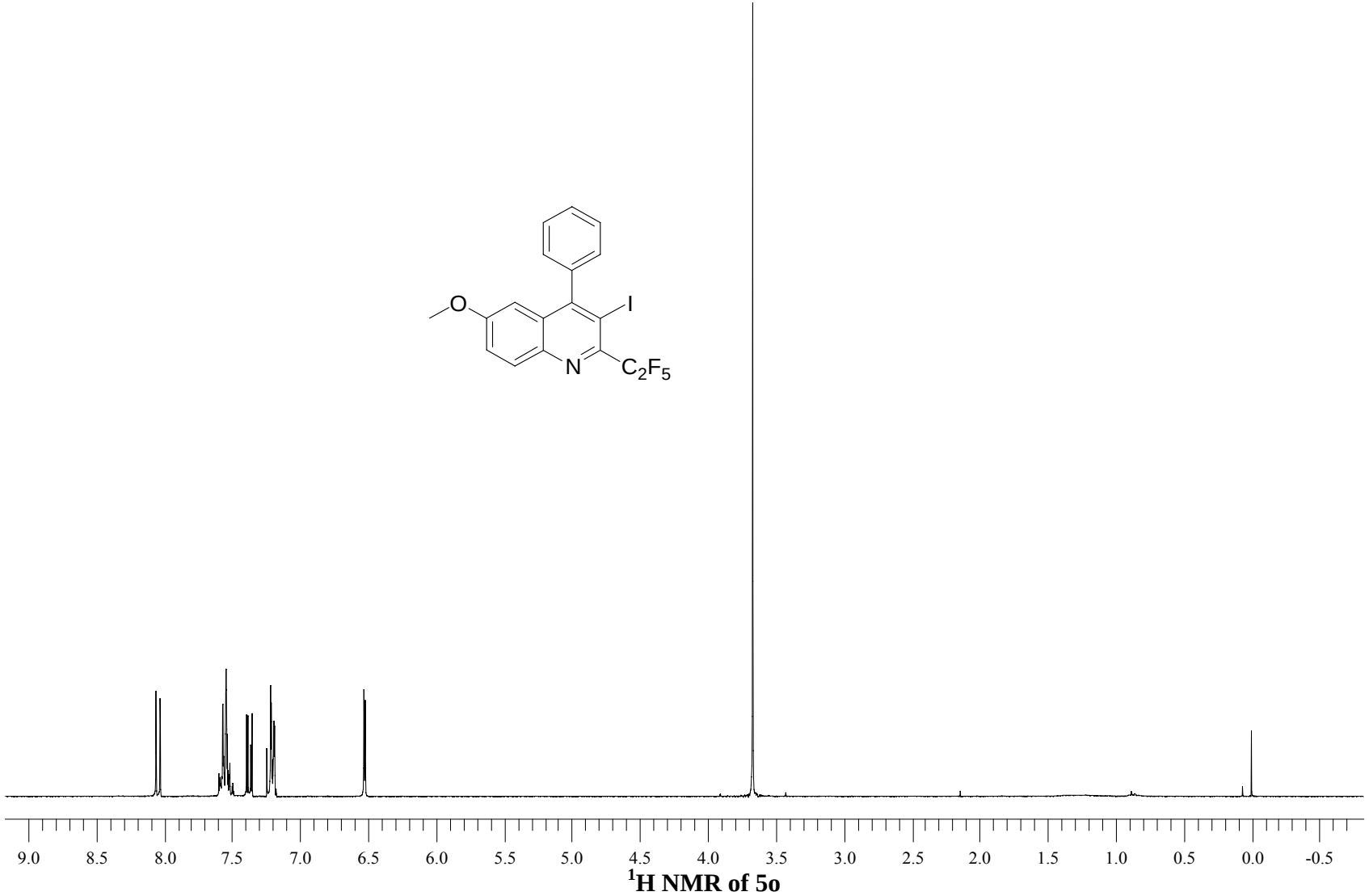
^{13}C NMR of 5m



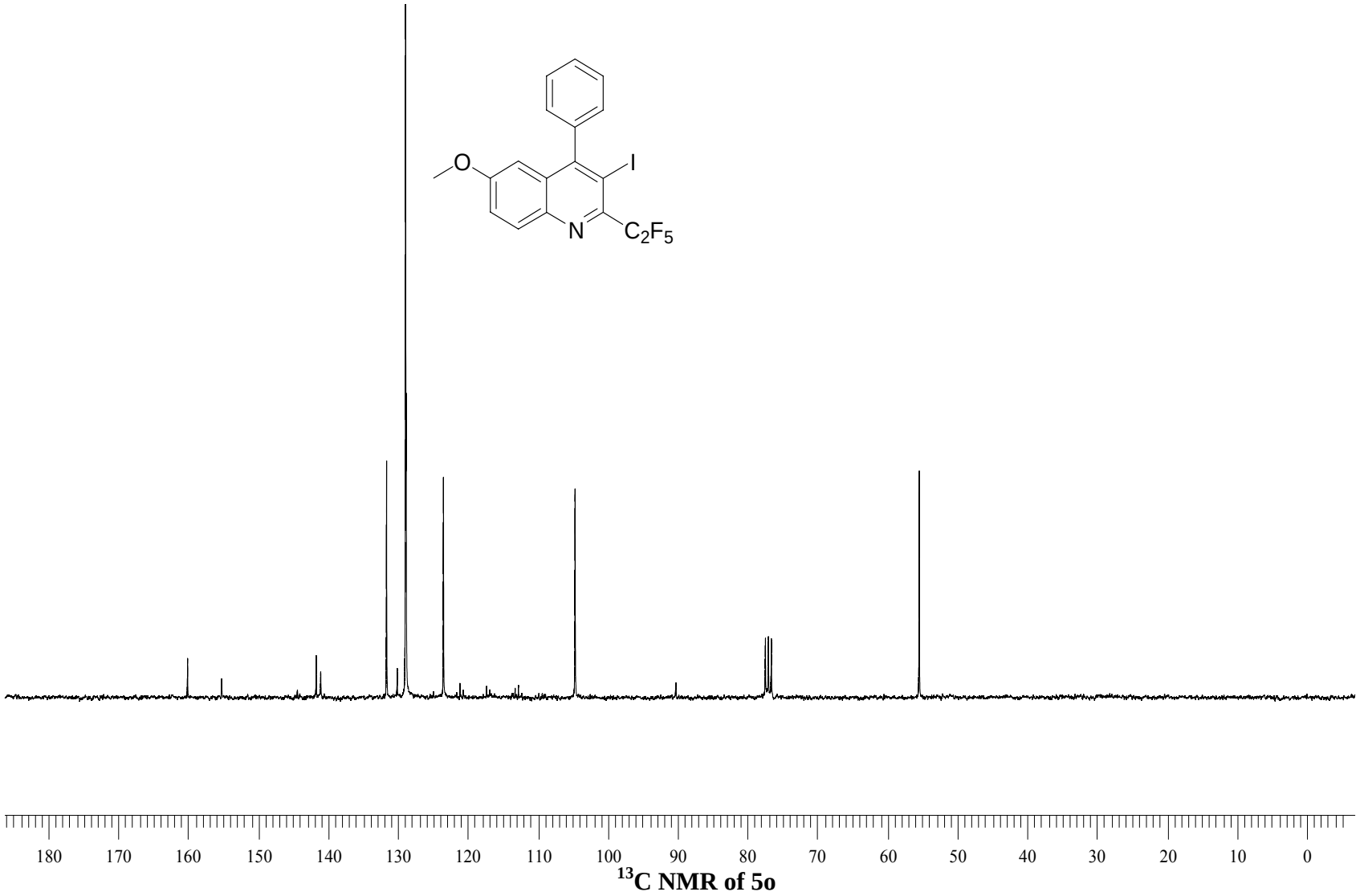
^{1}H NMR of 5n



^{13}C NMR of 5n



^{1}H NMR of 5o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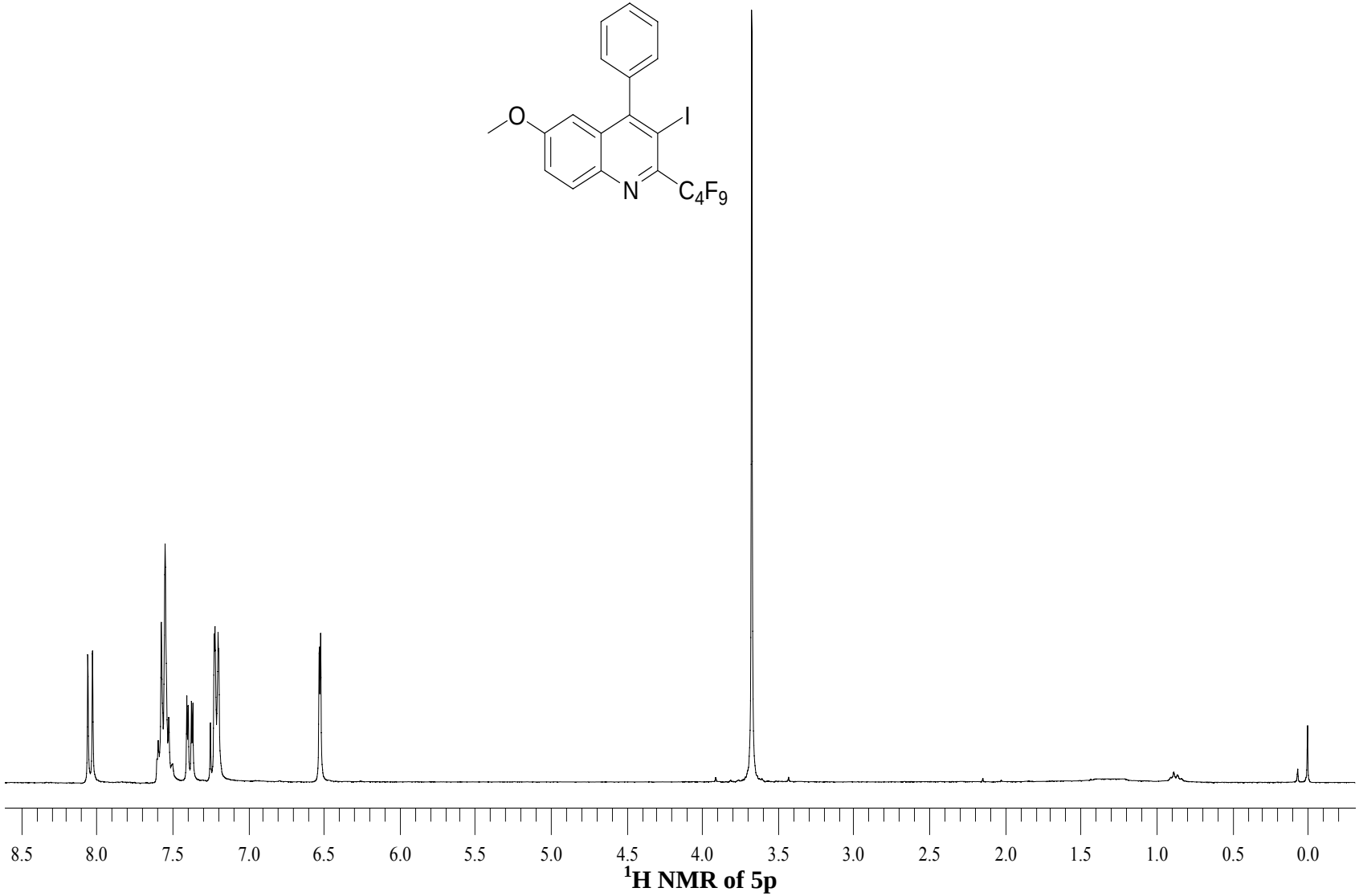
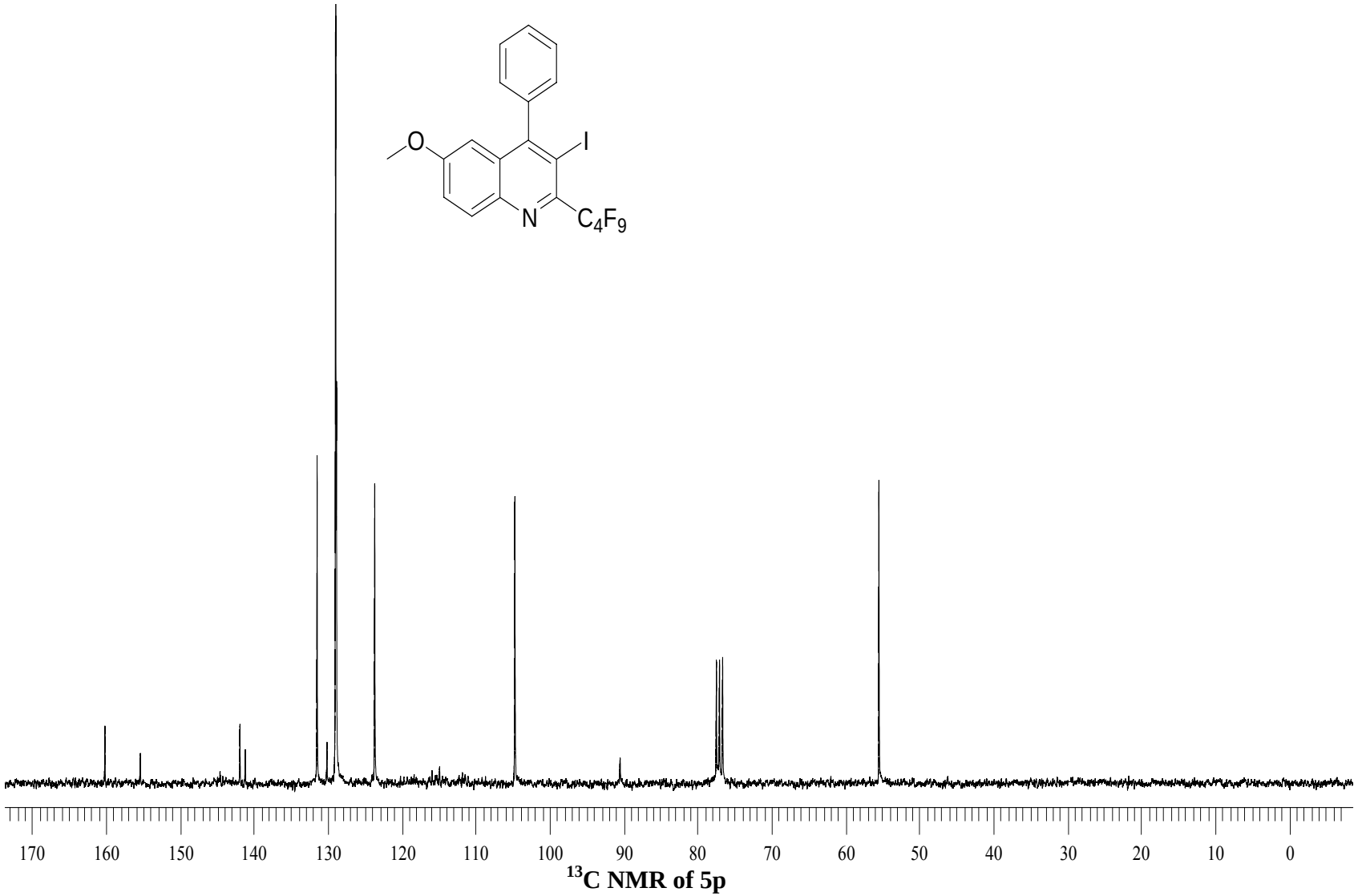
^{13}C NMR of 5o



^{1}H NMR of 5p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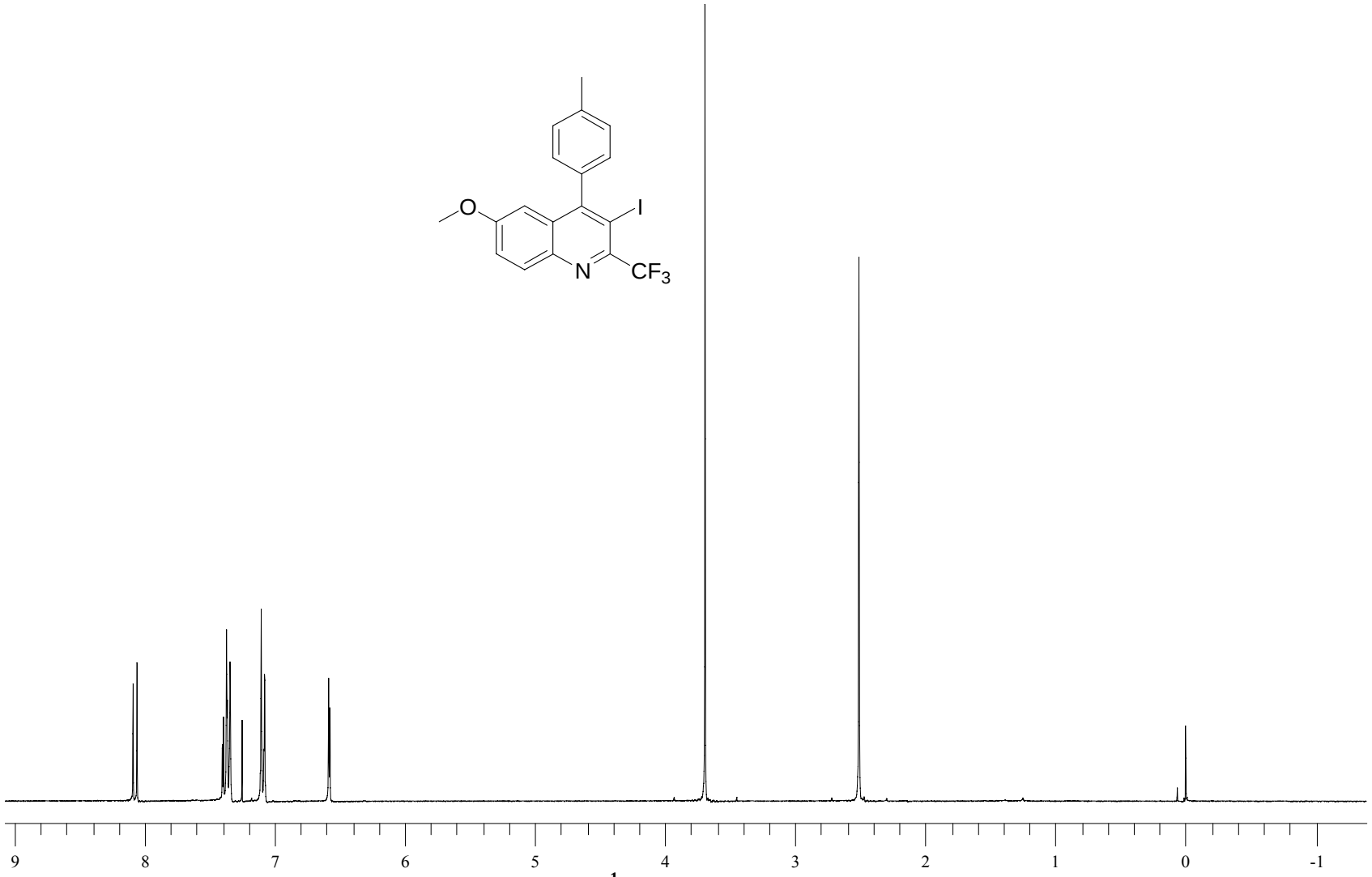
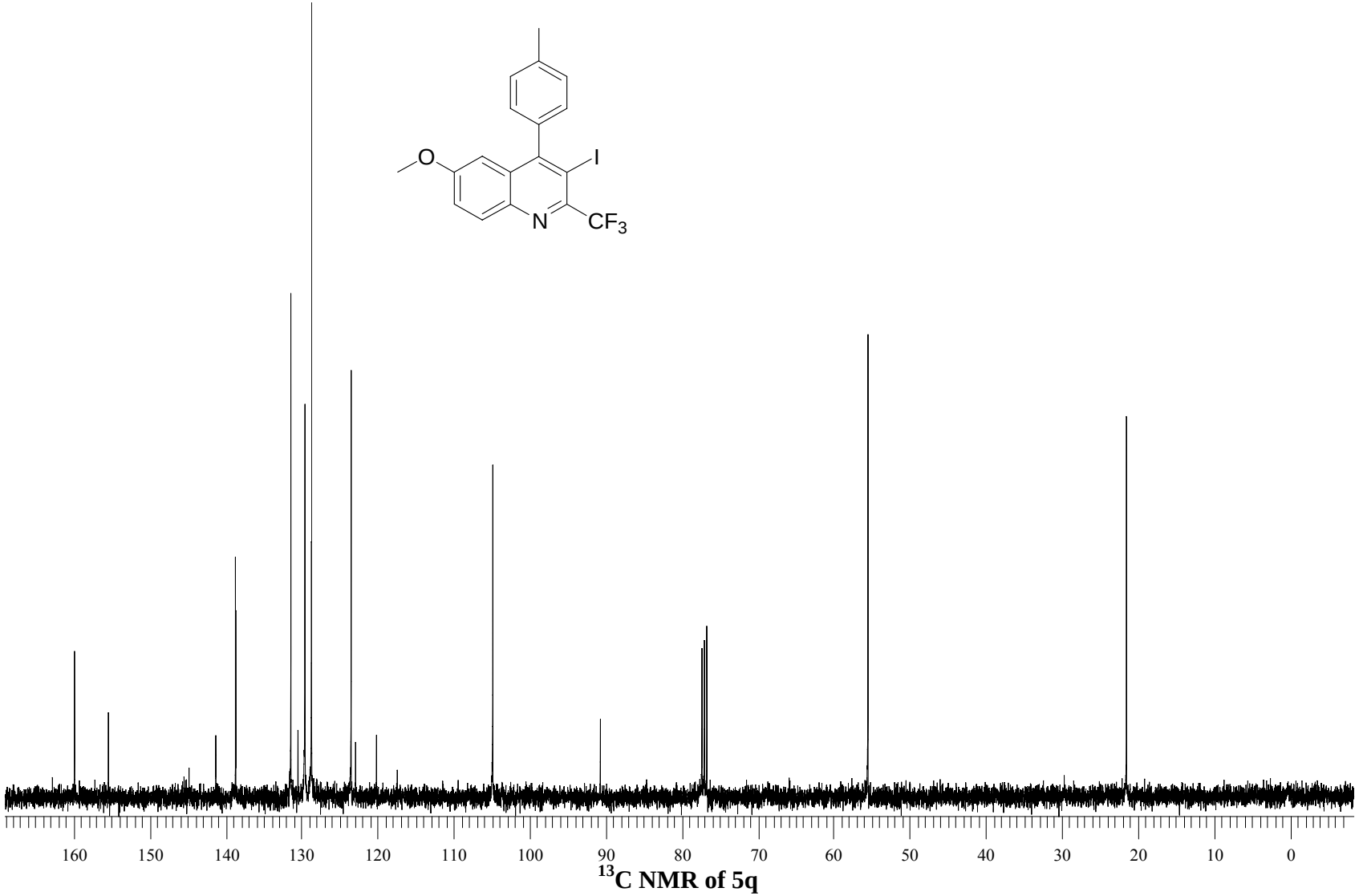
^{13}C NMR of 5p



^{1}H NMR of 5q



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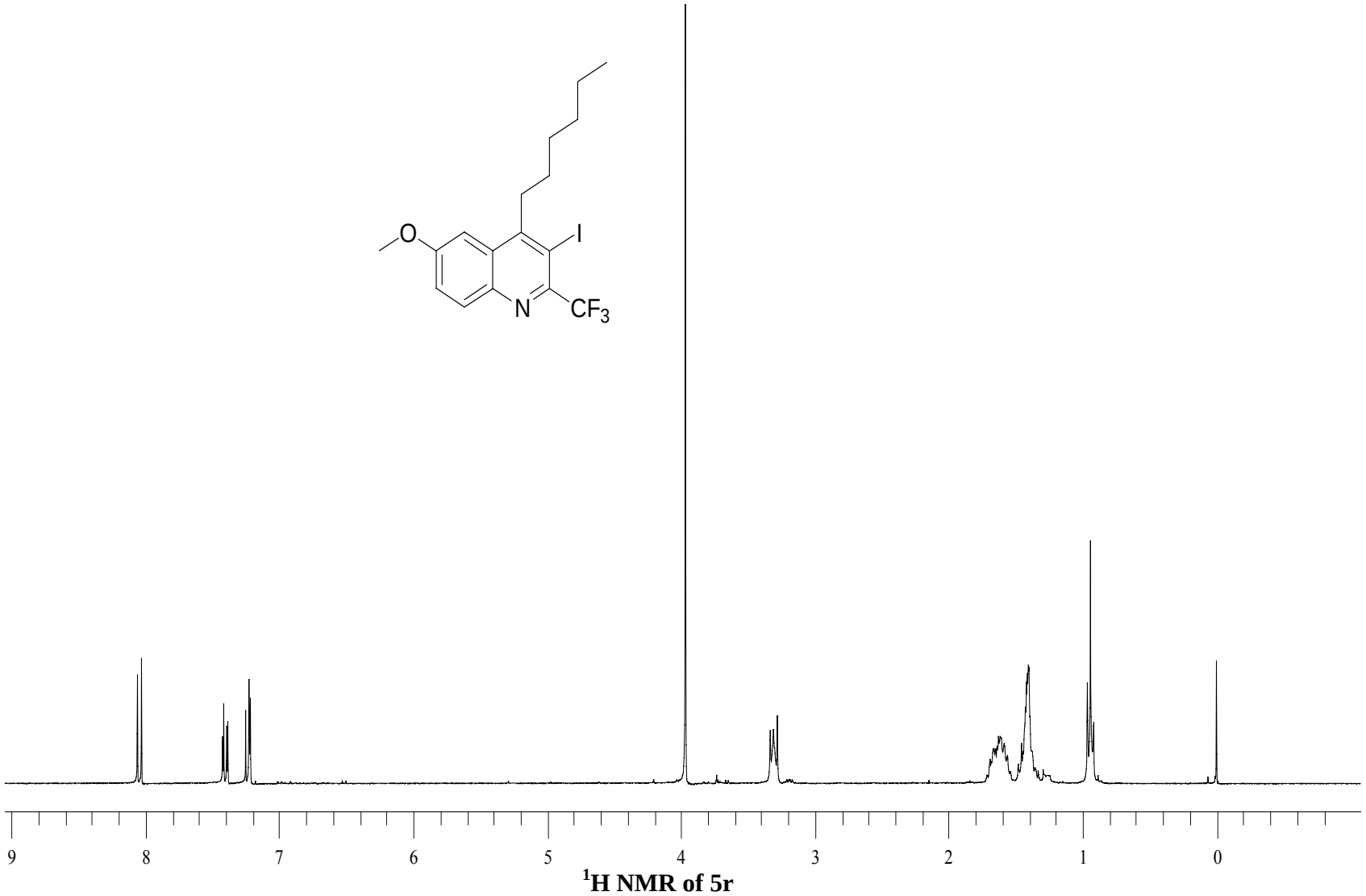
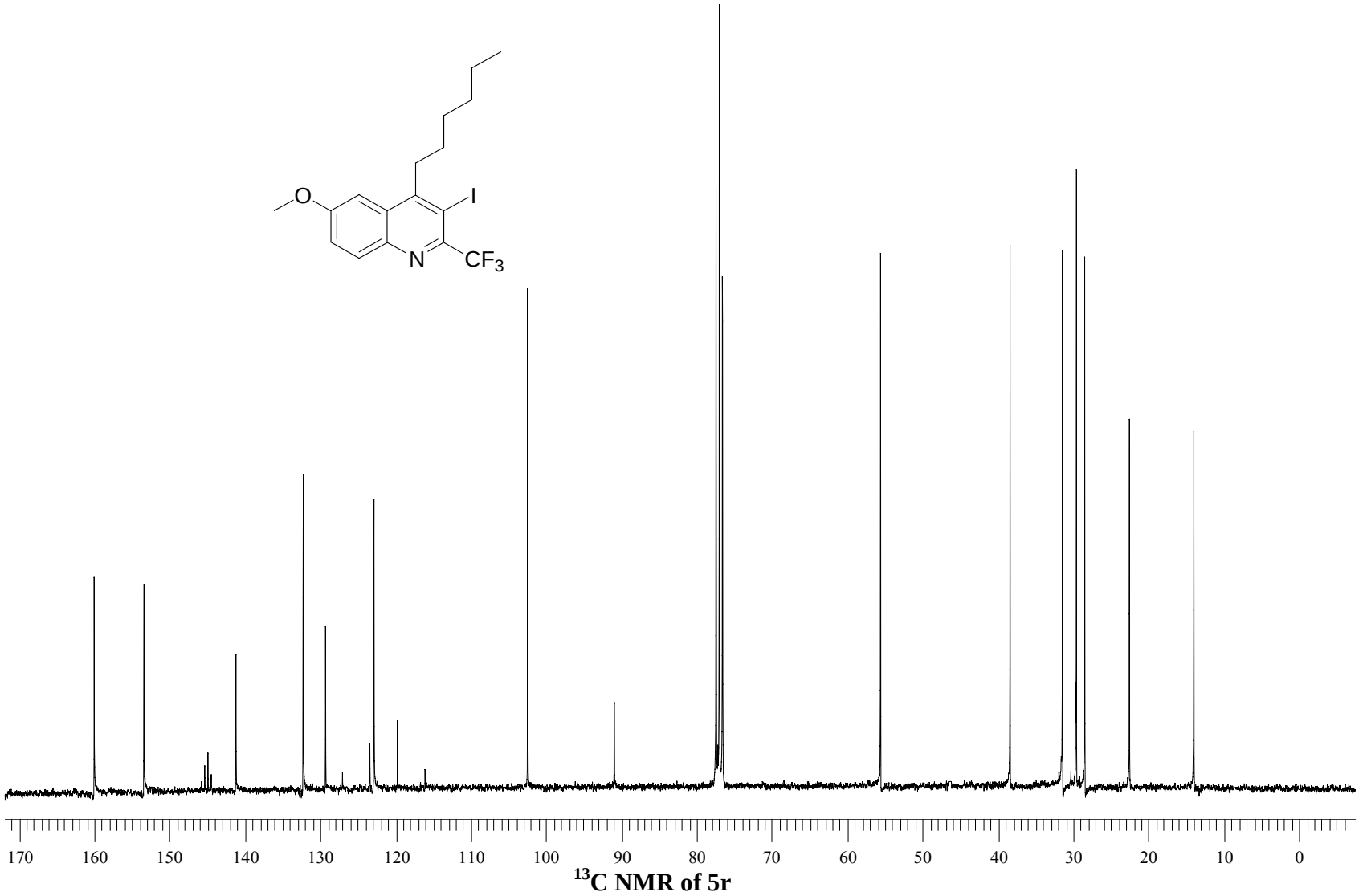
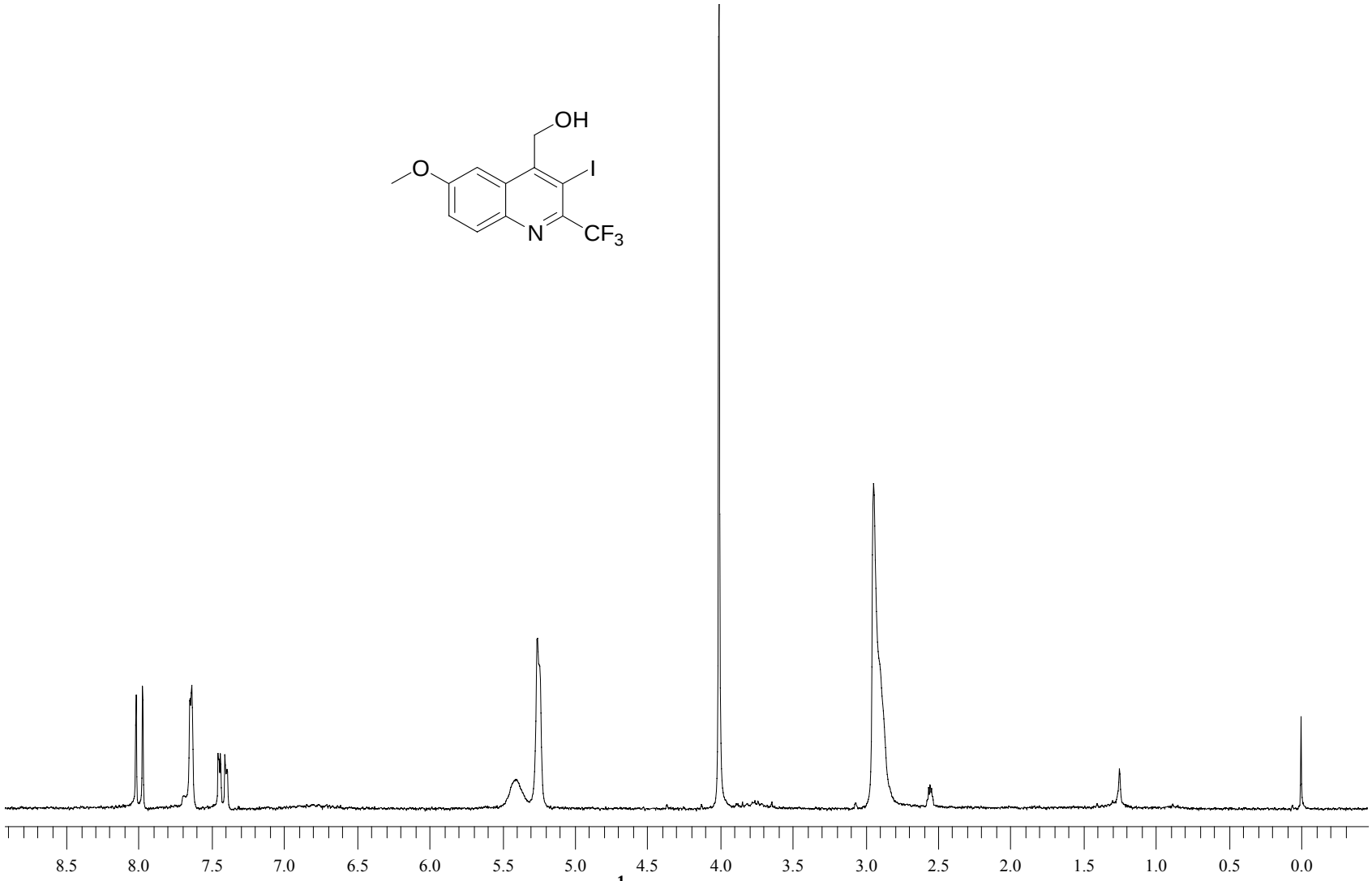


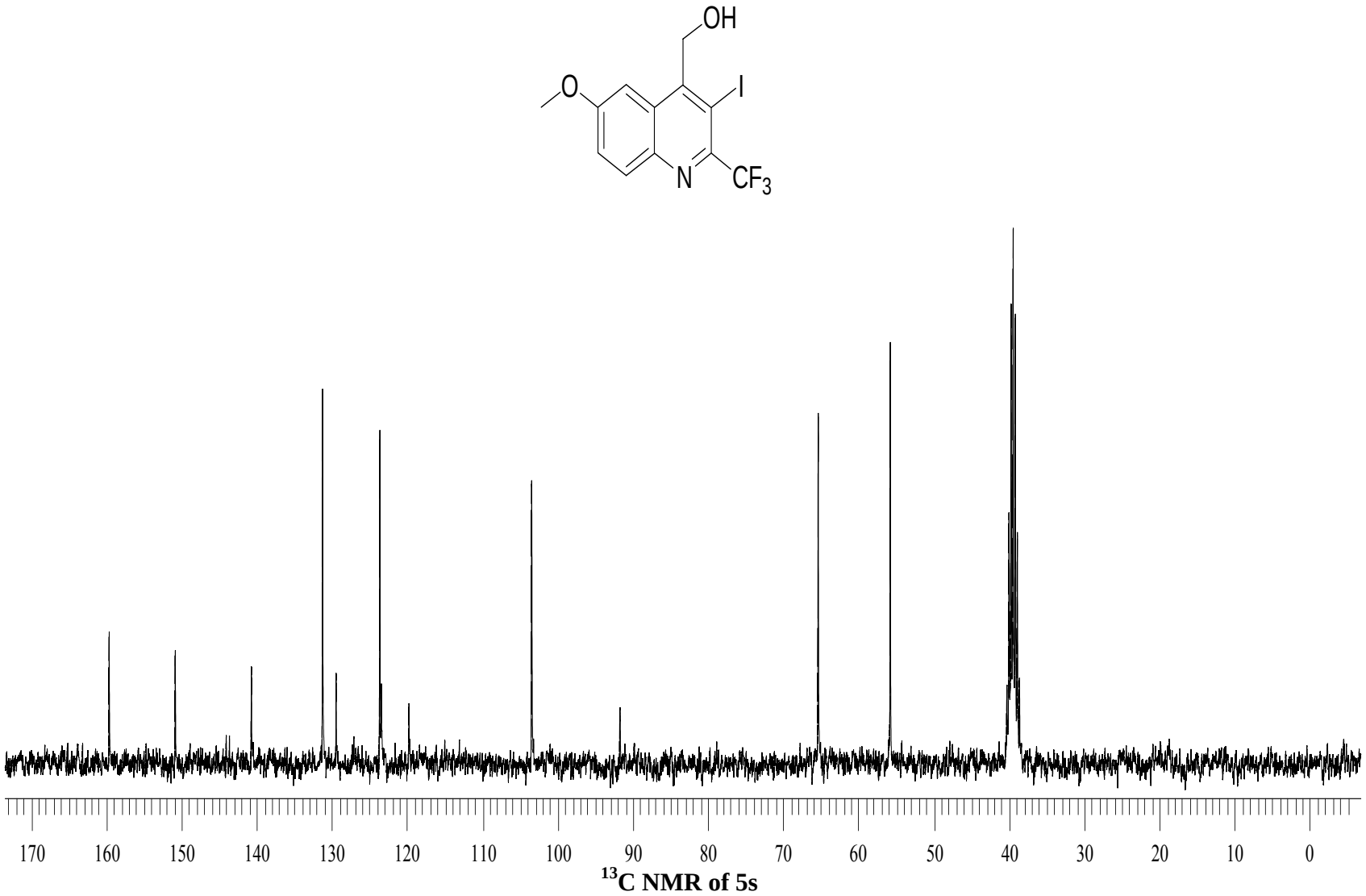
^{1}H NMR of 5r



^{13}C NMR of 5r



^{1}H NMR of 5s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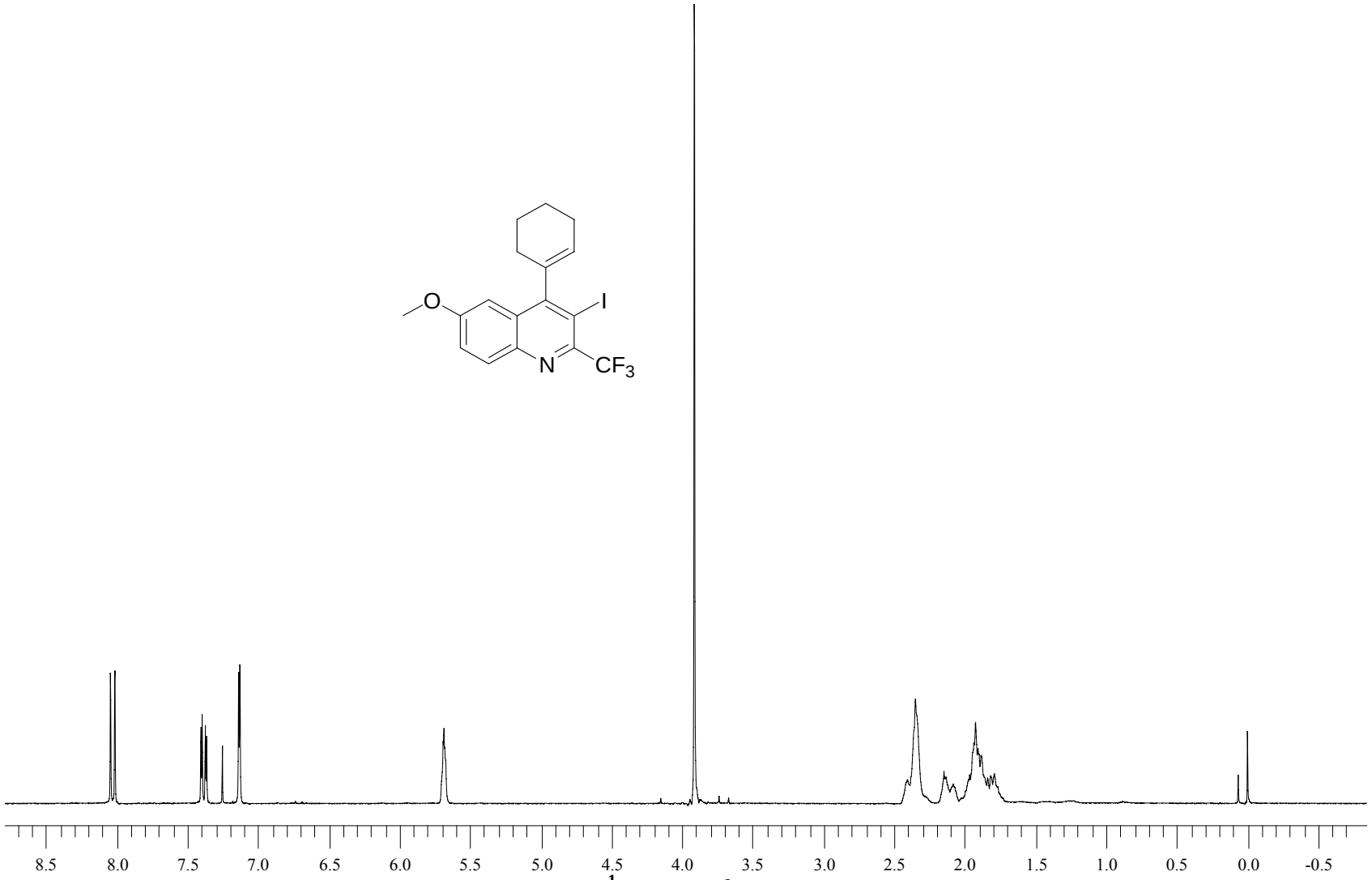
^{13}C NMR of 5s



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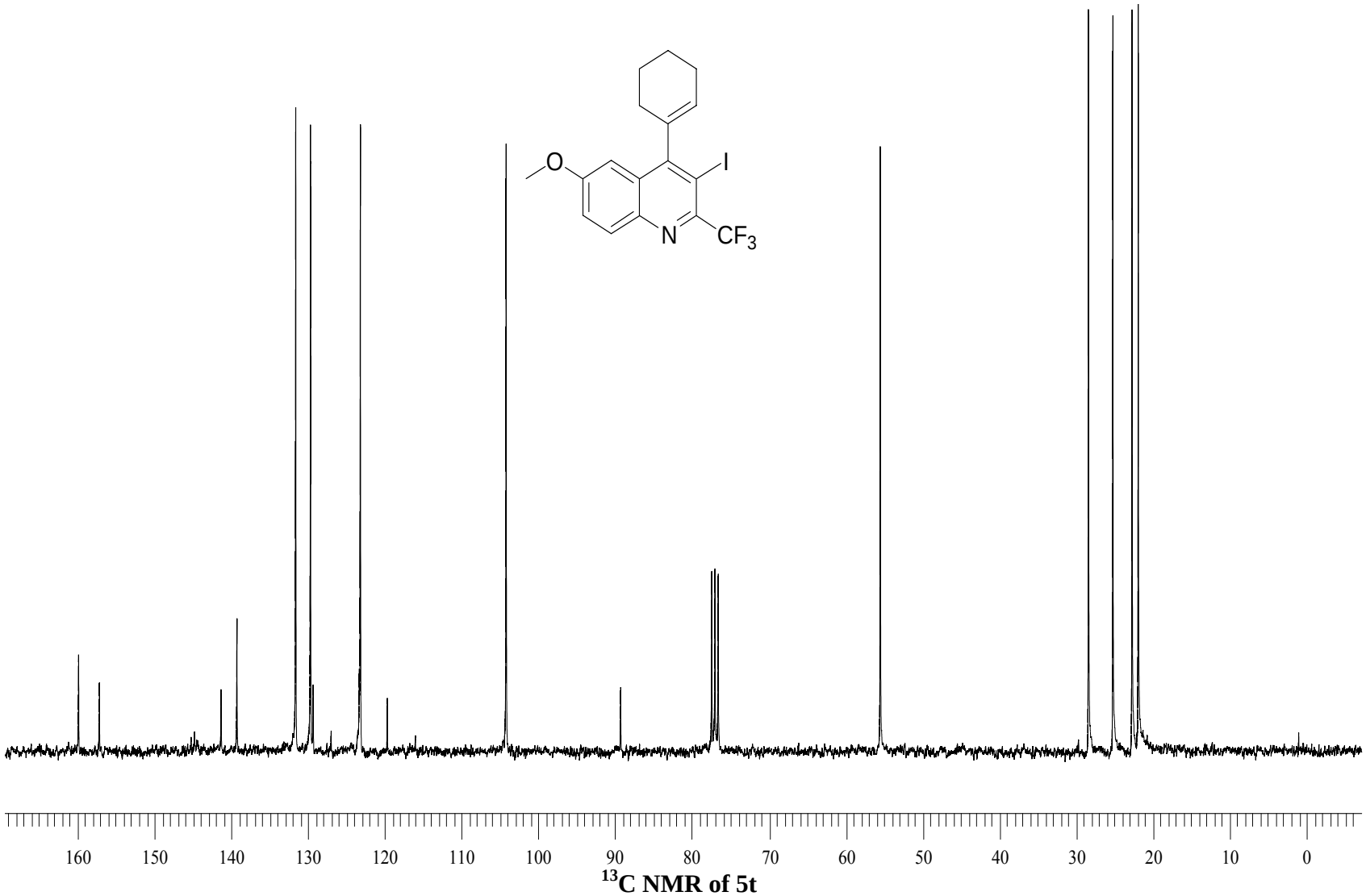
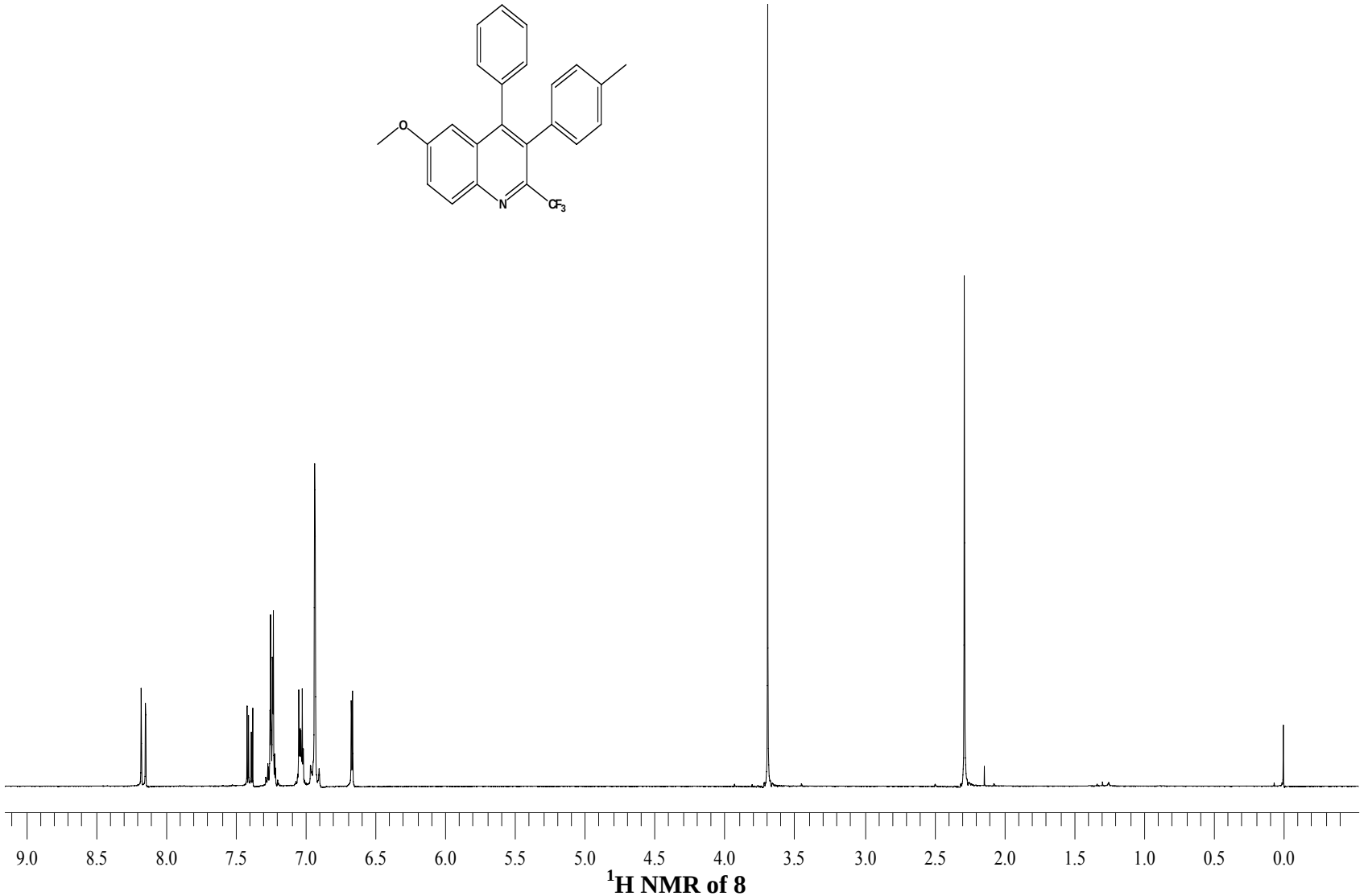
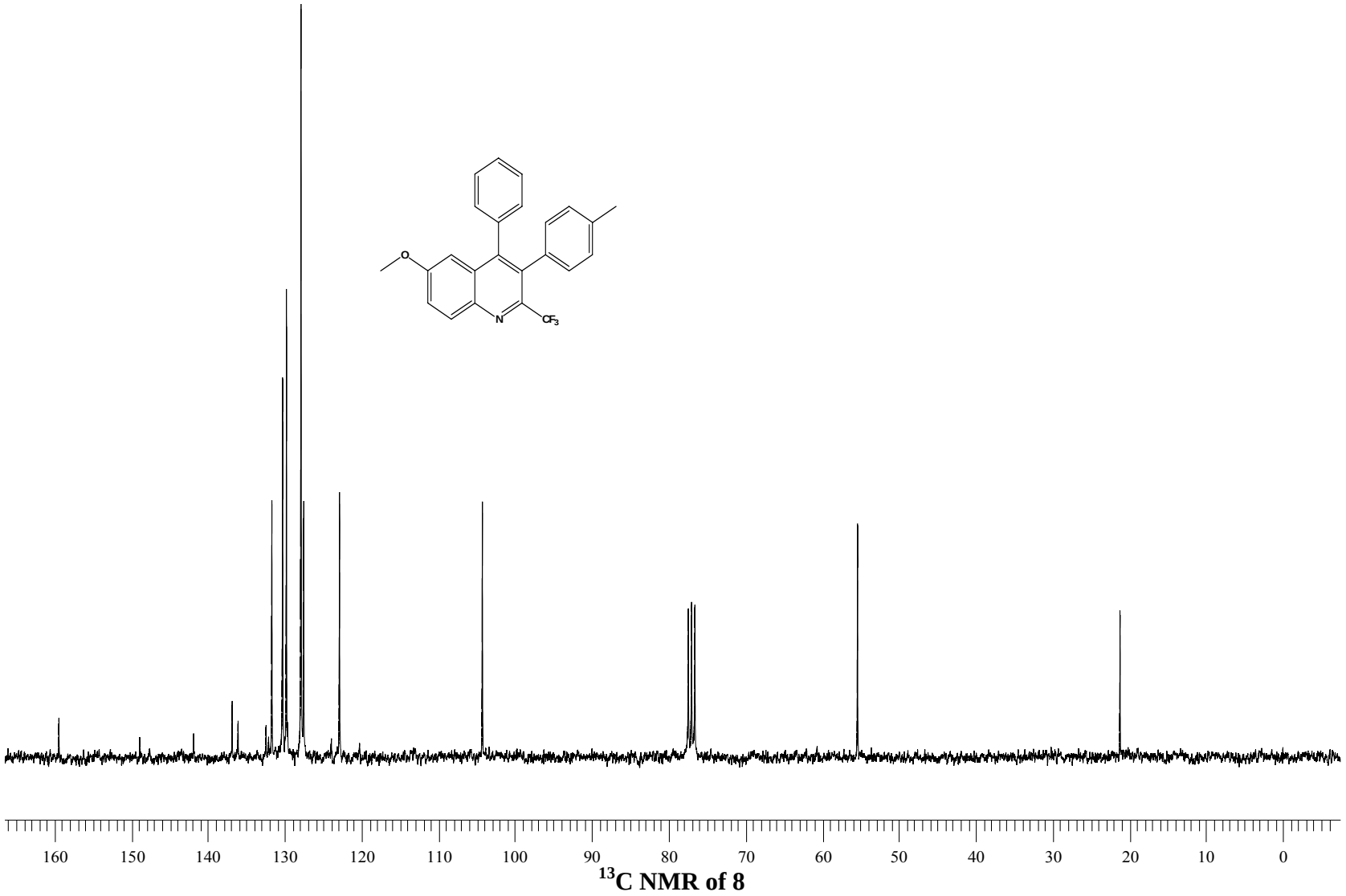


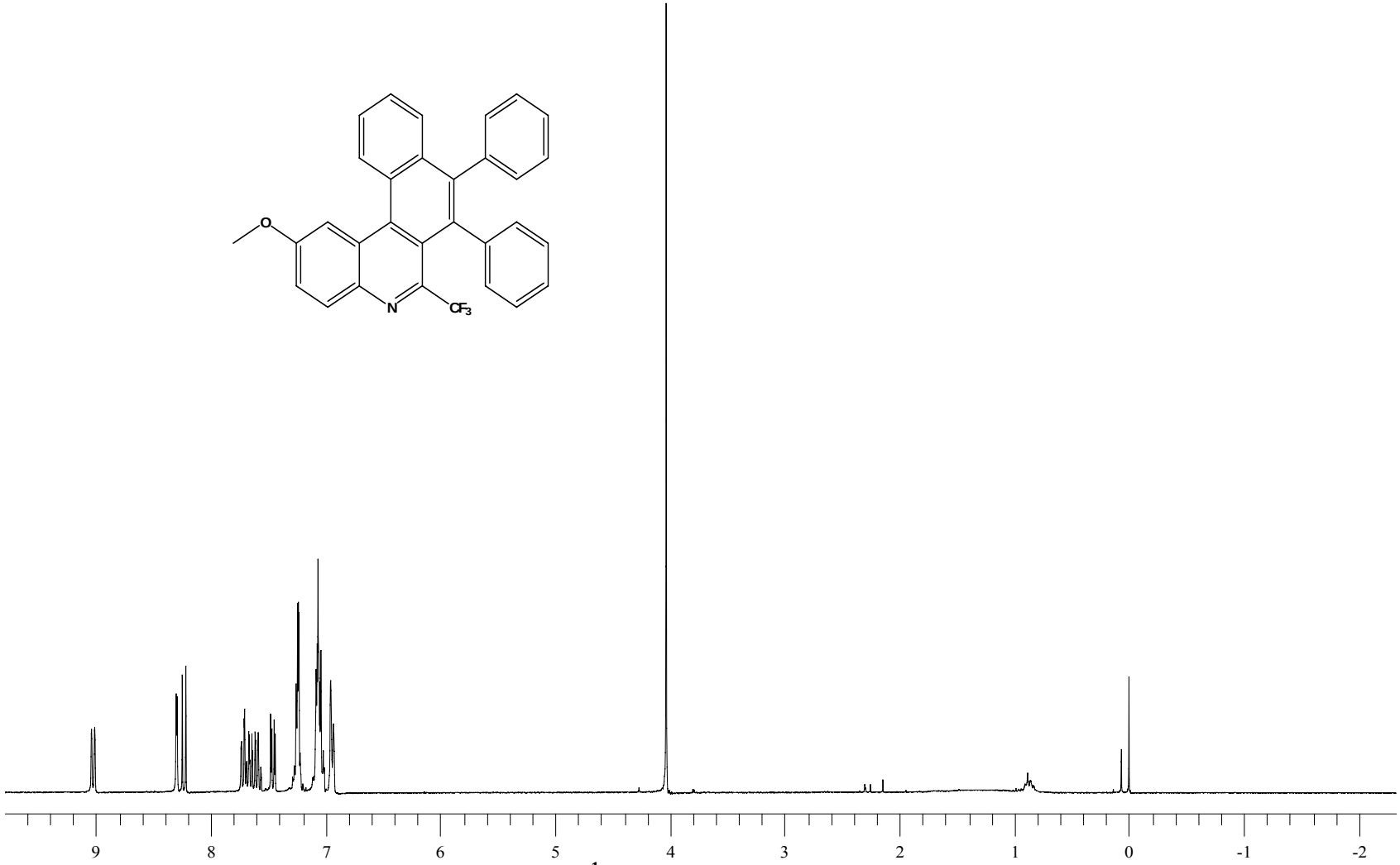
^{13}C NMR of 5t



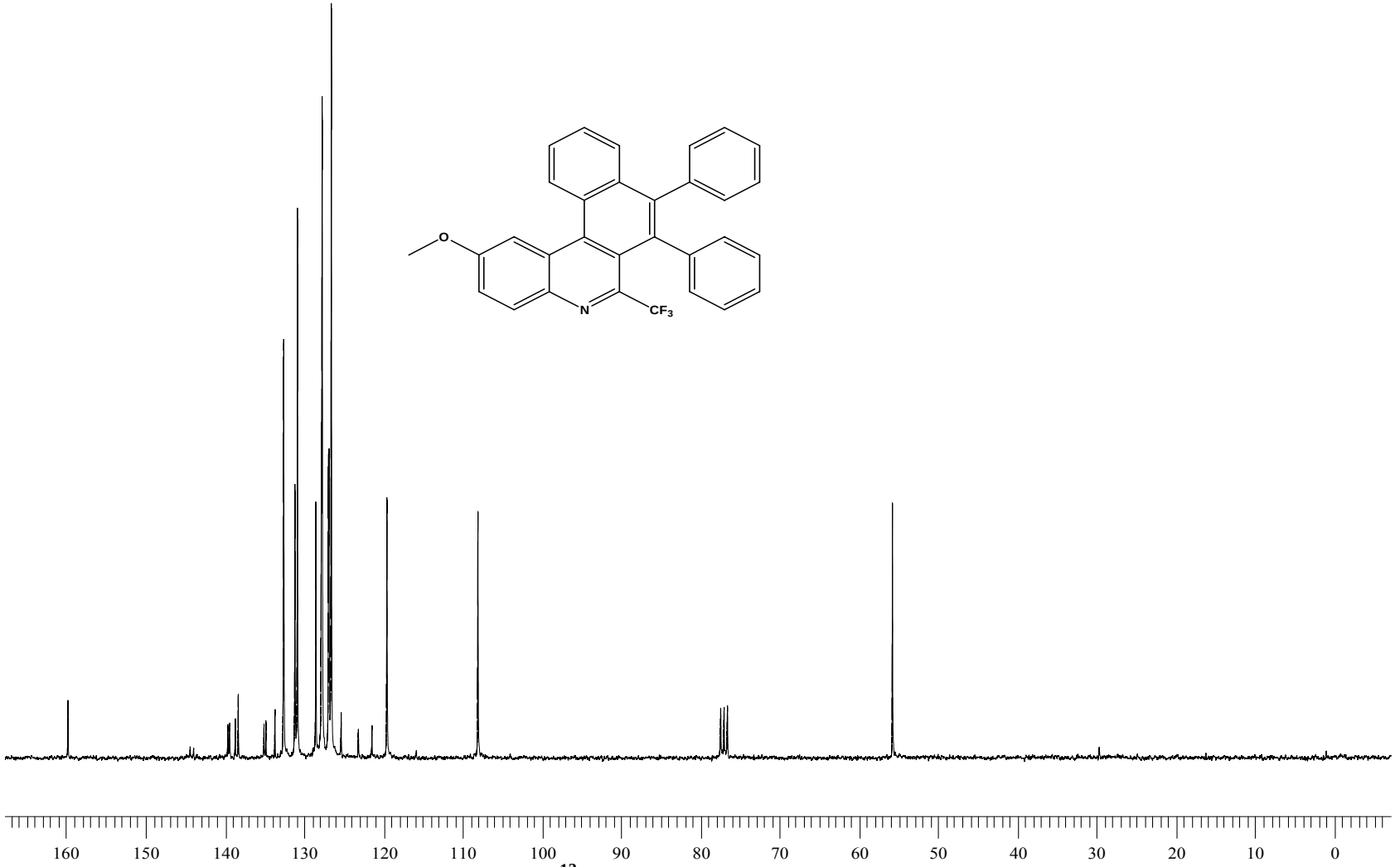
^{1}H NMR of 8



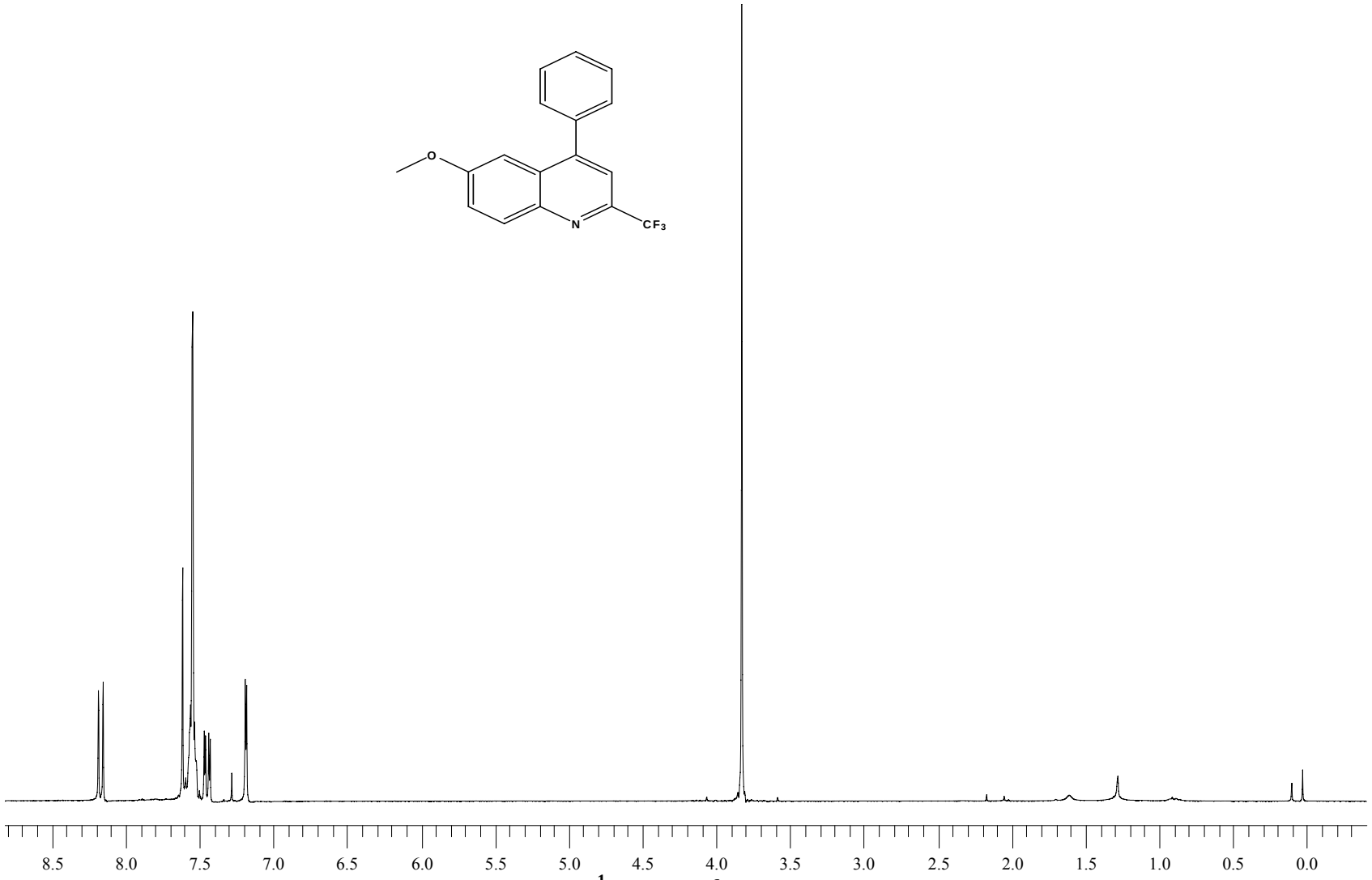
^{13}C NMR of 8



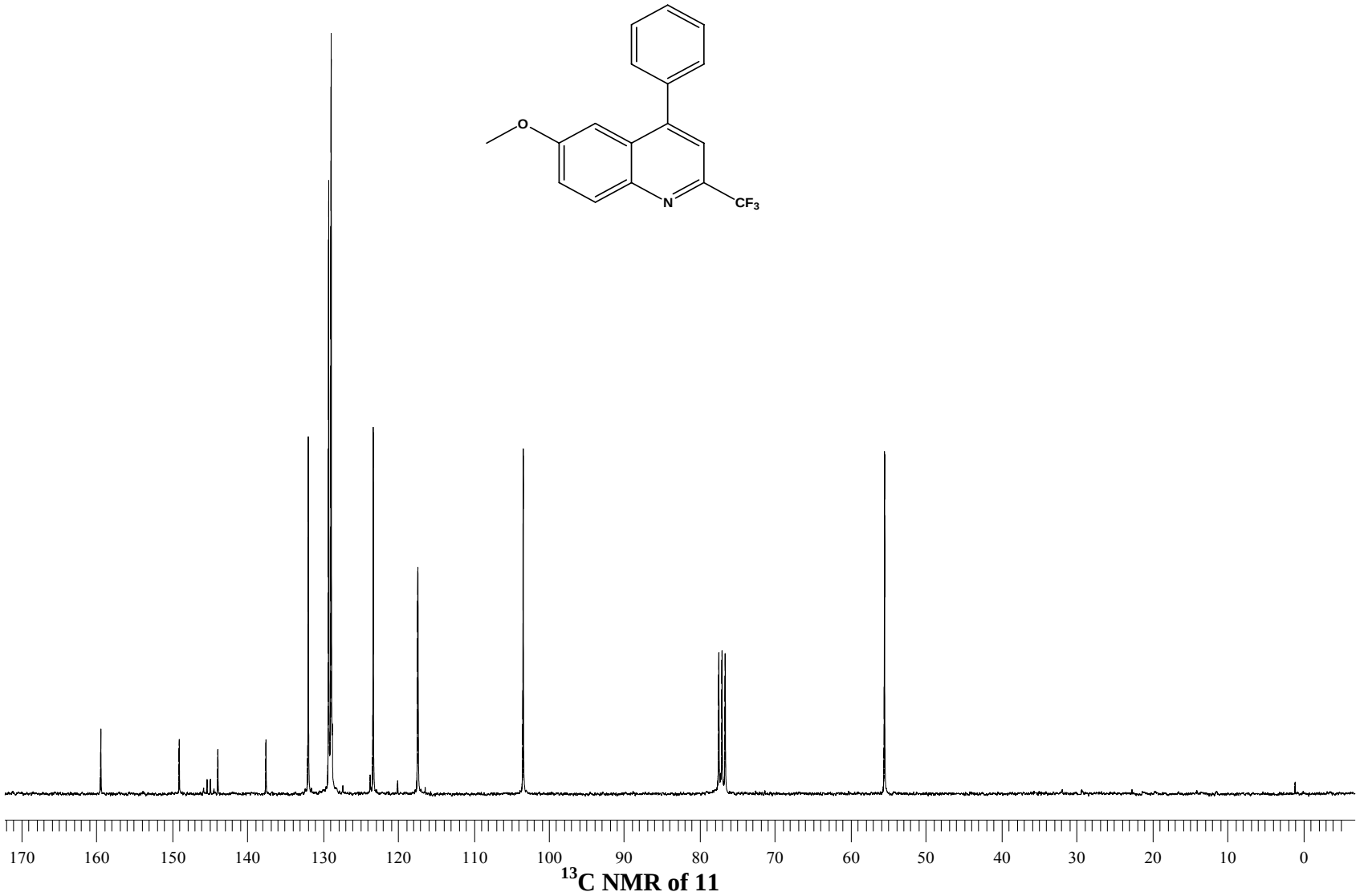
^{1}H NMR of 10



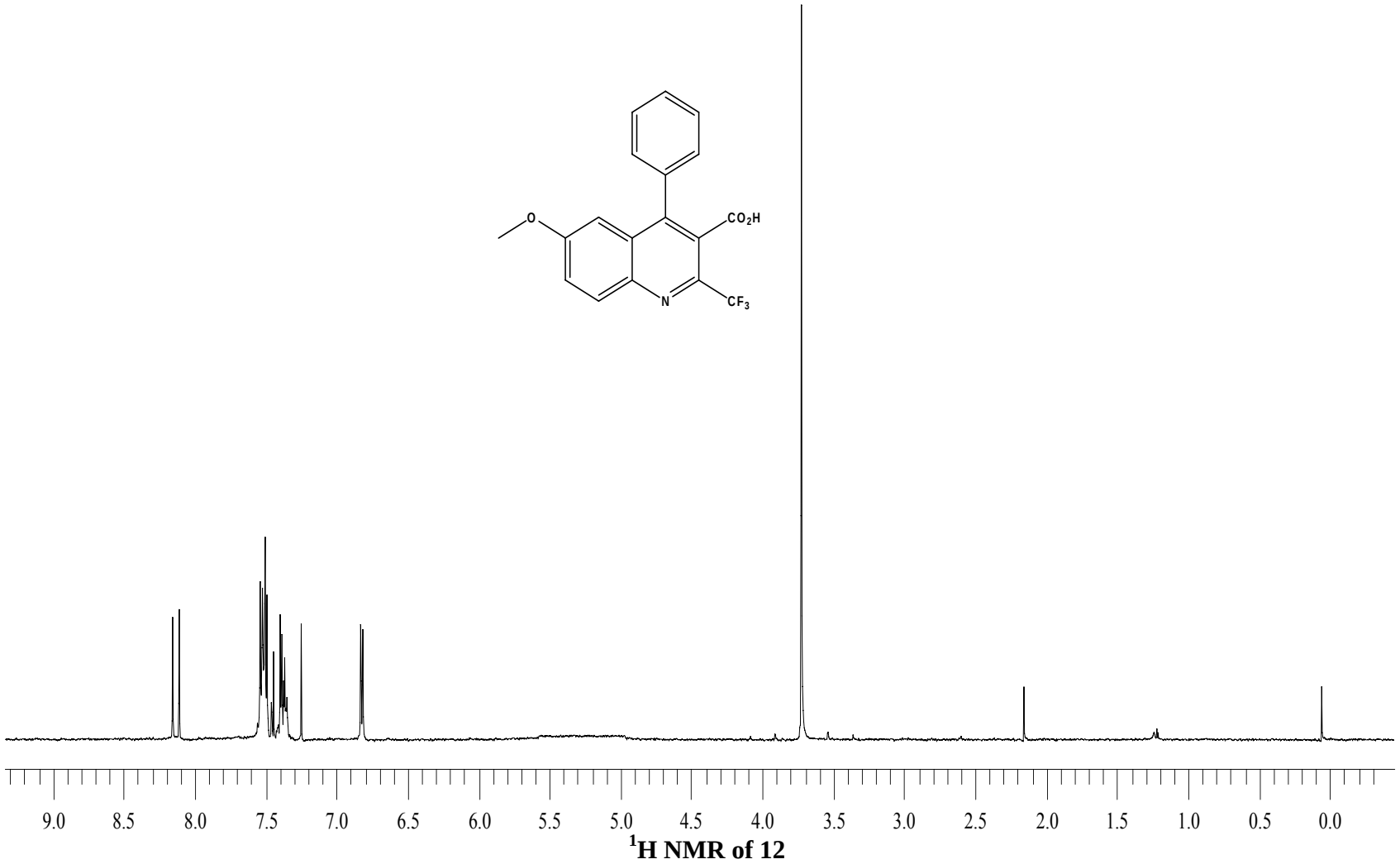
^{13}C NMR of 10



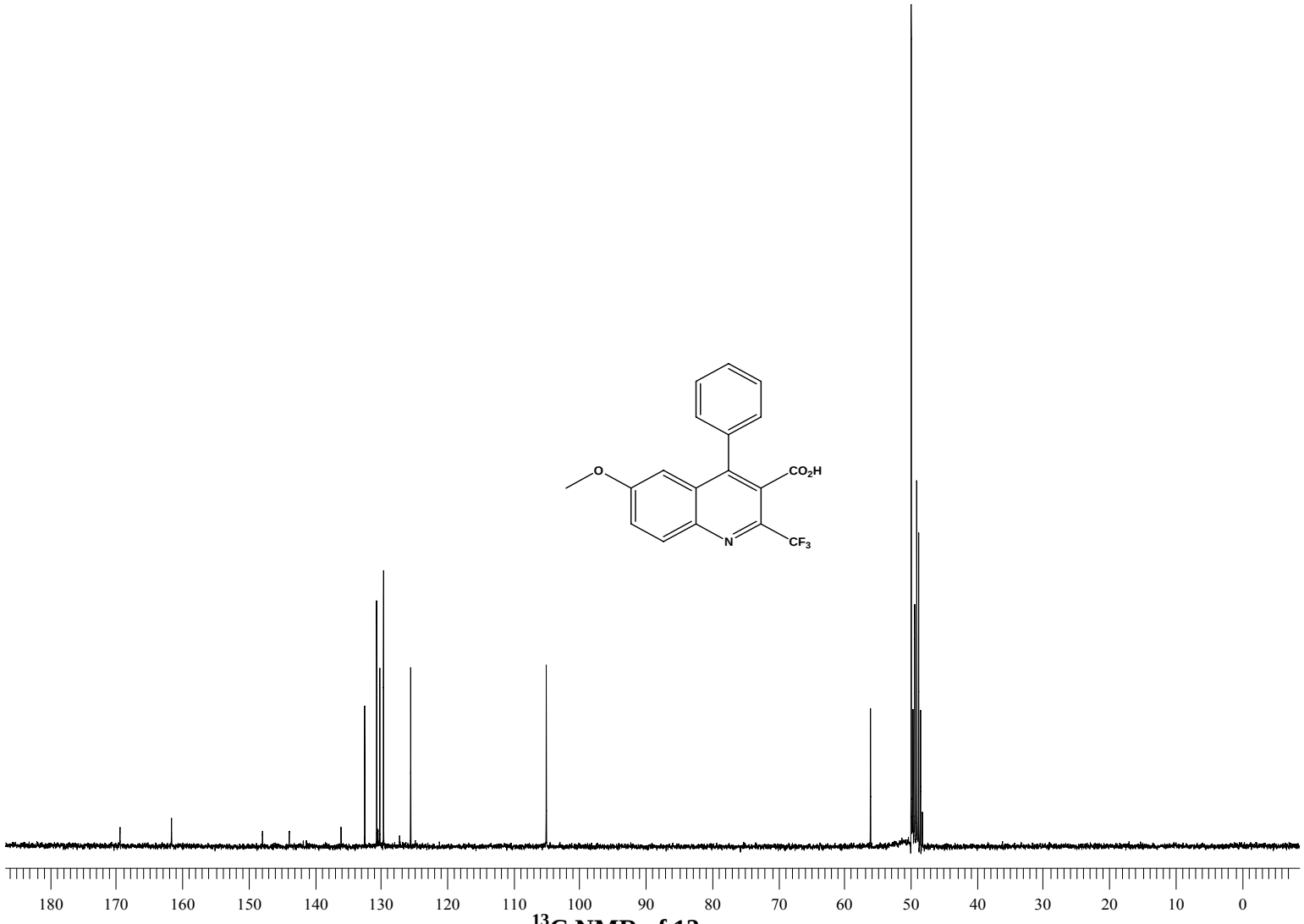
^{1}H NMR of 11



^{13}C NMR of 11



^{1}H NMR of 12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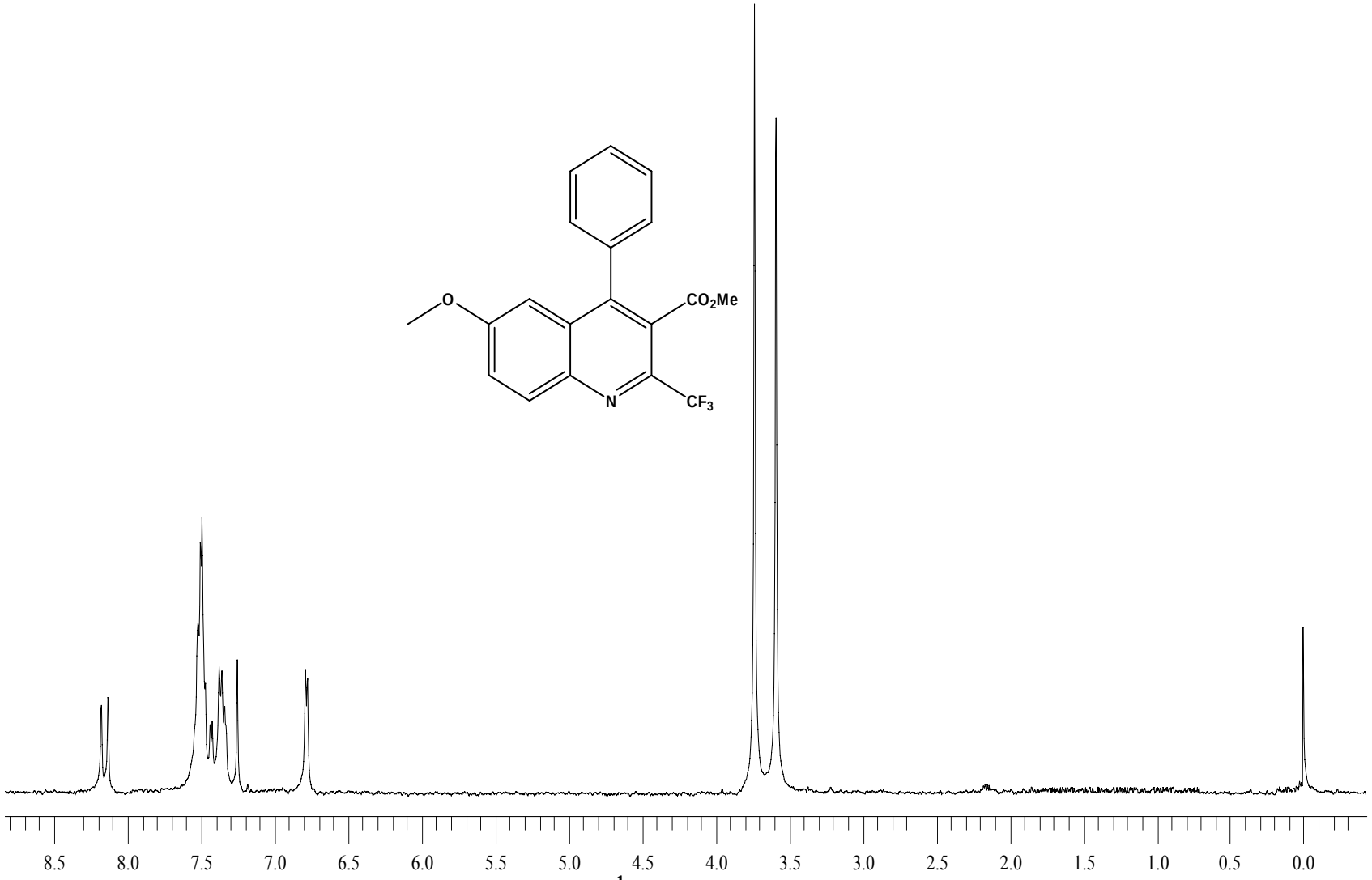
^{13}C NMR of 12



^{1}H NMR of 13

Antimalarial activity of perfluoroalkyl quinolines.

The antimalarial activity of some compounds (**5a, 5c, 5e, 5k, 5o, 5p, 5r, 8 & 10**) against the Plasmodium falciparum strain (FDL-B) has been examined at different doses, starting from 250 µg/ml onwards with 5-fold serial dilutions up to 0.016 µg/ml.[28] The doses were kept constant for all compounds in order to maintain the comparative profile of their activities. The compounds, **5a** and **5o** showed substantial *in vitro* activity for total parasite growth inhibition.

Table 1:

Antimalarial activity in vitro in *Plasmodium falciparum*							
Parasite Growth Inhibition assay							
		Percent Parasite Growth Inhibition					
Compounds			**Concentration: µg/ml**				
	250	50	10	2	0.4	0.08	0.016
5k	77.4	45.2	12.9	0	0	0	0
5a	90.3	74.2	48.4	12.9	0	0	0
5c	67.7	32.3	0	0	0	0	0
5e	35.5	0	0	0	0	0	0
5o	80.6	58.1	32.3	0	0	0	0

5p	67.7	35.2	0	0	0	0	0
5r	71	35.5	0	0	0	0	0
8	64.5	26.1	0	0	0	0	0
10	74.2	42	10.5	0	0	0	0