

Supporting Information
for
Palladium-catalyzed substitution of (coumarinyl)methyl acetates with
C-, N-, and S-nucleophiles

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**Experimental data and ¹H, ¹³C, and IR, and HRMS data for new compounds
produced in batch.**

Table of Contents:

General information:	1
Experimental procedures:	2
Spectral data for compounds 2a-h, 3a-f, 4a-e, 5a-k:	3
Library experimental/representative spectral data and NMR reprints:	18

General information:

All reactions were run in flame-dried glassware under an Ar atmosphere using standard Schlenk techniques. Commercially available reagents were used without additional purification. Compound purification was effected by flash chromatography using 230 × 400 mesh, 60 Å porosity silica gel. ¹H NMR and ¹³C NMR spectra were obtained on a Bruker Avance 400 and 500 DRX spectrometer and referenced to residual protio solvent signals. Structural assignments are based on ¹H, ¹³C, IR, and HRMS spectroscopies.

General Procedure for decarboxylative benzylation (DcB) reaction of coumarinyl acetates:

In a flame-dried Schlenk tube under argon, Pd(PPh₃)₄ (5 mol %) was added to a acetonitrile solution (1.5 mL) of coumarinyl acetate (0.16 mmol), and the solution was stirred at room temperature for 12–15 h. The reaction mixture was then concentrated in vacuo and purified directly by column chromatography with hexane/ethyl acetate (90:10) as eluent.

General procedure for the Suzuki-coupling of coumarinyl acetates and aryl/vinyl boronic acids:

In a flame-dried Schlenk tube under argon, Pd(PPh₃)₄ (5 mol %) was added a dioxane solution (2 mL) of (coumarinyl)methyl acetates (0.5 mmol), boronic acid (2 equiv), K₂CO₃ (1.5 equiv), and the solution was stirred at 90 °C for 12–15 min. The reaction mixture was then concentrated in vacuo and purified directly by column chromatography with hexane/ethyl acetate as eluent.

General procedure for the Pd-catalyzed coupling of coumarinyl acetates and sulfinates:

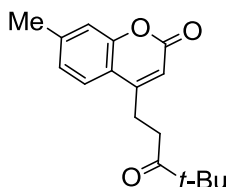
In a flame-dried Schlenk tube under argon, Pd(PPh₃)₄ (5 mol %) was added to a dioxane solution (2 mL) of (coumarinyl)methyl acetates (0.5 mmol) and sodium salt of arylsulfinate, and the solution stirred at 90 °C for 12 h. The reaction mixture was then concentrated in vacuo and purified directly by column chromatography with hexane/ethyl acetate as eluent.

General procedure for the Pd-catalyzed coupling of coumarinyl acetates and amines:

In a flame-dried Schlenk tube under argon, Pd(PPh₃)₄ (10 mol %) was added a dioxane solution (2 mL) of (coumarinyl)methyl acetates (0.5 mmol), amine (2 equiv), K₂CO₃ (2 equiv), and the solution stirred at 90 °C for 12–15 h (secondary amine) or 24 h (primary amine). The reaction mixture was then concentrated in vacuo and purified directly by column chromatography with hexane/ethyl acetate as eluent.

Spectral data for compounds 2a–h, 3a–f

2a: yellow viscous liquid



^1H NMR (400 MHz, CDCl_3):

δ ppm 7.53 (d, $J = 8$ Hz, 1H), 7.28–7.12 (m, 2H), 6.20 (s, 1H), 3.05–3.01 (m, 2H), 2.91–2.88 (m, 2H), 2.46 (s, 3H), 1.18 (s, 9H)

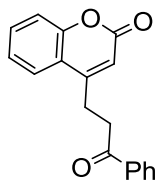
^{13}C NMR (125 MHz, CDCl_3):

δ ppm 213.56, 161.11, 155.35, 153.79, 143.05, 125.54, 123.82, 117.52, 116.62, 112.81, 44.20, 34.67, 26.41, 25.56, 21.58

IR (CH_2Cl_2): ν_{max} 1718, 1620 cm^{-1}

HRMS: Calcd. for $\text{C}_{17}\text{H}_{21}\text{O}_3$ ($\text{M} + \text{H}$), 273.1491; Found, 273.1365

2b: viscous liquid



^1H NMR (500 MHz, CDCl_3):

δ ppm 7.91–7.89 (m, 2H), 7.62 (dd, $J = 8, 1.5$ Hz, 1H), 7.53–7.39 (m, 4H), 7.28–7.22 (m, 2H), 6.25 (s, 1H), 3.35–3.32 (m, 2H), 3.20–3.17 (m, 2H)

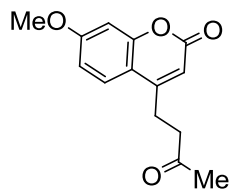
^{13}C NMR (100 MHz, CDCl_3):

δ ppm 195.11, 158.47, 152.71, 151.42, 133.96, 131.33, 129.60, 126.52, 125.75, 122.12, 121.89, 116.78, 115.13, 111.81, 34.08, 23.18.

IR (CH_2Cl_2): 1724, 1685 cm^{-1}

HRMS: Calcd. for $\text{C}_{18}\text{H}_{14}\text{O}_3\text{Na}$ ($\text{M} + \text{Na}$), 301.0841; Found, 301.0815

2c: viscous liquid



¹H NMR (400 MHz, CDCl₃):

δ ppm 7.45–7.43 (m, 1H), 6.78–6.76 (m, 1H), 6.70 (s, 1H), 5.98 (s, 1H), 3.78 (s, 3H), 2.94–2.91 (m, 2H), 2.79–2.76 (m, 2H), 2.15 (s, 3H).

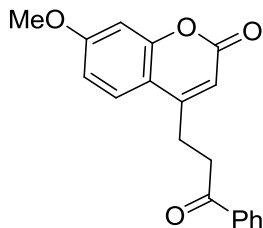
¹³C NMR (100 MHz, CDCl₃):

δ ppm 206.02, 162.69, 161.23, 155.49, 154.98, 125.12, 112.53, 112.45, 110.71, 101.11, 55.79, 41.20, 30.08, 25.08.

IR (CH₂Cl₂): 1720, 1605 cm⁻¹.

HRMS: Calcd. for C₁₄H₁₅O₄ (M + H), 247.0970; Found, 247.0963

2d: yellow viscous liquid



¹H NMR (500 MHz, CDCl₃):

δ ppm 7.91–7.89 (m, 2H), 7.53–7.50 (m, 2H), 7.42–7.39 (m, 2H), 6.79 (dd, *J* = 10.0, 5.0 Hz, 1H), 6.75 (s, 1H), 6.09 (s, 1H), 3.79 (s, 3H), 3.33–3.30 (m, 2H), 3.14–3.11 (m, 2H).

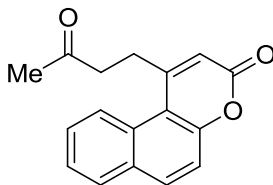
¹³C NMR (125 MHz, CDCl₃):

δ ppm 197.53, 162.70, 161.26, 155.52, 155.26, 136.28, 133.58, 128.79, 128.03, 125.20, 112.62, 112.47, 110.84, 101.14, 55.78, 36.51, 25.55.

IR (CH₂Cl₂): ν_{max} 1720, 1683, 1612 cm⁻¹.

HRMS: Calcd. for C₁₉H₁₆O₄Na (M + Na), 331.0946; Found, 331.0927.

2e: yellow viscous liquid



^1H NMR (500 MHz, CDCl_3):

δ ppm 8.31 (d, $J = 5$ Hz, 1H), 7.88 (d, $J = 10$ Hz, 1H), 7.83 (dd, $J = 8, 1.5$ Hz, 1H), 7.57–7.54 (m, 1H), 7.48–7.45 (m, 1H), 7.36 (d, $J = 10$ Hz, 1H), 6.27 (s, 1H), 3.45–3.42 (m, 2H), 2.85–2.82 (m, 2H). 2.14 (s, 3H).

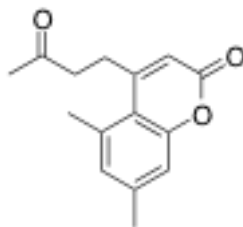
^{13}C NMR (125 MHz, CDCl_3):

δ ppm 204.33, 158.64, 155.08, 153.30, 132.27, 129.76, 128.29, 127.90, 126.65, 123.89, 122.96, 116.33, 113.70, 111.93, 40.20, 29.56, 28.51.

IR (CH_2Cl_2): ν_{max} 1718, 1421 cm^{-1} .

HRMS: Calcd. for $\text{C}_{17}\text{H}_{15}\text{O}_3$ ($\text{M} + \text{H}$), 267.1021; Found, 267.1083.

2f: yellow viscous liquid



^1H NMR (500 MHz, CDCl_3):

δ ppm; 6.95 (s, 1H), 6.83 (s, 1H), 6.04 (s, 1H), 3.15–3.12 (m, 2H), 2.75–2.72 (m, 2H), 2.60 (s, 3H), 2.30 (s, 3H), 2.16 (s, 3H).

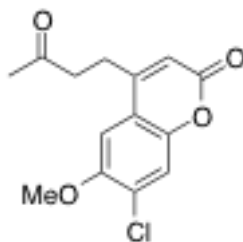
^{13}C NMR (125 MHz, CDCl_3):

δ ppm 205.89, 160.66, 156.75, 155.33, 141.97, 135.74, 130.12, 116.45, 116.03, 113.86, 42.36, 30.13, 29.37, 24.34, 21.13.

IR (CH_2Cl_2): ν_{max} 1735, 1714, 1604 cm^{-1} .

HRMS: Calcd. for $\text{C}_{15}\text{H}_{17}\text{O}_3$ ($\text{M} + \text{H}$), 245.1178; Found, 245.1159.

2g: viscous liquid



¹H NMR (500 MHz, CDCl₃):

δ ppm 7.52 (s, 1H), 7.14 (s, 1H), 6.13 (s, 1H), 2.95–2.92 (m, 2H), 2.81–2.78 (m, 2H), 2.38 (s, 3H), 2.17 (s, 3H)

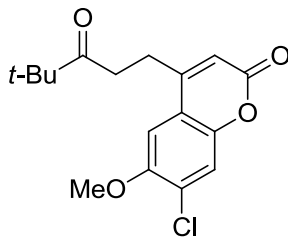
¹³C NMR (125 MHz, CDCl₃):

δ ppm 205.67, 160.37, 153.70, 151.94, 140.74, 130.28, 123.94, 191.21, 118.14, 113.79, 40.77, 30.07, 24.82, 20.50.

IR (CH₂Cl₂): 1731, 1701, 1610 cm⁻¹.

HRMS: Calcd. for C₁₄H₁₃ClO₃Na (M + Na), 287.0451; Found, 287.0444

2h: yellow viscous liquid



¹H NMR (500 MHz, CDCl₃):

δ ppm 7.54 (s, 1H), 6.78 (s, 1H), 6.05 (s, 1H), 3.89 (s, 3H), 2.91–2.88 (m, 2H) 2.84–2.81 (m, 2H), 1.11 (s, 9H).

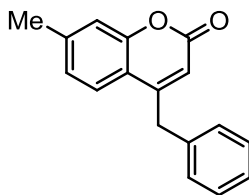
¹³C NMR (125 MHz, CDCl₃):

δ ppm 211.92, 159.17, 156.19, 153.17, 152.37, 123.53, 117.70, 111.46, 110.05, 99.17, 55.23, 42.76, 32.86, 24.98, 23.98.

IR (CH₂Cl₂): ν_{max} 1720, 1690, 1610 cm⁻¹.

HRMS: Calcd. for C₁₇H₂₀ClO₄ (M + H), 323.1050; Found, 323.1036.

3a: Colorless viscous liquid



^1H NMR (400, CDCl_3):

δ 7.53 (d, $J = 8.0$ Hz, 1H), 7.36–7.22 (m, 5H), 7.13 (s, 1H), 7.07 (d, $J = 8.0$ Hz, 1H), 6.07 (s, 1H), 4.09 (s, 2H), 2.43 (s, 3H) ppm.

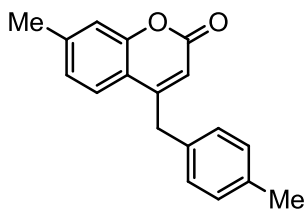
^{13}C NMR (100 MHz, CDCl_3):

δ 161.25, 154.73, 153.78, 142.96, 136.13, 129.08, 128.97, 127.22, 125.47, 124.40, 117.34, 116.83, 114.53, 38.02, 21.60 ppm.

IR (CH_2Cl_2): ν_{max} 3028, 1712, 1620 cm^{-1}

HRMS: Calcd. for $\text{C}_{17}\text{H}_{14}\text{O}_2\text{Na}$ ($\text{M} + \text{Na}$) 273.0892; Found 273.0883.

3b: Colorless viscous liquid;



^1H NMR (400, CDCl_3):

δ 7.55 (d, $J = 8.0$ Hz, 1H), 7.17–7.07 (m, 6H), 6.09 (s, 1H), 4.06 (s, 2H), 2.45 (s, 3H), 2.36 (s, 3H) ppm.

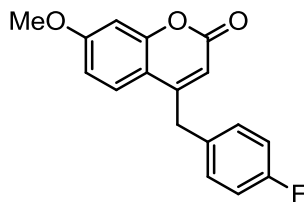
^{13}C NMR (100 MHz, CDCl_3):

δ 161.32, 154.94, 153.81, 142.88, 136.86, 133.00, 129.64, 128.92, 125.42, 124.39, 117.35, 116.88, 114.46, 37.66, 21.60, 21.07 ppm.

IR (CH_2Cl_2): ν_{max} 3010, 1712, 1620 cm^{-1}

HRMS: Calcd. for $\text{C}_{18}\text{H}_{16}\text{O}_2\text{Na}$ ($\text{M} + \text{Na}$) 287.1048; Found 287.1025.

3c: Colorless solid



^1H NMR (400, CDCl_3):

δ 7.51 (d, $J = 8.0$ Hz, 1H), 7.21–7.17 (m, 2H), 7.04–7.00 (m, 2H), 6.83–6.81 (m, 2H), 5.95 (s, 1H), 4.05 (s, 2H), 3.87 (s, 3H) ppm.

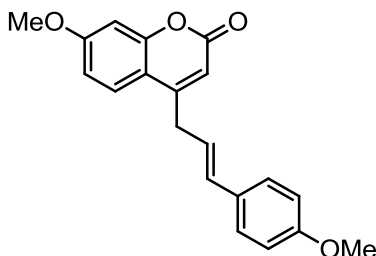
^{13}C NMR (100 MHz, CDCl_3):

δ 162.65, 161.94 (d, $J_{\text{C-F}} = 244$ Hz), 161.29, 155.53, 154.57, 131.84 (d, $J_{\text{C-F}} = 4$ Hz), 130.57 (d, $J_{\text{C-F}} = 8$ Hz), 125.55, 115.85 (d, $J_{\text{C-F}} = 22$ Hz), 112.59, 112.42, 112.40, 101.03, 55.76, 37.29 ppm.

IR (CH_2Cl_2): ν_{max} 1711, 1611 cm^{-1} .

HRMS: Calcd. for $\text{C}_{17}\text{H}_{14}\text{FO}_3$ (M + H) 285.0927; Found 285.0902.

3d: Colorless viscous liquid



^1H NMR (400, CDCl_3):

δ 7.60 (d, $J = 8$ Hz, 1H), 7.32–7.28 (m, 2H), 6.88–6.85 (m, 4H), 6.51 (d, $J = 16.0$ Hz, 1H), 6.23–6.13 (m, 2H), 3.89 (s, 3H), 3.82 (s, 3H), 3.63 (d, $J = 8$ Hz, 2H) ppm.

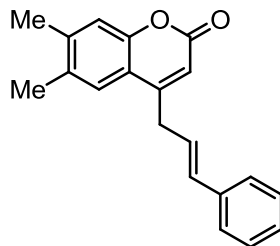
^{13}C NMR (100 MHz, CDCl_3):

δ 162.62, 161.48, 159.34, 155.55, 154.66, 133.45, 129.35, 127.44, 125.51, 121.70, 114.04, 112.80, 112.40, 111.53, 101.02, 55.77, 55.32, 35.15 ppm.

IR (CH_2Cl_2): ν_{max} 2956, 1718, 1610 cm^{-1}

HRMS: Calcd. for $\text{C}_{20}\text{H}_{19}\text{O}_4$ (M + H) 323.1283; Found 323.1280.

3e: Colorless viscous liquid



^1H NMR (400, CDCl_3):

δ 7.38–7.26 (m, 6H), 7.13 (s, 1H), 6.57 (d, $J = 16.0$ Hz, 1H), 6.37–6.29 (m, 2H), 3.66 (d, $J = 8$ Hz, 2H), 2.35 (s, 3H), 2.33 (s, 3H) ppm.

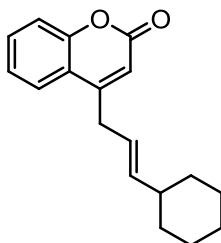
^{13}C NMR (100 MHz, CDCl_3):

δ 161.44, 154.28, 152.09, 141.84, 136.61, 132.98, 128.65, 127.80, 126.28, 124.54, 124.01, 117.74, 116.85, 113.56, 34.88, 20.21, 19.55 ppm.

IR (CH_2Cl_2): ν_{max} 3024, 1714, 1622 cm^{-1} .

HRMS: Calcd. for $\text{C}_{20}\text{H}_{19}\text{O}_2$ ($\text{M} + \text{H}$) 291.1385; Found 291.1357.

3f: Colorless viscous liquid



^1H NMR (400, CDCl_3):

δ 7.66 (d, $J = 4.0$ Hz, 1H), 7.56–7.52 (m, 1H), 7.37–7.28 (m, 2H), 6.32 (s, 1H), 5.66–5.61 (m, 1H), 5.55–5.49 (m, 1H), 3.48 (d, $J = 8$ Hz, 2H), 2.00 (bs, 1H), 1.75–1.65 (m, 4H), 1.33–1.05 (m, 6H) ppm.

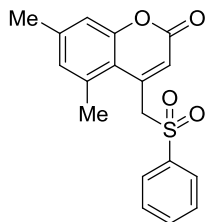
^{13}C NMR (100 MHz, CDCl_3):

δ 161.14, 155.11, 153.65, 141.77, 131.62, 124.46, 124.12, 121.13, 119.34, 117.22, 114.28, 40.74, 34.79, 32.82, 26.09, 25.96 ppm.

IR (CH_2Cl_2): ν_{max} 1728, 1604, 1413 cm^{-1} .

HRMS: Calcd. for $\text{C}_{18}\text{H}_{21}\text{O}_2$ ($\text{M} + \text{H}$) 269.1542; Found 269.1519.

4a: yellow viscous liquid



^1H NMR (500, CDCl_3):

δ ppm 7.74–7.72 (m, 2H), 7.64–7.61 (m, 1H), 7.51–7.48 (m, 2H), 6.95 (s, 1H), 6.84 (s, 1H), 5.89 (s, 1H), 4.65 (s, 2H), 2.73 (s, 3H), 2.30 (s, 3H).

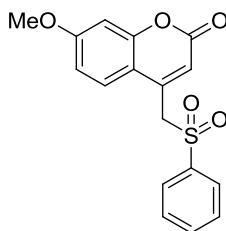
^{13}C NMR (125 MHz, CDCl_3):

δ 159.22, 155.42, 143.31, 142.92, 137.39, 135.79, 134.70, 130.61, 129.54, 128.57, 120.26, 116.55, 114.95, 61.11, 24.66, 21.24 ppm.

IR (CH_2Cl_2): ν_{max} 1718, 1618, 1446 cm^{-1} .

HRMS: Calcd. for $\text{C}_{18}\text{H}_{16}\text{O}_4\text{SNa}$ (M + Na) 351.0667; Found 351.0642

4b: yellow viscous liquid



^1H NMR (500, CDCl_3):

δ ppm 7.76–7.74 (m, 2H), 7.61–7.58 (m, 1H), 7.48–7.43 (m, 3H), 6.77–6.72 (m, 2H), 5.78 (s, 1H), 4.39 (s, 1H), 3.80 (s, 3H).

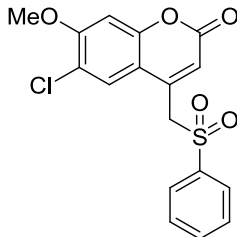
^{13}C NMR (125 MHz, CDCl_3):

δ 163.20, 159.88, 155.68, 142.73, 137.29, 134.67, 129.47, 128.55, 126.35, 116.13, 112.64, 111.54, 101.14, 58.60, 55.87 ppm.

IR (CH_2Cl_2): ν_{max} 1710, 1610 cm^{-1} .

HRMS: Calcd. for $\text{C}_{17}\text{H}_{14}\text{O}_5\text{SNa}$ (M + Na) 353.0460; Found 353.0466

4c: yellow viscous liquid



¹H NMR (500, CDCl₃ DMSO-D6):

δ 7.78 (d, *J* = 8 Hz, 2H), 7.62 (t, *J* = 7.5 Hz, 1H), 7.50–7.46 (m, 3H), 6.80 (s, 1H), 5.99 (s, 1H), 4.50 (s, 2H), 3.90 (s, 3H) ppm.

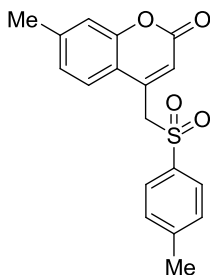
¹³C NMR (125 MHz, CDCl₃):

δ 157.44, 156.16, 152.11, 140.38, 135.64, 132.88, 127.62, 126.63, 124.23, 117.33, 115.37, 109.95, 98.63, 56.29, 54.93 ppm.

IR (CH₂Cl₂): ν_{max} 1718, 1635 cm⁻¹.

HRMS: Calcd. for C₁₇H₁₄ClO₅S (M + H) 365.0251; Found 365.0243

4d: yellow viscous liquid



¹H NMR (500, CDCl₃):

δ 7.70 (d, *J* = 8.5 Hz, 2H), 7.55 (d, *J* = 8 Hz, 1H), 7.34 (d, *J* = 8.5 Hz, 2H), 7.15–7.11 (m, 2H), 5.93 (s, 1H), 4.48 (s, 2H), 2.46 (s, 3H), 2.45 (s, 3H); ppm.

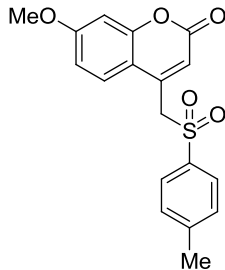
¹³C NMR (125 MHz, CDCl₃):

δ 159.78, 153.89, 145.94, 143.99, 142.91, 134.29, 130.09, 128.59, 125.70, 125.11, 118.36, 117.45, 115.63, 58.55, 21.74, 21.67.

IR (CH₂Cl₂): ν_{max} 1716, 1620 cm⁻¹.

HRMS: Calcd. for C₁₈H₁₇O₄S (M + H) 329.0848; Found 329.0862

4e: yellow viscous liquid



^1H NMR (500, CDCl_3):

δ 7.61 (d, $J = 8.5$ Hz, 2H), 7.48 (d, $J = 8.5$ Hz, 1H), 7.25 (d, $J = 8.5$ Hz, 2H), 6.78–6.74 (m, 2H), 5.74 (s, 1H), 4.36 (s, 2H), 3.80 (s, 3H), 2.36 (s, 3H) ppm.

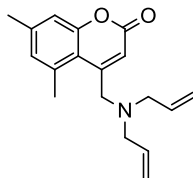
^{13}C NMR (125 MHz, CDCl_3):

δ 161.07, 157.82, 153.56, 143.78, 140.82, 132.19, 127.94, 126.44, 124.38, 113.90, 110.46, 109.49, 99.02, 56.60, 53.74, 19.60 ppm.

IR (CH_2Cl_2): ν_{max} 1716, 1608 cm^{-1} .

HRMS: Calcd. for $\text{C}_{18}\text{H}_{16}\text{O}_5\text{SNa}$ ($\text{M} + \text{Na}$) 367.0616; Found 367.0604

5a: yellow solid



^1H NMR (CDCl_3):

δ 6.93 (s, 1H), 6.79 (s, 1H), 6.74 (s, 1H), 5.81–5.74 (m, 2H), 5.15–5.07 (m, 4H), 3.75 (s, 2H), 3.10–3.08 (m, 4H), 2.58 (s, 3H), 2.28 (s, 3H) ppm.

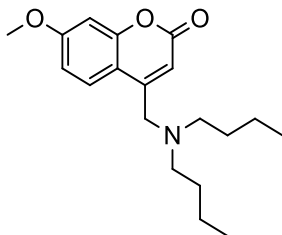
^{13}C NMR (125 MHz, CDCl_3):

δ 161.98, 156.37, 155.98, 142.23, 136.56, 135.60, 130.28, 118.66, 116.82, 116.76, 114.61, 57.76, 57.60, 25.13, 21.77 ppm.

IR (CH_2Cl_2): ν_{max} 3018, 1724 cm^{-1}

HRMS: Calcd. for $\text{C}_{18}\text{H}_{22}\text{NO}_2$ ($\text{M} + \text{H}$) 284.1651; Found 284.1627.

5b: yellow liquid



^1H NMR (CDCl_3):

δ ppm 7.67 (d, $J = 8.5$ Hz, 1H), 6.76–6.74 (m, 2H), 6.39 (s, 1H), 3.79 (s, 3H), 3.57 (s, 2H), 2.39 (t, $J = 7$ Hz, 4H), 1.38–1.35 (m, 4H), 1.24–1.29 (m, 4H), 0.81 (t, $J = 7.5$ Hz, 6H).

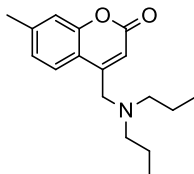
^{13}C NMR (125 MHz, CDCl_3):

δ 160.38, 159.78, 153.50, 152.46, 123.65, 110.59, 110.01, 109.41, 98.74, 53.85, 53.69, 52.36, 27.25, 18.57, 12.04 ppm

IR (CH_2Cl_2): ν_{max} 3018, 1724, 1612 cm^{-1}

HRMS: Calcd. for $\text{C}_{19}\text{H}_{28}\text{NO}_3$ ($M + H$) 318.2069, Found 318.2058.

5c: yellow liquid



^1H NMR (CDCl_3):

δ 7.61 (d, $J = 8$ Hz, 1H), 7.06 (s, 1H), 7.00–6.98 (m, 1H), 6.50 (s, 1H), 3.60 (s, 3H), 2.38–2.35 (m, 7H), 1.44–1.39 (m, 4H), 0.79 (t, $J = 7.5$ Hz, 6H) ppm.

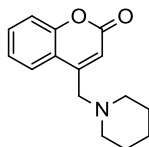
^{13}C NMR (125 MHz, CDCl_3):

δ 161.66, 154.30, 153.77, 142.57, 125.10, 124.18, 117.14, 116.57, 113.37, 56.63, 55.67, 21.60, 20.31, 11.85 ppm.

IR (CH_2Cl_2): ν_{max} 2958, 1724 cm^{-1} .

HRMS: Calcd. for $\text{C}_{17}\text{H}_{24}\text{NO}_2$ ($M + H$) 274.1807; Found 274.1875.

5d: Yellow viscous liquid



¹H NMR (500, CDCl₃):

δ 7.76 (dd, *J* = 8, 1.5 Hz, 1H), 7.45–7.41 (m, 1H), 7.26–7.17 (m, 2H), 6.47 (s, 1H), 3.51 (s, 1H), 2.40 (bs, 4H), 1.55–1.50 (m, 4H), 1.39–1.38 (m, 2H) ppm.

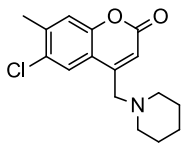
¹³C NMR (125 MHz, CDCl₃):

δ 161.19, 153.74, 152.67, 131.50, 124.77, 124.01, 119.04, 116.98, 114.59, 59.63, 55.02, 26.01, 24.09 ppm.

IR (CH₂Cl₂): ν_{max} 3010, 1730 cm⁻¹

HRMS: Calcd. for C₁₅H₁₈NO₂ (M + H) 244.1338; Found 244.1308.

5e: yellow liquid



¹H NMR (CDCl₃):

δ 7.76 (s, 1H), 7.13 (s, 1H), 6.44 (s, 1H), 3.47 (s, 2H), 2.39–2.38 (m, 7H), 1.56–1.52 (m, 4H), 1.40–1.39 (m, 2H) ppm.

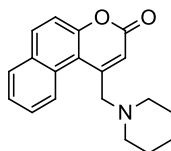
¹³C NMR (125 MHz, CDCl₃):

δ 158.67, 149.97, 149.54, 138.17, 127.74, 122.57, 116.67, 115.95, 112.49, 57.44, 52.81, 23.81, 21.89, 18.39 ppm.

IR (CH₂Cl₂): ν_{max} 1733, 1521 cm⁻¹.

HRMS: Calcd. for C₁₆H₁₉ClNO₂ (M + H) 292.1104; Found 292.1070.

5f: yellow viscous liquid



^1H NMR (400, CDCl_3):

δ ppm 8.68 (d, $J = 8.4$ Hz, 1H), 7.98 (d, $J = 8.8$, 1H), 7.92 (dd, $J = 8, 1.6$ Hz, 1H), 7.68–7.64 (m, 1H), 7.59–7.55 (m, 1H), 7.49 (d, $J = 8.8$ Hz, 1H), 6.86 (s, 1H), 3.93 (s, 2H), 2.60 (m, 4H), 1.66 (m, 4H), 1.53 (m, 2H).

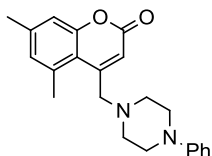
^{13}C NMR (125 MHz, CDCl_3):

δ ppm 160.92, 154.89, 154.19, 133.49, 131.28, 129.79, 129.33, 127.62, 126.65, 125.46, 117.79, 116.20, 114.62, 63.71, 54.68, 26.01, 24.19.

IR (CH_2Cl_2): ν_{max} 3018, 1730 cm^{-1} .

HRMS: Calcd. for $\text{C}_{19}\text{H}_{20}\text{NO}_2$ (M + H) 294.1494; Found 294.1482.

5g: yellow solid;



^1H NMR (400, CDCl_3):

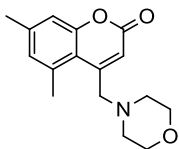
δ 7.31–7.27 (m, 2H), 7.05 (s, 1H), 6.95–6.88 (m, 4H), 6.56 (s, 1H), 3.74 (s, 2H), 3.23 (t, $J = 4.8$ Hz, 4H), 2.79 (s, 3H), 2.72 (t, $J = 4.8$ Hz, 4H), 2.39 (s, 3H) ppm.

^{13}C NMR (100 MHz, CDCl_3) δ 160.97, 155.61, 153.12, 151.13, 141.89, 136.61, 129.78, 129.16, 119.90, 116.15, 115.99, 115.84 ppm.

IR (CH_2Cl_2): ν_{max} 2821, 1722 cm^{-1} .

HRMS: Calcd. for $\text{C}_{22}\text{H}_{25}\text{N}_2\text{O}_2$ (M + H) 349.1916; Found 349.1908.

5h: yellow solid liquid



^1H NMR (500, CDCl_3):

δ 6.93 (s, 1H), 6.83 (s, 1H), 6.43 (s, 1H), 3.64 (t, $J = 4.5$ Hz, 4H), 3.59 (s, 2H), 2.67 (s, 3H), 2.46 (s, 4H), 2.29 (s, 3H) ppm.

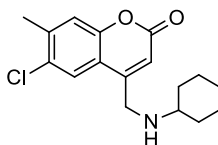
^{13}C NMR (125 MHz, CDCl_3):

δ 160.82, 155.58, 152.72, 141.89, 136.51, 129.74, 116.08, 115.90, 115.85, 66.87, 62.56, 53.63, 23.42, 21.14 ppm.

IR (CH_2Cl_2): ν_{max} 3018, 1724, 1618 cm^{-1} .

HRMS: Calcd. for $\text{C}_{16}\text{H}_{20}\text{N}_3$ (M + H) 274.1443; Found 274.1422.

5i: yellow viscous liquid



^1H NMR (400, CDCl_3):

δ 7.67 (s, 1H), 7.22 (s, 1H), 6.58 (s, 1H), 3.96 (s, 2H), 2.57–2.51 (m, 1H), 2.47 (s, 3H), 1.98–1.95 (m, 2H), 1.79–1.76 (m, 2H), 1.35–1.12 (m, 6H) ppm.

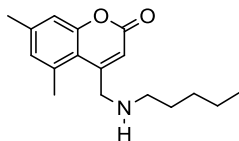
^{13}C NMR (100 MHz, CDCl_3):

δ 160.86, 153.66, 152.02, 140.32, 130.01, 123.92, 119.02, 117.79, 113.36, 56.72, 46.55, 33.65, 26.04, 24.92, 20.53 ppm.

IR (CH_2Cl_2): ν_{max} 3681, 3018, 1521 cm^{-1} .

HRMS: Calcd. for $\text{C}_{17}\text{H}_{21}\text{ClNO}_2$ (M + H) 306.1261; Found 306.1241

5j: yellow viscous liquid



^1H NMR (CDCl_3):

δ 7.03 (s, 1H), 6.90 (s, 1H), 6.55 (s, 1H), 4.03 (s, 2H), 2.73–2.69 (m, 4H), 2.38 (s, 3H), 1.55 (t, $J = 9$ Hz, 2H), 1.36–1.33 (m, 4H), 0.92 (m, 3H) ppm.

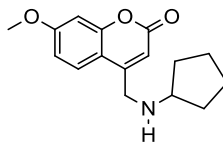
^{13}C NMR (125 MHz, CDCl_3):

δ 161.18, 155.93, 155.43, 141.68, 136.08, 129.71, 116.14, 115.88, 113.51, 53.42, 49.87, 29.87, 29.48, 23.74, 22.61, 21.14, 14.06 ppm.

IR (CH_2Cl_2): ν_{max} 1724, 1691 cm^{-1} .

HRMS: Calcd. for $\text{C}_{17}\text{H}_{24}\text{NO}_2$ ($\text{M} + \text{H}$) 274.1807 Found 274.1766.

5k: yellow viscous liquid;



^1H NMR (400, CDCl_3):

7.60 (d, $J = 8$ Hz, 1H), 6.87–6.82 (m, 2H), 6.41 (s, 1H), 3.91 (s, 2H), 3.88 (s, 3H), 3.20–3.17 (m, 1H), 1.91–1.85 (m, 2H), 1.76–1.70 (m, 2H), 1.61–1.55 (m, 2H), 1.45–1.38 (m, 2H) ppm.

^{13}C NMR (125 MHz, CDCl_3):

δ 160.50, 159.61, 153.55, 152.34, 123.08, 110.35, 110.23, 108.40, 98.96, 57.79, 53.76, 46.40, 31.19, 21.97 ppm.

IR (CH_2Cl_2): ν_{max} 17,20, 1612 cm^{-1} .

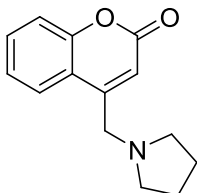
HRMS: Calcd. for $\text{C}_{16}\text{H}_{20}\text{NO}_3$ ($\text{M} + \text{H}$) 274.1443; Found 274.1396.

Library experimental/representative spectral data and NMR reprints

Experimental procedure

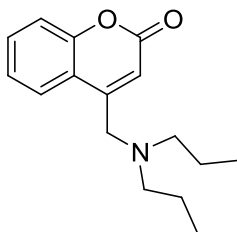
In the appropriate reactor position in the Chemspeed SLT1000 (4C × 16A = 64 member library) was added 96.7 mg of potassium carbonate (0.700 mmol), 2.50 mL of a 0.140 M (0.350 mmol) solution in dioxane of the coumarin (C), 3.30 mL of a 0.0105 M (0.0105 mmol) solution in dioxane of the tetrakis(triphenylphosphine)palladium and 0.66 mL of a 0.800 M (0.525 mmol) solution in dioxane of the amine (A), and the reaction mixture was vortex shaken at 90 °C for 16 hours. The reaction mixtures were concentrated, ethyl acetate (2 mL) was added to the residues and the resulting solutions were gravity filtered through SPE-Si (400 mg) into the appropriate CCT tubes. The process was repeated twice (2 × 2 mL), the filtrates were concentrated and the resulting residues were purified by LC-MS.

¹H, ¹³C NMR spectra were recorded on an Avance AV-III 500 with a dual carbon/proton (CPDUL) cryoprobe operating at 500 MHz and 125 MHz respectively. Infrared (IR) spectra were obtained using a Perkin-Elmer Spectrum 100 FT-IR spectrometer with a UATR application.



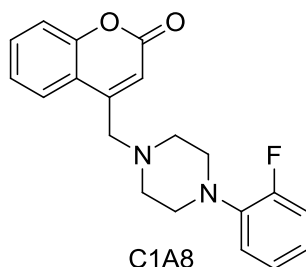
C1A5

4-(Pyrrolidin-1-ylmethyl)-2H-chromen-2-one: ¹H NMR (500 MHz, CDCl₃) δ 7.82–7.80 (m, 1H), 7.52–7.49 (m, 1H), 7.34–7.26 (m, 2H), 6.54 (d, *J* = 1 Hz, 1H), 3.79 (d, *J* = 1 Hz, 2H), 2.65–2.62 (m, 4H), 1.84–1.82 (m, 4H) ppm; ¹³C NMR (125 MHz, CDCl₃) δ 158.83, 151.32, 150.55, 129.22, 122.31, 121.76, 116.47, 114.66, 112.10, 54.10, 52.09, 21.32 ppm; IR (CH₂Cl₂): ν 1717, 1617 cm⁻¹; HRMS: Calcd for C₁₄H₁₆NO₂ (M + H) 230.1136; found: 230.1179.

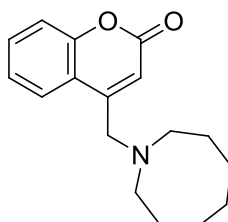


C1A7

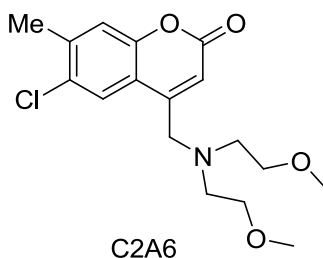
4-((Dipropylamino)methyl)-2H-chromen-2-one: ^1H NMR (500 MHz, CDCl_3) δ 7.83–7.81 (m, 1H), 7.52–7.49 (m, 1H), 7.33–7.25 (m, 2H), 6.66 (t, $J = 1\text{ Hz}$, 1H), 3.72 (d, $J = 1\text{ Hz}$, 2H), 2.46 (t, $J = 7.5\text{ Hz}$, 4H), 1.54–1.46 (m, 4H), 0.88 (t, $J = 7.5\text{ Hz}$, 6H) ppm; ^{13}C NMR (125 MHz, CDCl_3) δ 160.97, 153.90, 153.25, 131.11, 124.08, 123.58, 118.58, 116.60, 114.02, 56.24, 55.21, 19.91, 11.46 ppm; IR (CH_2Cl_2): ν 1724, 1623, 1550 cm^{-1} ; HRMS: Calcd for $\text{C}_{16}\text{H}_{22}\text{NO}_2$ (M + H) 260.1606; found 260.1649.



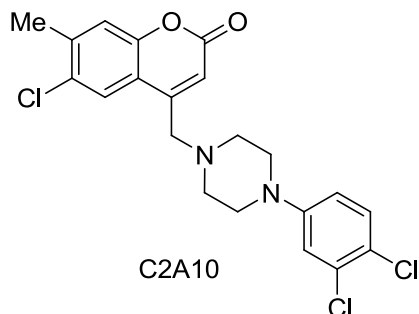
4-((4-(2-Fluorophenyl)piperazin-1-yl)methyl)-2H-chromen-2-one: ^1H NMR (500 MHz, CDCl_3) δ 7.85–7.83 (m, 1H), 7.55–7.52 (m, 1H), 7.36–7.34 (m, 1H), 7.31–7.17 (m, 1H), 7.05–6.93 (m, 4H), 6.60 (s, 1H), 3.72 (d, $J = 5\text{ Hz}$, 2H), 3.15–3.13 (m, 4H), 2.76–2.74 (m, 4H) ppm; ^{13}C NMR (125 MHz, CDCl_3) δ 161.03, 155.72 (d, $J_{\text{CF}} = 244\text{ Hz}$), 153.82, 151.86, 139.9 (d, $J_{\text{CF}} = 8.7\text{ Hz}$), 131.75, 124.75, 124.52 (d, $J_{\text{CF}} = 2.5\text{ Hz}$), 124.16, 122.64 (d, $J_{\text{CF}} = 7.5\text{ Hz}$), 118.93 (d, $J_{\text{CF}} = 17.5\text{ Hz}$), 118.86, 117.12, 116.15 (d, $J_{\text{CF}} = 20\text{ Hz}$), 114.94, 58.84, 53.60, 50.55, 50.52; IR (CH_2Cl_2): ν 1719, 1624, 1605 cm^{-1} ; HRMS: Calcd for $\text{C}_{20}\text{H}_{20}\text{FN}_2\text{O}_2$ (M + H) 339.1464; found 339.1526.



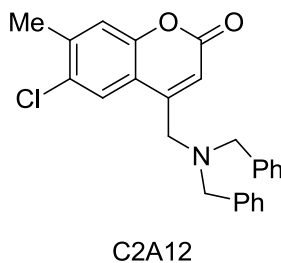
4-(Azocan-1-ylmethyl)-2H-chromen-2-one: ^1H NMR (500 MHz, CDCl_3) δ 7.89–7.87 (m, 1H), 7.52–7.49 (m, 1H), 7.34–7.27 (m, 2H), 6.50 (s, 1H), 3.75 (d, $J = 5\text{ Hz}$, 2H), 2.67–2.64 (m, 4H), 1.60–1.55 (m, 10H) ppm; ^{13}C NMR (125 MHz, CDCl_3) δ 160.19, 152.76, 152.74, 130.55, 124.31, 122.91, 118.04, 115.94, 113.98, 59.33, 53.95, 26.77, 26.36, 24.84 ppm; IR (CH_2Cl_2): ν 1720, 1623, 1605, cm^{-1} ; HRMS: Calcd for $\text{C}_{17}\text{H}_{22}\text{NO}_2$ (M + H) 272.1606; found: 272.1658.



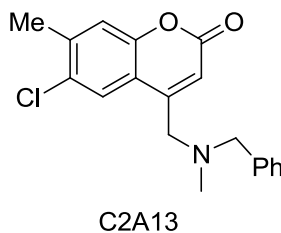
4-((bis(2-Methoxyethyl)amino)methyl)-6-chloro-7-methyl-2H-chromen-2-one: ^1H NMR (500 MHz, CDCl_3) δ 7.94 (s, 1H), 7.19 (d, $J = 1$ Hz, 1H), 6.59 (s, 1H), 3.89 (d, $J = 5$ Hz, 2H), 3.49 (t, $J = 5$ Hz, 4H), 3.33 (s, 6H), 2.82 (t, $J = 5$ Hz, 4H), 2.45 (s, 3H) ppm; ^{13}C NMR (125 MHz, CDCl_3) δ 160.90, 153.03, 152.06, 140.21, 129.86, 125.01, 118.69, 117.98, 114.70, 71.39, 58.82, 56.36, 54.42, 20.52 ppm; IR (CH_2Cl_2): ν 1731, 1616 cm^{-1} ; HRMS: Calcd for $\text{C}_{17}\text{H}_{23}\text{ClNO}_4$ (M + H) 340.1271; found: 340.1326.



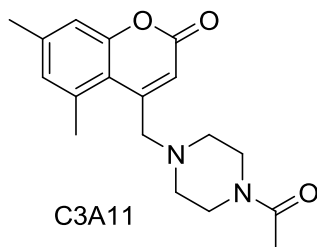
6-Chloro-4-((4-(3,4-dichlorophenyl)piperazin-1-yl)methyl)-7-methyl-2H-chromen-2-one: ^1H NMR (500 MHz, CDCl_3) δ 7.81 (s, 1H), 7.28–7.26 (m, 1H), 7.22 (s, 1H), 6.96 (d, $J = 3$ Hz, 1H), 6.75–6.73 (m, 1H), 6.53 (s, 1H), 3.65 (s, 2H), 3.21 (t, $J = 5$ Hz, 4H), 2.69 (t, $J = 5$ Hz, 4H), 2.46 (s, 3H) ppm; ^{13}C NMR (125 MHz, CDCl_3) δ 160.58, 152.17, 150.63, 150.47, 140.70, 132.82, 130.48, 130.07, 124.62, 122.44, 118.97, 117.78, 117.41, 115.45, 115.00, 58.77, 53.11, 48.74, 20.60 ppm; IR (CH_2Cl_2): ν 1728, 1616, 1592 cm^{-1} ; HRMS: Calcd for $\text{C}_{21}\text{H}_{20}\text{Cl}_3\text{N}_2\text{O}_2$ (M + H) 437.0546; found: 437.0567.



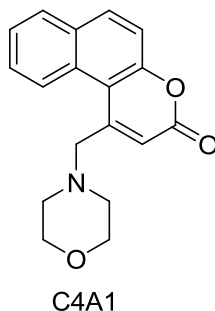
6-Chloro-4-((dibenzylamino)methyl)-7-methyl-2H-chromen-2-one: ^1H NMR (500 MHz, CDCl_3) δ 7.71 (s, 1H), 7.34–7.24 (m, 10H), 7.11 (s, 1H), 6.61 (s, 1H), 3.61–3.60 (s, 6H), 2.40 (s, 3H) ppm; ^{13}C NMR (125 MHz, CDCl_3) δ 159.63, 151.34, 151.07, 139.51, 137.19, 128.92, 128.05, 127.65, 126.57, 124.10, 117.77, 116.87, 114.24, 58.01, 53.88, 19.56 ppm; IR (CH_2Cl_2): ν 1731, 1617, 1548 cm^{-1} ; HRMS: Calcd for $\text{C}_{25}\text{H}_{23}\text{ClNO}_2$ (M + H) 404.1373; found: 404.1428.



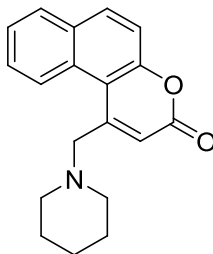
4-((Benzyl(methyl)amino)methyl)-6-chloro-7-methyl-2H-chromen-2-one: ^1H NMR (500 MHz, CDCl_3) δ 7.75 (s, 1H), 7.34–7.26 (m, 5H), 7.15 (s, 1H), 6.52 (s, 1H), 3.62 (s, 2H), 3.54 (s, 2H), 2.41 (s, 3H), 2.26 (s, 3H) ppm; ^{13}C NMR (125 MHz, CDCl_3) δ 158.77, 150.21, 150.08, 138.53, 136.26, 128.03, 127.15, 126.69, 125.65, 123.15, 116.85, 115.98, 113.22, 60.92, 55.97, 40.91, 18.64 ppm; IR (CH_2Cl_2): ν 1728, 1616 cm^{-1} ; HRMS: Calcd for $\text{C}_{19}\text{H}_{19}\text{ClNO}_2$ ($\text{M} + \text{H}$) 328.1060; found: 328.1118.



4-((4-Acetylpiperazin-1-yl)methyl)-5,7-dimethyl-2H-chromen-2-one: ^1H NMR (500 MHz, CDCl_3) δ 7.01 (s, 1H), 6.91 (s, 1H), 6.51 (s, 1H), 3.71 (s, 2H), 3.65 (t, $J = 5$ Hz, 2H), 3.49 (t, $J = 5$ Hz, 2H), 2.74 (s, 3H), 2.53 (q, $J = 5$ Hz, 4H), 2.38 (s, 3H), 2.10 (s, 3H) ppm; ^{13}C NMR (125 MHz, CDCl_3) δ 168.99, 160.77, 155.53, 152.76, 142.01, 136.38, 129.80, 116.08, 115.79, 115.62, 61.94, 53.07, 52.99, 46.15, 41.32, 23.52, 21.33, 21.15 ppm; IR (CH_2Cl_2): ν 1728, 1638, 1617 cm^{-1} ; HRMS: Calcd for $\text{C}_{18}\text{H}_{23}\text{N}_2\text{O}_3$ ($\text{M} + \text{H}$) 315.1664; found: 315.1728

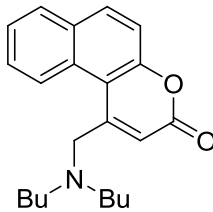


1-(Morpholinomethyl)-3H-benzo[*f*]chromen-3-one: ^1H NMR (500 MHz, CDCl_3) δ 8.65 (d, $J = 10$ Hz, 1H), 7.95 (d, $J = 5$ Hz, 1H), 7.90 (d, $J = 10$ Hz, 1H), 7.66–7.62 (m, 1H), 7.57–7.54 (m, 1H), 7.44 (d, $J = 10$ Hz, 2H), 6.82 (s, 1H), 3.96 (s, 2H), 3.78–3.76 (m, 4H), 2.66–2.65 (m, 4H) ppm; ^{13}C NMR (125 MHz, CDCl_3) 160.64, 154.93, 152.98, 133.73, 131.28, 129.59, 129.48, 127.77, 126.25, 125.59, 117.73, 116.24, 114.28, 66.89, 63.13, 53.59 ppm; IR (CH_2Cl_2): ν 1724, 1618, 1617 cm^{-1} ; HRMS: Calcd for $\text{C}_{18}\text{H}_{18}\text{NO}_3$ ($\text{M} + \text{H}$) 296.1242; found 296.1292.



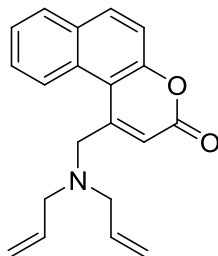
C4A2

1-(Piperidin-1-ylmethyl)-3H-benzo[f]chromen-3-one: ^1H NMR (500 MHz, CDCl_3) δ 8.62 (d, $J = 10$ Hz, 1H), 7.93 (d, $J = 10$ Hz, 1H), 7.89–7.87 (m, 1H), 7.64–7.61 (m, 1H), 7.55–7.52 (m, 1H), 7.44 (d, $J = 10$ Hz, 1H), 6.82 (s, 1H), 3.88 (s, 2H), 2.56 (bs, 4H), 1.65–1.61 (m, 4H), 1.50–1.47 (m, 2H) ppm; ^{13}C NMR (125 MHz, CDCl_3) δ 160.08, 154.01, 153.38, 132.65, 130.42, 128.92, 128.49, 126.81, 125.79, 124.64, 116.89, 115.28, 113.74, 62.84, 53.84, 25.19, 23.36 ppm; IR (CH_2Cl_2): ν 1726, 1624, 1550 cm^{-1} ; HRMS: Calcd for $\text{C}_{19}\text{H}_{20}\text{NO}_2$ ($\text{M} + \text{H}$) 294.1449; found: 294.1492.



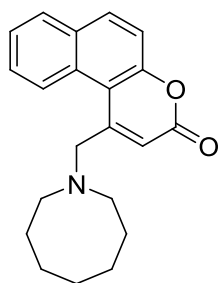
C4A3

1-((Dibutylamino)methyl)-3H-benzo[f]chromen-3-one: ^1H NMR (500 MHz, CDCl_3) δ 8.54 (d, $J = 10$ Hz, 1H), 7.94 (d, $J = 5$ Hz, 1H), 7.91–7.89 (m, 1H), 7.65–7.63 (m, 1H), 7.56–7.53 (m, 1H), 7.46 (d, $J = 5$ Hz, 1H), 7.09 (s, 1H), 4.09 (s, 2H), 2.56 (t, $J = 5$ Hz, 4H), 1.53–1.47 (m, 4H), 1.37–1.29 (m, 4H), 0.90 (t, $J = 5$ Hz, 6H) ppm; ^{13}C NMR (125 MHz, CDCl_3) δ 160.18, 155.60, 153.64, 132.34, 130.28, 128.73, 128.46, 126.59, 125.38, 124.40, 116.81, 114.28, 113.51, 59.10, 53.20, 28.36, 19.63, 13.08 ppm; IR (CH_2Cl_2): ν 1722, 1623, 1549 cm^{-1} ; HRMS: Calcd for $\text{C}_{22}\text{H}_{28}\text{NO}_2$ ($\text{M} + \text{H}$) 338.2075; found: 338.2119.



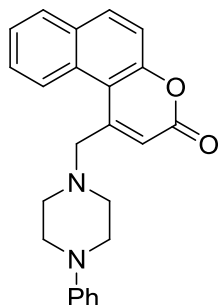
C4A4

1-((Diallylamino)methyl)-3H-benzo[f]chromen-3-one: ^1H NMR (500 MHz, CDCl_3) δ 8.44 (d, $J = 10$ Hz, 1H), 7.95 (d, $J = 10$ Hz, 1H), 7.91–7.89 (m, 1H), 7.63–7.61 (m, 1H), 7.56–7.53 (m, 1H), 7.47 (d, $J = 10$ Hz, 1H), 7.08 (t, $J = 1$ Hz, 1H), 5.96–5.88 (m, 2H), 5.28–5.18 (m, 4H), 4.14 (d, $J = 1$ Hz, 2H), 3.23 (d, $J = 5$ Hz, 4H) ppm; ^{13}C NMR (125 MHz, CDCl_3) δ 161.06, 155.78, 154.73, 134.88, 133.49, 131.31, 129.65, 129.53, 127.65, 126.19, 125.45, 118.24, 117.83, 115.18, 114.37, 58.22, 56.96 ppm; IR (CH_2Cl_2): ν 1727, 1551 cm^{-1} ; HRMS: Calcd for $\text{C}_{20}\text{H}_{20}\text{NO}_2$ ($\text{M} + \text{H}$) 306.1449; found: 306.1501.



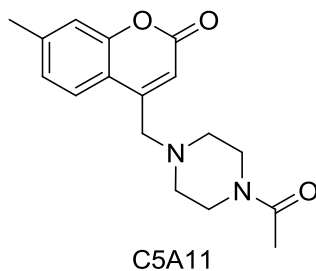
C4A14

1-(Azocan-1-ylmethyl)-3H-benzo[f]chromen-3-one: ^1H NMR (500 MHz, CDCl_3) δ 8.73 (d, $J = 10$ Hz, 1H), 7.96 (d, $J = 10$ Hz, 1H), 7.90–7.88 (m, 1H), 7.66–7.63 (m, 1H), 7.56–7.53 (m, 1H), 7.46 (d, $J = 10$ Hz, 1H), 6.73 (s, 1H), 4.03 (d, $J = 1$ Hz, 2H), 2.74 (t, $J = 5$ Hz, 4H), 1.55–1.52 (m, 10H) ppm; ^{13}C NMR (125 MHz, CDCl_3) δ 160.86, 155.26, 154.83, 133.56, 131.21, 129.76, 129.21, 127.59, 127.15, 125.53, 117.76, 116.98, 114.69, 64.11, 54.32, 27.94, 27.20, 25.83 ppm; IR (CH_2Cl_2): ν 1720, 1623, 1549 cm^{-1} ; HRMS: Calcd for $\text{C}_{21}\text{H}_{24}\text{NO}_2$ ($\text{M} + \text{H}$) 322.1762; found: 322.1790.

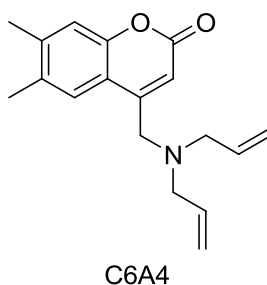


C4A16

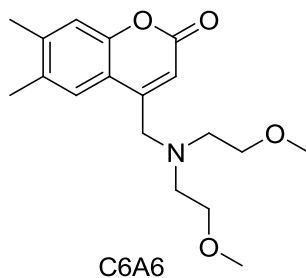
1-((4-Phenylpiperazin-1-yl)methyl)-3H-benzof[*h*]chromen-3-one: ^1H NMR (500 MHz, CDCl_3) δ 8.61 (d, $J = 10$ Hz, 1H), 7.97 (d, $J = 10$ Hz, 1H), 7.91–7.89 (m, 1H), 7.66–7.63 (m, 1H), 7.57–7.54 (m, 1H), 7.47 (d, $J = 10$ Hz, 1H), 7.28–7.25 (m, 2H), 6.94–6.93 (m, 2H), 6.88–6.85 (m, 2H), 4.02 (s, 2H), 3.25 (t, $J = 5$ Hz, 4H), 2.82 (t, $J = 5$ Hz, 4H) ppm; ^{13}C NMR (125 MHz, CDCl_3) δ 160.74, 154.99, 153.30, 151.13, 133.75, 131.32, 129.67, 129.48, 129.18, 127.78, 126.39, 125.61, 119.98, 117.79, 116.36, 116.21, 114.40, 62.83, 53.23, 49.22 ppm; IR (CH_2Cl_2): ν 1720, 1622, 1598 cm^{-1} ; HRMS: Calcd for $\text{C}_{24}\text{H}_{23}\text{N}_2\text{O}_2$ ($\text{M} + \text{H}$) 371.1715; found: 371.1732.



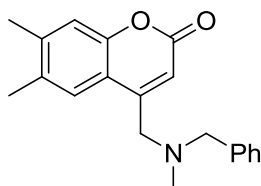
4-((4-Acetylpiperazin-1-yl)methyl)-7-methyl-2H-chromen-2-one: ^1H NMR (500 MHz, CDCl_3) δ 7.68 (d, $J = 10$ Hz, 1H), 7.14–7.10 (m, 2H), 6.48 (s, 1H), 3.67–3.65 (m, 4H), 3.51 (t, $J = 5$ Hz, 2H), 2.54 (q, $J = 5$ Hz, 4H), 2.45 (s, 3H), 2.11 (s, 3H) ppm; ^{13}C NMR (125 MHz, CDCl_3) δ 168.97, 161.15, 153.87, 151.47, 143.06, 125.37, 124.31, 117.22, 116.21, 113.78, 58.65, 53.35, 53.17, 46.20, 41.36, 21.63, 21.35 ppm; IR (CH_2Cl_2): ν 1717, 1618, 1557 cm^{-1} ; HRMS: Calcd for $\text{C}_{17}\text{H}_{21}\text{N}_2\text{O}_3$ ($\text{M} + \text{H}$) 301.1507; found: 301.1545.



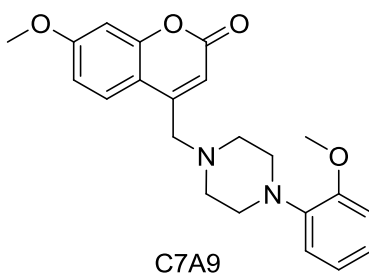
4-((Diallylamino)methyl)-6,7-dimethyl-2H-chromen-2-one: ^1H NMR (500 MHz, CDCl_3) δ 7.47 (s, 1H), 7.09 (s, 1H), 6.56 (s, $J = 1$ Hz, 1H), 5.89–5.84 (m, 2H), 5.25–5.17 (m, 4H), 3.69 (d, $J = 1$ Hz, 2H), 3.16 (d, $J = 5$ Hz, 4H), 2.33 (s, 3H), 2.31 (s, 3H) ppm; ^{13}C NMR (125 MHz, CDCl_3) δ 160.48, 152.26, 150.85, 140.27, 133.76, 131.41, 123.23, 116.94, 116.26, 115.27, 112.07, 56.0, 52.30, 18.95, 18.25 ppm; IR (CH_2Cl_2): ν 1713, 1623, 1557 cm^{-1} ; HRMS: Calcd for $\text{C}_{18}\text{H}_{22}\text{NO}_2$ ($\text{M} + \text{H}$) 284.1606; found: 284.1645.



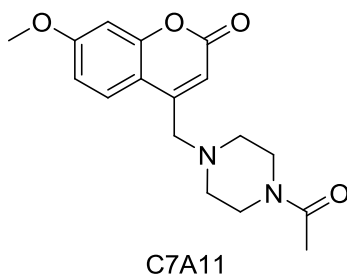
4-((bis(2-Methoxyethyl)amino)methyl)-6,7-dimethyl-2H-chromen-2-one: ^1H NMR (500 MHz, CDCl_3) δ 7.54 (s, 1H), 7.10 (s, 1H), 6.60 (s, 1H), 3.91 (d, $J = 1$ Hz, 2H), 3.51 (t, $J = 5$ Hz, 4H), 3.32 (s, 6H), 2.84 (t, $J = 5$ Hz, 4H), 2.33 (s, 3H), 2.31 (s, 3H) ppm; ^{13}C NMR (125 MHz, CDCl_3) δ 161.83, 153.97, 152.07, 141.40, 132.60, 124.58, 117.43, 116.51, 113.18, 71.44, 58.81, 56.15, 54.63, 20.17, 19.43 ppm; IR (CH_2Cl_2): ν 1717, 1623, 1557 cm^{-1} ; HRMS: Calcd for $\text{C}_{18}\text{H}_{26}\text{NO}_4$ ($\text{M} + \text{H}$) 320.1817; found: 320.1857.



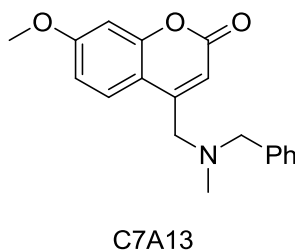
4-((Benzyl(methyl)amino)methyl)-6,7-dimethyl-2H-chromen-2-one: ^1H NMR (500 MHz, CDCl_3) δ 7.37–7.28 (m, 6H), 7.07 (s, 1H), 6.51 (s, 1H), 3.64 (s, 2H), 3.58 (s, 2H), 2.31 (s, 3H), 2.28 (s, 3H), 2.26 (s, 3H) ppm; ^{13}C NMR (125 MHz, CDCl_3) δ 160.41, 151.63, 150.97, 140.39, 137.22, 131.45, 127.83, 127.26, 126.22, 123.74, 116.22, 115.29, 112.72, 61.65, 56.43, 41.70, 18.97, 18.15 ppm; IR (CH_2Cl_2): ν 1714, 1623, 1557 cm^{-1} ; HRMS: Calcd for $\text{C}_{20}\text{H}_{22}\text{NO}_2$ ($\text{M} + \text{H}$) 308.1606; found: 308.1641.



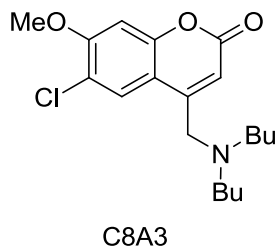
7-Methoxy-4-((4-(2-methoxyphenyl)piperazin-1-yl)methyl)-2H-chromen-2-one: ^1H NMR (500 MHz, CDCl_3) δ 7.79 (d, $J = 10$ Hz, 1H), 7.02–6.82 (m, 6H), 6.41 (s, 1H), 3.87 (s, 3H), 3.86 (s, 3H), 3.66 (s, 2H), 3.11 (bs, 4H), 2.74 (bs, 4H) ppm; ^{13}C NMR (125 MHz, CDCl_3) δ 162.55, 161.51, 155.65, 152.24, 141.10, 125.97, 123.07, 121.00, 118.24, 112.48, 112.23, 111.82, 111.17, 100.80, 59.22, 55.75, 55.38, 53.74, 50.65 ppm; IR (CH_2Cl_2): ν 1717, 1610, 1557 cm^{-1} ; HRMS: Calcd for $\text{C}_{22}\text{H}_{25}\text{N}_2\text{O}_4$ ($\text{M} + \text{H}$) 381.1770; found: 381.1804.



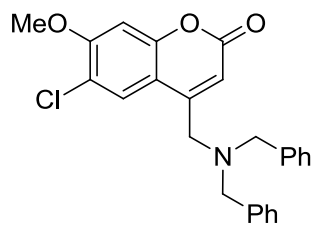
4-((4-Acetylpiperazin-1-yl)methyl)-7-methoxy-2H-chromen-2-one: ^1H NMR (500 MHz, CDCl_3) δ 7.73 (d, $J = 10$ Hz, 1H), 6.87–6.82 (m, 2H), 6.37 (s, 1H), 3.88 (s, 3H), 3.67–3.63 (m, 4H), 3.50 (t, $J = 5$ Hz, 2H), 2.55–2.52 (m, 4H), 2.11 (s, 3H) ppm; ^{13}C NMR (125 MHz, CDCl_3) δ 168.96, 162.64, 161.29, 155.63, 151.59, 125.75, 112.28, 112.18, 111.77, 100.84, 58.88, 55.76, 53.31, 53.14, 46.19, 41.35, 21.34 ppm; IR (CH_2Cl_2): ν 1713, 1608, 1557 cm^{-1} ; HRMS: Calcd for $\text{C}_{17}\text{H}_{21}\text{N}_2\text{O}_4$ (M + H) 317.1457; found: 317.1496.



4-((Benzyl(methyl)amino)methyl)-7-methoxy-2H-chromen-2-one: ^1H NMR (500 MHz, CDCl_3) δ 7.67 (d, $J = 10$ Hz, 1H), 7.33–7.25 (m, 5H), 6.82–6.79 (m, 2H), 6.42 (t, $J = 1$ Hz, 1H), 3.85 (s, 3H), 3.61 (s, 2H), 3.58 (d, $J = 1$ Hz, 2H), 2.26 (s, 3H) ppm; ^{13}C NMR (125 MHz, CDCl_3) δ 162.52, 161.55, 155.61, 153.10, 138.36, 128.94, 128.42, 127.39, 126.05, 112.44, 112.12, 111.86, 100.76, 62.57, 58.15, 55.72, 42.75 ppm; IR (CH_2Cl_2): ν 1716, 1611 cm^{-1} ; HRMS: Calcd for $\text{C}_{19}\text{H}_{20}\text{NO}_3$ (M + H) 310.1398; found: 310.1438.

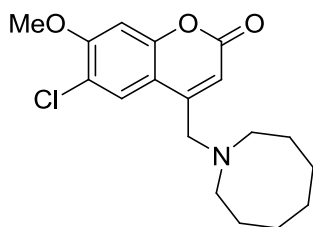


6-Chloro-4-((dibutylamino)methyl)-7-methoxy-2H-chromen-2-one: ^1H NMR (500 MHz, CDCl_3) δ 7.90 (s, 1H), 6.85 (s, 1H), 6.47 (s, 1H), 3.96 (s, 3H), 3.62 (d, $J = 5$ Hz, 1H), 2.47 (t, $J = 5$ Hz, 4H), 1.45–1.43 (m, 4H), 1.34–1.28 (m, 4H), .089 (t, $J = 5$ Hz, 6H) ppm; ^{13}C NMR (125 MHz, CDCl_3) δ 161.09, 157.34, 153.86, 153.62, 125.77, 118.59, 112.78, 112.40, 101.21, 56.56, 55.98, 54.23, 29.14, 20.56, 14.02 ppm; IR (CH_2Cl_2): ν 1729, 1607, 1557 cm^{-1} ; HRMS: Calcd for $\text{C}_{19}\text{H}_{27}\text{ClNO}_3$ (M + H) 352.1635; found: 352.1673.



C8A12

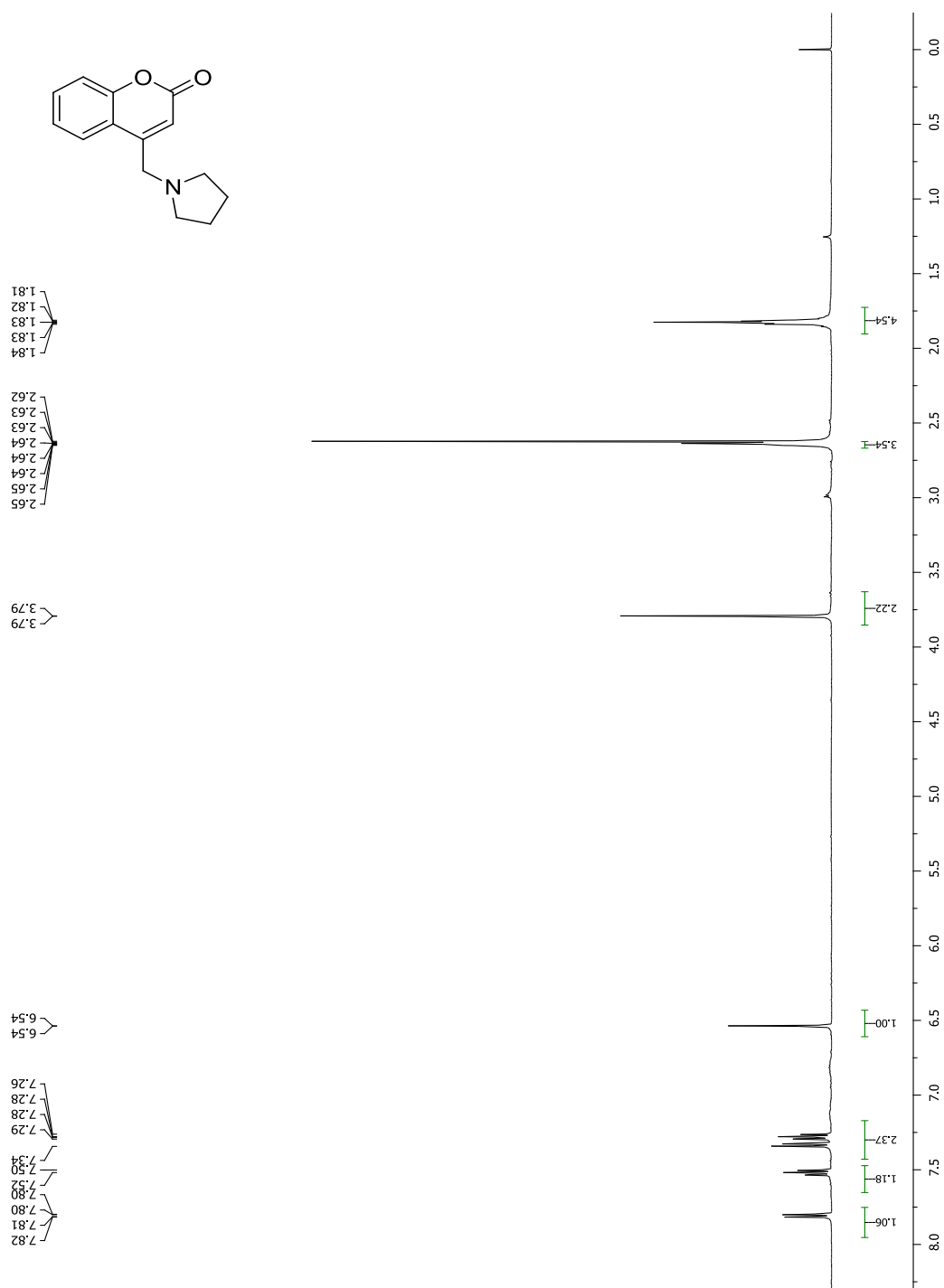
6-Chloro-4-((dibenzylamino)methyl)-7-methoxy-2H-chromen-2-one: ^1H NMR (500 MHz, CDCl_3) δ 7.79 (s, 1H), 7.34–7.25 (m, 10H), 6.80 (s, 1H), 6.51 (s, 1H), 3.93 (s, 3H), 3.61–3.60 (m, 6H) ppm; ^{13}C NMR (125 MHz, CDCl_3) δ 160.77, 157.50, 153.94, 152.56, 138.12, 129.01, 128.59, 127.52, 126.21, 118.69, 113.13, 112.57, 101.19, 58.94, 56.60, 55.08 ppm; IR (CH_2Cl_2): ν 1728, 1607, 1553 cm^{-1} ; HRMS: Calcd for $\text{C}_{25}\text{H}_{23}\text{ClNO}_3$ (M + H); 420.1322 found: 420.1357.



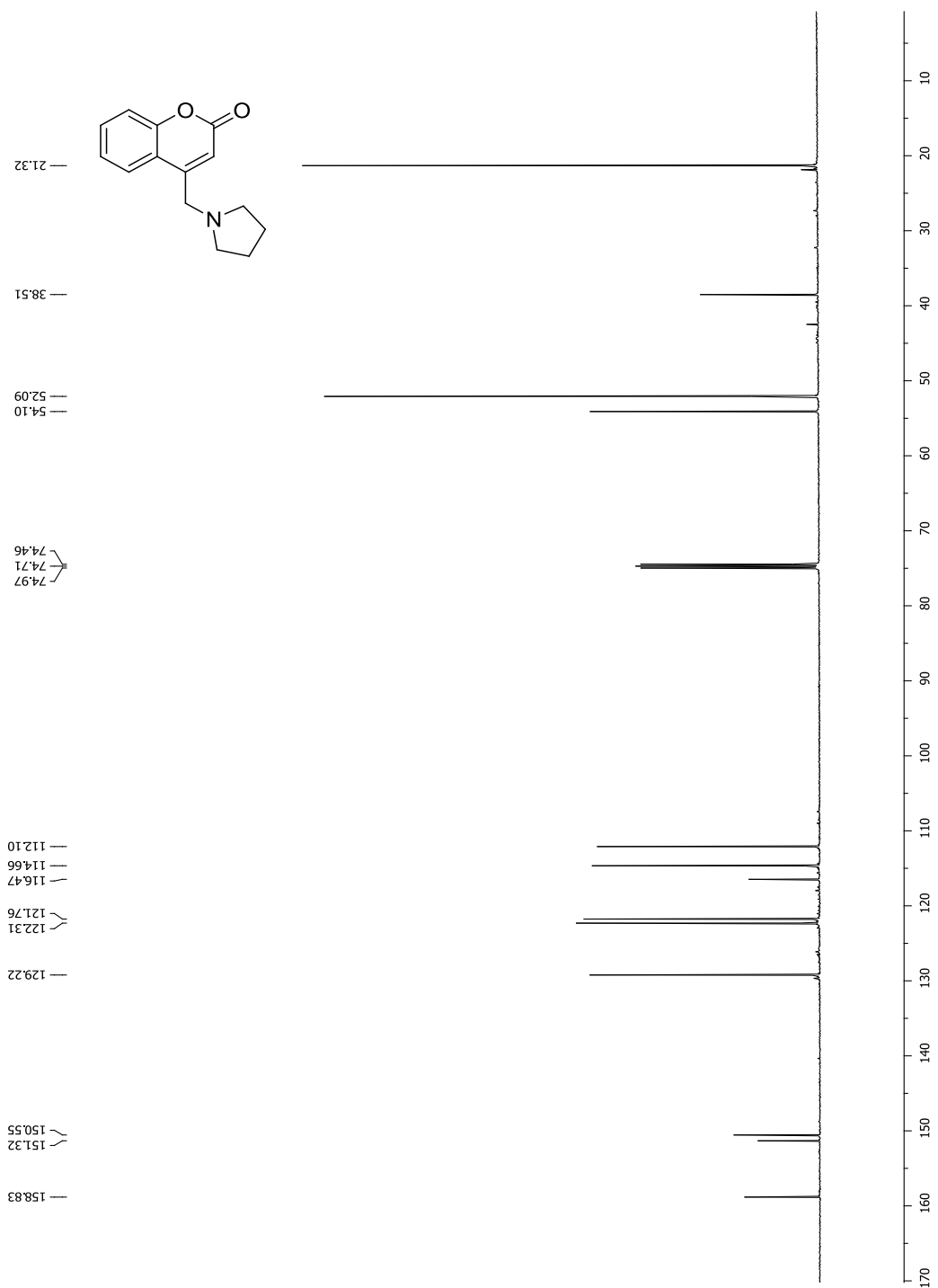
C8A14

4-(Azocan-1-ylmethyl)-6-chloro-7-methoxy-2H-chromen-2-one: ^1H NMR (500 MHz, CDCl_3) δ 8.01 (s, 1H), 6.85 (s, 1H), 6.33 (s, 1H), 3.97 (s, 3H), 3.66 (d, $J = 0.8$ Hz, 2H), 2.63 (bs, 4H), 1.61–1.55 (m, 10H) ppm; ^{13}C NMR (125 MHz, CDCl_3) δ 161.01, 157.41, 153.97, 153.09, 126.77, 118.61, 112.97, 112.85, 100.15, 60.86, 56.58, 55.01, 27.76, 27.38, 25.75 ppm; IR (CH_2Cl_2): ν 1729, 1607, 1555 cm^{-1} ; HRMS: Calcd for $\text{C}_{18}\text{H}_{23}\text{ClNO}_3$ (M + H); 336.1322 found: 336.1359.

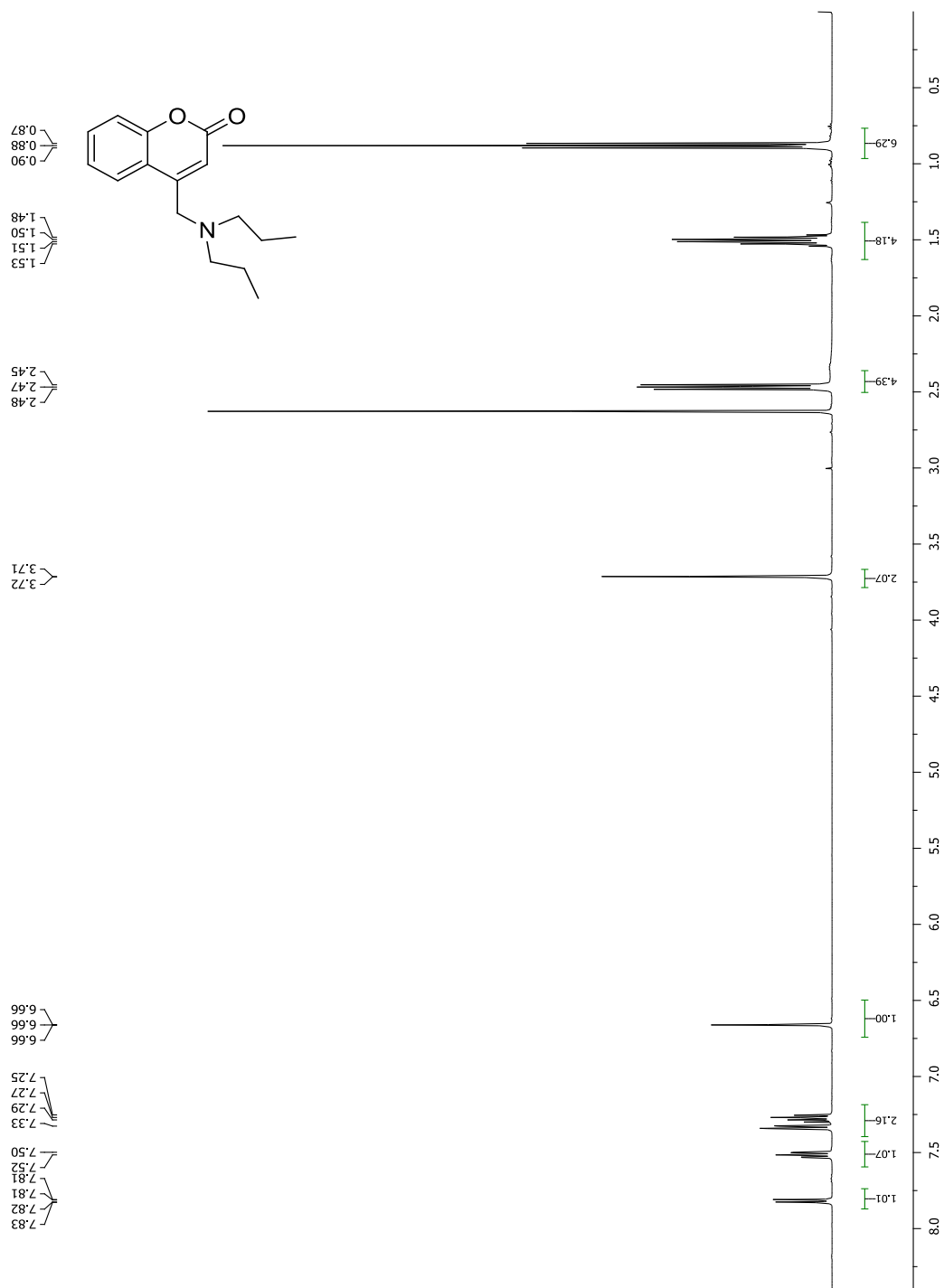
C1A5



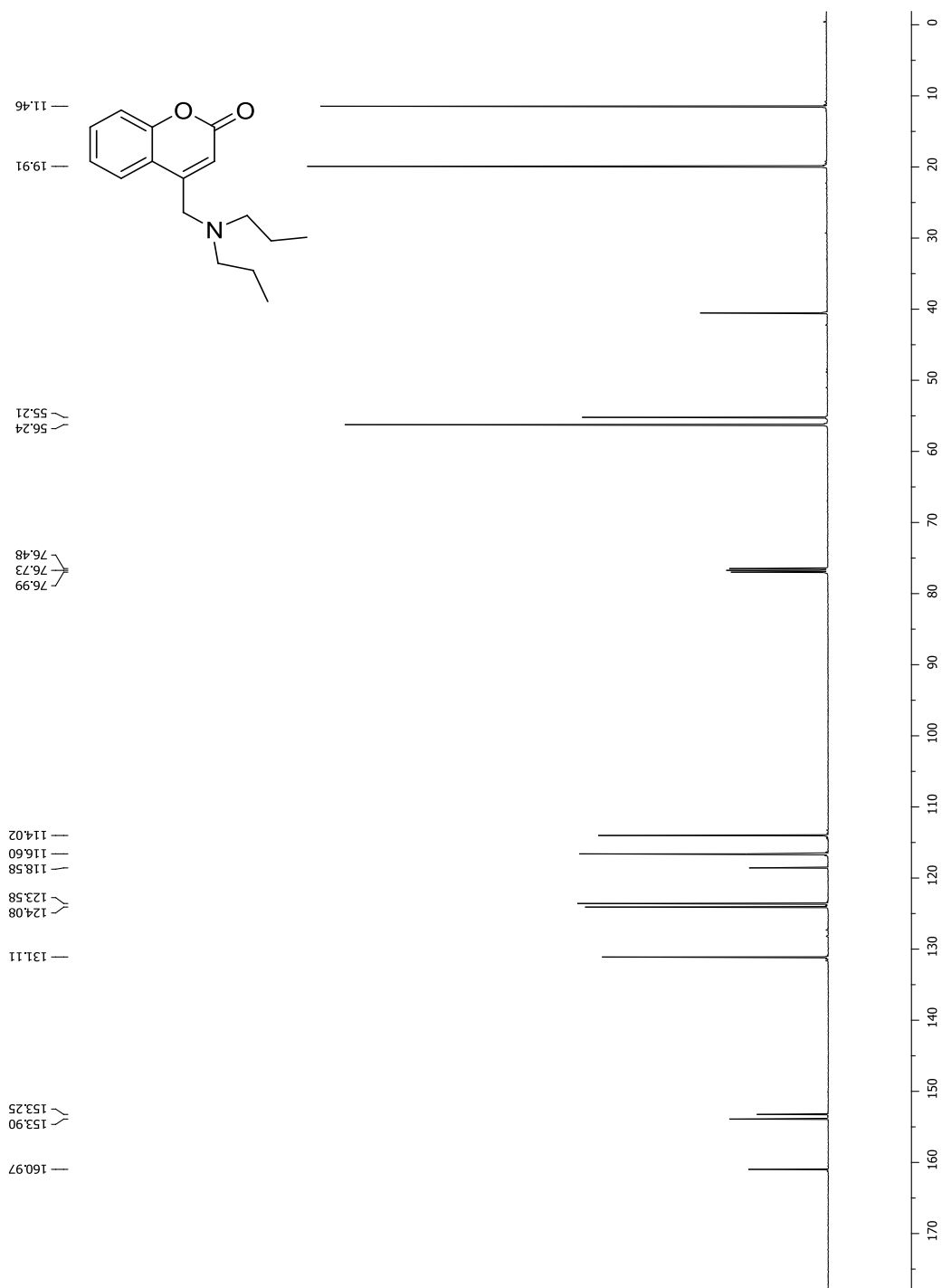
C1A5



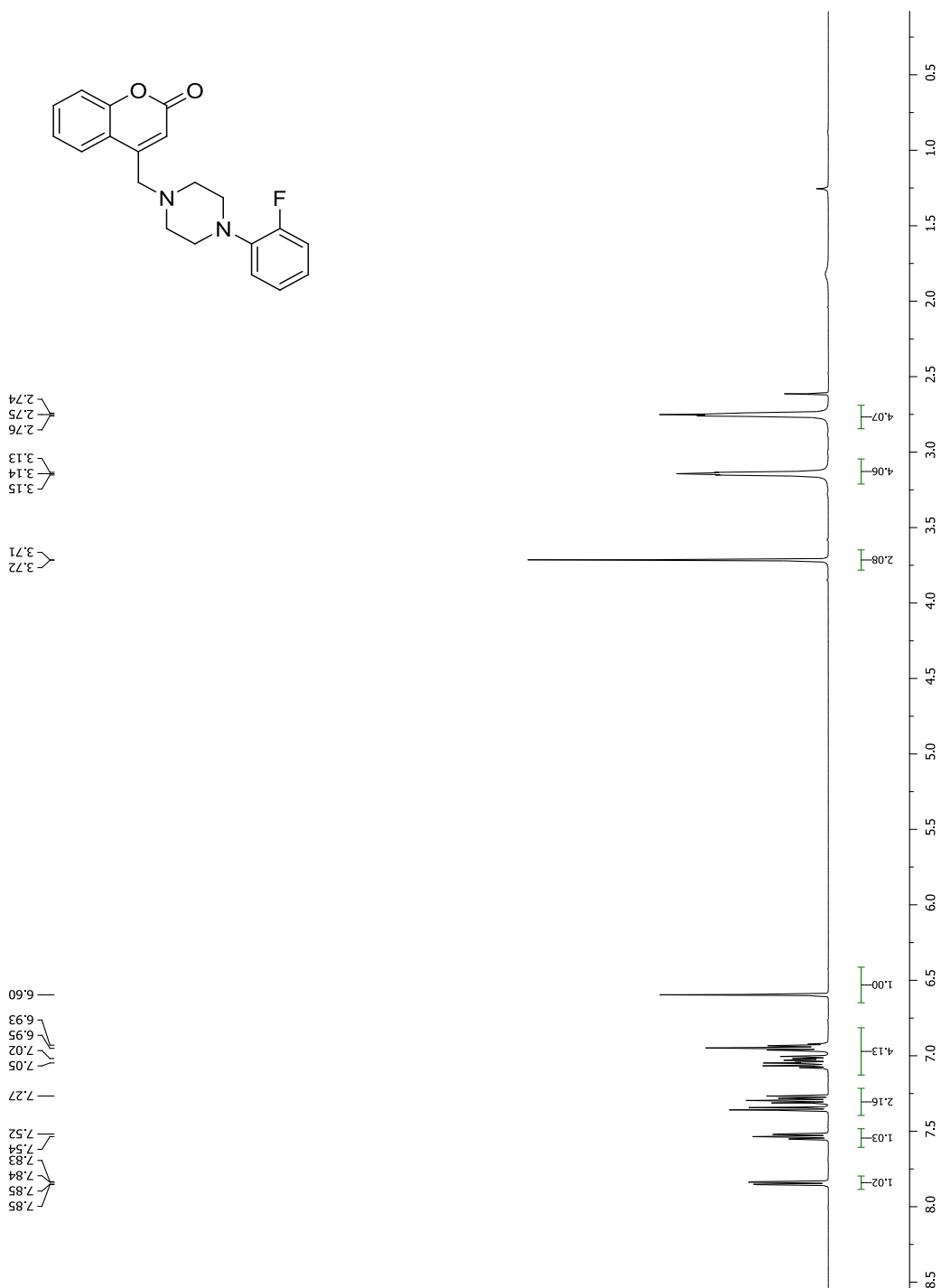
C1A7



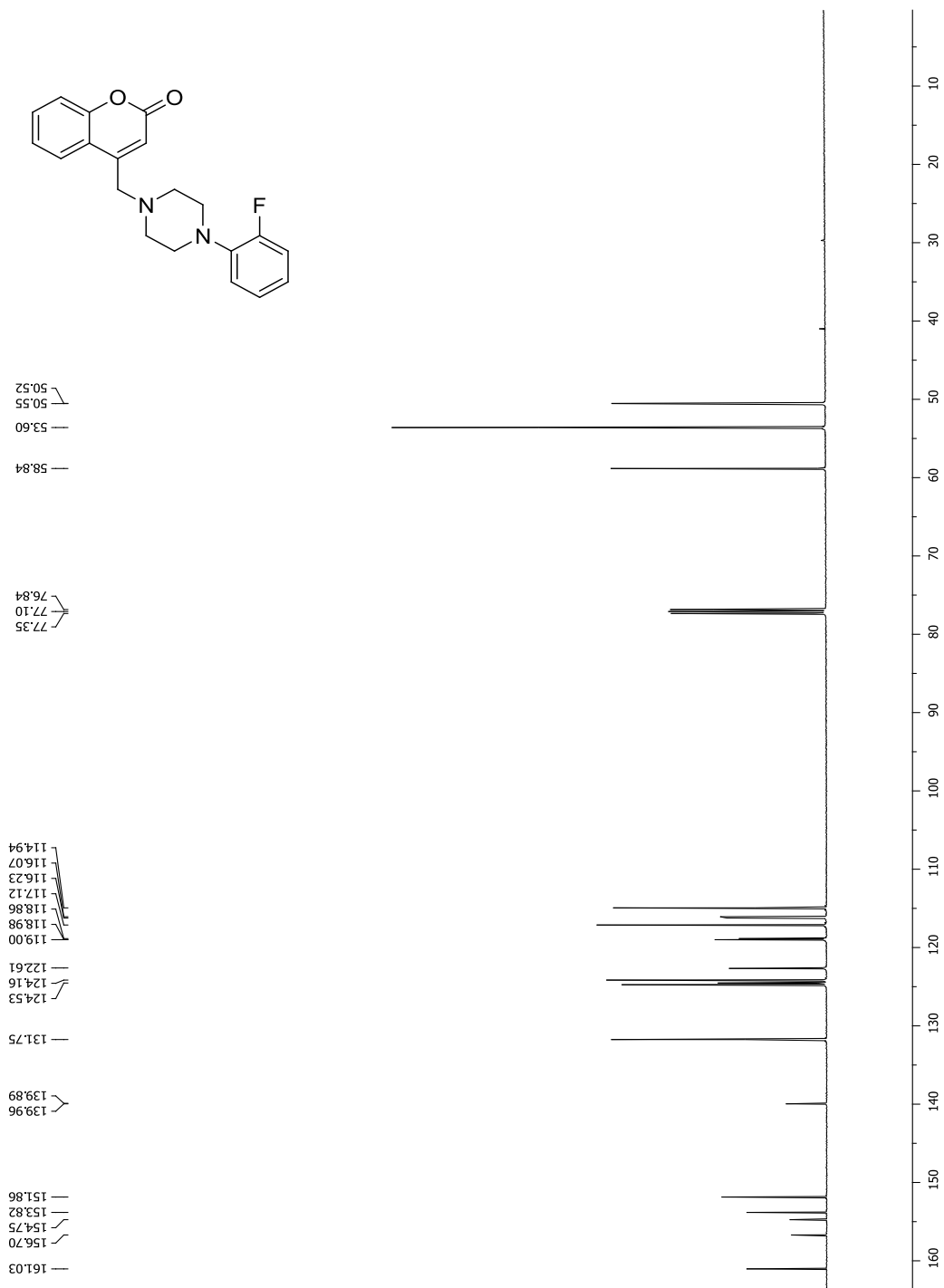
C1A7



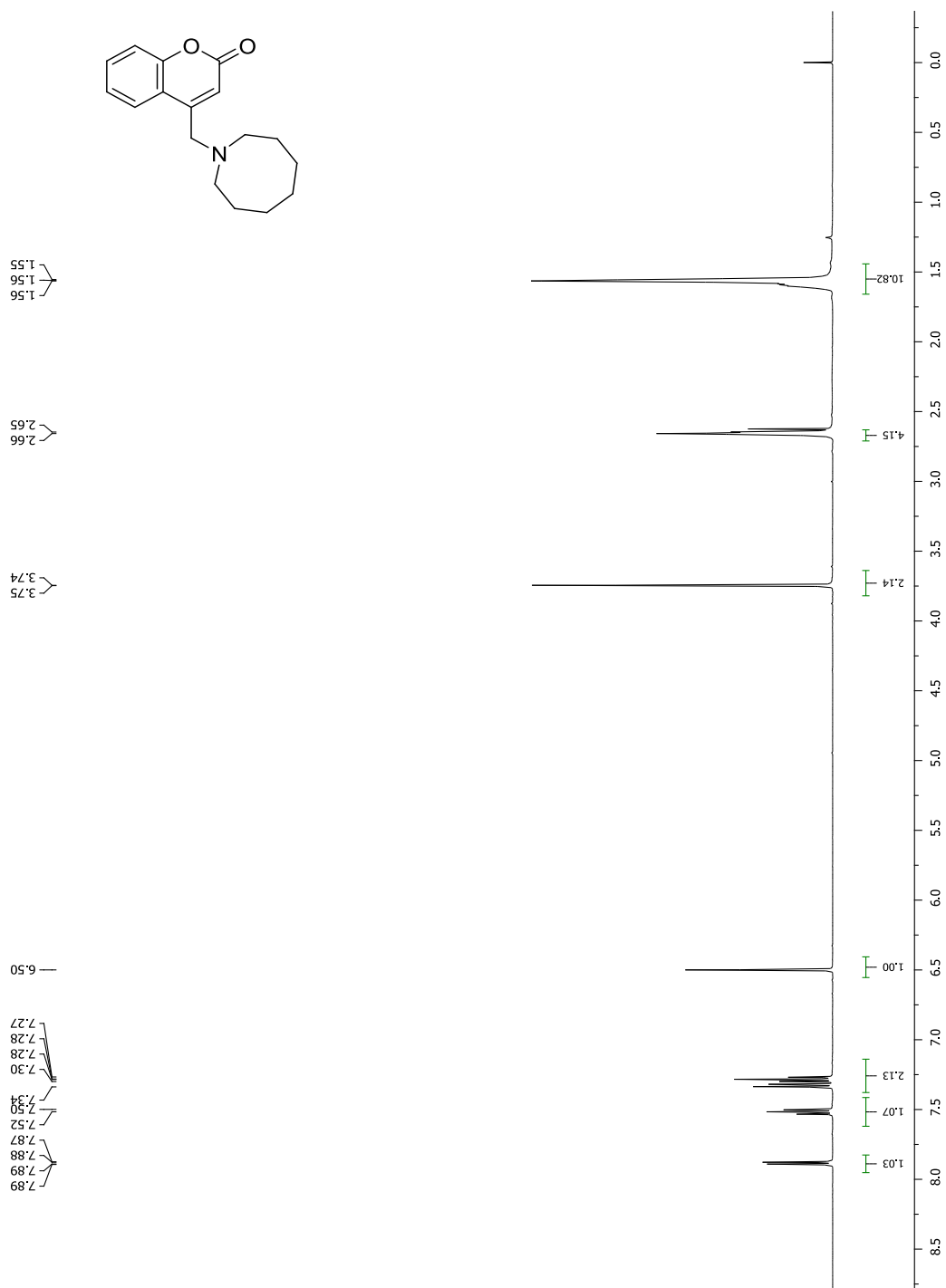
C1A8



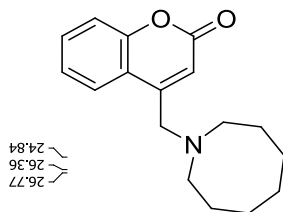
C1A8



C1A14



C1A14



26.77
26.36
24.84

53.95

59.33

76.33
76.08
75.82

113.98

118.04

115.94

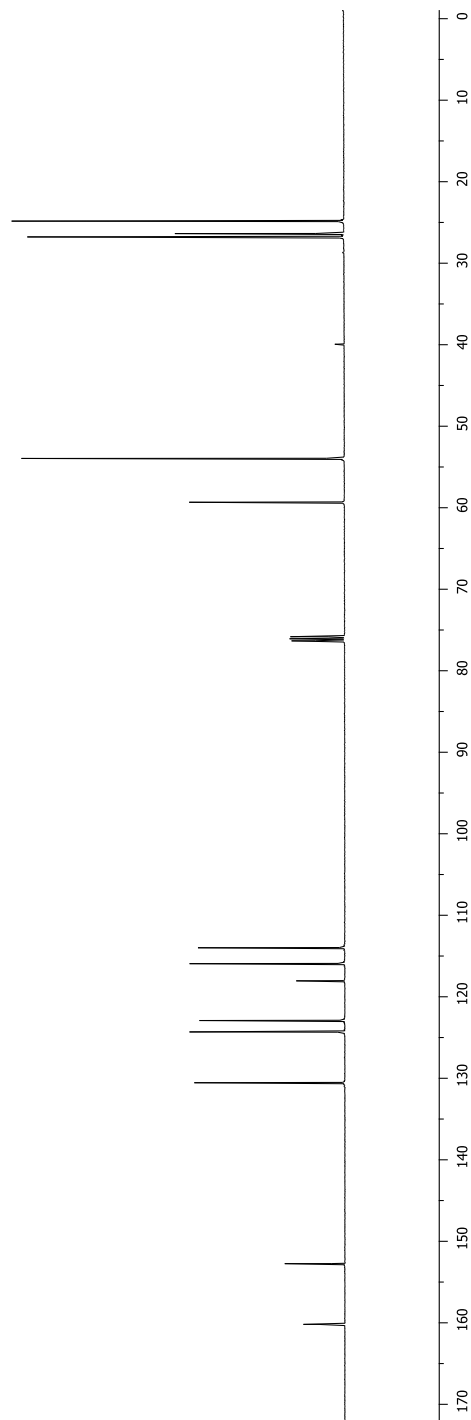
122.91

124.31

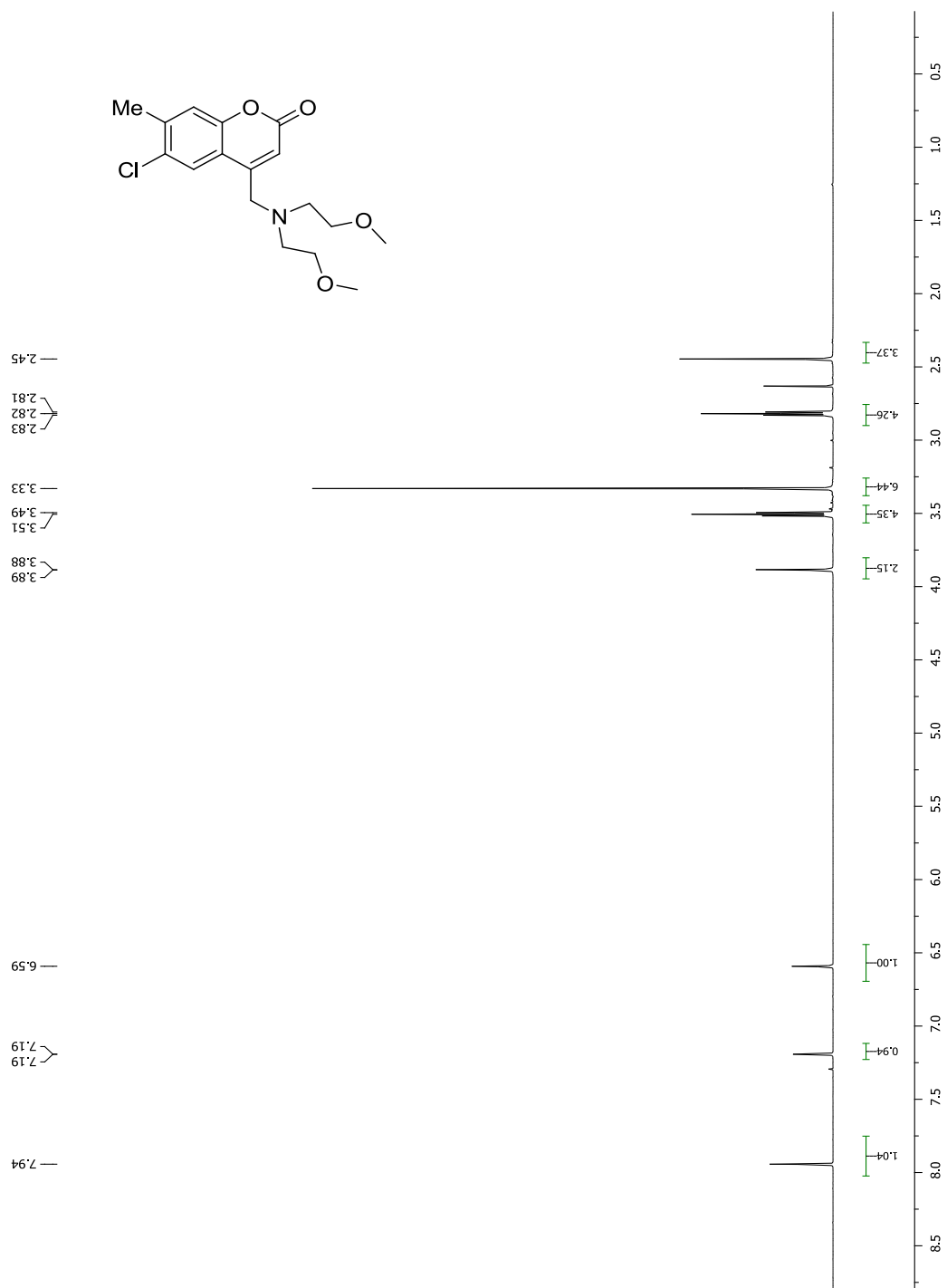
130.55

152.76
152.74

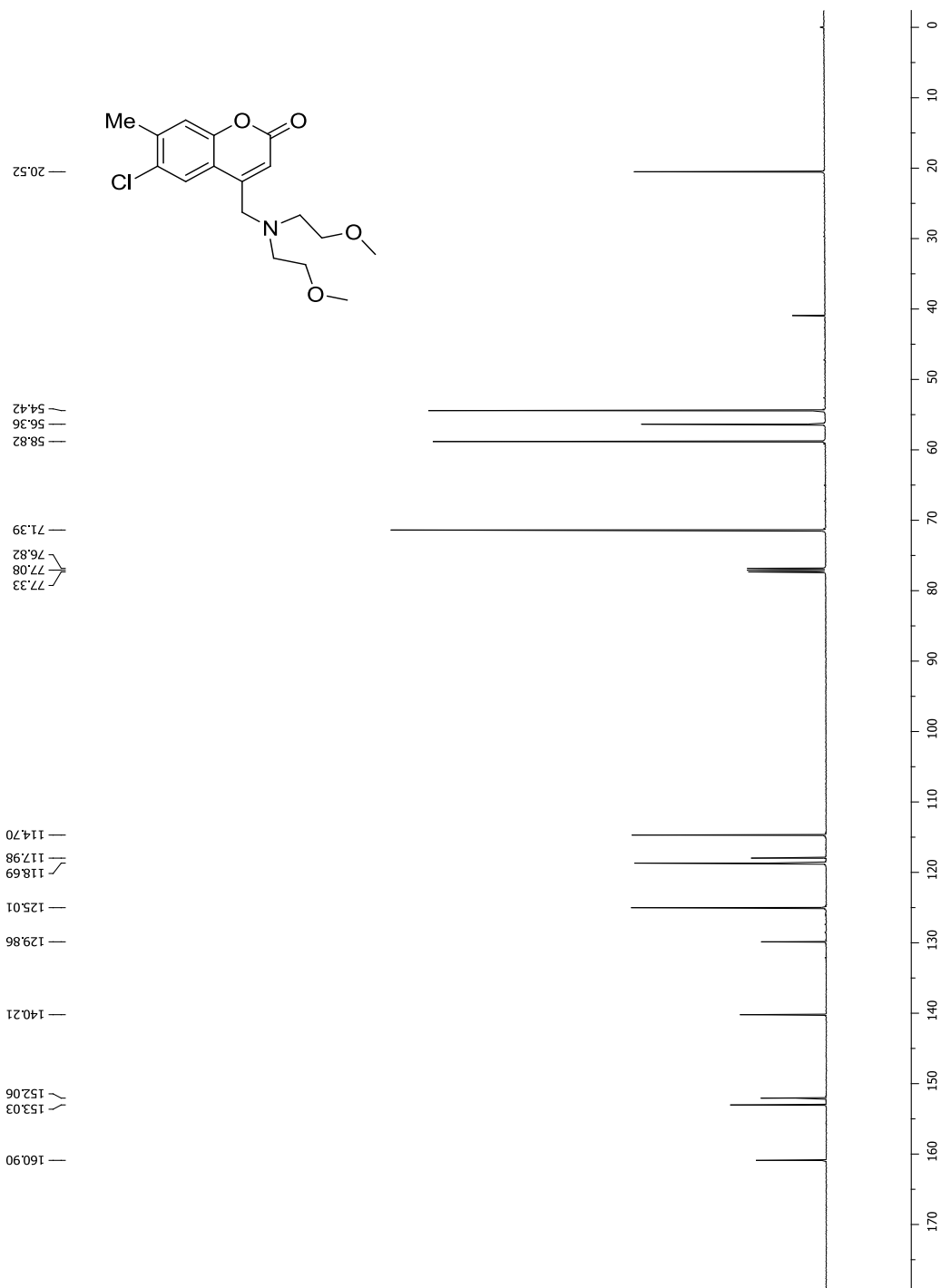
160.19



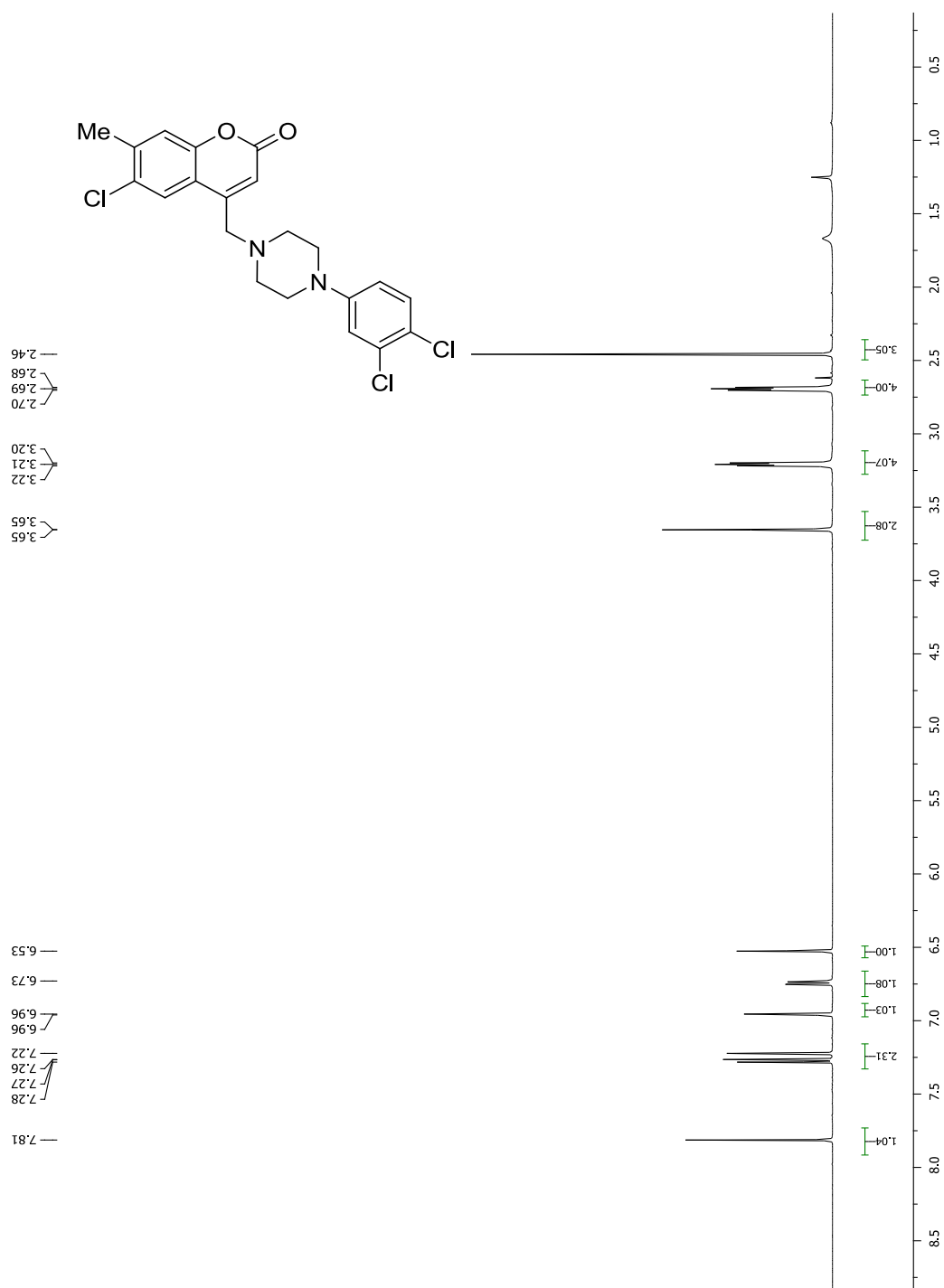
C2A6



C2A6



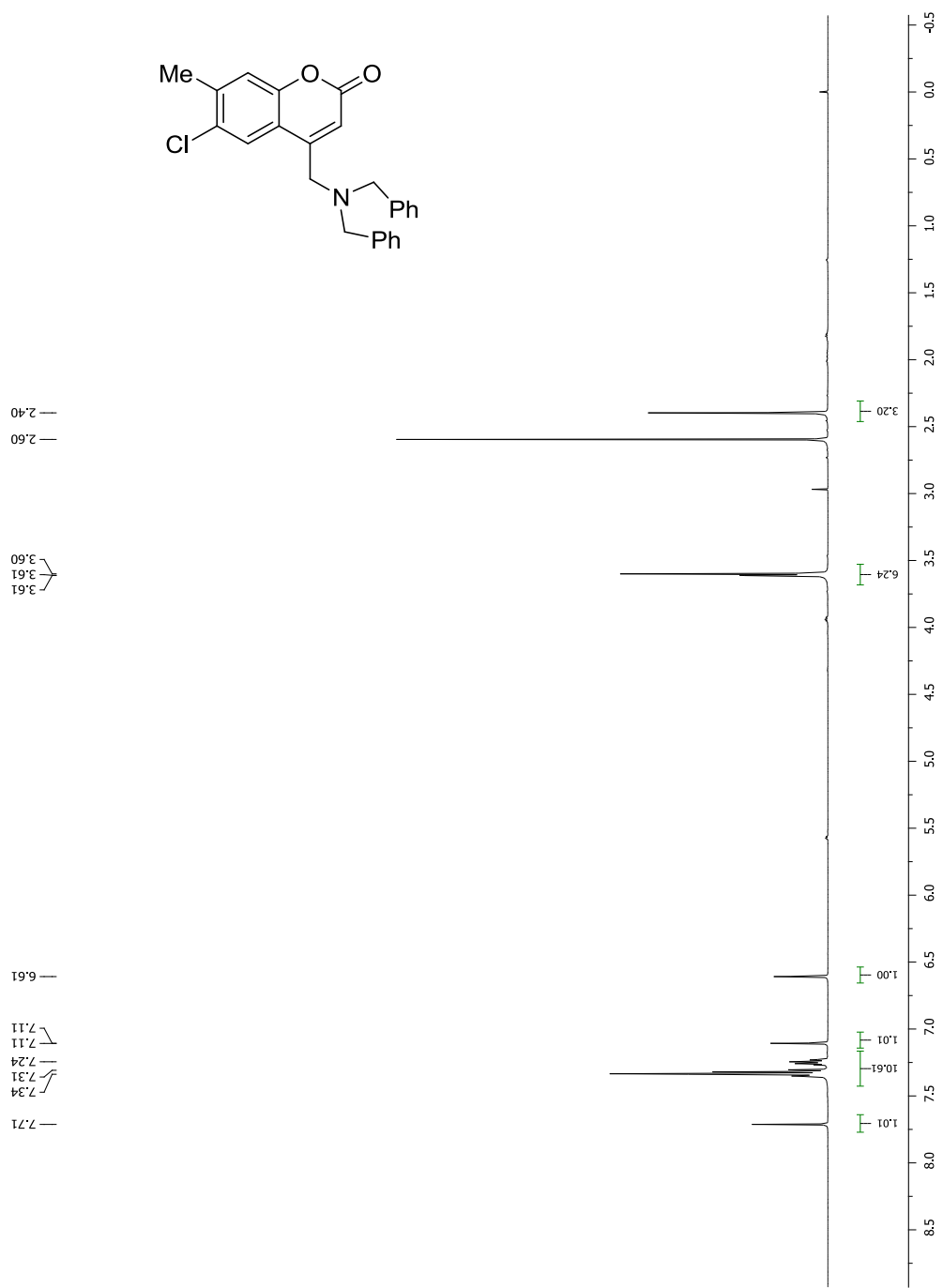
C2A10



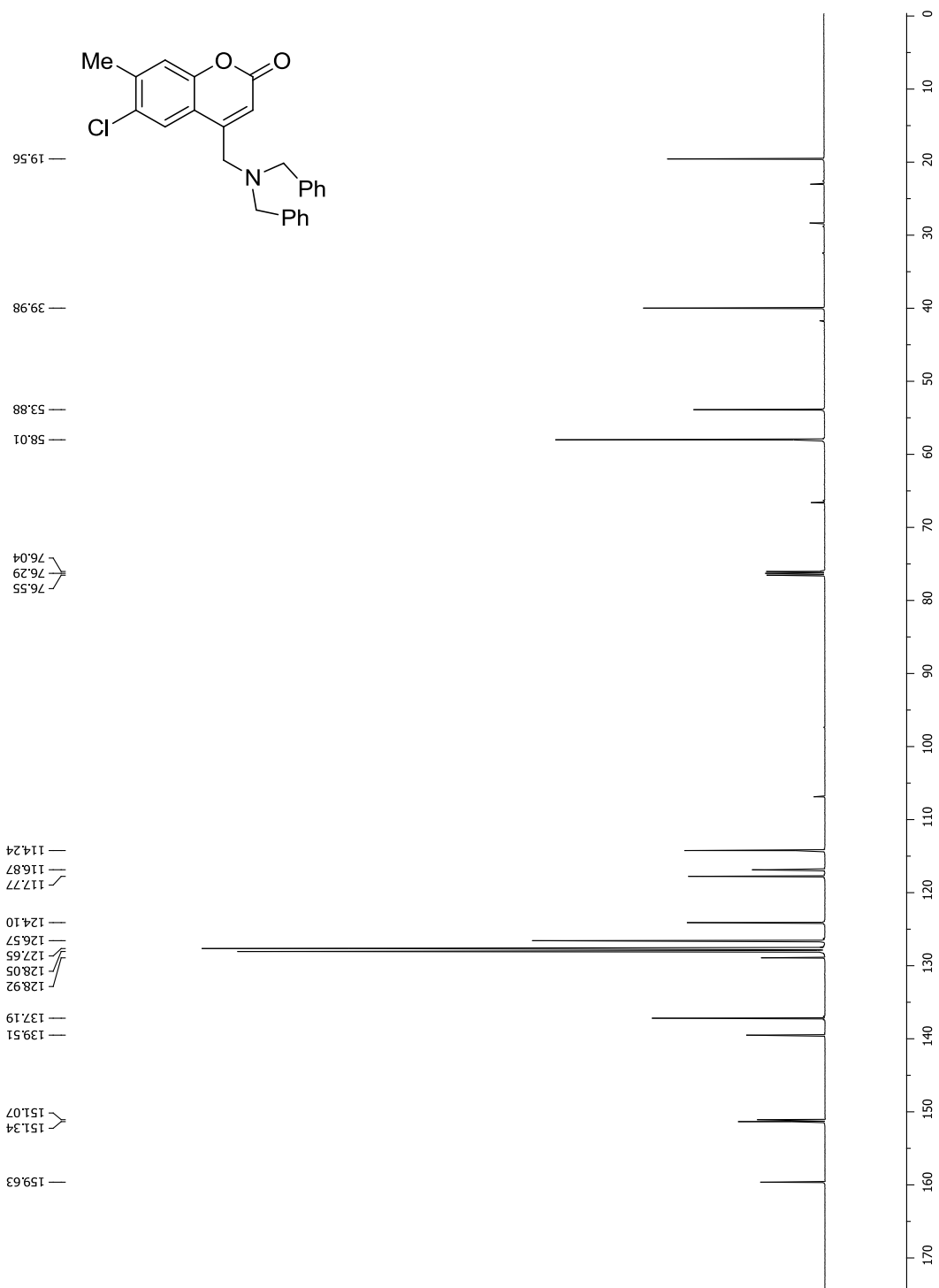
C2A10



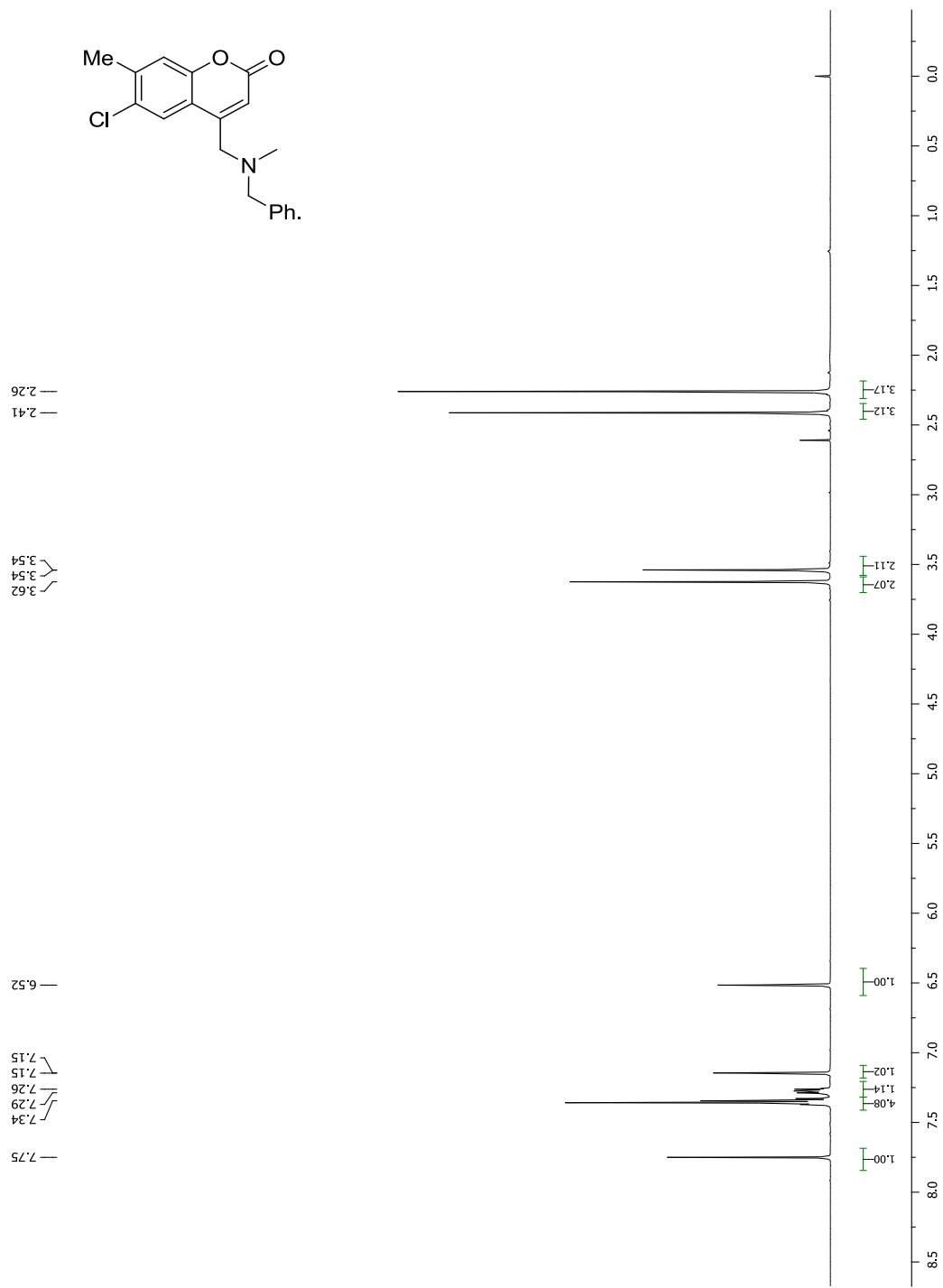
C2A12



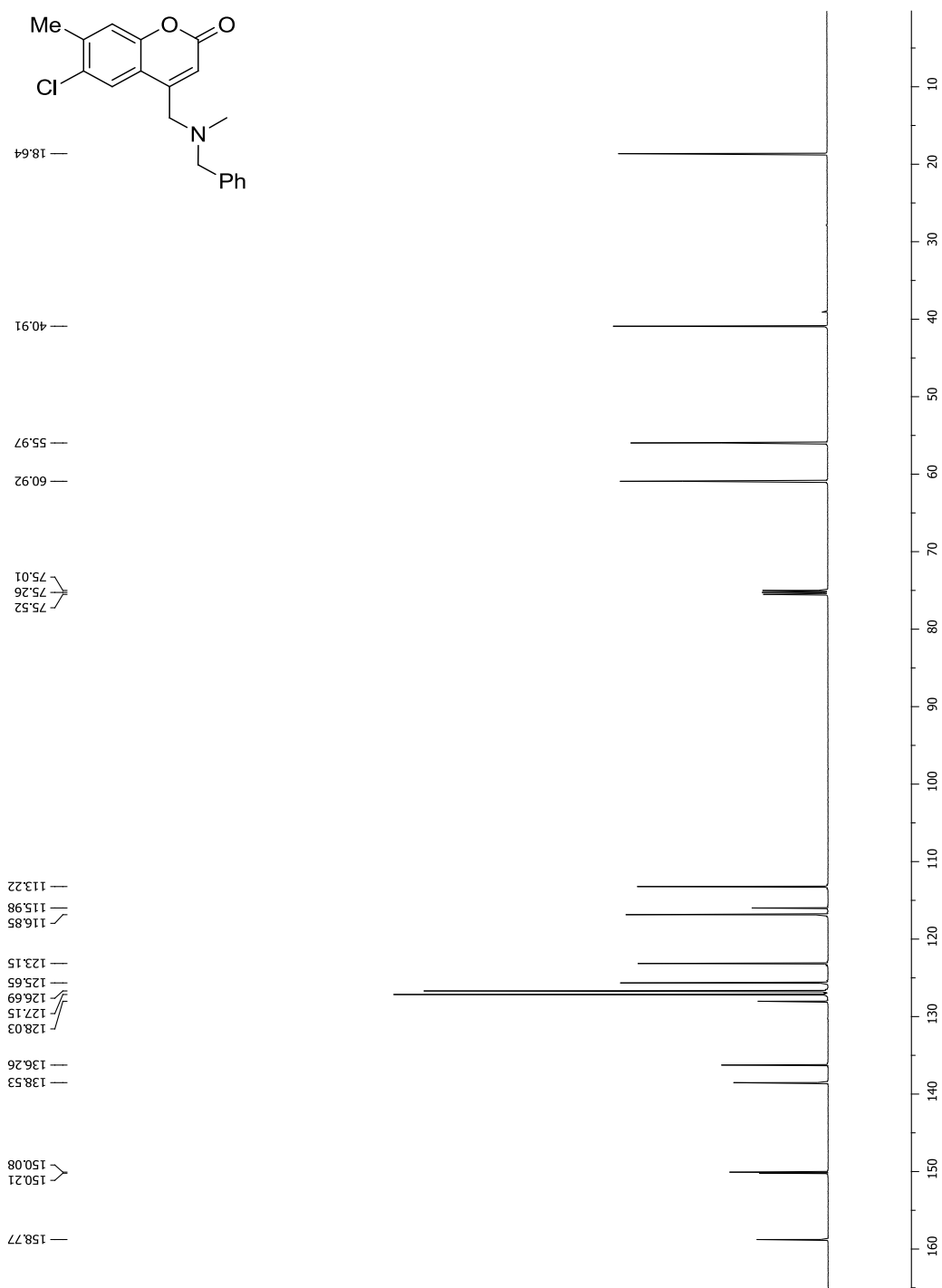
C2A12



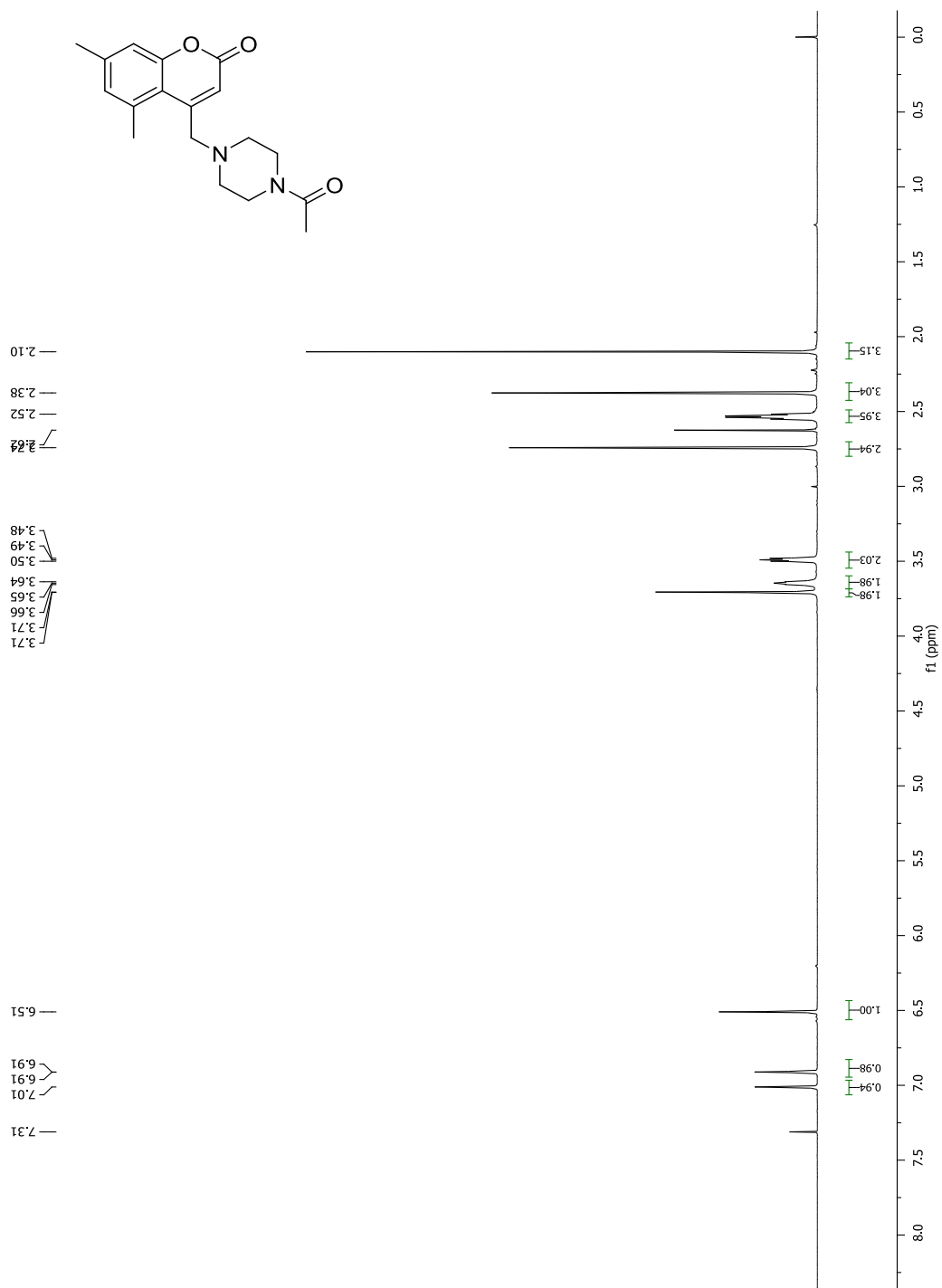
C2A13



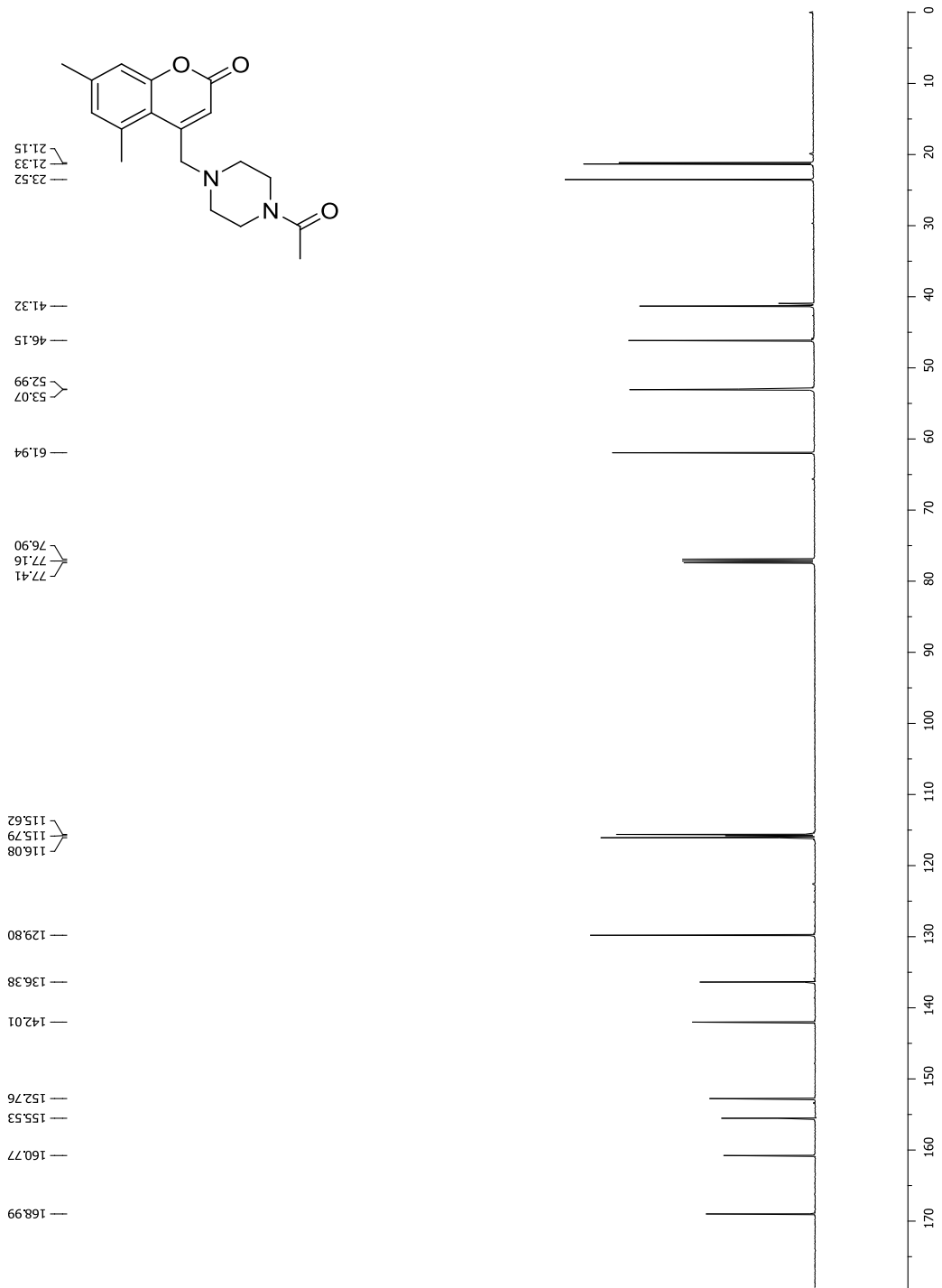
C2A13



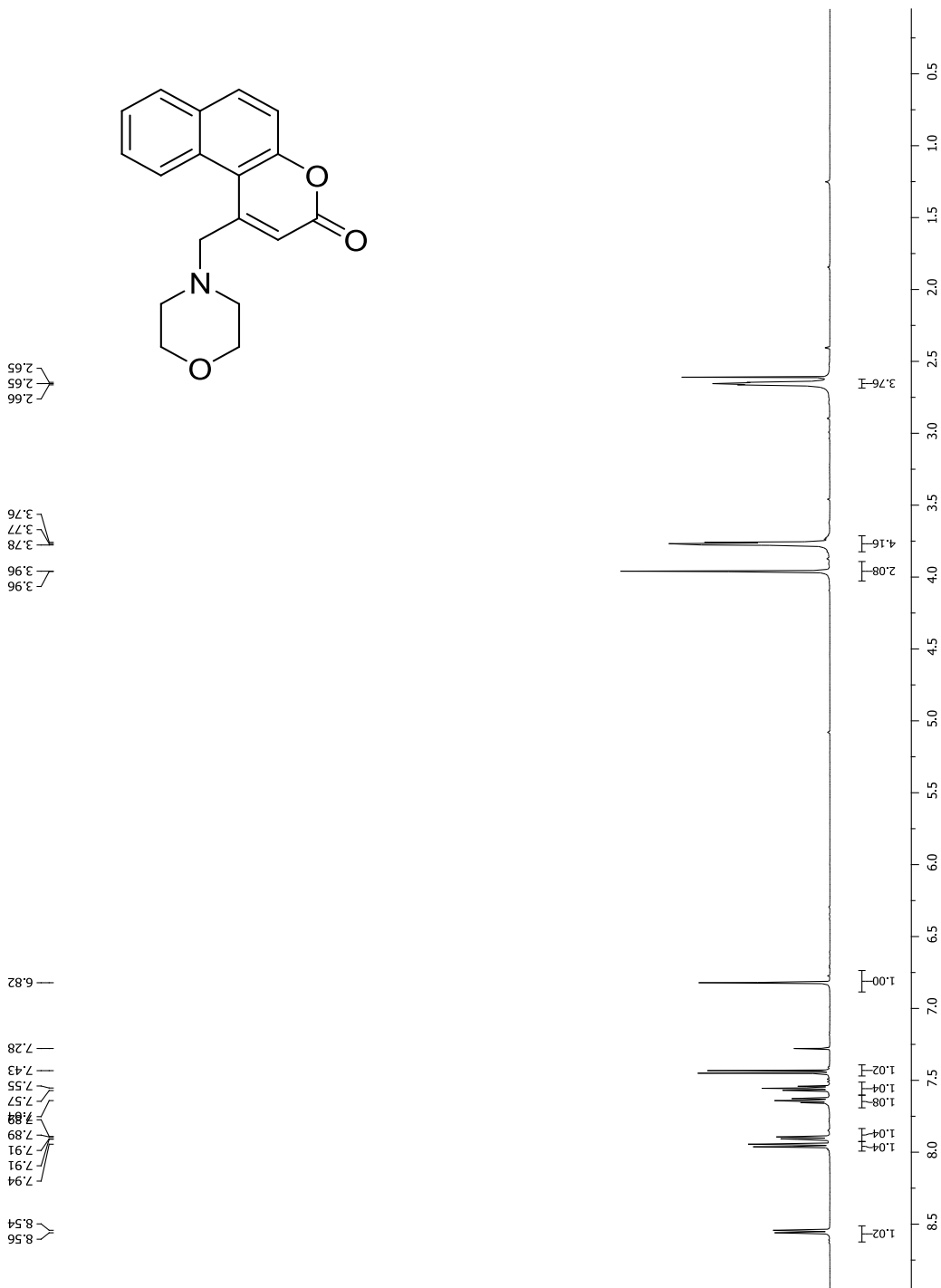
C3A11



C3A11



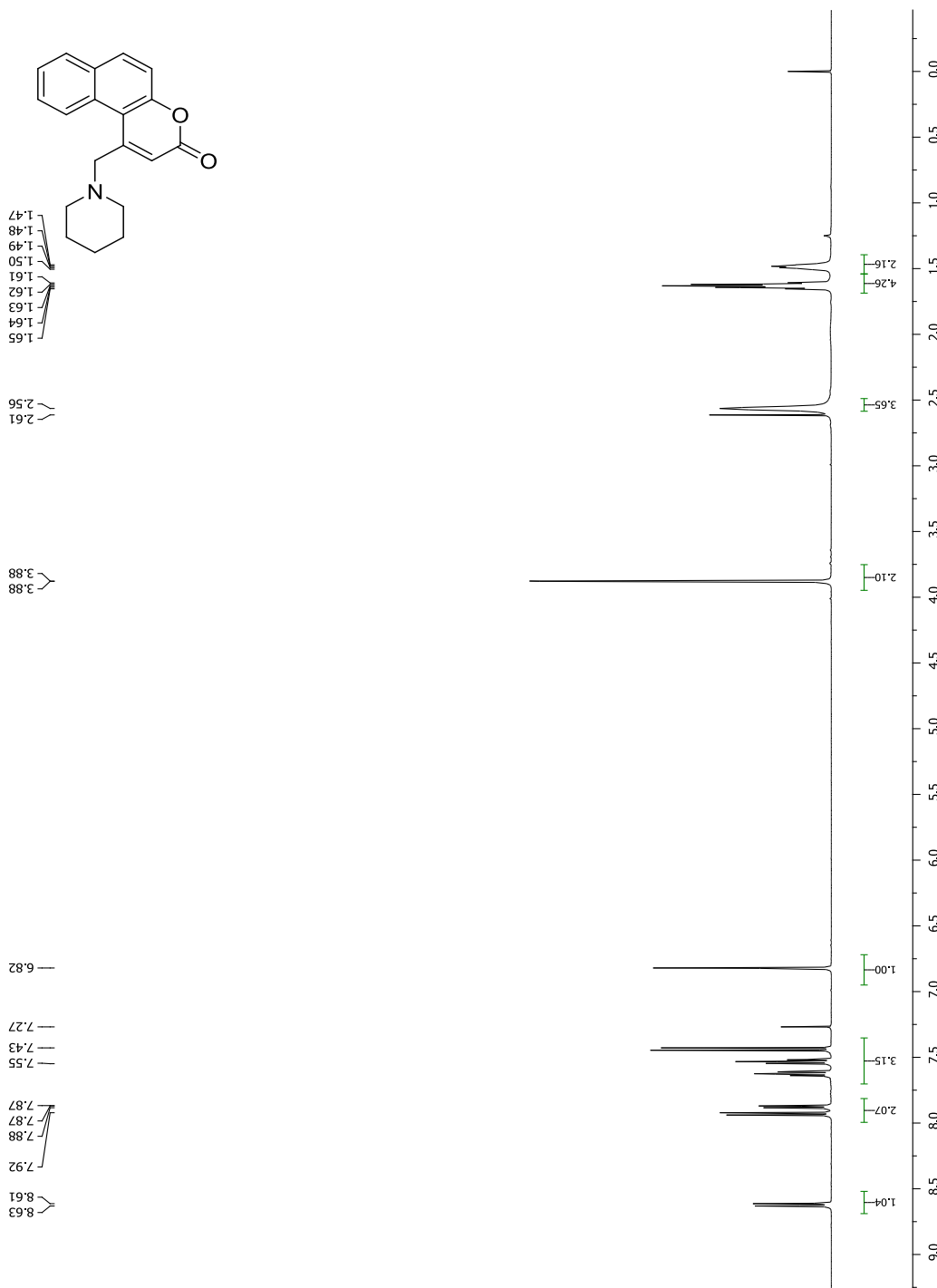
C4A1



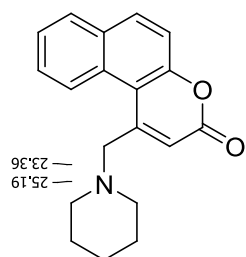
C4A1



C4A2



C4A2



25.19
23.36

53.84

62.84

76.02
76.27
76.53

113.74

115.28

116.89

124.64

125.79

126.81

128.49

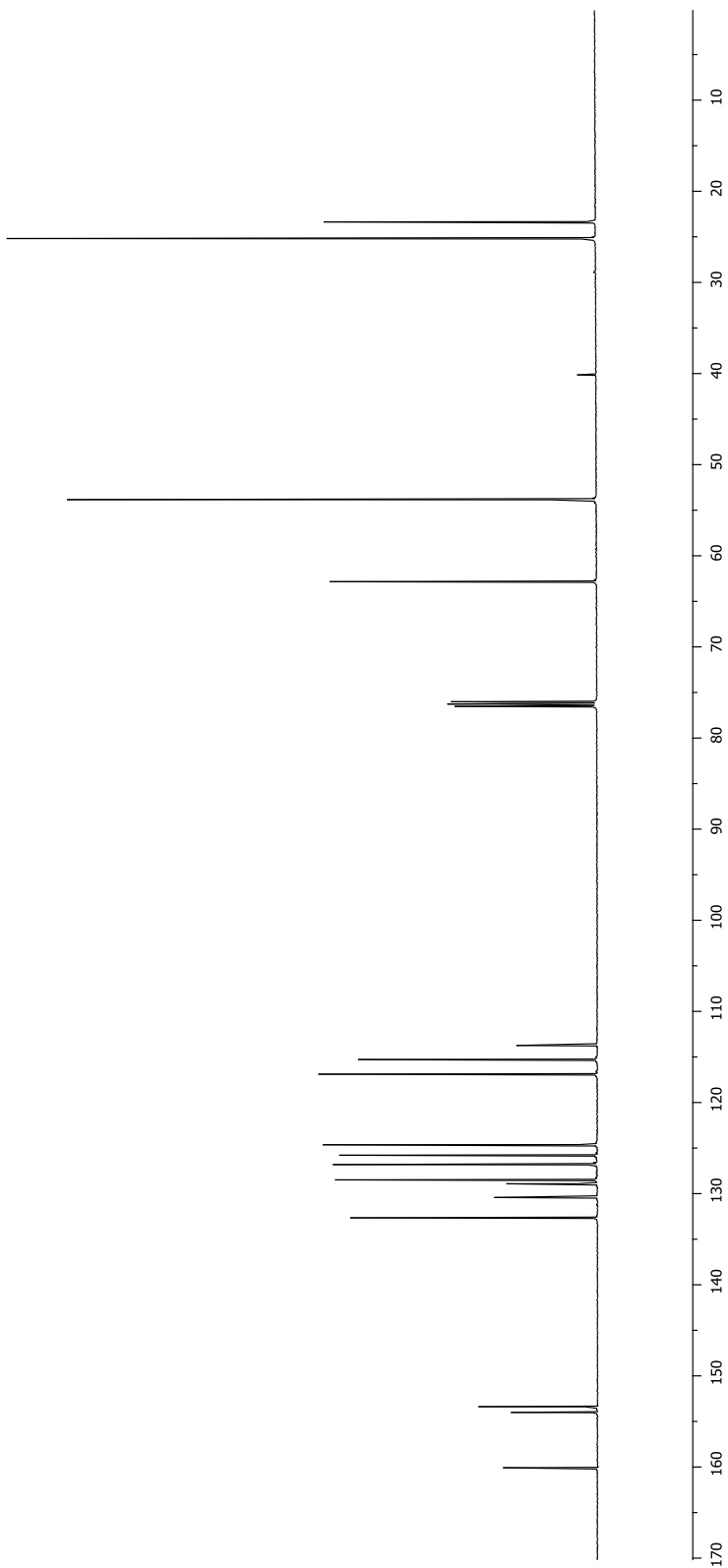
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132.65

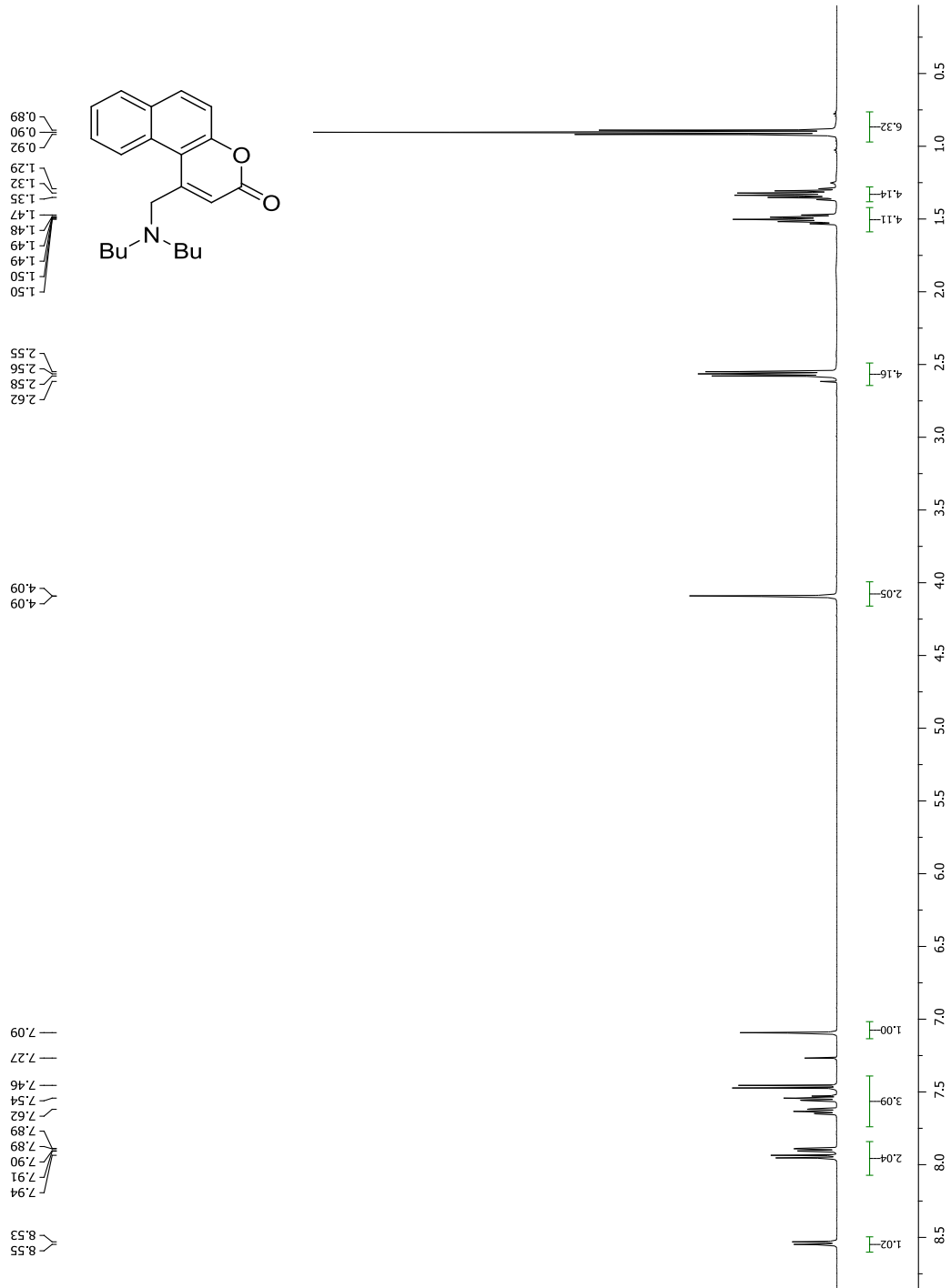
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154.01

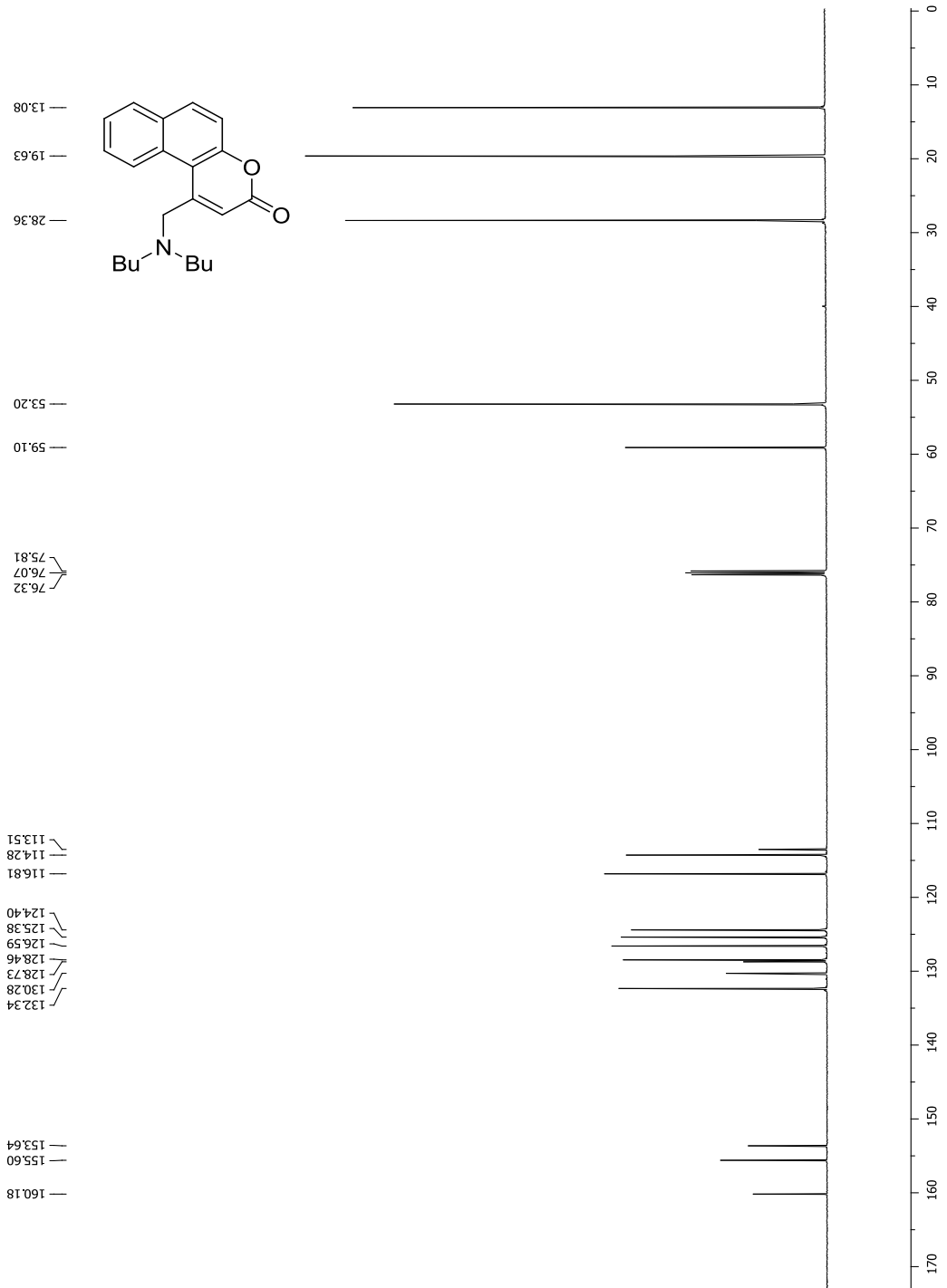
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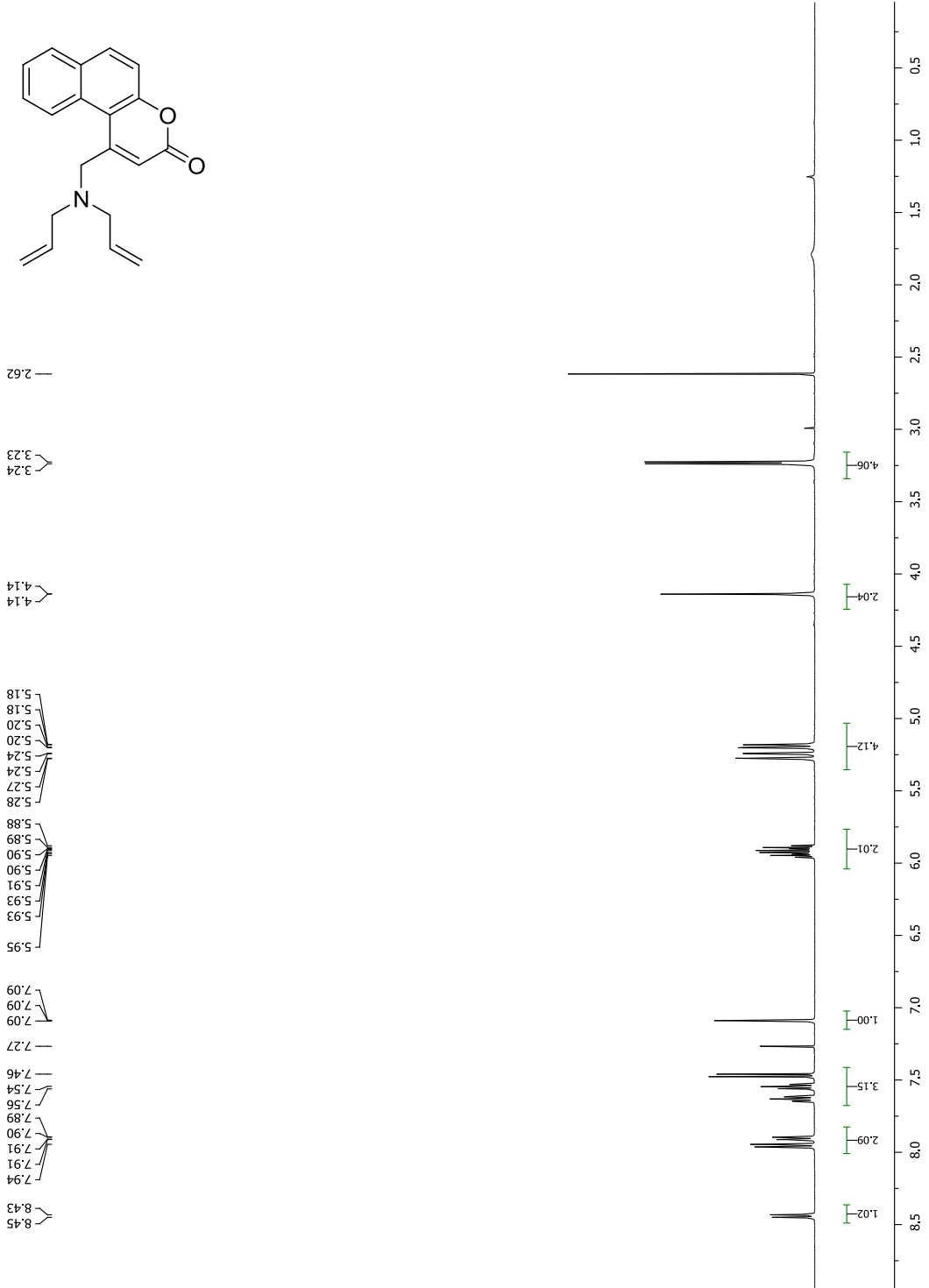
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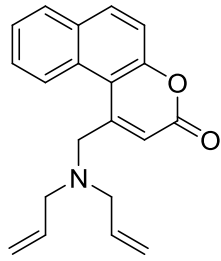
C4A3



C4A4



C4A4

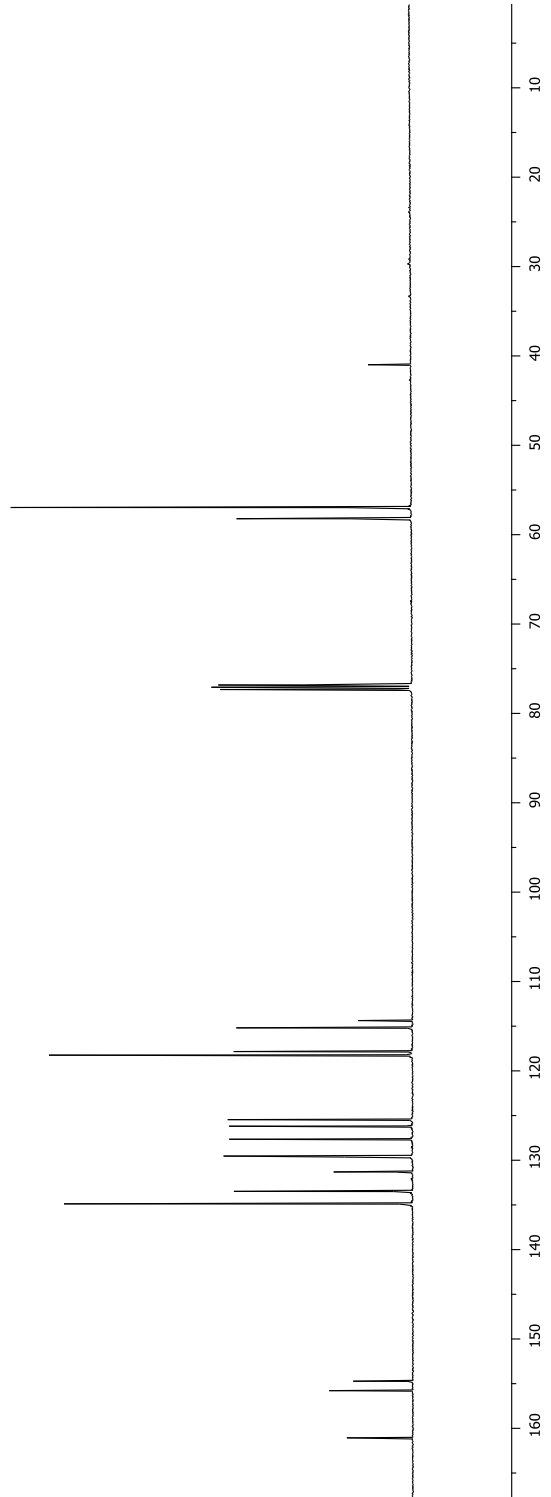


58.22
56.96

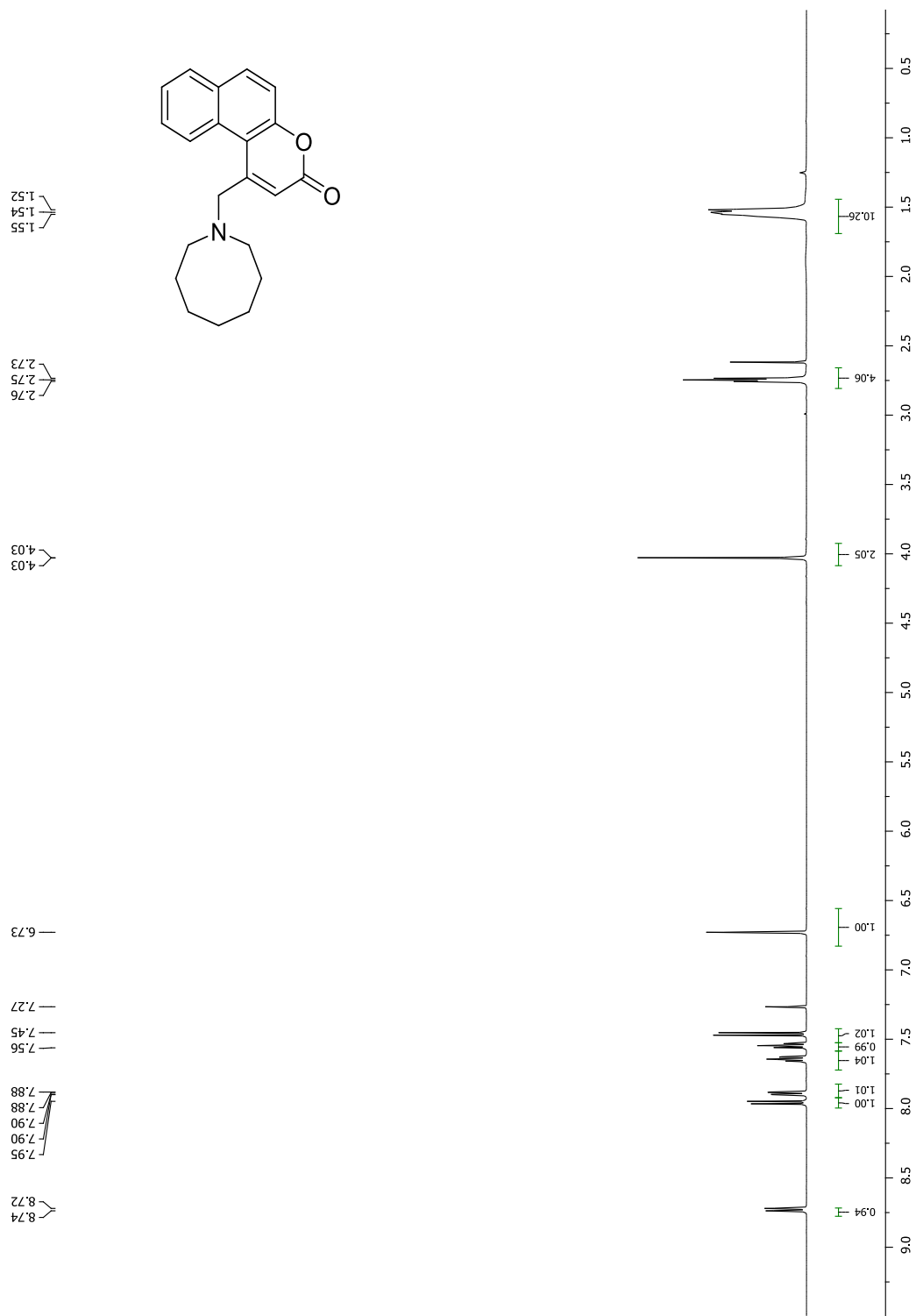
77.33
77.07
76.82

134.88
133.99
133.99
129.53
127.65
126.19
125.45
118.24
117.83
115.18
114.37

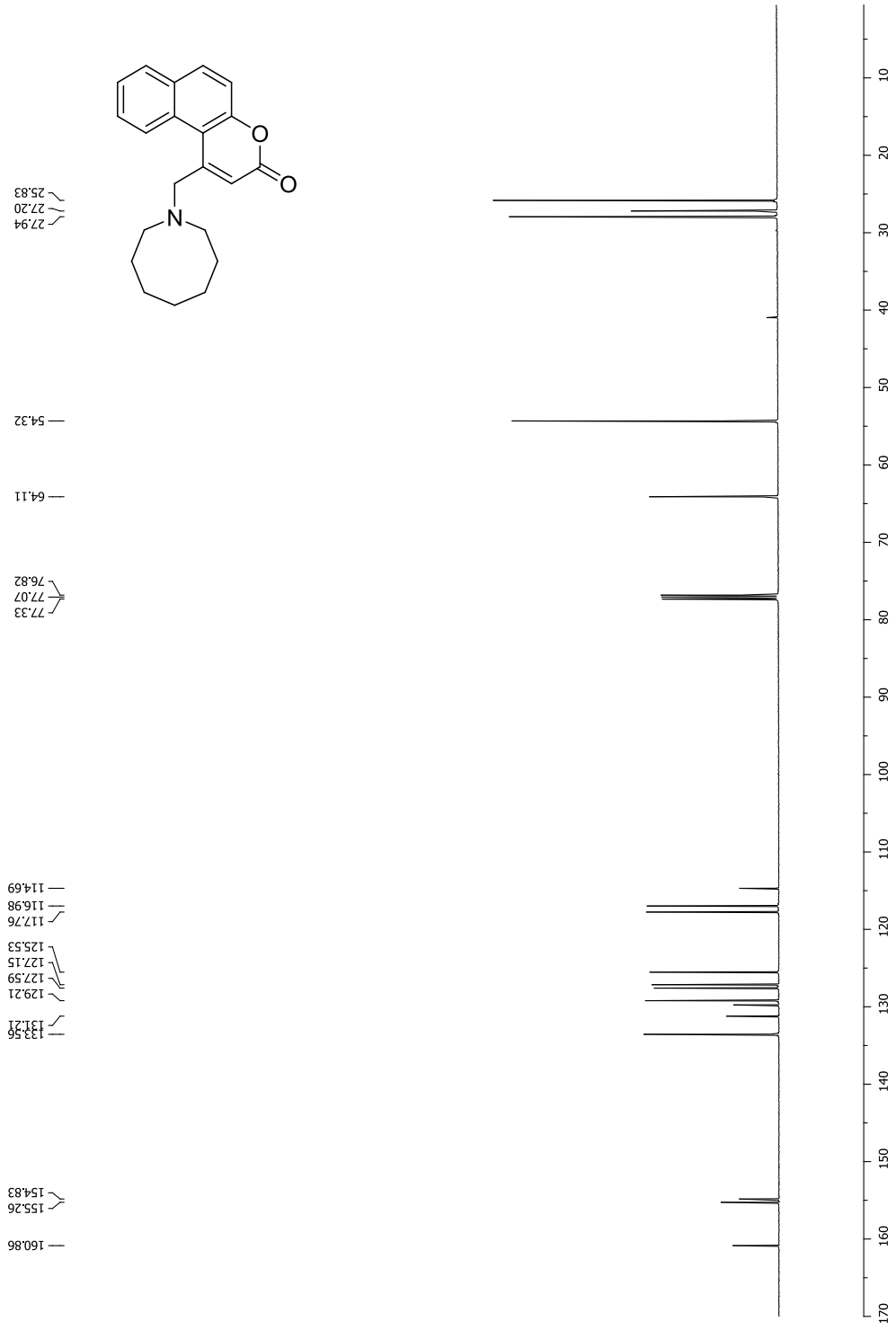
161.06
155.78
154.73



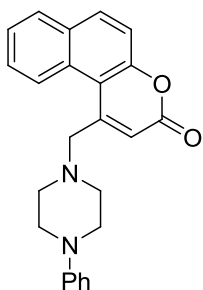
C4A14



C4A14



C4A16



2.83
2.82
2.81

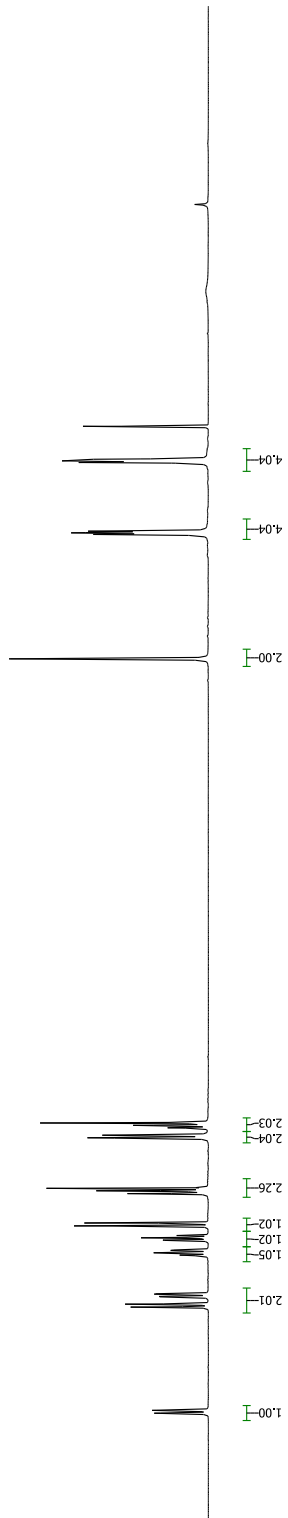
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4.02

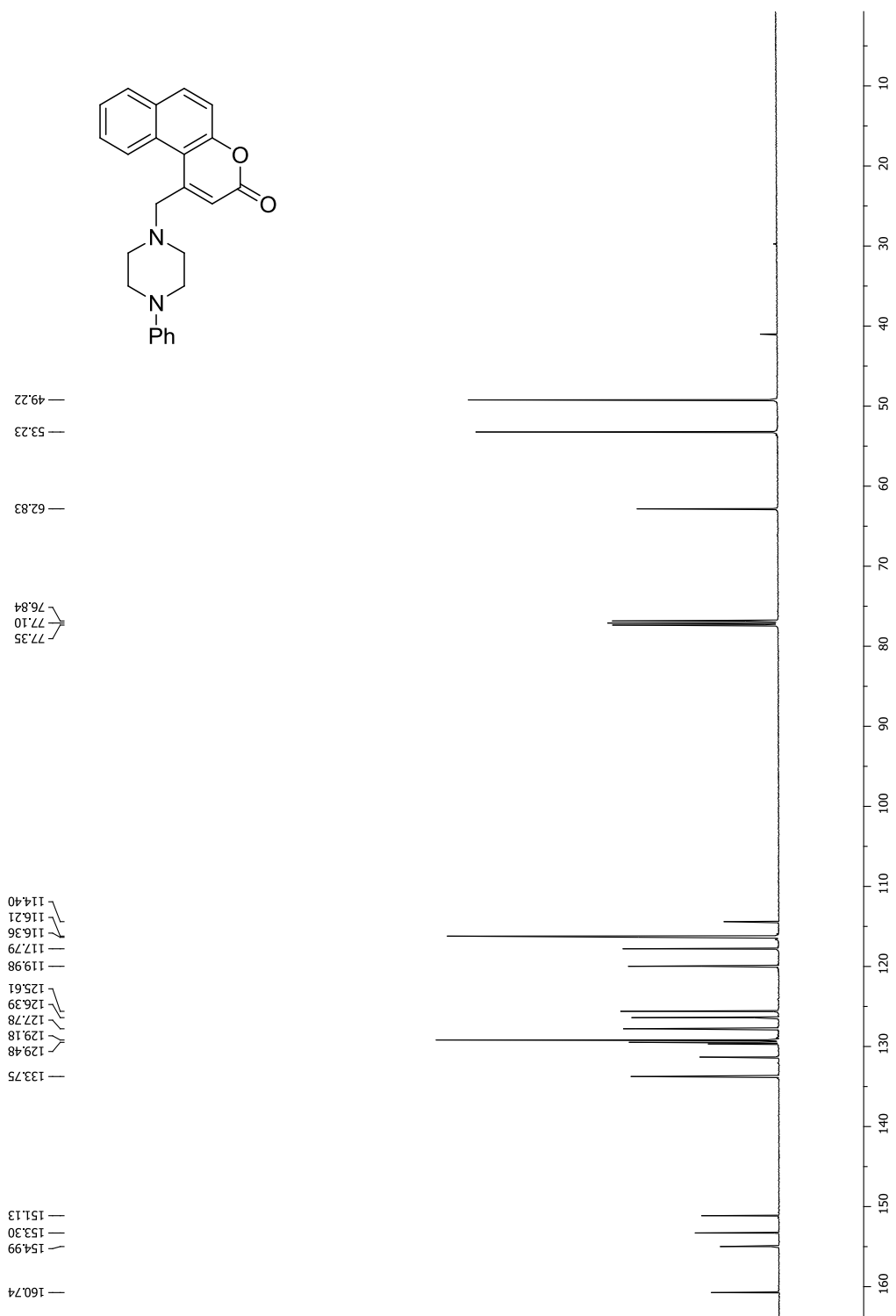
6.94
6.94
6.93
6.88
6.88
6.87
6.87
6.85

7.25
7.46
7.55
7.63
7.63
7.89
7.90
7.91
7.91
7.96

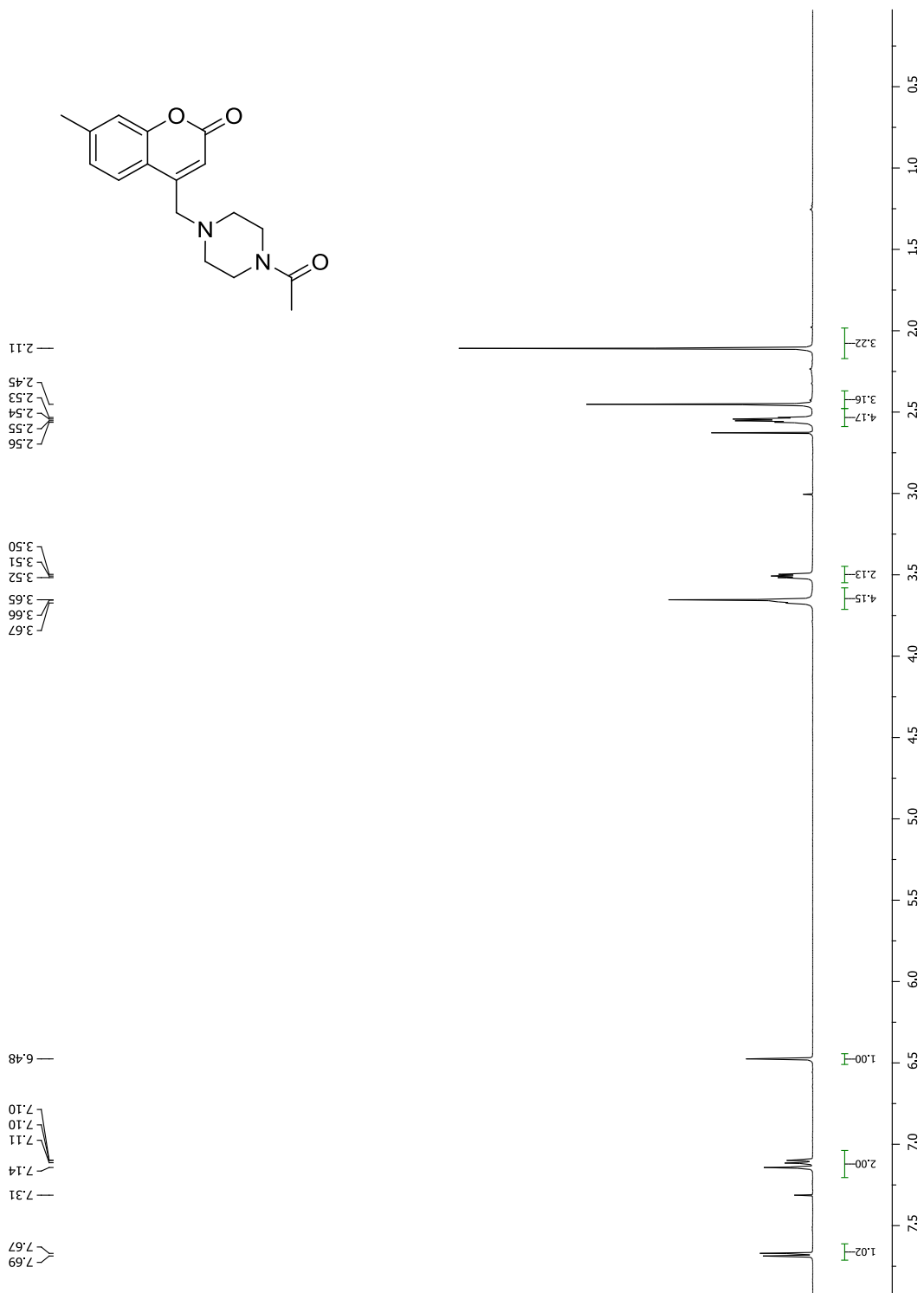
8.60
8.62



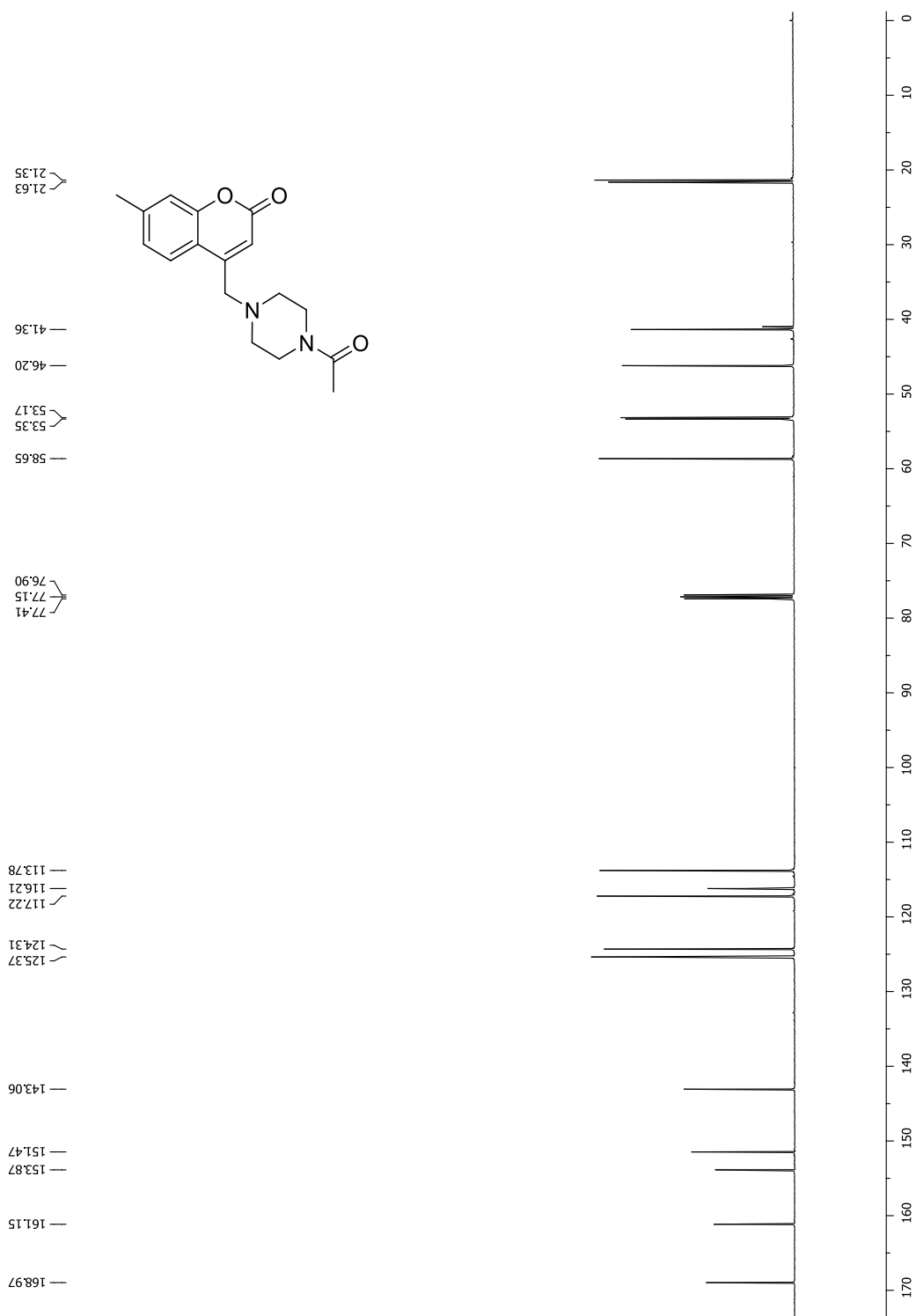
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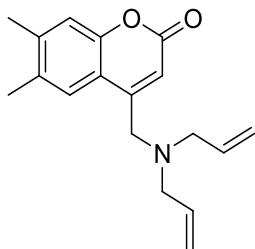
C5A11



C5A11



C6A4



2.33
2.31

3.17
3.16

3.69
3.69

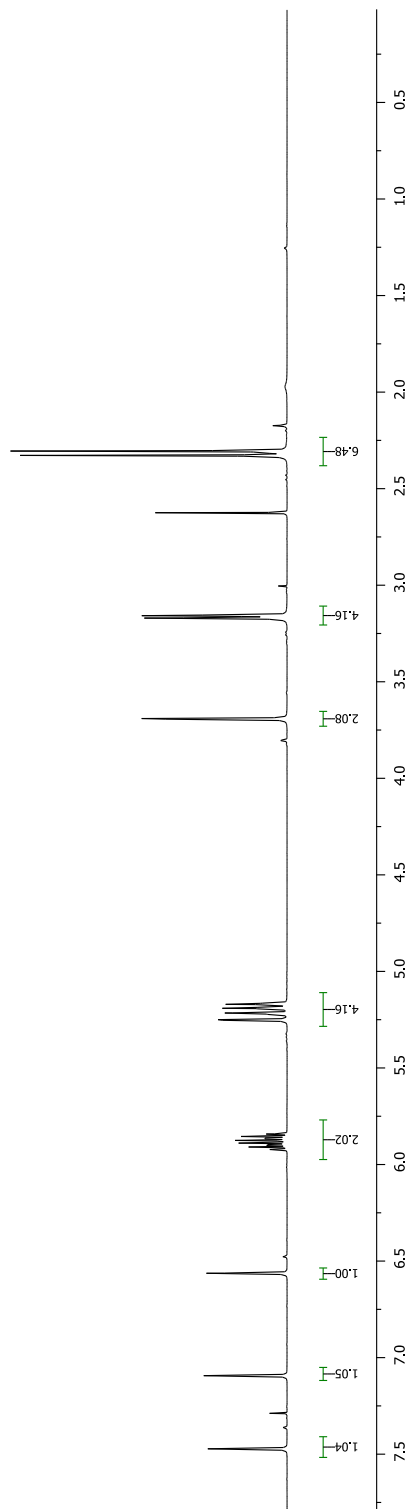
5.17
5.17
5.19
5.19
5.19
5.22
5.22
5.25
5.25

5.84
5.85
5.86
5.87
5.88
5.89

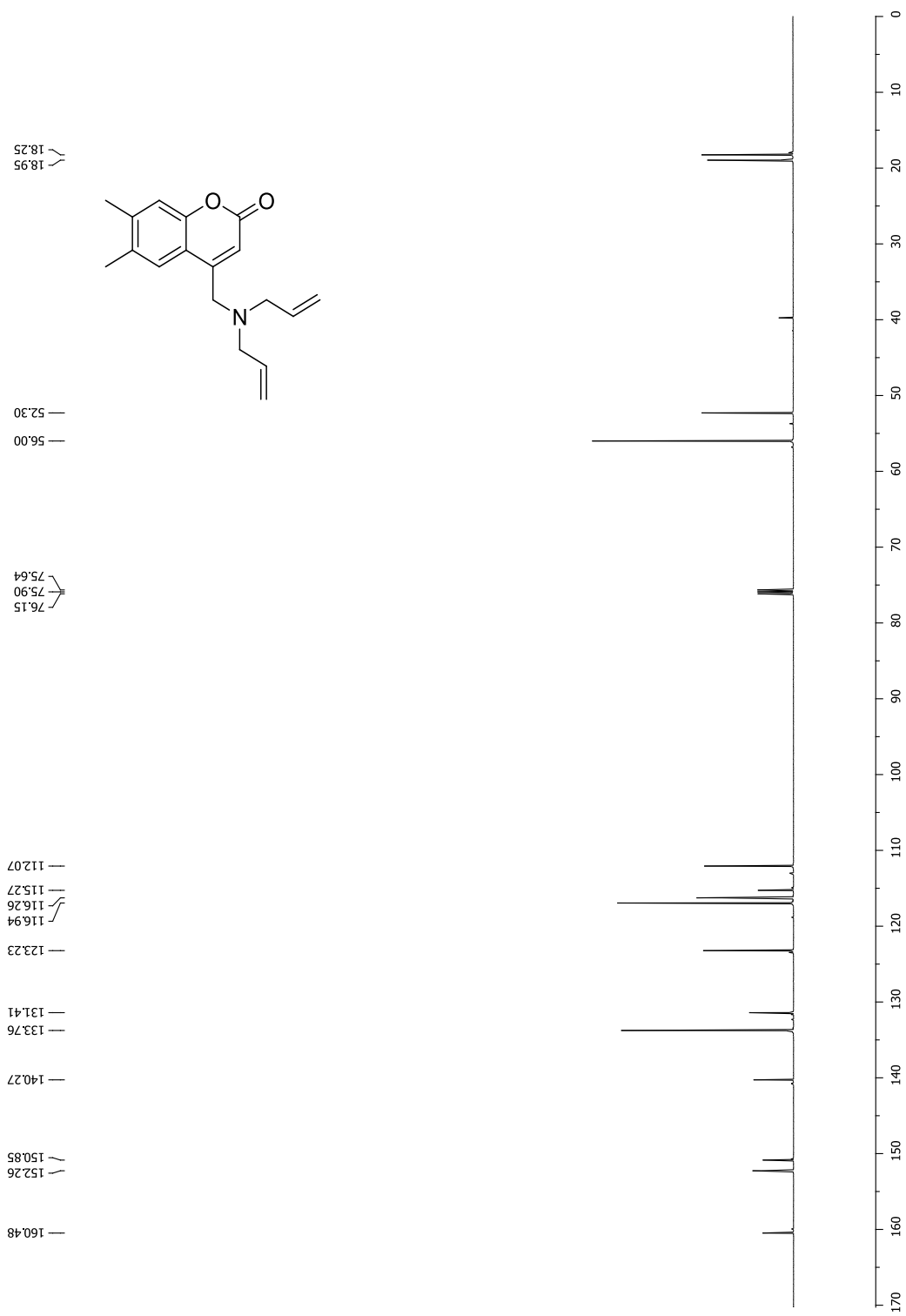
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6.56

7.09

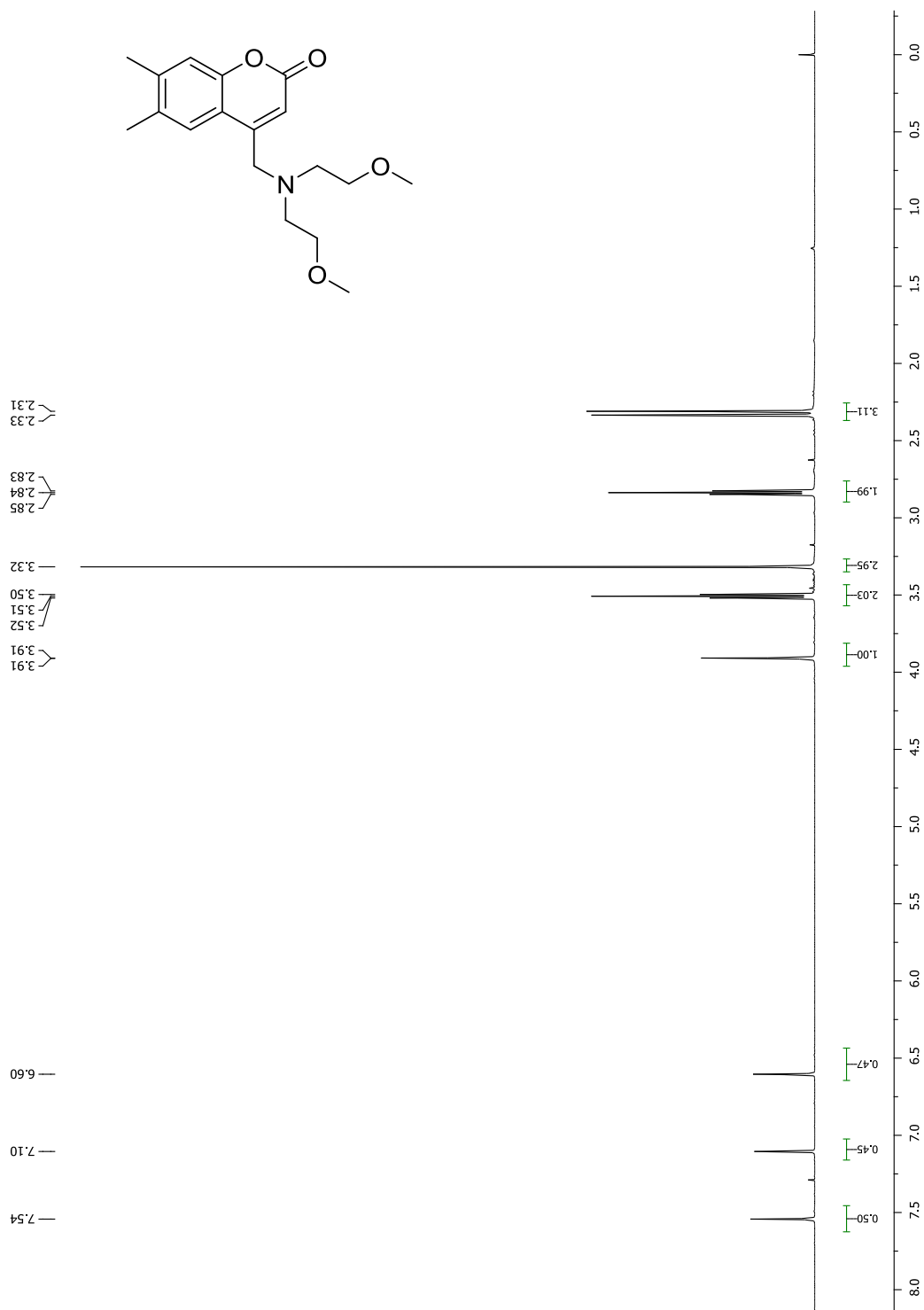
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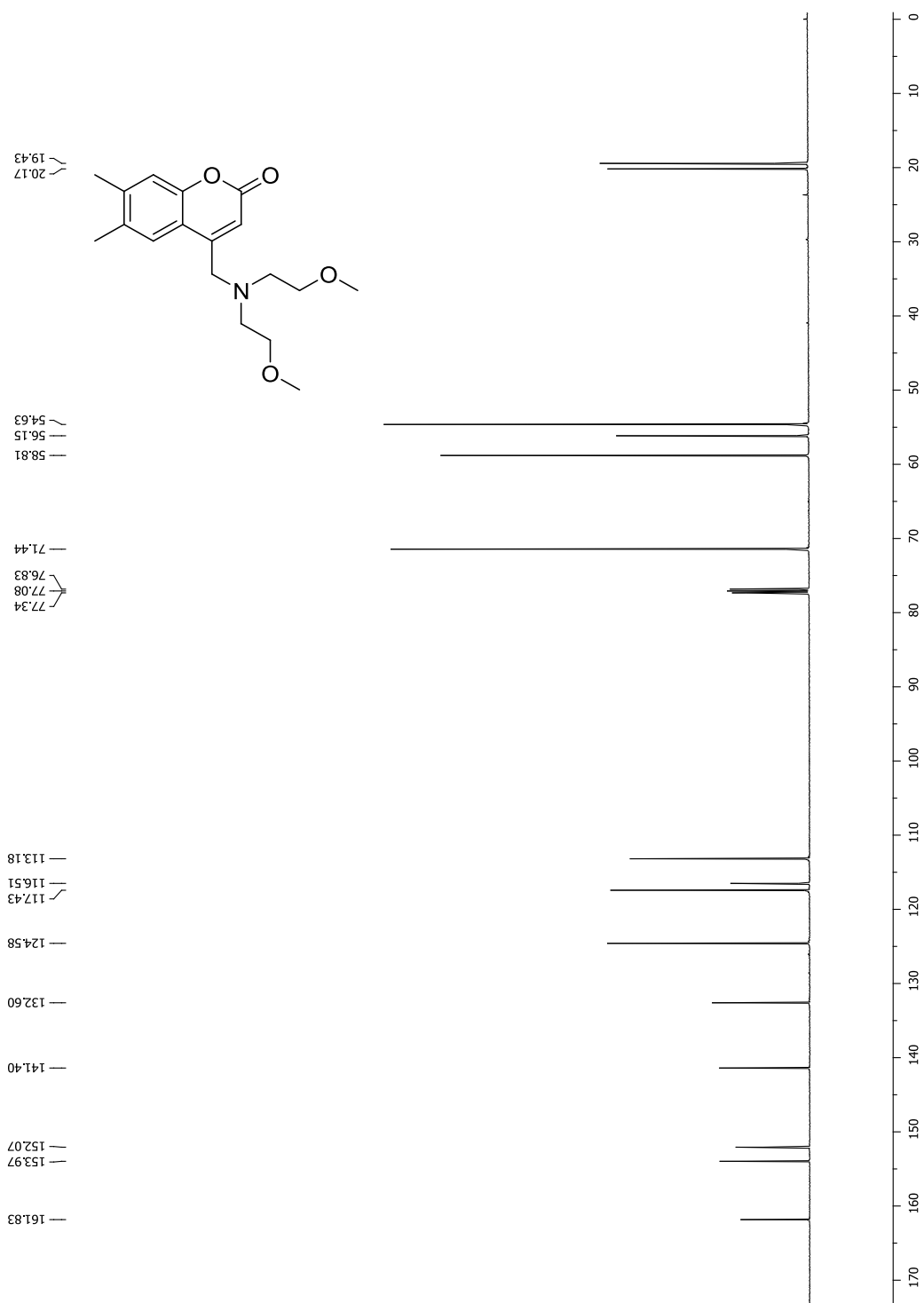
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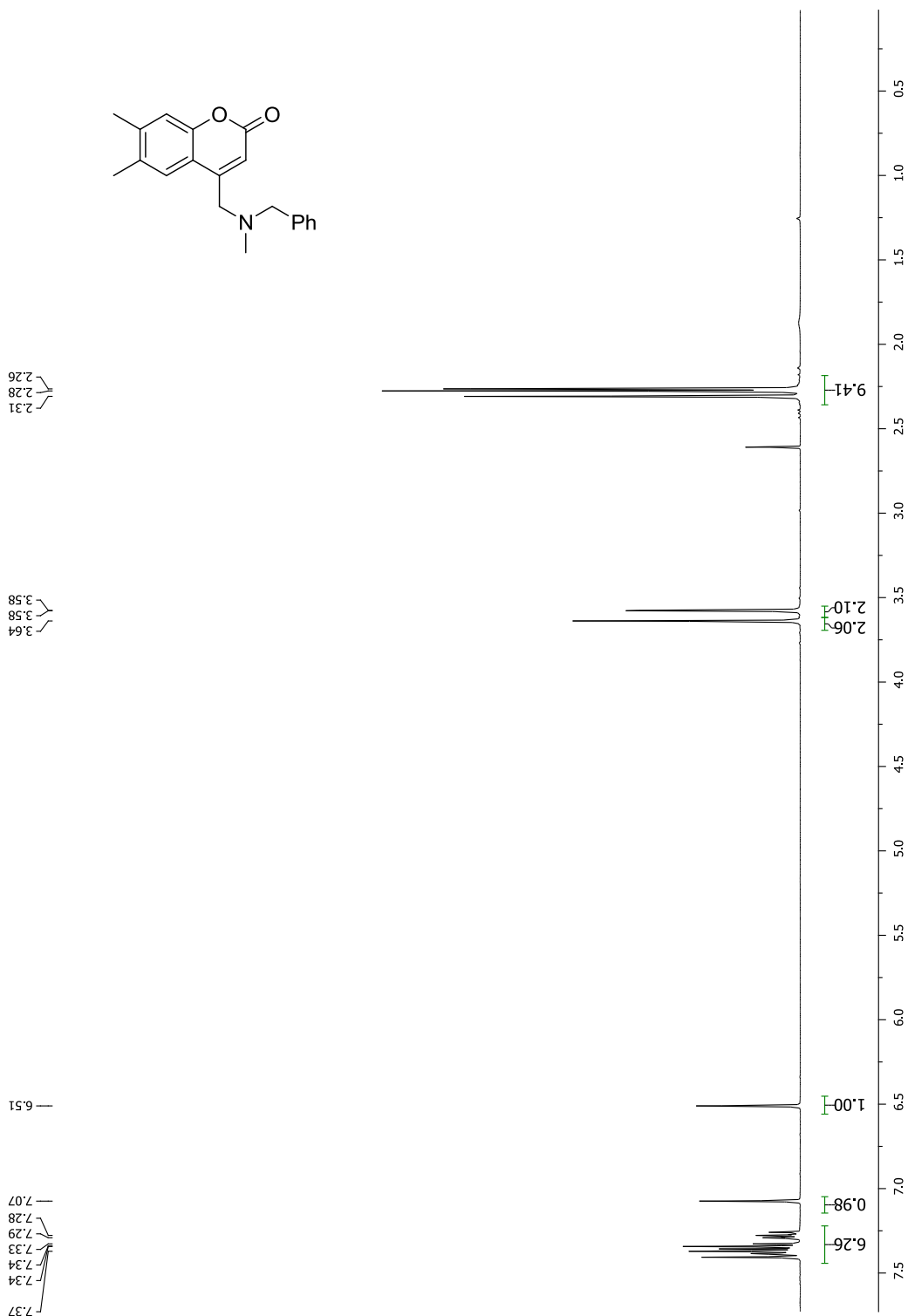
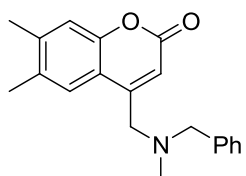
C6A6



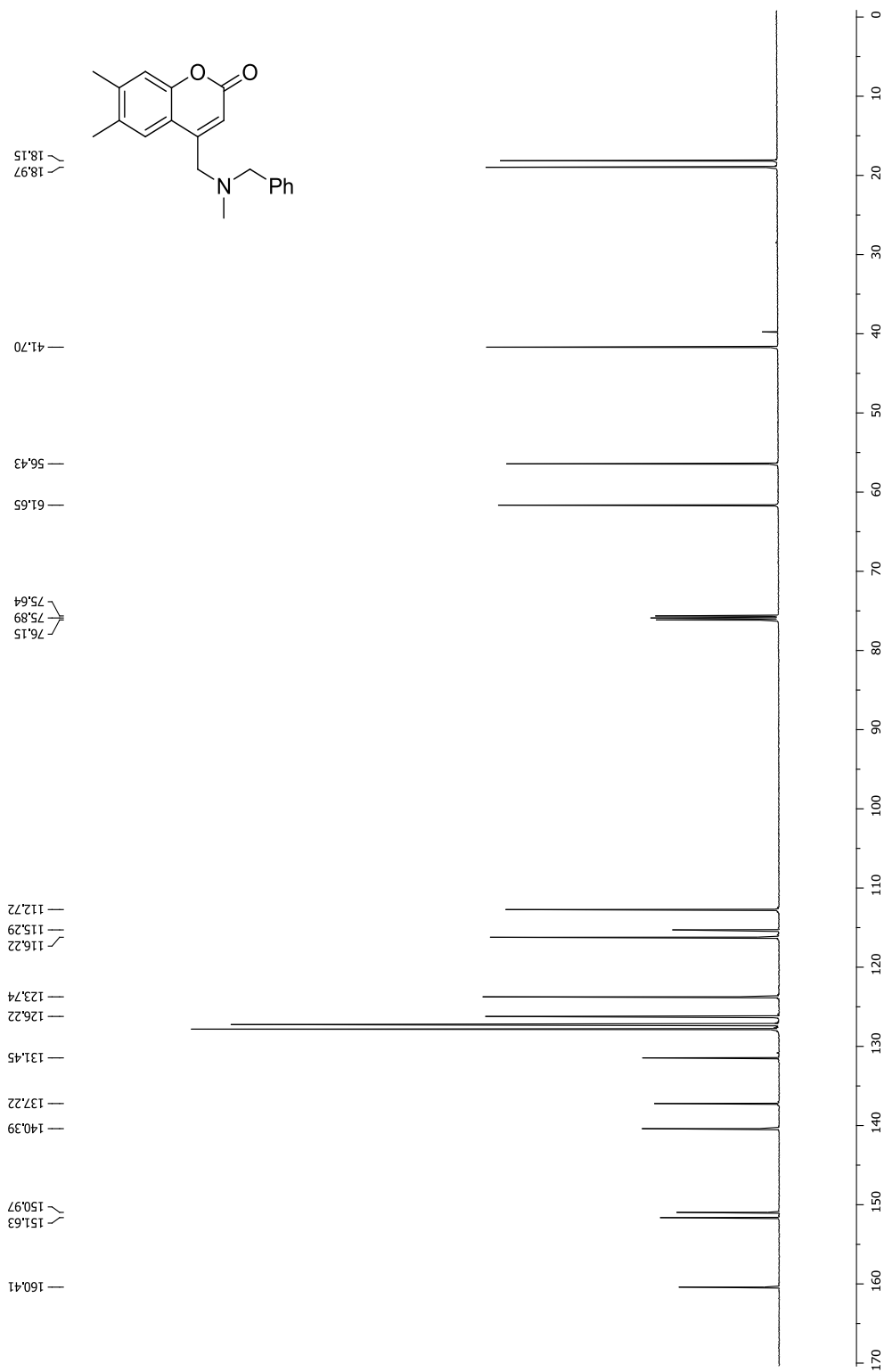
C6A6



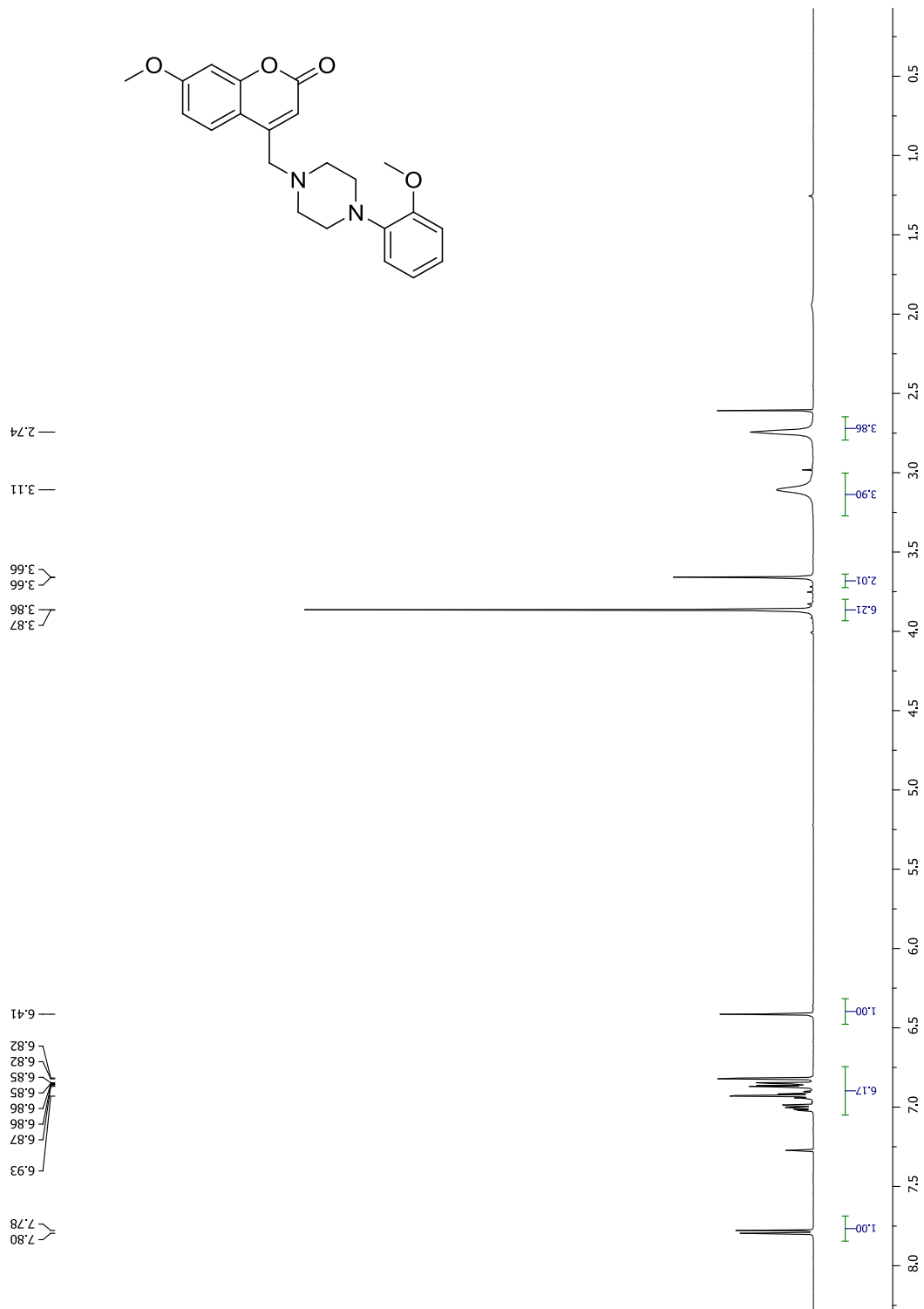
C6A13



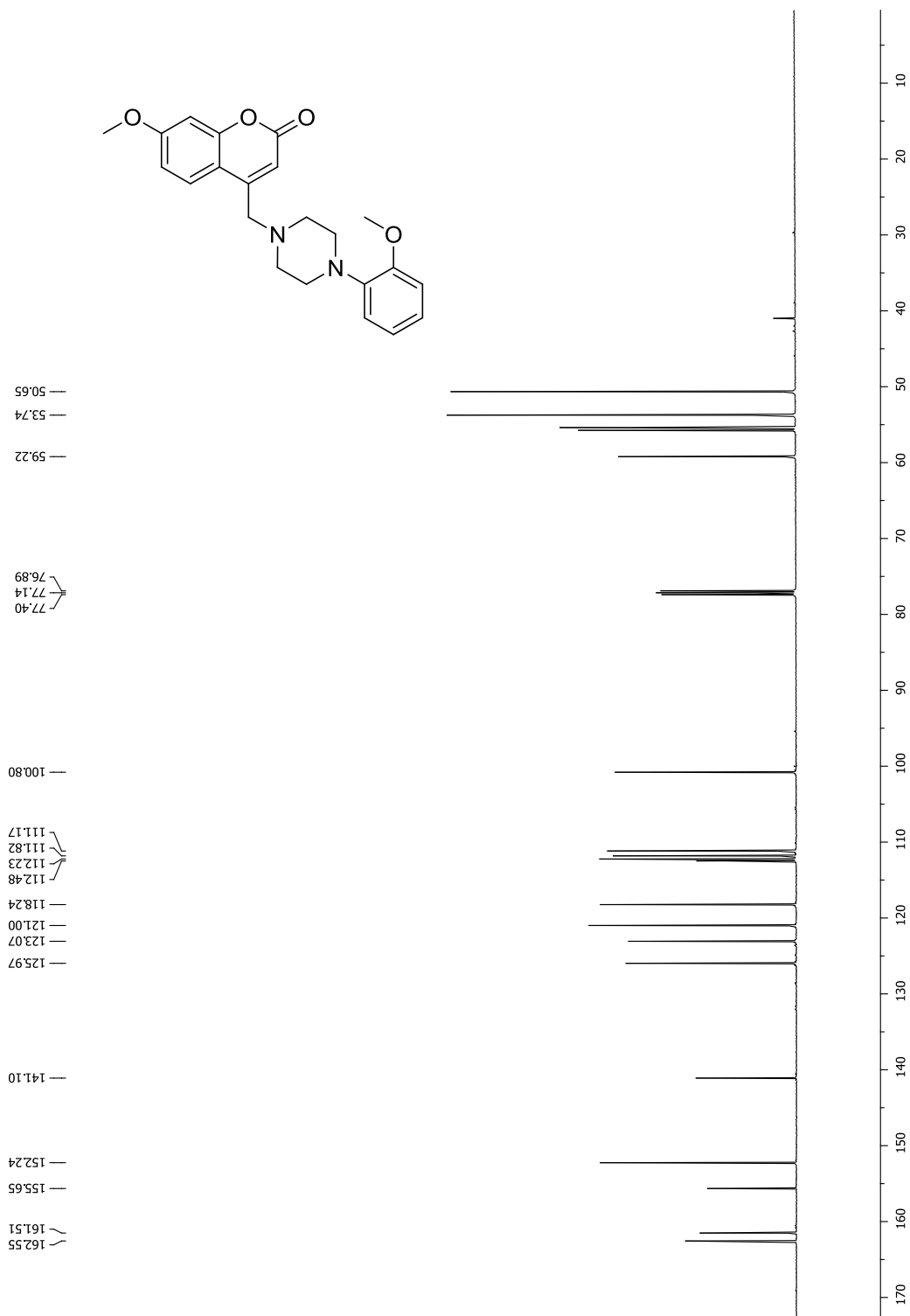
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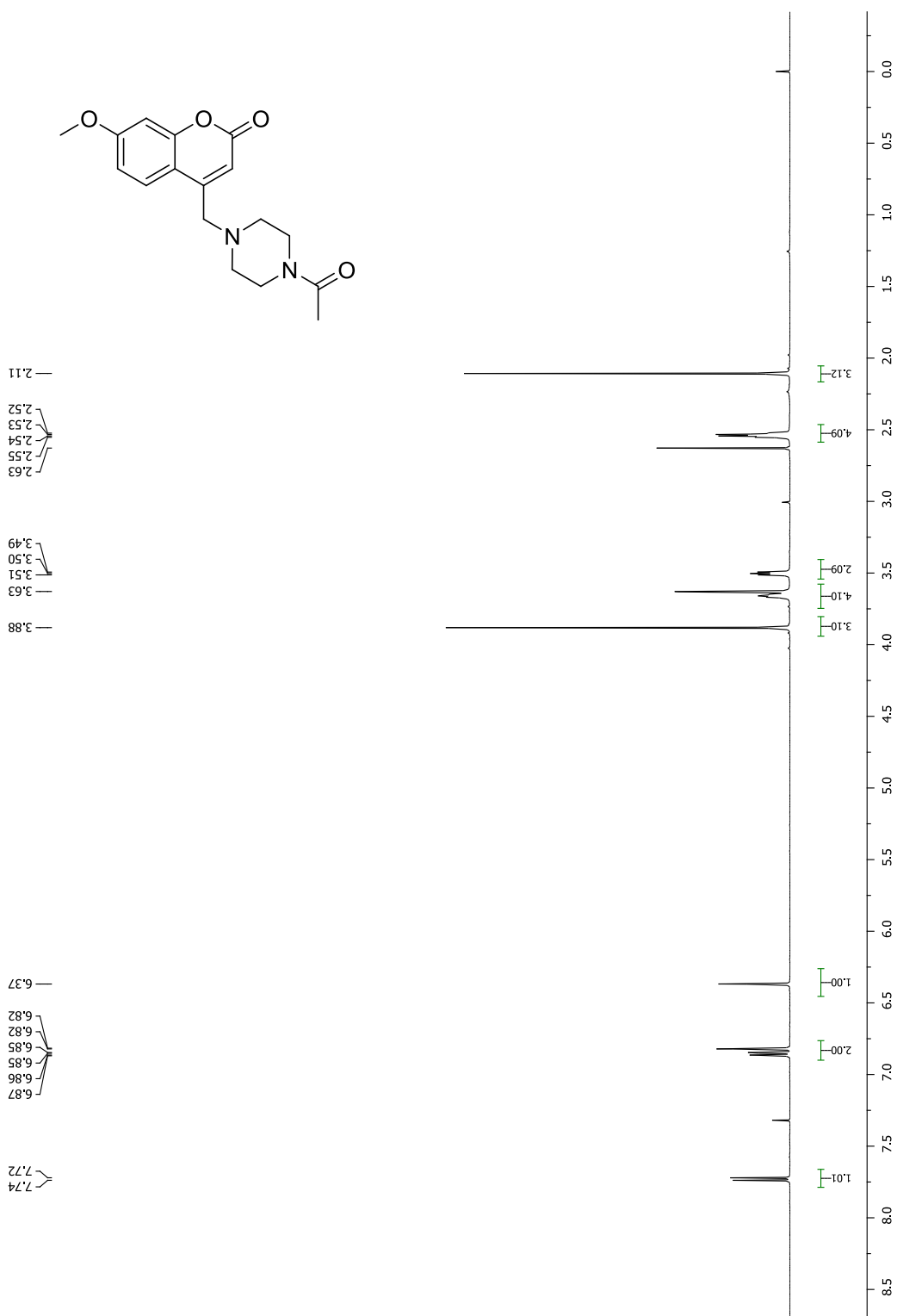
C7A9



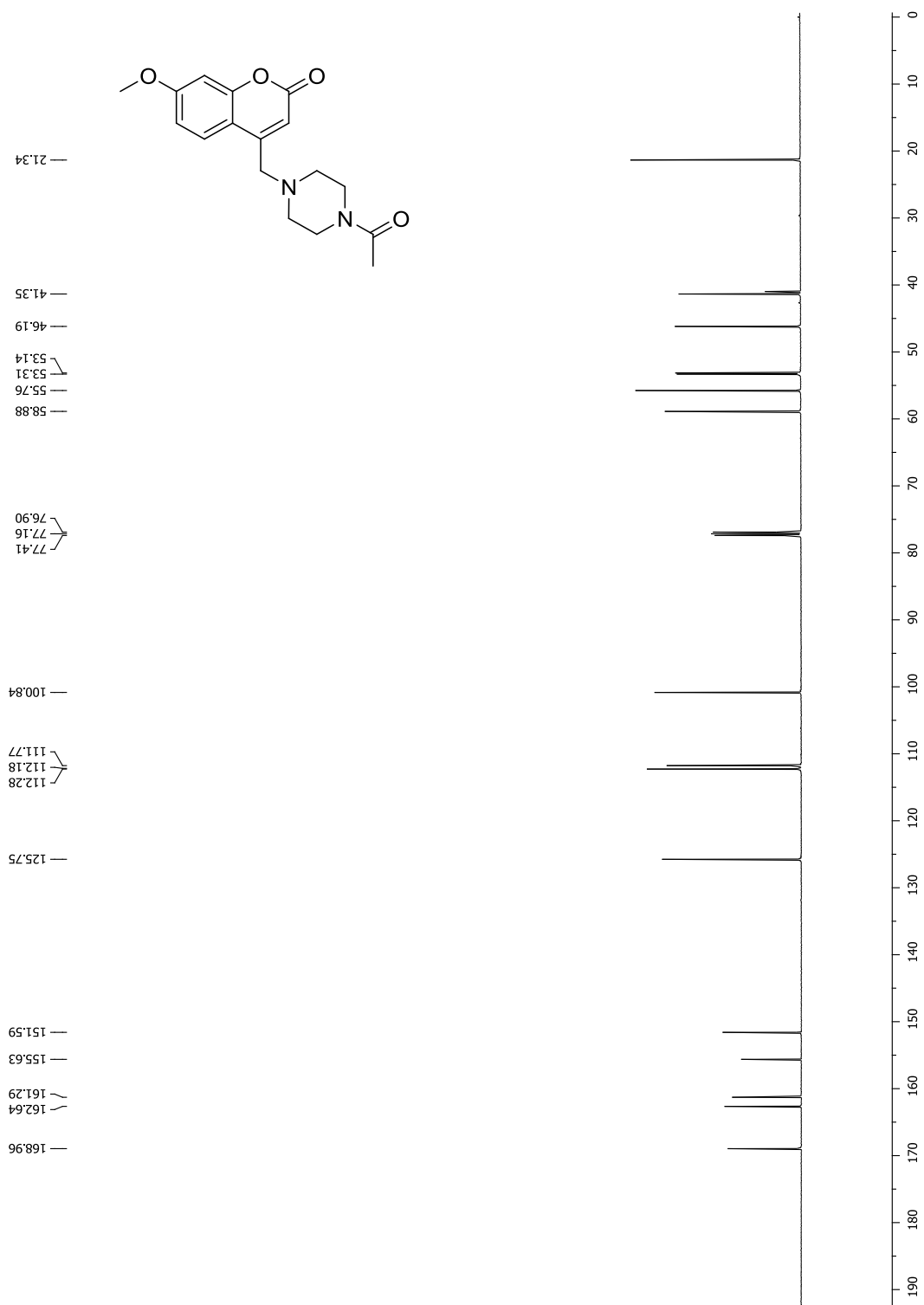
C7A9



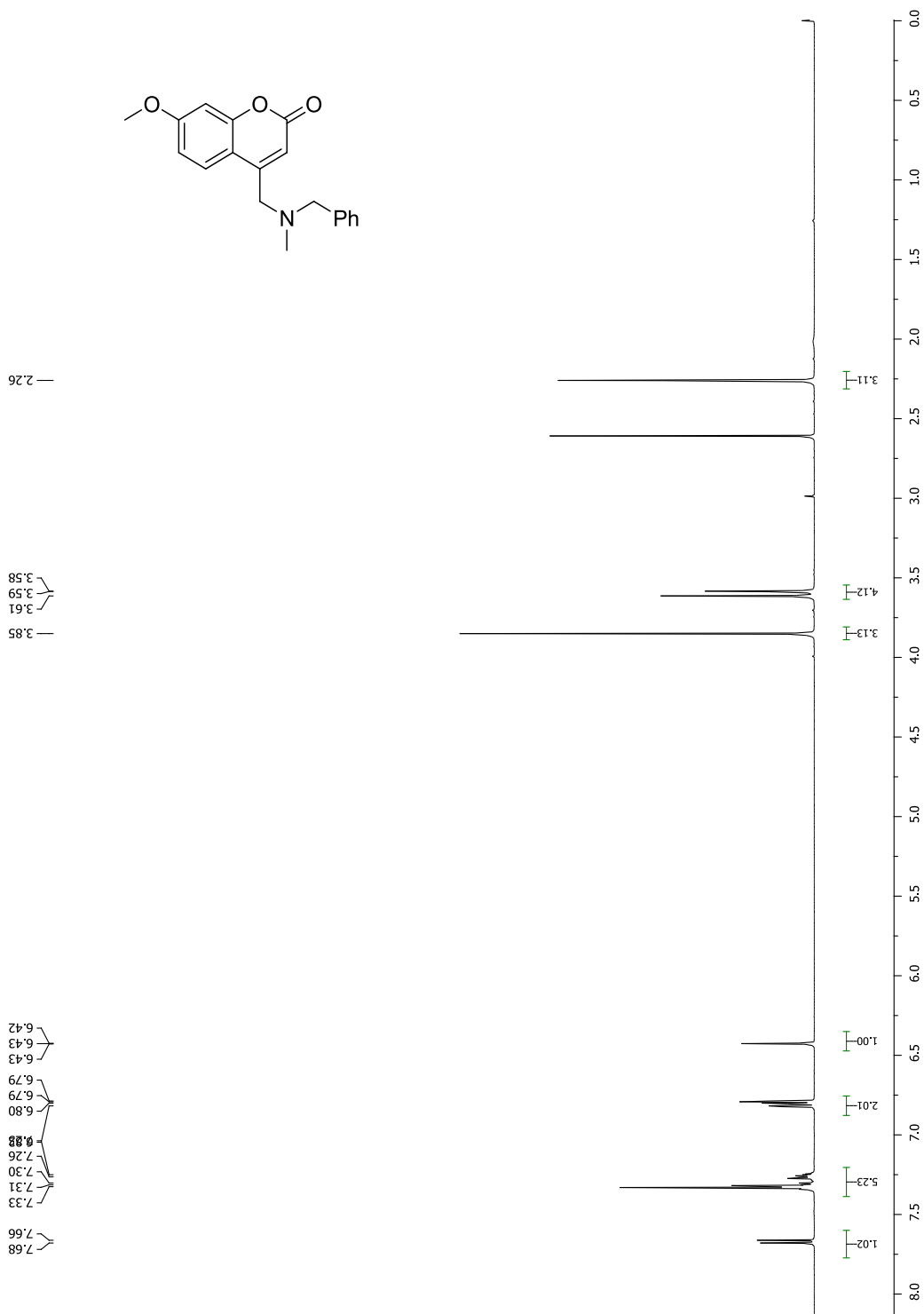
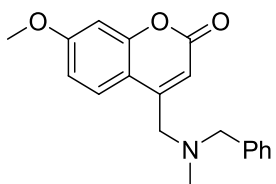
C7A11



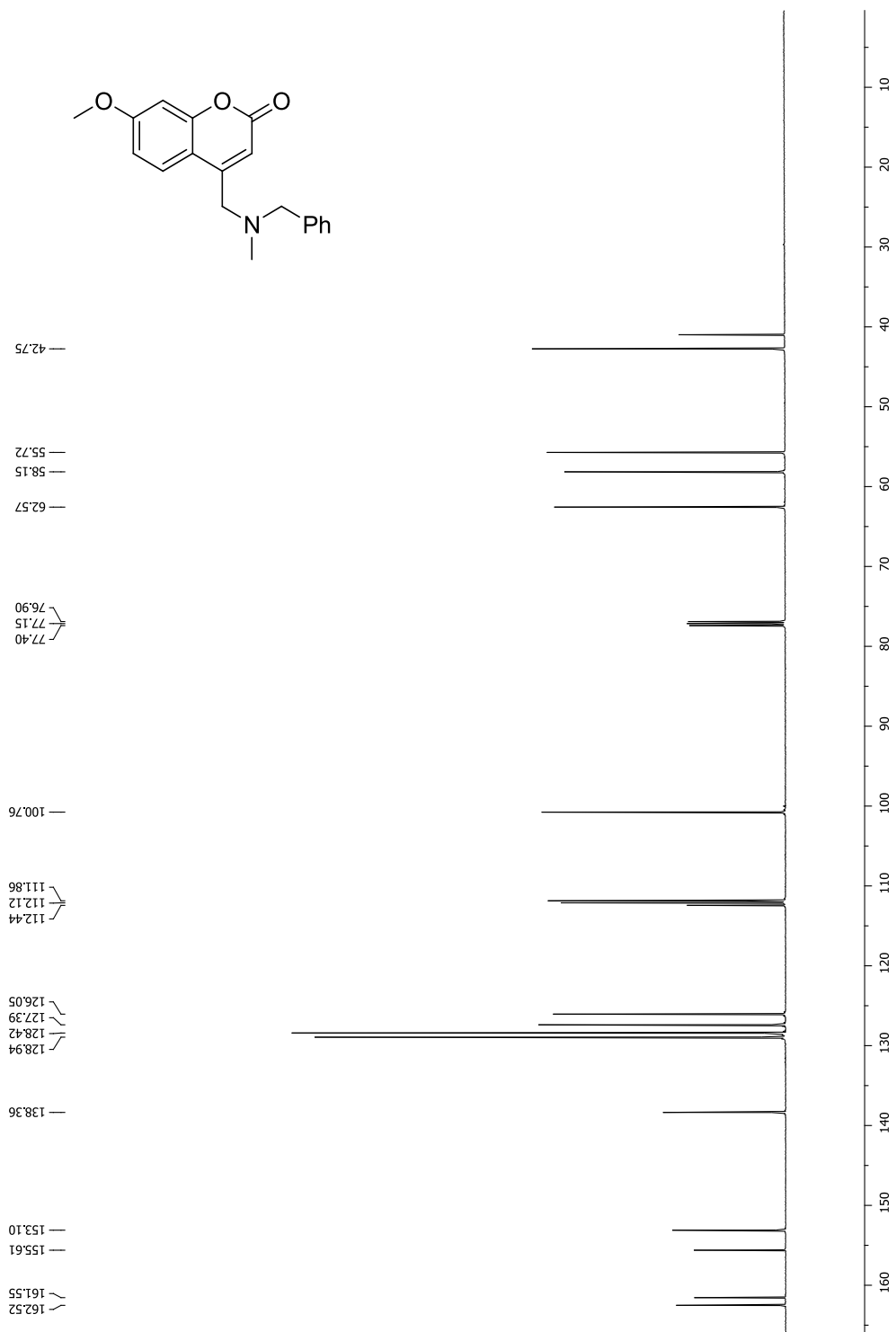
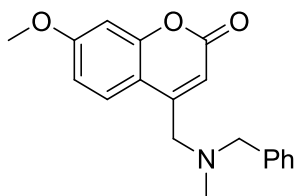
C7A11



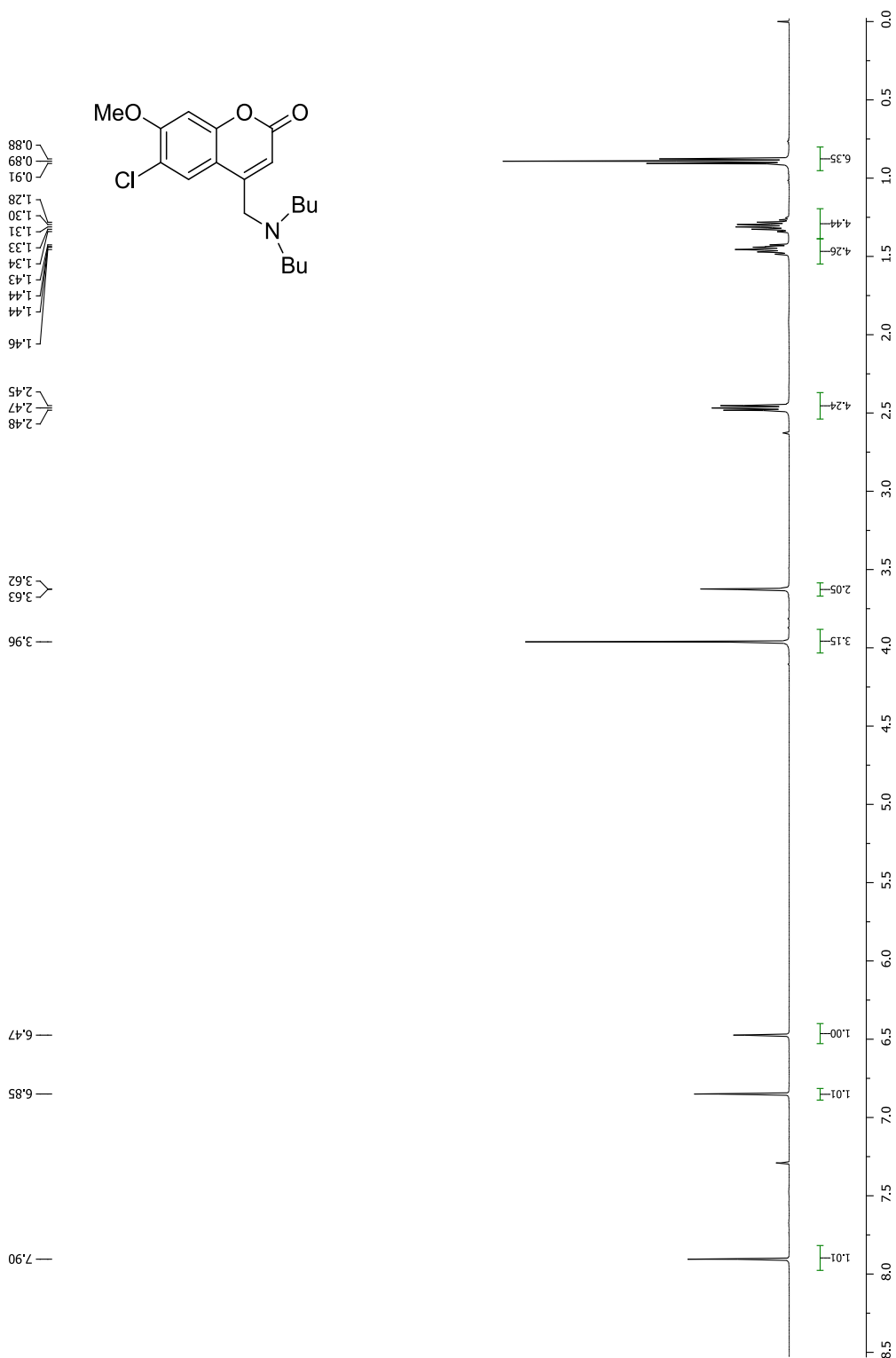
C7A13



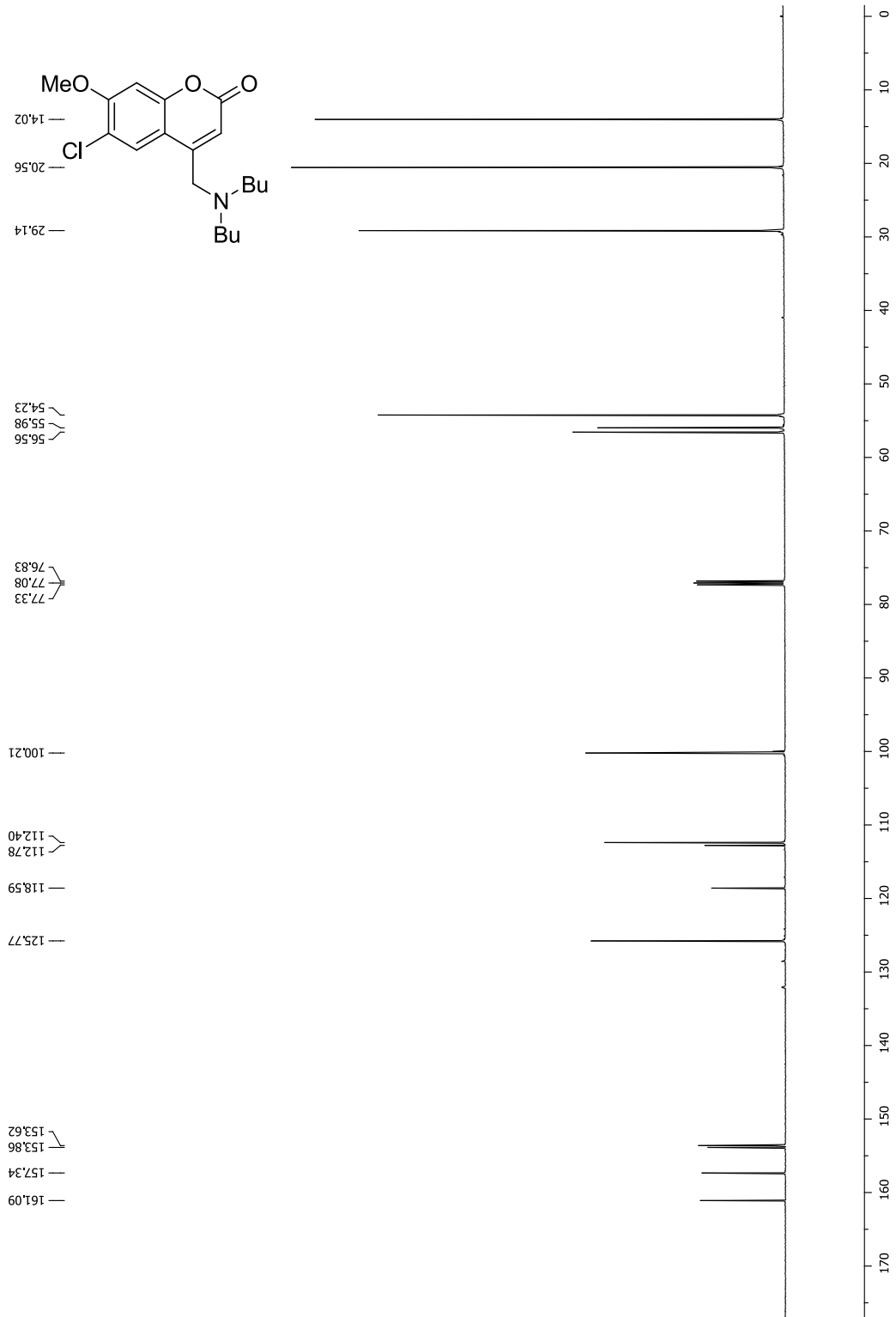
C7A13



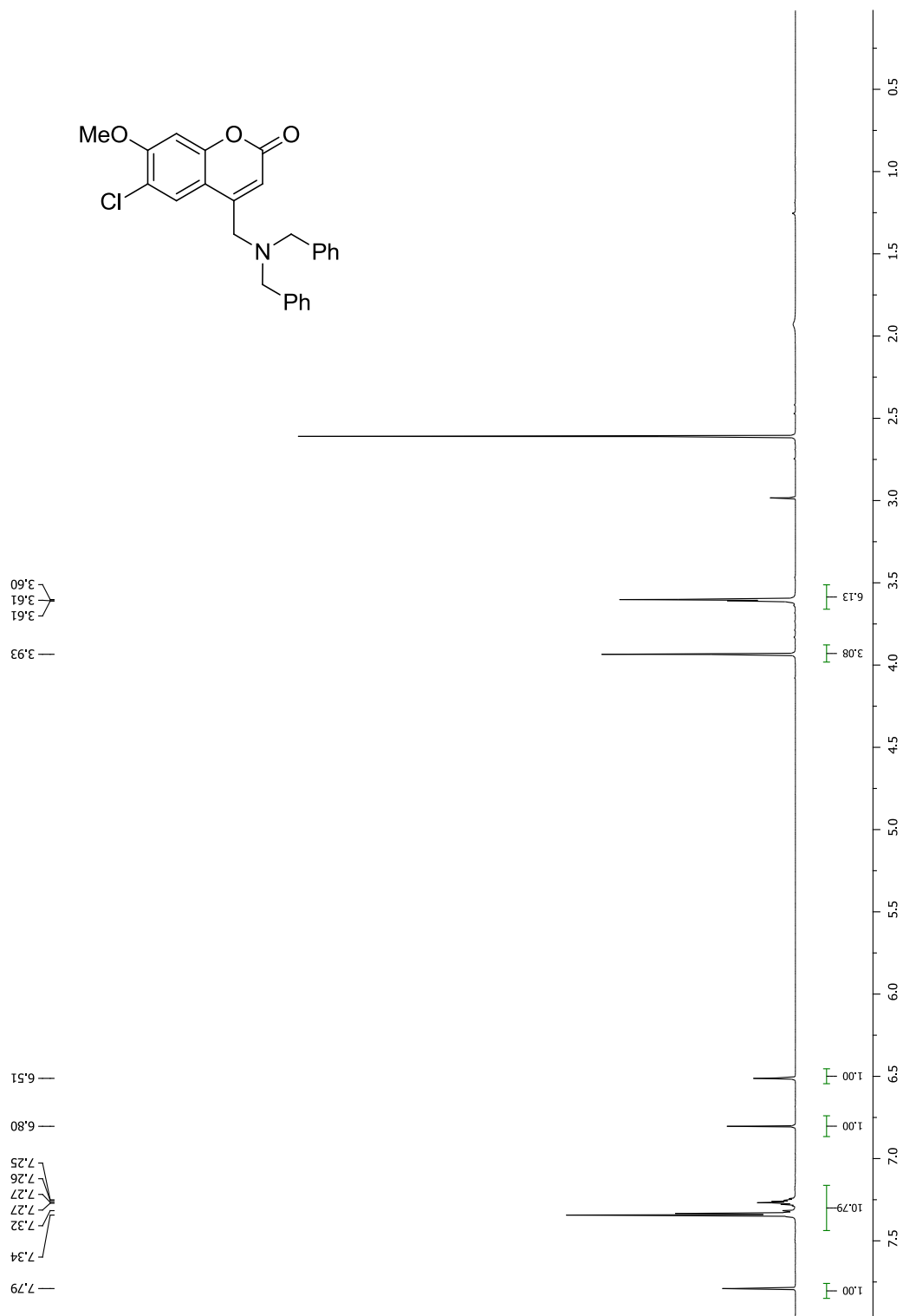
C8A3



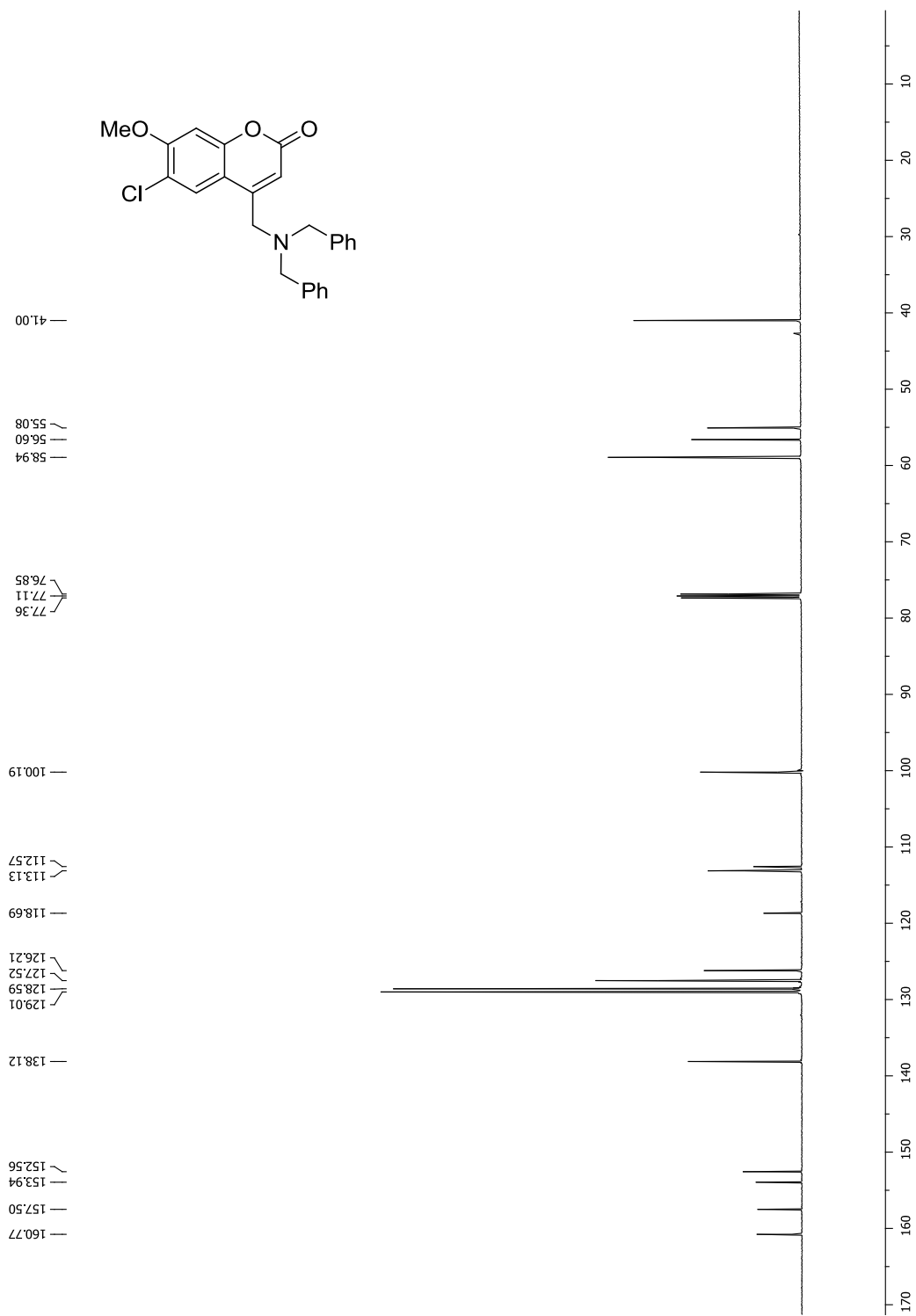
C8A3



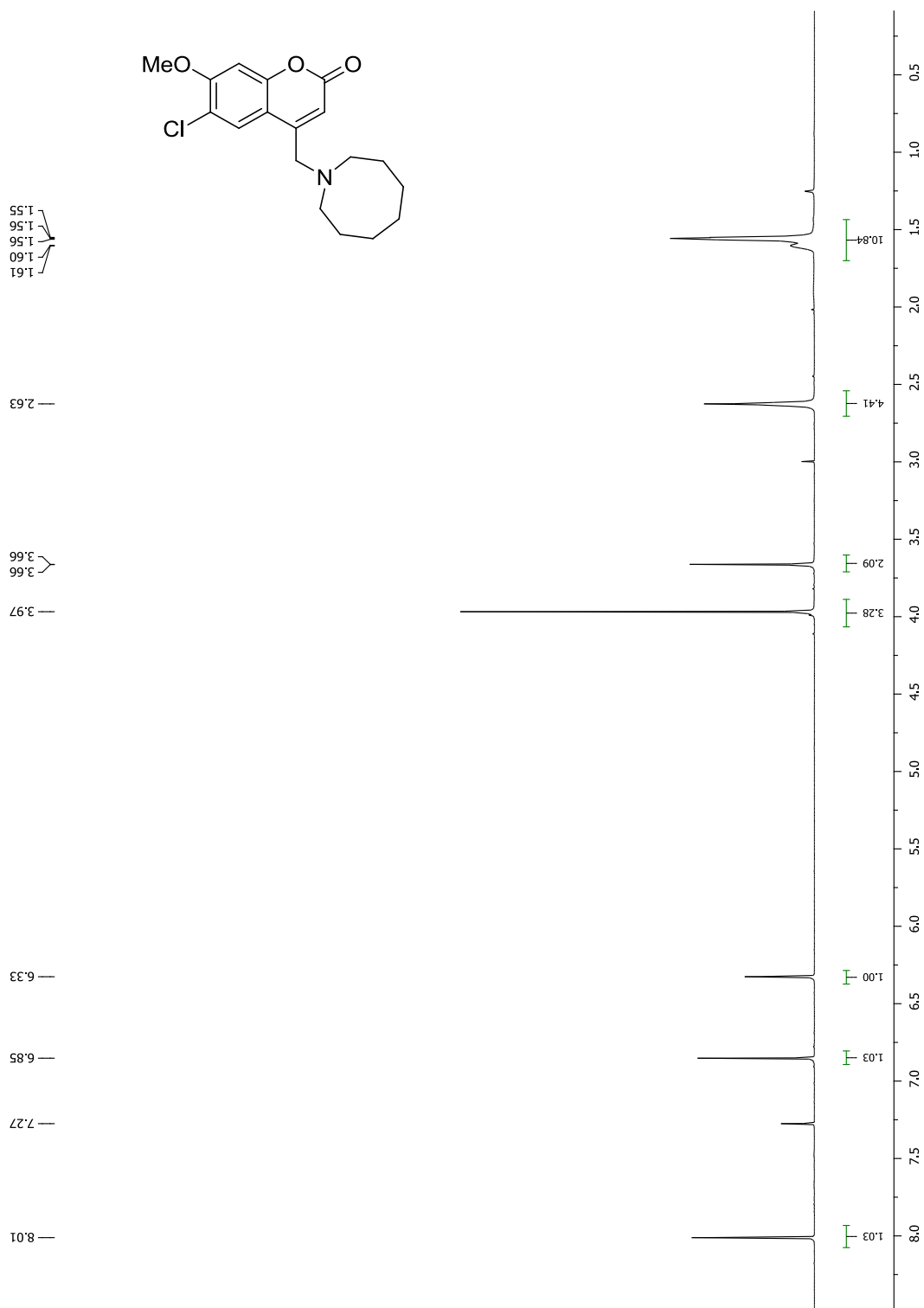
C8A12



C8A12



C8A14



C8A14

