Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Electronic Supporting Information

Practical Synthesis of Isoindolines Yields A Potent Colistin Potentiator in Multidrug-Resistant *Acinetobacter baumannii*

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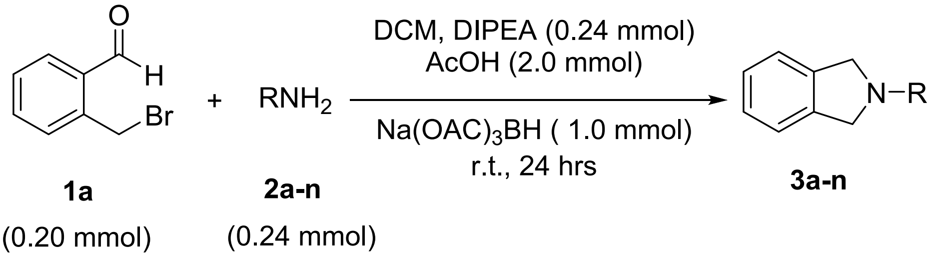
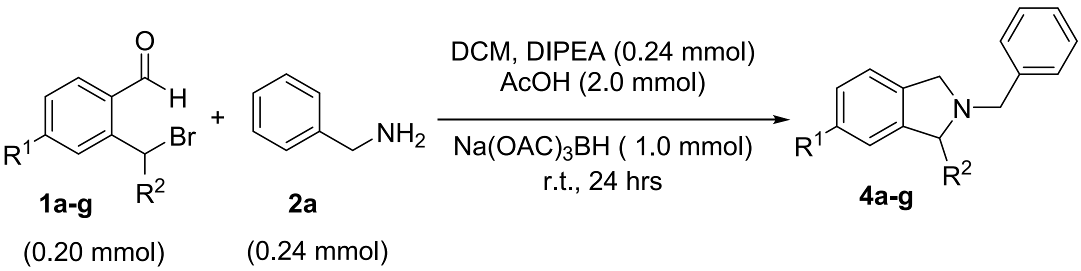
Table of Content

1.3. Procedure for synthesizing Isoindoline Derivatives

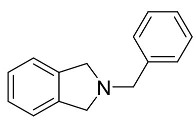




Different bromomethyl benzaldehyde precursors were synthesized using the reported protocol[S1]. The bromomethyl benzaldehyde (40.0 mg, 0.20mmol) was dissolved in dry dichloromethane (1mL) and stirred under argon atmosphere during the reaction at room temperature. After that, N, N-diisopropylethylamine (47 µL, 0.24 mmol) and different amines (0.24 mmol) were added consecutively and stirred for 1 hour at room temperature. Therefore, acetic acid* (114 µL, 2.0 mmol) and sodium triacetoxyborohydride (211mg, 1.0 mmol.) were added and stirred for overnight at room temperature. After that, the reaction mixture was quenched with aqueous sodium bicarbonate (5 mL) and washed with dichloromethane (5.0 mL × 3). The combined organic layer was dried over anhydrous sodium sulfate, filtered, and concentrated in vaccuo to obtain the crude product, which was purified by column chromatography on basic alumina using 3%(v/v) methanol-dichloromethane to afford compounds **4a-g**. For compounds **3a-n**, different amines were reacted with unsubstituted bromomethyl benzaldehyde following the above-mentioned procedure.

*Trifluoroacetic acid (TFA, 114 µL, 2.0 mmol) was used for bromomethyl benzaldehyde containing electronegative atoms (F, Cl, Br, CF_3).

2. Compound Characterization Data



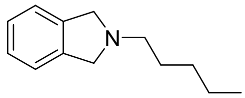
2-Benzyl-2,3-dihydro-1*H*-isoindole, **3a**; brown oil; 33 mg, 80% yield; TLC (3% methanol-dichloromethane) $R_f = 0.15$

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.47- 7.40 (m, 2 H), 7.38- 7. 31 (m, 2H), 7.21 (s, 4 H), 3.96 (s, 4H), 3.95 (s, 2H) ppm

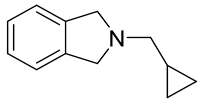
^{13}C NMR (75 MHz, CDCl3) δ 140.19, 139.08, 128.83, 128.42, 127.15, 126.70, 122.34, 60.33, 58.96 ppm

IR (cm^{-1}) 2860, 16200, 1230, 720

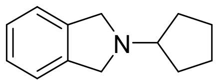
HRMS (ESI+) : *m/z* $[M+H]^+$ calculated for $C_{15}H_{15}N$: 210.120; found 210.121.



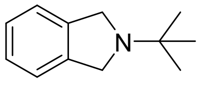
2-Pentyl-2,3-dihydro-1*H*-isoindole, **3b**; brown oil, 33 mg, 88% yield; TLC (3% methanol-dichloromethane) R_f= 0.15
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.21 (s, 4H), 3.94 (s, 4H), 2.73 (t, *J* = 6Hz, 2H), 1.61- 1.59 (m, 2H), 1.42-1.36 (m, 4H), 0.96- 0.94 (t, *J*= 6Hz, 3H) ppm
^{13}C NMR (75 MHz, $CDCl_3$) δ 140.17, 126.23, 122.26, 59.15, 56.31, 29.68, 28.68, 22.68, 14.00 ppm
IR (cm^{-1}) 2965, 1680, 1240, 720
HRMS (ESI+) : *m/z* $[M+H]^+$ calculated for $C_{13}H_{13}N$: 190.151; found 190.152.



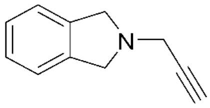
2-(Cyclopropylmethyl)-2,3-dihydro-1*H*-isoindole, **3c**; brown oil; 29 mg, 84% yield; TLC (3% methanol-dichloromethane) R_f= 0.15
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.21 (s, 4H), 4.00 (s, 4H), 2.62 (d, *J* = 6 Hz, 2H), 1.07- 1.00 (m,1H), 0.97-0.56 (m, 2H), 0.26- 0.21 (m, 2H) ppm
^{13}C NMR (75 MHz, $CDCl_3$) δ 140.14, 126.66, 122.27, 60.79, 59.15, 29.27, 10.13, 3.72 ppm
IR (cm^{-1}) 2865, 2150, 1870, 1650, 1230, 850, 720
HRMS (ESI+) : *m/z* $[M+H]^+$ calculated for $C_{12}H_{15}N$: 174.120; found 174.122.



2-Cyclopentyl-2,3-dihydro-1*H*-isoindole, **3d**; brown oil, 29 mg, 77% yield; TLC (3% methanol-dichloromethane) R_f= 0.15
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.20 (s, 4H), 3.96 (s, 4H), 2.95-1.90 (m, 1H), 1.89-1.80 (m, 2H), 1.79-1.74 (m, 2H), 1.69- 1.59 (m, 4H) ppm
^{13}C NMR (75 MHz, $CDCl_3$) δ 140.19, 126.66, 122.30, 66.65, 58.50, 32.08, 24.07 ppm
IR (cm^{-1}) 2965, 2260, 2550, 1450, 1335, 1230, 820, 700
HRMS (ESI+) calculated for $C_{13}H_{17}N$ $[M+H]^+$: 188.136, found 188.137.

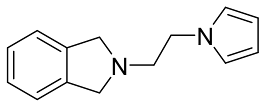


2-*tert*-butyl-2,3-dihydro-1*H*-isoindole, **3e**; brown oil, 29 mg, 84% yield; TLC (3% methanol-dichloromethane) R_f= 0.15
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.21 (s, 4H), 4.08 (s, 4H), 1.20 (s, 9H) ppm
^{13}C NMR (75 MHz, $CDCl_3$) δ 139.93, 126.56, 122.43, 52.65, 52.03, 26.06 ppm
IR (cm^{-1}) 2870, 2600, 1670, 1440, 1220, 720
HRMS (ESI+) : *m/z* $[M+H]^+$ calculated for $C_{12}H_{17}N$: 176.136; found 176.139.

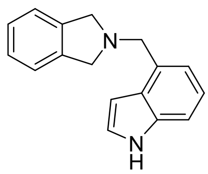


2-(Prop-2-yn-1-yl)-2,3-dihydro-1*H*-isoindole, **3f**; brown oil, 22 mg, 69% yield; TLC (3% methanol-dichloromethane) R_f= 0.15
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.23 (s, 4H), 4.09 (s, 4H), 3.66 (s, 2H), 2.31 (t, *J* = 3Hz, 1H) ppm
^{13}C NMR (75 MHz, $CDCl_3$) δ 139.95, 126.78, 122.35, 73.87, 57.16, 42.70, 29.26 ppm

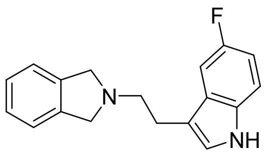
IR (cm^{-1}) 2850, 2230, 1650, 1230, 920, 720
HRMS (ESI+) : *m/z* $[M+H]^+$ calculated for $C_{11}H_{11}N$: 158.089; found 158.091.



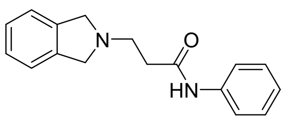
2-[2-(1H-pyrrol-1-yl)ethyl]-2,3-dihydro-1*H*-isoindole, **3g**; brown oil, 29 mg, 68% yield; TLC (3% methanol-dichloromethane) R_f= 0.15
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.06 (s, 1H), 7.23 (s, 4H), 7.05 (d, *J* = 10 Hz, 2H), 4.17 (t, *J* = 9Hz, 2H), 4.26 (s, 4H), 3.14(t, *J* = 5 Hz, 2H) ppm
^{13}C NMR (75 MHz, $CDCl_3$) δ 139.31, 137.22, 128.94, 126.99, 122.29, 119.30, 59.22, 56.39, 46.48 ppm
IR (cm^{-1}) 2850, 1950, 1530, 1230, 720
HRMS (ESI+) : *m/z* $[M+H]^+$ calculated for $C_{14}H_{16}N_2$: 214.131; found 214.134.



4-[(1,3-dihydro-2H-isoindol-2-yl)methyl]-1*H*-indole, **3h**; brown oil, 38 mg, 77% yield; TLC (3% methanol-dichloromethane) R_f= 0.15
^{1}H NMR (300 MHz, $CDCl_3$) δ 8.26 (s, 1H), 7.24 (d, *J* = 3 Hz, 1H), 7.23 (s, 1H), 7.21 (d, *J* = 3 Hz,1H), 7.19 (s, 4H), 6.79- 6.77 (m, 1H), 4.24 (s, 2H), 4.04 (s, 4H) ppm
^{13}C NMR (75 MHz, $CDCl_3$) δ 140.45, 135.89, 127.46, 126.57, 123.91, 122.32, 121.96, 119.96, 110.08, 101.34, 59.11, 57.99 ppm
IR (cm^{-1}) 3400, 2850,1650, 1230, 744, 720
HRMS (ESI+) : *m/z* $[M+H]^+$ calculated for $C_{17}H_{16}N_2$: 249.131; found 249.133.

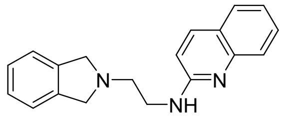


3-[2-(1,3-dihydro-2*H*-isoindol-2-yl)ethyl]-5-fluoro-1*H*-indole, **3i**; brown oil, 50 mg, 90% yield; TLC (3% methanol-dichloromethane) R_f= 0.15
^{1}H NMR (300 MHz, $CDCl_3$) δ 8.34 (s, 1H), 7.31 (d, *J* = 3 Hz, 1H), 7.28 (s, 1H), 7.24 (s, 4H), 7.11 (d, *J* = 3 Hz, 4H), 6.98-6.91 (m, 1H), 4.07 (s, 4H), 3.13- 3.00 (m, 4H) ppm
^{13}C NMR (75 MHz, $CDCl_3$) δ 159.24, 156.14, 140.02, 132.78, 126.78, 123.53, 122.33, 111.84, 110.06, 103.51, 59.16, 56.55, 24.96 ppm
^{19}F NMR (282 MHz, $CDCl_3$) δ -125.49(s) ppm
IR (cm^{-1}) 3400, 2960, 2250, 1950, 1695, 1395, 1230, 744, 720
HRMS (ESI+) : *m/z* $[M+H]^+$ calculated for $C_{18}H_{17}FN_2$:281.137; found 281.139.

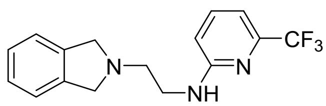


3-(1,3-dihydro-2*H*-isoindol-2-yl)-*N*-phenylpropanamide, **3j**; brown oil, 37 mg, 70% yield; TLC (3% methanol-dichloromethane) R_f= 0.15
^{1}H NMR (300 MHz, $CDCl_3$) δ 10.67 (s, 1H), 7.29 (s, 4H), 4.13 (s, 4H), 3.16 (t, *J* = 6 Hz, 2H), 2.66 (t, *J* =5 Hz, 2H) ppm

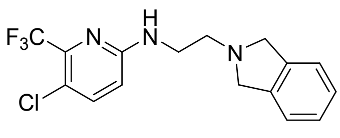
^{13}C NMR (75 MHz, $CDCl_3$) δ 170.63, 138.97, 128.86, 127.24, 123.73, 122.47, 119.94, 58.45, 51.69, 34.71 ppm
IR (cm^{-1}) 2980, 2400, 2650, 1680, 1460, 1230, 850, 720, 650
HRMS (ESI+) : *m/z* $[M+H]^+$ calculated for $C_{17}H_{18}N_2O$: 267.141; found 267.144.



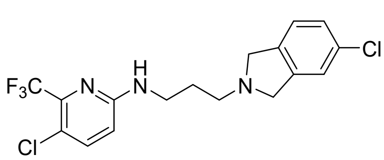
N-[2-(2,3-dihydro-1*H*-inden-2-yl)ethyl]quinolin-2-amine, **3k**; brown oil, 47 mg, 81% yield; TLC (3% methanol-dichloromethane) R_f= 0.15
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.79 (d, *J* = 9 Hz, 1H), 7.25 (d, *J* = 9 Hz, 1H), 7.61- 7.52 (m, 2H), 7.24 (s, 4H), 7.23- 7.19 (m, 1H), 6.66 (d, *J* = 9Hz, 1H), 5.46 (s,1H), 4.04 (s, 4H), 3.74 (q, *J* = 9 Hz, 2H), 3.09 (t, *J* = 6 Hz, 2H) ppm
^{13}C NMR (75 MHz, $CDCl_3$) δ 156.98, 148.11, 139.91, 137.02, 129.44, 127.44, 126.86, 126.15, 123.40, 122.34, 121.93, 112.27, 58.79, 54.49, 39.93 ppm
IR (cm^{-1}) 3300, 2985, 1680, 1342, 1270, 750, 720
HRMS (ESI+) : *m/z* $[M+H]^+$ calculated for $C_{20}H_{20}N_2$:290.157; found 290.159.



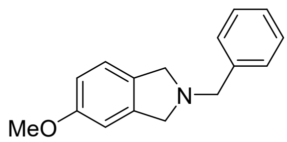
N-2-(2-Trifluoromethyl-6-aminopyridyl)ethyl isoindoline, **3l**;brown oil, 46 mg, 75% yield; TLC (3% methanol-dichloromethane) R_f= 0.15
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.51 (t, *J* = 7Hz, 1H), 7.24 (s, 4H), 6.93 (d, *J* = 4Hz, 1H), 6.56 (d, *J* = 4Hz, 1H), 5.44 (s,1H), 4.01 (s, 4H), 3.54 (q, *J* = 9Hz, 2H), 3.04 (t, *J* = 4Hz, 2H) ppm
^{13}C NMR (75 MHz, $CDCl_3$) δ 158.59, 143.28, 139.81, 137.76, 126.87, 122.31, 110.63, 108.68, 60.41, 58.76, 54.24, 40.15, 21.01, 14.20 ppm
^{19}F NMR (282 MHz, $CDCl_3$) δ -68.75(s) ppm
IR (cm^{-1}) 3300, 2985, 1680, 1342, 1270, 1245, 750, 720R
HRMS (ESI+) : *m/z* $[M+H]^+$ calculated for $C_{16}H_{16}F_3N_3$:308.129; found 308.131.



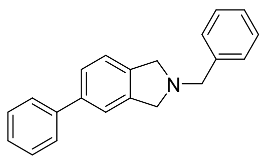
N-2-(2-Trifluoromethyl-3-chloro-6-aminopyridyl)ethyl isoindoline, **3m**; brown oil, 49 mg, 72 % yield; TLC (3% methanol-dichloromethane) R_f= 0.15
^{1}H NMR (300 MHz, $CDCl_3$) δ7.46 (d, *J* = 9Hz, 1H), 7.24 (s, 4H), 6.51 (d, *J* = 9Hz, 1H), 5.44 (s, 1H), 4.02 (s, 4H), 3.52 (q, *J* = 9Hz, 2H), 3.03 (t, *J* = 4Hz, 2H) ppm
^{13}C NMR (75 MHz, $CDCl_3$) δ 156.01, 140.43, 139.75, 126.88, 122.33, 119.40, 116.71, 111.56, 58.76, 54.23, 40.25 ppm
^{19}F NMR (282 MHz, $CDCl_3$) δ -66.16(s) ppm
IR(cm^{-1}) 3300, 2985, 1680, 1342, 1270, 1245, 830, 750, 720
HRMS (ESI+) : *m/z* $[M+H]^+$ calculated for $C_{16}H_{16}ClF_3N_3$:342.090; found 342.093.



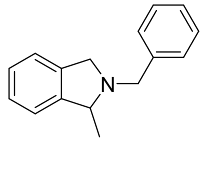
N-(2-Trifluoromethyl-3-chloro-6-aminopyridyl)propyl 4-chloroisoindoline, **3n**; brown oil, 36 mg, 47% yield; TLC (3% methanol-dichloromethane) R_f= 0.15
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.45 (d, *J* = 9Hz, 1H), 7.22- 7.19 (m, 2H), 7.15 (d, *J* = 9Hz, 1H), 6.46 (d, *J* = 9Hz, 1H), 5.50 (s,1H), 3.93 (d, *J* = 4Hz, 4H), 3.48 (q, *J* = 9Hz, 2H), 2.88 (t, *J* = 4Hz, 2H), 1.93-1.85 (m, 2H) ppm
^{13}C NMR (75 MHz, $CDCl_3$) δ 159.24, 156.14, 140.02, 132.72, 127.00, 126.78, 123.53, 122.33, 110.84, 110.06, 58.84, 59.16, 56.55, 24.96 ppm
^{19}F NMR (282 MHz, $CDCl_3$) δ -66.12(s) ppm
IR(cm^{-1}) 3300, 2985, 1680, 1342, 1270, 1245, 830, 750, 720
HRMS (ESI+) : *m/z* $[M+H]^+$ calculated for $C_{16}H_{16}Cl_2F_3N_3$:390.067; found 390.069.



2-Benzyl-5-methoxy-2,3-dihydro-1*H*-isoindole, **4a**; brown oil; 41 mg, 85% yield; TLC (3% methanol-dichloromethane) R_f= 0.15
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.45-7.42 (m, 2H), 7.38-7.36 (m, 1H), 7.35-7.30 (m, 2H), 7.09 (d, *J* = 9 Hz, 1H), 6.75 (d, *J* = 6 Hz, 2H), 3.93 (s, 4H), 3.90 (s, 2H), 3.80 (s, 3H) ppm
^{13}C NMR (75 MHz, $CDCl_3$) δ 158.98, 141.68, 139.09, 132.26, 128.83, 128.40, 127.13, 122.95, 112.47, 108.10, 60.36, 59.13, 58.37, 55.47 ppm
IR (cm^{-1}) 2965, 1650, 1260, 1220, 720
HRMS (ESI+) : *m/z* $[M+H]^+$ calculated for $C_{16}H_{17}NO$: 240.131; found 240.132.

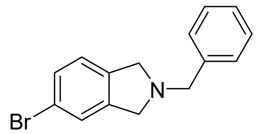


2-Benzyl-5-phenyl-2,3-dihydro-1*H*-isoindole, **4b**; brown oil; 43 mg, 76% yield; TLC (3% methanol-dichloromethane) R_f= 0.15
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.60-7.56 (m, *J* = 6 Hz, 2 H), 7.49-7.47 (m, 1H), 7.46-7.44 (m, 3H), 7.43-7.41 (m, 3H), 7.40-7.31 (m, 4H), 4.02 (d, *J* = 6 Hz, 4 H), 3.98 (s, 2H) ppm
^{13}C NMR (75 MHz, $CDCl_3$) δ 141.42, 140.81, 140.22, 139.26, 139.87, 128.86, 128.72, 128.46, 127.23, 127.19, 127.10, 125.99, 122.63, 121.21, 60.31, 58.93, 58.69 ppm
IR (cm^{-1}) 2865, 1650, 1230, 720
HRMS (ESI+) : *m/z* $[M+H]^+$ calculated for $C_{21}H_{19}N$: 286.151; found 286.154.



2-Benzyl-1-methyl-2,3-dihydro-1*H*-isoindole, **4c**; brown oil; 23 mg, 51% yield; TLC (3% methanol-dichloromethane) R_f= 0.15
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.46- 7.42 (m, 2H), 7.39- 7.34 (m, 2H), 7.33- 7.31 (m,1H), 7.25- 7.23 (m, 1H), 7.22-7.20 (m, 1H), 7.19-7.16 (m, 1H), 4.27 (d, *J* = 12 Hz, 1H), 4.07 (d, *J*= 15 Hz, 1H), 3.64 (d, *J* = 6 Hz, 1H), 3.60 (d, *J* = 6 Hz,1H), 1.51 (d, *J* =6 Hz, 3H) ppm
^{13}C NMR (75 MHz, $CDCl_3$) δ 128.39, 128.35, 127.00, 126.78, 122.18, 121.78, 63.70, 58.07, 57.85, 18.83 ppm
IR(cm^{-1}) 2964, 1650, 1210, 720

HRMS (ESI+) : *m/z* $[M+H]^+$ calculated for $C_{16}H_{17}N$: 224.136; found 224.139.



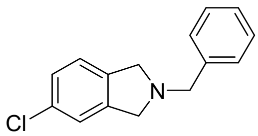
2-Benzyl-5-bromo-2,3-dihydro-1*H*-isoindole, **4d**; brown oil; 42 mg, 74% yield; TLC (3% methanol-dichloromethane) R_f= 0.15

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.42-7.40 (m, 2H), 7.38-7.37 (m, 1H), 7.35-7.33 (m, 3H), 7.06 (d, *J* =9 Hz, 2H), 3.93 (s, 4H), 3.91 (s, 2H) ppm

^{13}C NMR (75 MHz, $CDCl_3$) δ 142.57, 139.21, 138.69, 129.74, 128.77, 127.47, 127.27, 125.61, 123.88, 120.39, 60.13, 58.55, 58.42 ppm

IR (cm^{-1}) 2950, 1670, 1240, 680, 730

HRMS (ESI+) : *m/z* $[M+H]^+$ calculated for $C_{15}H_{14}BrN$: 288.031; found 288.033.



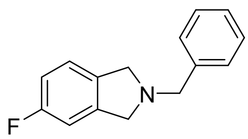
2-Benzyl-5-chloro-2,3-dihydro-1*H*-isoindole, **4e**; brown oil; 35 mg, 71% yield; TLC (3% methanol-dichloromethane) R_f= 0.15

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.42-7.39 (m, 2H), 7.38-7.37 (m, 1H), 7.35-7.30 (m, 2H), 7.20-7.16 (m, 2H), 7.13-7.06 (m, 1H), 3.92 (s, 4H), 3.91 (s, 2H) ppm

^{13}C NMR (75 MHz, $CDCl_3$) δ 142.23, 138.80, 132.40, 128.77, 128.46, 127.26, 126.84, 123.44, 122.68, 60.18, 58.65, 58.38 ppm

IR (cm^{-1}) 2950, 1660, 1240, 830, 720

HRMS (ESI+): *m/z* $[M+H]^+$ calculated for $C_{15}H_{14}ClN$: 243.081; found 243.084.



2-Benzyl-5-fluoro-2,3-dihydro-1*H*-isoindole, **4f**; brown oil; 26 mg, 58% yield; TLC (3% methanol-dichloromethane) R_f= 0.15

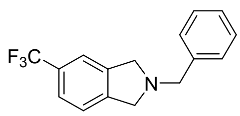
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.42-7.39 (m, 2H), 7.38-7.37 (m, 1H), 7.35-7.31 (m, 2H), 7.15-7.10 (m, 1H), 6.92-6.89 (m, 2H), 3.92 (s, 4H), 3.90 (s, 2H) ppm

^{13}C NMR (75 MHz, $CDCl_3$) δ 138.57, 135.75, 132.39, 128.66 (d, *J* = 28.50 Hz), 127.56 (t, *J* = 21.75 Hz), 123.36 (d, *J* = 9 Hz), 113.60 (d, *J* = 22.50 Hz), 109.68 (d, *J* = 23.25 Hz), 60.22, 58.81, 58.18, 30.93 ppm

^{19}F NMR (282 MHz, $CDCl_3$) δ -116.56(s) ppm

IR (cm^{-1}) 2950, 1660, 1420, 1240, 720

HRMS (ESI+): *m/z* $[M+H]^+$ calculated for $C_{15}H_{14}FN$: 228.111; found 228.112.



2-Benzyl-5-(trifluoromethyl)-2,3-dihydro-1*H*-isoindole, **4g**; brown oil; 23 mg, 42% yield; TLC (3% methanol-dichloromethane) R_f= 0.15

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.46-7.44 (m, 2H), 7.43-7.41 (m, 2H), 7.39-7.38 (m, 1H), 7.37-7.30 (m, 3H), 3.99 (s, 4H), 3.95 (s, 2H) ppm
^{13}C NMR (75 MHz, $CDCl_3$) δ 144.39, 141.15, 138.71, 128.74, 128.50, 127.30, 123.52 (q, J = 3.75 Hz), 119.36, 119.31, 60.10, 58.60, 58.54 ppm
^{19}F NMR (282 MHz, $CDCl_3$) δ -62.01(s) ppm
IR (cm^{-1}) 2860, 1650, 1390, 1220, 720
HRMS (ESI+) : *m/z* $[M+H]^+$ calculated for $C_{15}H_{14}CF_3N$: 278.107; found 278.110.

3. Biological Assay Protocol

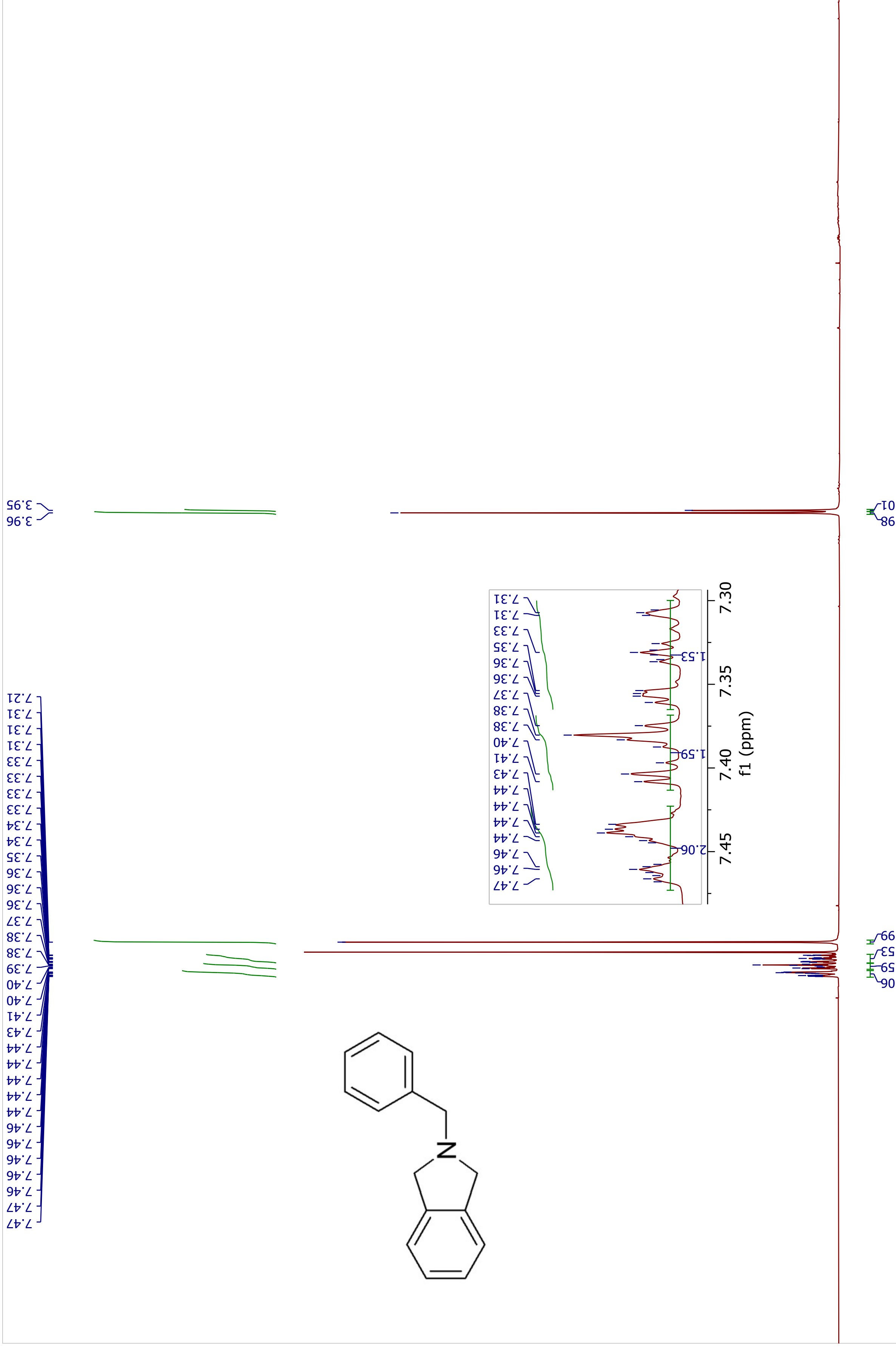
Bacteria were streaked on the BAP plate and incubated at 35 °C for 18 to 24 hours. Then, bacteria were cultured in the LB medium to the log phase and diluted to OD_{600} 0.002 in the MHB II medium. For two-fold serial microdilution, 100 µL of MHB II was added to each well in row A of clear 96-well microplates, and 50 µL of MHB II was added to each well in rows from B to H. Appropriate concentrated compounds or colistin were pipetted into the corresponding well in row A. Two-fold serial dilution of compounds or colistin was performed in the following rows from B to H using a 50 µL manual multichannel pipette. For MRCs, tests were performed similarly, except that the two-fold serial dilution was prepared in the MHB II medium supplemented with 4 µg/mL of colistin. All microplates were inoculated with 50 µL of diluted bacteria for a final inoculum concentration of OD_{600} 0.001 and then incubated at 35 °C with shaking for 18 hours. The MRCs were the lowest compound concentration inhibiting bacterial growth.

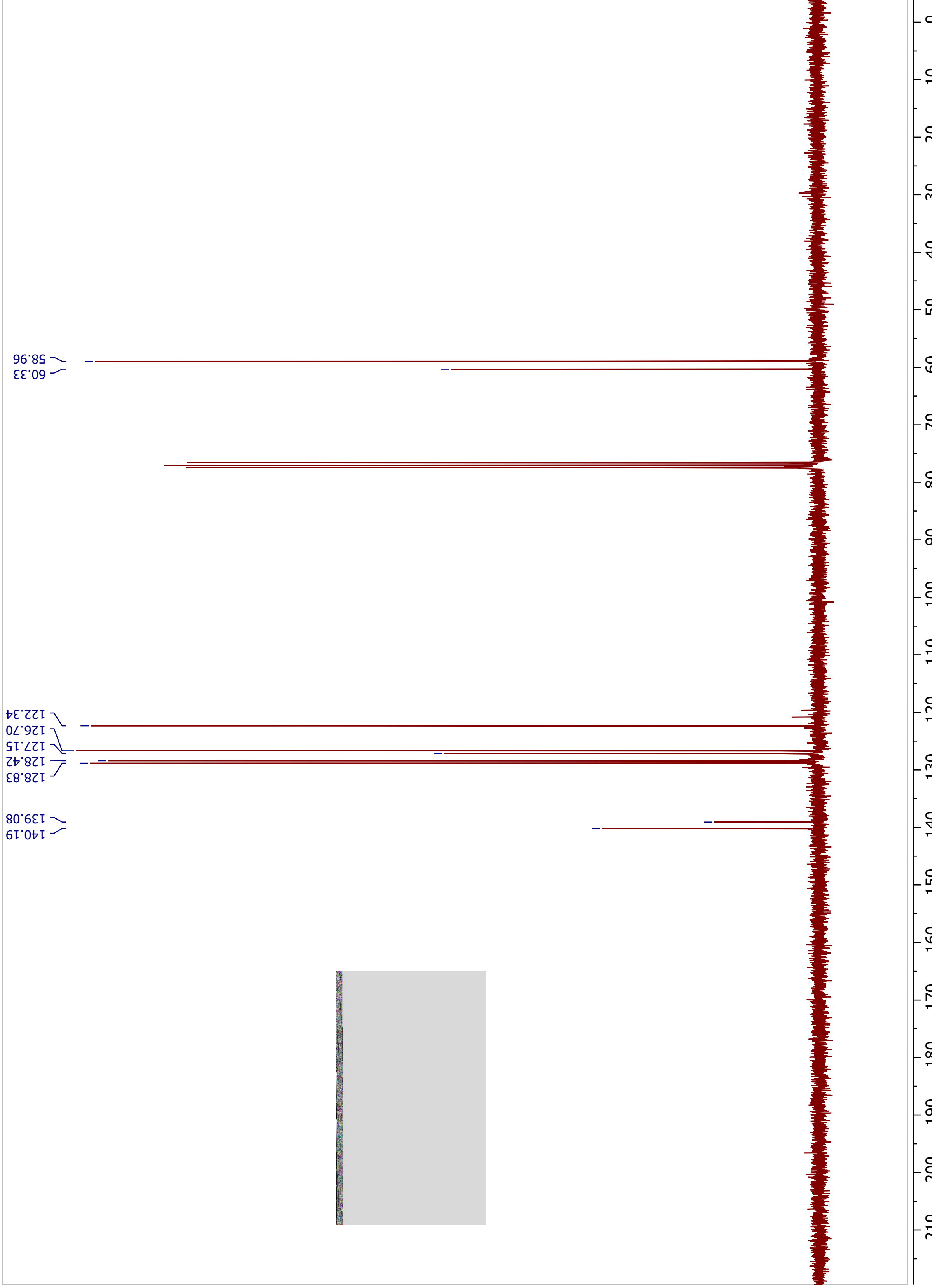
Table S1. Comparison of MIC data of isoindolines against *A. baumanni* AR-0289.

Entry	Compounds	MRC[a]
1	3h	4
2	3i	4
3	3k	0.5
4	3l	4
5	3n	2
6	4c	4

[a] MRC in µg/mL, in the presence of 1 µg/mL of compound and colistin, unless otherwise noted.

NMR Spectra

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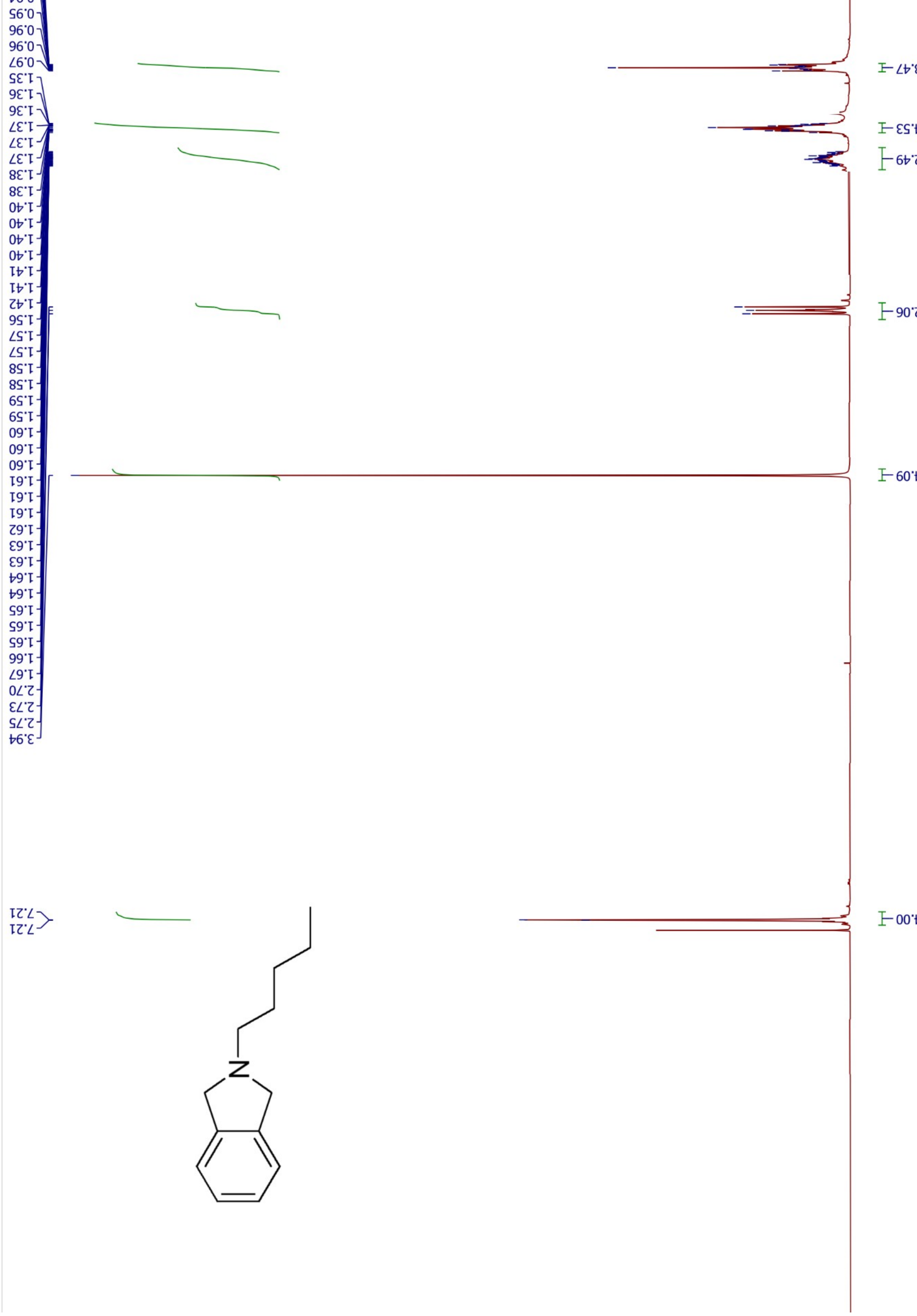
60.33
122.34
126.70
127.15
128.42
128.83
139.08
140.19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0.97
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1.37
1.37
1.37
1.38
1.38
1.40
1.40
1.40
1.40
1.41
1.41
1.42
1.56
1.57
1.57
1.58
1.58
1.59
1.59
1.60
1.60
1.60
1.61
1.61
1.61
1.62
1.63
1.63
1.64
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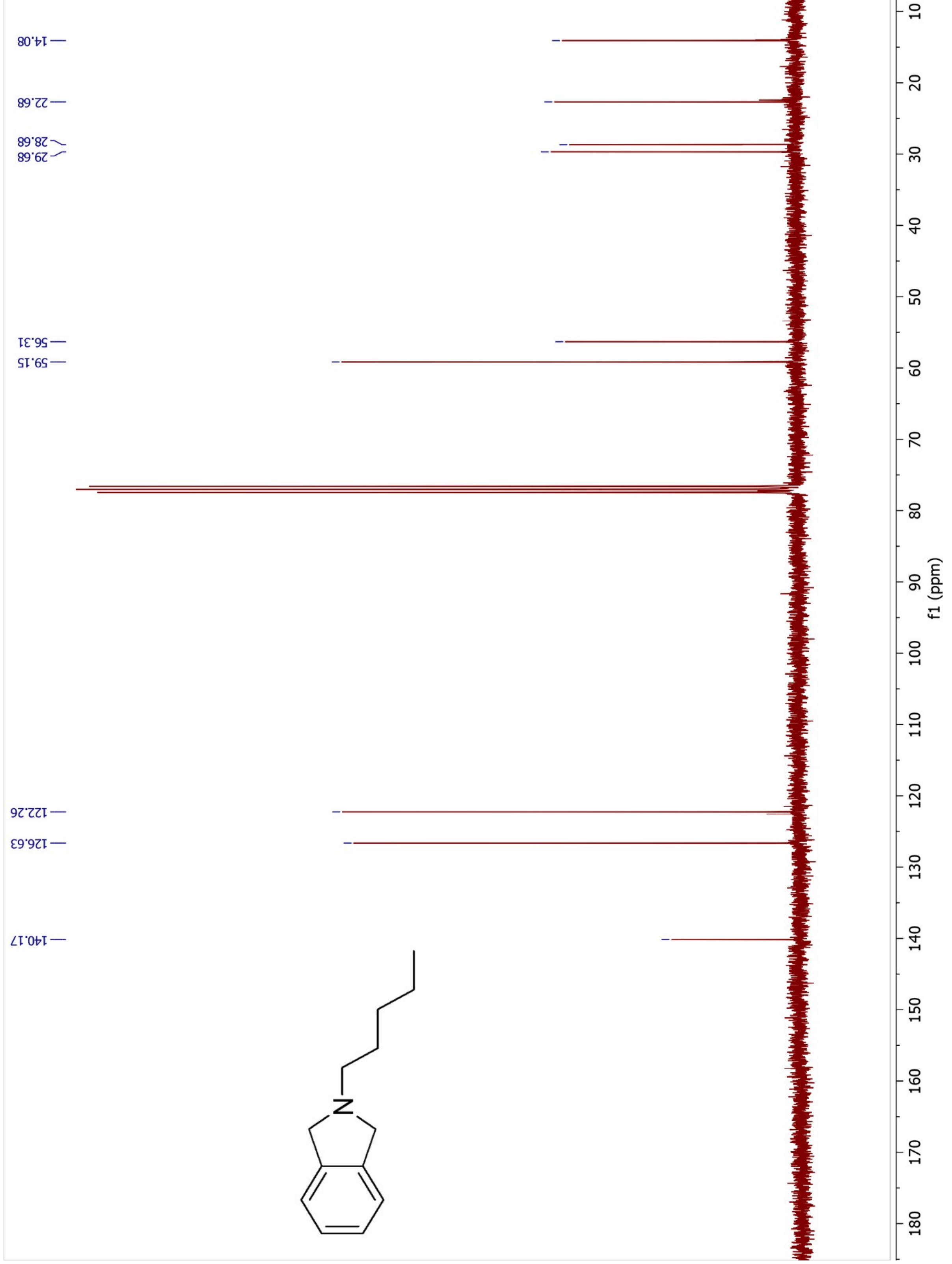
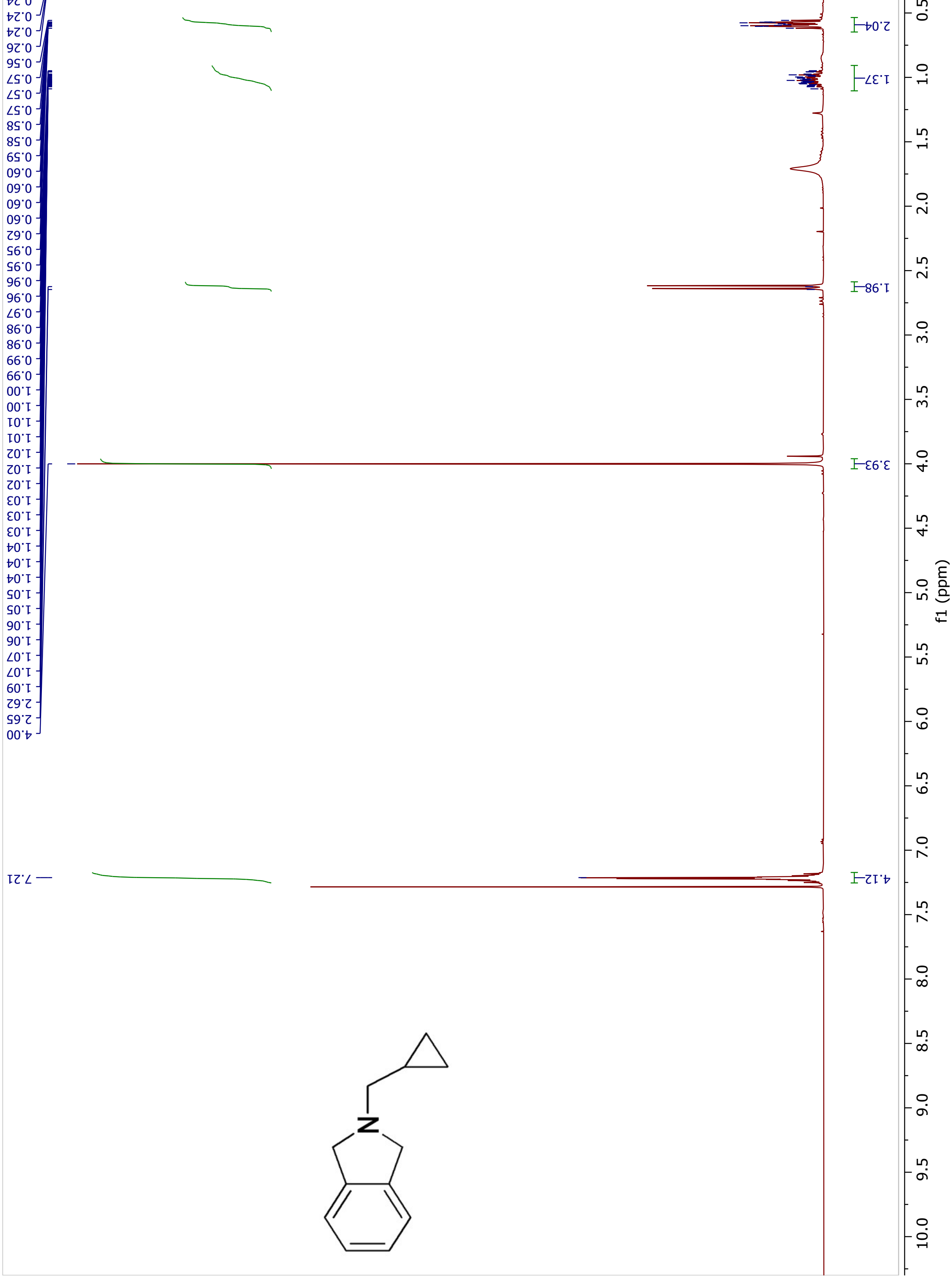
7.21
7.21
N


14.08
22.68
28.68
29.68
56.31
59.15
122.26
126.63
140.17
f1 (ppm)
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
N


f1 (ppm)
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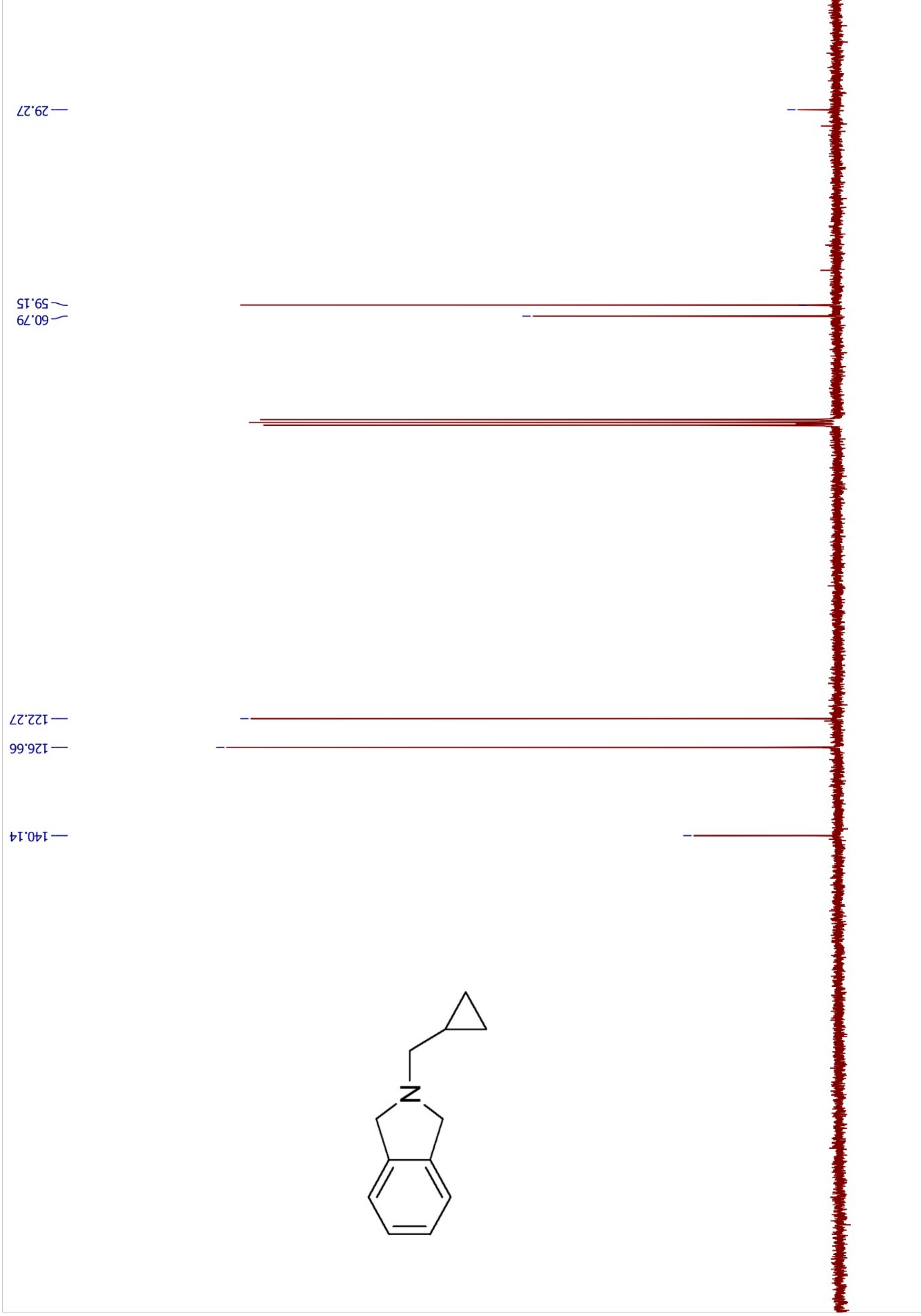
4.00
2.65
2.62
4.12
3.93
1.98
1.37
2.04
N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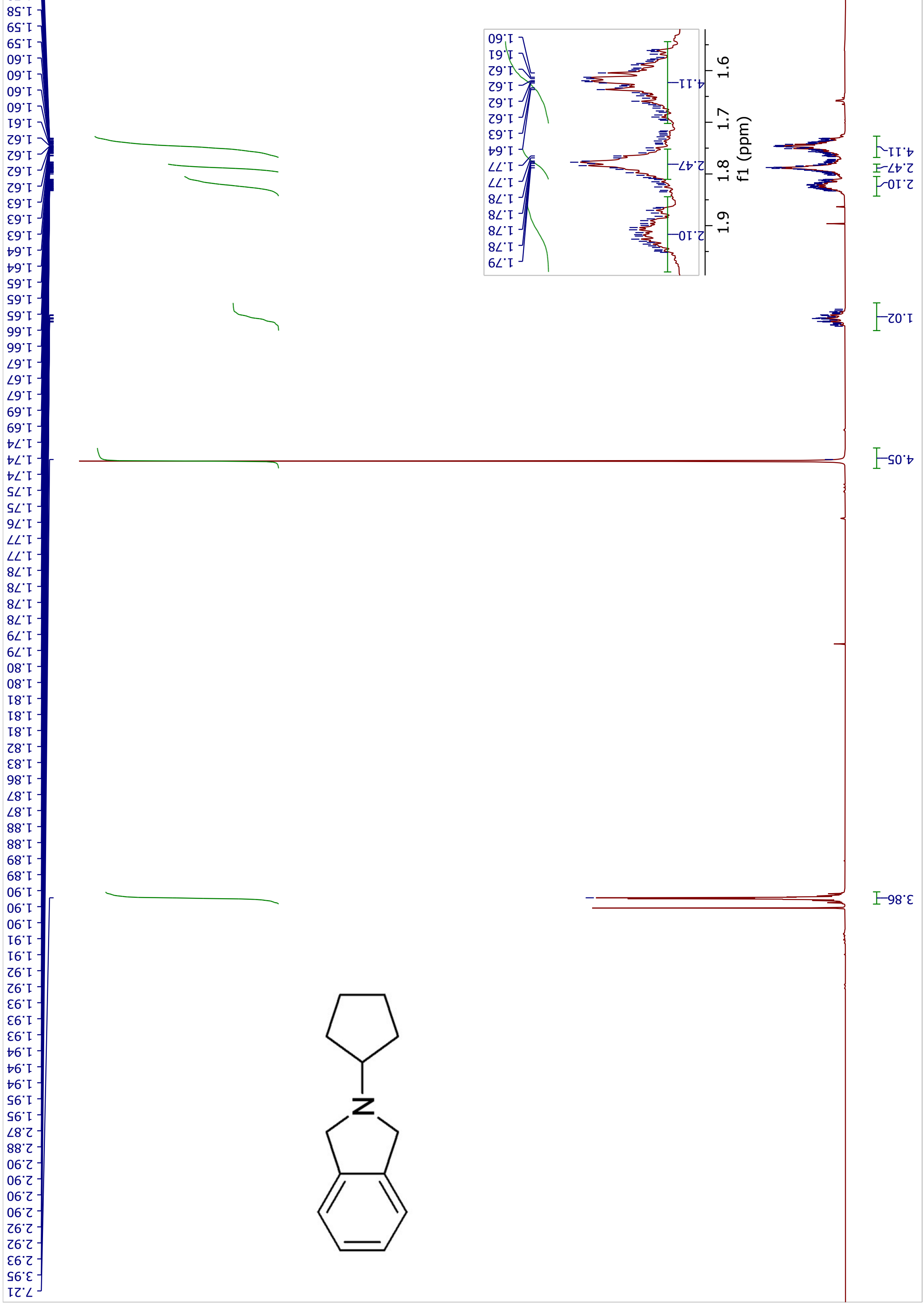
122.27
126.66
140.14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1.90
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1.92
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1.95
2.87
2.88
2.90
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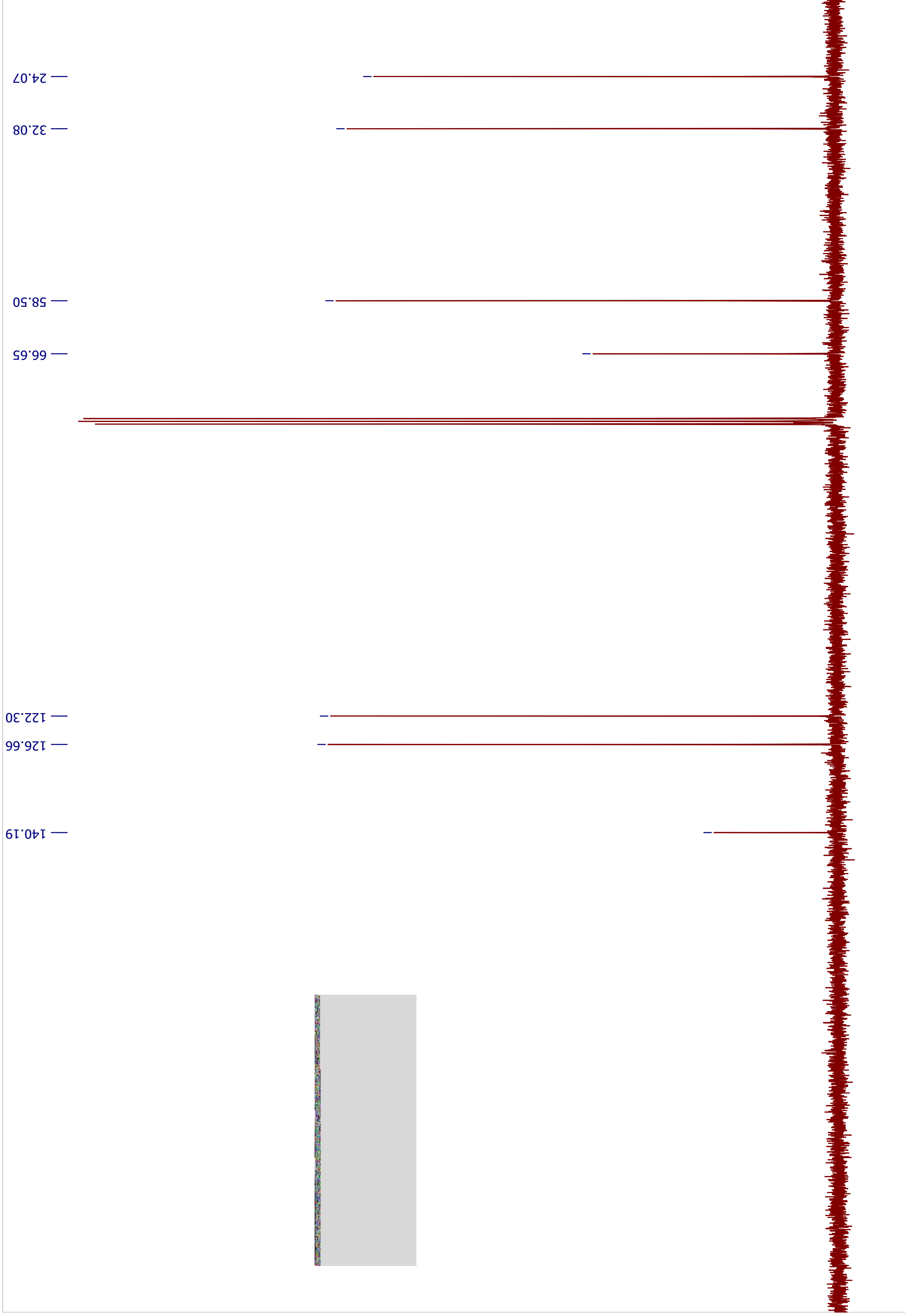
2.90
2.90
2.92
2.92
2.93
3.95
7.21
4.11
2.47
2.10
1.02
4.05
3.86
N
1.6
1.7
1.8
1.9
f1 (ppm)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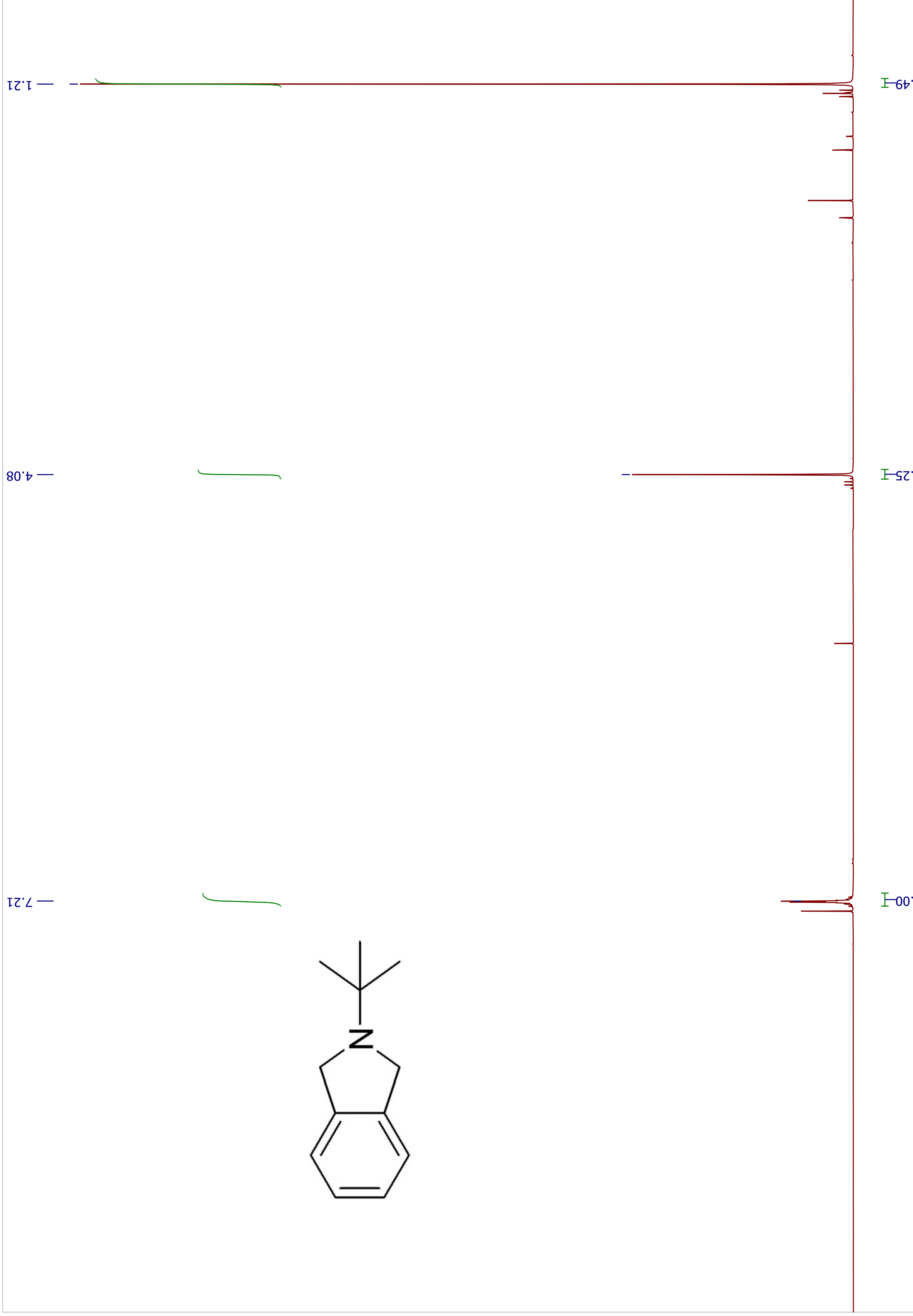
32.08
58.50
66.65
122.30
126.66
140.19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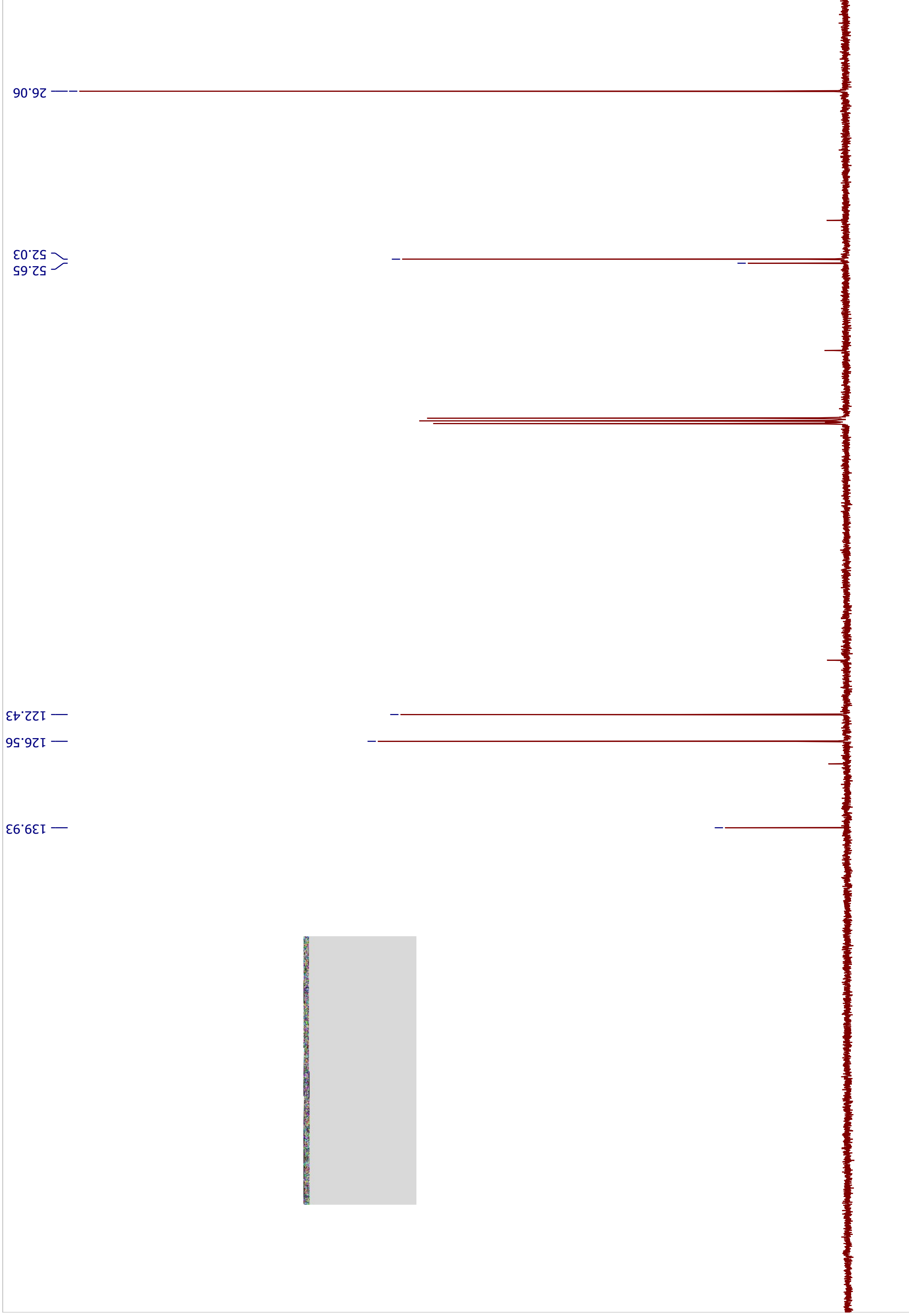
4.08
7.21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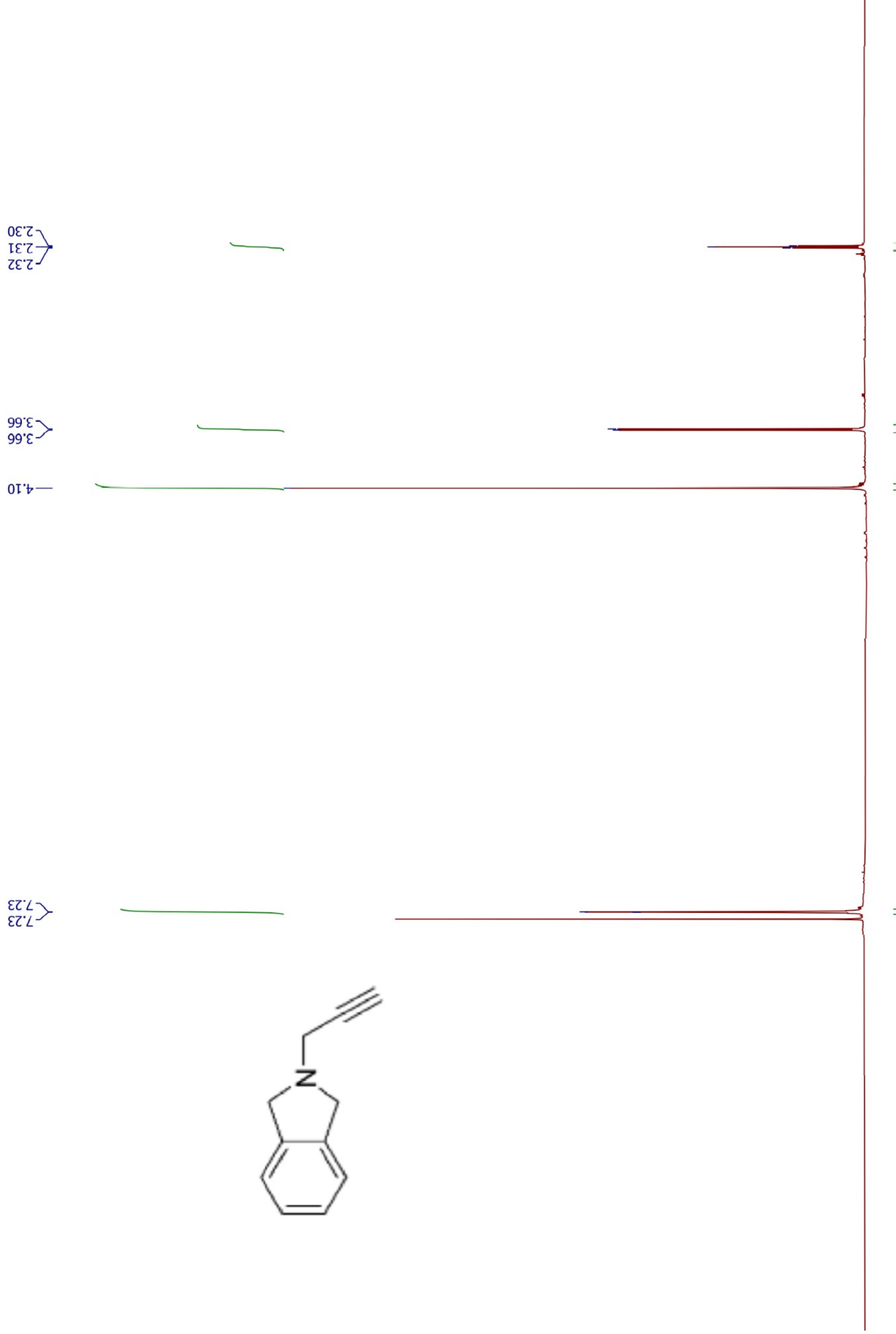
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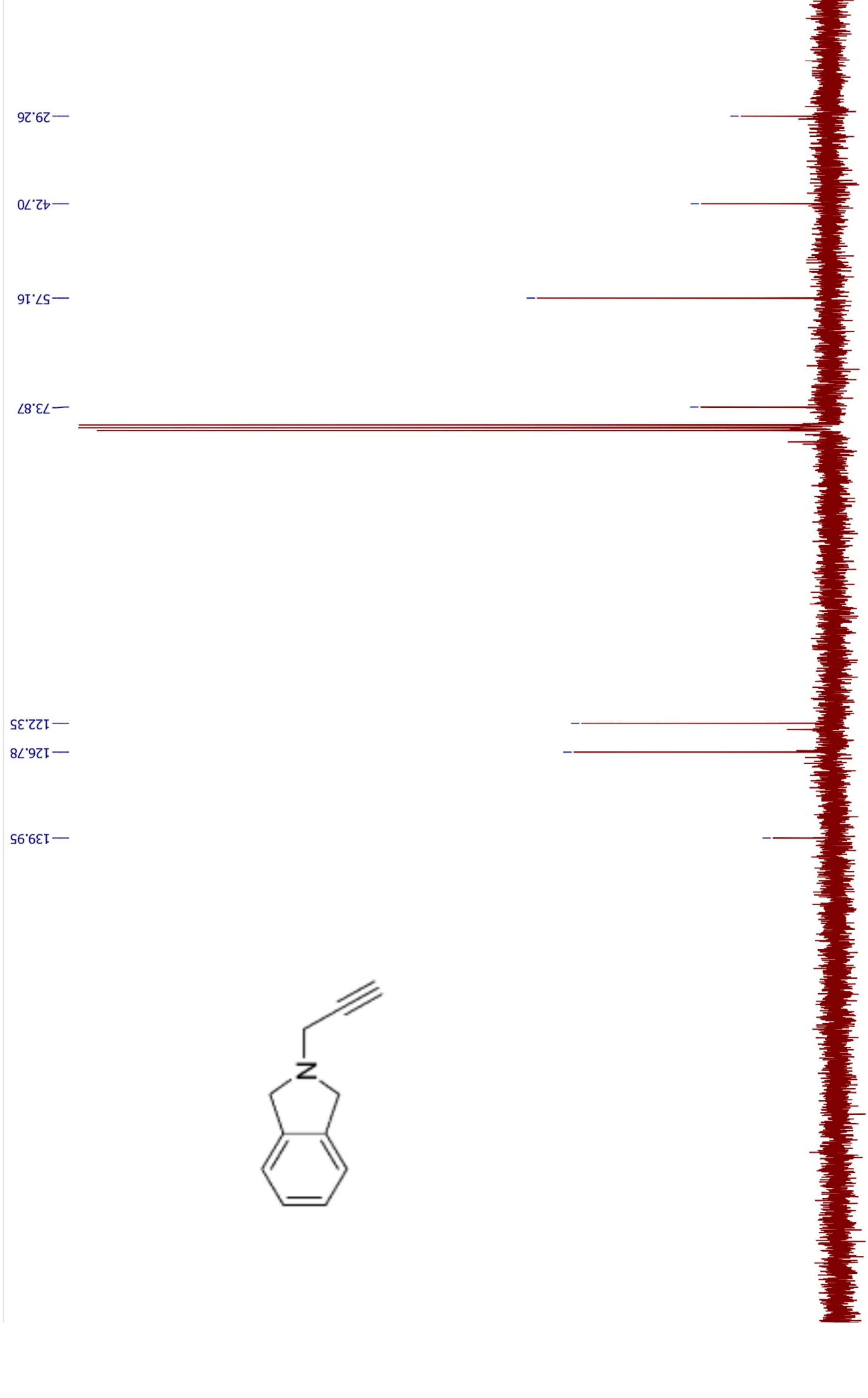
3.66
4.10
7.23
7.23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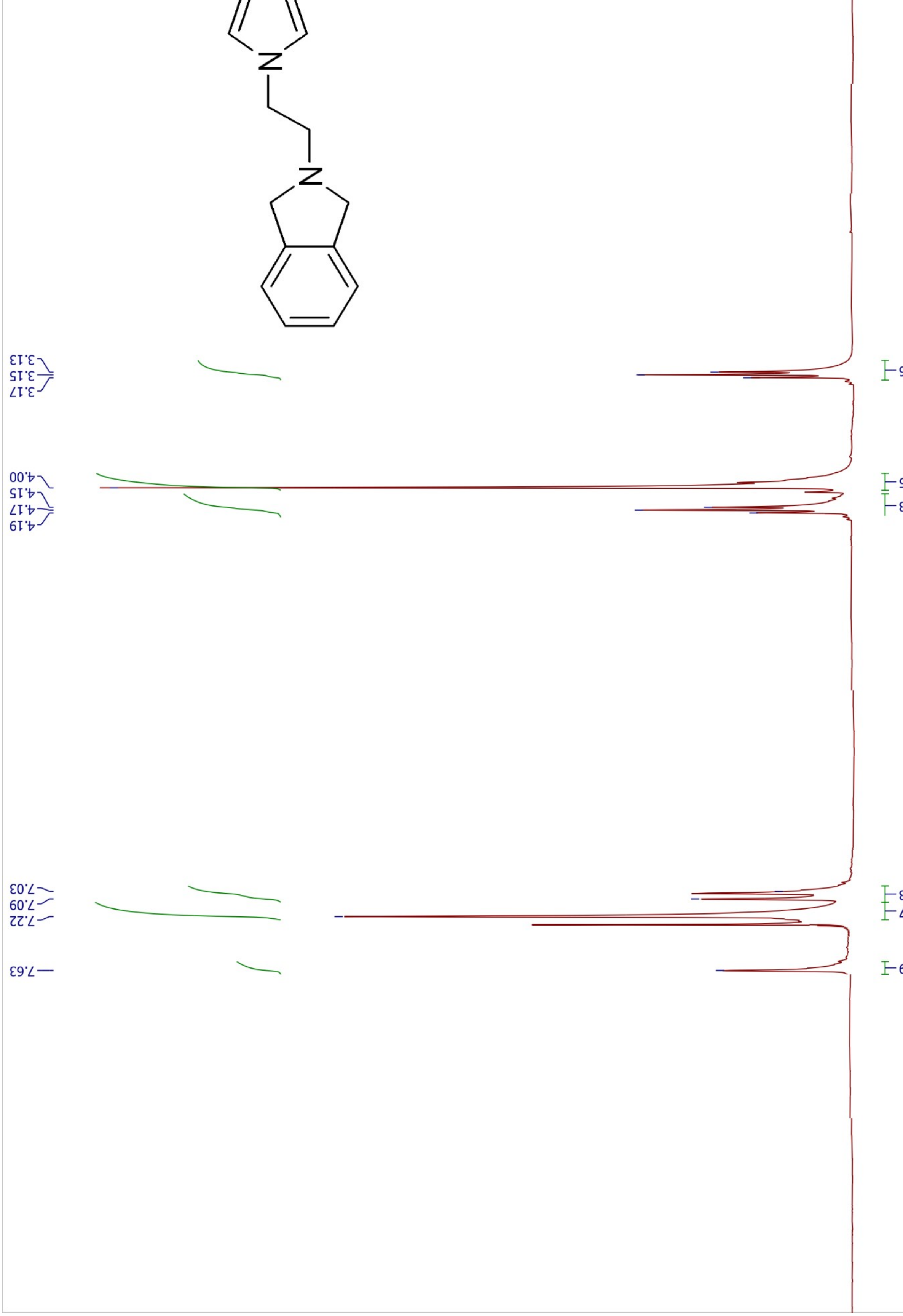
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4.19
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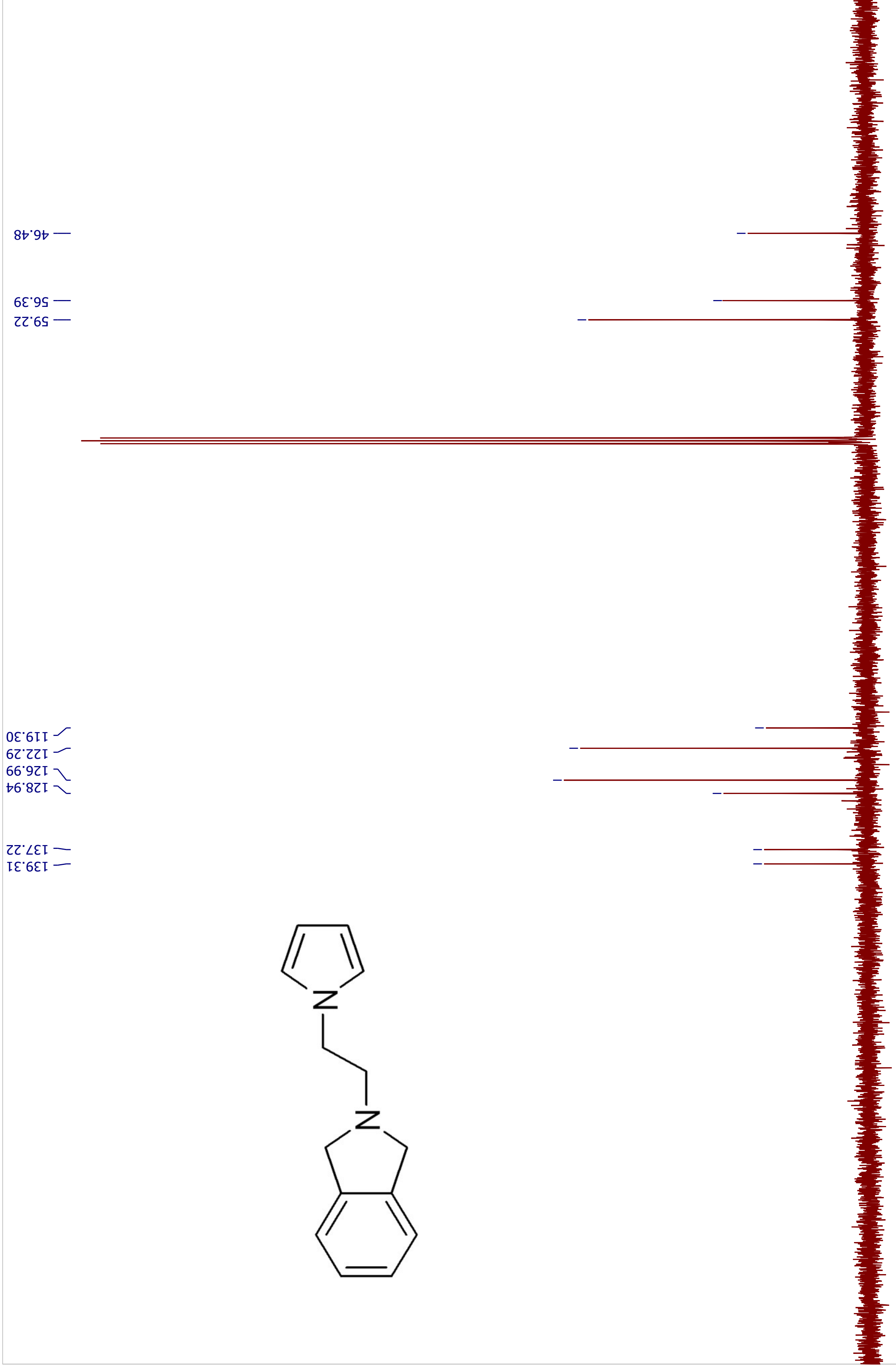
7.22
7.63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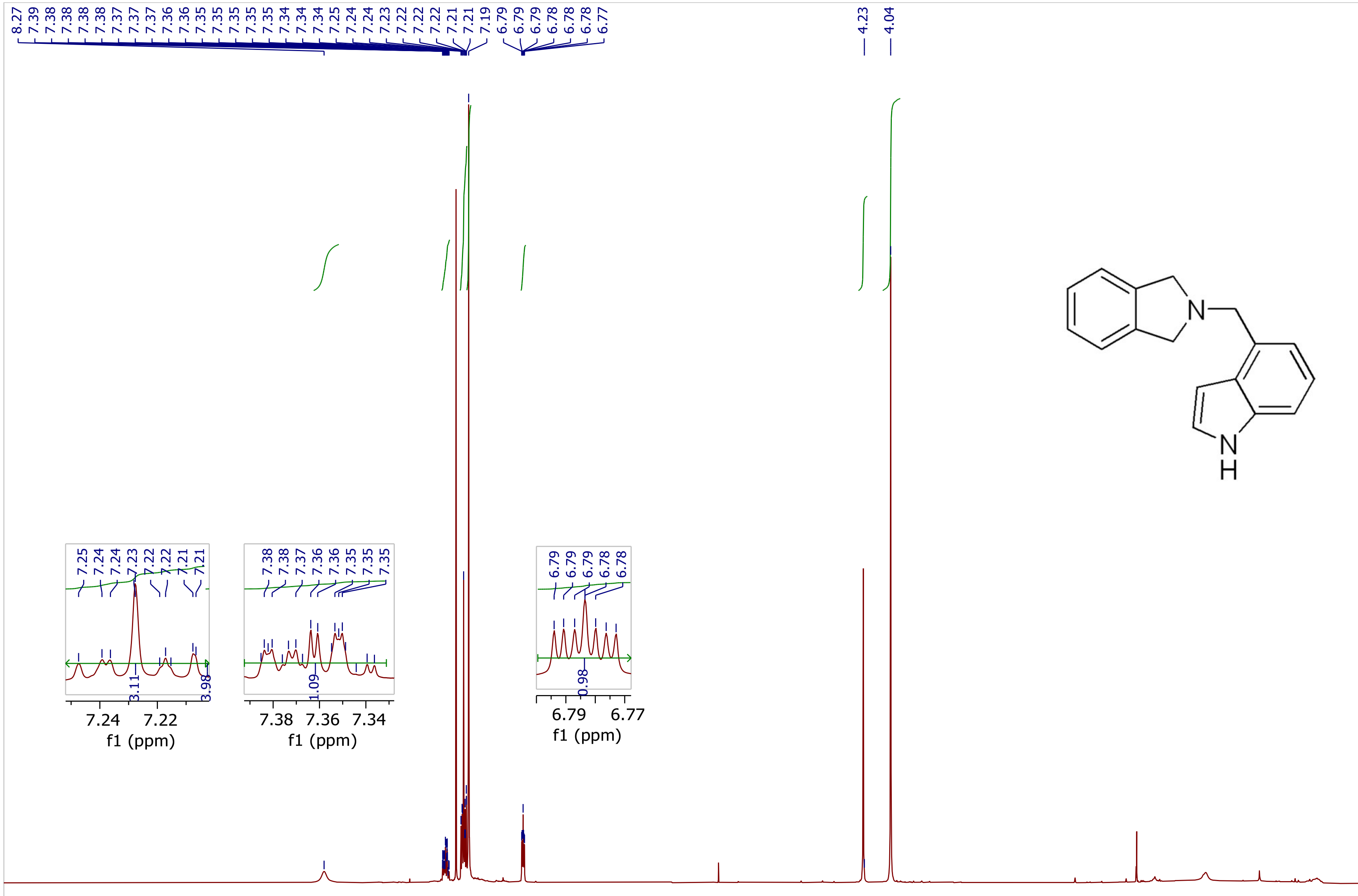
139.31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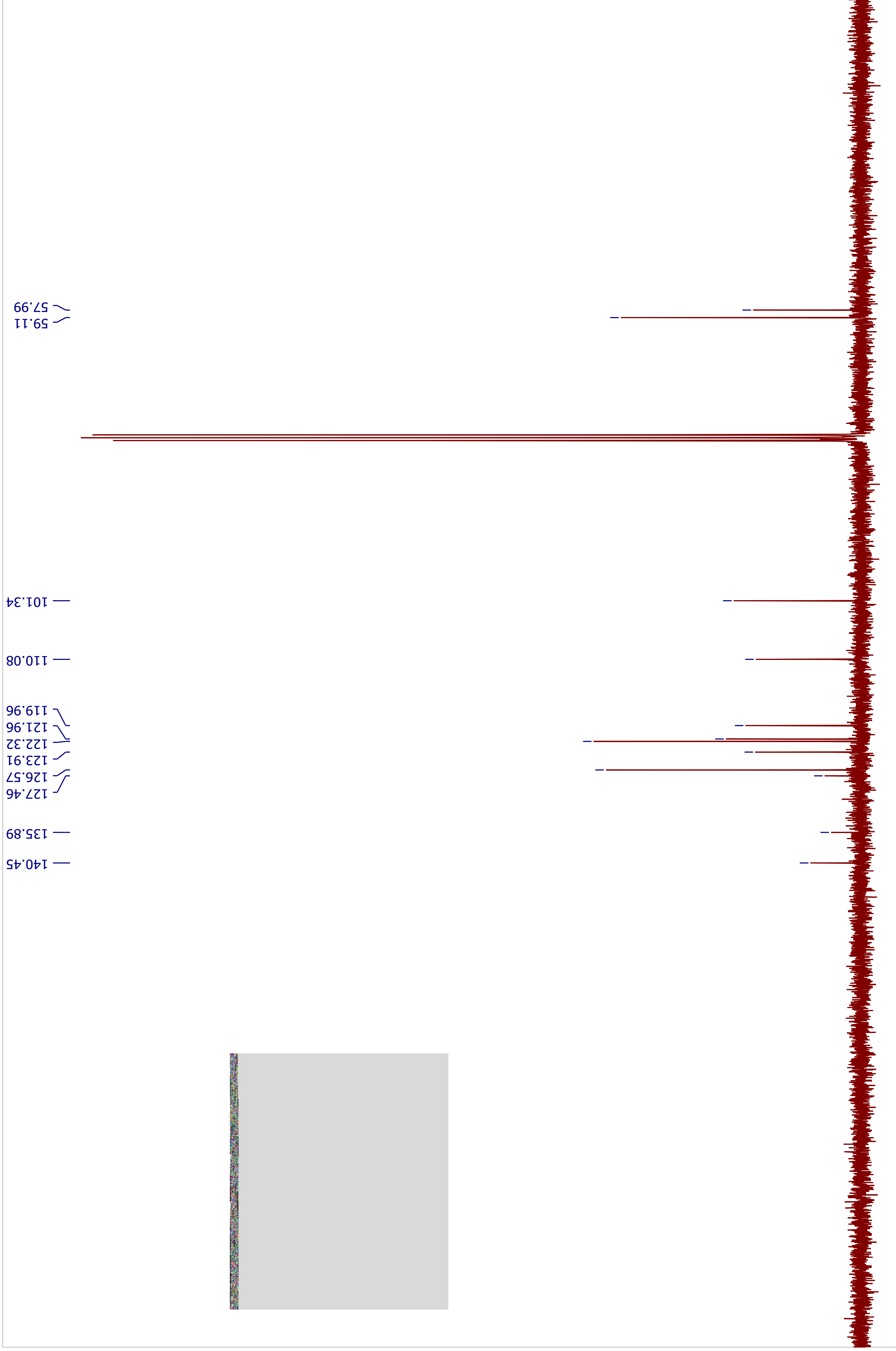
4.23
4.04
7.25 7.24 7.24 7.23 7.22 7.22 7.21 7.21
3.11
3.98
7.24 7.22
f1 (ppm)
7.38 7.38 7.37 7.36 7.36 7.35 7.35 7.35
1.09
7.38 7.36 7.34
f1 (ppm)
6.79 6.79 6.79 6.78 6.78
0.98
6.79 6.77
f1 (ppm)
N
N
H



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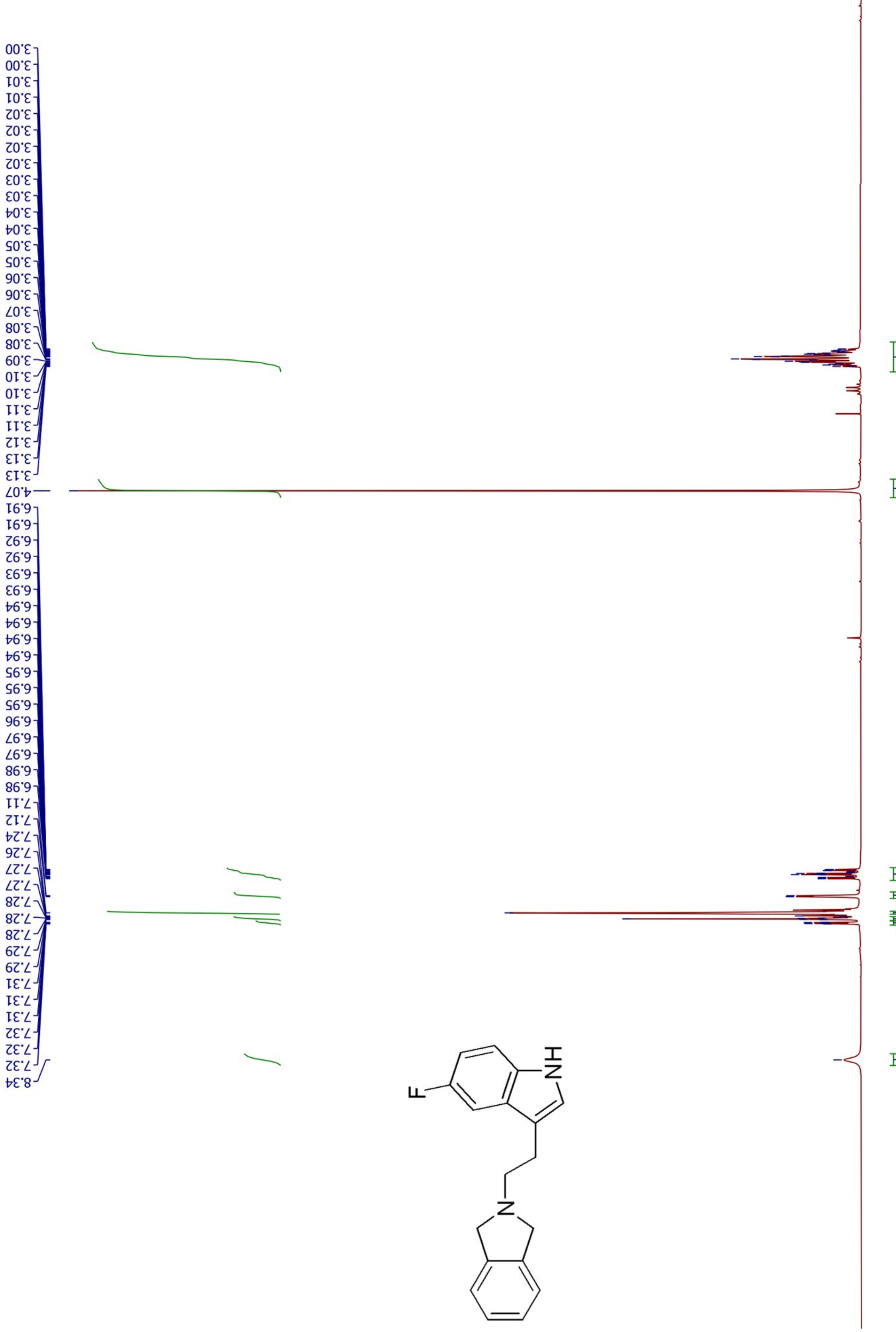
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3.06
3.06
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3.08
3.08
3.09
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3.10
3.11
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3.12
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3.13
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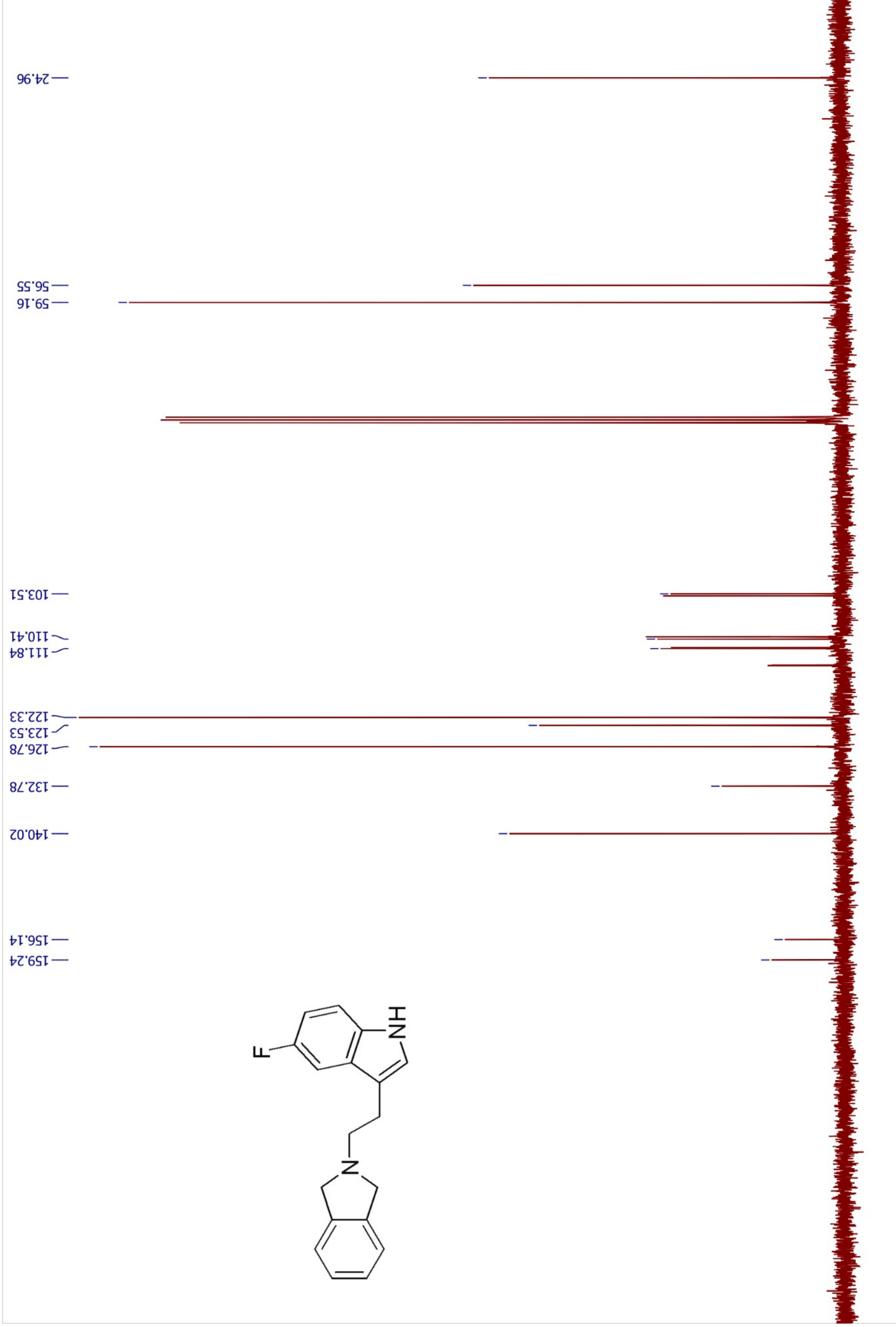
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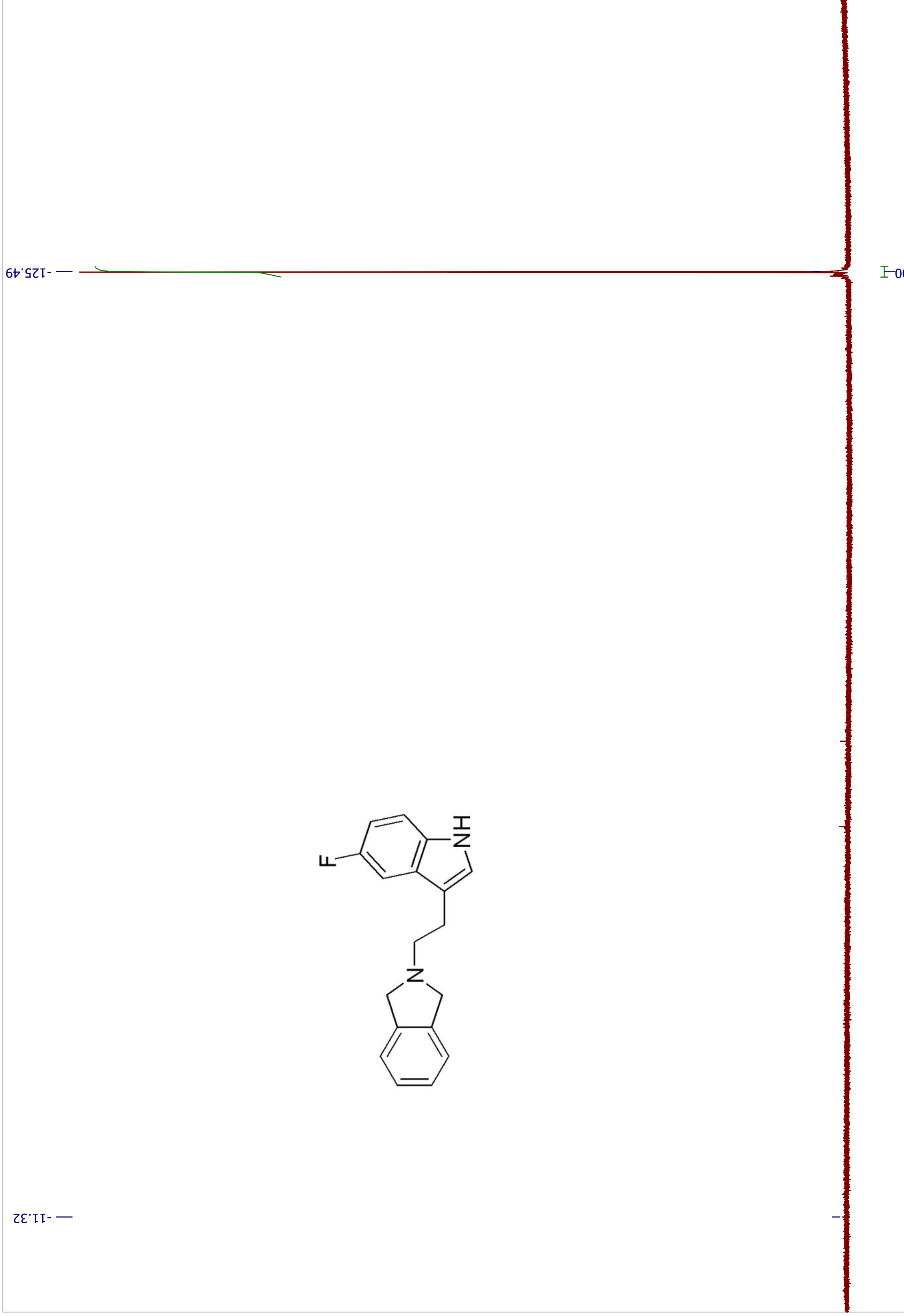
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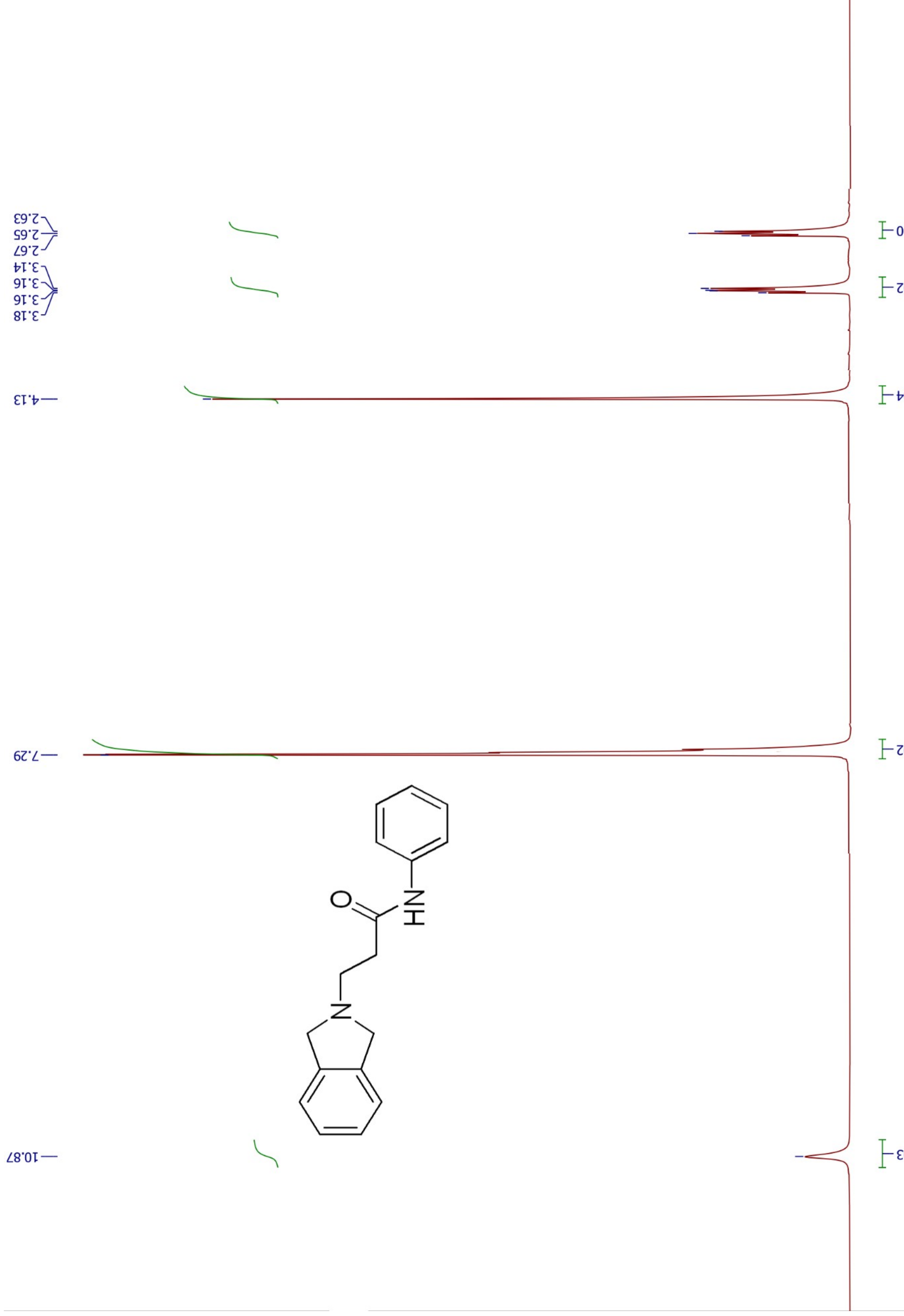
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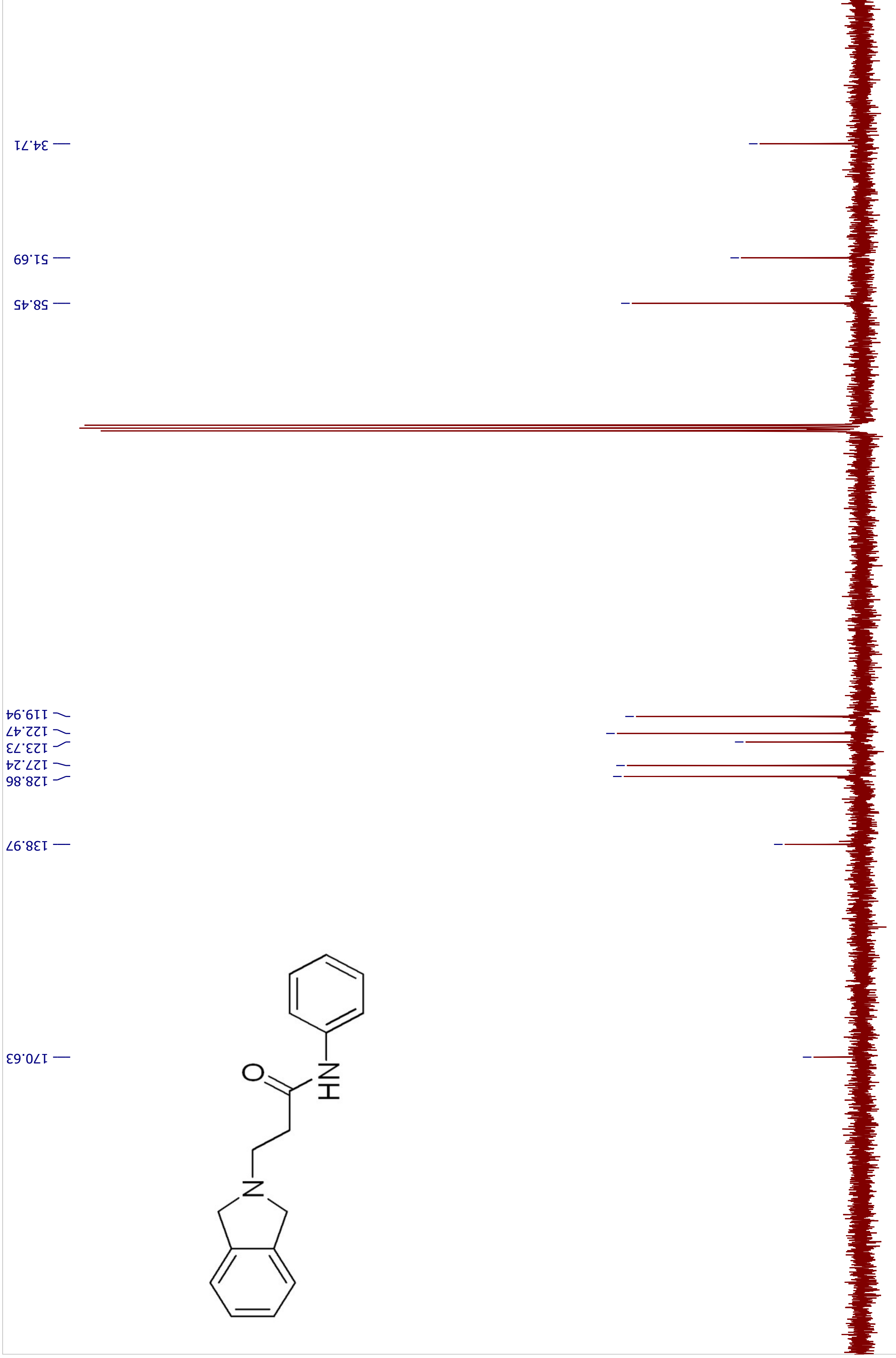
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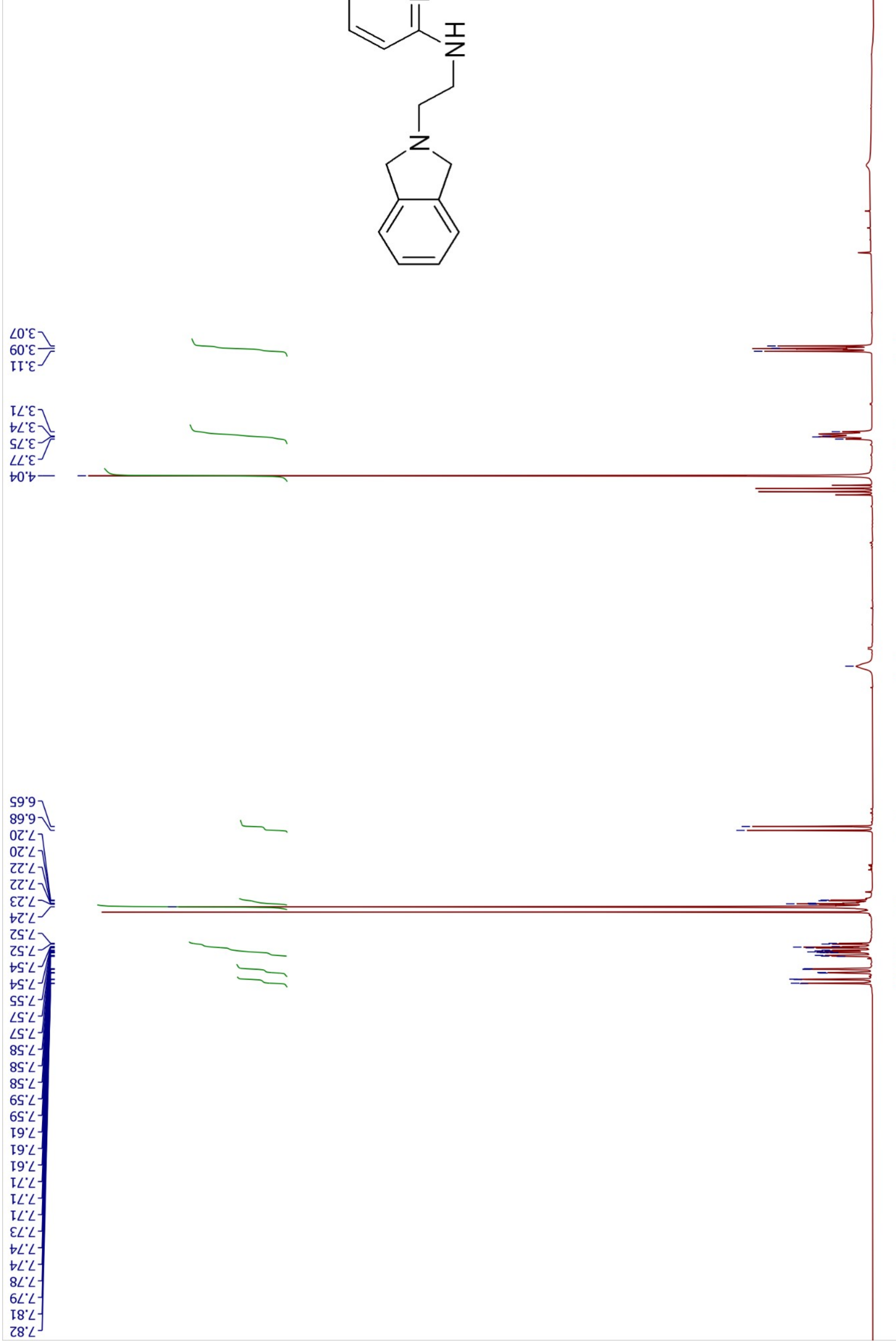
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N


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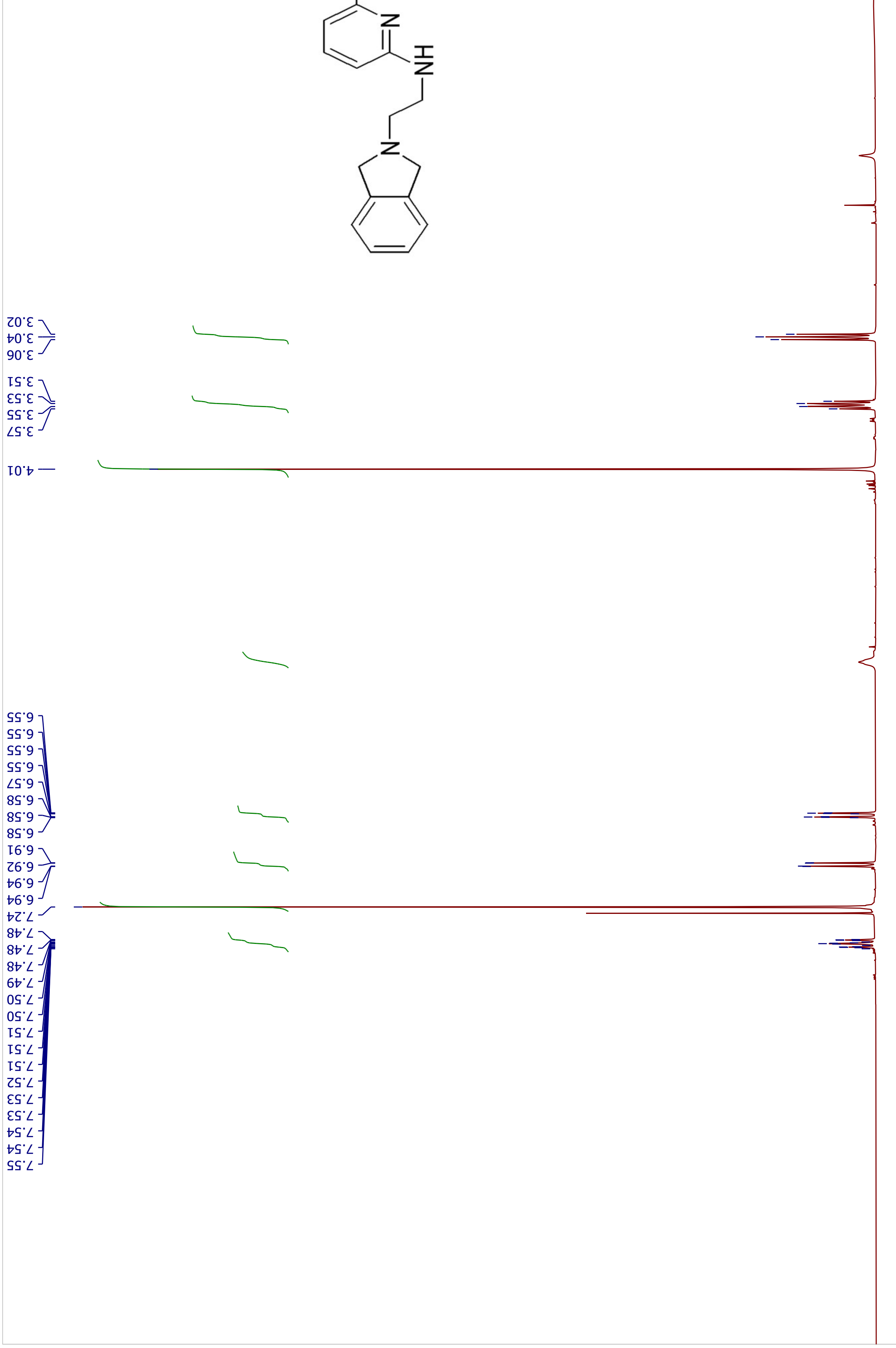

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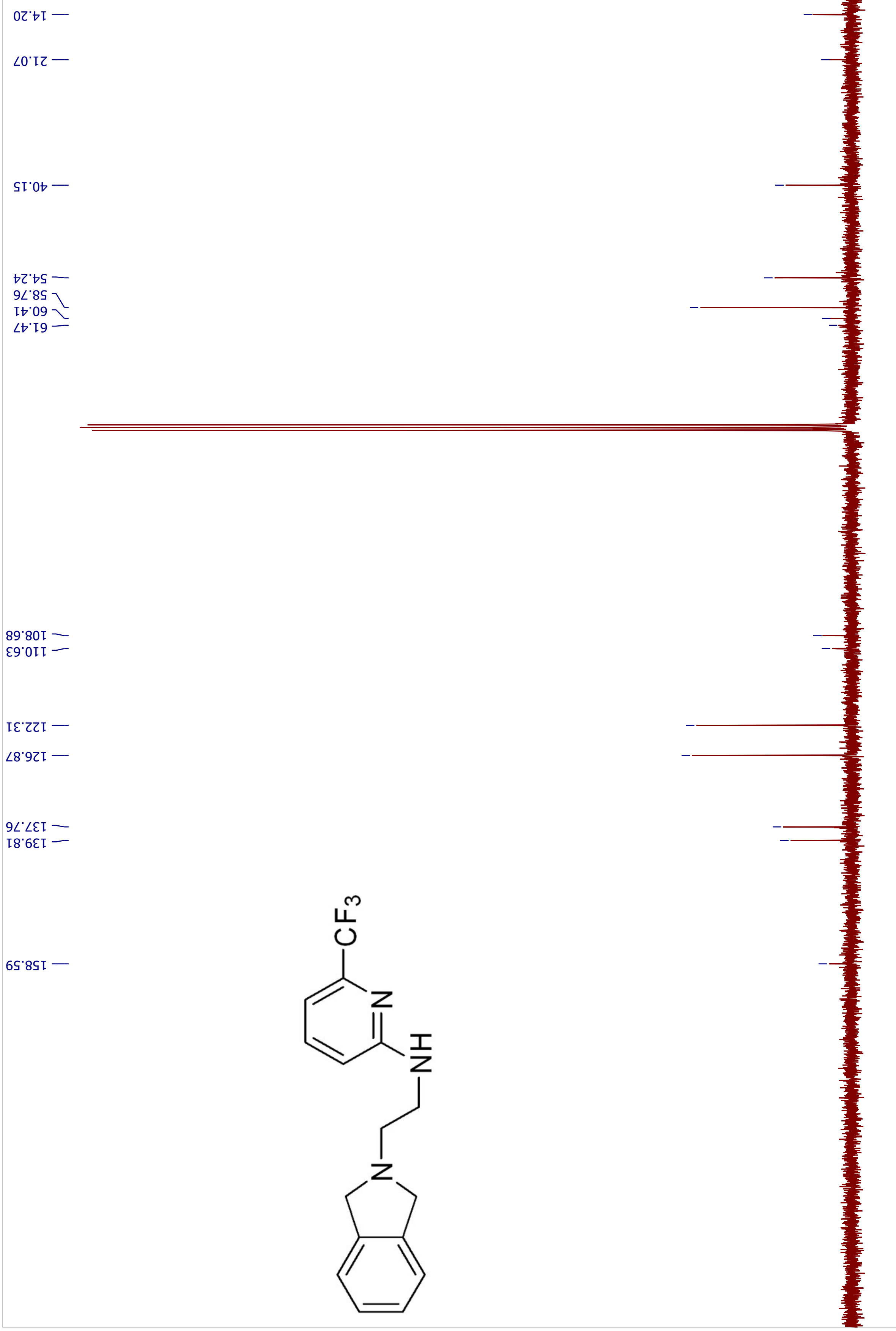
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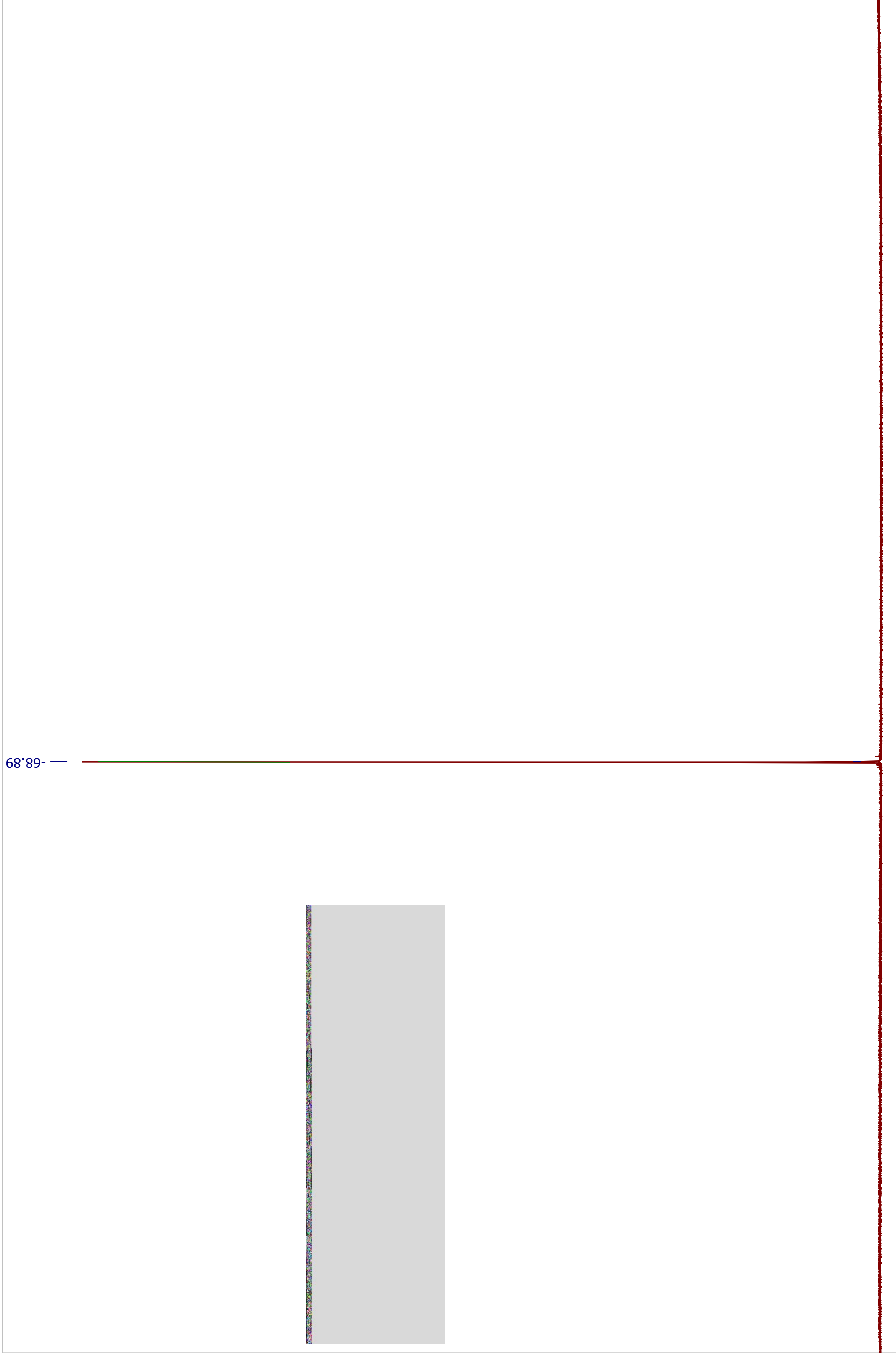
NH
N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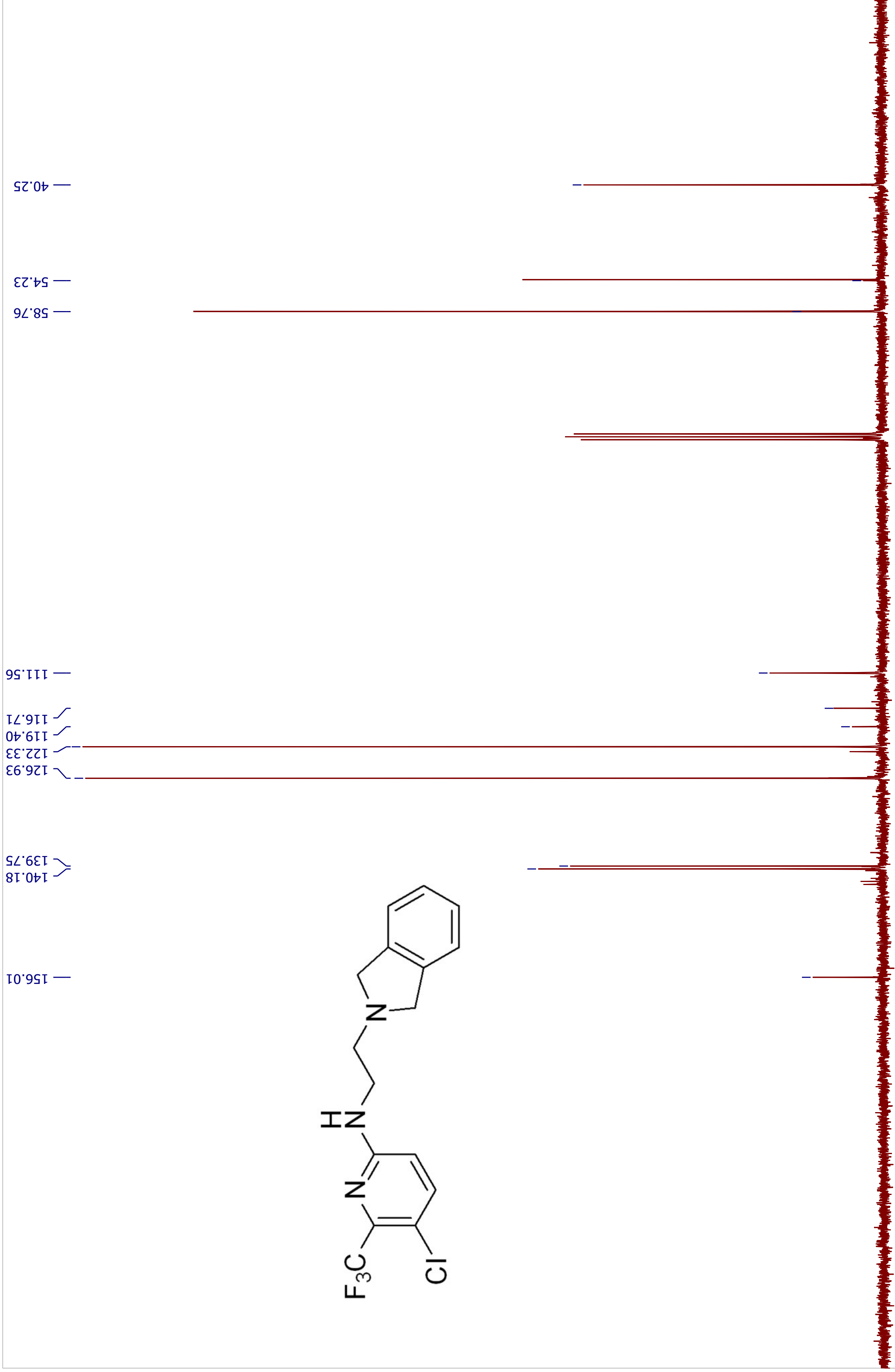
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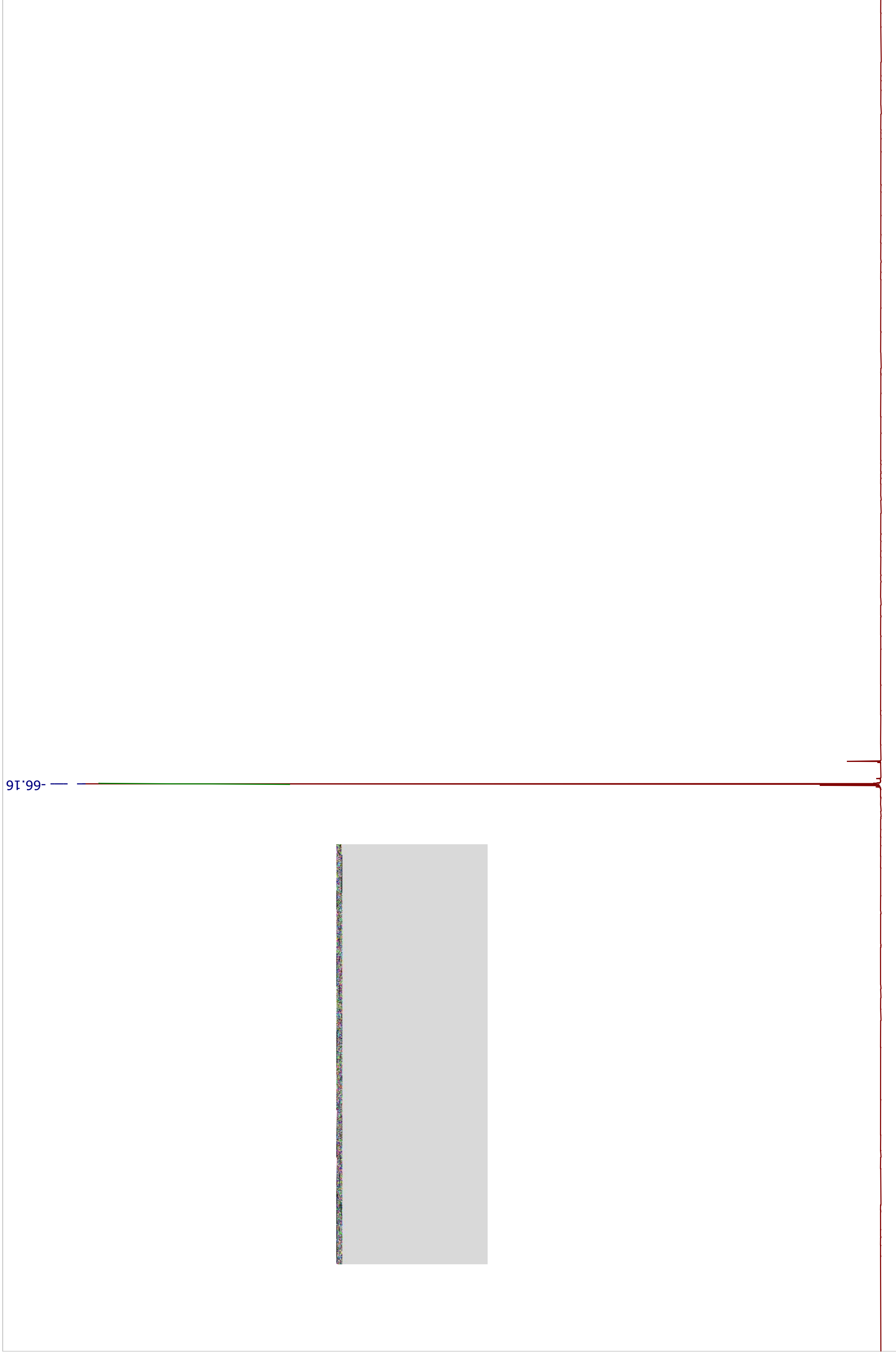
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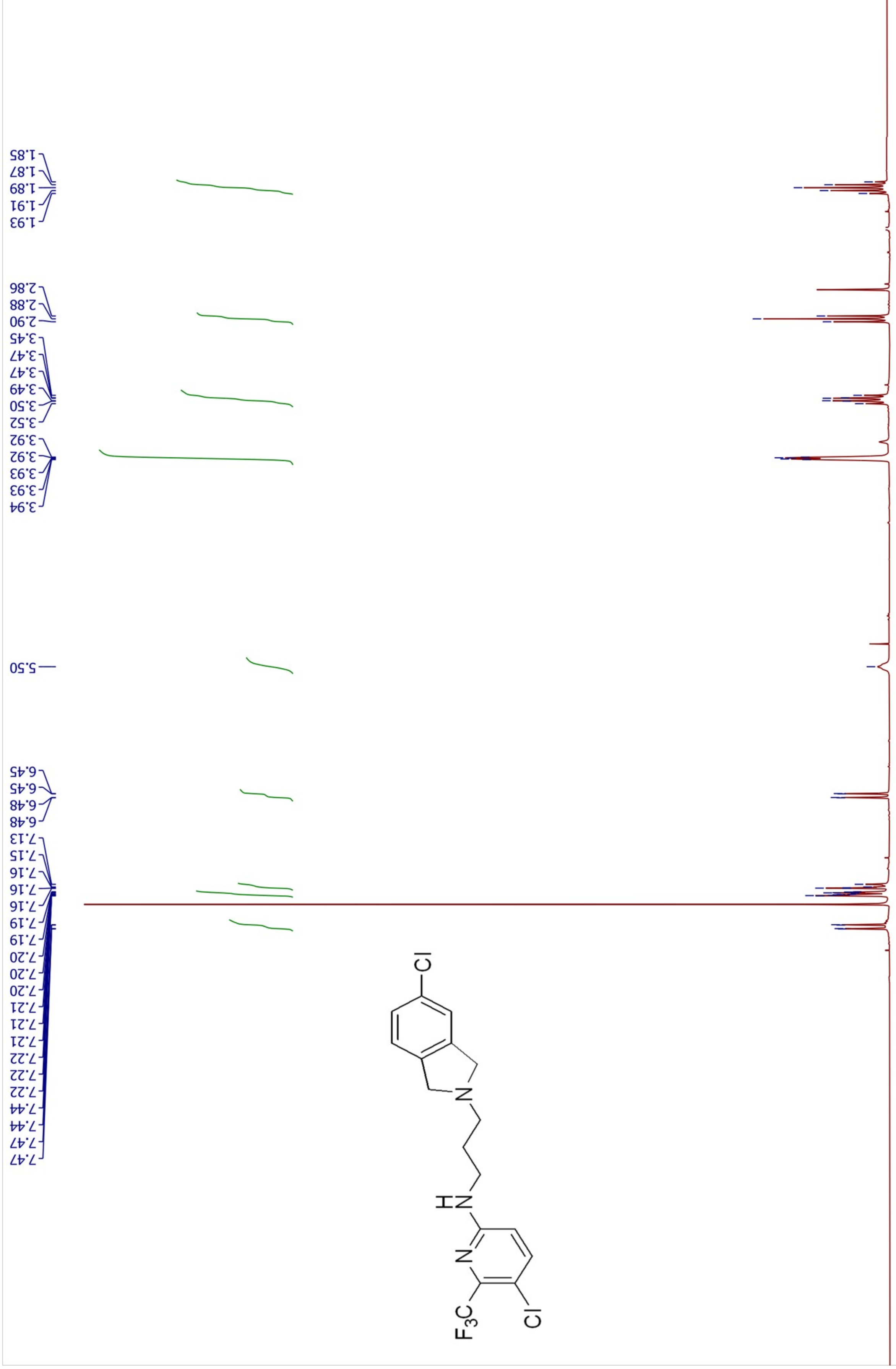

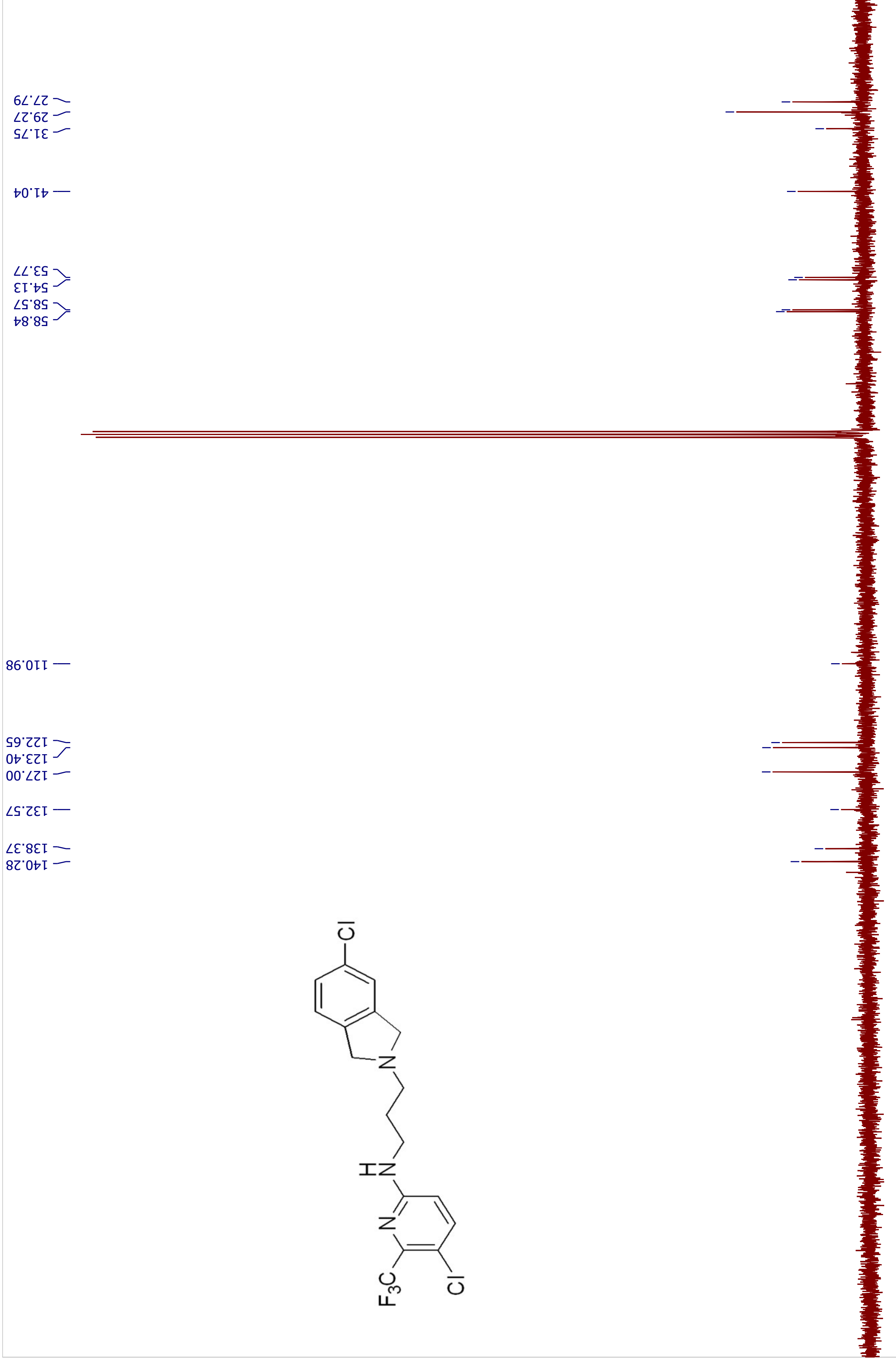
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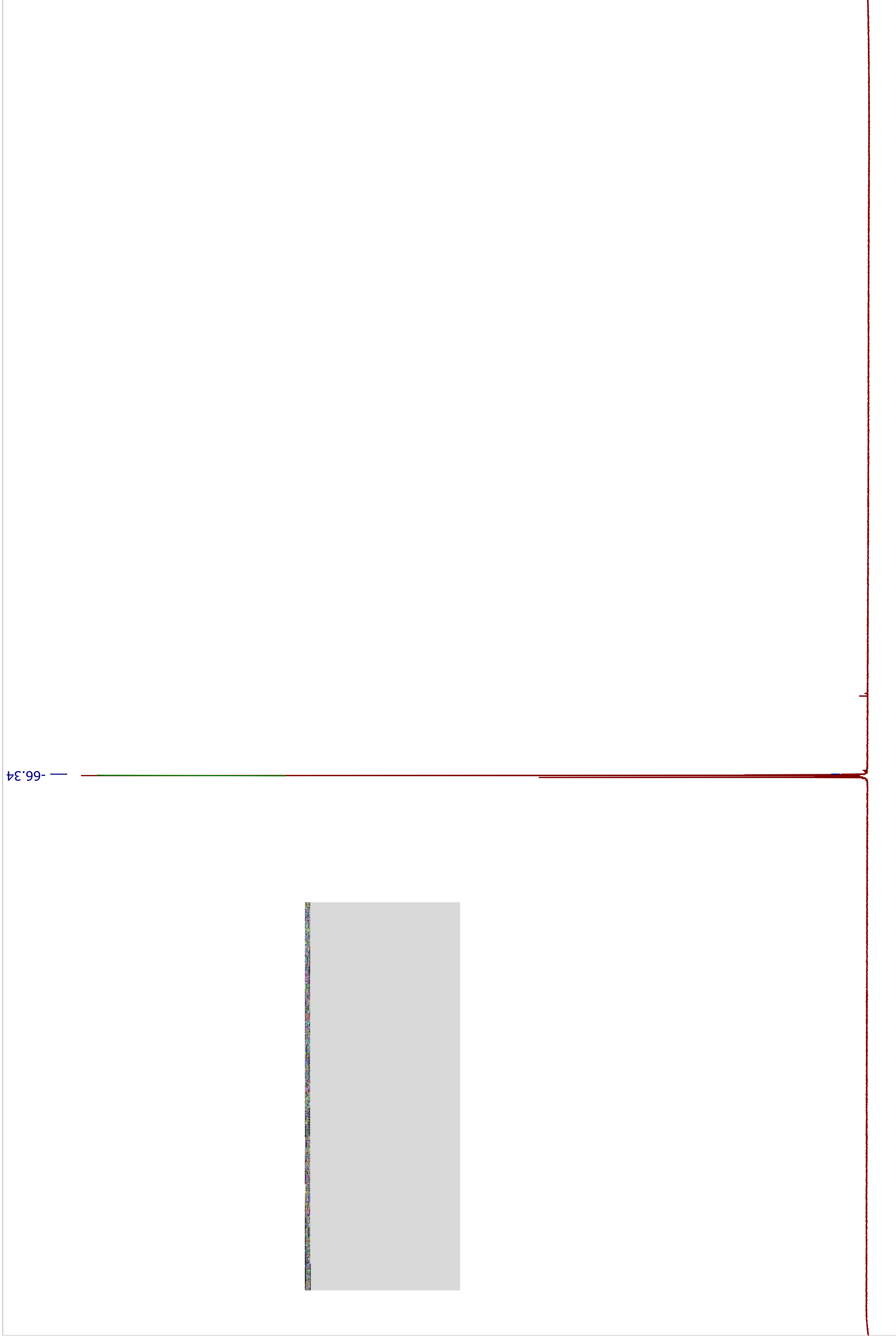
N
H
N
F3C
Cl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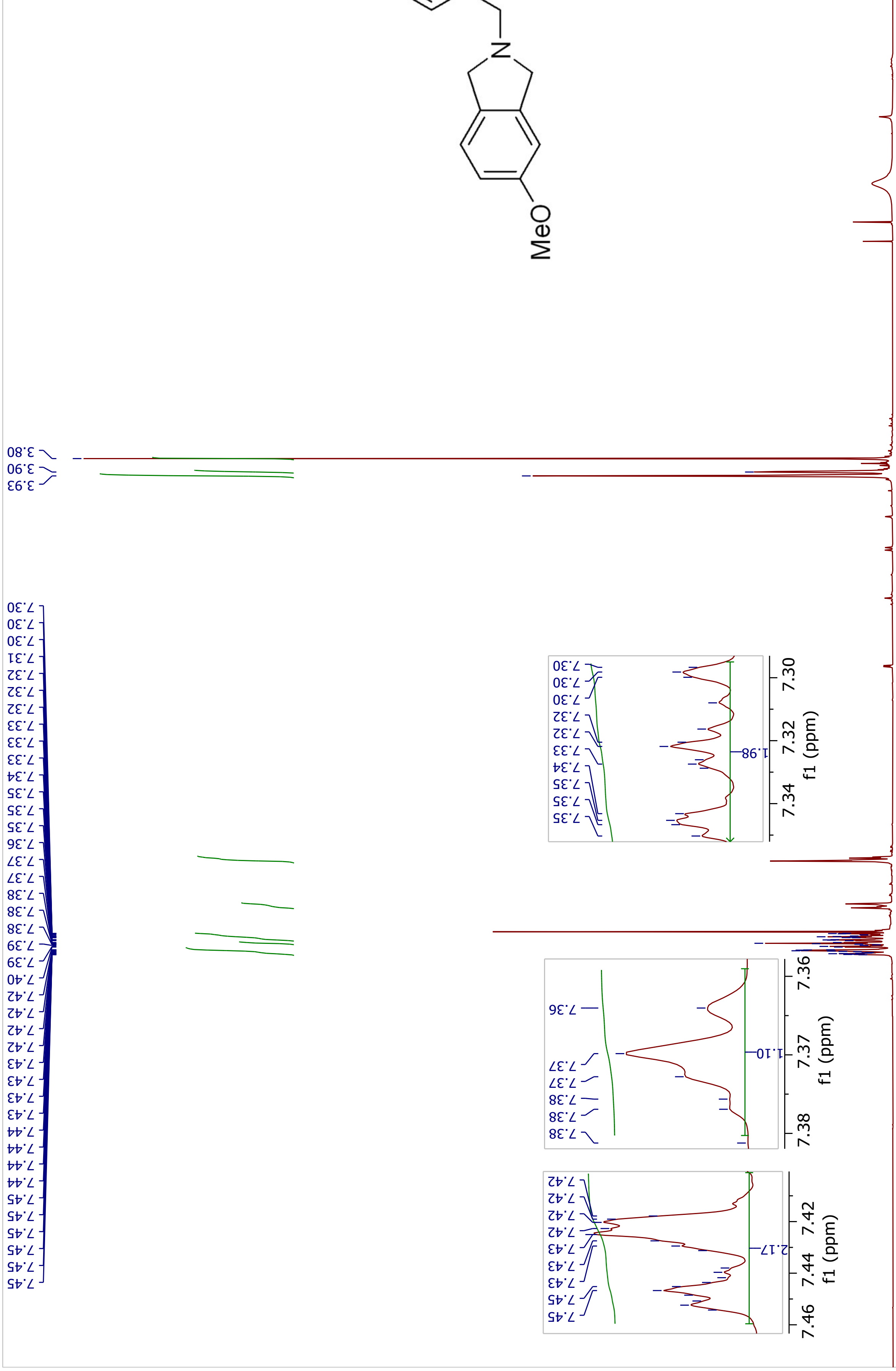

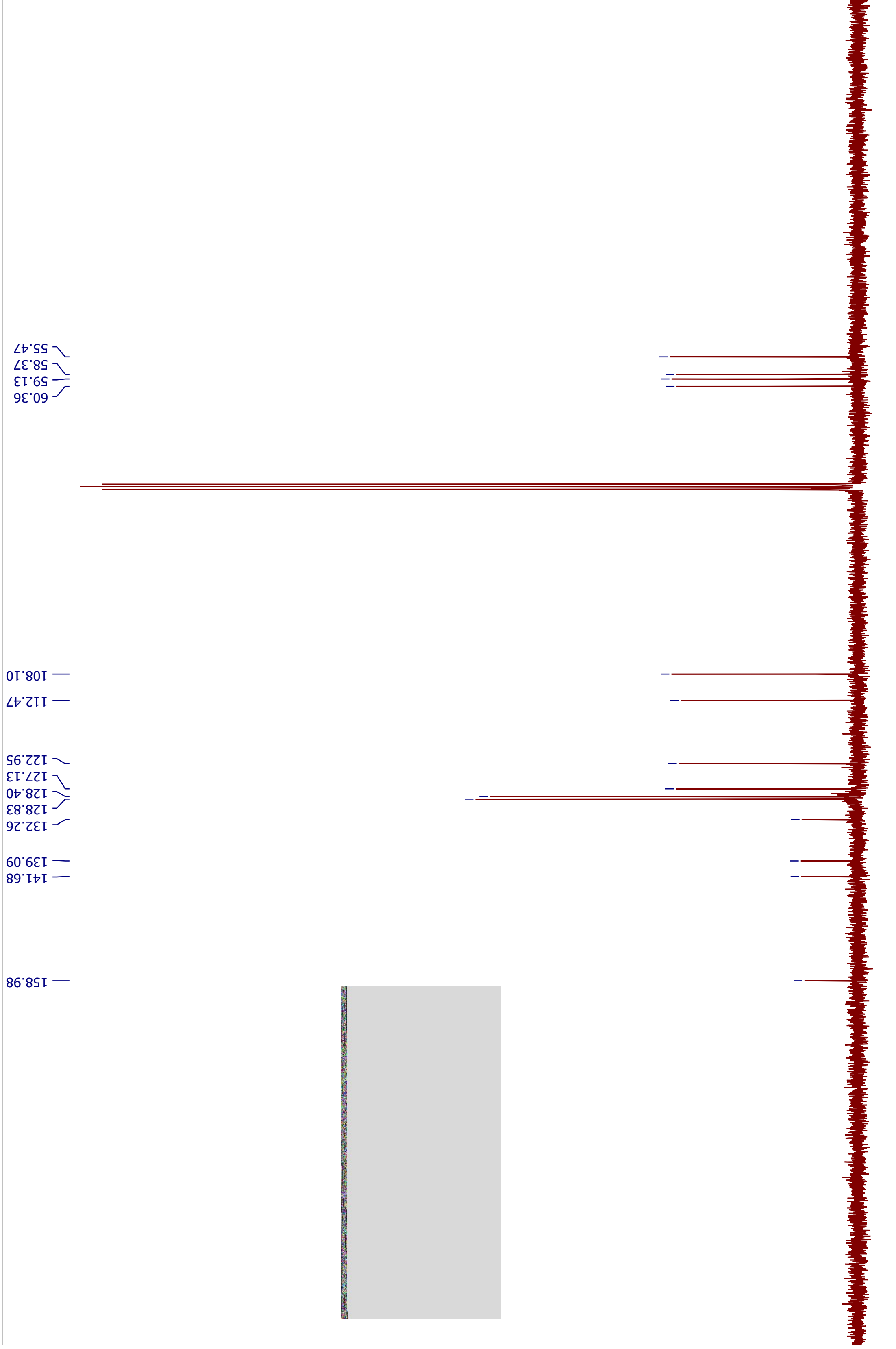
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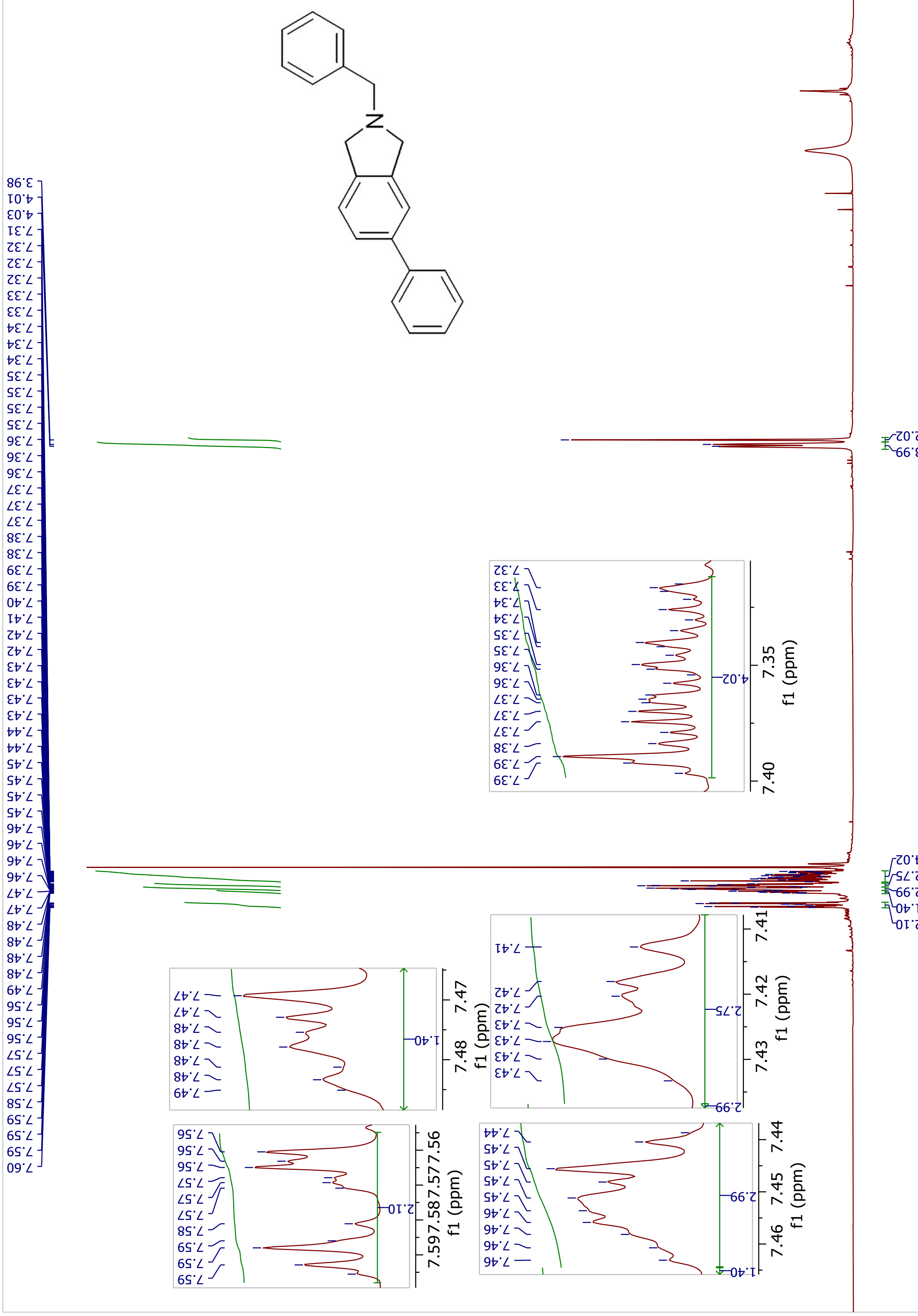
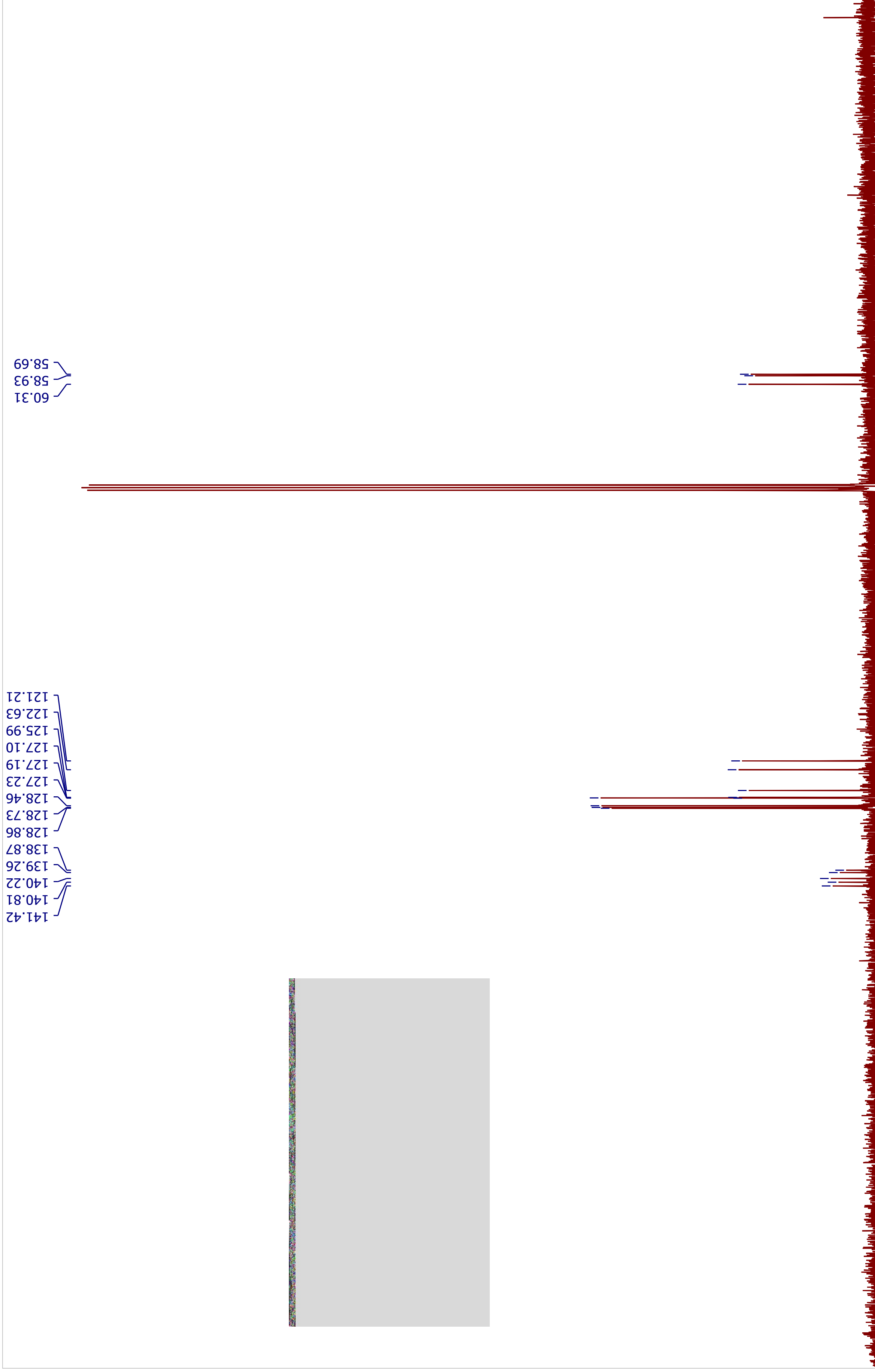
158.98

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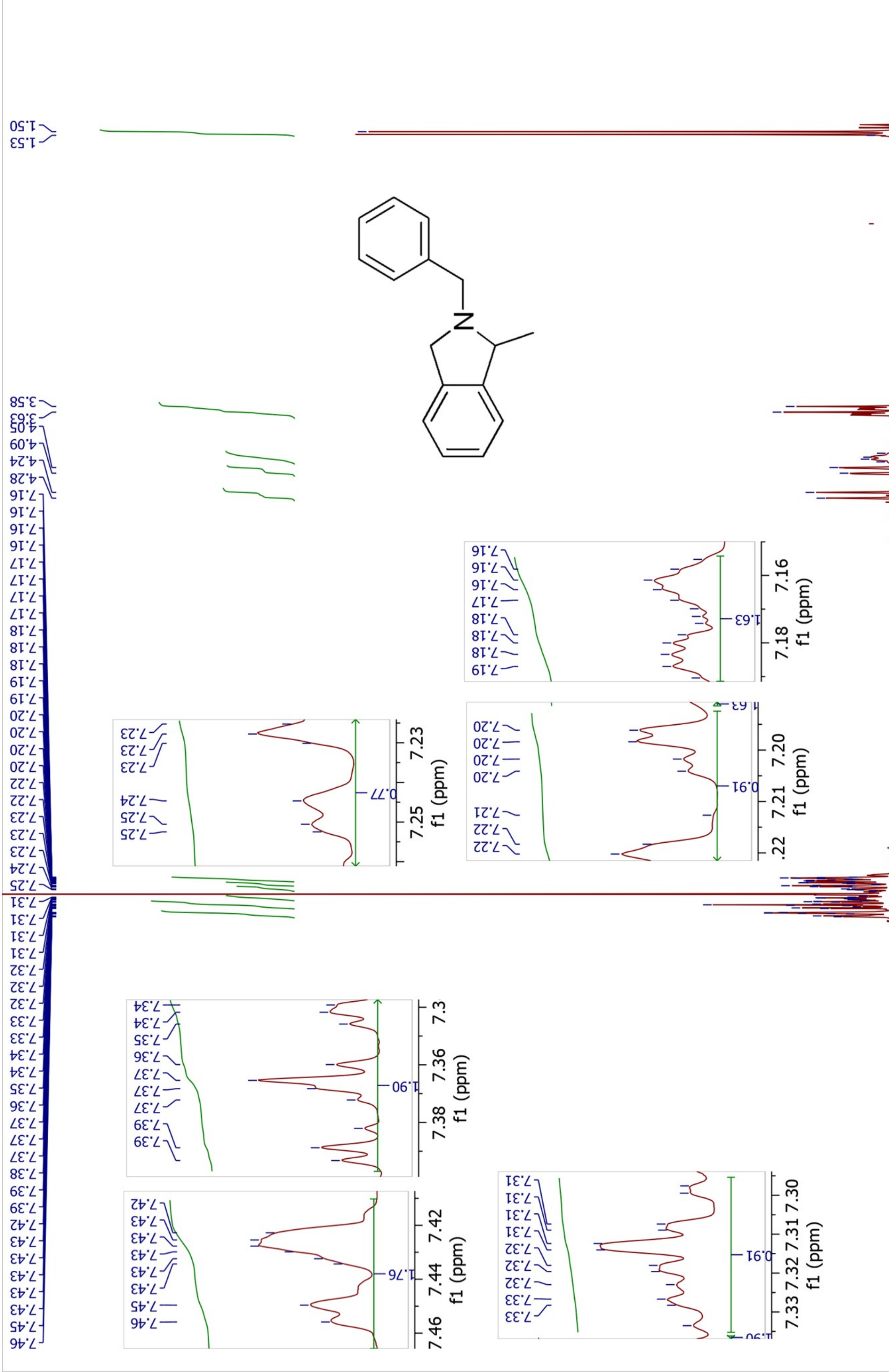
140.81
141.42



1.50
1.53
3.58
3.63
4.05
4.09
4.24
4.28
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7.18
7.19
7.20
7.22
7.23
7.24
7.25
7.31
7.32
7.33
7.34
7.35
7.36
7.37
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7.39
7.42
7.43
7.45
7.46
N
f1 (ppm)


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58.07
63.70
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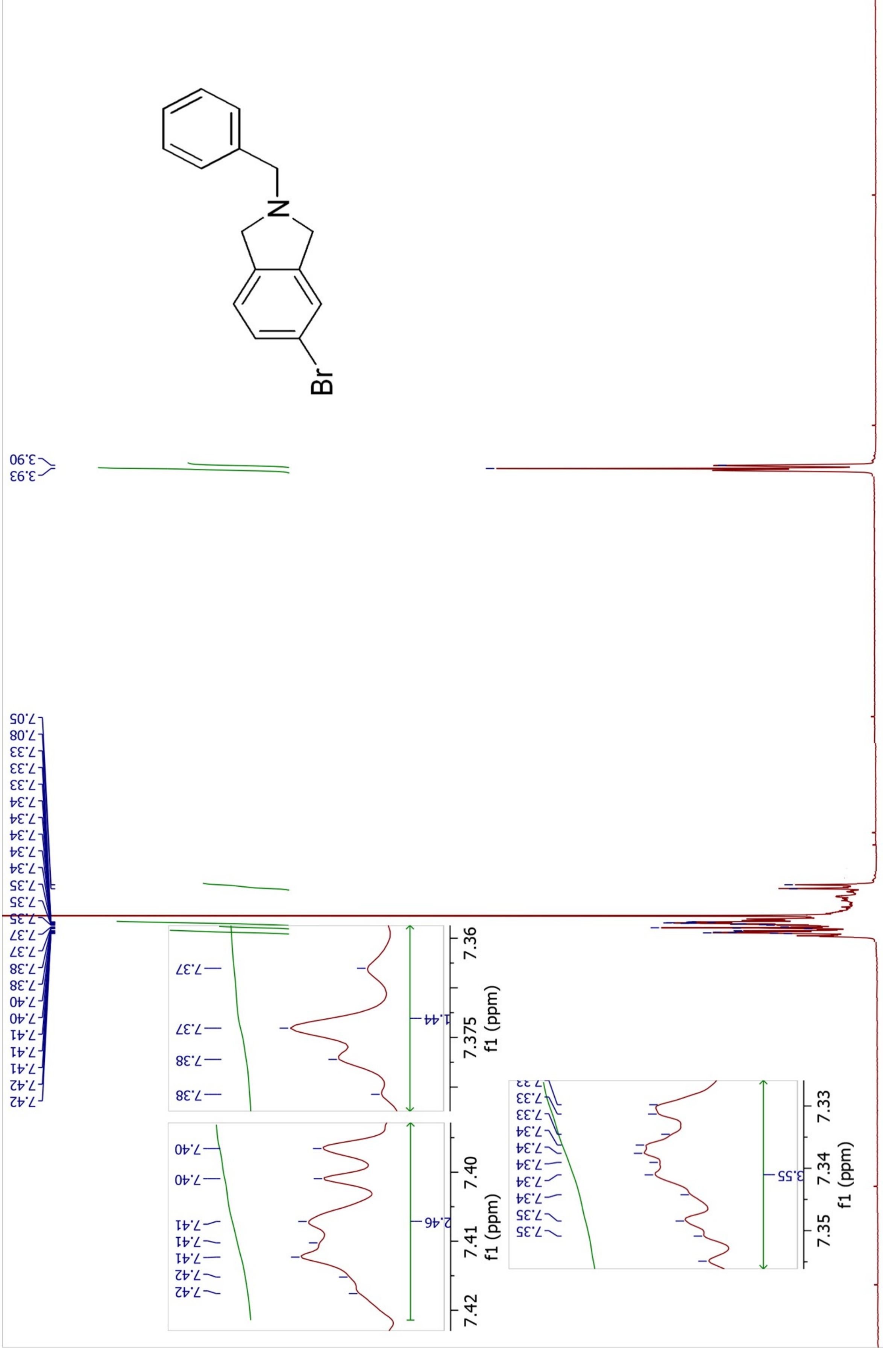
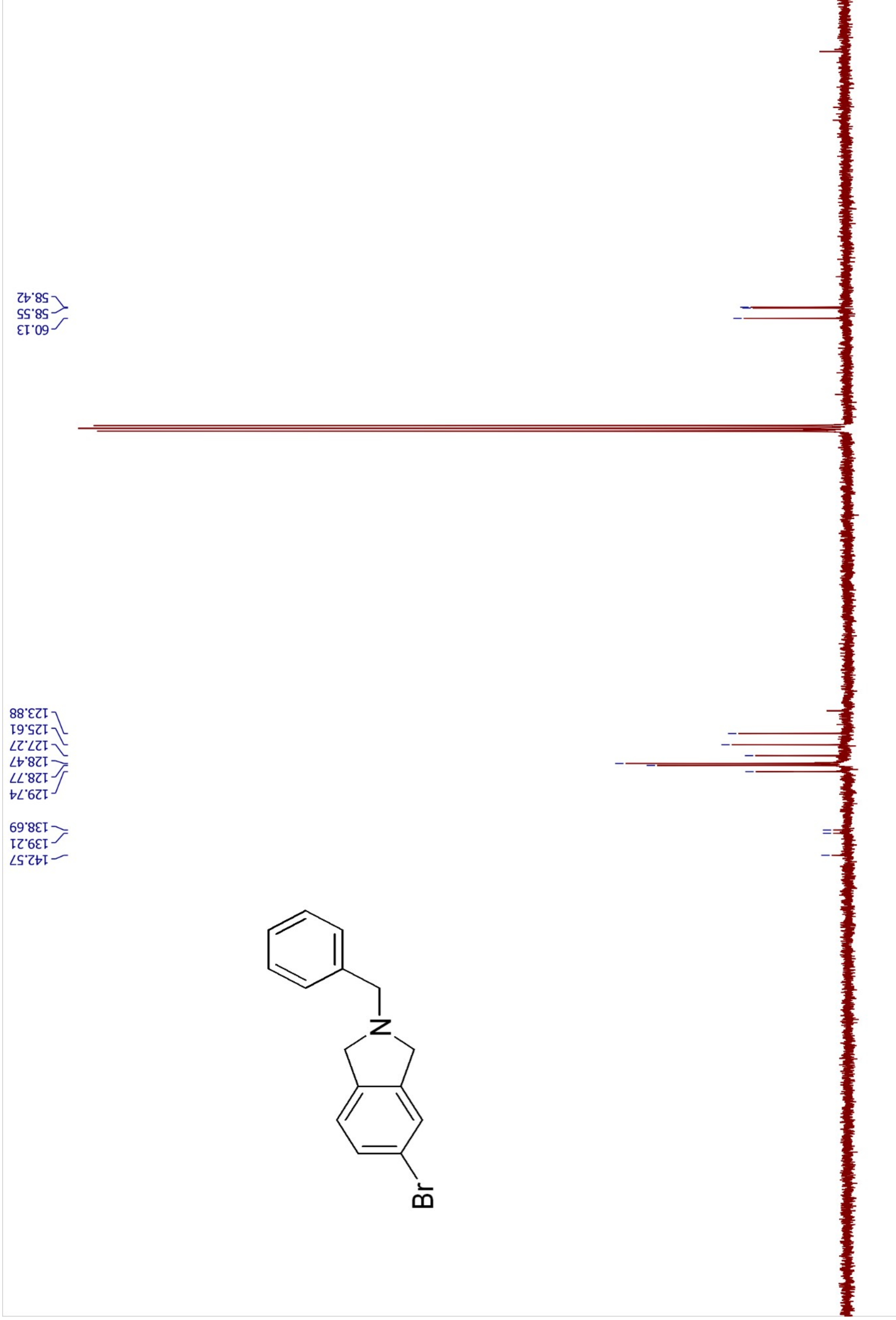
N


Br
N
f1 (ppm)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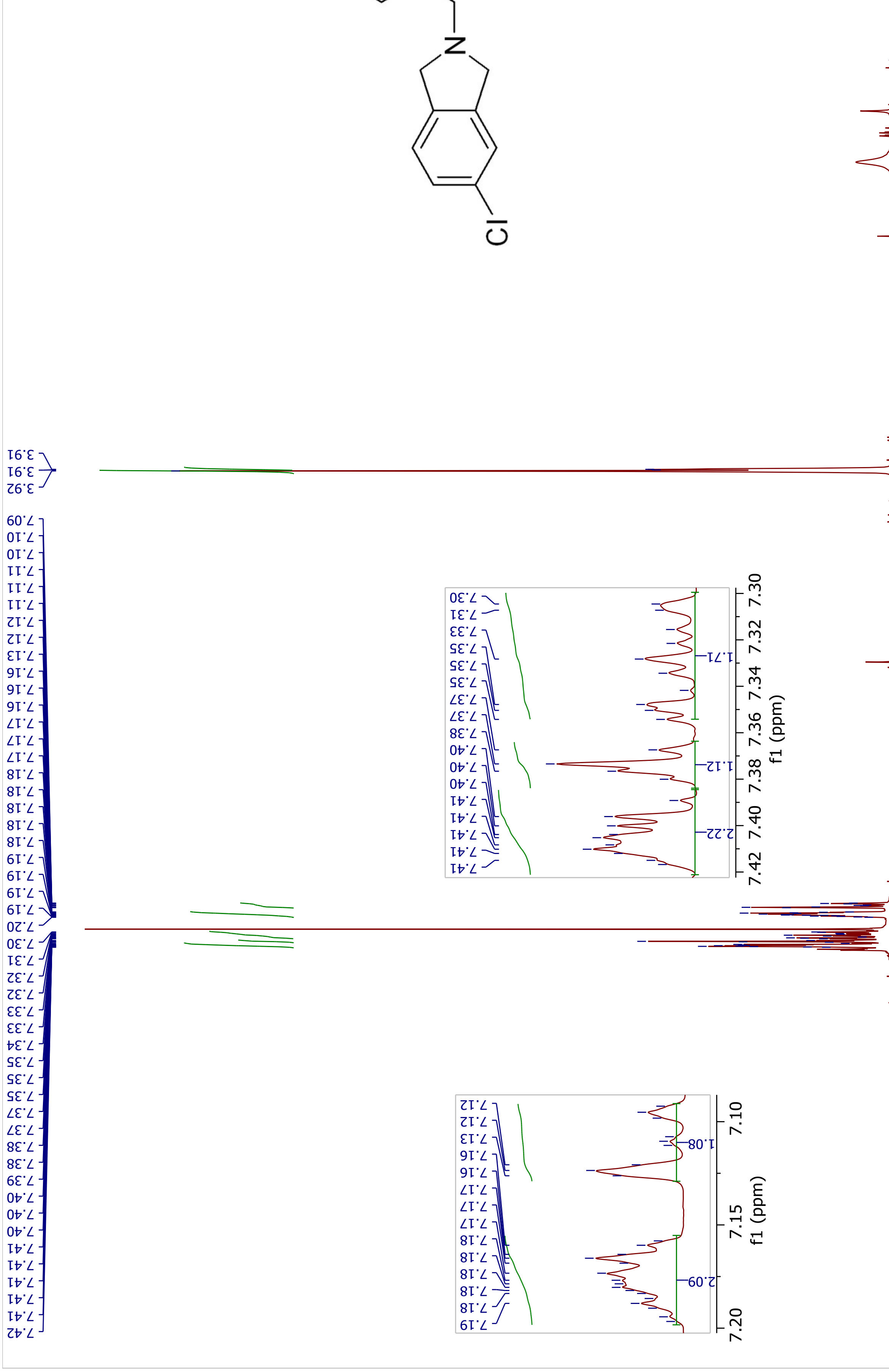
Br
N


Cl
N
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3.91
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7.10
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7.12
7.13
7.16
7.16
7.16
7.17
7.17
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7.40
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7.41
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7.42
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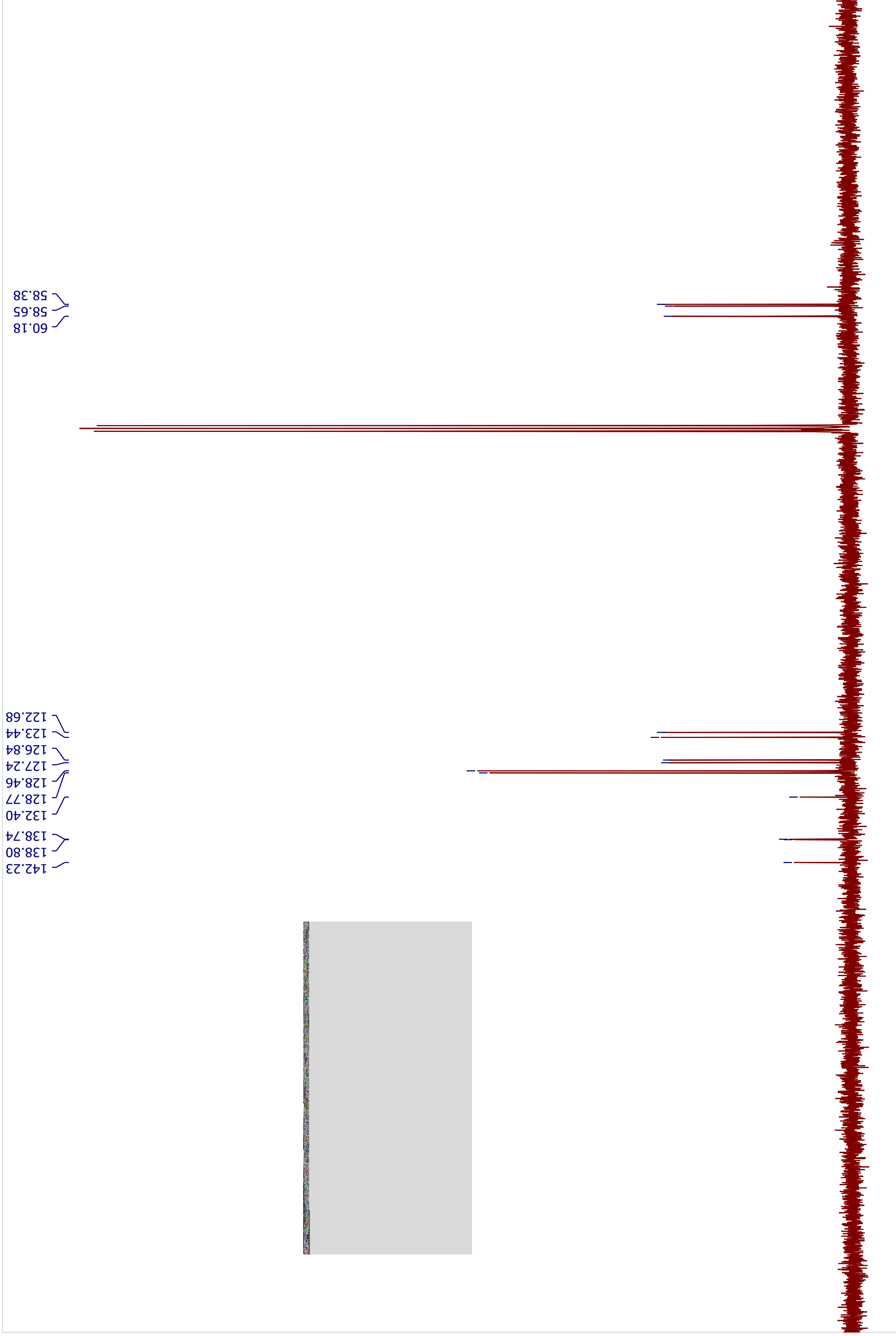
f1 (ppm)
1.08
2.09
f1 (ppm)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138.74
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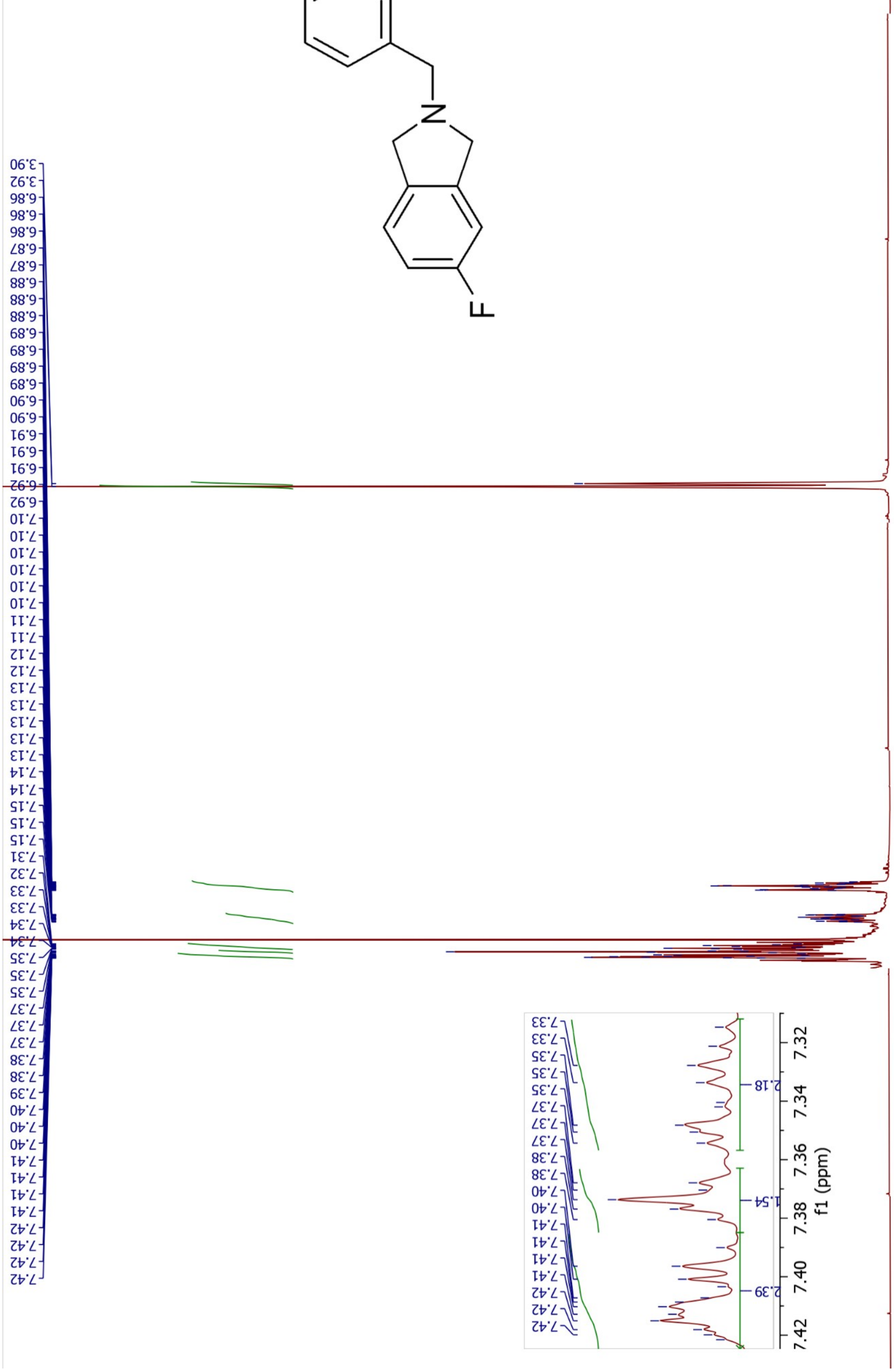
142.23


N
F
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7.42
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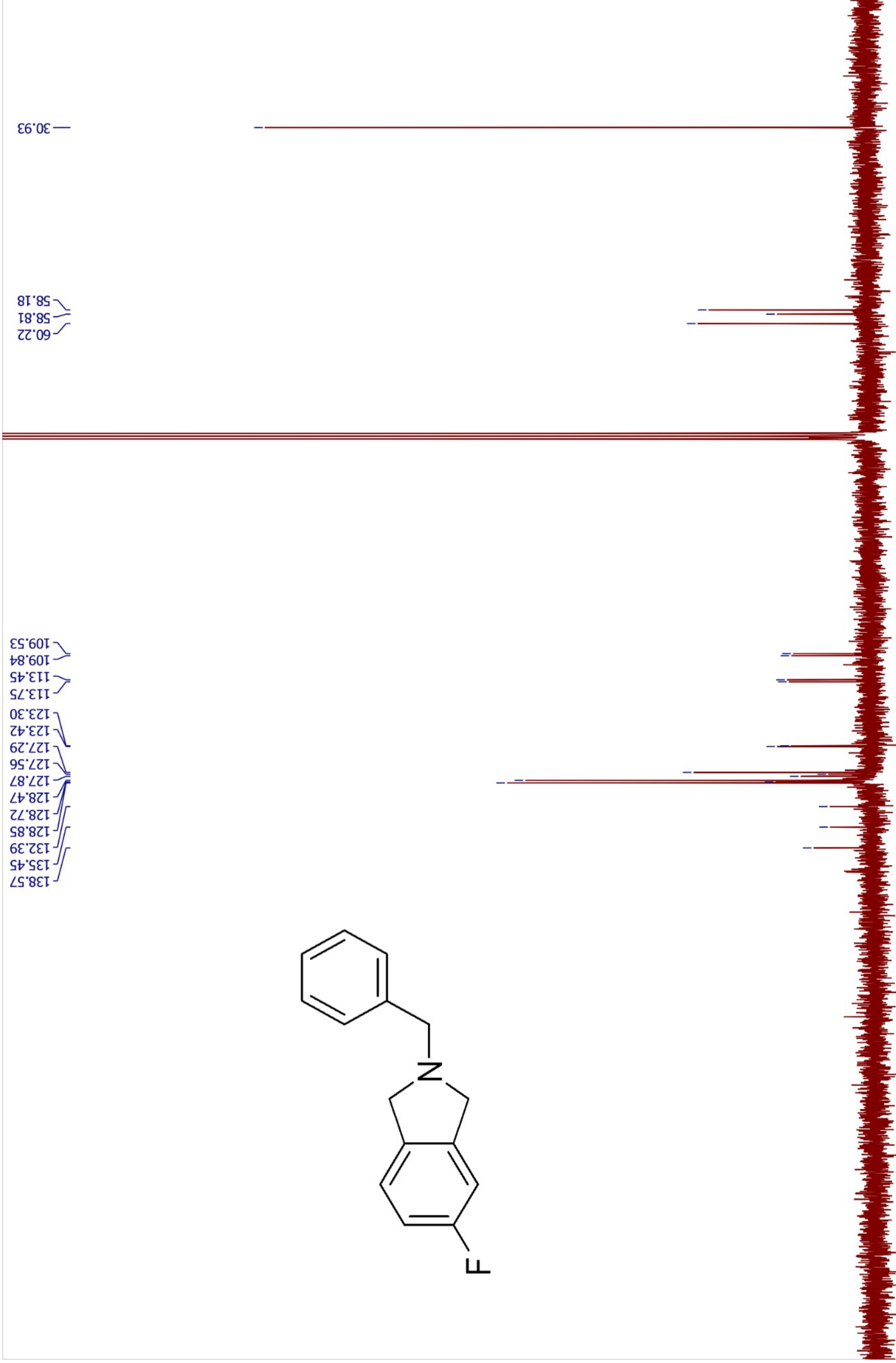
7.40
7.42
f1 (ppm)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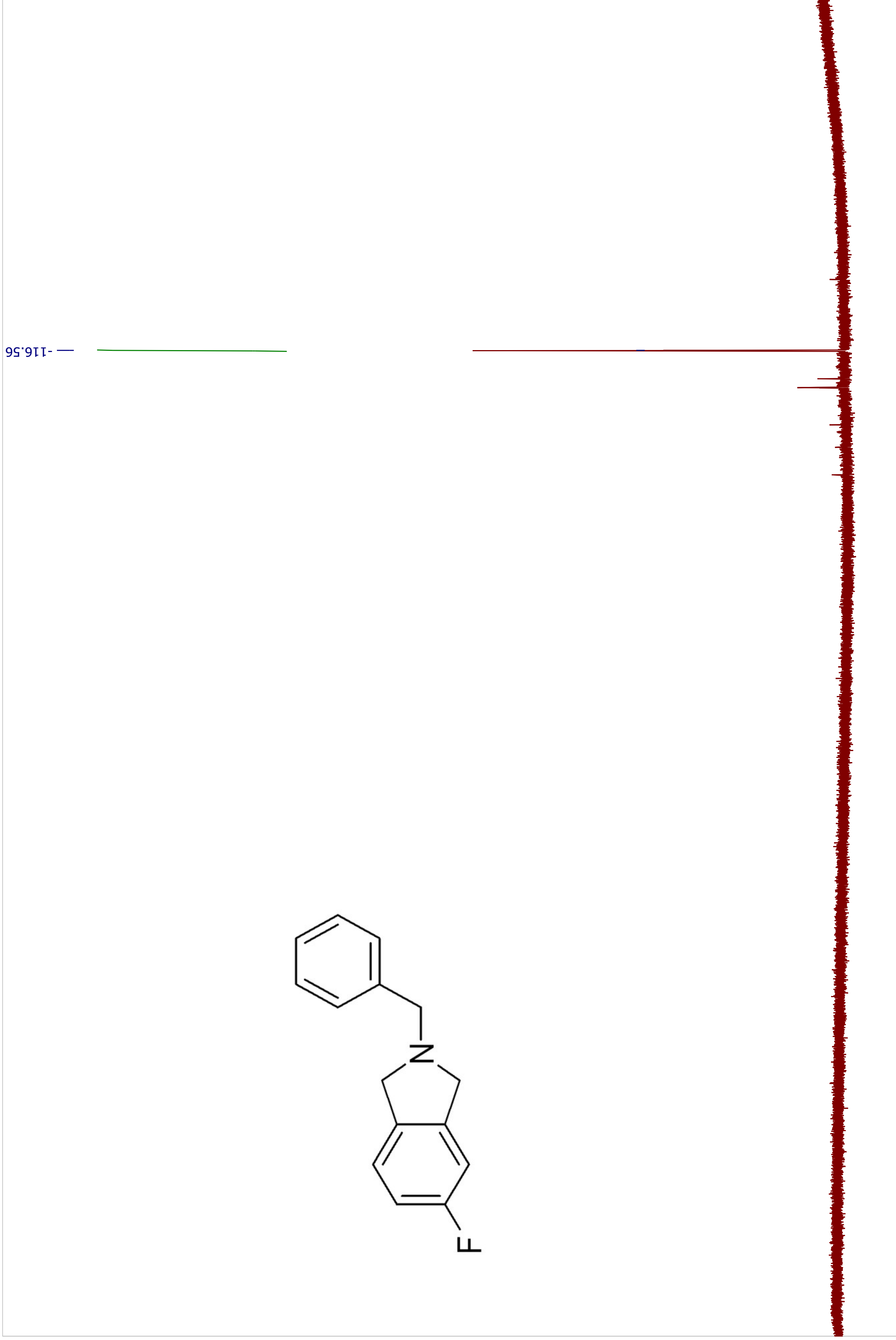
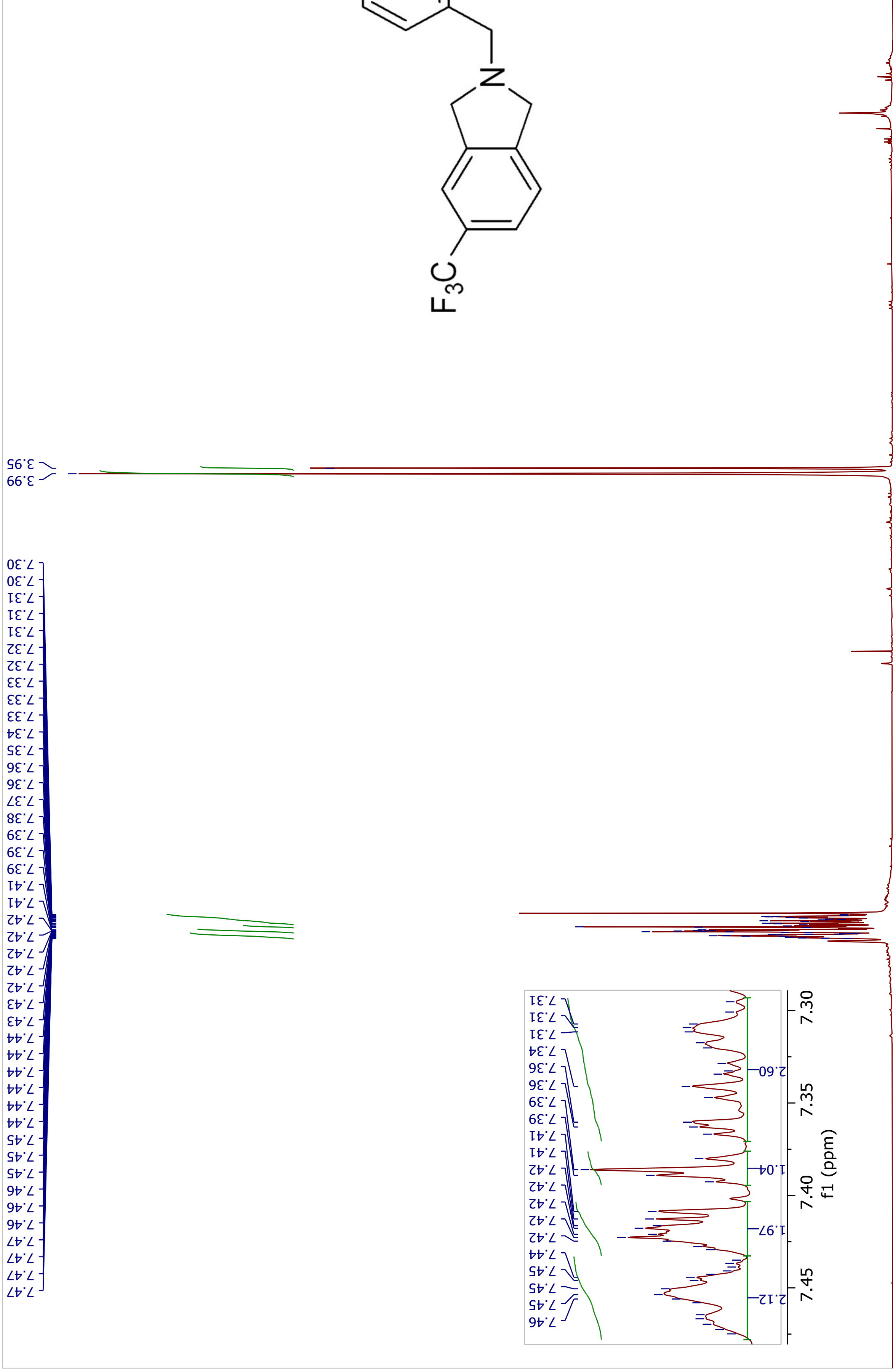
128.72
128.85
132.39
135.45
138.57
N
F


-116.56


F3C
N
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7.46
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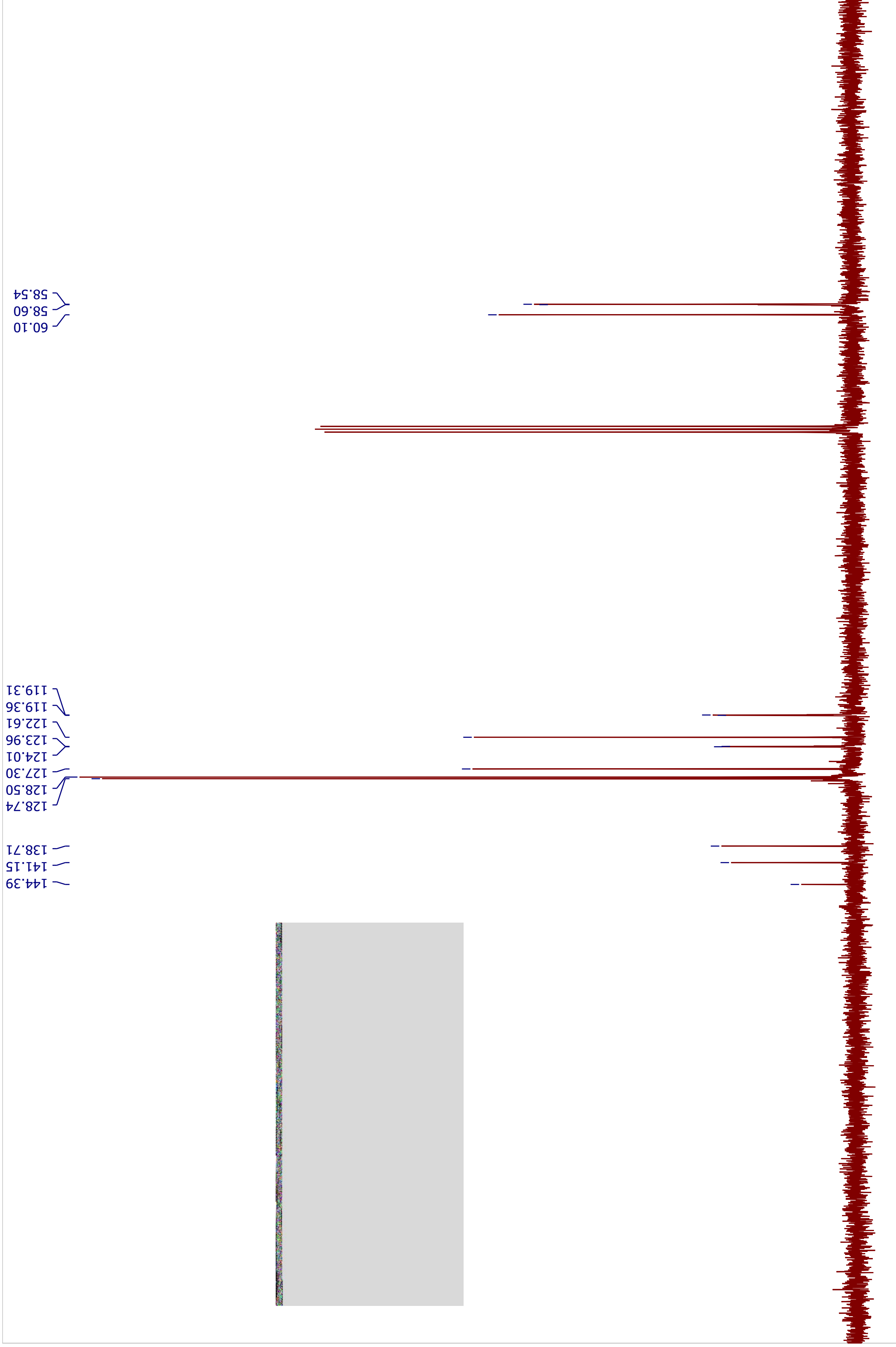
7.35
7.40
7.45
f1 (ppm)



58.54
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60.10
119.31
119.36
122.61
123.96
124.01
127.30
128.50
128.74
138.71
141.15
144.39

5.Reference.

[S1] S.Wang, Y. Zhou, H. Huang, *Org. Lett.* **2021**, *23*, 2125–2129