

– Supporting Information –

S1 Appendix

Pyrimidine analogs of C1 domain–targeted isophthalates as protein kinase C ligands: Structure-activity relationships and biological activities.

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NMR Spectra

Peak reports and multiplet assignments are provided for all ^1H , ^{13}C and ^{19}F NMR spectra. Compound peaks are highlighted in **green** and solvent peaks in **yellow**. All 2D-NMR spectra are edited to highlight the correlation peaks. ^{13}C -HSQC spectra include DEPT-135 information with $-\text{CH}-$ and $-\text{CH}_3$ correlation peaks in positive phase (**red**) while $-\text{CH}_2-$ correlation peaks in negative phase (**blue**). For some compounds also ^{15}N -HMBC NMR spectrum is available.

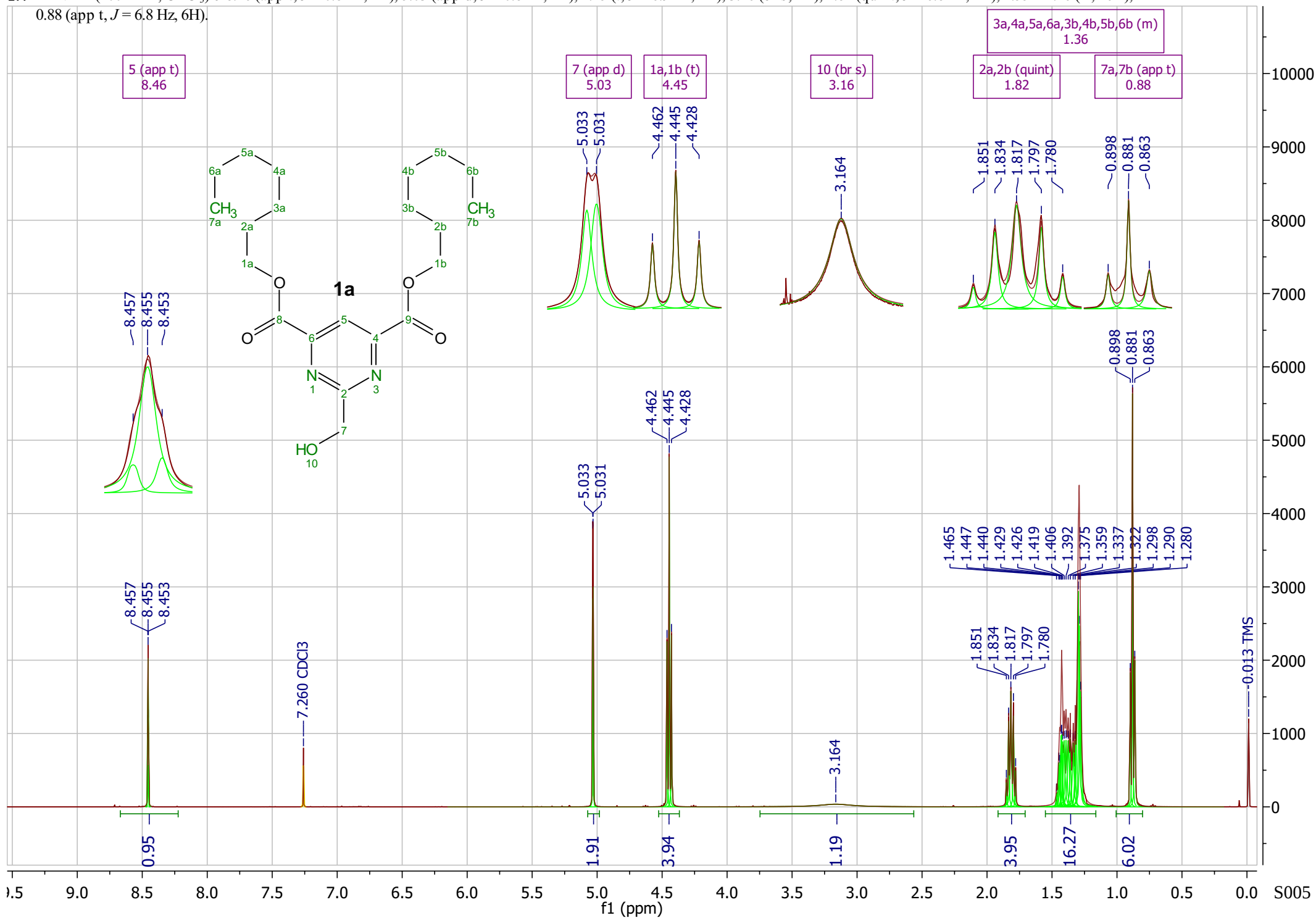
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Compounds			Page
Compound	1a		S005
Compound	1b		S011
Compound	1c		S017
Compound	1d		S022
Compound	1e		S026
Compound	1f		S032
Compound	1g		S038
Compound	1h		S045
Compound	2a		S049
Compound	2b		S053

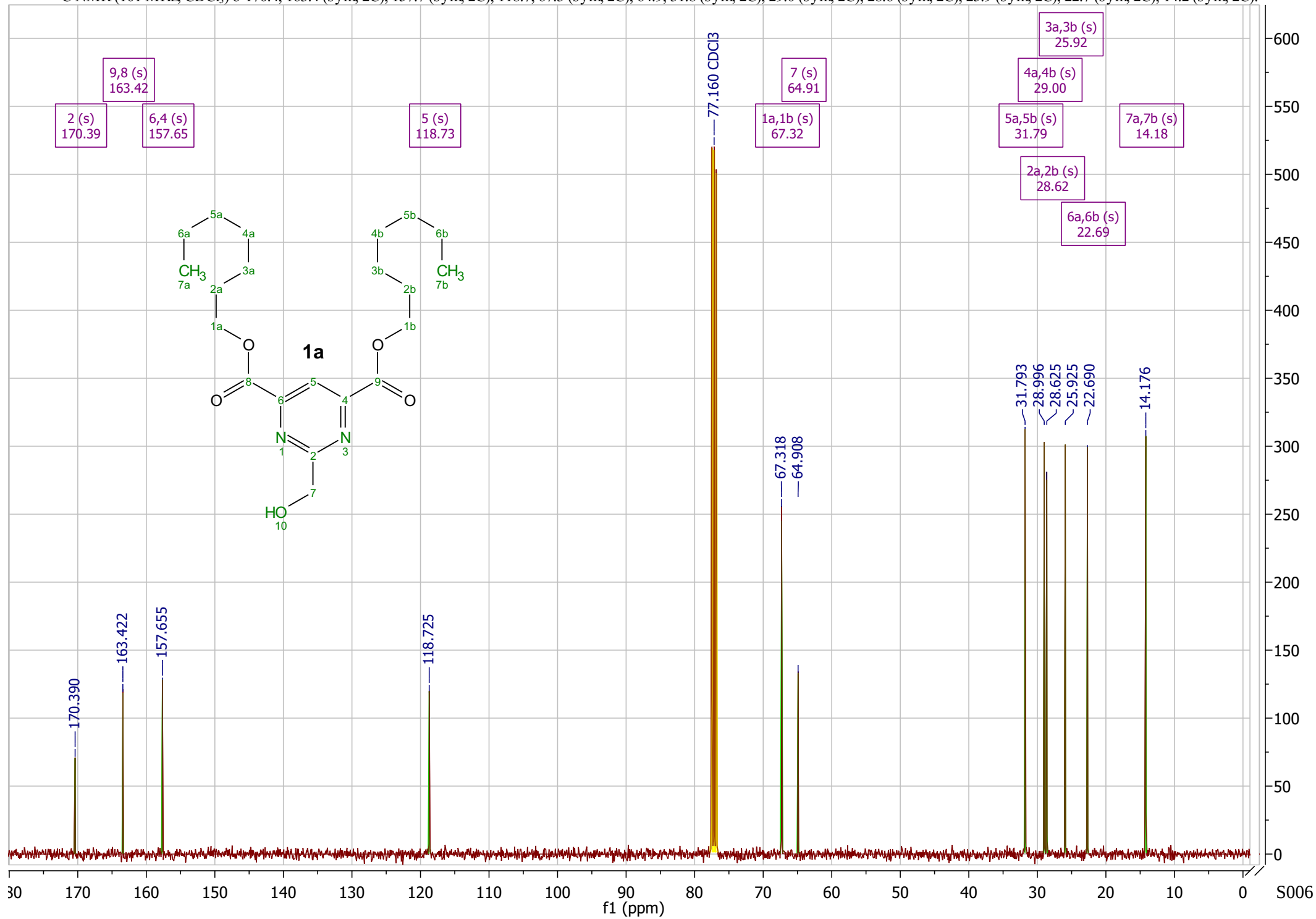
Compound	2c		S057
Compound	2d		S061
Compound	2e		S065
Compound	2f		S069
Compound	2g		S075
Compound	2h		S080
Compound	2i		S085
Compound	2j		S090
Compound	2k		S096
Compound	2l		S100
Compound	5		S105
Compound	6a		S111
Compound	6b		S117
Compound	6c		S123
Compound	6d		S129
Compound	6e		S133
Compound	6f		S136
Compound	6g		S142
Compound	9		S149

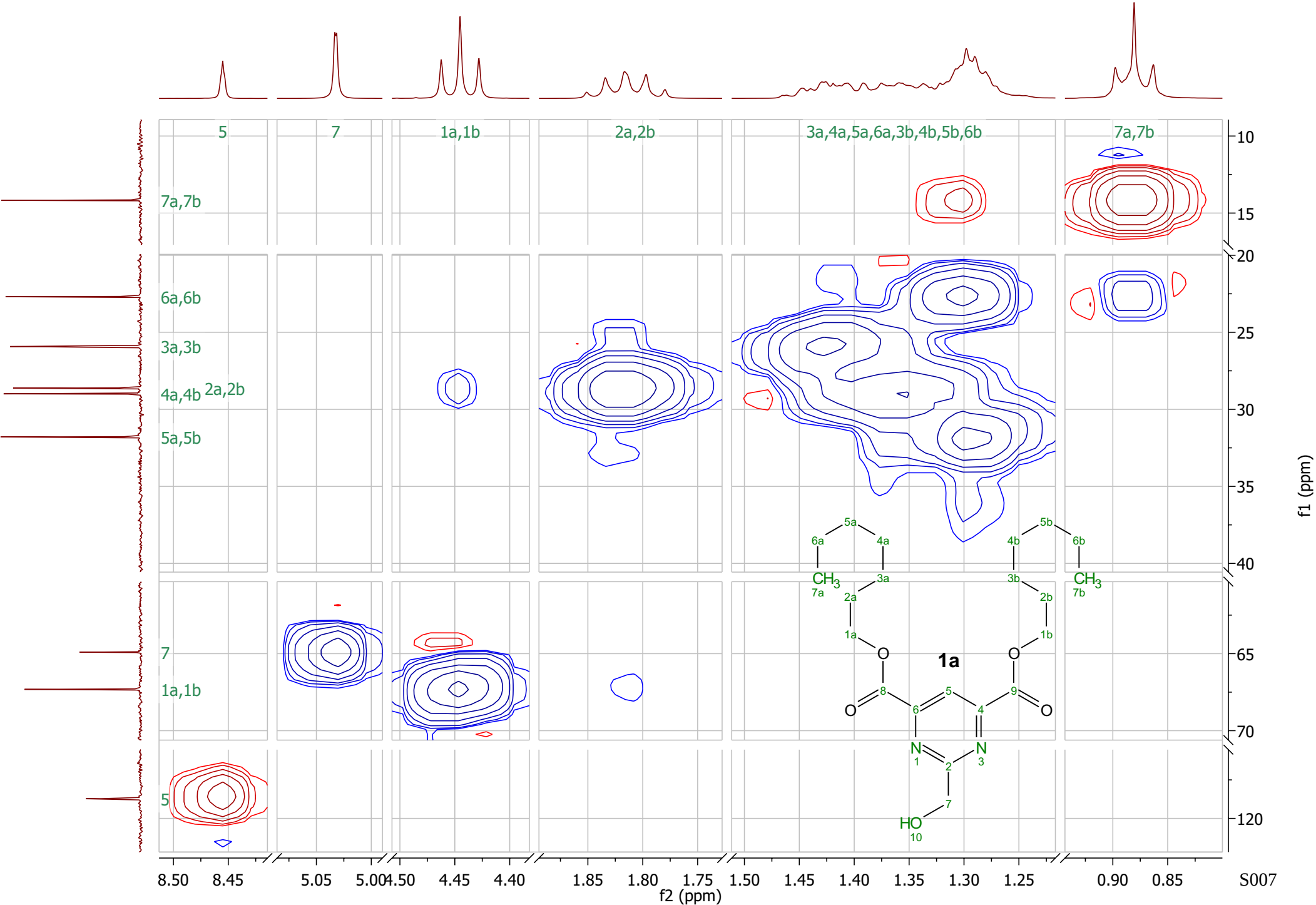
Compound	10		S153
Compound	11		S159
Compound	12		S163
Compound	13		S167
Compound	14		S171
Compound	15		S175
Compound	16		S179
Compound	17		S184
Compound	18		S188
Compound	19		S192
Compound	20		S196
Compound	21		S200
Compound	22		S204
Compound	23		S209
Compound	24		S213
Compound	25		S219
Compound	26		S226
Compound	27		S230

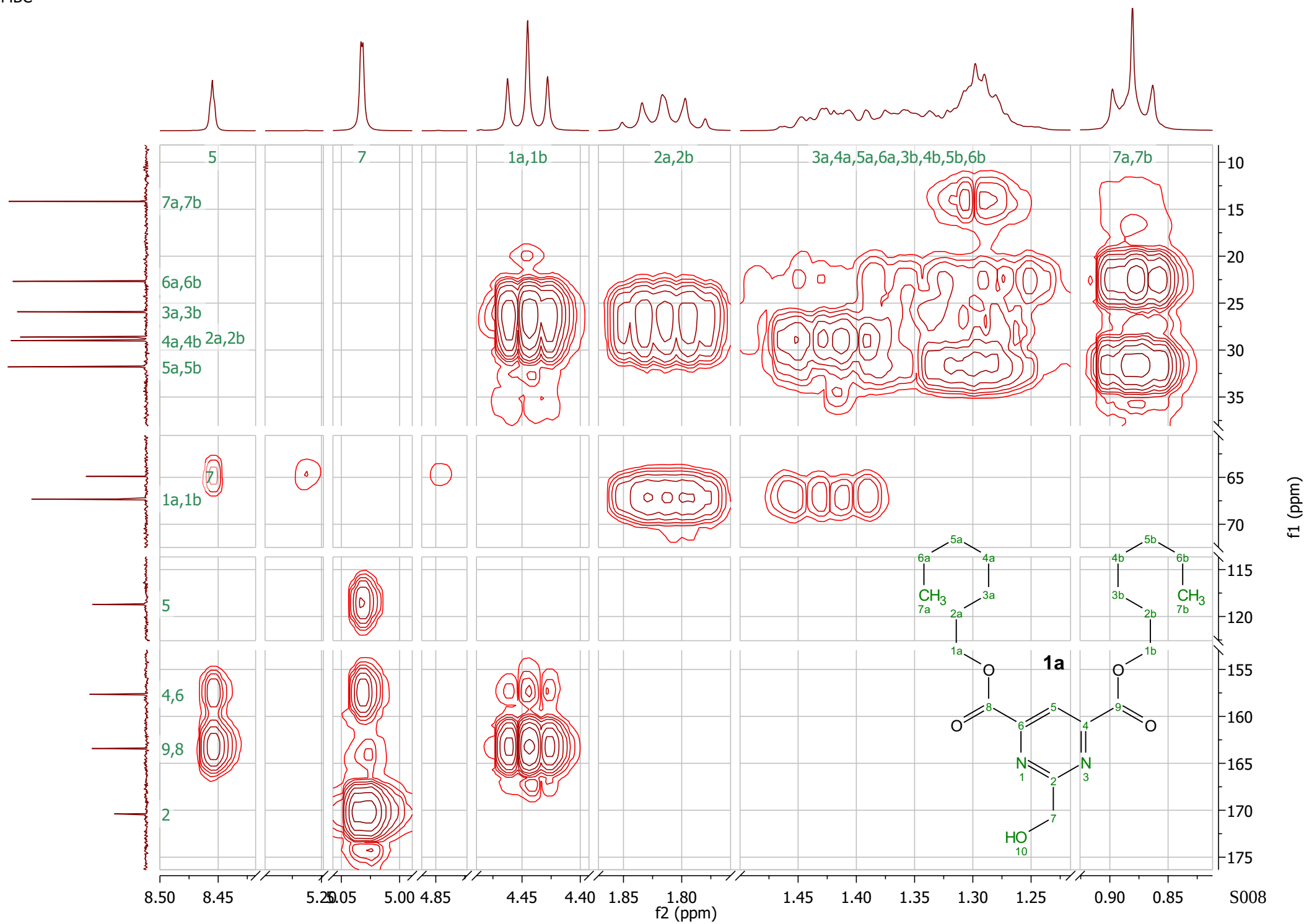
^1H NMR (400 MHz, CDCl_3) δ 8.46 (app t, $J = 0.8$ Hz, 1H), 5.03 (app d, $J = 0.8$ Hz, 2H), 4.45 (t, $J = 6.9$ Hz, 4H), 3.16 (br s, 1H), 1.82 (quint, $J = 6.8$ Hz, 4H), 1.55 – 1.16 (m, 16H), 0.88 (app t, $J = 6.8$ Hz, 6H).

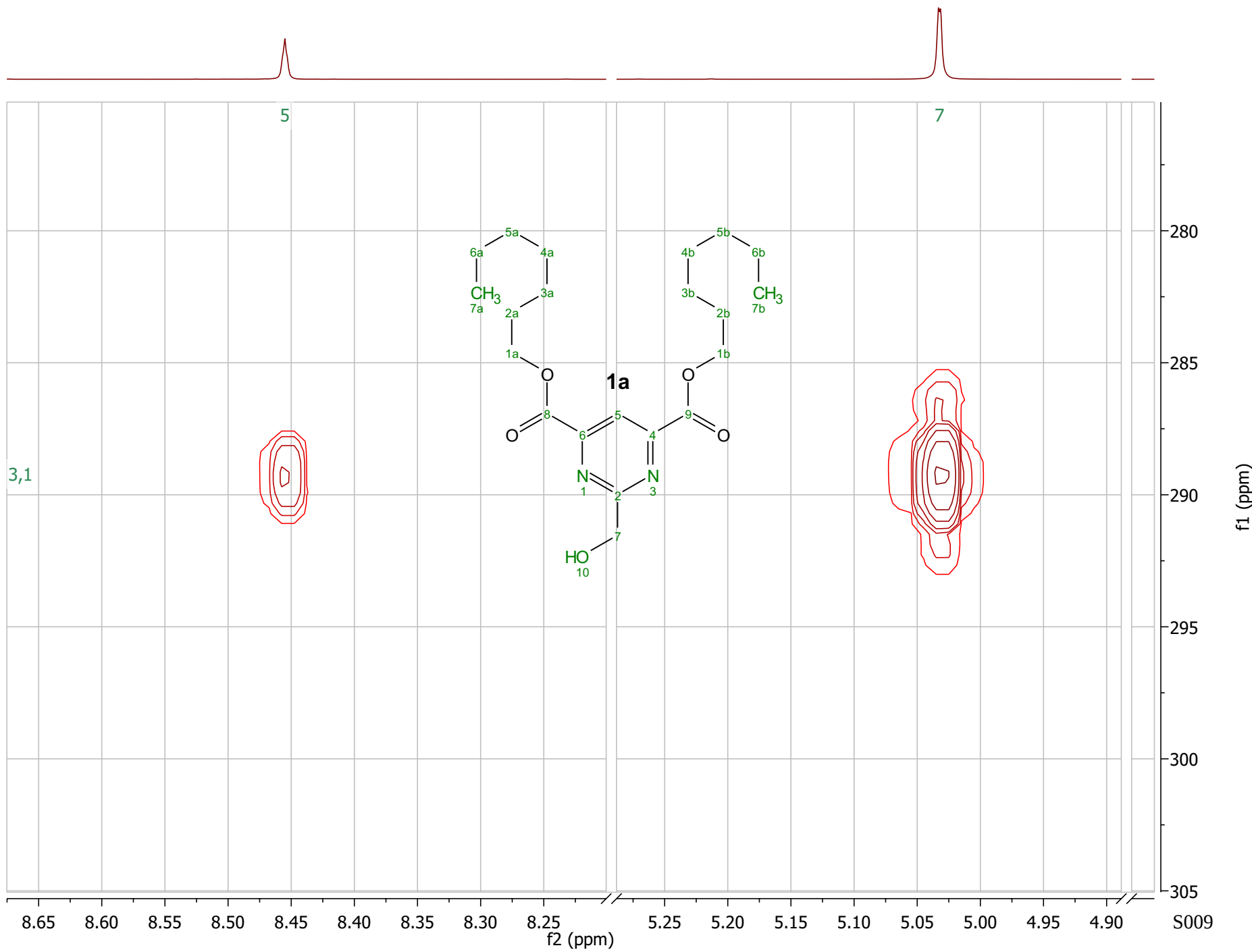


¹³C NMR (101 MHz, CDCl₃) δ 170.4, 163.4 (sym, 2C), 157.7 (sym, 2C), 118.7, 67.3 (sym, 2C), 64.9, 31.8 (sym, 2C), 29.0 (sym, 2C), 28.6 (sym, 2C), 25.9 (sym, 2C), 22.7 (sym, 2C), 14.2 (sym, 2C).

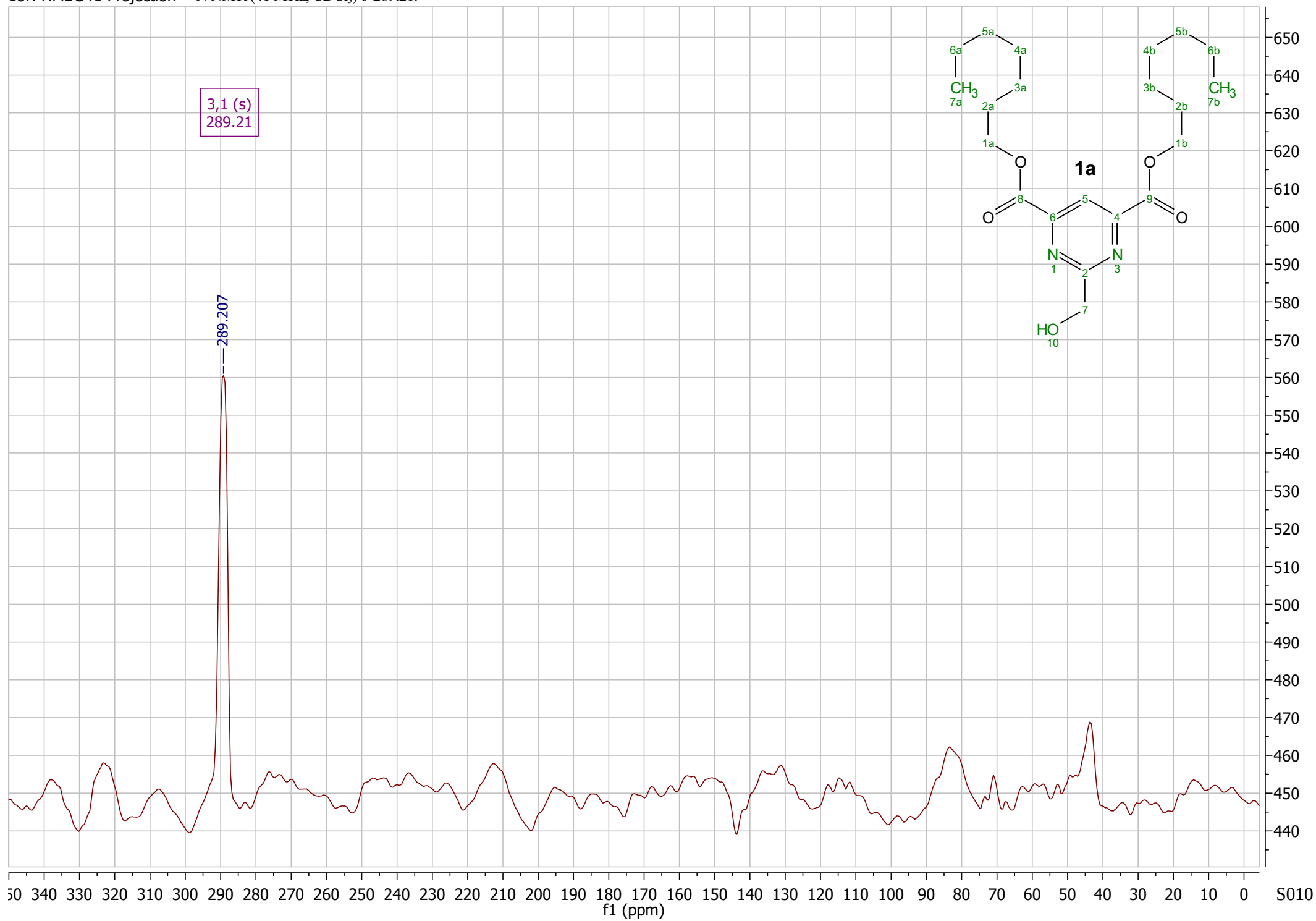




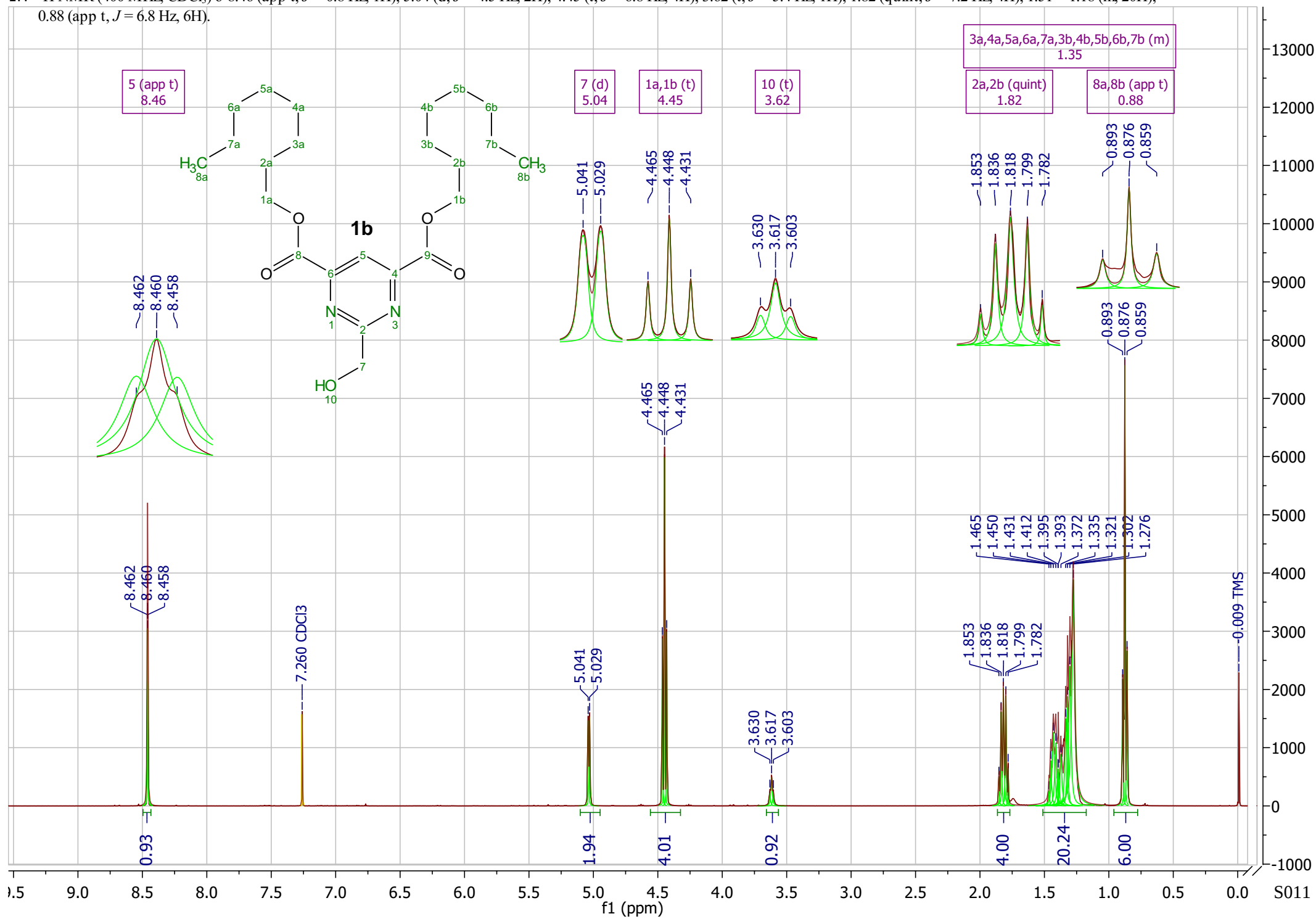




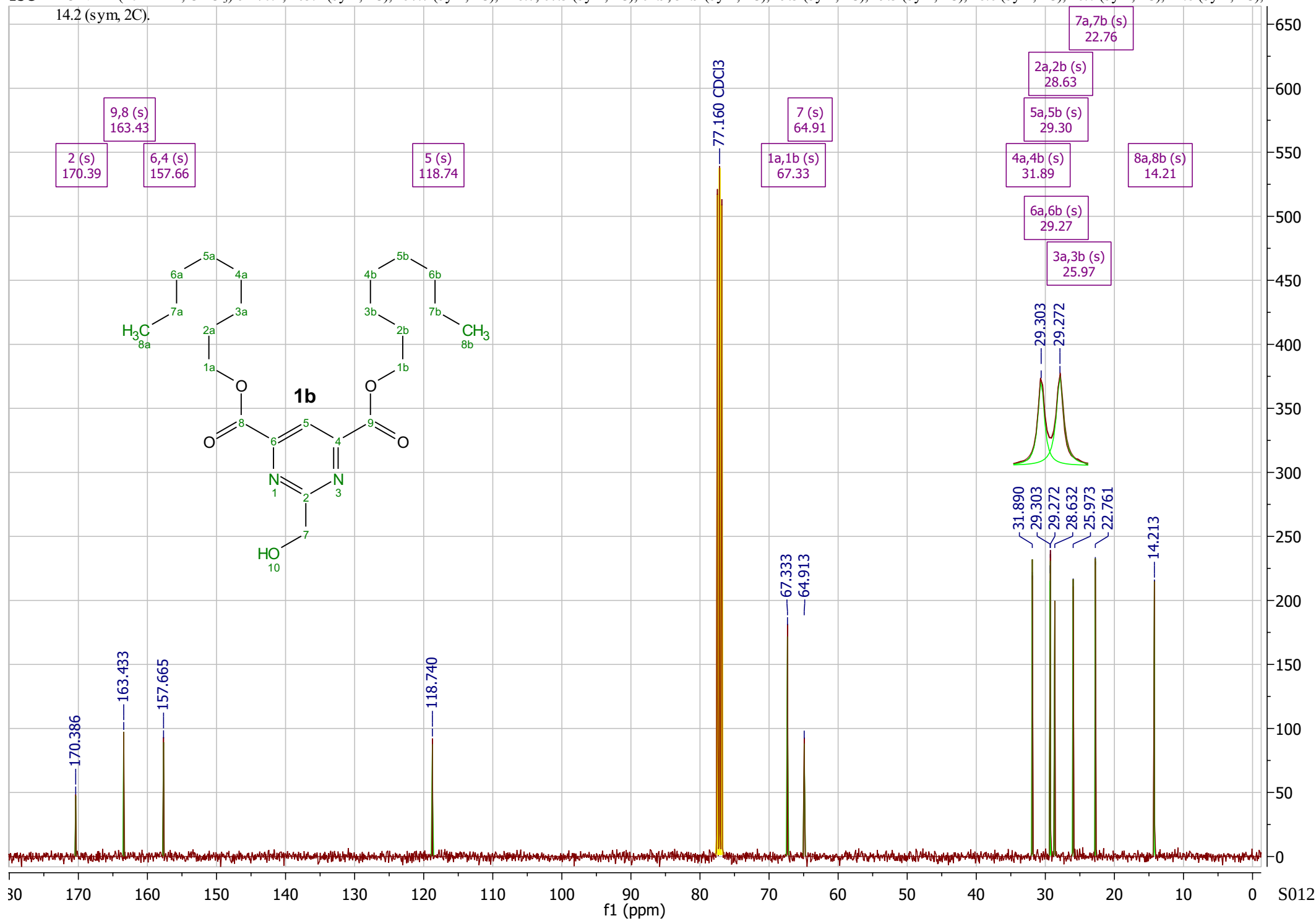
15N HMBC f1 Projection ¹⁵N NMR (41 MHz, CDCl₃) δ 289.21.

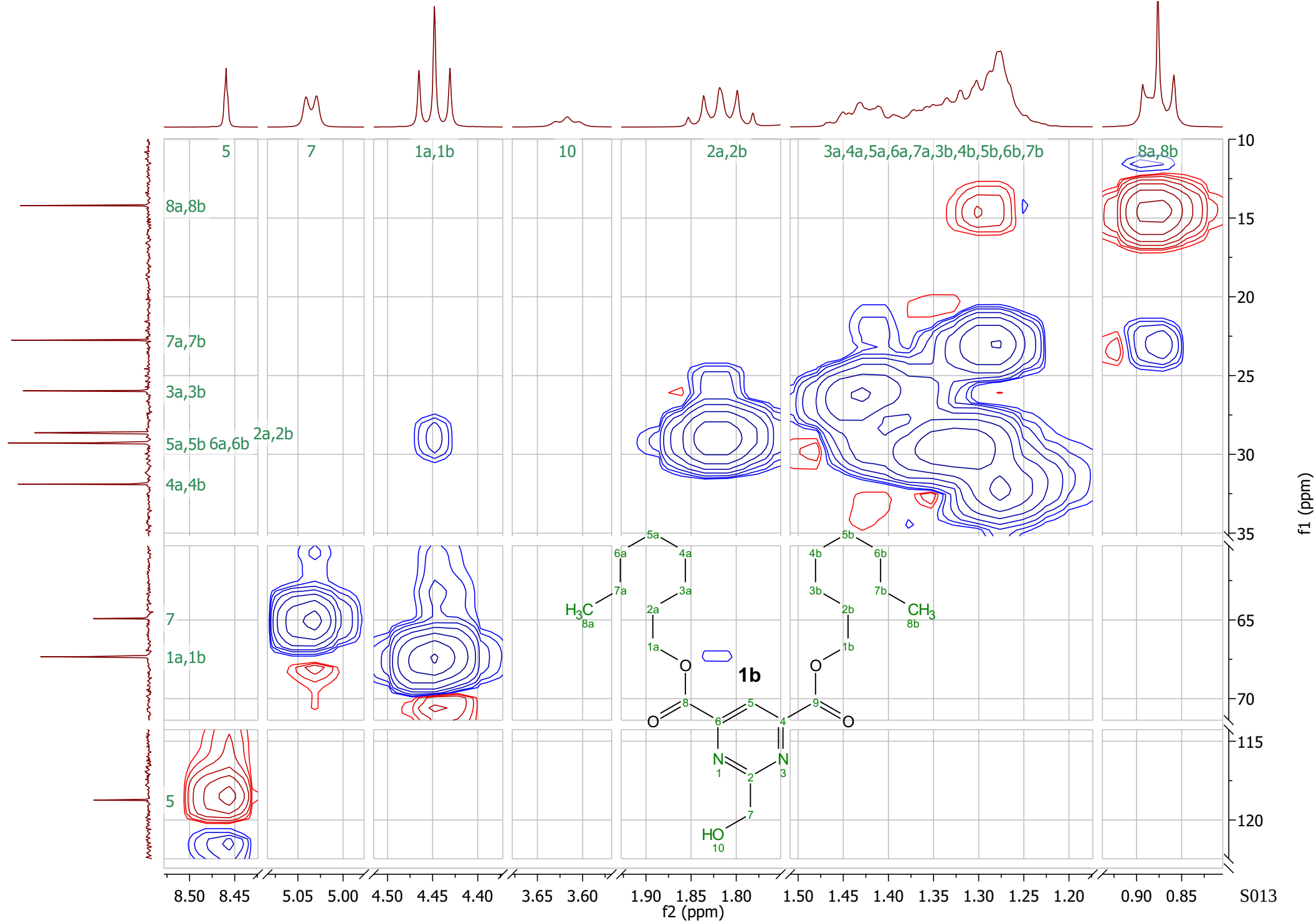


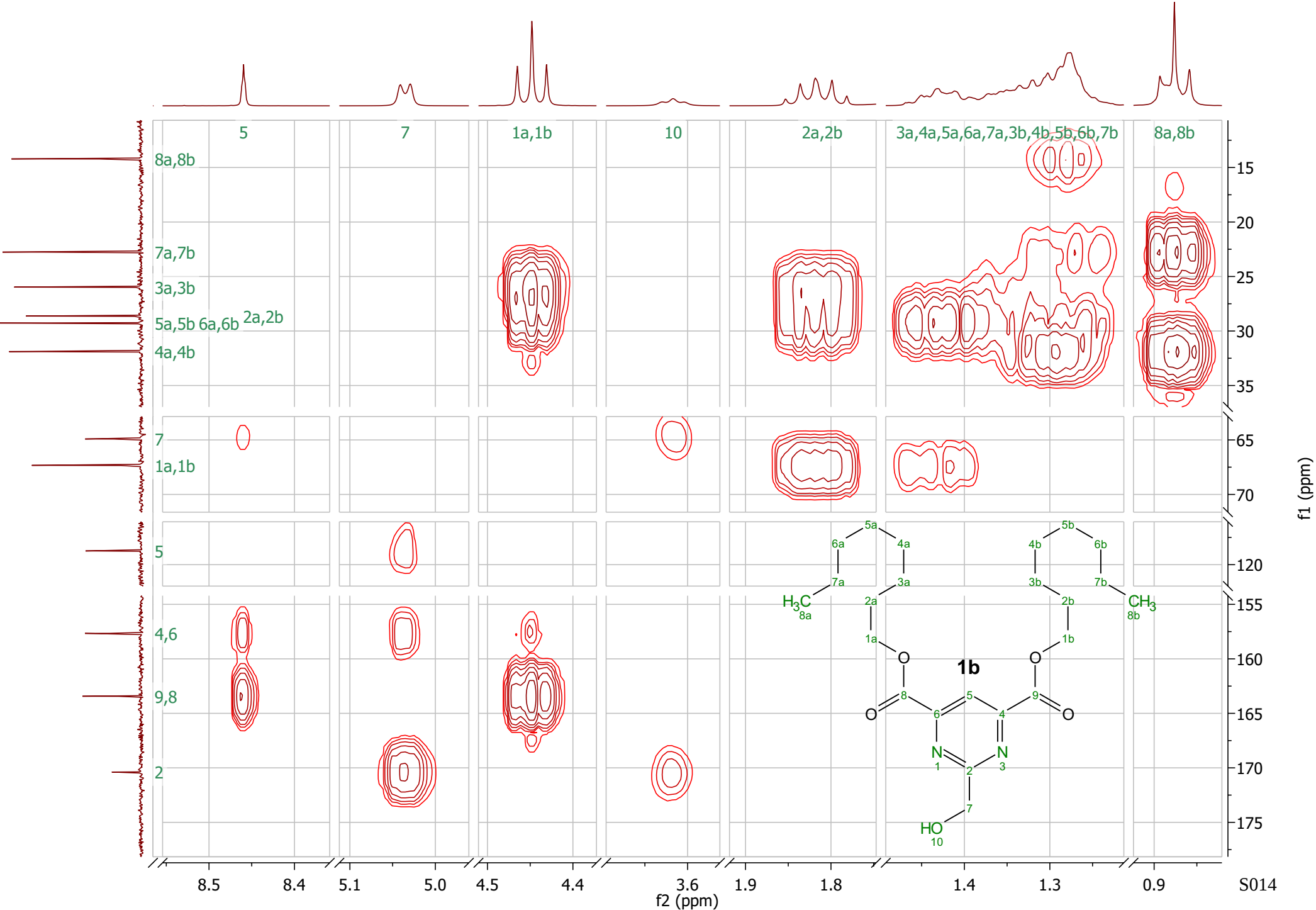
^1H NMR (400 MHz, CDCl_3) δ 8.46 (app t, $J = 0.8$ Hz, 1H), 5.04 (d, $J = 4.5$ Hz, 2H), 4.45 (t, $J = 6.8$ Hz, 4H), 3.62 (t, $J = 5.4$ Hz, 1H), 1.82 (quint, $J = 7.2$ Hz, 4H), 1.51 – 1.18 (m, 20H), 0.88 (app t, $J = 6.8$ Hz, 6H).

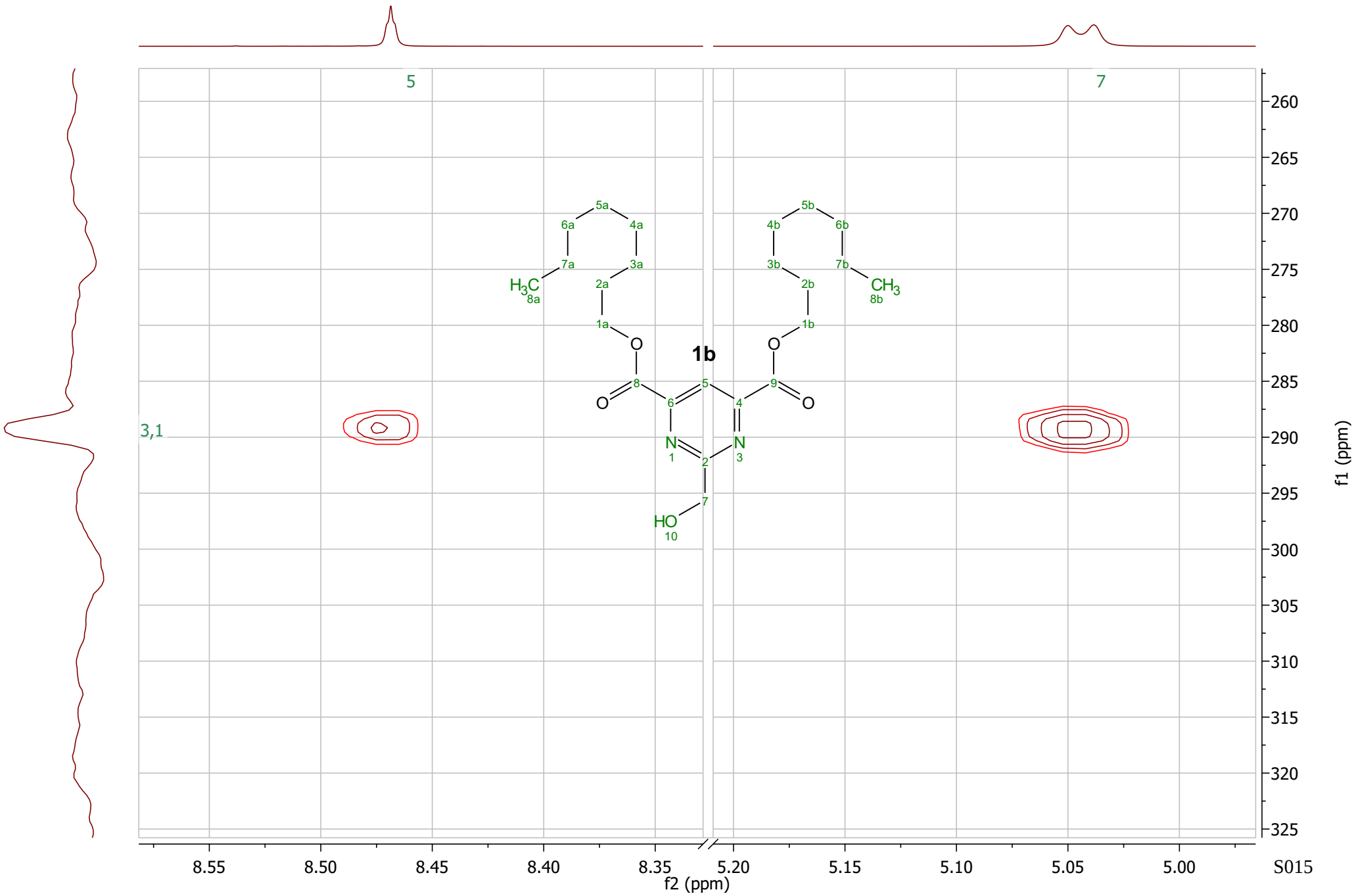


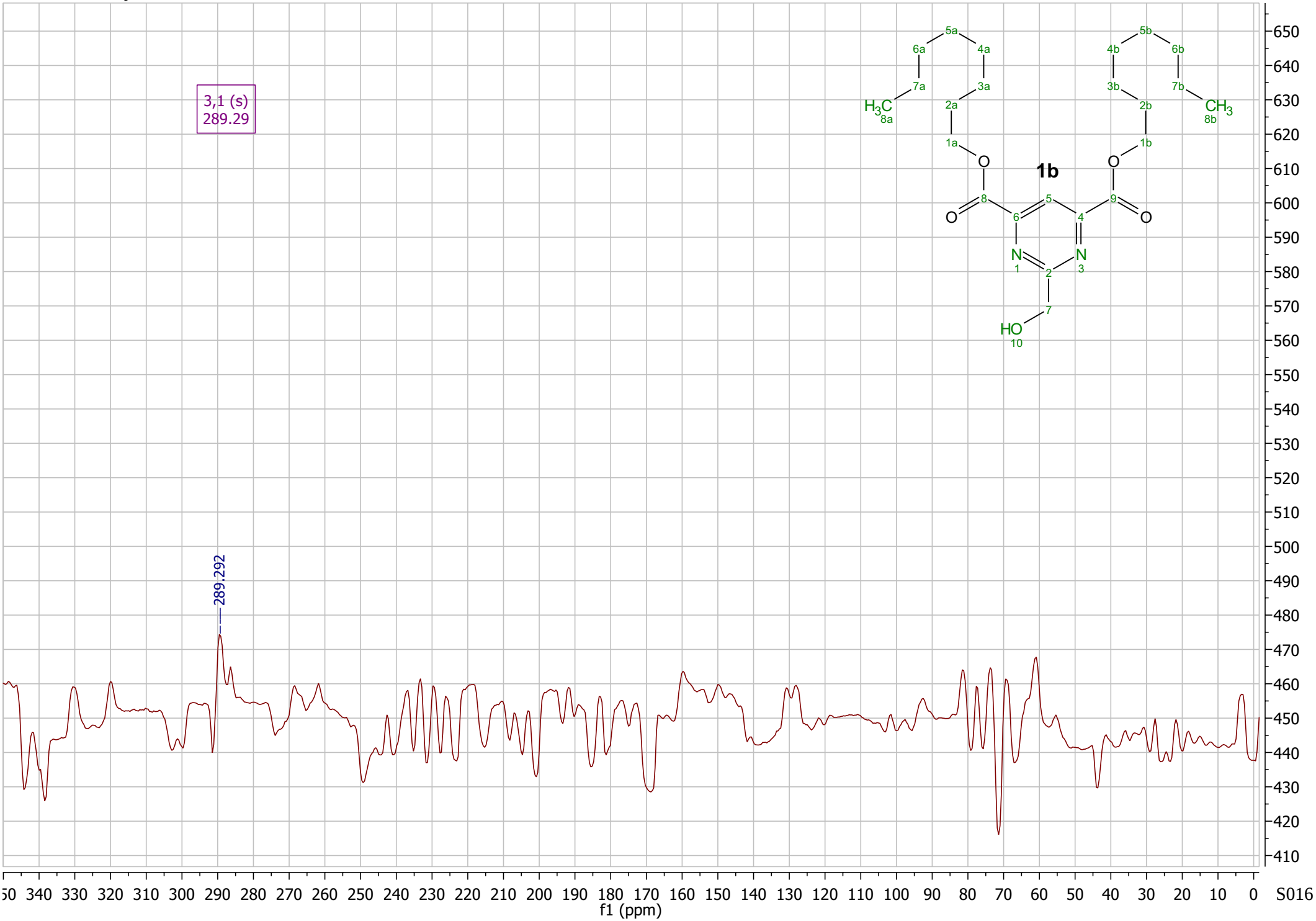
13C ¹³C NMR (101 MHz, CDCl₃) δ 170.4, 163.4 (sym, 2C), 157.7 (sym, 2C), 118.7, 67.3 (sym, 2C), 64.9, 31.9 (sym, 2C), 29.3 (sym, 2C), 29.3 (sym, 2C), 28.6 (sym, 2C), 26.0 (sym, 2C), 22.8 (sym, 2C), 14.2 (sym, 2C).



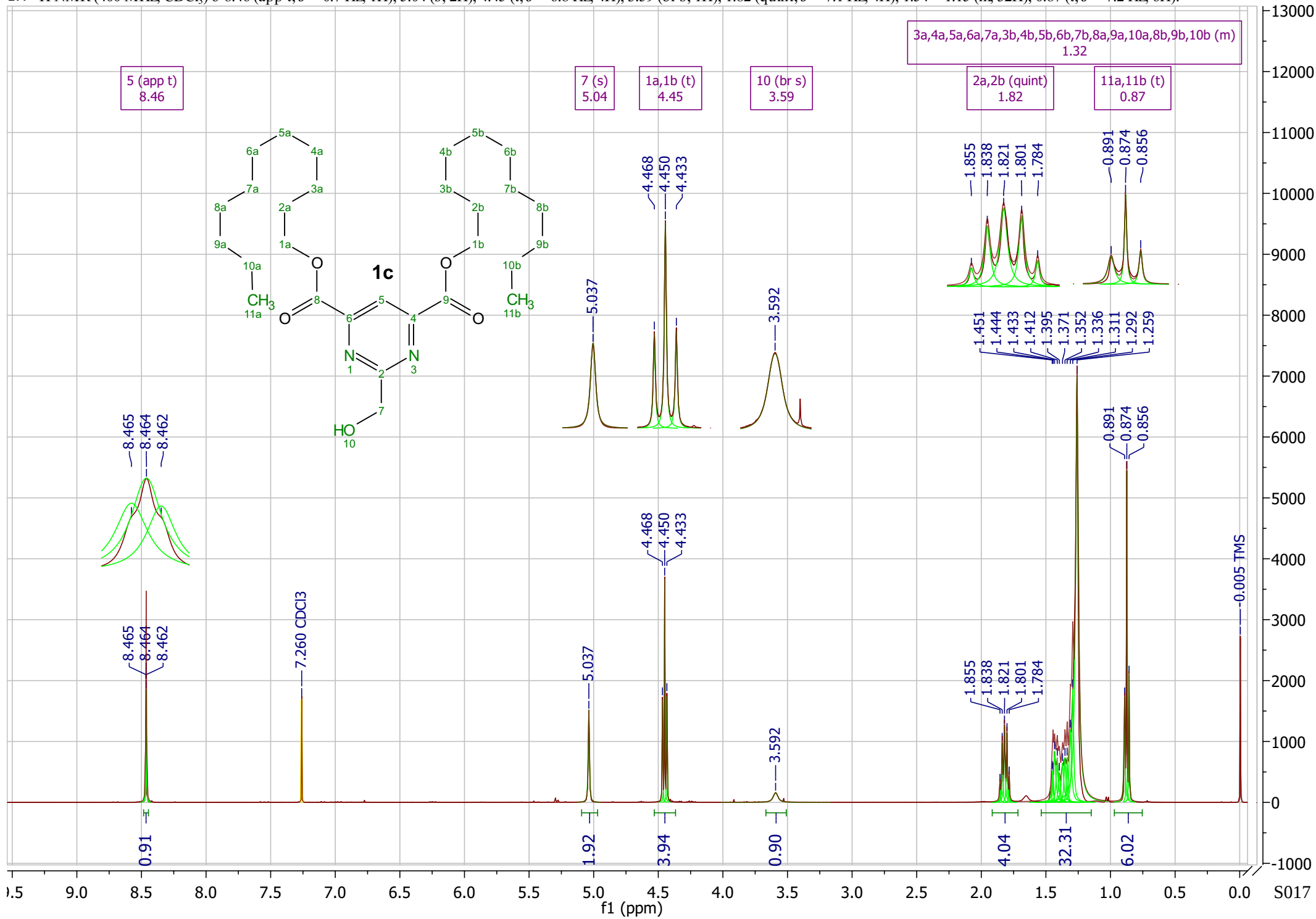




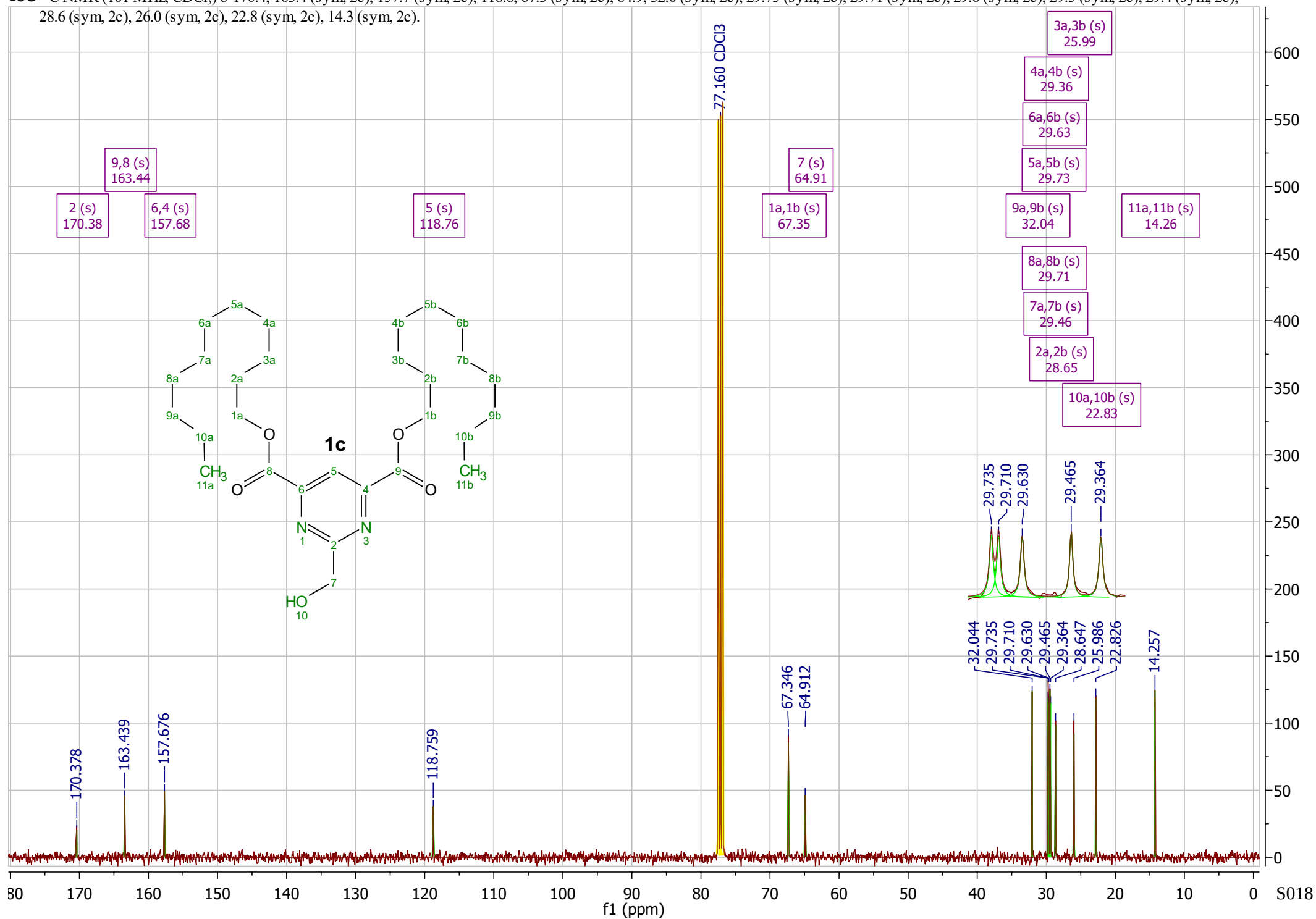


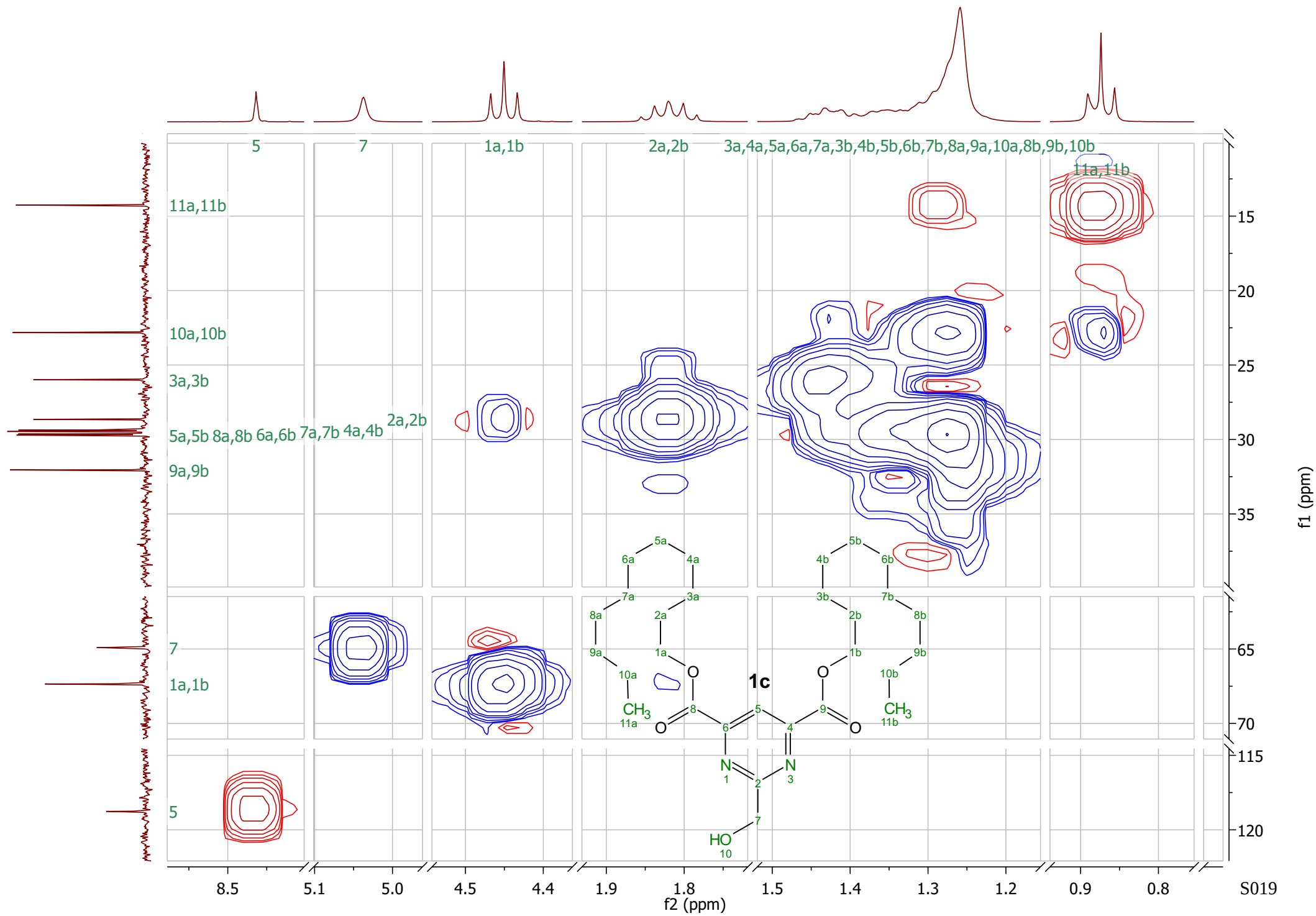


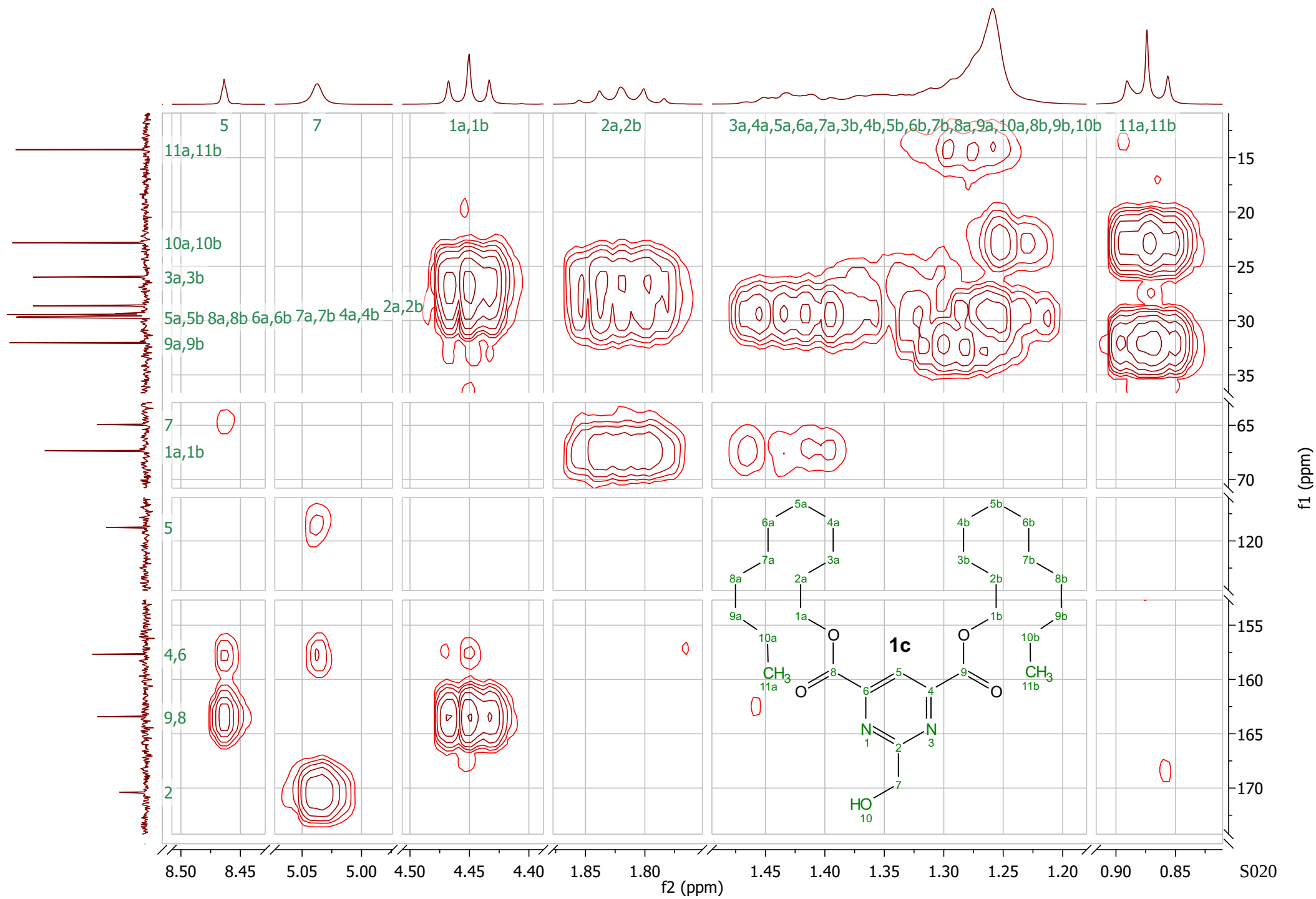
^1H NMR (400 MHz, CDCl_3) δ 8.46 (app t, $J = 0.7$ Hz, 1H), 5.04 (s, 2H), 4.45 (t, $J = 6.8$ Hz, 4H), 3.59 (br s, 1H), 1.82 (quint, $J = 7.1$ Hz, 4H), 1.54 – 1.15 (m, 32H), 0.87 (t, $J = 7.2$ Hz, 6H).

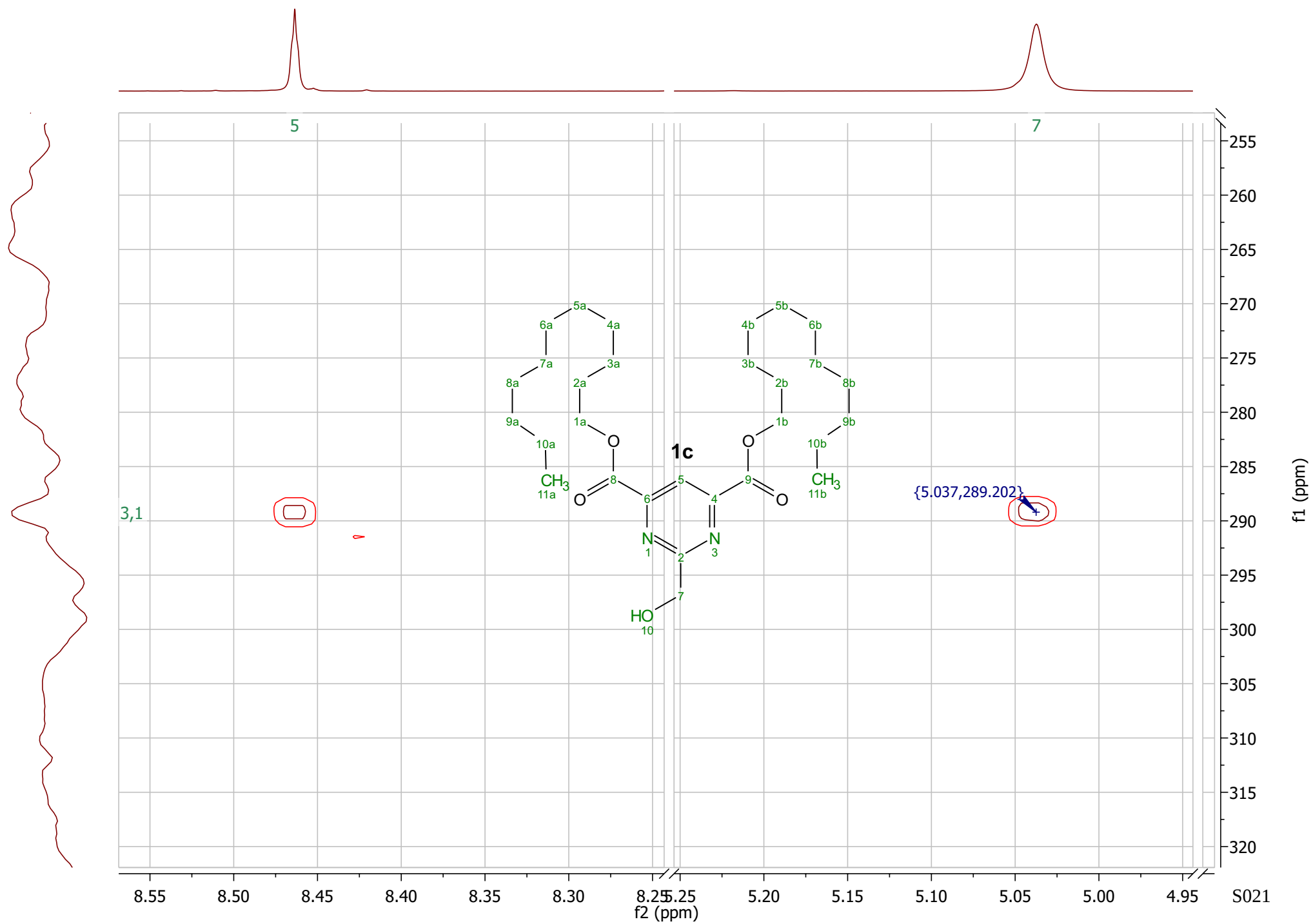


^{13}C NMR (101 MHz, CDCl_3) δ 170.4, 163.4 (sym, 2c), 157.7 (sym, 2c), 118.8, 67.3 (sym, 2c), 64.9, 32.0 (sym, 2c), 29.73 (sym, 2c), 29.71 (sym, 2c), 29.6 (sym, 2c), 29.5 (sym, 2c), 29.4 (sym, 2c), 28.6 (sym, 2c), 26.0 (sym, 2c), 22.8 (sym, 2c), 14.3 (sym, 2c).

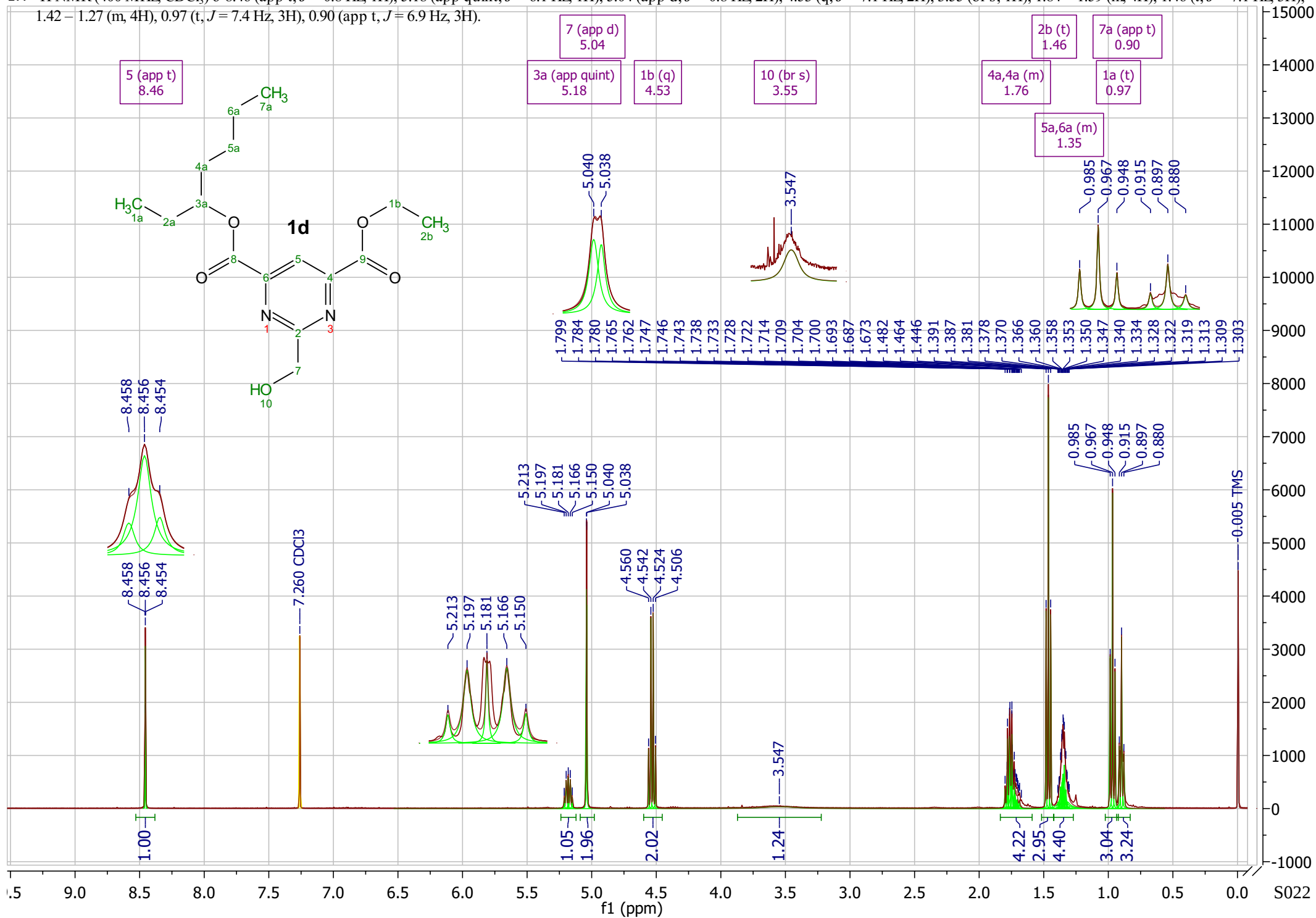




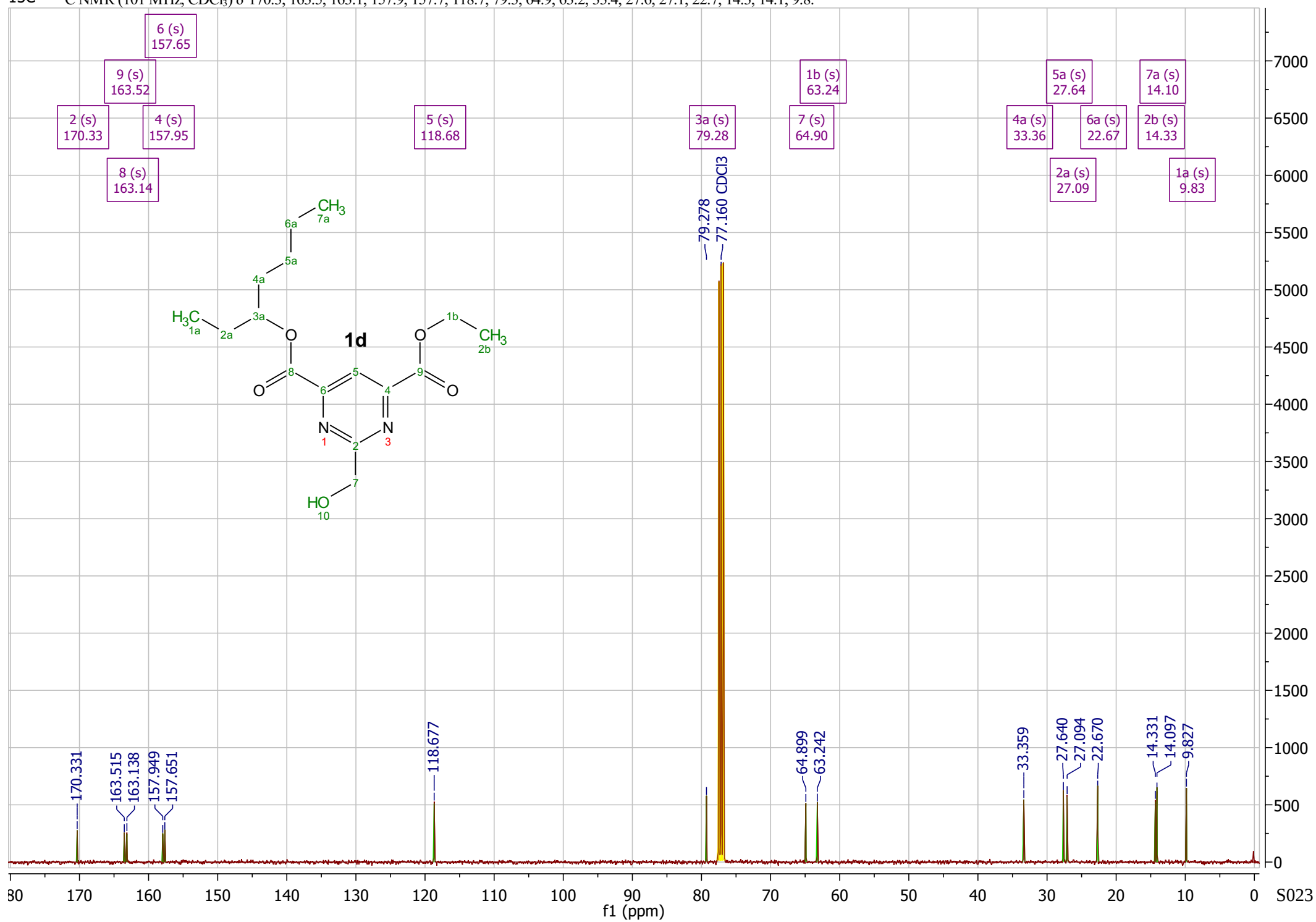


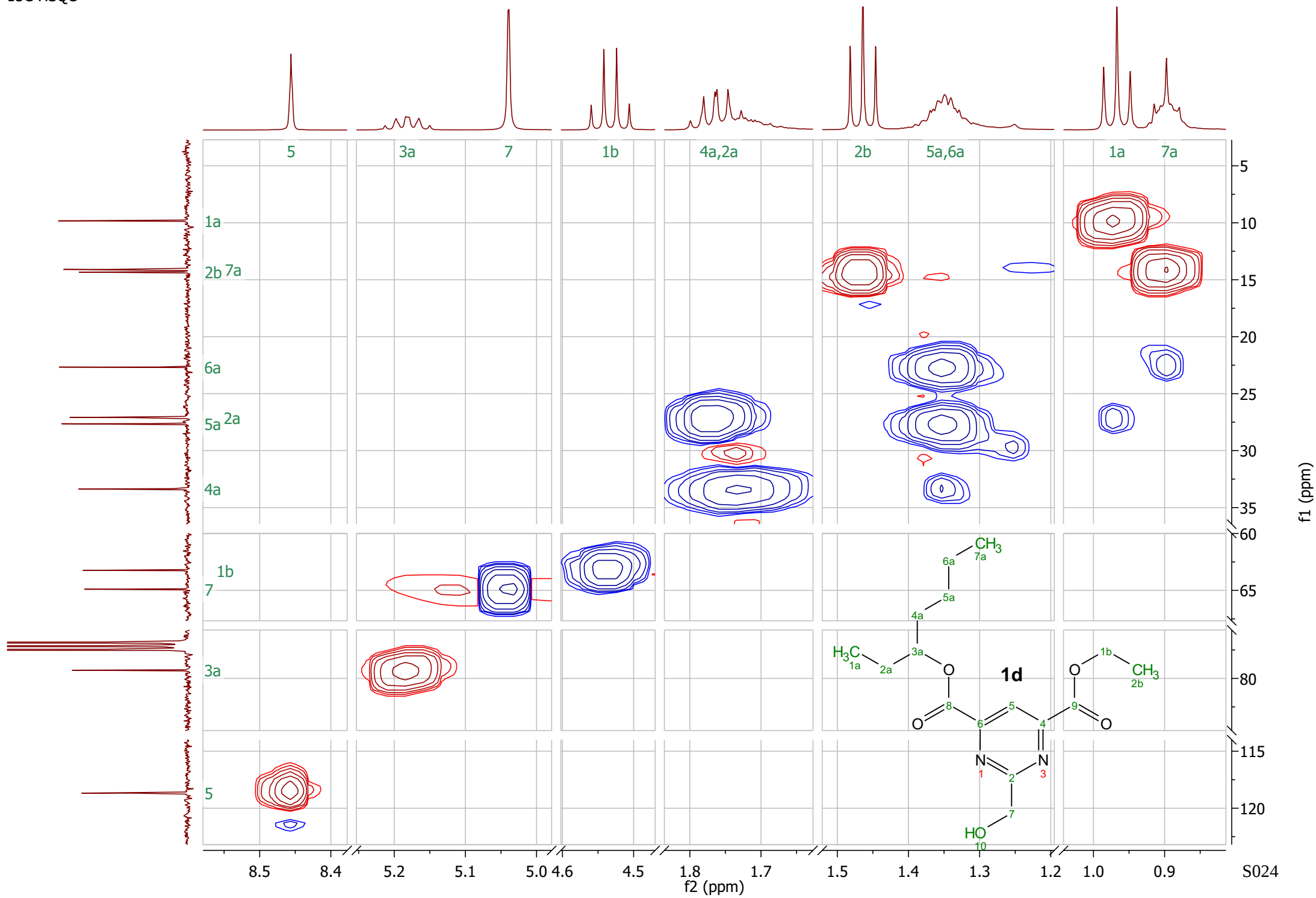


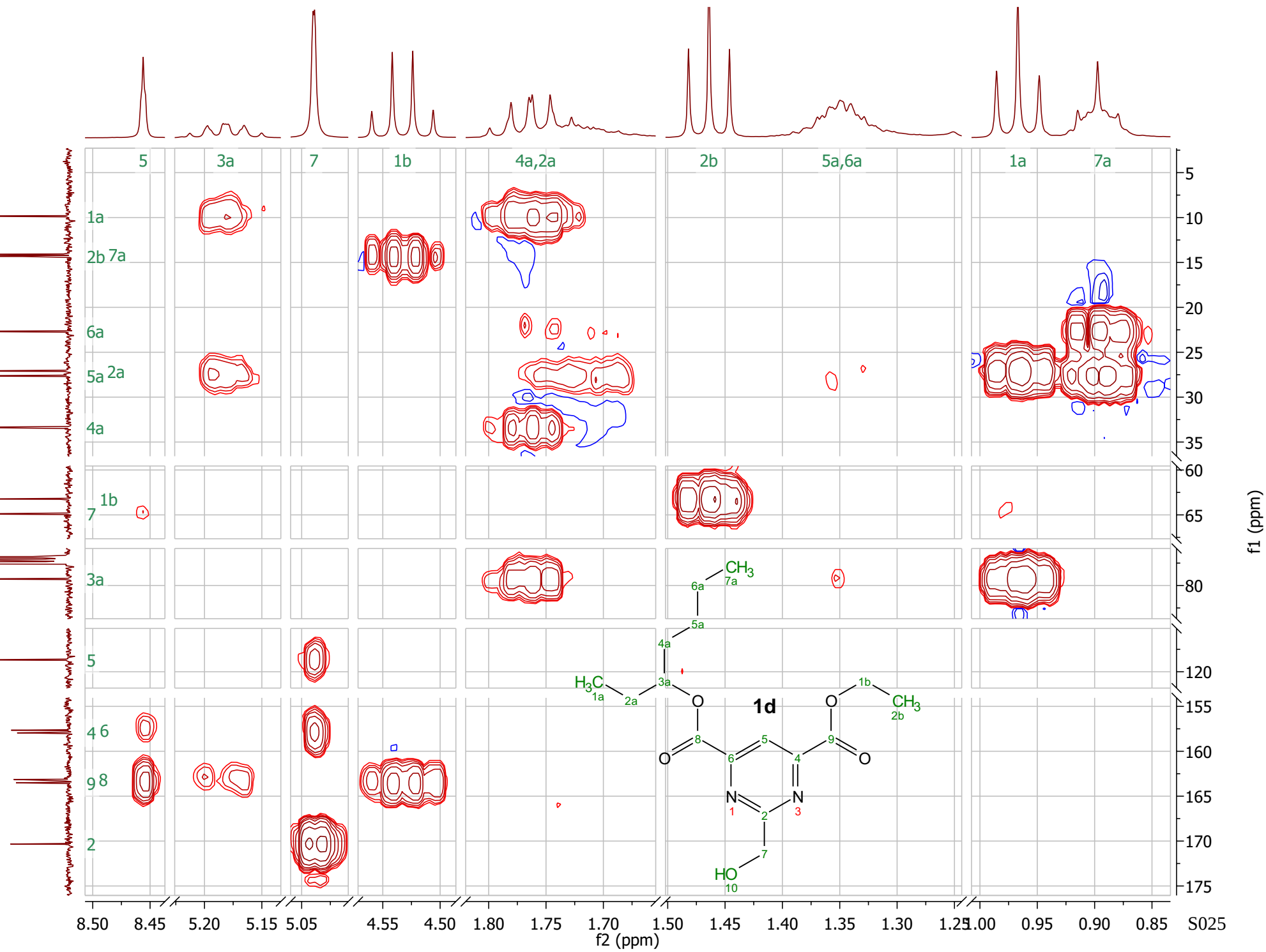
^1H NMR (400 MHz, CDCl_3) δ 8.46 (app t, $J = 0.8$ Hz, 1H), 5.18 (app quint, $J = 6.1$ Hz, 1H), 5.04 (app d, $J = 0.8$ Hz, 2H), 4.53 (q, $J = 7.1$ Hz, 2H), 3.55 (br s, 1H), 1.84 – 1.59 (m, 4H), 1.46 (t, $J = 7.1$ Hz, 3H), 1.42 – 1.27 (m, 4H), 0.97 (t, $J = 7.4$ Hz, 3H), 0.90 (app t, $J = 6.9$ Hz, 3H).



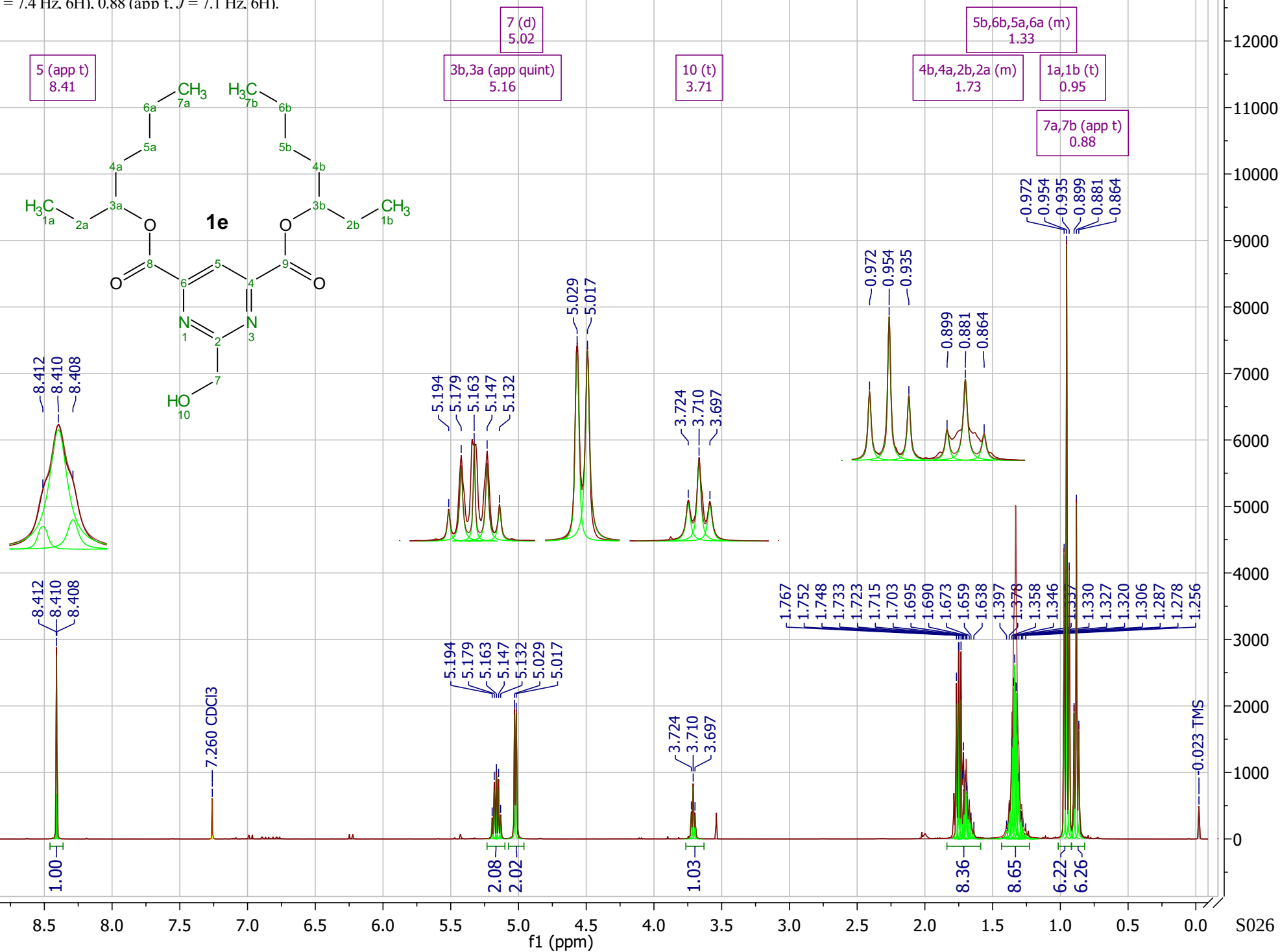
¹³C NMR (101 MHz, CDCl₃) δ 170.3, 163.5, 163.1, 157.9, 157.7, 118.7, 79.3, 64.9, 63.2, 33.4, 27.6, 27.1, 22.7, 14.3, 14.1, 9.8.



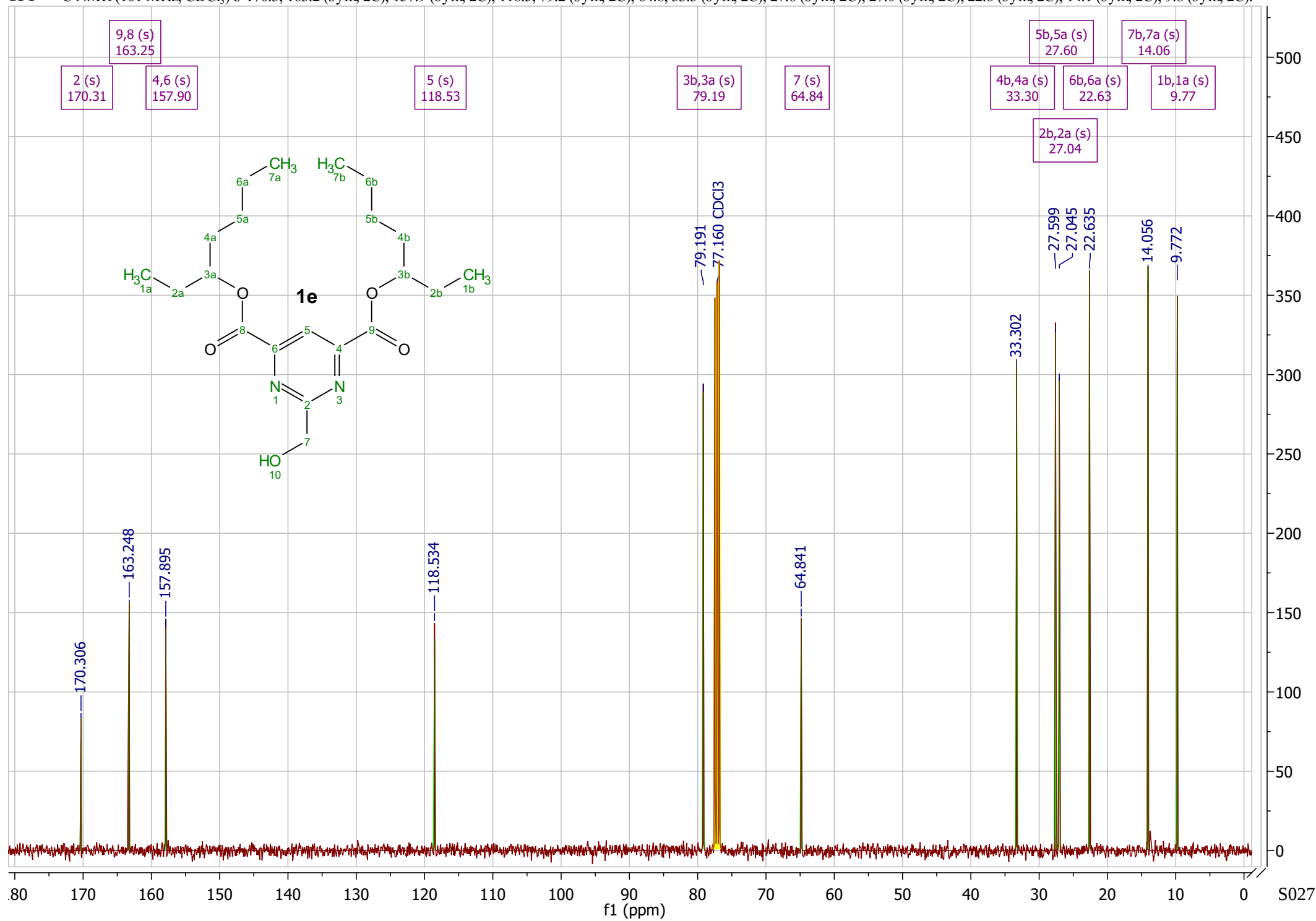


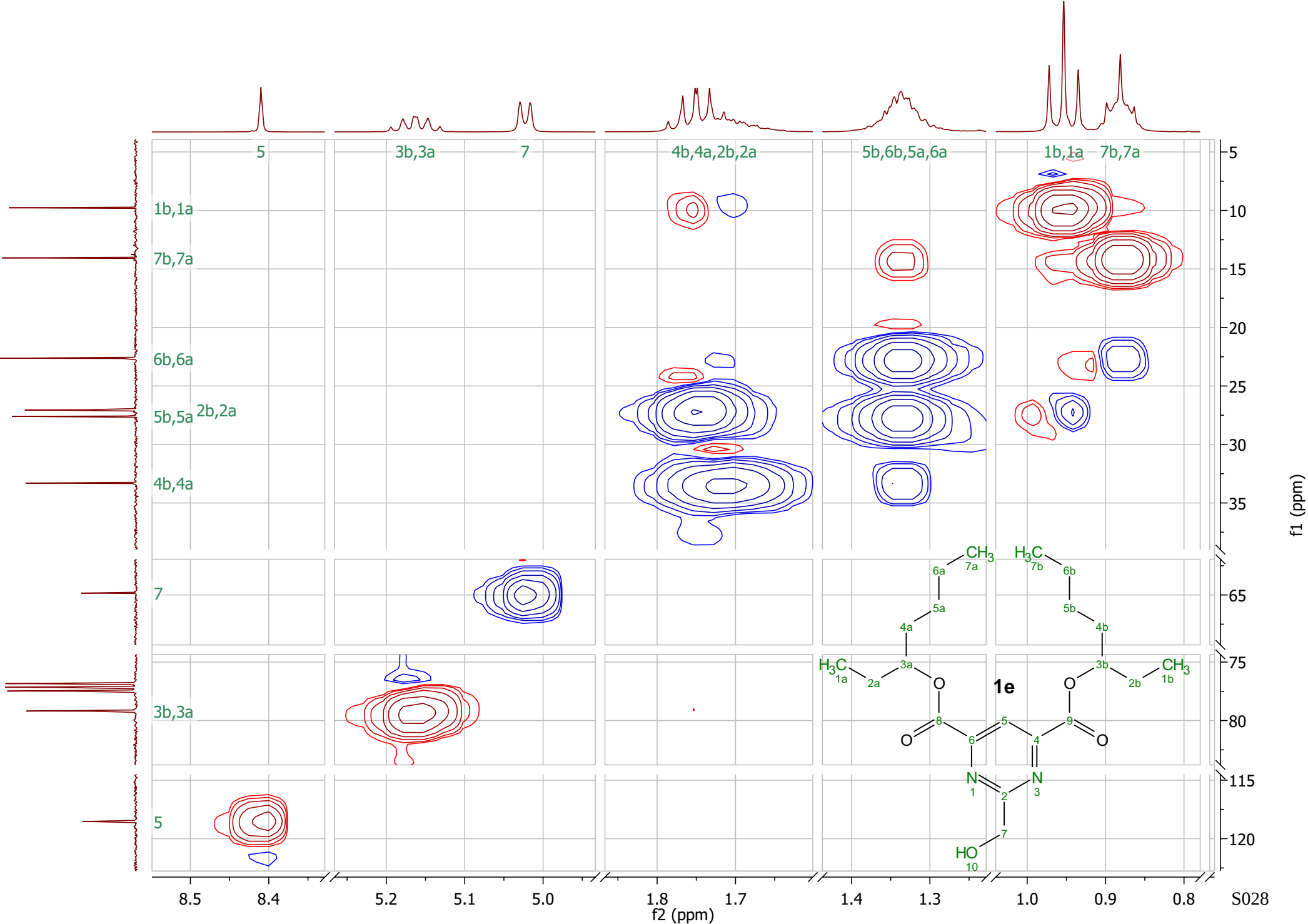


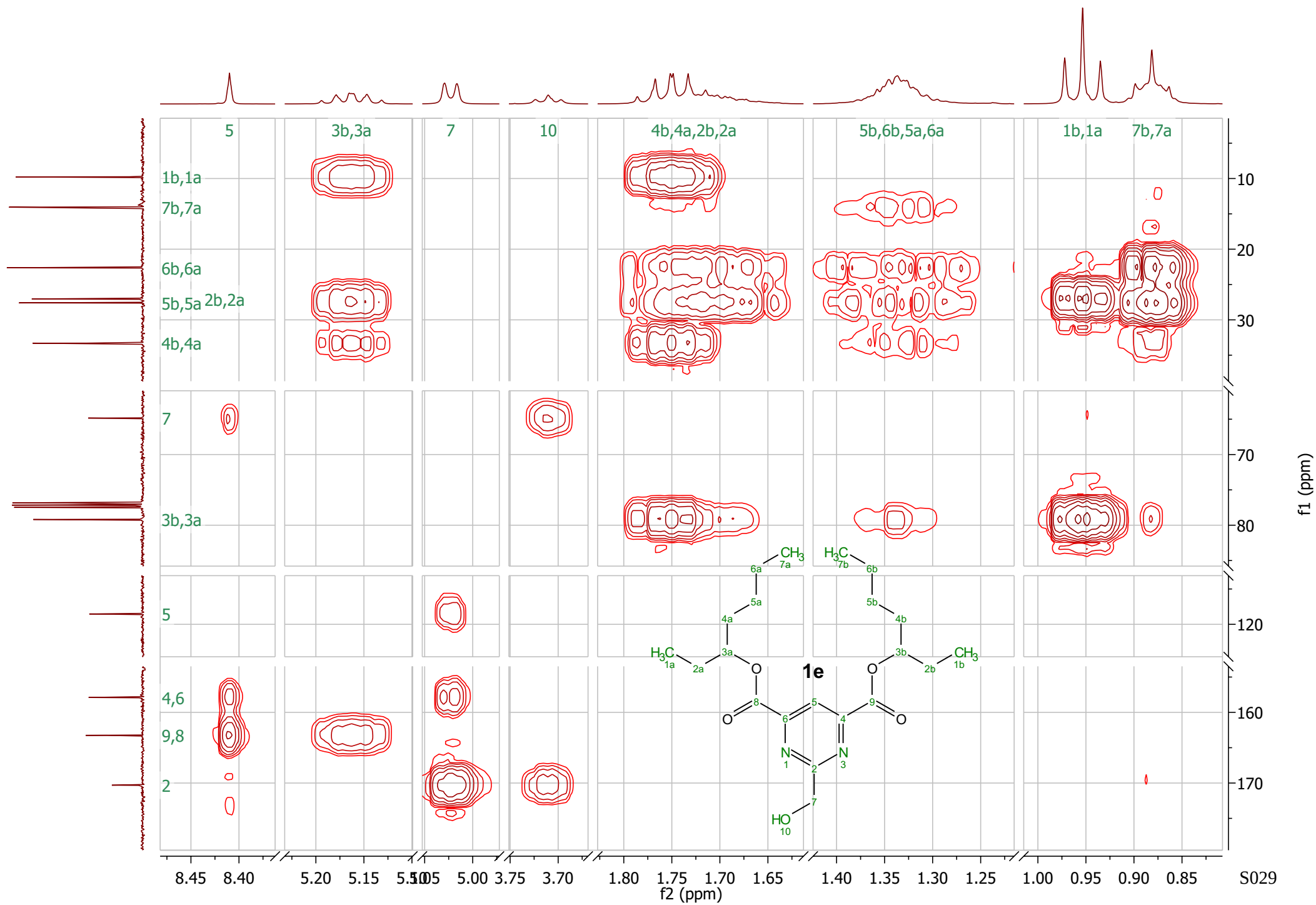
^1H NMR (400 MHz, CDCl_3) δ 8.41 (app t, $J = 0.8$ Hz, 1H), 5.16 (app quint, $J = 6.2$ Hz, 2H), 5.02 (d, $J = 5.3$ Hz, 2H), 3.71 (t, $J = 5.3$ Hz, 1H), 1.84 – 1.59 (m, 8H), 1.43 – 1.23 (m, 8H), 0.95 (t, $J = 7.4$ Hz, 6H), 0.88 (app t, $J = 7.1$ Hz, 6H).

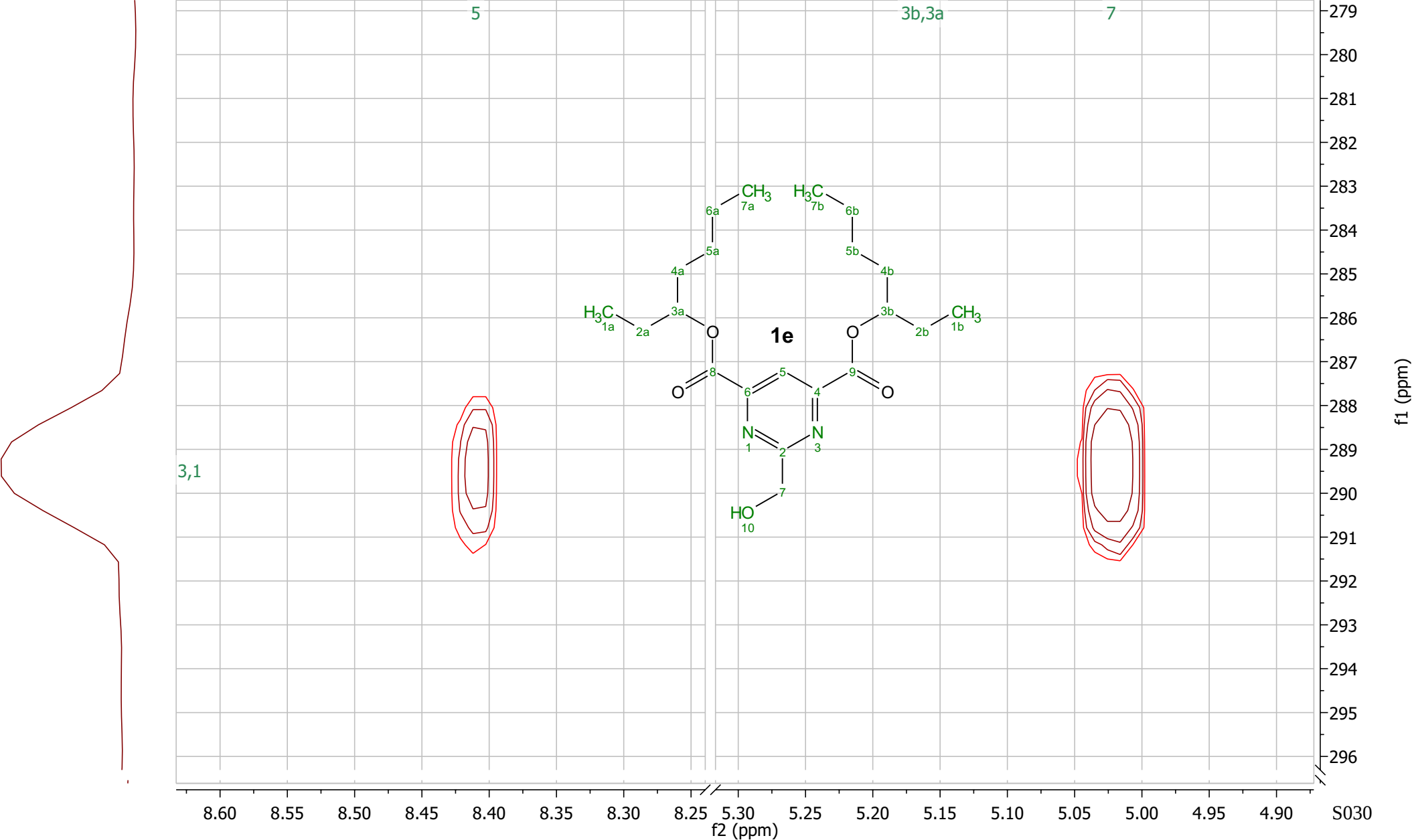


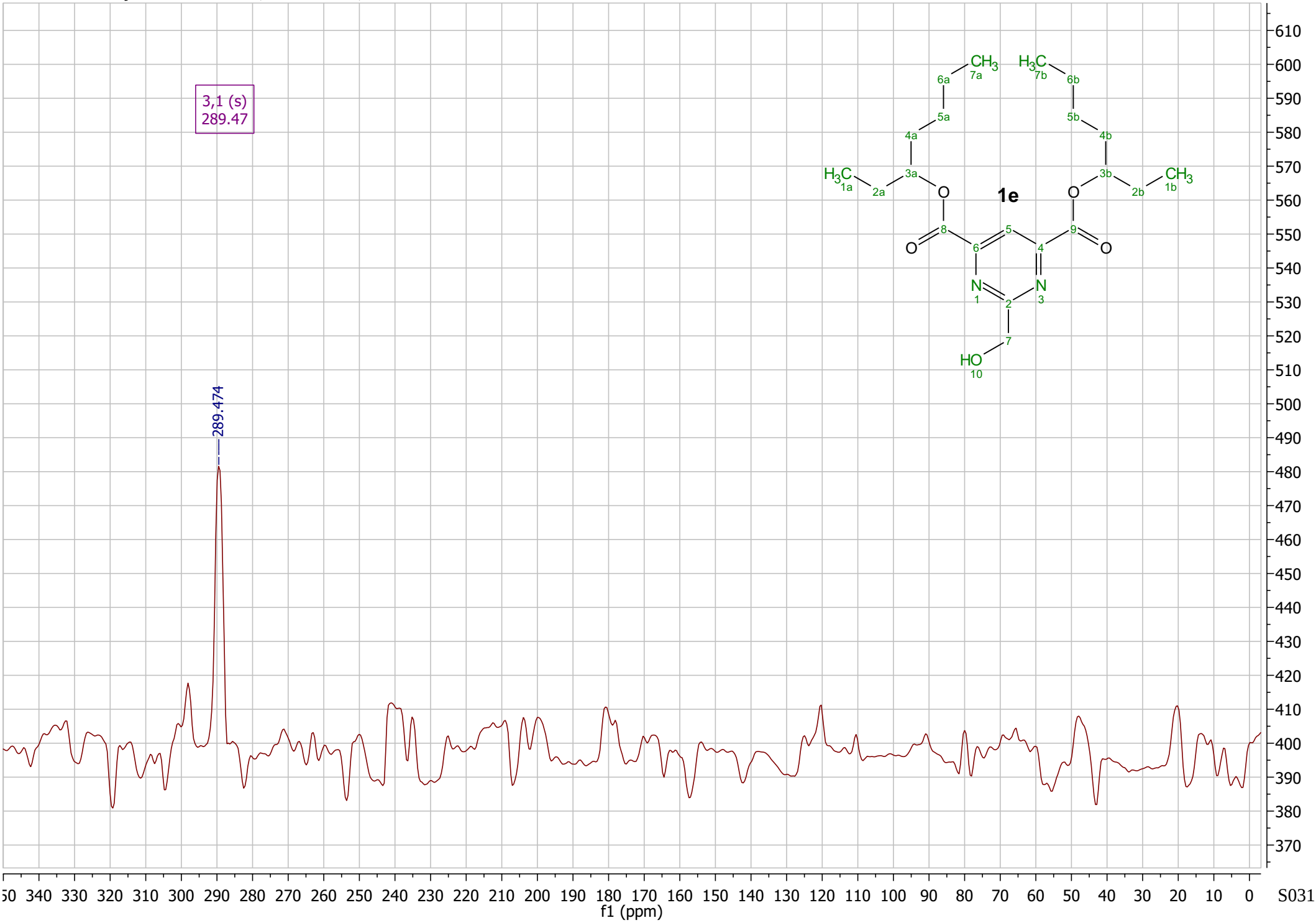
13C ^{13}C NMR (101 MHz, CDCl_3) δ 170.3, 163.2 (sym, 2C), 157.9 (sym, 2C), 118.5, 79.2 (sym, 2C), 64.8, 33.3 (sym, 2C), 27.6 (sym, 2C), 27.0 (sym, 2C), 22.6 (sym, 2C), 14.1 (sym, 2C), 9.8 (sym, 2C).



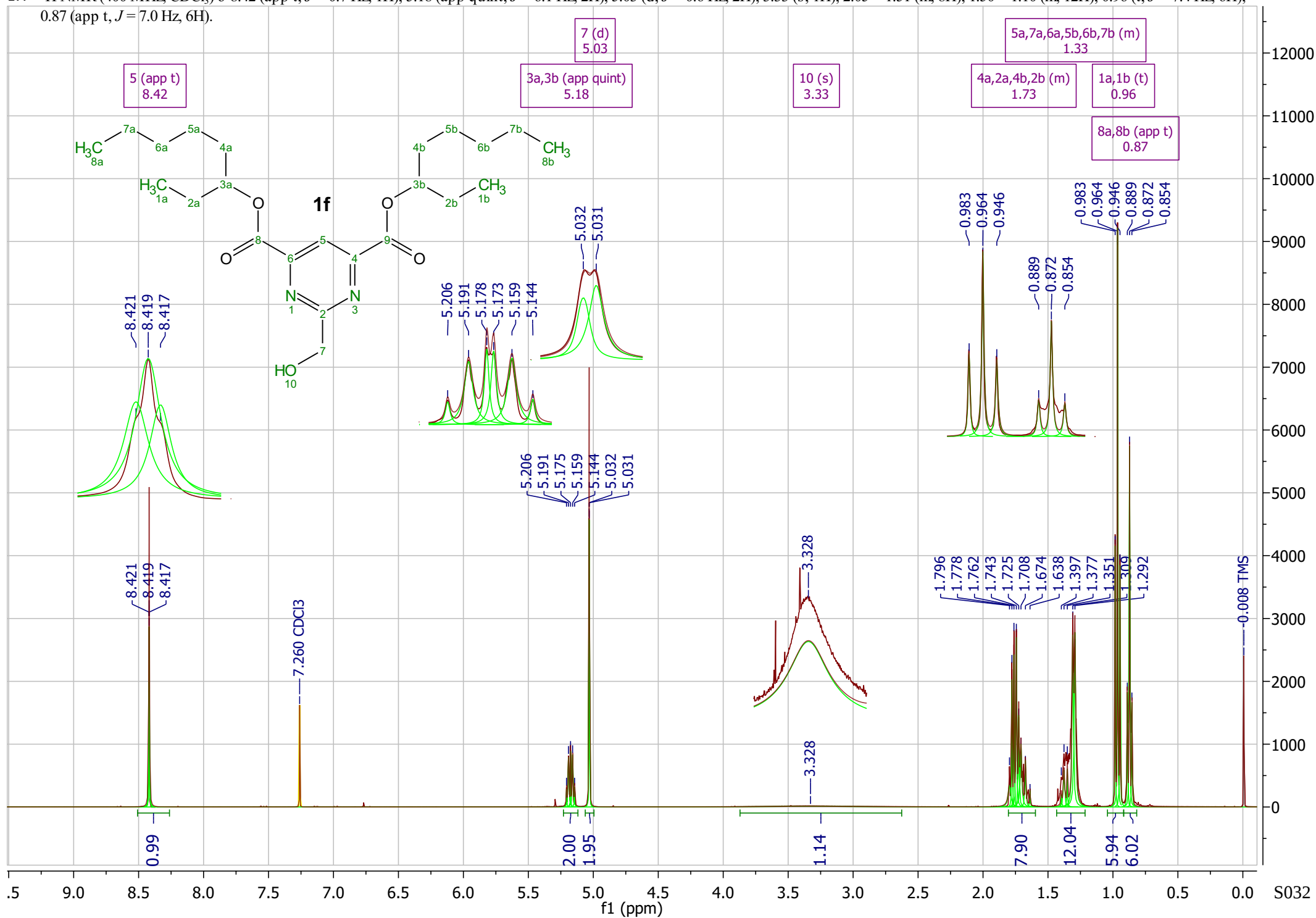




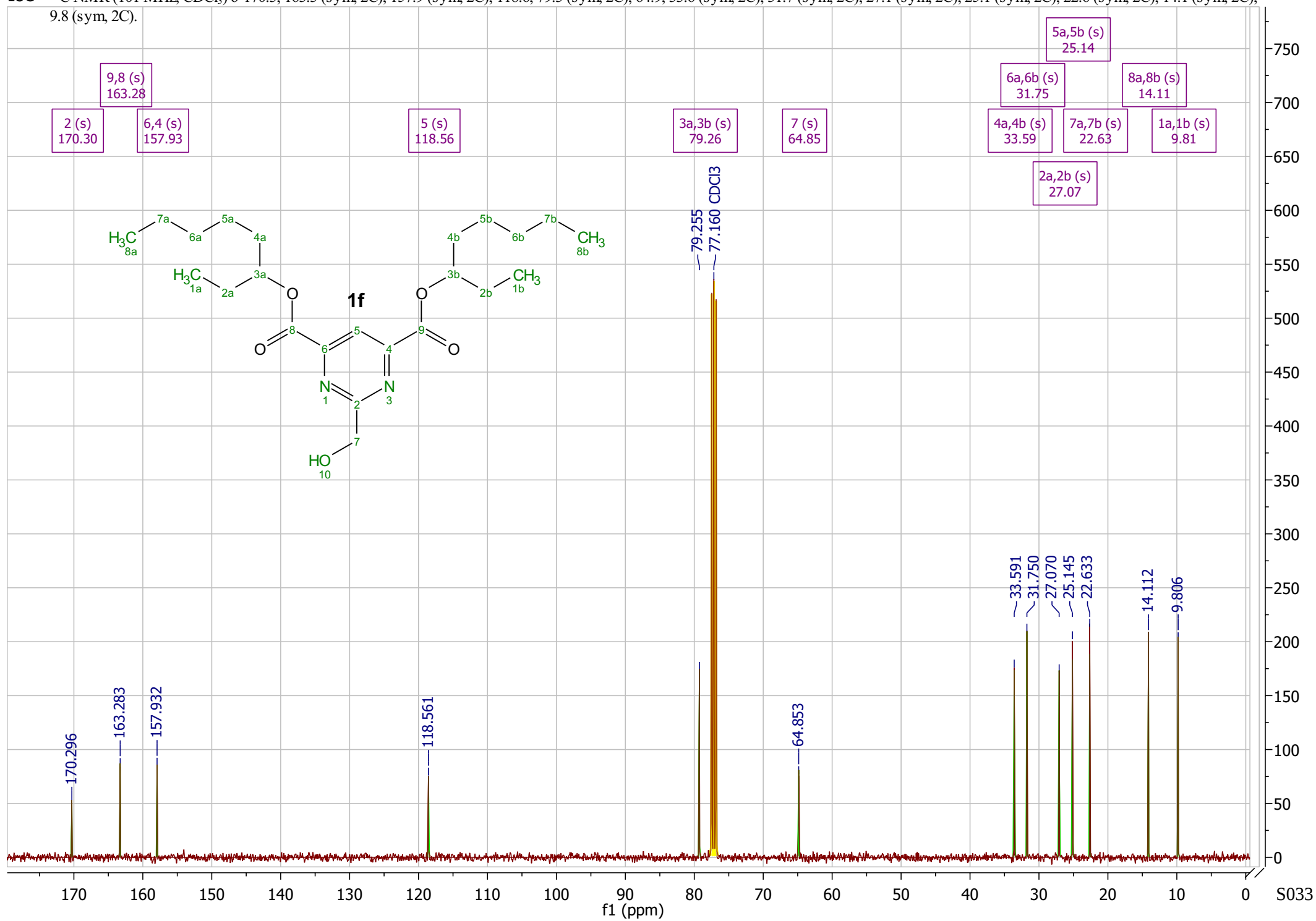


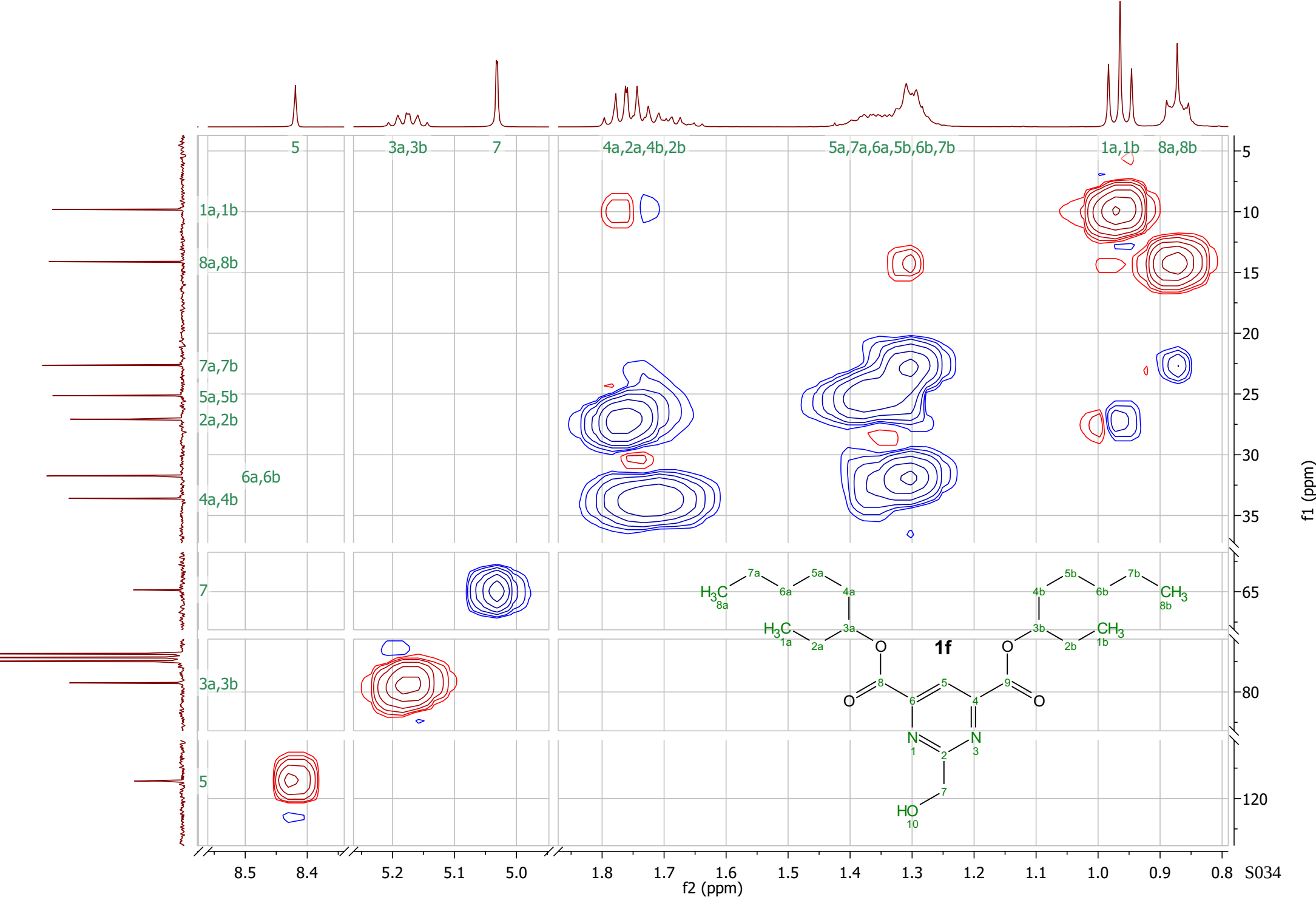


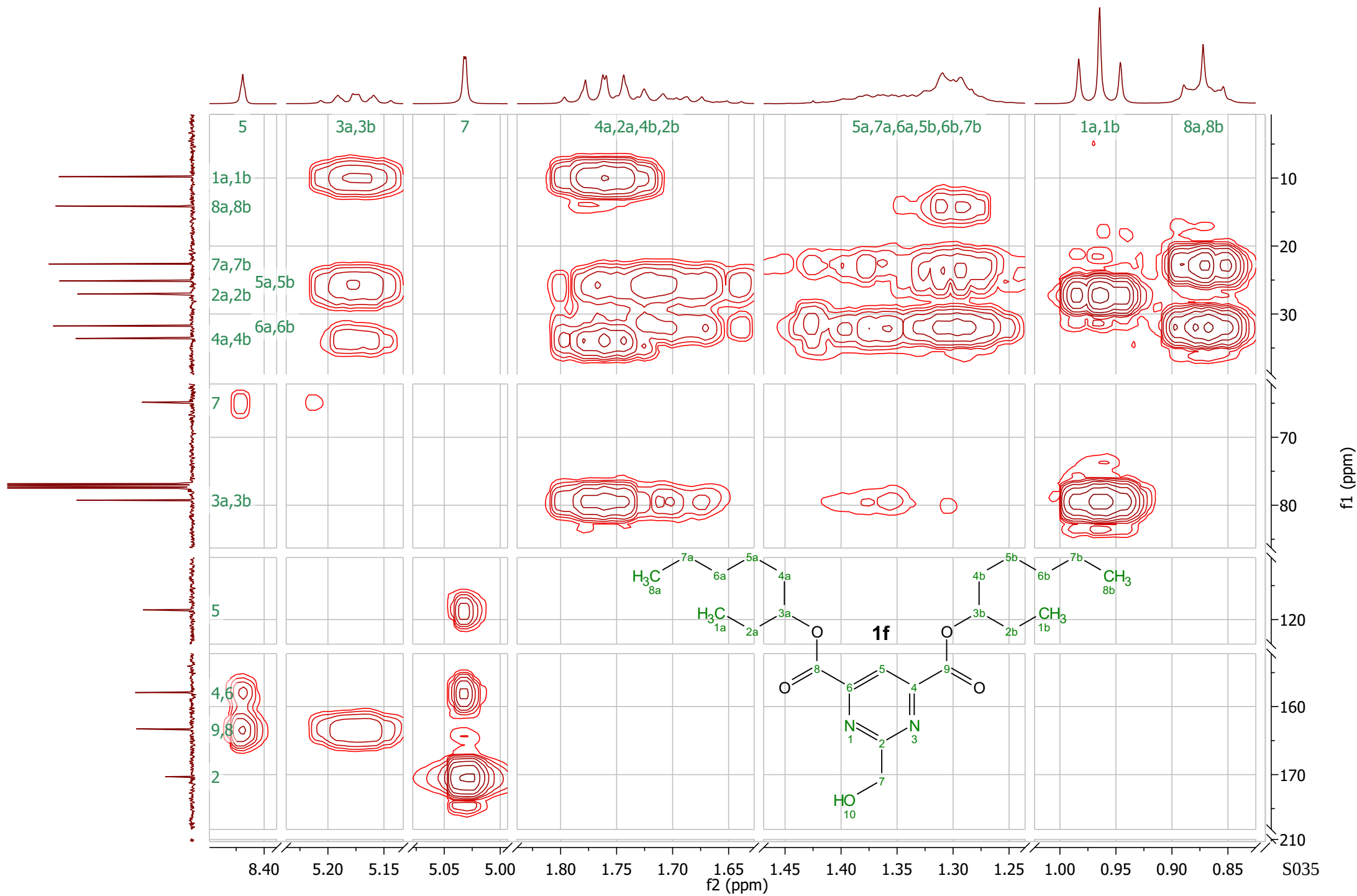
^1H NMR (400 MHz, CDCl_3) δ 8.42 (app t, $J = 0.7$ Hz, 1H), 5.18 (app quint, $J = 6.1$ Hz, 2H), 5.03 (d, $J = 0.6$ Hz, 2H), 3.33 (s, 1H), 2.05 – 1.51 (m, 8H), 1.50 – 1.10 (m, 12H), 0.96 (t, $J = 7.4$ Hz, 6H), 0.87 (app t, $J = 7.0$ Hz, 6H).

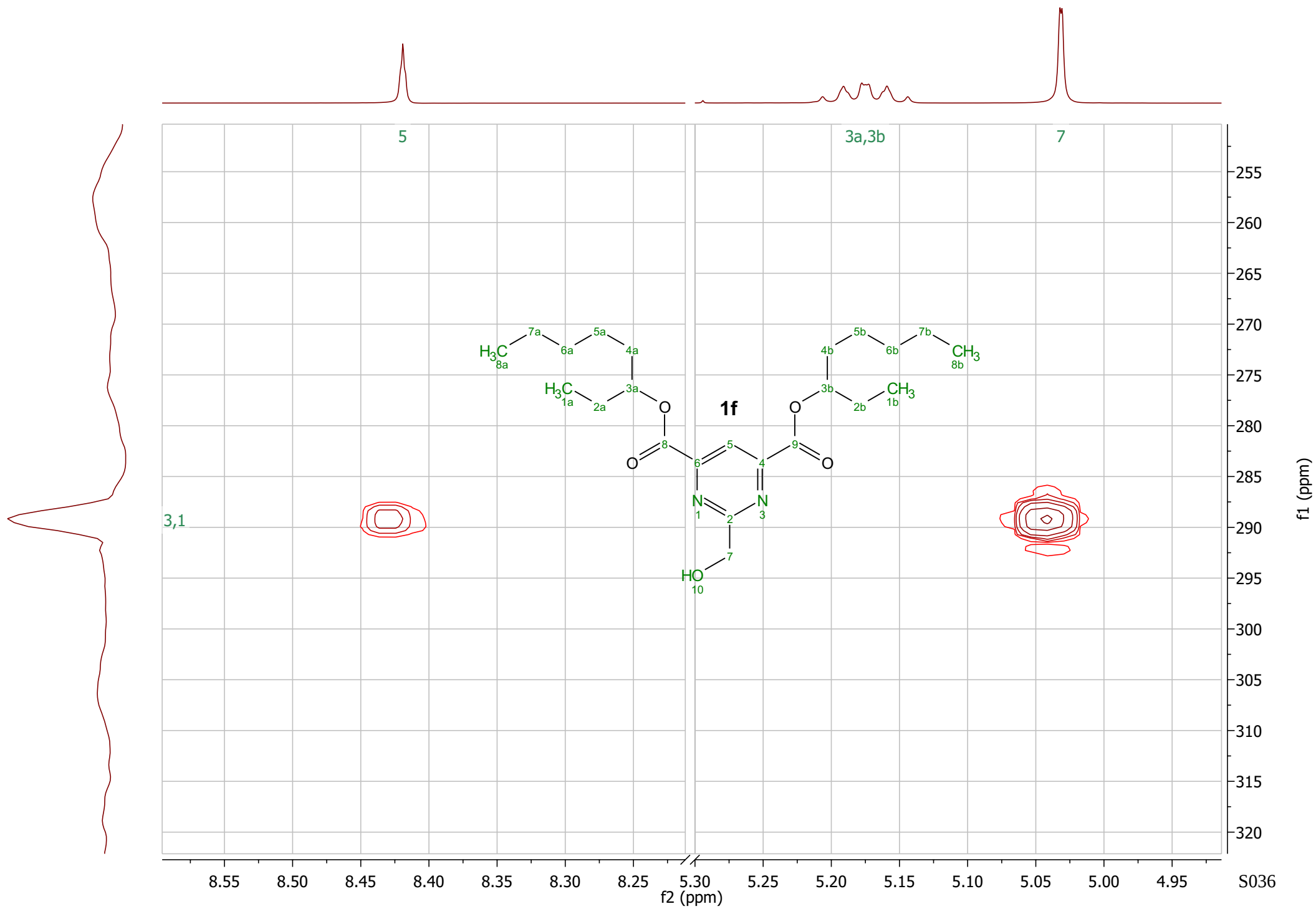


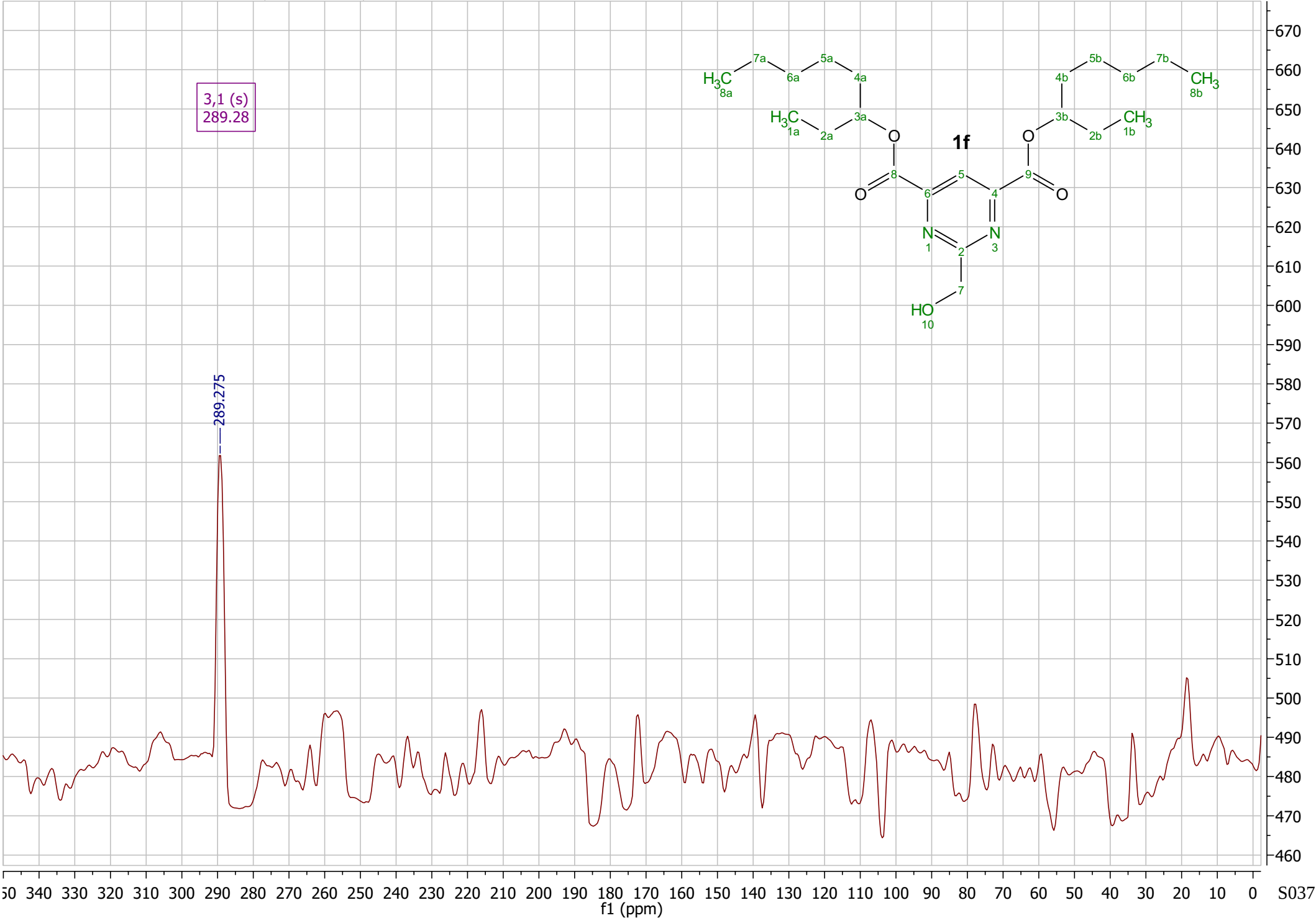
13C ¹³C NMR (101 MHz, CDCl₃) δ 170.3, 163.3 (sym, 2C), 157.9 (sym, 2C), 118.6, 79.3 (sym, 2C), 64.9, 33.6 (sym, 2C), 31.7 (sym, 2C), 27.1 (sym, 2C), 25.1 (sym, 2C), 22.6 (sym, 2C), 14.1 (sym, 2C), 9.8 (sym, 2C).



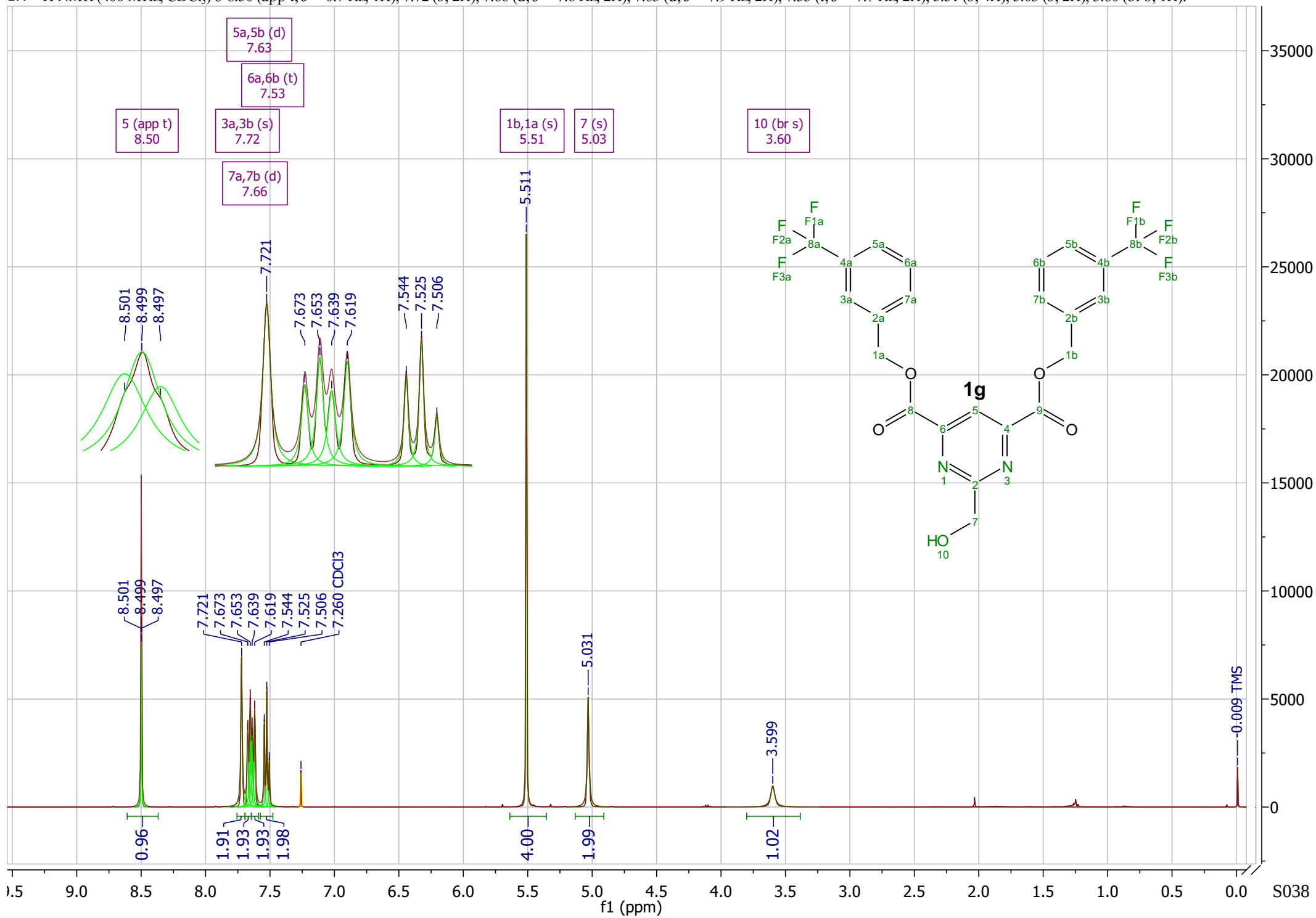




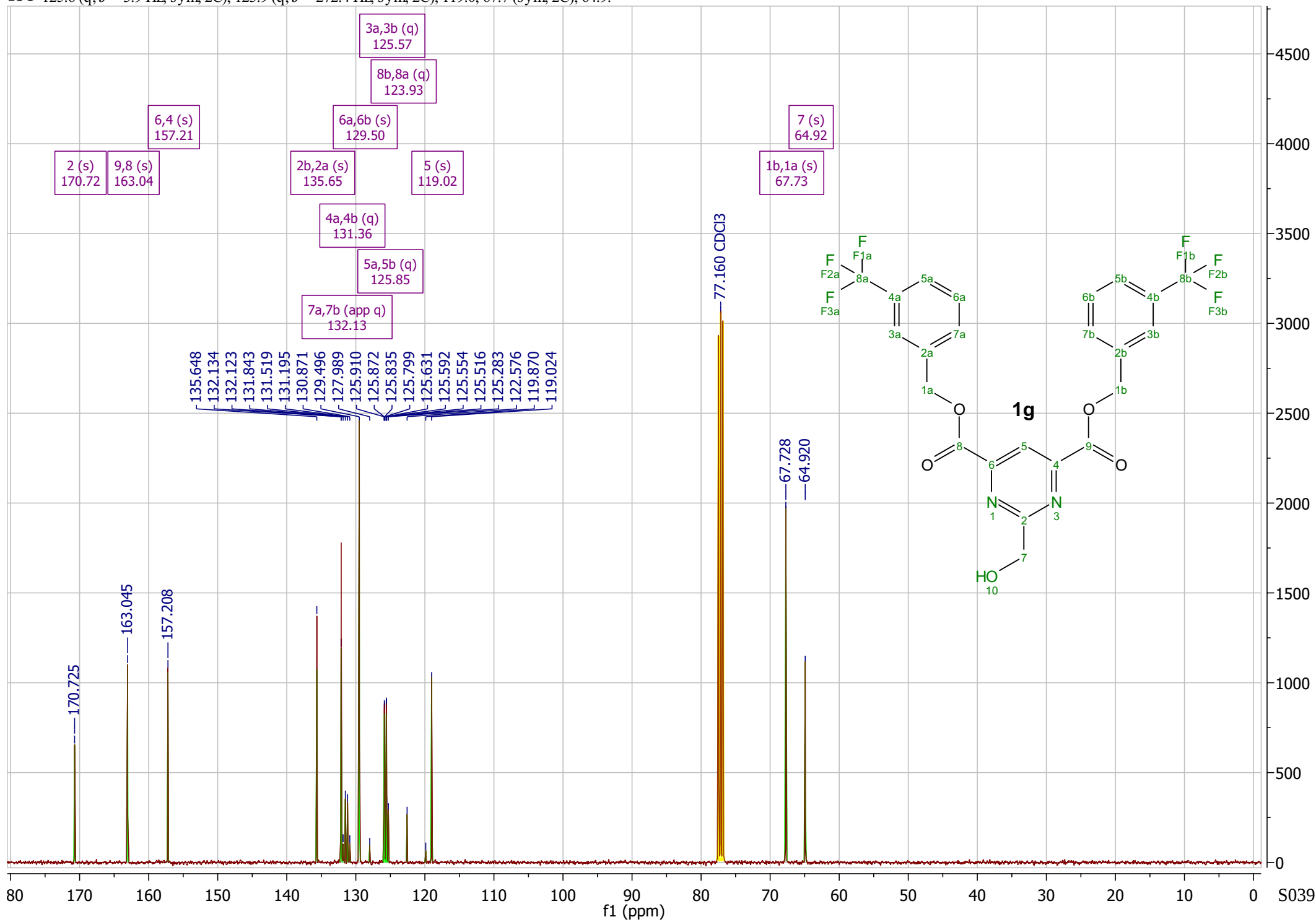




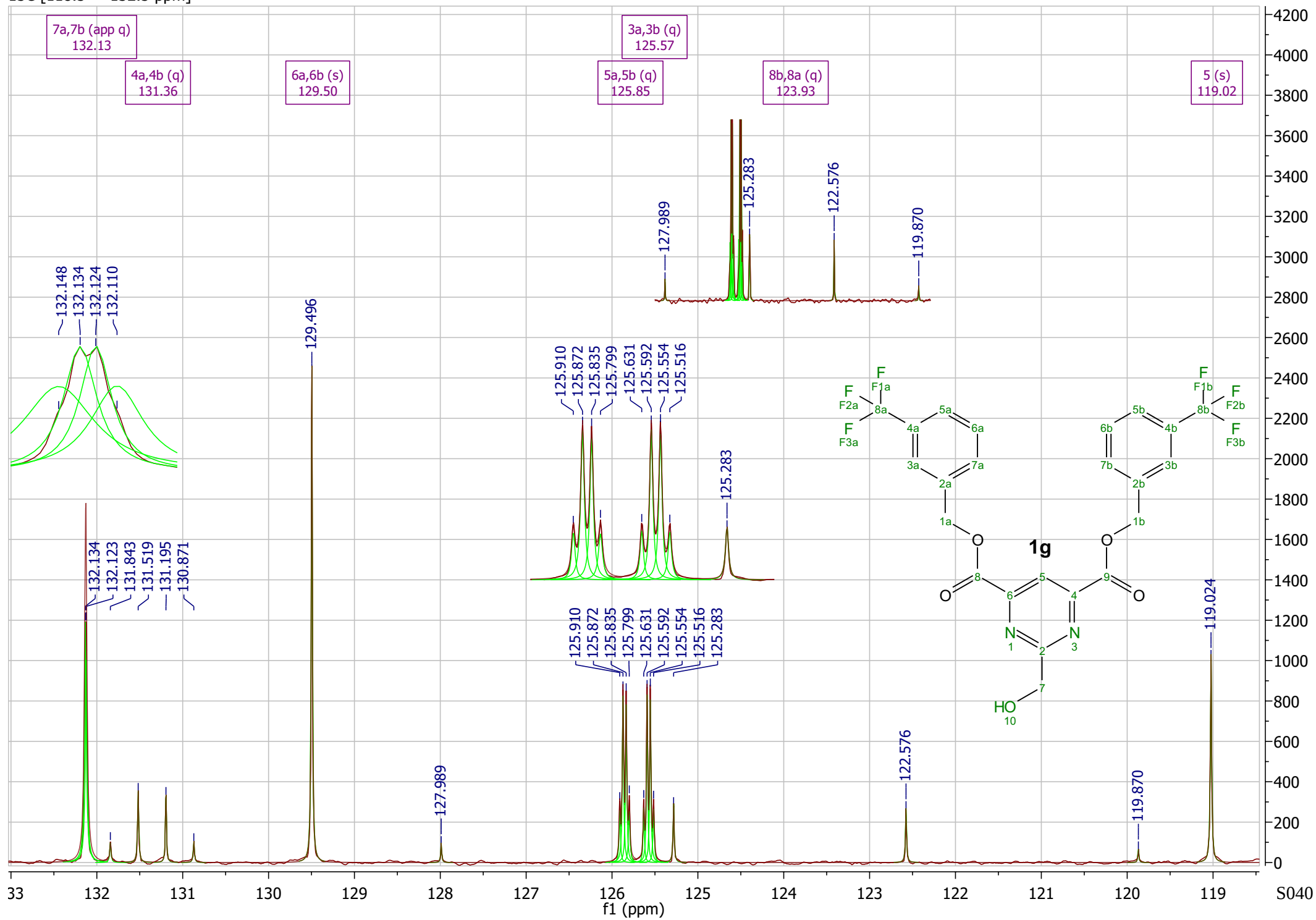
^1H NMR (400 MHz, CDCl_3) δ 8.50 (app t, $J = 0.7$ Hz, 1H), 7.72 (s, 2H), 7.66 (d, $J = 7.6$ Hz, 2H), 7.63 (d, $J = 7.9$ Hz, 2H), 7.53 (t, $J = 7.7$ Hz, 2H), 5.51 (s, 4H), 5.03 (s, 2H), 3.60 (br s, 1H).

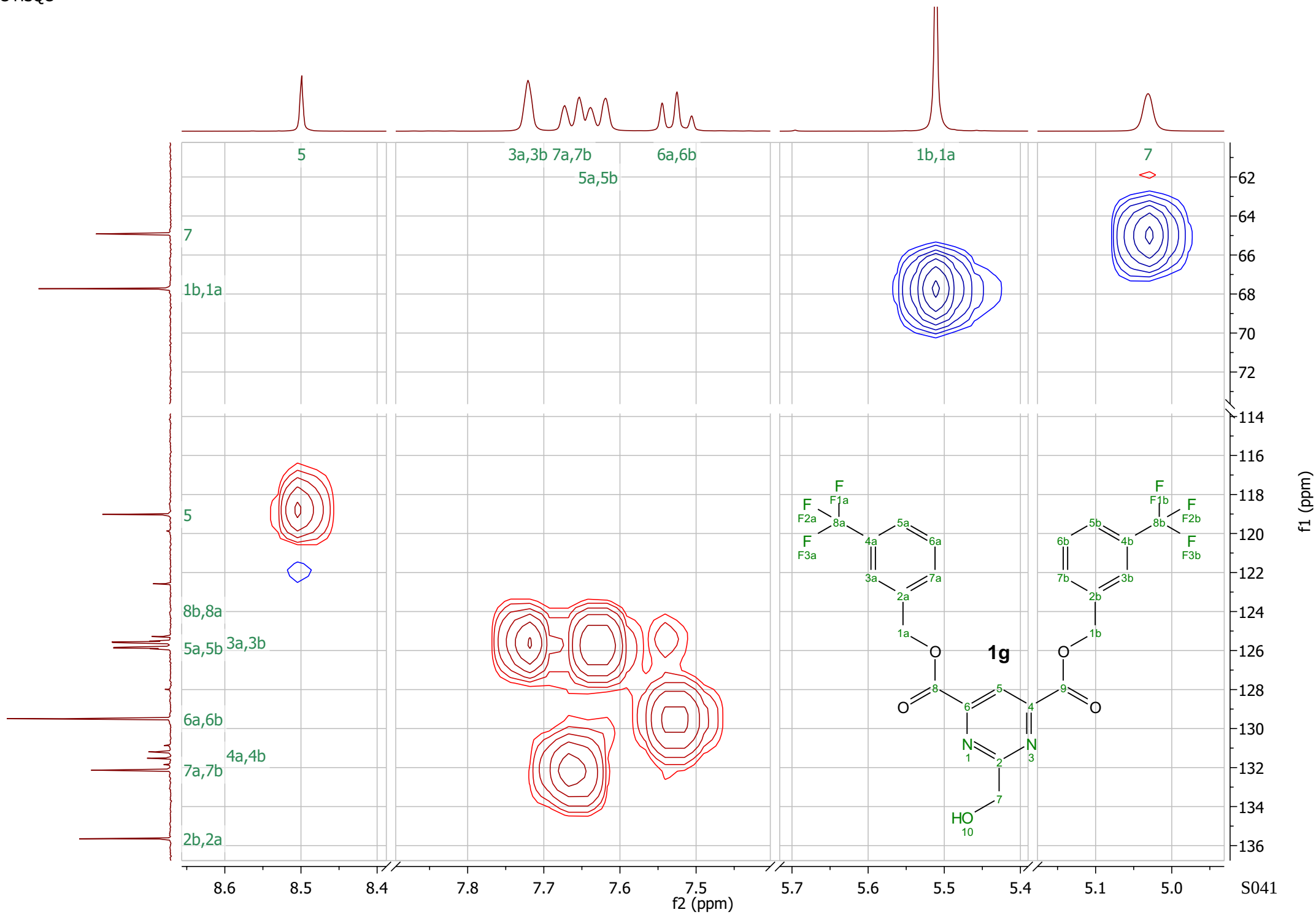


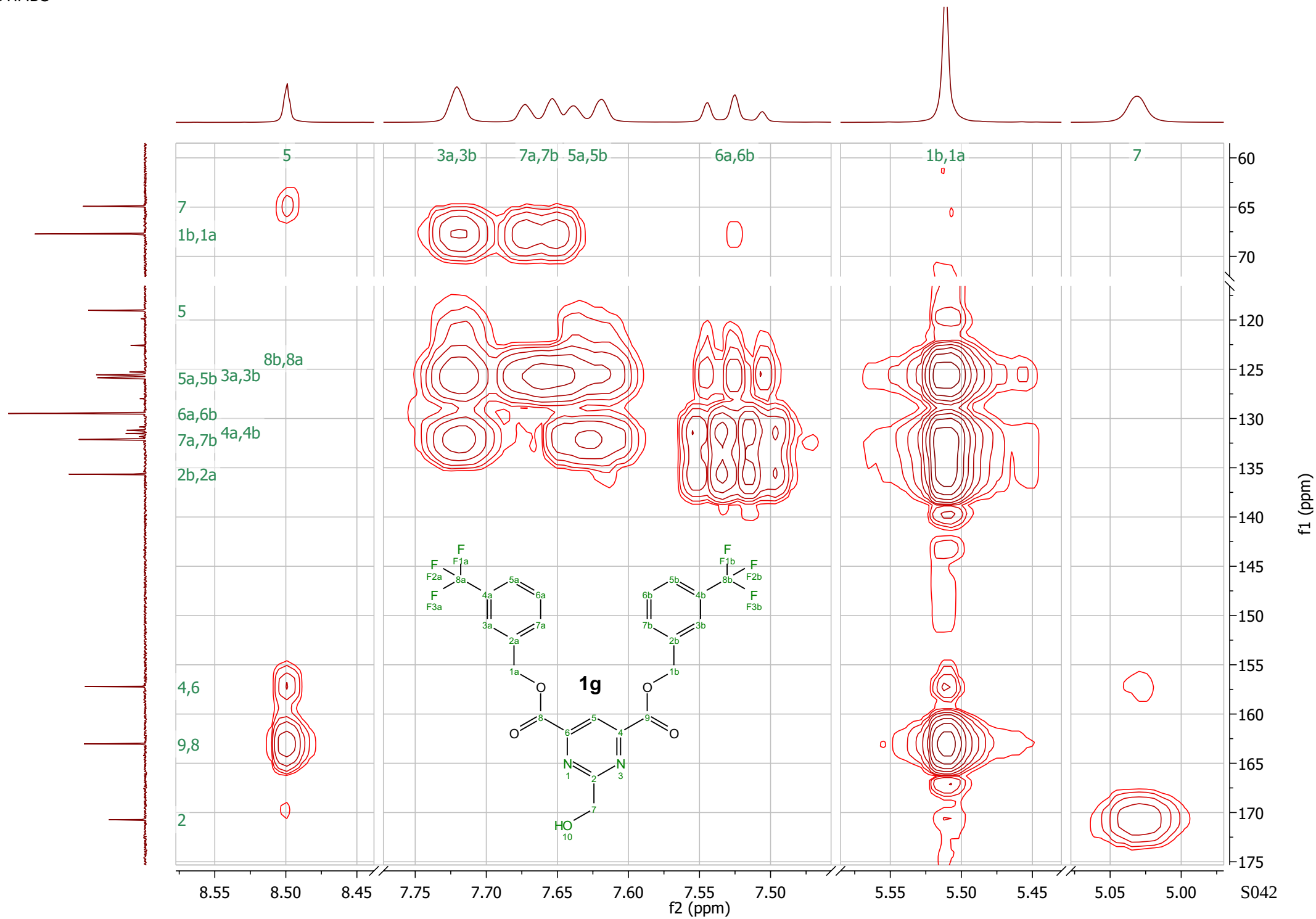
¹³C NMR (101 MHz, CDCl₃) δ 170.7, 163.0 (sym, 2C), 157.2 (sym, 2C), 132.1 (app q, *J* = 1.1 Hz, sym, 2C), 131.4 (q, *J* = 32.6 Hz, sym, 2C), 129.5 (sym, 2C), 125.9 (q, *J* = 3.7 Hz, sym, 2C), 125.6 (q, *J* = 3.9 Hz, sym, 2C), 123.9 (q, *J* = 272.4 Hz, sym, 2C), 119.0, 67.7 (sym, 2C), 64.9.

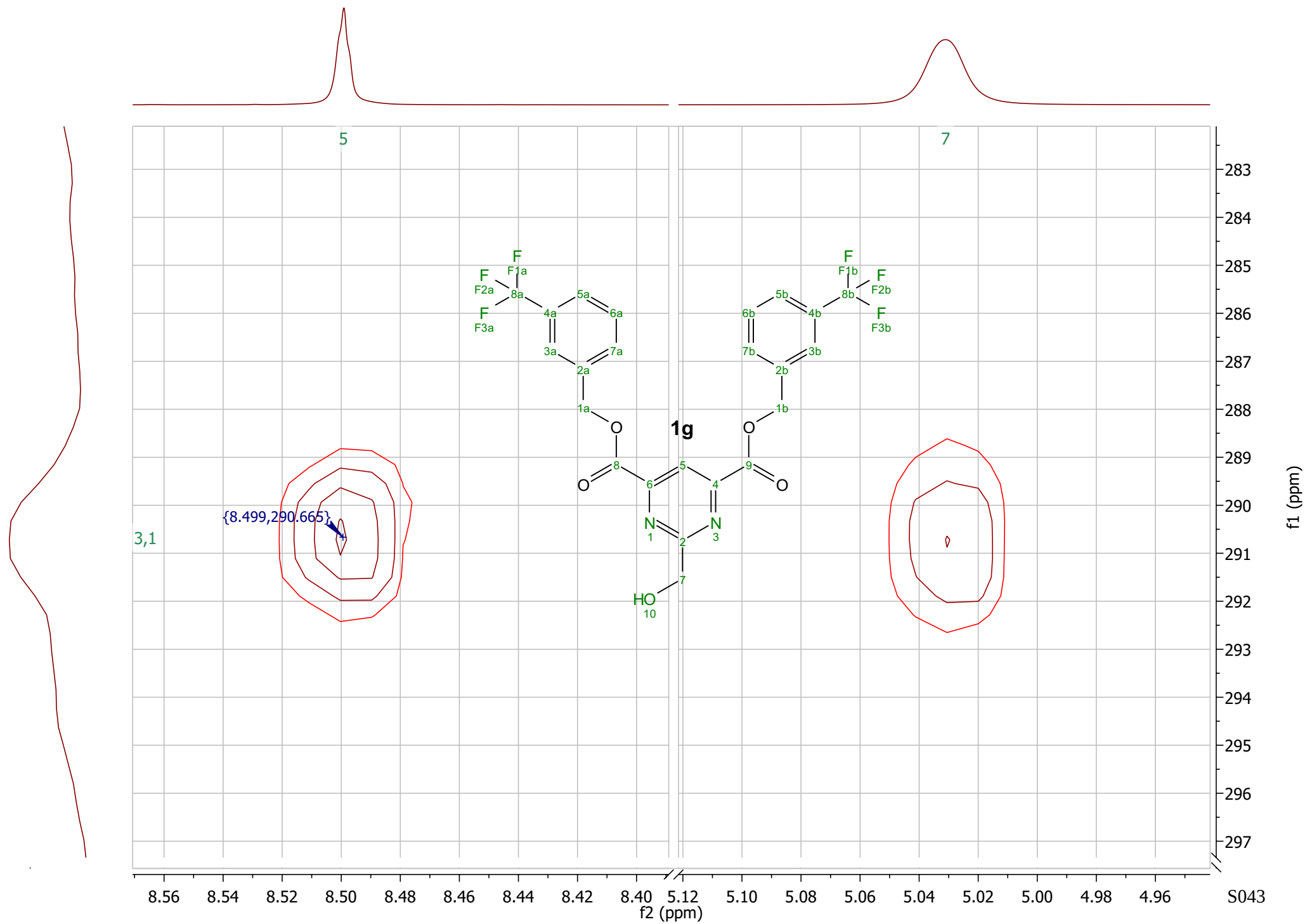


¹³C [118.5 — 132.5 ppm]

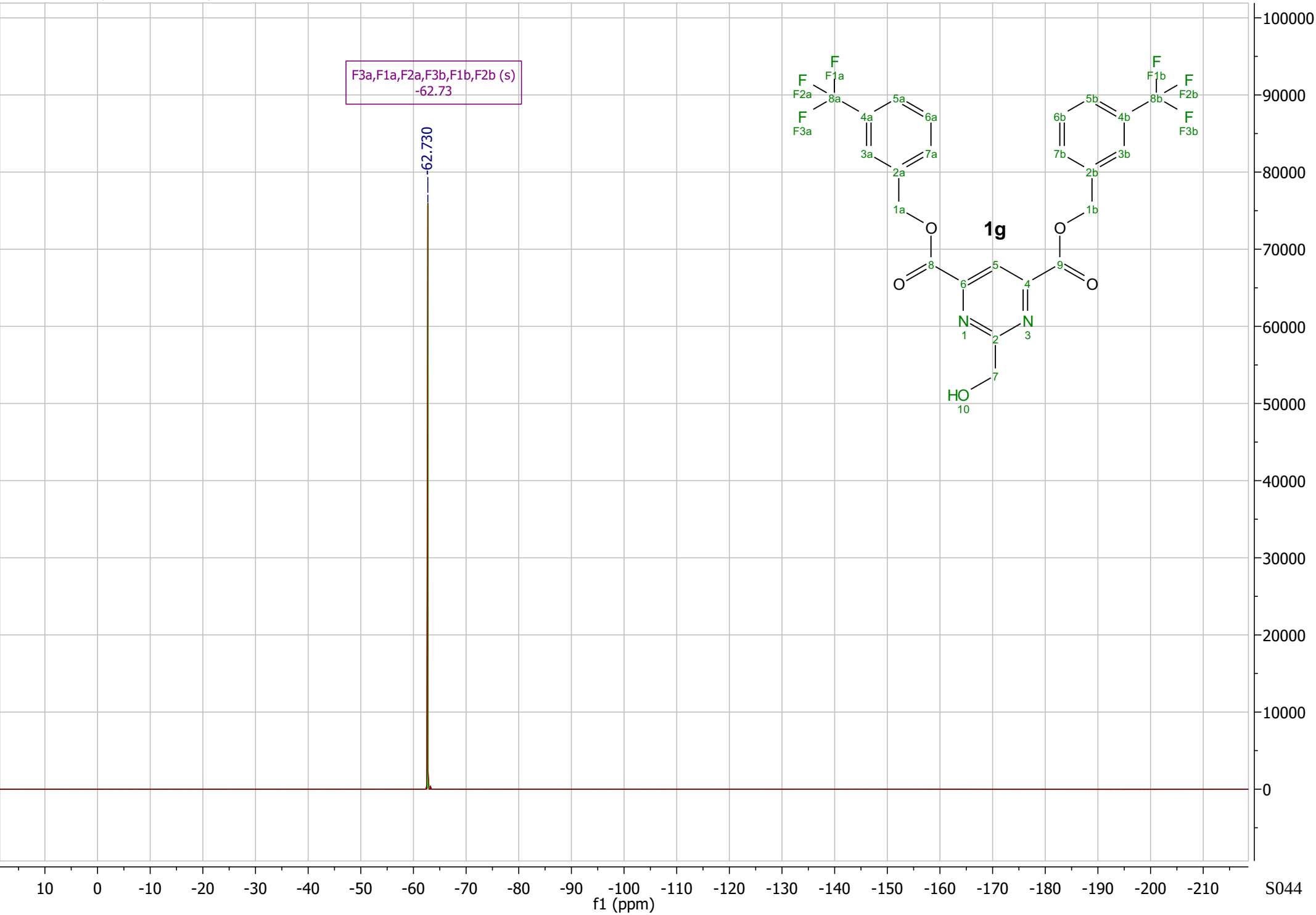




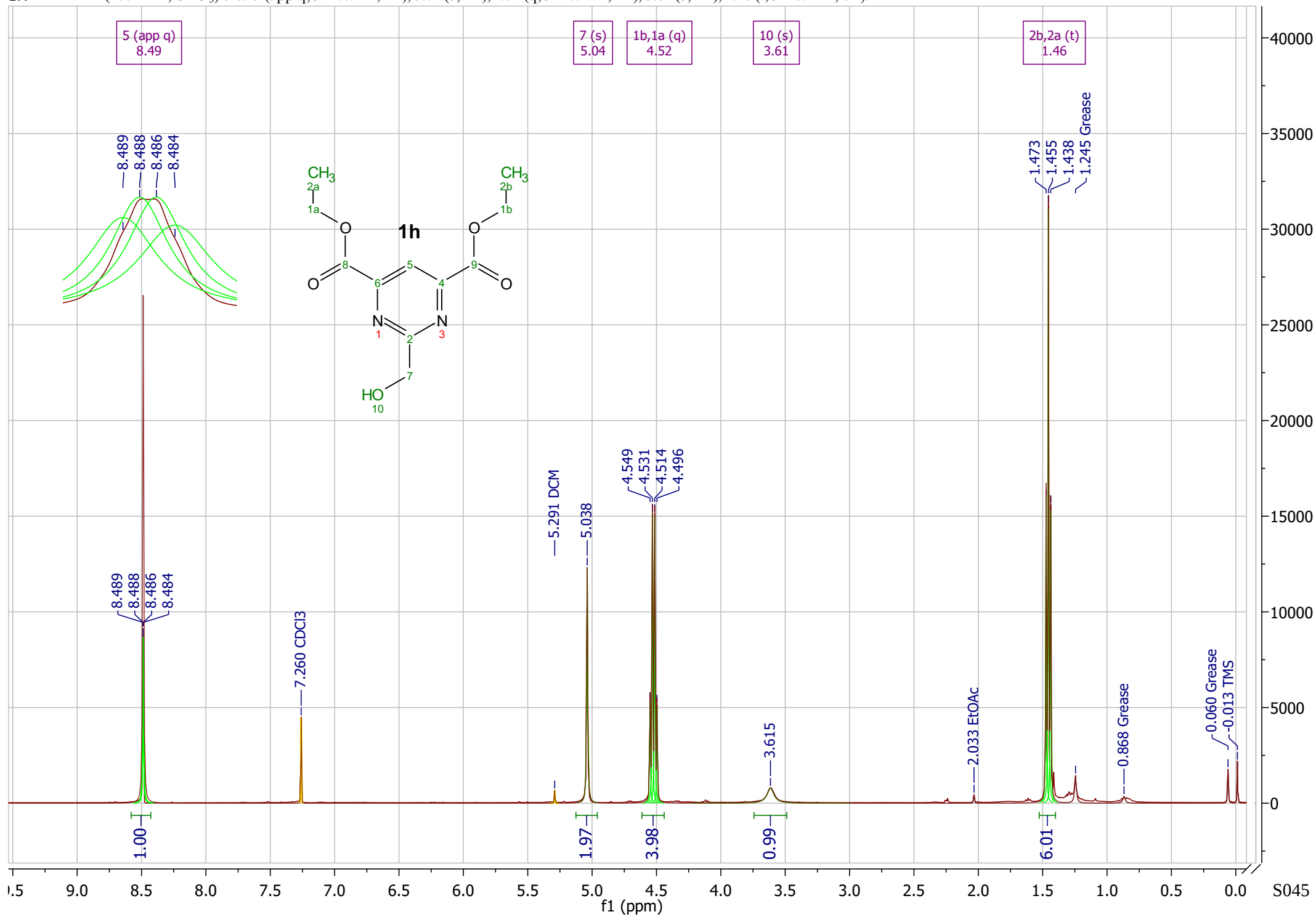




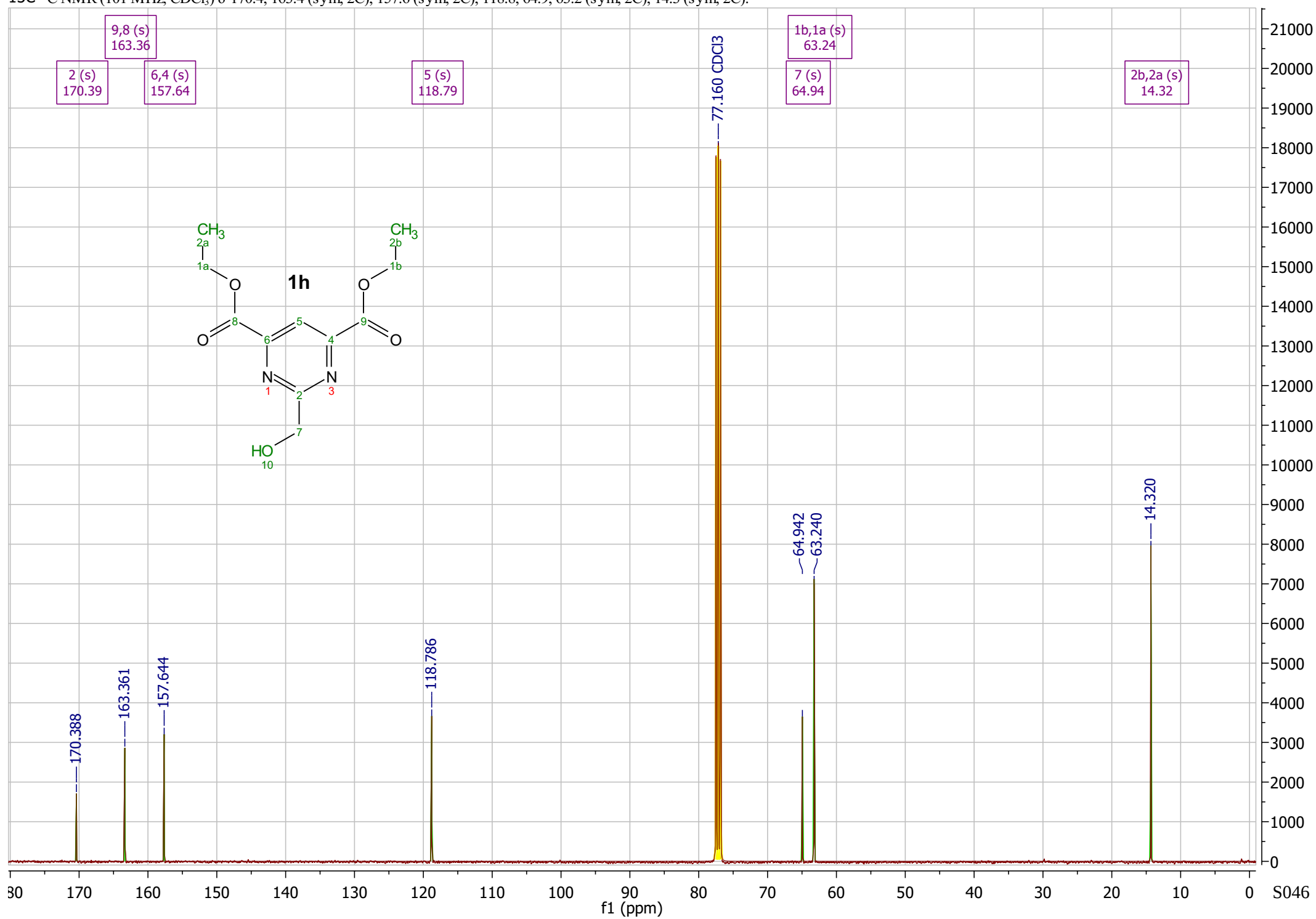
19F 19F NMR (376 MHz, CDCl3) δ -62.73.

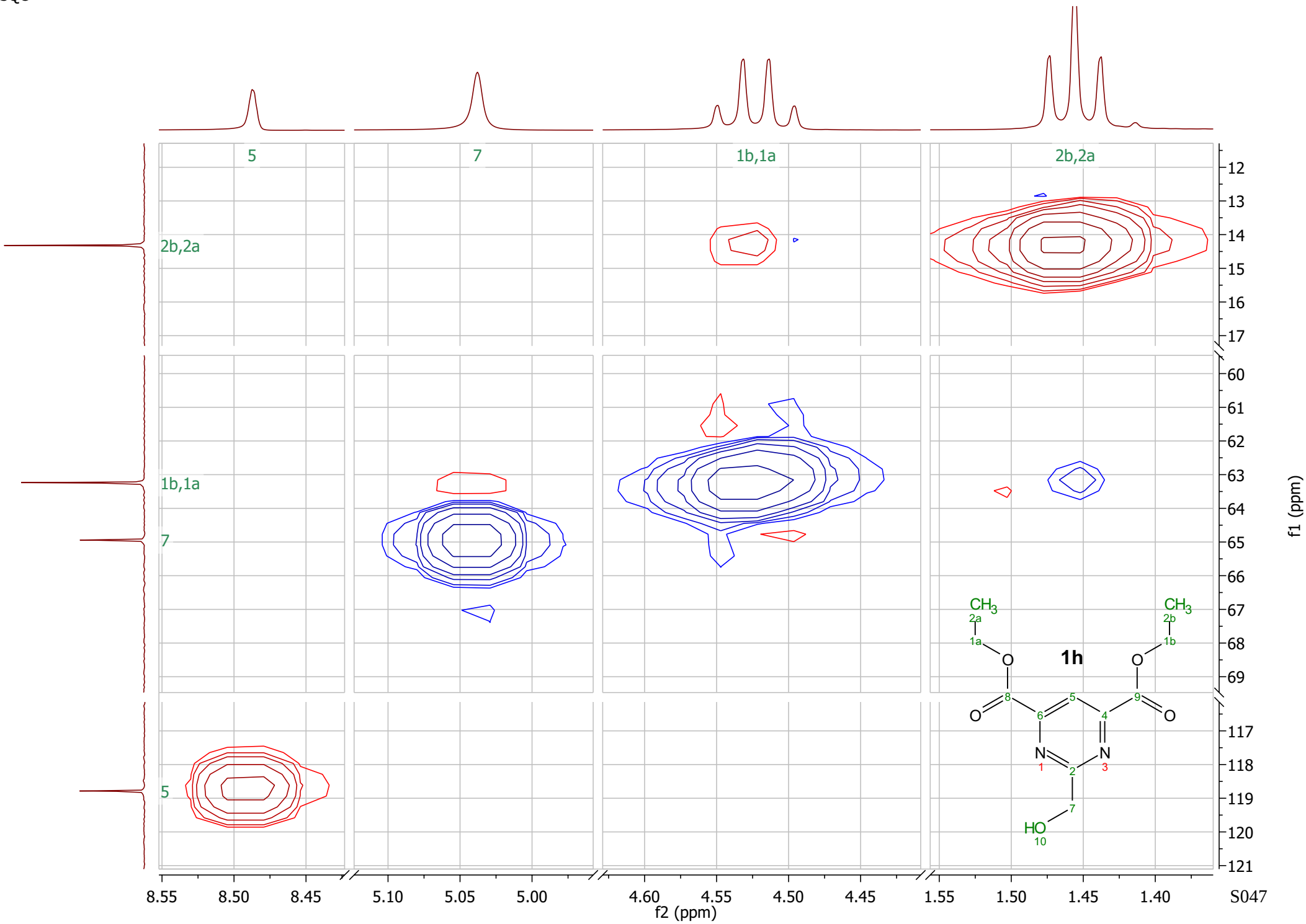


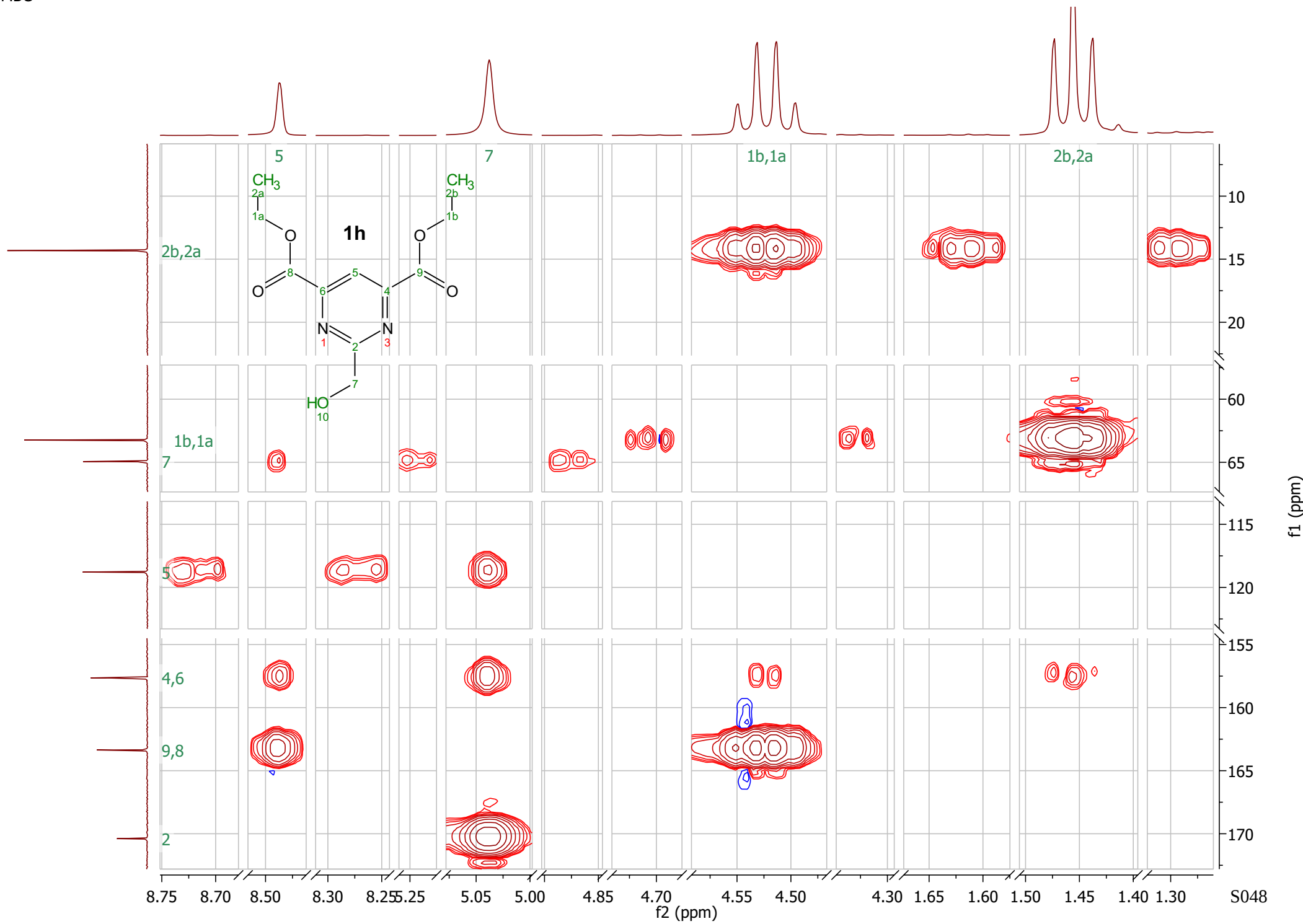
^1H NMR (400 MHz, CDCl_3) δ 8.49 (app q, $J = 0.7$ Hz, 1H), 5.04 (s, 2H), 4.52 (q, $J = 7.1$ Hz, 4H), 3.61 (s, 1H), 1.46 (t, $J = 7.1$ Hz, 6H).



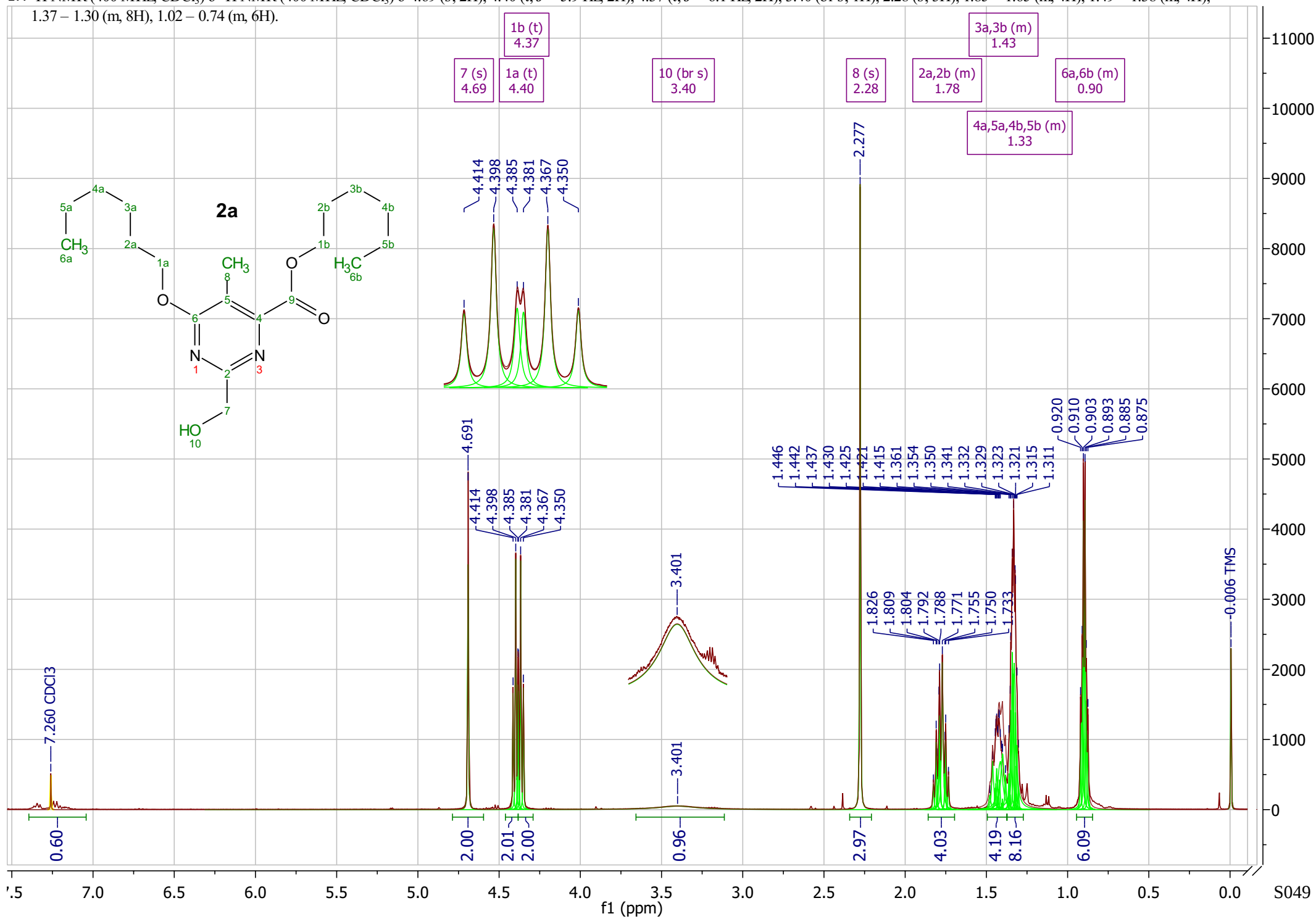
^{13}C NMR (101 MHz, CDCl_3) δ 170.4, 163.4 (sym, 2C), 157.6 (sym, 2C), 118.8, 64.9, 63.2 (sym, 2C), 14.3 (sym, 2C).



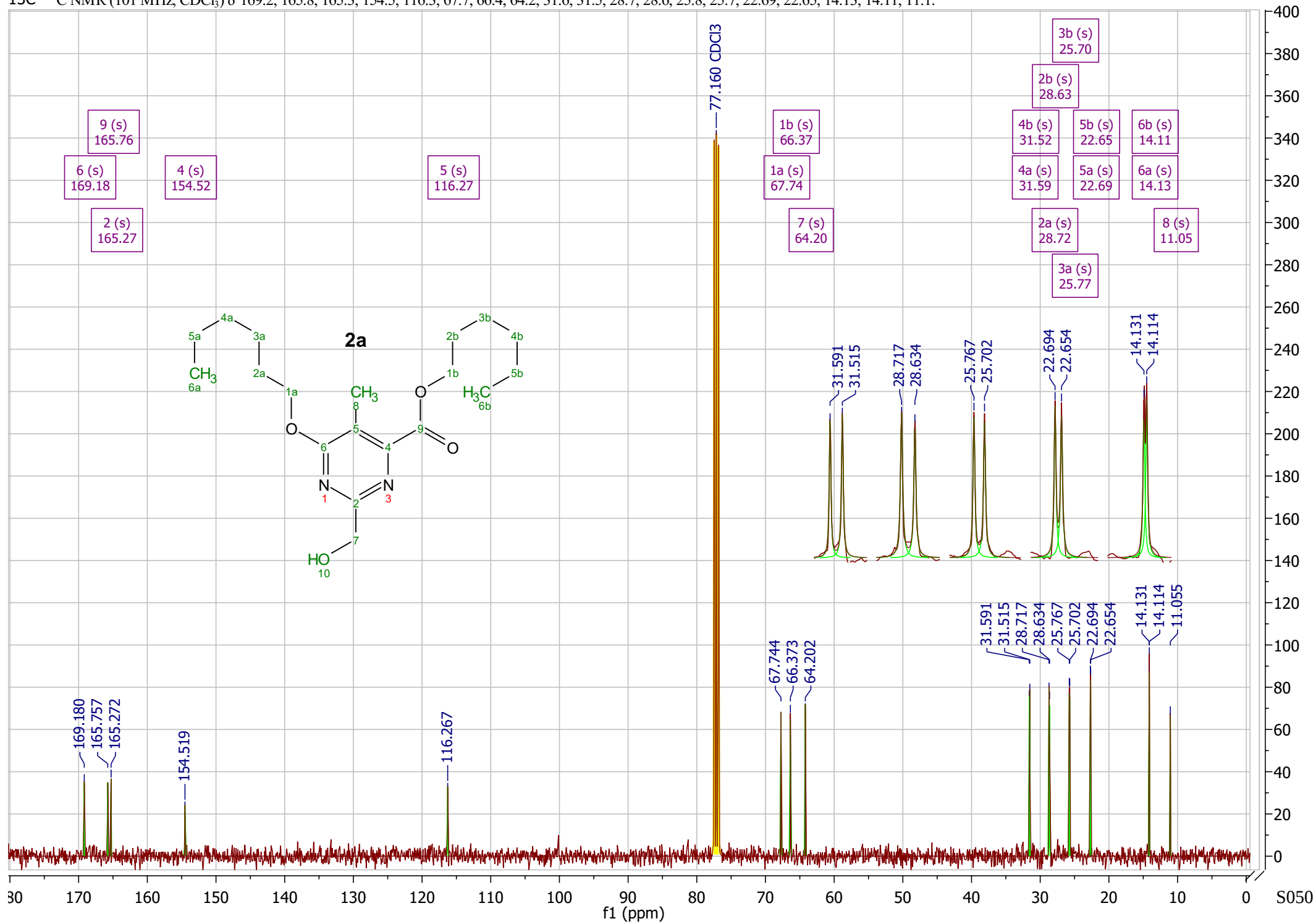


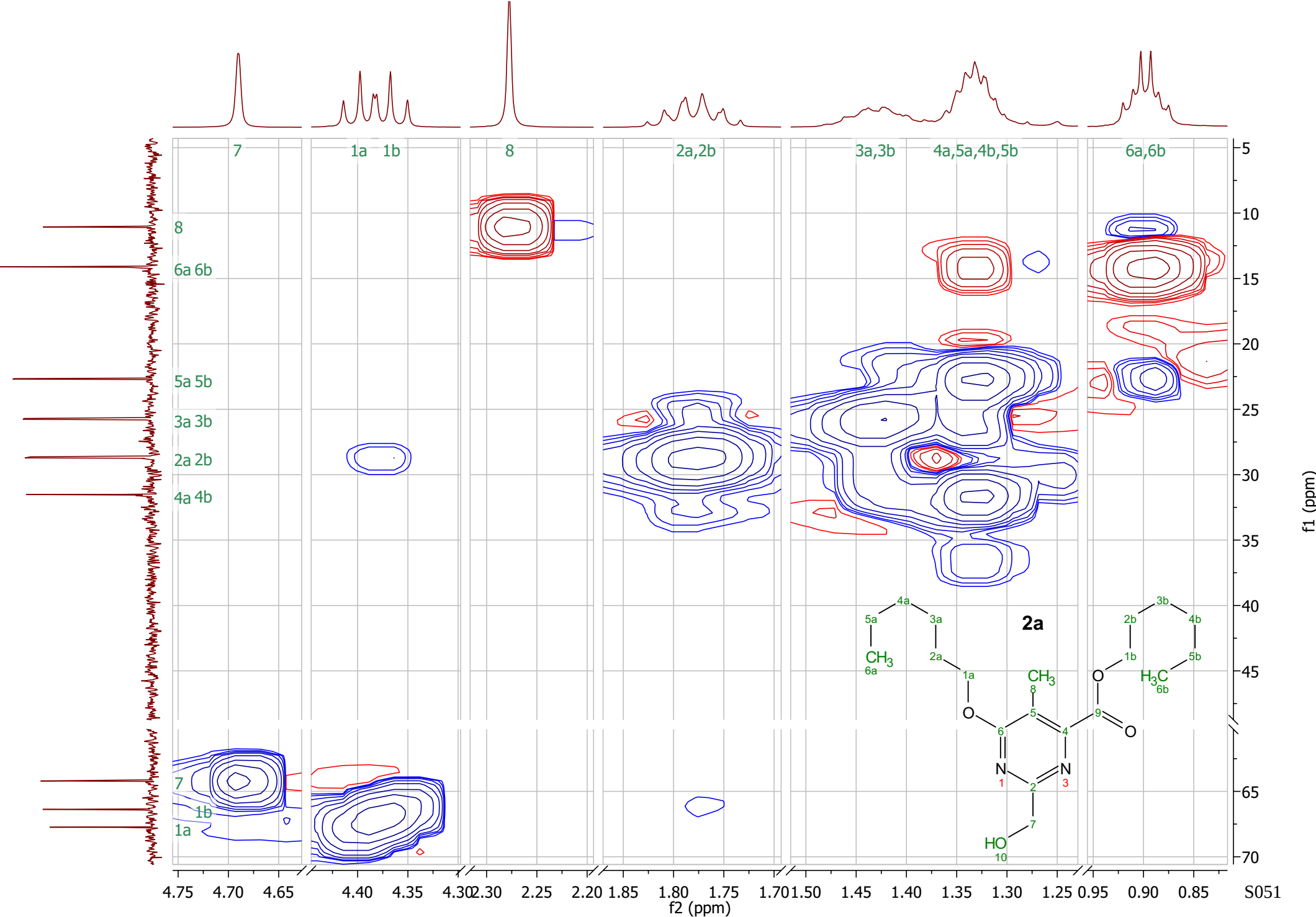


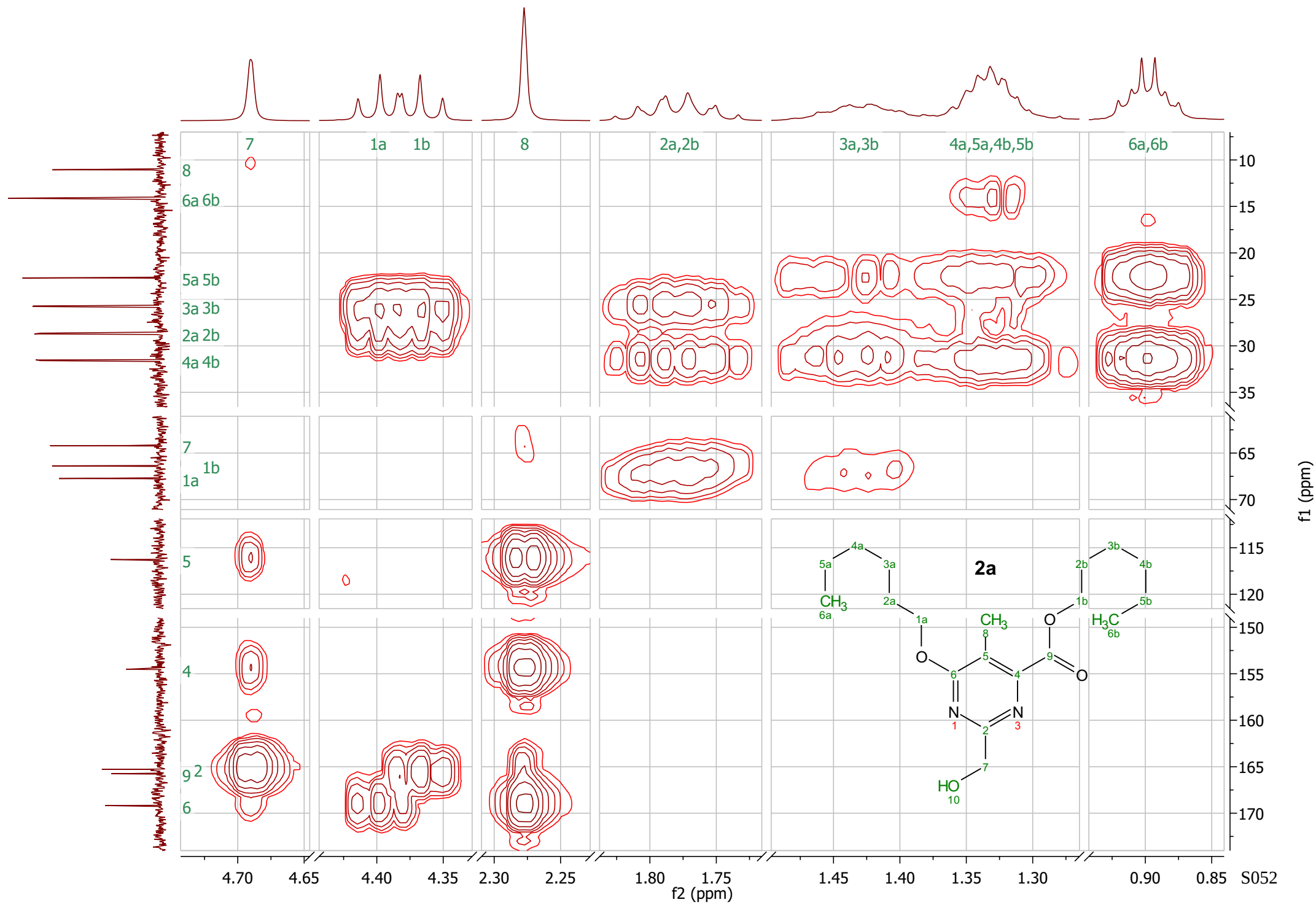
^1H NMR (400 MHz, CDCl_3) δ 4.69 (s, 2H), 4.40 (t, $J = 5.9$ Hz, 2H), 4.37 (t, $J = 6.1$ Hz, 2H), 3.40 (br s, 1H), 2.28 (s, 3H), 1.85 – 1.65 (m, 4H), 1.49 – 1.38 (m, 4H), 1.37 – 1.30 (m, 8H), 1.02 – 0.74 (m, 6H).



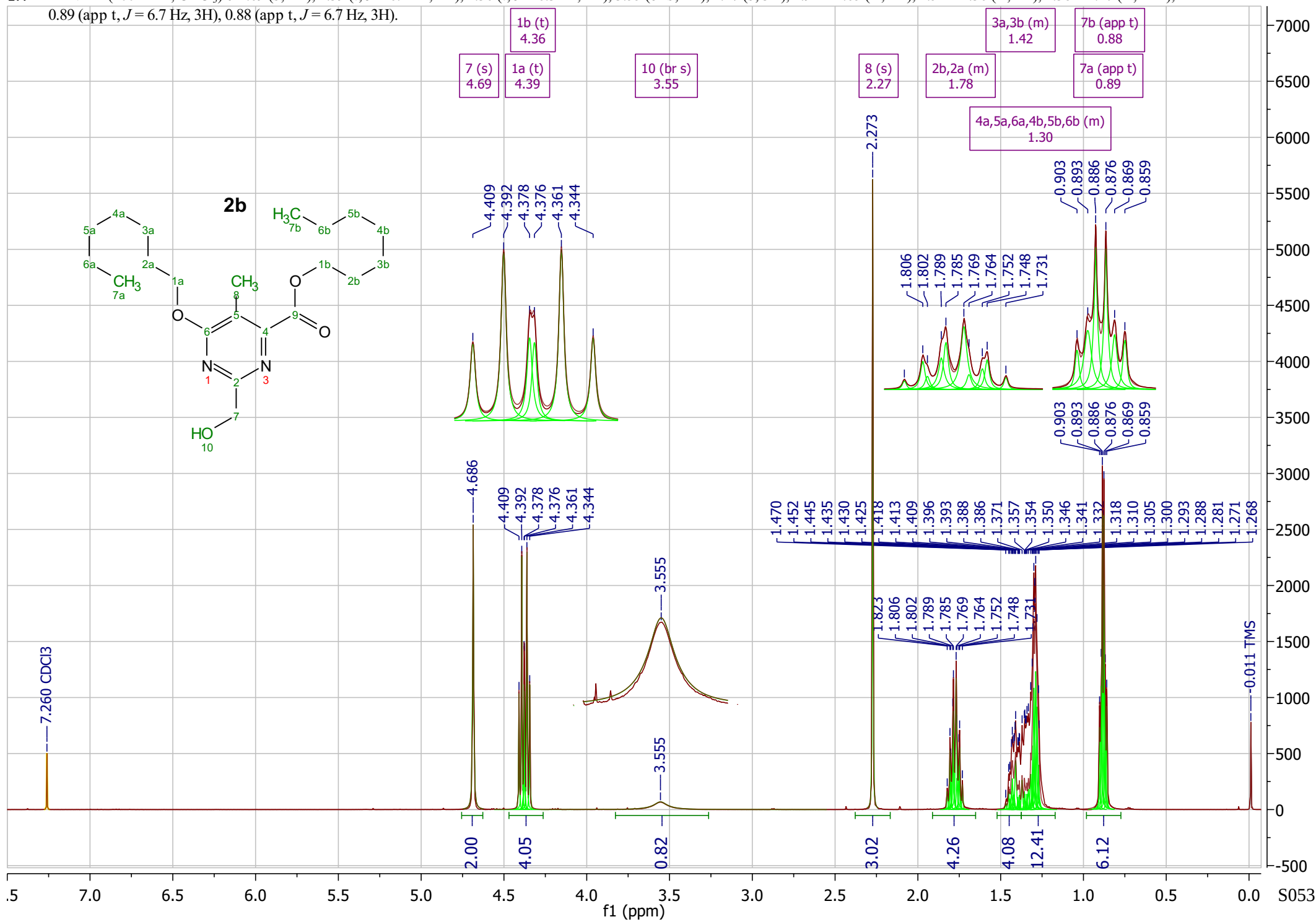
¹³C NMR (101 MHz, CDCl₃) δ 169.2, 165.8, 165.3, 154.5, 116.3, 67.7, 66.4, 64.2, 31.6, 31.5, 28.7, 28.6, 25.7, 22.69, 22.65, 14.13, 14.11, 11.1.



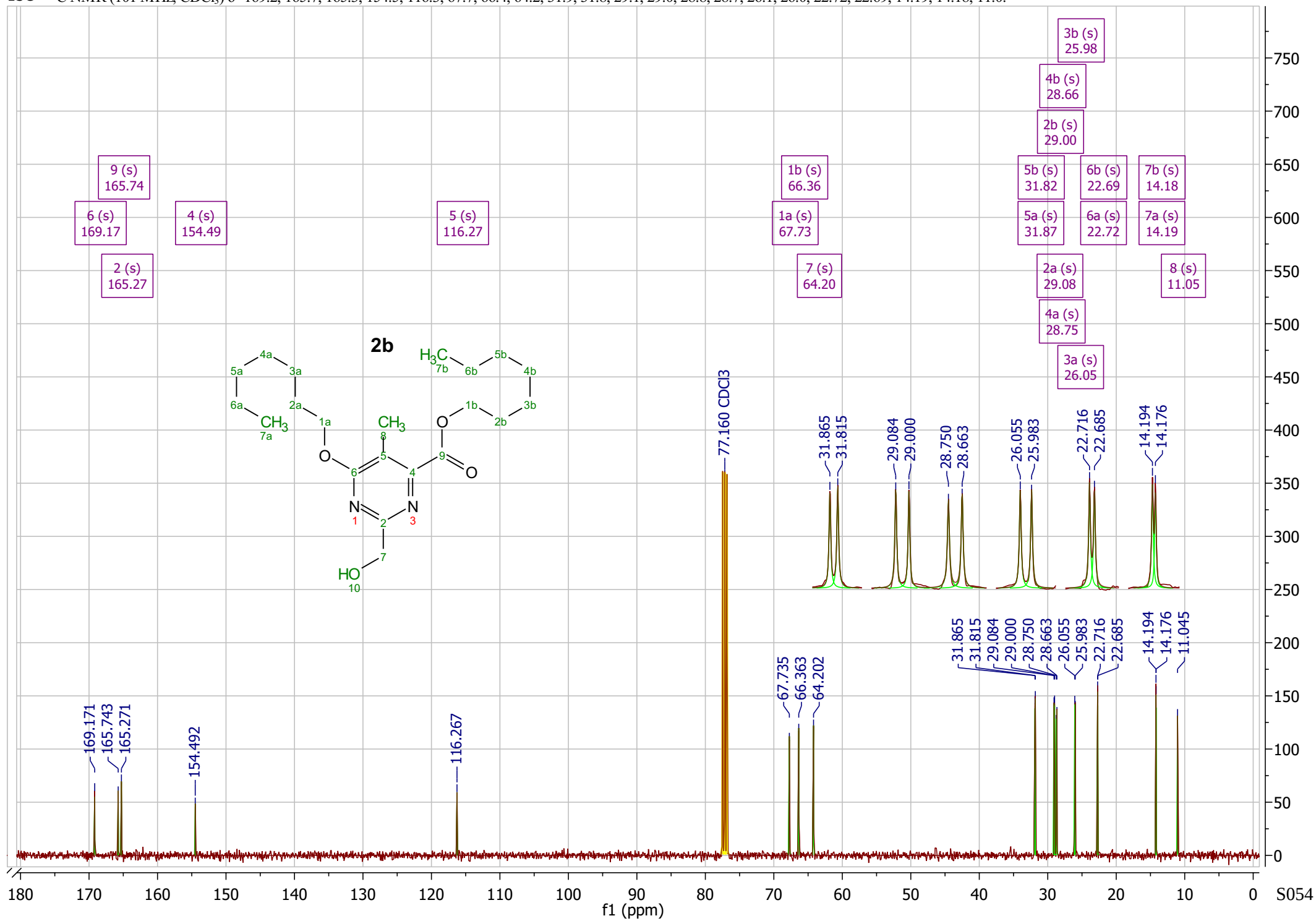


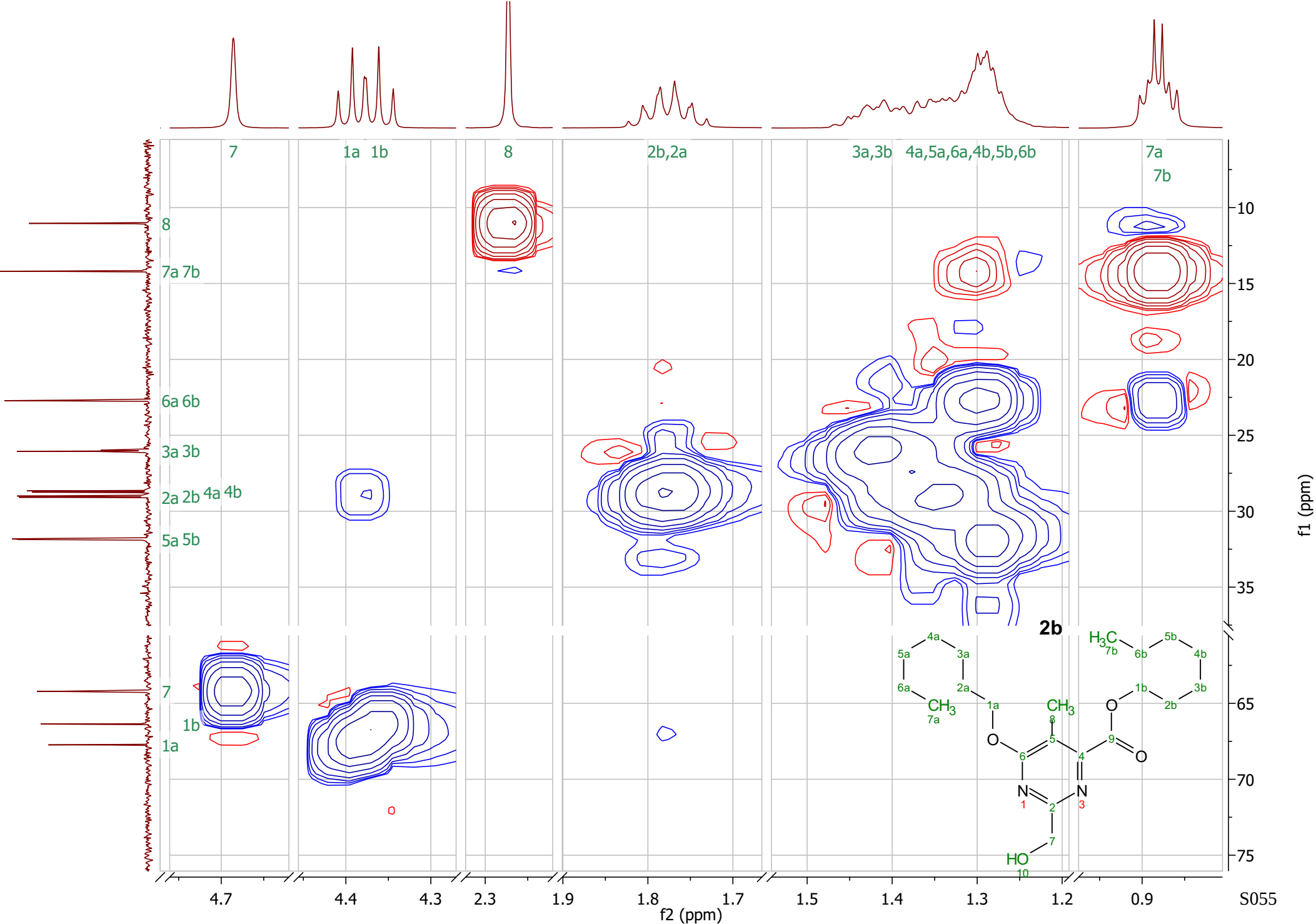


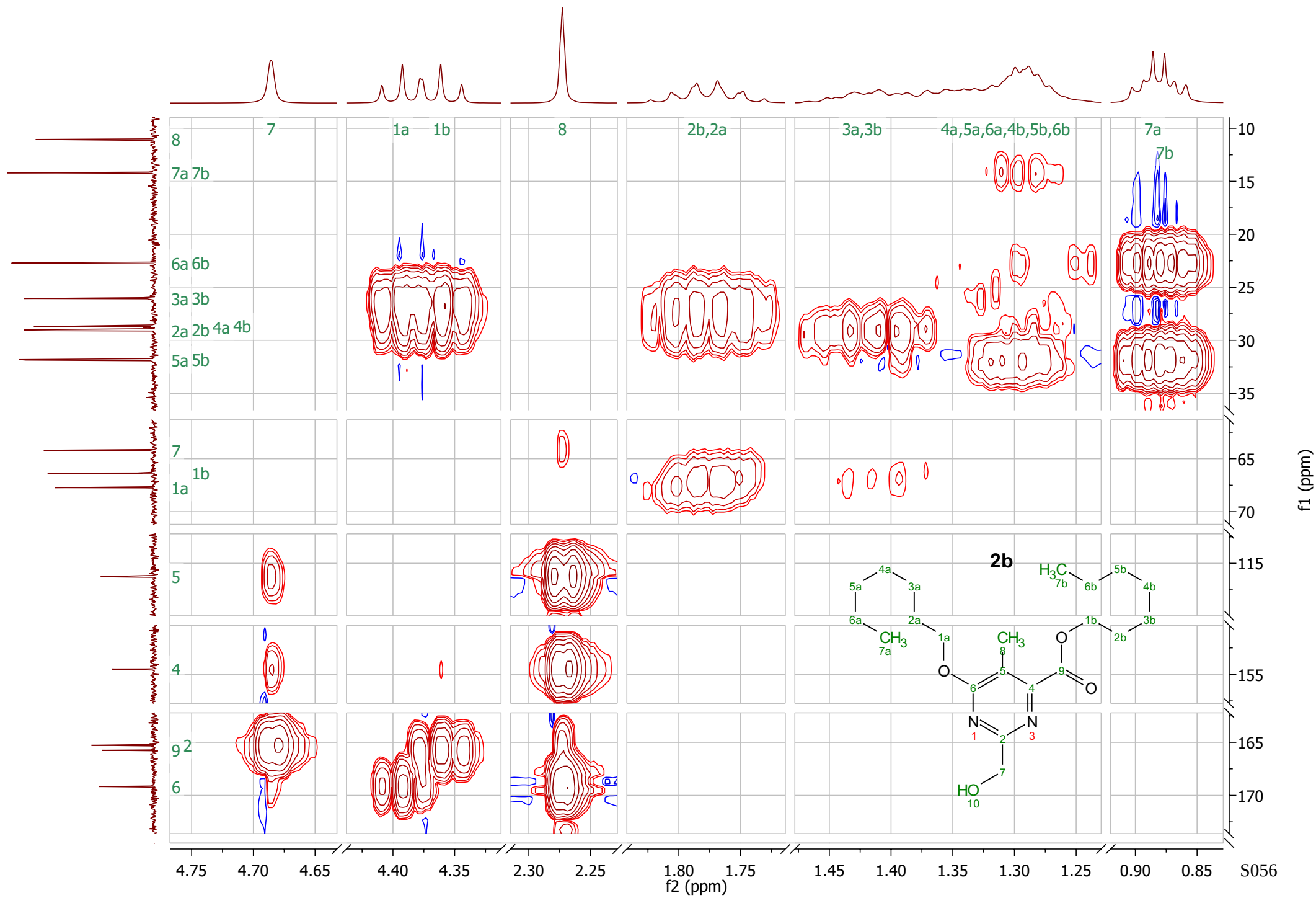
¹H NMR (400 MHz, CDCl₃) δ 4.69 (s, 2H), 4.39 (t, *J* = 6.1 Hz, 2H), 4.36 (t, *J* = 6.3 Hz, 2H), 3.55 (br s, 1H), 2.27 (s, 3H), 1.91 – 1.65 (m, 4H), 1.52 – 1.36 (m, 4H), 1.38 – 1.17 (m, 12H), 0.89 (app t, *J* = 6.7 Hz, 3H), 0.88 (app t, *J* = 6.7 Hz, 3H).



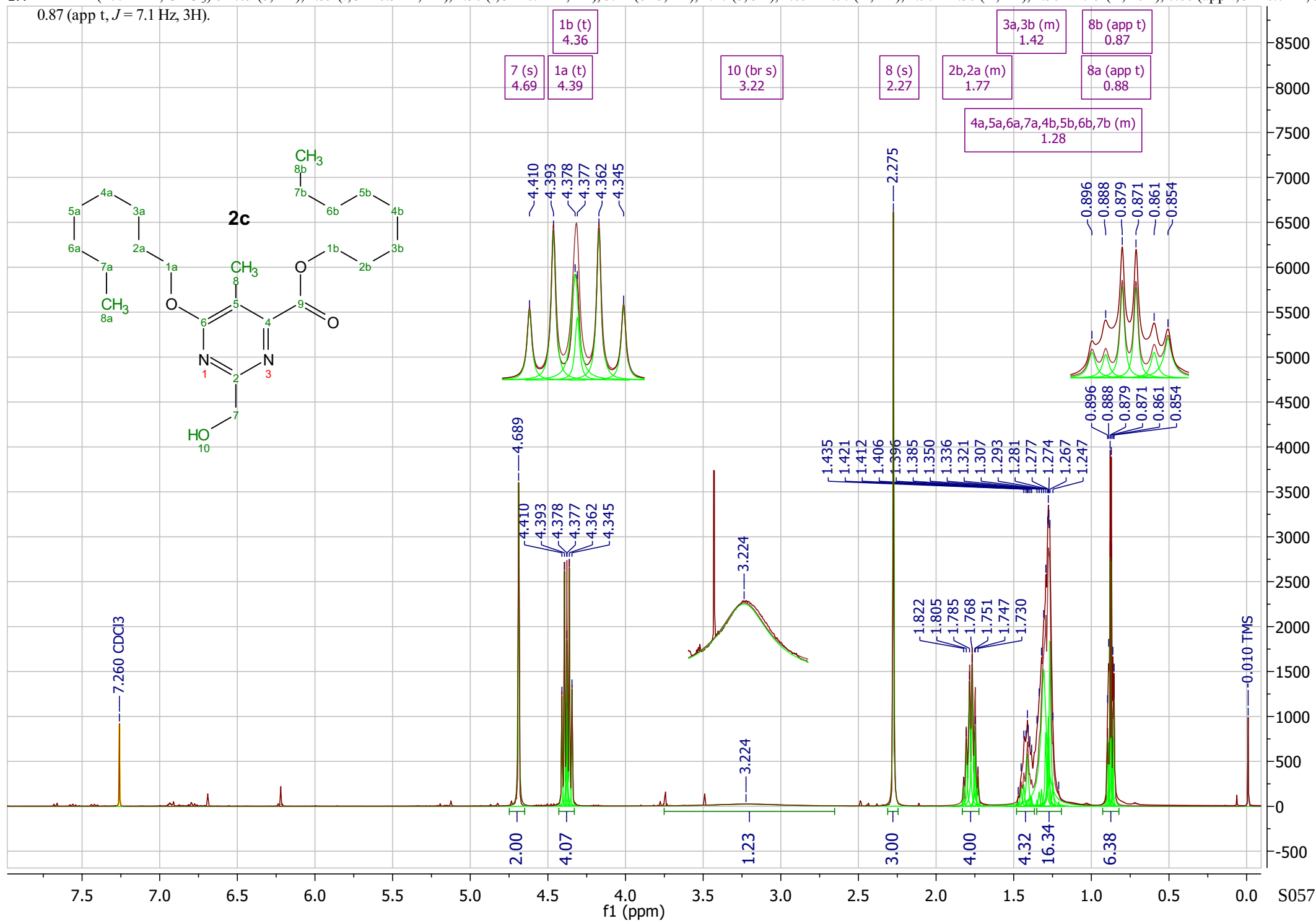
¹³C ¹³C NMR (101 MHz, CDCl₃) δ 169.2, 165.7, 165.3, 154.5, 116.3, 67.7, 66.4, 64.2, 31.9, 31.8, 29.1, 29.0, 28.8, 28.7, 26.1, 26.0, 22.72, 22.69, 14.19, 14.18, 11.0.



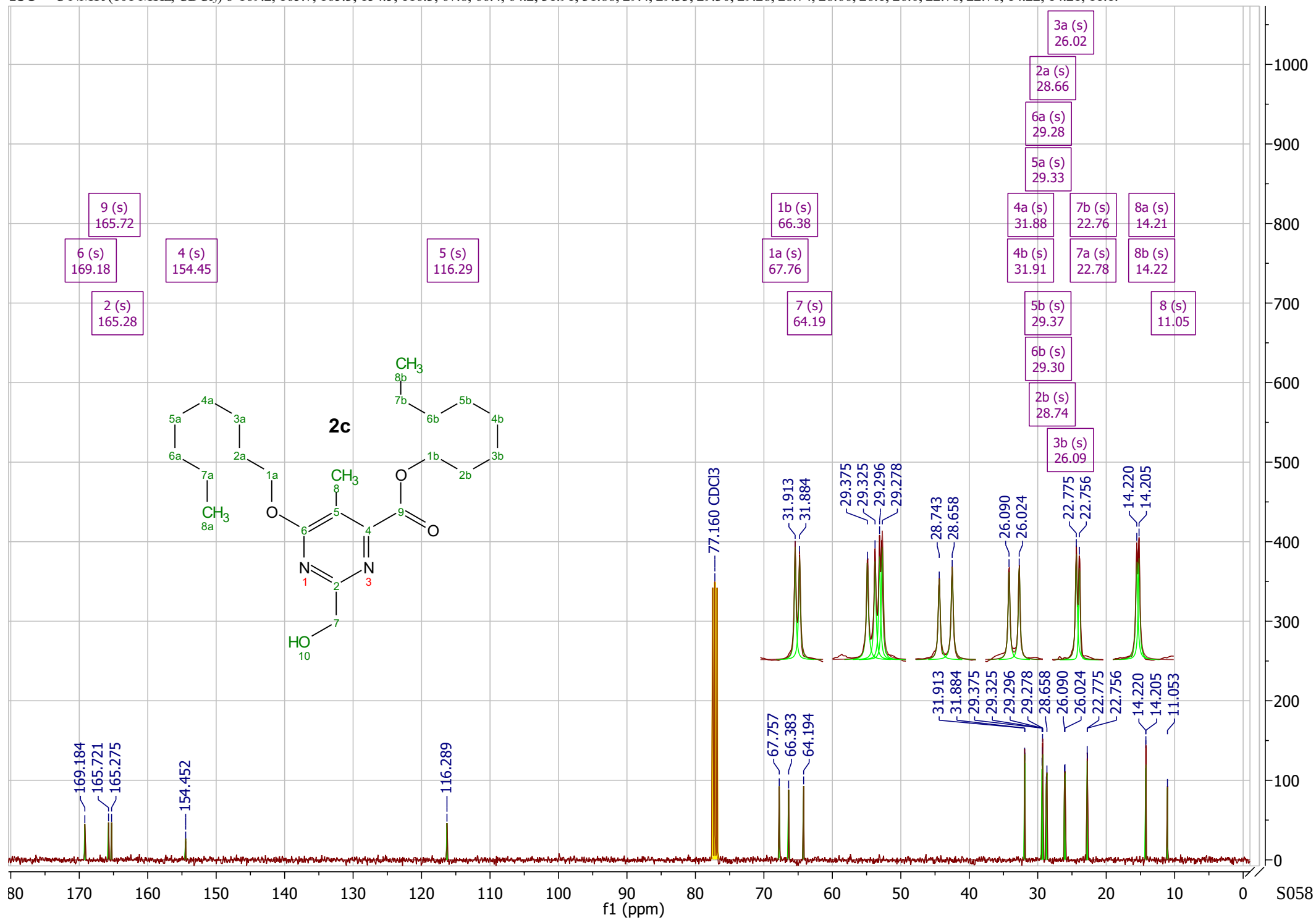


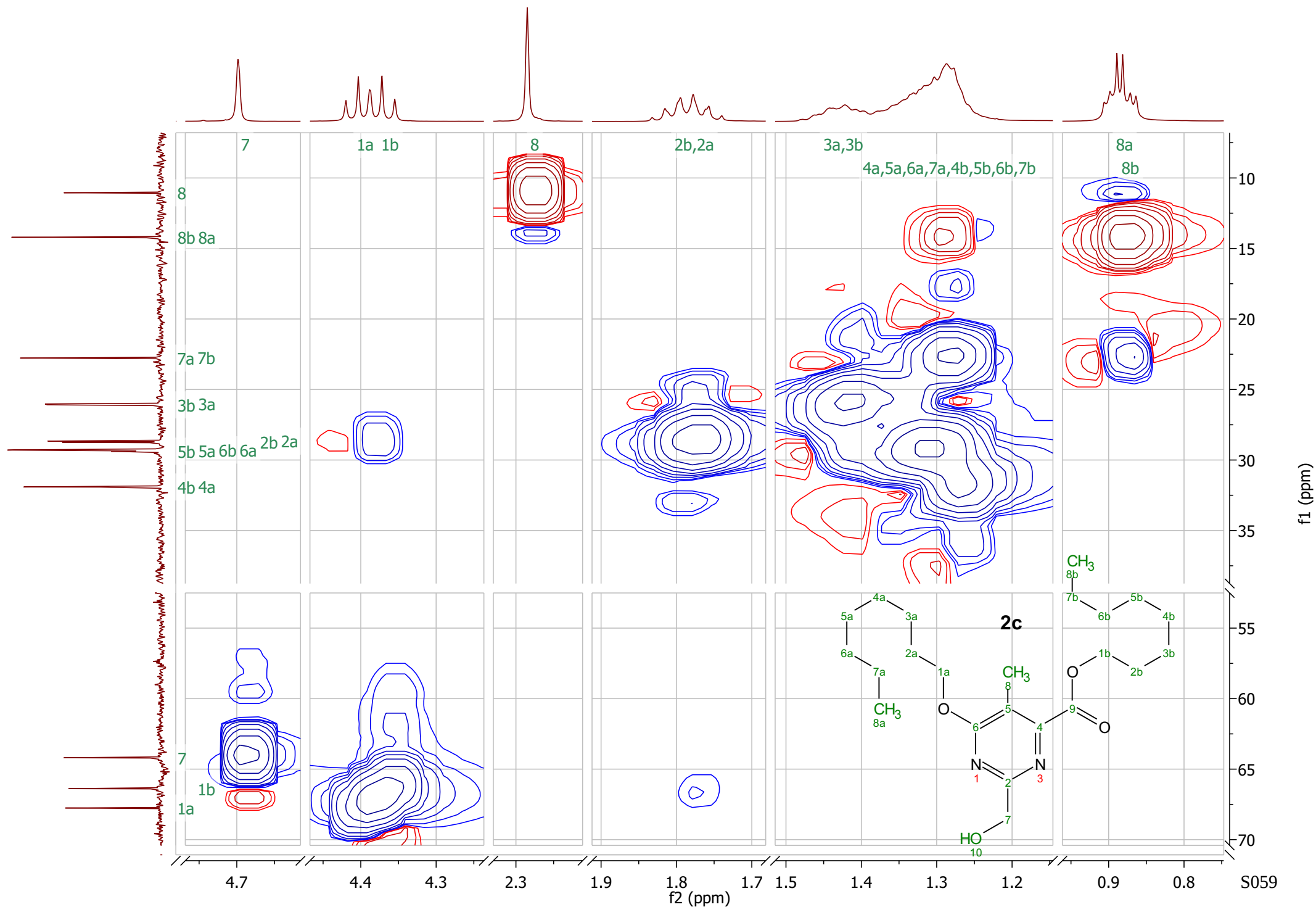


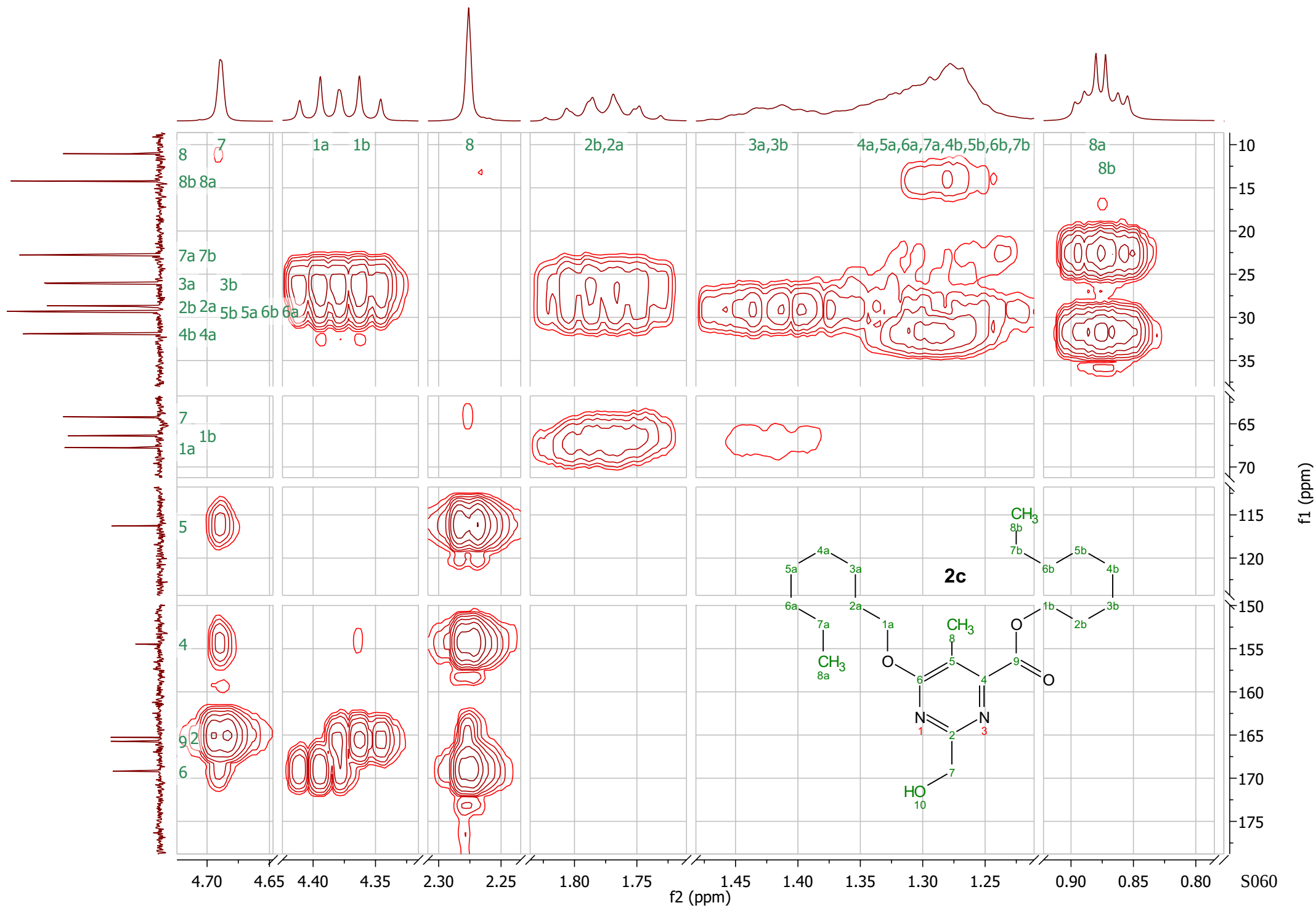
^1H NMR (400 MHz, CDCl_3) δ 4.69 (s, 2H), 4.39 (t, $J = 6.3$ Hz, 2H), 4.36 (t, $J = 6.4$ Hz, 2H), 3.22 (br s, 1H), 2.27 (s, 3H), 1.85 – 1.70 (m, 4H), 1.50 – 1.36 (m, 4H), 1.38 – 1.19 (m, 16H), 0.88 (app t, $J = 6.7$ Hz, 3H), 0.87 (app t, $J = 7.1$ Hz, 3H).



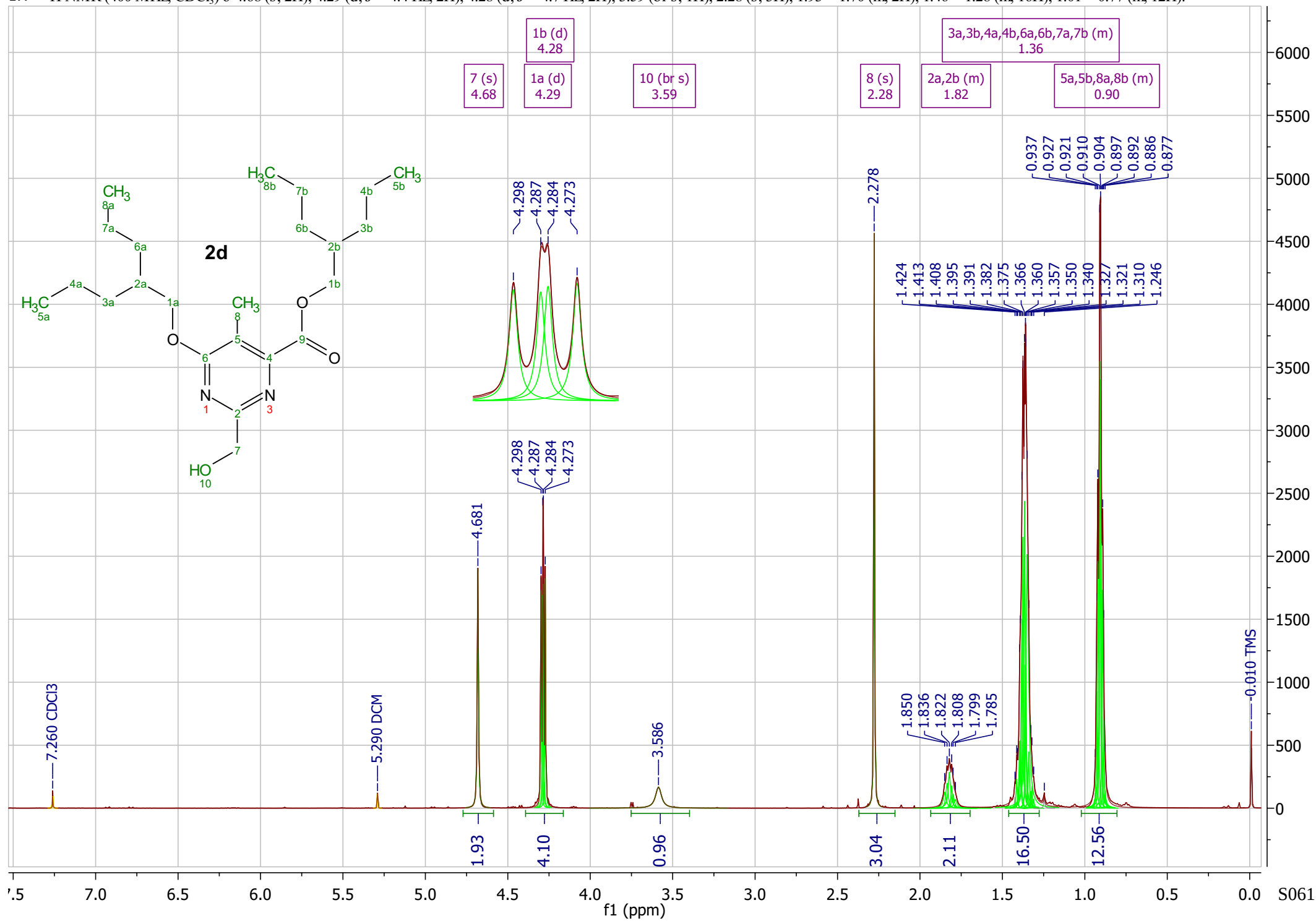
^{13}C ^{13}C NMR (101 MHz, CDCl_3) δ 169.2, 165.7, 165.3, 154.5, 116.3, 67.8, 66.4, 64.2, 31.91, 31.88, 29.4, 29.33, 29.28, 28.74, 28.66, 26.1, 26.0, 22.78, 22.76, 14.22, 14.21, 11.1.



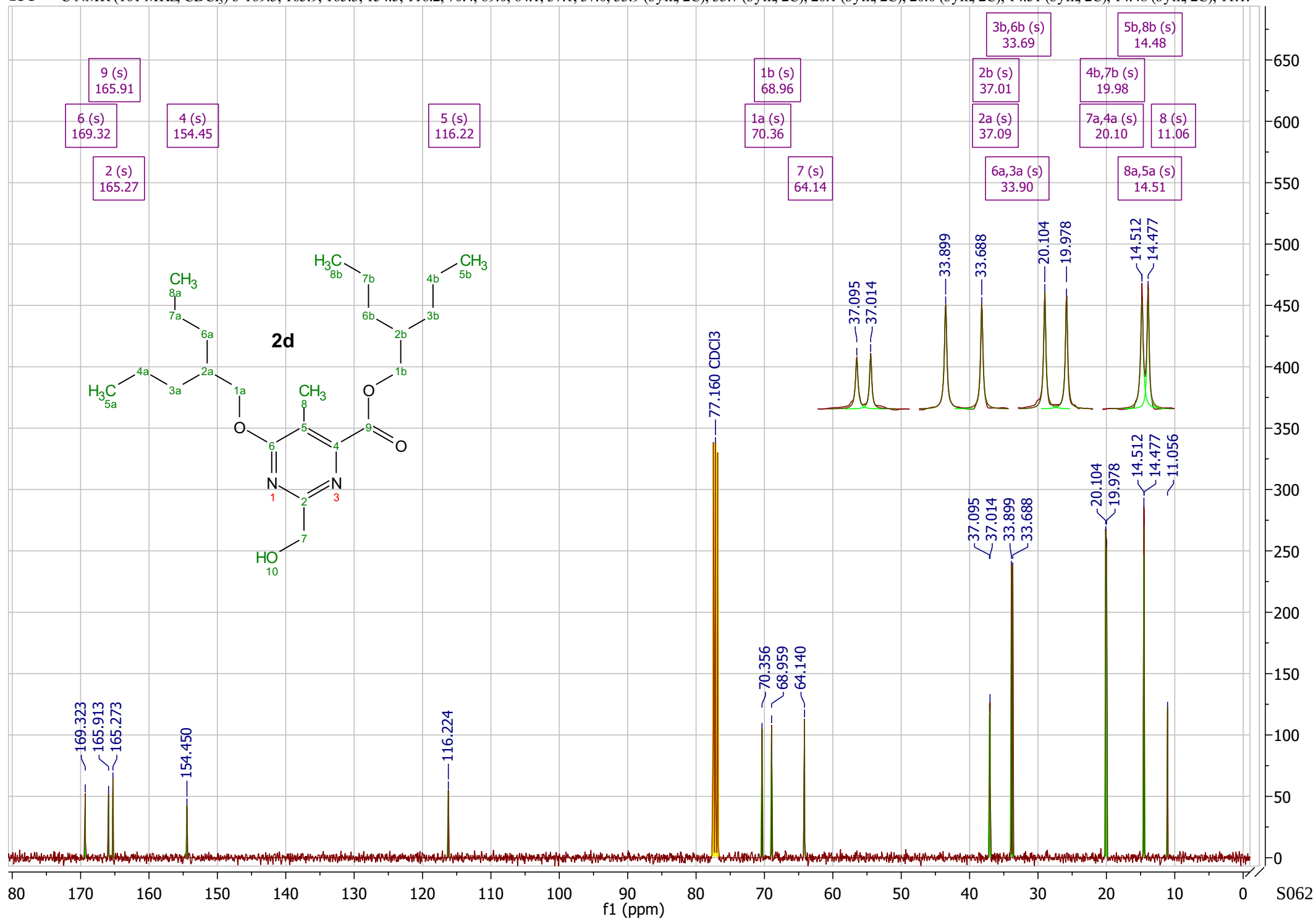


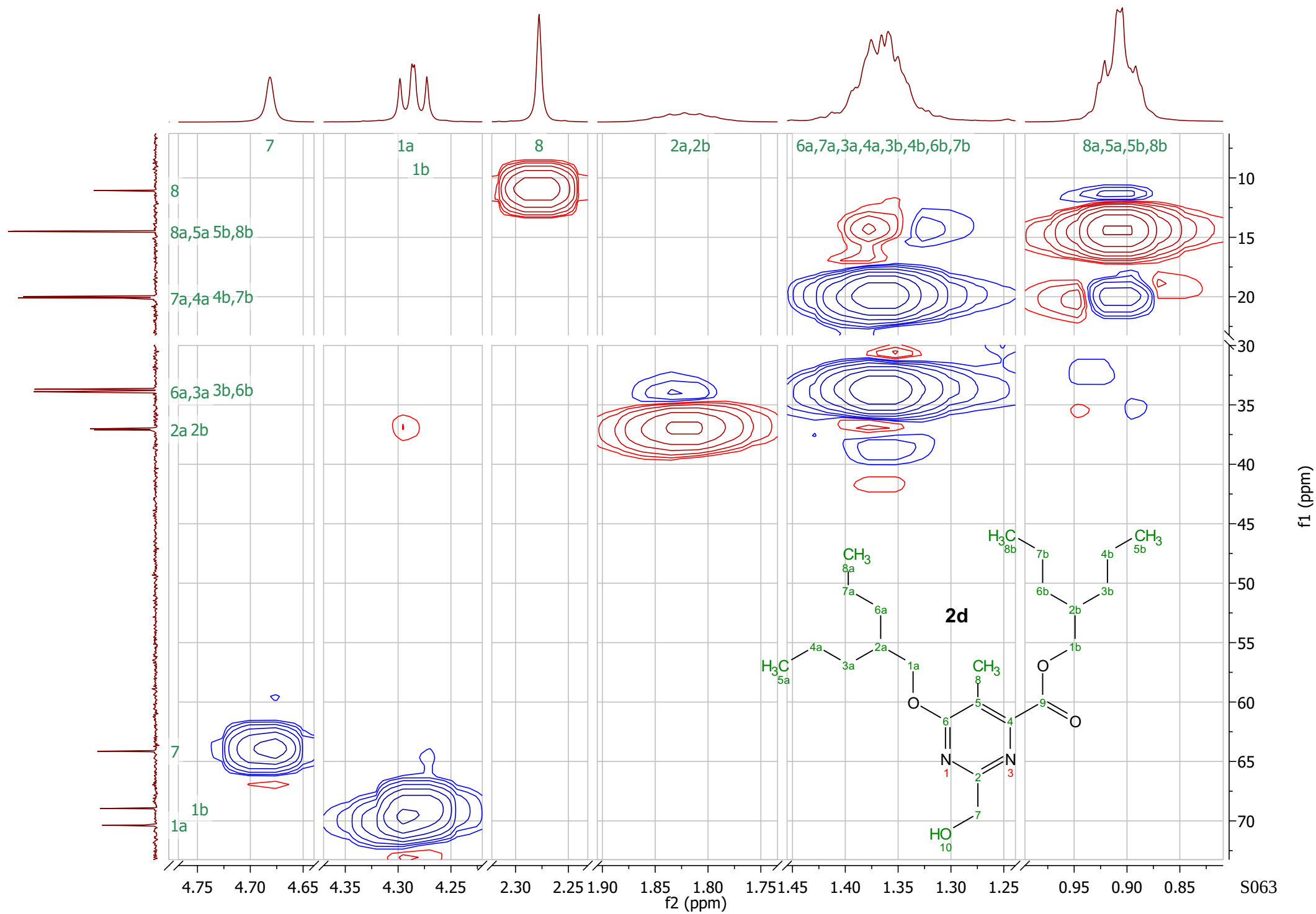


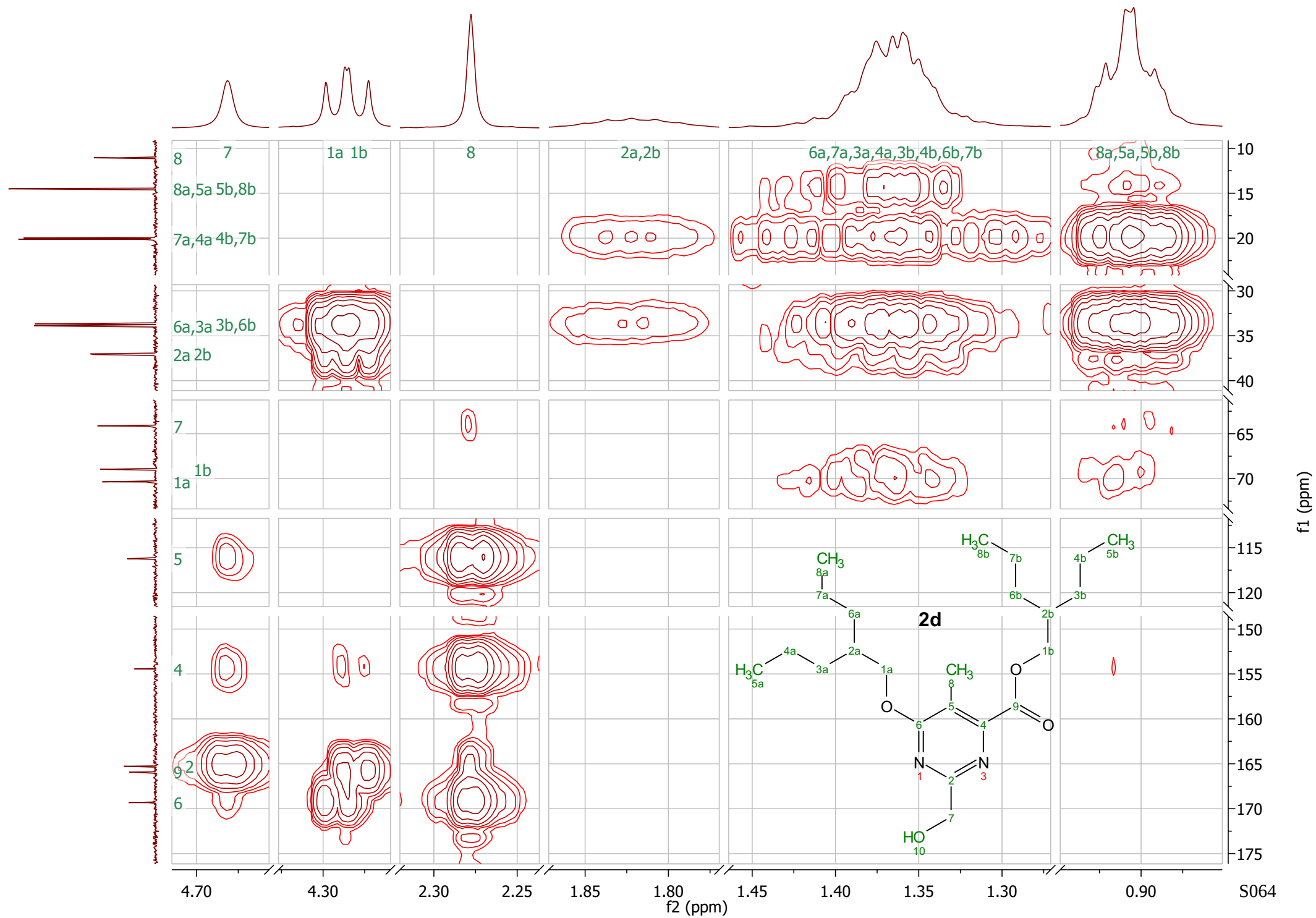
^1H NMR (400 MHz, CDCl_3) δ 4.68 (s, 2H), 4.29 (d, $J = 4.4$ Hz, 2H), 4.28 (d, $J = 4.7$ Hz, 2H), 3.59 (br s, 1H), 2.28 (s, 3H), 1.93 – 1.70 (m, 2H), 1.46 – 1.28 (m, 16H), 1.01 – 0.77 (m, 12H).



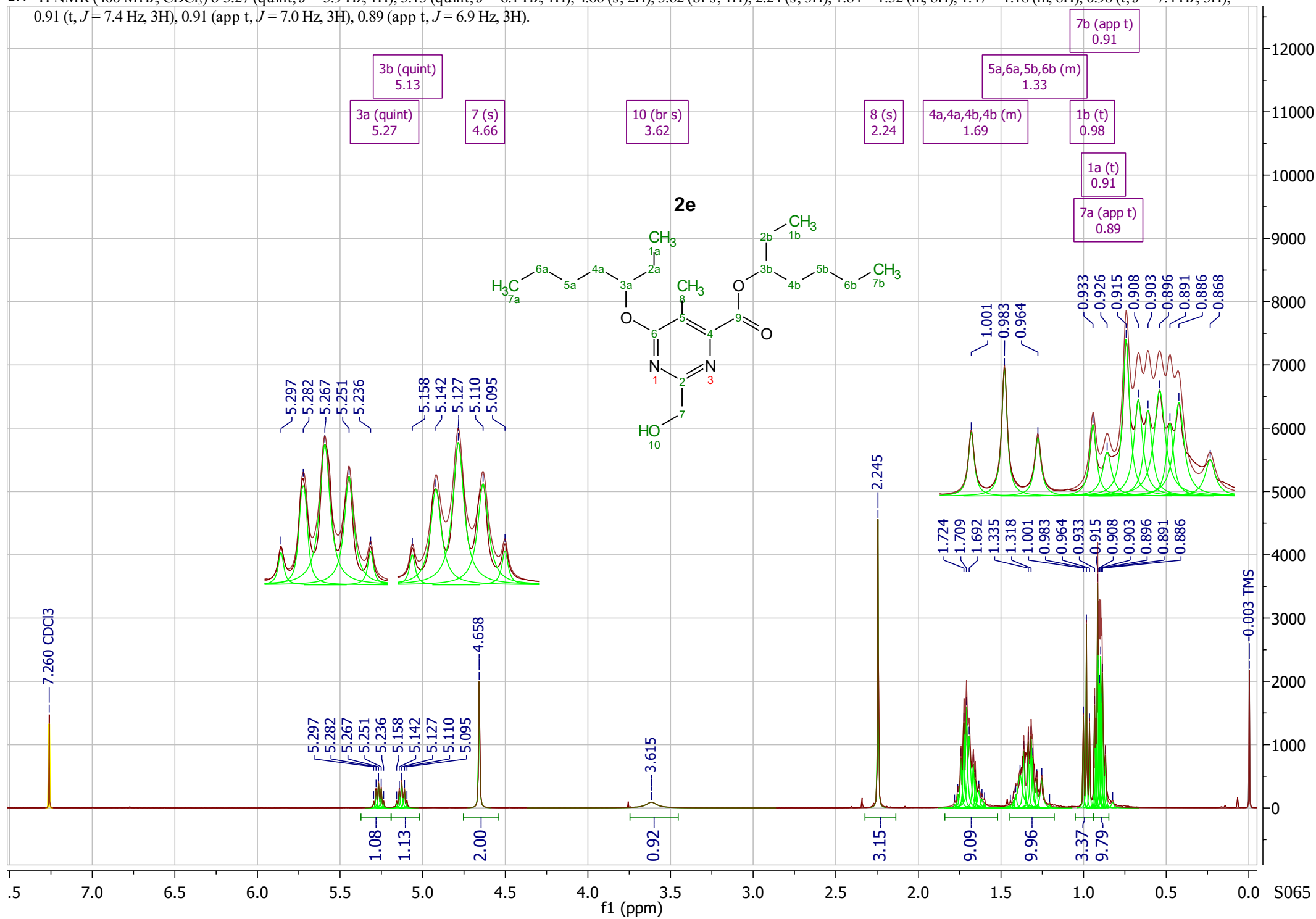
13C ^{13}C NMR (101 MHz, CDCl_3) δ 169.3, 165.9, 165.3, 154.5, 116.2, 70.4, 69.0, 64.1, 37.1, 37.0, 33.9 (sym, 2C), 33.7 (sym, 2C), 20.1 (sym, 2C), 20.0 (sym, 2C), 14.51 (sym, 2C), 14.48 (sym, 2C), 11.1.



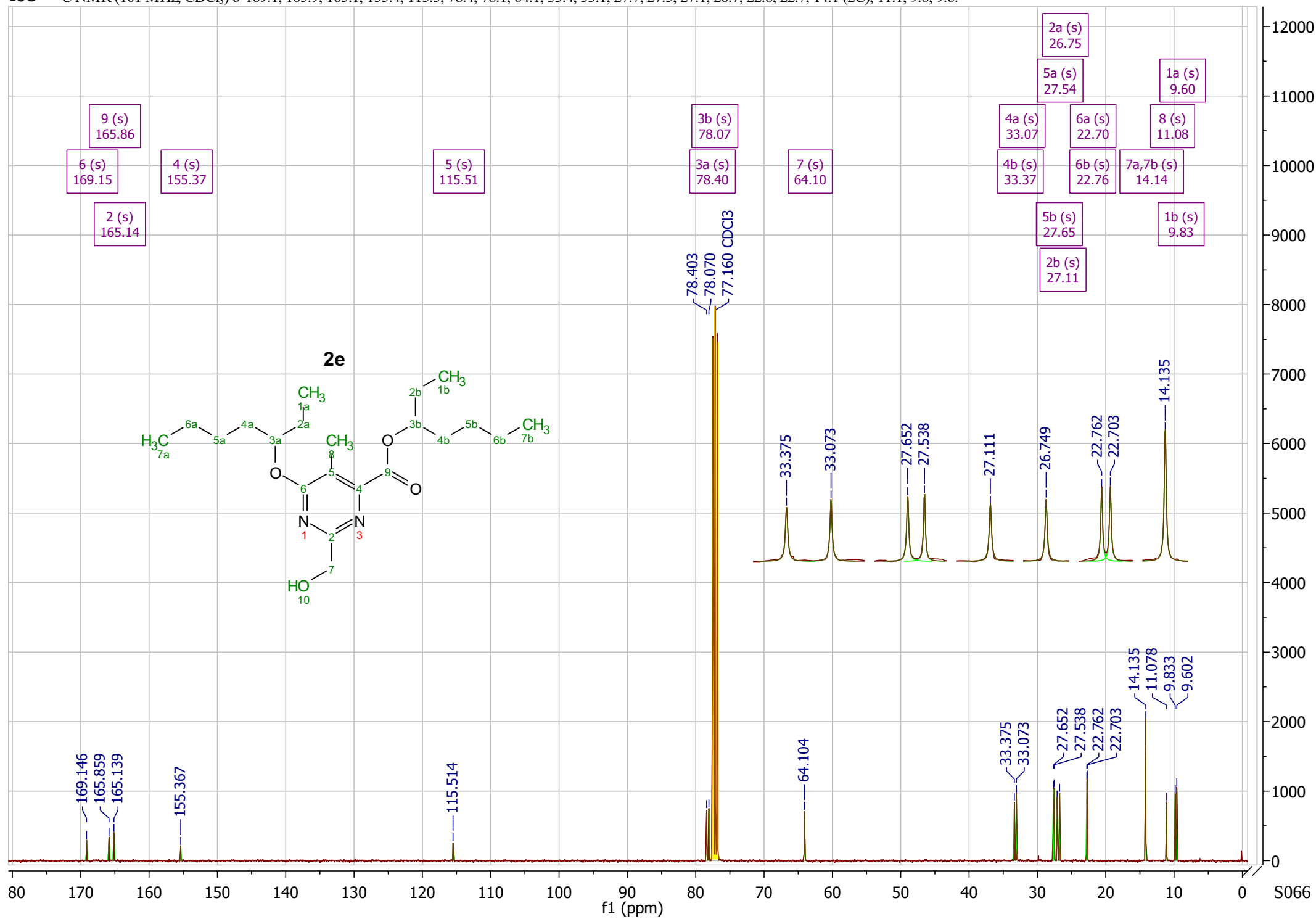


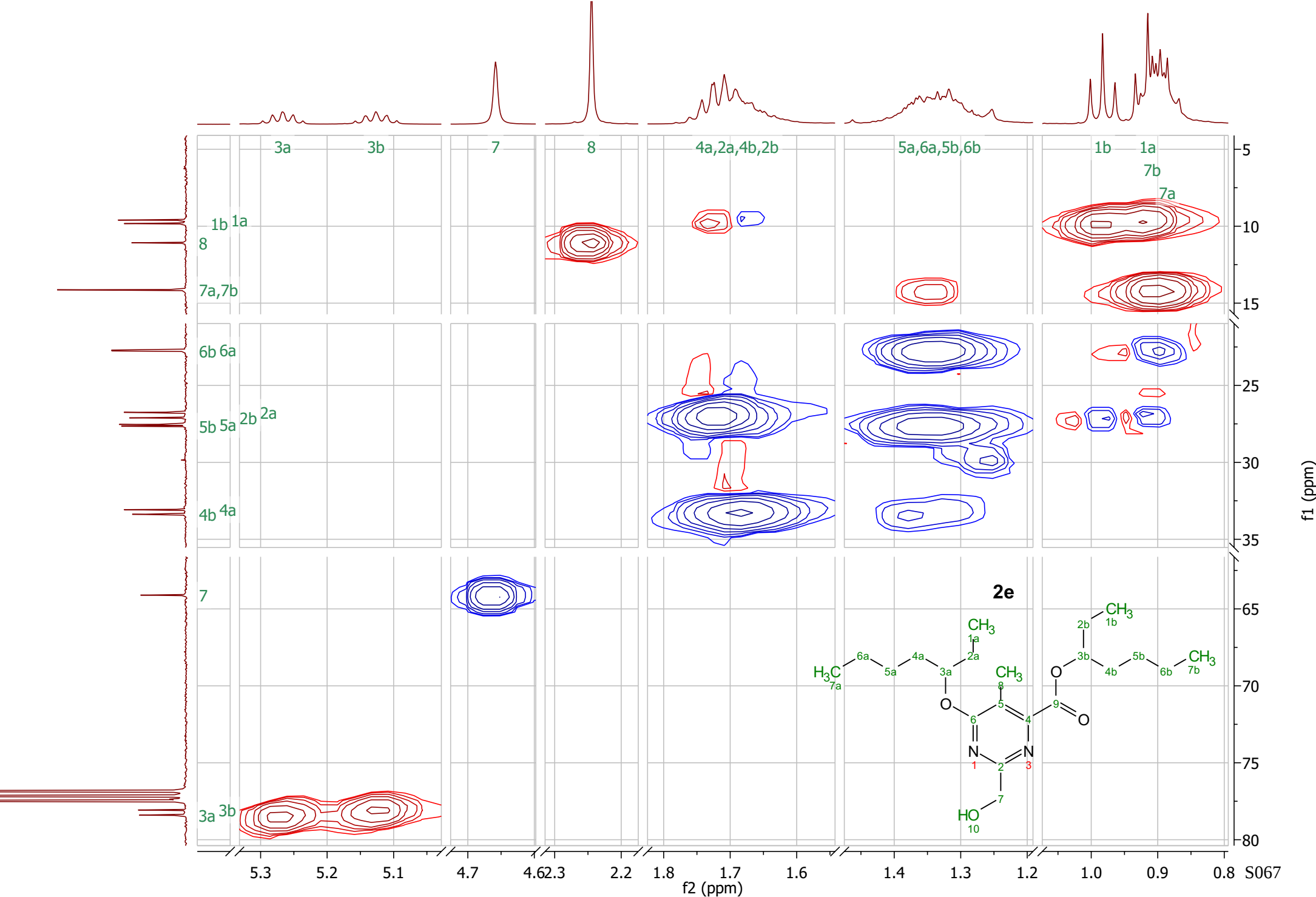


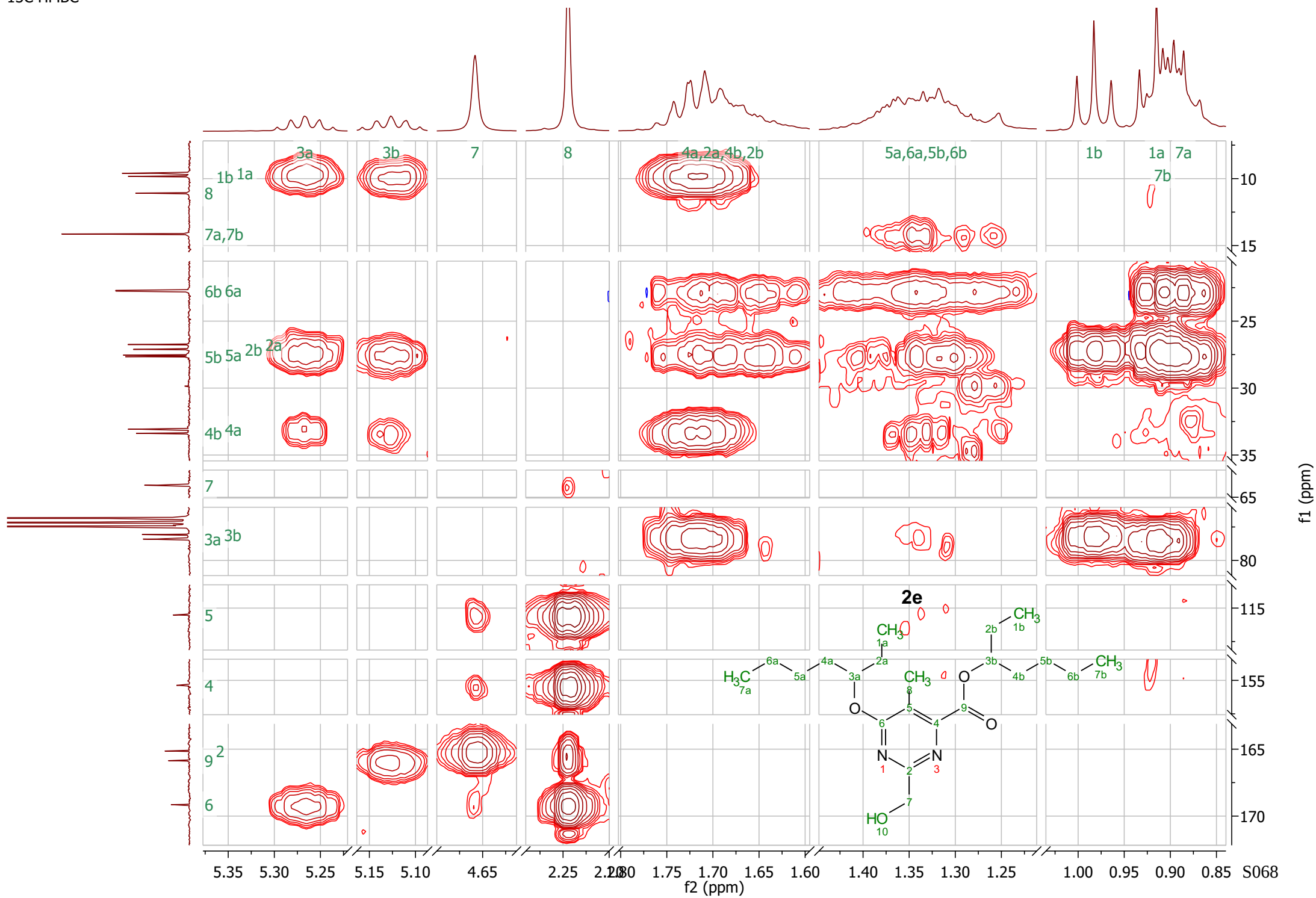
^1H NMR (400 MHz, CDCl_3) δ 5.27 (quint, $J = 5.9$ Hz, 1H), 5.13 (quint, $J = 6.1$ Hz, 1H), 4.66 (s, 2H), 3.62 (br s, 1H), 2.24 (s, 3H), 1.84 – 1.52 (m, 8H), 1.47 – 1.18 (m, 8H), 0.98 (t, $J = 7.4$ Hz, 3H), 0.91 (t, $J = 7.4$ Hz, 3H), 0.91 (app t, $J = 7.0$ Hz, 3H), 0.89 (app t, $J = 6.9$ Hz, 3H).



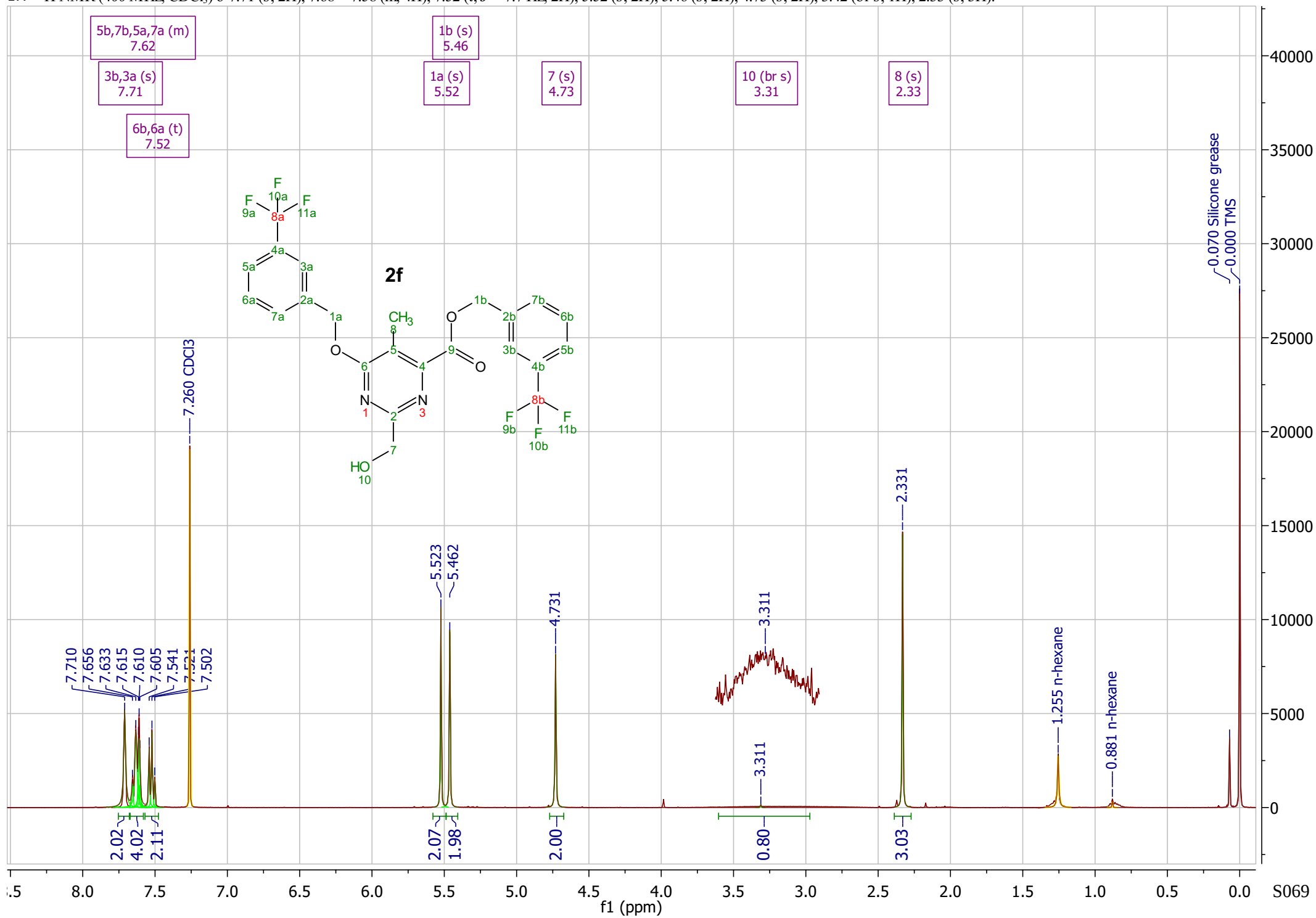
13C ^{13}C NMR (101 MHz, CDCl_3) δ 169.1, 165.9, 165.1, 155.4, 115.5, 78.4, 78.1, 64.1, 33.4, 33.1, 27.7, 27.5, 27.1, 26.7, 22.8, 22.7, 14.1 (2C), 11.1, 9.8, 9.6.



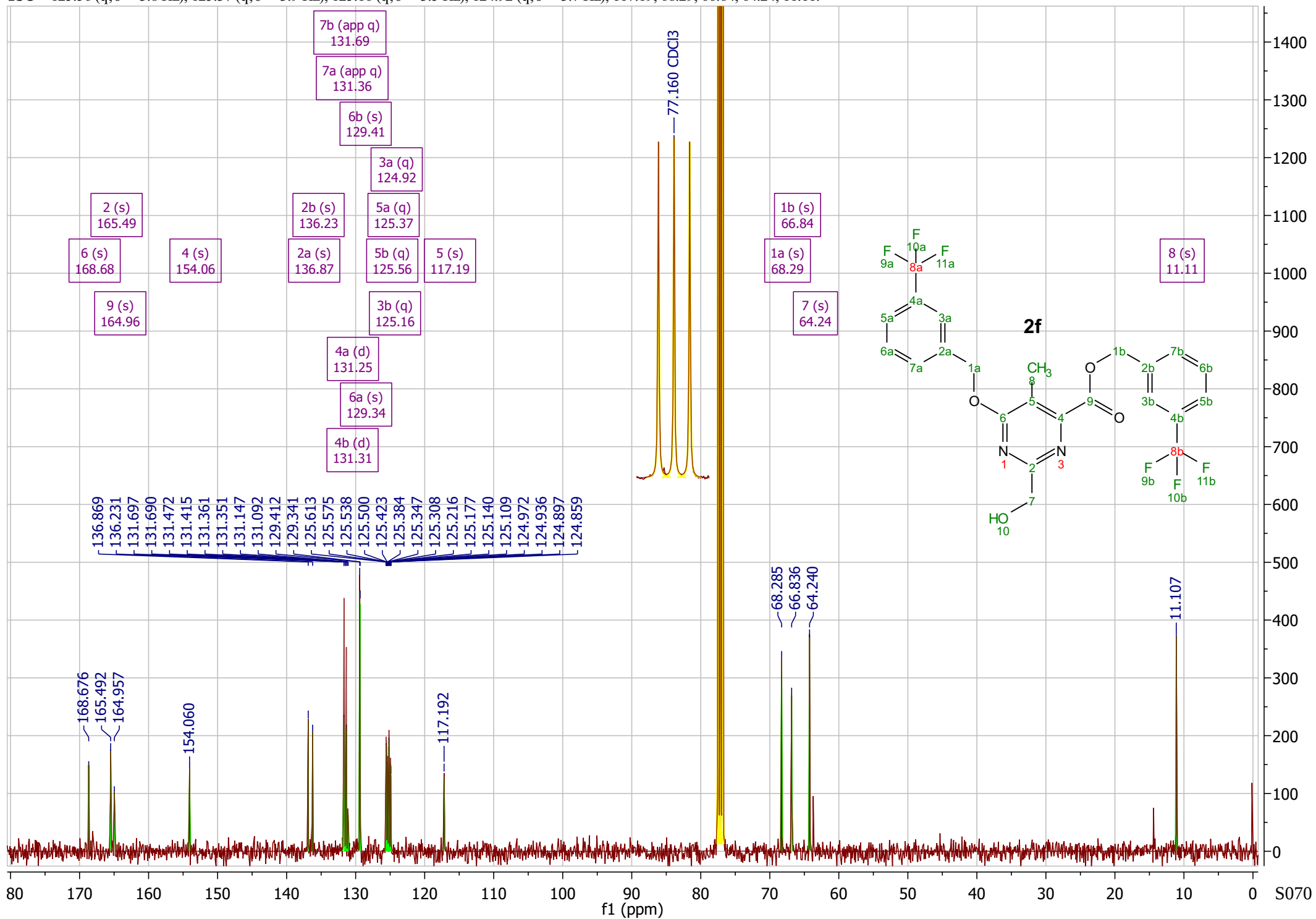




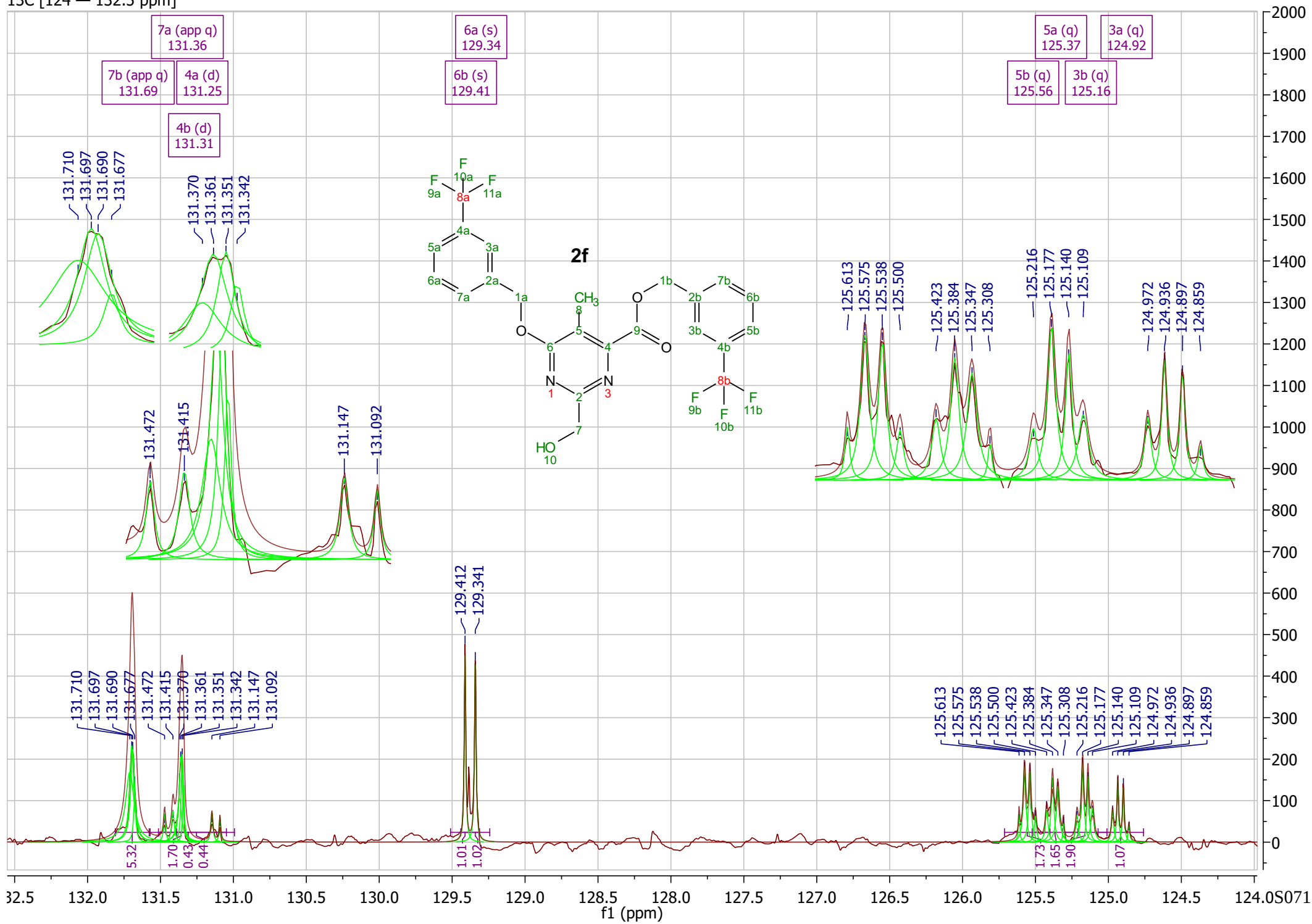
^1H NMR (400 MHz, CDCl_3) δ 7.71 (s, 2H), 7.68 – 7.58 (m, 4H), 7.52 (t, $J = 7.7$ Hz, 2H), 5.52 (s, 2H), 5.46 (s, 2H), 4.73 (s, 2H), 3.42 (br s, 1H), 2.33 (s, 3H).

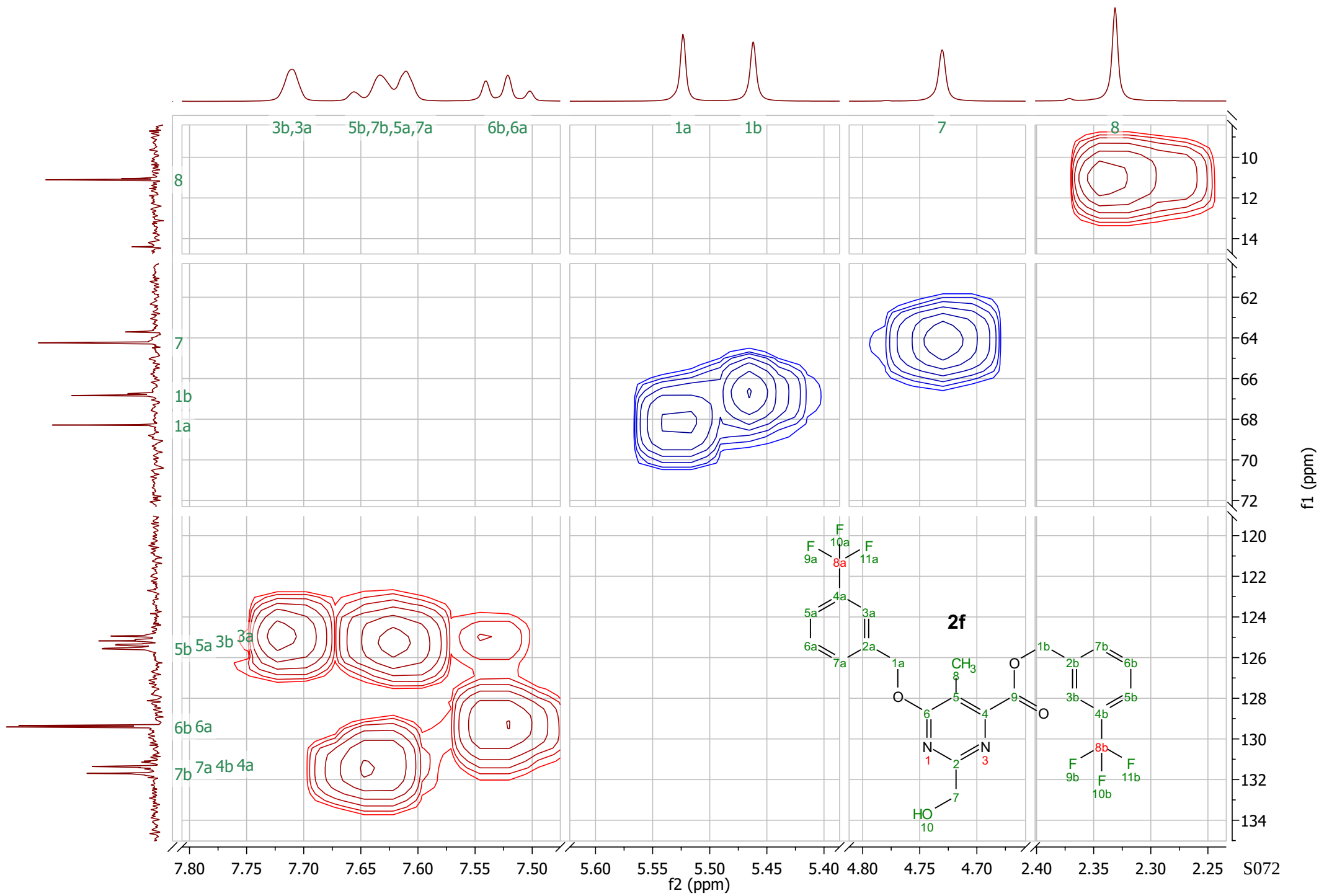


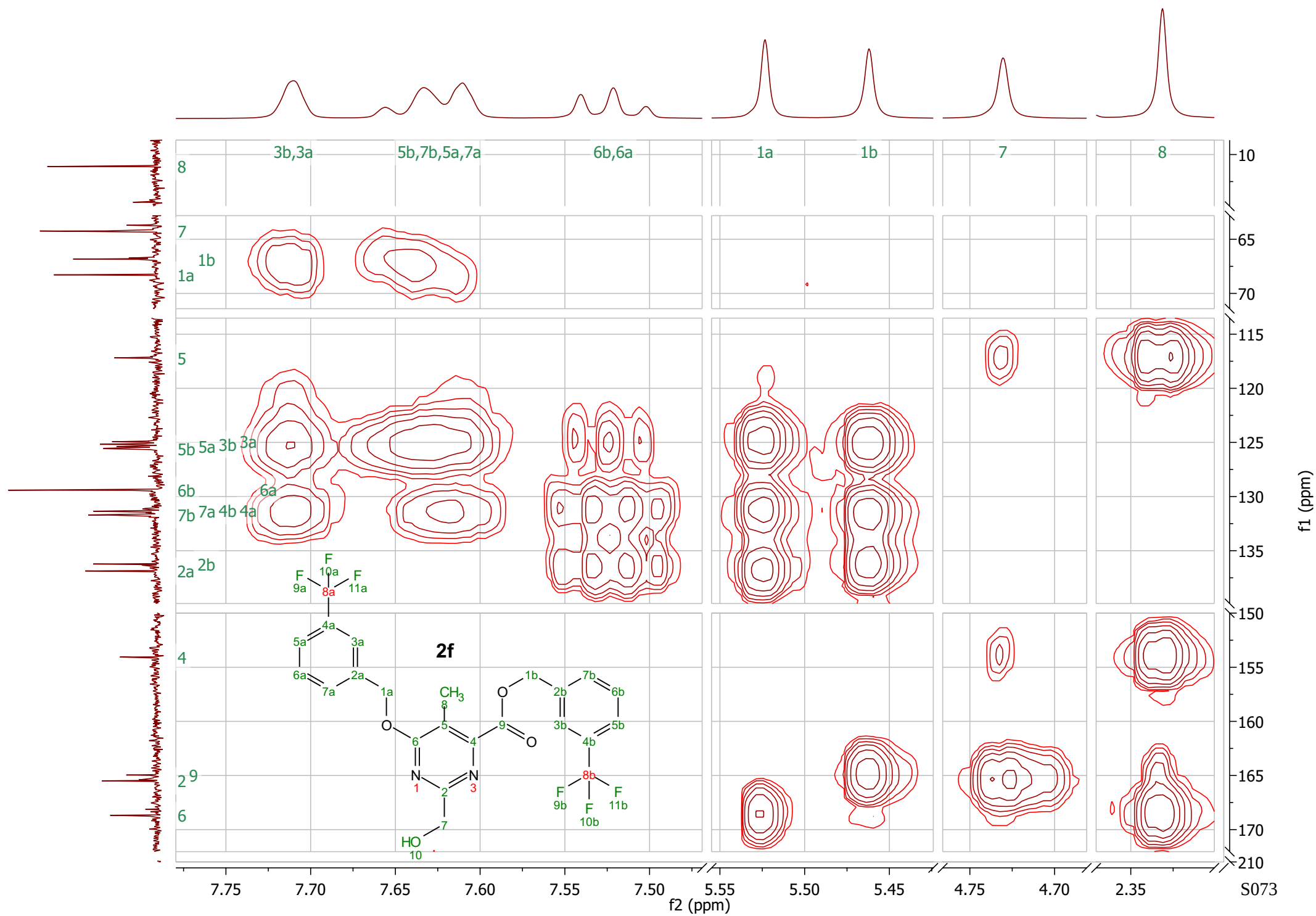
¹³C NMR (101 MHz, CDCl₃) δ 168.68, 165.49, 154.06, 136.87, 136.23, 131.69 (app q, *J* = 1.1 Hz), 131.36 (app q, *J* = 1.0 Hz), 131.31 (d, *J* = 32.7 Hz), 131.25 (d, *J* = 32.4 Hz), 129.41, 129.34, 125.56 (q, *J* = 3.8 Hz), 125.37 (q, *J* = 3.9 Hz), 125.16 (q, *J* = 3.5 Hz), 124.92 (q, *J* = 3.7 Hz), 117.19, 68.29, 66.84, 64.24, 11.11.



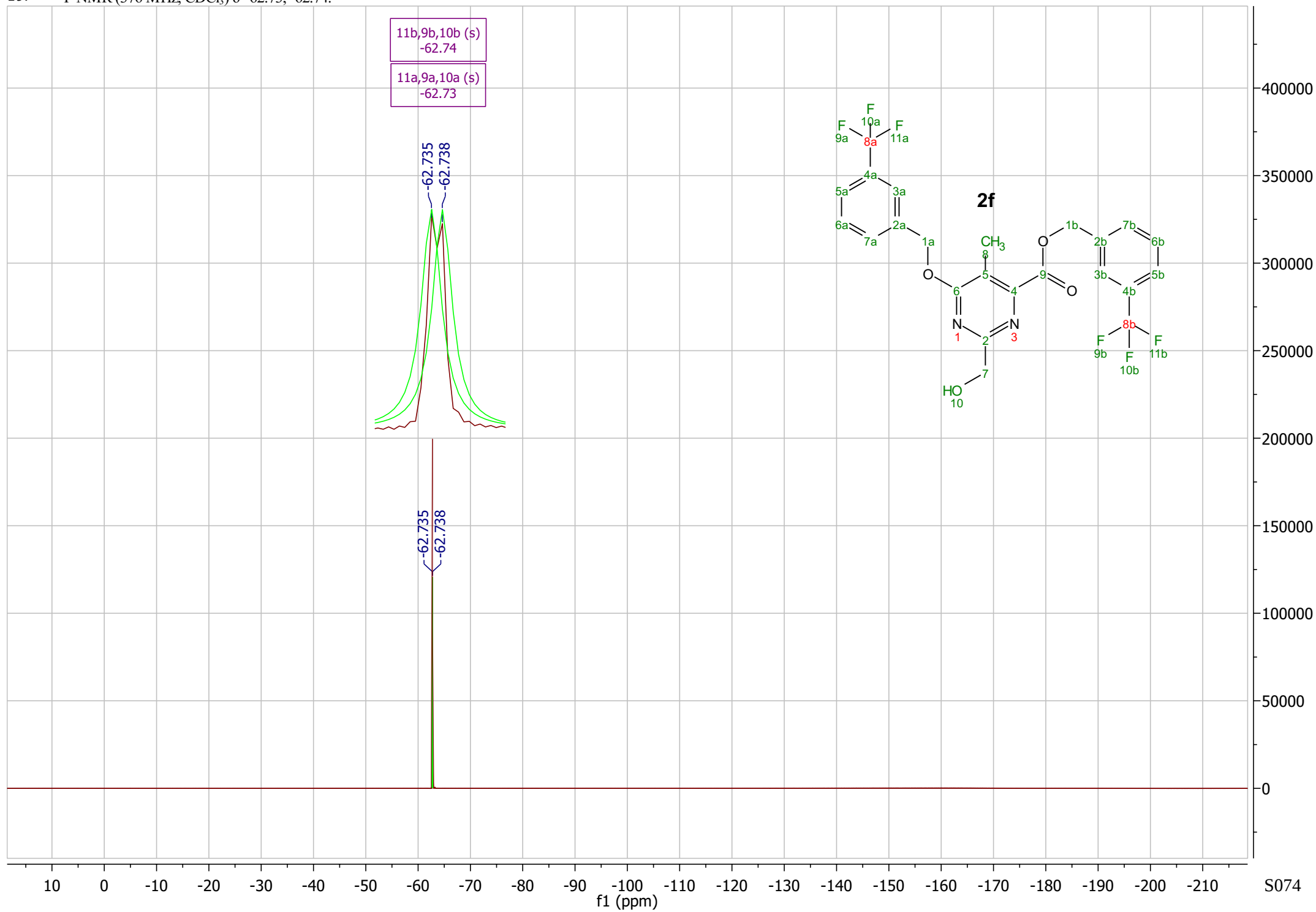
¹³C [124 — 132.5 ppm]



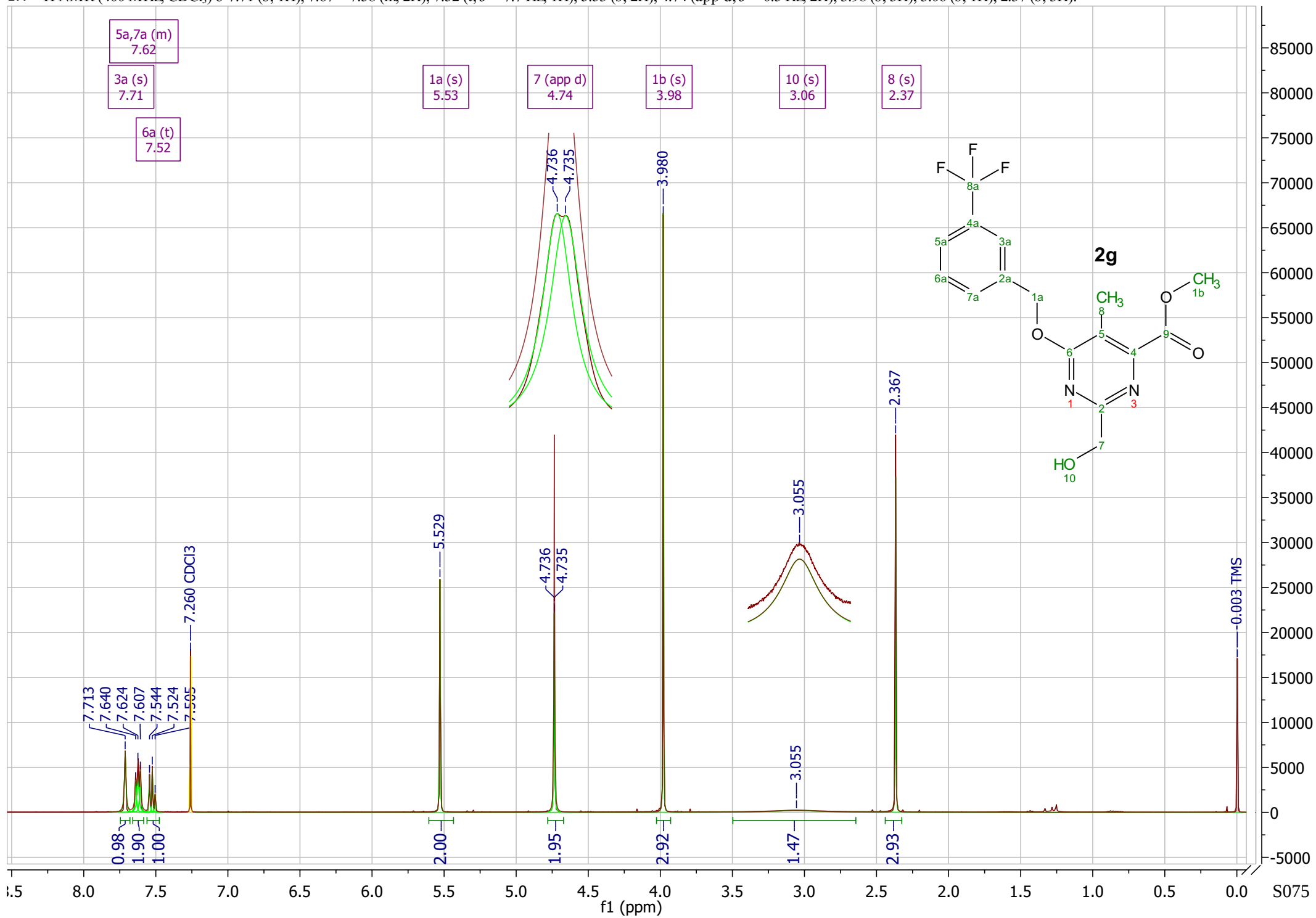




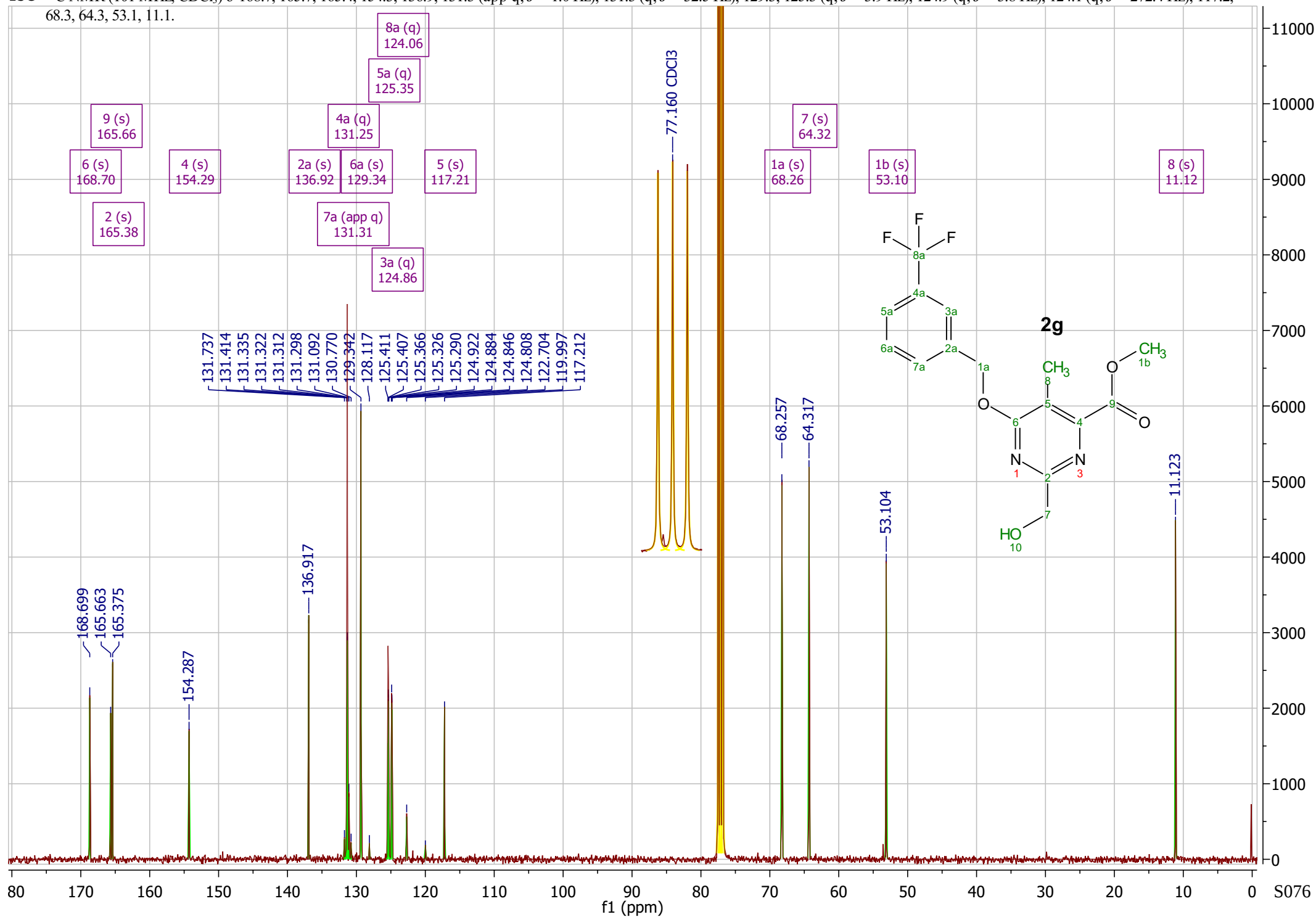
¹⁹F ¹⁹F NMR (376 MHz, CDCl₃) δ -62.73, -62.74.



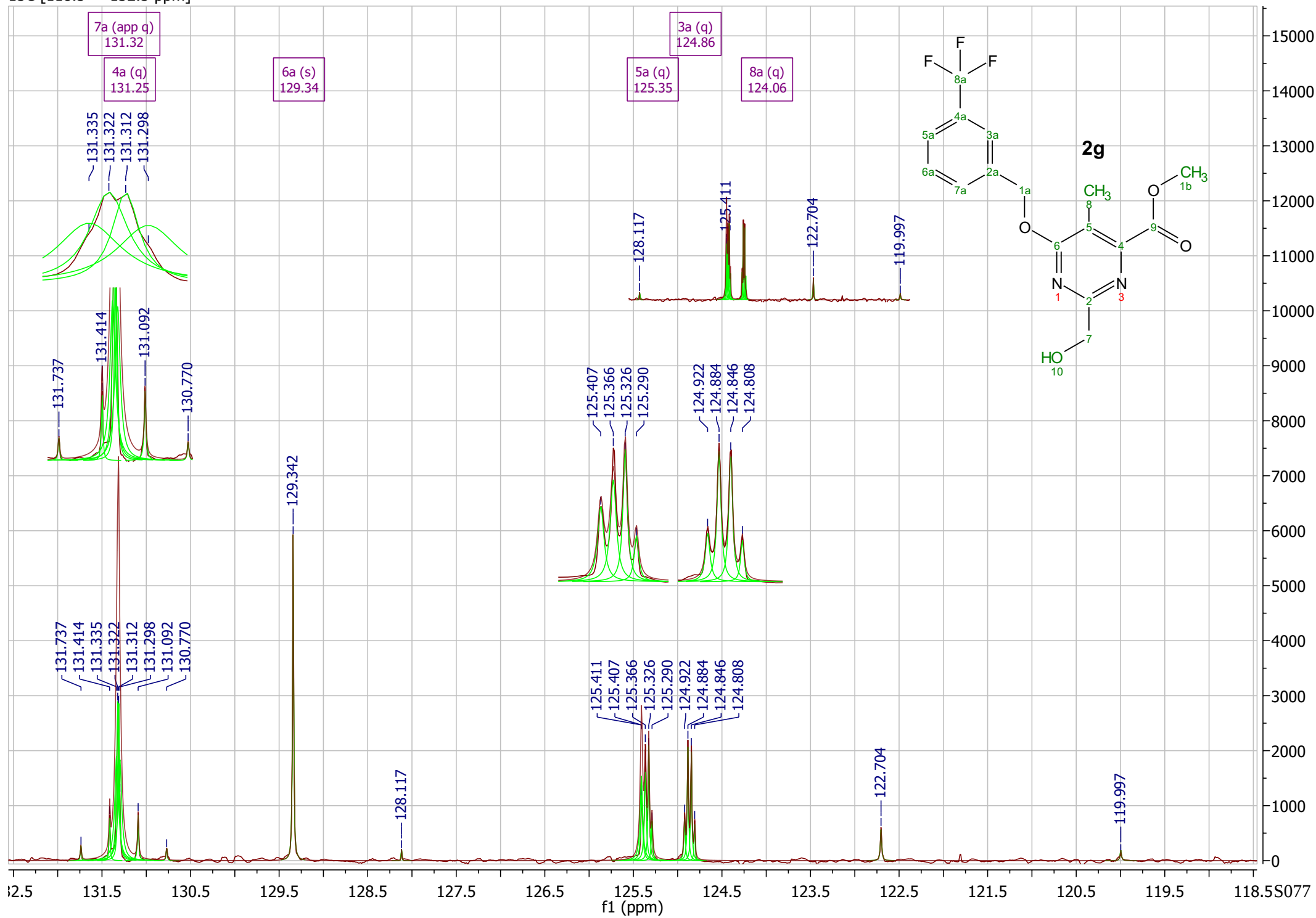
^1H NMR (400 MHz, CDCl_3) δ 7.71 (s, 1H), 7.67 – 7.58 (m, 2H), 7.52 (t, $J = 7.7$ Hz, 1H), 5.53 (s, 2H), 4.74 (app d, $J = 0.5$ Hz, 2H), 3.98 (s, 3H), 3.06 (s, 1H), 2.37 (s, 3H).

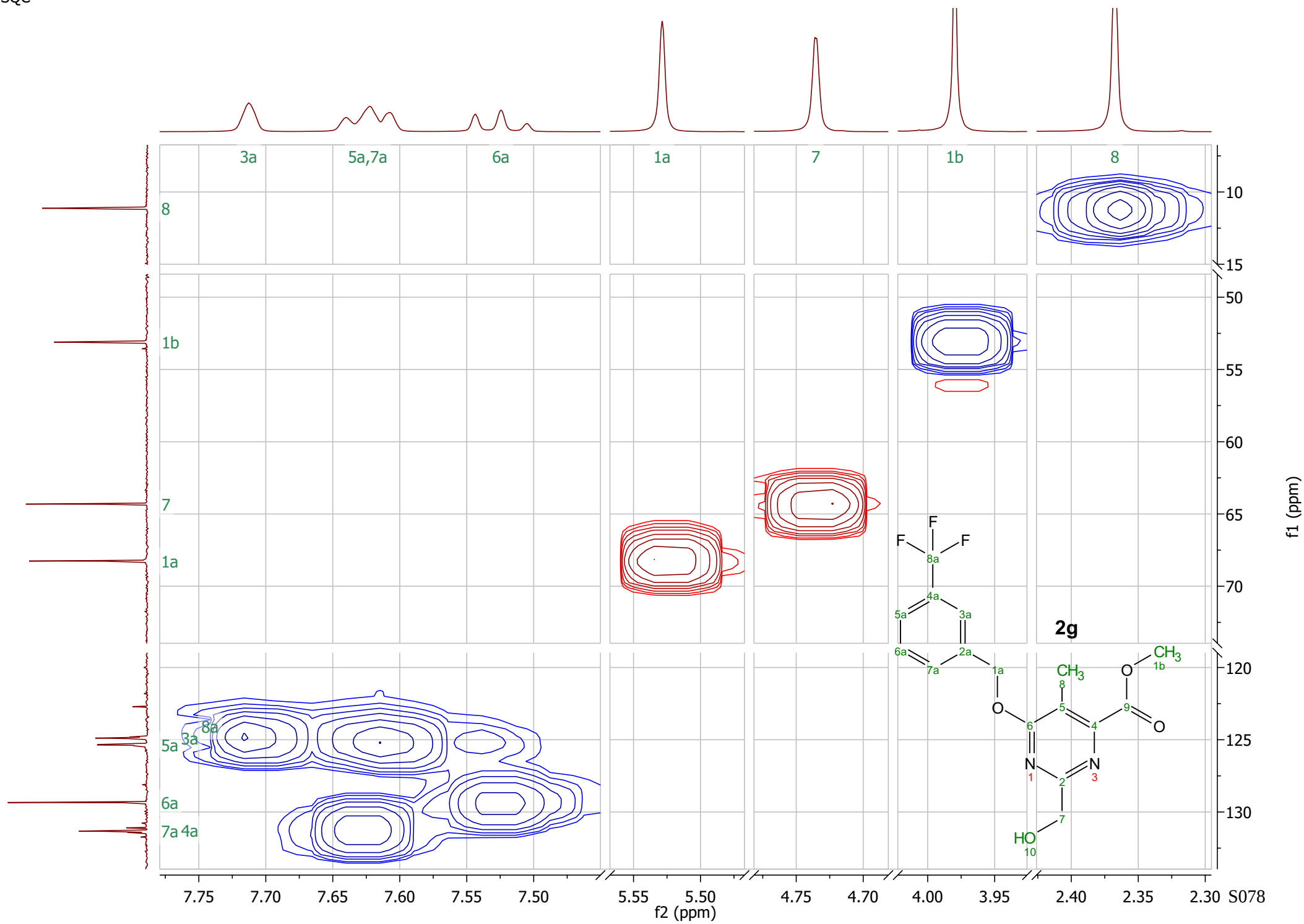


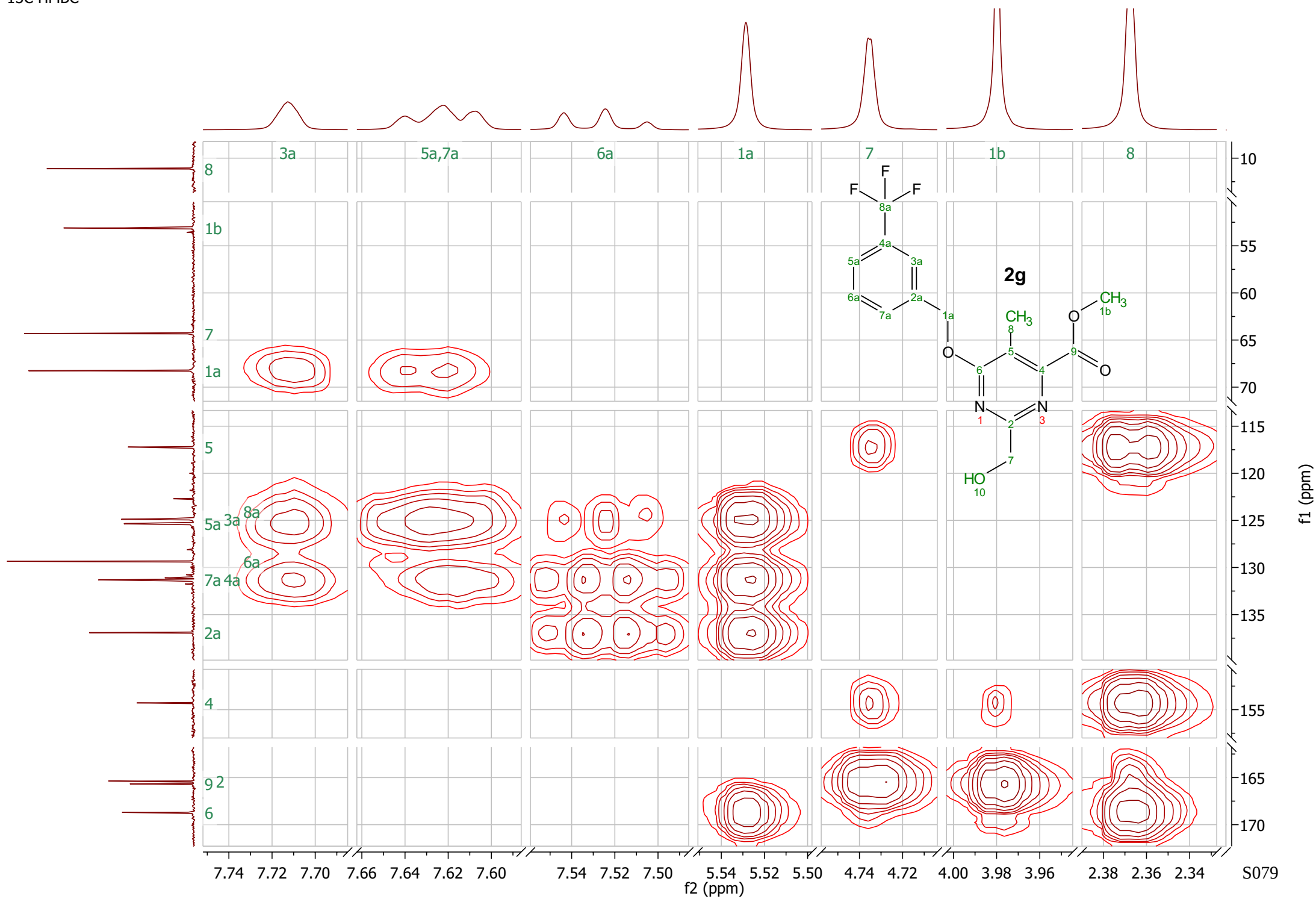
¹³C ¹³C NMR (101 MHz, CDCl₃) δ 168.7, 165.7, 165.4, 154.3, 136.9, 131.3 (app q, *J* = 1.0 Hz), 131.3 (q, *J* = 32.5 Hz), 129.3, 125.3 (q, *J* = 3.9 Hz), 124.9 (q, *J* = 3.8 Hz), 124.1 (q, *J* = 272.4 Hz), 117.2, 68.3, 64.3, 53.1, 11.1.



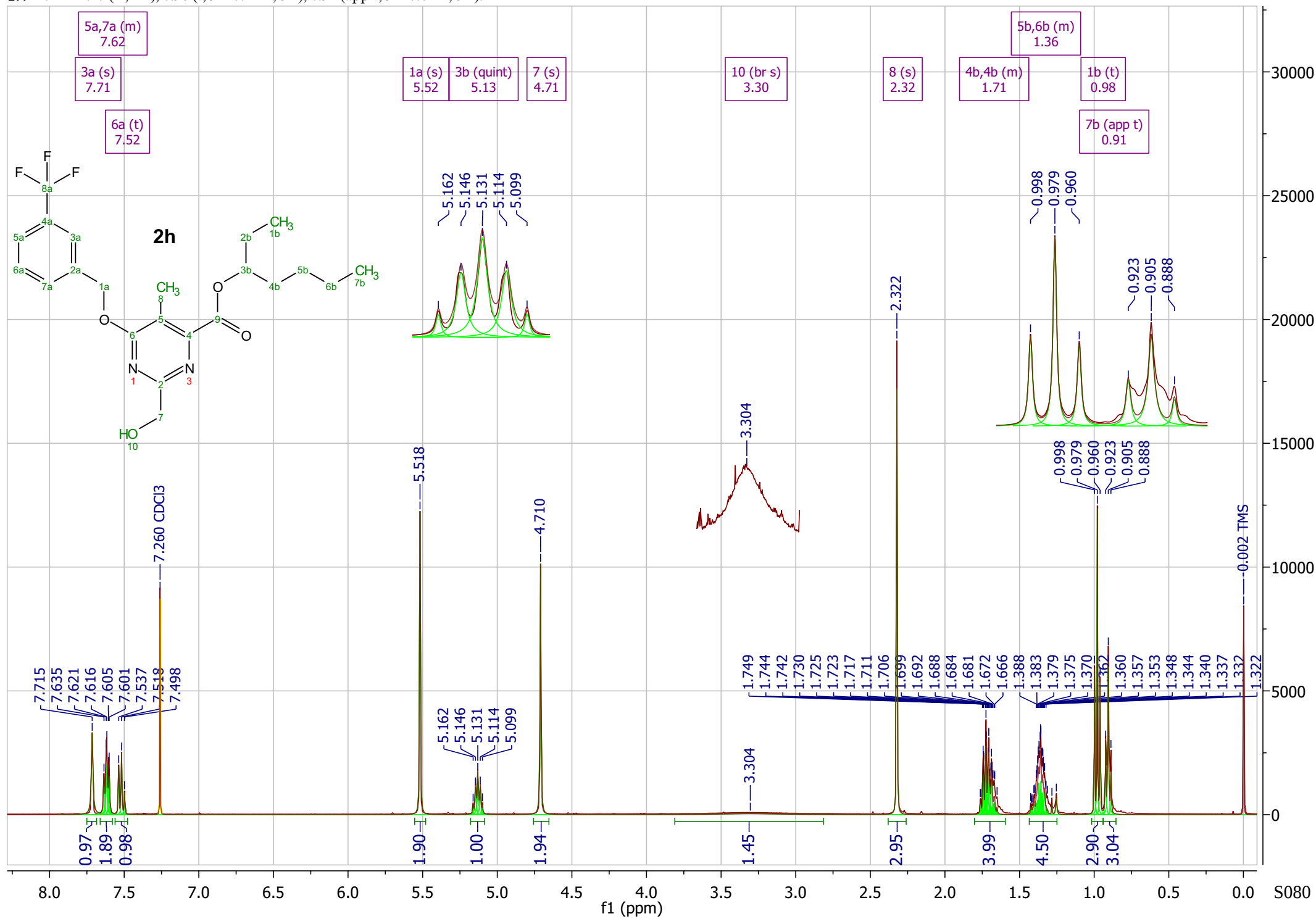
¹³C [118.5 — 132.5 ppm]



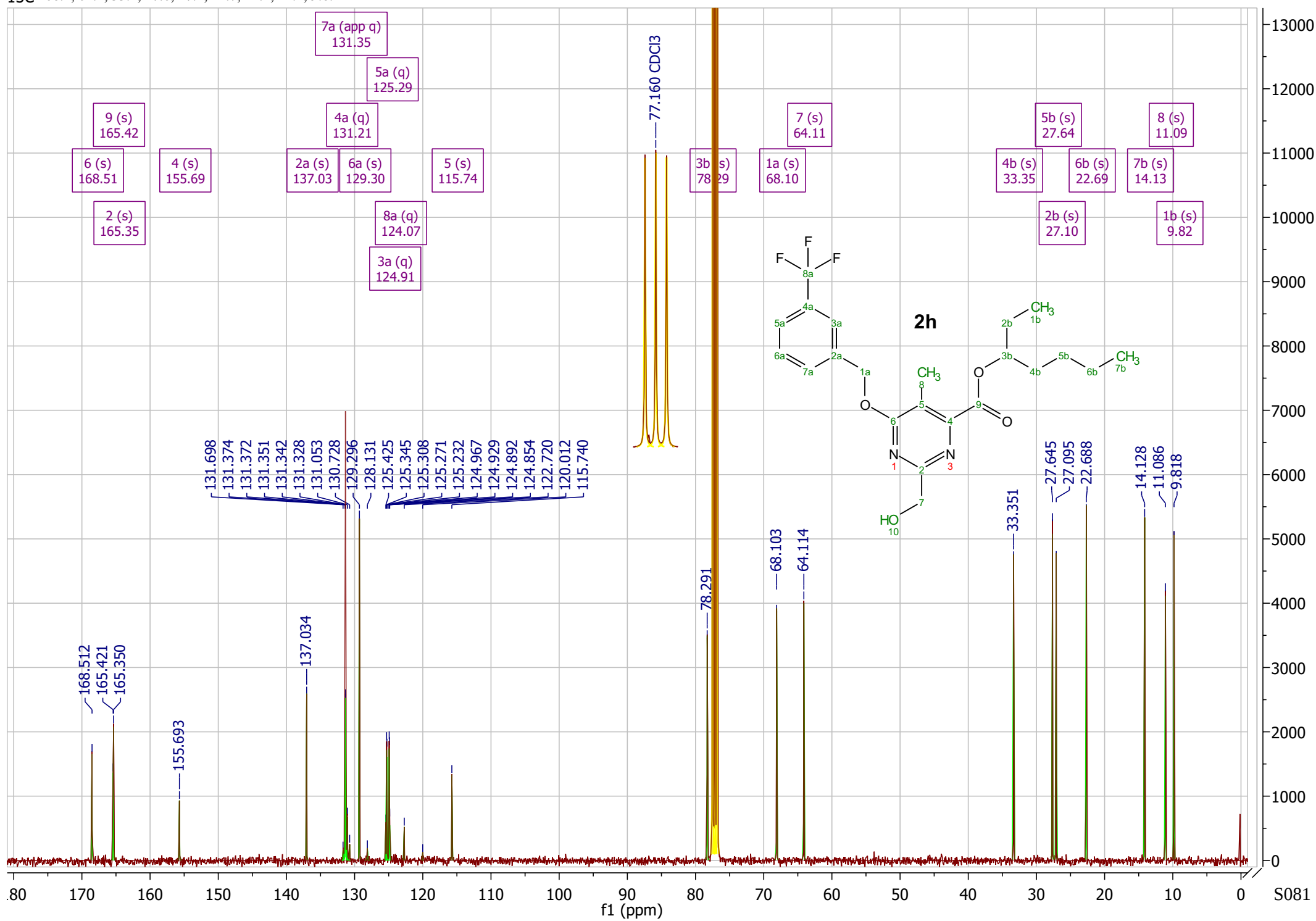




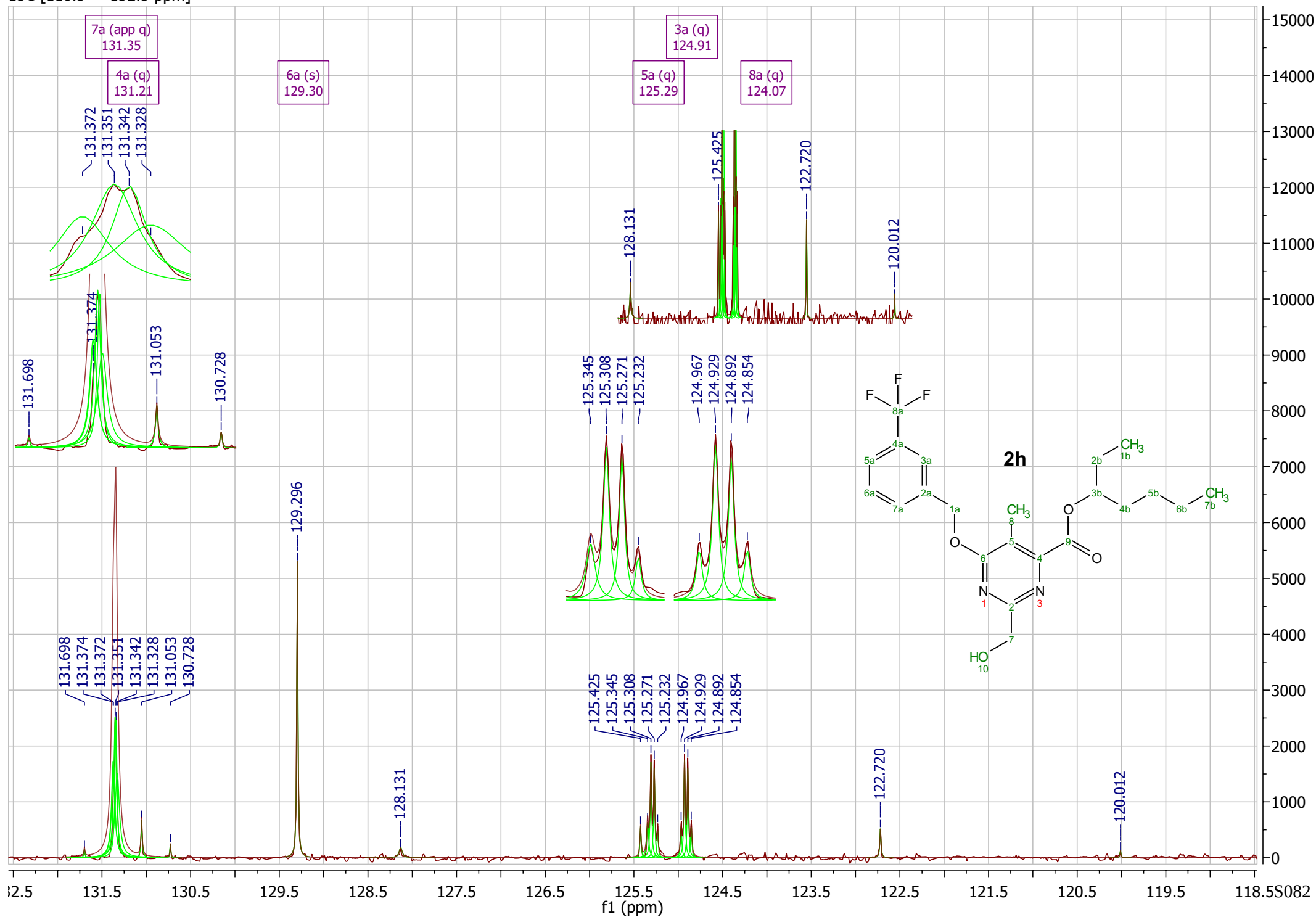
¹H NMR (400 MHz, CDCl₃) δ 7.71 (s, 1H), 7.66 – 7.58 (m, 2H), 7.52 (t, *J* = 7.7 Hz, 1H), 5.52 (s, 2H), 5.13 (quint, *J* = 6.1 Hz, 1H), 4.71 (s, 2H), 3.30 (br s, 1H), 2.32 (s, 3H), 1.81 – 1.59 (m, 4H), 1H 1.44 – 1.27 (m, 4H), 0.98 (t, *J* = 7.4 Hz, 3H), 0.91 (app t, *J* = 7.0 Hz, 3H).

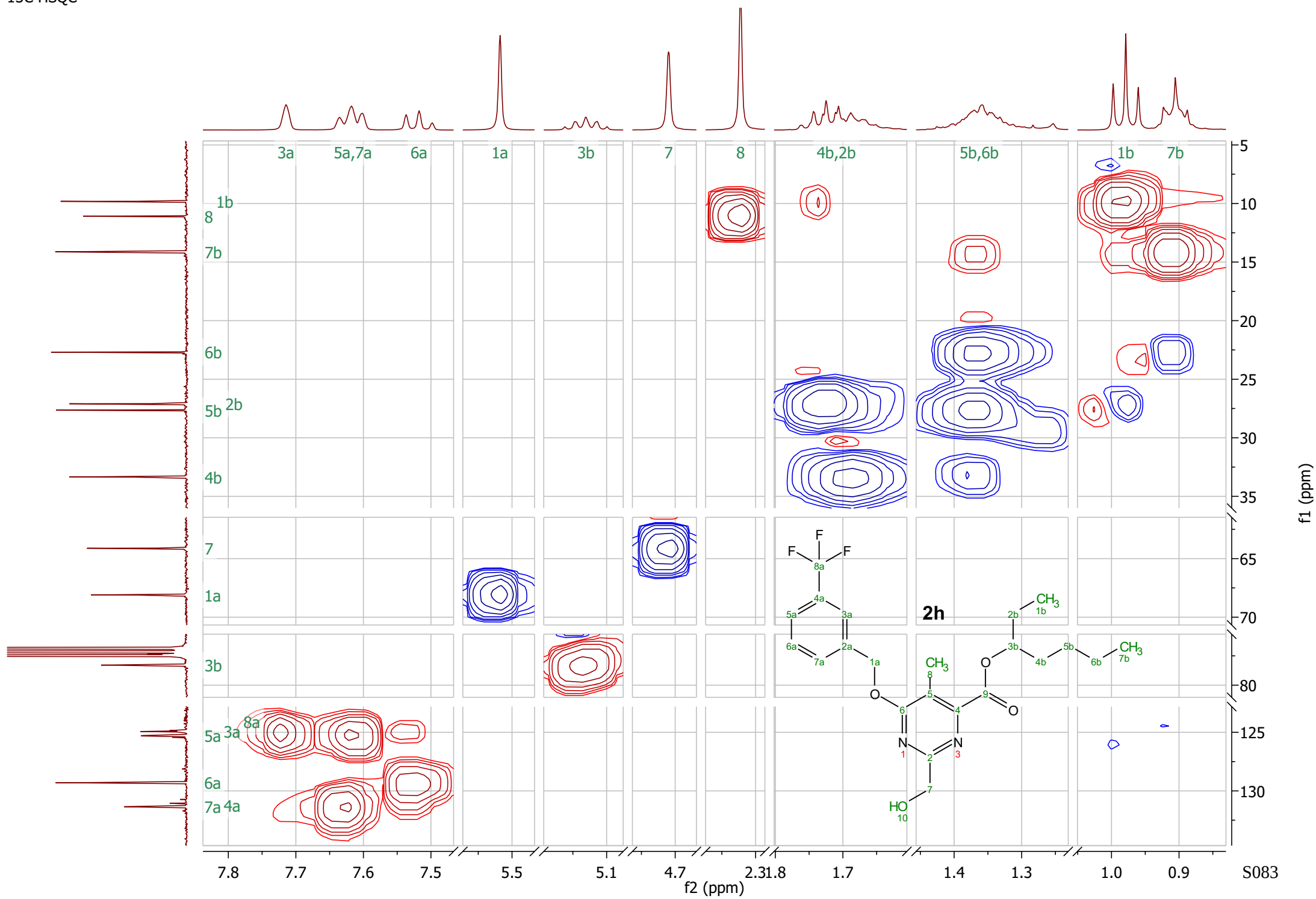


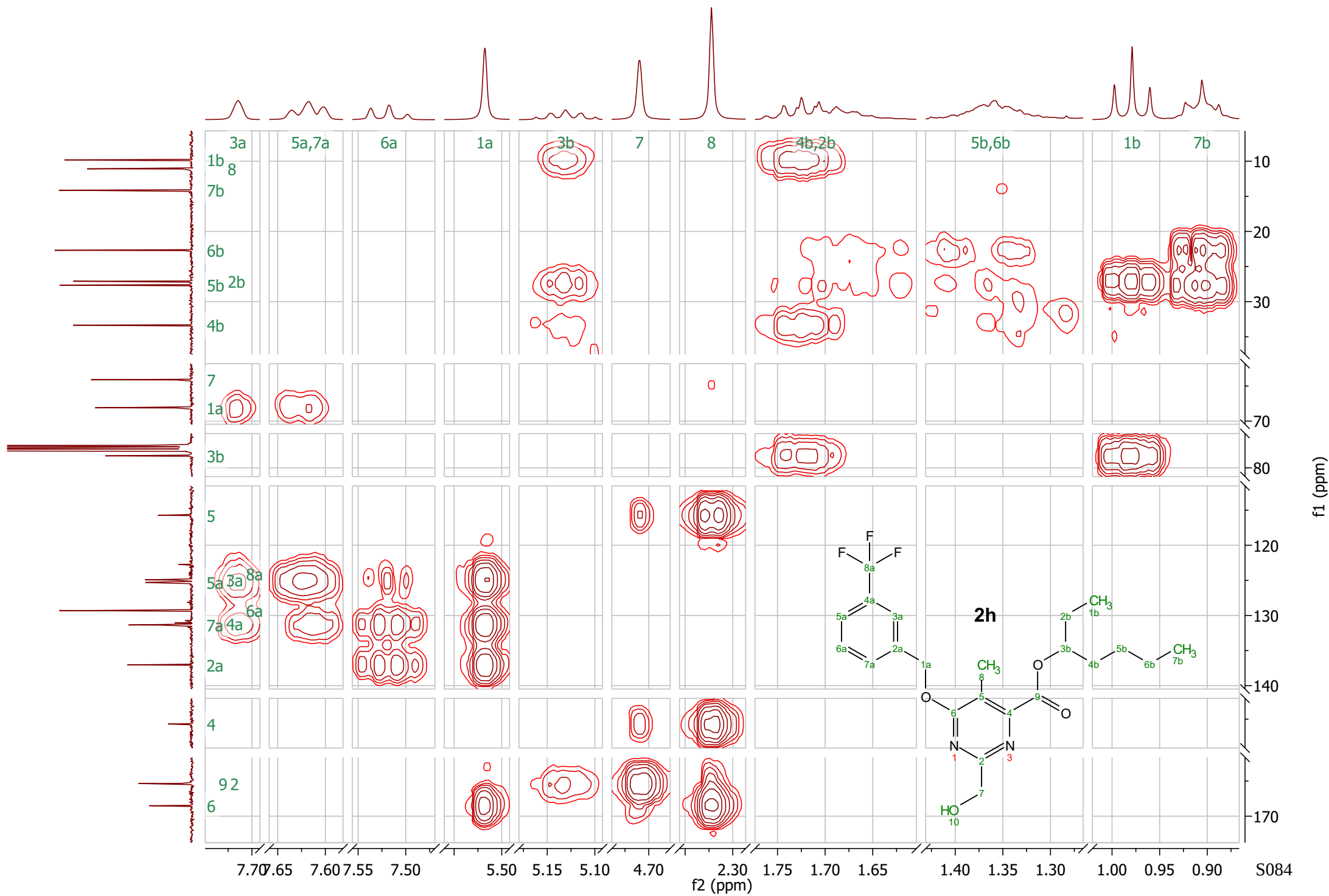
¹³C NMR (101 MHz, CDCl₃) δ 168.5, 165.4, 155.7, 137.0, 131.3 (app q, *J* = 1.3 Hz), 131.2 (q, *J* = 32.6 Hz), 129.3, 125.3 (q, *J* = 3.8 Hz), 124.9 (q, *J* = 3.8 Hz), 124.1 (q, *J* = 272.4 Hz), 115.7, 78.3, 13C 68.1, 64.1, 33.4, 27.6, 27.1, 22.7, 14.1, 11.1, 9.8.



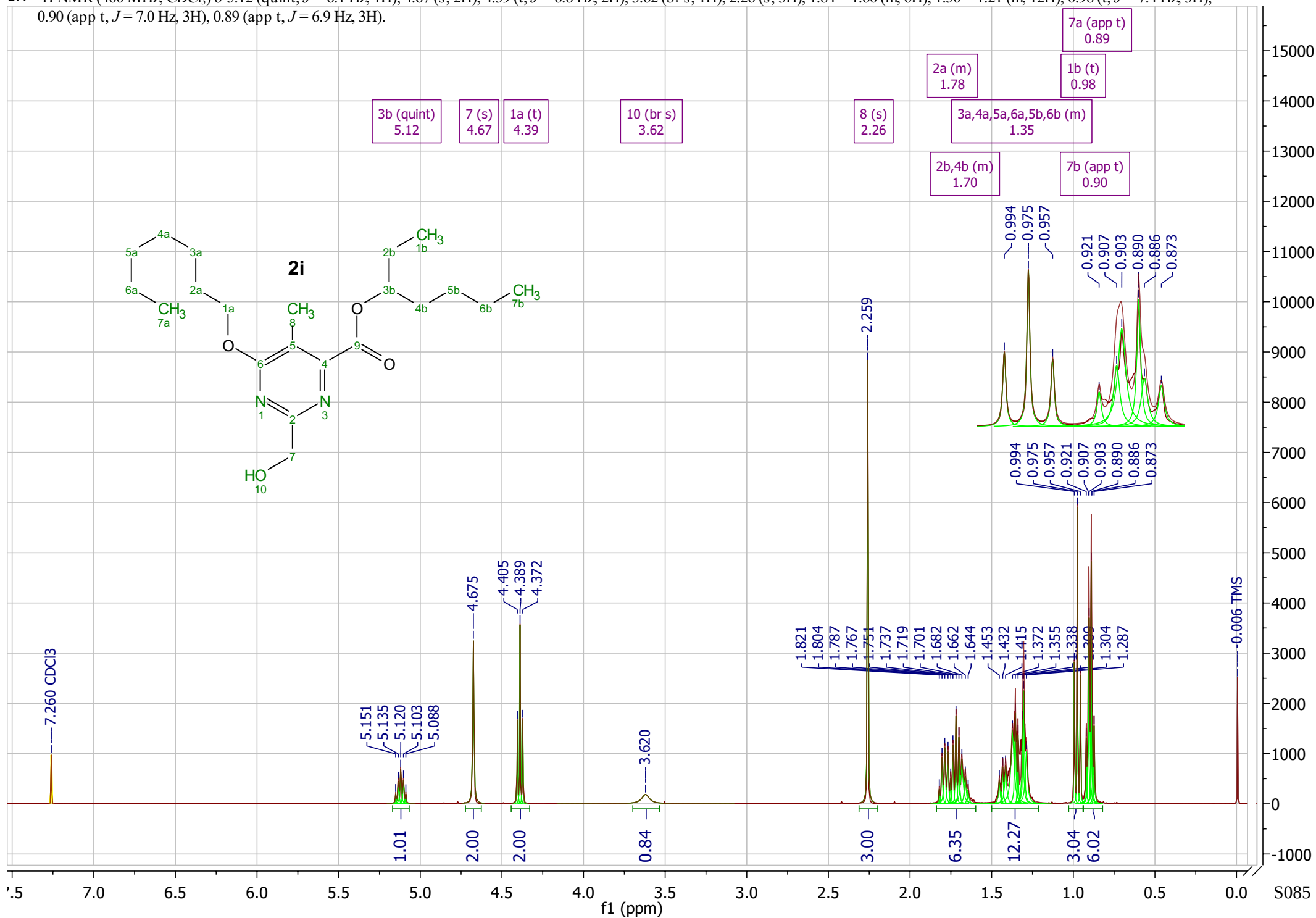
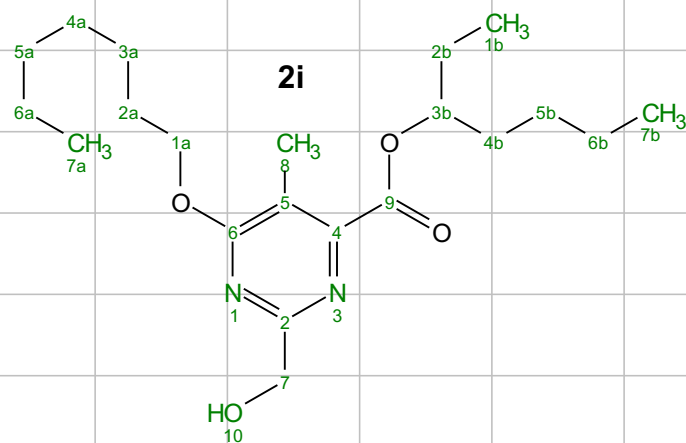
¹³C [118.5 — 132.5 ppm]



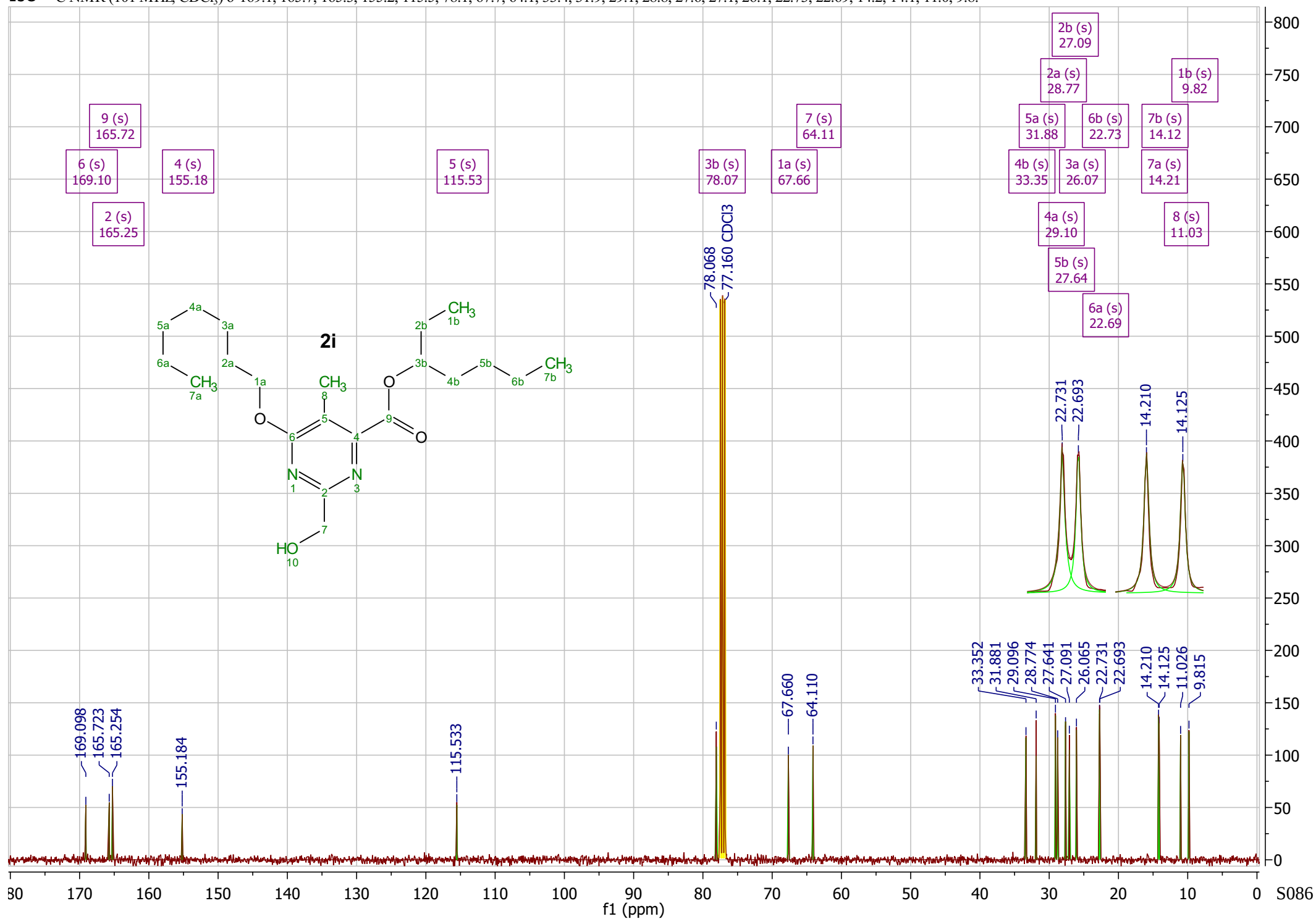


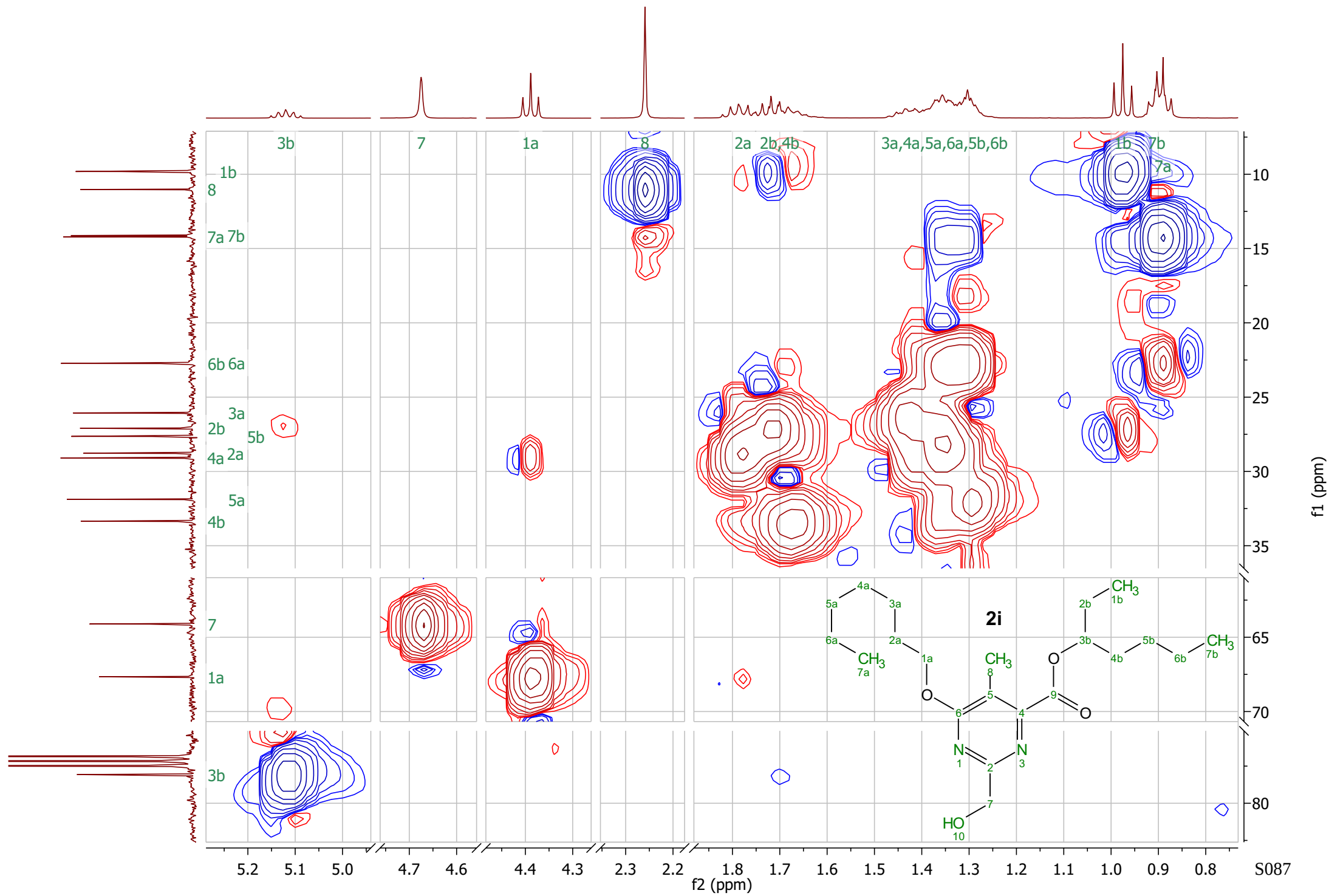


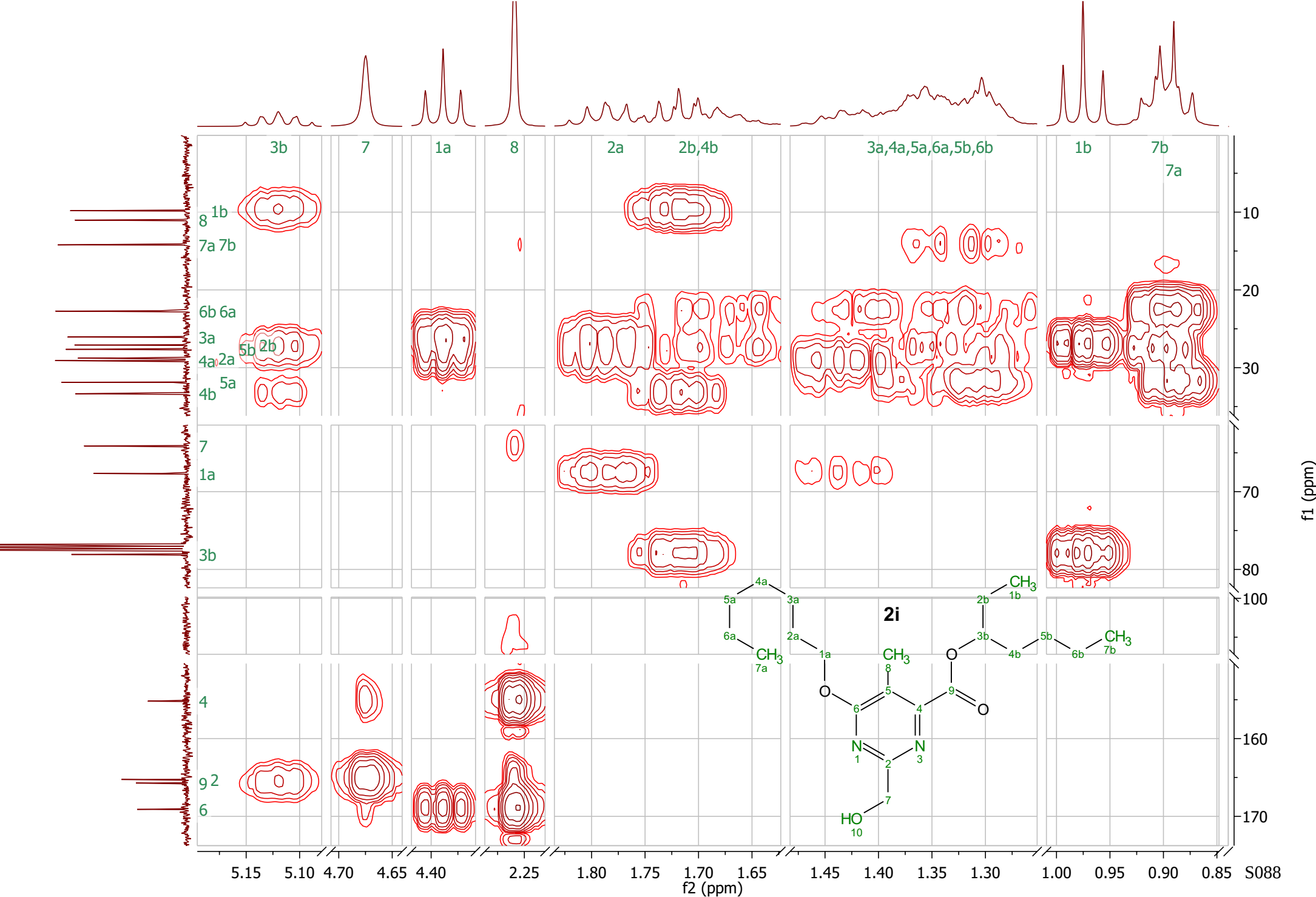
^1H NMR (400 MHz, CDCl_3) δ 5.12 (quint, $J = 6.1$ Hz, 1H), 4.67 (s, 2H), 4.39 (t, $J = 6.6$ Hz, 2H), 3.62 (br s, 1H), 2.26 (s, 3H), 1.84 – 1.60 (m, 6H), 1.50 – 1.21 (m, 12H), 0.98 (t, $J = 7.4$ Hz, 3H), 0.90 (app t, $J = 7.0$ Hz, 3H), 0.89 (app t, $J = 6.9$ Hz, 3H).



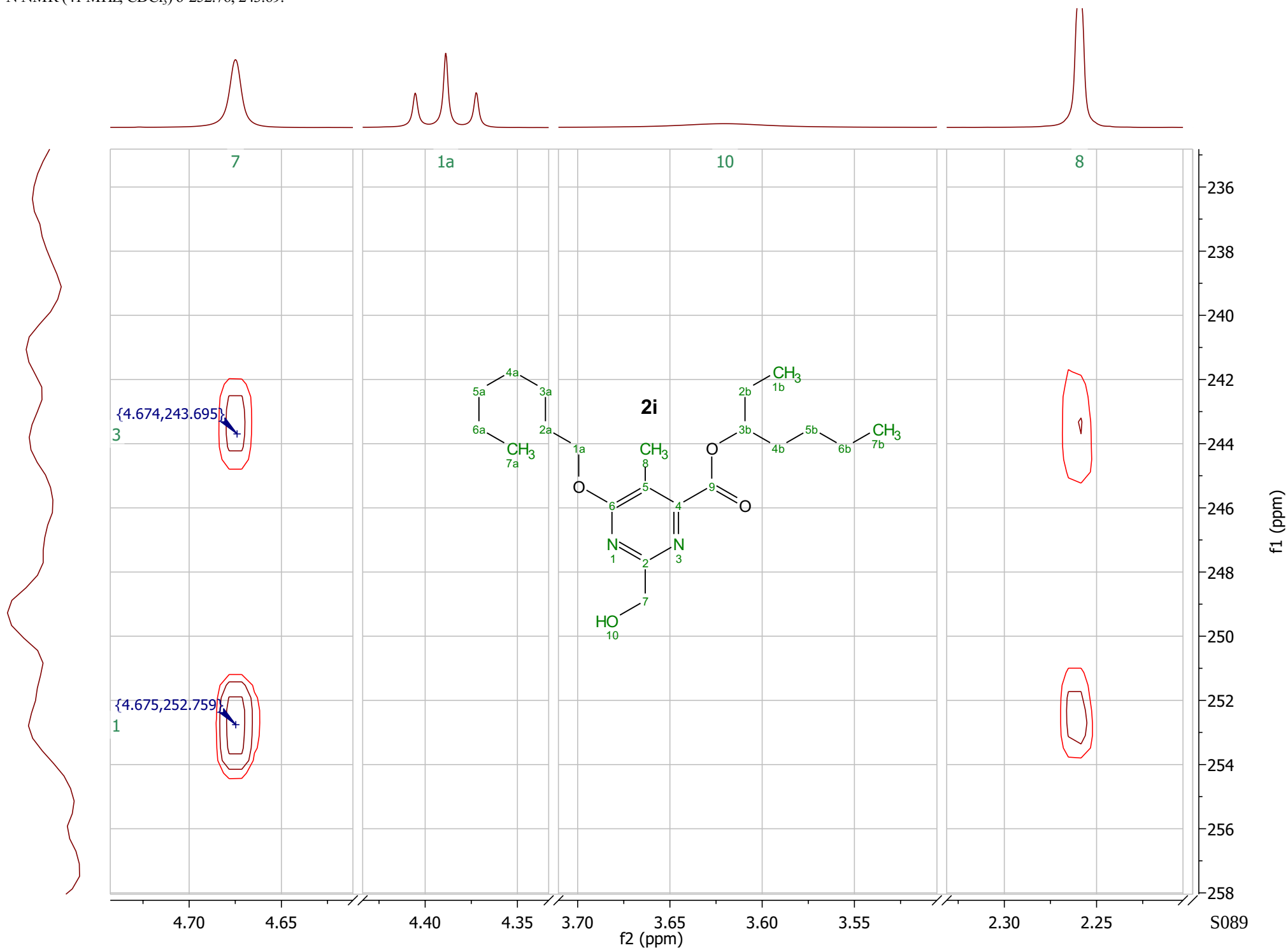
¹³C ¹³C NMR (101 MHz, CDCl₃) δ 169.1, 165.7, 165.3, 155.2, 115.5, 78.1, 67.7, 64.1, 33.4, 31.9, 29.1, 28.8, 27.6, 27.1, 26.1, 22.73, 22.69, 14.2, 14.1, 11.0, 9.8.



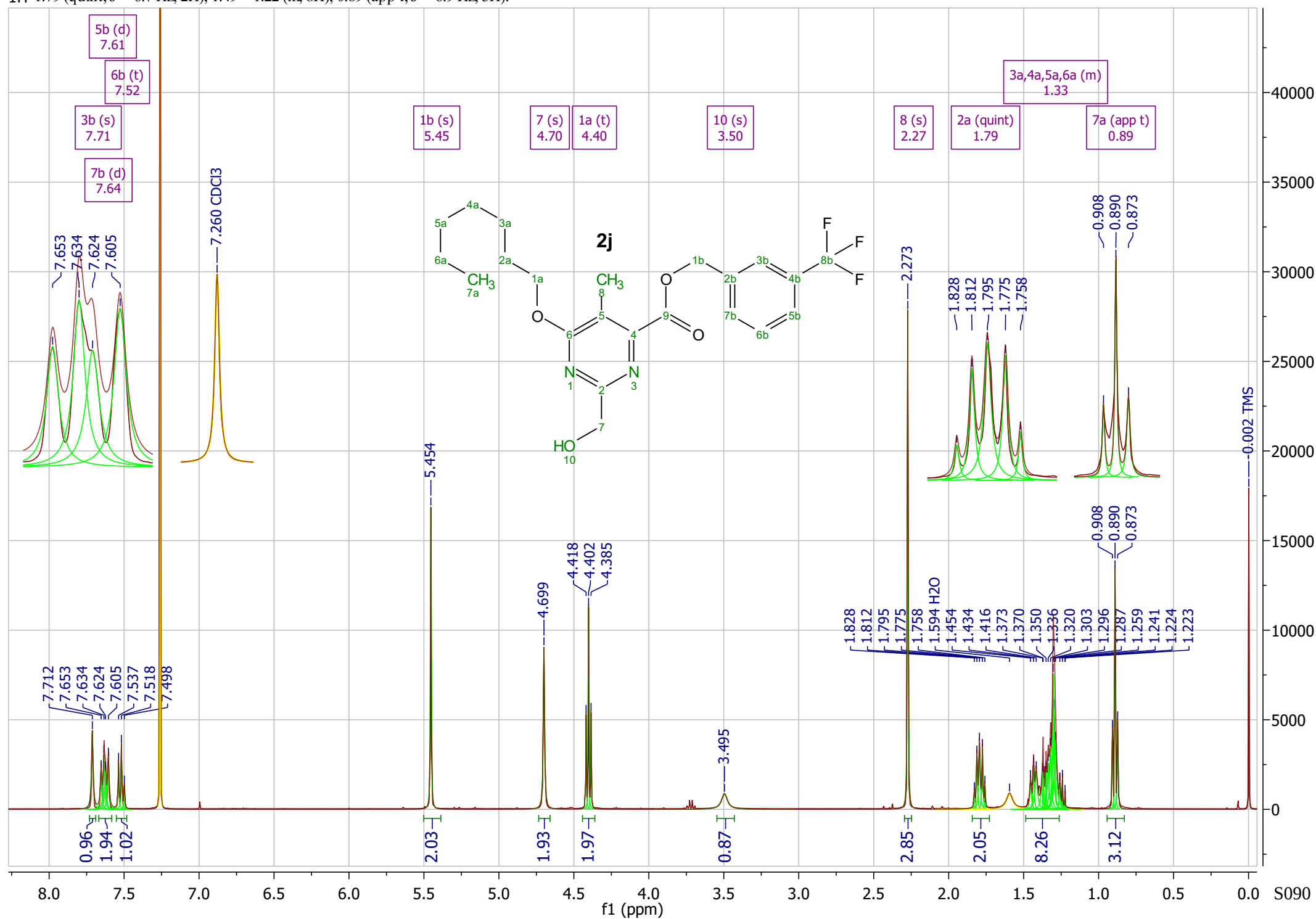




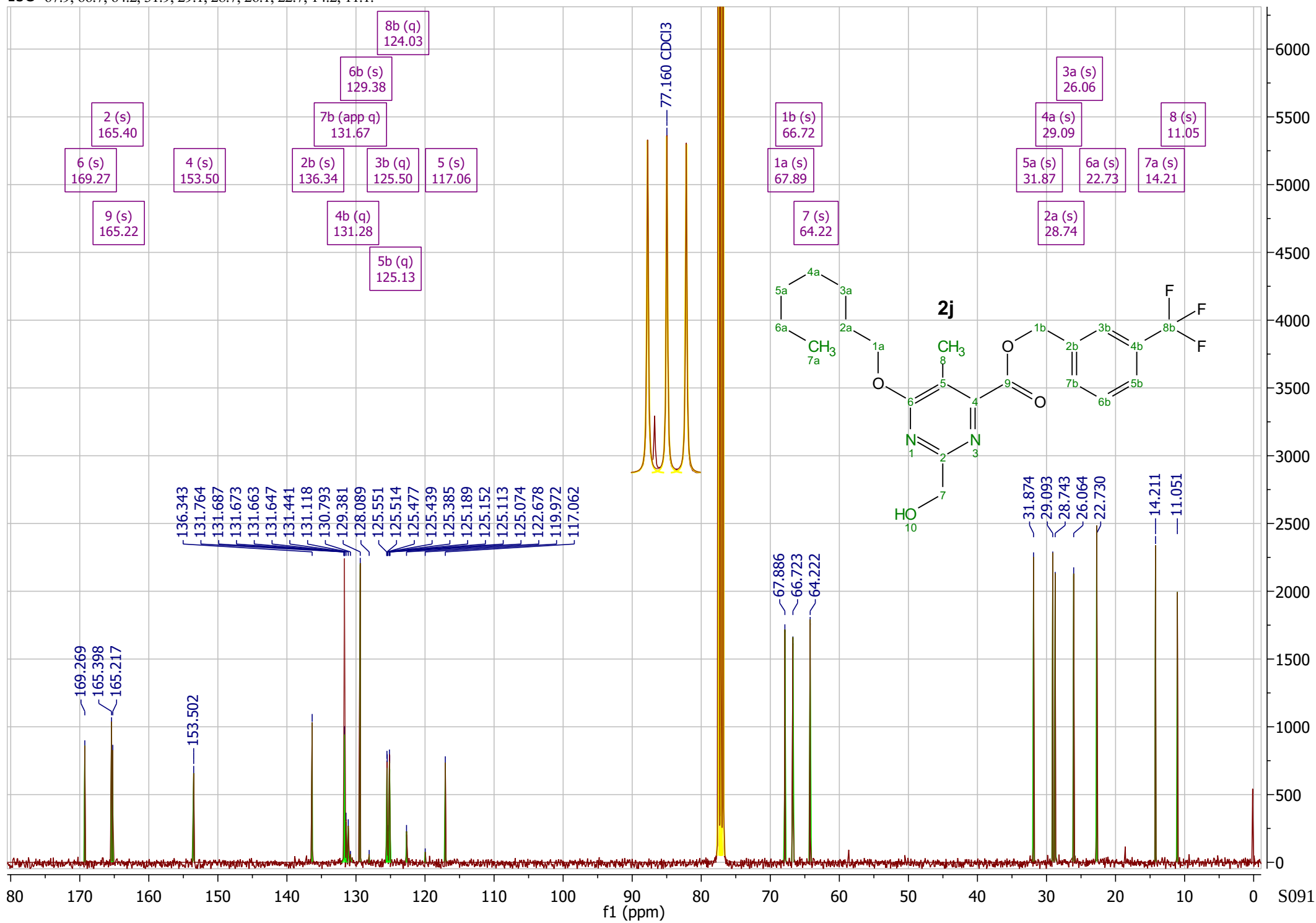
15N HMBC ¹⁵N NMR (41 MHz, CDCl₃) δ 252.76, 243.69.



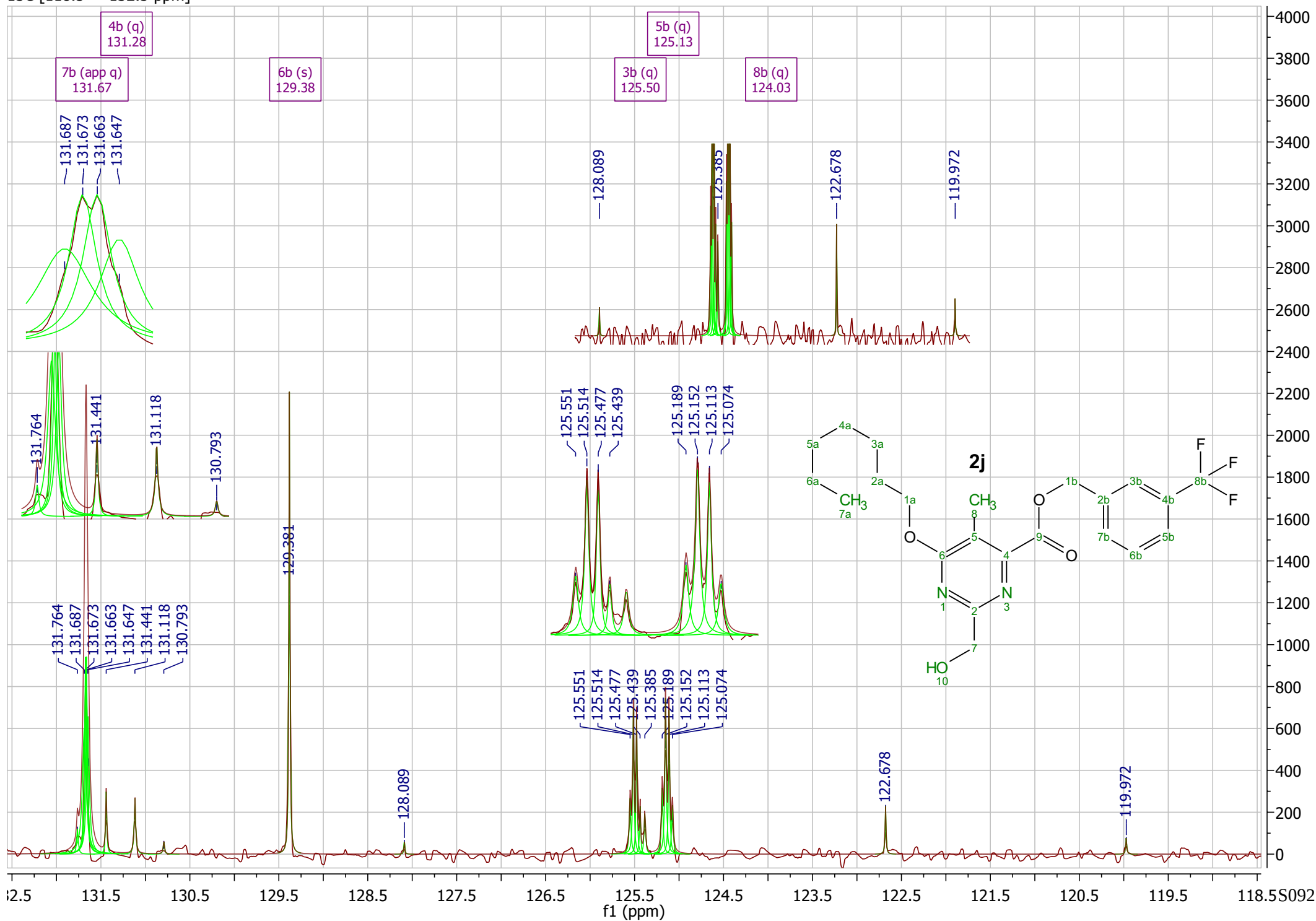
¹H NMR (400 MHz, CDCl₃) δ 7.71 (s, 1H), 7.64 (d, *J* = 7.6 Hz, 1H), 7.61 (d, *J* = 7.7 Hz, 1H), 7.52 (t, *J* = 7.7 Hz, 1H), 5.45 (s, 2H), 4.70 (s, 2H), 4.40 (t, *J* = 6.6 Hz, 2H), 3.50 (s, 1H), 2.27 (s, 3H), 1.79 (quint, *J* = 6.7 Hz, 2H), 1.49 – 1.22 (m, 8H), 0.89 (app t, *J* = 6.9 Hz, 3H).

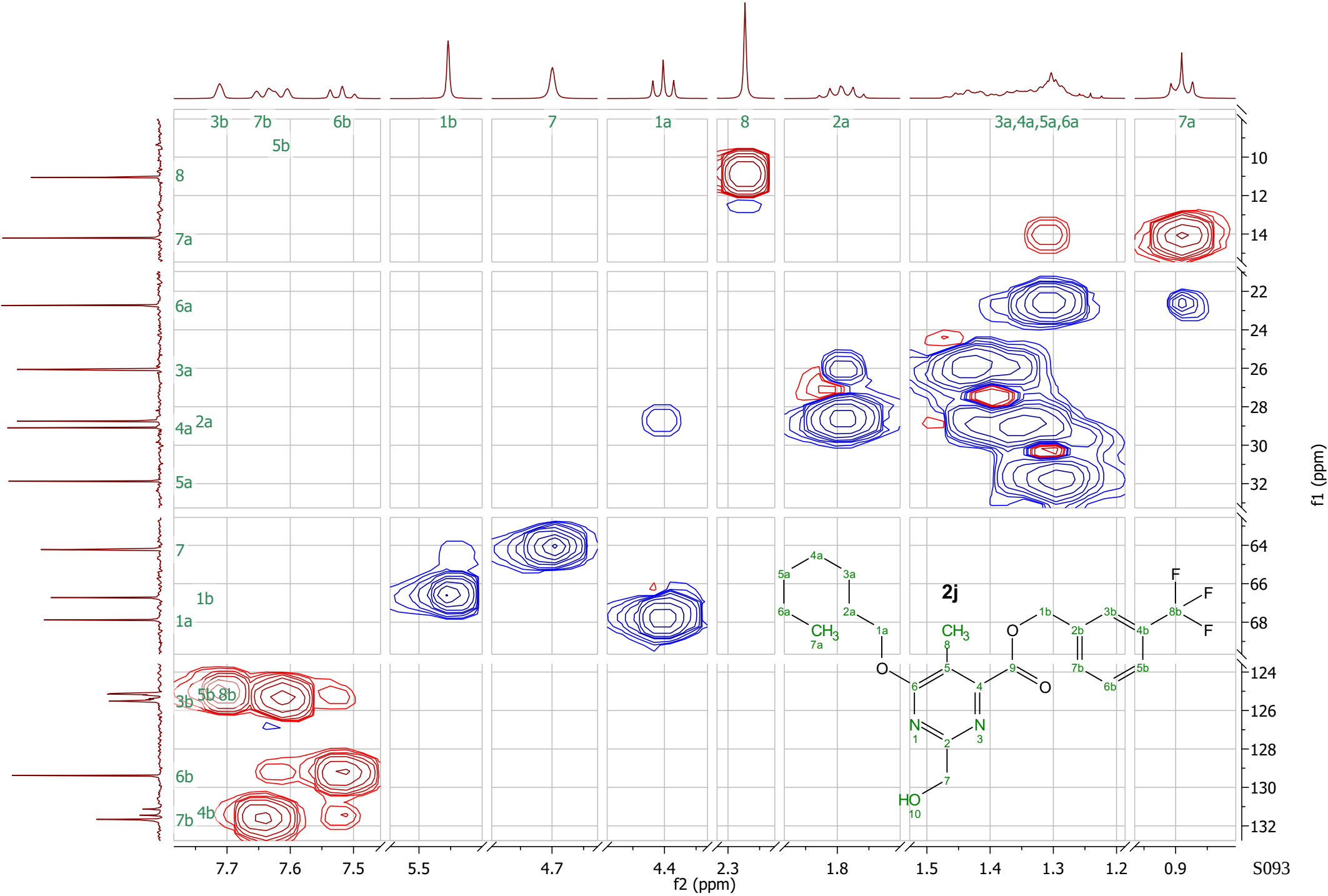


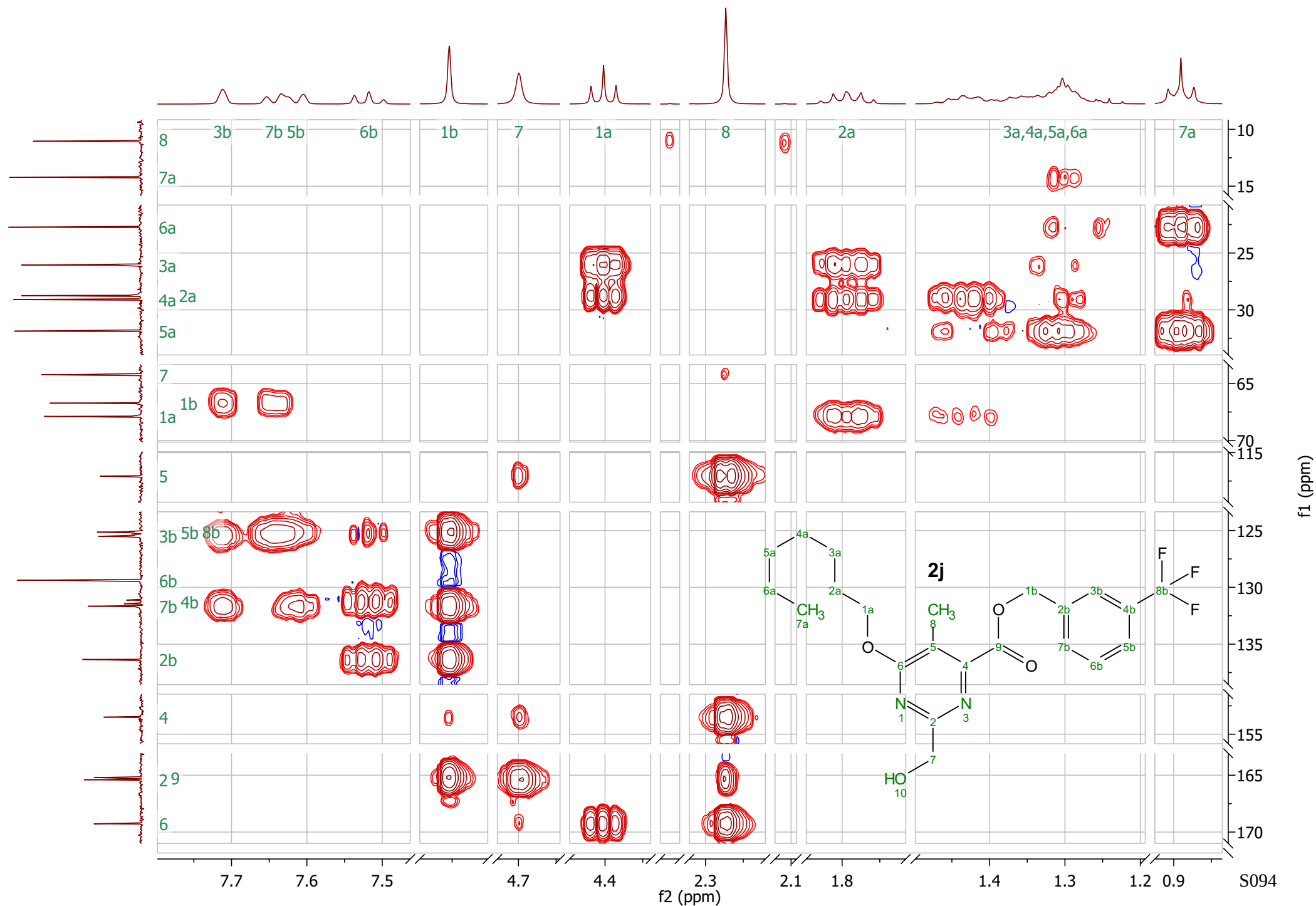
^{13}C NMR (101 MHz, CDCl_3) δ 169.3, 165.4, 165.2, 153.5, 136.3, 131.7 (app q, $J = 1.3$ Hz), 131.3 (q, $J = 32.8$ Hz), 129.4, 125.5 (q, $J = 3.8$ Hz), 125.1 (q, $J = 3.9$ Hz), 124.0 (q, $J = 272.2$ Hz), 117.1, 13C 67.9, 66.7, 64.2, 31.9, 29.1, 28.7, 26.1, 22.7, 14.2, 11.1.

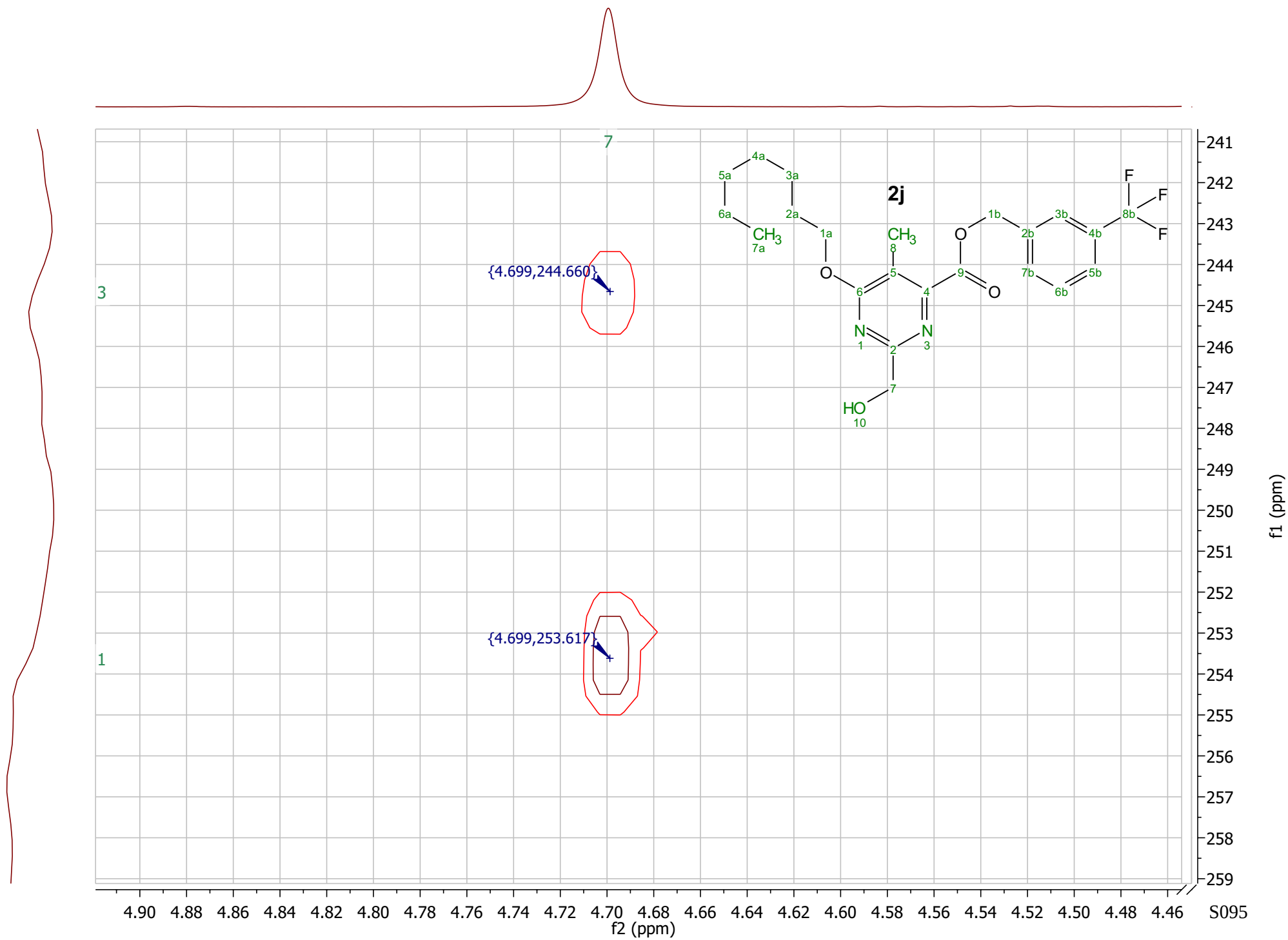


¹³C [118.5 — 132.5 ppm]

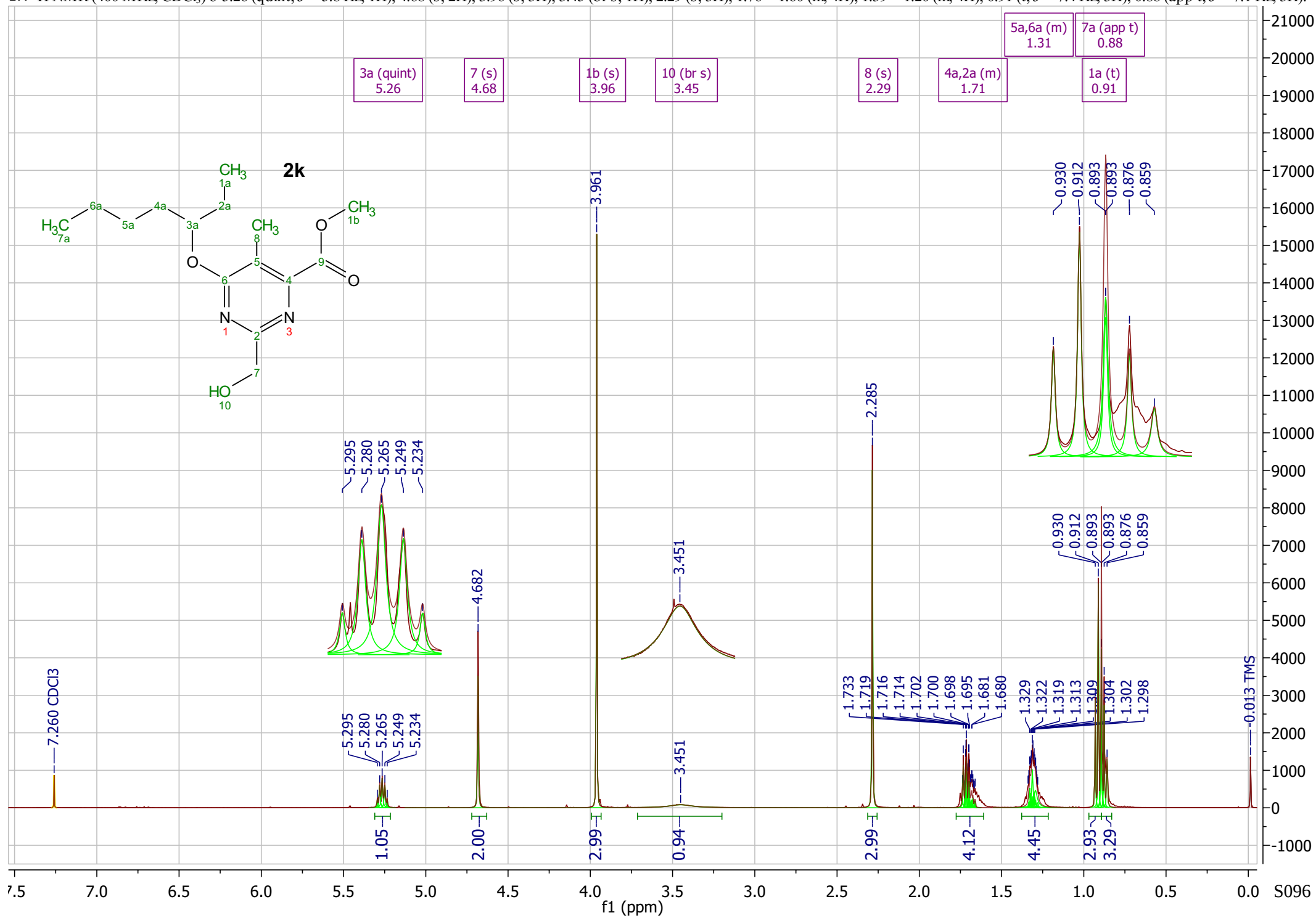




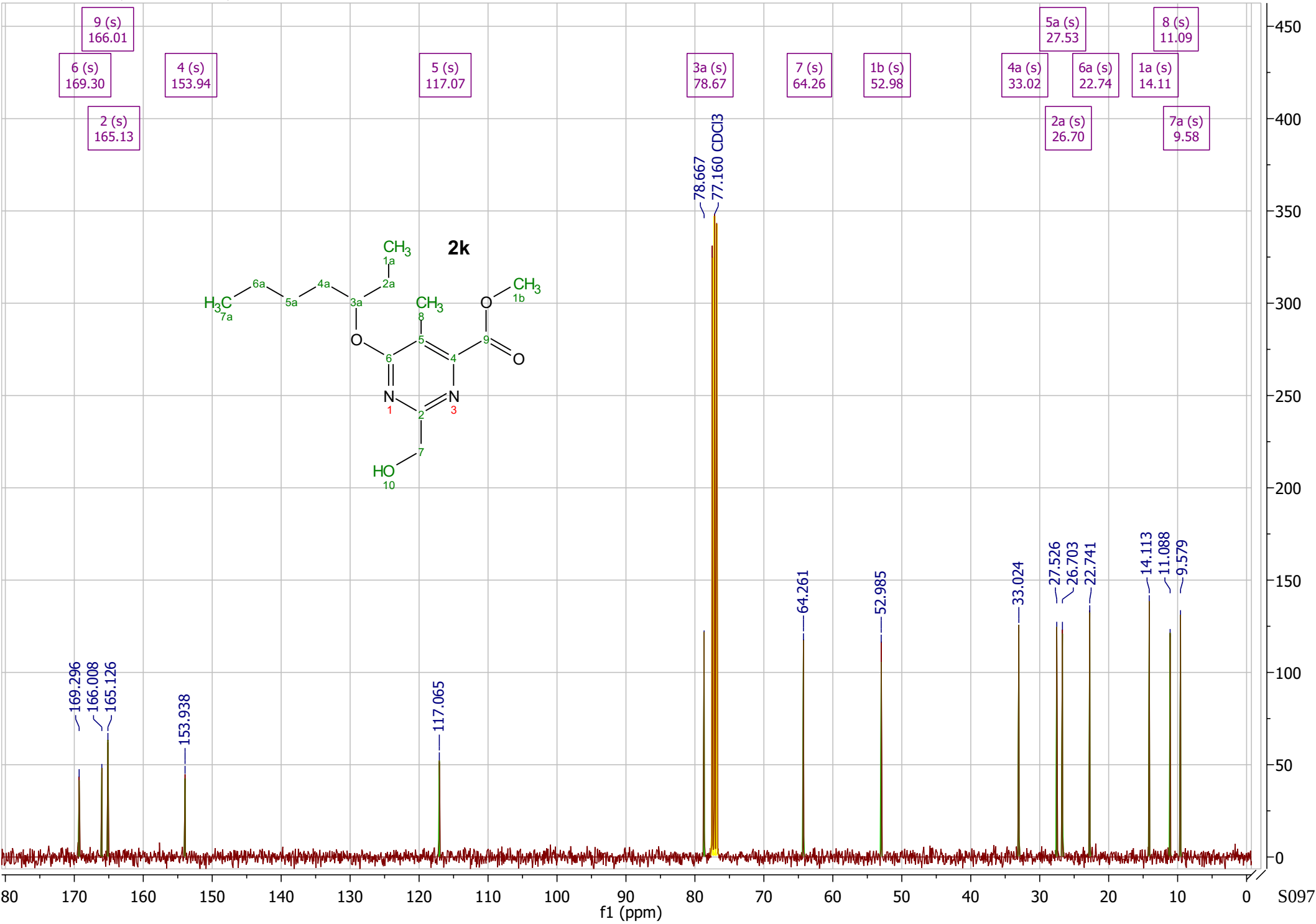


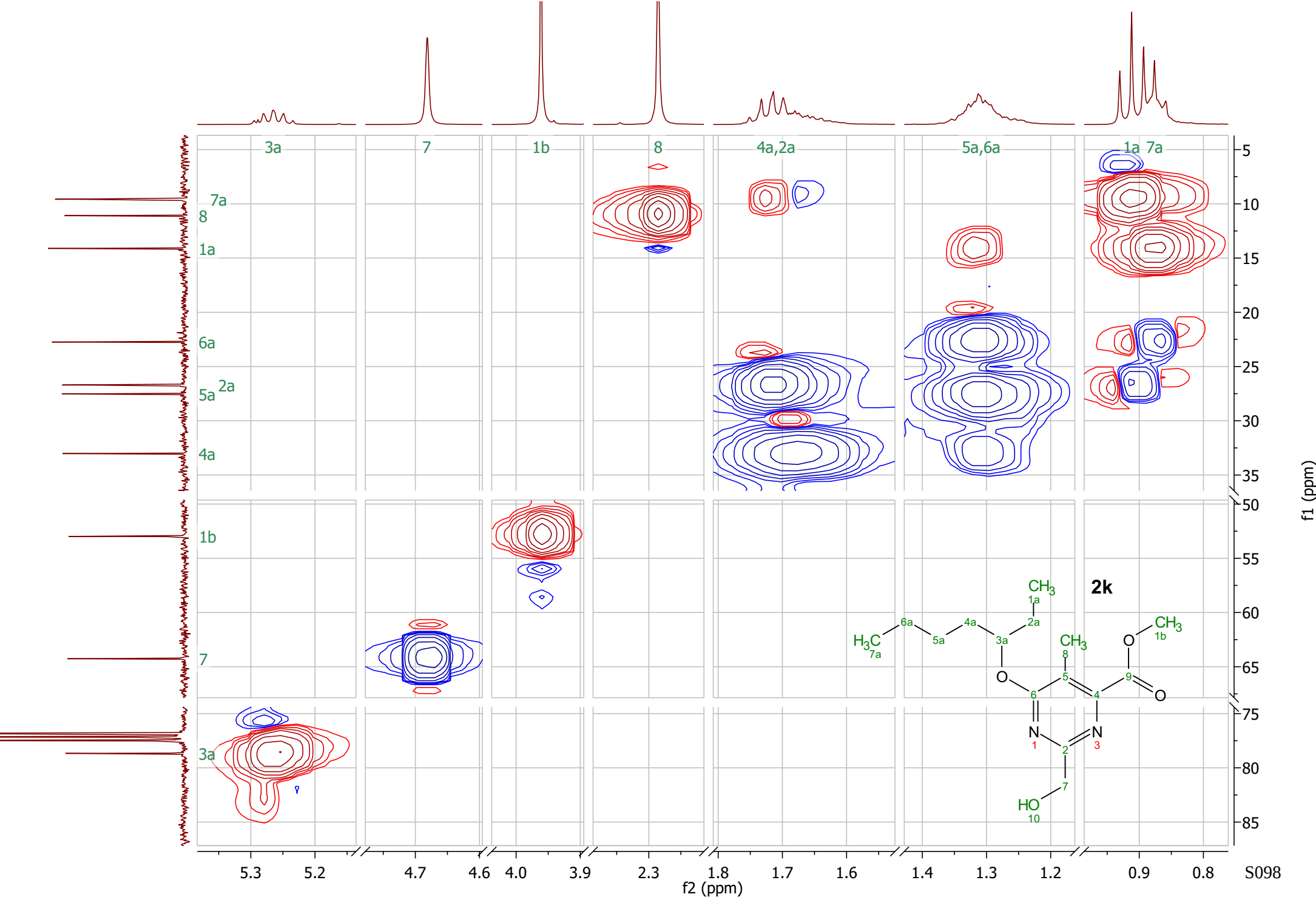


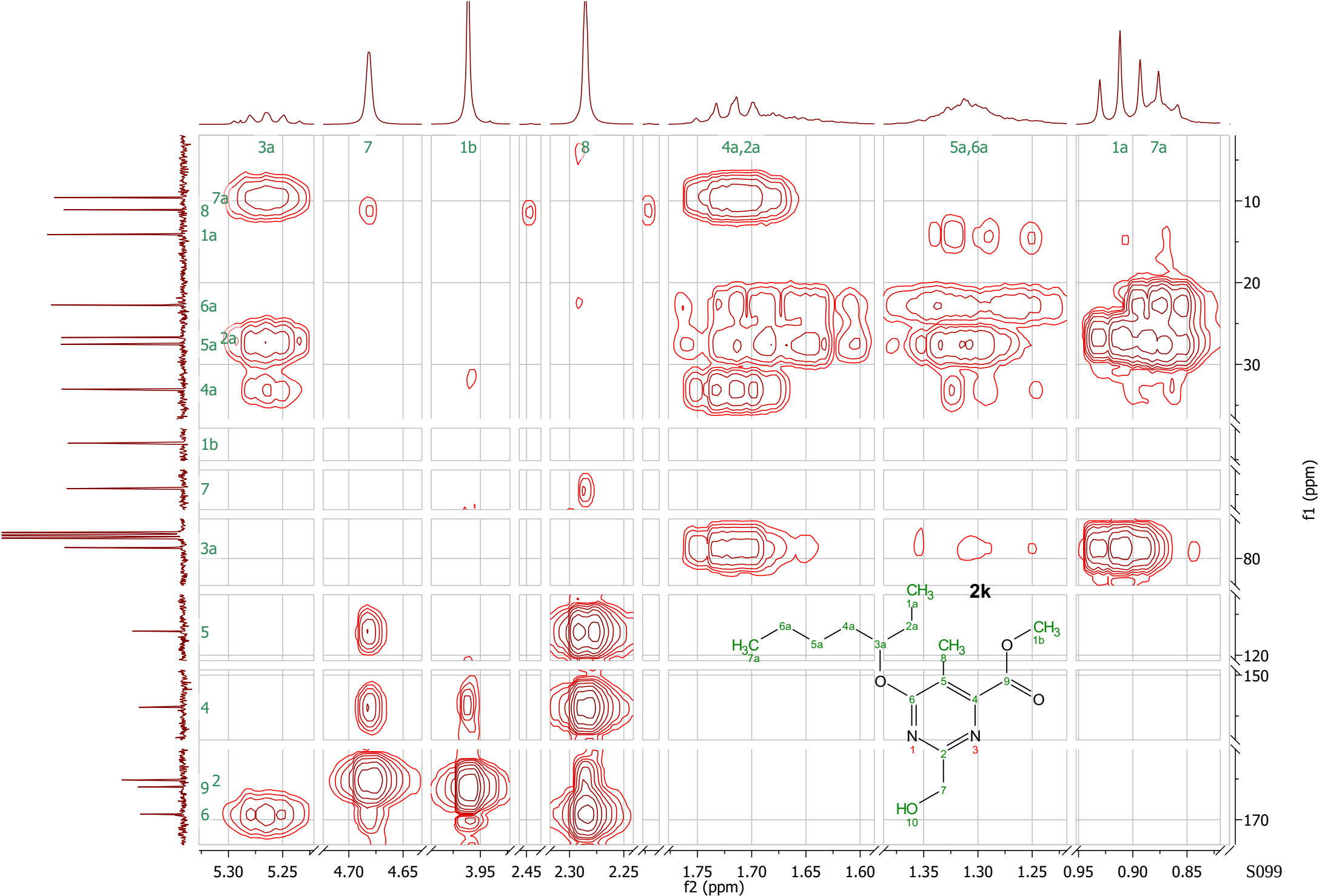
^1H NMR (400 MHz, CDCl_3) δ 5.26 (quint, $J = 5.8$ Hz, 1H), 4.68 (s, 2H), 3.96 (s, 3H), 3.45 (br s, 1H), 2.29 (s, 3H), 1.76 – 1.60 (m, 4H), 1.39 – 1.20 (m, 4H), 0.91 (t, $J = 7.4$ Hz, 3H), 0.88 (app t, $J = 7.1$ Hz, 3H).



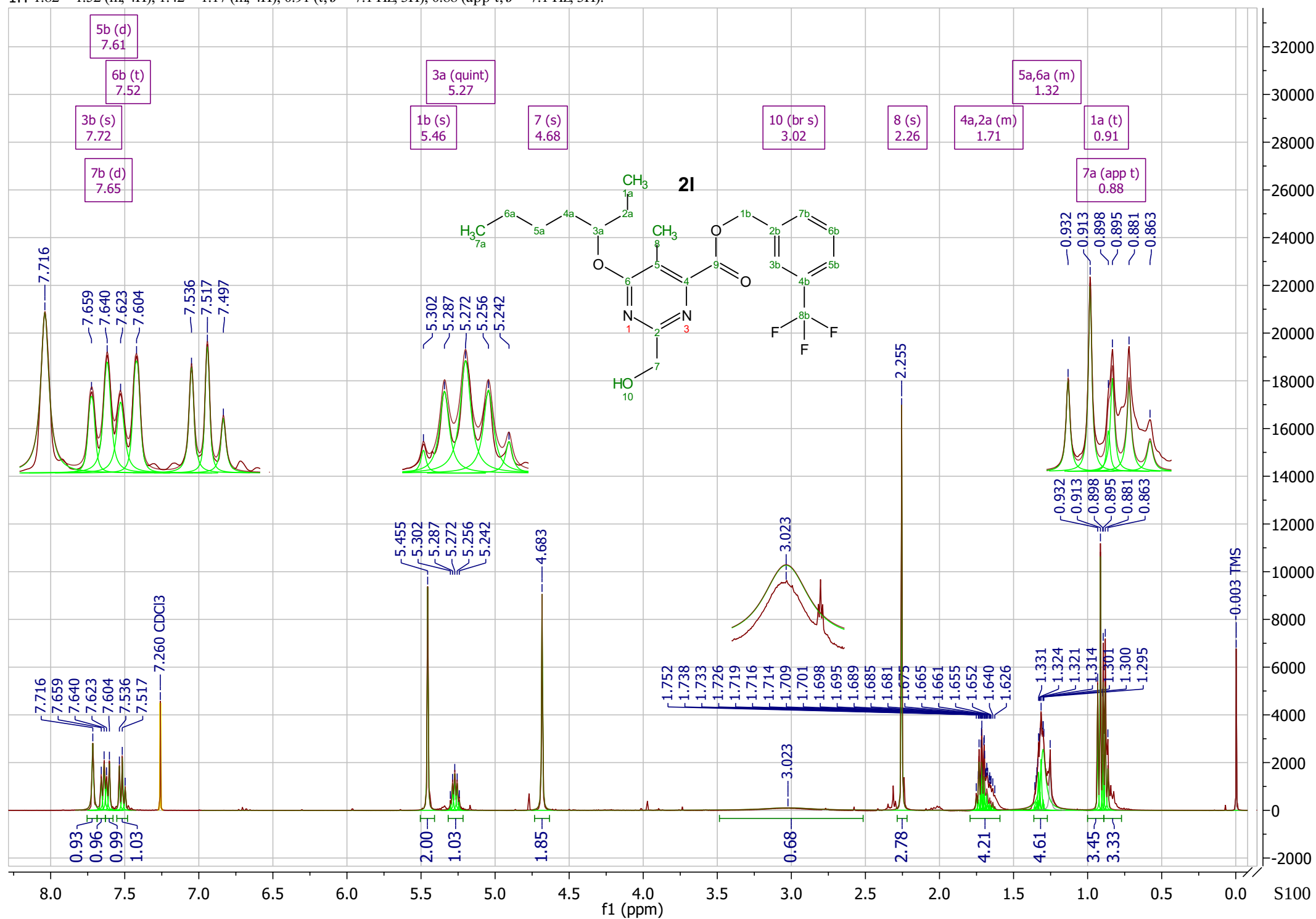
13C ¹³C NMR (101 MHz, CDCl₃) δ 169.3, 166.0, 165.1, 153.9, 117.1, 78.7, 64.3, 53.0, 33.0, 27.5, 26.7, 22.7, 14.1, 11.1, 9.6.



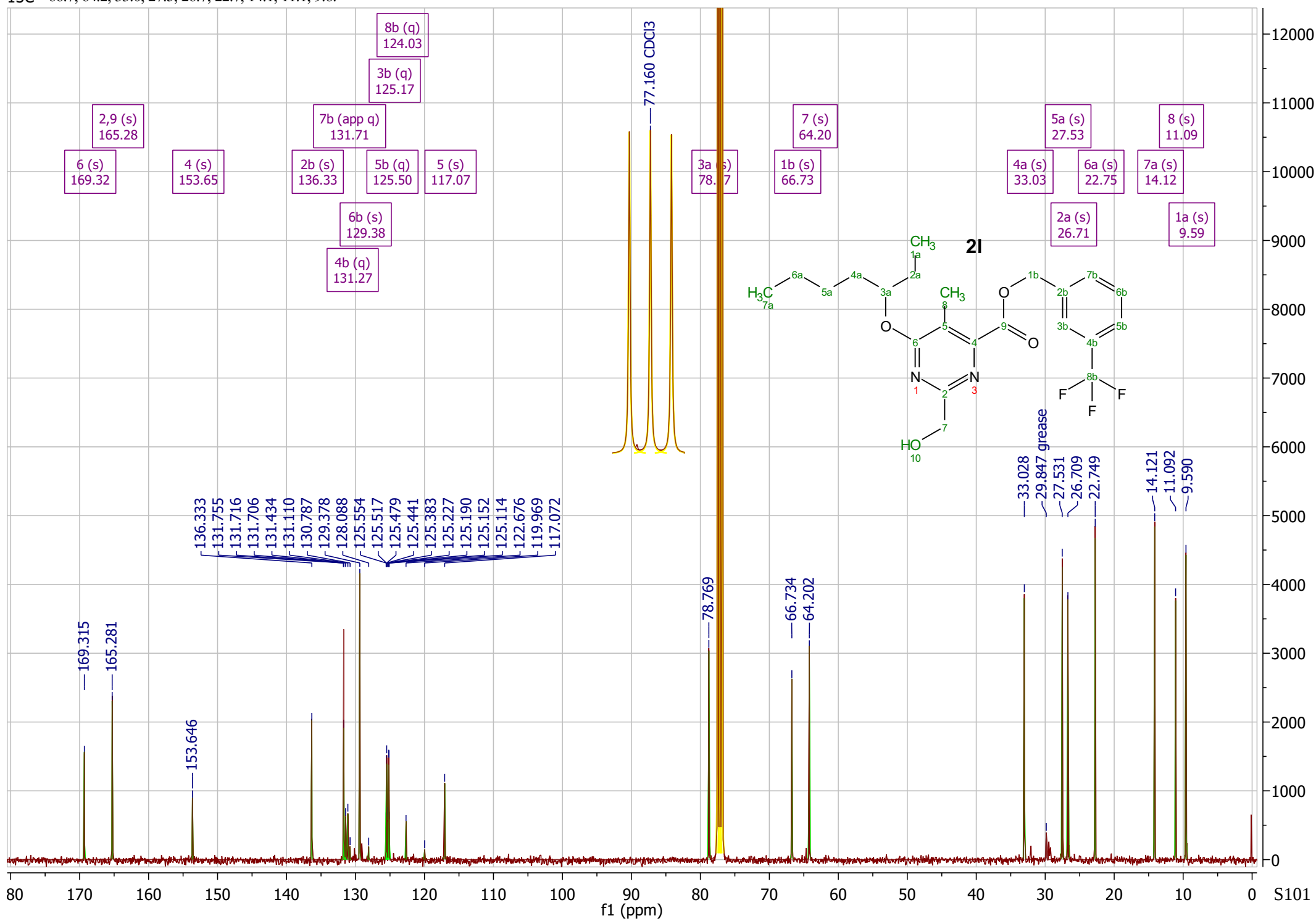




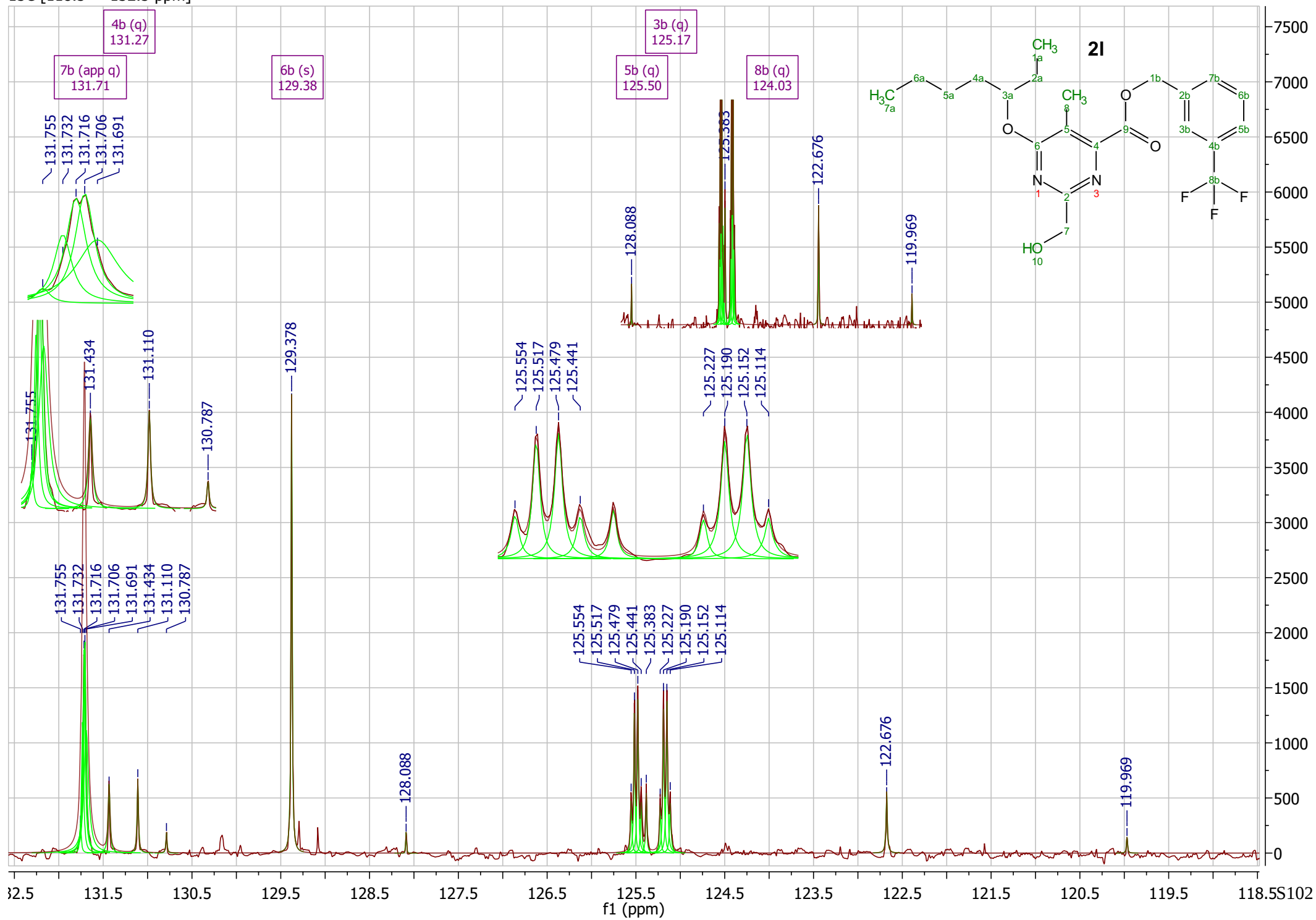
^1H NMR (400 MHz, CDCl_3) δ 7.72 (s, 1H), 7.65 (d, $J = 7.7$ Hz, 1H), 7.61 (d, $J = 7.8$ Hz, 1H), 5.46 (s, 2H), 5.27 (quint, $J = 5.9$ Hz, 1H), 4.68 (s, 2H), 3.02 (br s, 1H), 2.26 (s, 3H), 1H 1.82 – 1.52 (m, 4H), 1.42 – 1.17 (m, 4H), 0.91 (t, $J = 7.1$ Hz, 3H), 0.88 (app t, $J = 7.1$ Hz, 3H).

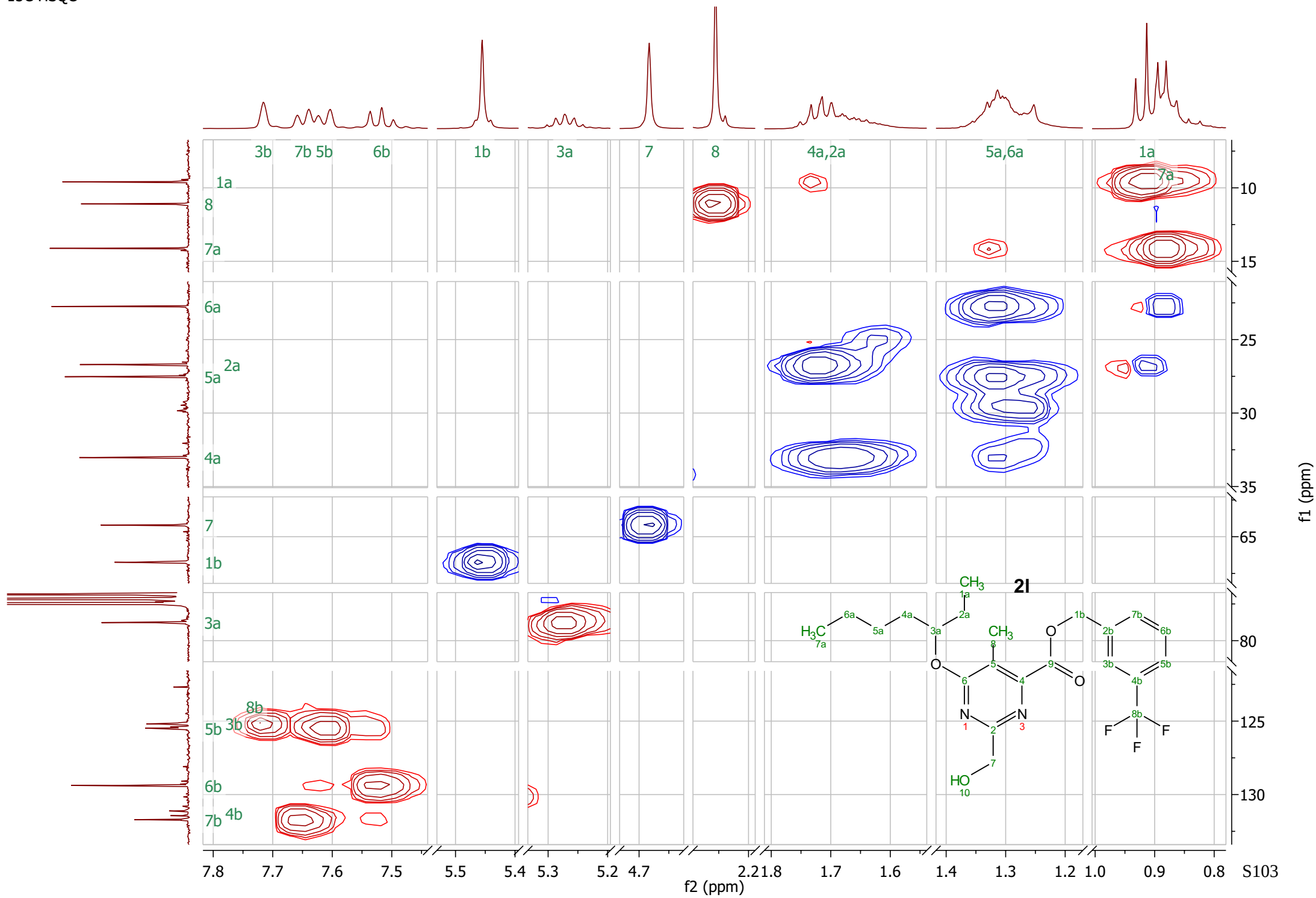


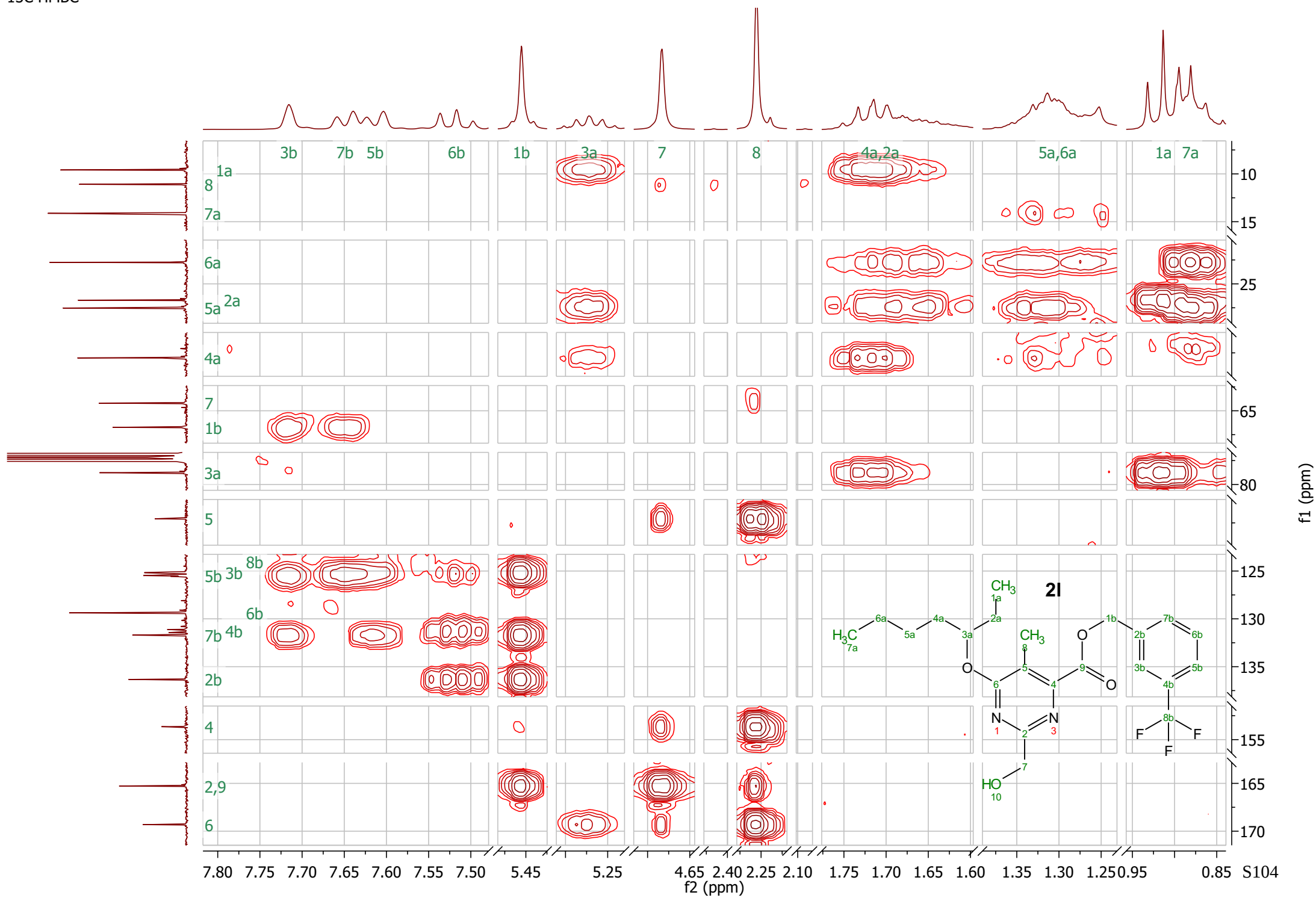
¹³C NMR (101 MHz, CDCl₃) δ 169.3, 165.3 (2C), 153.6, 136.3, 131.7 (app q, *J* = 1.1 Hz), 131.3 (q, *J* = 32.4 Hz), 129.4, 125.5 (q, *J* = 3.8 Hz), 125.2 (q, *J* = 3.8 Hz), 124.0 (q, *J* = 272.3 Hz), 117.1, 78.8, 13C 66.7, 64.2, 33.0, 27.5, 26.7, 22.7, 14.1, 11.1, 9.6.



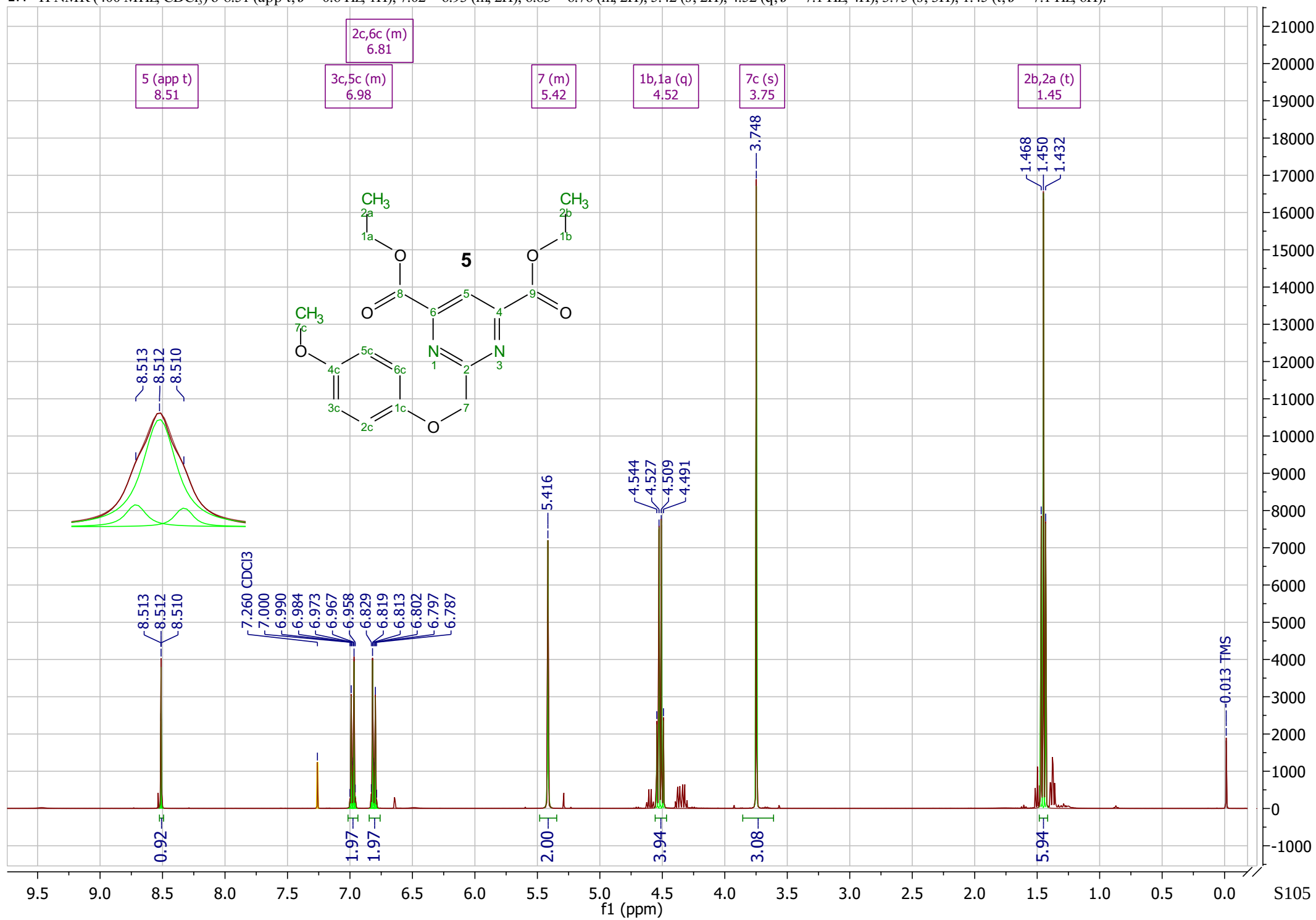
^{13}C [118.5 — 132.5 ppm]



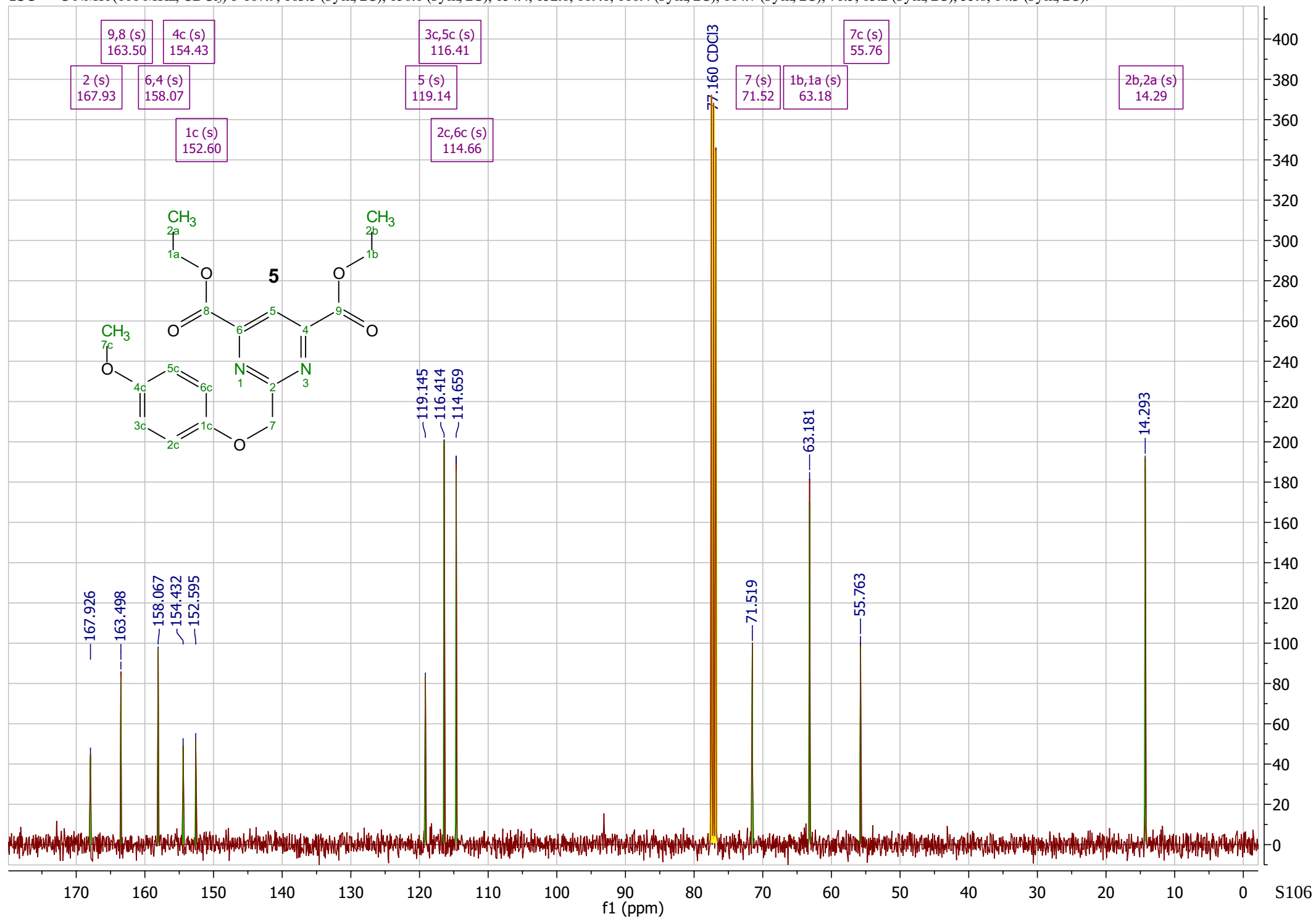


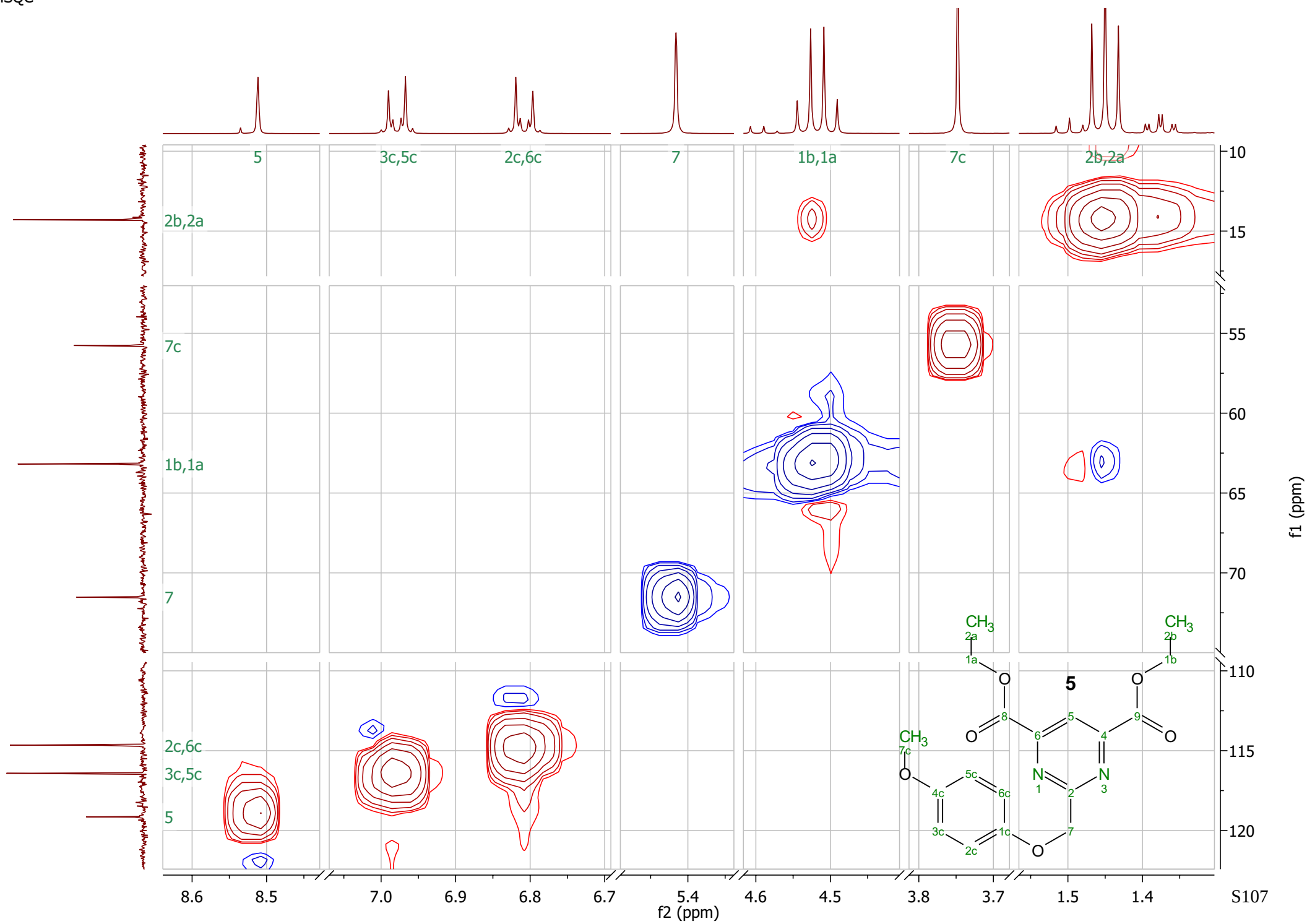


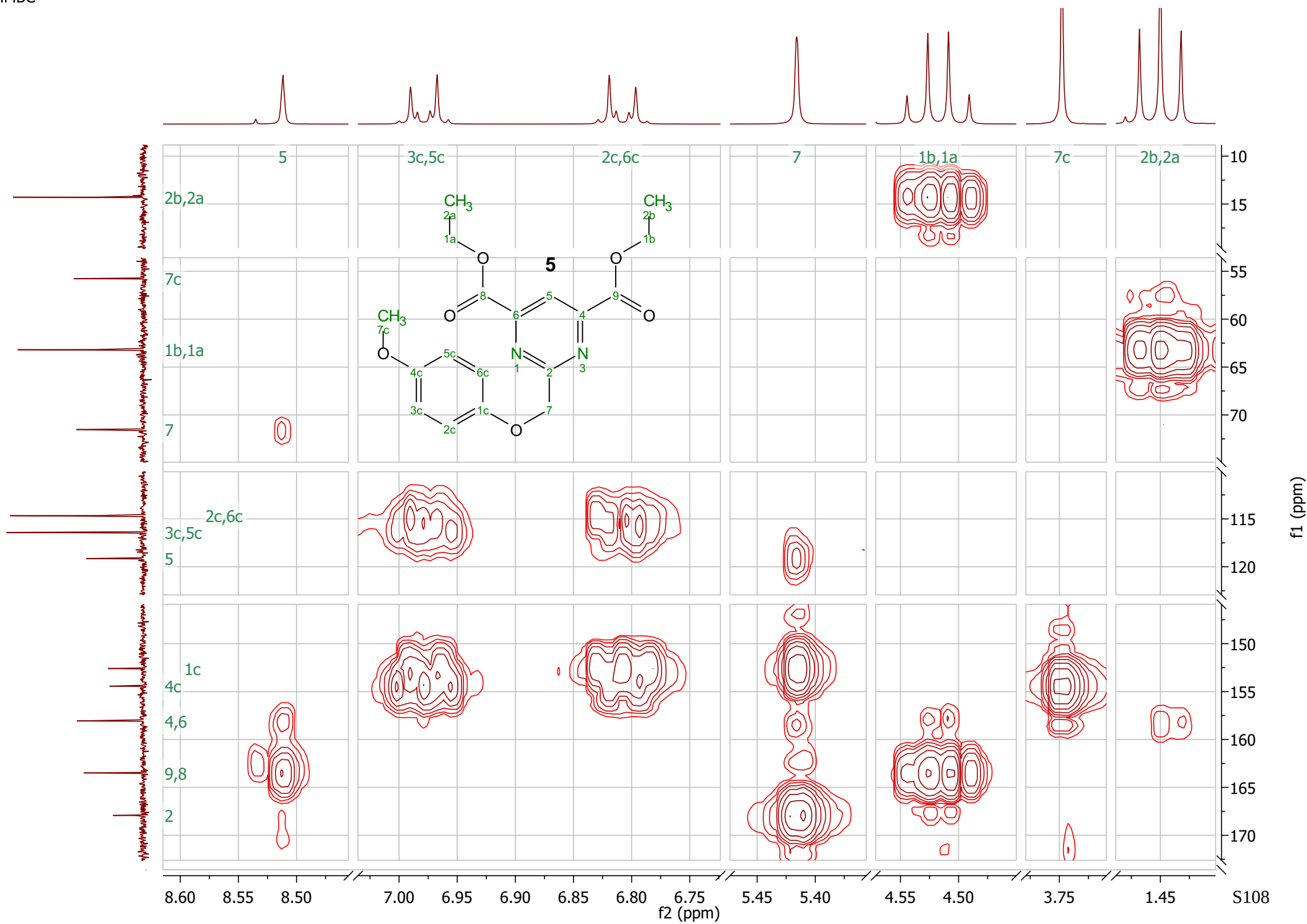
^1H NMR (400 MHz, CDCl_3) δ 8.51 (app t, $J = 0.6$ Hz, 1H), 7.02 – 6.93 (m, 2H), 6.85 – 6.76 (m, 2H), 5.42 (s, 2H), 4.52 (q, $J = 7.1$ Hz, 4H), 3.75 (s, 3H), 1.45 (t, $J = 7.1$ Hz, 6H).

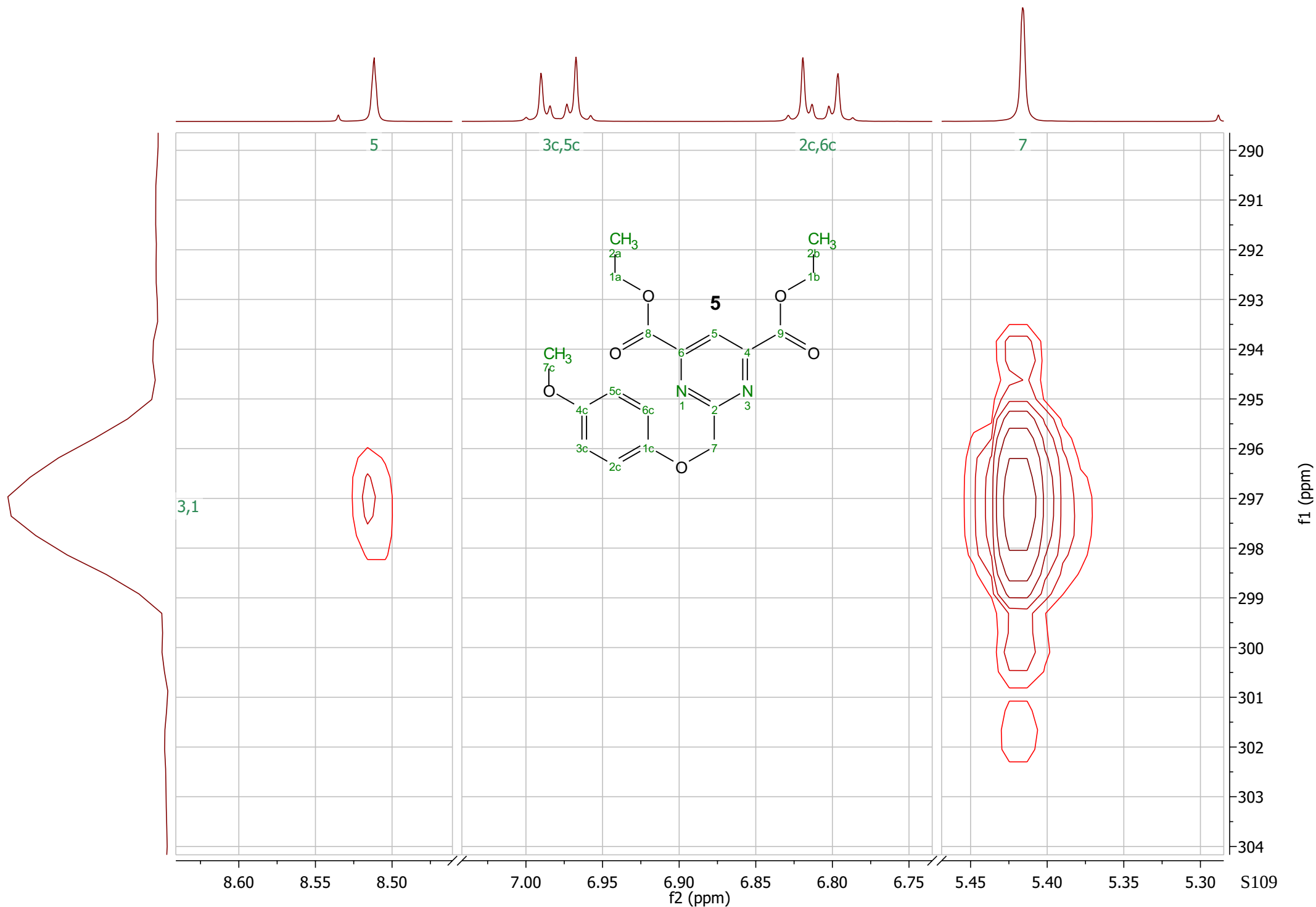


13C ^{13}C NMR (101 MHz, CDCl_3) δ 167.9, 163.5 (sym, 2C), 158.1 (sym, 2C), 154.4, 152.6, 119.1, 116.4 (sym, 2C), 114.7 (sym, 2C), 71.5, 63.2 (sym, 2C), 55.8, 14.3 (sym, 2C).





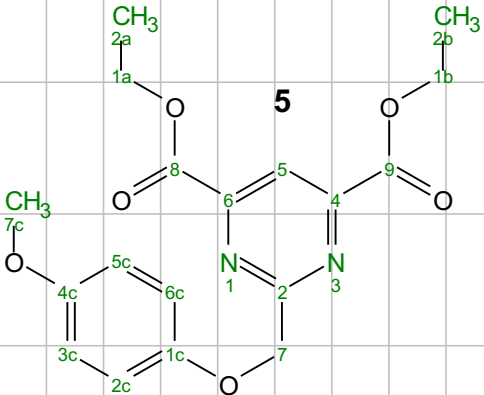




15N HMBC f1 Projection ¹⁵N NMR (41 MHz, CDCl₃) δ 297.15.

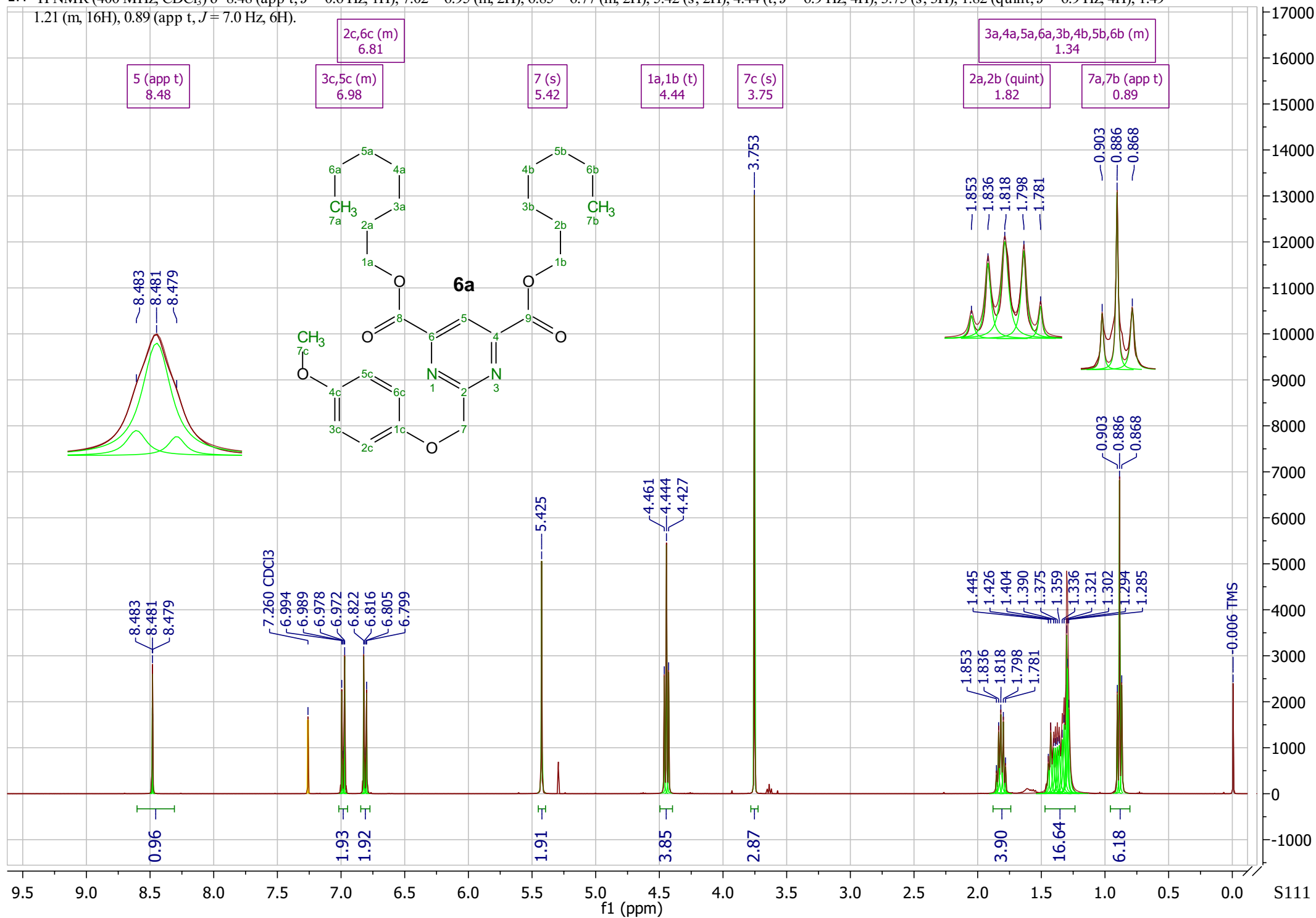
1,3 (s)
297.15

297.150

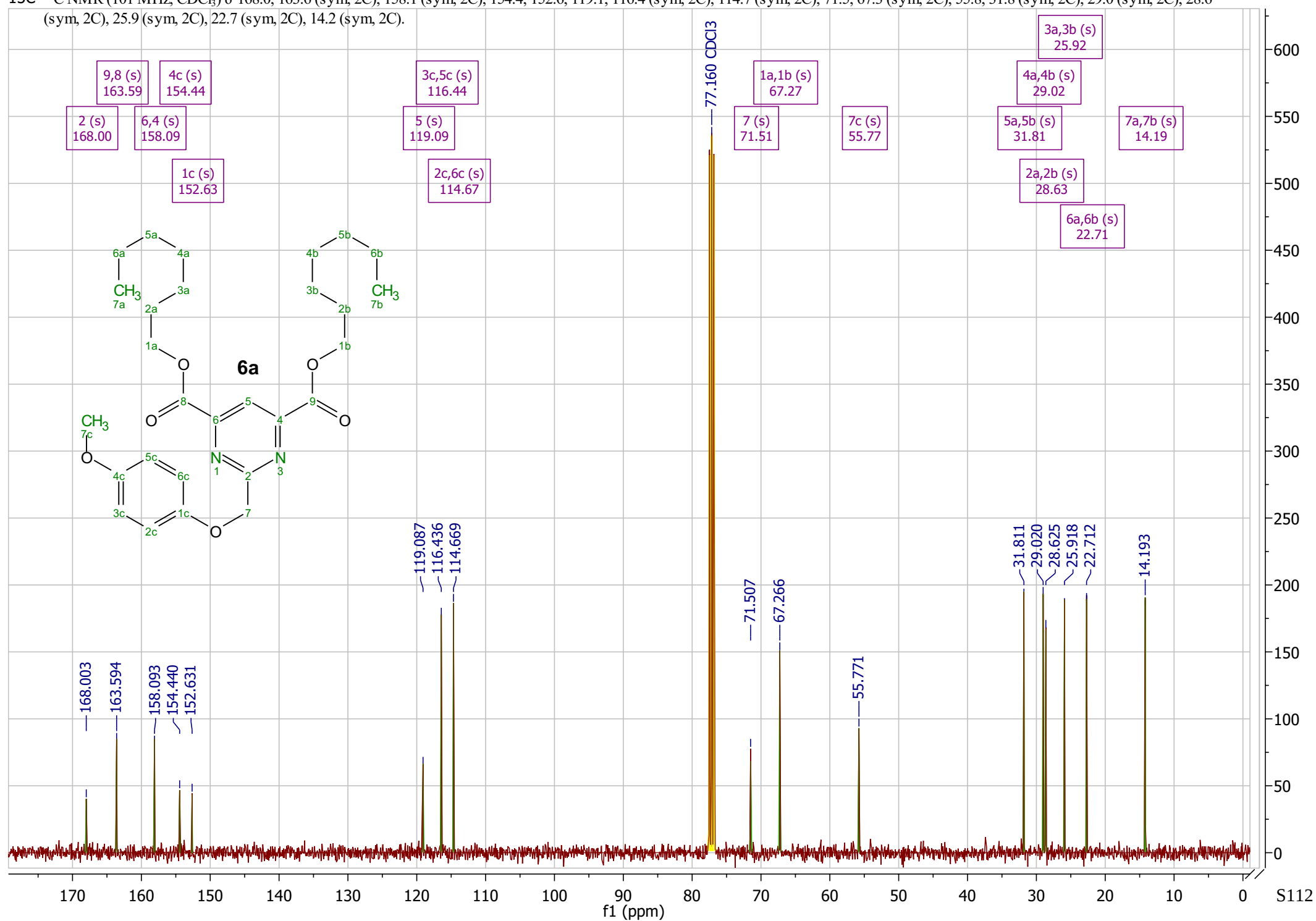


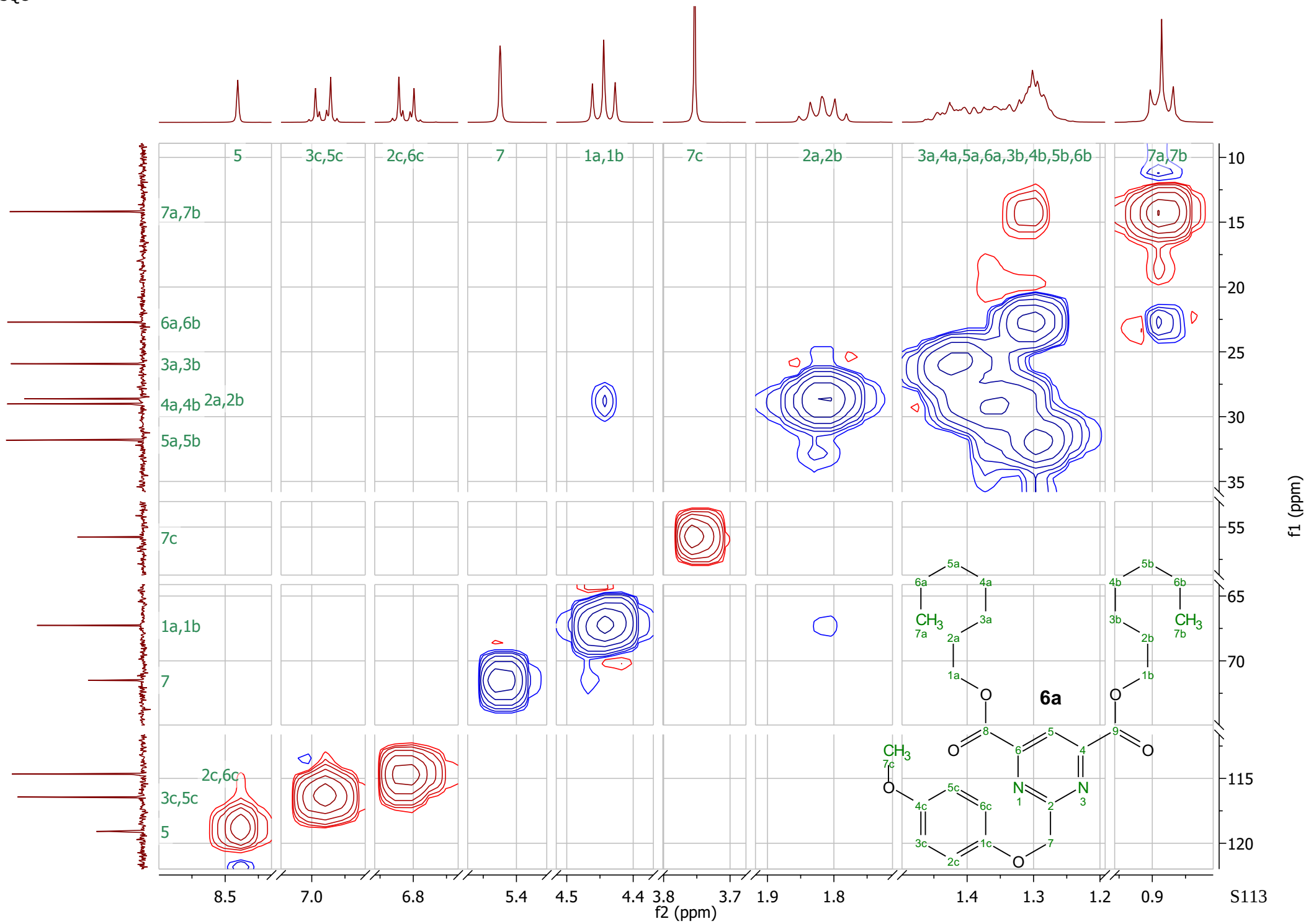
50 340 330 320 310 300 290 280 270 260 250 240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 S110
f1 (ppm)

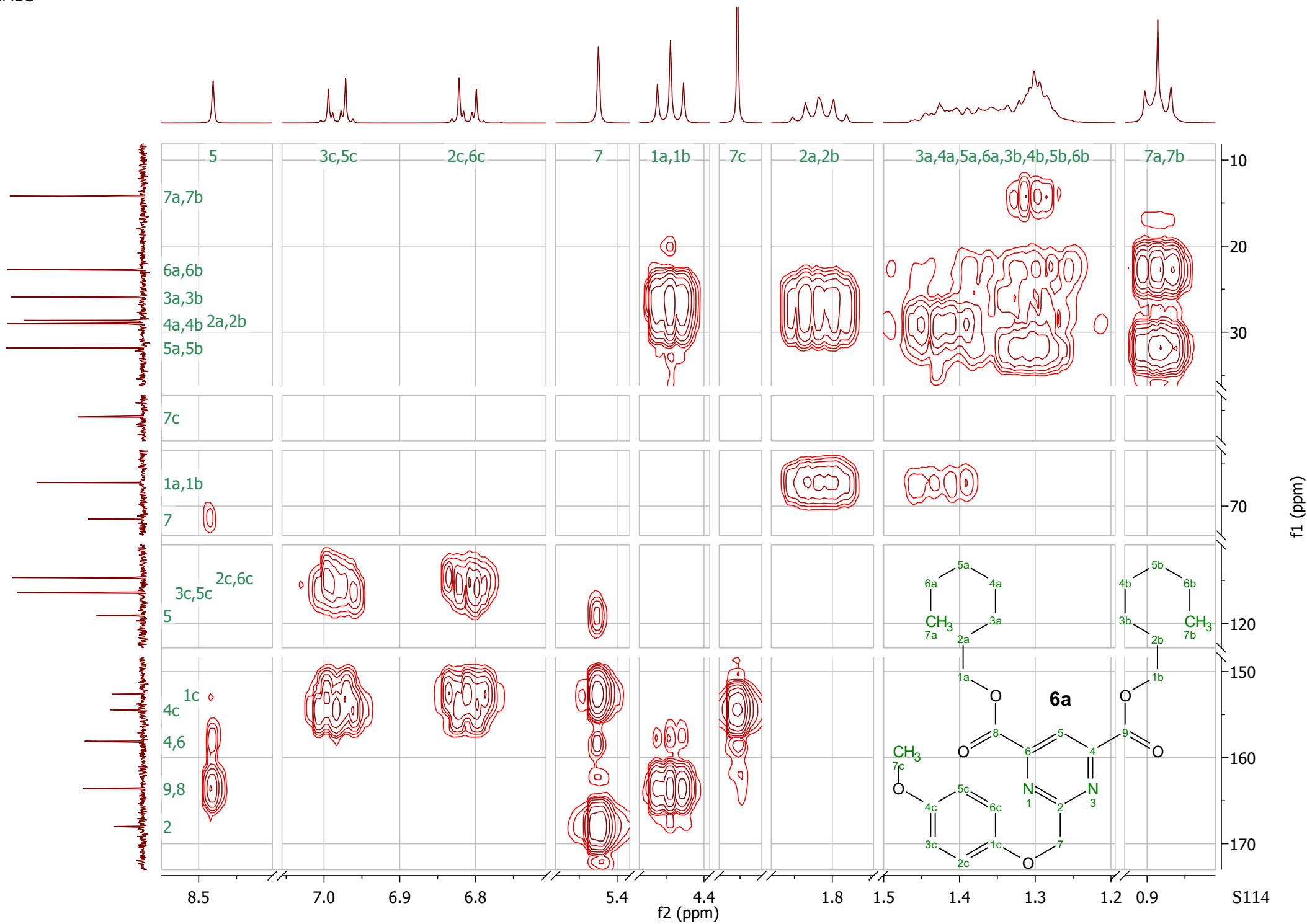
^1H ^1H NMR (400 MHz, CDCl_3) δ 8.48 (app t, $J = 0.6$ Hz, 1H), 7.02 – 6.95 (m, 2H), 6.85 – 6.77 (m, 2H), 5.42 (s, 2H), 4.44 (t, $J = 6.9$ Hz, 4H), 3.75 (s, 3H), 1.82 (quint, $J = 6.9$ Hz, 4H), 1.49 – 1.21 (m, 16H), 0.89 (app t, $J = 7.0$ Hz, 6H).

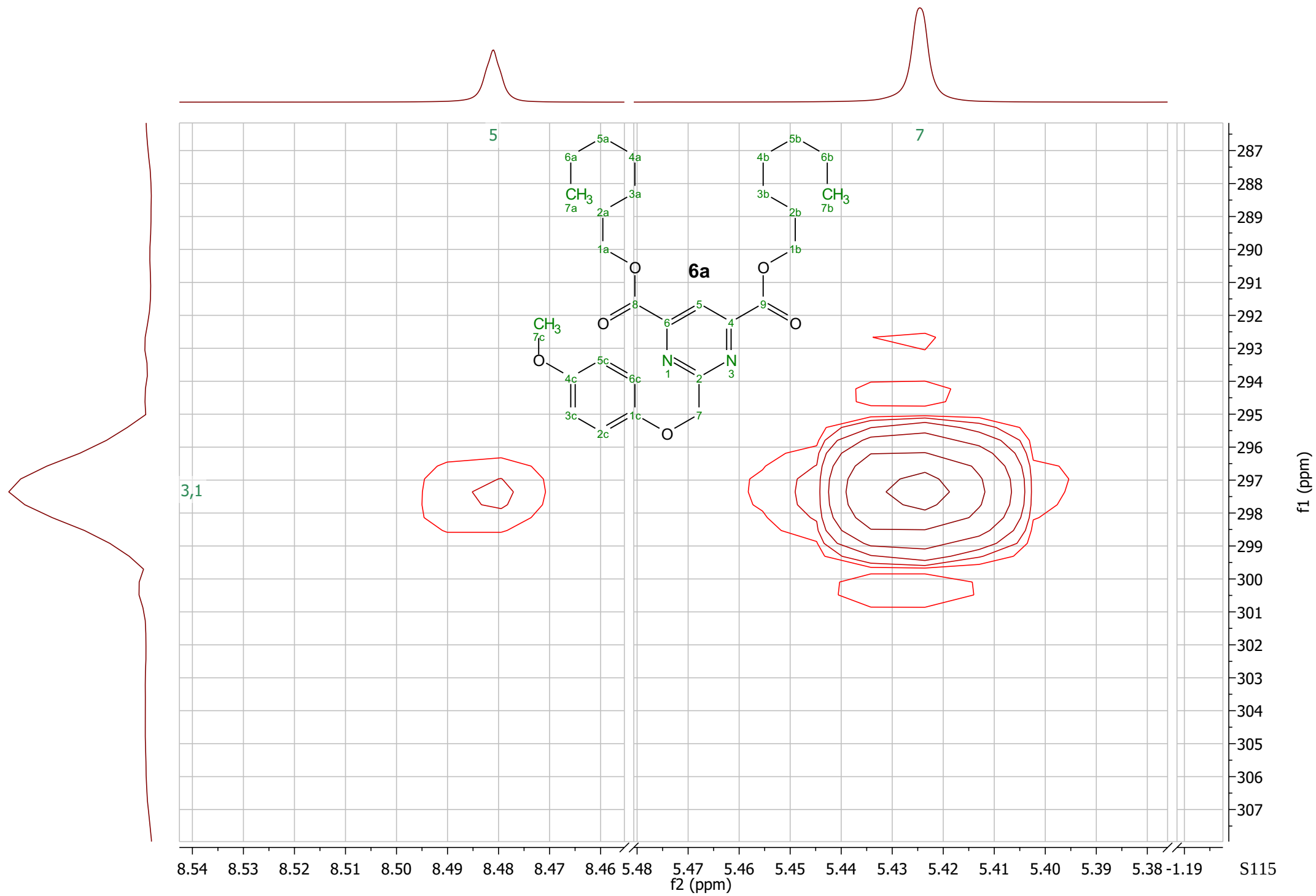


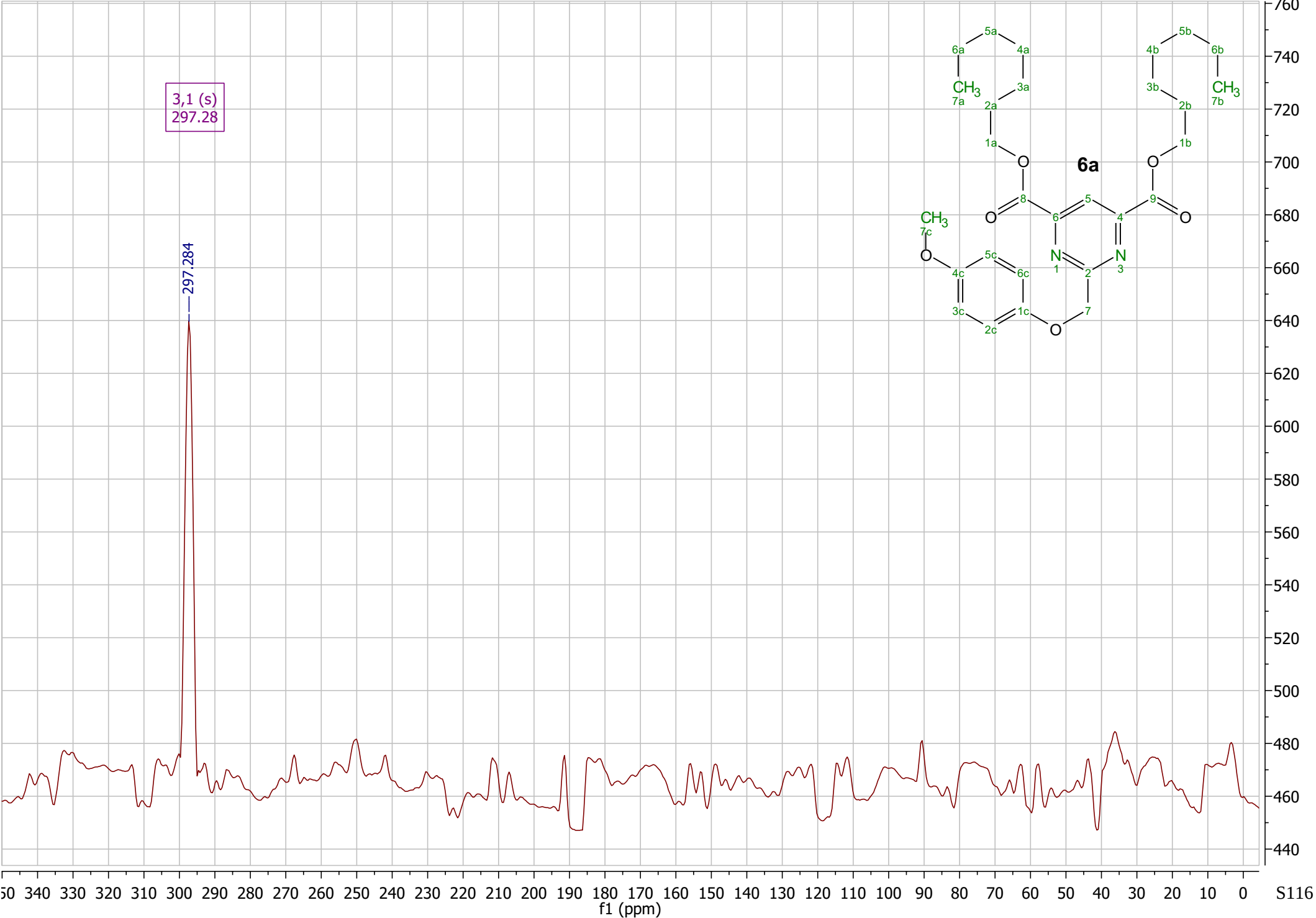
¹³C ¹³C NMR (101 MHz, CDCl₃) δ 168.0, 163.6 (sym, 2C), 158.1 (sym, 2C), 154.4, 152.6, 119.1, 116.4 (sym, 2C), 114.7 (sym, 2C), 71.5, 67.3 (sym, 2C), 55.8, 31.8 (sym, 2C), 29.0 (sym, 2C), 28.6 (sym, 2C), 25.9 (sym, 2C), 22.7 (sym, 2C), 14.2 (sym, 2C).



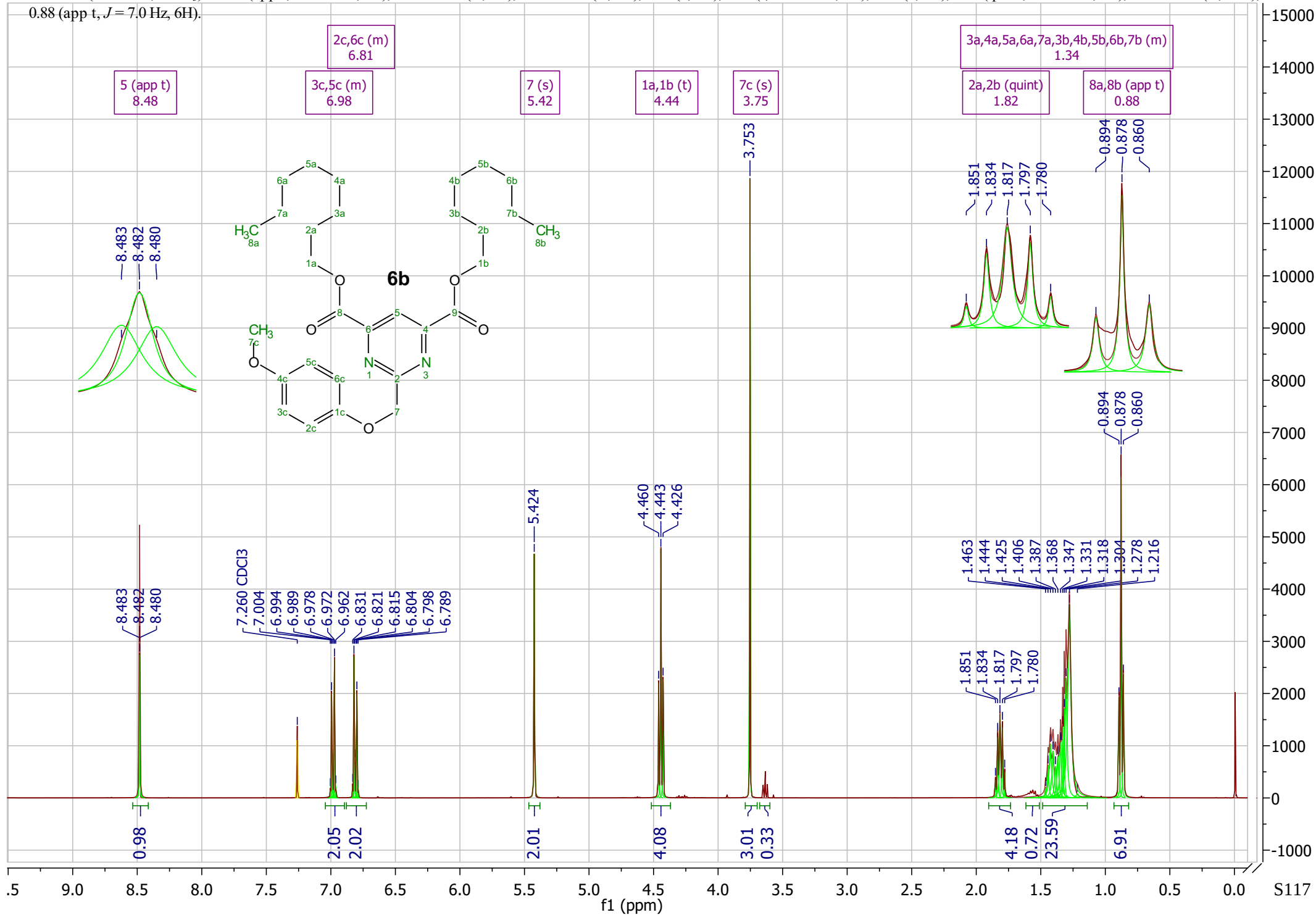




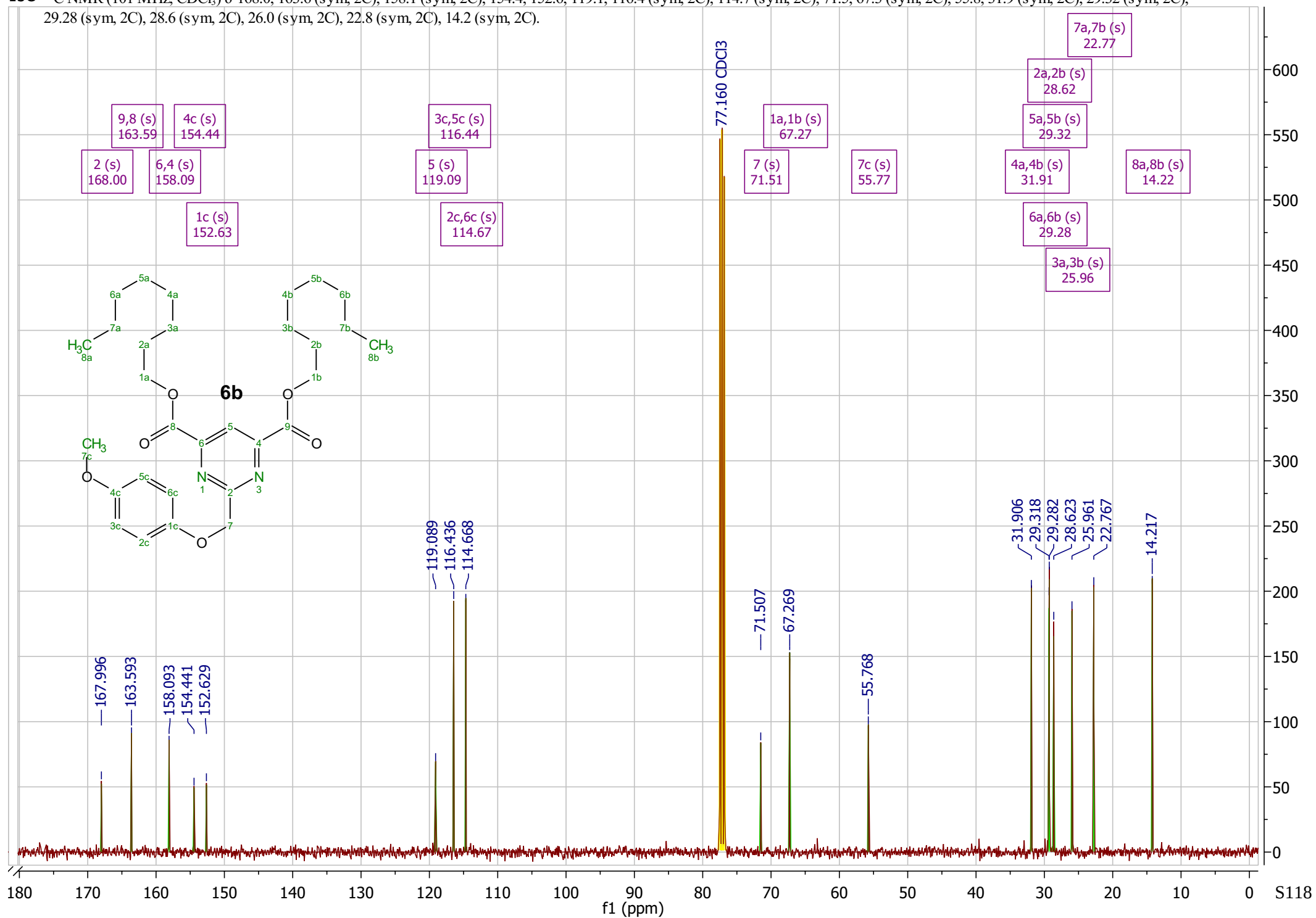


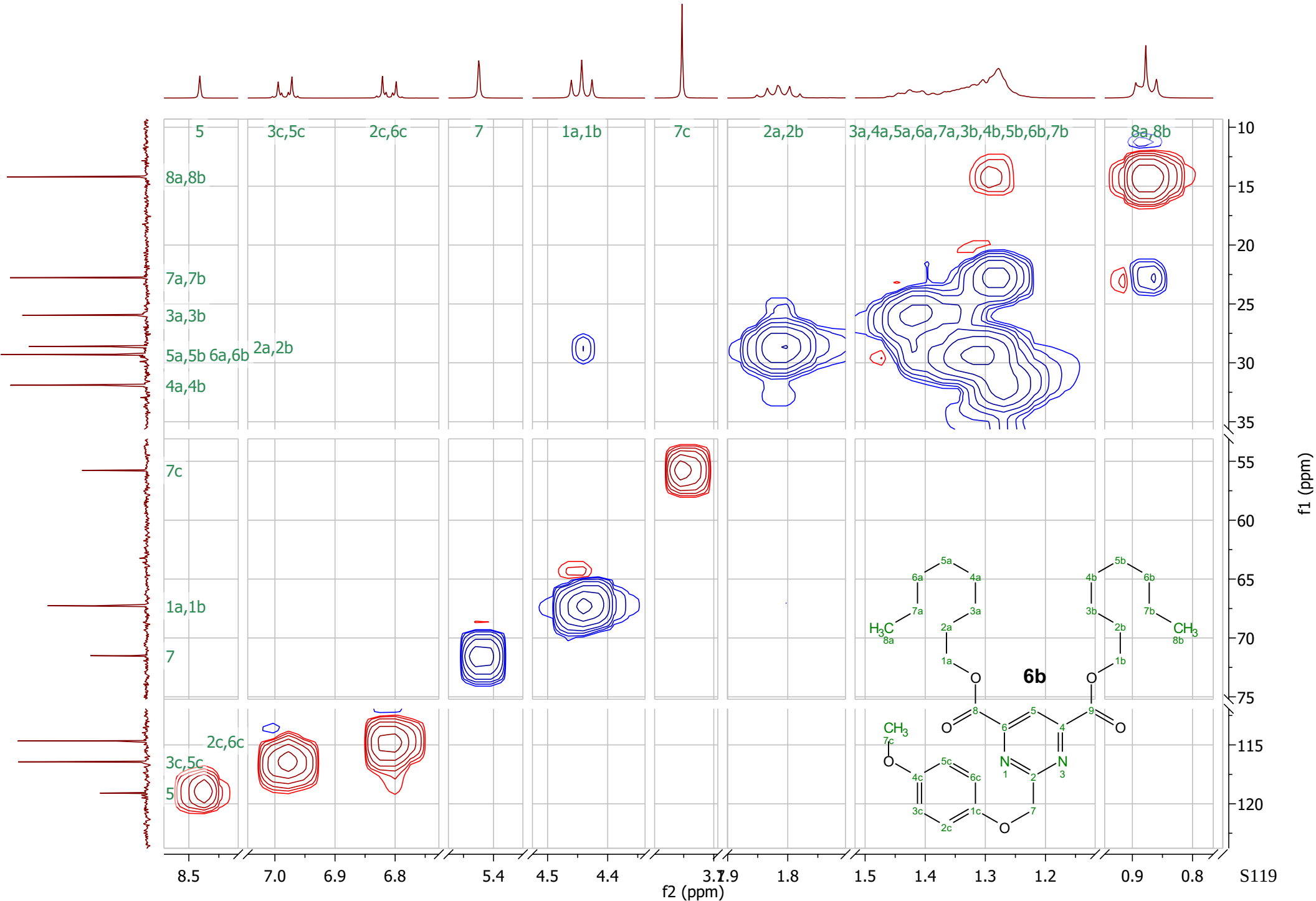


^1H NMR (400 MHz, CDCl_3) δ 8.48 (app t, $J = 0.6$ Hz, 1H), 7.04 – 6.89 (m, 2H), 6.88 – 6.73 (m, 2H), 5.42 (s, 2H), 4.44 (t, $J = 6.9$ Hz, 4H), 3.75 (s, 3H), 1.82 (quint, $J = 6.9$ Hz, 4H), 1.49 – 1.14 (m, 20H), 0.88 (app t, $J = 7.0$ Hz, 6H).

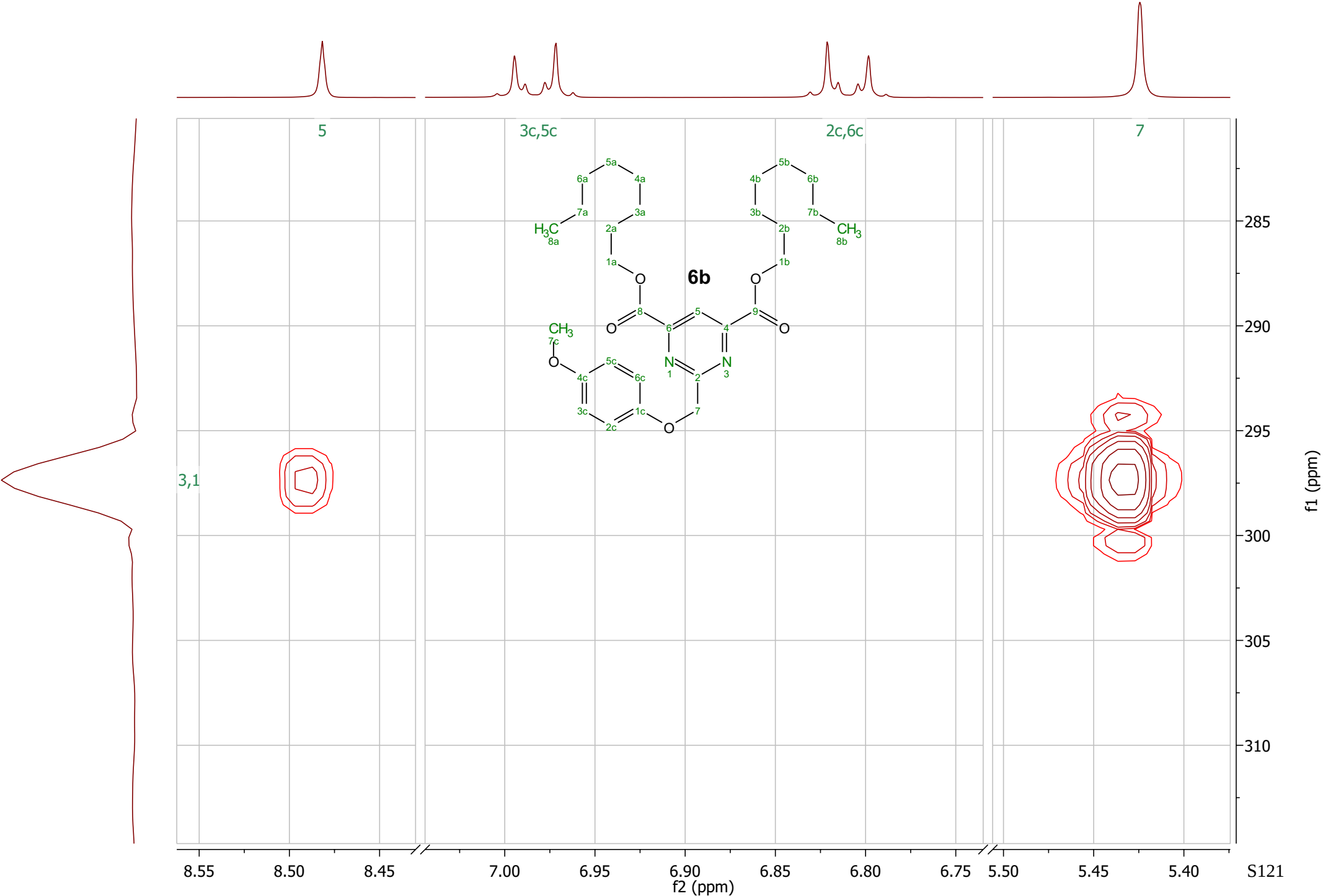


¹³C ¹³C NMR (101 MHz, CDCl₃) δ 168.0, 163.6 (sym, 2C), 158.1 (sym, 2C), 154.4, 152.6, 119.1, 116.4 (sym, 2C), 114.7 (sym, 2C), 71.5, 67.3 (sym, 2C), 55.8, 31.9 (sym, 2C), 29.32 (sym, 2C), 29.28 (sym, 2C), 28.6 (sym, 2C), 26.0 (sym, 2C), 22.8 (sym, 2C), 14.2 (sym, 2C).

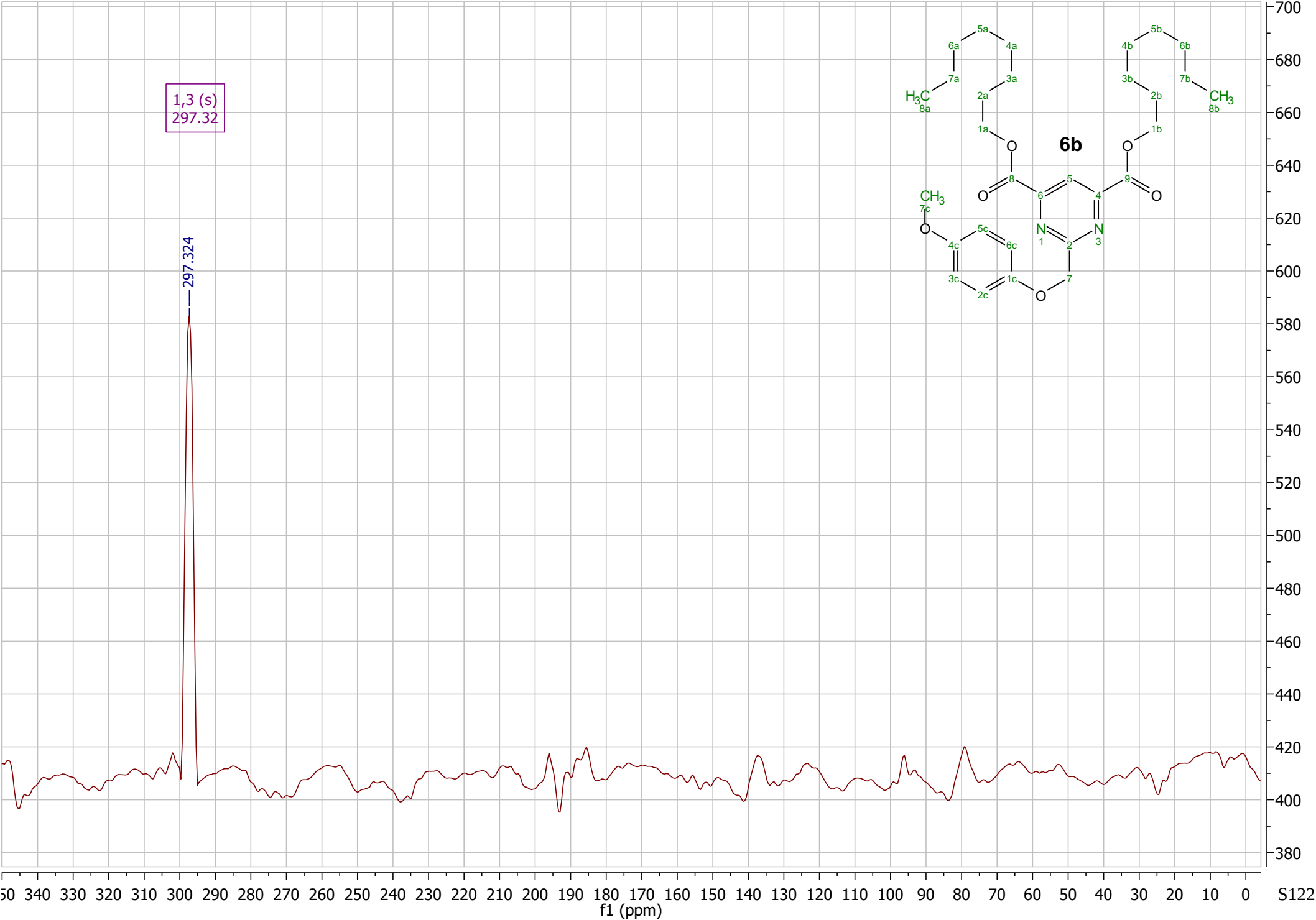




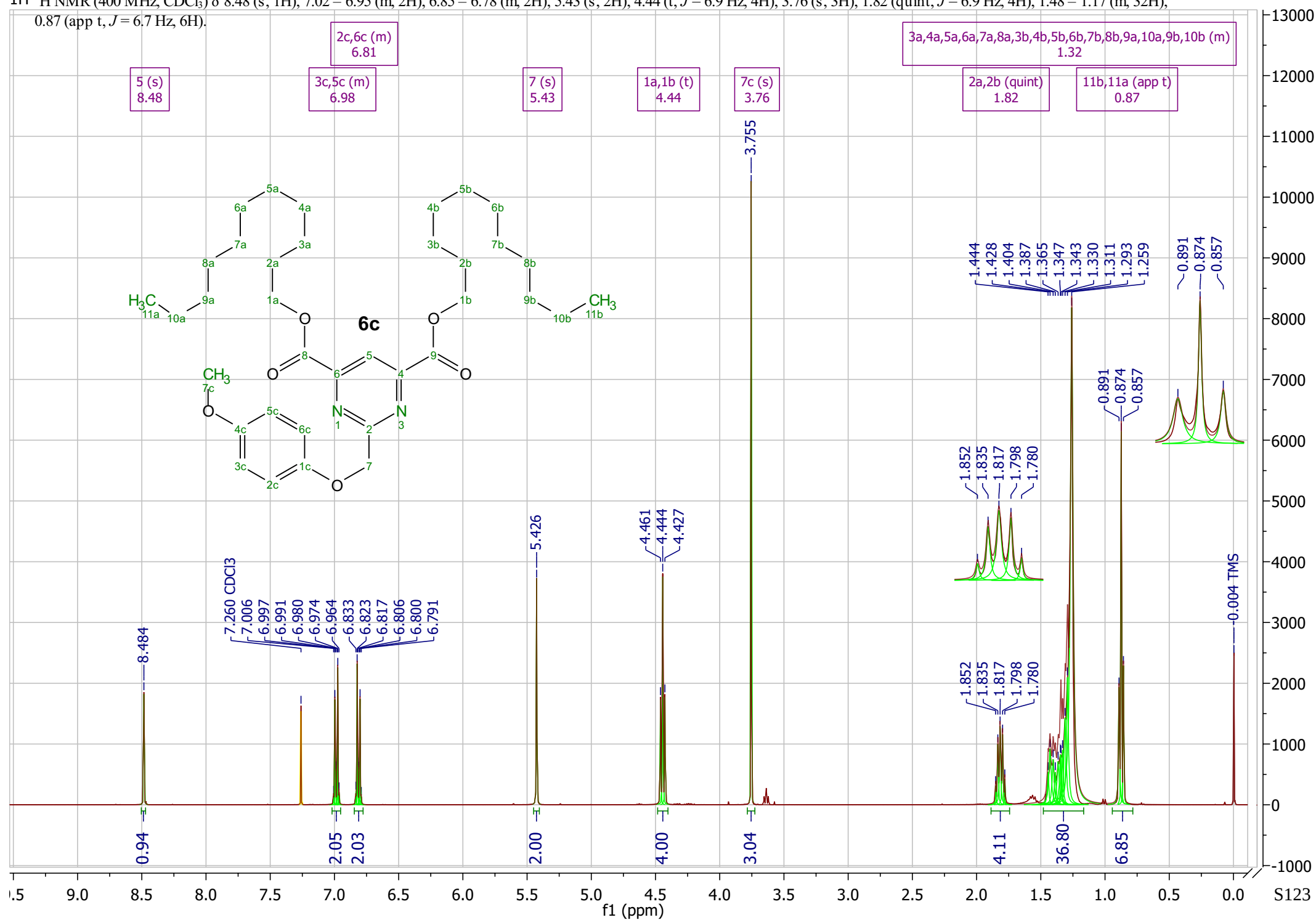
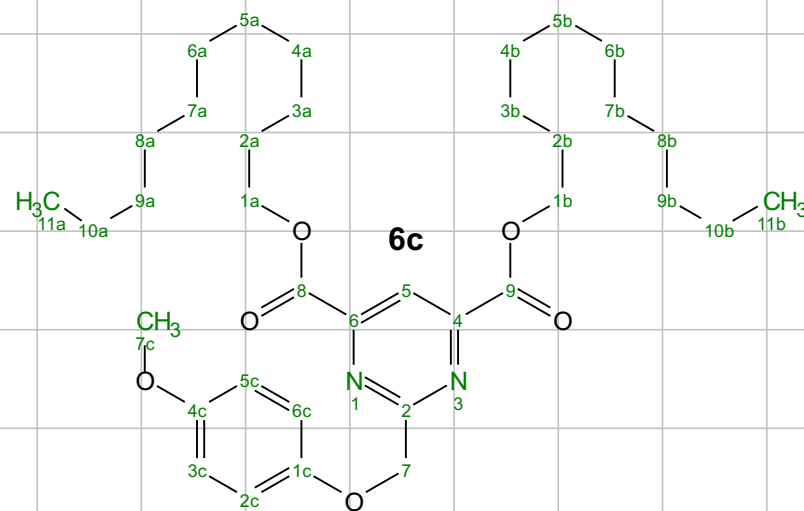




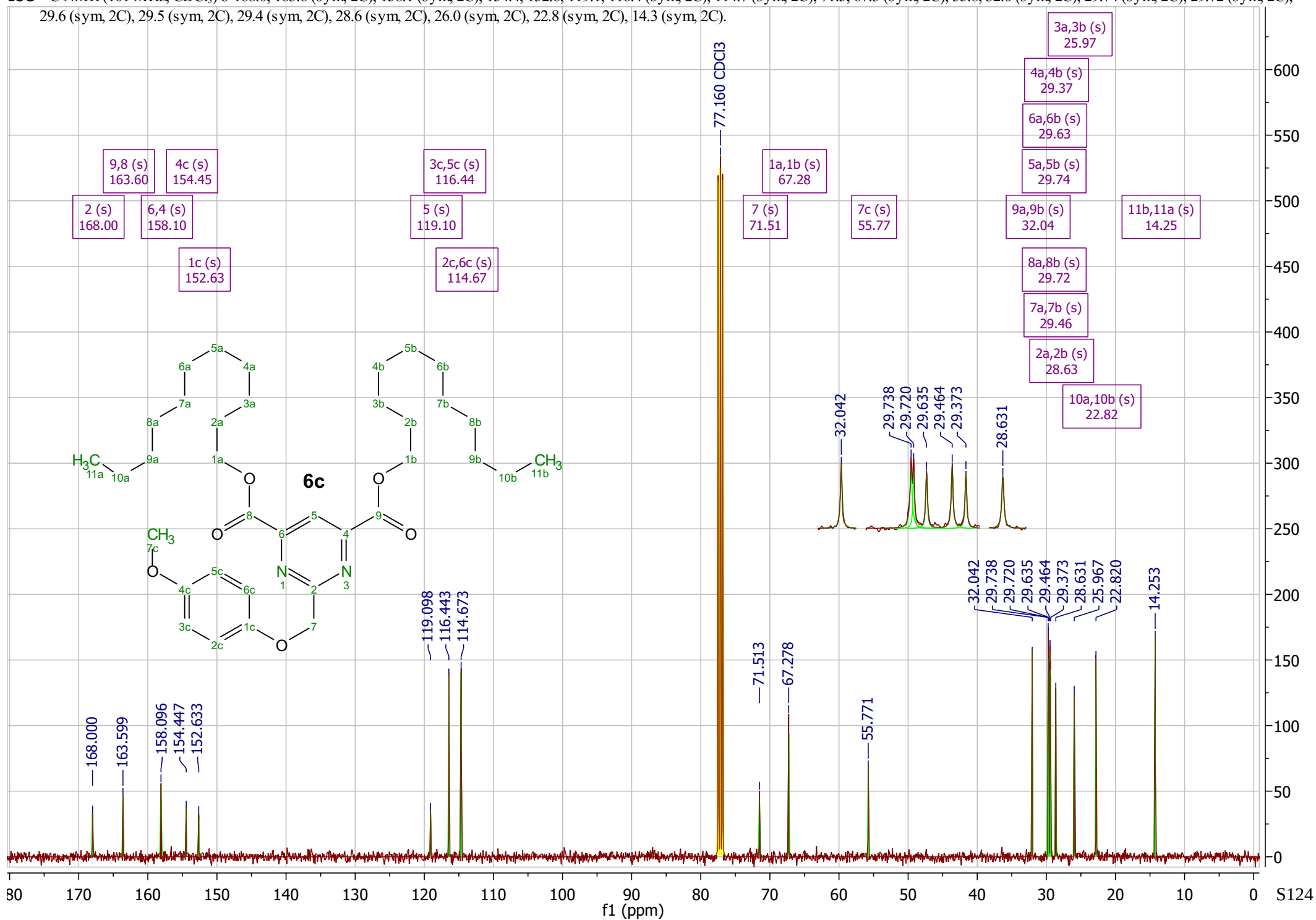
15N HMBC f1 Projection ¹⁵N NMR (41 MHz, CDCl₃) δ 297.32.

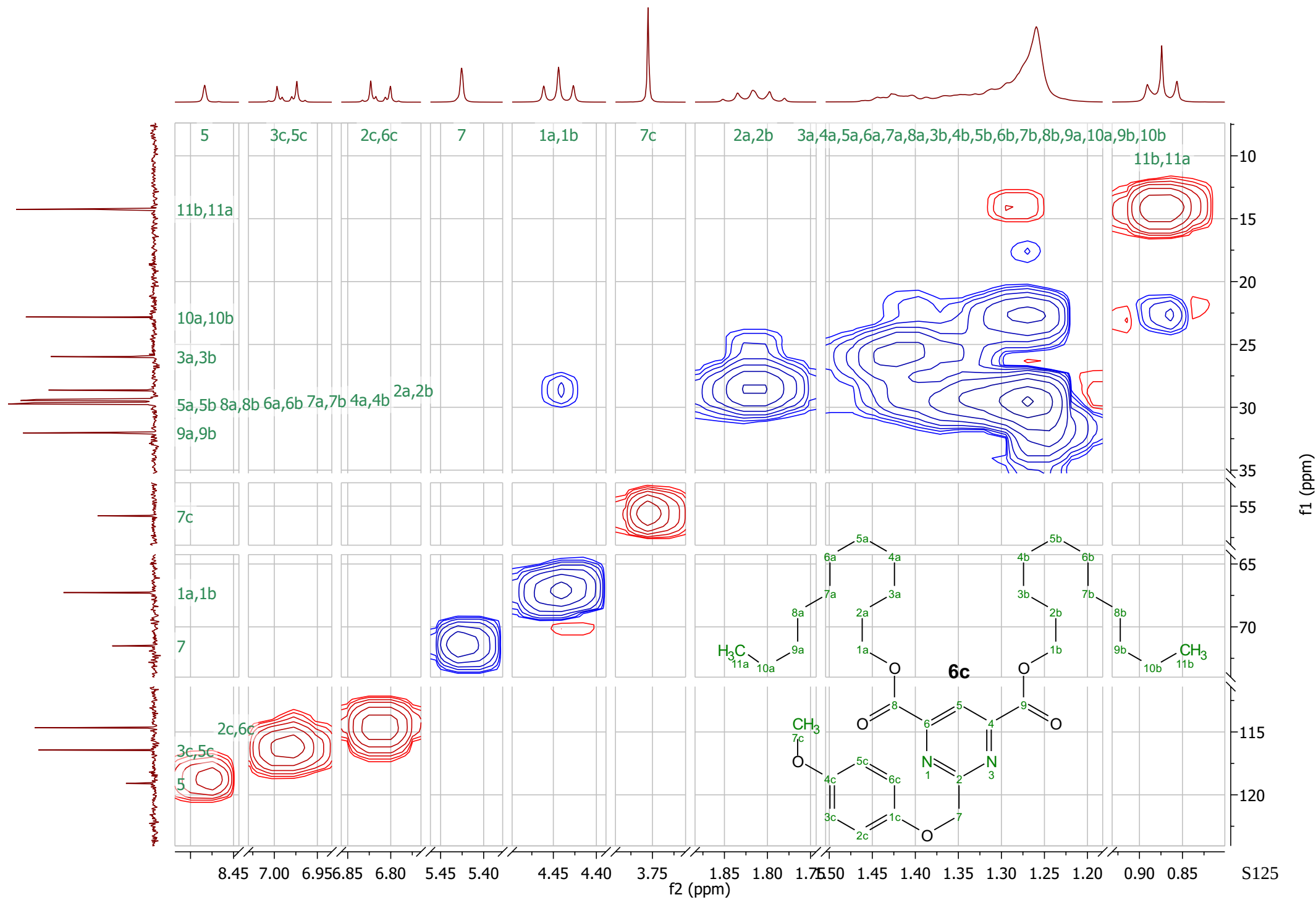


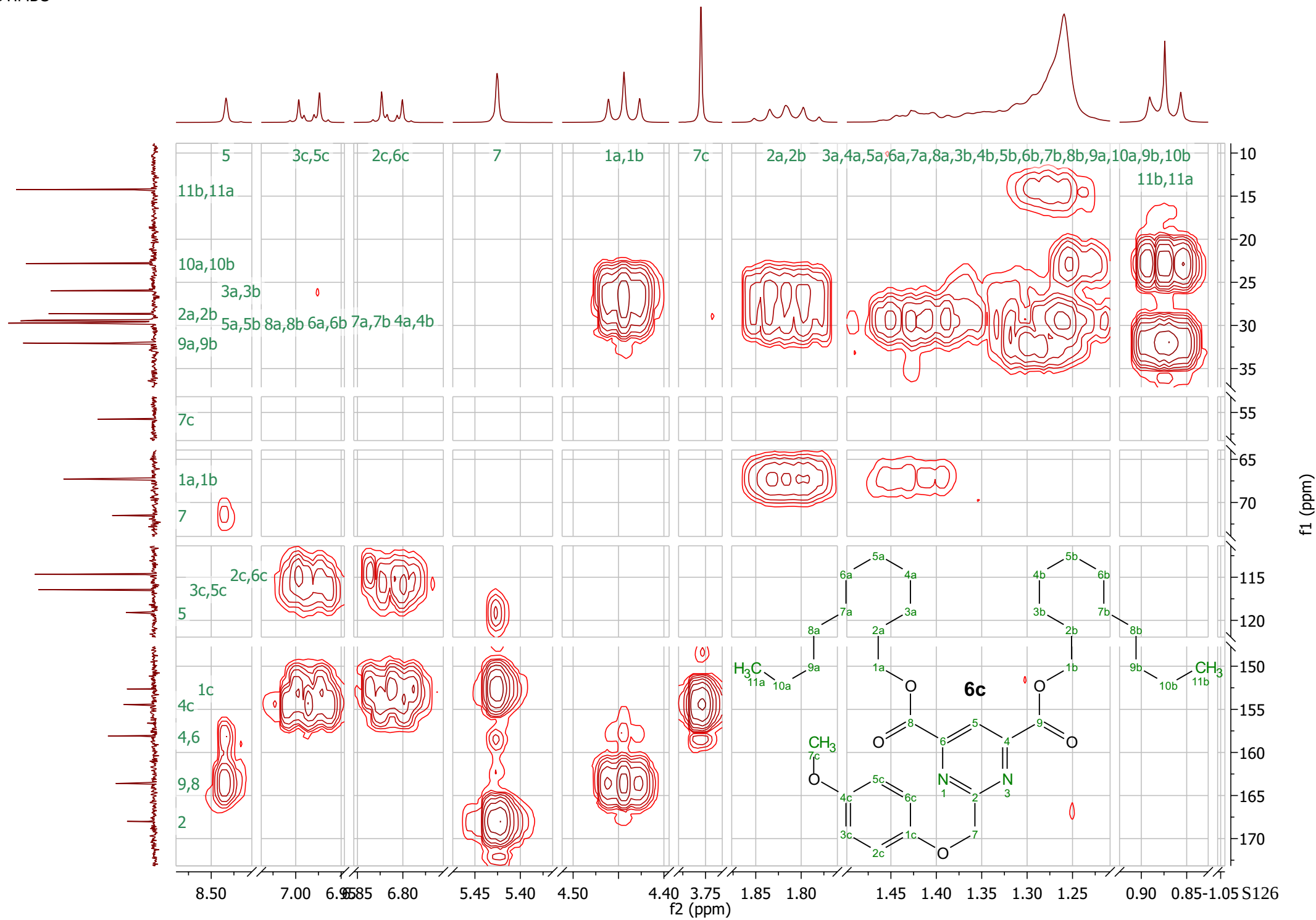
^1H NMR (400 MHz, CDCl_3) δ 8.48 (s, 1H), 7.02 – 6.95 (m, 2H), 6.85 – 6.78 (m, 2H), 5.43 (s, 2H), 4.44 (t, $J = 6.9$ Hz, 4H), 3.76 (s, 3H), 1.82 (quint, $J = 6.9$ Hz, 4H), 1.48 – 1.17 (m, 32H), 0.87 (app t, $J = 6.7$ Hz, 6H).

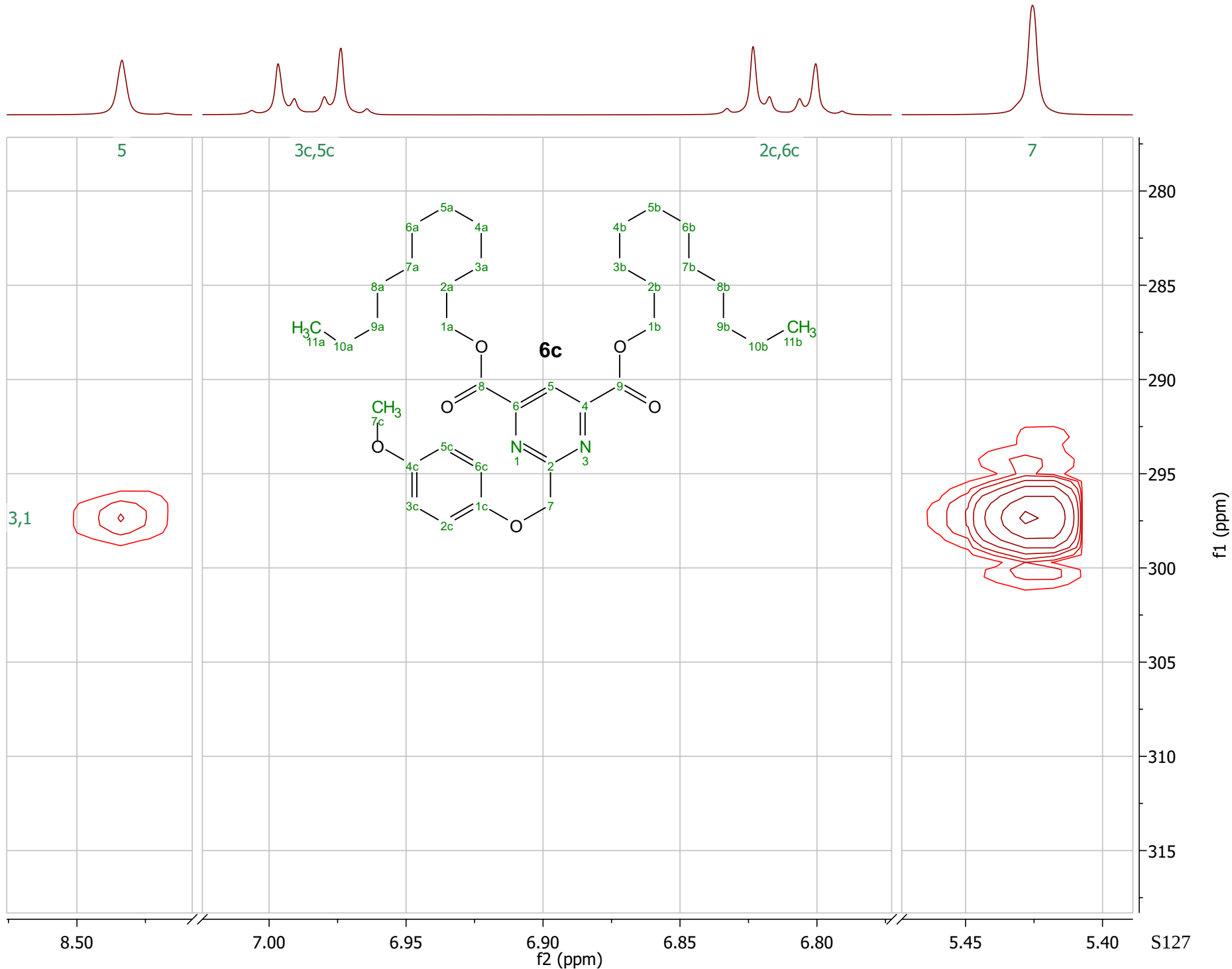


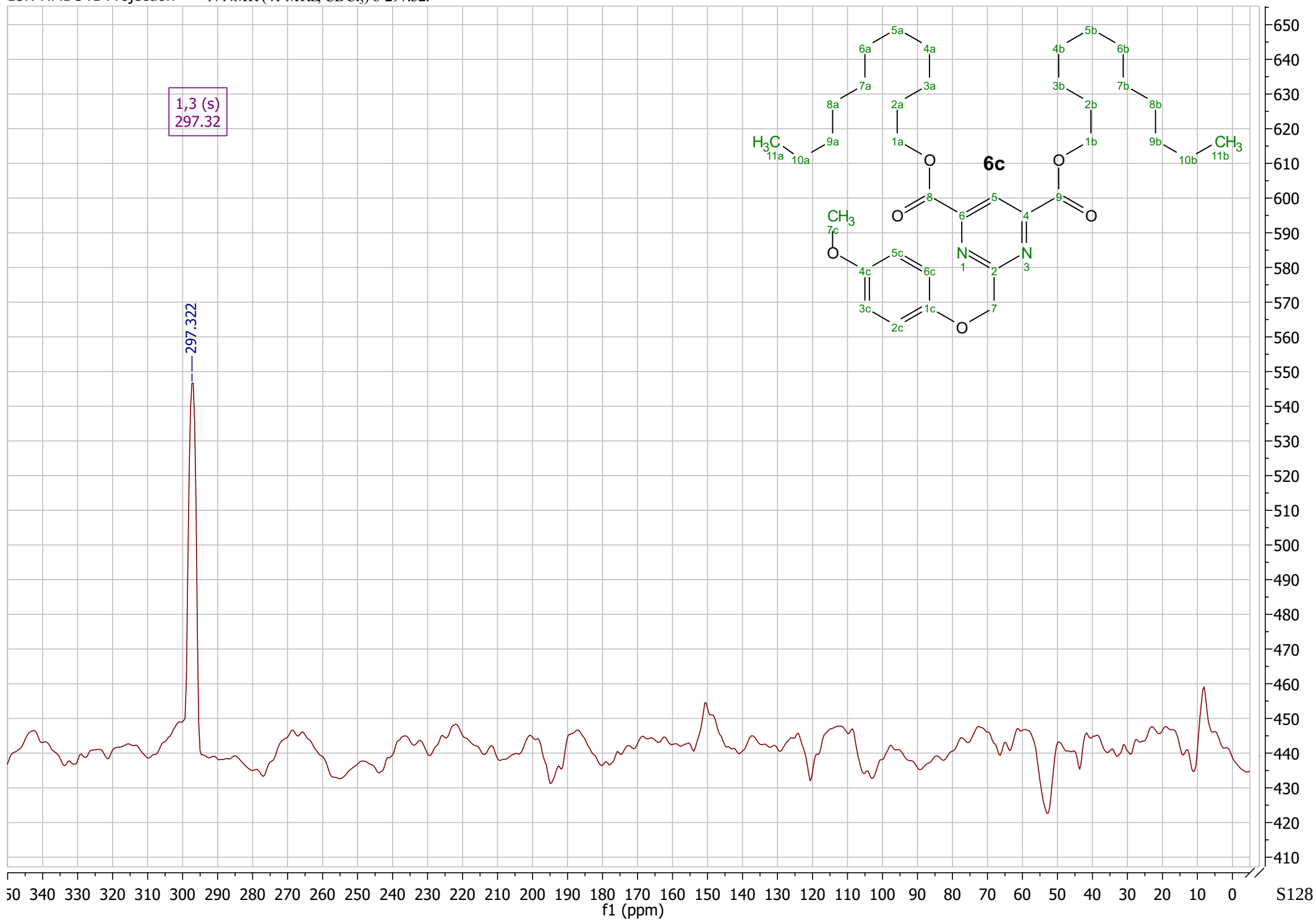
¹³C ¹³C NMR (101 MHz, CDCl₃) δ 168.0, 163.6 (sym, 2C), 158.1 (sym, 2C), 154.4, 152.6, 119.1, 116.4 (sym, 2C), 114.7 (sym, 2C), 71.5, 67.3 (sym, 2C), 55.8, 32.0 (sym, 2C), 29.74 (sym, 2C), 29.72 (sym, 2C), 29.6 (sym, 2C), 29.5 (sym, 2C), 29.4 (sym, 2C), 28.6 (sym, 2C), 26.0 (sym, 2C), 22.8 (sym, 2C), 14.3 (sym, 2C).



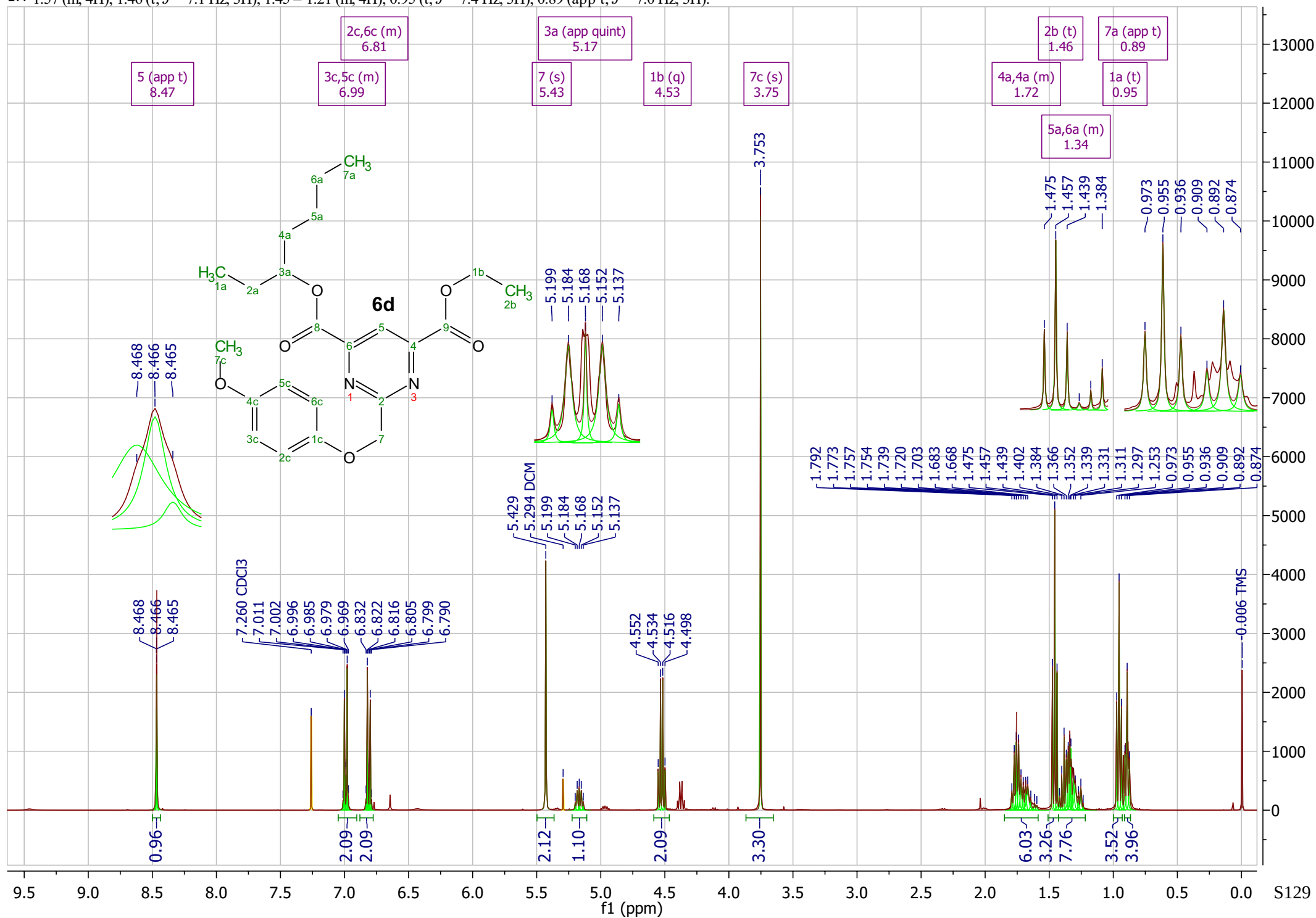




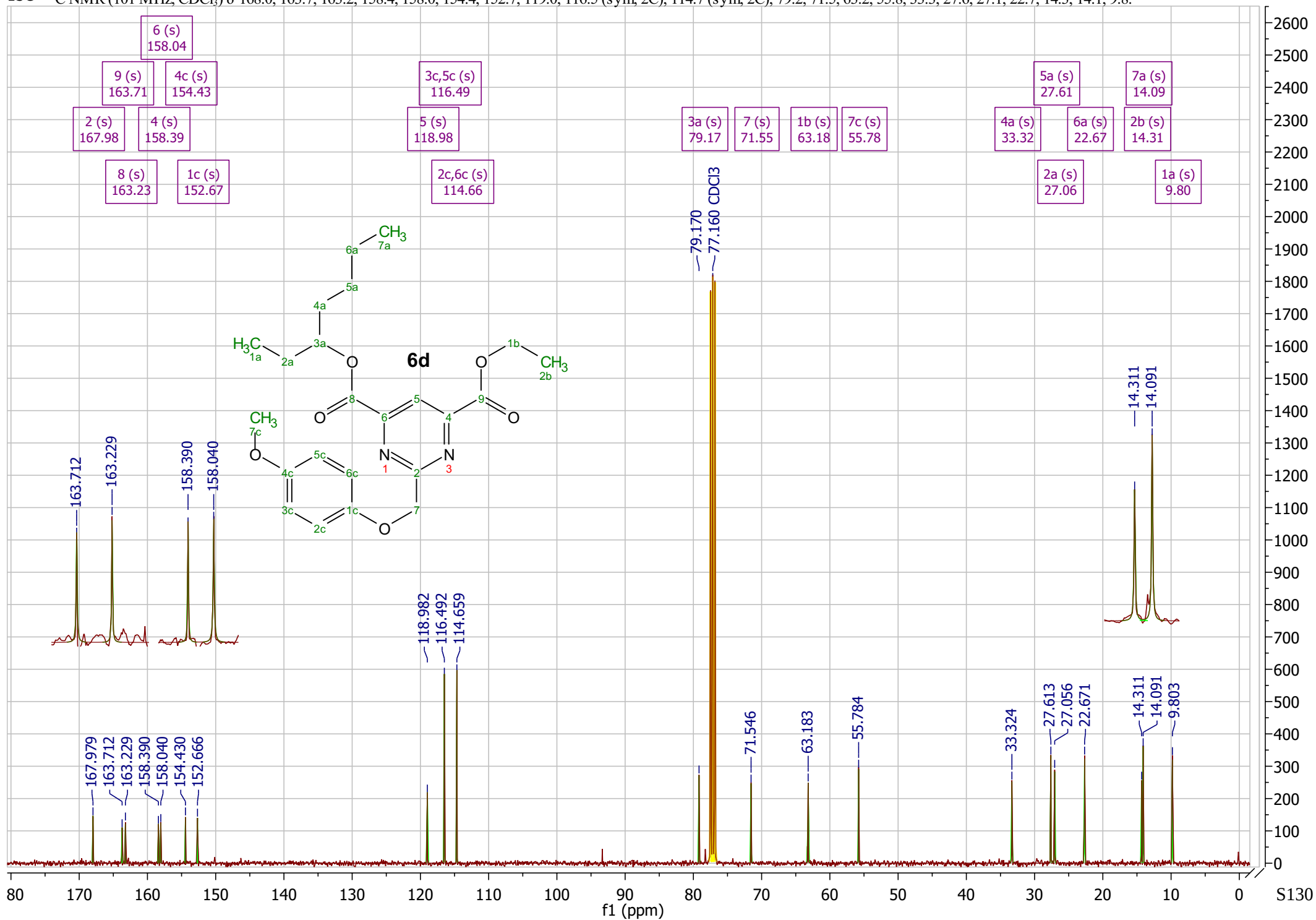


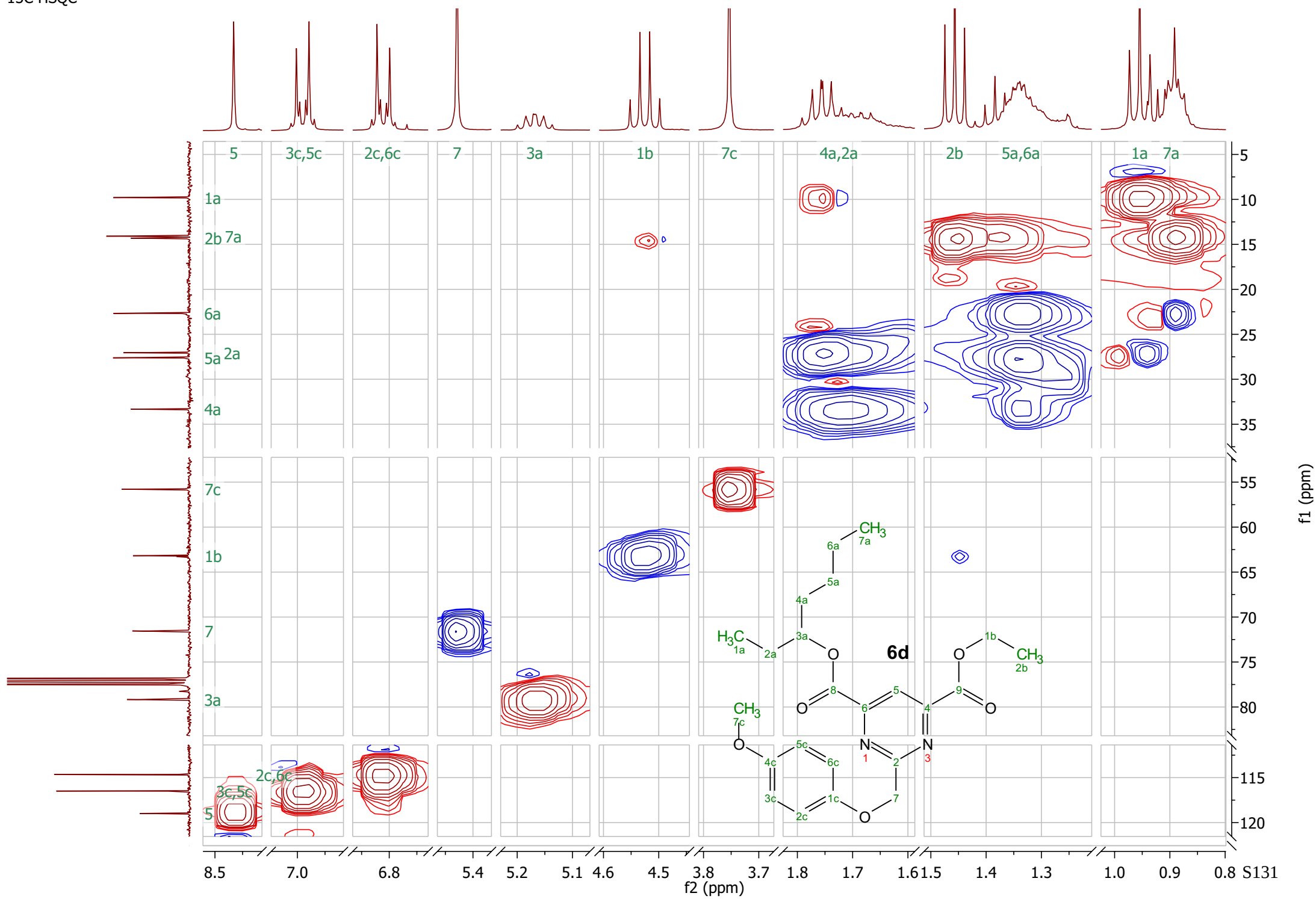


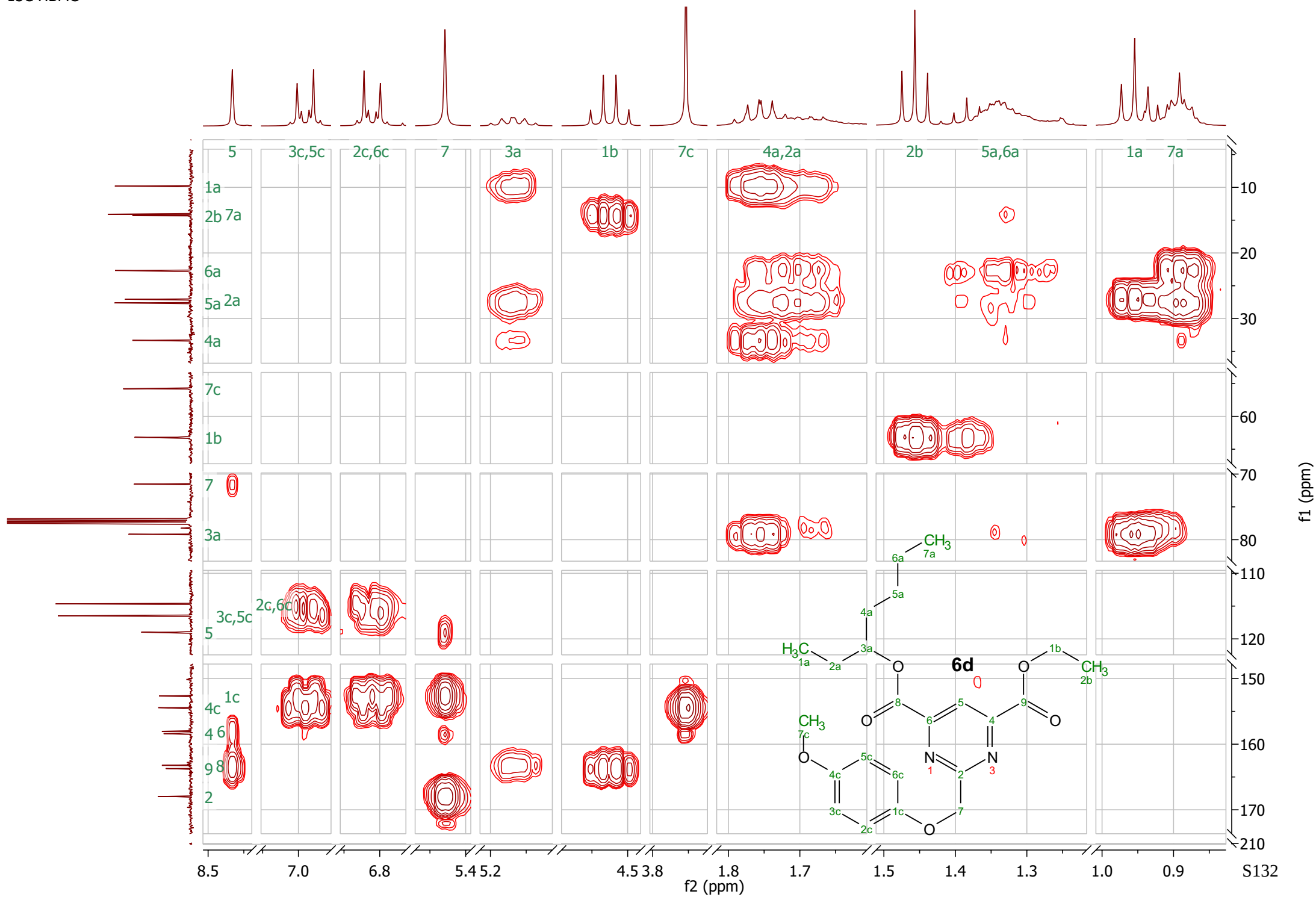
¹H NMR (400 MHz, CDCl₃) δ 8.47 (app t, *J* = 0.6 Hz, 1H), 7.05 – 6.90 (m, 2H), 6.88 – 6.76 (m, 2H), 5.43 (s, 2H), 5.17 (app quint, *J* = 6.1 Hz, 1H), 4.53 (q, *J* = 7.1 Hz, 2H), 3.75 (s, 3H), 1.85 – 1.57 (m, 4H), 1.46 (t, *J* = 7.1 Hz, 3H), 1.45 – 1.21 (m, 4H), 0.95 (t, *J* = 7.4 Hz, 3H), 0.89 (app t, *J* = 7.0 Hz, 3H).



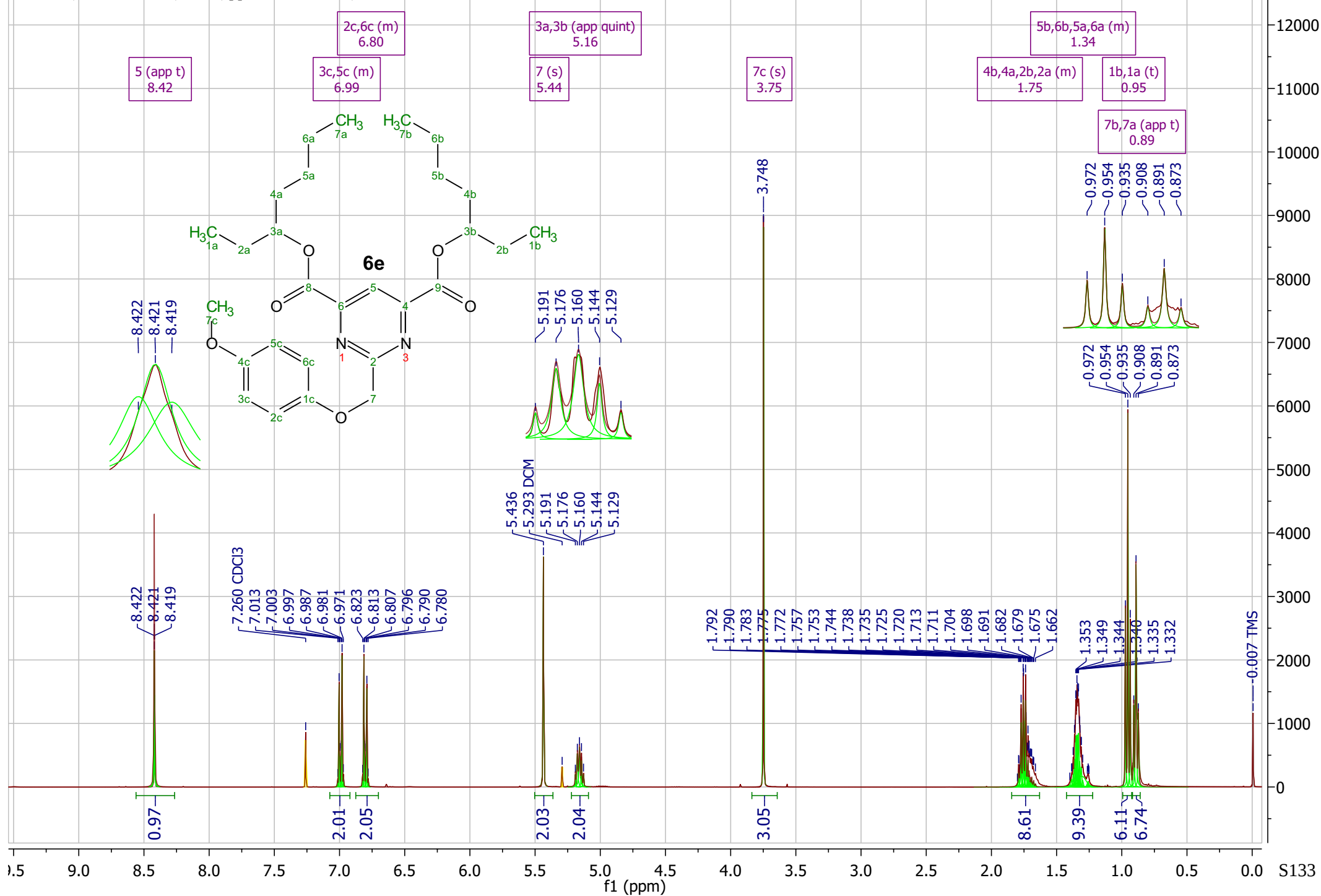
^{13}C ^{13}C NMR (101 MHz, CDCl_3) δ 168.0, 163.7, 163.2, 158.4, 158.0, 154.4, 152.7, 119.0, 116.5 (sym, 2C), 114.7 (sym, 2C), 79.2, 71.5, 63.2, 55.8, 33.3, 27.6, 27.1, 22.7, 14.3, 14.1, 9.8.



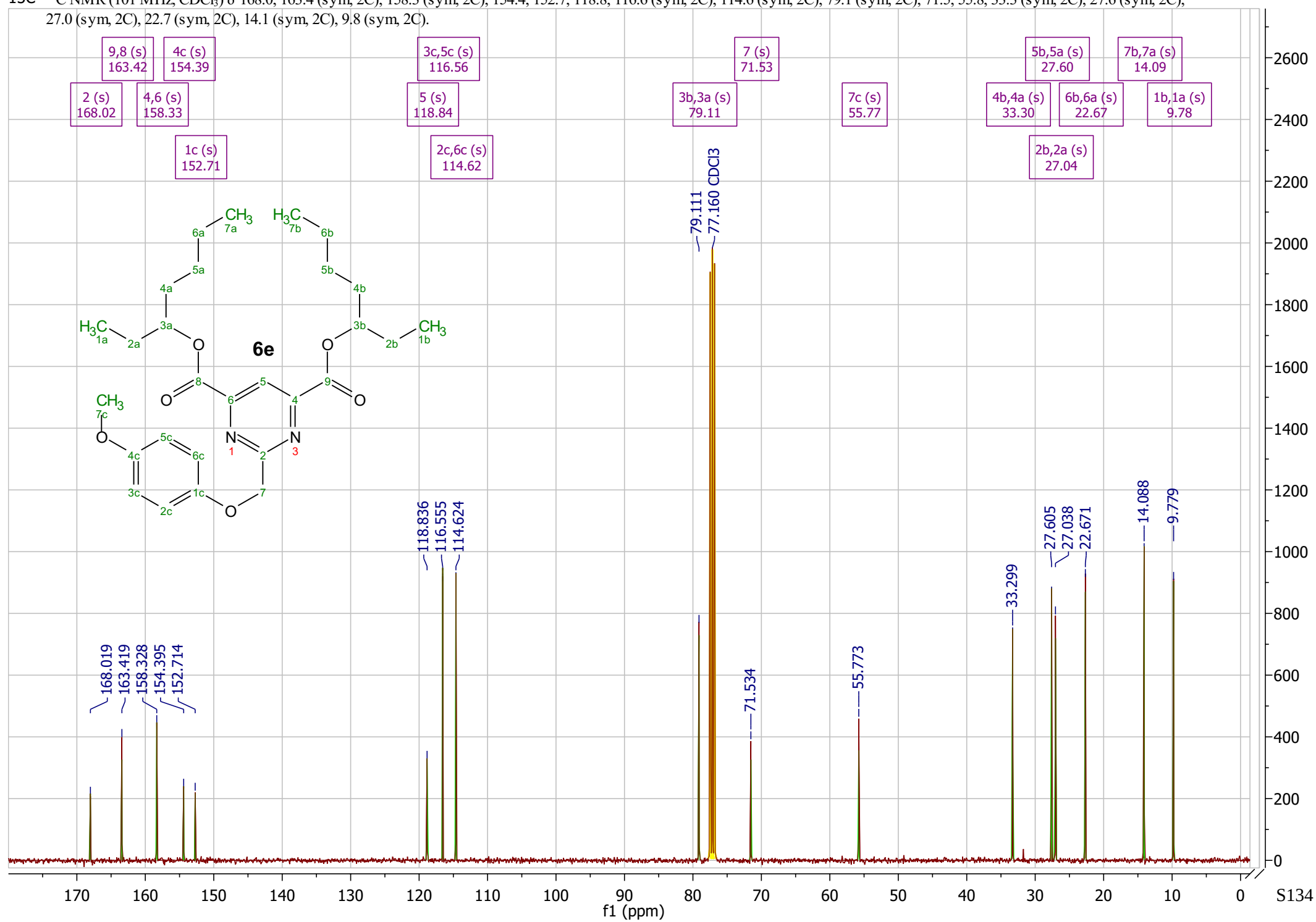


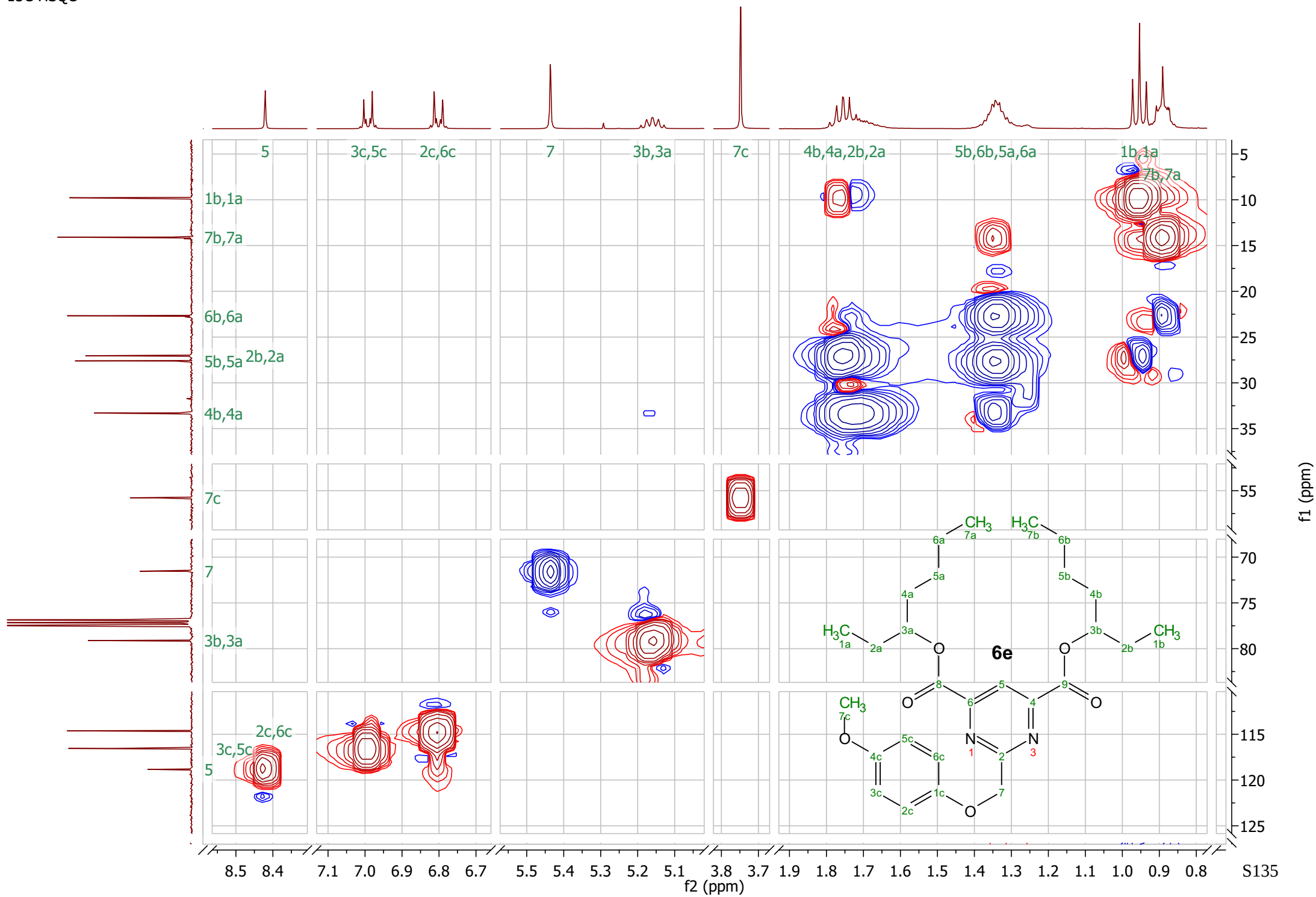


^1H NMR (400 MHz, CDCl_3) δ 8.42 (app t, $J = 0.6$ Hz, 1H), 7.07 – 6.92 (m, 2H), 6.88 – 6.70 (m, 2H), 5.44 (s, 2H), 5.16 (app quint, $J = 6.1$ Hz, 2H), 3.75 (s, 3H), 1.92 – 1.55 (m, 8H), 1.42 – 1.22 (m, 8H), 0.95 (t, $J = 7.4$ Hz, 6H), 0.89 (app t, $J = 7.1$ Hz, 6H).

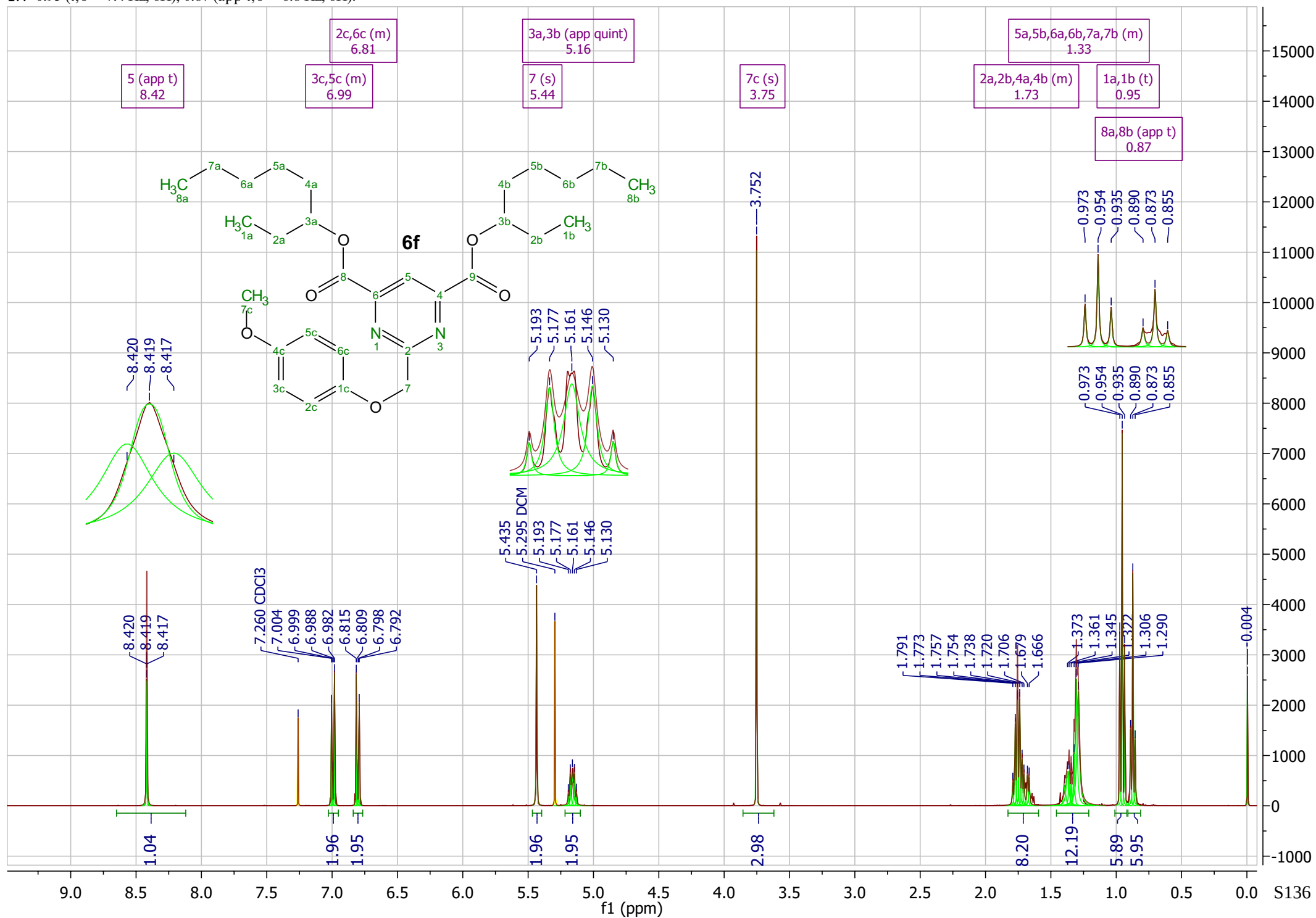


13C ¹³C NMR (101 MHz, CDCl₃) δ 168.0, 163.4 (sym, 2C), 158.3 (sym, 2C), 154.4, 152.7, 118.8, 116.6 (sym, 2C), 114.6 (sym, 2C), 79.1 (sym, 2C), 71.5, 55.8, 33.3 (sym, 2C), 27.6 (sym, 2C), 27.0 (sym, 2C), 22.7 (sym, 2C), 14.1 (sym, 2C), 9.8 (sym, 2C).

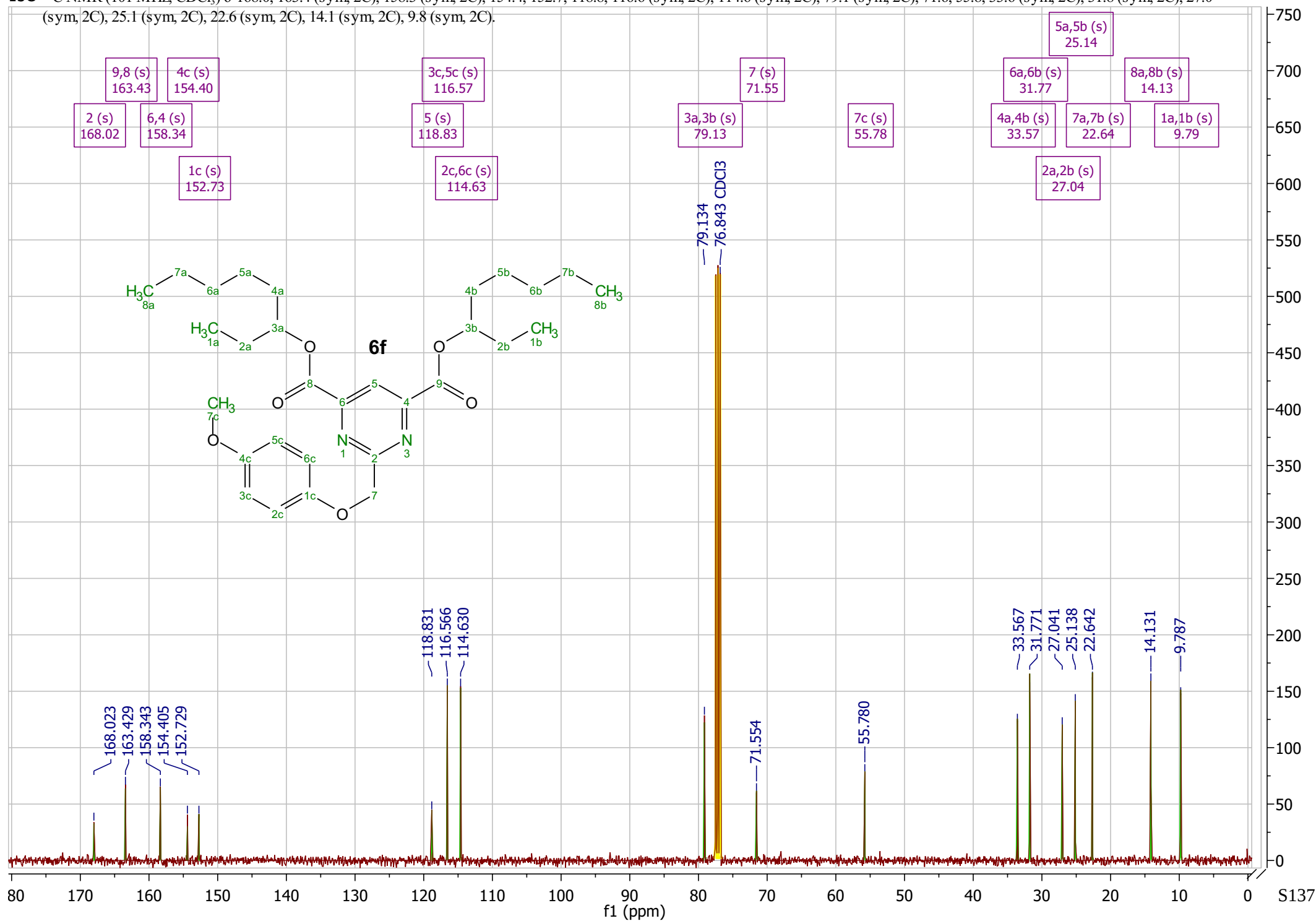


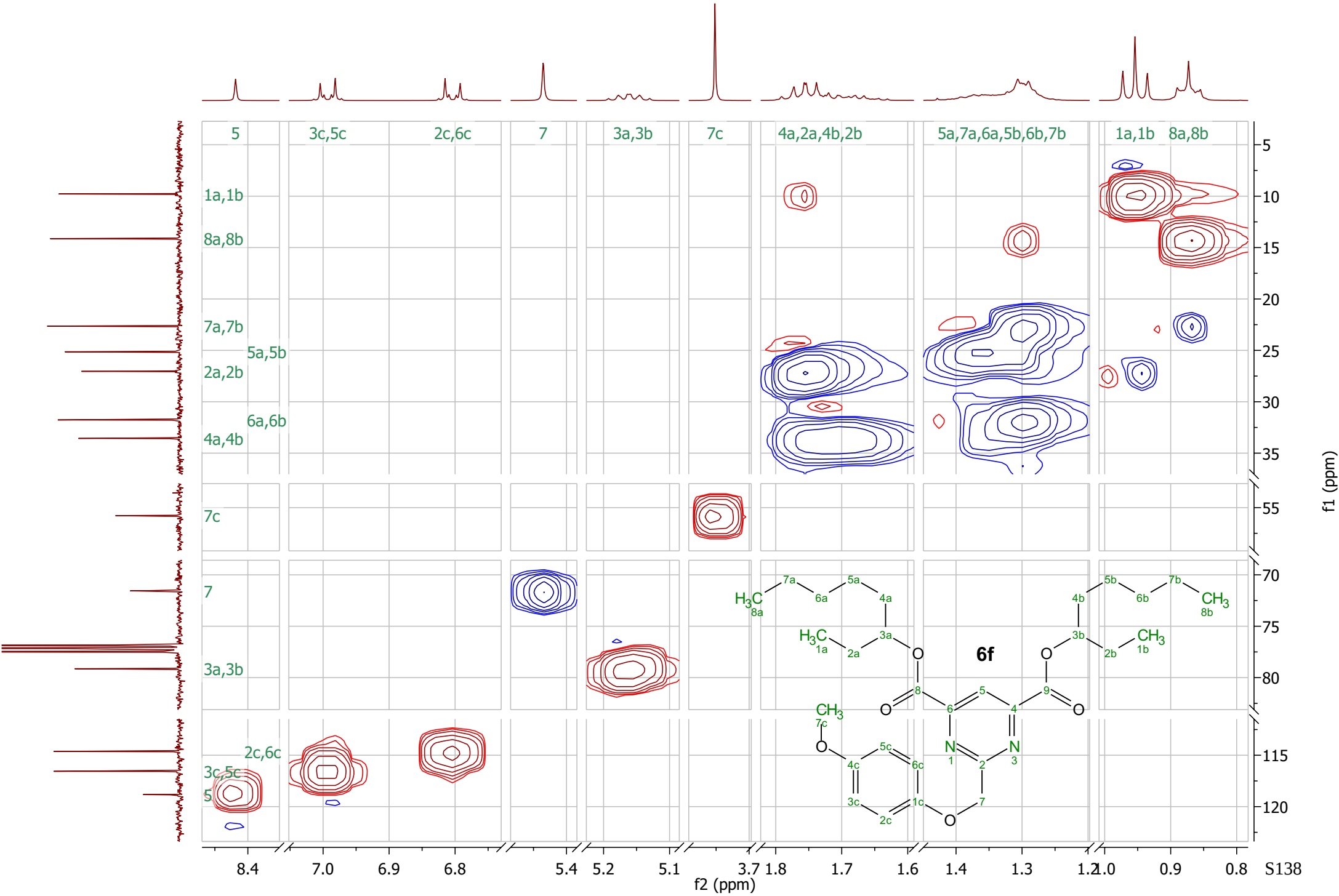


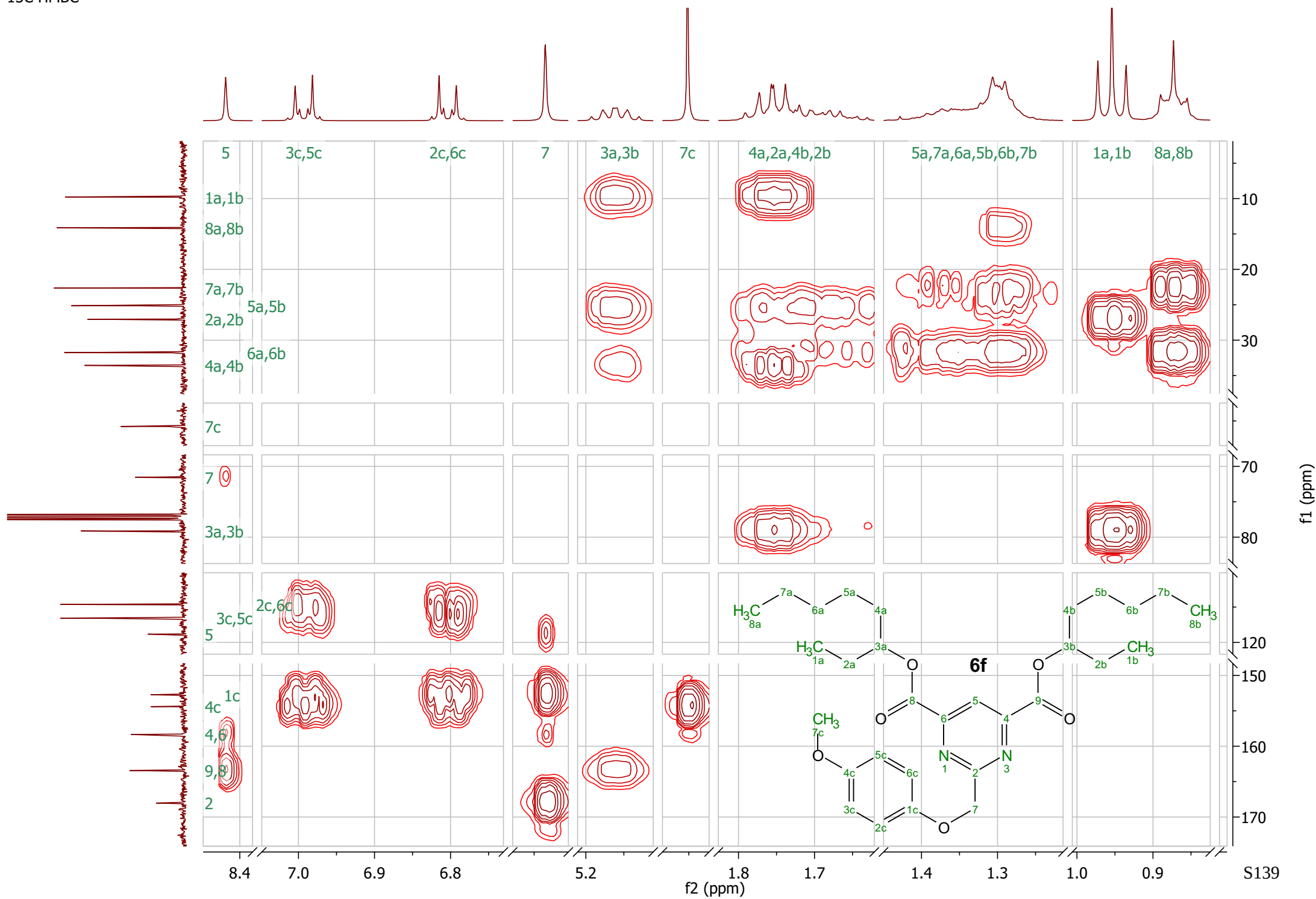
¹H NMR (400 MHz, CDCl₃) δ 8.42 (app t, *J* = 0.6 Hz, 1H), 7.03 – 6.95 (m, 2H), 6.84 – 6.77 (m, 2H), 5.44 (s, 2H), 5.16 (app quint, *J* = 6.2 Hz, 2H), 3.75 (s, 3H), 1.83 – 1.59 (m, 8H), 1.46 – 1.21 (m, 12H), 1H 0.95 (t, *J* = 7.4 Hz, 6H), 0.87 (app t, *J* = 6.8 Hz, 6H).

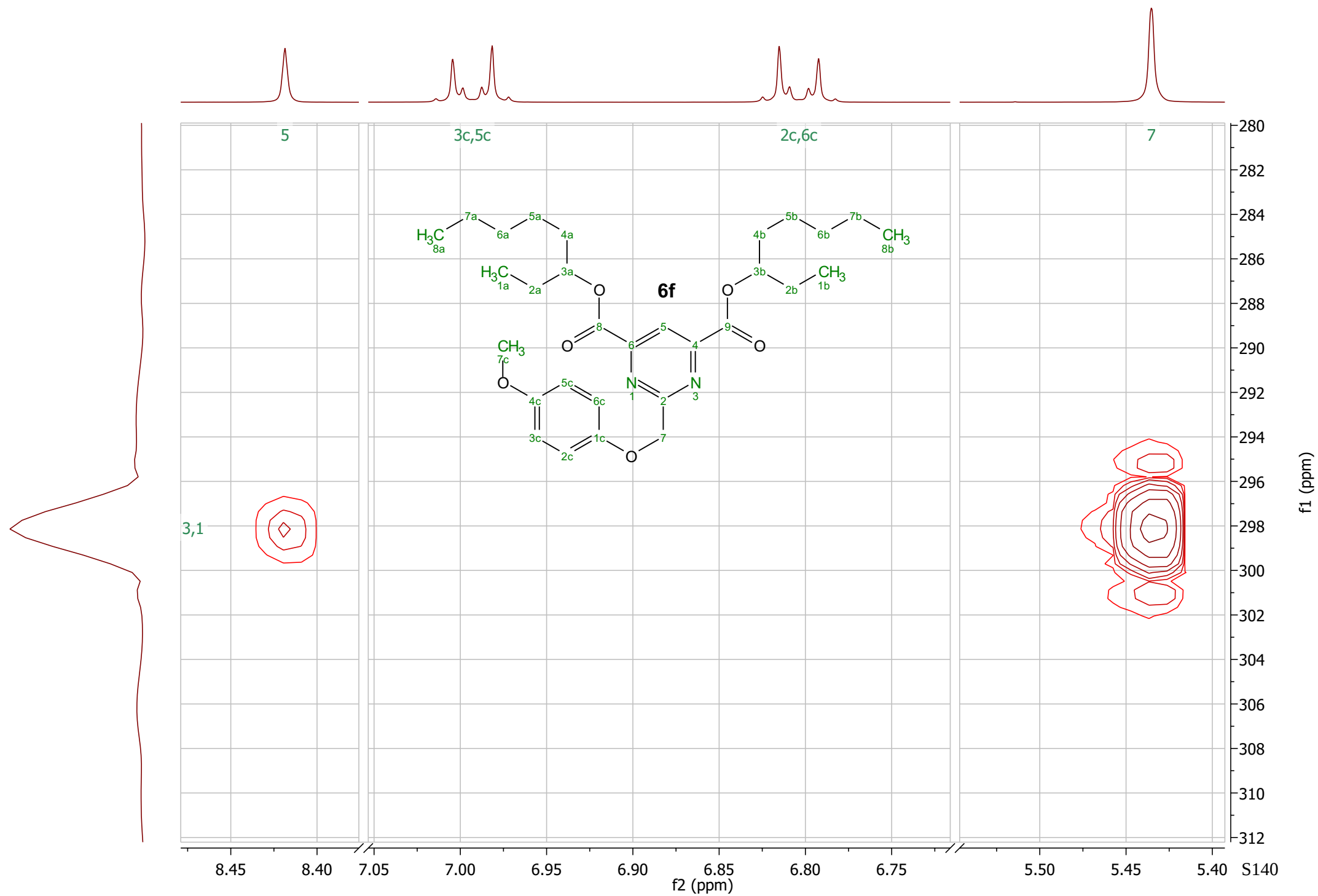


^{13}C NMR (101 MHz, CDCl_3) δ 168.0, 163.4 (sym, 2C), 158.3 (sym, 2C), 154.4, 152.7, 118.8, 116.6 (sym, 2C), 114.6 (sym, 2C), 79.1 (sym, 2C), 71.6, 55.8, 33.6 (sym, 2C), 31.8 (sym, 2C), 27.0 (sym, 2C), 25.1 (sym, 2C), 22.6 (sym, 2C), 14.1 (sym, 2C), 9.8 (sym, 2C).



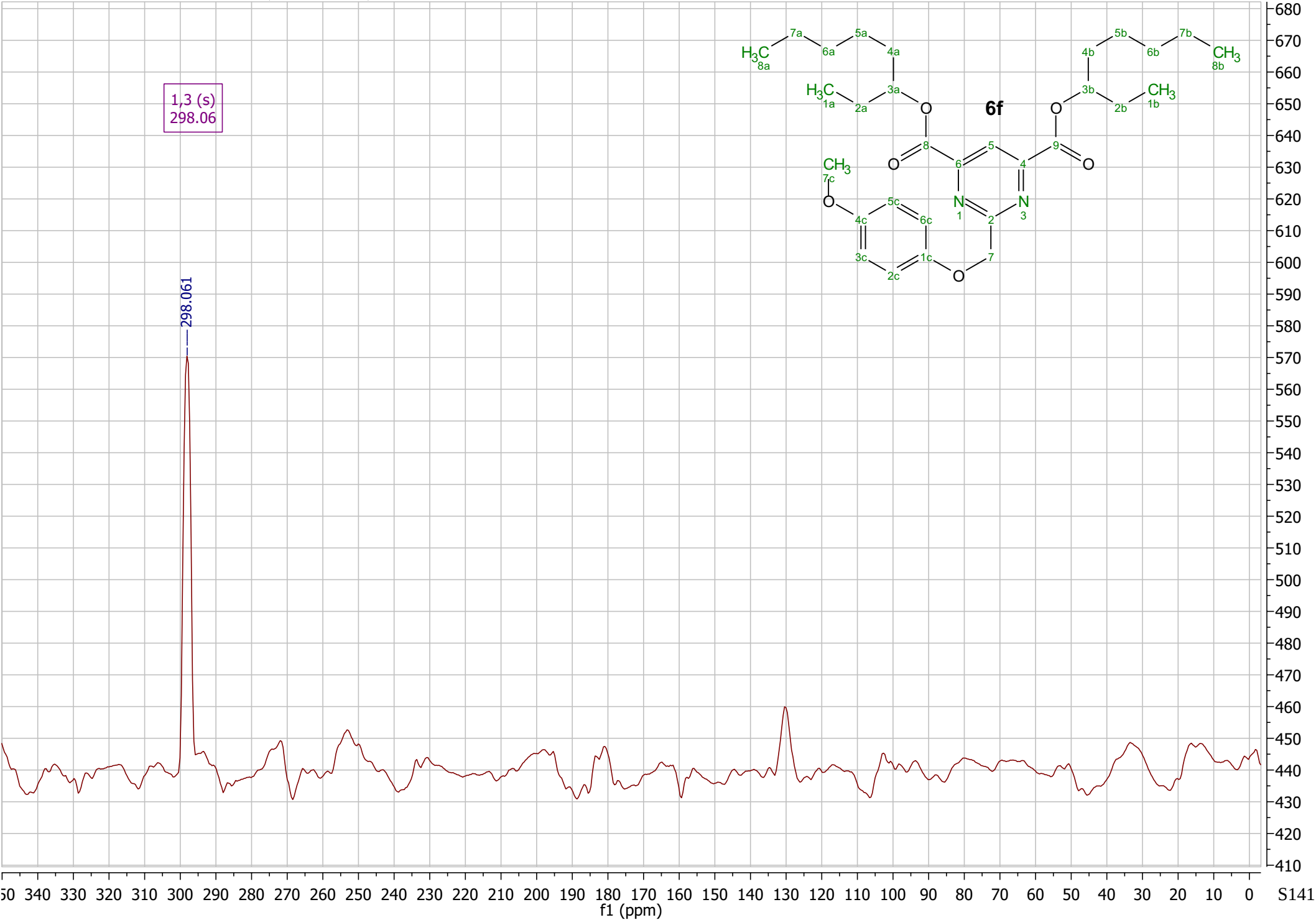
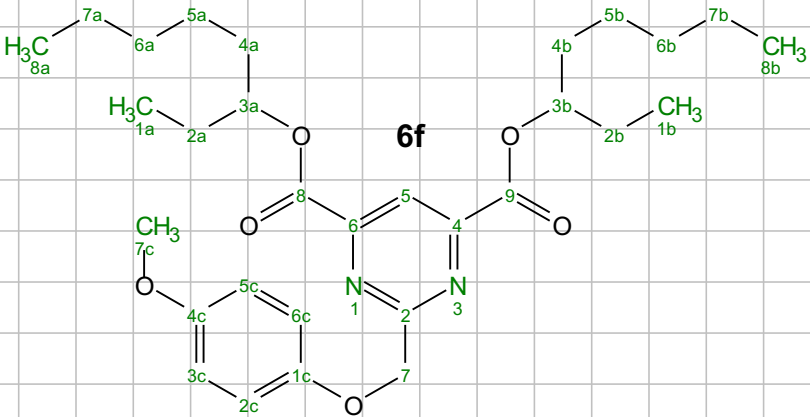




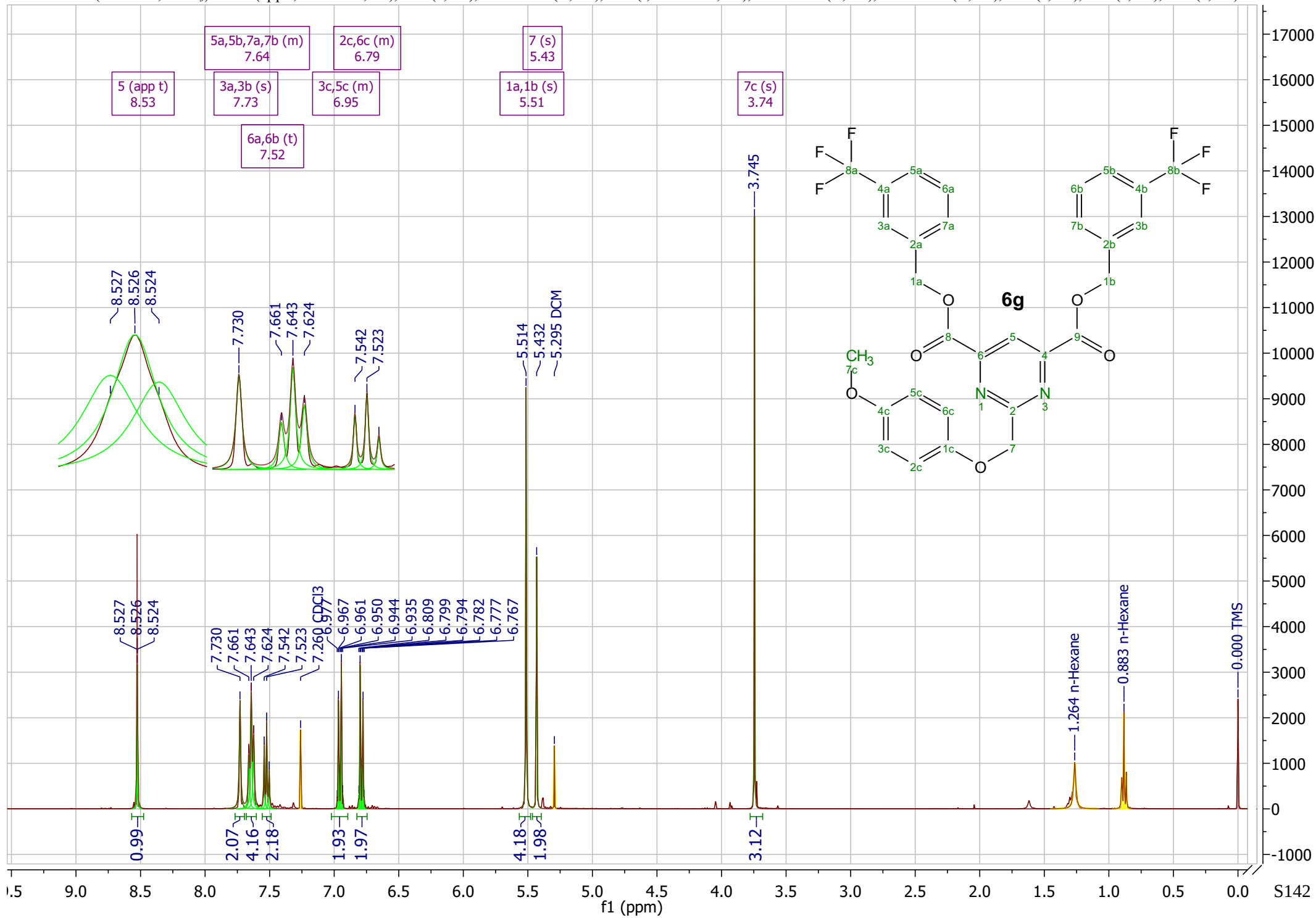


1,3 (s)
298.06

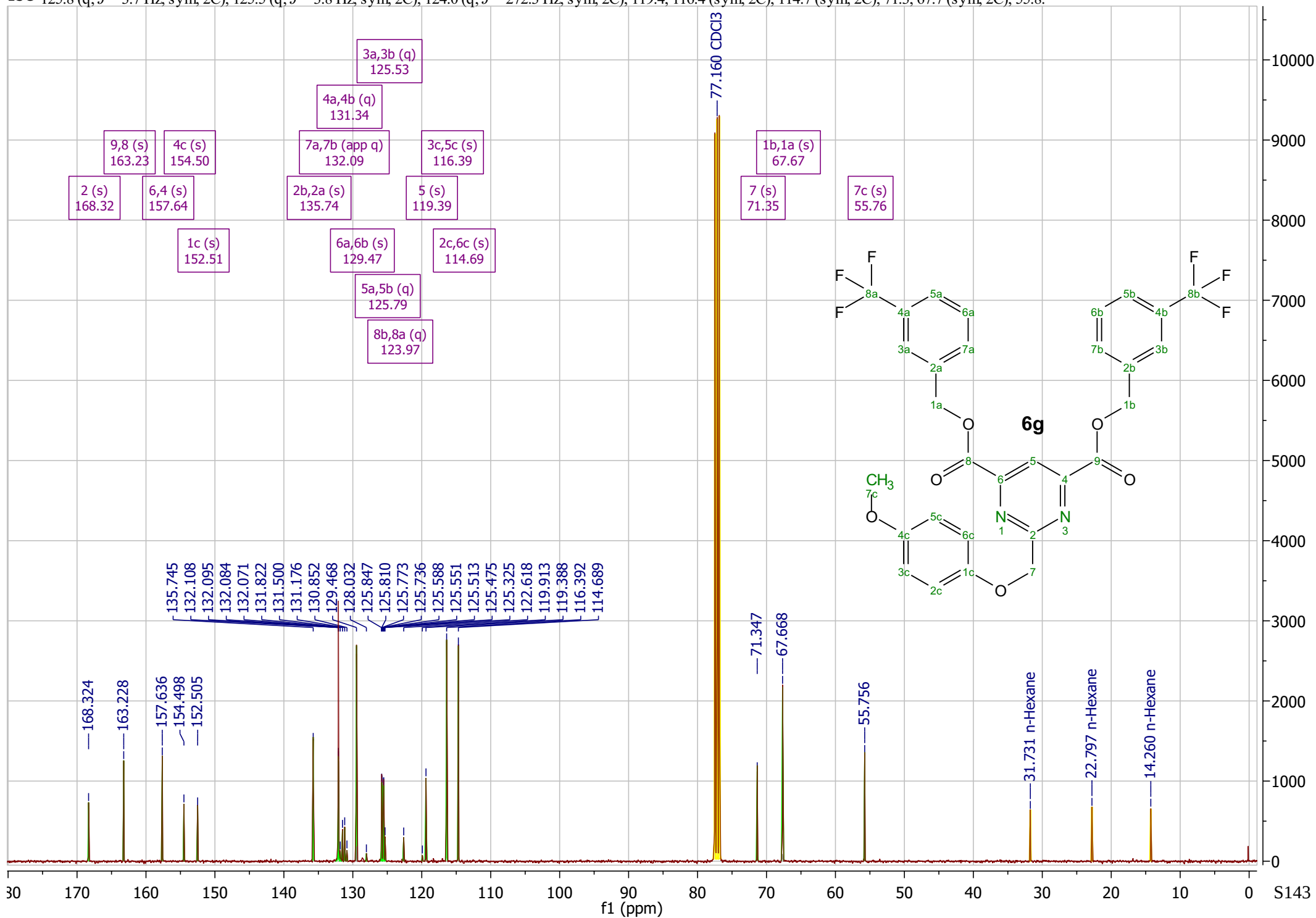
298.061



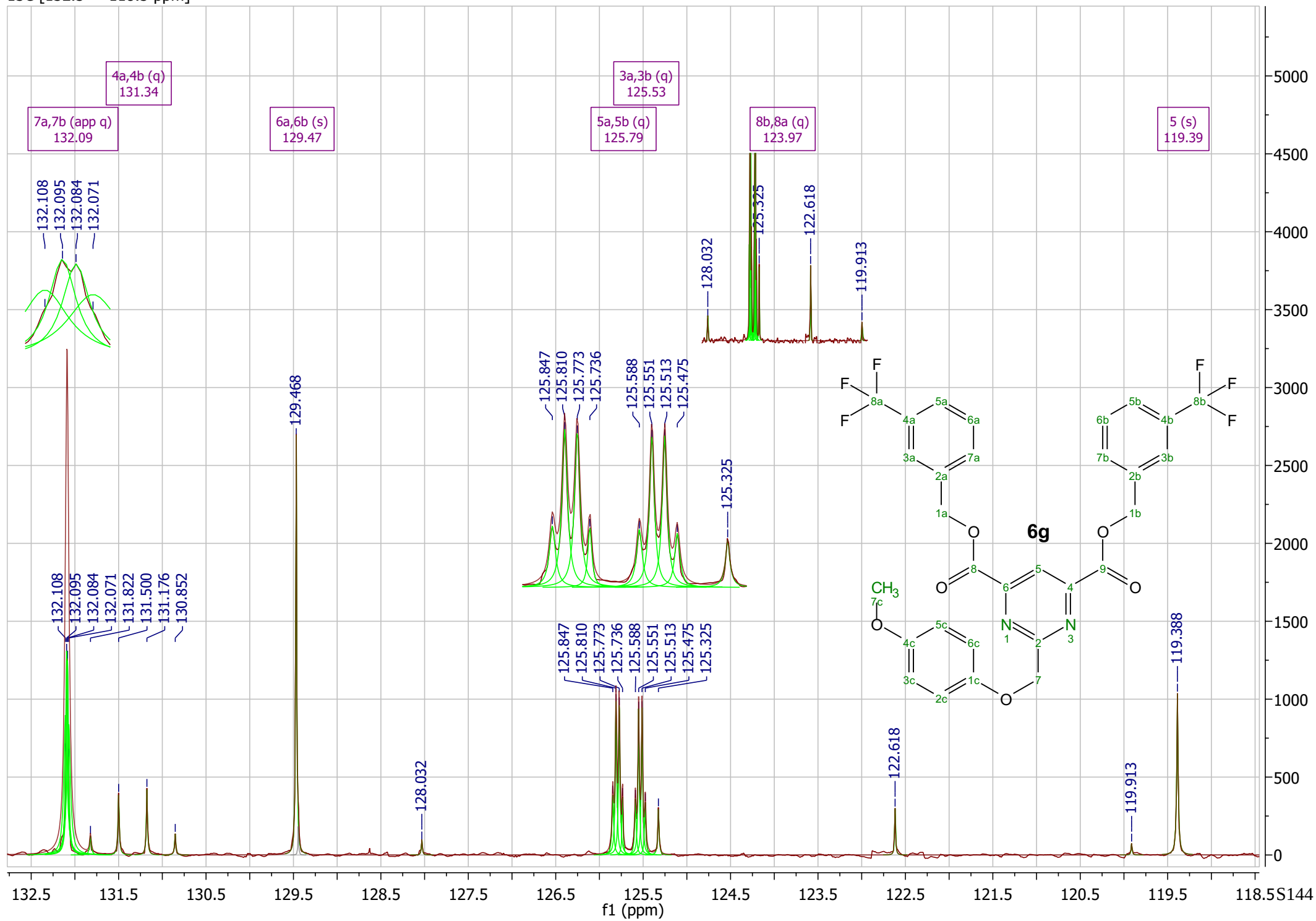
^1H NMR (400 MHz, CDCl_3) δ 8.53 (app t, $J = 0.6$ Hz, 1H), 7.73 (s, 2H), 7.69 – 7.60 (m, 4H), 7.52 (t, $J = 7.7$ Hz, 2H), 7.02 – 6.89 (m, 2H), 6.83 – 6.74 (m, 2H), 5.51 (s, 4H), 5.43 (s, 2H), 3.74 (s, 3H).

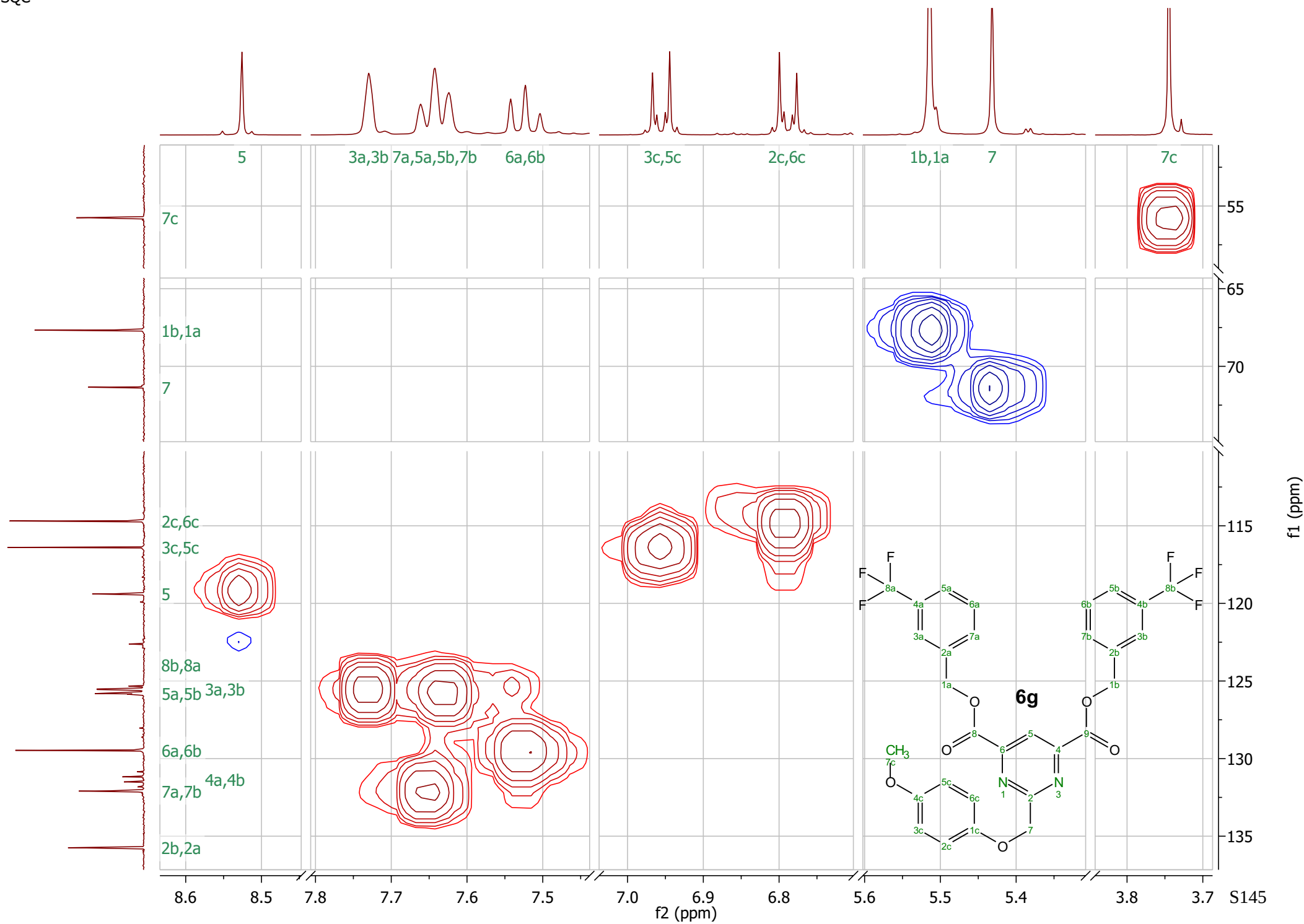


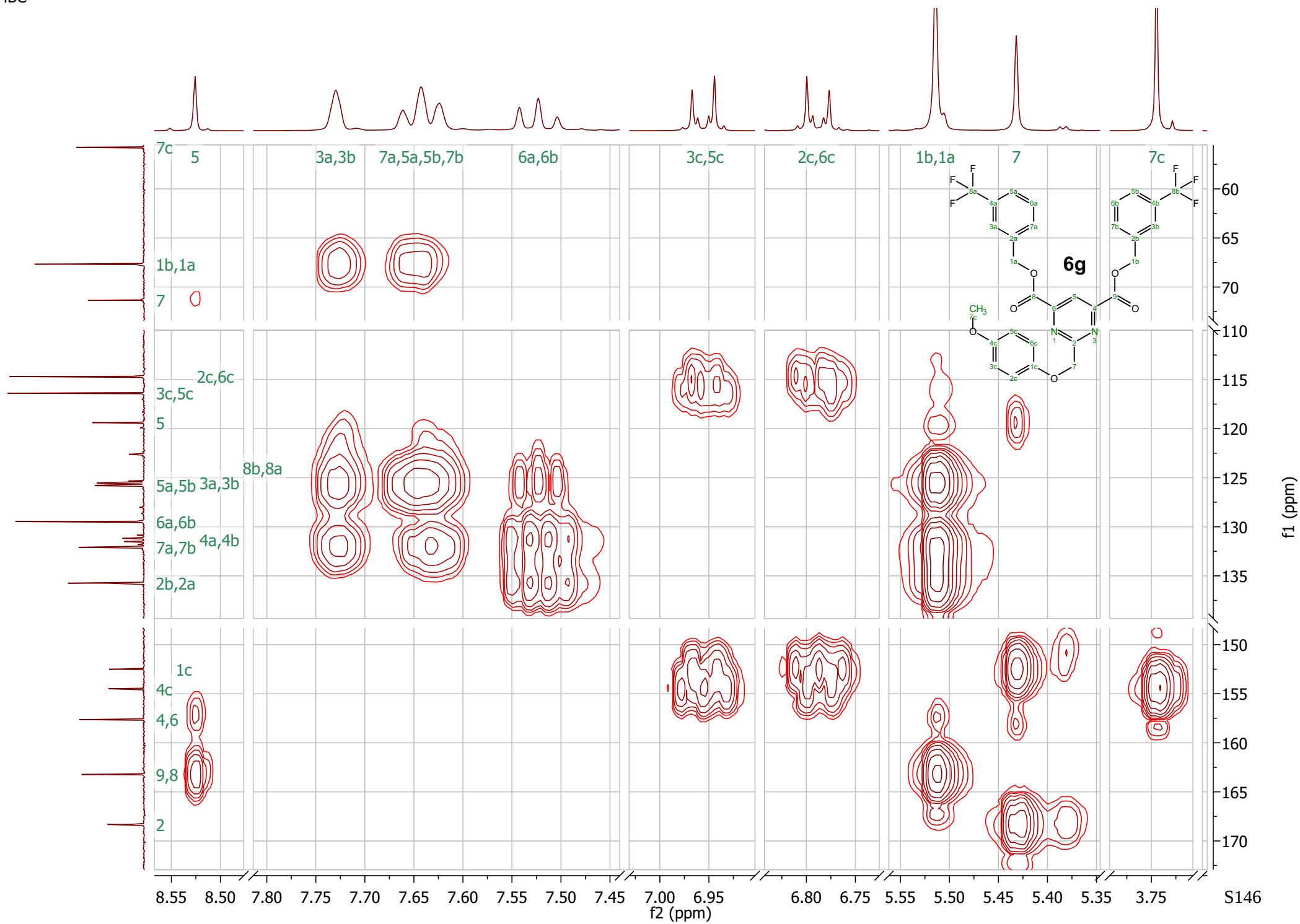
^{13}C NMR (101 MHz, CDCl_3) δ 168.3, 163.2 (sym, 2C), 157.6 (sym, 2C), 154.5, 152.5, 135.7 (sym, 2C), 132.1 (app q, $J = 1.1$ Hz, sym, 2C), 131.3 (q, $J = 32.5$ Hz, sym, 2C), 129.5 (sym, 2C), 125.8 (q, $J = 3.7$ Hz, sym, 2C), 125.5 (q, $J = 3.8$ Hz, sym, 2C), 124.0 (q, $J = 272.3$ Hz, sym, 2C), 119.4, 116.4 (sym, 2C), 114.7 (sym, 2C), 71.3, 67.7 (sym, 2C), 55.8.

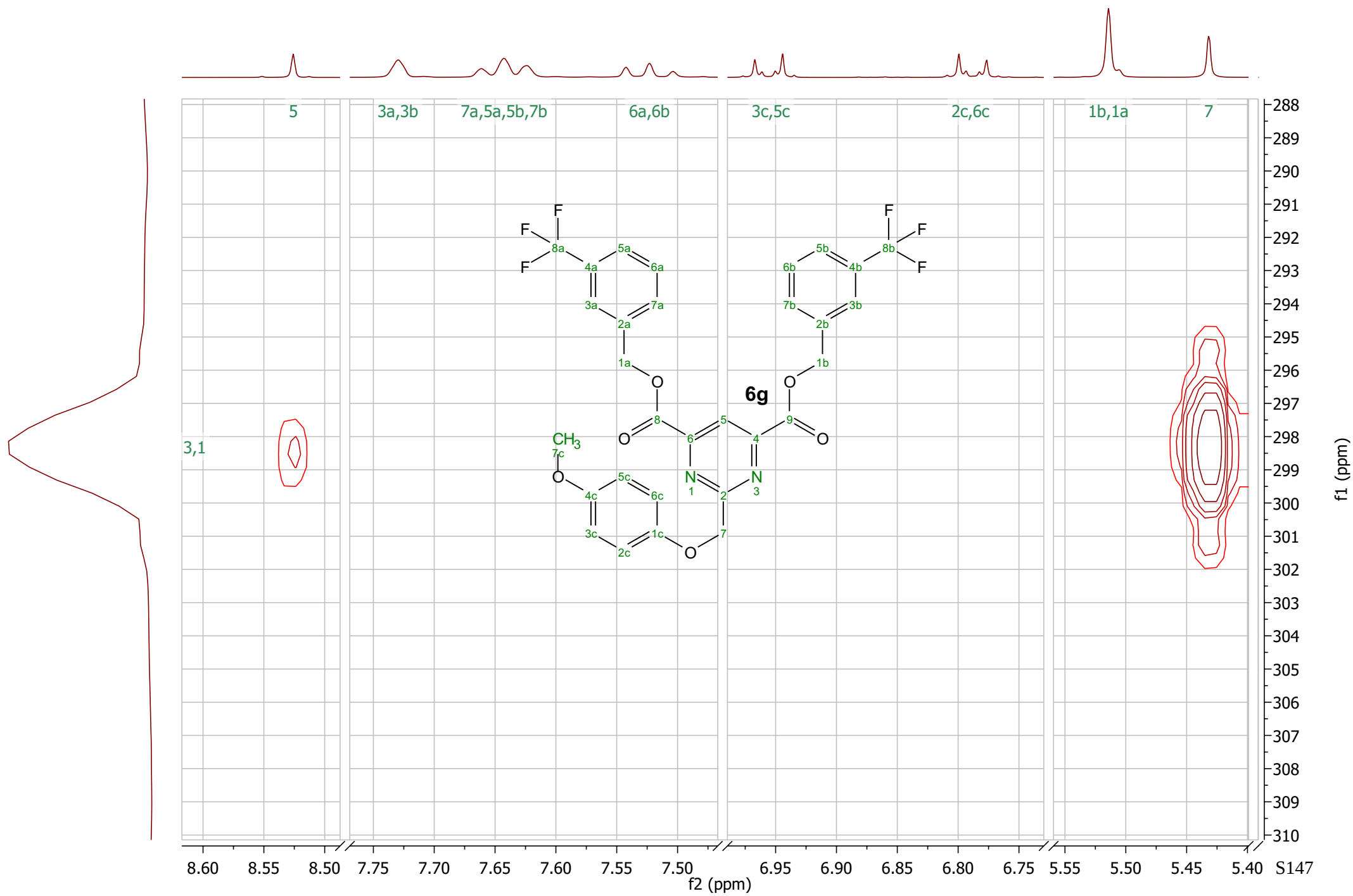


¹³C [132.5 — 118.5 ppm]





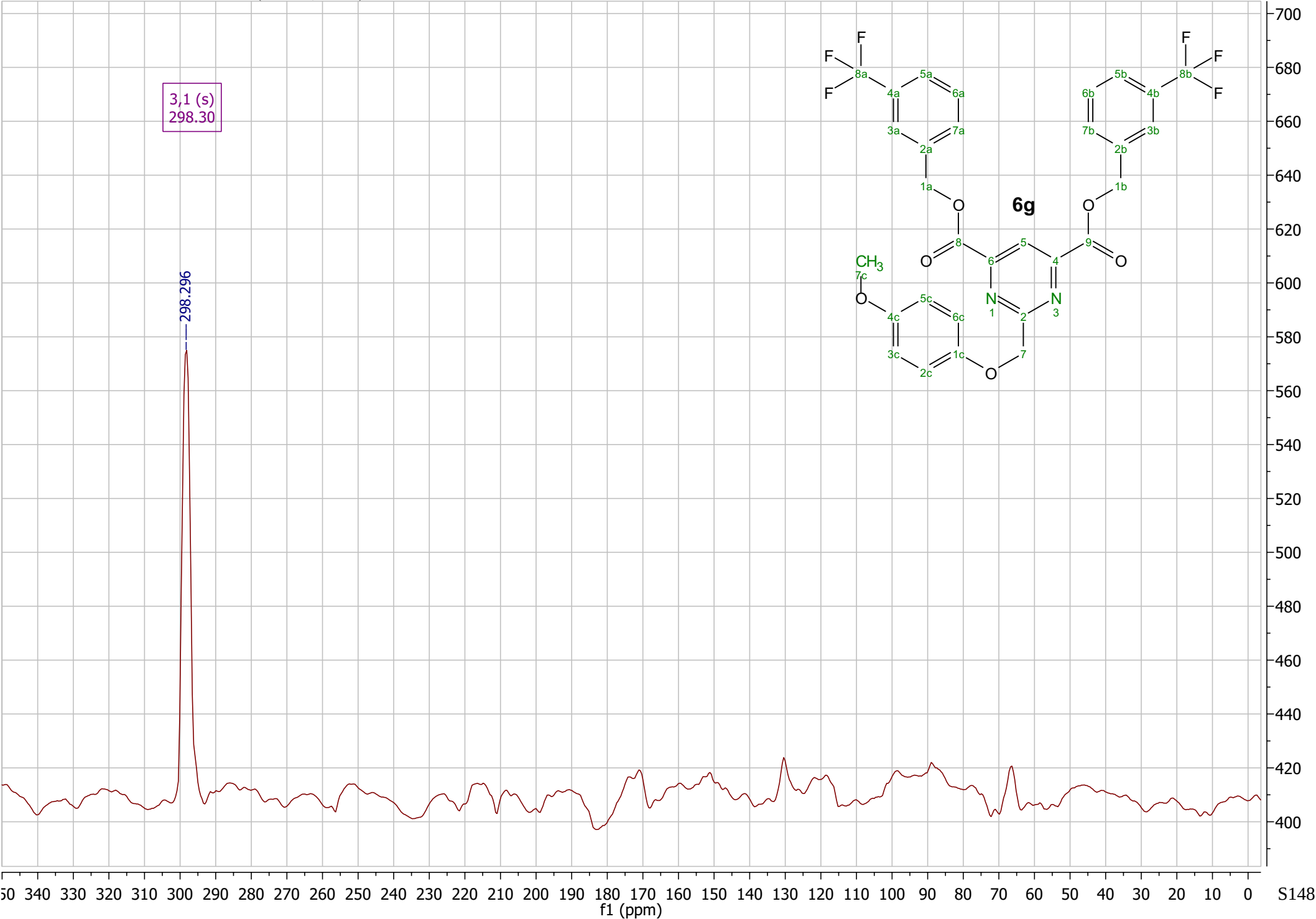




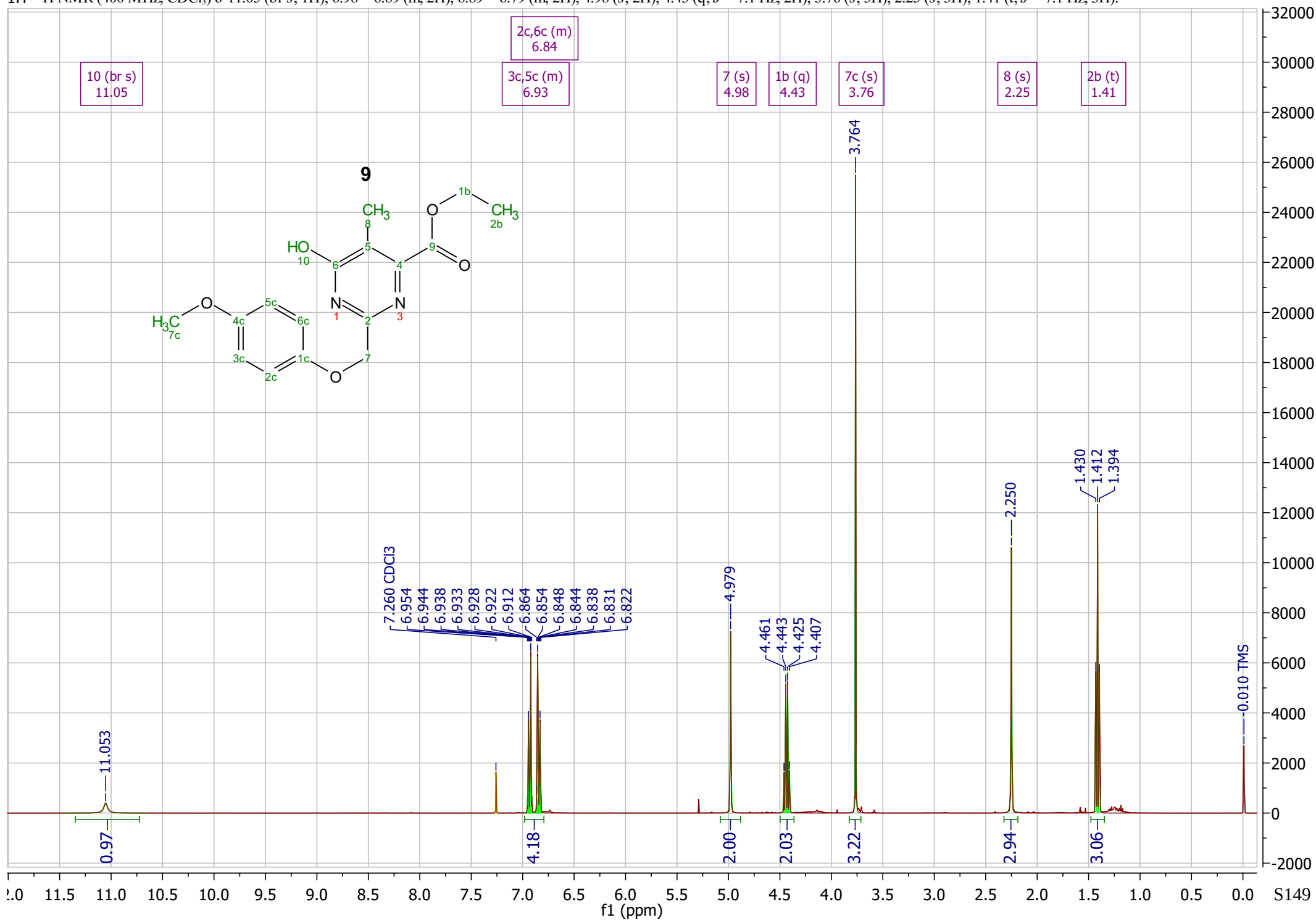
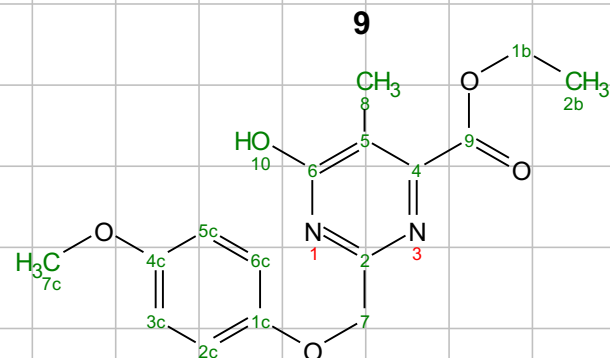
15N HMBC f1 Projection ¹⁵N NMR (41 MHz, CDCl₃) δ 298.30.

3,1 (s)
298.30

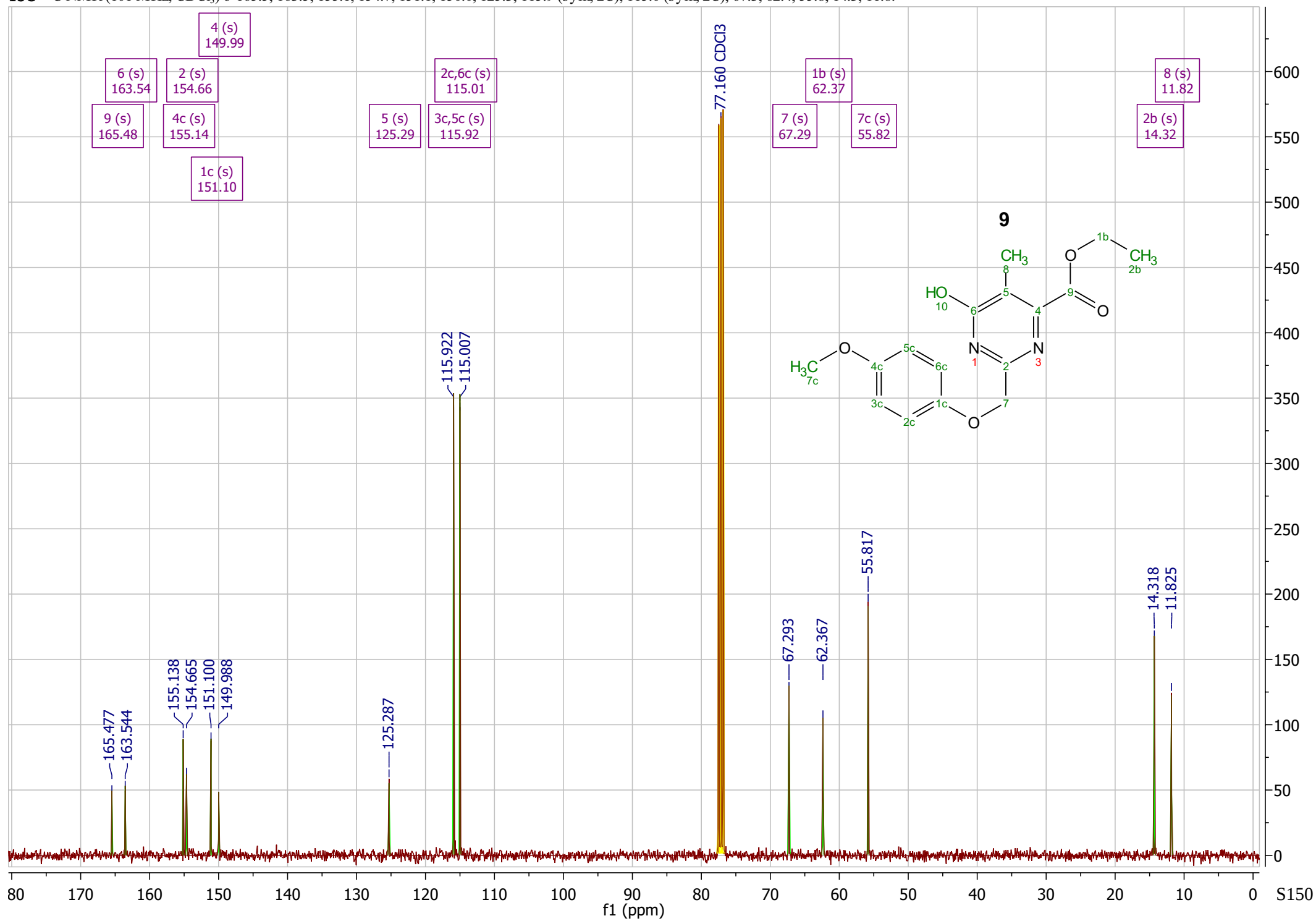
298.296

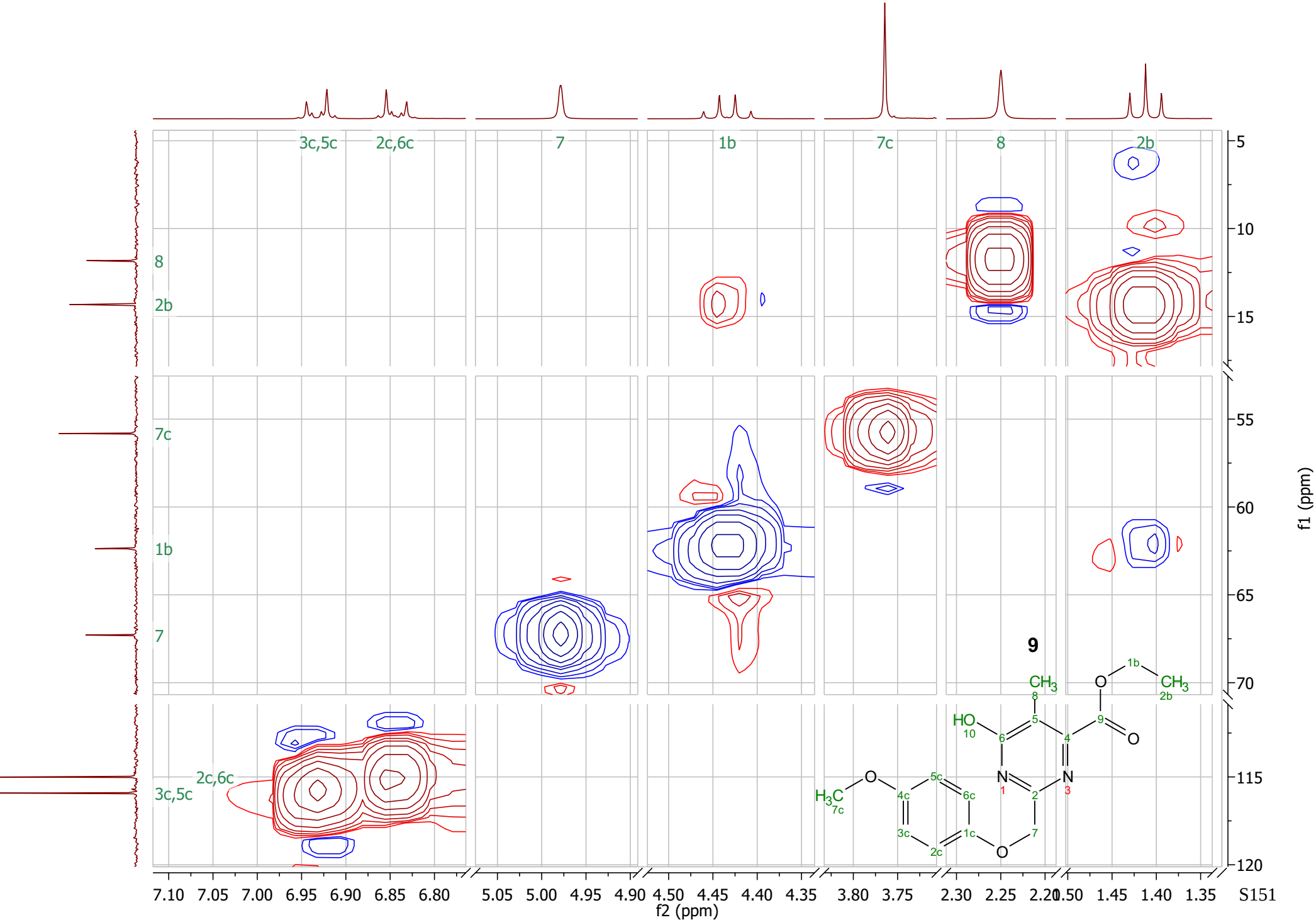


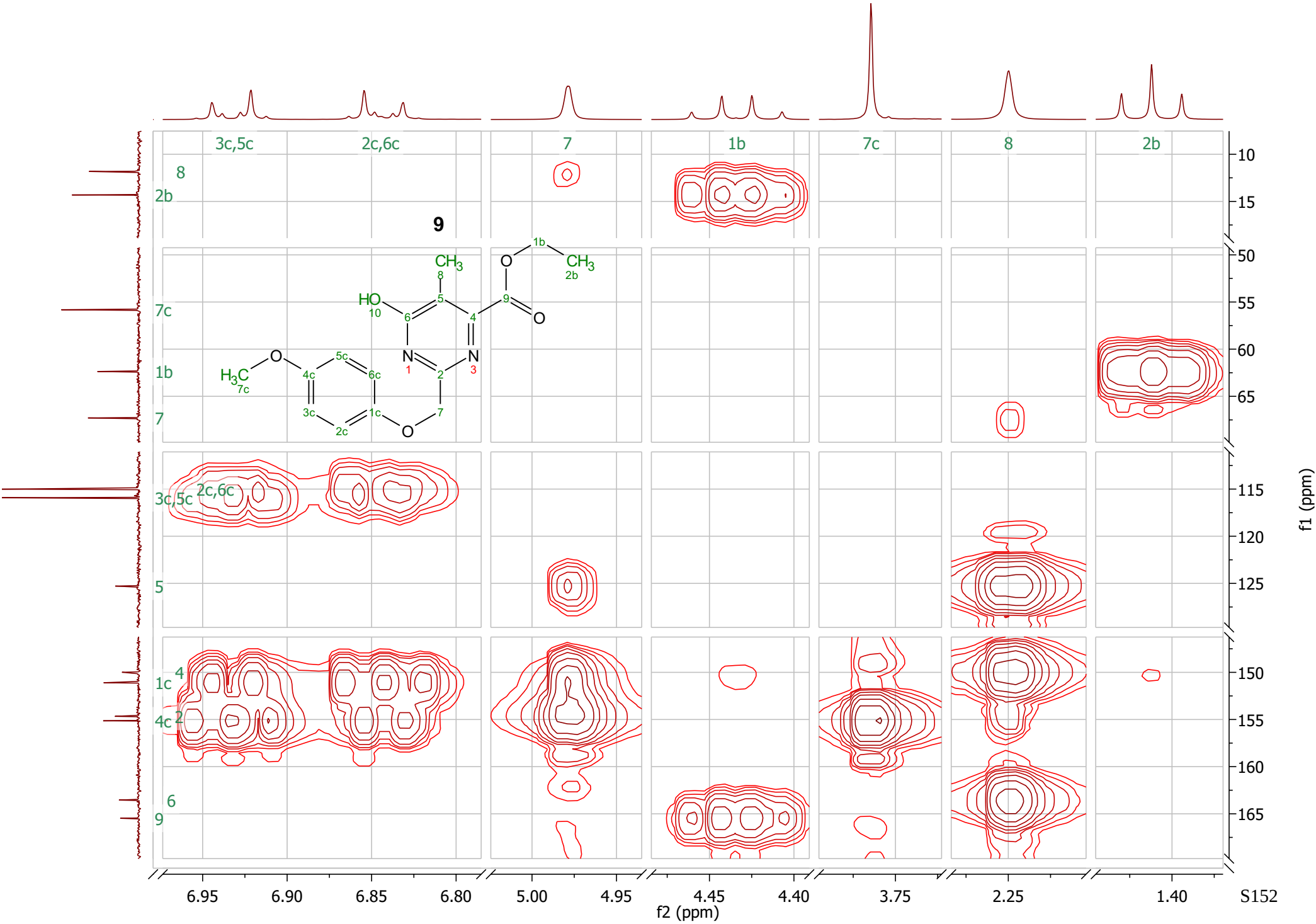
^1H NMR (400 MHz, CDCl_3) δ 11.05 (br s, 1H), 6.98 – 6.89 (m, 2H), 6.89 – 6.79 (m, 2H), 4.98 (s, 2H), 4.43 (q, $J = 7.1$ Hz, 2H), 3.76 (s, 3H), 2.25 (s, 3H), 1.41 (t, $J = 7.1$ Hz, 3H).



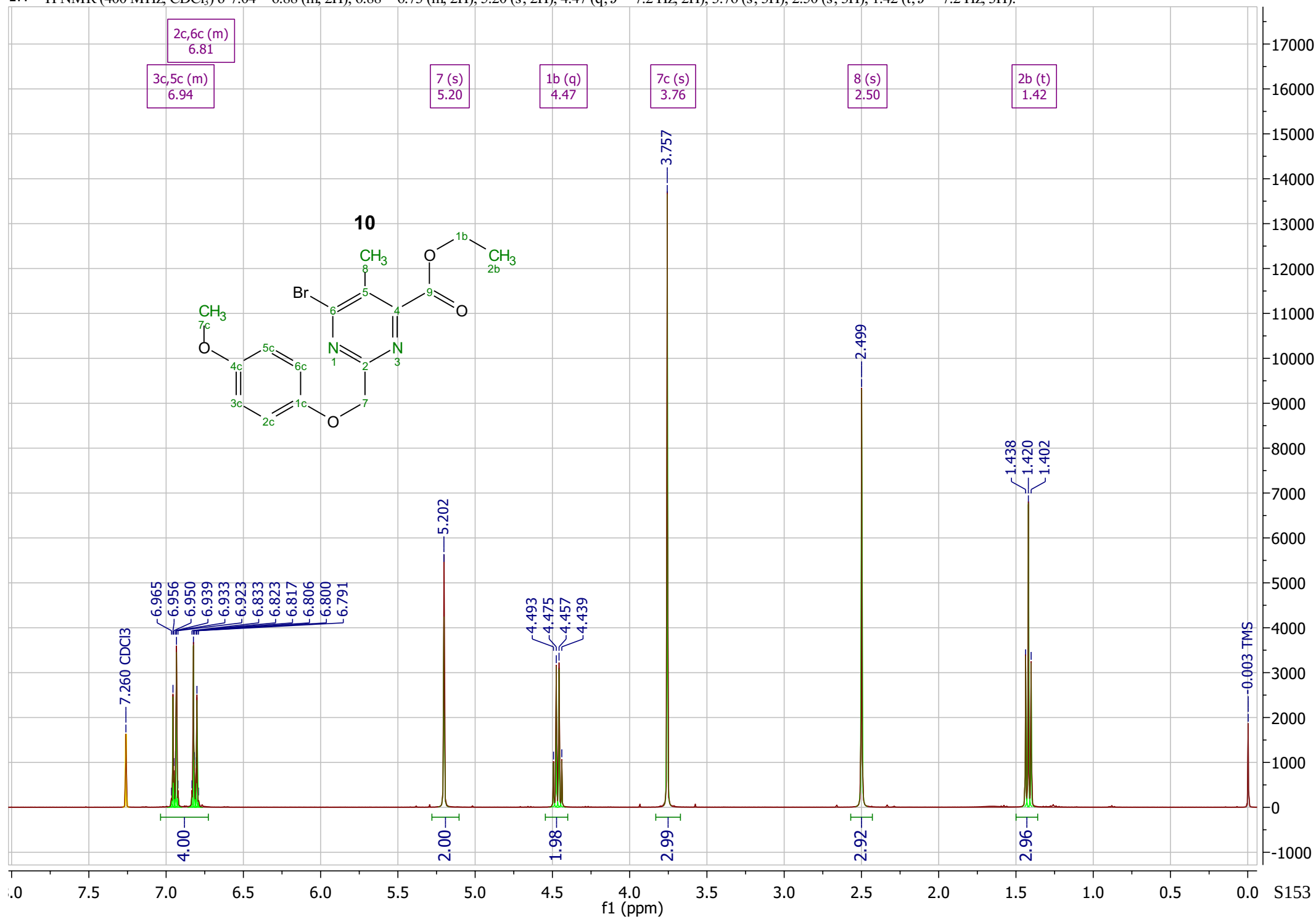
¹³C ¹³C NMR (101 MHz, CDCl₃) δ 165.5, 163.5, 155.1, 154.7, 151.1, 150.0, 125.3, 115.9 (sym, 2C), 115.0 (sym, 2C), 67.3, 62.4, 55.8, 14.3, 11.8.



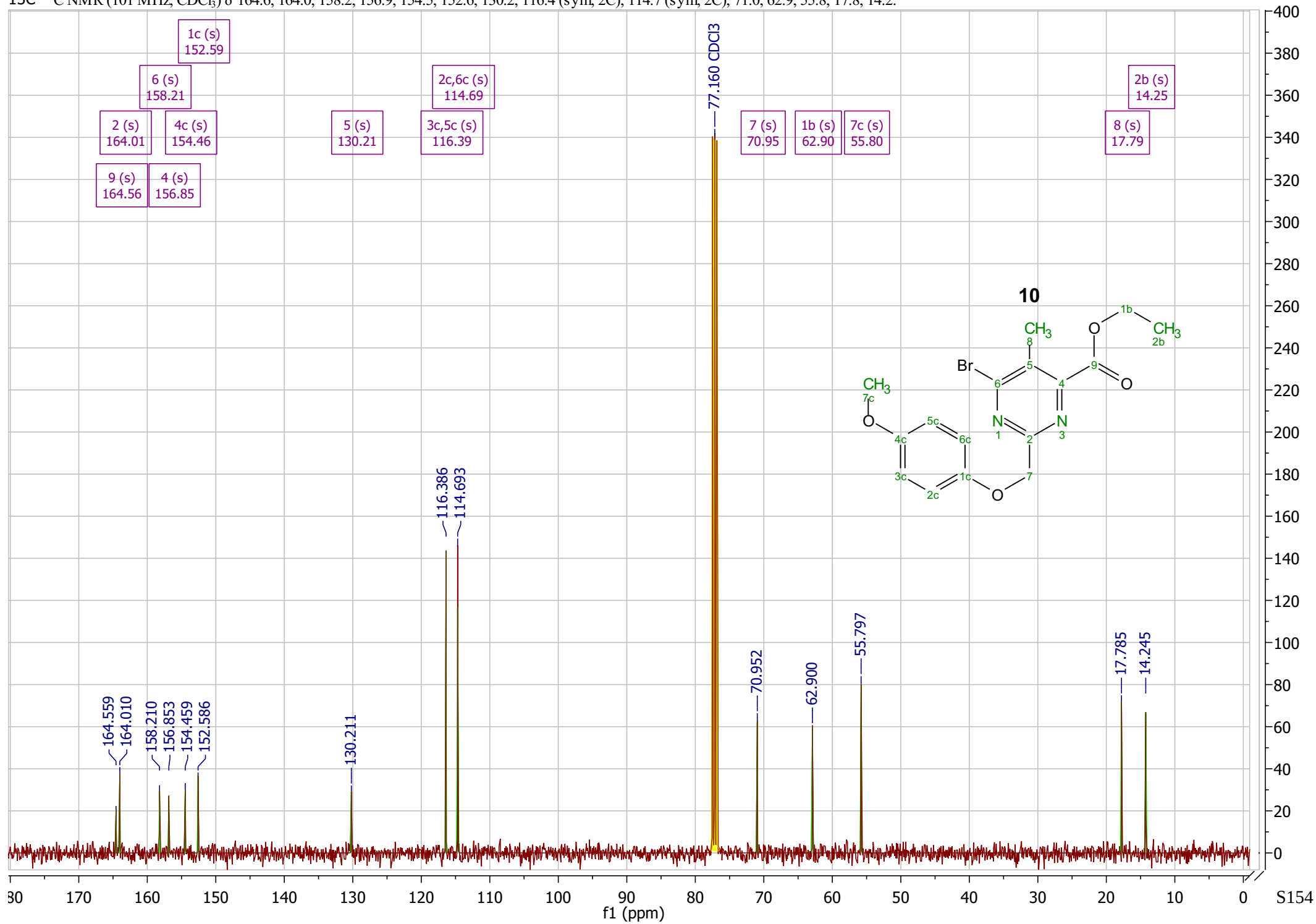


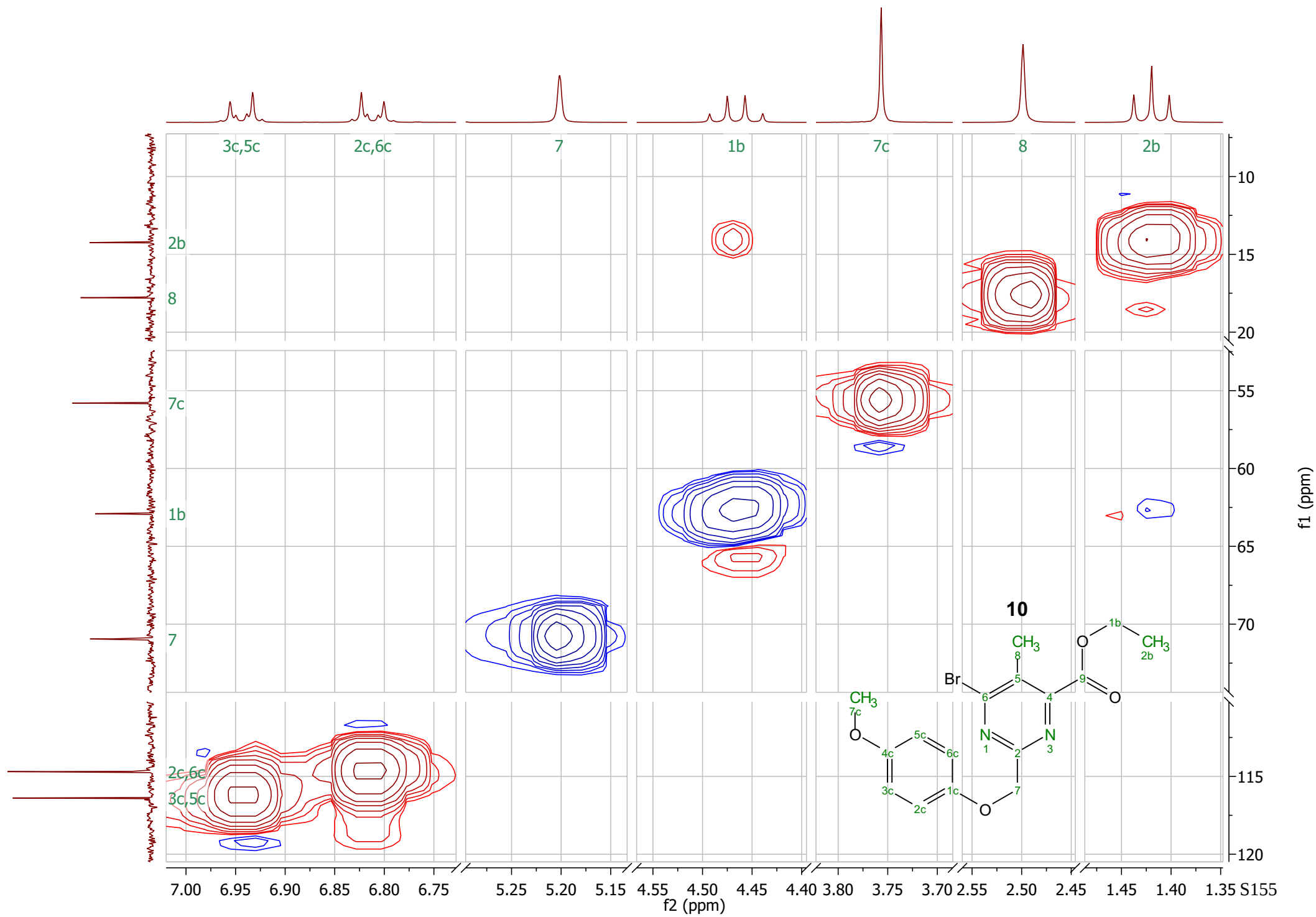


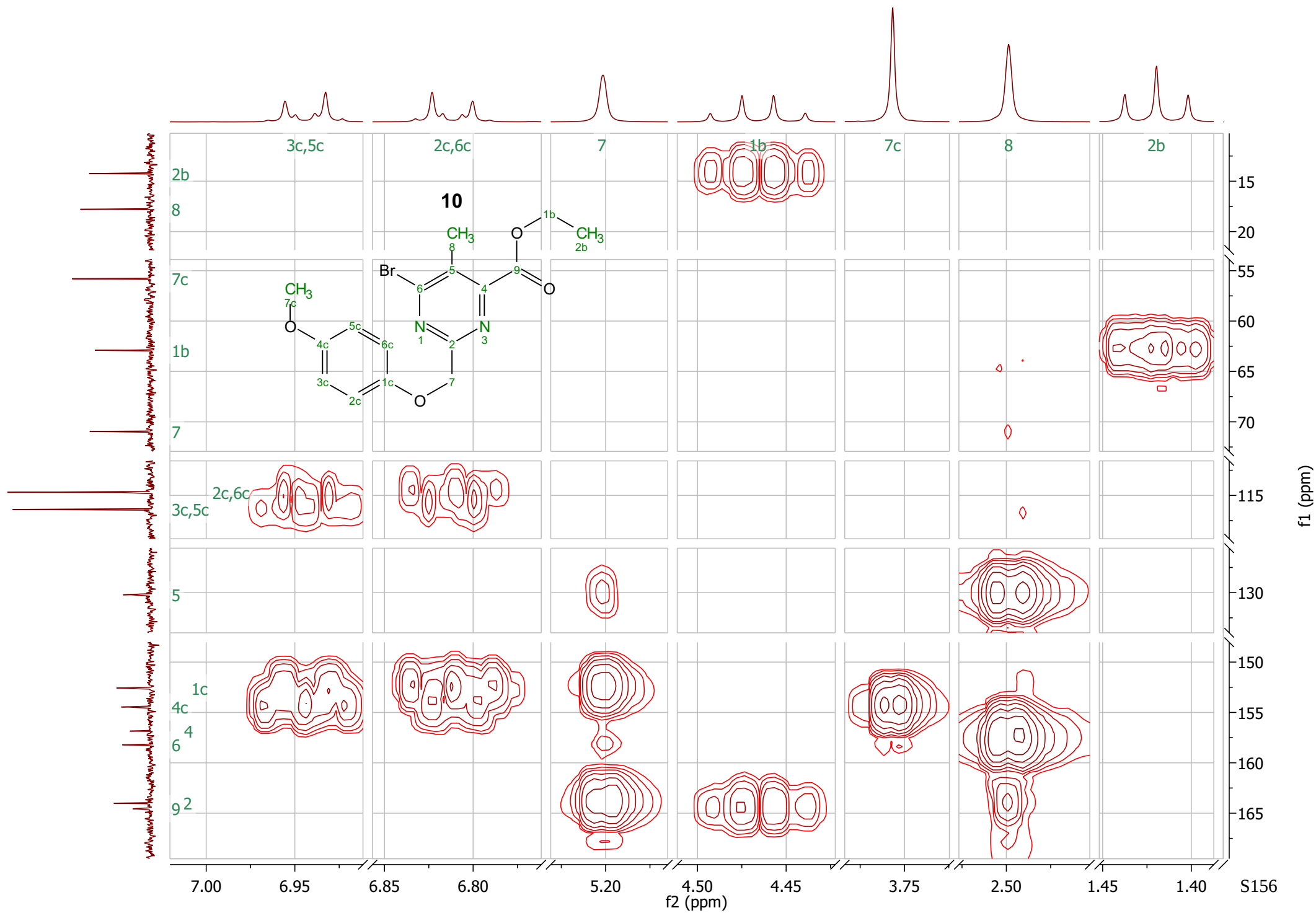
^1H NMR (400 MHz, CDCl_3) δ 7.04 – 6.88 (m, 2H), 6.88 – 6.73 (m, 2H), 5.20 (s, 2H), 4.47 (q, $J = 7.2$ Hz, 2H), 3.76 (s, 3H), 2.50 (s, 3H), 1.42 (t, $J = 7.2$ Hz, 3H).

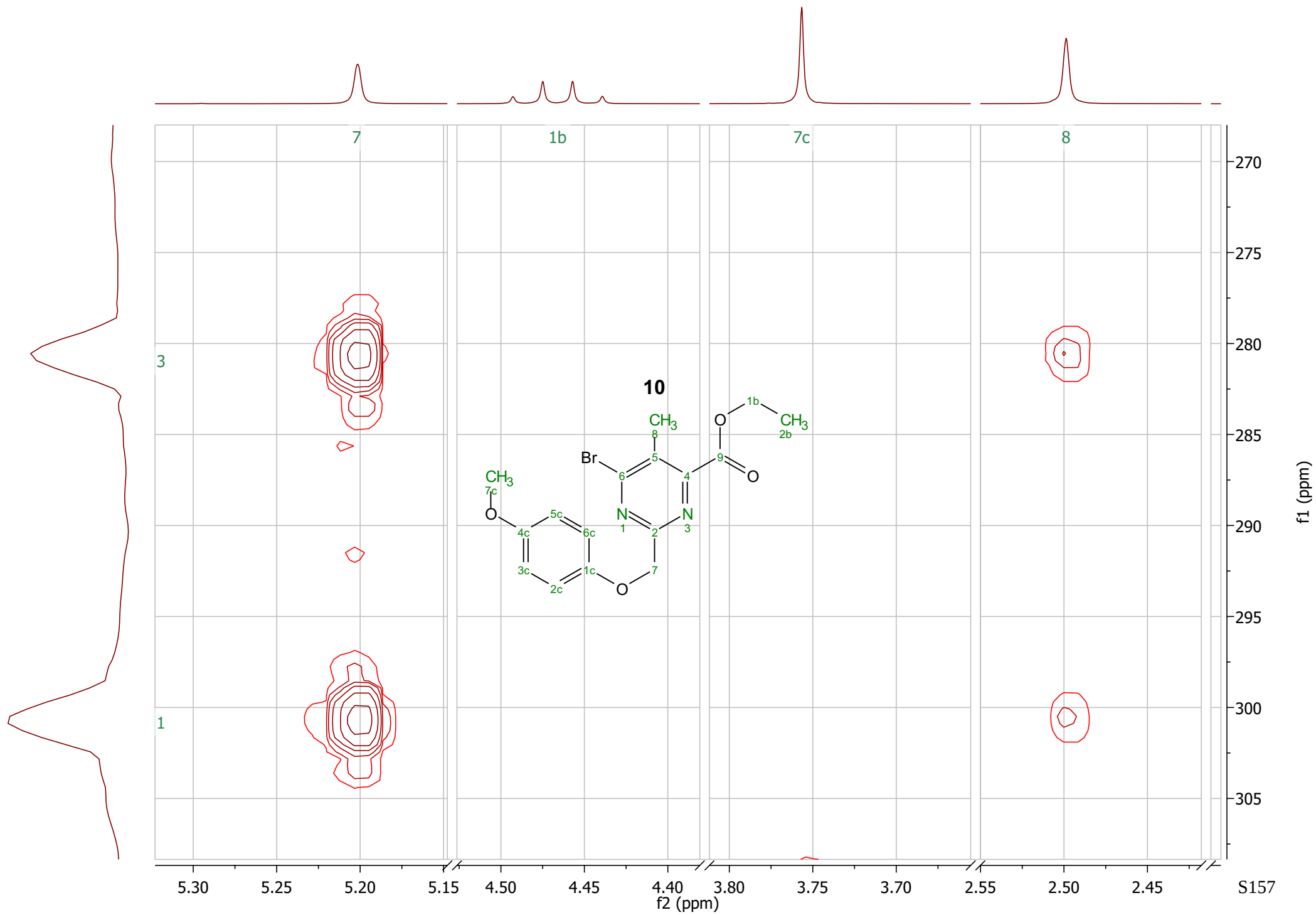


^{13}C NMR (101 MHz, CDCl_3) δ 164.6, 164.0, 158.2, 156.9, 154.5, 152.6, 130.2, 116.4 (sym, 2C), 114.7 (sym, 2C), 71.0, 62.9, 55.8, 17.8, 14.2.

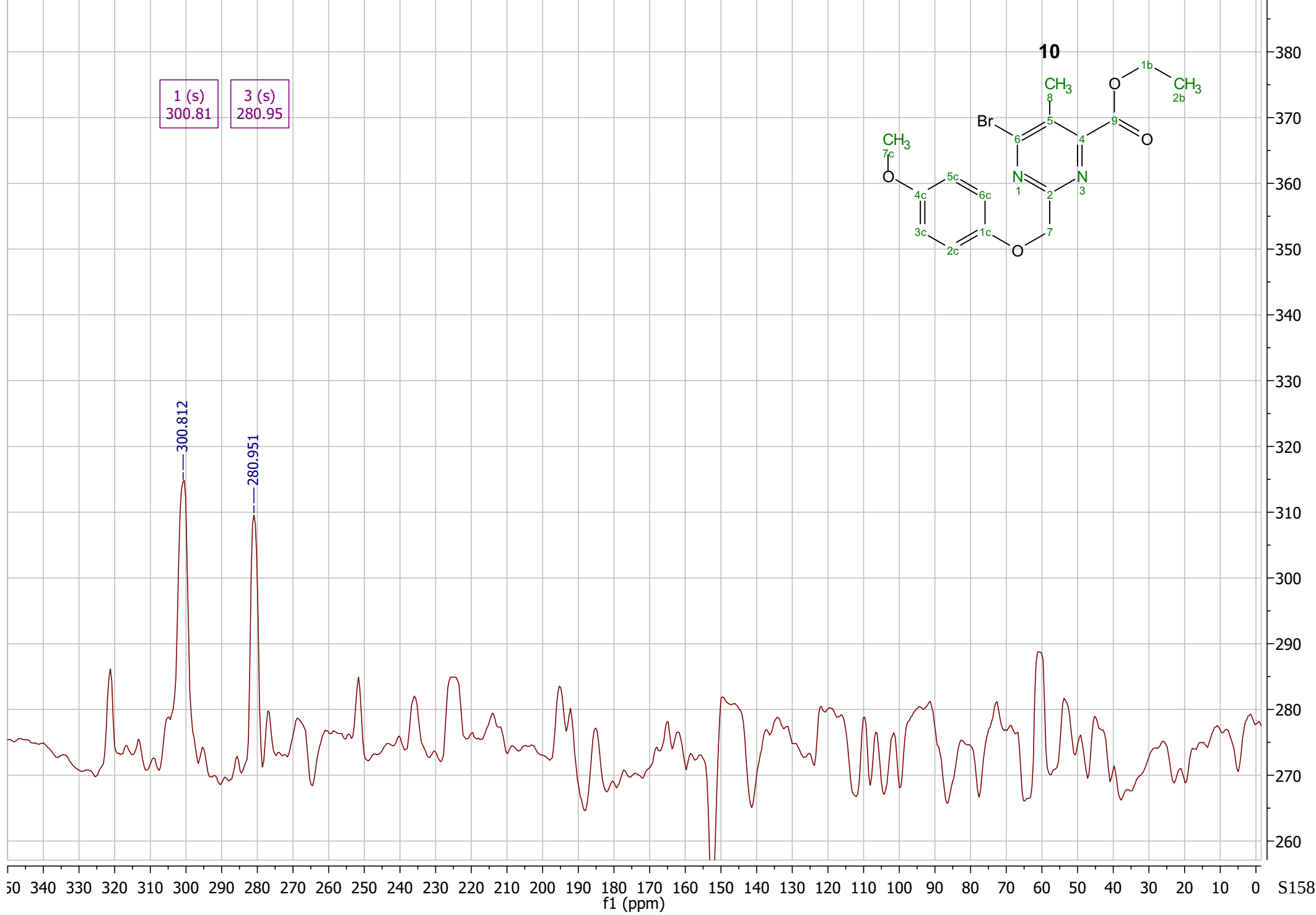




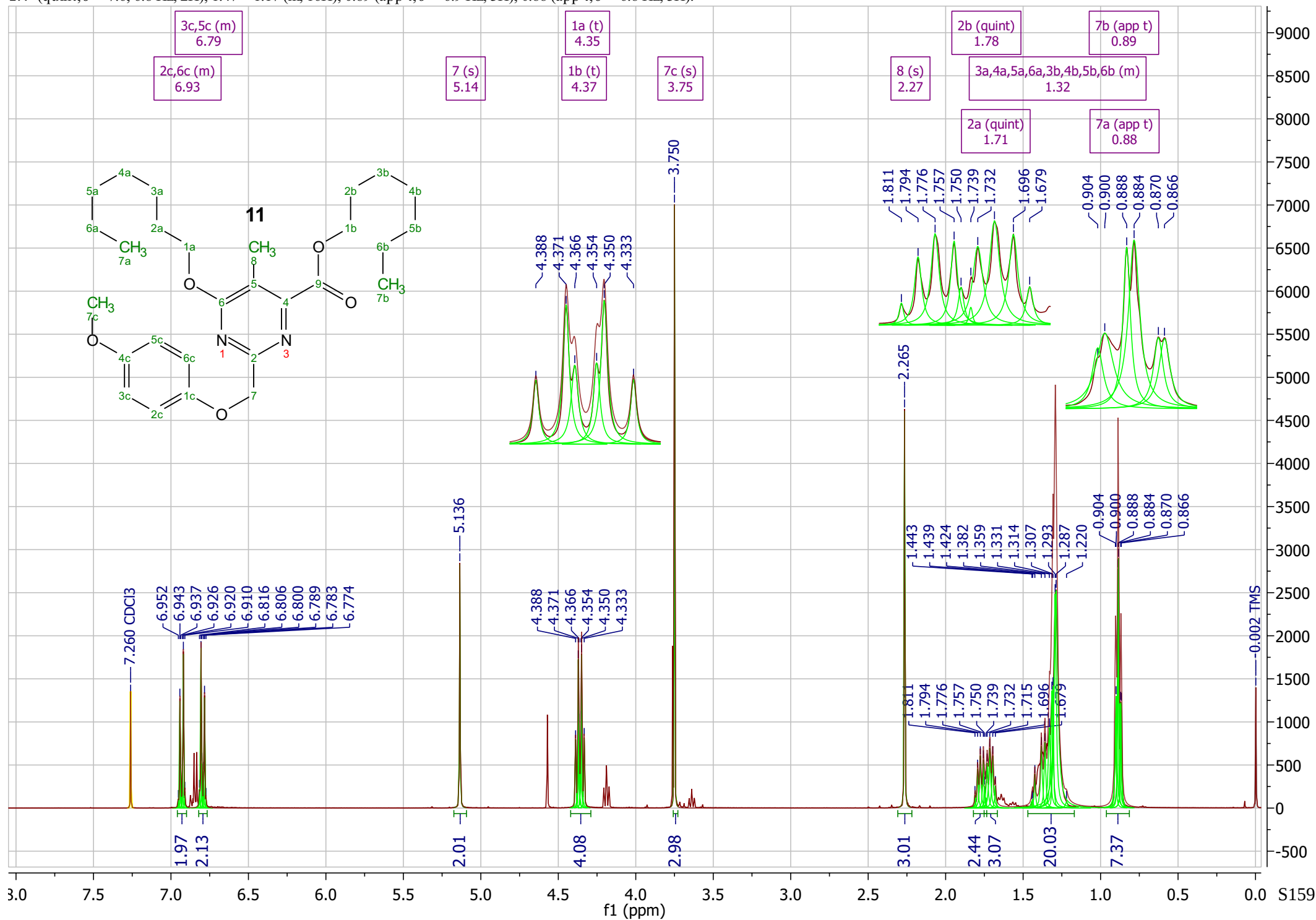




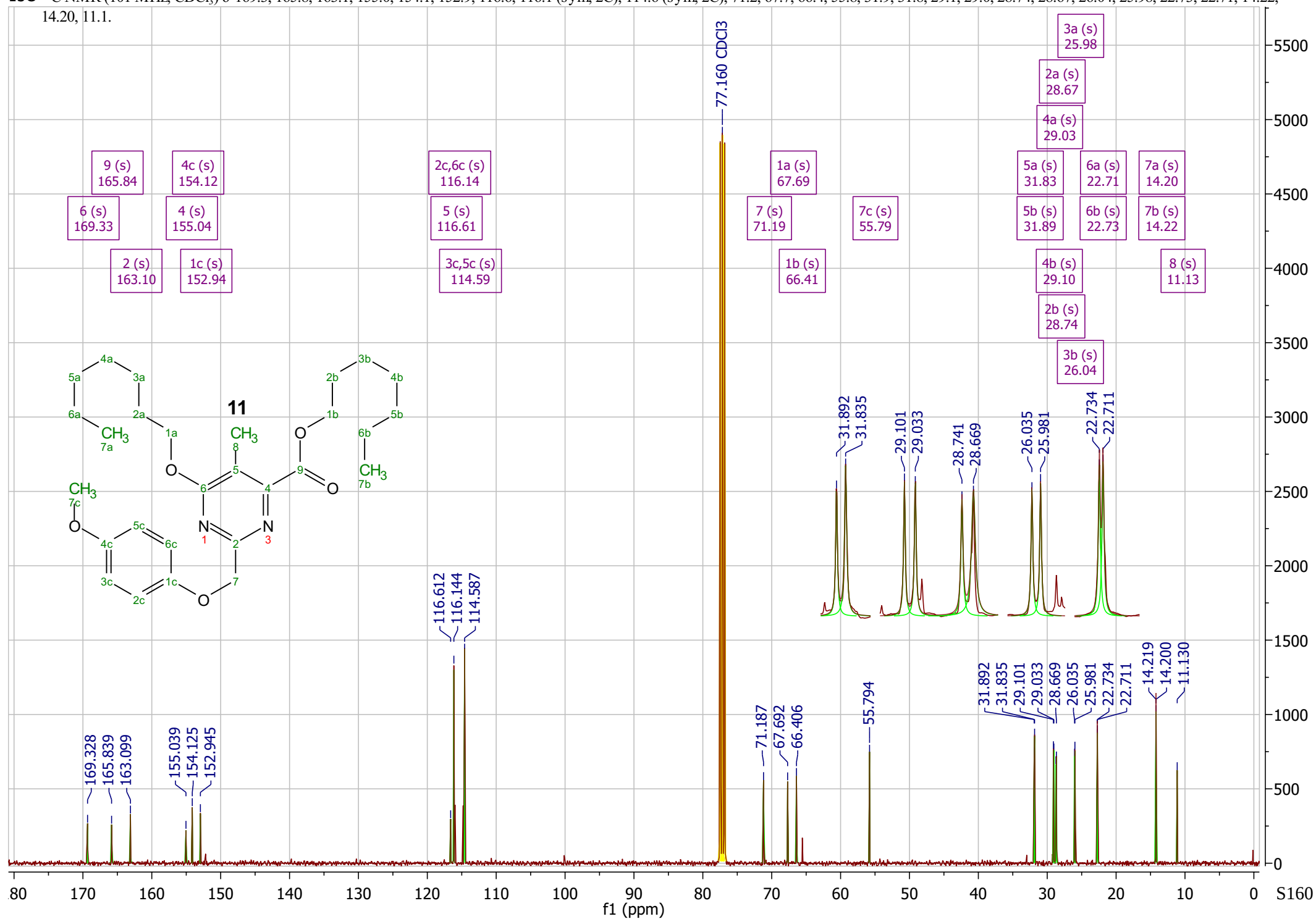
15N HMBC f1 Projection ¹⁵N NMR (41 MHz, CDCl₃) δ 300.81, 280.95.

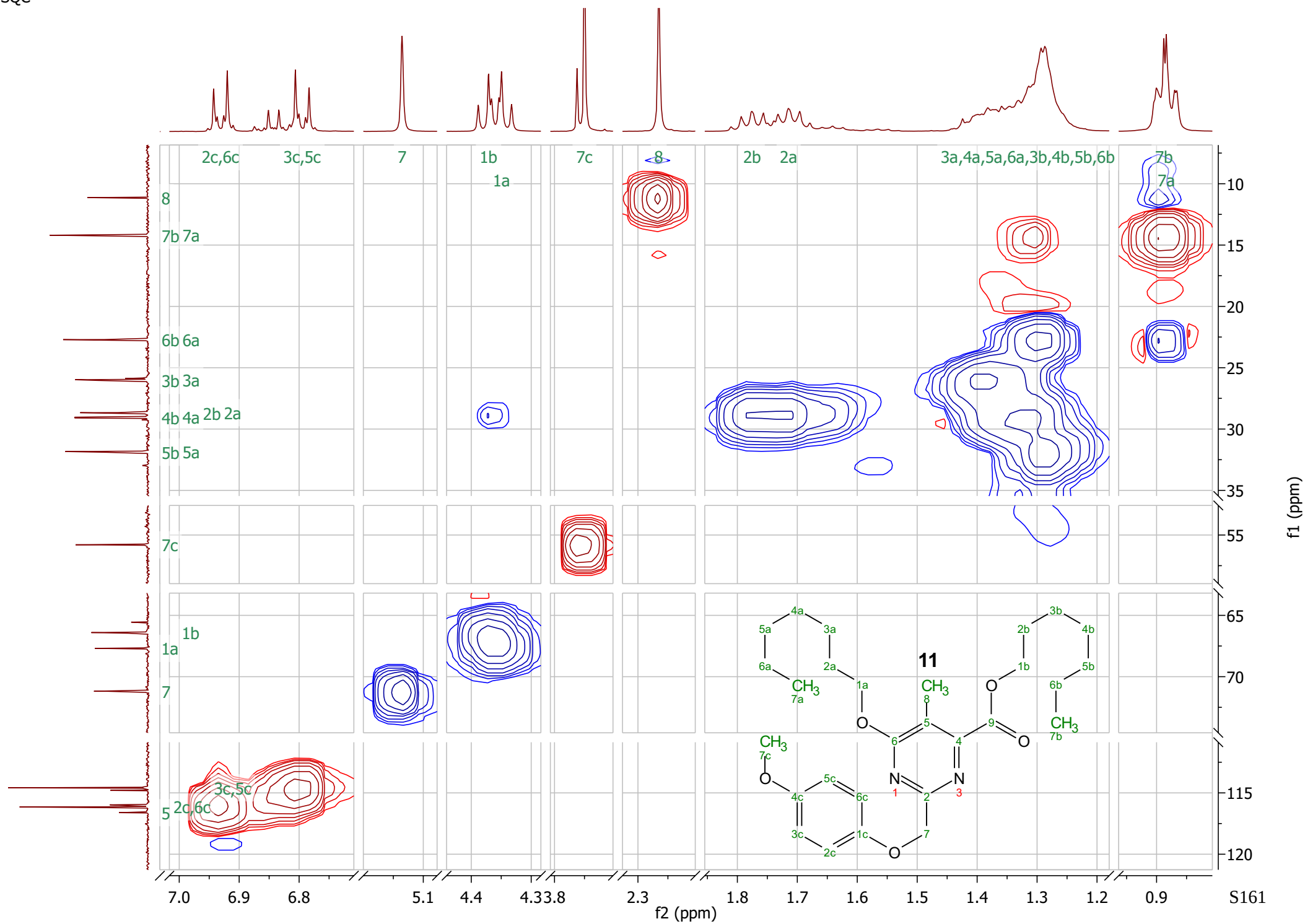


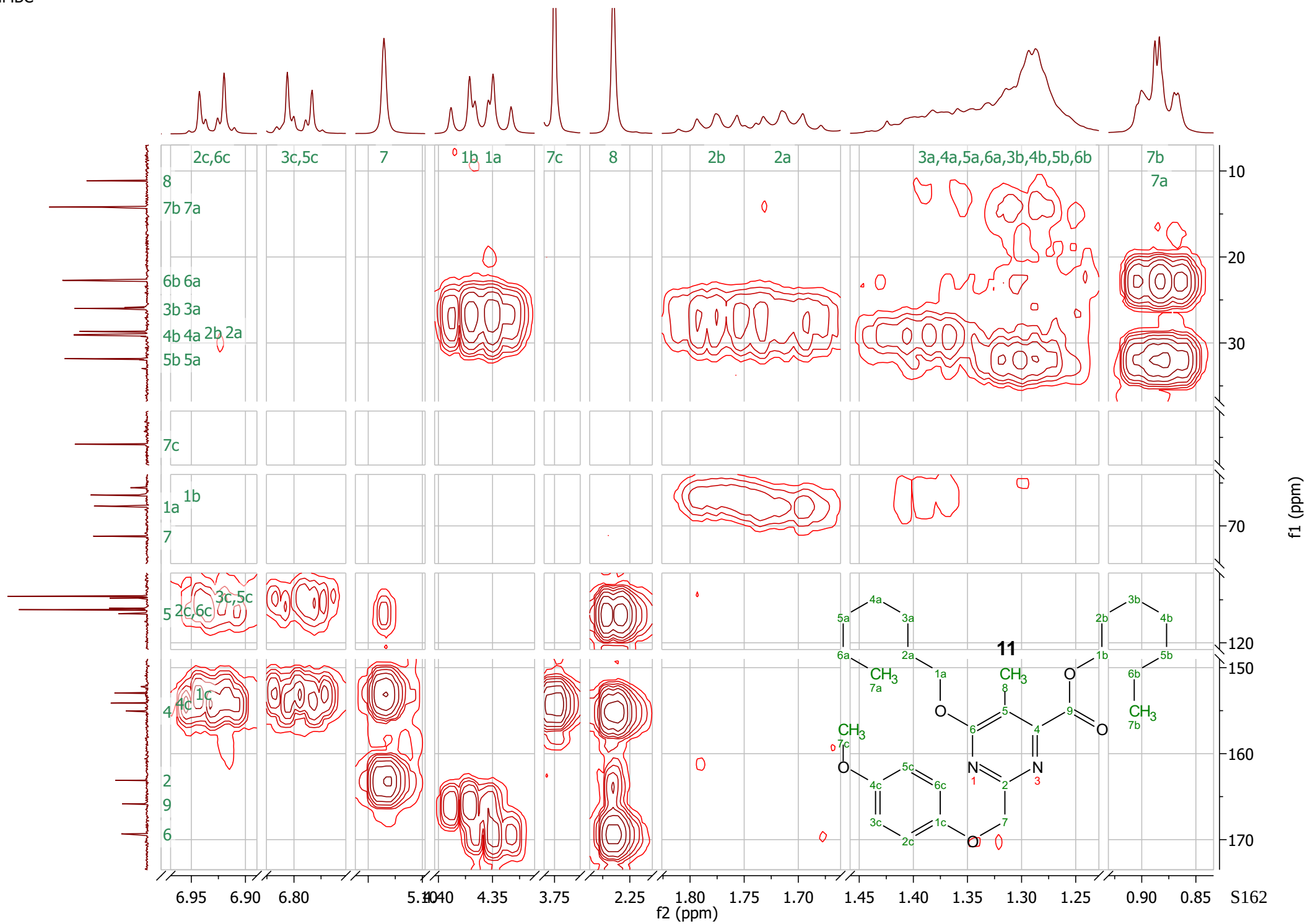
¹H NMR (400 MHz, CDCl₃) δ_{ppm} 6.98 – 6.86 (m, 2H), 6.86 – 6.75 (m, 2H), 5.14 (s, 2H), 5.14 (s, 2H), 4.35 (t, *J* = 6.7 Hz, 2H), 4.35 (t, *J* = 6.7 Hz, 2H), 3.75 (s, 3H), 2.27 (s, 3H), 1.78 (quint, *J* = 6.9 Hz, 2H), 1.71 (quint, *J* = 7.6, 6.8 Hz, 2H), 1.47 – 1.17 (m, 16H), 0.89 (app t, *J* = 6.9 Hz, 3H), 0.88 (app t, *J* = 6.8 Hz, 3H).



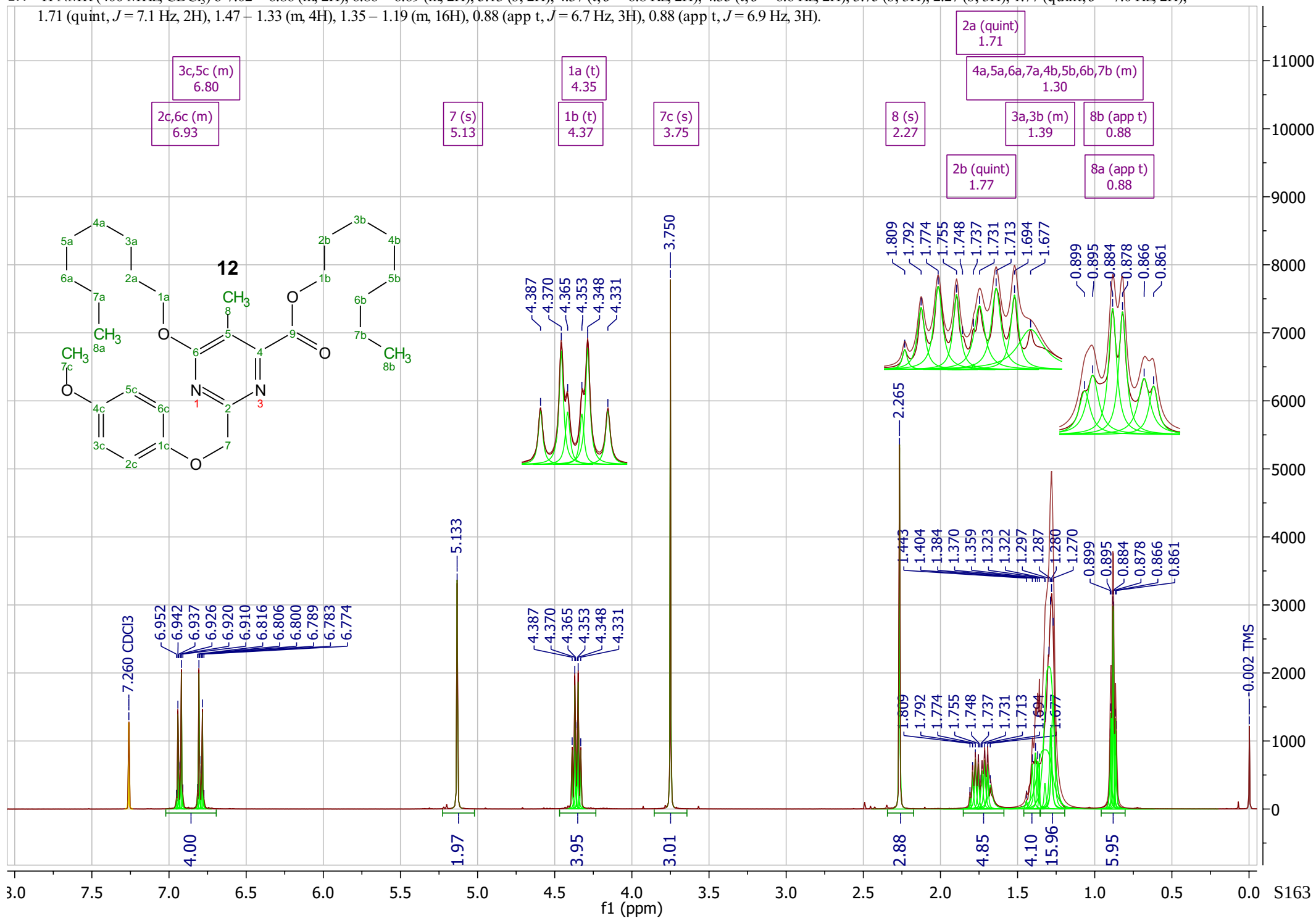
^{13}C NMR (101 MHz, CDCl_3) δ 169.3, 165.8, 163.1, 155.0, 154.1, 152.9, 116.6, 116.1 (sym, 2C), 114.6 (sym, 2C), 71.2, 67.7, 66.4, 55.8, 31.9, 31.8, 29.1, 29.0, 28.74, 28.67, 26.04, 25.98, 22.73, 22.71, 14.22, 14.20, 11.1.



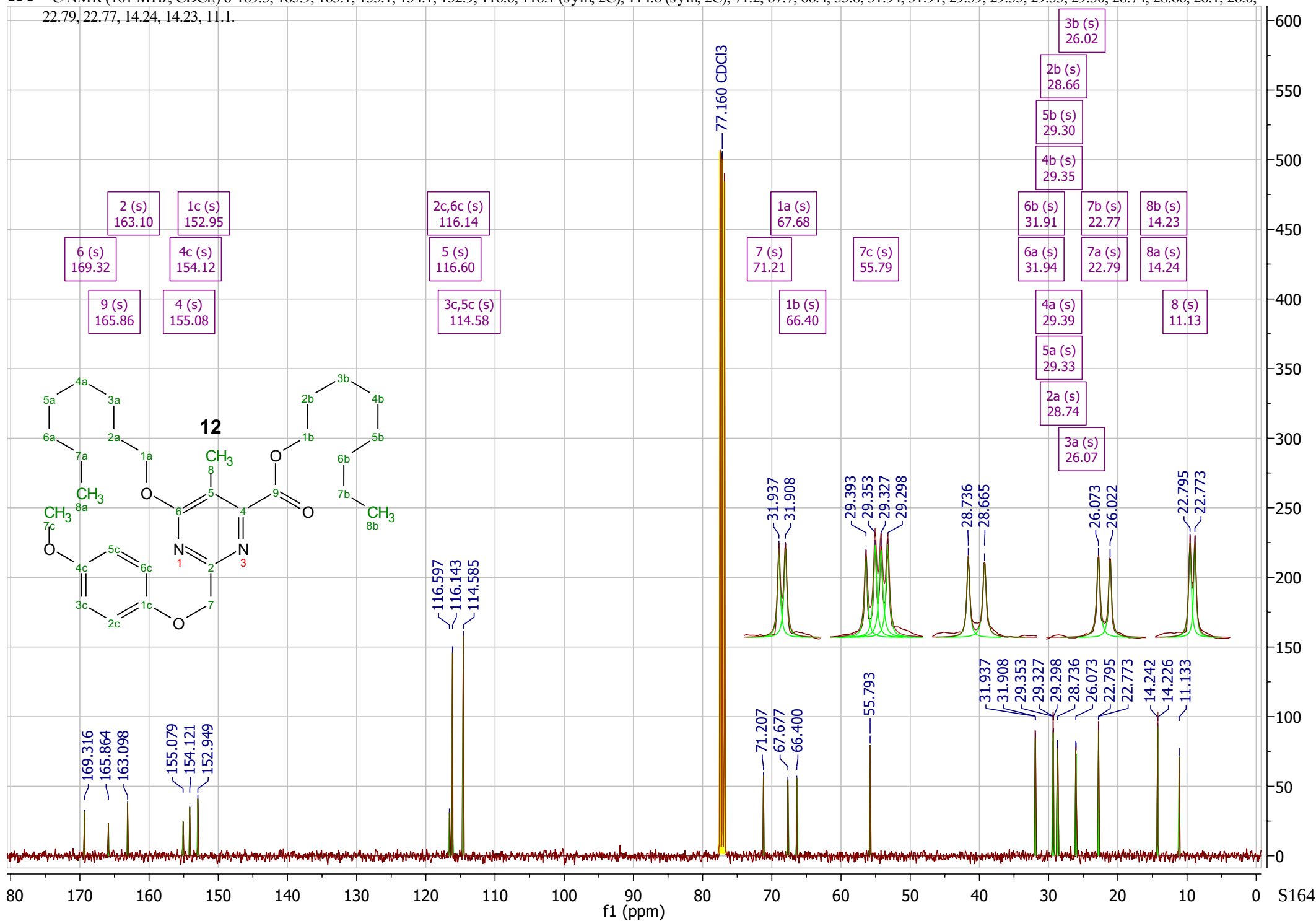


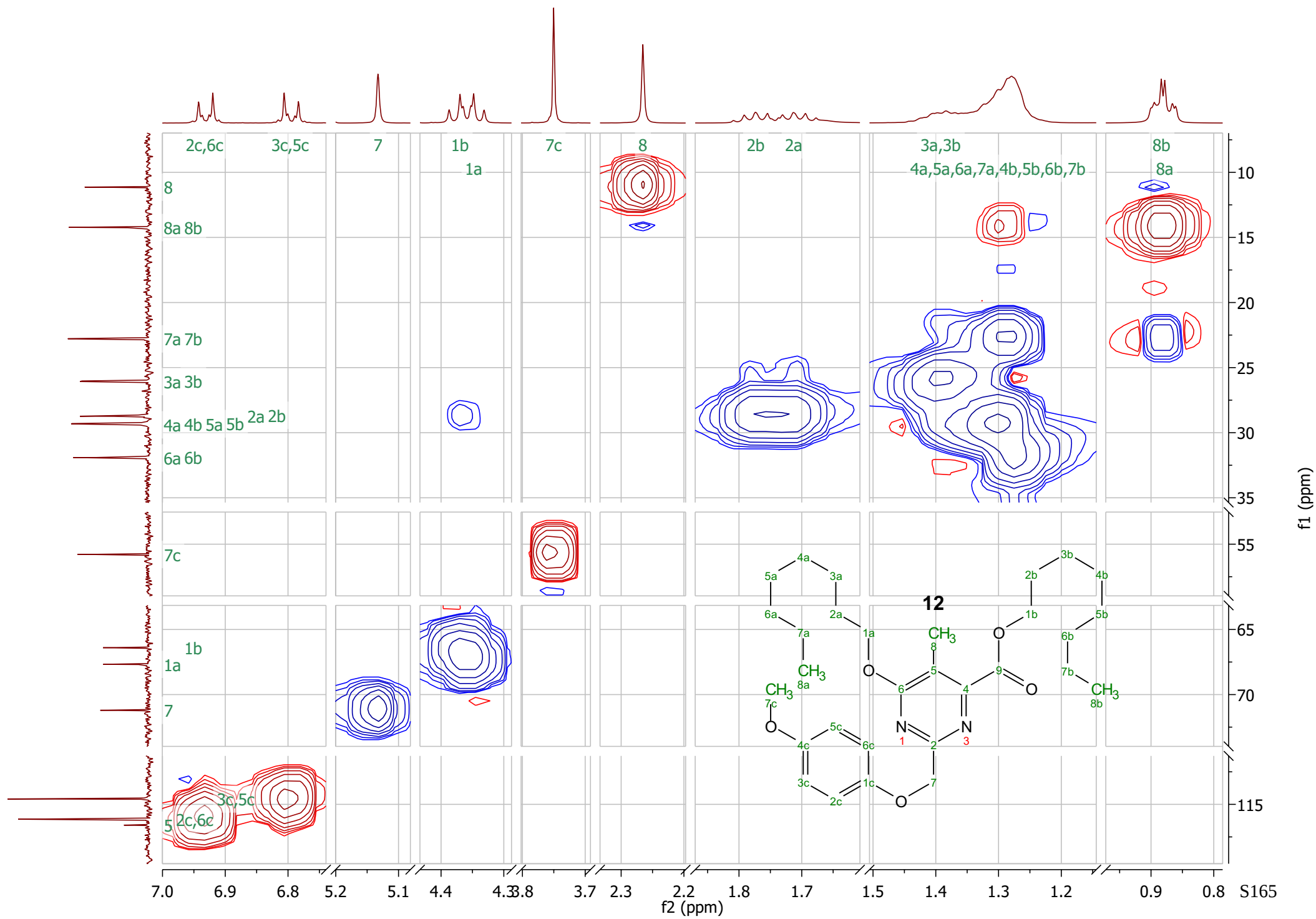


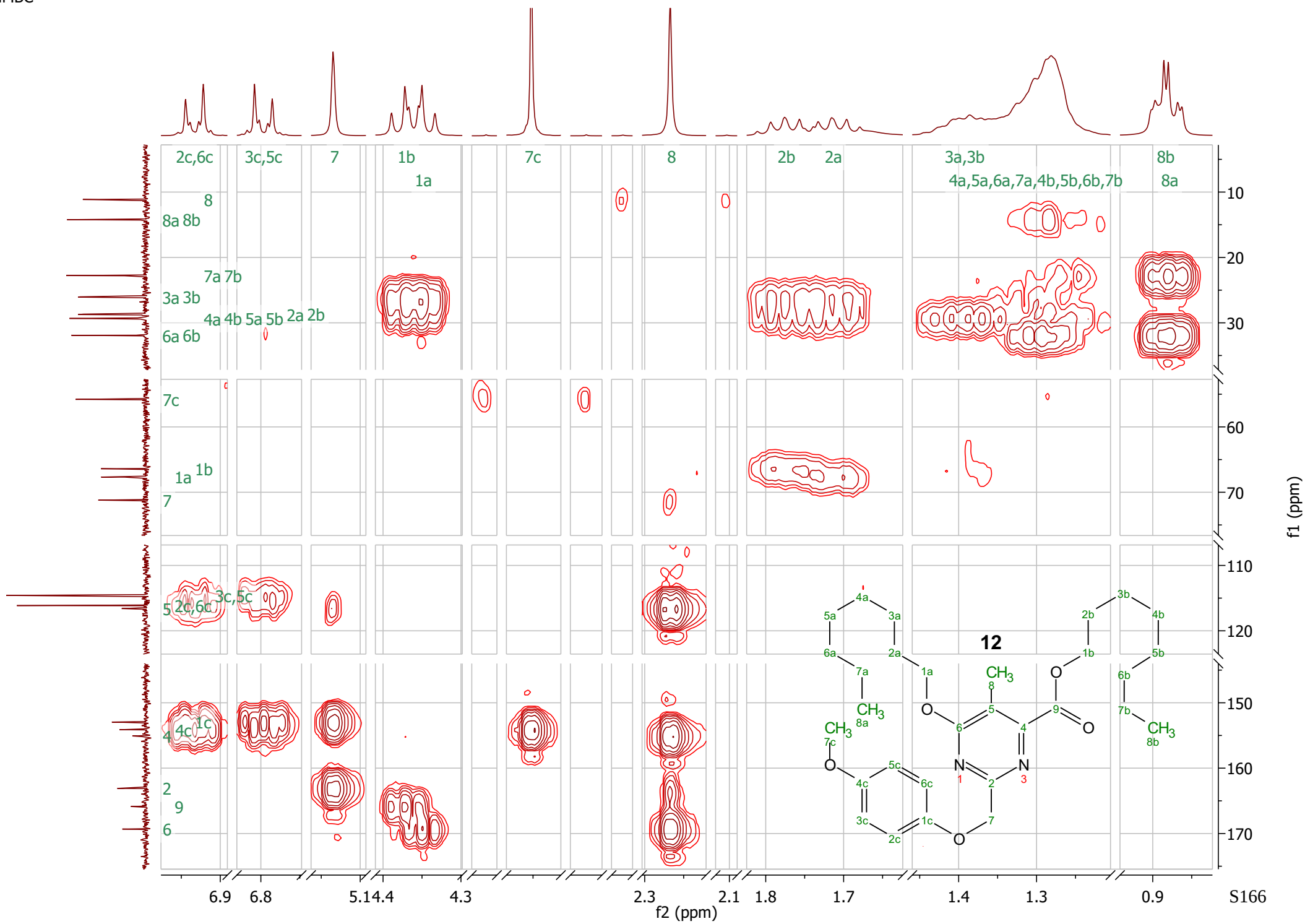
^1H NMR (400 MHz, CDCl_3) δ 7.02 – 6.86 (m, 2H), 6.86 – 6.69 (m, 2H), 5.13 (s, 2H), 4.37 (t, J = 6.8 Hz, 2H), 4.35 (t, J = 6.6 Hz, 2H), 3.75 (s, 3H), 2.27 (s, 3H), 1.77 (quint, J = 7.0 Hz, 2H), 1.71 (quint, J = 7.1 Hz, 2H), 1.47 – 1.33 (m, 4H), 1.35 – 1.19 (m, 16H), 0.88 (app t, J = 6.7 Hz, 3H), 0.88 (app t, J = 6.9 Hz, 3H).



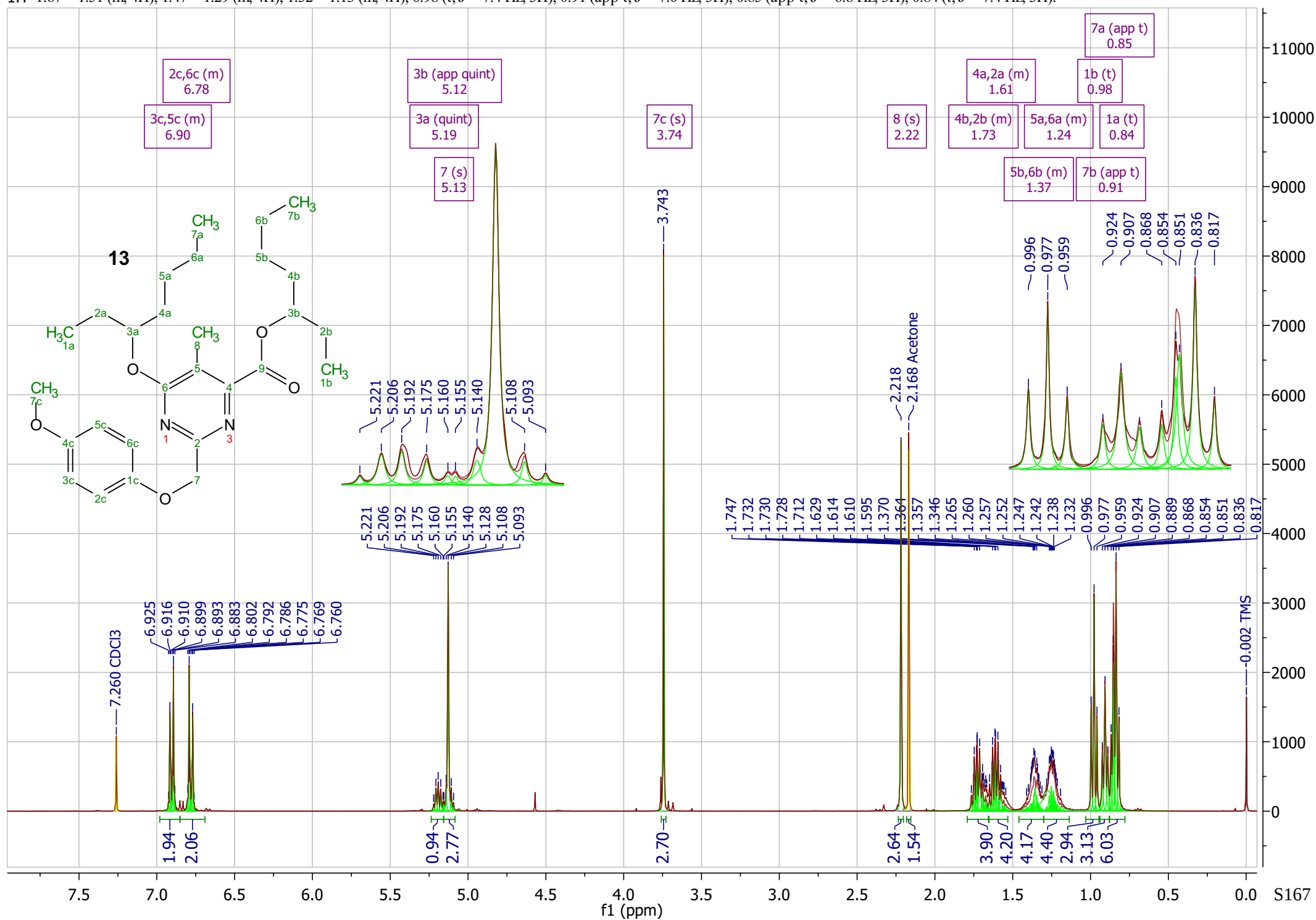
¹³C ¹³C NMR (101 MHz, CDCl₃) δ 169.3, 165.9, 163.1, 155.1, 154.1, 152.9, 116.6, 116.1 (sym, 2C), 114.6 (sym, 2C), 71.2, 67.7, 66.4, 55.8, 31.94, 31.91, 29.39, 29.35, 29.33, 29.30, 28.74, 28.66, 26.1, 26.0, 22.79, 22.77, 14.24, 14.23, 11.1.





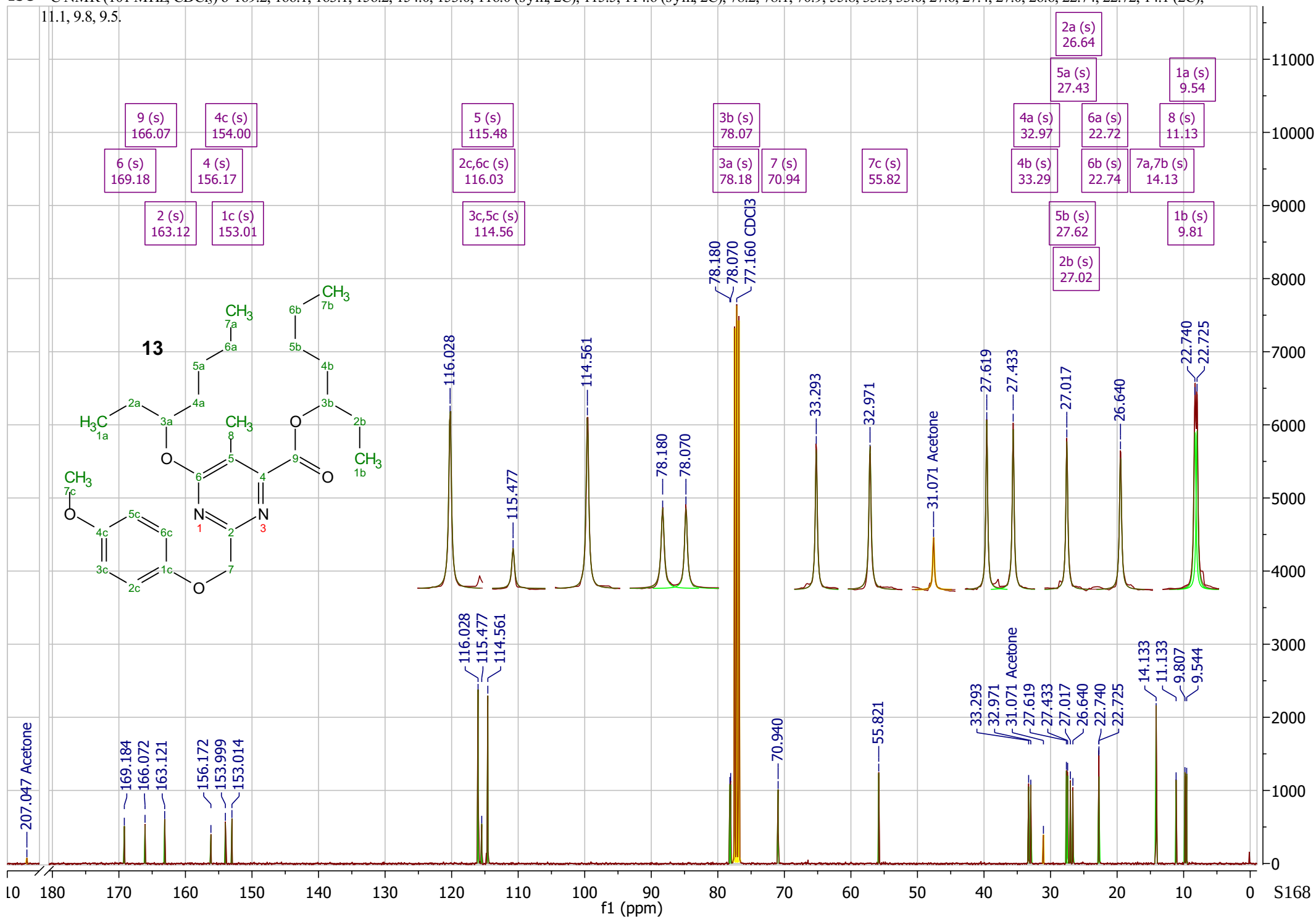


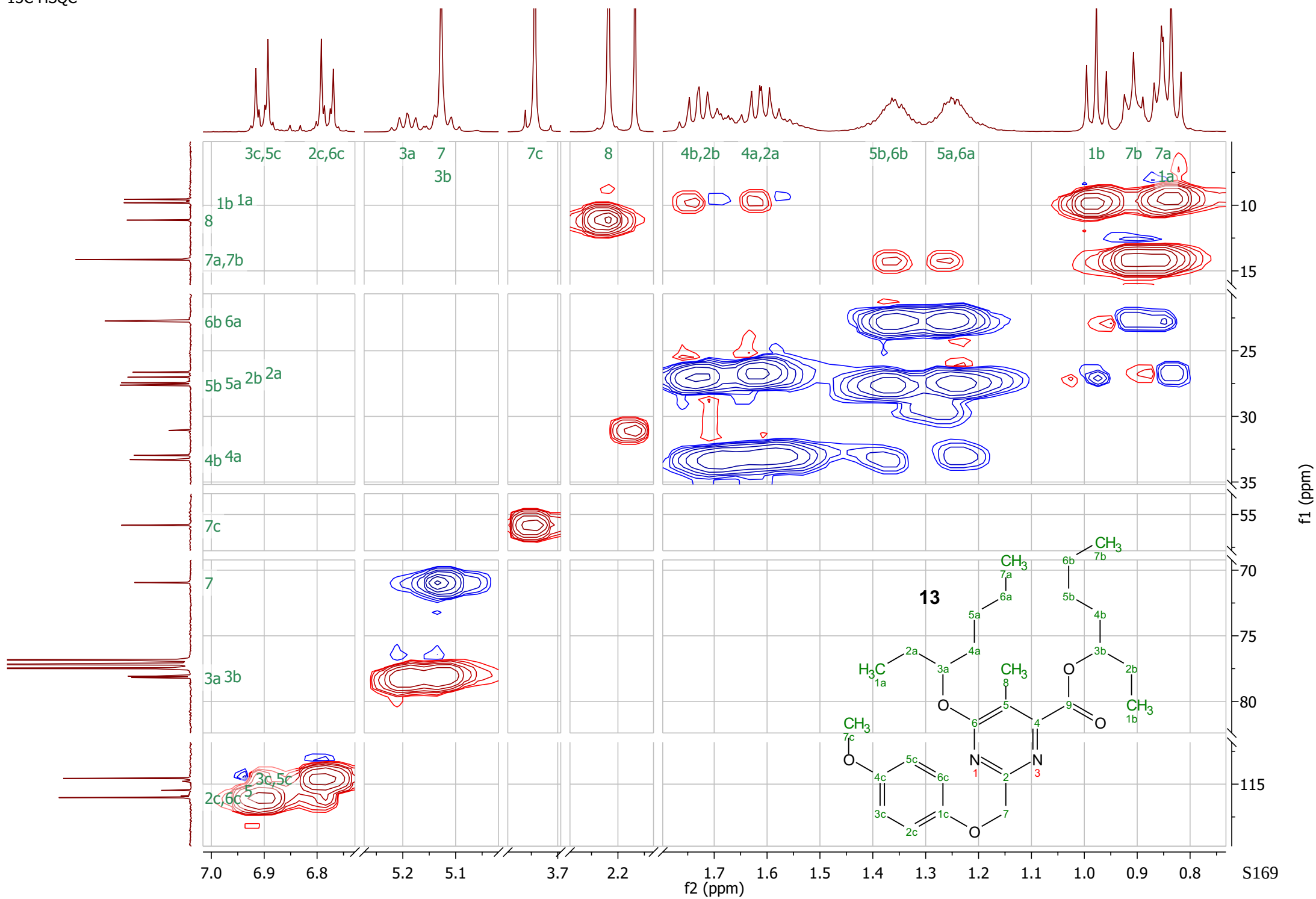
¹H NMR (400 MHz, CDCl₃) δ 6.98 – 6.84 (m, 2H), 6.84 – 6.69 (m, 2H), 5.13 (s, 2H), 5.12 (app quint, *J* = 5.9 Hz, 1H), 3.74 (s, 2H), 2.22 (s, 3H), 1.79 – 1.63 (m, 4H), 1H 1.67 – 1.51 (m, 4H), 1.47 – 1.29 (m, 4H), 1.32 – 1.13 (m, 4H), 0.98 (t, *J* = 7.4 Hz, 3H), 0.91 (app t, *J* = 7.0 Hz, 3H), 0.85 (app t, *J* = 6.8 Hz, 3H), 0.84 (t, *J* = 7.4 Hz, 3H).

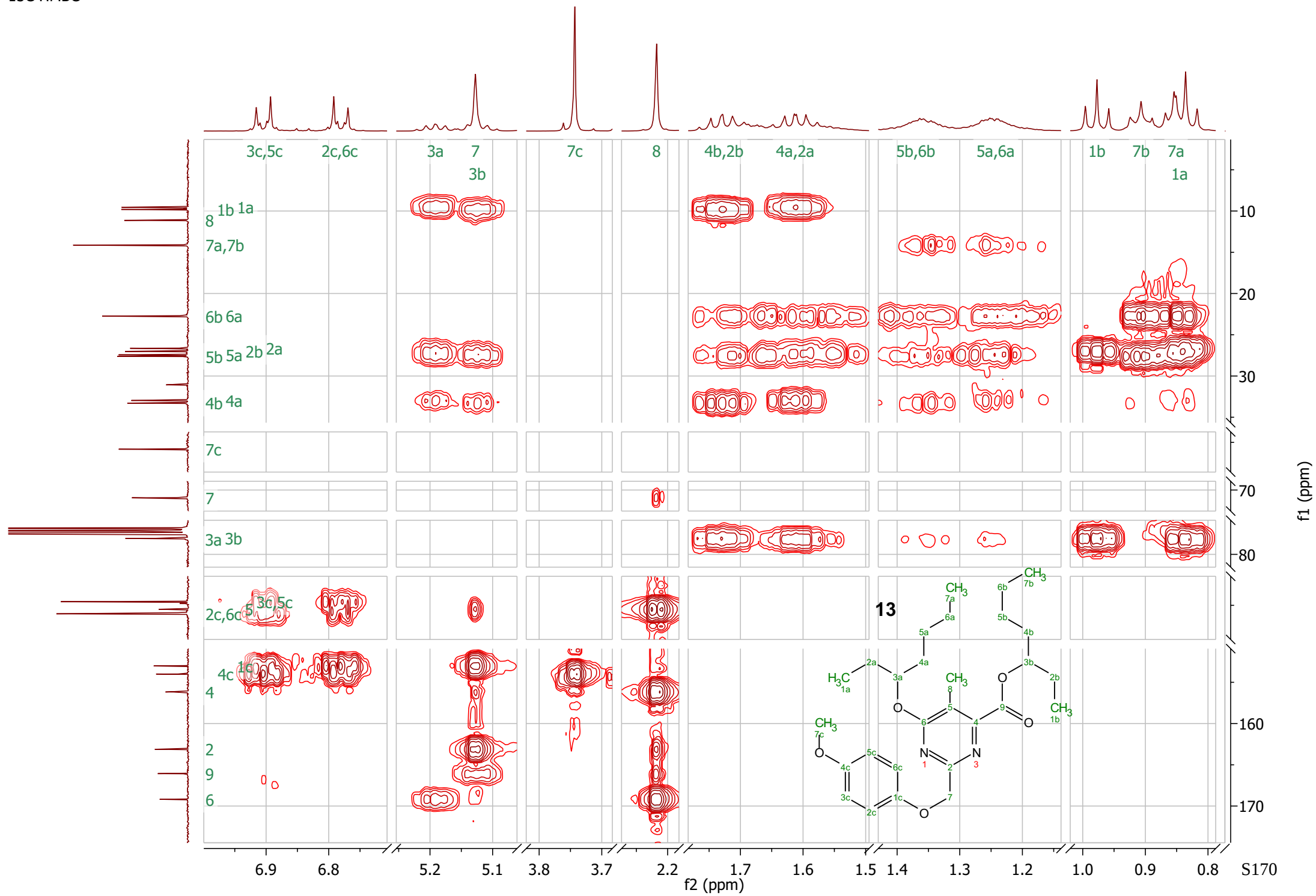


^{13}C NMR (101 MHz, CDCl_3) δ 169.2, 166.1, 163.1, 156.2, 154.0, 153.0, 116.0 (sym, 2C), 115.5, 114.6 (sym, 2C), 78.2, 78.1, 70.9, 55.8, 33.3, 33.0, 27.6, 27.4, 27.0, 26.6, 22.74, 22.72, 14.1 (2C),

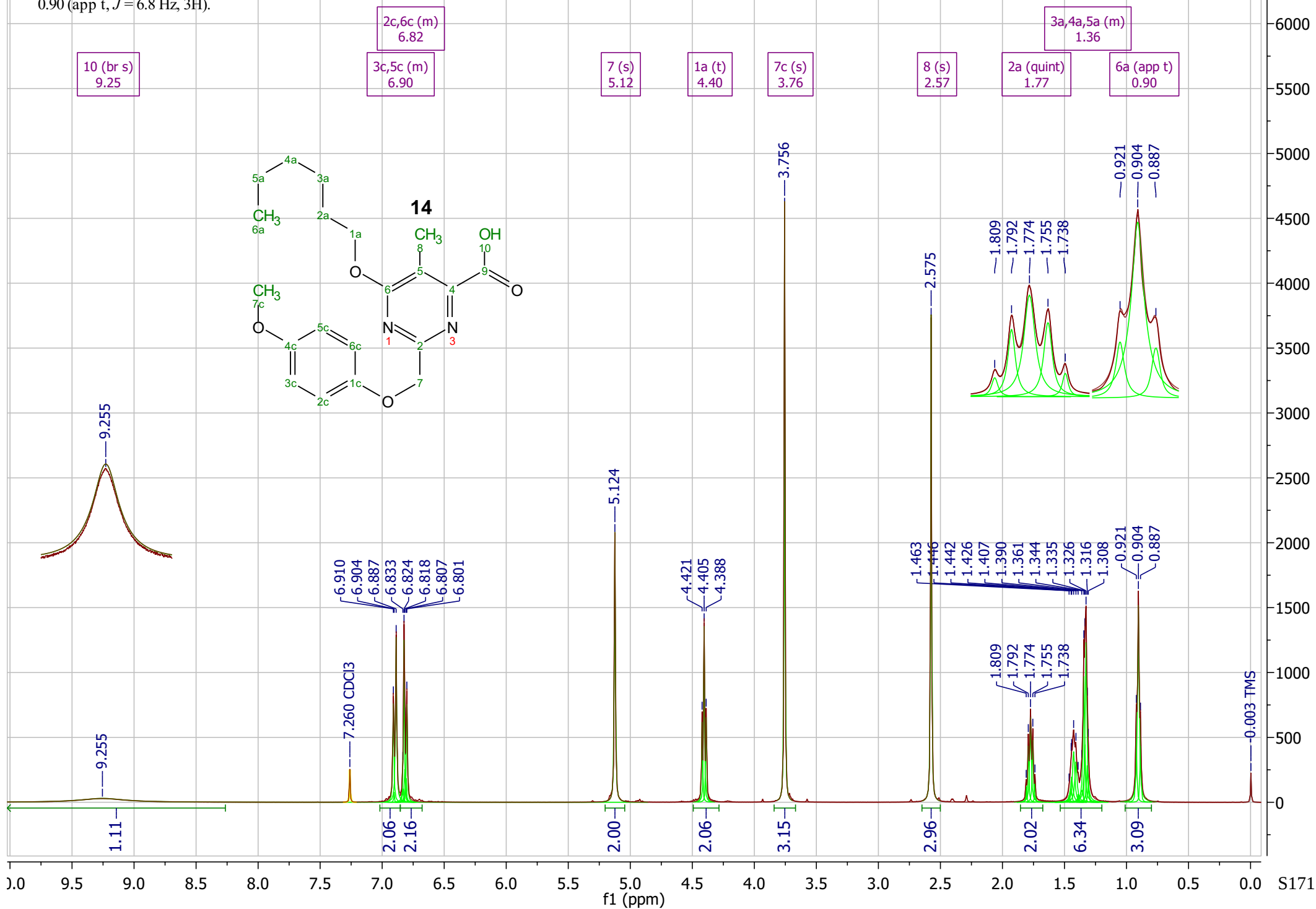
11.1, 9.8, 9.5.



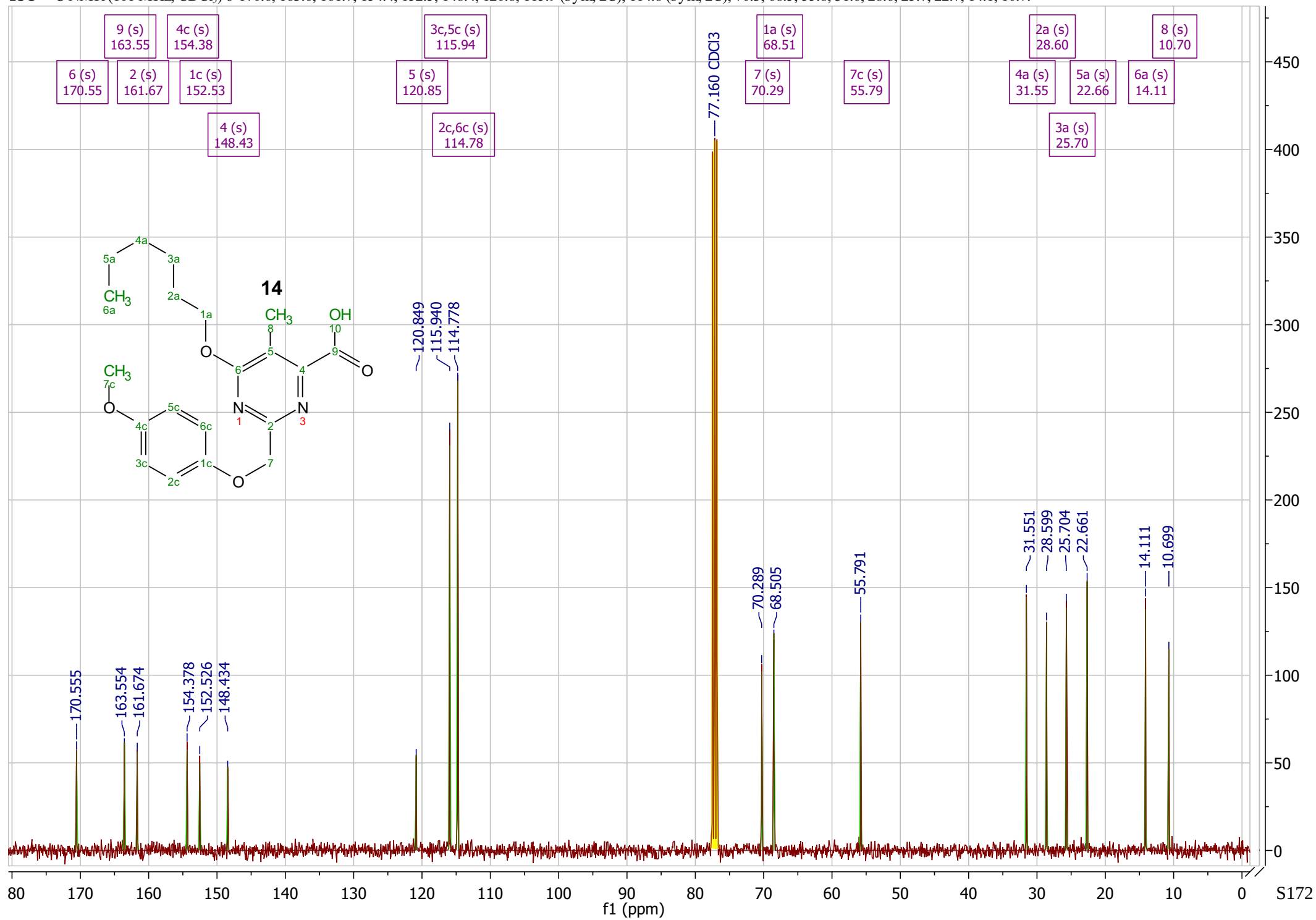


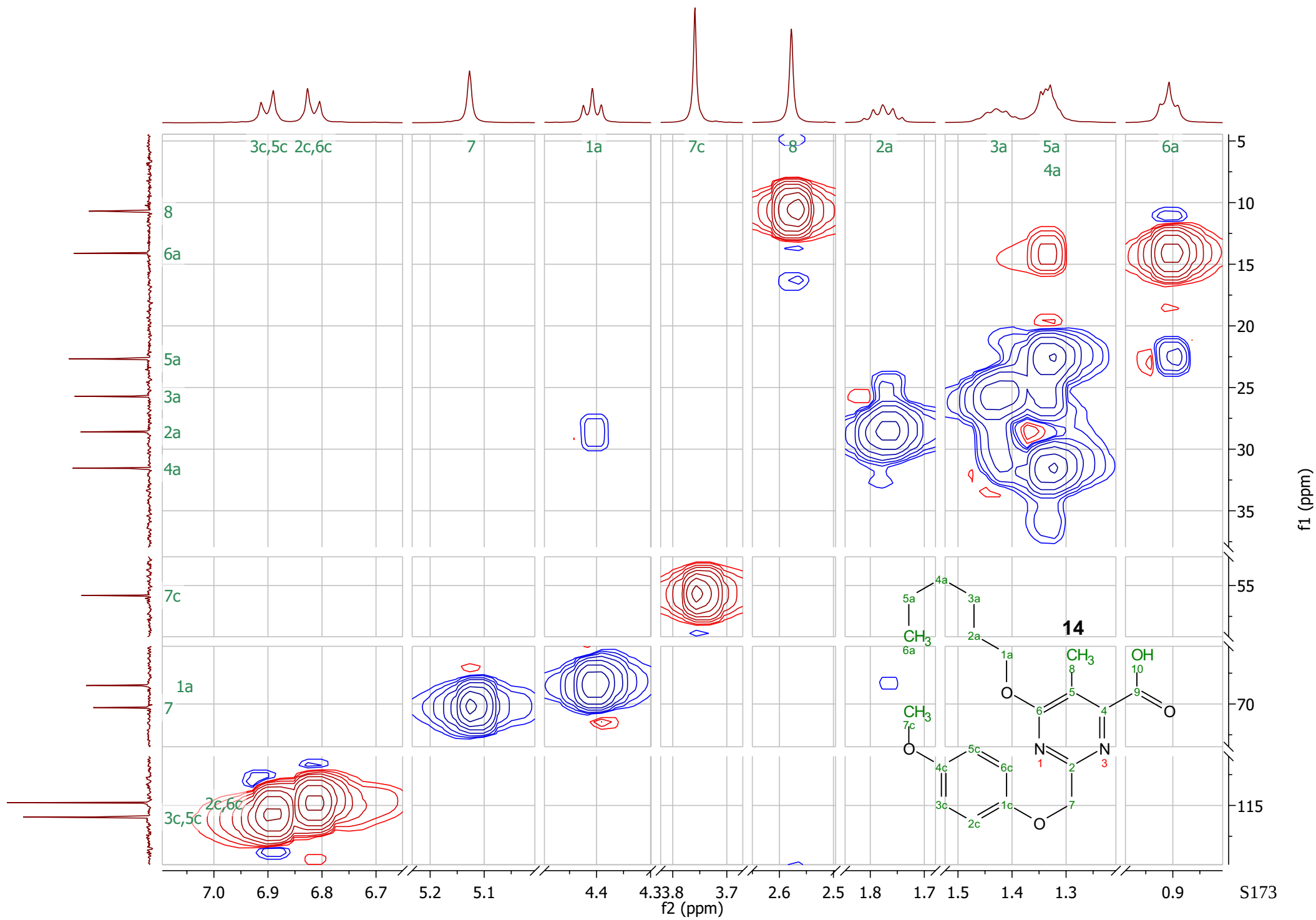


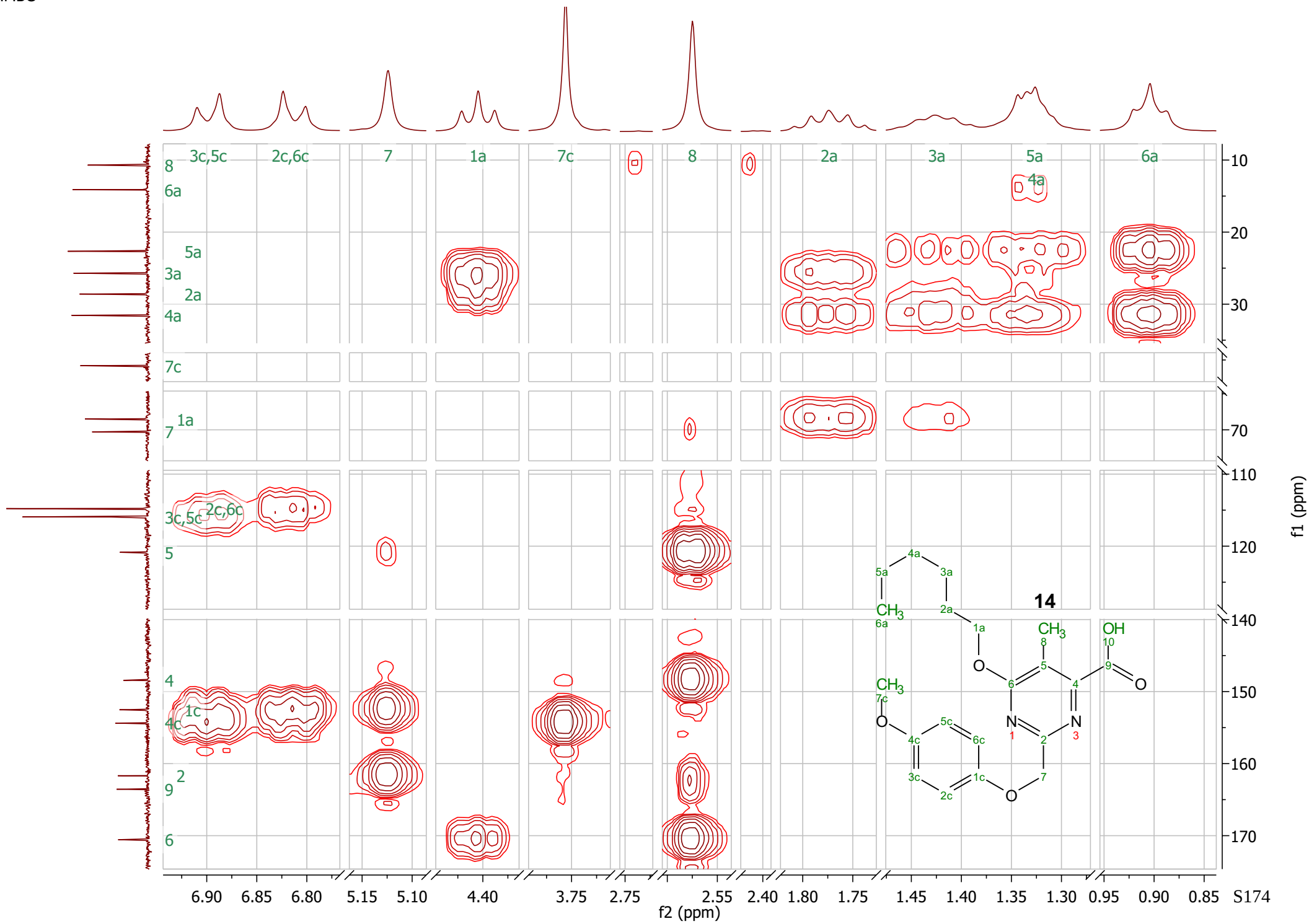
^1H NMR (400 MHz, CDCl_3) δ 9.25 (br s, 1H), 7.02 – 6.85 (m, 2H), 6.85 – 6.68 (m, 2H), 5.12 (s, 2H), 4.40 (t, $J = 6.6$ Hz, 2H), 3.76 (s, 3H), 2.57 (s, 3H), 1.77 (quint, $J = 6.8$ Hz, 2H), 1.53 – 1.20 (m, 6H), 0.90 (app t, $J = 6.8$ Hz, 3H).



13C ^{13}C NMR (101 MHz, CDCl_3) δ 170.6, 163.6, 161.7, 154.4, 152.5, 148.4, 120.8, 115.9 (sym, 2C), 114.8 (sym, 2C), 70.3, 68.5, 55.8, 31.6, 28.6, 25.7, 22.7, 14.1, 10.7.

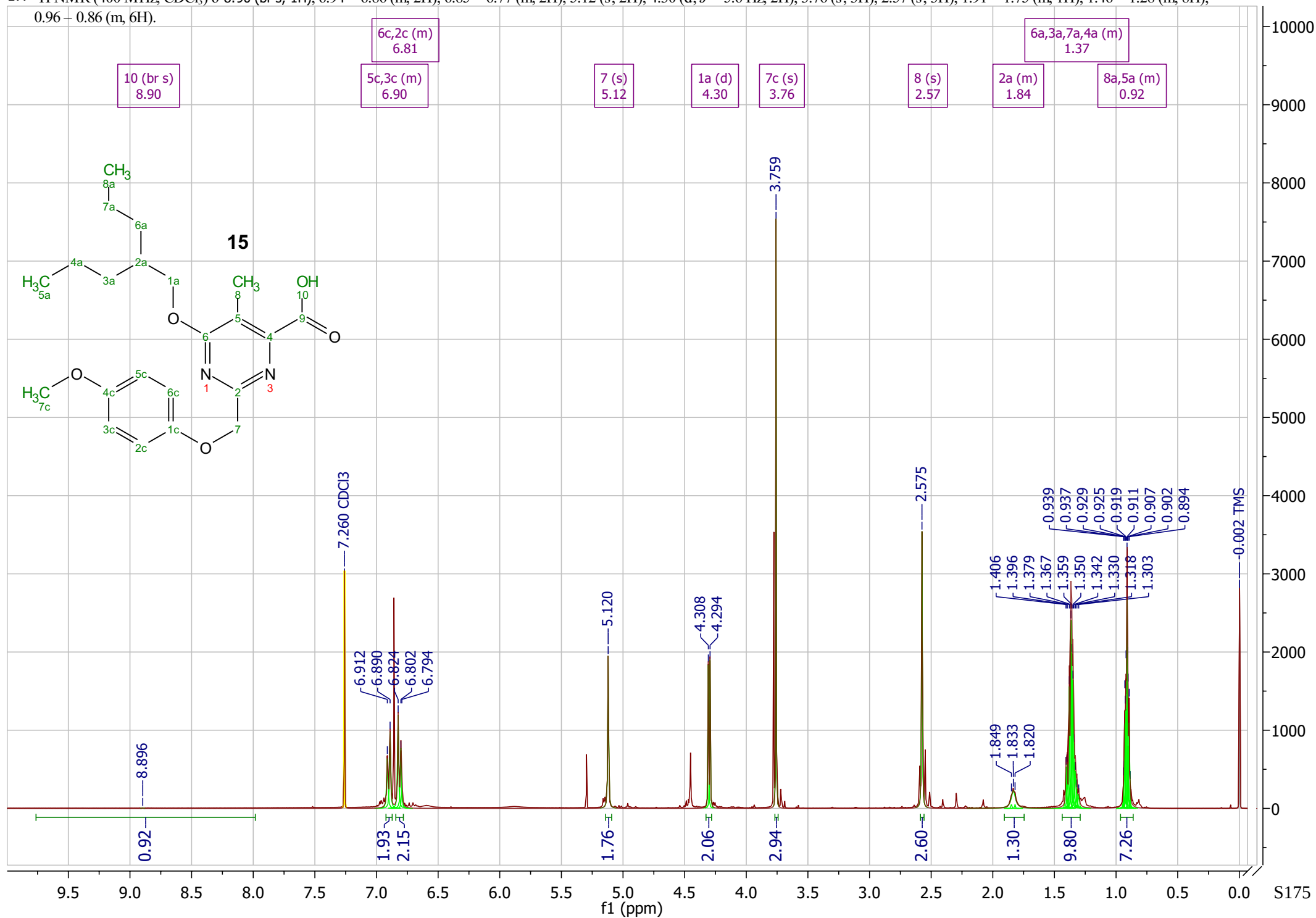
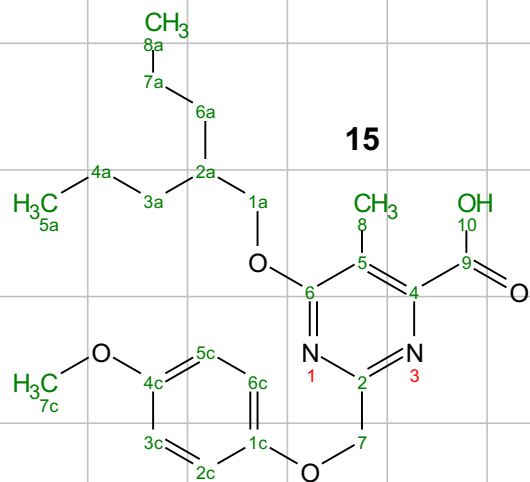




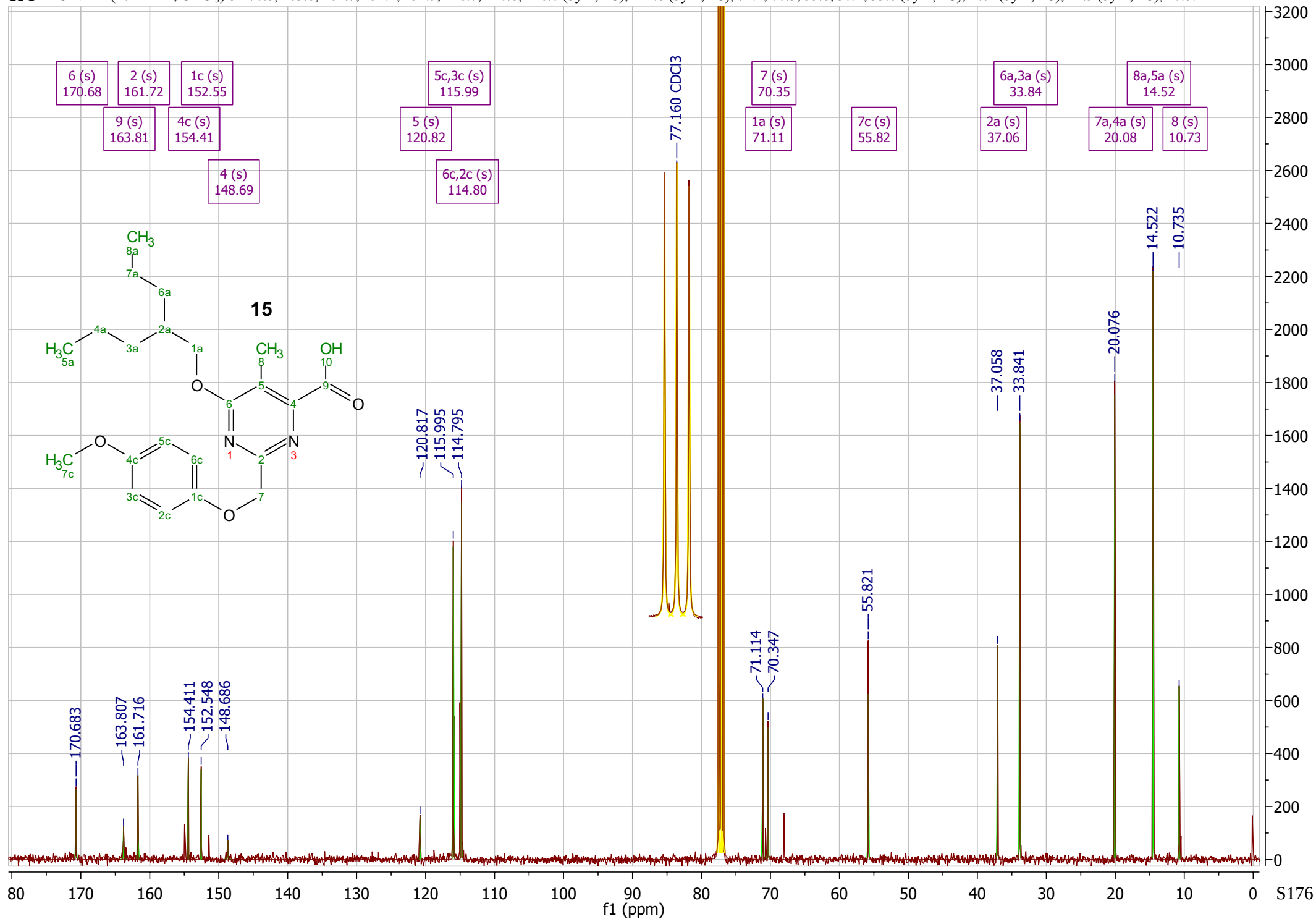


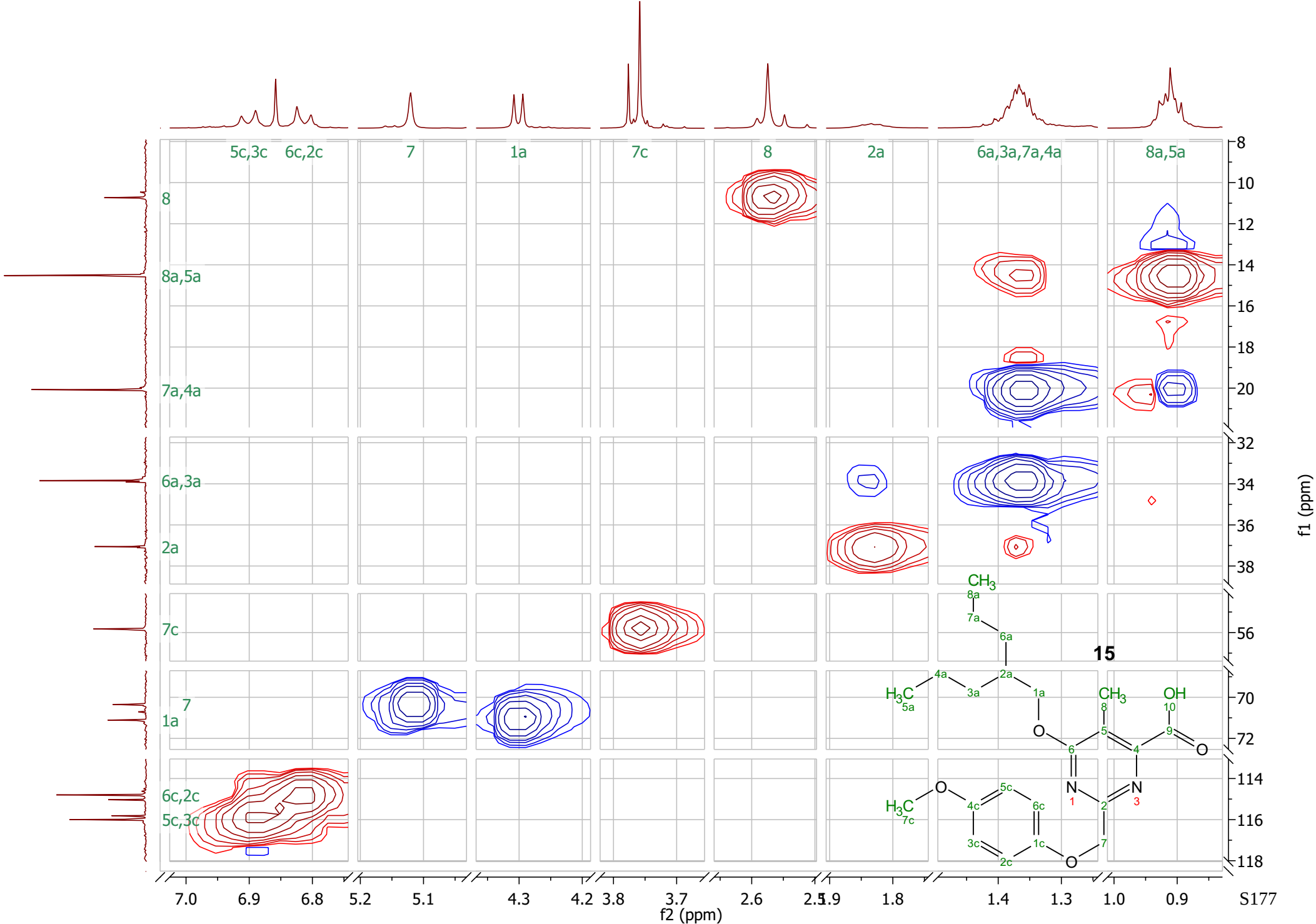
^1H NMR (400 MHz, CDCl_3) δ 8.90 (br s, 1H), 6.94 – 6.86 (m, 2H), 6.85 – 6.77 (m, 2H), 5.12 (s, 2H), 4.30 (d, $J = 5.6$ Hz, 2H), 3.76 (s, 3H), 2.57 (s, 3H), 1.91 – 1.75 (m, 1H), 1.46 – 1.28 (m, 8H),

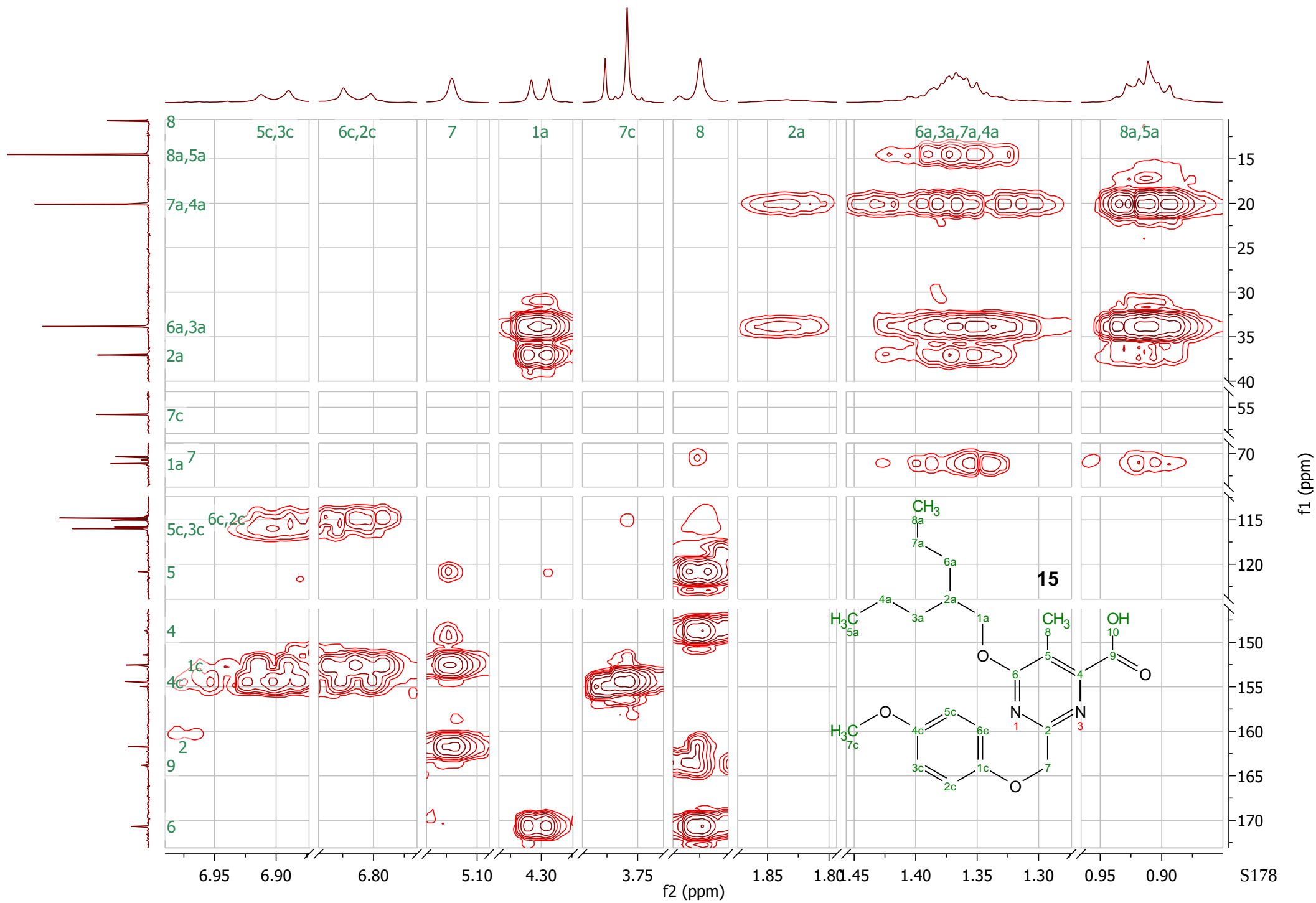
0.96 – 0.86 (m, 6H).



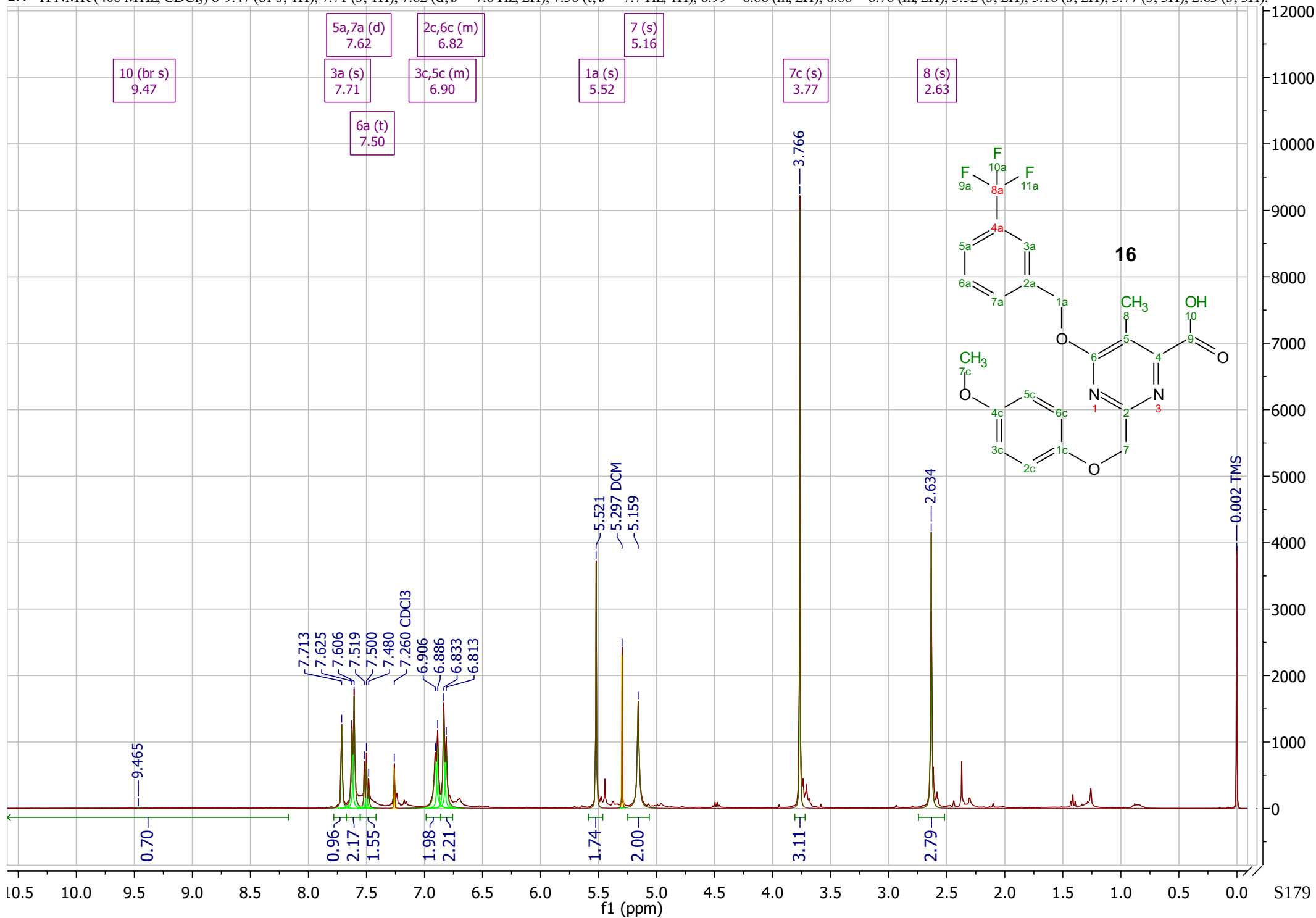
13C ^{13}C NMR (101 MHz, CDCl_3) δ 170.7, 163.8, 161.7, 154.4, 152.5, 148.7, 120.8, 116.0 (sym, 2C), 114.8 (sym, 2C), 71.1, 70.3, 55.8, 37.1, 33.8 (sym, 2C), 20.1 (sym, 2C), 14.5 (sym, 2C), 10.7.



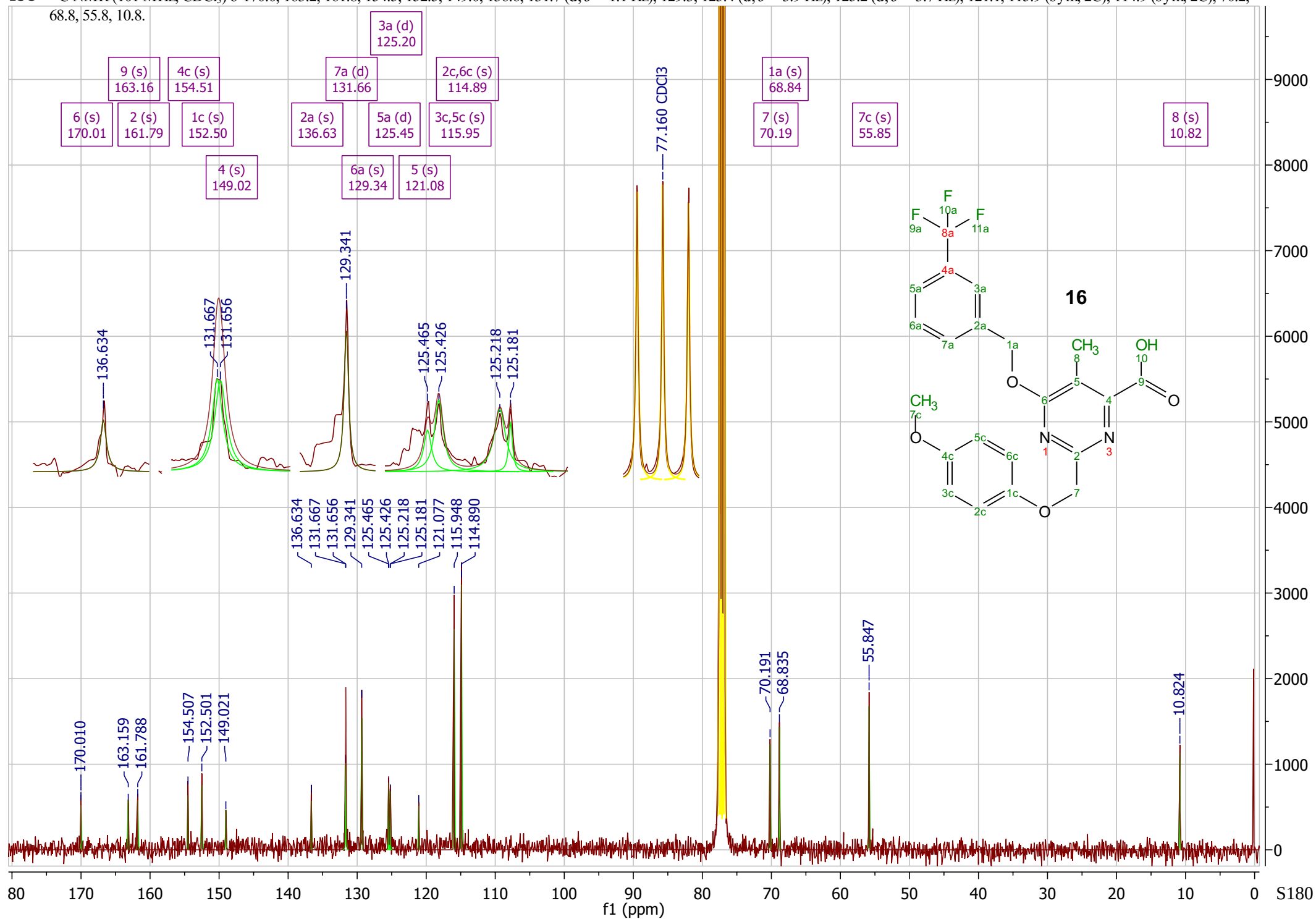


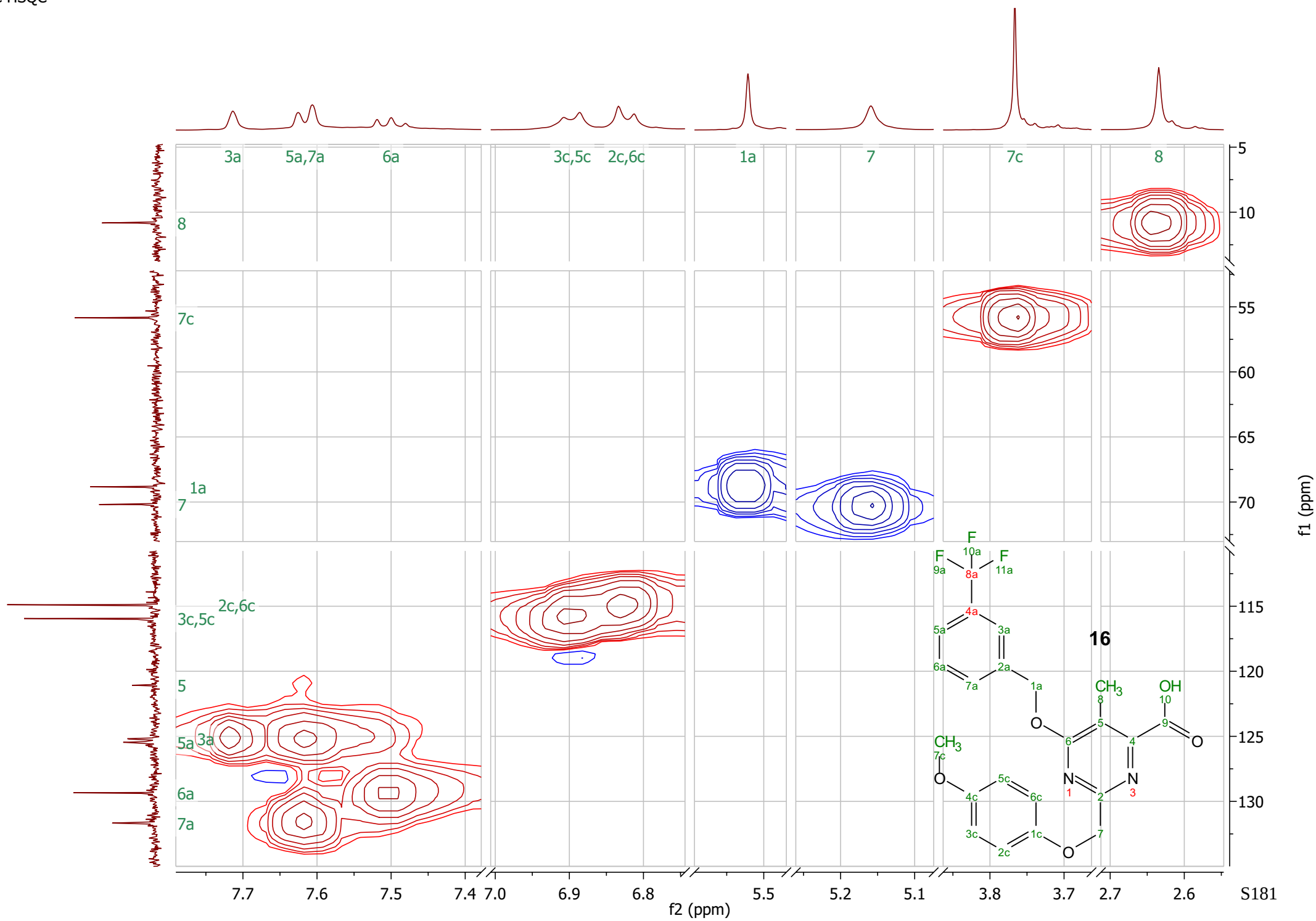


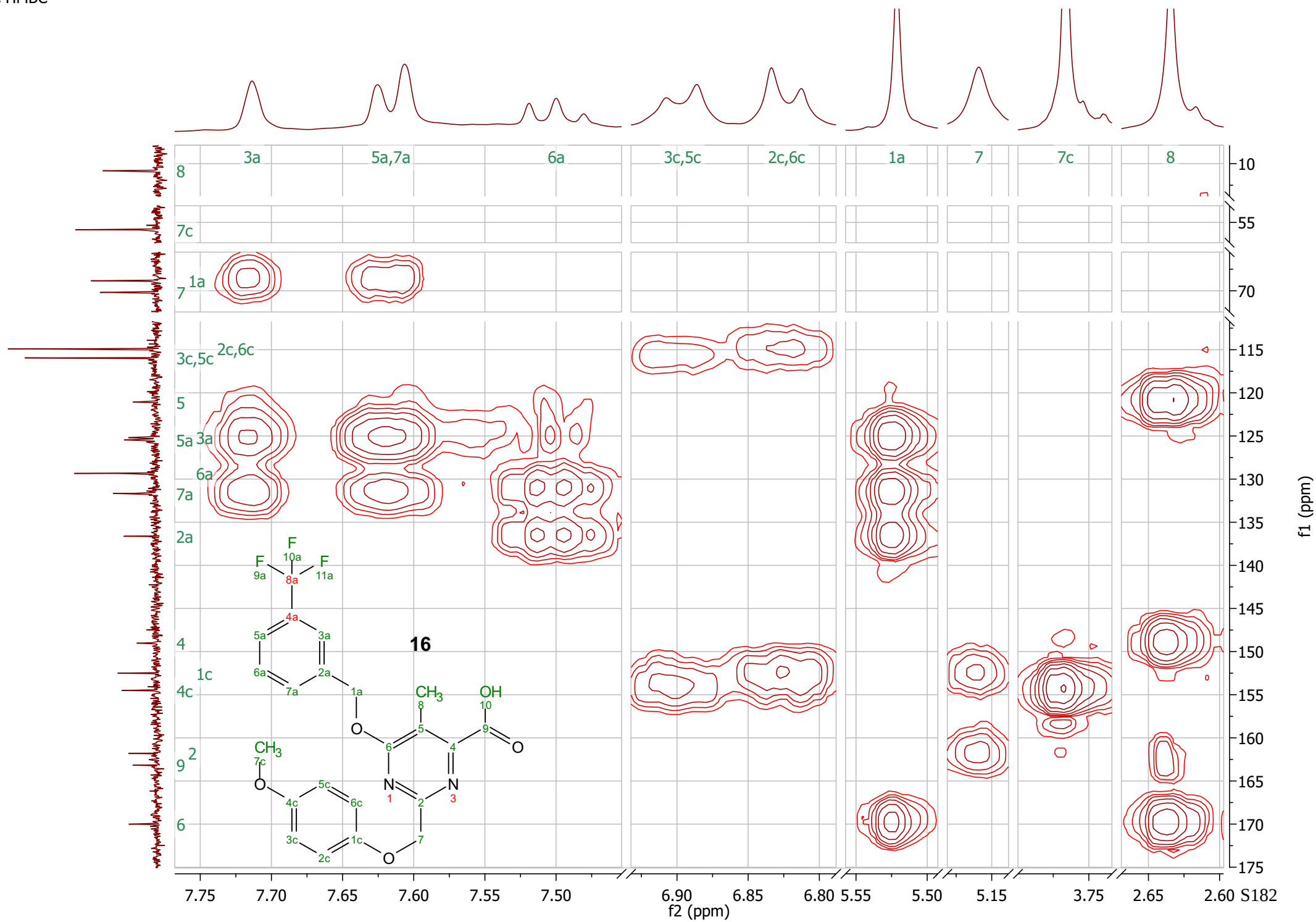
^1H NMR (400 MHz, CDCl_3) δ 9.47 (br s, 1H), 7.71 (s, 1H), 7.62 (d, $J = 7.6$ Hz, 2H), 7.50 (t, $J = 7.7$ Hz, 1H), 6.99 – 6.86 (m, 2H), 6.86 – 6.76 (m, 2H), 5.52 (s, 2H), 5.16 (s, 2H), 3.77 (s, 3H), 2.63 (s, 3H).



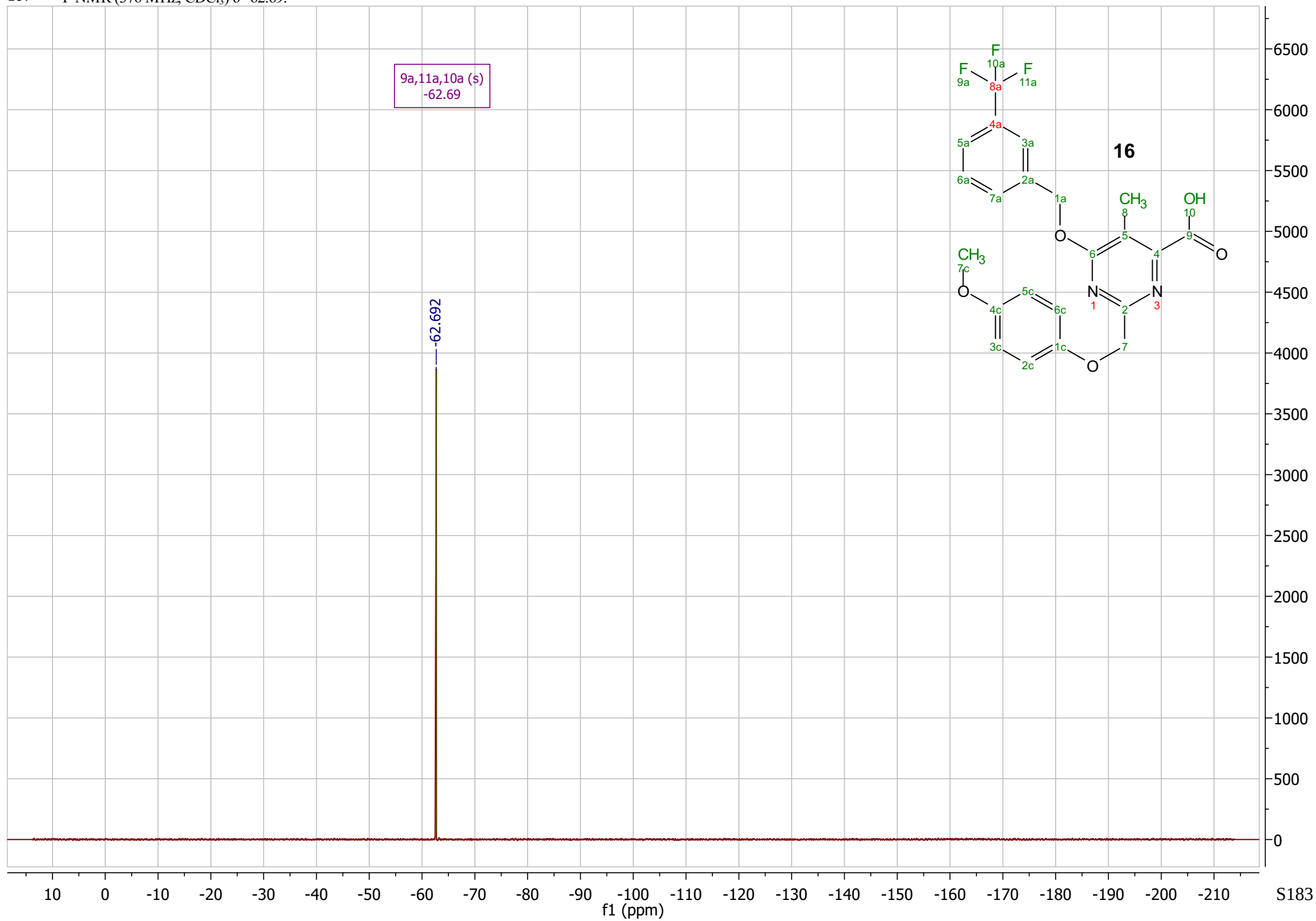
¹³C ¹³C NMR (101 MHz, CDCl₃) δ 170.0, 163.2, 161.8, 154.5, 152.5, 149.0, 136.6, 131.7 (d, *J* = 1.1 Hz), 129.3, 125.4 (d, *J* = 3.9 Hz), 125.2 (d, *J* = 3.7 Hz), 121.1, 115.9 (sym, 2C), 114.9 (sym, 2C), 70.2, 68.8, 55.8, 10.8.



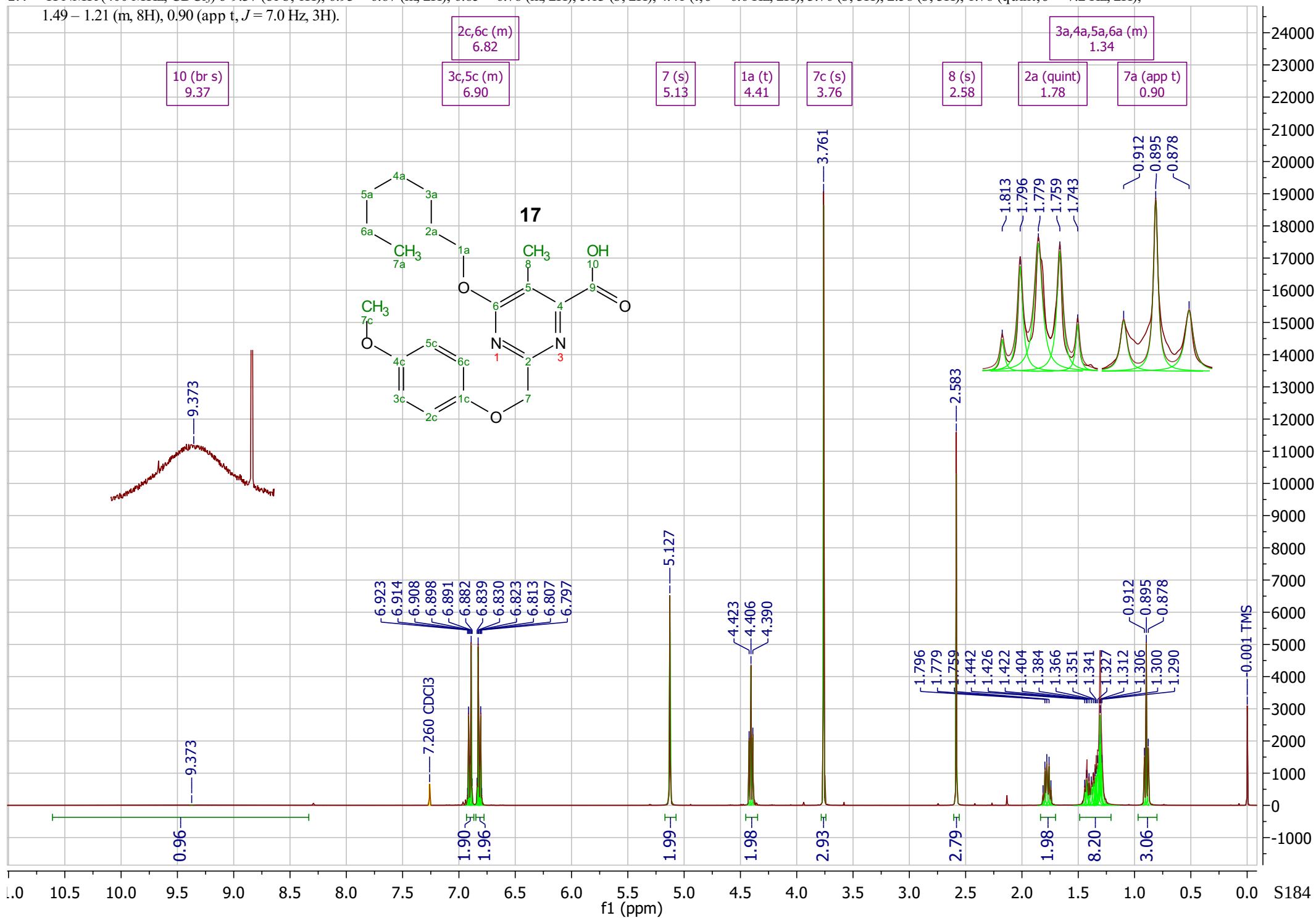




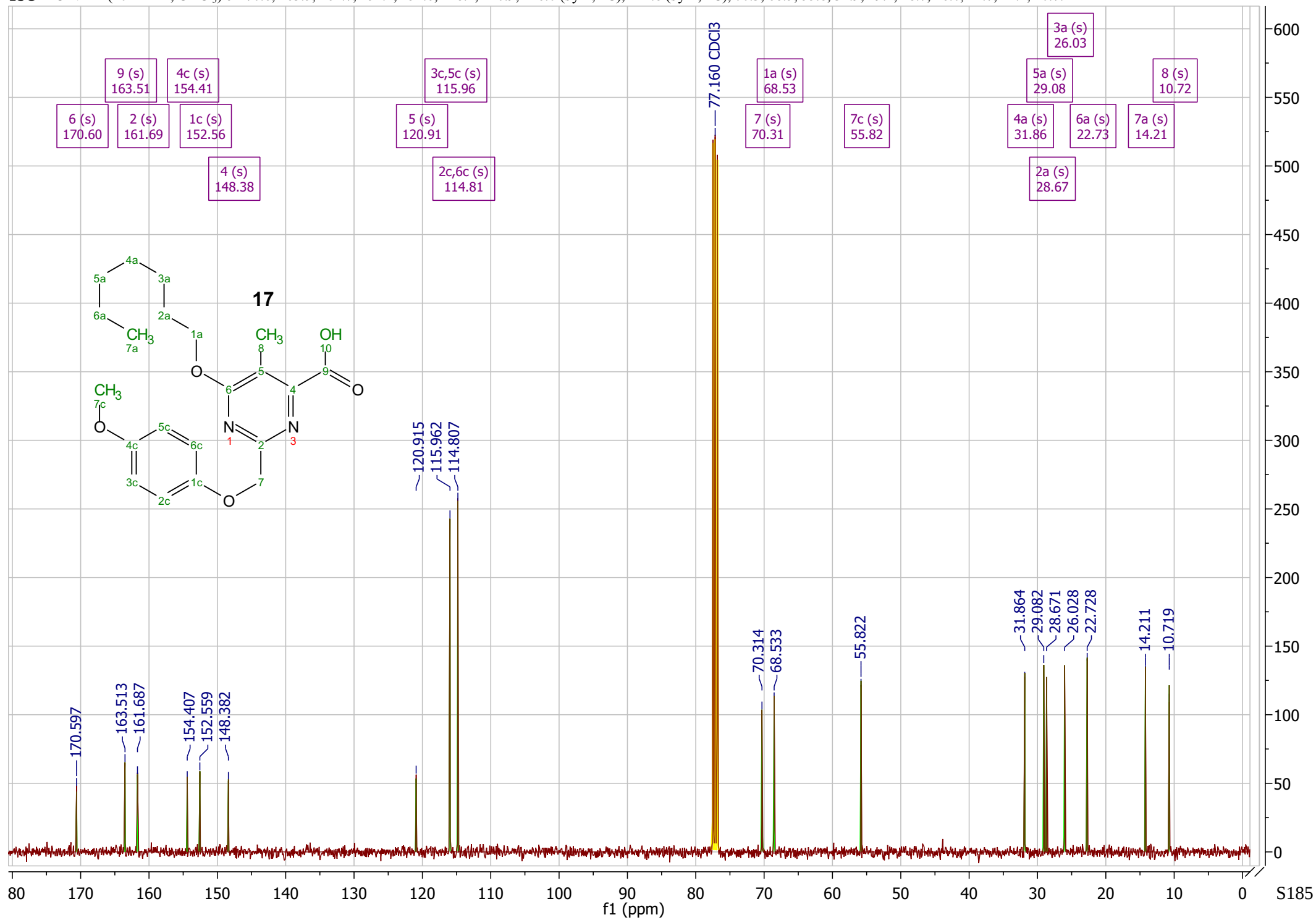
19F ^{19}F NMR (376 MHz, CDCl_3) δ -62.69.

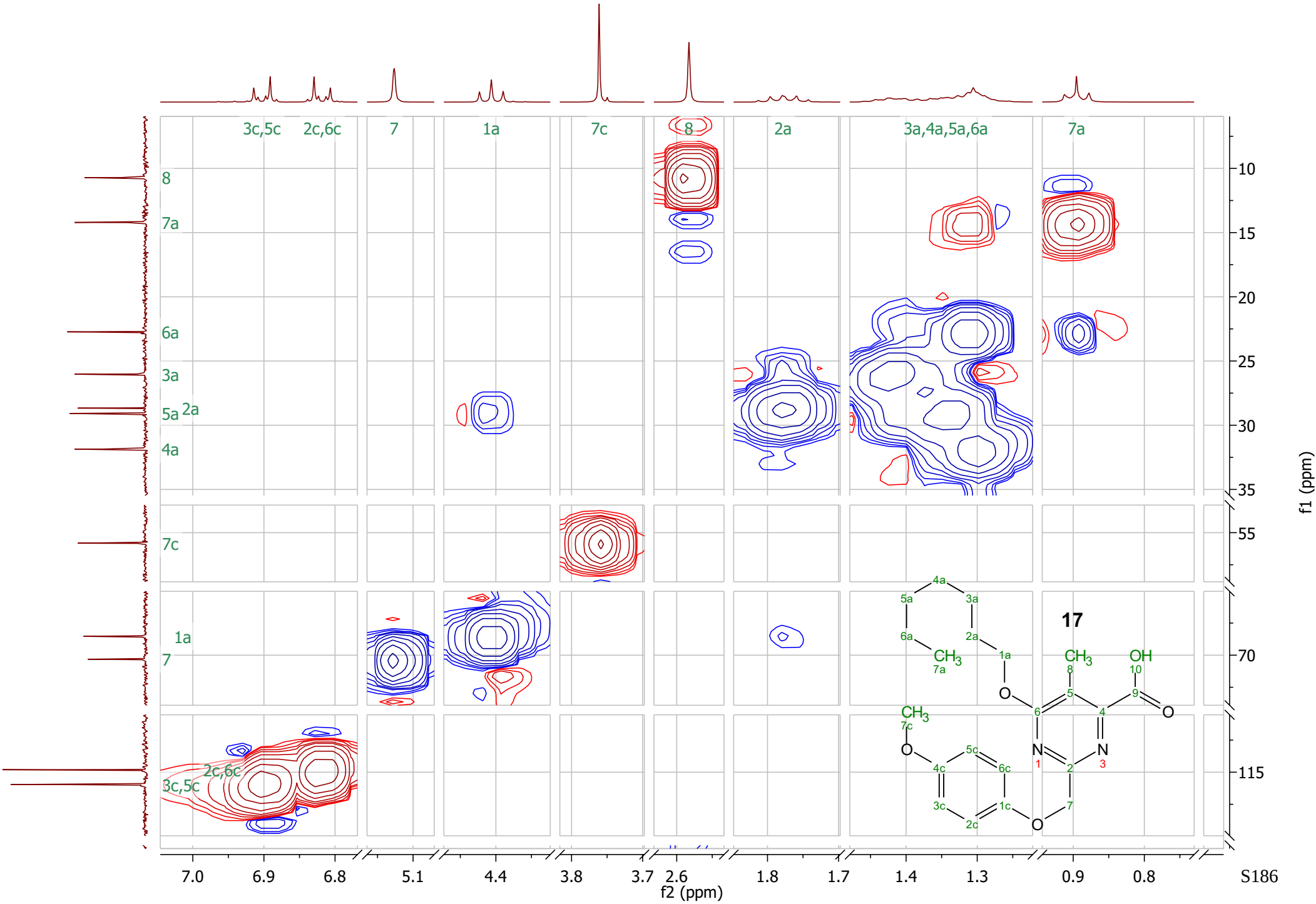


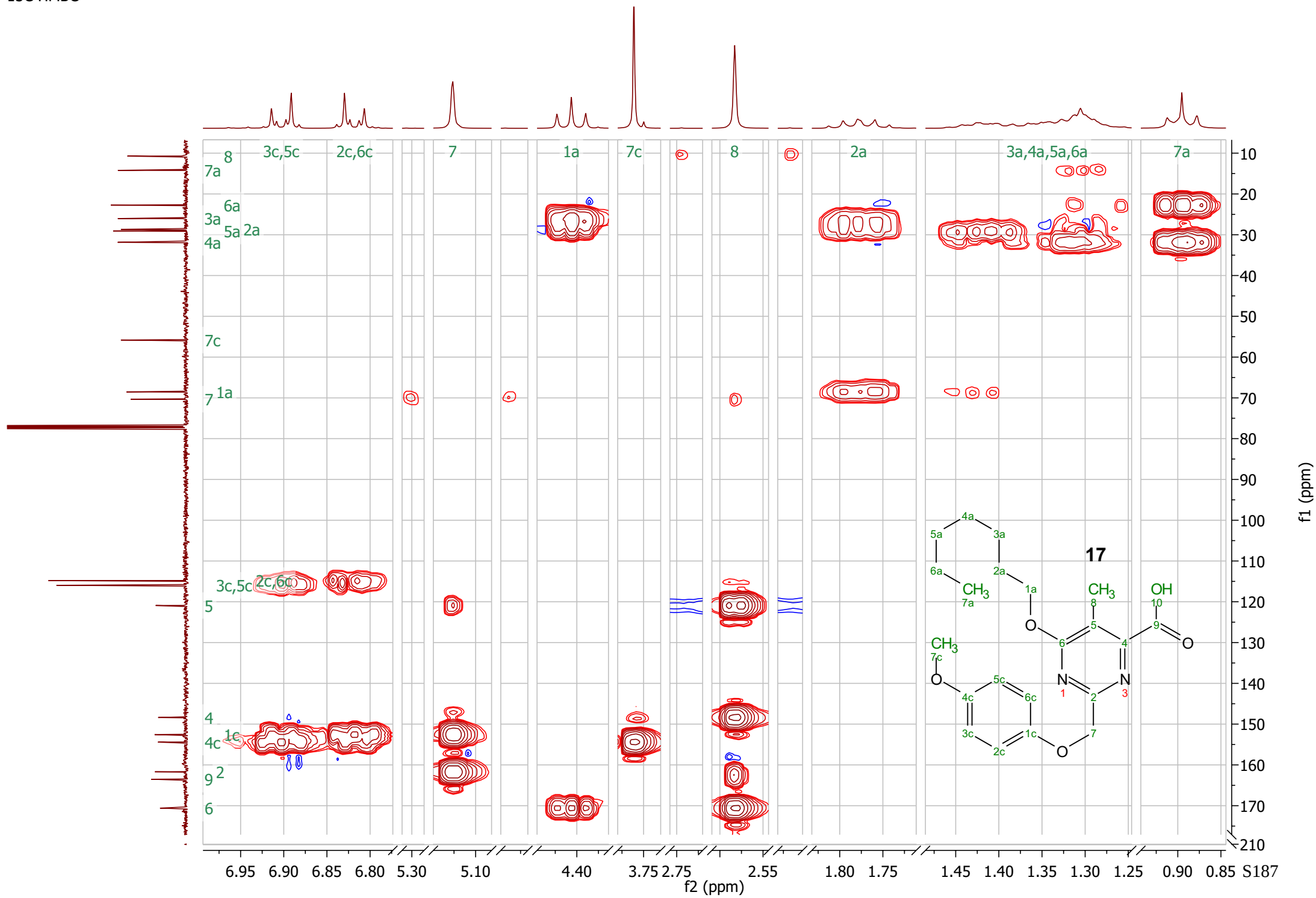
^1H NMR (400 MHz, CDCl_3) δ 9.37 (br s, 1H), 6.93 – 6.87 (m, 2H), 6.85 – 6.78 (m, 2H), 5.13 (s, 2H), 4.41 (t, $J = 6.6$ Hz, 2H), 3.76 (s, 3H), 2.58 (s, 3H), 1.78 (quint, $J = 7.2$ Hz, 2H), 1.49 – 1.21 (m, 8H), 0.90 (app t, $J = 7.0$ Hz, 3H).



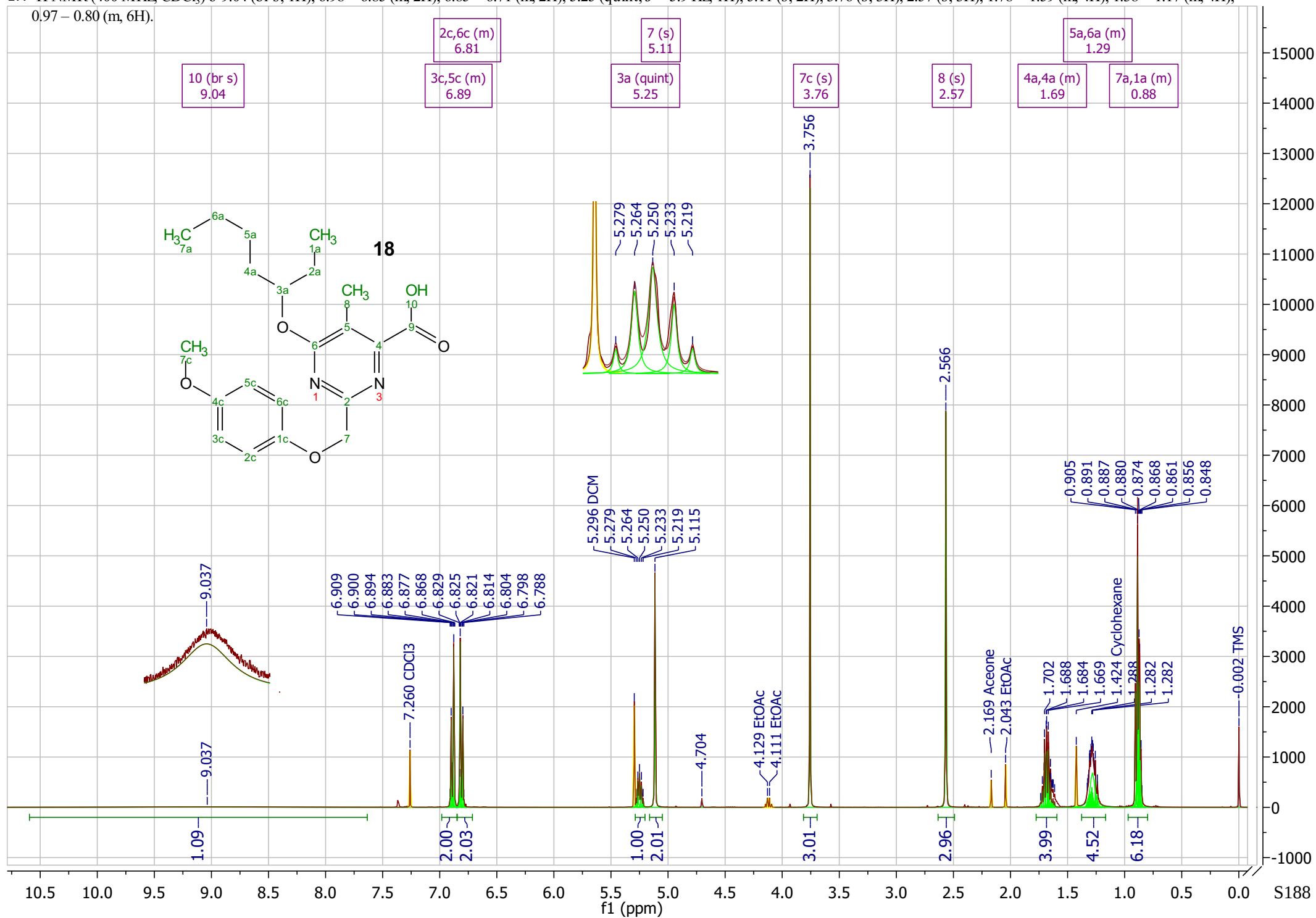
13C ¹³C NMR (101 MHz, CDCl₃) δ 170.6, 163.5, 161.7, 154.4, 152.6, 148.4, 120.9, 116.0 (sym, 2C), 114.8 (sym, 2C), 70.3, 68.5, 55.8, 31.9, 29.1, 28.7, 26.0, 22.7, 14.2, 10.7.



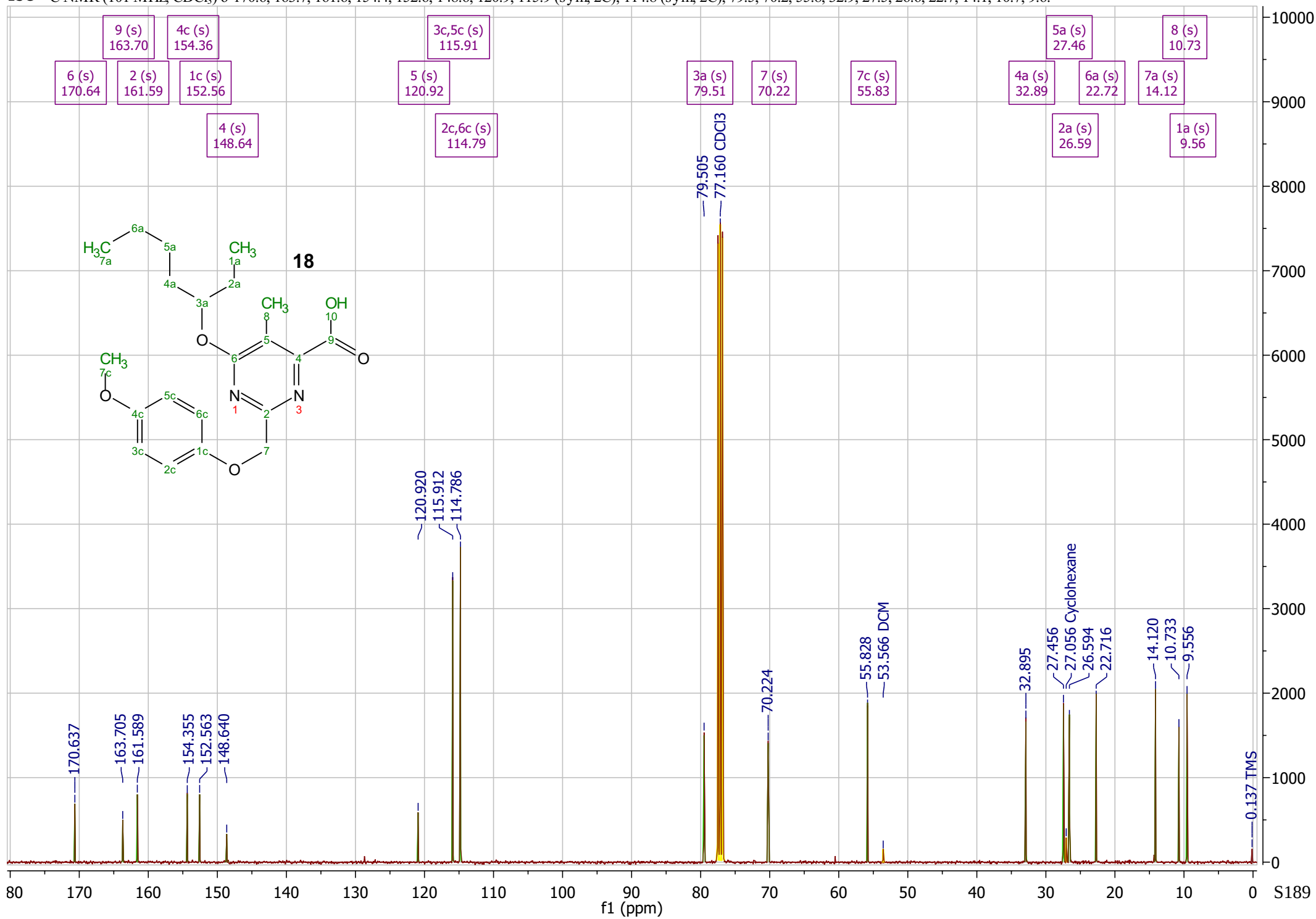


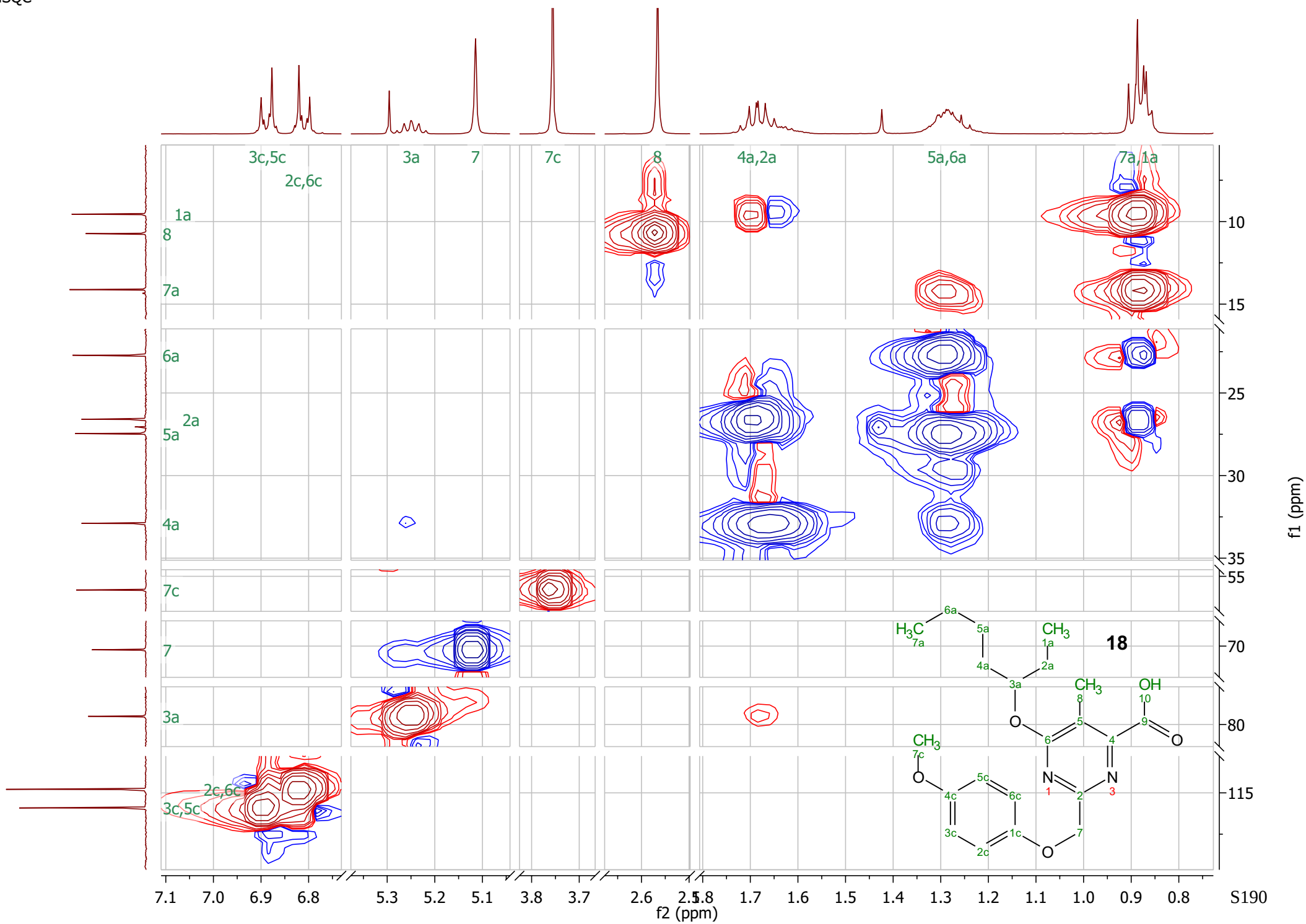


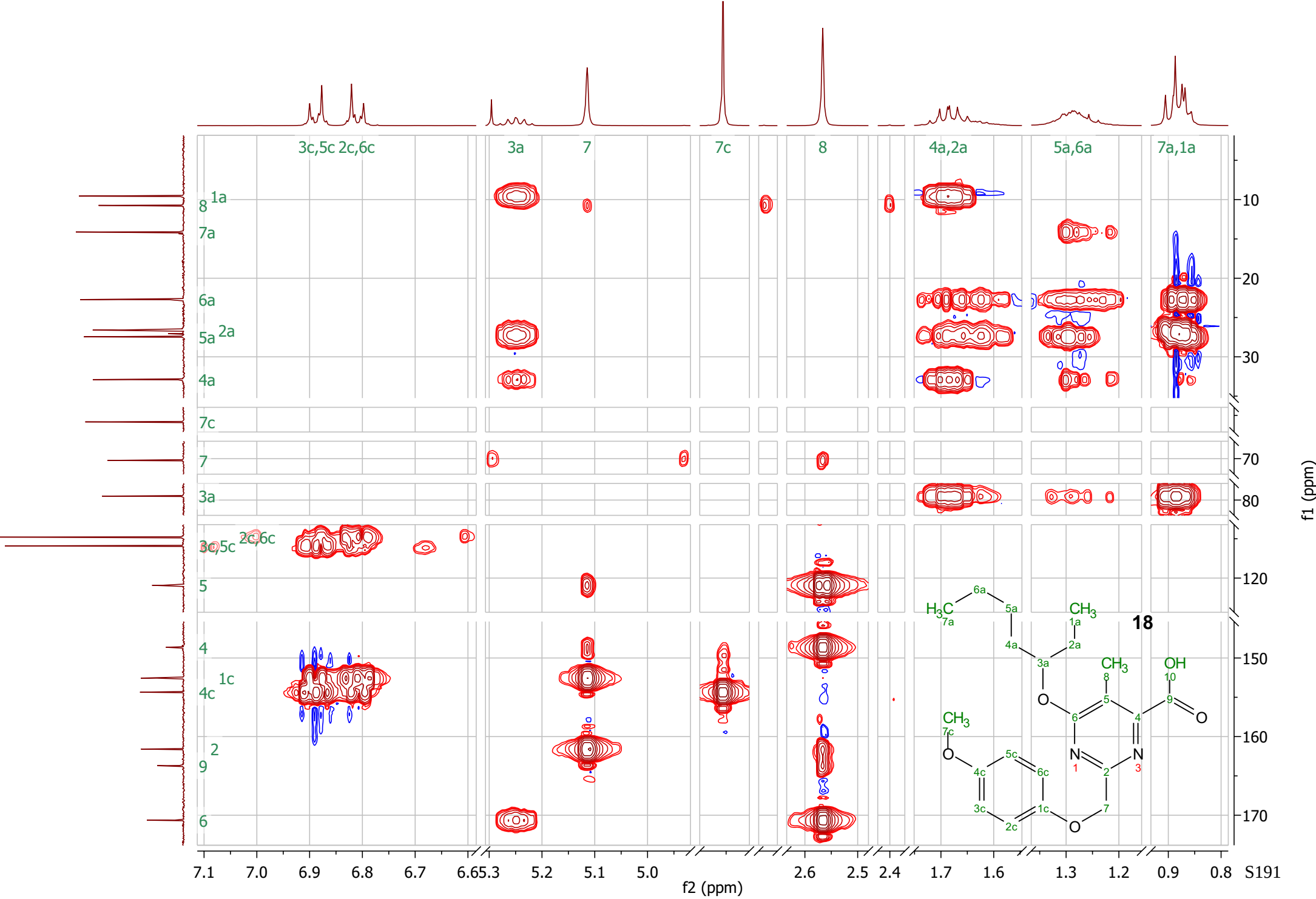
^1H NMR (400 MHz, CDCl_3) δ 9.04 (br s, 1H), 6.98 – 6.85 (m, 2H), 6.85 – 6.71 (m, 2H), 5.25 (quint, $J = 5.9$ Hz, 1H), 5.11 (s, 2H), 3.76 (s, 3H), 2.57 (s, 3H), 1.78 – 1.59 (m, 4H), 1.38 – 1.17 (m, 4H), 0.97 – 0.80 (m, 6H).



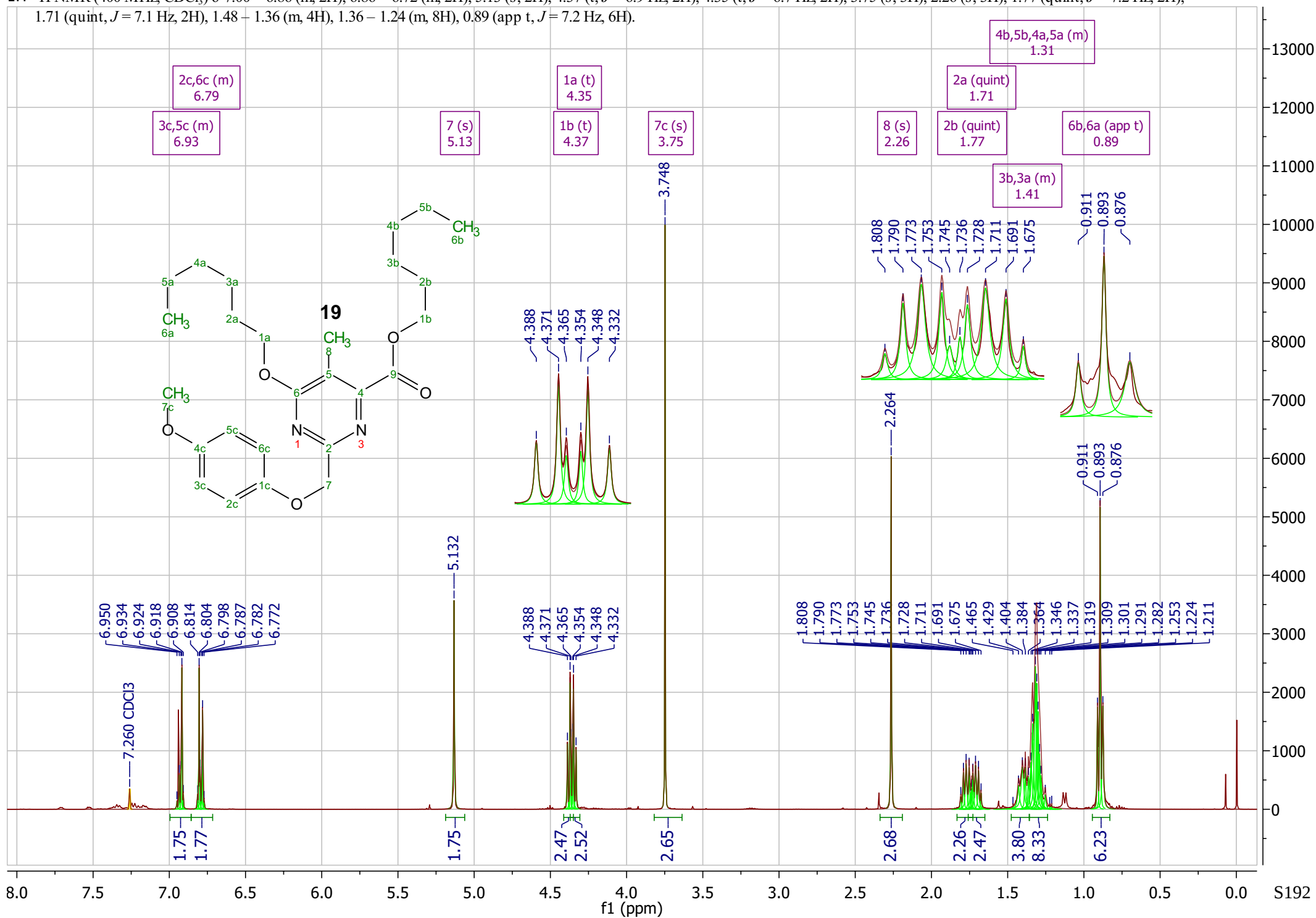
^{13}C NMR (101 MHz, CDCl_3) δ 170.6, 163.7, 161.6, 154.4, 152.6, 148.6, 120.9, 115.9 (sym, 2C), 114.8 (sym, 2C), 79.5, 70.2, 55.8, 32.9, 27.5, 26.6, 22.7, 14.1, 10.7, 9.6.



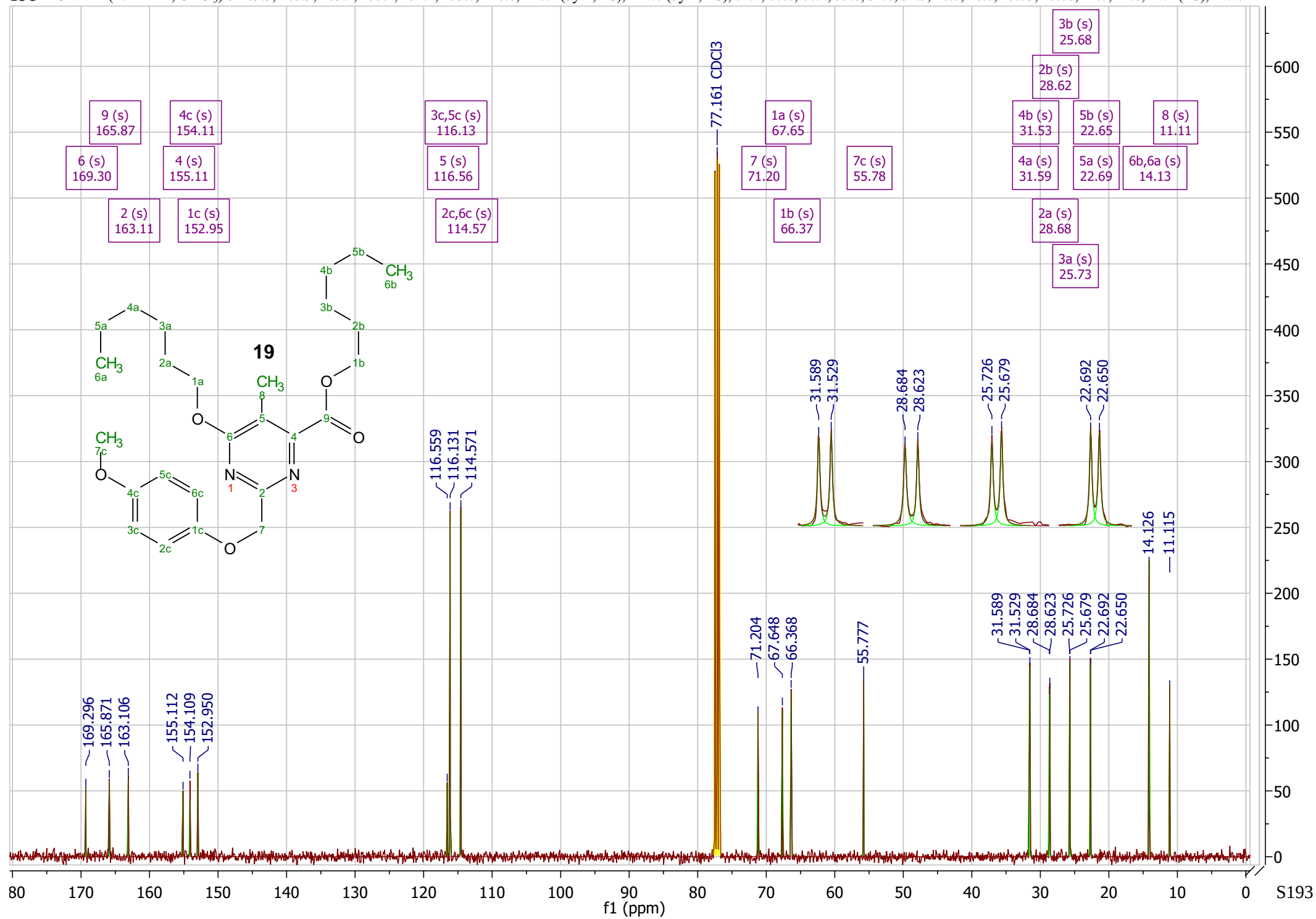


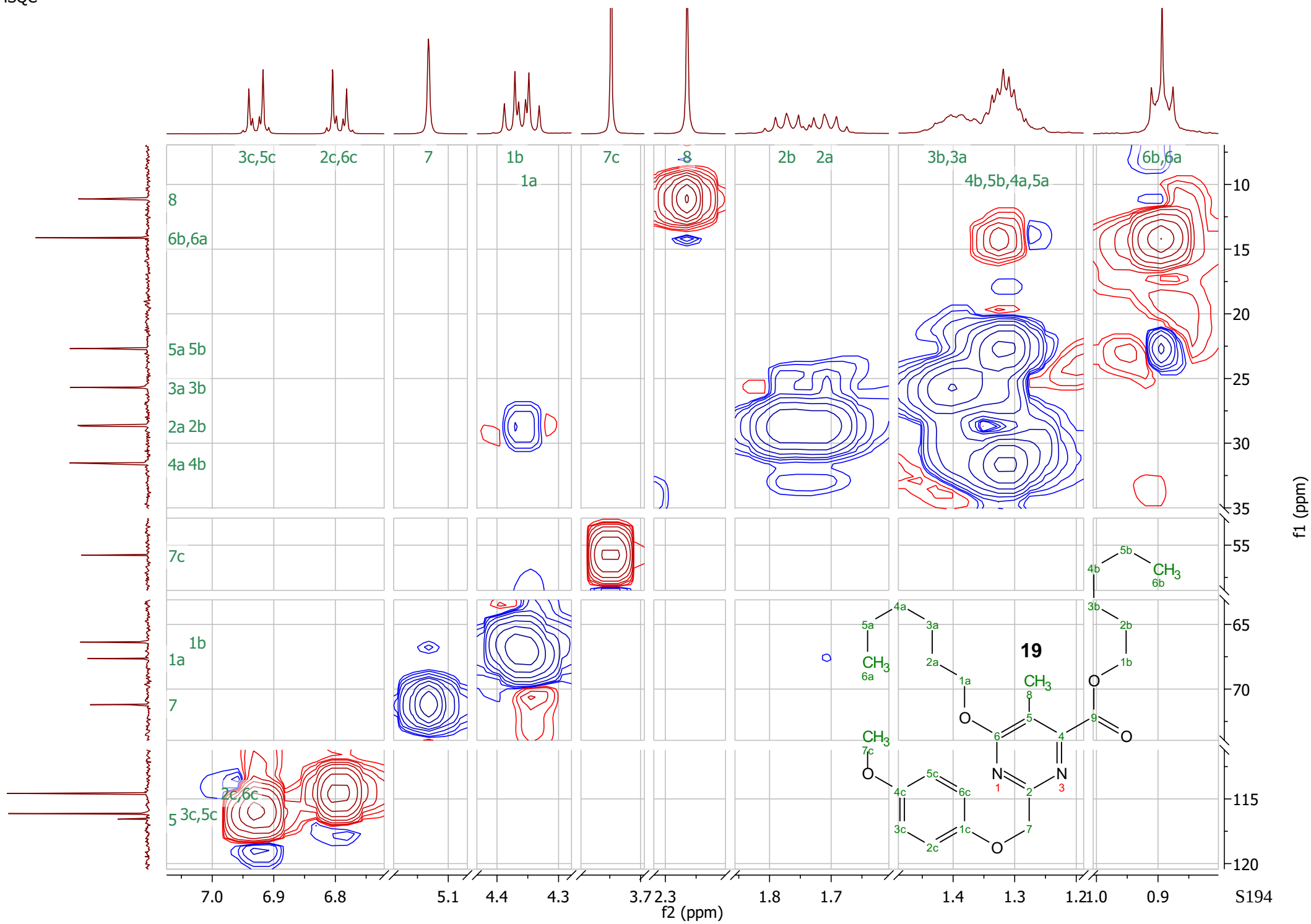


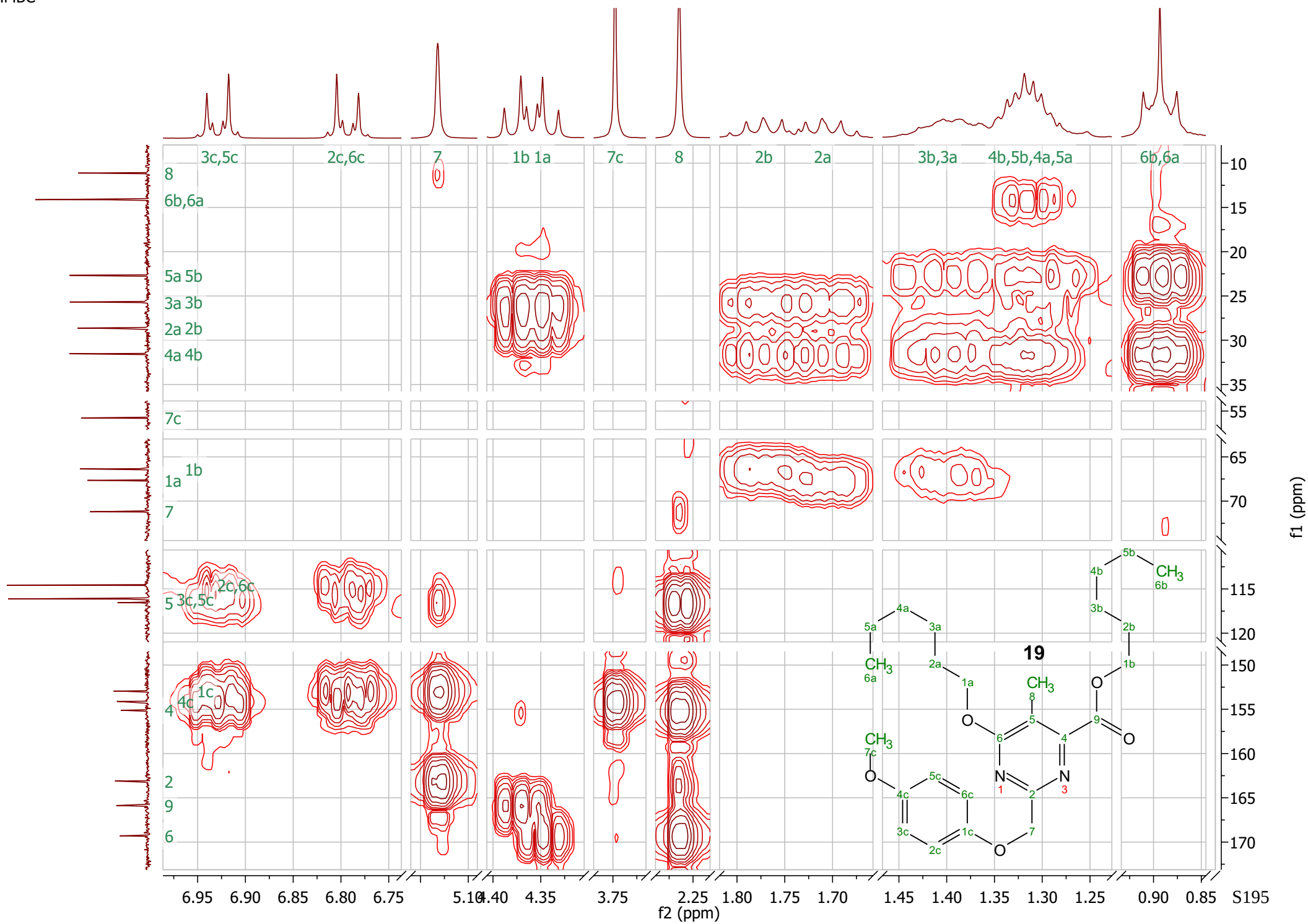
^1H NMR (400 MHz, CDCl_3) δ 7.00 – 6.86 (m, 2H), 6.86 – 6.72 (m, 2H), 5.13 (s, 2H), 4.37 (t, $J = 6.9$ Hz, 2H), 4.35 (t, $J = 6.7$ Hz, 2H), 3.75 (s, 3H), 2.26 (s, 3H), 1.77 (quint, $J = 7.2$ Hz, 2H), 1.71 (quint, $J = 7.1$ Hz, 2H), 1.48 – 1.36 (m, 4H), 1.36 – 1.24 (m, 8H), 0.89 (app t, $J = 7.2$ Hz, 6H).



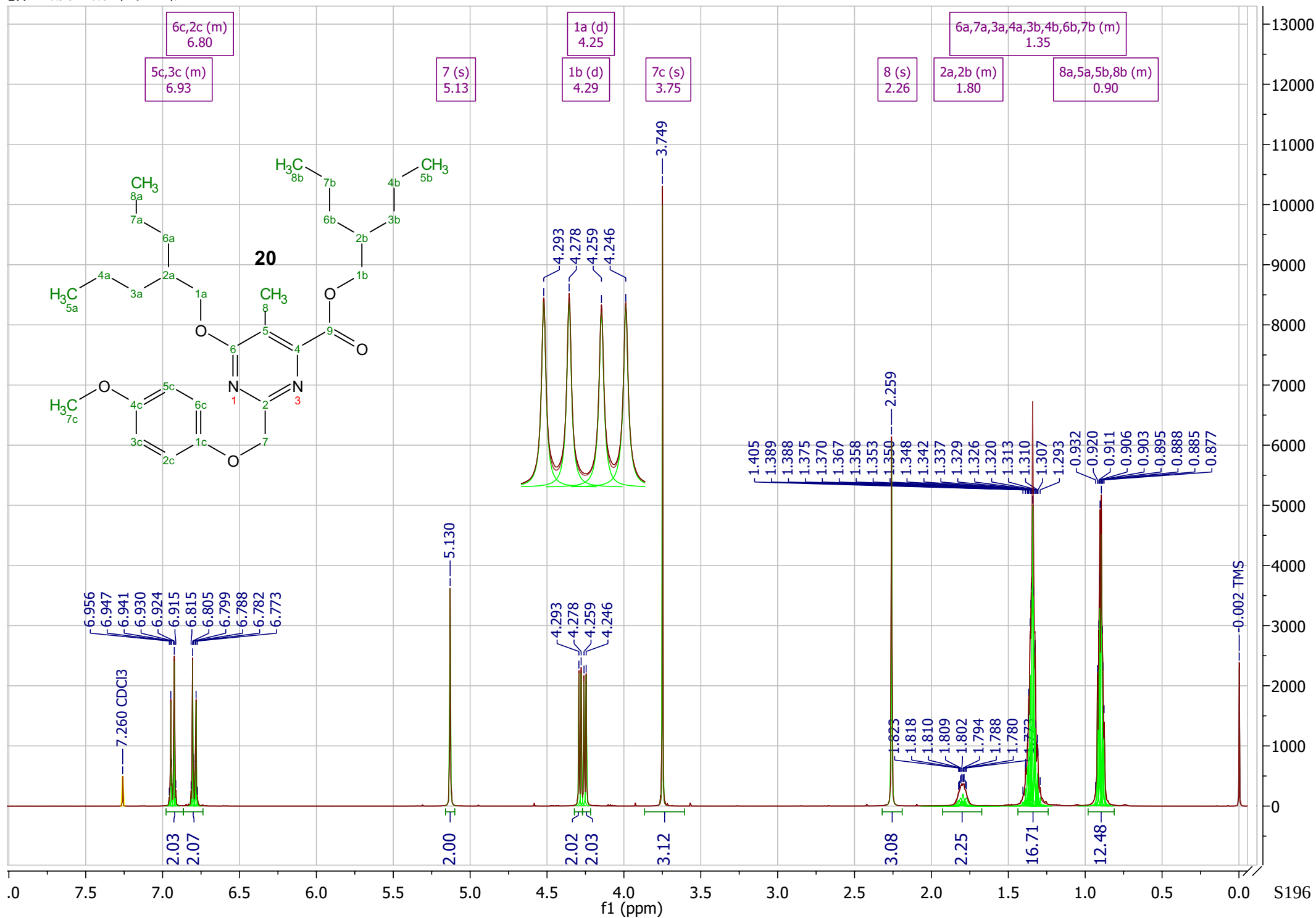
13C ¹³C NMR (101 MHz, CDCl₃) δ 169.3, 165.9, 163.1, 155.1, 154.1, 153.0, 116.6, 116.1 (sym, 2C), 114.6 (sym, 2C), 71.2, 67.6, 66.4, 55.8, 31.6, 31.5, 28.7, 28.6, 25.73, 25.68, 22.7, 22.6, 14.1 (2C), 11.1.



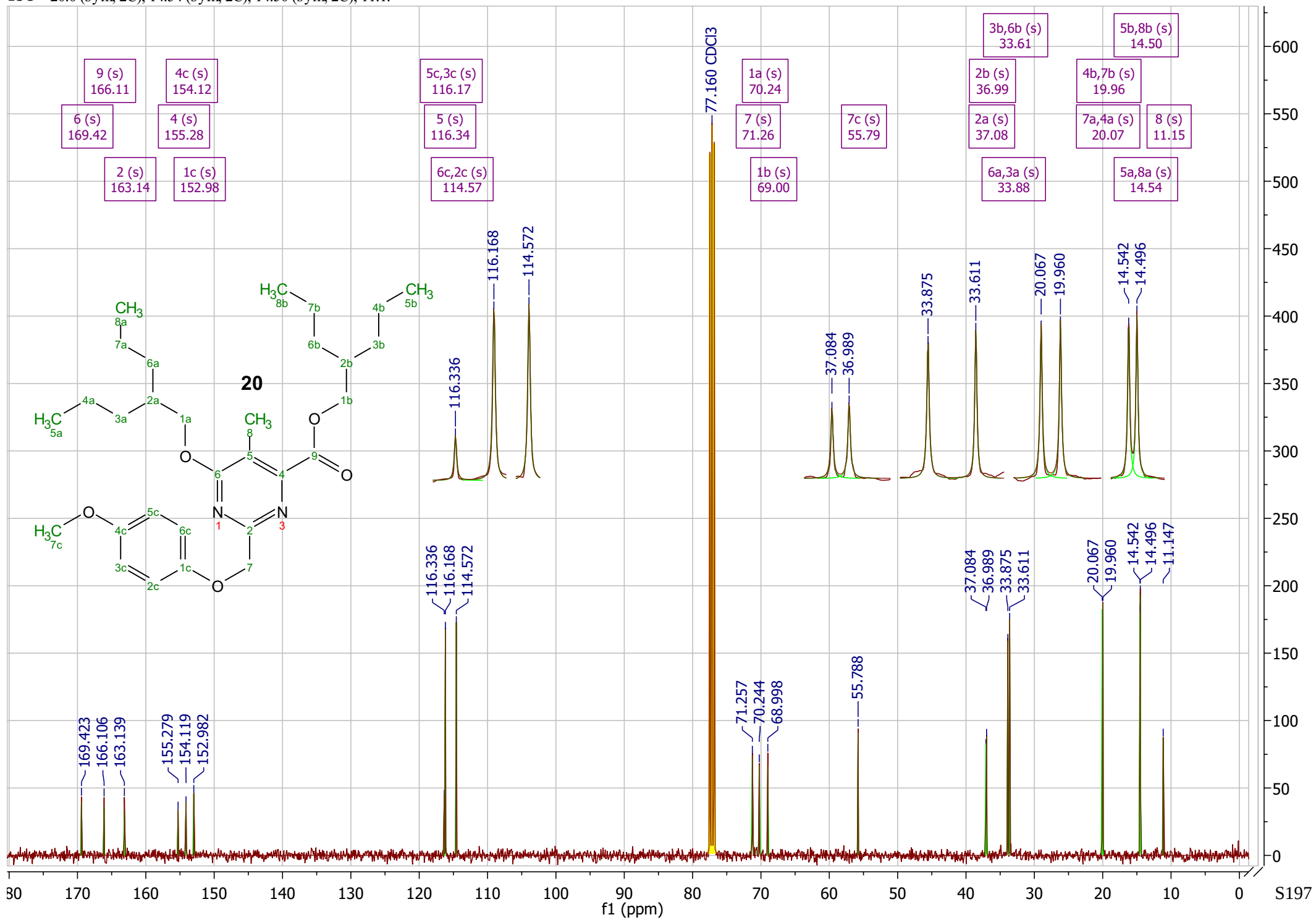


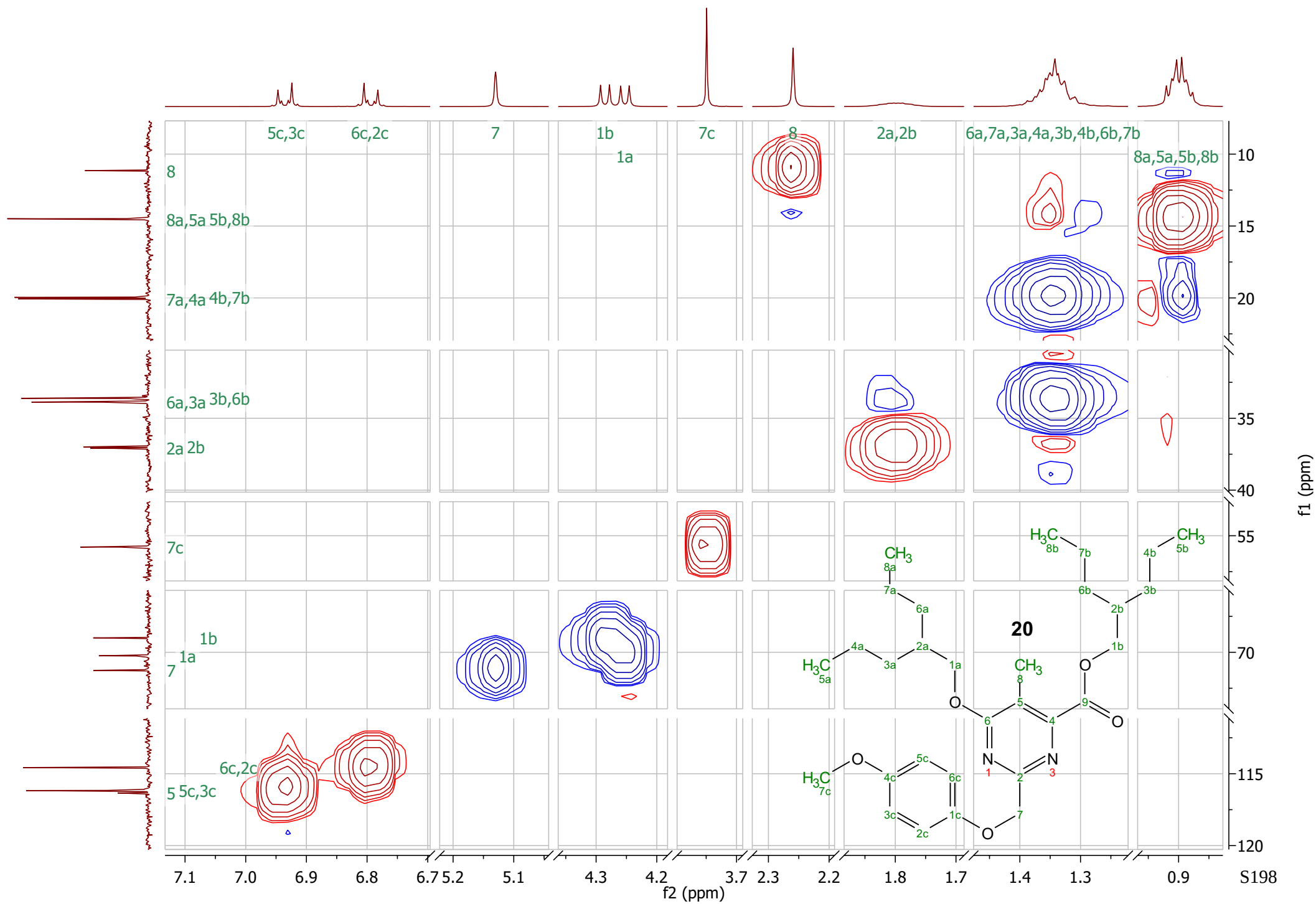


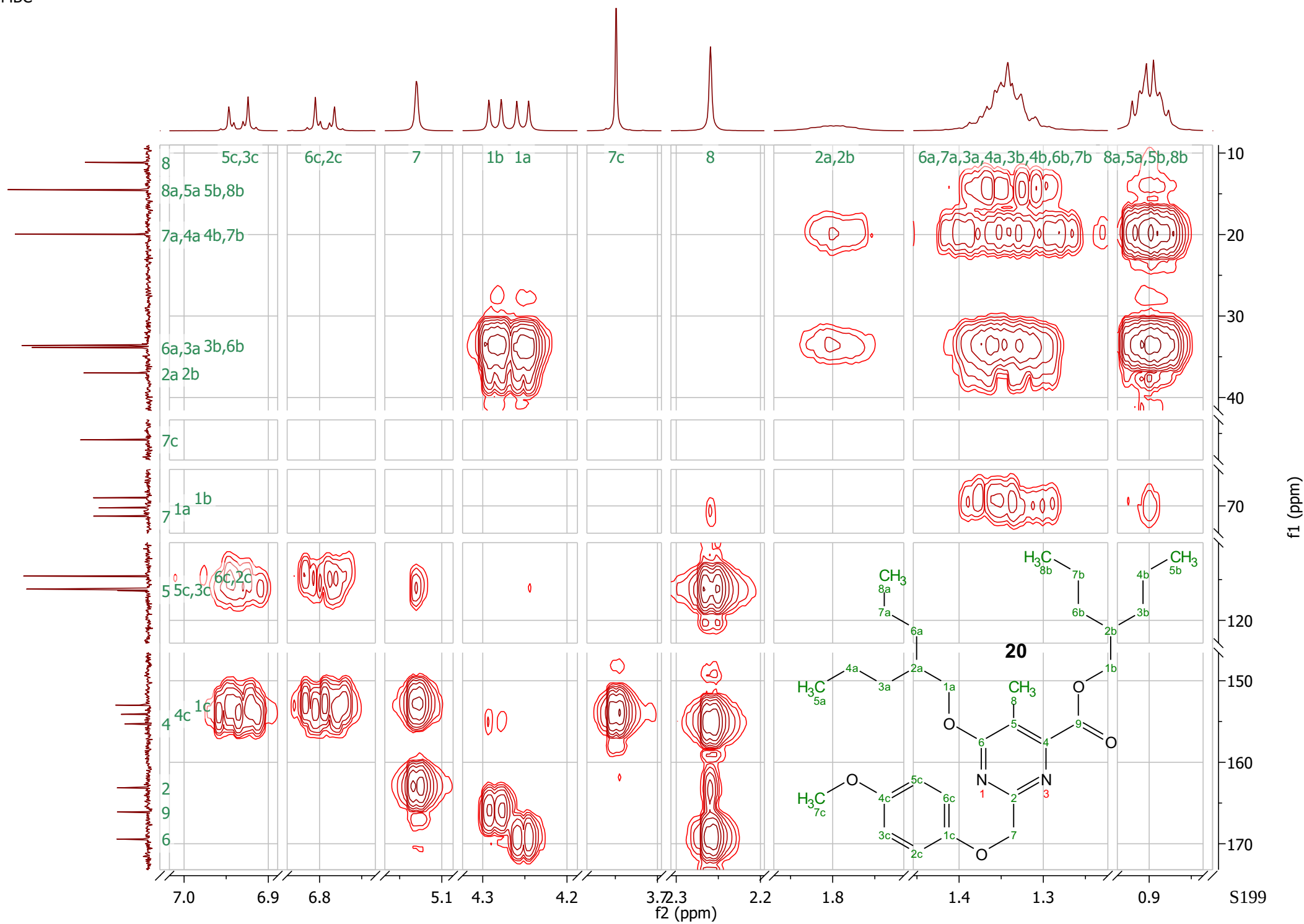
¹H NMR (400 MHz, CDCl₃) δ 6.98 – 6.86 (m, 2H), 6.86 – 6.74 (m, 2H), 5.13 (s, 2H), 4.29 (d, *J* = 5.8 Hz, 2H), 4.25 (d, *J* = 5.6 Hz, 2H), 3.75 (s, 3H), 2.26 (s, 3H), 1.93 – 1.67 (m, 2H), 1.44 – 1.24 (m, 16H), 0.98 – 0.81 (m, 12H).



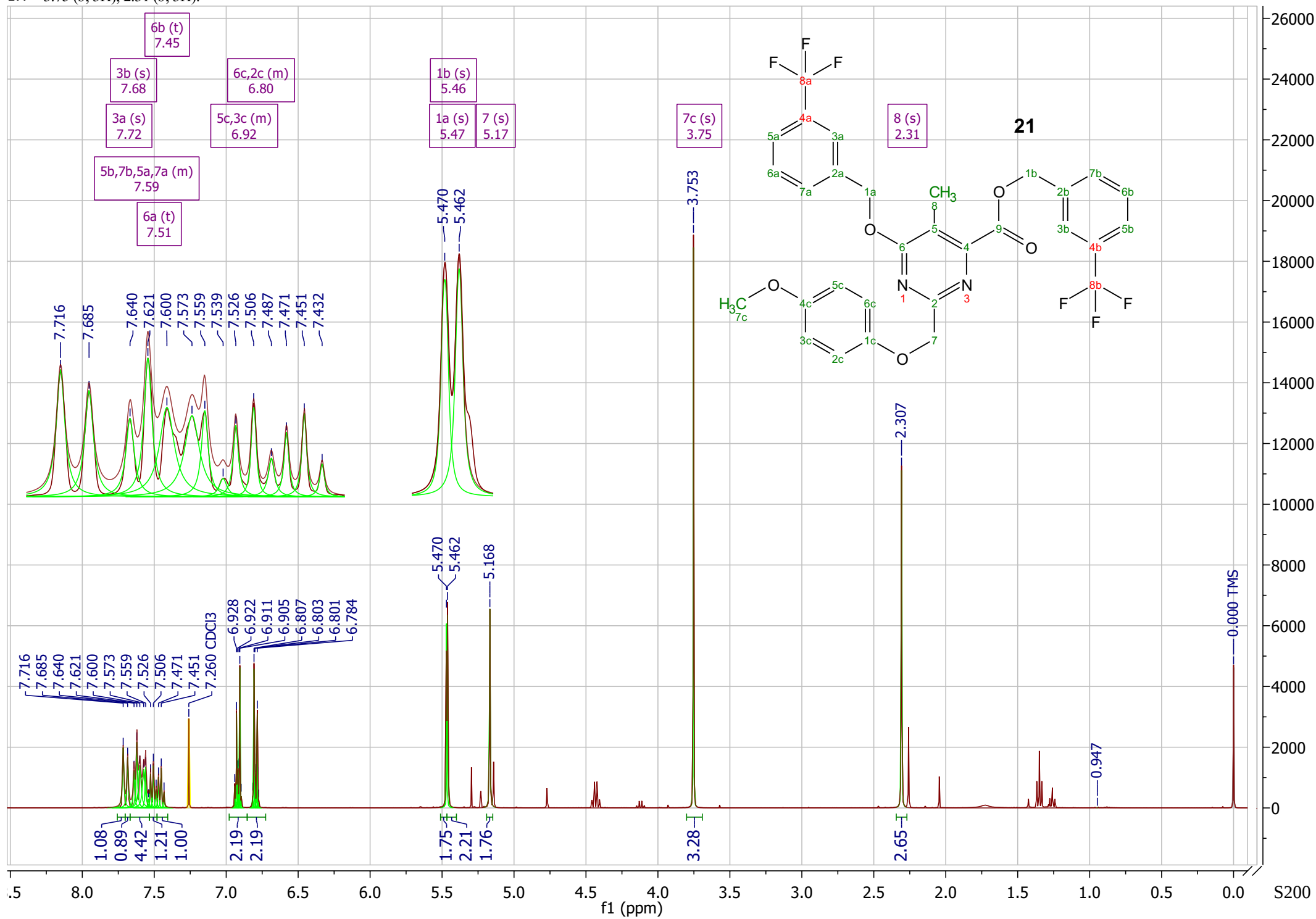
¹³C NMR (101 MHz, CDCl₃) δ 169.4, 166.1, 163.1, 155.3, 154.1, 153.0, 116.3, 116.2 (sym, 2C), 114.6 (sym, 2C), 71.3, 70.2, 69.0, 55.8, 37.1, 37.0, 33.9 (sym, 2C), 33.6 (sym, 2C), 20.1 (sym, 2C), 20.0 (sym, 2C), 14.54 (sym, 2C), 14.50 (sym, 2C), 11.1.



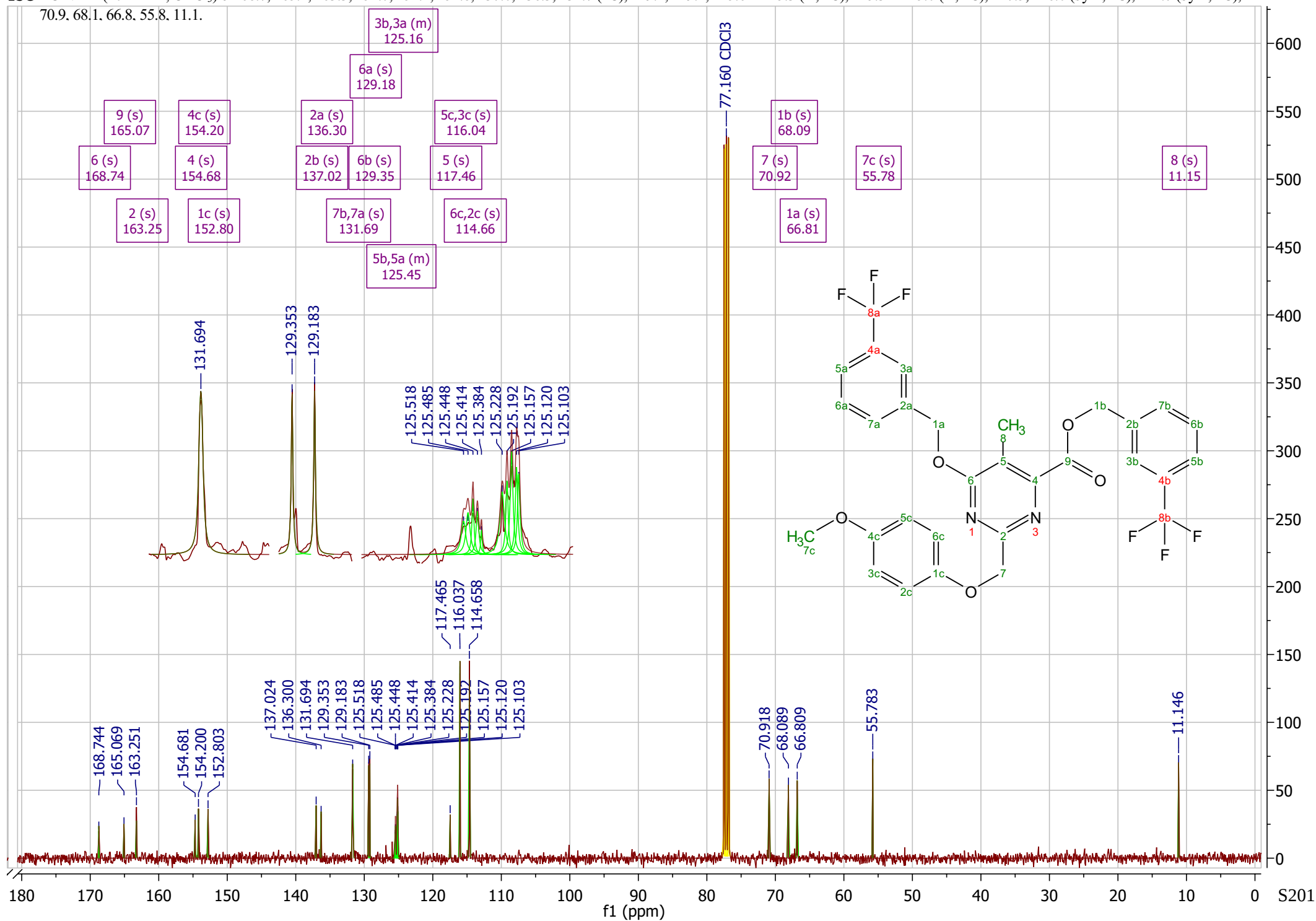


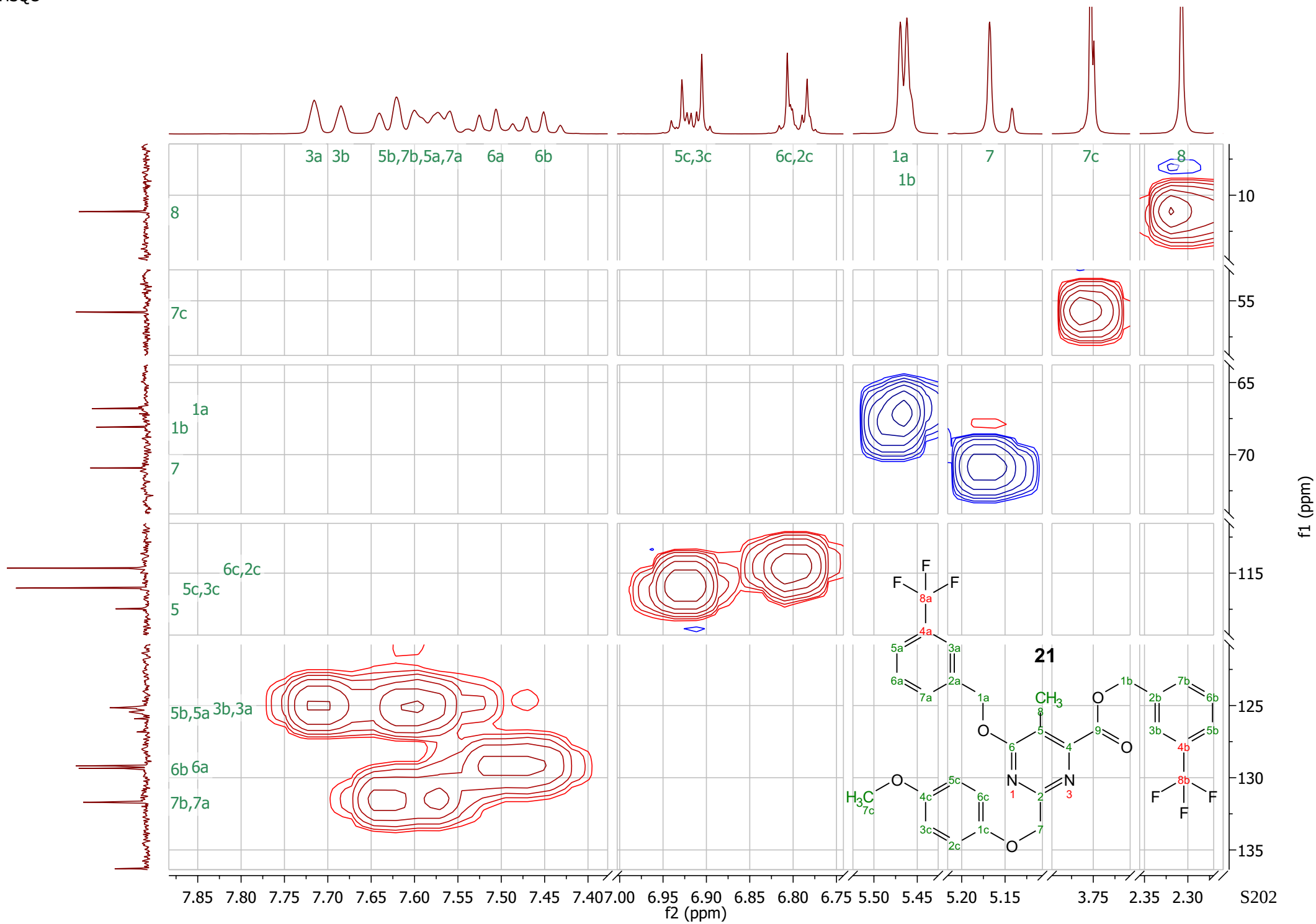


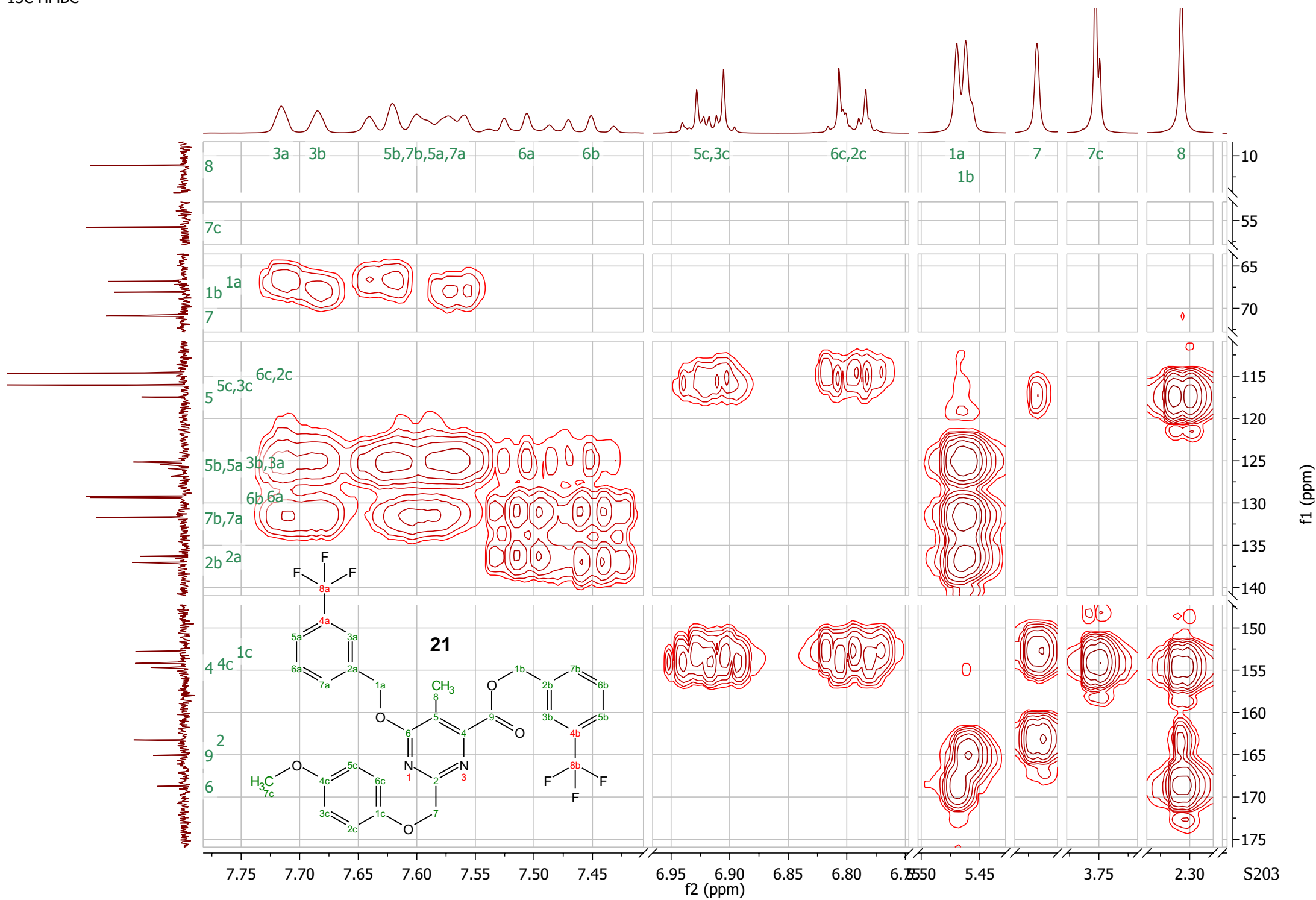
¹H NMR (400 MHz, CDCl₃) δ 7.72 (s, 1H), 7.68 (s, 1H), 7.67 – 7.48 (m, 4H), 7.51 (t, *J* = 7.7 Hz, 1H), 7.45 (t, *J* = 7.7 Hz, 1H), 7.00 – 6.85 (m, 2H), 6.85 – 6.70 (m, 2H), 5.47 (s, 2H), 5.46 (s, 2H), 5.17 (s, 2H), 3.75 (s, 3H), 2.31 (s, 3H).



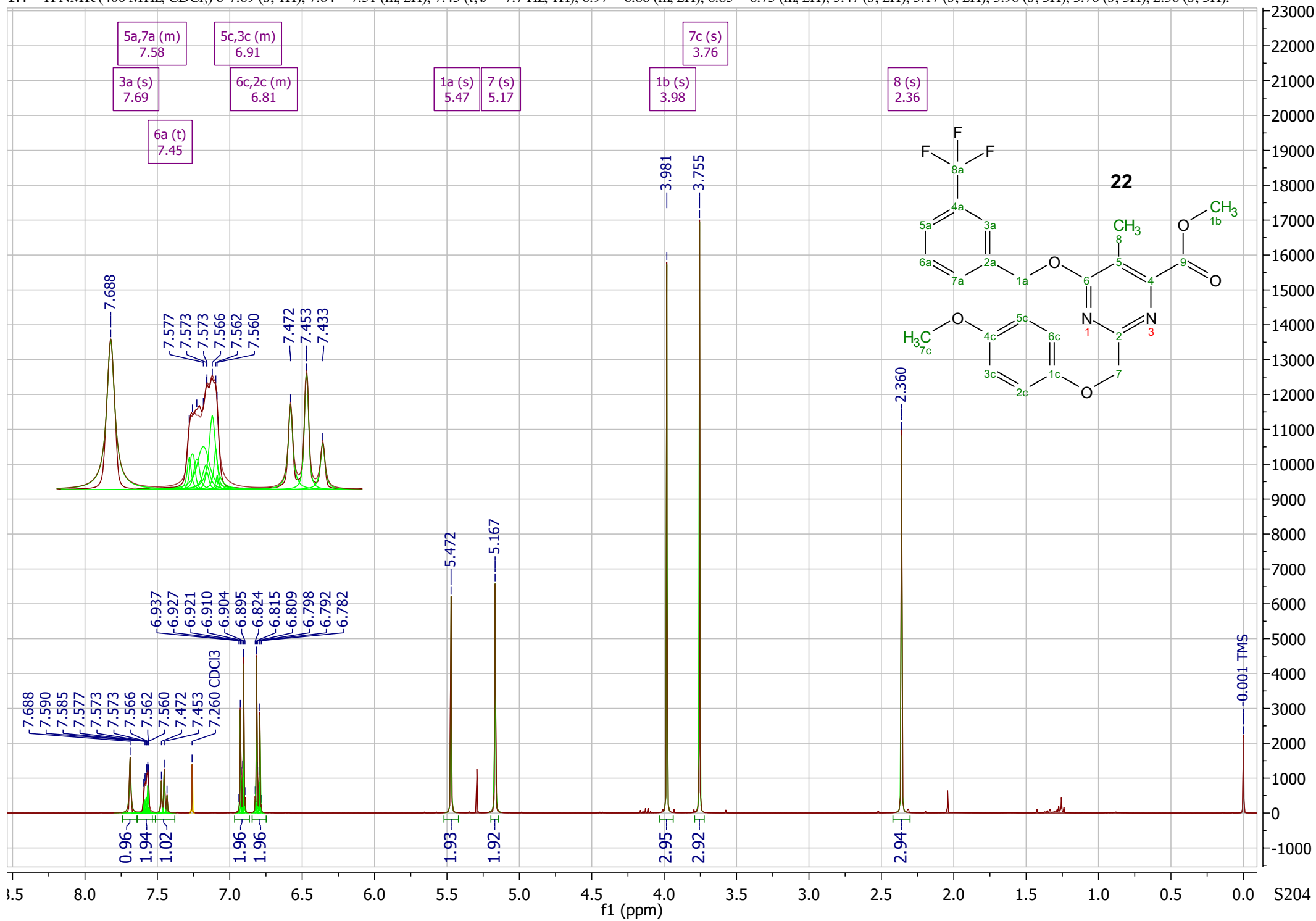
13C ¹³C NMR (101 MHz, CDCl₃) δ 168.7, 165.1, 163.3, 154.7, 154.2, 152.8, 137.0, 136.3, 131.7 (2C), 129.4, 129.2, 125.6 – 125.3 (m, 2C), 125.3 – 125.0 (m, 2C), 117.5, 116.0 (sym, 2C), 114.7 (sym, 2C), 70.9, 68.1, 66.8, 55.8, 11.1.



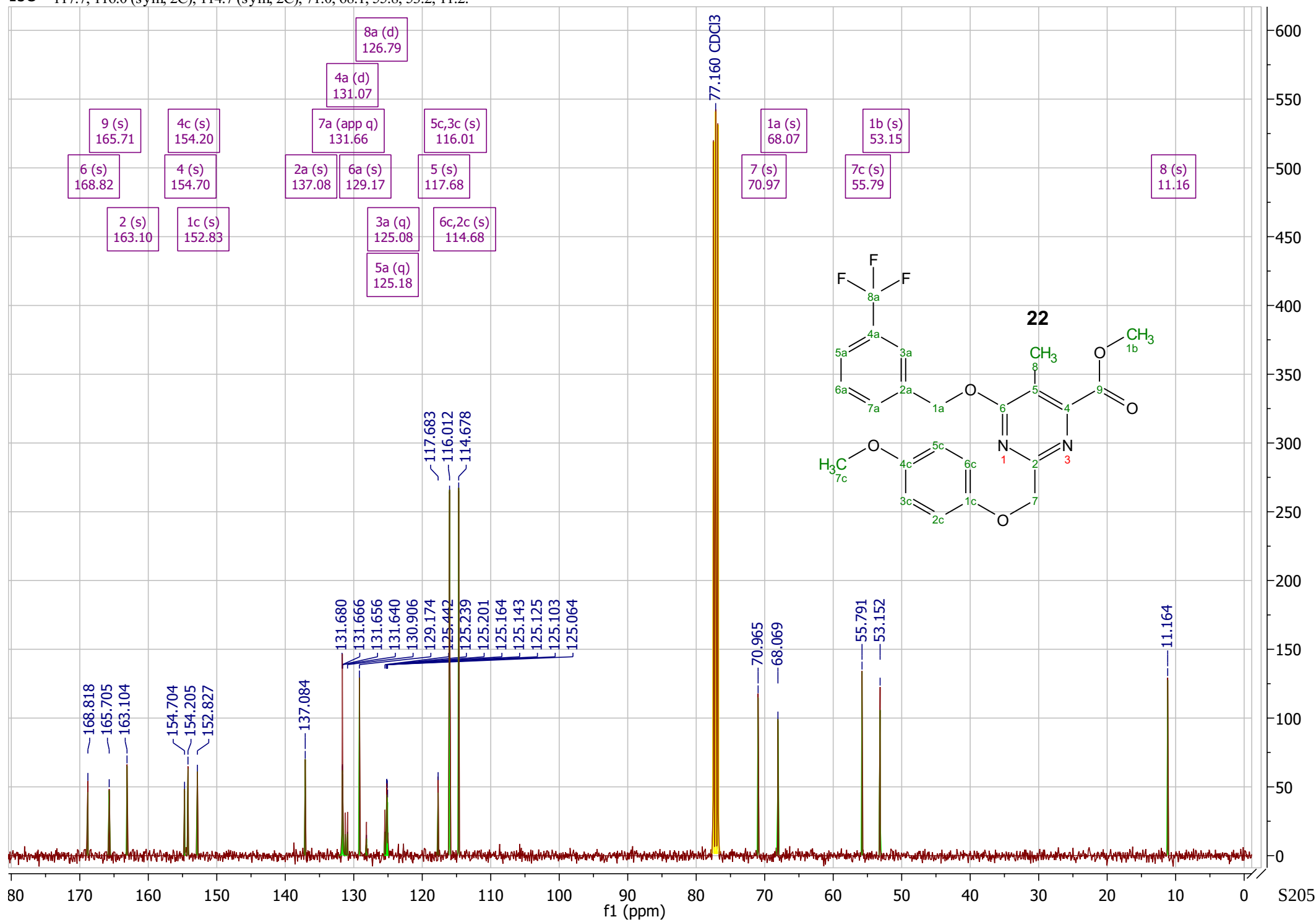




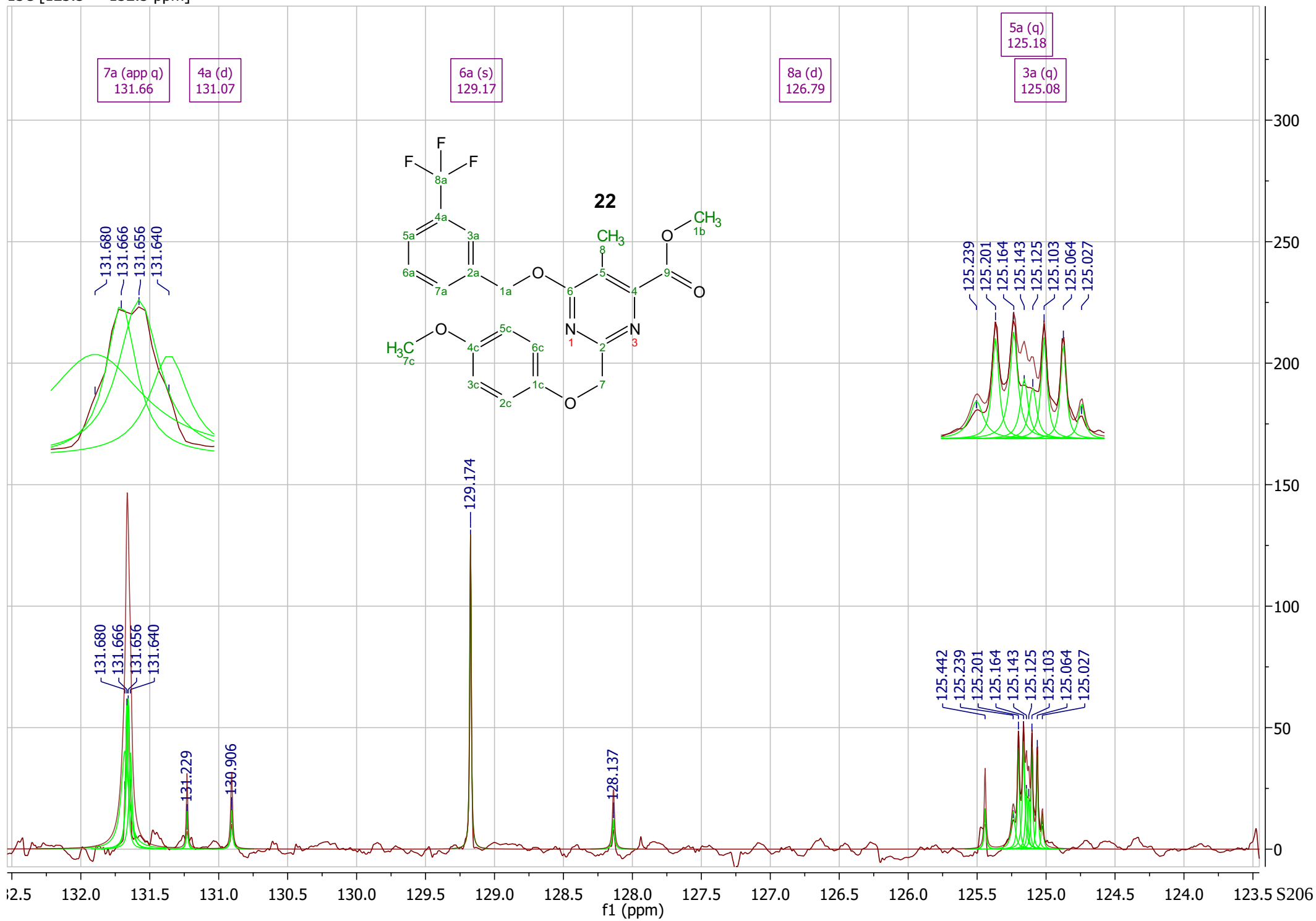
^1H NMR (400 MHz, CDCl_3) δ 7.69 (s, 1H), 7.64 – 7.51 (m, 2H), 7.45 (t, $J = 7.7$ Hz, 1H), 6.97 – 6.86 (m, 2H), 6.85 – 6.75 (m, 2H), 5.47 (s, 2H), 5.17 (s, 2H), 3.98 (s, 3H), 3.76 (s, 3H), 2.36 (s, 3H).

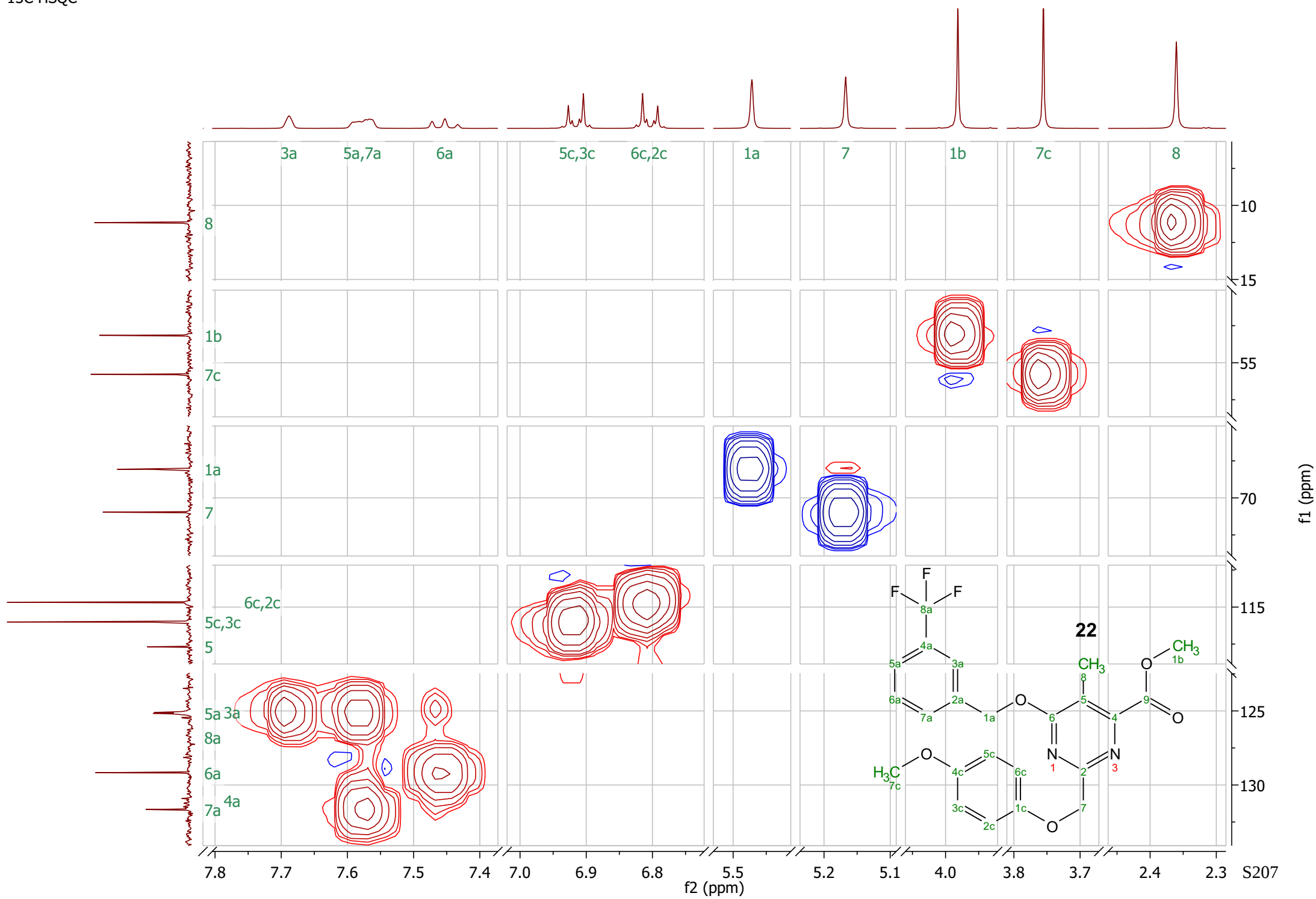


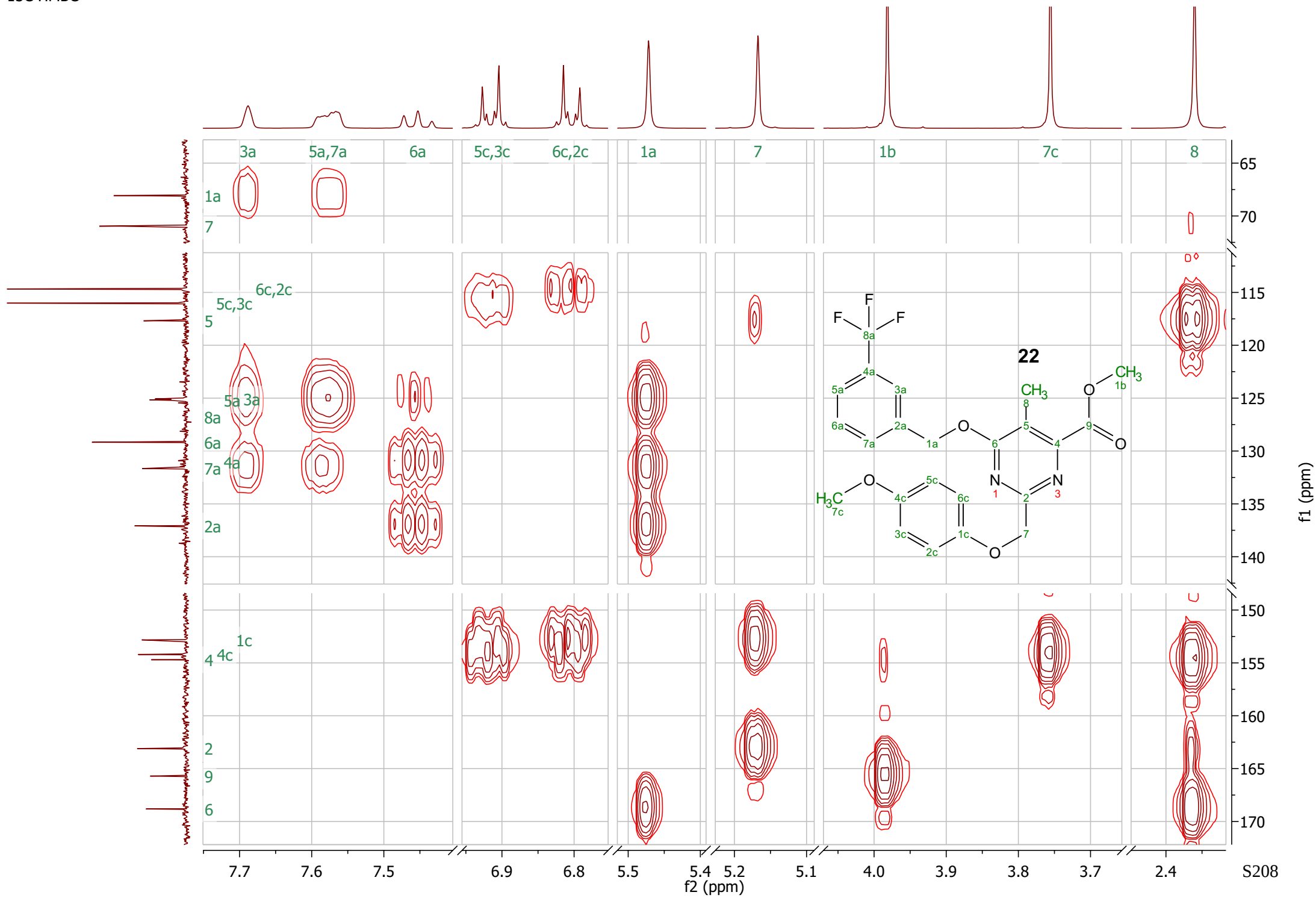
¹³C NMR (101 MHz, CDCl₃) δ 168.8, 165.7, 163.1, 154.7, 154.2, 152.8, 137.1, 131.7 (app q, *J* = 1.2 Hz), 131.1 (d, *J* = 32.4 Hz), 129.2, 126.8 (d, *J* = 271.1 Hz), 125.2 (q, *J* = 3.9 Hz), 125.1 (q, *J* = 3.9 Hz), 117.7, 116.0 (sym, 2C), 114.7 (sym, 2C), 71.0, 68.1, 55.8, 53.2, 11.2.



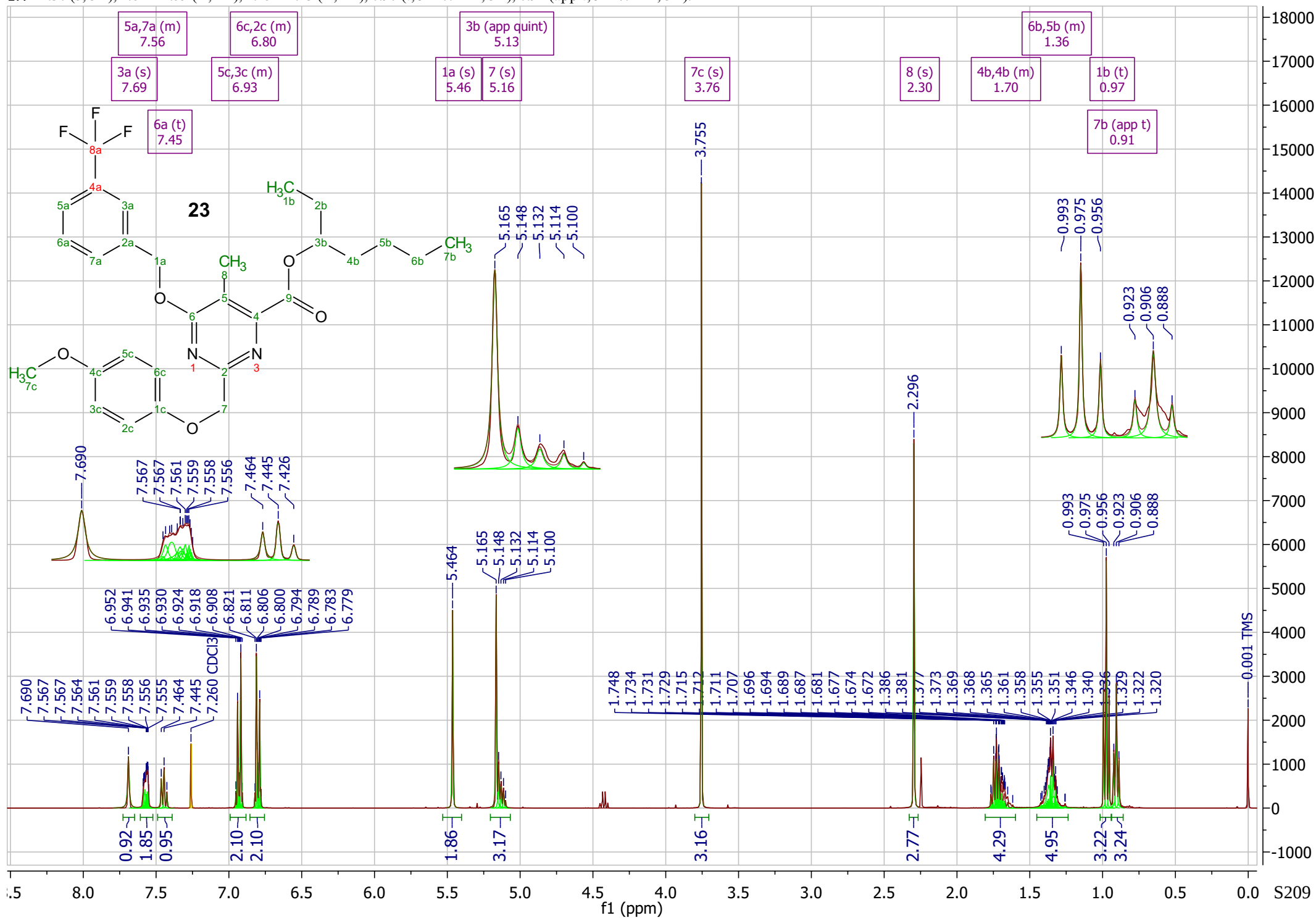
¹³C [123.5 — 132.5 ppm]



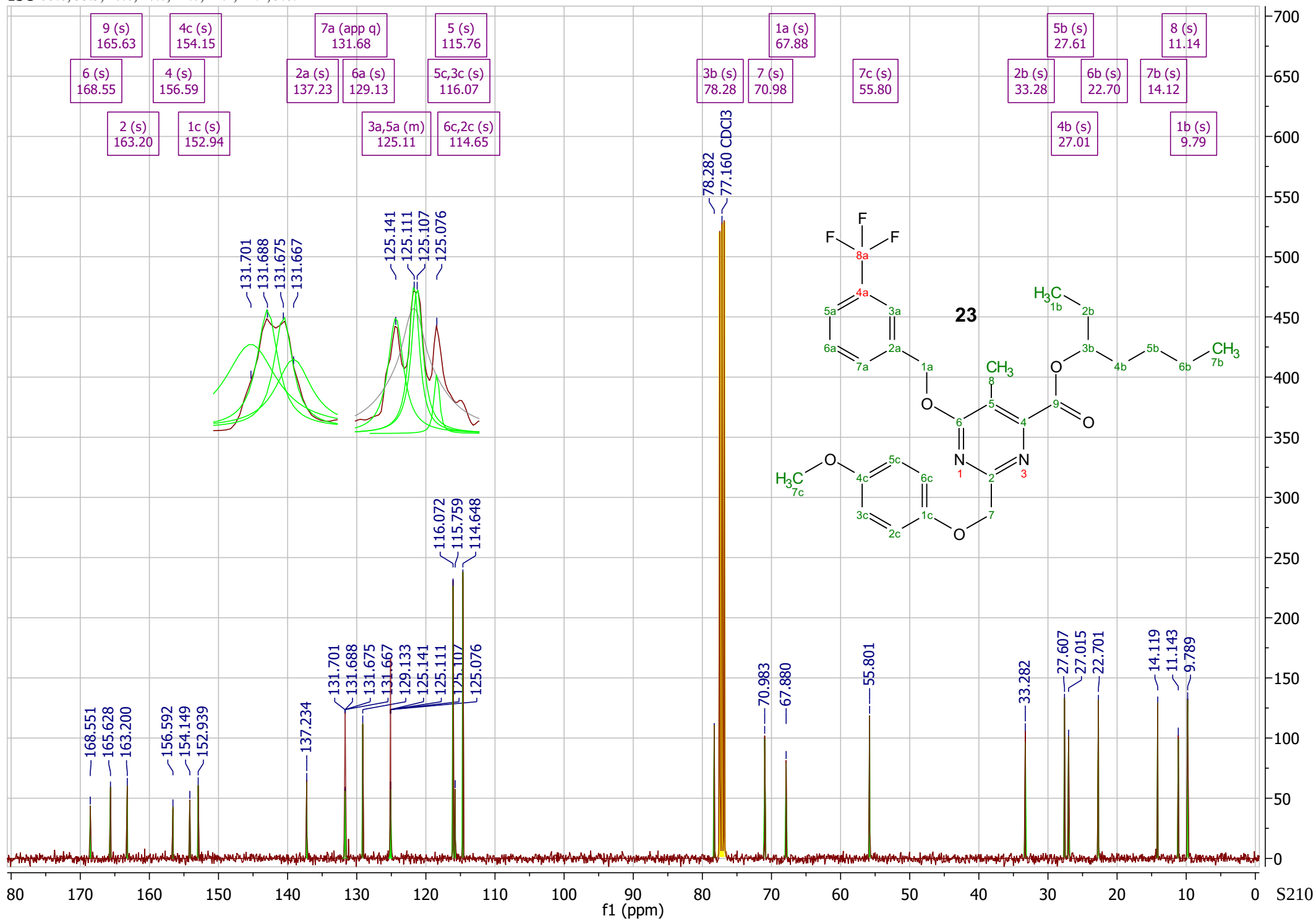


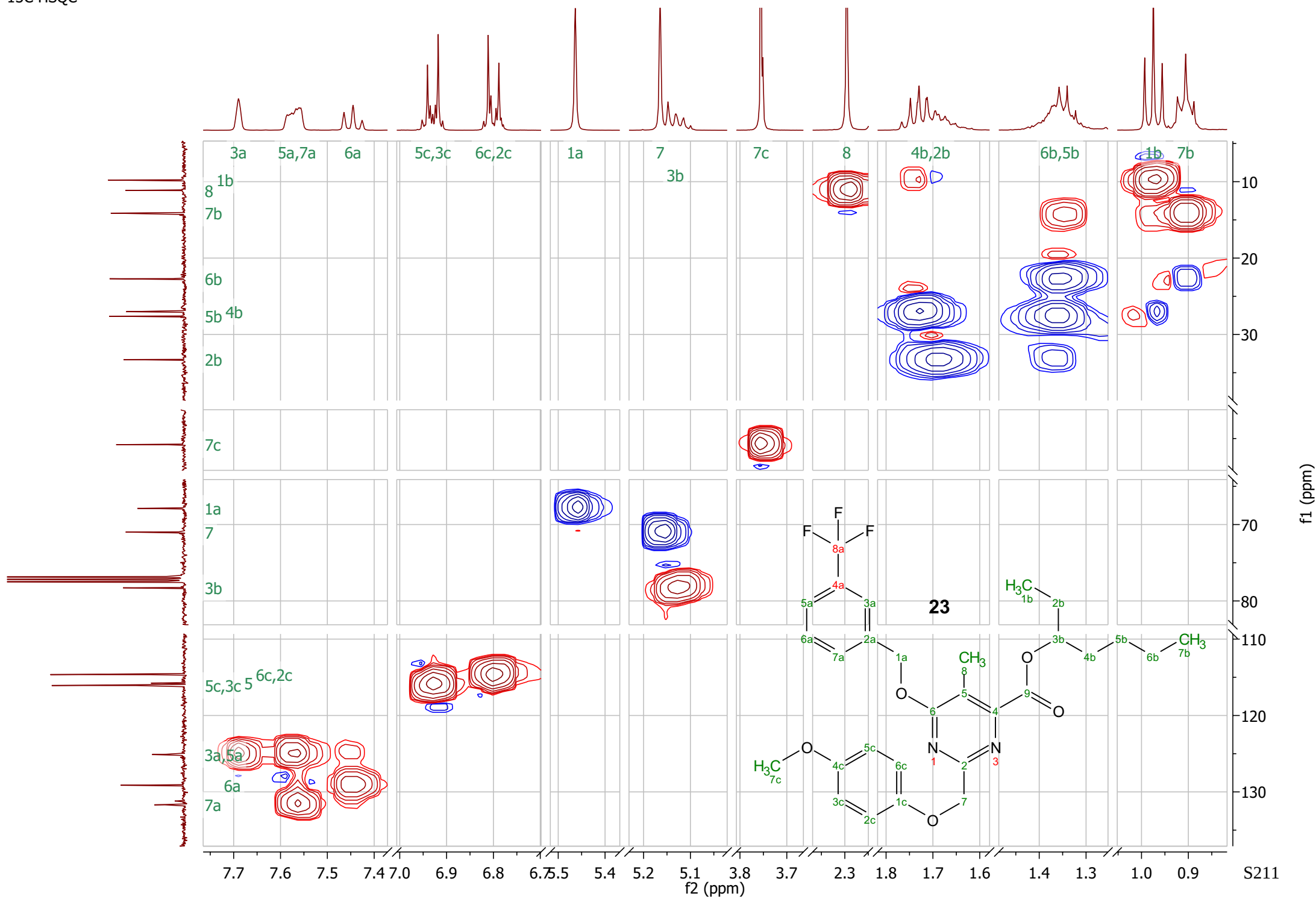


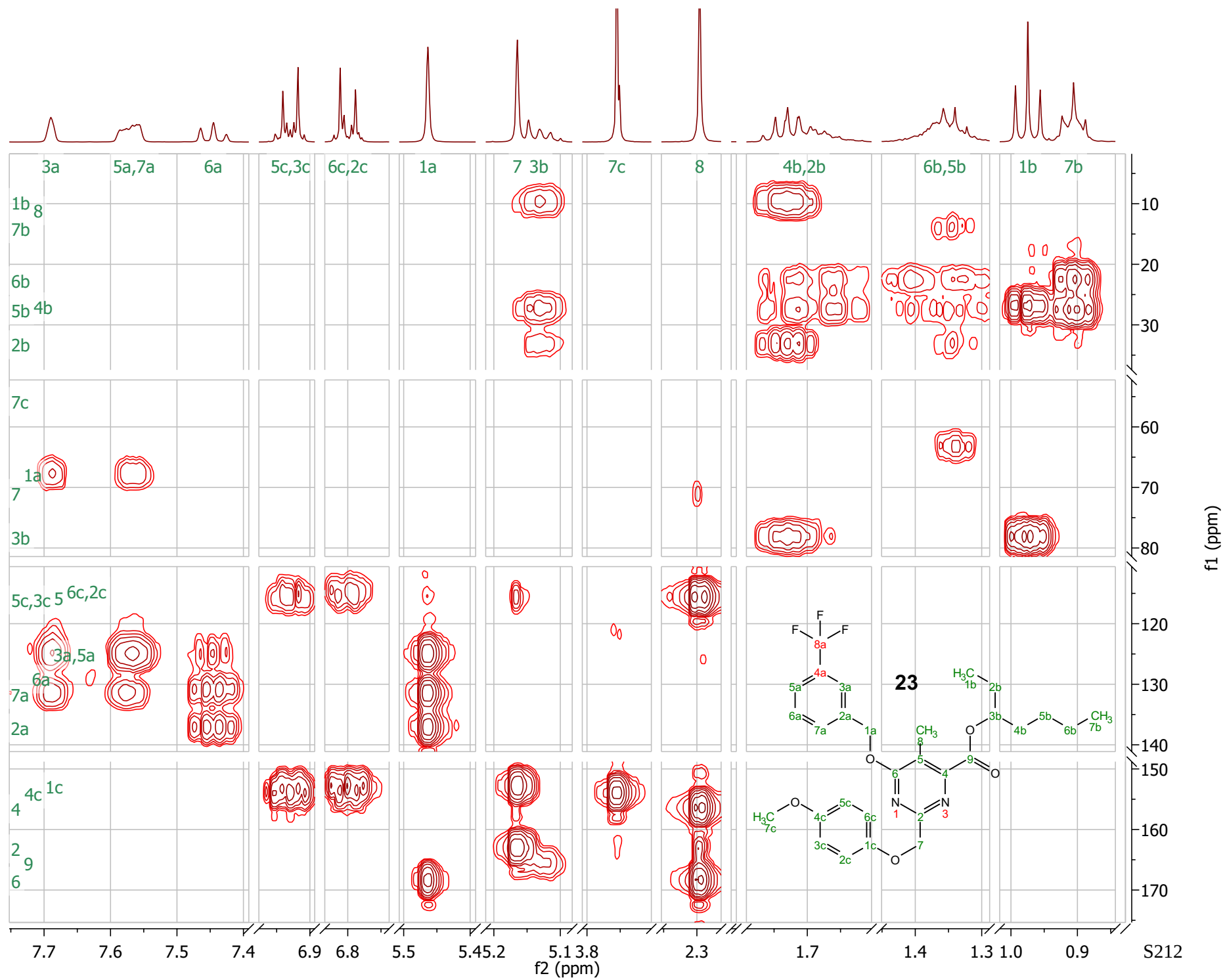
¹H NMR (400 MHz, CDCl₃) δ 7.69 (s, 1H), 7.61 – 7.52 (m, 2H), 7.45 (t, *J* = 7.7 Hz, 1H), 6.99 – 6.88 (m, 2H), 6.86 – 6.75 (m, 2H), 5.46 (s, 2H), 5.16 (s, 2H), 5.13 (app quint, *J* = 6.5 Hz, 1H), 3.76 (s, 3H), 2.30 (s, 3H), 1.81 – 1.59 (m, 4H), 1.45 – 1.23 (m, 4H), 0.97 (t, *J* = 7.4 Hz, 3H), 0.91 (app t, *J* = 7.1 Hz, 3H).



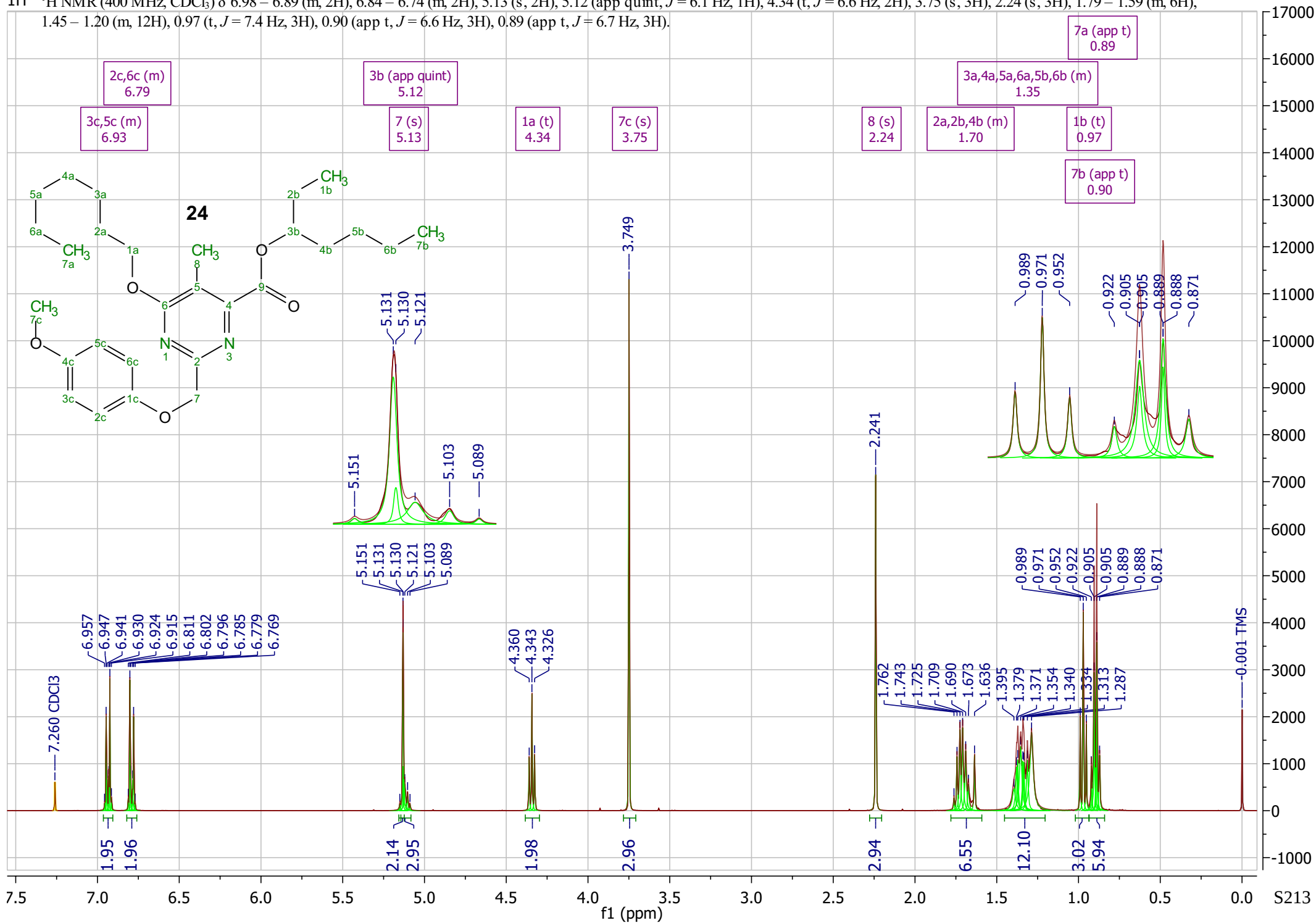
^{13}C NMR (101 MHz, CDCl_3) δ 168.6, 165.6, 154.1, 152.9, 137.2, 131.7 (app q, $J = 1.3, 0.9$ Hz), 129.1, 125.2 – 125.0 (m, 2C), 116.1 (sym, 2C), 115.8, 114.6 (sym, 2C), 78.3, 71.0, 67.9, 13C 55.8, 33.3, 27.6, 27.0, 22.7, 14.1, 11.1, 9.8.



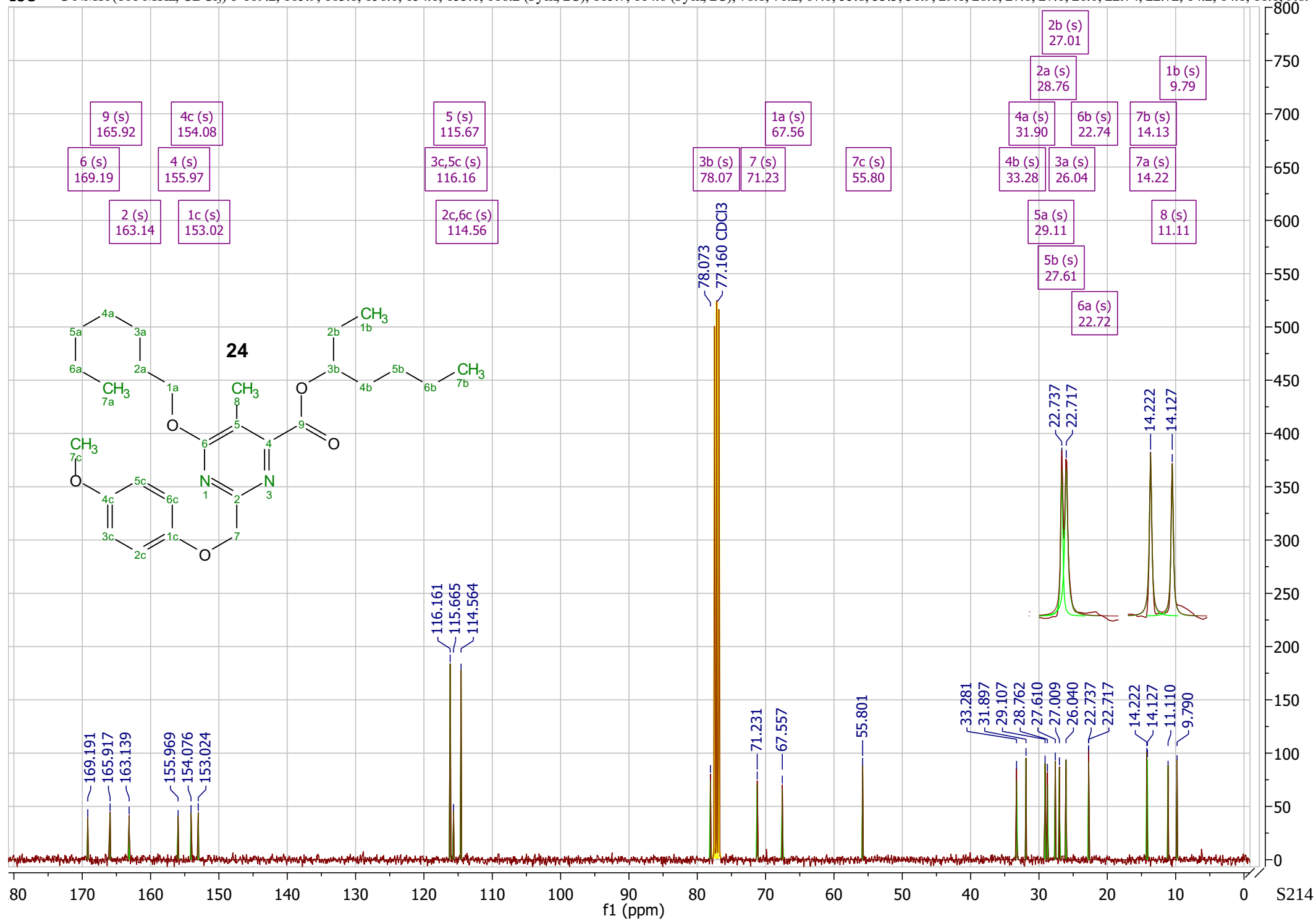


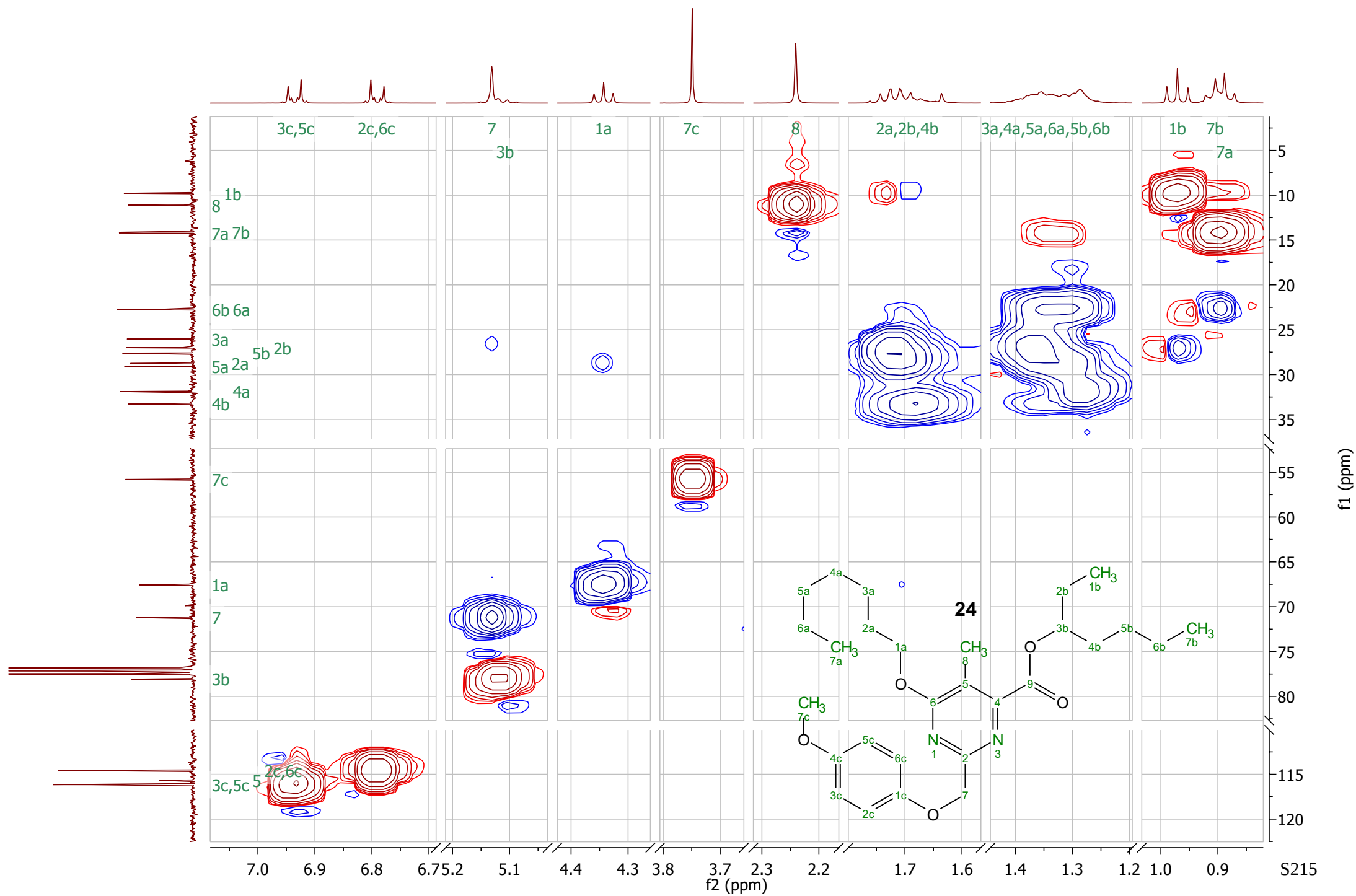


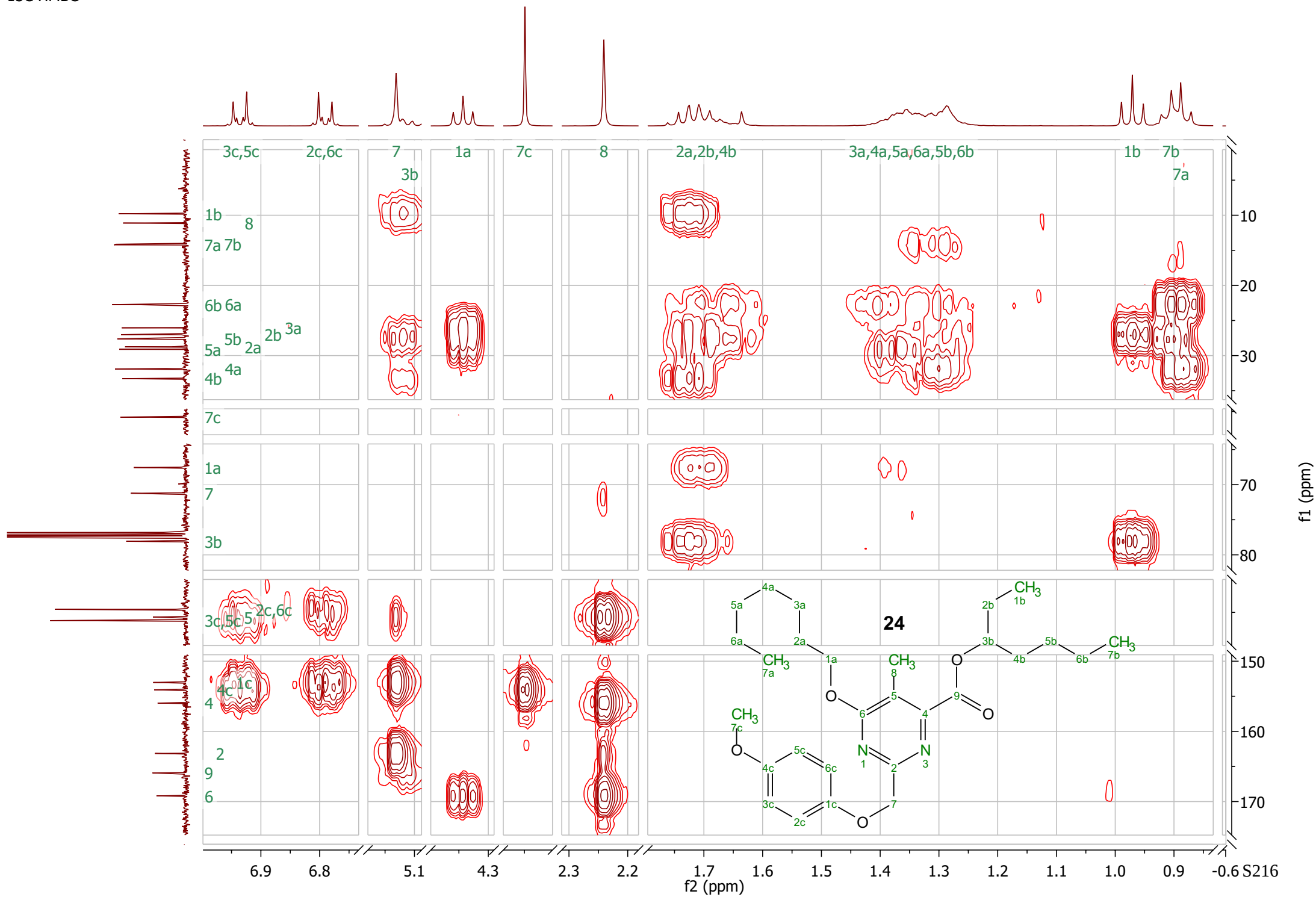
^1H NMR (400 MHz, CDCl_3) δ 6.98 – 6.89 (m, 2H), 6.84 – 6.74 (m, 2H), 5.13 (s, 2H), 5.12 (app quint, $J = 6.1$ Hz, 1H), 4.34 (t, $J = 6.6$ Hz, 2H), 3.75 (s, 3H), 2.24 (s, 3H), 1.79 – 1.59 (m, 6H), 1.45 – 1.20 (m, 12H), 0.97 (t, $J = 7.4$ Hz, 3H), 0.90 (app t, $J = 6.6$ Hz, 3H), 0.89 (app t, $J = 6.7$ Hz, 3H).

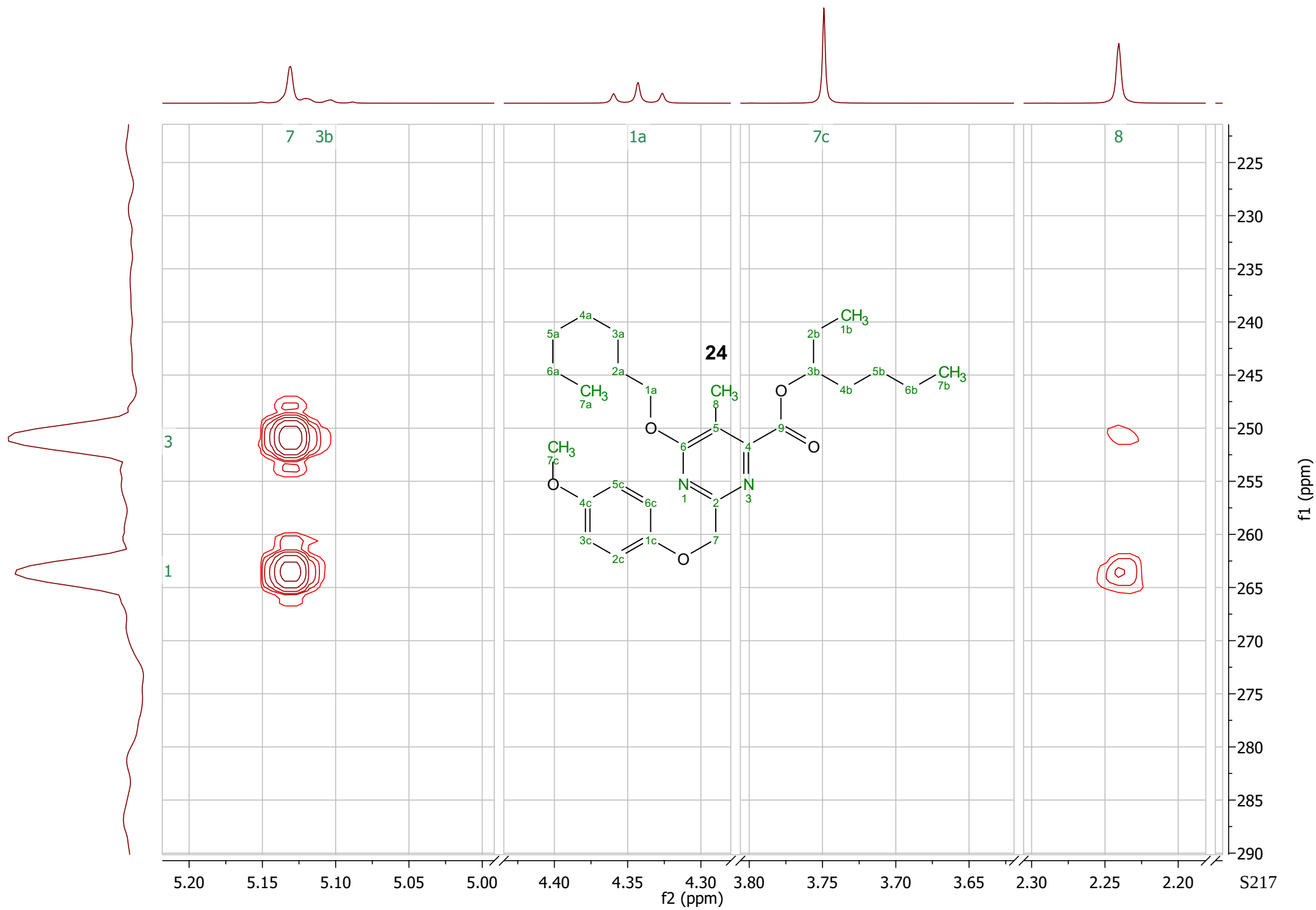


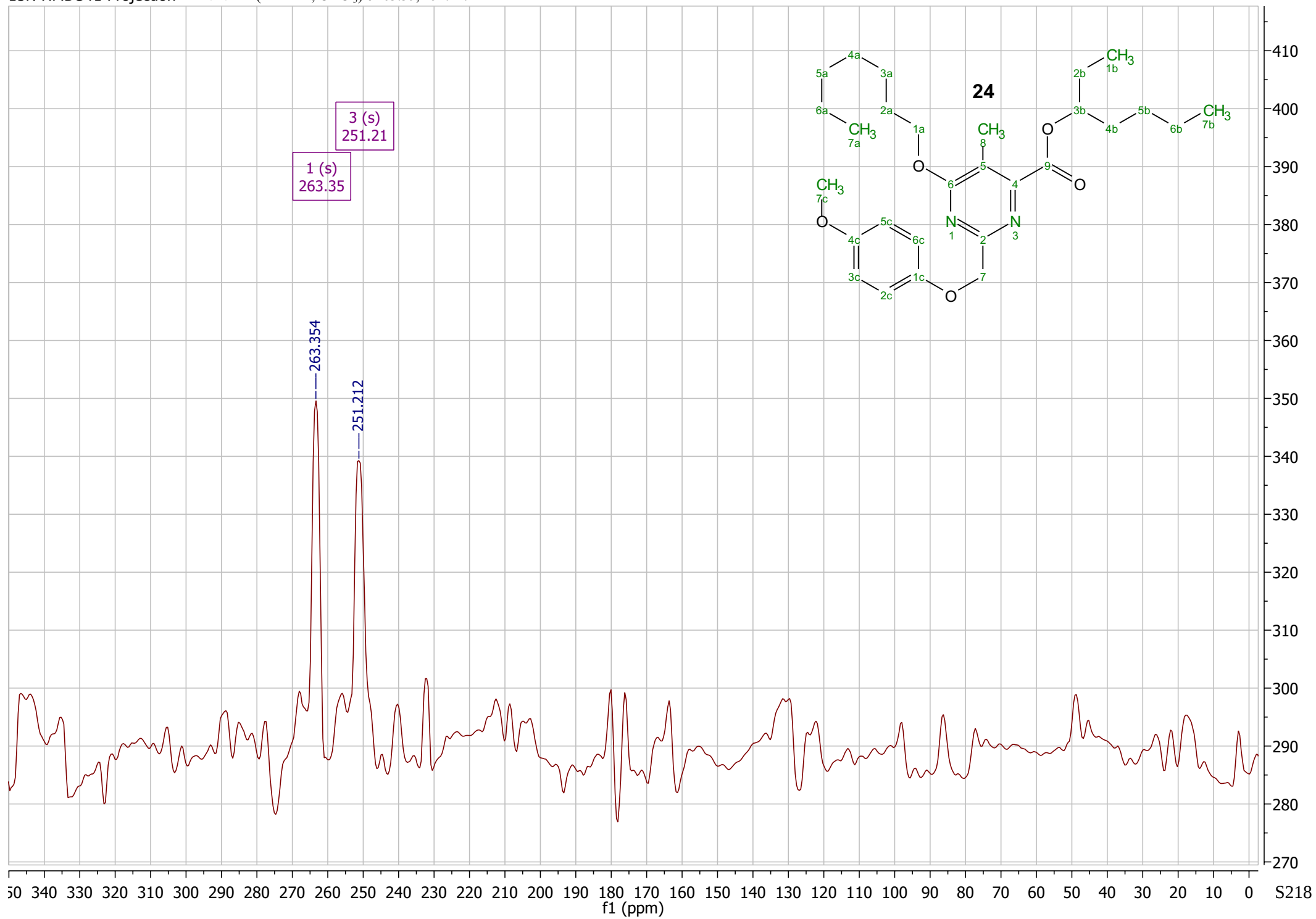
13C ^{13}C NMR (101 MHz, CDCl_3) δ 169.2, 165.9, 163.1, 156.0, 154.1, 153.0, 116.2 (sym, 2C), 115.7, 114.6 (sym, 2C), 78.1, 71.2, 67.6, 55.8, 33.3, 31.9, 29.1, 28.8, 27.6, 27.0, 26.0, 22.74, 22.72, 14.2, 14.1, 11.1, 9.8.



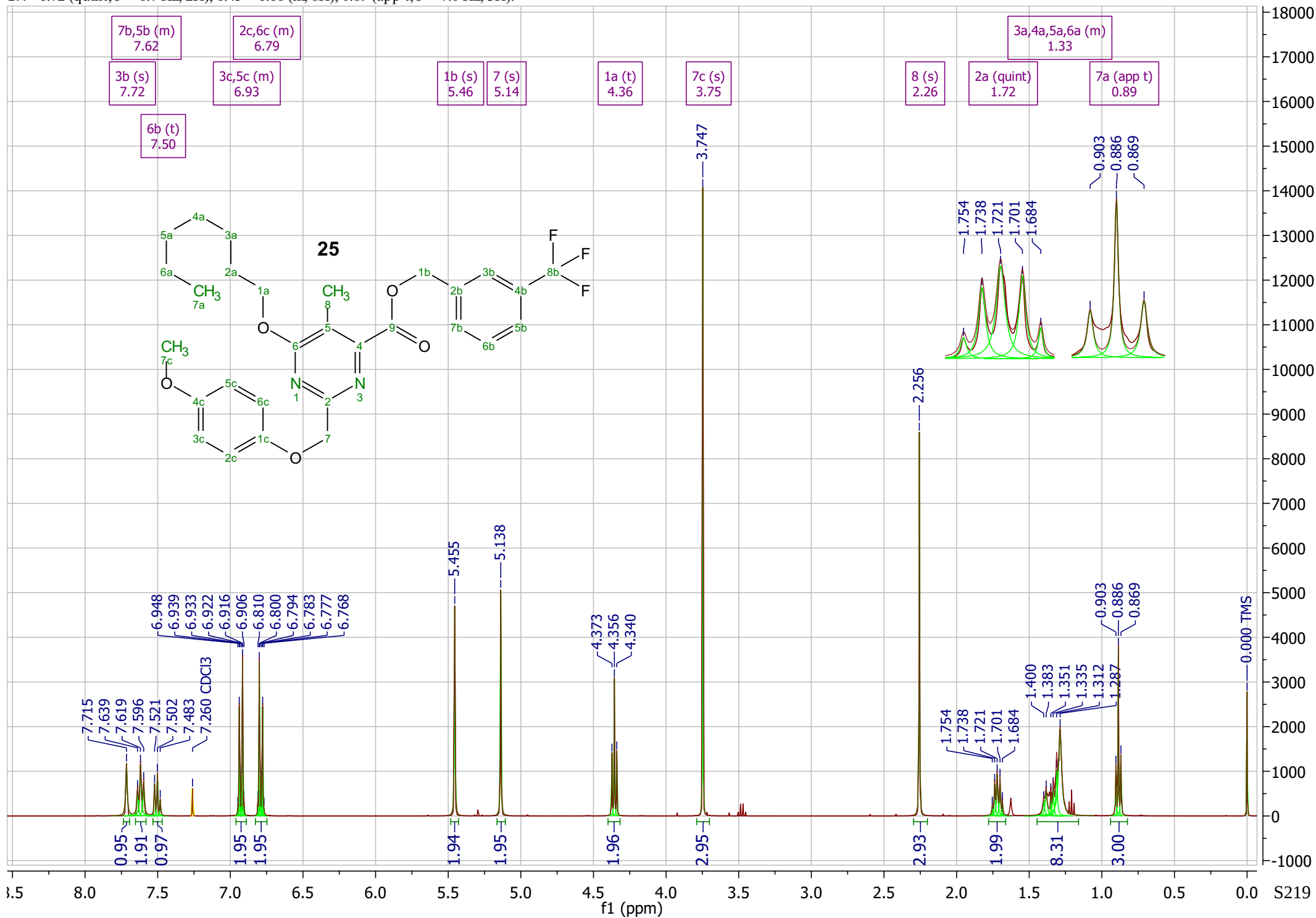




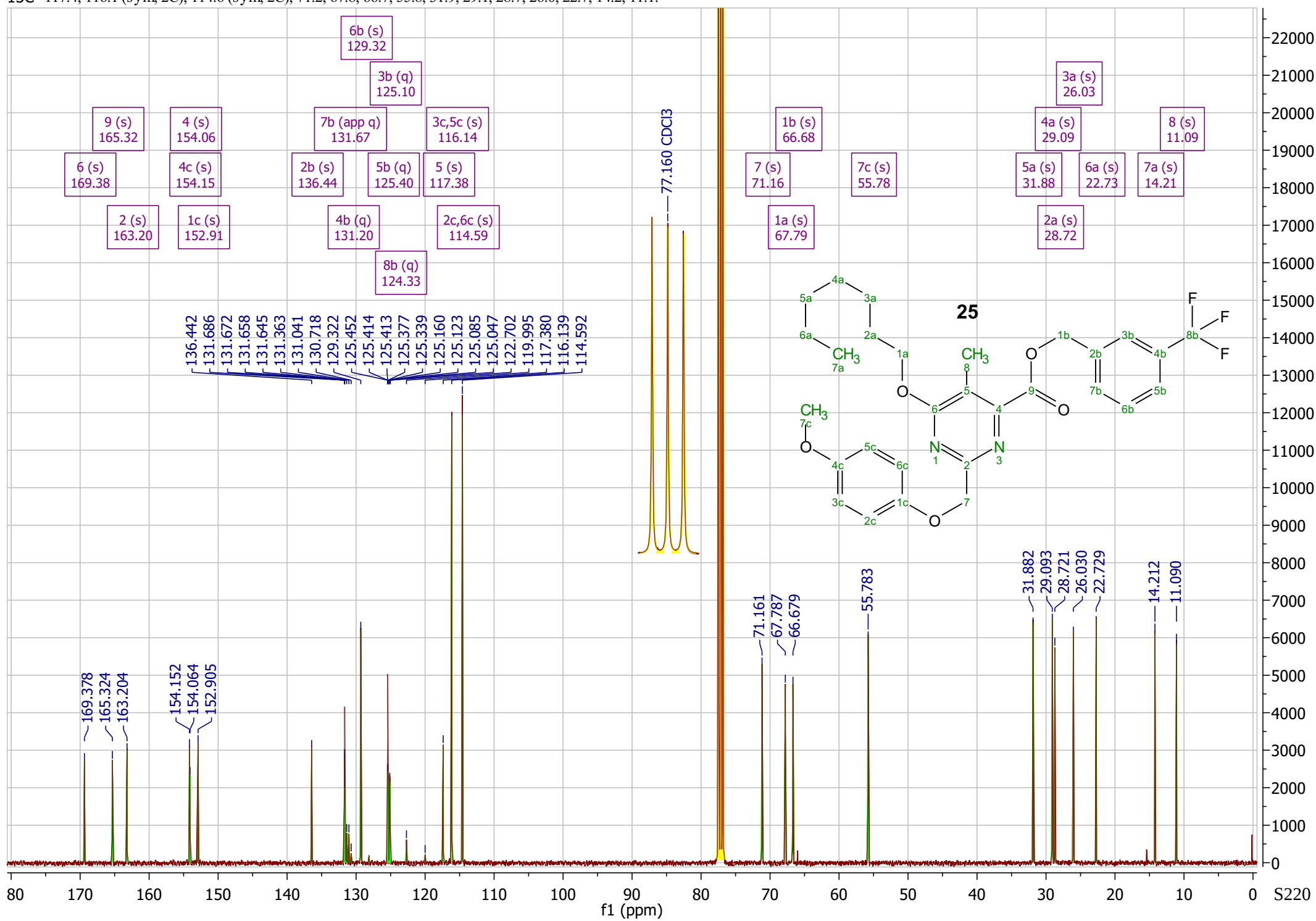




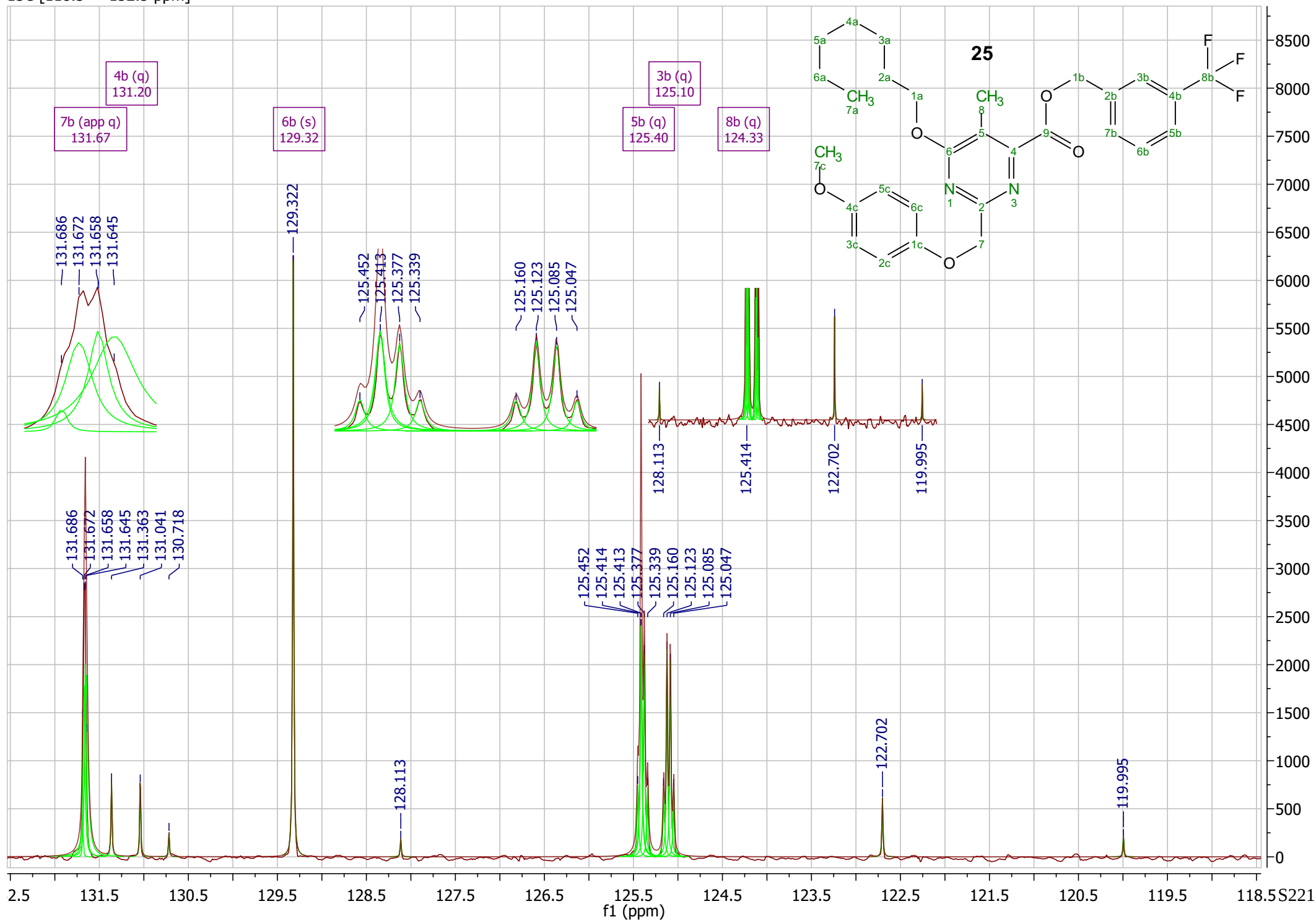
¹H NMR (400 MHz, CDCl₃) δ 7.72 (s, 1H), 7.65 – 7.58 (m, 2H), 7.50 (t, *J* = 7.7 Hz, 1H), 6.96 – 6.89 (m, 2H), 6.83 – 6.75 (m, 2H), 5.46 (s, 2H), 5.14 (s, 2H), 4.36 (s, 2H), 5.14 (s, 2H), 4.36 (t, *J* = 6.6 Hz, 2H), 3.75 (s, 3H), 2.26 (s, 3H), 1.72 (quint, *J* = 6.7 Hz, 2H), 1.45 – 1.16 (m, 8H), 0.89 (app t, *J* = 7.0 Hz, 3H).

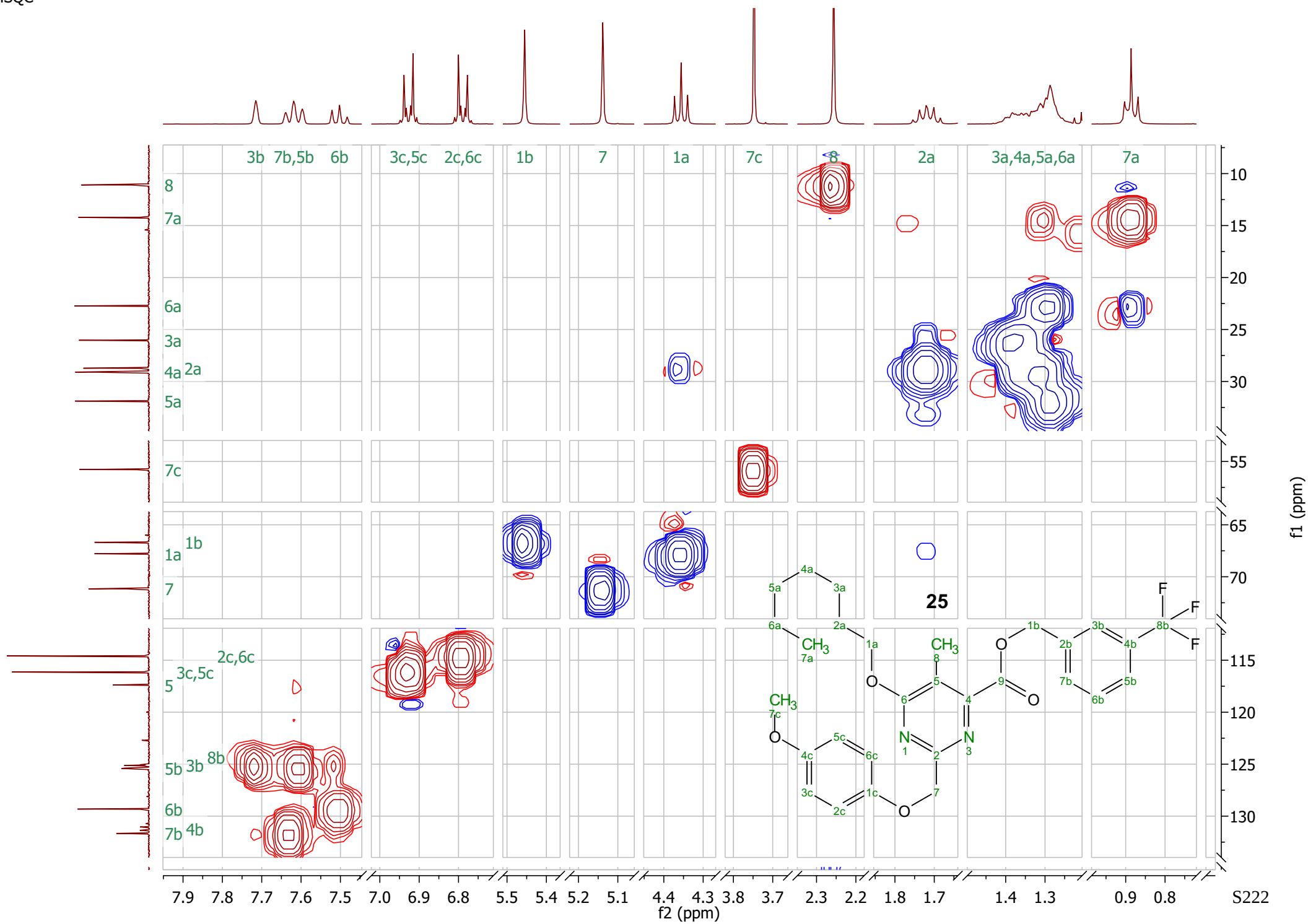


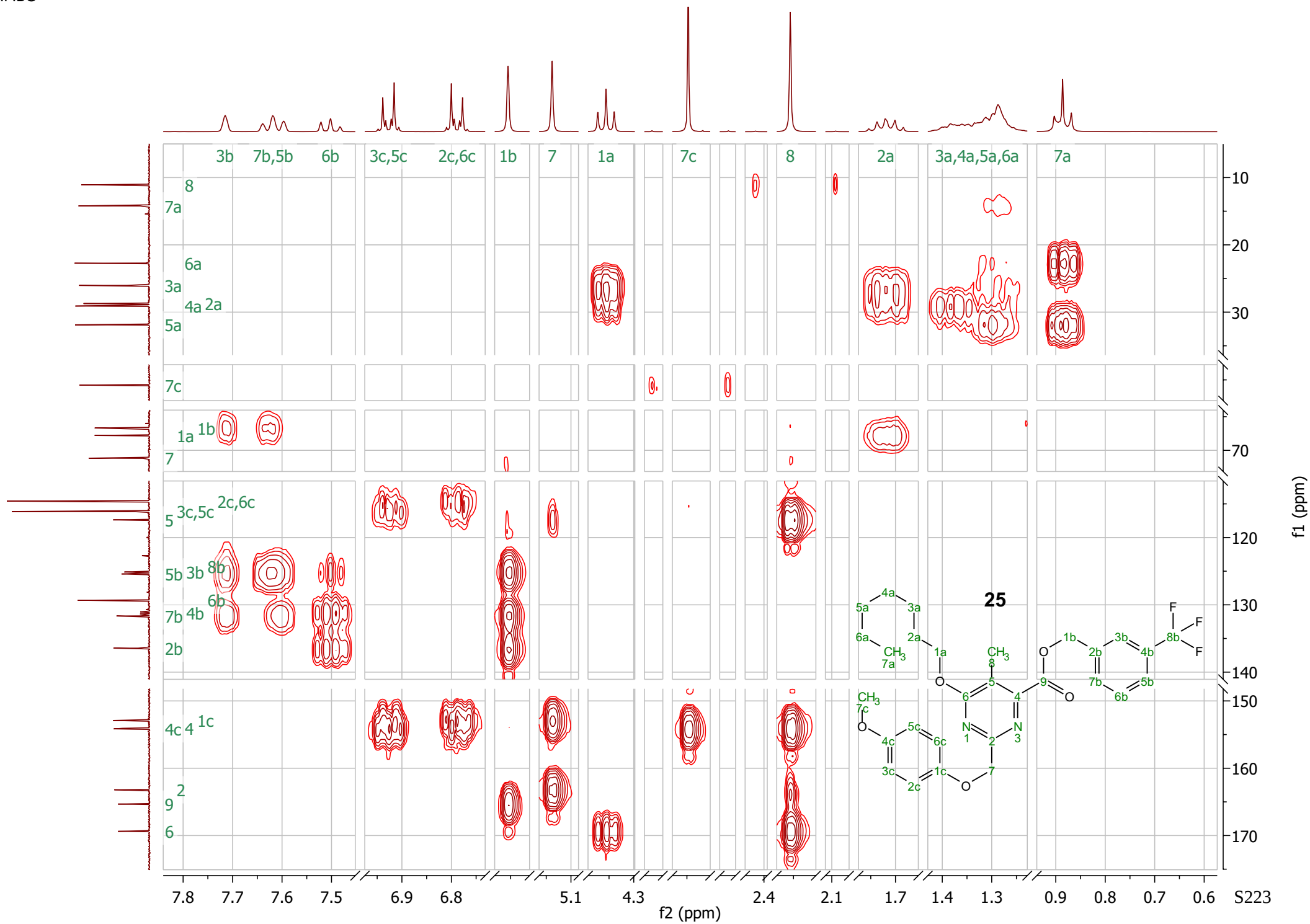
^{13}C NMR (101 MHz, CDCl_3) δ 169.4, 165.3, 163.2, 154.2, 152.9, 154.1, 152.9, 136.4, 131.7 (app q, $J = 1.5$ Hz), 131.2 (q, $J = 3.6$ Hz), 129.3, 125.4 (q, $J = 3.6$ Hz), 125.1 (q, $J = 3.7$ Hz), 124.3 (q, $J = 272.5$ Hz), 117.4, 116.1 (sym, 2C), 114.6 (sym, 2C), 71.2, 67.8, 66.7, 55.8, 31.9, 29.1, 28.7, 26.0, 22.7, 14.2, 11.1.

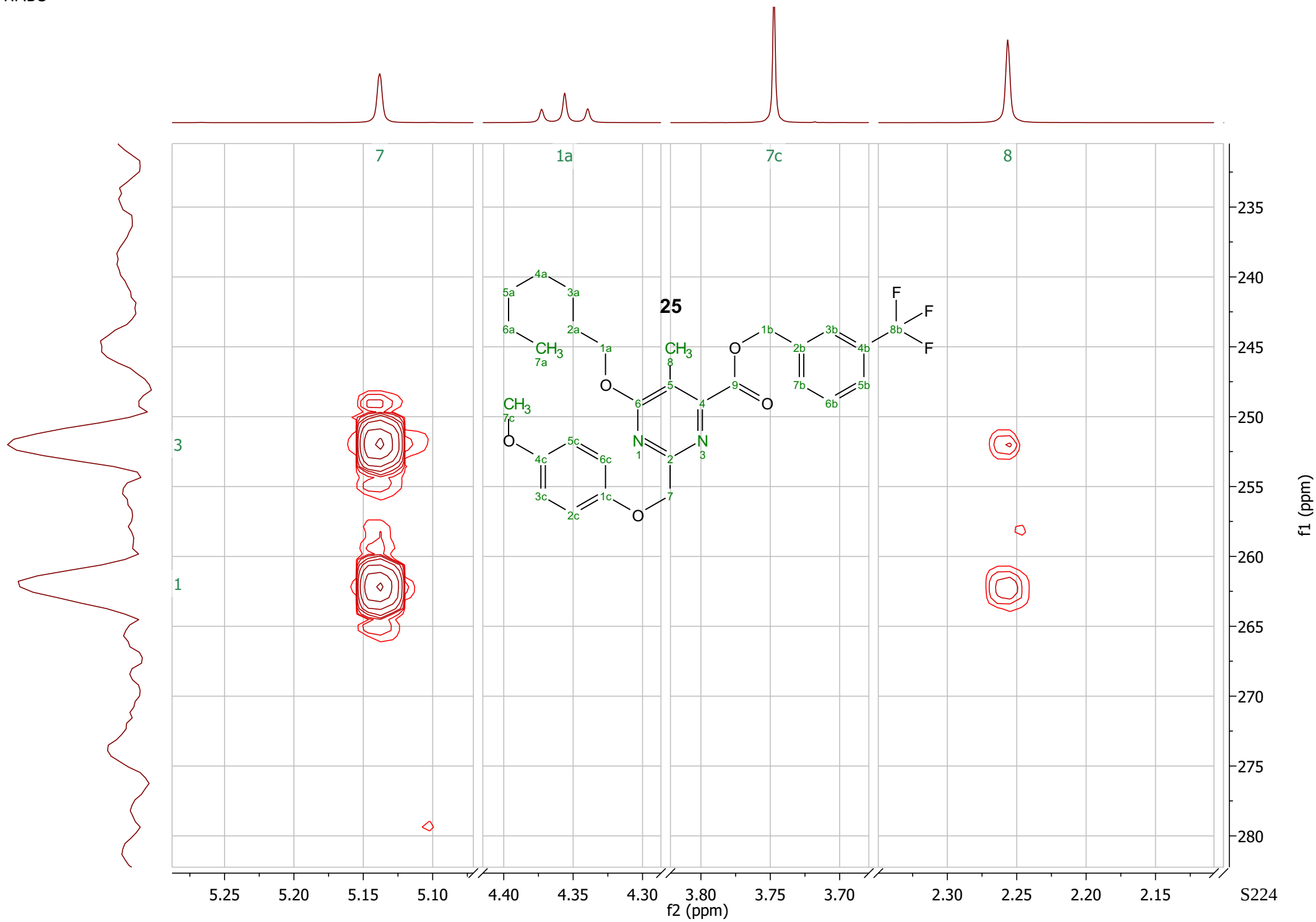


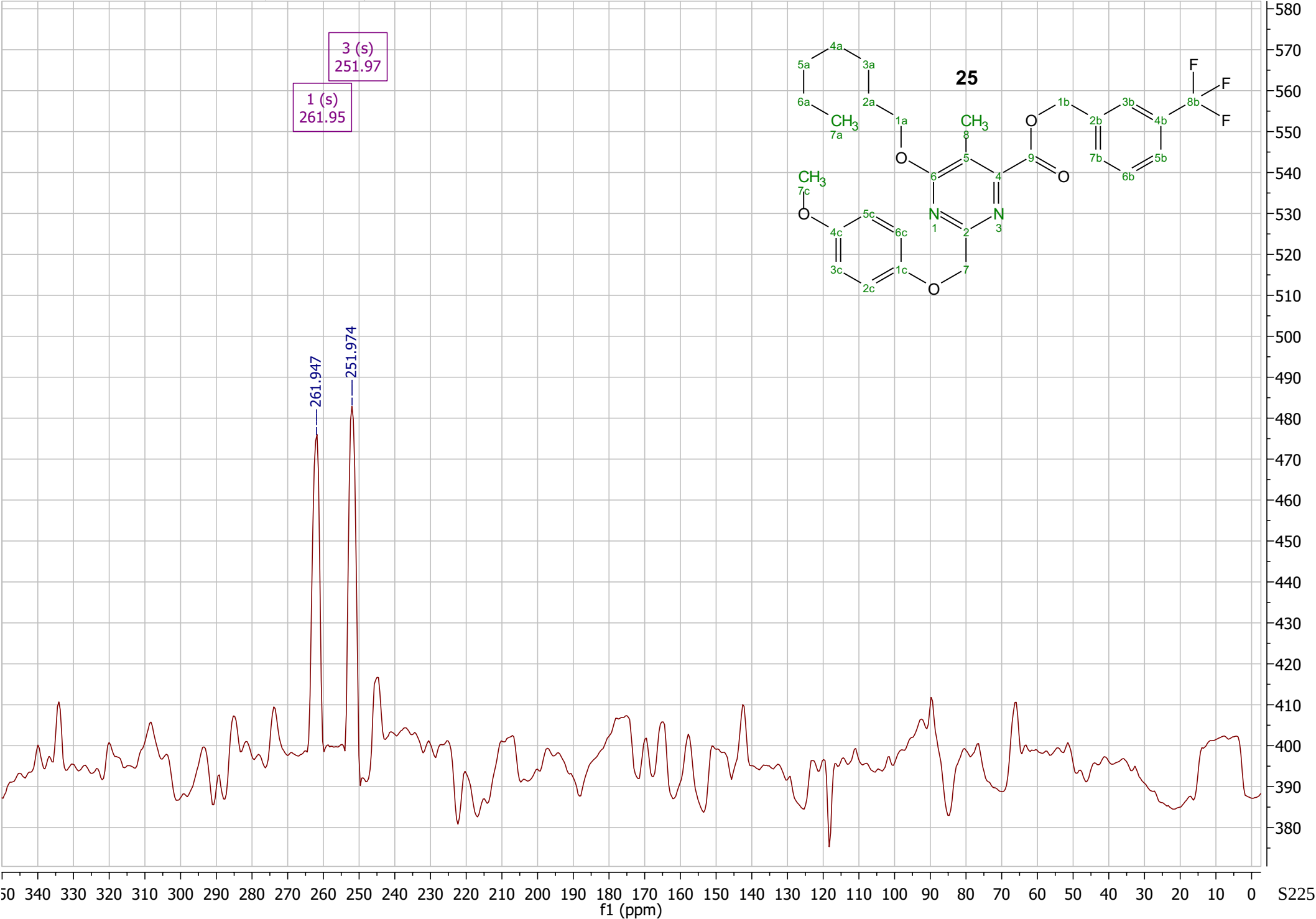
¹³C [118.5 — 132.5 ppm]



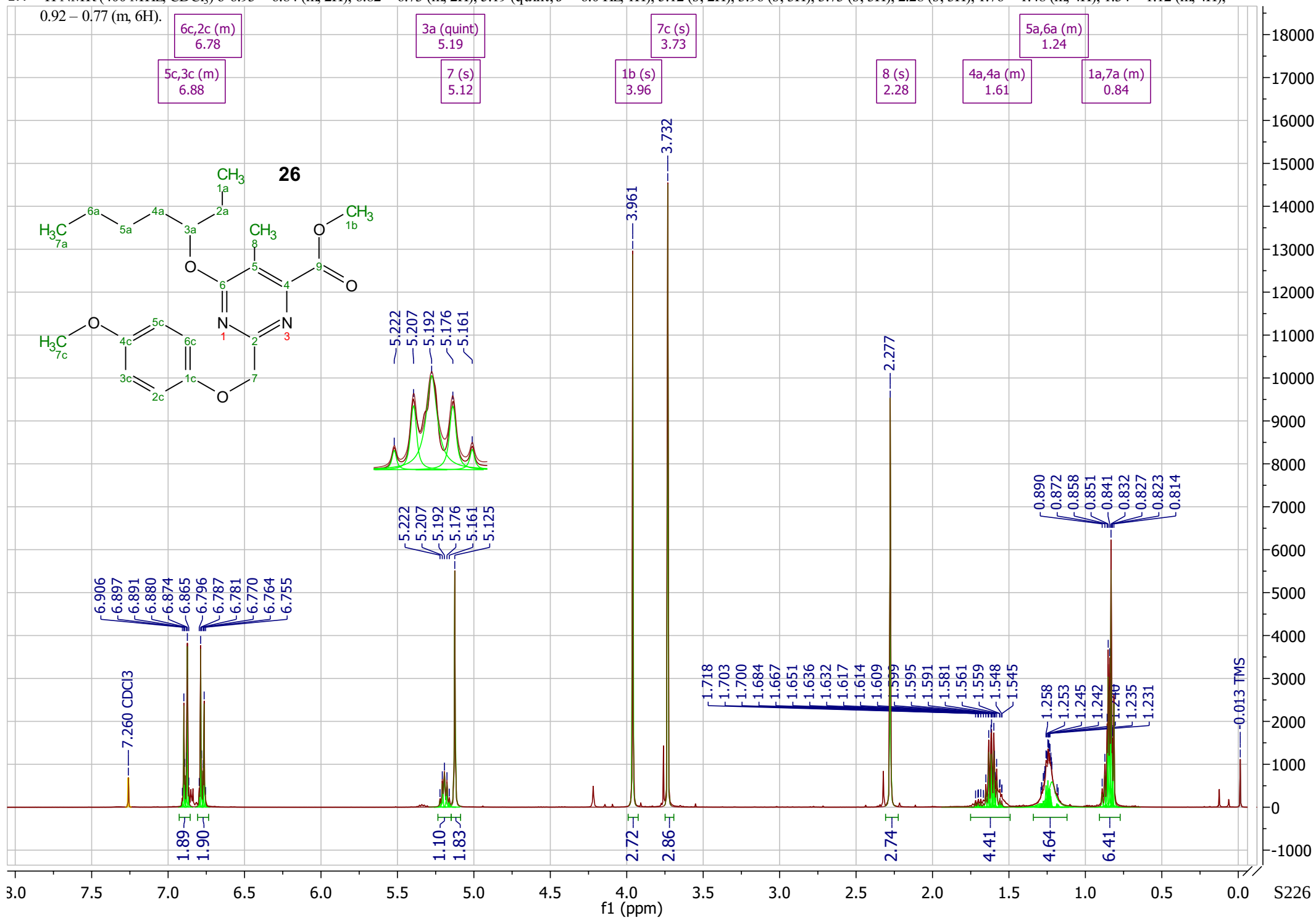




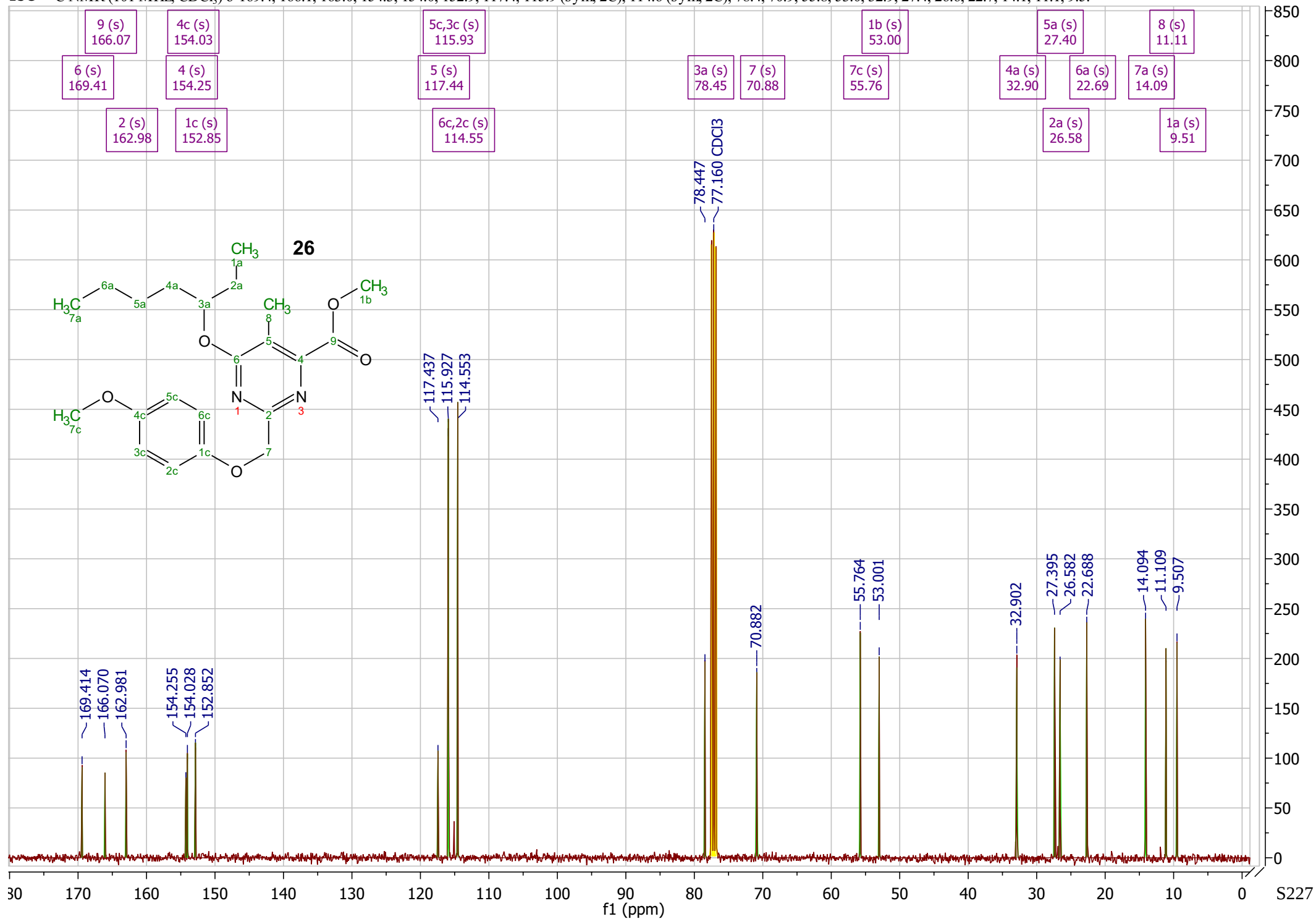


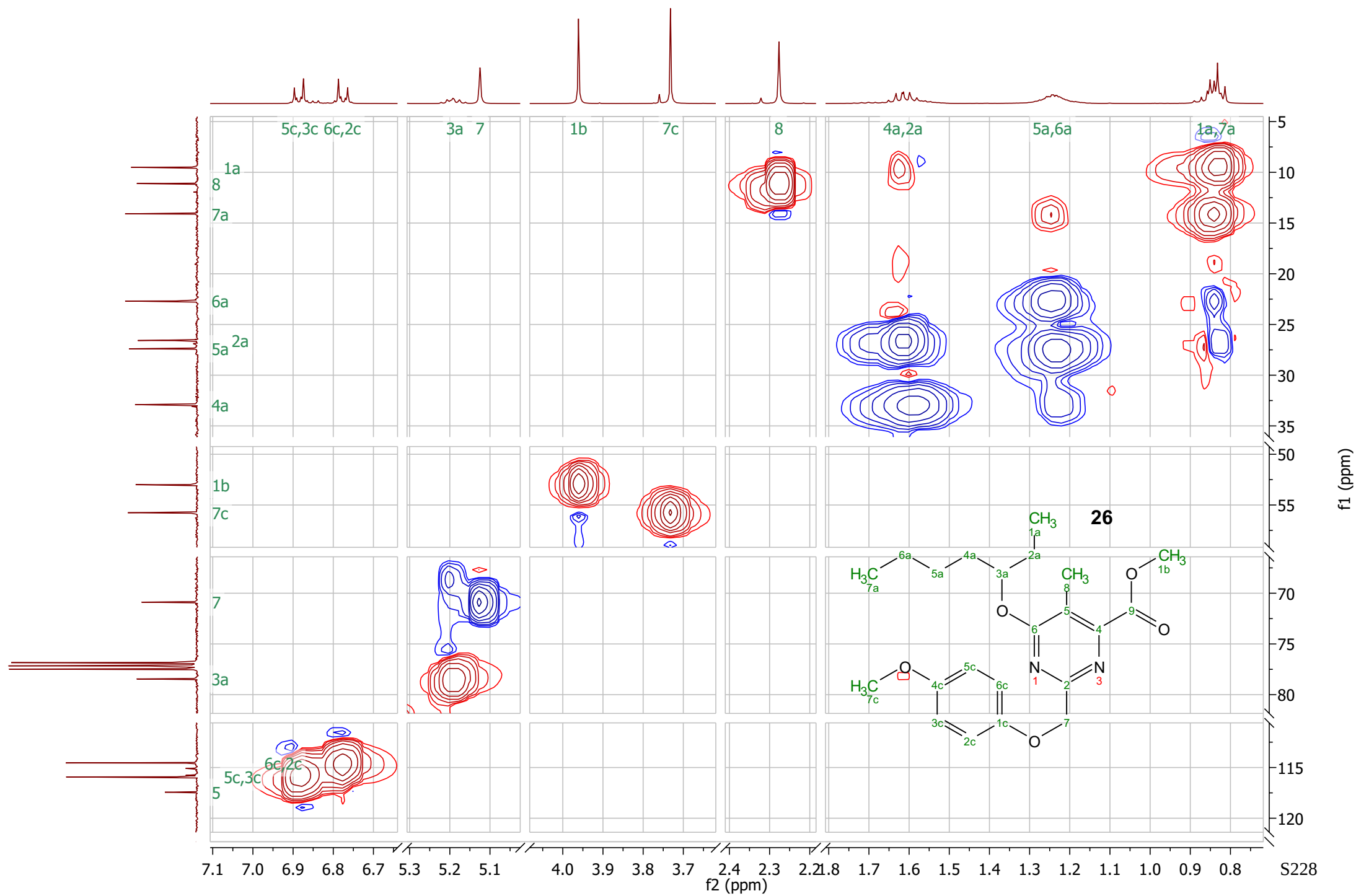


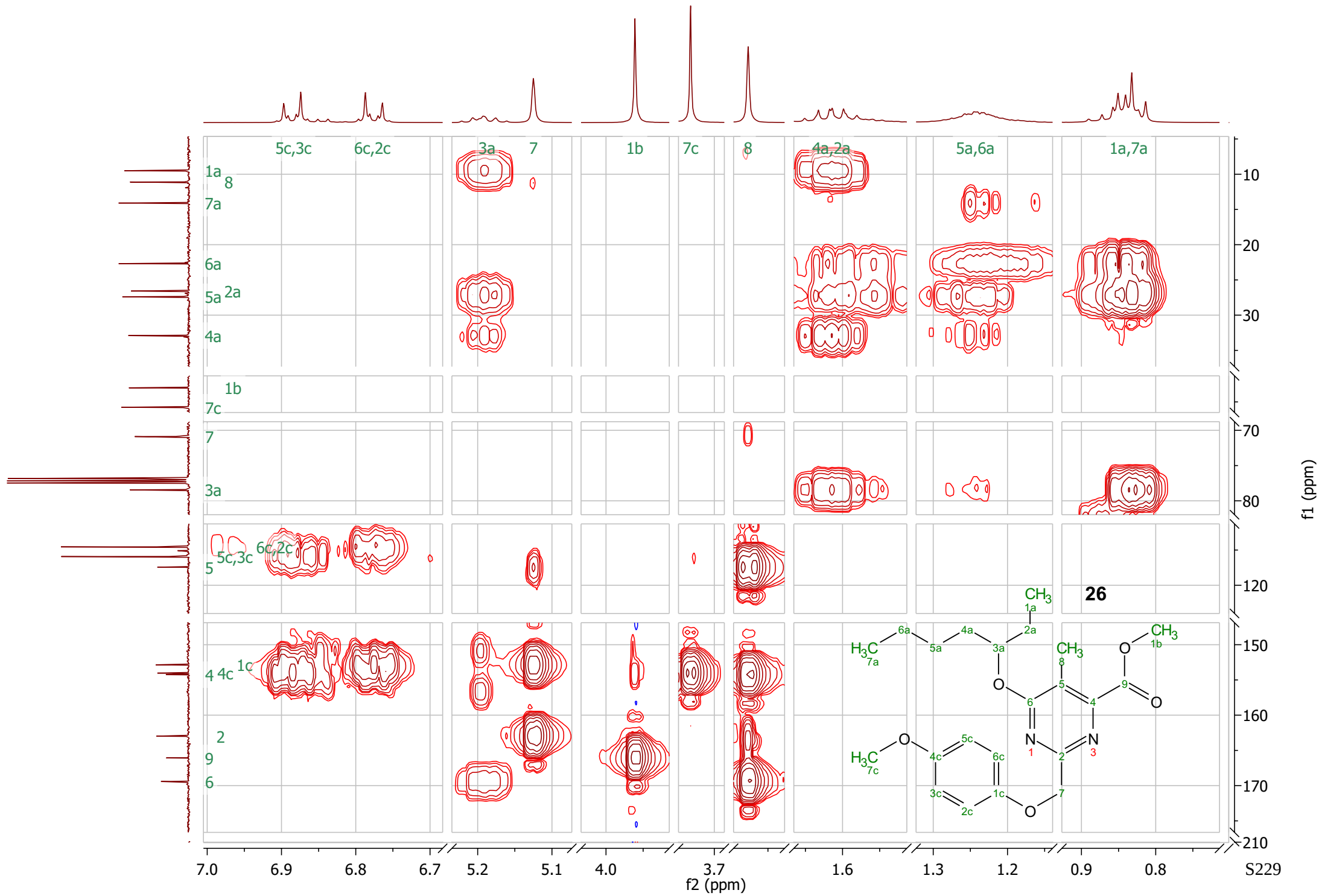
^1H NMR (400 MHz, CDCl_3) δ 6.93 – 6.84 (m, 2H), 6.82 – 6.73 (m, 2H), 5.19 (quint, $J = 6.0$ Hz, 1H), 5.12 (s, 2H), 3.96 (s, 3H), 3.73 (s, 3H), 2.28 (s, 3H), 1.76 – 1.48 (m, 4H), 1.34 – 1.12 (m, 4H), 0.92 – 0.77 (m, 6H).



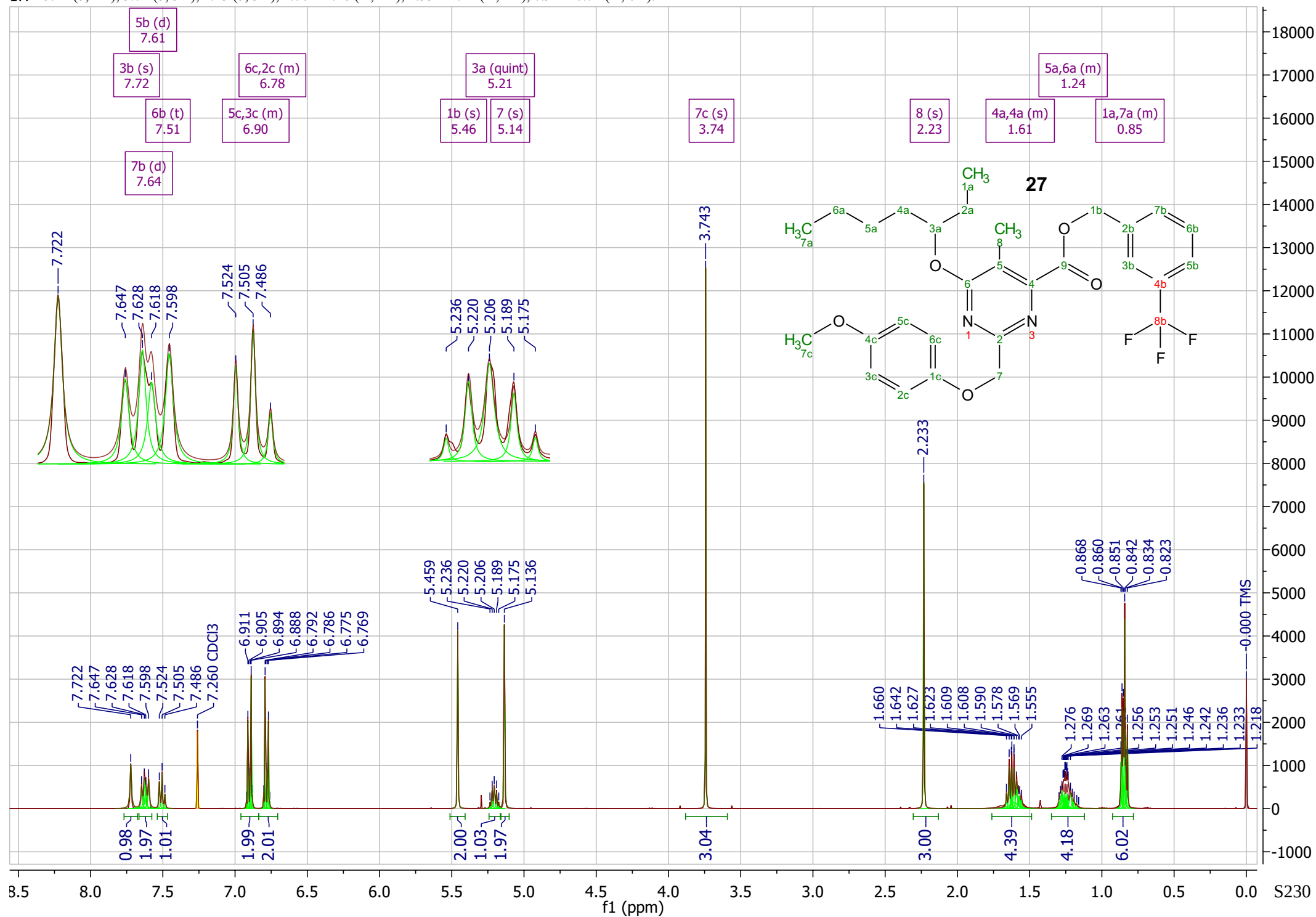
13C ¹³C NMR (101 MHz, CDCl₃) δ 169.4, 166.1, 163.0, 154.3, 154.0, 152.9, 117.4, 115.9 (sym, 2C), 114.6 (sym, 2C), 78.4, 70.9, 55.8, 53.0, 32.9, 27.4, 26.6, 22.7, 14.1, 11.1, 9.5.







^1H NMR (400 MHz, CDCl_3) δ 7.72 (s, 1H), 7.64 (d, $J = 7.6$ Hz, 1H), 7.61 (d, $J = 7.9$ Hz, 1H), 7.51 (t, $J = 7.7$ Hz, 1H), 6.97 – 6.84 (m, 2H), 6.84 – 6.71 (m, 2H), 5.46 (s, 2H), 5.21 (quint, $J = 5.9$ Hz, 1H), 1H 5.14 (s, 2H), 3.74 (s, 3H), 2.23 (s, 3H), 1.76 – 1.48 (m, 4H), 1.33 – 1.11 (m, 4H), 0.92 – 0.74 (m, 6H).



¹³C NMR (101 MHz, CDCl₃) δ 169.4, 165.5, 163.2, 154.3, 154.1, 152.9, 136.4, 131.7 (app q, *J* = 0.9 Hz), 129.3, 125.4 (q, *J* = 3.8 Hz), 125.2 (q, *J* = 3.8 Hz), 117.2, 116.0 (sym, 2C), 114.6 (sym, 2C), 13C 78.5, 70.9, 66.7, 55.8, 32.9, 27.4, 26.6, 22.7, 14.1, 11.1, 9.5.

