Electronic Supplementary Material (ESI) for Chemical Communications

SUPPORTING INFORMATION

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1. General.

Aldehydes were distilled prior to use for the elaboration of the iminoesters. Melting points were determined with a Reichert Thermovar hot plate apparatus and are uncorrected. Only the structurally most important peaks of the IR spectra (recorded on a Nicolet 510 P-FT and on a Jasco FTIR 4100) are listed. ^{1}H NMR (300 MHz) and ^{13}C NMR (75 MHz) spectra were obtained on a Bruker AC-300 using $CDCl_3$ as solvent and TMS as internal standard, unless otherwise stated. Optical rotations were measured on a Perkin Elmer 341 polarimeter. Low-resolution electron impact (EI) mass spectra were obtained at 70eV on a Shimadzu QP-5000 and high-resolution mass spectra were obtained on a Finnigan VG Platform. HRMS (EI) were recorded on a Finnigan MAT 95S. Microanalyses were performed on a Perkin Elmer 2400 and a Carlo Erba EA1108. Analytical TLC was performed on Schleicher & Schuell F1400/LS silica gel plates and the spots were visualized under UV light (λ=254 nm). For flash chromatography we employed Merck silica gel 60 (0.040-0.063 mm). Complexes were prepared according to the reported procedure (see text). All of the transformations performed with silver catalysts were performed in the absence of light.

2. General procedure for the synthesis of compounds 3 and 4 in the absence of AgOAc.

Methyl ester L-proline hydrochloride (82.8 mg, 0.5 mmol) or L-4-hydroxyproline methyl ester hydrochloride (92.1 mg, 0.5 mmol), the corresponding alkene (0.5 mmol), the aldehyde (0.5 mmol) and triethylamine (90 µL, 0.55 mmol) were dissolved in toluene (3mL). The resulting mixture was stirred for times described in Table 1 and 2. Then the solvent was evaporated under reduced pressure and the residue was purified by flash chromatography (silica gel) to afford the corresponding product **3** or **4**.

3. General procedure for the synthesis of compounds 3 and 4 in the presence of AgOAc.

Methyl ester L-proline hydrochloride (82.8 mg, 0.5 mmol) or L-4-Hydroxyproline methyl ester hydrochloride (92.1 mg, 0.5 mmol), silver acetate (4.15 mg, 0.025 mmol), the corresponding alkene (0.5 mmol), the aldehyde (0.5 mmol) and triethylamine (90 µL, 0.55 mmol) were dissolved in toluene (3mL). The resulting suspension was stirred for the corresponding times (see Tables 1 and 2) avoiding the light exposure. Then the solvent was evaporated under reduced pressure. and the residue was purified by flash chromatography (silica gel) to afford the corresponding product **3** or **4**.

4. Physical and spectroscopic data of compounds 3 and 4

(2*S,3*S**,7a*R**)-Dimethyl 3-[*(E)*-styryl]hexahydro-*1H*-pyrrolizine-2,7a-dicarboxylate 3a:** Pale orange needles, mp: 107-110ºC; IR (neat) ν_{max} 2985, 2939, 2305, 1714, 1691 cm^{-1}; ^1H NMR δ_H: 1.72–1.93 (m, 3H, C*H*$_2$CH$_2$N, C*H*HCCO$_2$Me), 2.22 (deform. dd, *J* = 13.0, 12.8 Hz, 1H, C*H*HCHCO$_2$Me), 2.31 (deform. ddd, *J* = 8.6, 6.9 Hz, 1H, C*H*HCCO$_2$Me), 2.64 (dd, *J* = 13.0, 6.7 Hz, 1H, C*H*HCHCO$_2$Me), 2.89 (deform. ddd, *J* = 11.2, 6.7, 2.3 Hz, 1H, C*H*HN), 3.10 (m, 1H, C*H*HN), 3.51-3.58 (m, 4H, CHCO$_2$Me, CHCO$_2$C*H*$_3$), 3.75 (s, 3H, CCO$_2$CH$_3$), 4.19 (dd, *J* = 10.4, 6.4 Hz, 1H, CHN), 5.98 (dd, *J* = 15.5, 10.4 Hz, 1H, C*H*CHN), 6.56 (d, *J* = 15.5 Hz, 1H, C*H*Ph), 7.28-7.35 (m, 5H, Ar*H*); ^{13}C NMR δ_C: 28.0 (*C*H$_2$CH$_2$N), 36.5 (*C*H$_2$CCO$_2$Me), 37.2 (*C*H$_2$CHCO$_2$Me), 48.8 (CH$_2$N), 50.0 (*C*HCO$_2$Me), 51.9 (CHCO$_2$*C*H$_3$), 52.6 (CCO$_2$*C*H$_3$), 67.4 (CHN), 76.4 (*C*CO$_2$Me), 125.7 (*C*HCHN), 126.7, 128.0, 128.7, 136.5 (Ar*C*), 135.5 (*C*HPh), 172.2 (CH*C*O$_2$Me), 177.0 (C*C*O$_2$Me); MS (EI-GC) *m/z*: 329 (M^+, 3%), 271 (19), 270 (100), 243 (13), 238 (21), 210 (17), 184 (40), 123 (10), 115 (10); Microanalysis calculated for $C_{19}H_{23}NO_4$: C, 69.3; H, 7.0; N, 4.3%; found: C, 69.5; H, 7.2; N, 4.5%.

(2*S,3*S**,7a*R**)-2-allyl 7a-methyl 2-methyl-3-(*(E)*-styryl)hexahydro-*1H*-pyrrolizine-2,7a-dicarboxylate 3b:** Brown-yellow solid, mp: 90-95ºC; IR (neat) ν_{max} 2983, 1720, 1699, 2310, 1270 cm^{-1}; ^1H NMR δ_H: 1.44 (s, 3H, CCH$_3$), 1.69-2.02 (m, 3H, C*H*$_2$CH$_2$N, C*H*HCCO$_2$Me), 2.15-2.24 (m, 1H, C*H*HCCO$_2$Me), 2.51 [d, *J* = 13.7 Hz, 1H, C*H*HC(CH$_3$)CO$_2$Allyl], 2.64 [d, *J* = 13.7 Hz, 1H, C*H*HC(CH$_3$)CO$_2$Allyl], 2.92-3.01 (m, 1H, C*H*HN), 3.08-3.16 (m, 1H, C*H*HN), 3.77 (s, 3H, CCO$_2$CH$_3$), 3.80 (d, *J* = 10.4, Hz, 1H, CHN), 4.43-4.45 (m, 2H, CO$_2$C*H*$_2$CHCH$_2$), 5.07 (ddd, *J* = 10.4, 2.6, 1.2 Hz, 1H, CO$_2$CH$_2$CHC*H*H), 5.19 (ddd, *J* = 17.2, 2.6, 1.2 Hz, 1H, CO$_2$CH$_2$CHC*H*H), 5.75 (ddt, *J* = 17.2, 10.4, 5.9 Hz, 1H, CO$_2$CH$_2$C*H*CH$_2$), 5.95 (dd, *J* = 15.6, 10.4 Hz, 1H, C*H*CHN), 6.53 (d, *J* = 15.6 Hz, 1H, C*H*Ph), 7.23-7.34 (m, 5H, Ar*H*); ^{13}C NMR δ_C: 23.5 (C*C*H$_3$), 27.5 (*C*H$_2$CH$_2$N), 39.2 (*C*H$_2$CCO$_2$Me), 43.9 [*C*H$_2$C(CH$_3$)CO$_2$Allyl], 49.0 (CH$_2$N), 52.7 (CCO$_2$*C*H$_3$),

55.5 (CCO_2CH_3), 65.7 ($CO_2CH_2CHCH_2$), 74.6 (CHN), 77.4 [$C(CH_3)CO_2$Allyl], 118.6 ($CO_2CH_2CHCH_2$), 126.1 (*C*HCHN), 126.7, 127.9, 128.7, 136.6 (Ar*C*), 132.1 ($CO_2CH_2CHCH_2$), 135.4 (*C*HPh), 174.4 (CO_2Allyl), 178.0 (CO_2Me); MS (EI-GC) *m/z*: 369 (M^+, <1%), 310 (33), 243 (34), 185 (15), 184 (100), 115 (11); Microanalysis calculated for $C_{22}H_{27}NO_4$: C, 71.5; H, 7.4; N, 3.8%; found: C, 72.2; H, 7.1; N, 4.2%.

(3a*S,4*S**,8a*R**,8b*R**)-methyl 2-methyl-1,3-dioxo-4-((*E*)-styryl)decahydropyrrolo[3,4-a]pyrrolizine-8a-carboxylate 3c:** Sticky brown oil IR (neat) ν_{max} 2360, 2341, 1699, 1265 cm^{-1}; ^{1}H NMR δ_H: 1.73-1.85, 1.95-2.08 (m, 2H, C*H*$_2$CH$_2$N), 2.31-2.40, 2.46-2.59 (m, 3H, C*H*$_2$CCO$_2$Me, C*H*HN), 2.97 (s, 3H, NCH_3), 3.08 (m, 1H, C*H*HN), 3.46 (deform. dd, *J* = 8.1 Hz, 1H, C*H*CHN), 3.81 (s, 3H, CO_2CH_3), 3.89 (d, *J* = 8.1 Hz, 1H, CHCCO$_2$Me), 4.20 (dd, *J* = 9.0, 8.1 Hz, 1H, CHN), 6.37 (dd, *J* = 15.6, 9.0 Hz, 1H, C*H*CHN), 6.76 (d, *J* = 15.6 Hz, 1H, C*H*Ph), 7.21-7.42 (m, 5H, Ar*H*); ^{13}C NMR δ_C: 25.0 (N*C*H$_3$), 25.3 (*C*H$_2$CH$_2$N), 30.3 (*C*H$_2$CCO$_2$Me), 48.3 (*C*H$_2$N), 51.2 (*C*HCCO$_2$Me), 52.3 (*C*HCHCCO$_2$Me), 53.2 (CCO$_2$*C*H$_3$), 64.6 (CHN), 78.9 (*C*CO$_2$CH$_3$), 123.4 (*C*HCHN), 126.9, 128.1, 128.6, 136.7 (Ar*C*), 135.9 (*C*HPh), 174.1, 176.7 (2xCON), 177.1 (CO_2Me); MS (EI-GC) *m/z*: 354 (M^+, <1%), 296 (25), 295 (100), 243 (30), 242 (10), 241 (10), 228 (11), 184 (13), 115 (12), 91 (11); Microanalysis calculated for $C_{20}H_{22}N_2O_4$: C, 67.8; H, 6.3; N, 7.9%; found: C, 68.2; H, 6.3; N, 8.0%.

(3a*S,4*S**,8a*R**,8b*R**)-methyl 2-methyl-1,3-dioxo-4-((*E*)-styryl)decahydropyrrolo[3,4-a]pyrrolizine-8a-carboxylate 3c´:** Sticky brown oil; IR (neat) ν_{max} 2370, 2328, 1715 cm^{-1}; ^{1}H NMR δ_H: 1.83-2.02 (m, 3H, C*H*$_2$CH$_2$N, C*H*HCCO$_2$Me), 2.72-2.81(m, 1H, C*H*HCCO$_2$Me), 2.98 (s, 3H, NCH_3), 3.02-3.09 (m, 2H, C*H*$_2$N), 3.40 (d, *J* = 9.5 Hz, 1H, C*H*CCO$_2$Me), 3.56 (dd, *J* = 9.5, 7.5 Hz, 1H, C*H*CHN), 3.71 (s, 3H, CO_2CH_3), 4.42 (deform. dd, *J* = 7.5, 7.0 Hz, 1H, CHN), 6.32 (dd, *J* = 15.9, 7.0 Hz, 1H, C*H*CHN), 6.85 (d, *J* = 15.9 Hz, 1H, C*H*Ph), 7.22-7.42 (m, 5H, Ar*H*); ^{13}C NMR δ_C: 25.0 (N*C*H$_3$), 25.3 (*C*H$_2$CH$_2$N), 36.3 (*C*H$_2$CCO$_2$Me), 49.3 (*C*H$_2$N), 51.1 (*C*HCCO$_2$Me), 52.7 (*C*HCHCCO$_2$Me), 57.1 (CCO$_2$*C*H$_3$), 67.3 (CHN), 78.8 (*C*CO$_2$CH$_3$), 125.3 (*C*HCHN), 126.7, 128.1, 128.6, 136.3 (Ar*C*), 134.9 (*C*HPh), 172.1, 176.1 (2xCON), 176.3 (CO_2Me); MS (EI-GC) *m/z*: 354 (M^+, <1%), 296 (31), 295 (100), 243 (28), 242 (11), 228 (15), 184 (12), 183 (10), 115 (14); Microanalysis calculated for $C_{20}H_{22}N_2O_4$: C, 67.8; H, 6.3; N, 7.9%; found: C, 68.6; H, 6.5; N, 8.1%.

(1*R,2*R**,3*S**,7a*R**)-trimethyl 3-((*E*)-styryl)hexahydro-*1H*-pyrrolizine-1,2,7a-tricarboxylate 3d:** Sticky yellow oil; IR (neat) ν_{max} 2965, 2915, 2306, 1715, 1713, 1699 cm^{-1}; ^{1}H NMR δ_H: 1.76–1.86 (m, 1H, C*H*HCH$_2$N), 1.93–2.03 (m, 1H, C*H*HCH$_2$N), 2.08–2.17 (m, 1H, C*H*HCCO$_2$Me), 2.52–2.61 (m, 1H, C*H*HCCO$_2$Me), 2.83 (deform. ddd, *J* = 10.8, 6.6, 6.5 Hz, 1H, C*H*HN), 3.09 (deform. ddd, *J* = 10.8, 6.6, 6.5 Hz, 1H, C*H*HN), 3.42 (d, *J* = 11.7 Hz, 1H, C*H*CCO$_2$Me), 3.58, 3.69 (s, 6H, 2xCHCO$_2$C*H*$_3$), 3.70 (s, 3H, CCO$_2$C*H*$_3$), 4.02 (dd, *J* = 11.7, 8.2 Hz, 1H, C*H*CHN), 4.28 (dd, *J* = 10.4, 8.2 Hz, 1H, C*H*N), 5.96 (dd, *J* = 15.5, 10.4 Hz, 1H, C*H*CHN), 6.56 (d, *J* = 15.5 Hz, 1H, C*H*Ph), 7.25-7.35 (m, 5H, Ar*H*); ^{13}C NMR δ_C: 27.6 (*C*H$_2$CH$_2$N), 35.8 (*C*H$_2$CCO$_2$Me), 48.8 (CH$_2$N), 52.1, 52.2 (2x*C*HCO$_2$Me), 52.4, 52.6, 53.6 (3xCO$_2$*C*H$_3$), 65.7 (CHN), 78.2 (*C*CO$_2$Me), 125.3 (*C*HCHN), 126.7, 128.2, 128.7, 136.3 (Ar*C*), 135.8 (*C*HPh), 171.1, 171.7 (2xCH*C*O$_2$Me), 174.1 (C*C*O$_2$Me); MS (EI-GC) *m/z*: 387 (M^+, <1%), 271 (19), 270 (100), 243 (13), 238 (21), 210 (17), 184 (40), 123 (10), 115 (10); Microanalysis calculated for $C_{21}H_{25}NO_6$: C, 65.1; H, 6.5; N, 3.6 %; found: C, 65.4; H, 7.0; N, 3.9%.

(1*S,2*S**,3*S**,7a*R*)-methyl 2-nitro-1-phenyl-3-((*E*)-styryl)hexahydro-*1H*-pyrrolizine-7a-carboxylate 3e:** Sticky brown oil; IR (neat) ν_{max} 3003, 2983, 2872, 1726, 1536 cm^{-1}; ^1H NMR δ_H: 1.86–2.10 (m, 3H, C*H*$_2$CH$_2$N, C*H*HCCO$_2$Me), 2.68-2.76 (m, 1H, C*H*HCCO$_2$Me), 2.92 (ddd, *J* = 10.1, 6.7, 4.5 Hz, 1H, C*H*HN), 3.25 (ddd, *J* = 10.1, 7.5, 6.3 Hz, 1H, C*H*HN), 3.37 (s, 3H, CCO$_2$CH$_3$), 4.17 (d, *J* = 11.3 Hz, 1H, C*H*CCO$_2$Me), 4.79 (dd, *J* = 10.2, 7.9 Hz, 1H, C*H*N), 6.10 (dd, *J* = 11.3, 7.8 Hz, 1H, C*H*NO$_2$), 6.14 (dd, *J* = 15.5, 10.3 Hz, 1H, C*H*CHN), 6.72 (d, *J* = 15.5 Hz, 1H, C*H*Ph), 7.23-7.40 (m, 10H, Ar*H*); ^{13}C NMR δ_C: 27.4 (*C*H$_2$CH$_2$N), 35.5 (*C*H$_2$CCO$_2$Me), 48.6 (CH$_2$N), 52,1 (CCO$_2$*C*H$_3$), 55.4 (*C*HCCO$_2$CH$_3$), 66.2 (CHN), 80.5 (*C*CO$_2$Me), 91.9 (*C*HNO$_2$), 122.7 (*C*HCHN), 127.1, 127.3, 128.3, 128.6, 128.7, 128.9, 134.1, 135.8 (Ar*C*), 138.3 (*C*HPh), 173.6 (C*C*O$_2$Me); MS (EI-GC) *m/z*: 392 (M^+, <1%), 243 (11), 185 (14), 184 (100), 156 (16); HRMS calculated for $C_{23}H_{24}N_2O_4$+1: 393.1814 found: 393.1800.

(1*R,2*S**,3*S**,7a*R**)-methyl 1-nitro-2-phenyl-3-((E)-styryl)hexahydro-1H-pyrrolizine-7a-carboxylate 3e´:** Sticky brown oil; IR (neat) ν_{max} 3015, 2979, 2872, 1725, 1530 cm^{-1}; ^1H NMR δ_H: 1.57-1.63 (m, 1H, C*H*HCH$_2$N), 1.96-2.02 (m, 2H, C*H*HCH$_2$N, C*H*HCCO$_2$Me), 2.46-2.52 (m, 1H, C*H*HCCO$_2$Me), 3.03 (ddd, *J* = 10.8, 8.7, 6.1 Hz, 1H, C*H*HN), 3.13-3.19 (m, 1H, C*H*HN), 4.06 (dd, *J* = 11.6, 10.2 Hz, 1H, C*H*Ph), 4.23 (ddd, *J* = 11.6, 7.6, 0.5 Hz, 1H, C*H*N), 5.94 (d, *J* = 10.2 Hz, 1H, C*H*NO$_2$), 6.18 (dd, *J* = 15.9, 7.6 Hz, 1H, C*H*CHN), 6.44 (dd, *J* = 15.9, 0.5 Hz, 1H, C*H*Ph), 7.24-7.40 (m, 10H, Ar*H*); ^{13}C NMR δ_C: 26.0 (*C*H$_2$CH$_2$N), 32.1 (*C*H$_2$CCO$_2$Me), 50.7 (CH$_2$N), 51.0 (CCO$_2$*C*H$_3$), 53.6 (*C*HPh), 67.8 (CHN), 76.2 (*C*CO$_2$Me), 97.1 (*C*HNO$_2$), 123.8 (*C*HCHN), 126.6, 127.9, 128.0, 128.2, 128.7, 129.2, 136.1, 136.2 (Ar*C*), 136.4 (*C*HPh), 173.5 (C*C*O$_2$Me); MS (EI-GC) *m/z*: 392 (M^+, <1%), 243 (10), 185 (15), 184 (100), 156 (17), 115 (10); HRMS calculated for $C_{23}H_{24}N_2O_4$+1: 393.1814 found: 393.1806.

(1*R,2*R**,3*S**,7a*S**)-methyl 1,2-bis(phenylsulfonyl)-3-((*E*)-styryl)hexahydro-*1H*-pyrrolizine-7a-carboxylatetricarboxylate 3f:** Sticky pale yellow oil; IR (neat) ν_{max} 2991, 2934, 1708, 1310, 1141 cm^{-1}; ^1H NMR δ_H: 1.99–2.05 (m, 2H, C*H*$_2$CH$_2$N), 2.14-2.22 (m, 1H, C*H*HCCO$_2$Me), 3.03-3.07 (m, 1H, C*H*HCCO$_2$Me), 3.14-3.21 (m, 1H, C*H*HN), 3.32-3.38 (m, 1H, C*H*HN), 3.87 (s, 3H, CCO$_2$CH$_3$), 4.51 (d, *J* = 8.1 Hz, 1H, C*H*CCO$_2$Me), 4.71 (dd, *J* = 10.0, 8.2 Hz, 1H, CHN), 5.04 (deform. dd, *J* = 8.2, 8.1 Hz, 1H, CHN), 6.20 (d, *J* = 15.7 Hz, 1H, C*H*Ph), 6.47 (dd, *J* = 15.7, 10.0 Hz, 1H, C*H*CHN), 7.13-8.04 (m, 15H, Ar*H*); ^{13}C NMR δ_C: 25.6 (*C*H$_2$CH$_2$N), 35.1 (*C*H$_2$CCO$_2$Me), 49.1 (CH$_2$N), 53.1 (CHCO$_2$*C*H$_3$), 65.7 (CHN), 73.7 [*C*H(SO$_2$Ph)CH], 74.5 [*C*H(SO$_2$Ph)CCO$_2$Me], 78.8 (*C*CO$_2$Me), 122.7 (*C*HCHN), 126.9, 128.3, 128.6, 128.9, 129.0, 129.6, 133.6, 133.9, 134.5, 135.9, 139.2, 141.5 (Ar*C*), 136.7 (*C*HPh), 170.9 (C*C*O$_2$Me); MS (EI-GC) *m/z*: 493 (10), 492 (11), 410 (10), 310 (11), 244 (31), 243 (100), 128 (15), 115 (17); HRMS calculated for $C_{29}H_{29}NO_6S_2$ +1: 552.1514 found: 552.1548.

(1*S,2*S**,3*S**,7a*S**)-methyl 1,2-bis(phenylsulfonyl)-3-((*E*)-styryl)hexahydro-1H-pyrrolizine-7a-carboxylatetricarboxylate 3f´:** Sticky yellow oil; IR (neat) ν_{max} 2979, 2910, 1715, 1300, 1148 cm^{-1}; ^1H NMR δ_H: 2.02–2.17 (m, 3H, C*H*$_2$CH$_2$N, C*H*HCCO$_2$Me), 2.94-3.16 (m, 3H, C*H*HCCO$_2$Me, C*H*$_2$N), 3.83 (s, 3H, CCO$_2$CH$_3$), 4.03 (deform dd, *J* = 4.3, 4.1 Hz, 1H, C*H*(SO$_2$Ph)CH), 4.38 (dd, *J* = 8.4, 4.3 Hz, 1H, CHN), 5.06 (d, *J* = 4.1 Hz, 1H, C*H*(SO$_2$Ph)CCO$_2$Me), 6.13-6.24 (m, 2H, C*H*CHN, C*H*Ph), 7.14-7.90 (m, 15H, Ar*H*); ^{13}C NMR δ_C: 26.4 (*C*H$_2$CH$_2$N), 32.4 (*C*H$_2$CCO$_2$Me), 47.2 (CH$_2$N), 53.3 (CHCO$_2$*C*H$_3$), 64.7 (CHN), 66.9 [*C*H(SO$_2$Ph)CH], 71.7 [*C*H(SO$_2$Ph)CCO$_2$Me], 79.8 (*C*CO$_2$Me), 125.9 (*C*HCHN), 126.7, 128.2,

128.6, 128.9, 128.9, 129.3, 129.3, 134.2, 134.3, 135.7, 137.0, 138.5 (Ar*C*), 135.2 (*C*HPh), 173.9 (C*C*O$_2$Me); MS (EI-GC) *m/z*: 551 (M$^+$, <1%), 492 (15), 410 (10), 311 (10), 310 (10), 244 (25), 243 (100), 128 (11), 115 (21); HRMS calculated for $C_{29}H_{29}NO_6S_2$ +1: 552.1514 found: 552.1565.

(2*S,3*S**,7a*R**)-dimethyl 3-((*E*)-prop-1-en-1-yl)hexahydro-*1H*-pyrrolizine-2,7a-dicarboxylatetricarboxylate 3g:** Sticky brown oil; IR (neat) ν_{max} 2985, 2939, 2305, 1714, 1691 cm^{-1}; ^{1}H NMR δ_H: 1.69 (d, *J* = 6.5 Hz, 3H, CHC*H*$_3$), 1.71–1.85 (m, 3H, C*H*$_2$CH$_2$N, C*H*HCCO$_2$Me), 2.02-2.12 (m, 1H, C*H*HCO$_2$Me), 2.20-2.23 (m, 1H, C*H*HCHCO$_2$Me), 2.55 (dd, *J* = 13.2, 6.7 Hz, 1H, C*H*HCHCO$_2$Me), 2.79-2.87 (m, 1H, C*H*HN), 3.02-3.07 (m, 1H, C*H*HN), 3.41 (deform. ddd, *J* = 12.7, 7.5, 6.7 Hz, 1H, C*H*CO$_2$Me), 3.61 (s, 3H, CHCO$_2$C*H*$_3$), 3.72 (s, 3H, CCO$_2$C*H*$_3$), 3.99 (dd, *J* = 10.3, 7.5 Hz, 1H, C*H*N), 5.25 (dd, *J* = 15.0, 10.3 Hz, 1H, C*H*CHN), 5.68 (dq, *J* = 15.0, 6.5 Hz, 1H, C*H*Me); ^{13}C NMR δ_C: 17.9 (CH*C*H$_3$), 27.6 (*C*H$_2$CH$_2$N), 36.4 (*C*H$_2$CHCO$_2$Me), 37.1 (*C*H$_2$CCO$_2$Me), 48.6 (CH$_2$N), 49.8 (*C*HCO$_2$Me), 51.7 (CHCO$_2$*C*H$_3$), 52.6 (CCO$_2$*C*H$_3$), 67.3 (CHN), 76.3 (*C*CO$_2$Me), 126.8 (*C*HCHN), 132.1 (*C*HMe), 172.5 (CH*C*O$_2$Me), 177.0 (C*C*O$_2$Me); MS (EI-GC) *m/z*: 267 (M$^+$, <1%), 208 (100), 207 (10), 181 (25), 59 (10); Microanalysis calculated for $C_{14}H_{21}NO_4$: C, 62.9; H, 7.9; N, 5.2%; found: C, 63.3; H, 7.4; N, 5.4%.

(2*S,3*R**,7a*R**)-dimethyl 3-phenylhexahydro-*1H*-pyrrolizine-2,7a-dicarboxylate 3h:** Sticky colorless oil; IR (neat) ν_{max} 2900, 1718, 1687 cm^{-1}; ^{1}H NMR δ_H: 1.81–2.00 (m, 3H, C*H*$_2$CH$_2$N, C*H*HCCO$_2$Me), 2.34-2.43 (m, 2H, C*H*HCCO$_2$Me, C*H*HCHCO$_2$Me), 2.54-2.61 (m, 1H, C*H*HCHCO$_2$Me), 2.64-2.76 (m, 2H, CH$_2$N), 3.23 (s, 3H, CHCO$_2$C*H*$_3$), 3.76 (s, 3H, CCO$_2$C*H*$_3$), 3.88 (ddd, *J* = 13.0, 8.8, 7.4 Hz, 1H, CHCO$_2$Me), 4.73 (d, *J* = 8.8 Hz, 1H, CHN), 7.15-7.17, 7.25-7.28 (m, 5H, Ar*H*); ^{13}C NMR δ_C: 28.3 (*C*H$_2$CH$_2$N), 36.3 (*C*H$_2$CHCO$_2$Me), 36.7 (*C*H$_2$CCO$_2$Me), 47.2 (CH$_2$N), 51.4 (*C*HCO$_2$Me), 52.7 (CHCO$_2$*C*H$_3$), 52.5 (CCO$_2$*C*H$_3$), 67.3 (CHN), 76.1 (*C*CO$_2$Me), 127.9, 128.2, 129.3, 138.0 (Ar*C*), 172.2 (CH*C*O$_2$Me), 177.3 (C*C*O$_2$Me); MS (EI-GC) *m/z*: 303 (M$^+$, <1%), 245 (11), 244 (100), 226 (21), 218 (10), 217 (17), 185 (26), 77 (15); HRMS calculated for $C_{17}H_{21}NO_4$ +1: 304.1549 found: 304.1553.

***(*3*R**,7a*R**)-dimethyl 3-phenylhexahydro-*1H*-pyrrolizine-1,7a-dicarboxylate 3h´:** Sticky colorless oil; IR (neat) ν_{max} 2935, 2903, 1720, 1705 cm^{-1}; ^{1}H NMR δ_H: 1.37–1.48 (m, 1H, C*H*HCCO$_2$Me), 1.65-1.86 (m, 2H, C*H*$_2$CH$_2$N), 2..18 (ddd, *J* = 12.1, 6.7, 4.1 Hz, 1H, C*H*HCHPh), 2.26-2.34 (m, 1H, C*H*HCCO$_2$Me), 2.41-2.55 (m, 3H, C*H*HCHPh, C*H*$_2$N), 3.72 (s, 3H, CHCO$_2$C*H*$_3$), 3.82 (s, 3H, CCO$_2$C*H*$_3$), 3.80 (dd, *J* = 12.1, 6.7 Hz, 1H, CHCO$_2$Me), 4.49 (dd, *J* = 12.8, 4.0 Hz, 1H, CHN), 7.27-7.45 (m, 5H, Ar*H*); ^{13}C NMR δ_C: 25.8 (*C*H$_2$CH$_2$N), 29.2 (*C*H$_2$CHPh), 33.0 (*C*H$_2$CCO$_2$Me), 50.7 (CH$_2$N), 51.0 (*C*HCO$_2$Me), 52.0 (CHCO$_2$*C*H$_3$), 52.9 (CCO$_2$*C*H$_3$), 64.8 (CHN), 76.4 (*C*CO$_2$Me), 127.7, 128.3, 128.9, 137.7 (Ar*C*), 173.1 (CH*C*O$_2$Me), 175.5 (C*C*O$_2$Me); MS (EI-GC) *m/z*: 303 (M$^+$, <1%), 245 (10), 244 (100), 243 (10), 227 (10), 226 (23), 217 (14), 185 (15), 77 (13); HRMS calculated for $C_{17}H_{21}NO_4$ +1: 304.1549 found: 304.1592.

(2*S,3*S**,7a*R**)-dimethyl 3-isobutylhexahydro-*1H*-pyrrolizine-2,7a-dicarboxylate 3i:** colorless oil; R_f 0.29 (*n*-hexane/ethyl acetate 7/3); IR (neat) ν_{max} 2986, 2956, 2903, 1716, 1700 cm^{-1}; ^{1}H NMR δ_H: 0.93 [d, 6H, *J* = 6.0 Hz, CH(C*H*$_3$)$_2$], 1.35-1.41 [m, 2H, C*H*HCH$_2$N, C*H*(CH$_3$)$_2$], 1.52-1.62 (m, 1H, C*H*HCH$_2$N), 1.74-1.83, 1.87-1.94 (m, 2H, C*H*$_2$CCO$_2$Me), 2.22 (dd, *J* = 13.7, 5.4 Hz, 1H, C*H*HCHCO$_2$Me), 2.41 (ddd, *J* = 12.6, 8.4, 4.0 Hz, 1H, C*H*HCHCO$_2$Me), 2.57 (dd, *J* = 13.7, 9.1 Hz, 1H, C*H*HCHCO$_2$Me), 2.92-3.15 (m, 3H, C*H*N, C*H*HN, C*H*CO$_2$Me), 3.68 (s, 3H, CHCO$_2$CH$_3$), 3.73 (s, 3H, CCO$_2$CH$_3$); ^{13}C NMR δ_C: 22.9 [CH(*C*H$_3$)$_2$], 25.0 (*C*H$_2$CH$_2$N), 26.1

[*C*H(CH$_3$)$_2$], 35.8 (*C*H$_2$CHN) 37.8 (*C*H$_2$CCO$_2$Me), 39.7 (C*H*$_2$CHCO$_2$Me), 47.4 (CH$_2$N), 48.6 (CHCO$_2$*C*H$_3$), 51.5 (CCO$_2$*C*H$_3$), 52.9 (*C*HCO$_2$Me), 62.9 (CHN), 76.1 (*C*CO$_2$Me), 176.2 (CH*C*O$_2$Me), 176.3 (C*C*O$_2$Me); MS (EI-GC) *m/z*: 283 (M$^+$, <1%), 225 (15), 224 (100), 198 (14), 197 (35), 165 (21), 128 (11), 127 (10); Microanalysis calculated for C$_{15}$H$_{25}$NO$_4$: C, 63.6; H, 8.9; N, 4.9%; found: C, 63.5; H, 8.4; N, 5.1%.

(1*S,3*R**,7a*R**)-3-ethyl 1,7a-dimethyl hexahydro-*1H*-pyrrolizine-1,3,7a-tricarboxylate 3j:** Sticky yellow oil; IR (neat) ν_{max} 2991, 2910, 1714, 1711, 1699 cm^{-1}; ^{1}H NMR δ_H: 1.30 (t, *J* = 7.1 Hz, 3H, CO$_2$CH$_2$C*H*$_3$), 1.41 (ddd, *J* = 12.7, 11.4, 7.6 Hz, 1H, C*H*HCCO$_2$Me), 1.80-1.90 (m, 2H, CH$_2$N), 2.15 (ddd, *J* = 12.7, 7.0, 4.8 Hz, 1H, C*H*HCHCO$_2$Et), 2.32-2.47 (m, 2H, C*H*HCHCO2Et, C*H*HCCO$_2$Me), 2.52-2.61 (m, 1H, C*H*HN), 3.11-3.16 (m, 1H, C*H*HN), 3.59 (dd, *J* = 12.2, 7.0 Hz, 1H, CHCO$_2$Me), 3.69 (s, 3H, CHCO$_2$C*H*$_3$), 3.76 (s, 3H, CCO$_2$C*H*$_3$), 4.00 (dd, *J* = 12.2, 4.8 Hz, 1H, CHCO$_2$Et), 4.24 (q, *J* = 7.1 Hz, 2H, CO$_2$C*H*$_2$CH$_3$); ^{13}C NMR δ_C: 14.3 (CO$_2$CH$_2$*C*H$_3$), 26.0 (*C*H$_2$CH$_2$N), 28.8 (*C*H$_2$CHCO$_2$Et), 32.4 (*C*H$_2$CCO$_2$Me), 50.3 (*C*HCO$_2$Me), 51.4 (CO$_2$*C*H$_2$CH$_3$), 52.1 (CHCO$_2$*C*H$_3$), 52.9 (CCO$_2$*C*H$_3$), 61.3 (CH$_2$N), 64.7 (CHN), 76.7 (*C*CO$_2$Me), 169.9, 172.3, 174.7 (2x*C*O$_2$Me, *C*O$_2$Et); MS (EI-GC) *m/z*: 299 (M$^+$, <1%), 241 (14), 240 (100), 226 (21), 212 (23), 166 (10), 108 (21); HRMS calculated for C$_{23}$H$_{24}$N$_2$O$_4$ +1: 300.1447 found: 300.1451.

(2*S*,3*S*,6*R*,7a*S*)-dimethyl 6-hydroxy-3-((*E*)-styryl)hexahydro-*1H*-pyrrolizine-2,7a-dicarboxylate 4a: Brown needles, mp: 99-102ºC; $[\alpha]_D^{20} = +81.2^o$ (*c* 1, CH$_2$Cl$_2$), IR (neat) ν_{max} 3322, 2950, 2305, 1715, 1707 cm^{-1}; ^{1}H NMR δ_H: 1.97 (dd, *J* = 13.5, 4.8 Hz, 1H, C*H*HCCO$_2$Me), 2.42 (deform. dd, *J* = 12.9, 12.3 Hz, 1H, C*H*HCHCO$_2$Me), 2.54-2.61 (m, 2H, C*H*HCHCO$_2$Me, C*H*HCCO$_2$Me), 3.07-3.16 (m, 2H, C*H*$_2$N), 3.50-3.56 (m, 4H, C*H*CO$_2$Me, CHCO$_2$C*H*$_3$), 3.73 (s, 3H, CCO$_2$CH$_3$), 4.21 (dd, *J* = 10.3, 7.8 Hz, 1H, CHN), 4.56 (deform. dddd, *J* = 5.1, 5.0, 4.8, 4.7 Hz, 1H, C*H*OH), 6.23 (dd, *J* = 15.5, 10.4 Hz, 1H, C*H*CHN), 6.51 (d, *J* = 15.5 Hz, 1H, C*H*Ph), 7.23-7.38 (m, 5H, Ar*H*); ^{13}C NMR δ_C: 36.9 (*C*H$_2$CCO$_2$Me), 45.0 (*C*H$_2$CHCO$_2$Me), 50.5 (*C*HCO$_2$Me), 51.9 (CCO$_2$*C*H$_3$), 52.7 (*C*HCO$_2$Me), 56.2 (CH$_2$N), 66.9 (CHN), 74.2 (CHOH), 75.9 (*C*CO$_2$Me), 126.7, 128.0, 128.7, 136.7 (Ar*C*), 127.5 (*C*HCHN), 136.7 (*C*HPh), 172.4 (CH*C*O$_2$Me), 176.5 (C*C*O$_2$Me); MS (EI-GC) *m/z*: 345 (M$^+$, <1%), 269 (11), 268 (100), 243 (11), 241 (15), 209 (15), 126 (11), 105 (13); Microanalysis calculated for C$_{19}$H$_{23}$NO$_5$: C, 66.1; H, 6.7; N, 4.1%; found: C, 66.5; H, 7.0; N, 4.3%.

(2*R*,3*R*,6*R*,7a*R*)-dimethyl 6-hydroxy-3-((*E*)-styryl)hexahydro-*1H*-pyrrolizine-2,7a-dicarboxylate 4a´: Brown needles, mp: 95-97ºC; $[\alpha]_D^{20} = +34.7^o$ (*c* 1, CH$_2$Cl$_2$); IR (neat) ν_{max} 3396, 2944, 2315, 1717, 1698 cm^{-1}; ^{1}H NMR δ_H: 2.06 (dd, *J* = 14.0, 6.1 Hz, 1H, C*H*HCCO$_2$Me), 2.24 (dd, *J* = 13.4, 11.7 Hz, 1H, C*H*HCHCO$_2$Me), 2.50 (dd, *J* = 14.0, 1.8 Hz, 1H, C*H*HCCO$_2$Me), 2.63 (dd, *J* = 13.4, 7.0 Hz, 1H, C*H*HCHCO$_2$Me), 2.92 (dd, *J* = 11.7, 2.5 Hz, 1H, C*H*HN), 3.50-3.53 (m, 4H, C*H*CO$_2$Me, CHCO$_2$C*H*$_3$), 3.76 (s, 3H, CCO$_2$CH$_3$), 4.16 (dd, *J* = 10.4, 7.4 Hz, 1H, CHN), 4.44 (m, 1H, C*H*OH), 5.87 (dd, *J* = 15.6, 10.4 Hz, 1H, C*H*CHN), 6.57 (d, *J* = 15.5 Hz, 1H, C*H*Ph), 7.27-7.31 (m, 5H, Ar*H*); ^{13}C NMR δ_C: 36.9 (*C*H$_2$CCO$_2$Me), 46.5 (*C*H$_2$CHCO$_2$Me), 50.7 (*C*HCO$_2$Me), 52.0 (CCO$_2$*C*H$_3$), 53.0 (*C*HCO$_2$Me), 57.0 (CH$_2$N), 66.5 (CHN), 75.0 (CHOH), 75.5 (*C*CO$_2$Me), 125.3 (*C*HCHN), 126.7, 128.2, 128.8, 136.3 (Ar*C*), 136.0 (*C*HPh), 172.3 (CH*C*O$_2$Me), 177.3 (C*C*O$_2$Me); MS (EI-GC) *m/z*: 345 (M$^+$, <1%), 269 (13), 268 (100), 243 (10), 241 (31), 209 (22), 105 (11), 59 (10); Microanalysis calculated for C$_{19}$H$_{23}$NO$_5$: C, 66.1; H, 6.7; N, 4.1%; found: C, 66.4; H, 6.9; N, 4.1%.

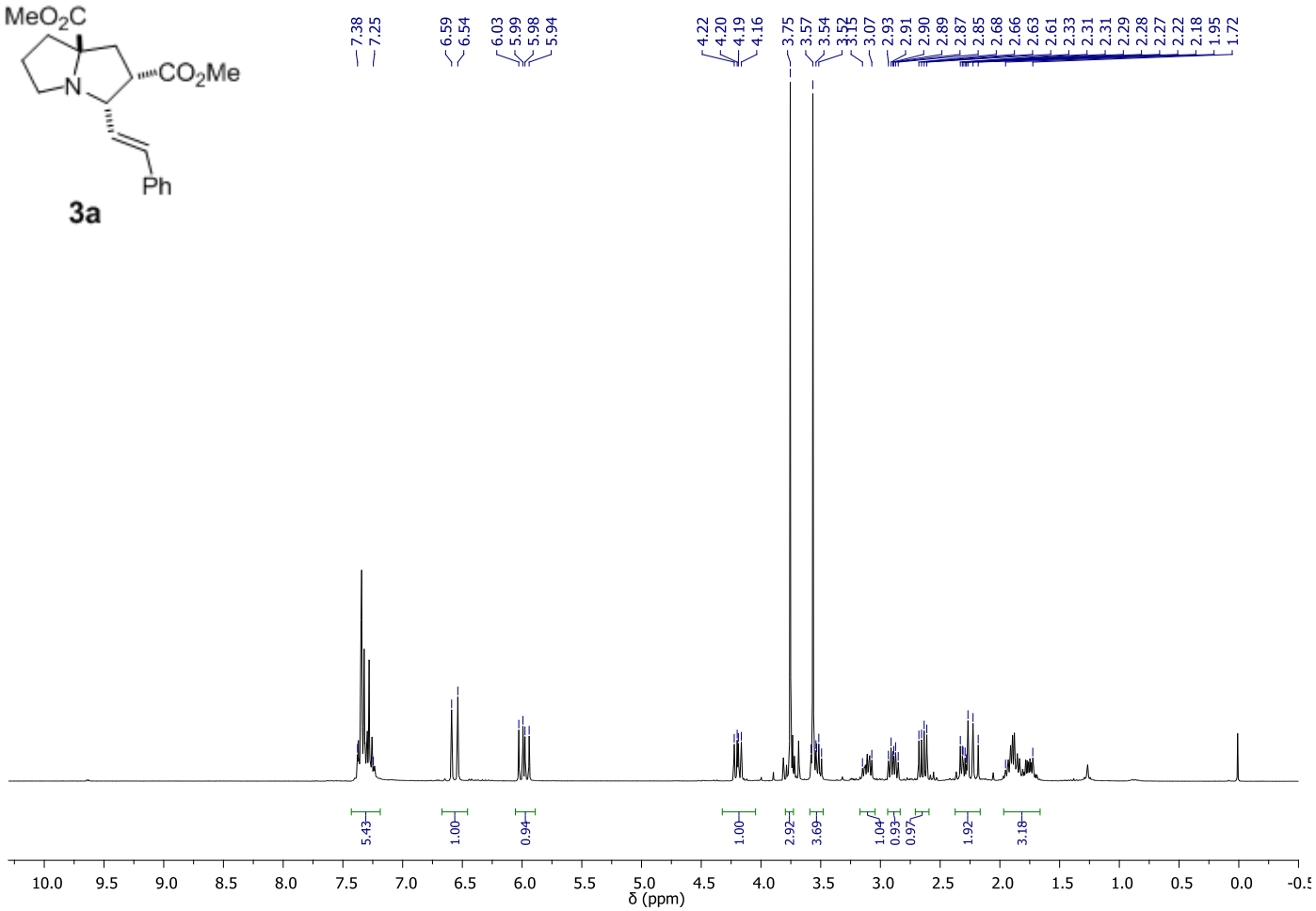
(2*S*,3*S*,6*R*,7a*S*)-dimethyl 6-((*tert*-butyldimethylsilyl)oxy)-3-((*E*)-styryl)hexahydro-*1H*-pyrrolizine-2,7a-dicarboxylate 4b: Sticky orange oil; $[\alpha]_D^{20} = +4.2^o$ (*c* 1, CH_2Cl_2); IR (neat) ν_{max} 3396, 2944, 2315, 1717, 1698 cm^{-1}; ^1H NMR δ_H: -0.04 (s, 6H, OTBS), 0.81 (s, 9H, OTBS), 1.95 (dd, *J* = 13.0, 6.0 Hz, 1H, C*H*HCCO$_2$Me), 2.28 (deform. dd, *J* = 13.2, 13.0 Hz, 1H, C*H*HCHCO$_2$Me), 2.40-2.51 (m, 2H, C*H*HCHCO$_2$Me, C*H*HCCO$_2$Me), 2.8 (dd, *J* = 11.6, 4.7 Hz, 1H, C*H*HN), 3.20 (dd, *J* = 11.6, 5.4 Hz, 1H, C*H*HN), 3.49-3.56 (m, 4H, C*H*CO$_2$Me, CHCO$_2$C*H*$_3$), 3.74 (s, 3H, CCO$_2$CH$_3$), 4.18 (dd, *J* = 10.5, 7.2 Hz, 1H, CHN), 4.56 (deform. dddd, *J* = 6.0, 5.4, 5.3, 4.7 Hz, 1H, C*H*OH), 5.85 (dd, *J* = 15.6, 10.5 Hz, 1H, C*H*CHN), 6.54 (d, *J* = 15.6 Hz, 1H, C*H*Ph), 7.24-7.30 (m, 5H, Ar*H*); ^{13}C NMR δ_C: -4.8, -4.9 (OTBS), 18.2 (OTBS), 25.9 (OTBS), 37.5 (*C*H$_2$CCO$_2$Me), 46.4 (*C*H$_2$CHCO$_2$Me), 49.4 (*C*HCO$_2$Me), 51.9 (CCO$_2$*C*H$_3$), 52.7 (*C*HCO$_2$Me), 56.3 (CH$_2$N), 66.9 (CHN), 74.5 (CHOH), 74.7 (*C*CO$_2$Me), 125.4 (*C*HCHN), 126.7, 128.2, 128.7, 136.4 (Ar*C*), 136.0 (*C*HPh), 171.9 (CH*C*O$_2$Me), 176.9 (C*C*O$_2$Me); MS (EI-GC) *m/z*: 459 (M^+, <1%), 327 (10), 268 (100), 267 (11), 243 (15), 242 (10), 241 (21), 209 (17), 208 (10), 106 (10), 105 (10); HRMS calculated for $C_{25}H_{37}NO_5Si$ +1: 460.2519 found: 460.2522.

(2*S*,3*S*,6*R*,7a*S*)-2-*tert*-butyl 7a-methyl 6-hydroxy-3-((*E*)-styryl)hexahydro-*1H*-pyrrolizine-2,7a-dicarboxylate 4c: Sticky yellow oil; $[\alpha]_D^{20} = -124.7^o$ (*c* 1, CH_2Cl_2); IR (neat) ν_{max} 2985, 2939, 2305, 1714, 1691 cm^{-1}; ^1H NMR δ_H: 1.26 [s, 1H, CO$_2$C(C*H*$_3$)$_3$], 1.94 (dd, *J* = 13.4, 5.1 Hz, 1H, C*H*HCCO$_2$Me), 2.37 (deform. dd, *J* = 12.6, 12.3 Hz, 1H, C*H*HCHCO$_2$Bu^t), 2.50-2.59 (m, 2H, C*H*HCHCO$_2$Bu^t, C*H*HCCO$_2$Me), 3.08-3.15 (m, 2H, C*H*$_2$N), 3.44 (ddd, *J* = 12.3, 7.5, 6.7 Hz, 1H, C*H*CO$_2$Bu^t), 3.72 (s, 3H, CCO$_2$C*H*$_3$), 4.16 (dd, *J* = 10.4, 7.5 Hz, 1H, CHN), 4.54 (deform. dddd, *J* = 5.5, 5.3, 5.1, 4.9 Hz, 1H, C*H*OH), 6.24 (dd, *J* = 15.6, 10.4 Hz, 1H, C*H*CHN), 6.51 (d, *J* = 15.6 Hz, 1H, C*H*Ph), 7.20-7.38 (m, 5H, Ar*H*); ^{13}C NMR δ_C: 28.2 [CO$_2$C(C*H*$_3$)$_3$], 36.9 (*C*H$_2$CCO$_2$Me), 45.2 (*C*H$_2$CHCO$_2$Bu^t), 51.2 (CCO$_2$*C*H$_3$), 52.6 (*C*HCO$_2$Bu^t), 56.0 (CH$_2$N), 66.9 (CHN), 74.3 (CHOH), 75.7 (*C*CO$_2$Me), 80.9 [CO$_2$*C*(CH$_3$)$_3$], 126.7, 127.9, 128.7, 136.6 (Ar*C*), 127.7 (*C*HCHN), 134.9 (*C*HPh), 171.1 (CH*C*O$_2$Bu^t), 176.7 (C*C*O$_2$Me); MS (EI-GC) *m/z*: 387 (M^+, <1%), 369 (11), 329 (10), 310 (15), 268 (30), 209 (100), 241 (11), 240 (17), 105 (12);Microanalysis calculated for $C_{22}H_{29}NO_5$: C, 68.2; H, 7.5; N, 3.6%; found: C, 68.5; H, 7.3; N, 3.7%.

(2*R*,3*R*,6*R*,7a*R*)-2-*tert*-butyl 7a-methyl 6-hydroxy-3-((*E*)-styryl)hexahydro-*1H*-pyrrolizine-2,7a-dicarboxylate 4c´: Sticky brown oil; $[\alpha]_D^{20} = +43.3^o$ (*c* 1, CH_2Cl_2); IR (neat) ν_{max} 3002, 2955, 2315, 1721, 1708 cm^{-1}; ^1H NMR δ_H: 1.30 [s, 1H, CO$_2$C(C*H*$_3$)$_3$], 2.03 (dd, *J* = 13.9, 6.1 Hz, 1H, C*H*HCCO$_2$Me), 2.16 (dd, *J* = 13.4, 11.9 Hz, 1H, C*H*HCHCO$_2$ Bu^t), 2.49 (dd, *J* = 14.0, 2.0 Hz, 1H, C*H*HCCO$_2$Me), 2.58 (dd, *J* = 13.4, 6.9 Hz, 1H, C*H*HCHCO$_2$Bu^t), 2.91 (dd, *J* = 11.7, 2.5 Hz, 1H, C*H*HN), 3.37 (dd, *J* = 11.7, 5.4 Hz, 1H, C*H*HN), 3.49 (dd, *J* = 11.9, 7.4 Hz, 1H, C*H*CO$_2$Bu^t), 3.78 (s, 3H, CCO$_2$CH$_3$), 4.11 (dd, *J* = 10.4, 7.4 Hz, 1H, CHN), 4.40 (m, 1H, C*H*OH), 5.88 (dd, *J* = 15.6, 10.4 Hz, 1H, C*H*CHN), 6.57 (d, *J* = 15.5 Hz, 1H, C*H*Ph), 7.26-7.37 (m, 5H, Ar*H*); ^{13}C NMR δ_C: 28.2 [CO$_2$C(C*H*$_3$)$_3$], 36.8 (*C*H$_2$CCO$_2$Me), 46.5 (*C*H$_2$CHCO$_2$Bu^t), 51.4 (CCO$_2$*C*H$_3$), 53.0 (*C*HCO$_2$Bu^t), 57.1 (CH$_2$N), 66.6 (CHN), 75.2 (CHOH), 75.5 (*C*CO$_2$Me), 81.1 [CO$_2$*C*(CH$_3$)$_3$], 125.7 (*C*HCHN), 126.7, 128.2, 128.8, 136.0 (Ar*C*), 136.3 (*C*HPh), 171.0 (CH*C*O$_2$Bu^t), 176.5 (C*C*O$_2$Me); MS (EI-GC) *m/z*: 387 (M^+, <1%), 369 (10), 329 (10), 328 (11), 311 (15), 310 (13), 209 (100), 241 (13), 240 (21), 105 (10); Microanalysis calculated for $C_{22}H_{29}NO_5$: C, 68.2; H, 7.5; N, 3.6%; found: C, 68.6; H, 7.4; N, 3.5%.

(3a*S*,4*S*,7*R*,8a*R*,8b*R*)-methyl 7-hydroxy-2-methyl-1,3-dioxo-4-((*E*)-styryl)decahydropyrrolo[3,4-a]pyrrolizine-8a-carboxylate 4d: Sticky yellow oil; $[\alpha]_D^{20} = -78.1^o$ (*c* 1, CH_2Cl_2); IR (neat) ν_{max} 3005, 2980, 2305, 1714, 1710, 1698 cm^{-1}; ^1H NMR δ_H: 2.31-2.41 (m, 1H, C*H*HCCO$_2$Me), 2.71-2.83 (m, 3H, C*H*HCCO$_2$Me, C*H*$_2$N), 2.97 (s, 3H, NCH$_3$), 3.52 (deform. dd, *J* = 8.5, 8.1 Hz, 1H, C*H*CON), 3.85 (s, 3H, CO$_2$CH$_3$), 3.95 (d, *J* = 8.1 Hz, 1H, CHCCO$_2$Me), 4.21 (deform. dd, *J* = 9.1, 8.5 Hz, 1H, C*H*N), 4.36 (m, 1H, CHOH), 6.23 (dd, *J* = 15.6, 9.1 Hz, 1H, C*H*CHN), 6.76 (d, *J* = 15.6 Hz, 1H, C*H*Ph), 7.26-7.40 (m, 5H, Ar*H*); ^{13}C NMR δ_C: 26.1 (NC*H*$_3$), 37.3 (*C*H$_2$CCO$_2$Me), 52.3, 53.1, (2x*C*HCON), 54.4 (CCO$_2$*C*H$_3$), 55.1 (*C*H$_2$N), 65.7 (CHN), 75.3 (CHOH), 77.9 (*C*CO$_2$CH$_3$), 125.3 (*C*HCHN), 126.9, 128.2, 128.7, 135.7 (Ar*C*), 136.0 (*C*HPh), 176.2, 176.3 (2xCON), 177.1 (*C*O$_2$Me); MS (EI-GC) *m/z*: 370 (M^+, <1%), 352 (10), 312 (10), 293 (100), 243 (21), 210 (12), 182 (40), 115 (10); HRMS calculated for $C_{20}H_{22}N_2O_5$ +1: 371.1607 found: 371.1621.

5. NMR spectra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N
Ph
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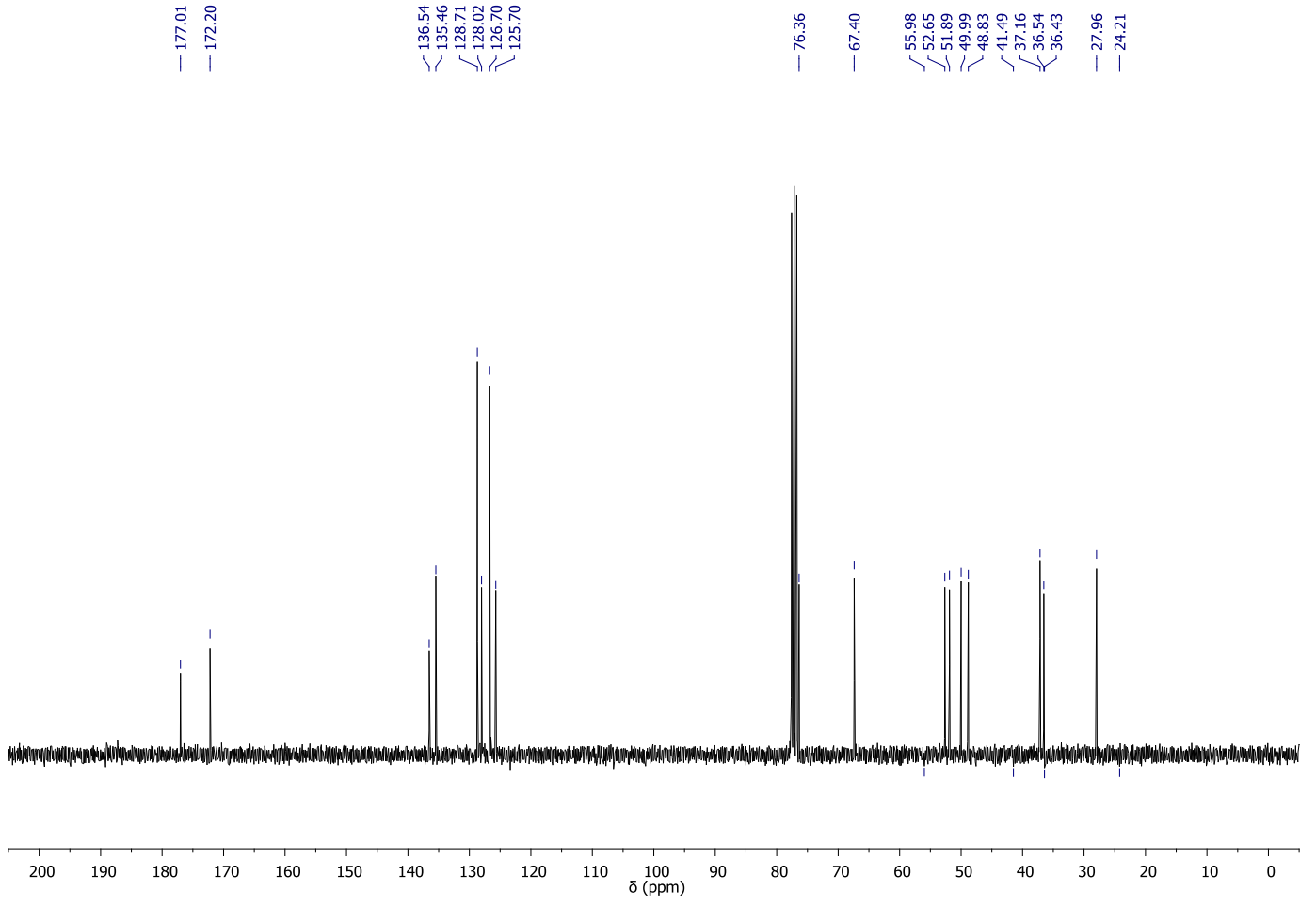
5.99
5.98
5.94
4.22
4.20
4.19
4.16
3.75
3.57
3.54
3.52
3.15
3.07
2.93
2.91
2.90
2.89
2.87
2.85
2.68
2.66
2.63
2.61
2.33
2.31
2.31
2.29
2.28
2.27
2.22
2.18
1.95
1.72
5.43
1.00
0.94
1.00
2.92
3.69
1.04
0.93
0.97
1.92
3.18
δ (ppm)


177.01
172.20
136.54
135.46
128.71
128.02
126.70
125.70
76.36
67.40
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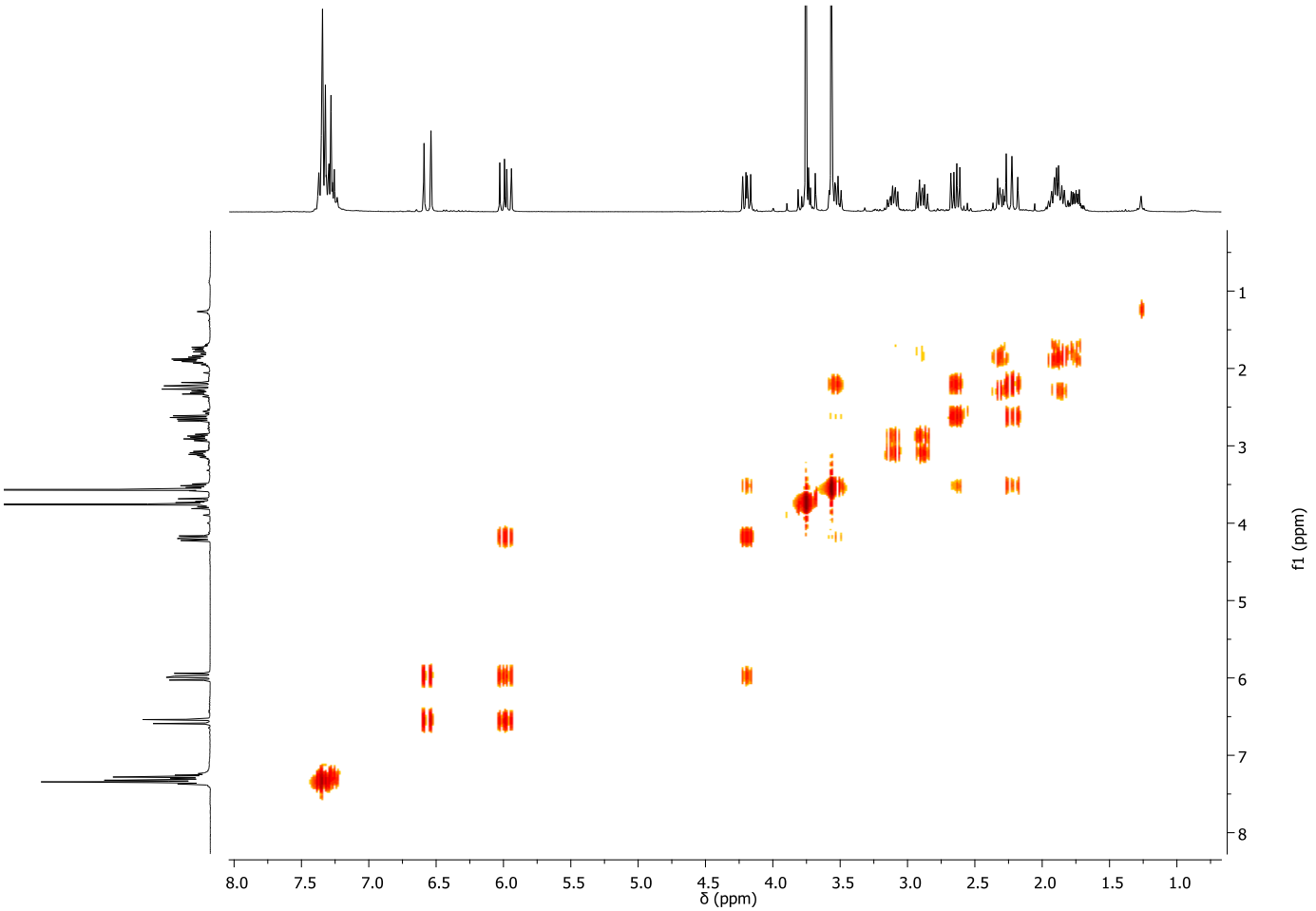
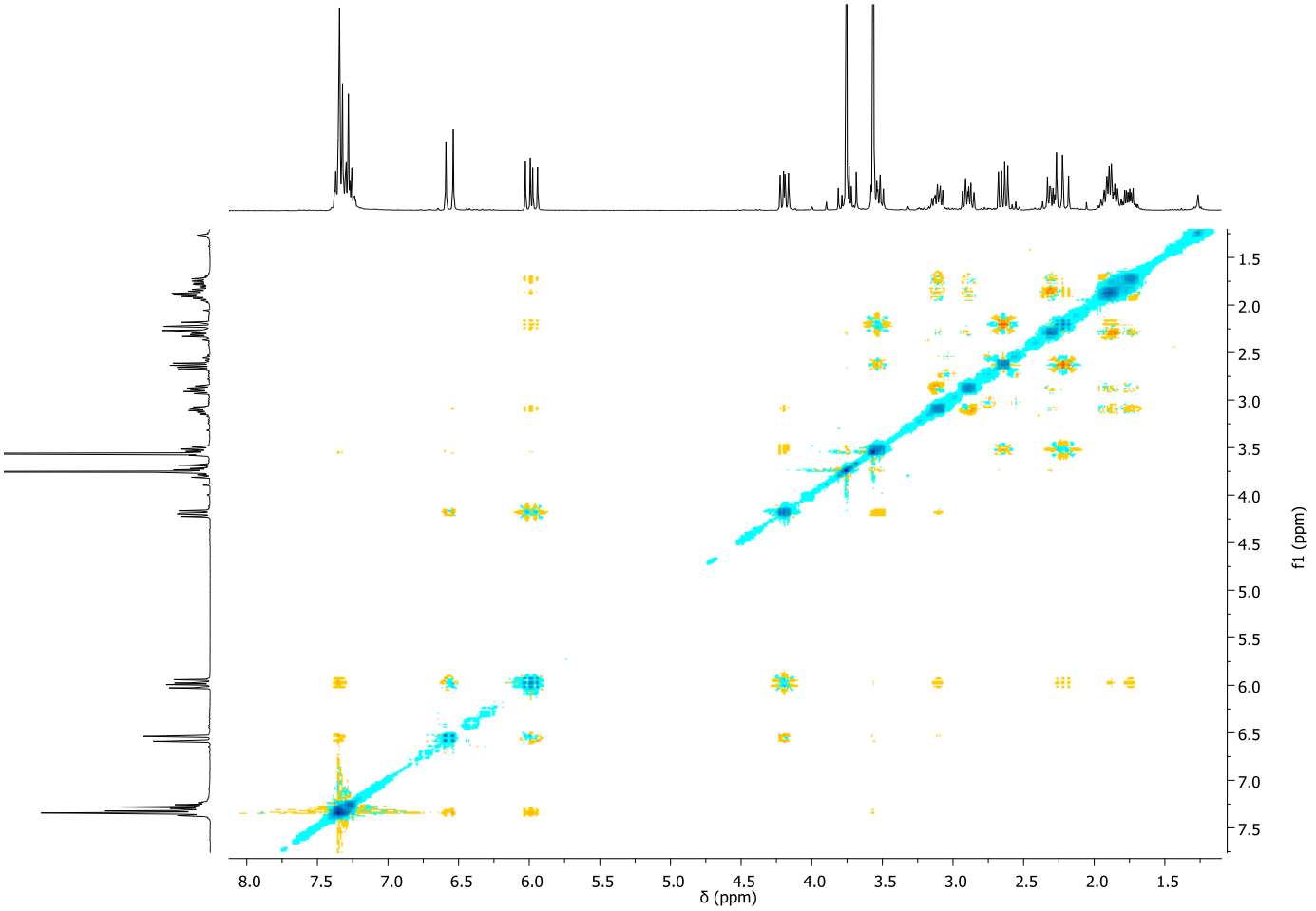
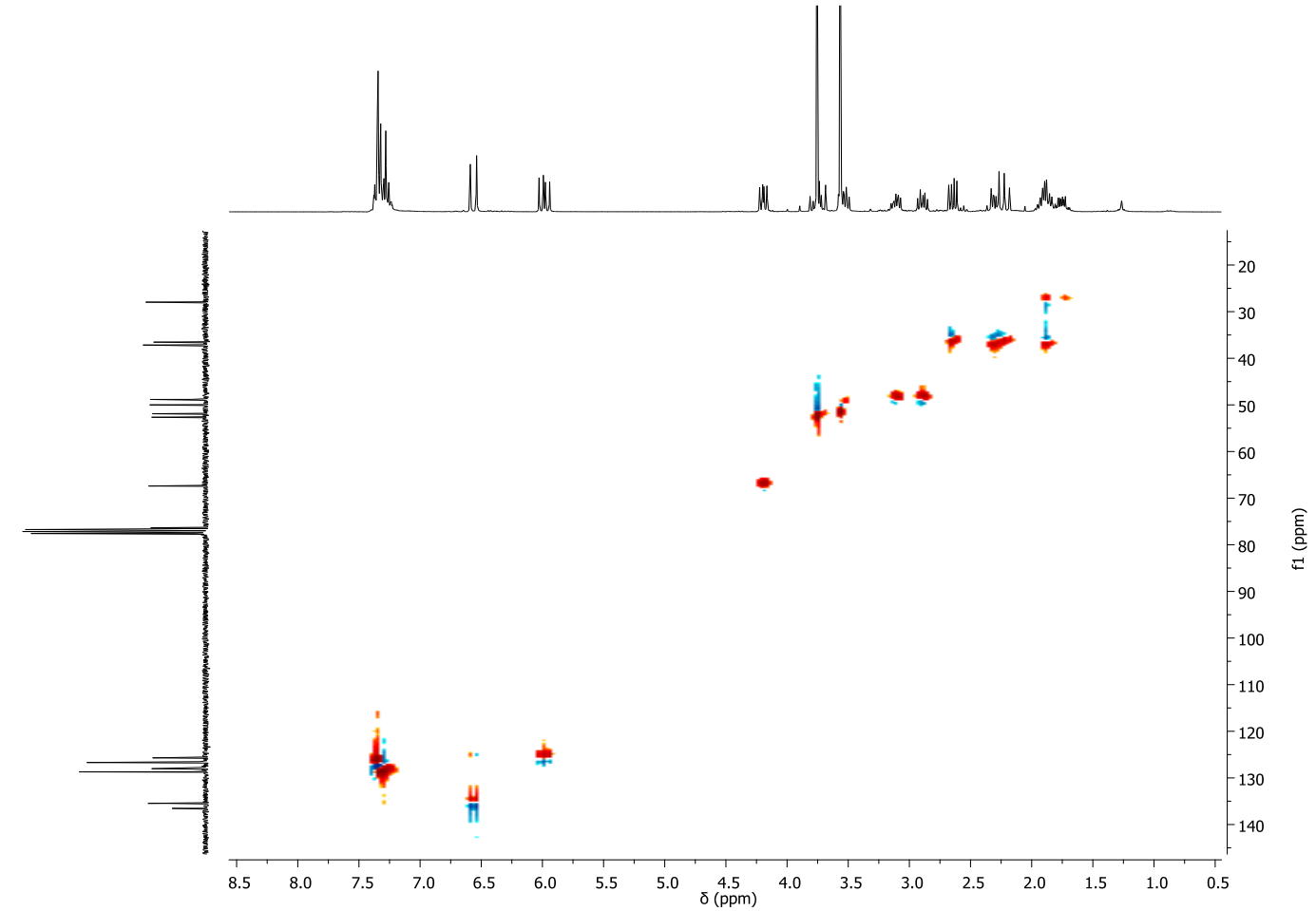
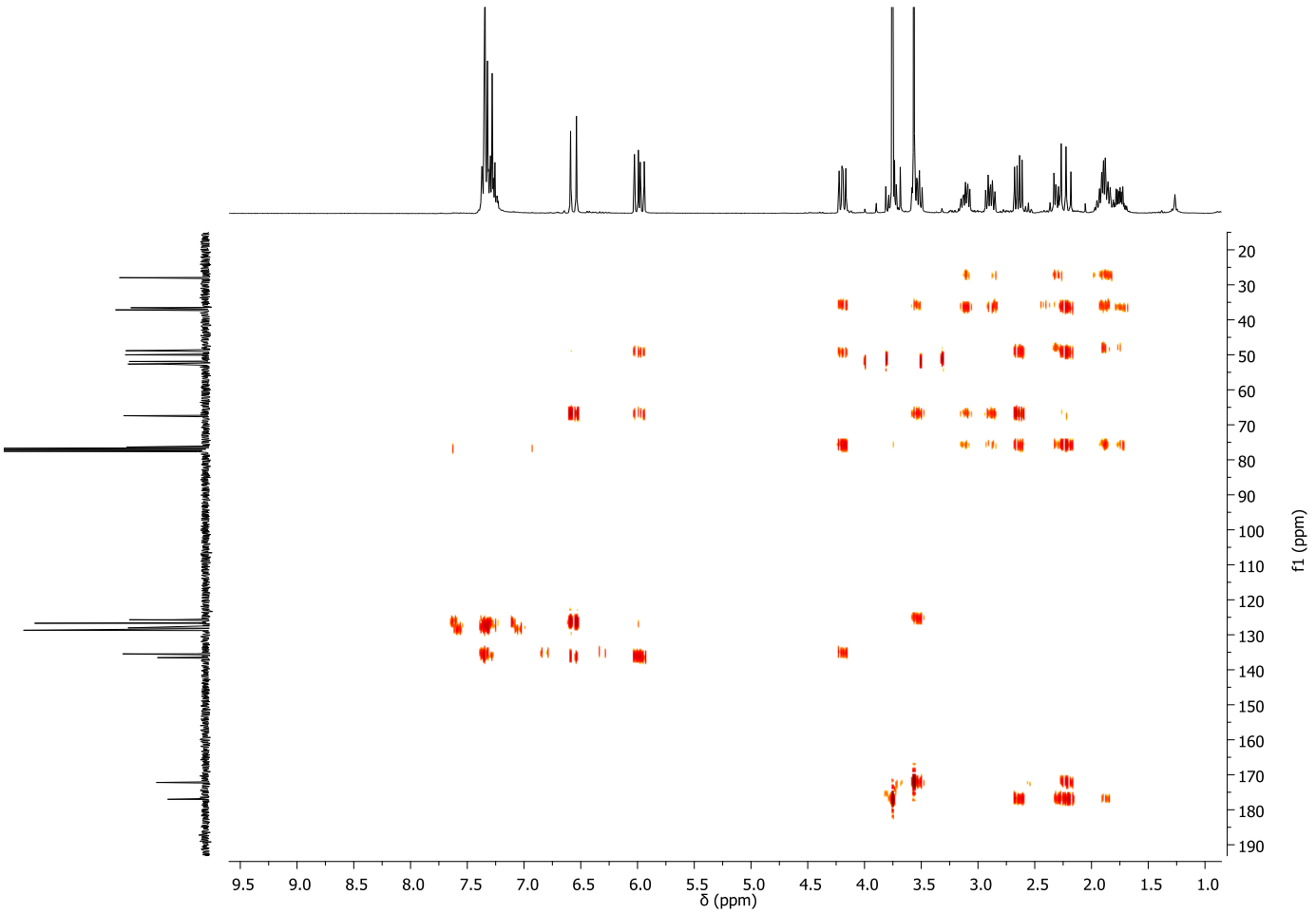
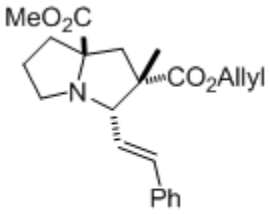
36.54
36.43
27.96
24.21
δ (ppm)







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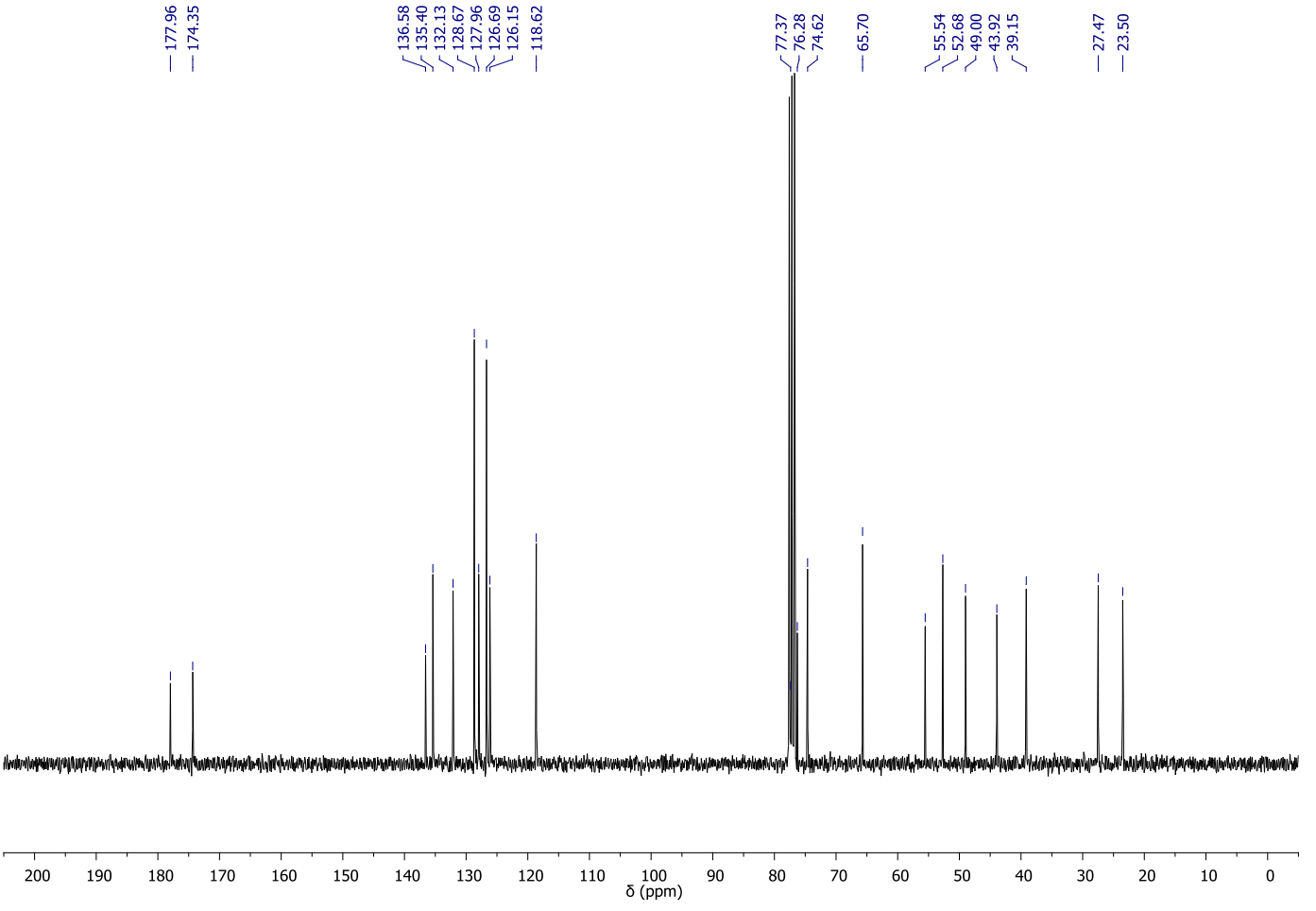
CO2Allyl
N
Ph

3b

7.34
7.23
6.55
6.50
5.99
5.96
5.94
5.91
5.74
5.70
5.22
5.22
5.09
5.08
4.45
4.44
4.43
3.81
3.78
3.77
3.16
3.08
3.01
2.92
2.66
2.62
2.54
2.49
2.24
2.15
2.02
1.70
1.69
1.44
4.23
0.57
1.00
1.00
0.99
0.99
0.99
1.97
3.97
1.00
0.99
0.98
0.99
1.00
3.52
2.99
δ (ppm)


177.96
174.35
136.58
135.40
132.13
128.67
127.96
126.69
126.15
118.62
77.37
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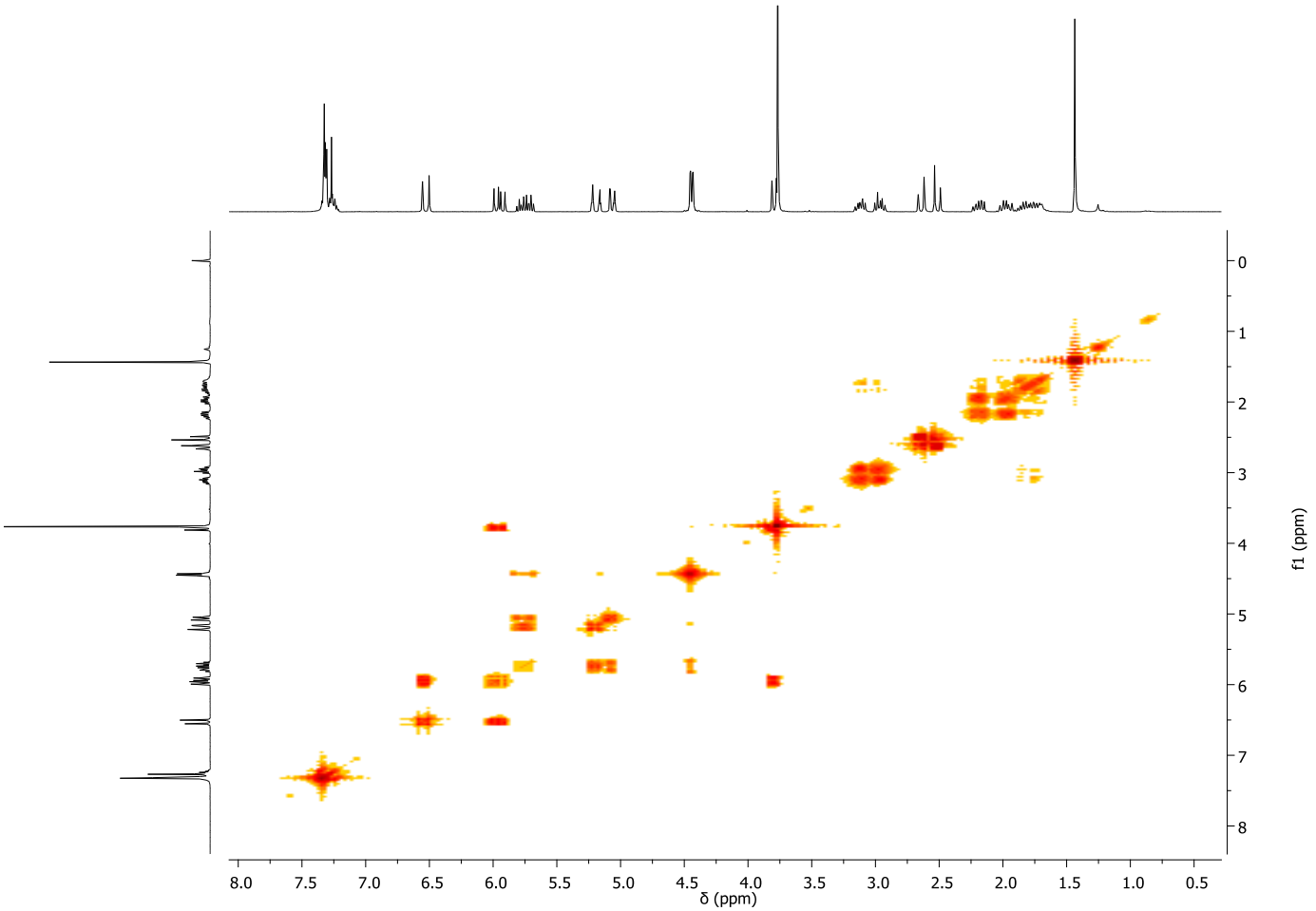
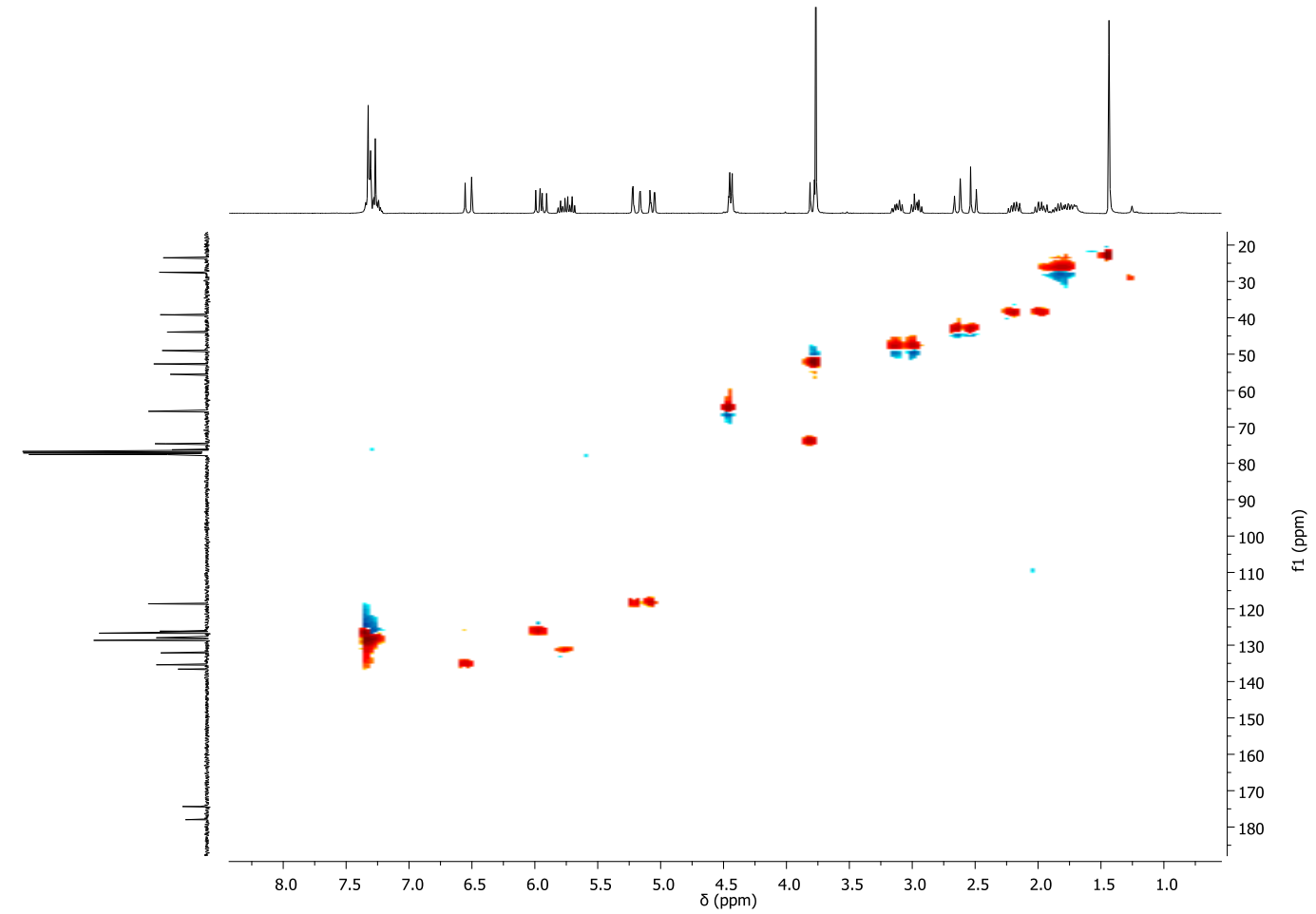
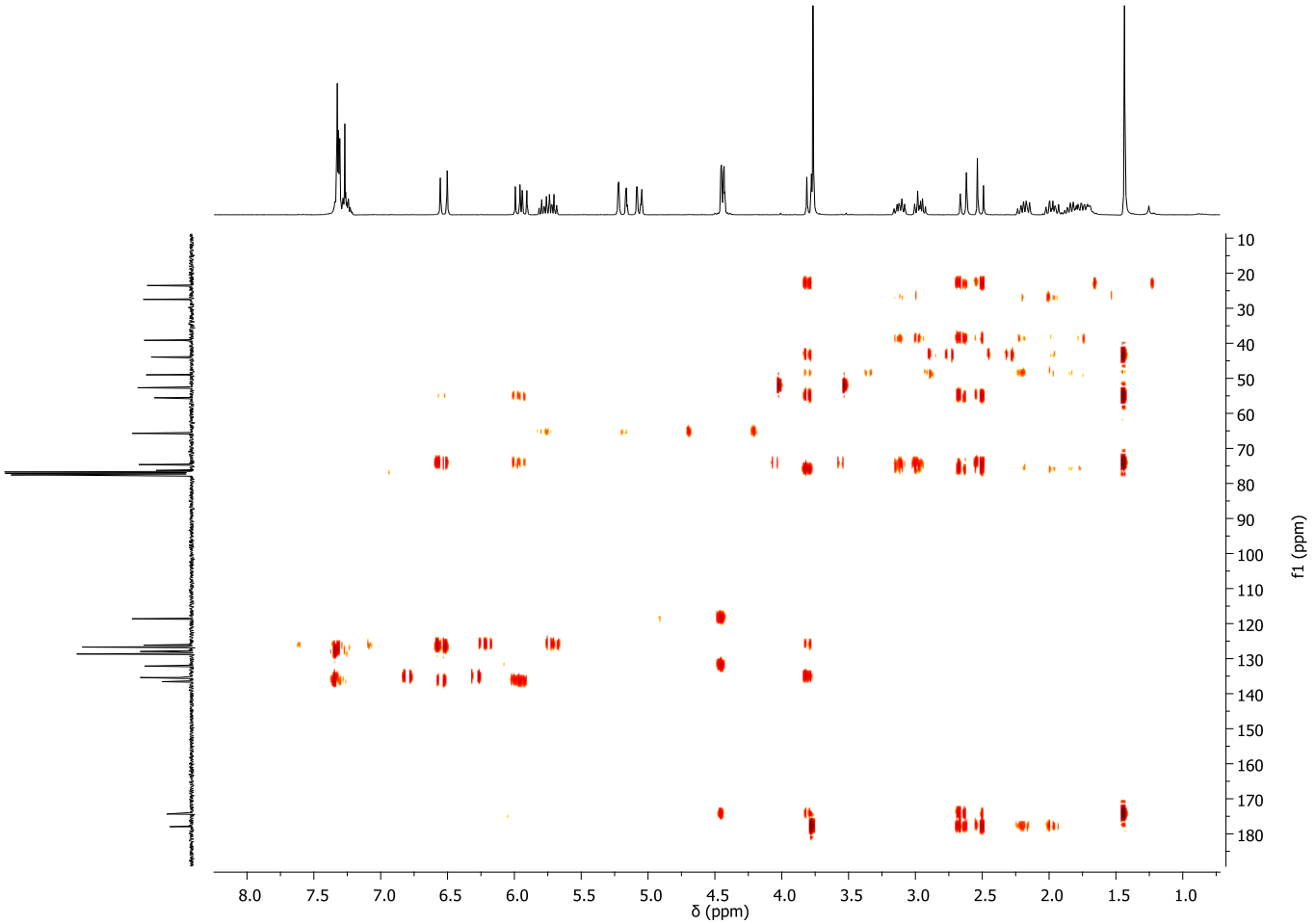
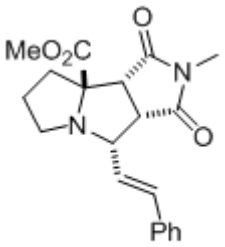
43.92
39.15
27.47
23.50
δ (ppm)








MeO2C
O
N
N
O
Ph

3c

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7.23
6.79
6.74
6.41
6.38
6.36
6.33
4.23
4.20
4.17
3.90
3.88
3.81
3.49
3.46
3.43
2.97
2.60
2.47
2.41
2.32
2.08
1.92
1.85
1.73
5.78
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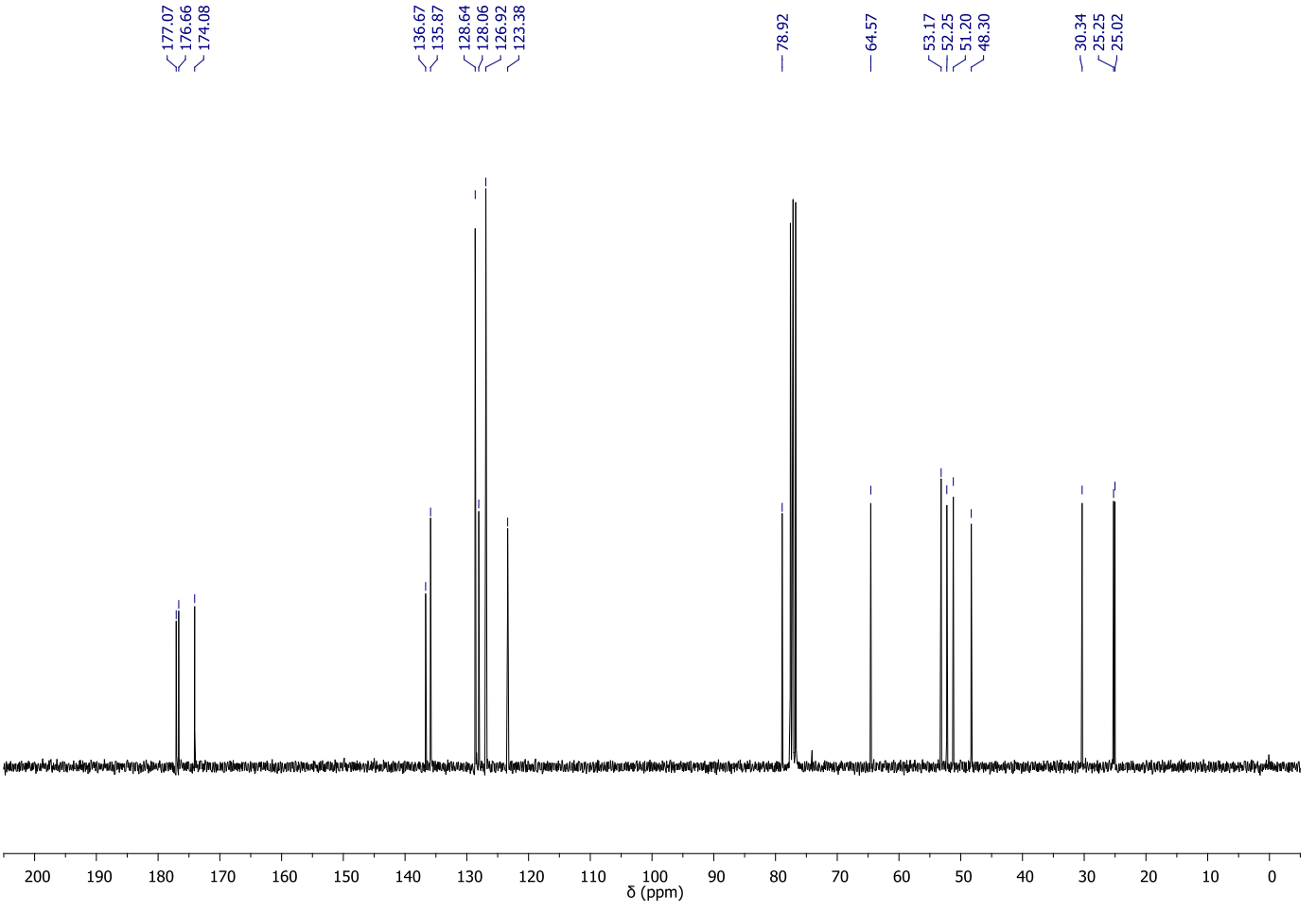
2.00
1.00
1.17
1.05
δ (ppm)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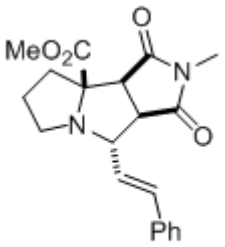
176.66
174.08
136.67
135.87
128.64
128.06
126.92
123.38
78.92
64.57
53.17
52.25
51.20
48.30
30.34
25.25
25.02
δ (ppm)


MeO2C
O
N
N
O
Ph

3c´

7.43
7.25
6.88
6.82
6.36
6.33
6.30
6.28
4.41
3.71
3.56
3.42
3.39
3.09
2.98
2.78
2.75
2.04
1.86
7.36
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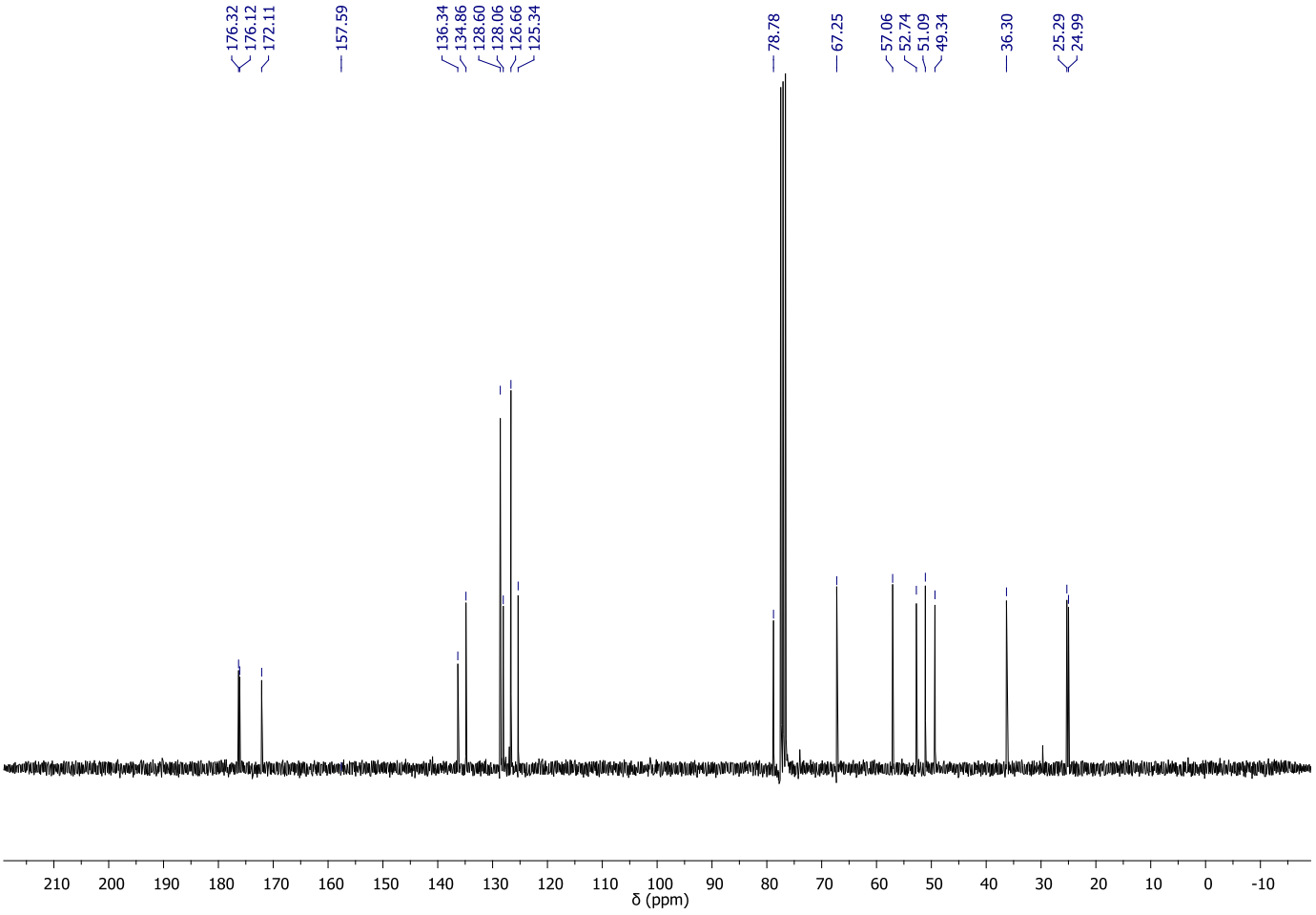
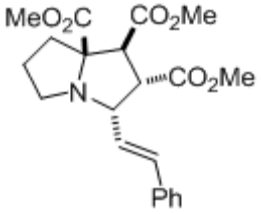
1.11
6.00
1.12
3.75
δ (ppm)


176.32
176.12
172.11
157.59
136.34
134.86
128.60
128.06
126.66
125.34
78.78
67.25
57.06
52.74
51.09
49.34
36.30
25.29
24.99
δ (ppm)


MeO2C
CO2Me
CO2Me
N
Ph

3d

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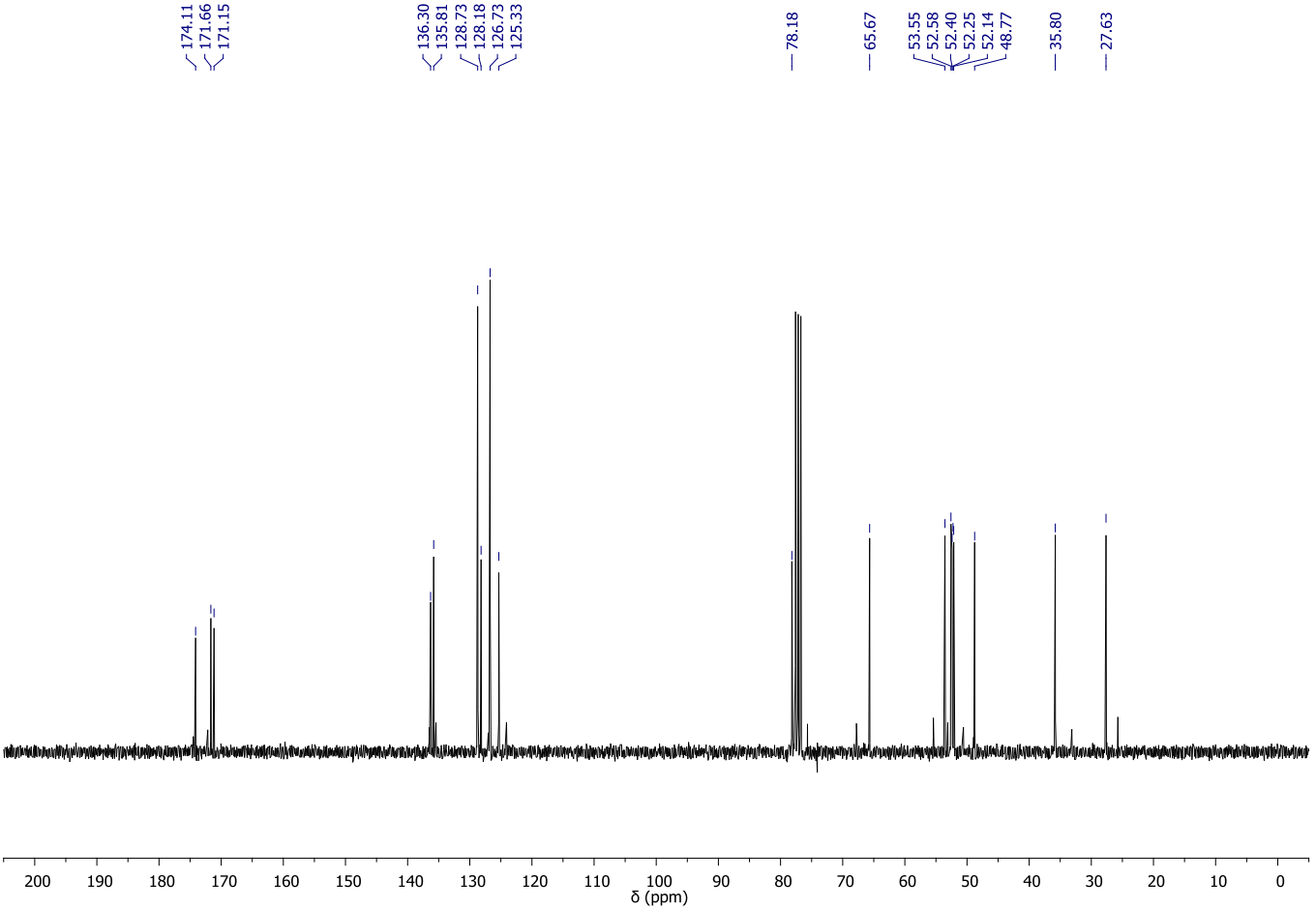
7.24
6.59
6.54
6.00
5.97
5.95
5.92
4.32
4.29
4.28
4.25
4.05
4.02
4.01
3.98
3.70
3.70
3.58
3.44
3.41
3.13
3.05
2.87
2.79
2.61
2.51
2.17
2.08
2.04
1.91
1.87
1.76
5.91
1.00
0.99
0.98
0.97
7.01
3.00
0.99
1.00
0.98
1.03
0.99
1.20
1.35
δ (ppm)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171.66
171.15
136.30
135.81
128.73
128.18
126.73
125.33
78.18
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53.55
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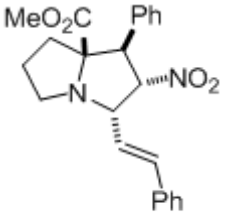
52.14
48.77
35.80
27.63
δ (ppm)


MeO2C
Ph
NO2
N
Ph

3e

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6.20
6.17
6.16
6.15
6.14
6.13
6.12
4.85
4.83
4.82
4.80
4.21
4.19
3.40
3.32
3.25
2.98
2.93
2.78
2.71
2.12
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1.99
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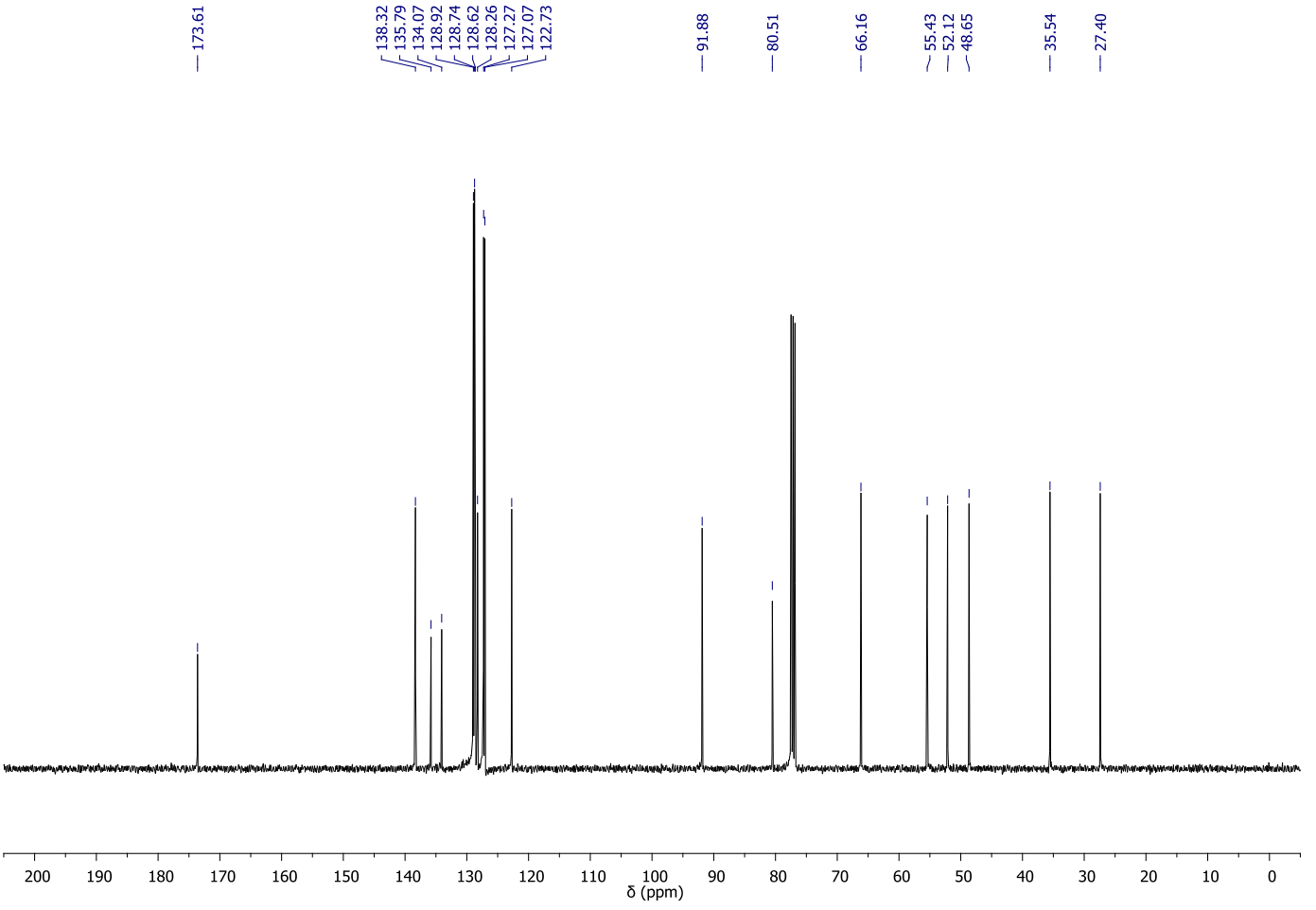
0.99
2.99
1.04
0.97
0.97
3.44
δ (ppm)


173.61
138.32
135.79
134.07
128.92
128.74
128.62
128.26
127.27
127.07
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91.88
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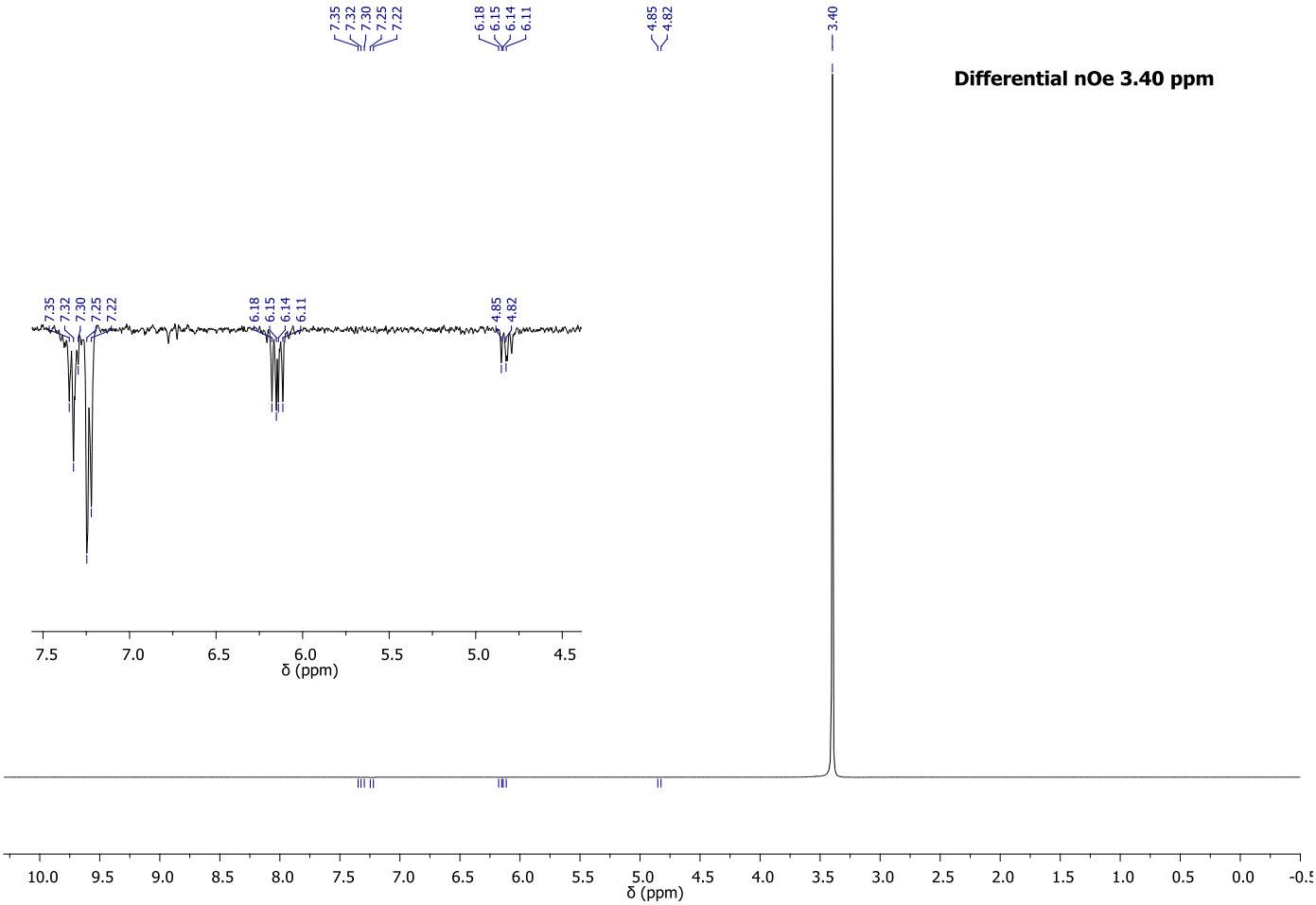
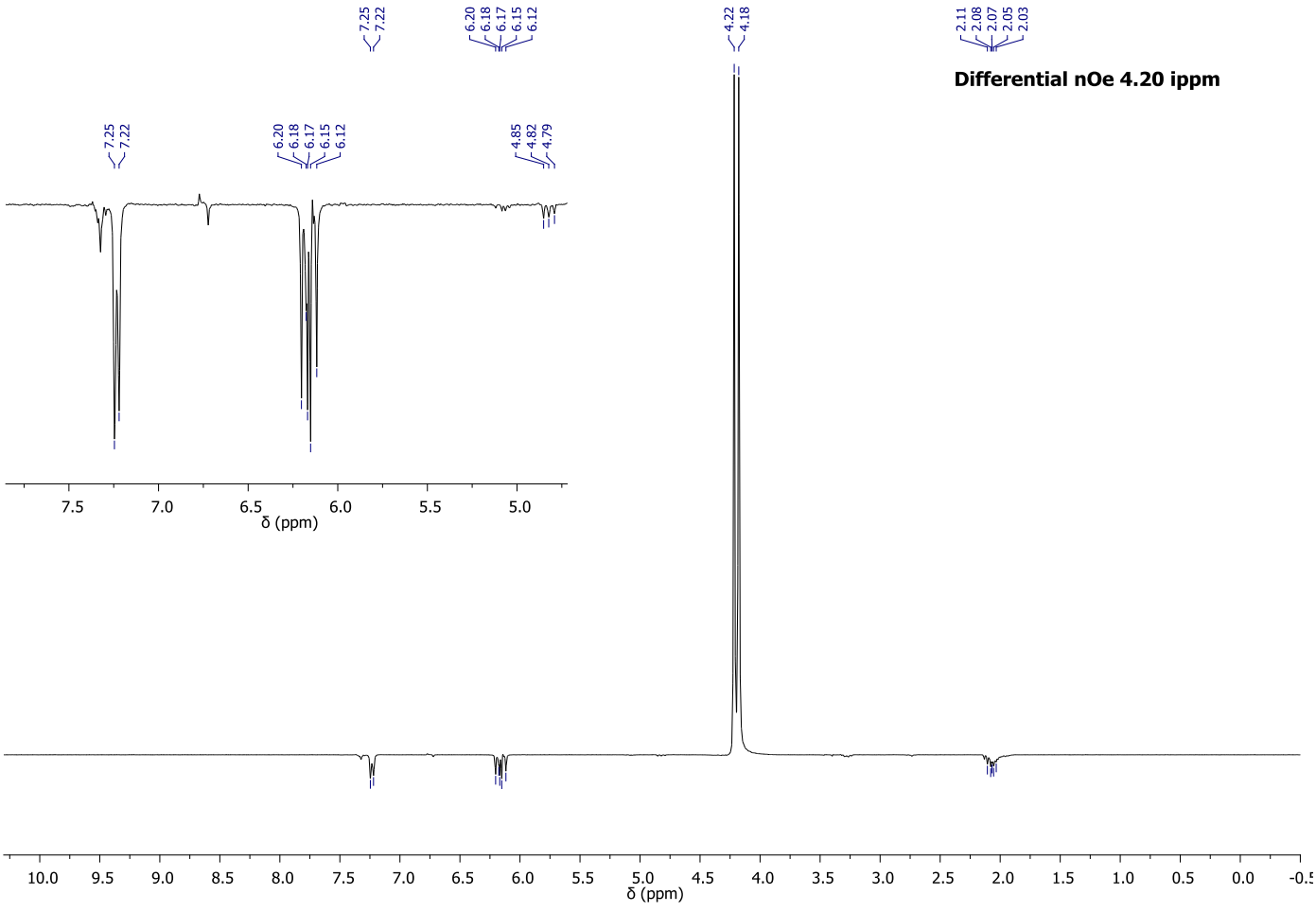
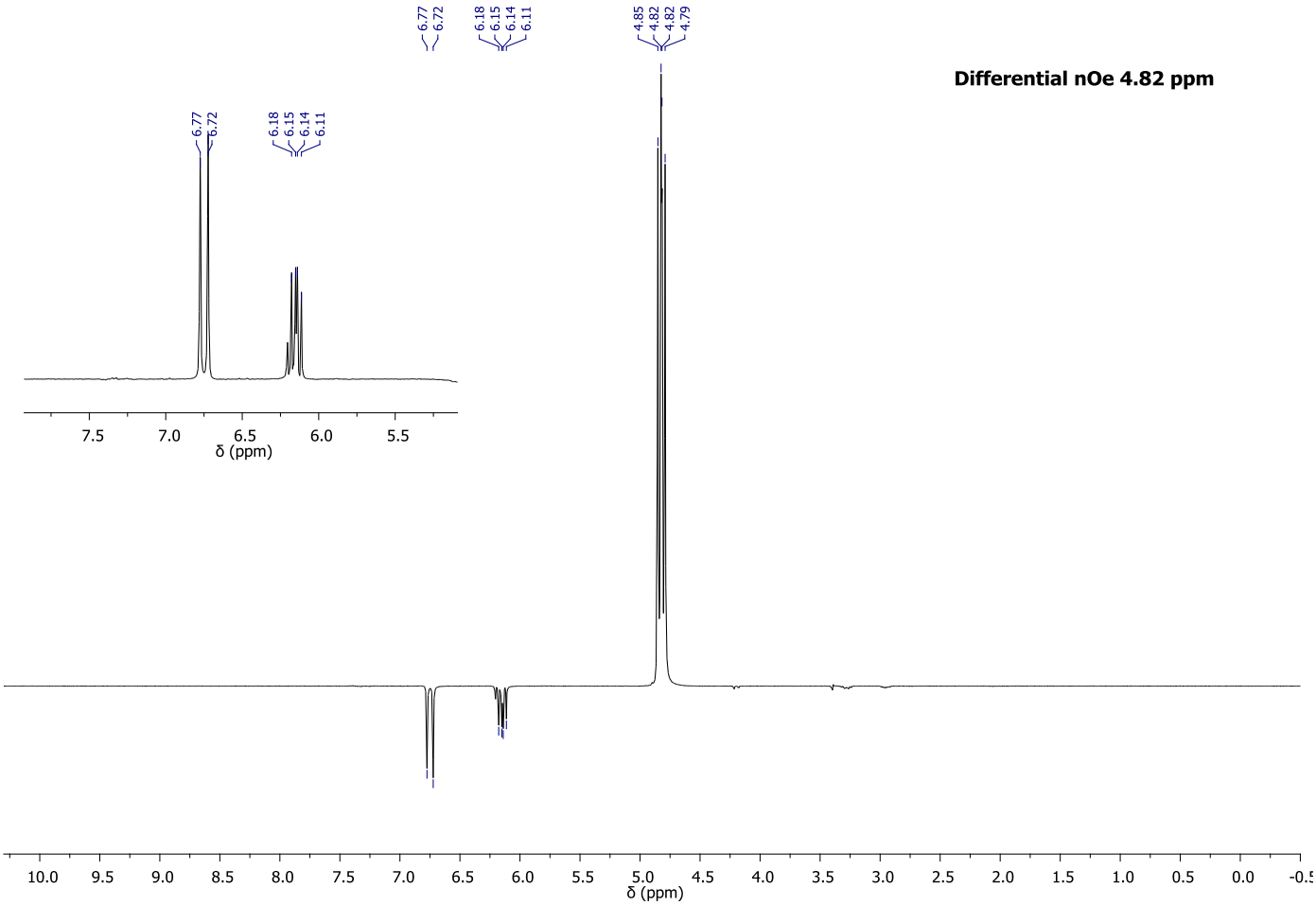
52.12
48.65
35.54
27.40
δ (ppm)



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6.72
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6.15
6.14
6.11
4.85
4.82
4.82
4.79
7.5
7.0
6.5
6.0
5.5
δ (ppm)
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
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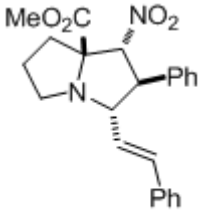
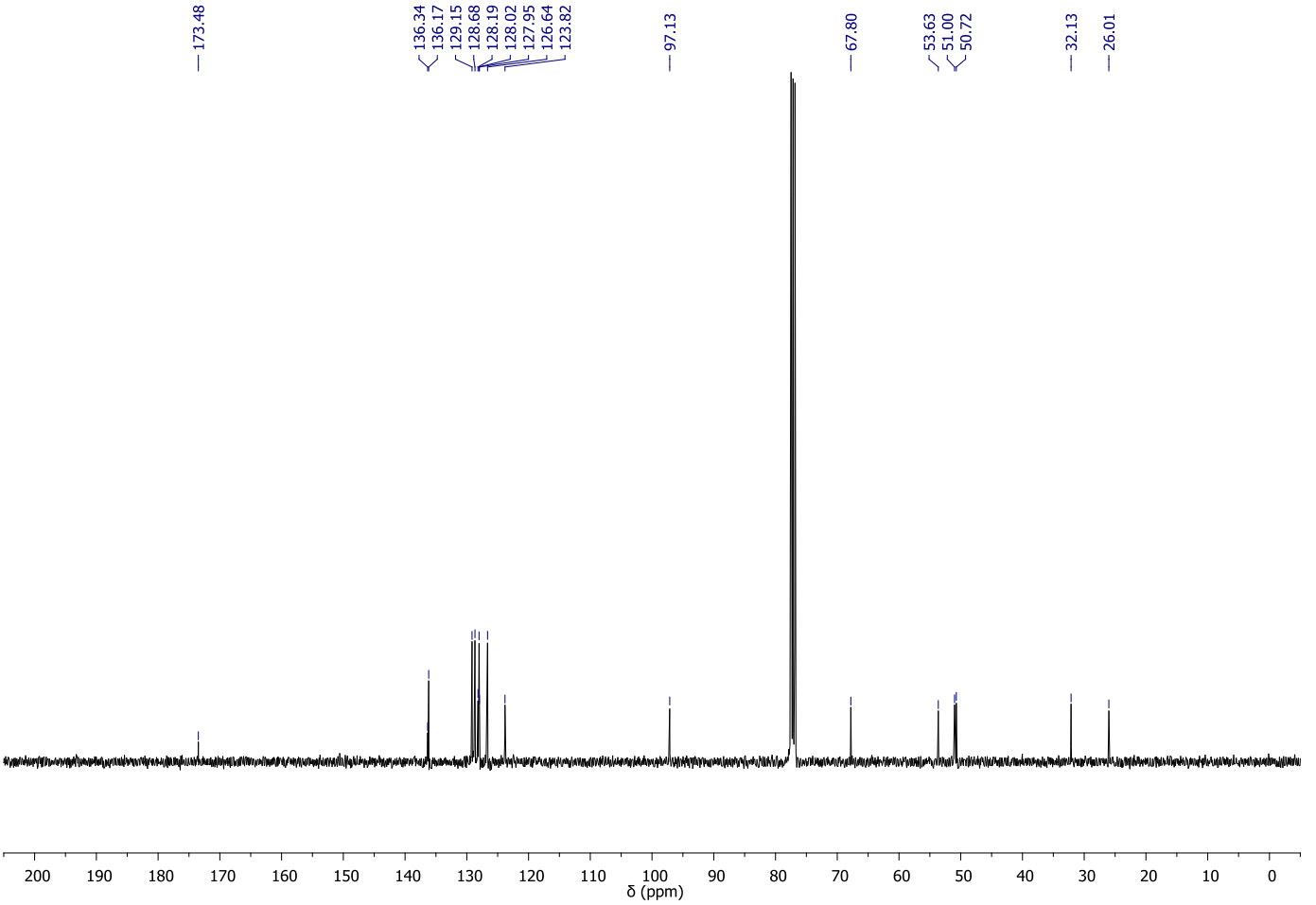
0.0
δ (ppm)


MeO2C
NO2
Ph
N
Ph

3e´

7.39
7.21
6.46
6.42
6.21
6.19
6.17
6.15
5.95
5.93
4.22
4.21
4.08
4.06
4.06
4.03
3.91
3.17
3.14
3.06
3.00
2.51
2.50
2.47
2.07
1.93
1.64
1.56
14.99
1.00
1.12
1.01
1.06
1.01
3.19
1.06
0.97
1.07
3.02
1.01
δ (ppm)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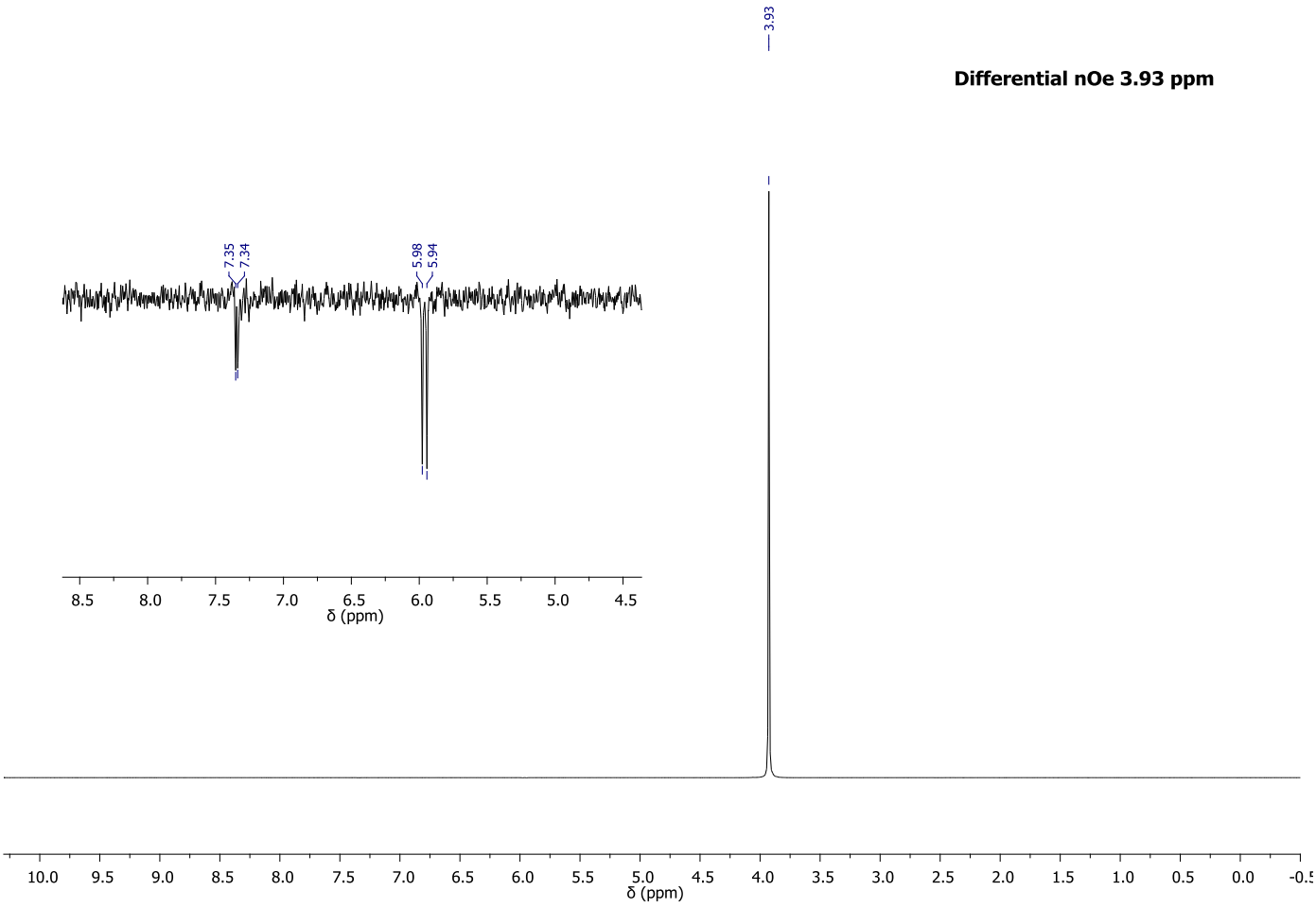
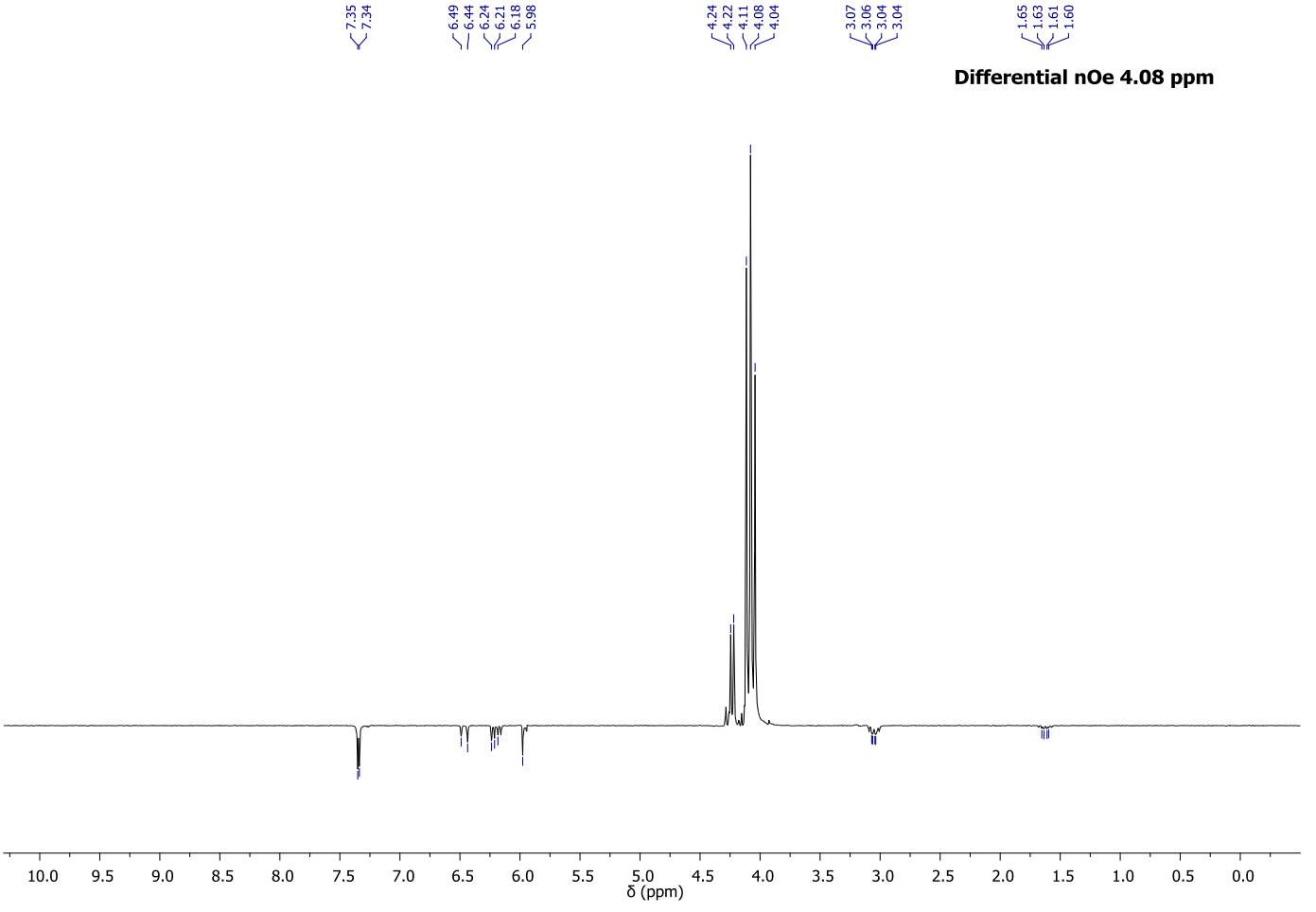
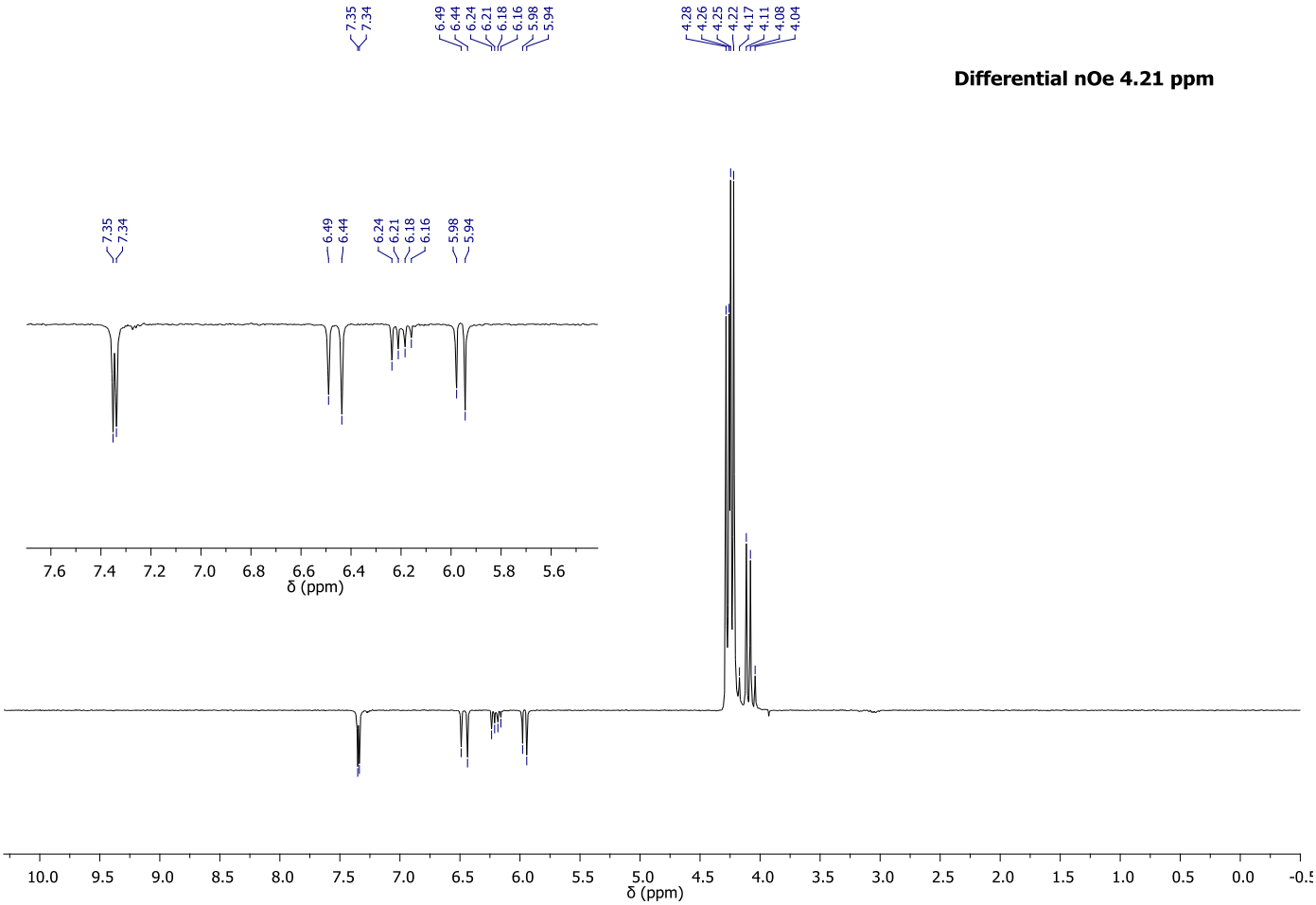
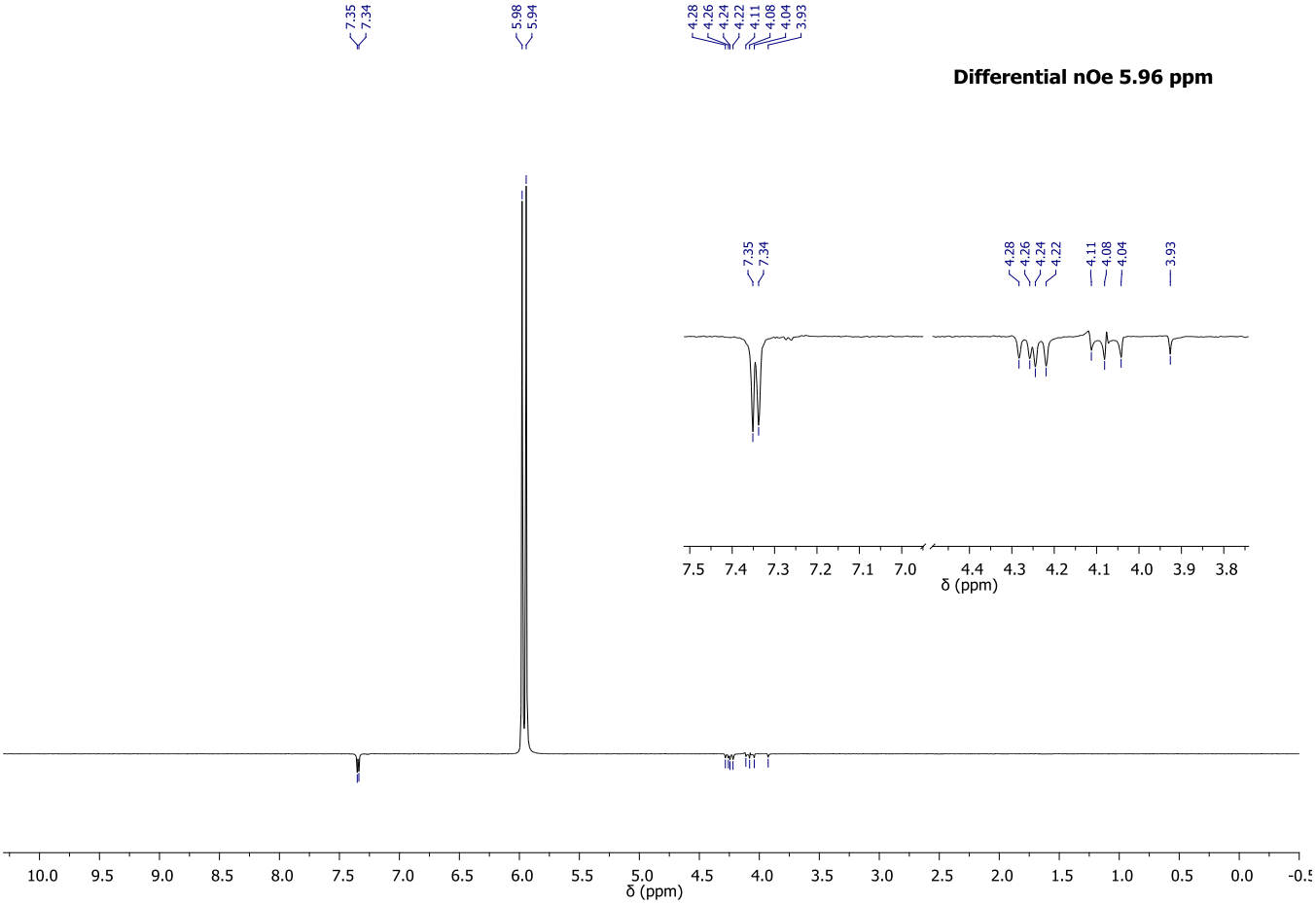
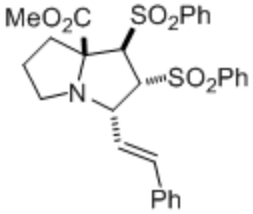
136.17
129.15
128.68
128.19
128.02
127.95
126.64
123.82
97.13
67.80
53.63
51.00
50.72
32.13
26.01
δ (ppm)


3.93
Differential nOe 3.93 ppm
7.35
7.34
5.98
5.94
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
δ (ppm)
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
δ (ppm)


7.35
7.34
6.49
6.44
6.24
6.21
6.18
5.98
4.24
4.22
4.11
4.08
4.04
3.07
3.06
3.04
3.04
1.65
1.63
1.61
1.60
Differential nOe 4.08 ppm
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
δ (ppm)

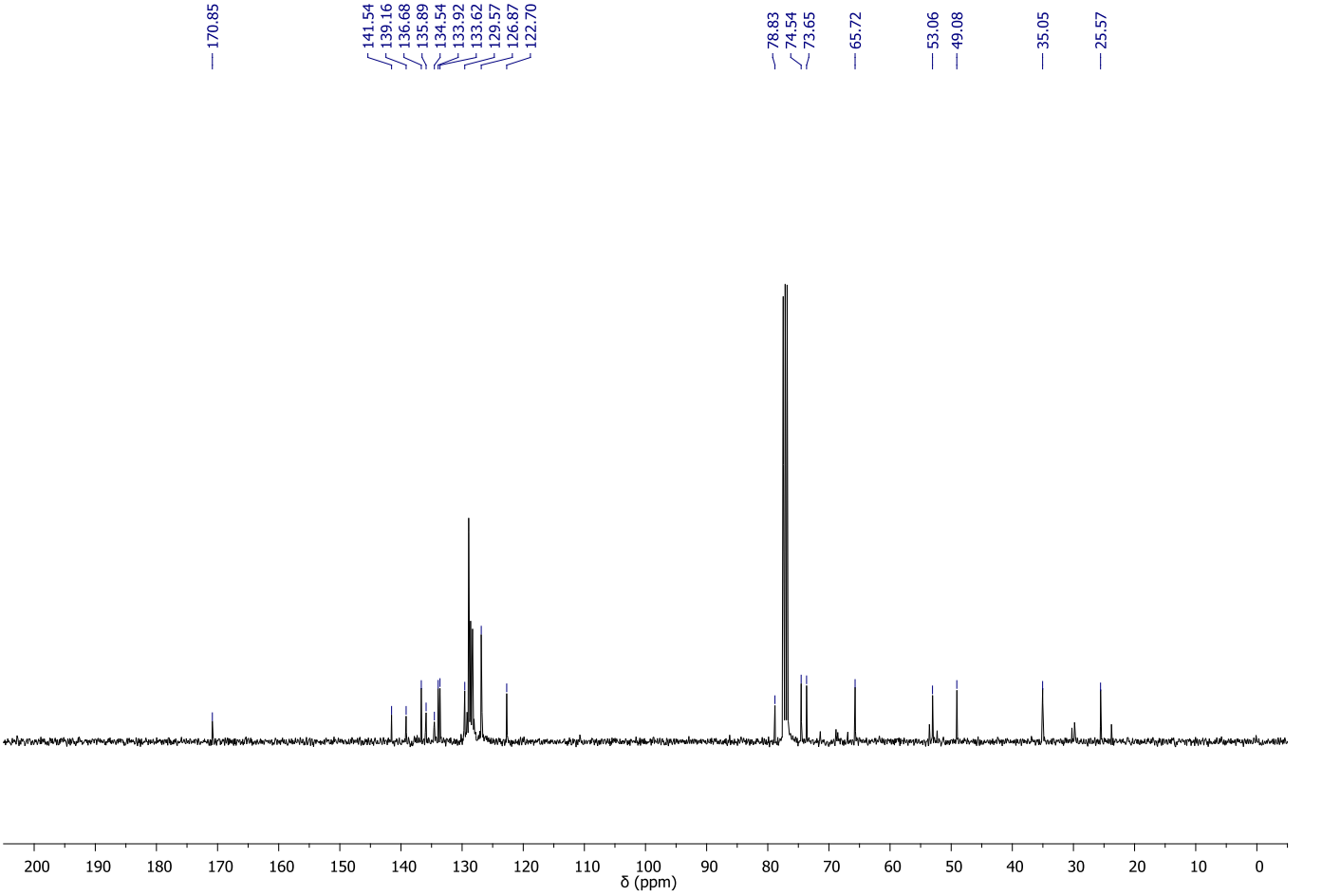

Differential nOe 4.21 ppm
7.35
7.34
6.49
6.44
6.24
6.21
6.18
6.16
5.98
5.94
4.28
4.26
4.25
4.22
4.17
4.11
4.08
4.04
δ (ppm)

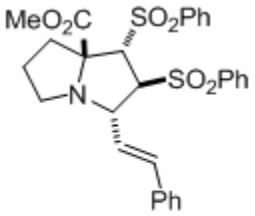

Differential nOe 5.96 ppm
7.35
7.34
5.98
5.94
4.28
4.26
4.24
4.22
4.11
4.08
4.04
3.93
δ (ppm)


MeO2C
SO2Ph
SO2Ph
N
Ph

3f

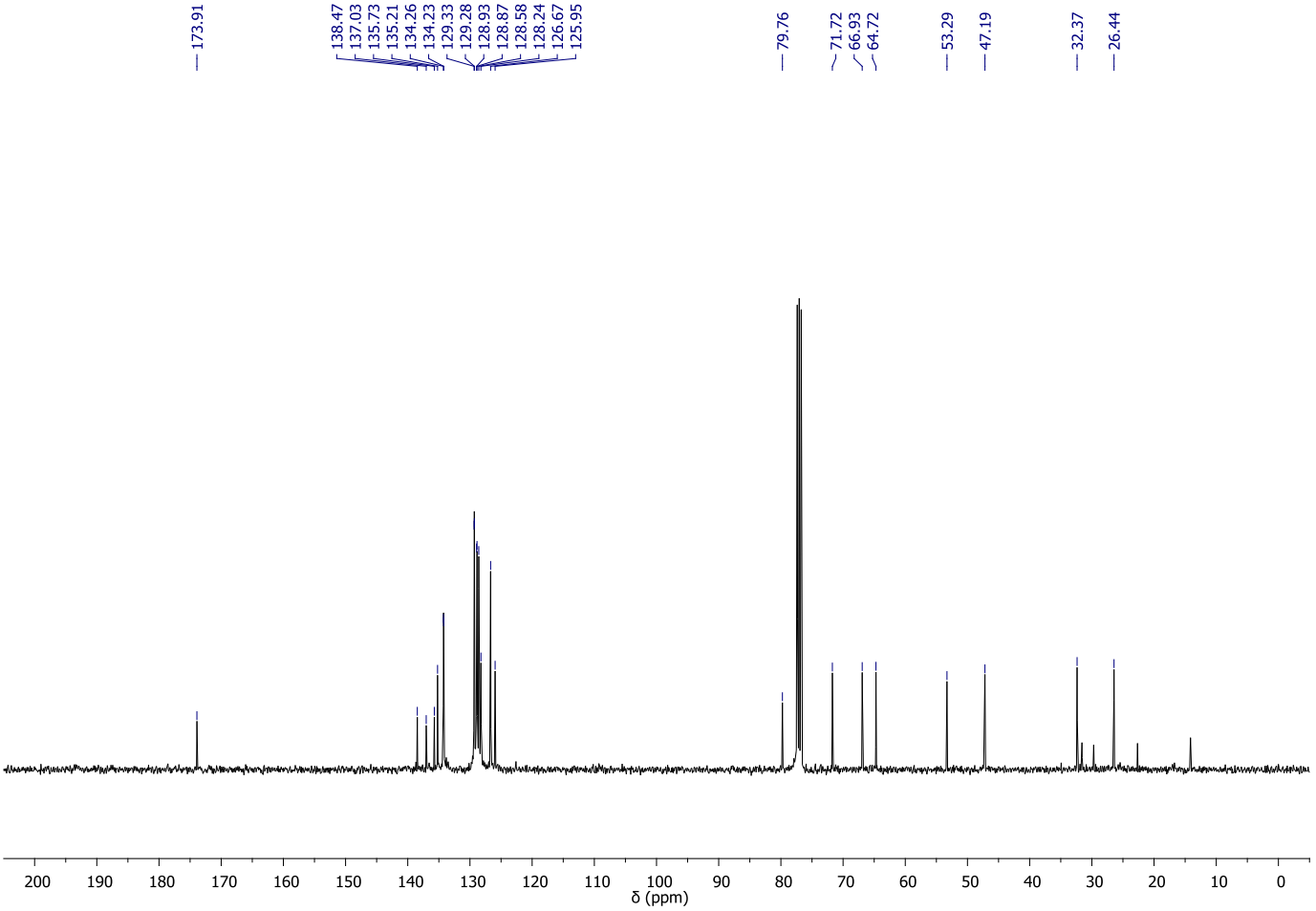
8.04
7.13
6.50
6.47
6.46
6.44
6.22
6.18
5.04
4.71
4.52
4.50
4.09
4.01
3.87
3.38
3.32
3.21
3.14
3.07
3.03
2.22
2.14
2.05
1.99
2.04
1.42
7.89
12.50
0.99
1.14
1.02
1.18
1.00
0.94
2.98
1.03
1.00
1.28
1.15
2.56
δ (ppm)

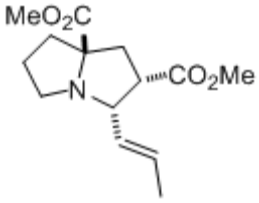

170.85
141.54
139.16
136.68
135.89
134.54
133.92
133.62
129.57
126.87
122.70
78.83
74.54
73.65
65.72
53.06
49.08
35.05
25.57
δ (ppm)


MeO2C
SO2Ph
SO2Ph
N
Ph

3f´

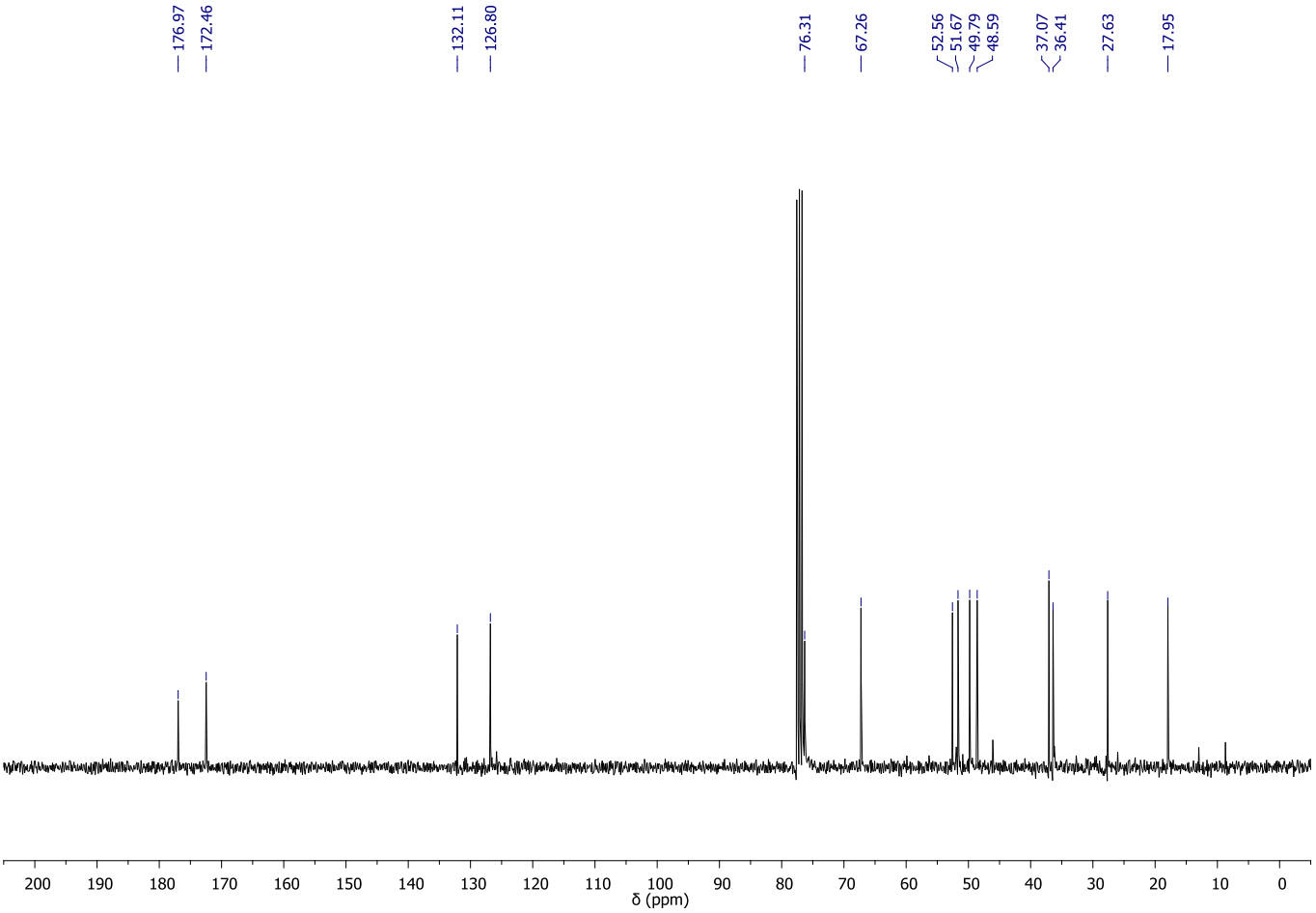
7.94
7.23
5.07
5.06
4.40
4.39
4.38
4.37
4.03
3.83
3.16
2.94
2.17
2.02
2.19
17.44
2.11
1.07
1.00
1.05
3.03
1.07
1.18
0.92
1.00
2.13
δ (ppm)

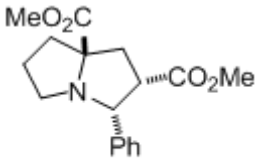

173.91
138.47
137.03
135.73
135.21
134.26
134.23
129.33
129.28
128.93
128.87
128.58
128.24
126.67
125.95
79.76
71.72
66.93
64.72
53.29
47.19
32.37
26.44
δ (ppm)


MeO2C
CO2Me
N

3g

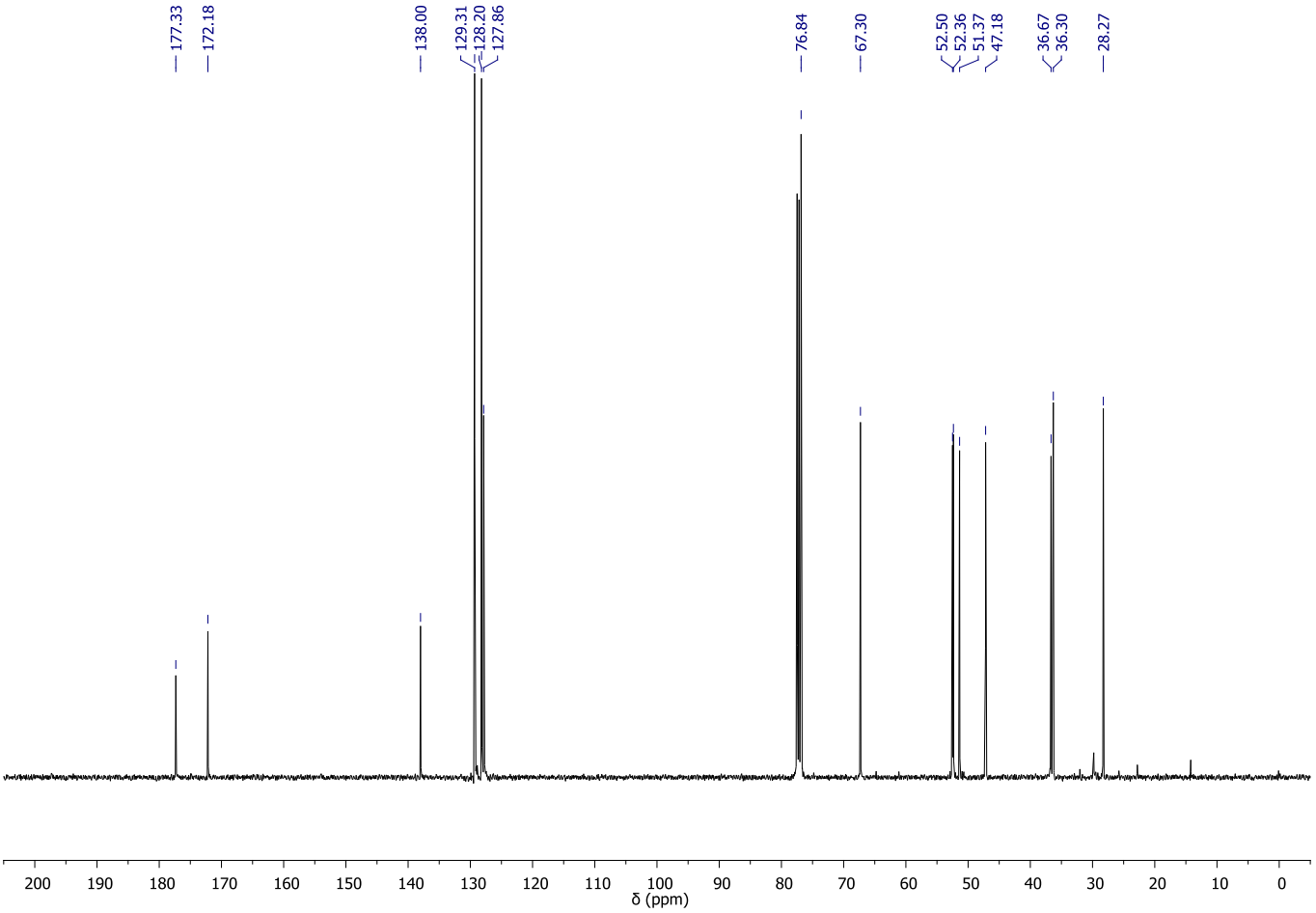
5.71
5.69
5.66
5.64
5.29
5.26
5.25
5.24
5.21
4.05
4.02
4.00
3.99
3.96
3.72
3.61
3.43
3.37
3.11
3.01
2.88
2.80
2.60
2.59
2.56
2.52
2.27
2.25
2.09
1.91
1.70
1.68
0.97
1.00
1.06
5.62
3.22
1.02
1.16
1.20
1.20
1.10
1.47
4.40
3.52
δ (ppm)

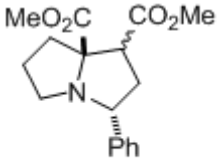

176.97
172.46
132.11
126.80
76.31
67.26
52.56
51.67
49.79
48.59
37.07
36.41
27.63
17.95
δ (ppm)


MeO2C
CO2Me
N
Ph

3h

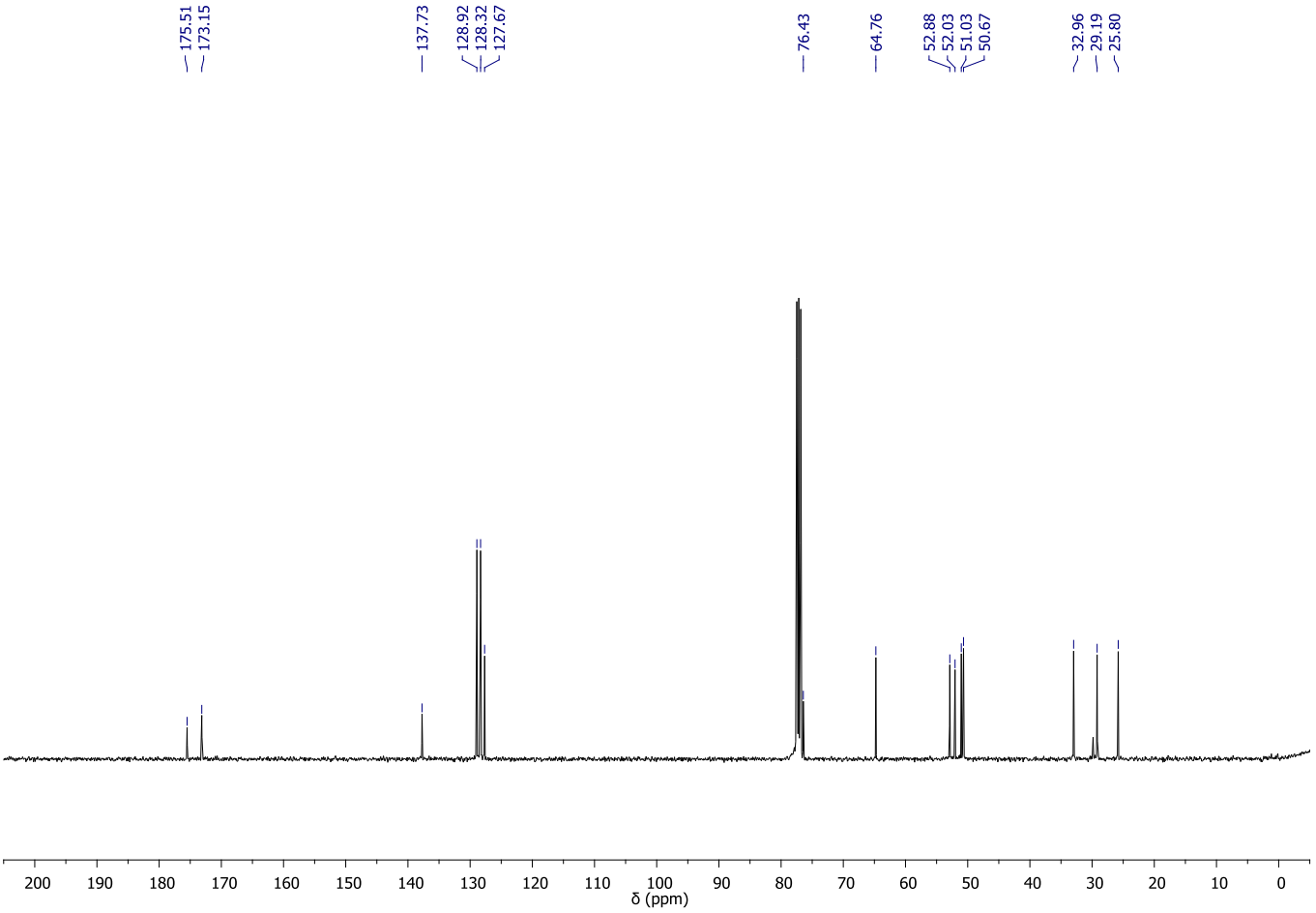
7.30
7.28
7.27
7.17
7.17
7.15
4.74
4.72
3.89
3.89
3.88
3.87
3.86
3.86
3.84
3.76
3.23
2.74
2.68
2.60
2.58
2.57
2.55
1.89
3.31
1.98
1.00
0.99
3.02
2.96
2.02
1.01
2.12
3.02
δ (ppm)

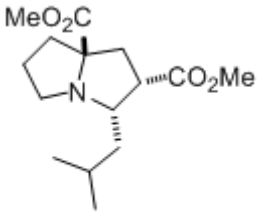

177.33
172.18
138.00
129.31
128.20
127.86
76.84
67.30
52.50
52.36
51.37
47.18
36.67
36.30
28.27
δ (ppm)


MeO2C
CO2Me
N
Ph

3h´

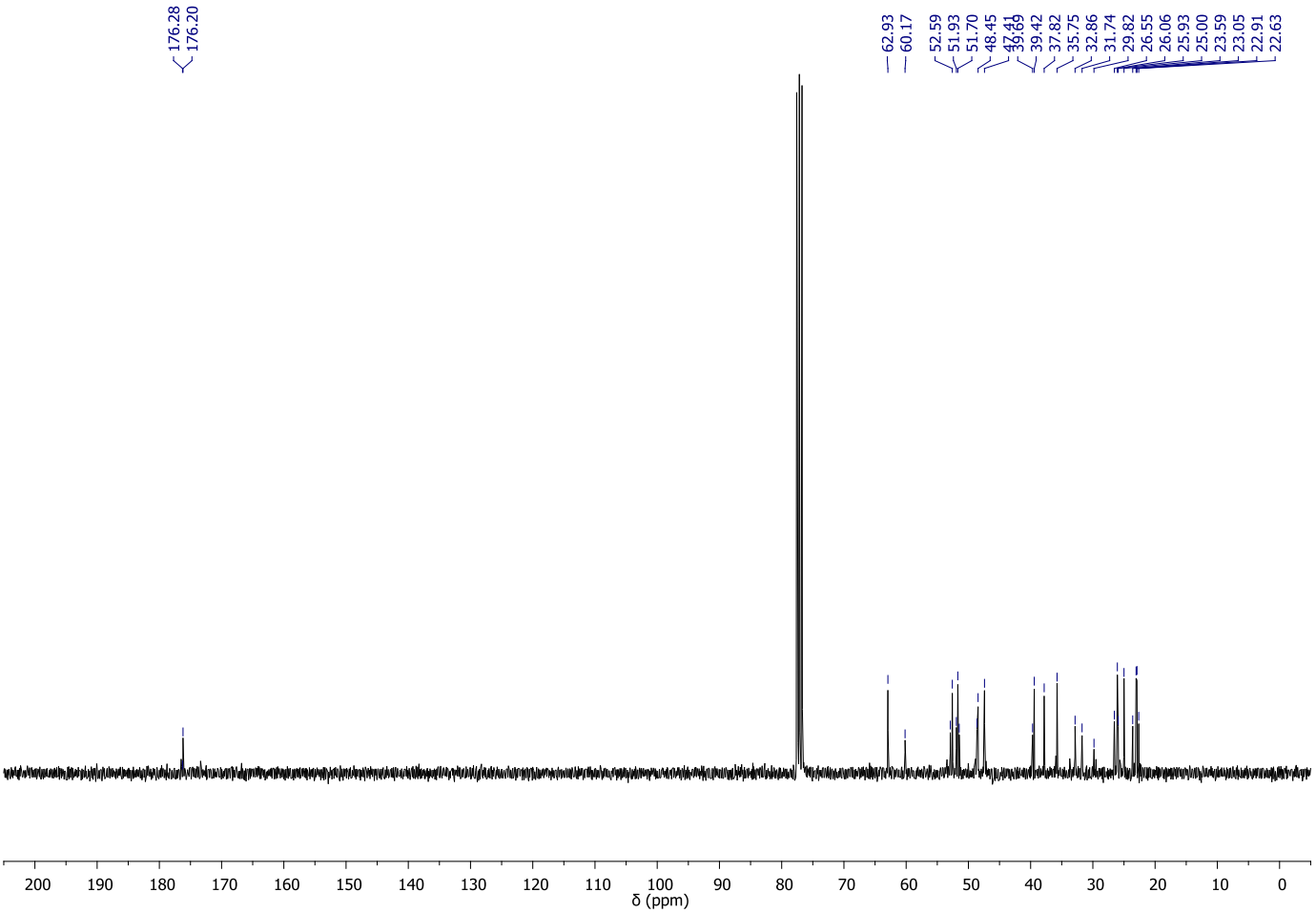
7.44
7.42
7.36
7.34
7.32
7.30
7.28
7.26
4.51
4.50
4.48
4.47
3.82
3.81
3.79
3.78
3.72
2.50
2.47
2.46
2.45
2.44
2.43
2.42
2.18
1.77
1.76
1.74
1.73
1.71
1.70
1.69
1.47
1.45
1.44
1.42
2.08
3.55
1.00
4.12
3.03
3.07
1.04
1.00
2.86
0.99
δ (ppm)

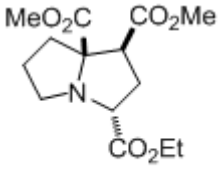

175.51
173.15
137.73
128.92
128.32
127.67
76.43
64.76
52.88
52.03
51.03
50.67
32.96
29.19
25.80
δ (ppm)


MeO2C
CO2Me
N

3i

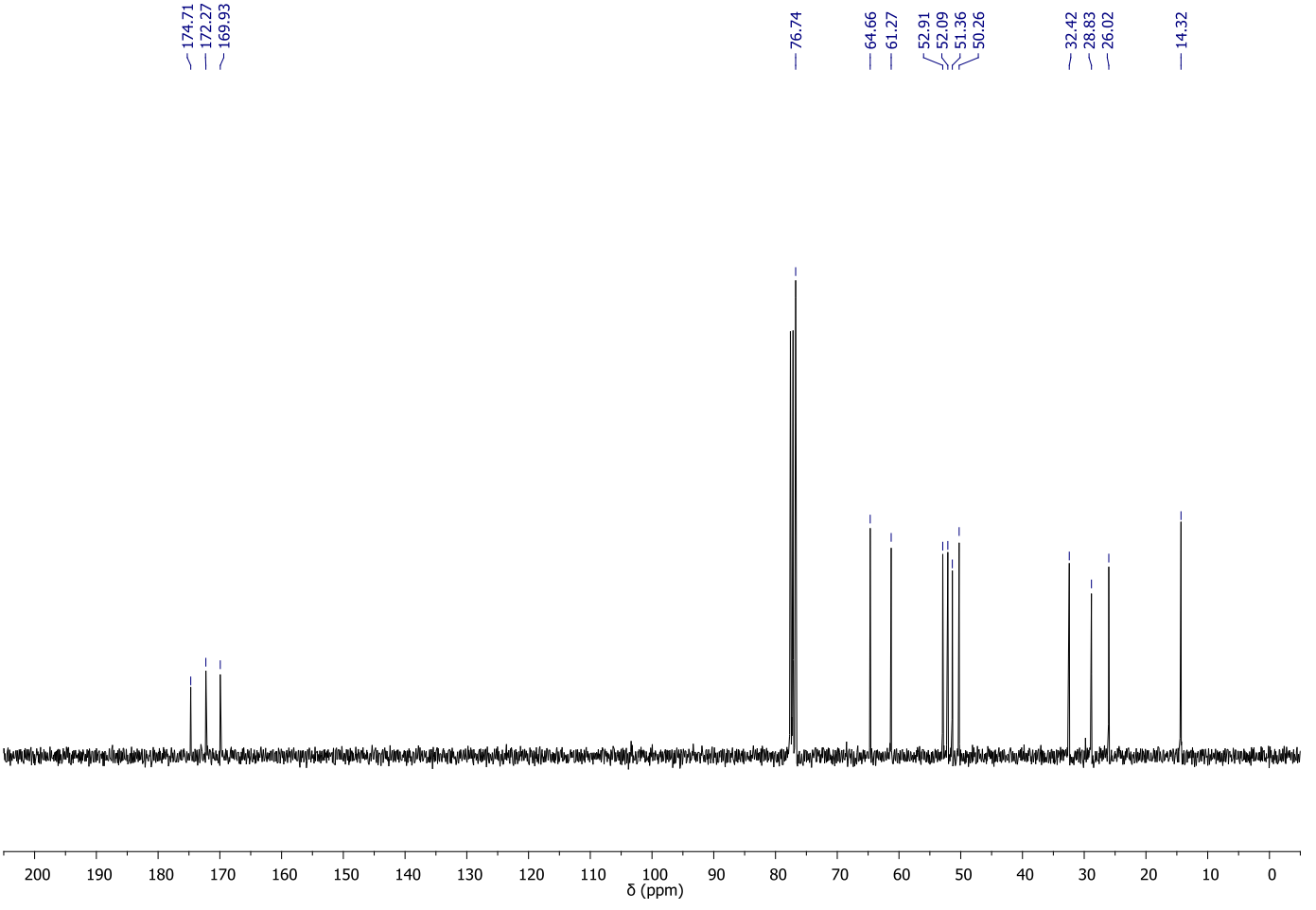
3.73
3.68
3.07
3.05
2.98
2.96
2.92
2.61
2.58
2.57
2.54
2.37
2.25
2.24
2.21
2.19
1.46
1.37
1.35
0.92
0.58
2.77
3.11
1.04
1.12
1.06
1.38
0.91
1.00
0.82
0.89
1.69
1.48
0.97
6.00
δ (ppm)

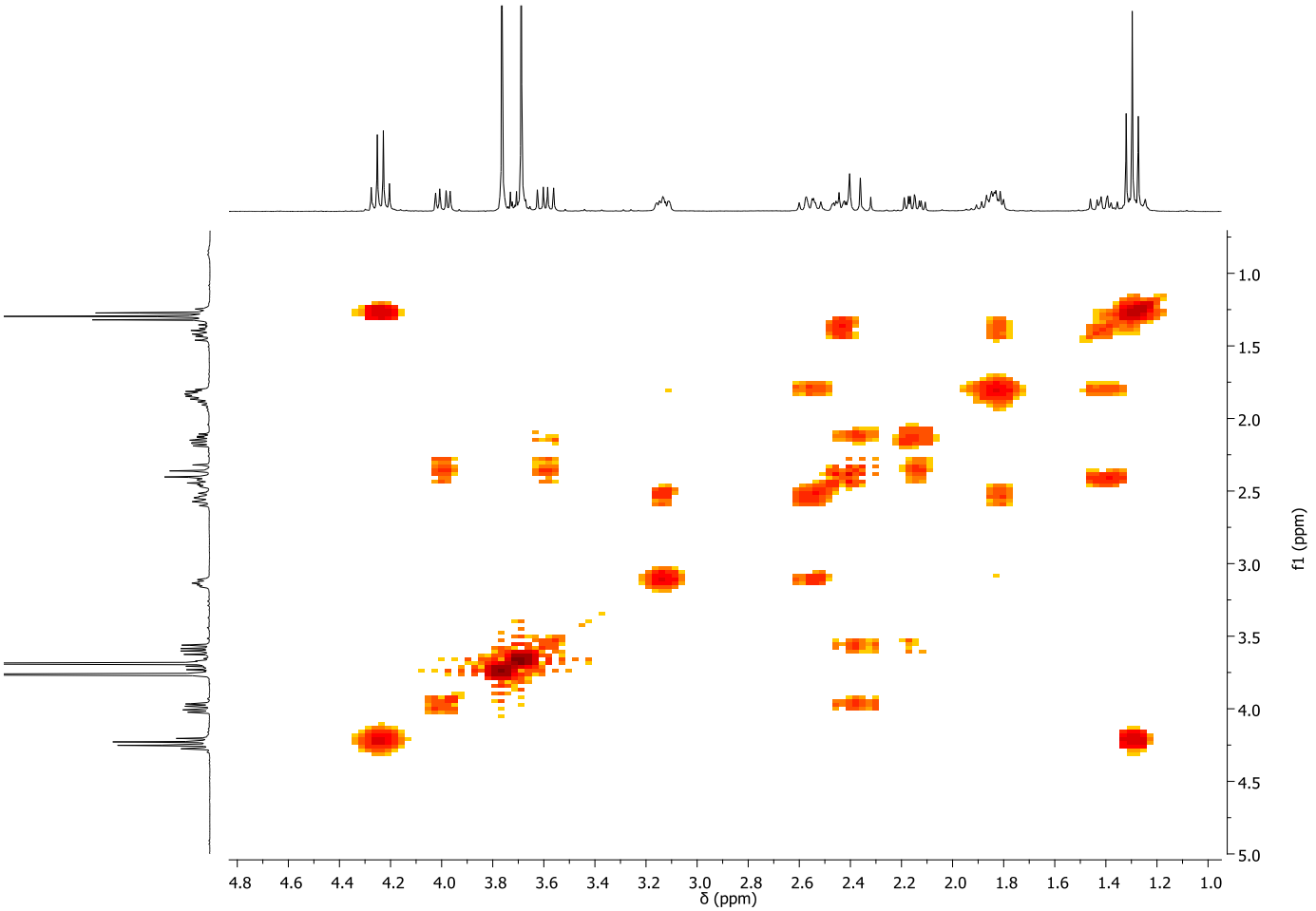

176.28
176.20
62.93
60.17
52.59
51.93
51.70
48.45
47.41
39.69
39.42
37.82
35.75
32.86
31.74
29.82
26.55
26.06
25.93
25.00
23.59
23.05
22.91
22.63
δ (ppm)

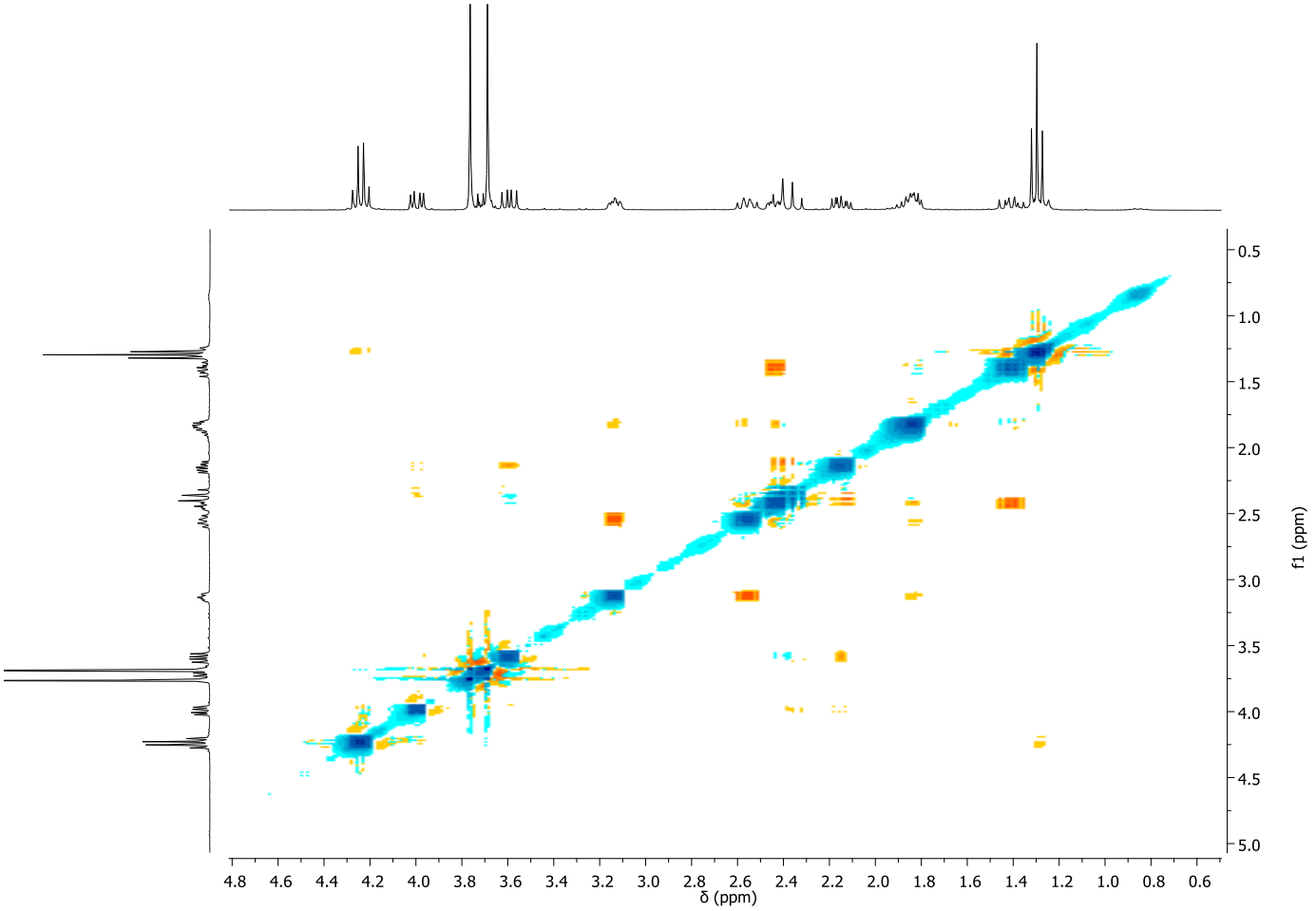

MeO2C
CO2Me
N
CO2Et

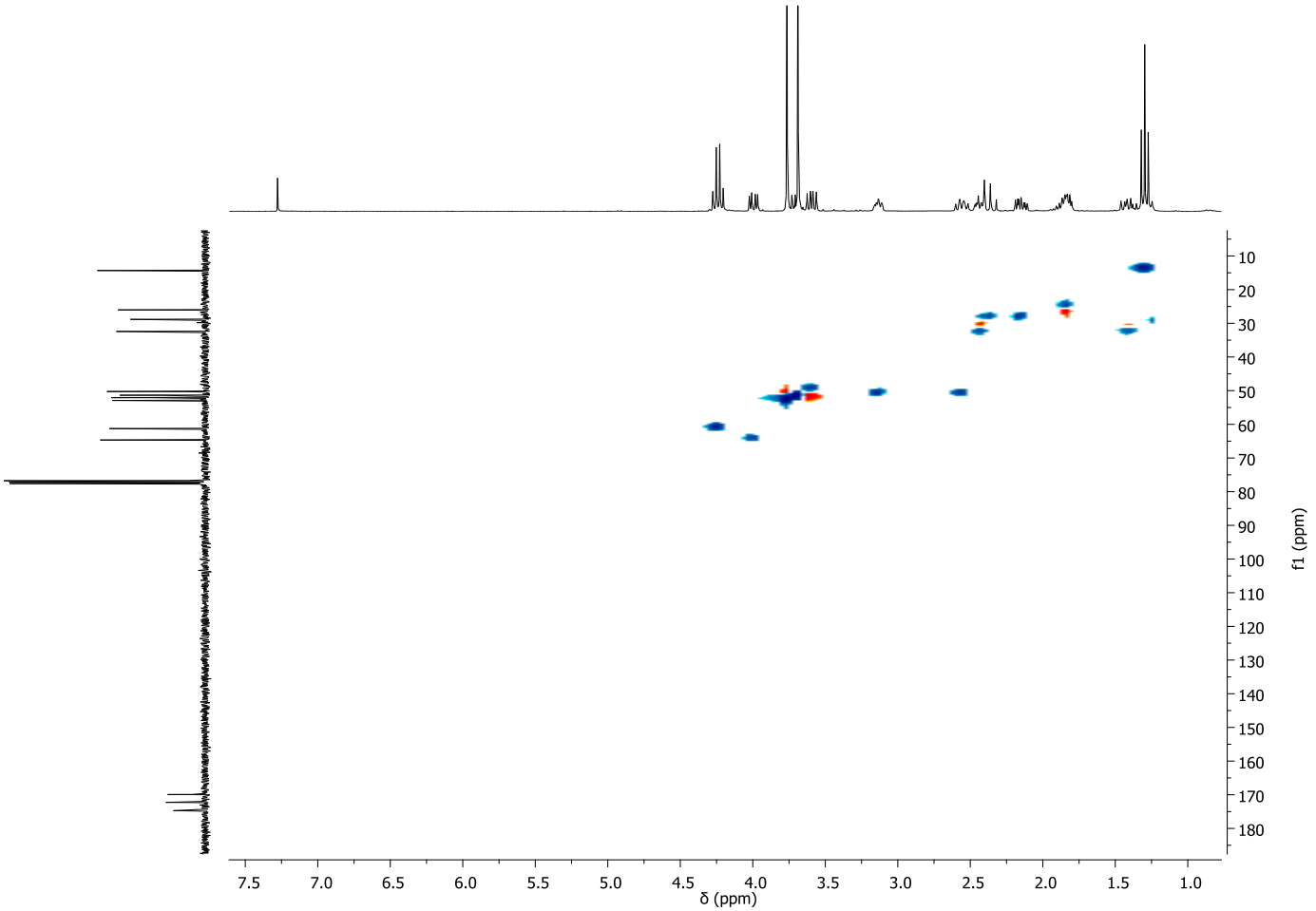
3j

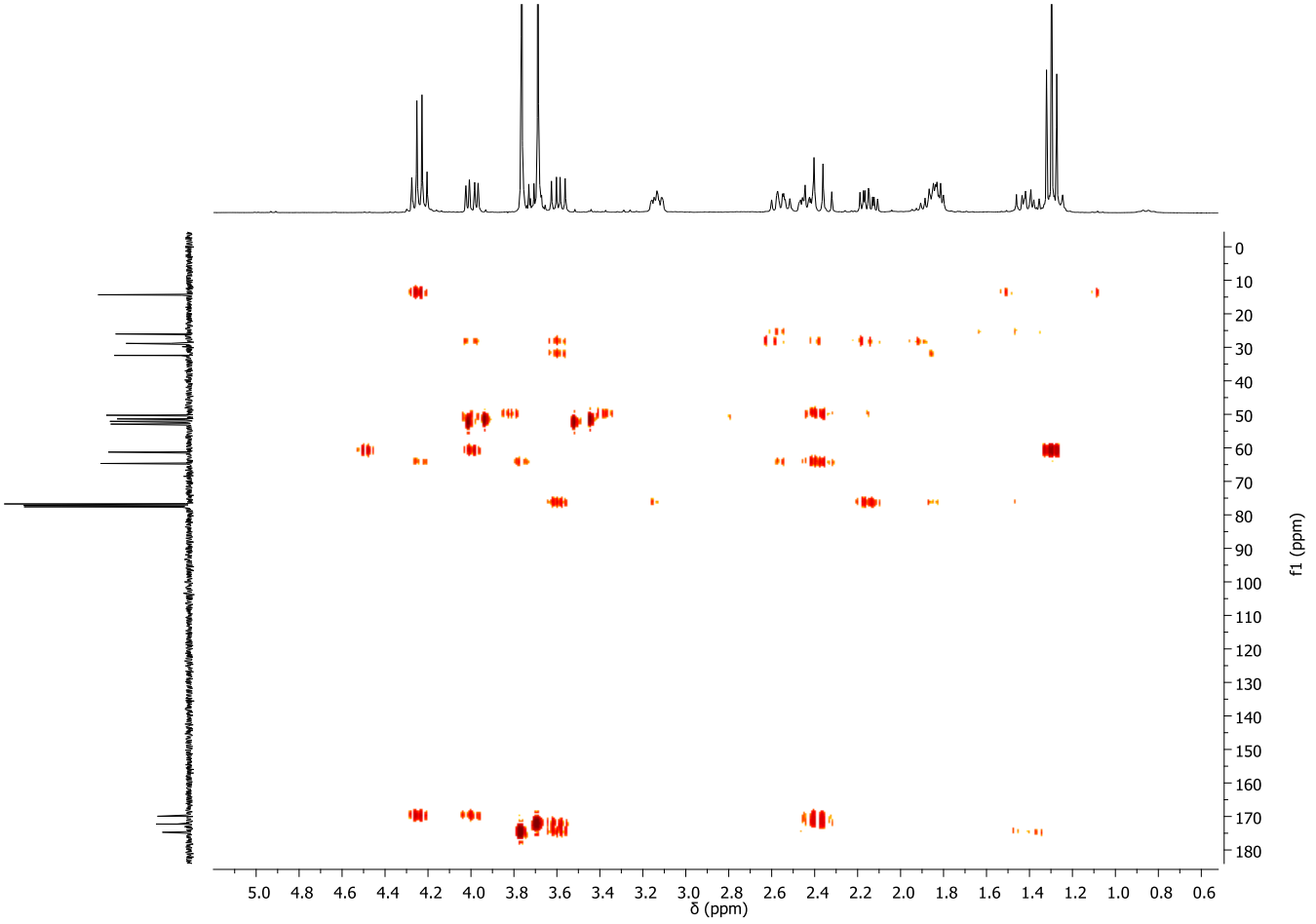
4.25
4.23
4.02
4.01
3.98
3.97
3.76
3.69
3.63
3.60
3.58
3.56
3.15
3.13
3.11
2.57
2.54
2.40
2.36
2.19
2.17
2.17
2.15
2.15
1.30
2.18
1.00
3.03
3.07
1.04
1.12
1.22
2.12
1.06
2.20
0.96
3.45
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
δ (ppm)

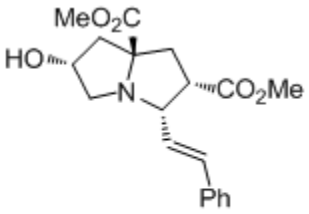

174.71
172.27
169.93
76.74
64.66
61.27
52.91
52.09
51.36
50.26
32.42
28.83
26.02
14.32
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
δ (ppm)


1.0
1.5
2.0
2.5
3.0
3.5
4.0
4.5
5.0
f1 (ppm)
4.8 4.6 4.4 4.2 4.0 3.8 3.6 3.4 3.2 3.0 2.8 2.6 2.4 2.2 2.0 1.8 1.6 1.4 1.2 1.0
δ (ppm)


0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0
4.5
5.0
f1 (ppm)
4.8 4.6 4.4 4.2 4.0 3.8 3.6 3.4 3.2 3.0 2.8 2.6 2.4 2.2 2.0 1.8 1.6 1.4 1.2 1.0 0.8 0.6
δ (ppm)

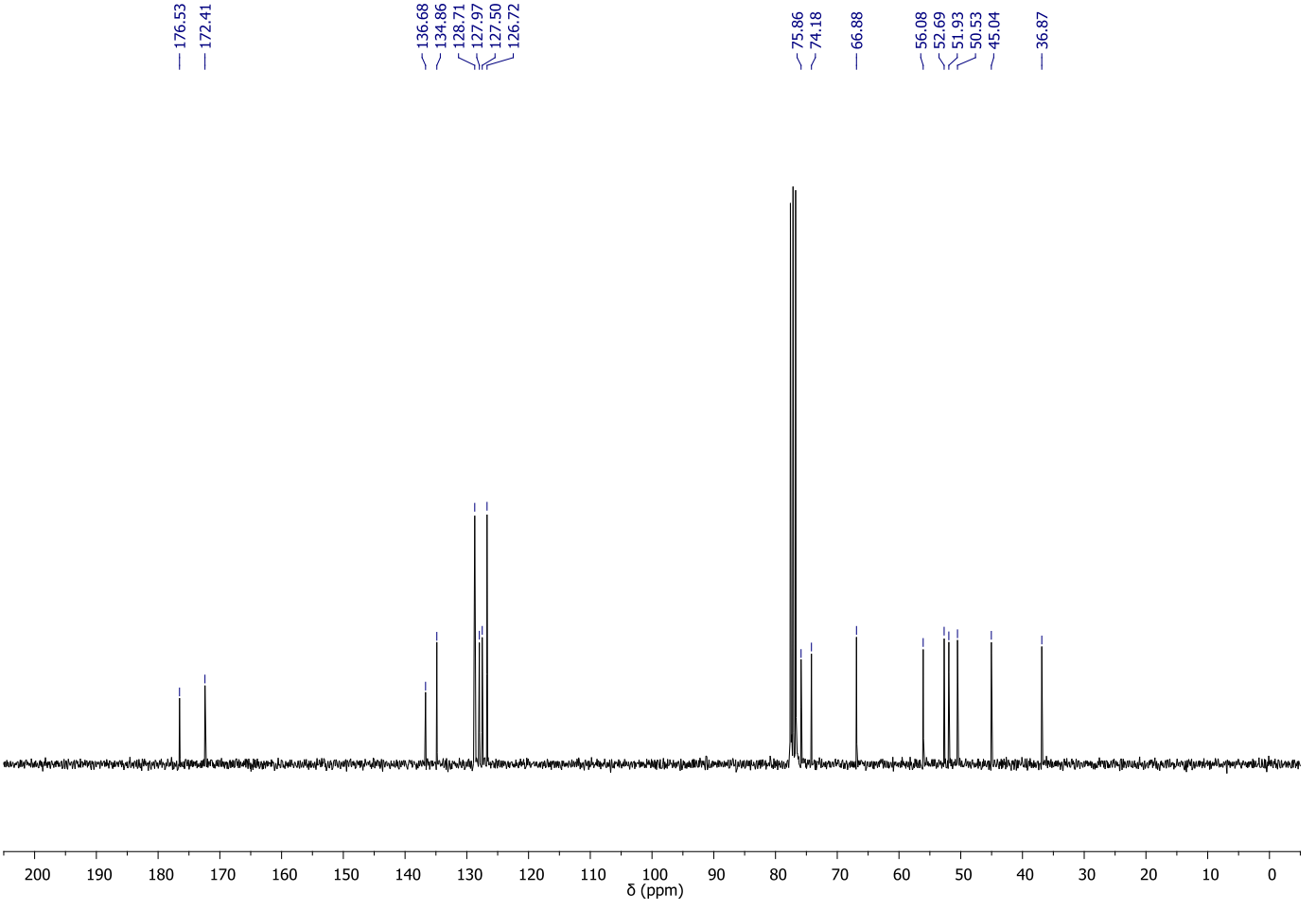

f1 (ppm)
δ (ppm)

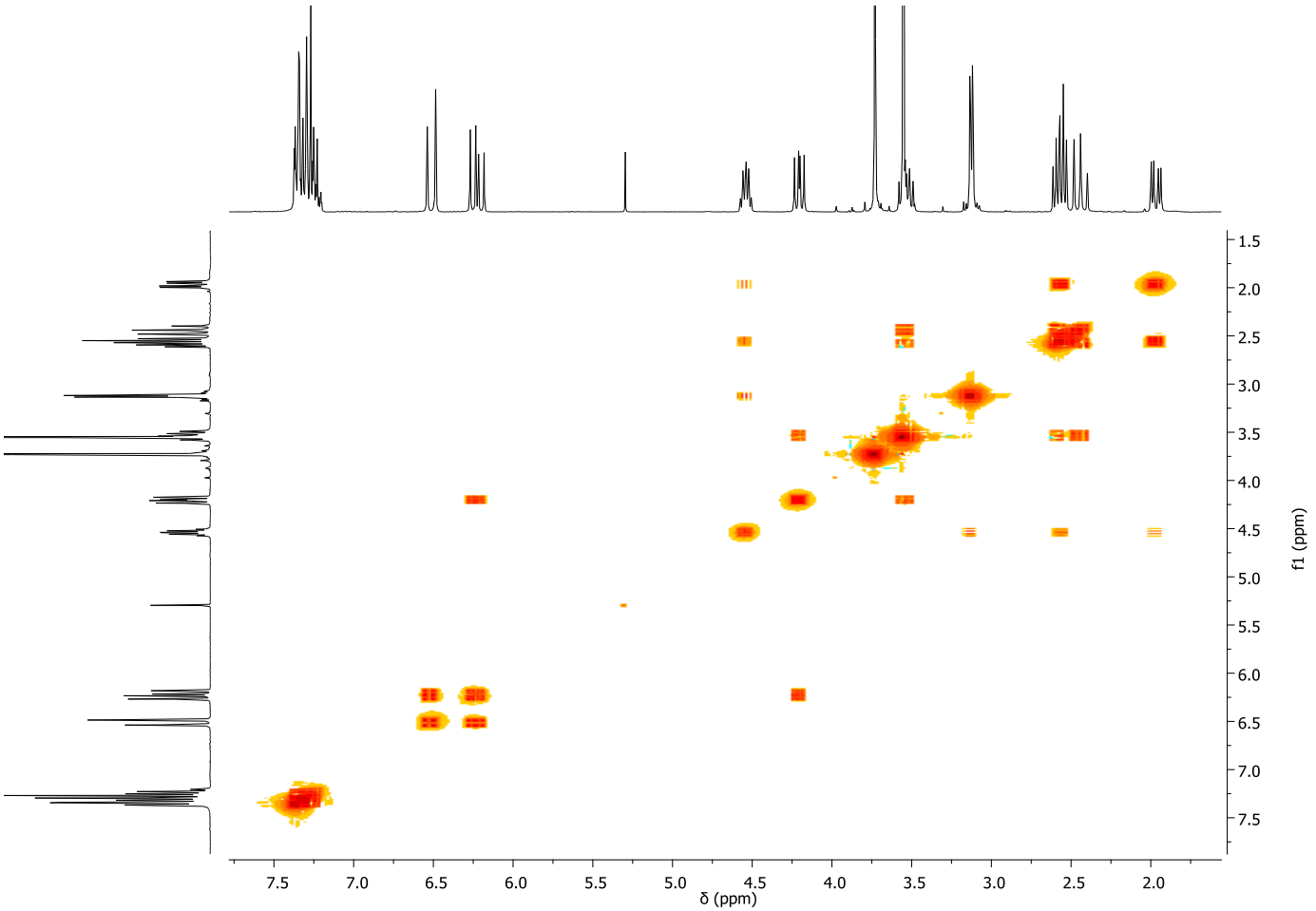

f1 (ppm)
δ (ppm)

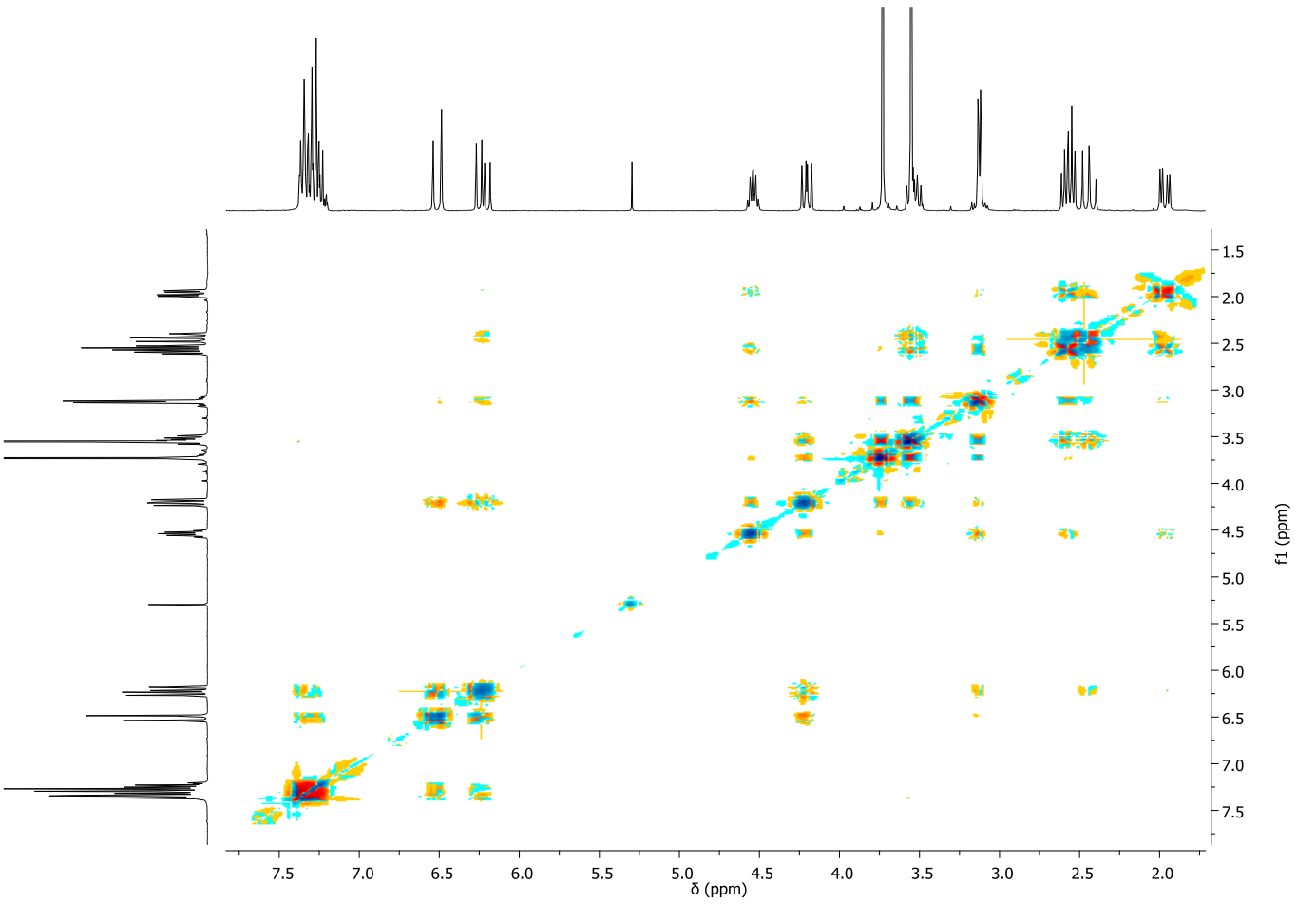

MeO2C
HO
N
CO2Me
Ph

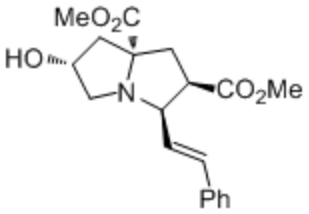
4a

7.37
7.21
6.54
6.49
6.27
6.23
6.22
6.18
4.57
4.56
4.54
4.54
4.52
4.51
4.23
4.21
4.20
4.17
3.73
3.55
3.54
3.52
3.51
2.59
2.57
2.57
2.55
2.44
2.00
1.98
1.95
1.94
5.42
1.00
1.00
0.99
1.00
3.00
4.00
2.00
1.98
1.00
1.00
δ (ppm)

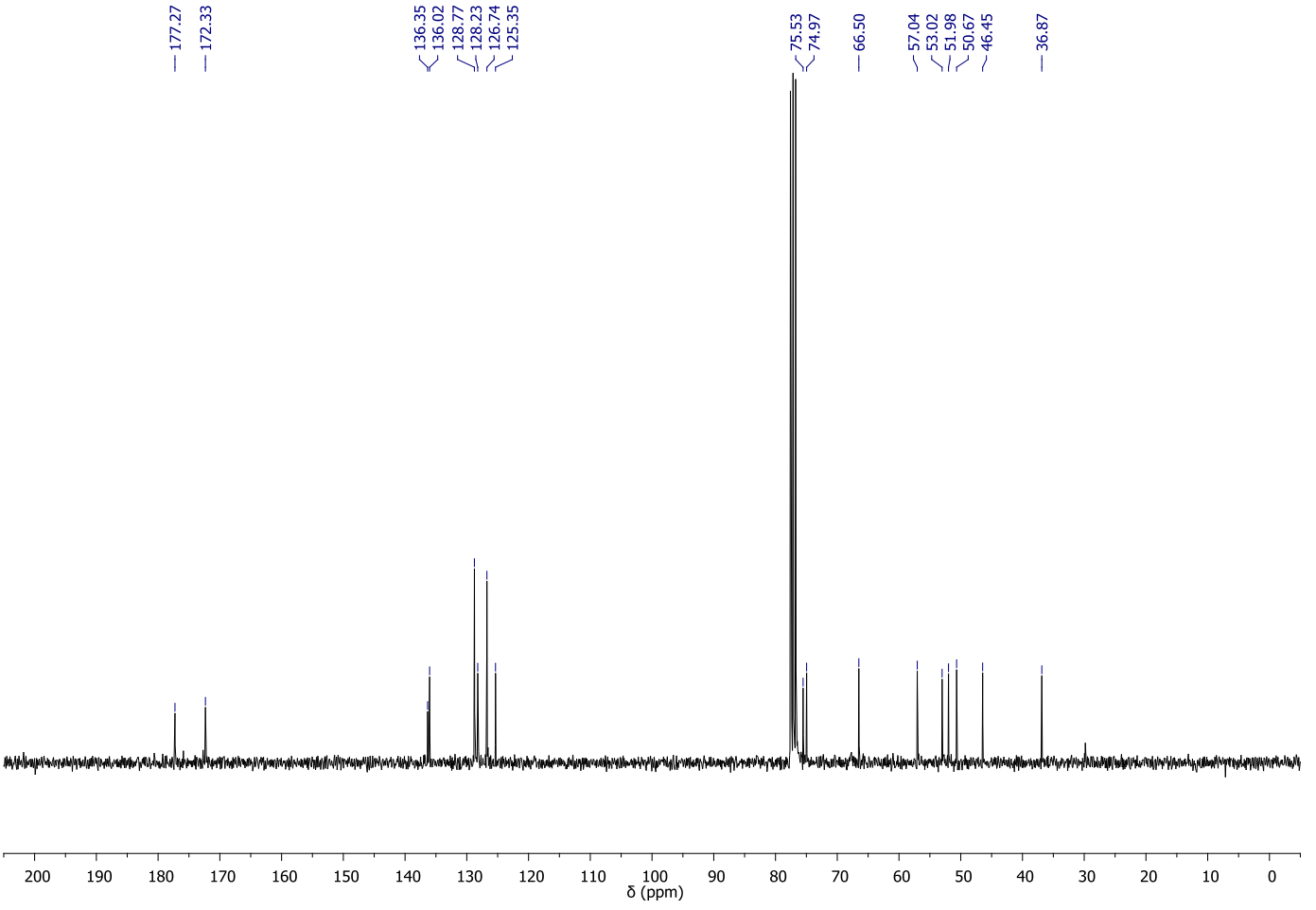

176.53
172.41
136.68
134.86
128.71
127.97
127.50
126.72
75.86
74.18
66.88
56.08
52.69
51.93
50.53
45.04
36.87
δ (ppm)

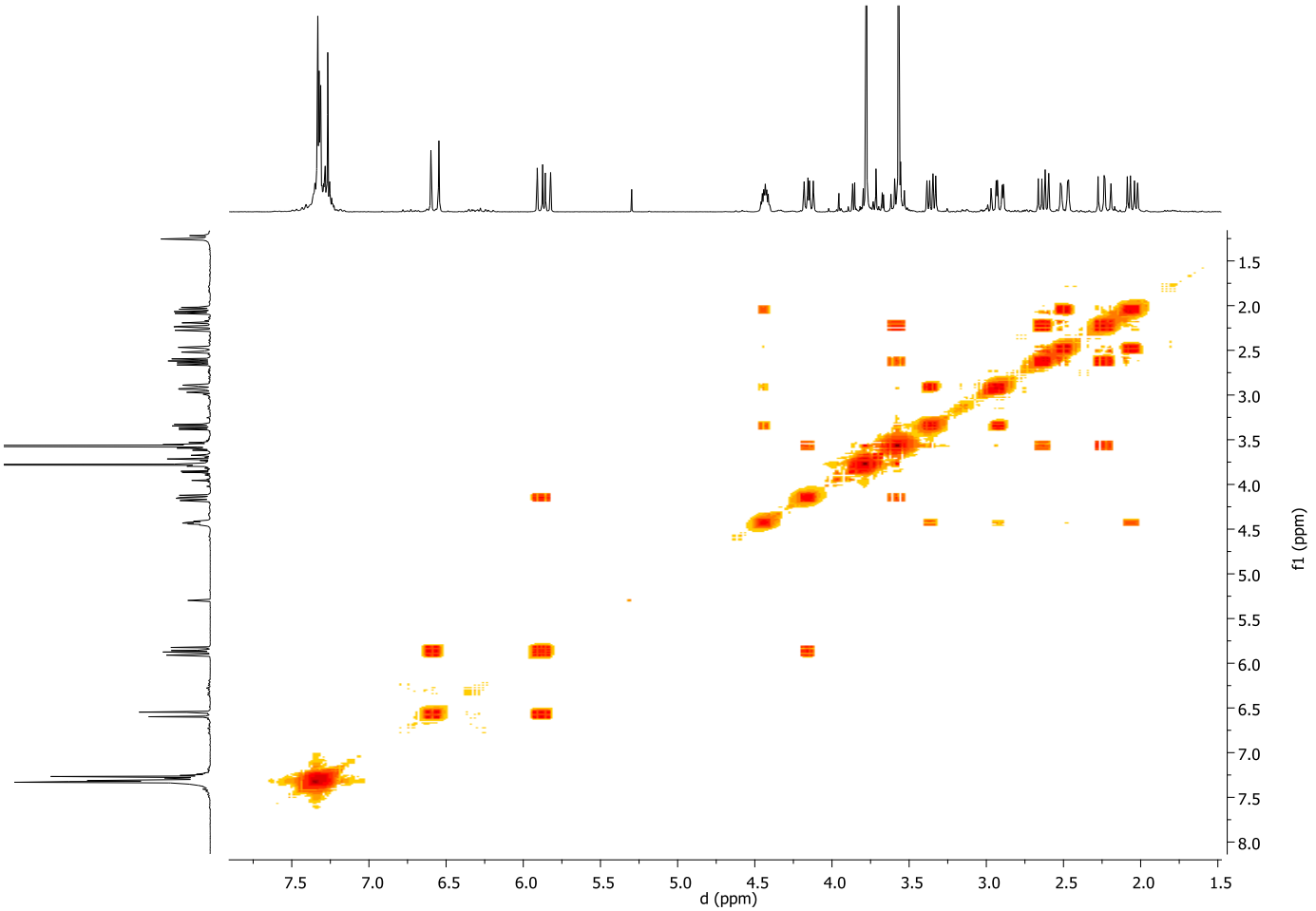

1.5
2.0
2.5
3.0
3.5
4.0
4.5
5.0
5.5
6.0
6.5
7.0
7.5
f1 (ppm)
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
δ (ppm)

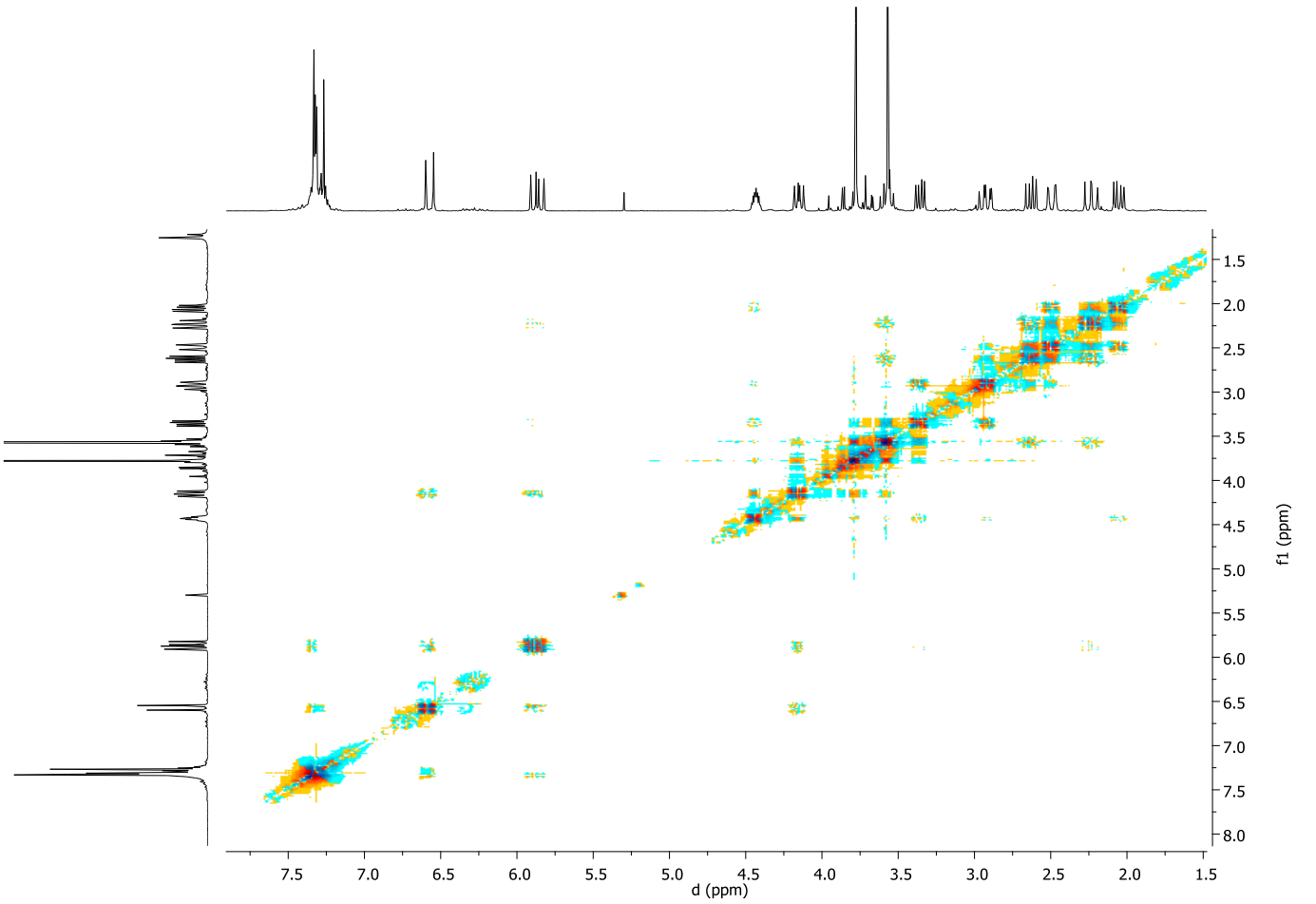

1.5
2.0
2.5
3.0
3.5
4.0
4.5
5.0
5.5
6.0
6.5
7.0
7.5
f1 (ppm)
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
δ (ppm)

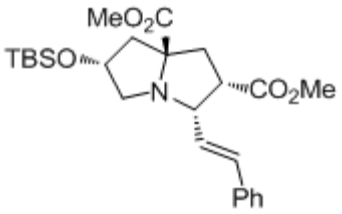


4a´



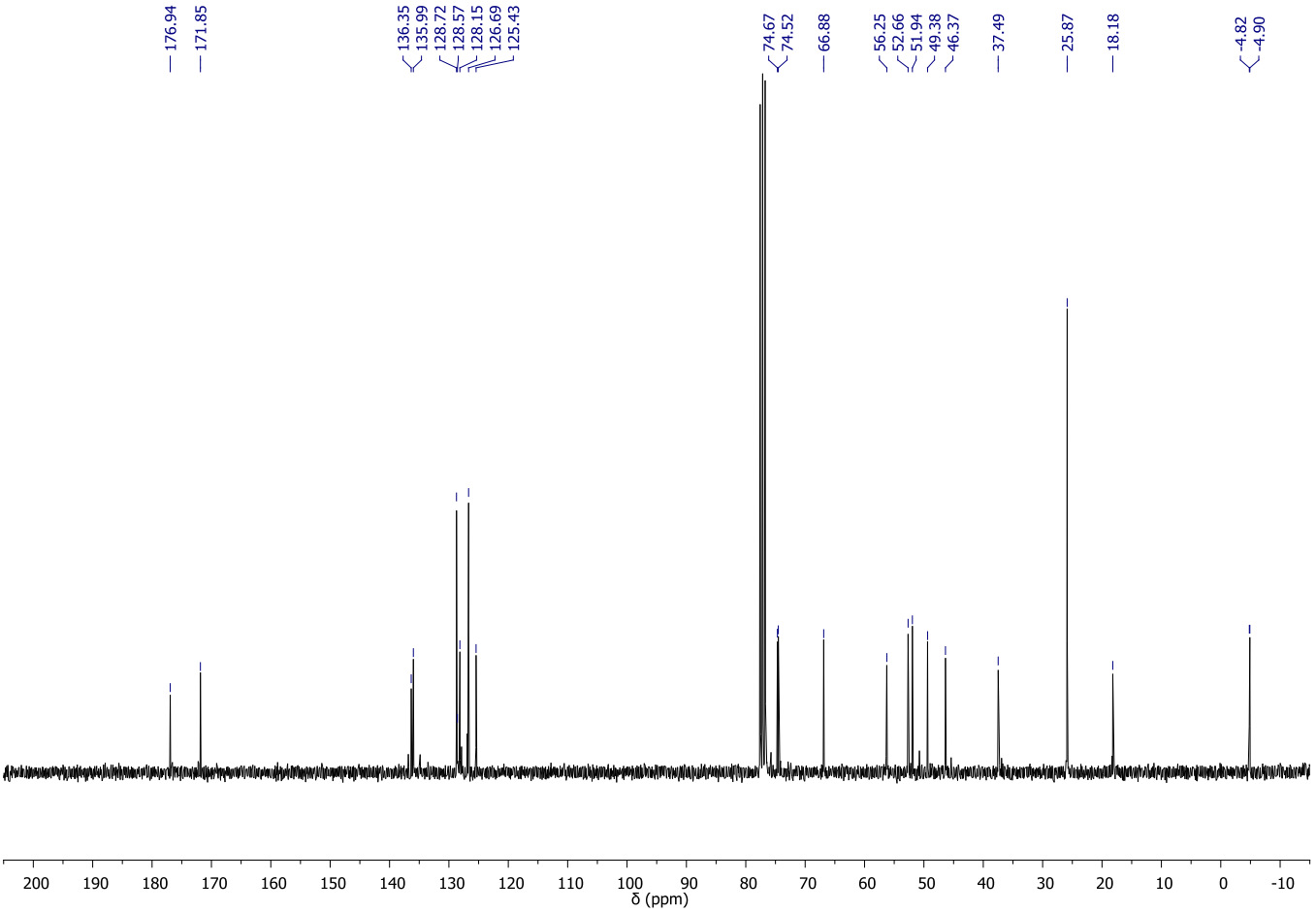


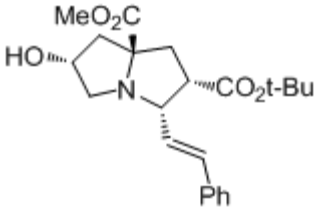



MeO2C
TBSO
N
CO2Me
Ph

4b

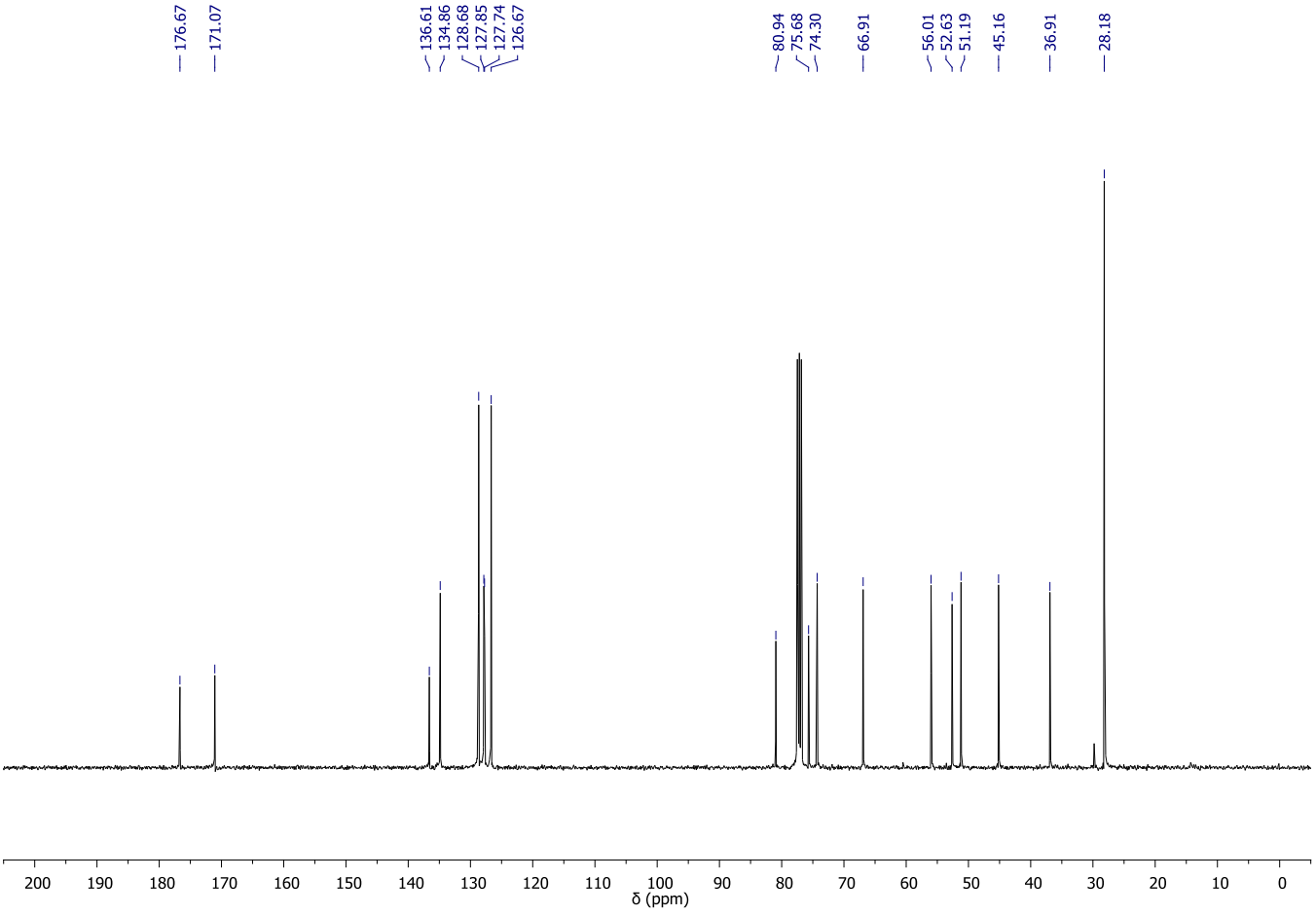
7.36
7.23
6.57
6.52
5.89
5.86
5.84
5.81
4.32
4.30
4.29
4.21
4.19
4.18
4.16
3.74
3.55
3.20
3.18
3.16
2.83
2.82
2.79
2.52
2.49
2.47
2.45
2.45
2.43
2.41
2.33
2.28
1.97
0.81
-0.04
5.26
1.16
1.00
1.13
1.17
3.43
4.66
1.01
0.26
1.02
2.45
1.12
1.18
9.19
5.79
δ (ppm)

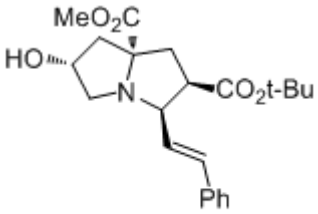

176.94
171.85
136.35
135.99
128.72
128.57
128.15
126.69
125.43
74.67
74.52
66.88
56.25
52.66
51.94
49.38
46.37
37.49
25.87
18.18
-4.82
-4.90
δ (ppm)


MeO2C
HO
N
CO2t-Bu
Ph

4c

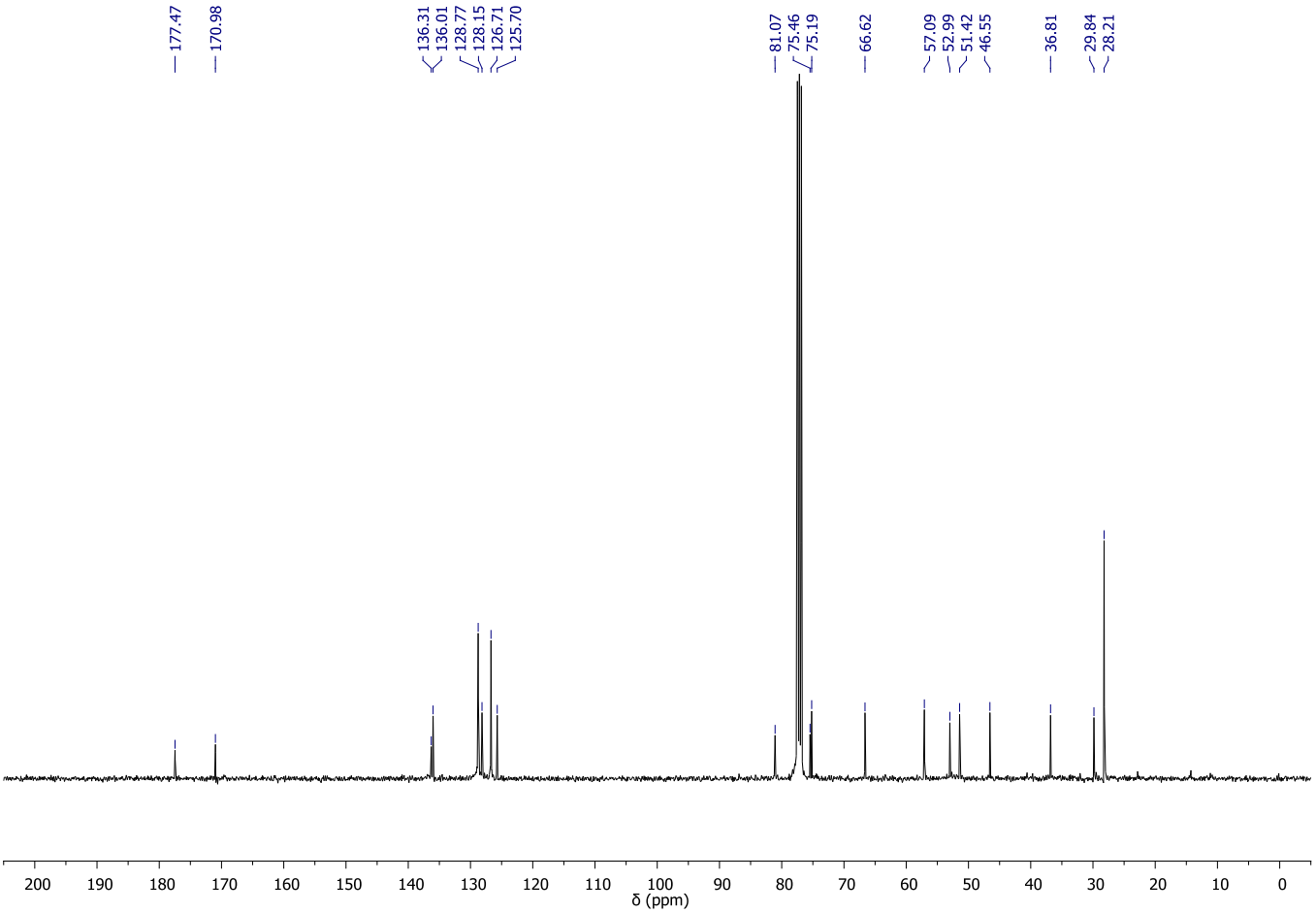
7.37
7.20
6.53
6.49
6.27
6.24
6.23
6.20
4.54
4.16
4.16
4.14
3.72
3.45
3.44
3.42
3.42
3.13
3.12
2.55
2.53
2.52
2.37
1.96
1.95
1.93
1.92
1.29
2.01
2.24
1.00
1.00
1.00
1.00
1.00
3.00
1.00
2.00
2.00
1.00
1.11
1.23
9.00
δ (ppm)

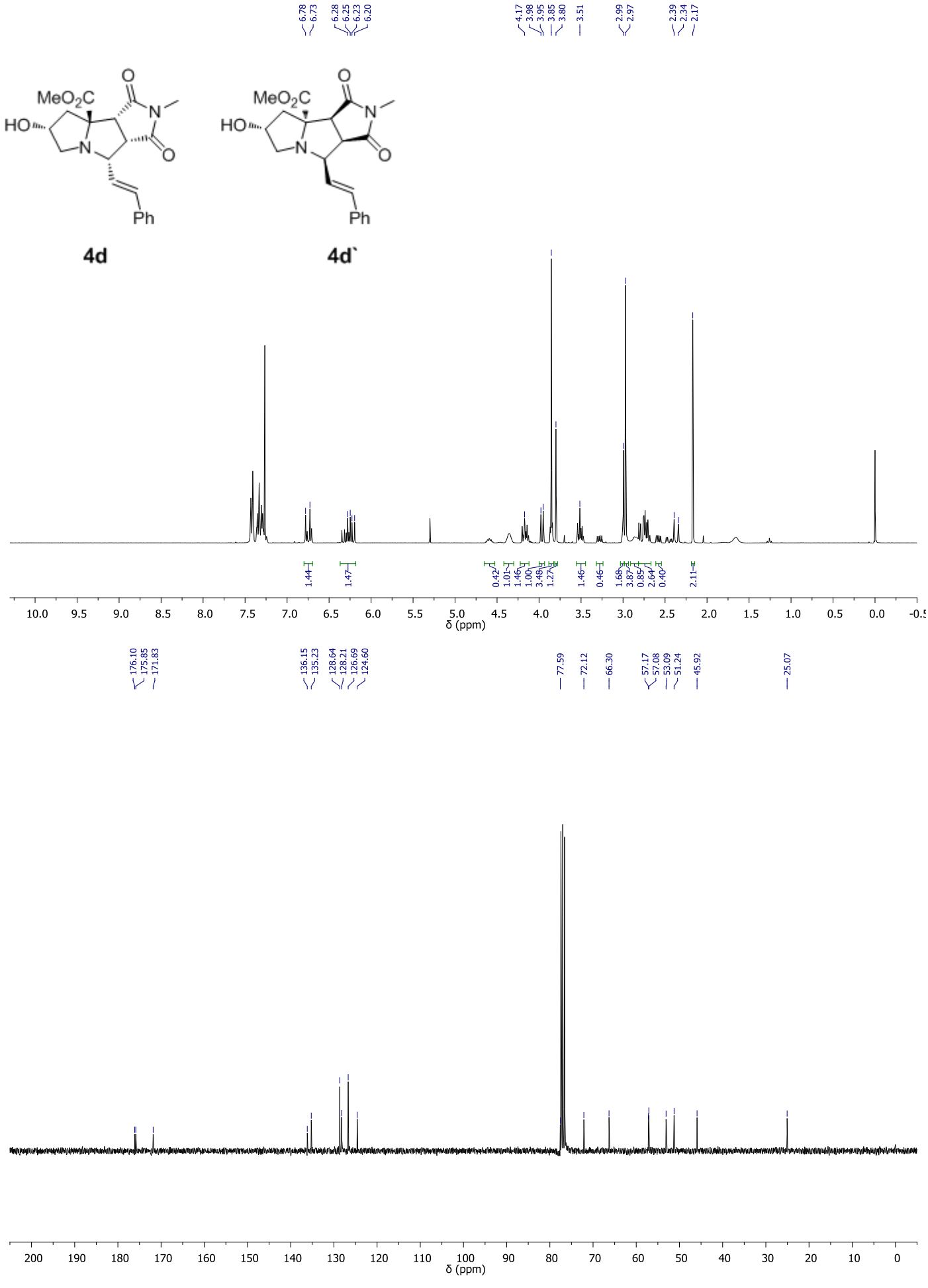

176.67
171.07
136.61
134.86
128.68
127.85
127.74
126.67
80.94
75.68
74.30
66.91
56.01
52.63
51.19
45.16
36.91
28.18
δ (ppm)


MeO2C
HO
N
CO2t-Bu
Ph

4c´

7.37
7.25
6.59
6.55
5.92
5.89
5.88
5.85
4.43
4.13
4.11
4.11
4.09
3.78
3.50
3.47
3.36
3.34
2.92
2.92
2.90
2.57
2.56
2.50
2.47
2.20
2.17
2.06
2.04
1.30
7.29
1.00
0.92
0.99
0.95
2.89
0.94
0.98
0.99
0.99
0.90
0.85
0.99
9.40
δ (ppm)


177.47
170.98
136.31
136.01
128.77
128.15
126.71
125.70
81.07
75.46
75.19
66.62
57.09
52.99
51.42
46.55
36.81
29.84
28.21
δ (ppm)


6.78
6.73
6.28
6.25
6.23
6.20
4.17
3.98
3.95
3.85
3.80
3.51
2.99
2.97
2.39
2.34
2.17
MeO2C
HO
N
O
Ph
4d
4d`
1.44
1.47
0.42
1.01
1.46
1.00
3.48
1.27
1.46
0.46
1.68
3.87
0.85
2.64
0.40
2.11
δ (ppm)
176.10
175.85
171.83
136.15
135.23
128.64
128.21
126.69
124.60
77.59
72.12
66.30
57.17
57.08
53.09
51.24
45.92
25.07
δ (ppm)

6. X-Ray diffraction analysis of 3a

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) x

No syntax errors found. CIF dictionary Interpreting this report

Datablock: x

```
Bond precision:  C-C = 0.0070 A          Wavelength=0.71073

Cell:            a=10.2542(17)     b=24.002(4)          c=14.842(2)
                 alpha=90          beta=104.390(5)      gamma=90
Temperature:     297 K
```

	Calculated	Reported
Volume	3538.3(10)	3538.3(10)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	?
Moiety formula	C19 H23 N O4	C19 H23 N O4
Sum formula	C19 H23 N O4	C19 H23 N O4
Mr	329.38	329.38
Dx,g cm-3	1.237	1.237
Z	8	8
Mu (mm-1)	0.086	0.086
F000	1408.0	1408.0
F000'	1408.70	
h,k,lmax	12,28,17	12,28,17
Nref	6320	6296
Tmin,Tmax	0.988,0.996	0.524,0.996
Tmin'	0.986	

```
Correction method= MULTI-SCAN

Data completeness= 0.996          Theta(max)= 25.130

R(reflections)= 0.0691( 2144)     wR2(reflections)= 0.1800( 6296)

S = 0.923                 Npar= 437
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level B

```
RINTA01_ALERT_3_B  The value of Rint is greater than 0.18
           Rint given   0.196
PLAT026_ALERT_3_B Ratio Observed / Unique Reflections too Low ....        34 Perc.
PLAT241_ALERT_2_B Check High      Ueq as Compared to Neighbors for        C6
```

Alert level C

```
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        C18
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        C37
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ..............     0.0070 Ang
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......     12.450
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......      3.036
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......      2.011
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L=  0.598         27
```

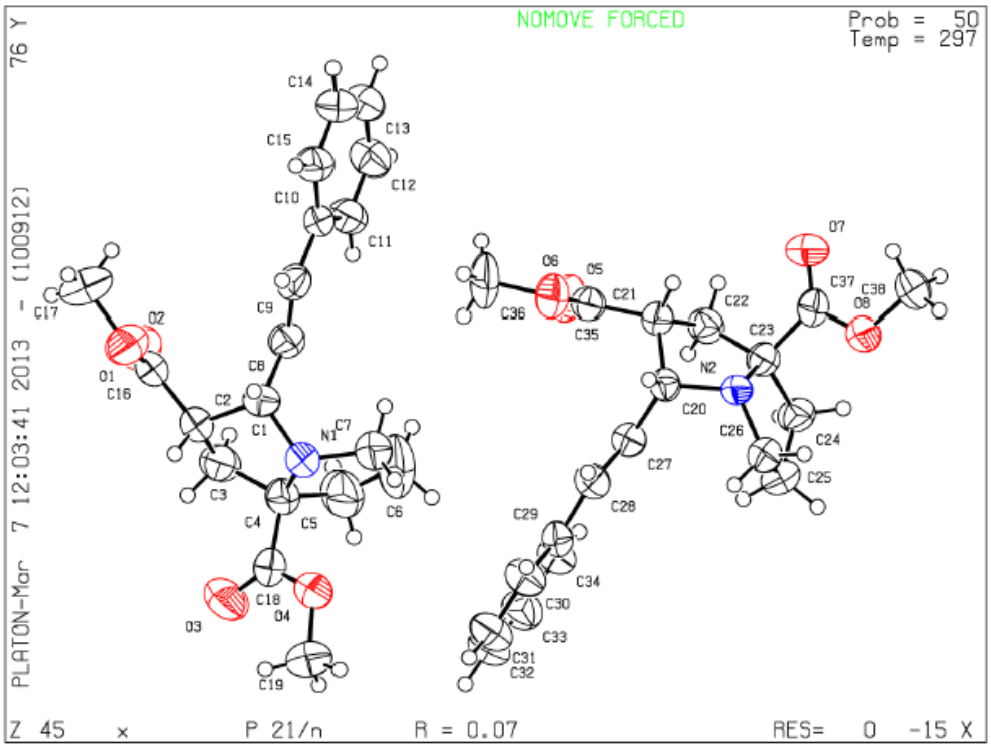
Alert level G

```
PLAT005_ALERT_5_G No _iucr_refine_instructions_details  in the CIF          ?
PLAT128_ALERT_4_G Alternate Setting of Space-group P21/c   .......      P21/n
PLAT793_ALERT_4_G The Model has Chirality at C1      (Verify) ....          S
PLAT793_ALERT_4_G The Model has Chirality at C2      (Verify) ....          S
PLAT793_ALERT_4_G The Model has Chirality at C4      (Verify) ....          R
PLAT793_ALERT_4_G The Model has Chirality at C20     (Verify) ....          R
PLAT793_ALERT_4_G The Model has Chirality at C21     (Verify) ....          R
PLAT793_ALERT_4_G The Model has Chirality at C23     (Verify) ....          S
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   3 ALERT level B = A potentially serious problem, consider carefully
   7 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   8 ALERT level G = General information/check it is not something unexpected

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   3 ALERT type 2 Indicator that the structure model may be wrong or deficient
   7 ALERT type 3 Indicator that the structure quality may be low
   7 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
```

Datablock x - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) x

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: x

Bond precision: C-C = 0.0060 A Wavelength=0.71073

Cell: a=11.1442(19) b=5.9143(10) c=13.609(2)
alpha=90 beta=94.567(4) gamma=90
Temperature: 298 K

	Calculated	Reported
Volume	894.1(3)	894.1(3)
Space group	P 21	P 21
Hall group	P 2yb	?
Moiety formula	C19 H23 N O5	C19 H23 N O5
Sum formula	C19 H23 N O5	C19 H23 N O5
Mr	345.38	345.38
Dx,g cm-3	1.283	1.283
Z	2	2
Mu (mm-1)	0.093	0.093
F000	368.0	368.0
F000'	368.19	
h,k,lmax	13,7,16	13,7,16
Nref	3159[1750]	3131
Tmin,Tmax	0.991,0.997	0.928,0.997
Tmin'	0.965	

Correction method= MULTI-SCAN

Data completeness= 1.79/0.99 Theta(max)= 25.060

R(reflections)= 0.0532(1784) wR2(reflections)= 0.1415(3131)

S = 1.002 Npar= 229

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

```
PLAT089_ALERT_3_C Poor Data / Parameter Ratio (Zmax  <   18) .....       7.64
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C4      --  C8       ..       6.3 su
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for         C8
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ...............    0.0060 Ang.
PLAT411_ALERT_2_C Short Inter H...H Contact  H3B    ..  H6       ..       2.06 Ang.
```

Alert level G

```
PLAT005_ALERT_5_G No _iucr_refine_instructions_details  in the CIF          ? Do !
PLAT007_ALERT_5_G Note: Number of Unrefined Donor-H Atoms ........          1
PLAT791_ALERT_4_G Note: The Model has Chirality at C2      (Verify)         R
PLAT791_ALERT_4_G Note: The Model has Chirality at C4      (Verify)         S
PLAT791_ALERT_4_G Note: The Model has Chirality at C6      (Verify)         S
PLAT791_ALERT_4_G Note: The Model has Chirality at C7      (Verify)         S
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   5 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   6 ALERT level G = General information/check it is not something unexpected

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   3 ALERT type 2 Indicator that the structure model may be wrong or deficient
   2 ALERT type 3 Indicator that the structure quality may be low
   4 ALERT type 4 Improvement, methodology, query or suggestion
   2 ALERT type 5 Informative message, check
```

PLATON version of 01/06/2013; check.def file version of 24/05/2013

Datablock x - ellipsoid plot