Synthesis of 1,2-diaminotruxinic δ-cyclobutanes by BF_3-controlled [2+2]-photocycloaddition of 5(4*H*)-oxazolones. Stereoselective expansion of δ-cyclobutanes to give highly substituted pyrrolidine-2,5-dicarboxylates

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Electronic Supplementary Information

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1.- Complete experimental section

General Methods. The [2+2]-photocycloaddition reactions were carried out under inert (Ar) atmosphere, using dry and deoxygenated methanol from a Pure Solv MD5 solvent purification system. The purification of the compounds was carried out by flash column liquid chromatographies using silica gel (70-230 μm) as support. ^{1}H, ^{13}C and ^{19}F NMR spectra of the isolated products **2** and **3** were recorded in $CDCl_3$ or CD_2Cl_2 solutions at 25 °C (other temperatures were specified) on Bruker AV300 and Bruker AV500 spectrometers (δ in ppm, *J* in Hz) at ^{1}H operating frequencies of 300.13 and 500.13 MHz, respectively. ^{1}H and ^{13}C NMR spectra were referenced using the solvent signal as internal standard, while ^{19}F NMR spectra were referenced to $CFCl_3$. The assignment of ^{1}H NMR peaks has been performed through standard 2D ^{1}H–COSY and selective 1D ^{1}H-SELNOE experiments. Typical mixing times in the case of selective 1D-SELNOE experiments were in the range 1.2-1.8 s, as a function of the irradiated signal. These values of optimized mixing times were set equal to the longitudinal relaxation time T_1, determined using the inversion–recovery sequence. The ^{13}C NMR peaks were identified using standard ^{1}H–^{13}C edited-HSQC and ^{1}H–^{13}C HMBC 2D-experiments. In both cases spectral widths of 10 ppm (^{1}H) and 200 ppm (^{13}C) were used, with averaged values of the coupling constants $^{1}J_{CH}$ = 145 Hz and long-range $^{n}J_{CH}$ = 10 Hz. ESI (ESI^+) mass spectra were recorded using an Esquire 3000 ion-trap mass spectrometer (Bruker Daltonic GmbH) equipped with a standard ESI/APCI source. HRMS and ESI (ESI^+) mass spectra were recorded using an MicroToF Q, API-Q-ToF ESI with a mass range from 20 to 3000 *m/z* and mass resolution 15000 (FWHM). The oxazolones **1** used as starting materials were synthesized according to published methods.[1] The compound $[Ru(bpy)_3](BF_4)_2$ was also prepared following published procedures,[2] and it was stored under protecting atmosphere (Ar) at 4 °C.

Irradiation setup. The irradation setup used in this case was a metallic cylindrical recipitent (16 cm internal diameter and 10.5 cm high) whose internal surface was covered with blue LEDs (222 diodes, 465 nm). This home-made system provided a electrical power of 18W and used a 12V power supply.

X-ray diffraction. Crystals of cyclobutanes **2n, 2o, 2s** and pyrrolidine **3r** of quality for X-ray measurements were grown by slow diffusion of *n*-pentane into CH_2Cl_2 (**2n**, **2o**, **2s**) or $CHCl_3$ (**3r**) solutions of the respective crude products at -18 °C for several weeks. One selected single crystal of each compound was mounted at the end of a quartz fiber in a random orientation, covered with perfluorinated oil and placed under a cold

stream of N_2 gas. The data collection were performed at 123 K (**2s**, **3r**) or 153 K (**2n, 2o**) on Oxford Diffraction Xcalibur Sapphire 3 (**2n**, **3r**), Bruker P4 (**2o**) o Bruker APEX Duo (**2s**) diffractometers, using graphite-monocromated Mo-Kα radiation (λ = 0.71073 Å). A hemisphere of data was collected based on ω-scan and ϕ-scan runs. The diffraction frames were integrated using the programs CrysAlis RED[3] or SAINT[4] and the integrated intensities were corrected for absorption with SADABS.[5] The structures were solved and developed by Fourier methods.[6] All non-hydrogen atoms were refined with anisotropic displacement parameters. The H atoms were placed at idealized positions and treated as riding atoms. Each H atom was assigned an isotropic displacement parameter equal to 1.2 times the equivalent isotropic displacement parameter of its parent atom. For structure solving and refinement the SHELX-97[7] Software Package was used. The structures were refined to F_o^2 and all reflections were used in the least-squares calculations.[8] CCDC-2177354 (**2o**), CCDC-2177355 (**2s**), and CCDC-2176207 (**3r**) contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif. The structure of cyclobutane **2n** could be solved, but the low quality of the data avoided a complete refinement, so the structure has to be considered only as a connectivity scheme. For the structure of **3r** it was found a disordered pentane molecule in (1/2, 1/2, 1/2), which was refined using geometrical restraints and constraints for the anisotropic thermal displacement parameters.

Computational details

All structures were optimized using density functional theory (DFT) as implemented in Gaussian 16,[9] with M06-2X[10] as functional, and 6-311+G(d,p) as basis set, introducing solvation factors with the IEF-PCM[11] method, and methanol as solvent, as in the optimized experimental conditions. The stationary points were characterized by frequency calculations in order to verify that they have the right number of imaginary frequencies.

Synthesis of the cyclobutane bis(amino acid)s δ-1,2-diaminotruxinic derivatives 2a-2u

All bis(amino acid)s containing the 1,2-diaminotruxinic core **2a-2u** have been prepared following the same experimental method, which is exemplified here for **2a**.

Synthesis of dimethyl-1,2-bis(benzamido)-3,4-diphenylcyclobutane-1,2-dicarboxylate **2a***.* The oxazolone **1a** (149.45 mg, 0.60 mmol) and $[Ru(bpy)_3](BF_4)_2$ (11.2 mg, 0.015 mmol) were suspended in deoxygenated and dry methanol (4 mL) under Ar atmosphere at room temperature. This suspension was treated with $BF_3{\cdot}Et_2O$ (34.1 mg, 0.24 mmol), and the resulting mixture was irradiated with blue light (465 nm, see irradiation setup) for 25 h at room temperature. After the reaction time the solvent was evaporated to dryness, and the solid residue was suspended in chloroform (10 mL). This suspension was washed with water (3 × 5 mL) and the organic phase was dried with anhydrous $MgSO_4$. The resulting solution, which contains cyclobutane **2a**, was purified by column chromatography using silica as support and a mixture ethyl acetate/n-hexane in gradient from 1/9 to 3/7 ratio. Cyclobutane **2a** was isolated as a white solid by solvent evaporation. Obtained 56.8 mg (34% yield). ^{1}H NMR ($CDCl_3$, 300.13 MHz) δ 8.30 (s, 1H, NH), 7.56 (m, 2H, H_o, CO-Ph), 7.46 (m, 3H, H_o, Ph + H_p, CO-Ph), 7.39-7.27 (m, 5H, H_m, Ph+ H_m, CO-Ph + H_p, Ph), 4.93 (s, 1H, CH), 3.73 (s, 3H, OCH_3). $^{13}C\{^1H\}$ NMR ($CDCl_3$, 75.5 MHz) δ 171.6, 166.7, 134.7, 133.3, 131.9, 129.1, 128.7, 128.6, 128.2, 127.0, 64.1, 53.1, 47.6. HRMS (ESI$^+$) m/z calcd for $C_{34}H_{30}N_2NaO_6$ $[M+Na]^+$: 585.2002, found: 585.1987.

Synthesis of dimethyl-1,2-bis(benzamido)-3,4-bis(4-methoxyphenyl)cyclobutane-1,2-dicarboxylate **2b.** Cyclobutane **2b** was prepared following the same procedure than that described for **2a**, with small modifications in the chromatographic purification. Oxazolone **1b** (167.45 mg, 0.60 mmol), $[Ru(bpy)_3](BF_4)_2$ (11.2 mg, 0.015 mmol) and $BF_3{\cdot}Et_2O$ (34.1 mg, 0.24 mmol) were irradiated in deoxygenated methanol (4 mL) to give **2b** as a white solid after chromatographic purification (ethyl acetate/n-hexane in 1/9 to 4/6 gradient ratio). Obtained: 64.4 mg (34 % yield). ^{1}H NMR ($CDCl_3$, 300.13 MHz) δ 8.29 (s, 1H, NH), 7.59 (m, 2H, H_o, Ph), 7.46 (tt, $^3J_{HH}$ = 7.4 Hz, $^4J_{HH}$ = 1.75 Hz, 1H, H_p, Ph), 7.41-7.33 (m, 4H, H_m, Ph + H_2, H_6, C_6H_4), 6.84 (m, 2H, H_3, H_5, C_6H_4), 4.80 (s, 1H, CH), 3.73 (s, 3H, CH_3O), 3.72 (s, 3H, $COOCH_3$). $^{13}C\{^1H\}$ NMR ($CDCl_3$, 75.5 MHz) δ 171.8, 166.7, 159.4, 133.4, 131.8, 130.2, 128.6, 127.0, 126.7, 114.1, 64.1, 55.3, 53.0, 47.3. HRMS (ESI$^+$) m/z calc for $C_{36}H_{34}N_2NaO_8$ $[M+Na]^+$: 645.2213, found: 645.2212.

Synthesis of dimethyl-1,2-bis(benzamido)-3,4-di-p-tolylcyclobutane-1,2-dicarboxylate **2c.**

Cyclobutane **2c** was prepared following the same procedure than that described for **2a**, with small modifications in the chromatographic purification. Oxazolone **1c** (157.85 mg, 0.60 mmol), $[Ru(bpy)_3](BF_4)_2$ (11.2 mg, 0.015 mmol) and $BF_3{\cdot}Et_2O$ (34.1 mg, 0.24 mmol) were irradiated in deoxygenated methanol (4

mL) to give **2c** as a white solid after chromatographic purification (ethyl acetate/n-hexane in 2/8 to 3/7 gradient ratio). Obtained: 80.0 mg (45 % yield). ^{1}H NMR ($CDCl_3$, 300.13 MHz) δ 8.33 (s, 1H, NH), 7.60 (m, 2H, H_o, C_6H_5), 7.47 (tt, $^{3}J_{HH}$ = 7.3 Hz, $^{4}J_{HH}$ = 1.5 Hz, 1H, H_p, C_6H_5), 7.38 (m, 2H, H_m, C_6H_5), 7.36 (m, 2H, H_2, H_6, C_6H_4), 7.12 (m, 2H, H_3, H_5, C_6H_4), 4.86 (s, 1H, CH), 3.72 (s, 3H, $COOCH_3$), 2.28 (s, 3H, CH_3). $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 75.5 MHz) δ 171.7, 166.7, 137.8, 133.4, 131.7, 131.6, 129.4, 128.9, 128.5, 127.0, 64.1, 52.9, 47.4, 21.1. HRMS (ESI^+) m/z calc for $C_{36}H_{34}N_2NaO_6$ $[M+Na]^+$ 613.2315, found: 613.2326.

Synthesis of dimethyl-1,2-bis(benzamido)-3,4-bis(4-chlorophenyl)cyclobutane-1,2-dicarboxylate **2d.** Cyclobutane **2d** was prepared following the same procedure than that described for **2a**. Oxazolone **1d** (170.45 mg, 0.60 mmol), $[Ru(bpy)_3](BF_4)_2$ (11.2 mg, 0.015 mmol) and $BF_3{\cdot}Et_2O$ (34.1 mg, 0.24 mmol) were irradiated in deoxygenated methanol (4 mL) to give **2d** as a white solid after chromatographic purification (ethyl acetate/n-hexane in 1/9 to 3/7 gradient ratio). Obtained: 53.4 mg (28 % yield). ^{1}H NMR ($CDCl_3$, 300.13 MHz) δ 8.17 (s, 1H, NH), 7.58 (m, 2H, H_o, C_6H_5), 7.50 (tt, $^{3}J_{HH}$ = 7.3 Hz, $^{4}J_{HH}$ = 1.4 Hz, 1H, H_p, C_6H_5), 7.41 (m, 2H, H_m, C_6H_5), 7.35-7.38 (m, 2H, $H_{2\text{-}6}$, C_6H_4Cl), 7.28 (m, 2H, $H_{3\text{-}5}$, C_6H_4Cl), 4.84 (s, 1H, CH), 3.74 (s, 3H, $COOCH_3$). $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 75.5 MHz) δ 171.3, 166.9, 134.3, 133.0, 132.9, 132.1, 130.3, 129.0, 128.8, 126.9, 64.3, 53.2, 46.9. HRMS (ESI^+) m/z calc for $C_{34}H_{28}Cl_2N_2NaO_6$ $[M+Na]^+$ 653.1222, found: 653.1198.

Synthesis of dimethyl-1,2-bis(benzamido)-3,4-bis(4-fluorophenyl)cyclobutane-1,2-dicarboxylate **2e.** Cyclobutane **2e** was prepared following the same procedure than that described for **2a**. Oxazolone **1e** (160.85 mg, 0.60 mmol), $[Ru(bpy)_3](BF_4)_2$ (11.2 mg, 0.015 mmol) and $BF_3{\cdot}Et_2O$ (34.1 mg, 0.24 mmol) were irradiated in deoxygenated methanol (4 mL) to give **2e** as a white solid after chromatographic purification (ethyl acetate/n-hexane in 1/9 to 3/7 gradient ratio). Obtained: 41 mg (23 % yield). ^{1}H NMR ($CDCl_3$, 300.13 MHz) δ 8.16 (s, 1H, NH), 7.57 (m, 2H, H_o, C_6H_5), 7.49 (tt, $^{3}J_{HH}$ = 7.3 Hz, $^{4}J_{HH}$ = 1.5 Hz, 1H, H_p, C_6H_5), 7.45-7.35 (m, 4H, H_m, C_6H_5 + $H_{2\text{-}6}$, C_6H_4F), 7.00 (t, $^{3}J_{HH}$ = $^{3}J_{FH}$ = 8.7 Hz, 2H, $H_{3\text{-}5}$, C_6H_4F), 4.84 (s, 1H, CH), 3.74 (s, 3H, $COOCH_3$). $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 75.5 MHz) δ 171.5, 166.8, 162.7, 133.1, 132.1, 130.7, 130.3, 128.8, 127.0, 115.8, 64.2, 53.2, 47.1. $^{19}F\{^{1}H\}$ NMR ($CDCl_3$, 282.40 MHz) δ -113.54 (s). HRMS (ESI^+) m/z calc for $C_{34}H_{28}F_2N_2NaO_6$ $[M+Na]^+$ 621.1813, found: 621.1780.

Synthesis of dimethyl-1,2-bis(benzamido)-3,4-bis(4-bromophenyl)cyclobutane-1,2-dicarboxylate **2f.** Cyclobutane **2f** was prepared following the same procedure than that described for **2a**, with slight

deviations in the chromatographic purification. Oxazolone **1f** (160.85 mg, 0.60 mmol), $[Ru(bpy)_3](BF_4)_2$ (11.2 mg, 0.015 mmol) and $BF_3{\cdot}Et_2O$ (34.1 mg, 0.24 mmol) were irradiated for 48 h in deoxygenated methanol (4 mL) to give **2f** as a white solid after chromatographic purification (ethyl acetate/n-hexane in 3/7 to 7/3 gradient ratio). Obtained: 35.7 mg (16 % yield). ^{1}H NMR ($CDCl_3$, 300.13 MHz): δ = 8.13 (s, 1H, NH), 7.57 (m, 2H, H_o, C_6H_5), 7.52-7.49 (m, 1H, H_p, C_6H_5), 7.45-7.39 (m, 4H, H_m, C_6H_5 + $H_{3\text{-}5}$, C_6H_4Br), 7.29 (m, 2H, $H_{2\text{-}6}$, C_6H_4Br), 4.80 (s, 1H, CH), 3.73 (s, 3H, $COOCH_3$). $^{13}C\{^1H\}$ NMR ($CDCl_3$, 75.5 MHz): δ 171.3, 167.0, 133.5, 133.1, 132.2, 132.0, 130.7, 128.8, 127.0, 122.6, 64.3, 53.3, 47.0. HRMS (ESI^+) m/z calc for $C_{34}H_{28}Br_2N_2NaO_6$ $[M+Na]^+$ 741.0314, found: 741.0170.

Synthesis of dimethyl-1,2-bis(benzamido)-3,4-bis(4-cyanophenyl)cyclobutane-1,2-dicarboxylate **2g.** Cyclobutane **2g** was prepared following the same procedure than that described for **2a**, with minor changes in the chromatographic purification. Oxazolone **1g** (164.4 mg, 0.60 mmol), $[Ru(bpy)_3](BF_4)_2$ (11.2 mg, 0.015 mmol) and $BF_3{\cdot}Et_2O$ (34.1 mg, 0.24 mmol) were irradiated for 25 h in deoxygenated methanol (4 mL) to give **2g** as a white solid after chromatographic purification (ethyl acetate/n-hexane in 3/7 to 7/3 gradient ratio). Obtained: 66.5 mg (36 % yield). ^{1}H NMR ($CDCl_3$, 300.13 MHz) δ 7.94 (s, 1H, NH), 7.61-7.48 (m, 7H, H_o, H_p, C_6H_5 + $H_{2\text{-}6}$, $H_{3\text{-}5}$, C_6H_4), 7.40 (m, 2H, H_m, C_6H_5), 4.97 (s, 1H, CH), 3.77 (s, 3H, $COOCH_3$). $^{13}C\{^1H\}$ NMR ($CDCl_3$, 75.5 MHz) δ 170.7, 166.9, 139.6 ($2C_i$), 132.5, 132.4, 129.7, 128.9, 126.9, 118.5, 112.3, 64.7, 53.6, 46.8. HRMS (ESI^+) m/z calc for $C_{36}H_{28}N_4NaO_6$ $[M+Na]^+$ 635.1907, found: 635.1871.

Synthesis of dimethyl-1,2-bis(benzamido)-3,4-bis(4-trifluoromethylphenyl)cyclobutane-1,2-dicarboxylate **2h.** Cyclobutane **2h** was prepared following the same procedure than that described for **2a**, with minor changes in the chromatographic purification. Oxazolone **1h** (190.24 mg, 0.60 mmol), $[Ru(bpy)_3](BF_4)_2$ (11.2 mg, 0.015 mmol) and $BF_3{\cdot}Et_2O$ (34.1 mg, 0.24 mmol) were irradiated for 25 h in deoxygenated methanol (4 mL) to give **2h** as a white solid after chromatographic purification (ethyl acetate/n-hexane in 1/9 to 4/6 gradient ratio). Obtained: 57.7 mg (28 % yield). ^{1}H NMR ($CDCl_3$, 300.13 MHz) δ 8.09 (s, 1H, NH), 7.57 (s, 4H, $H_{2\text{-}6}$ + $H_{3\text{-}5}$, C_6H_4-CF_3), 7.56-7.47 (m, 3H, H_o + H_p, C_6H_5), 7.39 (m, 2H, H_m, C_6H_5), 4.99 (s, 1H, CH), 3.77 (s, 3H, $COOCH_3$). $^{13}C\{^1H\}$ NMR ($CDCl_3$, 75.5 MHz) δ 171.1, 167.0, 138.4, 132.8, 132.3, 130.6, 129.4, 128.8, 126.9, 125.7, 120.4, 64.6, 53.4, 47.0. $^{19}F\{^1H\}$ NMR ($CDCl_3$, 282.40 MHz) δ -62.71 (s). HRMS (ESI^+) m/z calc for $C_{36}H_{28}F_6N_2NaO_6$ $[M+Na]^+$ 721.1749, found: 721.1745.

Synthesis of dimethyl-1,2-bis(benzamido)-3,4-bis(m-tolyl)cyclobutane-1,2-dicarboxylate **2i.** Cyclobutane **2i** was prepared following the same procedure than that described for **2a**, with minor changes in the chromatographic purification. Oxazolone **1i** (157.85 mg, 0.60 mmol), $[Ru(bpy)_3](BF_4)_2$ (11.2 mg, 0.015 mmol) and $BF_3{\cdot}Et_2O$ (34.1 mg, 0.24 mmol) were irradiated for 25 h in deoxygenated methanol (4 mL) to give **2i** as a white solid after chromatographic purification (ethyl acetate/n-hexane in 3/7 to 6/4 gradient ratio). Obtained: 88.31 mg (50 % yield). ^{1}H NMR ($CDCl_3$, 300.13 MHz) δ 8.33 (s, 1H, NH), 7.57 (m, 2H, H_o, C_6H_5), 7.47 (tt, $^3J_{HH}$ = 7.3 Hz, $^4J_{HH}$ = 1.4 Hz, 1H, H_p, C_6H_5), 7.37 (m, 2H, H_m, C_6H_5), 7.30-7.26 (m, 1H, H_6, C_6H_4), 7.24-7.17 (m, 2H, H_2, H_5, C_6H_4), 7.08-7.04 (m, 1H, H_4, C_6H_4), 4.85 (s, 1H, CH), 3.72 (s, 3H, $COOCH_3$), 2.26 (s, 3H, CH_3). $^{13}C\{^1H\}$ NMR ($CDCl_3$, 75.5 MHz) δ 171.7, 166.7, 138.4, 134.7, 133.4, 131.9, 129.9, 129.0, 128.7, 128.6, 127.0, 126.3, 64.1, 53.1, 47.7, 21.5. HRMS (ESI^+) m/z calc for $C_{36}H_{34}N_2NaO_6$ $[M+Na]^+$ 613.2315, found: 613.2281.

Synthesis of dimethyl-1,2-bis(benzamido)-3,4-bis(3-chlorophenyl)cyclobutane-1,2-dicarboxylate **2j.** Cyclobutane **2j** was prepared following the same procedure than that described for **2a**, with minor changes in the chromatographic purification. Oxazolone **1j** (170.45 mg, 0.60 mmol), $[Ru(bpy)_3](BF_4)_2$ (11.2 mg, 0.015 mmol) and $BF_3{\cdot}Et_2O$ (34.1 mg, 0.24 mmol) were irradiated for 25 h in deoxygenated methanol (4 mL) to give **2j** as a white solid after chromatographic purification (ethyl acetate/n-hexane in 2/8 to 5/5 gradient ratio). Obtained: 67 mg (35 % yield). ^{1}H NMR ($CDCl_3$, 300.13 MHz) δ 8.15 (s, 1H, NH), 7.56 (m, 2H, H_o, C_6H_5), 7.45 (tt, $^3J_{HH}$ = 7.4 Hz, $^4J_{HH}$ = 1.5 Hz, 1H, H_p, C_6H_5), 7.40-7.32 (m, 4H, H_m, C_6H_5 + H_2, H_6, C_6H_4Cl), 7.22 (m, 2H, H_4, H_5, C_6H_4Cl), 4.81 (s, 1H, CH), 3.72 (s, 3H, $COOCH_3$). $^{13}C\{^1H\}$ NMR ($CDCl_3$, 75.5 MHz) δ 171.2, 166.9, 136.5, 134.7, 133.0, 132.1, 130.0, 129.0, 128.7, 128.6, 127.3, 126.9, 64.2, 53.3, 47.0. HRMS (ESI^+) m/z calc for $C_{34}H_{28}Cl_2N_2NaO_6$ $[M+Na]^+$ 653.1222, found: 653.1195.

Synthesis of dimethyl-1,2-bis(benzamido)-3,4-bis(3-fluorophenyl)cyclobutane-1,2-dicarboxylate **2k.** Cyclobutane **2k** was prepared following the same procedure than that described for **2a**, with minor changes in the chromatographic purification. Oxazolone **1k** (180.14 mg, 0.60 mmol), $[Ru(bpy)_3](BF_4)_2$ (11.2 mg, 0.015 mmol) and $BF_3{\cdot}Et_2O$ (34.1 mg, 0.24 mmol) were irradiated for 25 h in deoxygenated methanol (4 mL) to give **2k** as a white solid after chromatographic purification (ethyl acetate/n-hexane in 3/7 to 7/3 gradient ratio). Obtained: 63.6 mg (35 % yield). ^{1}H NMR ($CDCl_3$, 300.13 MHz) δ 8.20 (s, 1H, NH), 7.58 (m, 2H, H_o, C_6H_5), 7.49

(m, 1H, H_p, C_6H_5), 7.39 (m, 2H, H_m, C_6H_5), 7.32-7.23 (m, 2H, H_6, H_5, C_6H_4F), 7.14 (m, 1H, H_2, C_6H_4F), 6.97 (m, 1H, H_4, C_6H_4F), 4.85 (s, 1H, CH), 3.74 (s, 3H, $COOCH_3$). $^{13}C\{^1H\}$ NMR ($CDCl_3$, 75.5 MHz) δ 171.3, 166.9, 162.9, 137.1, 133.1, 132.1, 130.4, 128.8, 127.0, 124.8, 116.1, 115.4, 64.3, 53.3, 47.2. $^{19}F\{^1H\}$ NMR ($CDCl_3$, 282.40 MHz) δ -112.12 (s). HRMS (ESI^+) m/z calc for $C_{34}H_{28}F_2N_2NaO_6$ $[M+Na]^+$ 621.1813, found 621.1873.

Synthesis of dimethyl-1,2-bis(benzamido)-3,4-bis(3-bromophenyl)cyclobutane-1,2-dicarboxylate **2l.** Cyclobutane **2l** was prepared following the same procedure than that described for **2a**, with minor changes in the chromatographic purification. Oxazolone **1l** (197.40 mg, 0.60 mmol), $[Ru(bpy)_3](BF_4)_2$ (11.2 mg, 0.015 mmol) and $BF_3{\cdot}Et_2O$ (34.1 mg, 0.24 mmol) were irradiated for 25 h in deoxygenated methanol (4 mL) to give **2l** as a white solid after chromatographic purification (ethyl acetate/n-hexane in 3/7 to 5/5 gradient ratio). Obtained: 93.5 mg (43 % yield). ^1H NMR ($CDCl_3$, 300.13 MHz) δ 8.16 (s, 1H, NH), 7.61-7.55 (m, 3H, H_o, C_6H_5 + H_2, C_6H_4Br), 7.49 (tt, $^3J_{HH}$ = 7.3 Hz, $^4J_{HH}$ = 1.3 Hz, 1H, H_p, C_6H_5), 7.43-7.37 (m, 4H, H_m, C_6H_5 + H_4, H_6, C_6H_4Br), 7.20 (m, 1H, H_5, C_6H_4Br), 4.82 (s, 1H, CH), 3.75 (s, 3H, $COOCH_3$). $^{13}C\{^1H\}$ NMR ($CDCl_3$, 75.5 MHz) δ 171.1, 166.9, 136.7, 133.0, 132.1, 131.9, 131.5, 130.3, 128.8, 127.9, 127.0, 122.9, 64.2, 53.3, 47.0. HRMS (ESI^+) m/z calc for $C_{34}H_{28}Br_2N_2NaO_6$ $[M+Na]^+$ 741.0212, found 741.0228.

Synthesis of dimethyl-1,2-bis(benzamido)-3,4-bis(3-trifluoromethylphenyl)cyclobutane-1,2-dicarboxylate **2m.** Cyclobutane **2m** was prepared following the same procedure than that described for **2a**, with minor changes in the chromatographic purification. Oxazolone **1m** (190.24 mg, 0.60 mmol), $[Ru(bpy)_3](BF_4)_2$ (11.2 mg, 0.015 mmol) and $BF_3{\cdot}Et_2O$ (34.1 mg, 0.24 mmol) were irradiated for 25 h in deoxygenated methanol (4 mL) to give **2m** as a white solid after chromatographic purification (ethyl acetate/n-hexane in 3/7 to 5/5 gradient ratio). Obtained: 80.5 mg (38 % yield). ^1H NMR ($CDCl_3$, 300.13 MHz) δ 8.08 (s, 1H, NH), 7.71-7.66 (m, 2H, H_6 + H_2, C_6H_4-CF_3), 7.57-7.45 (m, 5H, H_o + H_p, C_6H_5 + H_4 + H_5, C_6H_4-CF_3), 7.38 (m, 2H, H_m, C_6H_5), 4.98 (s, 1H, CH), 3.77 (s, 3H, $COOCH_3$). $^{13}C\{^1H\}$ NMR ($CDCl_3$, 75.5 MHz) δ 171.1, 166.9, 135.5, 132.9, 132.8, 132.3, 131.1, 129.4, 128.8, 126.9, 125.4, 125.3, 123.9, 64.4, 53.4, 47.0. $^{19}F\{^1H\}$ NMR ($CDCl_3$, 282.40 MHz) δ -62.72. HRMS (ESI^+) m/z calc for $C_{36}H_{28}F_6N_2NaO_6$ $[M+Na]^+$ 721.1749, found 721.1712.

Synthesis of dimethyl-1,2-bis(benzamido)-3,4-bis(2-methoxyphenyl)cyclobutane-1,2-dicarboxylate **2n.** Cyclobutane **2n** was prepared following the same procedure than that described for **2a**, with minor changes in the chromatographic purification and using an optimized reaction time. Oxazolone **1n** (167.45 mg, 0.60

mmol), $[Ru(bpy)_3](BF_4)_2$ (11.2 mg, 0.015 mmol) and $BF_3{\cdot}Et_2O$ (34.1 mg, 0.24 mmol) were irradiated for 60 h in deoxygenated methanol (4 mL) to give **2n** as a white solid after chromatographic purification (ethyl acetate/n-hexane in 3/7 to 5/5 gradient ratio). Obtained: 78.4 mg (42 % yield). ^{1}H NMR ($CDCl_3$, 300.13 MHz) δ 8.39 (s, 1H, NH), 7.61(m, 3H, H_o, C_6H_5), 7.48-7.35 (m, 4H, H_m + H_p, C_6H_5 + H_6, C_6H_4), 7.23 (m, 1H, H_4, C_6H_4), 6.87 (m, 2H, H_3 + H_5, C_6H_4), 5.38 (s, 1H, CH), 3.87 (s, 3H, CH_3O), 3.67 (s, 3H, $COOCH_3$). $^{13}C\{^1H\}$ NMR ($CDCl_3$, 75.5 MHz) δ 171.2, 166.8, 158.8, 134.1, 131.6, 129.4, 128.8, 128.6, 127.1, 123.5, 120.7, 111.2, 64.6, 56.1, 52.8, 40.8. HRMS (ESI$^+$) m/z calc for $C_{36}H_{34}N_2NaO_8$ $[M+Na]^+$ 645.2213, found 645.2253.

Synthesis of dimethyl-1,2-bis(benzamido)-3,4-bis(2-fluorophenyl)cyclobutane-1,2-dicarboxylate **2o.** Cyclobutane **2o** was prepared following the same procedure than that described for **2a**, with minor changes in the chromatographic purification and using an optimized reaction time. Oxazolone **1o** (160.85 mg, 0.60 mmol), $[Ru(bpy)_3](BF_4)_2$ (11.2 mg, 0.015 mmol) and $BF_3{\cdot}Et_2O$ (34.1 mg, 0.24 mmol) were irradiated for 48 h in deoxygenated methanol (4 mL) to give **2o** as a white solid after chromatographic purification (ethyl acetate/n-hexane in 3/7 to 4/6 gradient ratio). Obtained: 55.8 mg (31 % yield). ^{1}H NMR ($CDCl_3$, 300.13 MHz): δ 8.29 (s, 1H, NH), 7.61 (m, 2H, H_o, C_6H_5), 7.55-7.46 (m, 2H, H_p, C_6H_5 + H_5, C_6H_4F), 7.39 (m, 2H, H_m, C_6H_5), 7.30-7.22 (m, 1H, H_4, C_6H_4F), 7.11-7.02 (m, 2H, H_3 + H_6, C_6H_4F), 5.29 (s, 1H, CH), 3.71 (s, 3H, $COOCH_3$). $^{13}C\{^1H\}$ NMR ($CDCl_3$, 75.5 MHz) δ 170.9, 167.0, 162.0, 133.4, 132.0, 130.2, 129.1, 128.7, 127.1, 124.3, 121.7, 115.9, 64.4, 53.1, 40.0. $^{19}F\{^1H\}$ NMR ($CDCl_3$, 282.40 MHz) δ -114.71. HRMS (ESI$^+$) m/z calc for $C_{34}H_{28}F_2N_2NaO_6$ $[M+Na]^+$ 621.1813, found 621.1783.

Synthesis of dimethyl-1,2-bis(benzamido)-3,4-bis(3,4-dimethoxyphenyl)cyclobutane-1,2-dicarboxylate **2p.** Cyclobutane **2p** was prepared following the same procedure than that described for **2a**, with minor changes in the chromatographic purification. Oxazolone **1p** (185.46 mg, 0.60 mmol), $[Ru(bpy)_3](BF_4)_2$ (11.2 mg, 0.015 mmol) and $BF_3{\cdot}Et_2O$ (34.1 mg, 0.24 mmol) were irradiated for 25 h in deoxygenated methanol (4 mL) to give **2p** as a white solid after chromatographic purification (ethyl acetate/n-hexane in 2/8 to 5/5 gradient ratio). Obtained: 94.2 mg (46 % yield). ^{1}H NMR ($CDCl_3$, 300.13 MHz): δ 8.31 (s, 1H, NH), 7.58 (m, 2H, H_o, C_6H_5), 7.45 (tt, $^3J_{HH}$ = 7.5 Hz, $^4J_{HH}$ = 1.4 Hz, 1H, H_p, C_6H_5), 7.38-7.32 (m, 2H, H_m, C_6H_5), 7.01 (dd, $^3J_{HH}$ = 8.2 Hz, $^4J_{HH}$ = 2.1 Hz, 1H, H_6, C_6H_3), 6.94 (d, $^4J_{HH}$ = 2.1 Hz, 1H, H_2, C_6H_3), 6.80 (d, $^3J_{HH}$ = 8.2 Hz, 1H, H_5, C_6H_3), 4.74 (s, 1H, CH), 3.79 (s, 3H, CH_3O), 3.75 (s, 3H, CH_3O), 3.70 (s, 3H, $COOCH_3$). $^{13}C\{^1H\}$ NMR ($CDCl_3$, 75.5 MHz) δ 171.7, 166.6, 149.0,

148.9, 133.2, 131.9, 128.6, 127.2, 126.9, 121.3, 112.1, 111.1, 64.1, 55.8, 55.8, 52.9, 47.8. HRMS (ESI^+) m/z calc for $C_{38}H_{38}N_2NaO_{10}$ $[M+Na]^+$ 705.2424, found 705.2393.

Synthesis of dimethyl-1,2-bis(benzamido)-3,4-bis(3,4-dimethylphenyl)cyclobutane-1,2-dicarboxylate **2q.** Cyclobutane **2q** was prepared following the same procedure than that described for **2a**, with minor changes in the chromatographic purification. Oxazolone **1q** (166.25 mg, 0.60 mmol), $[Ru(bpy)_3](BF_4)_2$ (11.2 mg, 0.015 mmol) and $BF_3{\cdot}Et_2O$ (34.1 mg, 0.24 mmol) were irradiated for 25 h in deoxygenated methanol (4 mL) to give **2q** as a white solid after chromatographic purification (ethyl acetate/n-hexane in 3/7 to 6/4 gradient ratio). Obtained: 56.8 mg (31 % yield). ^1H NMR ($CDCl_3$, 300.13 MHz): δ 8.36 (s, 1H, NH), 7.60 (m, 2H, H_o, C_6H_5), 7.47 (tt, $^3J_{HH}$ = 7.4 Hz, $^4J_{HH}$ = 1.5 Hz, 1H, H_p, C_6H_5), 7.39-7.34 (m, 2H, H_m, C_6H_5), 7.23-7.17 (m, H_2 + H_6, C_6H_3), 7.06 (d, $^3J_{HH}$ = 7.3 Hz, 1H, H_5, C_6H_3), 4.80 (s, 1H, CH), 3.71 (s, 3H, $COOCH_3$), 2.17 (s, 6H, 2 CH_3). $^{13}C\{^1H\}$ NMR ($CDCl_3$, 75.5 MHz): δ 171.8, 166.7, 136.8, 136.5, 133.6, 132.1, 131.7, 130.4, 130.0, 128.6, 127.0, 126.5, 64.1, 52.9, 47.7, 19.9, 19.5. HRMS (ESI^+) m/z calc for $C_{38}H_{38}N_2NaO_6$ $[M+Na]^+$ 641.2630, found 641.2627.

Synthesis of dimethyl-1,2-bis(benzamido)-3,4-bis(3,4-dichlorophenyl)cyclobutane-1,2-dicarboxylate **2r.** Cyclobutane **2r** was prepared following the same procedure than that described for **2a**, with minor changes in the chromatographic purification. Oxazolone **1r** (380.5 mg, 1.20 mmol), $[Ru(bpy)_3](BF_4)_2$ (22.4 mg, 0.030 mmol) and $BF_3{\cdot}Et_2O$ (68.2 mg, 0.48 mmol) were irradiated for 25 h in deoxygenated methanol (8 mL) to give **2r** as a white solid after chromatographic purification (ethyl acetate/n-hexane in 3/7 to 6/4 gradient ratio). Obtained: 205.2 mg (49 % yield). ^1H NMR ($CDCl_3$, 300.13 MHz) δ 8.06 (s, 1H, NH), 7.58 (m, 2H, H_o, C_6H_5), 7.51 (tt, $^3J_{HH}$ = 7.4 Hz, $^4J_{HH}$ = 1.5 Hz, 1H, H_p, C_6H_5), 7.48 (d, $^4J_{HH}$ = 2.1 Hz, 1H, H_2, $C_6H_3Cl_2$), 7.41 (m, 2H, H_m, C_6H_5), 7.38 (d, $^3J_{HH}$ = 8.2 Hz, 1H, H_5, $C_6H_3Cl_2$), 7.29 (dd, $^3J_{HH}$ = 8.2 Hz, $^4J_{HH}$ = 2.1 Hz, 1H, H_6, $C_6H_3Cl_2$), 4.77 (s, 1H, CH), 3.75 (s, 3H, $COOCH_3$). $^{13}C\{^1H\}$ NMR ($CDCl_3$, 75.5 MHz) δ 170.9, 167.0, 134.5, 133.0, 132.7, 132.7, 132.3, 130.7, 128.8, 128.3, 126.9, 64.4, 53.4, 46.5. HRMS (ESI^+) m/z calc for $C_{34}H_{26}Cl_4N_2NaO_6$ $[M+Na]^+$ 721.0437, found 721.0427.

Synthesis of dimethyl-1,2-bis(benzamido)-3,4-bis(3,5-difluorophenyl)cyclobutane-1,2-dicarboxylate **2s.** Cyclobutane **2s** was prepared following the same procedure than that described for **2a**, with minor changes in the chromatographic purification. Oxazolone **1s** (171.04 mg, 0.60 mmol), $[Ru(bpy)_3](BF_4)_2$ (11.2 mg, 0.015 mmol) and $BF_3{\cdot}Et_2O$ (34.1 mg, 0.24 mmol) were irradiated for 25 h in deoxygenated methanol (4 mL) to give

2r as a white solid after chromatographic purification (ethyl acetate/n-hexane in 2/8 to 7/3 gradient ratio). Obtained: 73.6 mg (38 % yield). ^{1}H NMR ($CDCl_3$, 300.13 MHz) δ 8.08 (s, 1H, NH), 7.60 (m, 2H, H_o, C_6H_5), 7.52 (tt, $^{3}J_{HH}$ = 7.3 Hz, $^{4}J_{HH}$ = 1.3 Hz, 1H, H_p, C_6H_5), 7.42 (m, 2H, H_m, C_6H_5), 6.96 (m, 2H, $H_{2\text{-}6}$, $C_6H_3F_2$), 6.73 (tt, $^{3}J_{HH}$ = 8.8 Hz, $^{4}J_{HH}$ = 2.3 Hz, 1H, H_4, $C_6H_3F_2$), 4.77 (s, 1H, CH), 3.76 (s, 3H, $COOCH_3$). $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 75.5 MHz) δ 170.9, 167.1, 163.2, 138.2, 132.8, 132.4, 128.9, 127.0, 112.0, 104.1, 64.4, 53.5, 47.0. $^{19}F\{^{1}H\}$ NMR ($CDCl_3$, 282.40 MHz): δ -108.42. HRMS (ESI^+) m/z calc for $C_{34}H_{26}F_4N_2NaO_6$ $[M+Na]^+$ 657.1625, found 657.1628.

Synthesis of dimethyl-1,2-bis(benzamido)-3,4-bis(3,4,5-trimethoxyphenyl)cyclobutane-1,2-dicarboxylate **2t.** Cyclobutane **2t** was prepared following the same procedure than that described for **2a**, with minor changes in the chromatographic purification. Oxazolone **1t** (203.47 mg, 0.60 mmol), $[Ru(bpy)_3](BF_4)_2$ (11.2 mg, 0.015 mmol) and $BF_3{\cdot}Et_2O$ (34.1 mg, 0.24 mmol) were irradiated for 25 h in deoxygenated methanol (4 mL). After the reaction time a precipitate was formed, which was removed by filtration and characterized as the dispyrocyclobutane **2t***. Yellow solid. Obtained: 38 mg (19% yield) The alcoholic solution was evaporated to dryness and the usual work-up of the resulting residue gave **2t** as a white solid after chromatographic purification (ethyl acetate/n-hexane in 1/9 to 6/4 gradient ratio). Obtained: 96.1 mg (43 % yield).

Characterization of 2t*: ^{1}H NMR ($CDCl_3$, 300.13 MHz) δ 8.04 (m, 2H, H_o, C_6H_5), 7.59 (tt, $^{3}J_{HH}$ = 7.4 Hz, $^{4}J_{HH}$ = 1.4 Hz, 1H, H_p, C_6H_5), 7.49 (m, 2H, H_m, C_6H_5), 6.94 (m, 2H, H_2, H_6, C_6H_2), 4.81 (s, 1H, CH), 3.88 (s, 6H, CH_3O-$C_{3\text{-}5}$), 3.82 (s, 3H, CH_3O-C_4). $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 75.5 MHz) δ 176.1, 161.6, 152.8, 138.3, 133.4, 129.0, 128.2, 127.3, 125.6, 108.1, 73.3, 60.9, 57.2, 56.3. HRMS (ESI^+) m/z calc for $C_{38}H_{34}N_2NaO_{10}$ $[M+Na]^+$ 701.2111, found 701.2075. **Characterization of 2t**: ^{1}H NMR ($CDCl_3$, 300.13 MHz) δ 8.33 (s, 1H, NH), 7.60 (m, 2H, H_o, C_6H_5), 7.49 (tt, $^{3}J_{HH}$ = 7.4 Hz, $^{4}J_{HH}$ = 1.3 Hz, 1H, H_p, C_6H_5), 7.39 (m, 2H, H_m, C_6H_5), 6.68 (s, 2H, $H_{2\text{-}6}$, C_6H_2), 4.69 (s, 1H, CH), 3.77 (s, 3H, CH_3O), 3.76 (s, 6H, CH_3O), 3.73 (s, 3H, $COOCH_3$). $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 75.5 MHz) δ 171.8, 166.6, 153.5, 138.1, 133.2, 132.2, 130.6, 128.8, 126.9, 106.3, 64.2, 61.0, 56.3, 53.2, 48.9. HRMS (ESI^+) m/z calc for $C_{40}H_{42}N_2NaO_{12}$ $[M+Na]^+$ 765.2635, found 765.2638.

Synthesis of dimethyl-1,2-bis(benzamido)-3,4-di(2-thienyl)cyclobutane-1,2-dicarboxylate **2u.** Cyclobutane **2u** was prepared following the same procedure than that described for **2a**, with minor changes in the chromatographic purification and using an optimized reaction time. Oxazolone **1u** (153.02 mg, 0.60 mmol), $[Ru(bpy)_3](BF_4)_2$ (11.2 mg, 0.015 mmol) and $BF_3{\cdot}Et_2O$ (34.1 mg, 0.24 mmol) were irradiated for 48 h in

deoxygenated methanol (4 mL) to give **2r** as a white solid after chromatographic purification (ethyl acetate/n-hexane in 3/7 to 6/4 gradient ratio). Obtained: 53.6 mg (31 % yield). ^{1}H NMR ($CDCl_3$, 300.13 MHz) δ 8.32 (s, 1H, NH), 7.57 (m, 2H, H_o, C_6H_5), 7.41 (tt, $^{3}J_{HH}$ = 8.2 Hz, $^{4}J_{HH}$ = 1.2 Hz, 1H, H_p, C_6H_5), 7.35-7.28 (m, 2H, H_m, C_6H_5), 7.17 (dd, $^{3}J_{HH}$= 5.2 Hz, $^{4}J_{HH}$ = 1.2 Hz, 1H, H_3, SC_4H_3), 7.10 (dd, $^{3}J_{HH}$ = 3.6 Hz, $^{4}J_{HH}$ = 1.2 Hz, 1H, H_5, SC_4H_3), 6.89 (dd, $^{3}J_{HH}$ = 5.2 Hz, $^{3}J_{HH}$ = 3.6 Hz, H_4, SC_4H_3), 4.90 (s, 1H, CH), 3.64 (s, 3H, $COOCH_3$). $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 75.5 MHz) δ 171.0, 166.9, 137.3, 133.1, 132.0, 128.6, 127.6, 127.3, 127.1, 126.4, 64.2, 53.1, 46.4. HRMS (ESI$^+$) m/z calc for $C_{30}H_{27}N_2O_6S_2$ $[M+H]^+$ 575.1311, found 575.1295.

Expansion of the cyclobutane ring of δ-1,2-diaminotruxínics: synthesis of pyrrolidines 3.

All pyrrolidine-2,5-dicarboxylate derivatives **3** have been prepared following the same experimental method, which is detailed here for **3a**.

Synthesis of dimethyl-2-benzamido-1-benzoyl-3,4-diphenylpyrrolidine-2,5-dicarboxylate **3a***.* A solution of δ-cyclobutane **2a** (41.8 mg, 0.074 mmol) in methanol (5 mL) was treated with NaOMe (4.06 mg, 0.075 mmol), and the resulting mixture was heated at 110 °C for 1 h in a J-Young Sample Flask. Once cooled, the resulting solution was evaporated to dryness and the solid residue extracted with CH_2Cl_2 (3×5 mL). Any insoluble solid was removed at this point by filtration through Celite. The resulting clear solution was evaporated to dryness to give impure pyrrolidine **3a**, which was purified by crystallization from CH_2Cl_2/pentane to give **3a** as a white solid. Obtained: 21.2 mg (51% yield). Pyrrolidine **3a** was characterized by NMR methods as the mixture of two diastereoisomers in 1:0.45 molar ratio. Only the major isomer could be fully characterized by NMR. ^{1}H NMR ($CDCl_3$, 300.13 MHz) δ 8.14 (s, 1H, NH), 7.91 (m, 2H, H_o, NHCO-C_6H_5), 7.59-7.12 (m, 18H, C_6H_5), 5.28 (d, $^{3}J_{HH}$ = 10 Hz, 1H, H-C_5), 5.27 (d, $^{3}J_{HH}$ = 13.1 Hz, 1H, H-C_3), 4.27 (dd, $^{3}J_{HH}$ = 13.1 Hz, $^{3}J_{HH}$ = 10 Hz, 1H, H-C_4), 3.70 (s, 3H, C_2-$COOCH_3$), 3.10 (s, 3H, C_5-$COOCH_3$). $^{13}C\{^{1}H\}$NMR ($CDCl_3$, 75.5 MHz) δ 170.9, 170.8, 169.0, 167.4, 136.2, 135.2, 134.6, 133.0, 132.2, 130.9, 129.0, 129.0, 128.9, 128.7, 128.6, 128.6, 128.4, 128.2, 128.2, 127.4, 81.4, 69.7, 53.4, 53.4, 51.9, 51.8. HRMS (ESI$^+$) m/z calc for $C_{34}H_{30}N_2NaO_6$ $[M+Na]^+$ 585.2002, found 585.2003.

Synthesis of dimethyl-2-benzamido-1-benzoyl-3,4-bis(4-chlorophenyl)pyrrolidine-2,5-dicarboxylate **3d***.* The synthesis of **3d** was carried out following the same synthetic method than that detailed for **3a**. Therefore, δ-cyclobutane **2d** (79.4 mg, 0.126 mmol) was reacted with NaOMe (6.75 mg, 0.125 mmol) in MeOH (110

°C) for 1h to give **3d** as a single diastereoisomer after crystallization from CH_2Cl_2/pentane. Obtained: 40.1 mg (50% yield). White solid. ^{1}H NMR ($CDCl_3$, 300.13 MHz) δ 8.12 (s, 1H, NH), 7.89 (m, 2H, H_o, NHCO-C_6H_5), 7.63-7.55 (m, 3H, H_p, NHCO-C_6H_5 + H_o, N_1CO-C_6H_5), 7.50 (m, 2H, H_m, NHCO-C_6H_5), 7.38-7.30 (m, 7H, H_p, H_m, N_1CO-C_6H_5 + H_o, H_m, C_4-C_6H_4), 7.22 (m, 2H, H_m, C_3-C_6H_4), 7.12 (m, 2H, H_o, C_3-C_6H_4), 5.22 (d, $^3J_{HH}$ = 10 Hz, 1H, H-C_5), 5.20 (d, $^3J_{HH}$ = 13 Hz, 1H, H-C_3), 4.17 (dd, $^3J_{HH}$ = 13 Hz, $^3J_{HH}$ = 10 Hz, 1H, H-C_4), 3.73 (s, 3H, C_2-$COOCH_3$), 3.10 (s, 3H, C_5-$COOCH_3$). ^{13}C{^{1}H}NMR ($CDCl_3$, 75.5 MHz) δ 170.6, 169.0, 168.7, 167.6, 135.0, 134.5, 134.4, 134.3, 134.1, 131.3, 132.5, 131.1, 129.8, 129.4, 129.4, 129.0, 128.4, 128.2, 127.3, 81.1, 69.3, 53.6, 52.8, 52.1, 51.4. HRMS (ESI$^+$) m/z calc for $C_{34}H_{28}Cl_2N_2NaO_6$ $[M+Na]^+$ 653.1222; found: 653.1179.

Synthesis of dimethyl-2-benzamido-1-benzoyl-3,4-bis(4-fluorophenyl)pyrrolidine-2,5-dicarboxylate **3e***.* The synthesis of **3e** was carried out following the same synthetic method than that detailed for **3a**. Therefore, δ-cyclobutane **2e** (46.7 mg, 0.078 mmol) was reacted with NaOMe (4.3 mg, 0.08 mmol) in MeOH (110 °C) for 1h to give **3e** as a single diastereoisomer after crystallization from CH_2Cl_2/pentane. Obtained: 21.5 mg (46% yield). ^{1}H NMR ($CDCl_3$, 300.13 MHz) δ 8.12 (s, 1H, NH), 7.89 (m, 2H, H_o, NHCO-C_6H_5), 7.58-7.52 (m, 3H, H_p, NHCO-C_6H_5 + H_o, N_1CO-C_6H_5), 7.48 (m, 2H, H_m, NHCO-C_6H_5), 7.42-7.31 (m, 5H, H_p, H_m, N_1CO-C_6H_5 + H_o, C_4-C_6H_4), 7.17 (m, 2H, H_o, C_3-C_6H_4), 6.95 (m, 4H, H_m, C_6H_4), 5.22 (d, $^3J_{HH}$ = 10.1 Hz, 1H, H-C_5), 5.20 (d, $^3J_{HH}$ = 13.1 Hz, 1H, H-C_3), 4.18 (dd, $^3J_{HH}$ = 13.1 Hz, $^3J_{HH}$ = 10.1 Hz, 1H, H-C_4), 3.72 (s, 3H, C_2-$COOCH_3$), 3.10 (s, 3H, C_5-$COOCH_3$). ^{13}C NMR ($CDCl_3$, 75.5 MHz) δ 170.7, 169.0, 168.8, 167.6, 162.7, 162.5, 135.1, 134.4, 132.4, 131.7, 131.0, 130.1, 129.7, 129.0, 128.6, 128.4, 128.2, 127.3, 116.1, 115.8, 81.2, 69.5, 53.5, 52.8, 52.0, 51.4. ^{19}F NMR ($CDCl_3$, 282.4 MHz) δ -113.47 (m), -113.86 (m). HRMS (ESI$^+$) m/z calc for $C_{34}H_{28}F_2N_2NaO_6$ $[M+Na]^+$ 621.1813, found 621.1792.

Synthesis of dimethyl-2-benzamido-1-benzoyl-3,4-bis(4-cyanophenyl)pyrrolidine-2,5-dicarboxylate **3g***.* The synthesis of **3g** was carried out following the same synthetic method than that detailed for **3a**. Therefore, δ-cyclobutane **2g** (62 mg, 0.10 mmol) was reacted with NaOMe (5.9 mg, 0.10 mmol) in MeOH (110 °C) for 1h to give **3g** as a mixture of two different diastereoisomers (3.3/1 molar ratio) after crystallization from CH_2Cl_2/pentane. Obtained: 41.5 mg (67% yield). Only the major isomer could be fully characterized by NMR spectroscopy. ^{1}H NMR ($CDCl_3$, 400.13 MHz) δ 8.12 (s, 1H, NH), 7.89 (m, 2H, H_o, NHCO-C_6H_5), 7.60-7.47 (m, 14H, C_6H_5 + C_6H_4), 7.34-7.29 (m, 4H, C_6H_5 + C_6H_4), 5.36 (d, $^3J_{HH}$ = 12.9 Hz, 1H, H-C_3), 5.27 (d, $^3J_{HH}$ = 9.9 Hz, 1H,

H-C_5), 4.29 (dd, $^3J_{HH}$ = 12.9 Hz, $^3J_{HH}$ = 10 Hz, 1H, H-C_4), 3.71 (s, 3H, C_2-$COOCH_3$), 3.11 (s, 3H, C_5-$COOCH_3$). $^{13}C\{^1H\}$NMR ($CDCl_3$, 100.6 MHz) δ 170.1, 169.0, 168.2, 167.9, 141.0, 138.0, 134.7, 133.9, 133.1, 132.5, 132.7, 129.2, 129.1 (2C), 128.9, 128.5, 128.1, 127.3, 118.3, 118.2, 112.8, 112.6, 81.1, 69.1, 53.7, 53.1, 52.3, 51.6. HRMS (ESI^+) m/z calc for $C_{36}H_{28}N_4NaO_6$ $[M+Na]^+$ 635.1907, found: 635.1903.

Synthesis of dimethyl-2-benzamido-1-benzoyl-3,4-bis(4-(trifluoromethyl)phenyl)pyrrolidine-2,5-dicarboxylate **3h***.* The synthesis of **3h** was carried out following the same synthetic method than that detailed for **3a**. Therefore, δ-cyclobutane **2h** (41.5 mg, 0.06 mmol) was reacted with NaOMe (3.2 mg, 0.06 mmol) in MeOH (110 °C) for 1h to give **3h** as a single diastereoisomer after crystallization from CH_2Cl_2/pentane. Obtained: 16.1 mg (39% yield). ^1H NMR ($CDCl_3$, 300.13 MHz) δ 8.14 (s, 1H, NH), 7.90 (m, 2H, H_o, NHCO-C_6H_5), 7.58-7.52 (m, 3H, H_p, NHCO-C_6H_5 + H_o, N_1CO-C_6H_5), 7.48 (m, 2H, H_m, NHCO-C_6H_5), 7.42-7.31 (m, 5H, H_p, H_m, N_1CO-C_6H_5 + H_o, C_4-C_6H_4), 7.17 (m, 2H, H_o, C_3-C_6H_4), 6.95 (m, 4H, H_m, C_6H_4), 5.37 (d, $^3J_{HH}$ = 13 Hz, 1H, H-C_3), 5.29 (d, $^3J_{HH}$ = 9.9 Hz, 1H, H-C_5), 4.32 (dd, $^3J_{HH}$ = 13 Hz, $^3J_{HH}$ = 9.9 Hz, 1H, H-C_4), 3.71 (s, 3H, C_2-$COOCH_3$), 3.12 (s, 3H, C_5-$COOCH_3$). ^{13}C NMR ($CDCl_3$, 75.5 MHz) δ 170.4, 169.0, 168.5, 167.8, 139.9, 136.8, 134.9, 134.1, 132.6, 131.2, 130.8, 130.6, 129.1, 128.9, 128.5, 128.5, 128.2, 127.3, 126.2, 125.7, 120.3, 120.3, 81.2, 69.3, 53.6, 53.1, 52.2, 51.5. ^{19}F NMR ($CDCl_3$, 282.4 MHz) δ -62.71 (s), -62.75 (s). HRMS (ESI^+) m/z calc for $C_{36}H_{28}F_6N_2NaO_6$ $[M+Na]^+$ 721.1752, found 721.1744.

Synthesis of dimethyl-2-benzamido-1-benzoyl-3,4-bis(3-fluorophenyl)pyrrolidine-2,5-dicarboxylate **3k***.* The synthesis of **3k** was carried out following the same synthetic method than that detailed for **3a**. Therefore, δ-cyclobutane **2k** (107.4 mg, 0.18 mmol) was reacted with NaOMe (9.8 mg, 0.18 mmol) in MeOH (110 °C) for 1h to give **3k** as a mixture of two different diastereoisomers (2/1 molar ratio) after crystallization from CH_2Cl_2/pentane. Obtained: 78.4 mg (73% yield). Only the major isomer could be fully characterized by NMR spectroscopy. ^1H NMR ($CDCl_3$, 300.13 MHz) δ 8.12 (s, 1H, NH), 7.90 (m, 2H, H_o, NHCO-C_6H_5), 7.58-7.53 (m, 3H, H_p, NHCO-C_6H_5 + H_o, N_1CO-C_6H_5), 7.49 (m, 2H, H_m, NHCO-C_6H_5), 7.38-7.35 (m, 3H, H_p, H_m, N_1CO-C_6H_5), 7.24-7.20 (m, 2H, C_6H_4F), 7.18-7.13 (m, 2H, C_6H_4F), 7.01-6.98 (m, 1H, C_6H_4F), 6.94-6.91 (m, 3H, C_6H_4F), 5.25 (d, $^3J_{HH}$ = 10 Hz, 1H, H-C_5), 5.23 (d, $^3J_{HH}$ = 13.3 Hz, 1H, H-C_3), 4.19 (dd, $^3J_{HH}$ = 13. Hz, $^3J_{HH}$ = 10 Hz, 1H, H-C_4), 3.74 (s, 3H, C_2-$COOCH_3$), 3.12 (s, 3H, C_5-$COOCH_3$). ^{13}C NMR ($CDCl_3$, 75.5 MHz) δ 170.5, 169.0, 168.7, 167.6, 163.1, 162.8, 138.4, 135.4, 135.0, 134.3, 132.4, 131.0, 130.7, 130.2, 129.0, 128.4, 128.2, 127.3, 124.5, 123.8, 115.4,

115.1, 81.1, 69.3, 53.5, 53.0, 52.1, 51.6. ^{19}F NMR ($CDCl_3$, 282.4 MHz) δ -112.00 (m), -112.26 (m). HRMS (ESI^+) m/z calc for $C_{34}H_{28}F_2N_2NaO_6$ $[M+Na]^+$ 621.1813, found 621.1812.

Synthesis of dimethyl-2-benzamido-1-benzoyl-3,4-bis(3-bromophenyl)pyrrolidine-2,5-dicarboxylate **3l**. The synthesis of **3l** was carried out following the same synthetic method than that detailed for **3a**. Therefore, δ-cyclobutane **2l** (88.0 mg, 0.12 mmol) was reacted with NaOMe (6.7 mg, 0.12 mmol) in MeOH (110 °C) for 1h to give **3l** as a single diastereoisomer after crystallization from CH_2Cl_2/pentane. Obtained: 60.5 mg (69% yield). ^{1}H NMR ($CDCl_3$, 300.13 MHz) δ 8.10 (s, 1H, NH), 7.89 (m, 2H, H_o, NHCO-C_6H_5), 7.58-7.53 (m, 4H, H_p, NHCO-C_6H_5 + H_o, N_1CO-C_6H_5 + H, C_6H_4Br), 7.48 (m, 2H, H_m, NHCO-C_6H_5), 7.39-7.33 (m, 7H, H_m, H_p, N_1CO-C_6H_5 + C_6H_4Br), 7.20-7.12 (m, 3H, C_6H_4Br), 5.23 (d, $^3J_{HH}$ = 10 Hz, 1H, H-C_5), 5.18 (d, $^3J_{HH}$ = 13.1Hz, 1H, H-C_3), 4.15 (dd, $^3J_{HH}$ = 13.1 Hz, $^3J_{HH}$ = 10 Hz, 1H, H-C_4), 3.76 (s, 3H, C_2-$COOCH_3$), 3.12 (s, 3H, C_5-$COOCH_3$). ^{13}C{^{1}H}NMR ($CDCl_3$, 75.5 MHz) δ 170.5, 169.0, 168.6, 167.6, 138.1, 135.0, 134.9, 134.3, 132.4, 131.7, 131.3, 131.1, 131.6, 131.0, 130.7, 130.3, 129.0, 128.4, 128.2, 127.6, 127.3, 126.7, 123.1, 122.8, 81.2, 69.2, 53.6, 53.0, 52.1, 51.4. HRMS (ESI^+) m/z calc for $C_{34}H_{28}Br_2N_2NaO_6$ $[M+Na]^+$ 741.0212, found 741.0222.

Synthesis of dimethyl-2-benzamido-1-benzoyl-3,4-bis(3-(trifluoromethyl)phenyl)pyrrolidine-2,5-dicarboxylate **3m**. The synthesis of **3m** was carried out following the same synthetic method than that detailed for **3a**. Therefore, δ-cyclobutane **2m** (80.5 mg, 0.13 mmol) was reacted with NaOMe (7.1 mg, 0.13 mmol) in MeOH (110 °C) for 1h to give **3m** as a single diastereoisomer after crystallization from CH_2Cl_2/pentane. Obtained: 16.4 mg (20% yield). ^{1}H NMR ($CDCl_3$, 300.13 MHz): δ 8.12 (s, 1H, NH), 7.90 (m, 2H, H_o, NHCO-C_6H_5), 7.73 (m, 1H, C_6H_4), 7.59-7.45 (m, 10H, C_6H_5 + C_6H_4), 7.39-7.31 (m, 5H, C_6H_5 + C_6H_4), 5.34 (d, $^3J_{HH}$ = 13.1 Hz, 1H, H-C_3), 5.29 (d, $^3J_{HH}$ = 10Hz, 1H, H-C_5), 4.32 (dd, $^3J_{HH}$ = 13.1 Hz, $^3J_{HH}$ = 10 Hz, 1H, H-C_4), 3.73 (s, 3H, C_2-$COOCH_3$), 3.12 (s, 3H, C_5-$COOCH_3$). ^{13}C{^{1}H}NMR ($CDCl_3$, 75.5 MHz) δ 170.4, 169.0, 168.6, 167.7, 136.7, 134.9, 134.2, 133.8, 132.5, 131.1, 132.7, 130.9, 129.9, 129.4, 129.0, 128.5, 128.2, 127.3, 125.4, 124.5, 81.1, 69.2, 53.6, 52.9, 52.1, 51.6. ^{19}F NMR ($CDCl_3$, 282.4 MHz) δ -62.67 (s), -62.73 (s). HRMS (ESI^+) m/z calc for $C_{36}H_{28}F_6N_2NaO_6$ $[M+Na]^+$ 721.1749, found 721.1757.

Synthesis of dimethyl-2-benzamido-1-benzoyl-3,4-bis(2-fluorophenyl)pyrrolidine-2,5-dicarboxylate **3o**. The synthesis of **3o** was carried out following the same synthetic method than that detailed for **3a**. Therefore, δ-cyclobutane **2o** (62 mg, 0.10 mmol) was reacted with NaOMe (5.7 mg, 0.10 mmol) in MeOH (110 °C) for

1h to give **3o** as a mixture of two different diastereoisomers (2/1 molar ratio) after crystallization from CH_2Cl_2/pentane. Obtained: 37.7 mg (61% yield). Only the major isomer could be fully characterized by NMR spectroscopy. ^{1}H NMR ($CDCl_3$, 400.13 MHz): δ =8.05 (s, 1H, NH), 7.87 (m, 2H, H_o, NHCO-C_6H_5), 7.76 (m, 1H, H_6, C_4-C_6H_4F), 7.59 (m, 2H, H_o, N_1CO-C_6H_5), 7.52 (m, 1H, H_p, NHCO-C_6H_5), 7.45 (m, 2H, H_m, NHCO-C_6H_5), 7.38-7.29 (m, 5H, H_p, H_m, N_1CO-C_6H_5 + C_6H_4F), 7.17 (m, 2H, H_5, H_4, C_6H_4F), 7.05 (m, 1H, H_5, C_6H_4F), 6.95 (m, 2H, H_3, C_6H_4F), 5.79 (d, $^3J_{HH}$ = 13.3 Hz, 1H, H-C_3), 5.29 (d, $^3J_{HH}$ = 10 Hz, 1H, H-C_5), 4.70 (dd, $^3J_{HH}$ = 13.3 Hz, $^3J_{HH}$ = 10 Hz, 1H, H-C_4), 3.73 (s, 3H, C_2-$COOCH_3$), 3.13 (s, 3H, C_5-$COOCH_3$). ^{13}C {^{1}H} NMR ($CDCl_3$, 100.6 MHz): δ = 170.2, 169.0, 168.9, 167.7, 162.2, 161.3, 135.2, 134.8, 132.0, 130.9, 130.0, 129.6, 128.8, 128.4, 128.4, 128.1, 128.0, 127.3, 125.2, 124.2, 122.9, 120.2, 116.0, 115.5, 80.7, 68.7, 53.4, 52.1, 45.4, 42.8. ^{19}F NMR ($CDCl_3$, 376.5 MHz) δ -115.15 (m), -119.45 (m). HRMS (ESI$^+$) m/z calc for $C_{34}H_{28}F_2N_2NaO_6$ $[M+Na]^+$ 621.1813, found 621.1820.

Synthesis of dimethyl-2-benzamido-1-benzoyl-3,4-bis(3,4-dichlorophenyl)pyrrolidine-2,5-dicarboxylate **3r**. The synthesis of **3r** was carried out following the same synthetic method than that detailed for **3a**. Therefore, δ-cyclobutane **2r** (115.3 mg, 0.18 mmol) was reacted with NaOMe (10.0 mg, 0.18 mmol) in MeOH (110 °C) for 1h to give **3r** as a single diastereoisomer after column chromatography (silica, $CHCl_3$ as eluent) and crystallization from CH_2Cl_2/pentane. Obtained: 62.5 mg (54% yield). ^{1}H NMR ($CDCl_3$, 500.13 MHz) δ 8.11 (s, 1H, NH), 7.91 (m, 2H, H_o, NHCO-C_6H_5), 7.63-7.54 (m, 3H, H_p, NHCO-C_6H_5 + H_o, N_1CO-C_6H_5), 7.54-7.47 (m, 3H, H_m, NHCO-C_6H_5 + H_2, C_3-$C_6H_3Cl_2$), 7.45-7.34 (m, 5H, H_p, H_m, N_1CO-C_6H_5 + H_5, C_4-$C_6H_3Cl_2$ + H_5, C_3-$C_6H_3Cl_2$), 7.33-7.29 (m, 2H, H_2, H_6, C_4-$C_6H_3Cl_2$), 7.05 (dd, 1H, H_6, C_3-$C_6H_3Cl_2$), 5.23 (d, $^3J_{HH}$ = 16.4 Hz, 1H, H-C_5), 5.18 (d, $^3J_{HH}$ = 10.2 Hz, 1H, H-C_3), 4.13 (dd, $^3J_{HH}$ = 16.4 Hz, $^3J_{HH}$ = 10.2 Hz, 1H, H-C_4), 3.81 (s, 3H, C_2-C(O)OCH_3), 3.16 (s, 3H, C_5-C(O)OCH_3). ^{13}C{^{1}H}NMR ($CDCl_3$, 125.7 MHz) δ 170.1, 168.8, 168.3, 167.6, 135.8, 134.7, 134.0, 133.3, 133.0, 132.9, 132.7, 132.6, 132.4, 131.1, 131.0, 130.7, 130.1, 129.9, 128.9, 128.3, 128.0, 127.9, 127.2, 127.1, 80.9, 68.9, 53.5, 52.5, 52.1, 51.0. HRMS (ESI$^+$) m/z calc for $C_{34}H_{26}Cl_4N_2NaO_6$ $[M+Na]^+$ 721.0437, found 721.0418.

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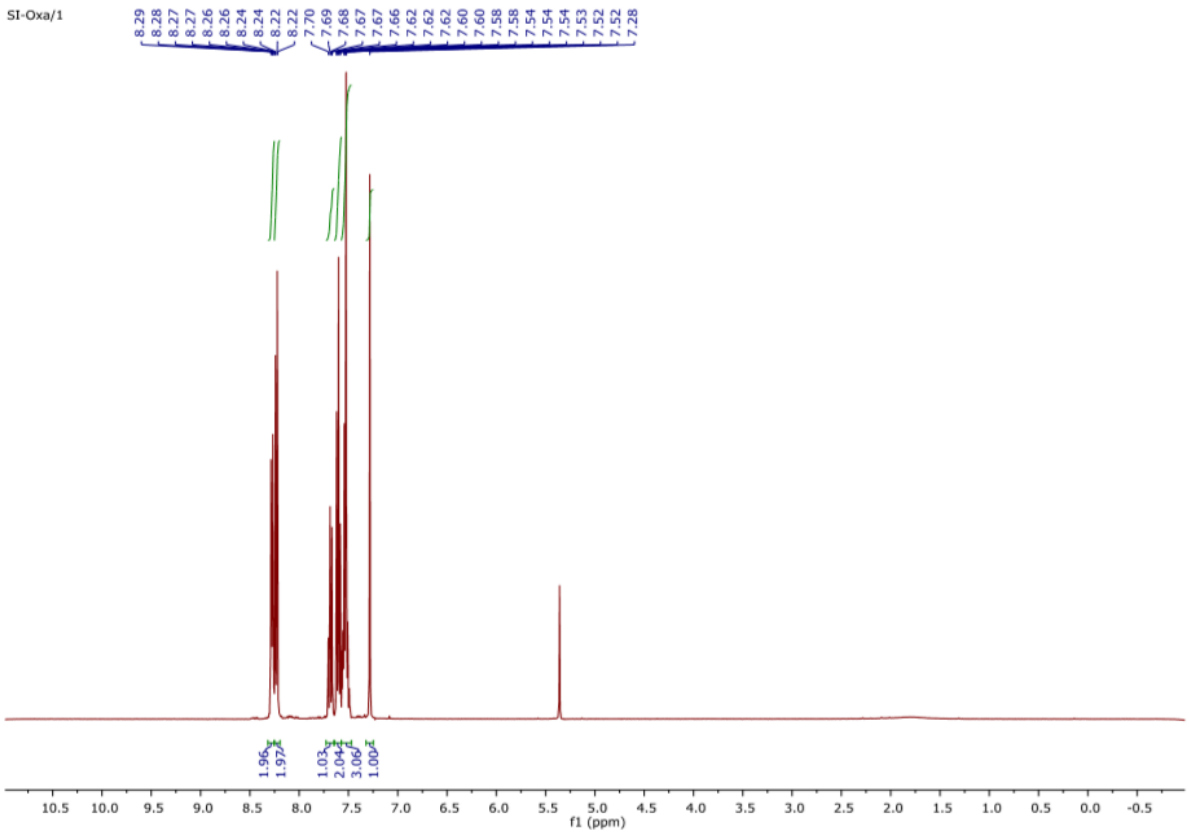
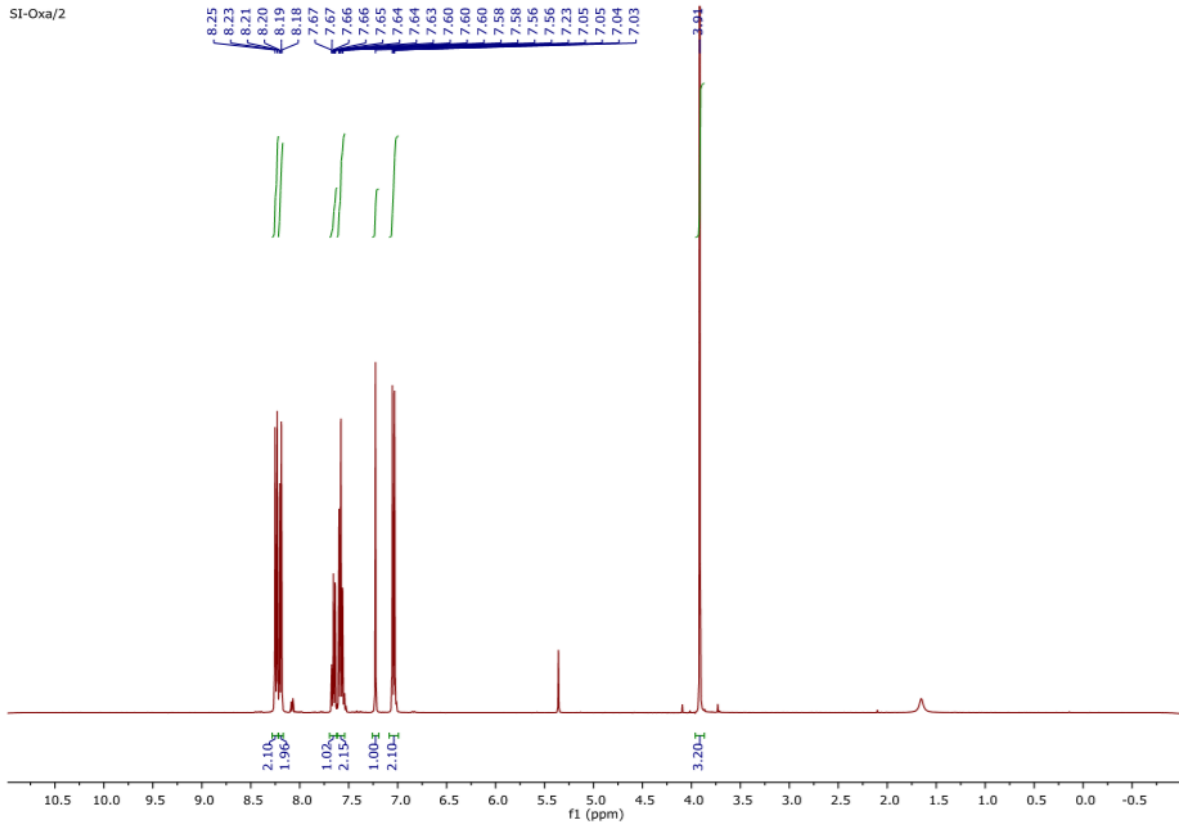
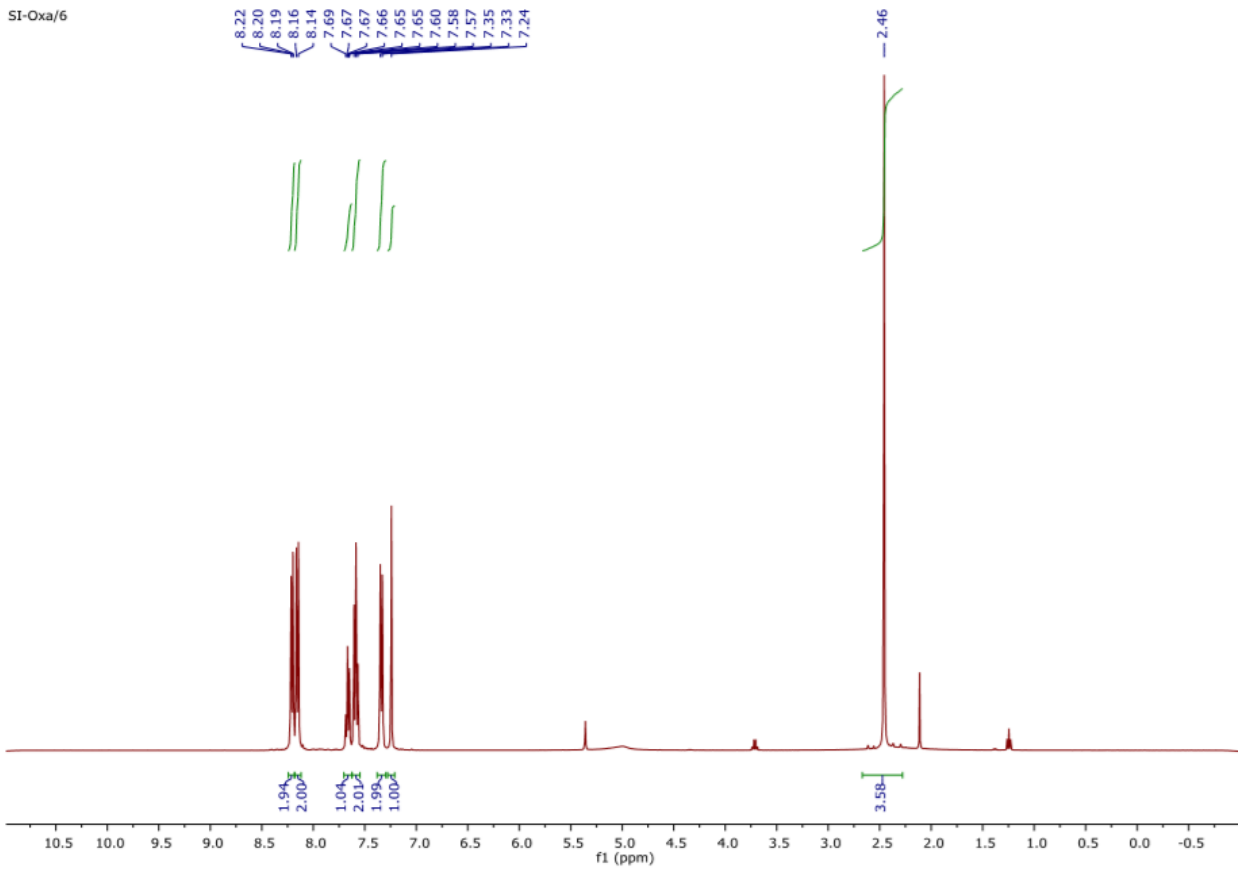
3.- ^{1}H NMR control spectra of starting (*Z*)-4-arylidene-2-phenyl-5(4*H*)-oxazolones 1a-1u



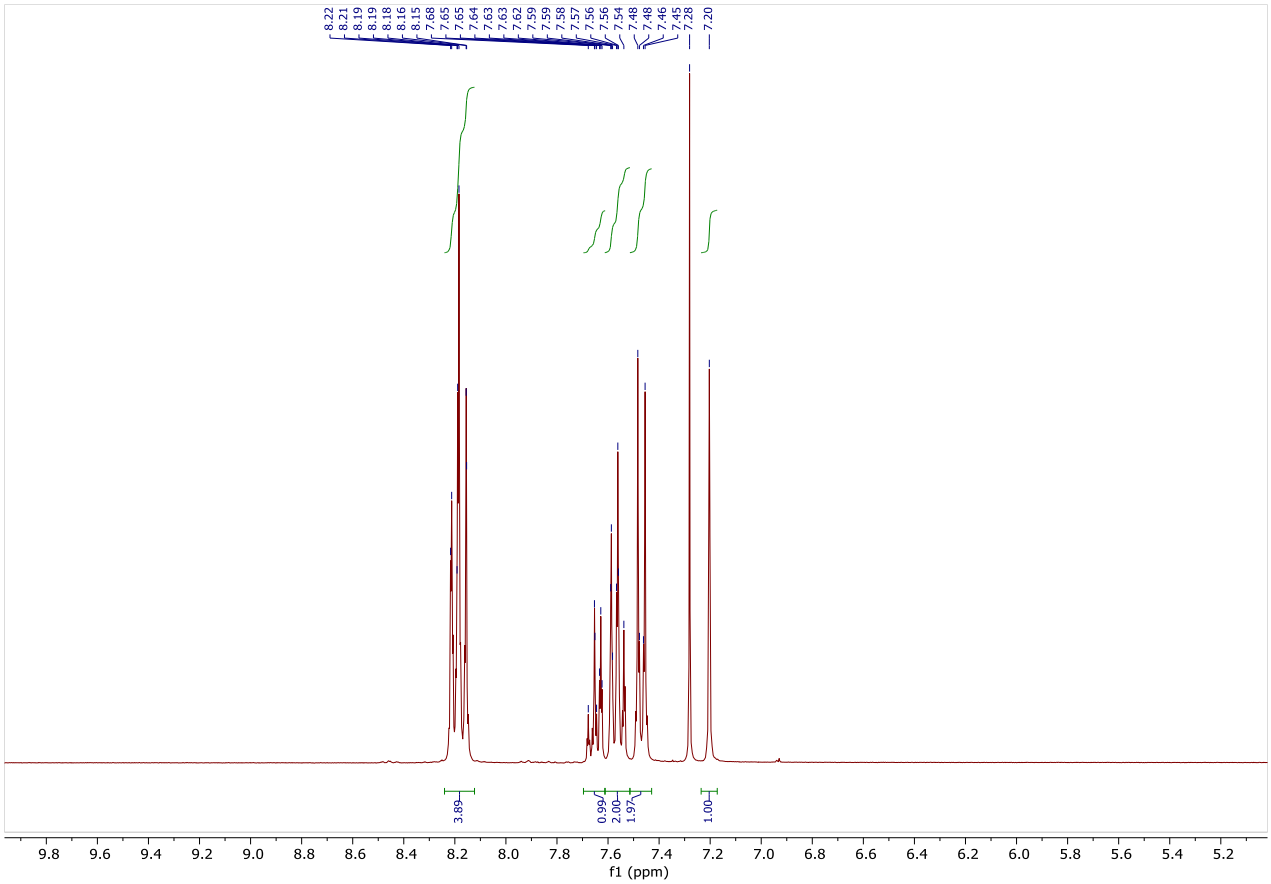
^{1}H NMR (CD_2Cl_2, 300.13 MHz) spectrum of oxazolone **1a**



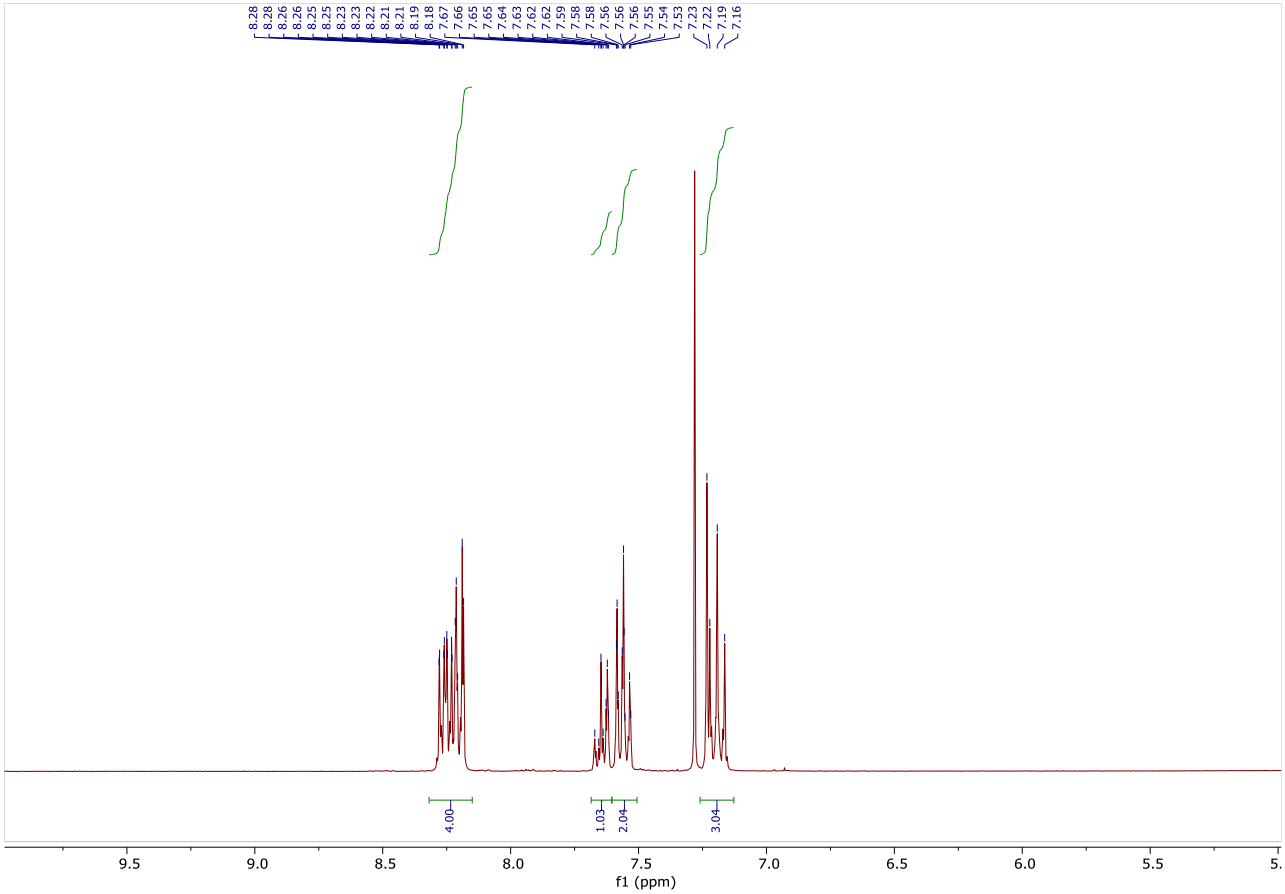
^{1}H NMR (CD_2Cl_2, 300.13 MHz) spectrum of oxazolone **1b**



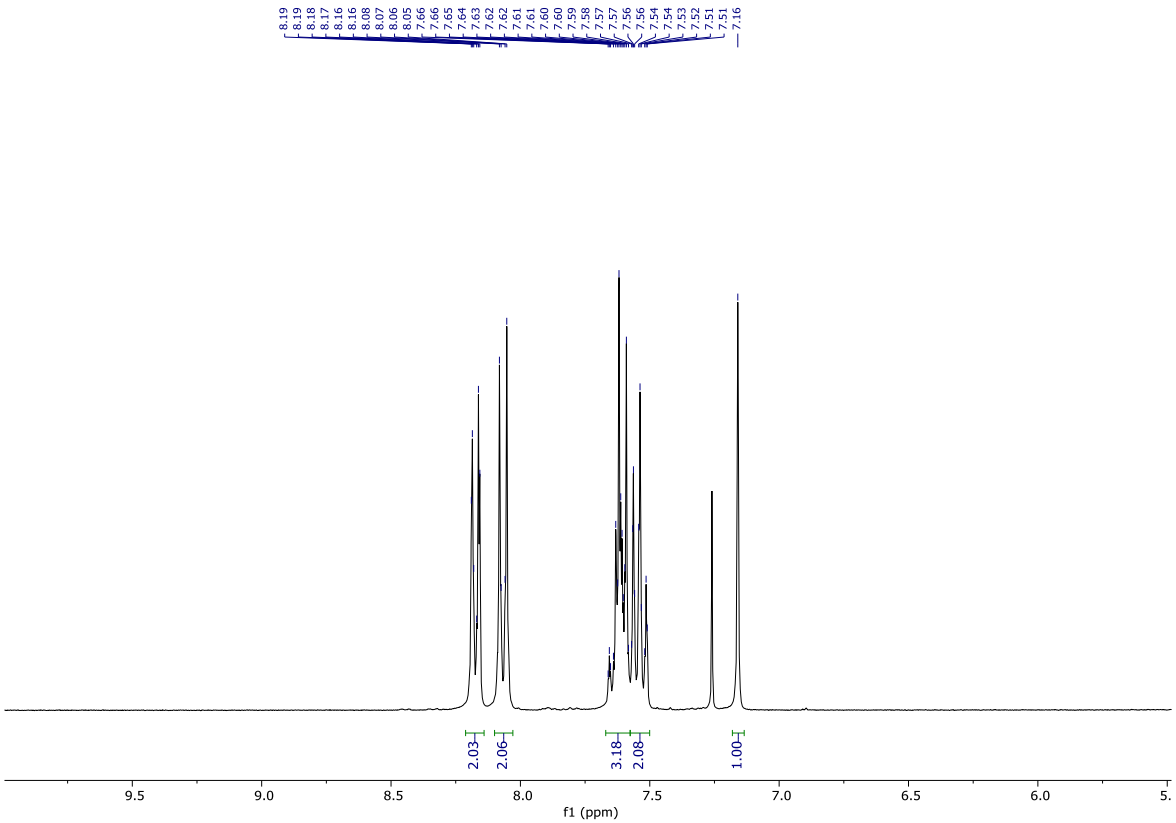
^{1}H NMR (CD_2Cl_2, 300.13 MHz) spectrum of oxazolone **1c**



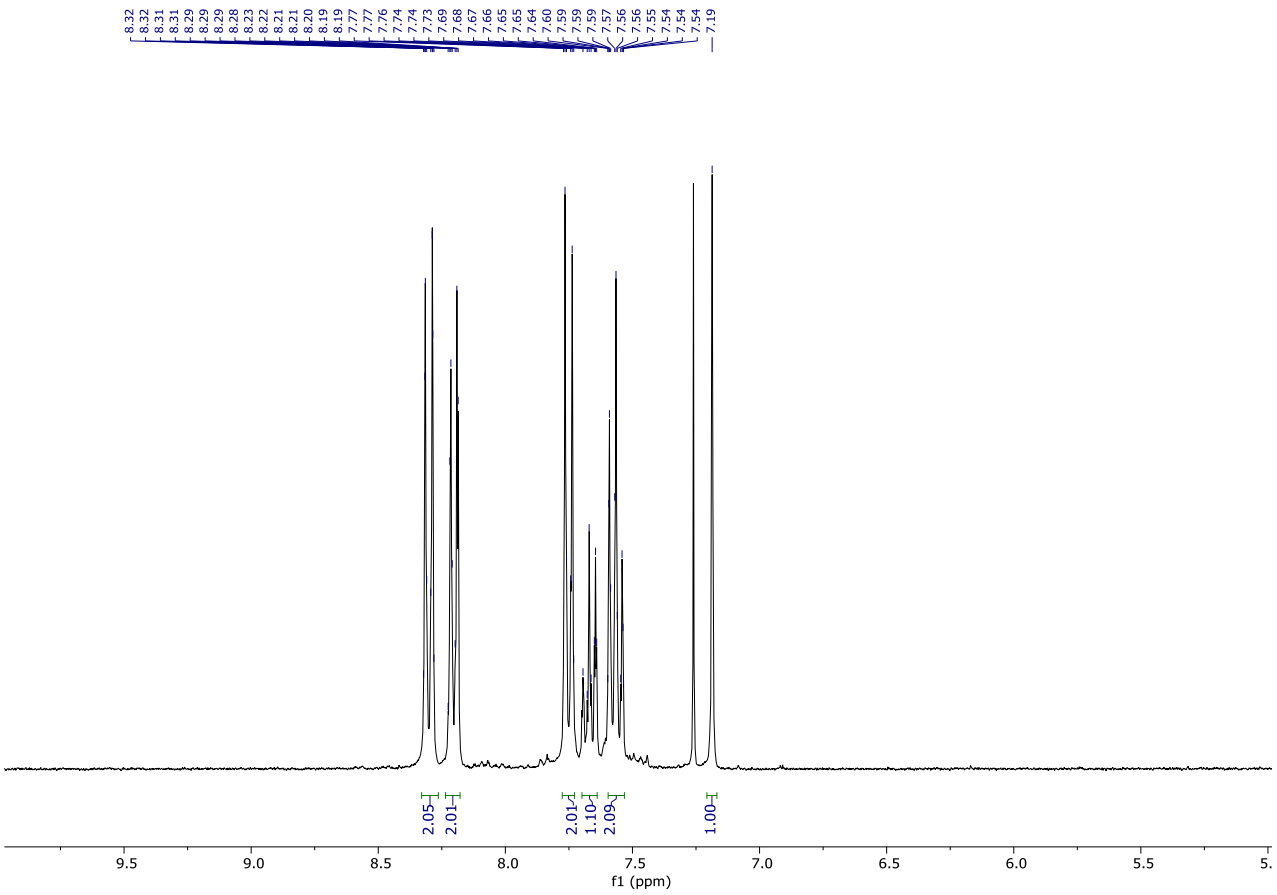
^{1}H NMR ($CDCl_3$, 300.13 MHz) spectrum of oxazolone **1d**



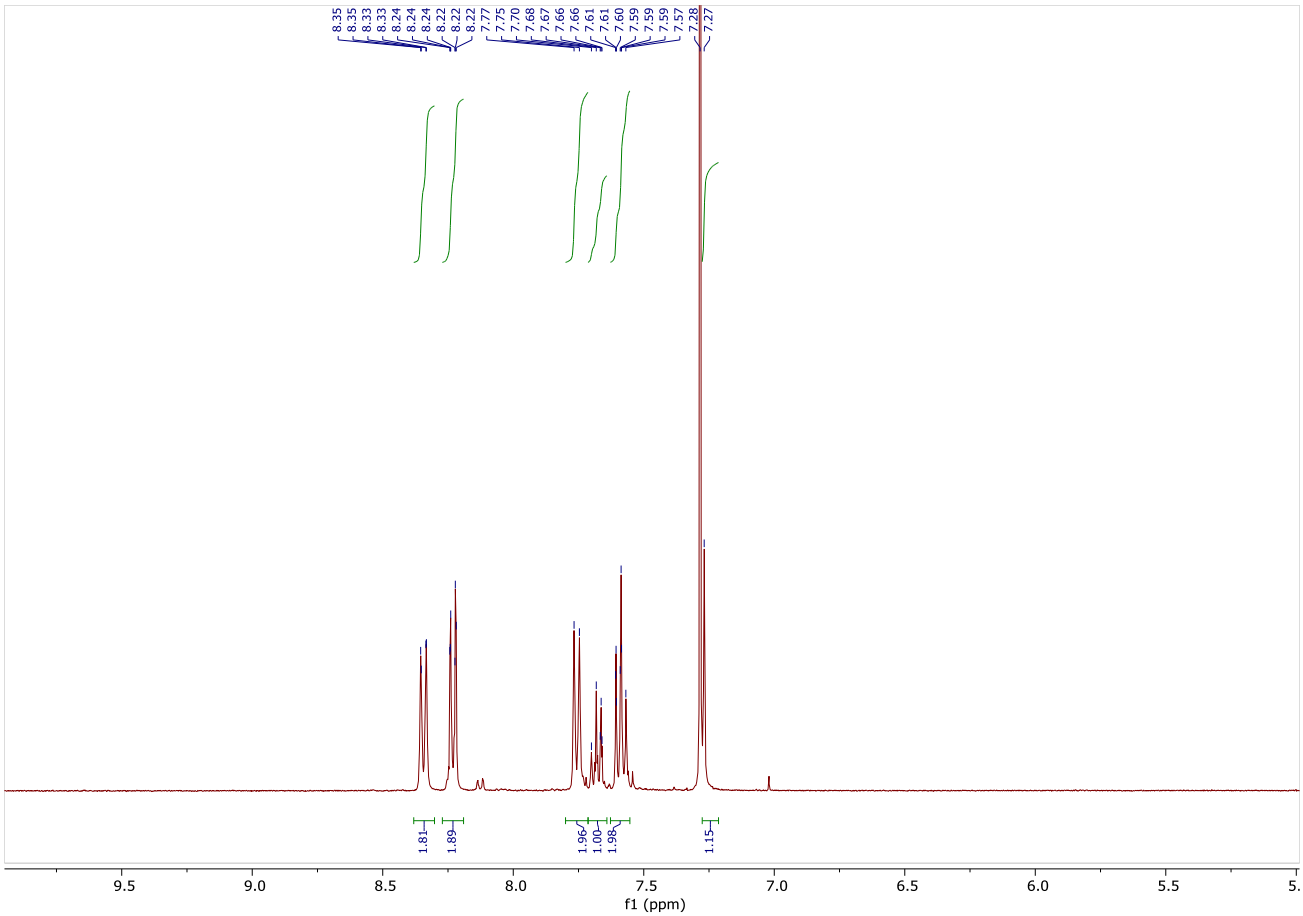
^{1}H NMR ($CDCl_3$, 300.13 MHz) spectrum of oxazolone **1e**



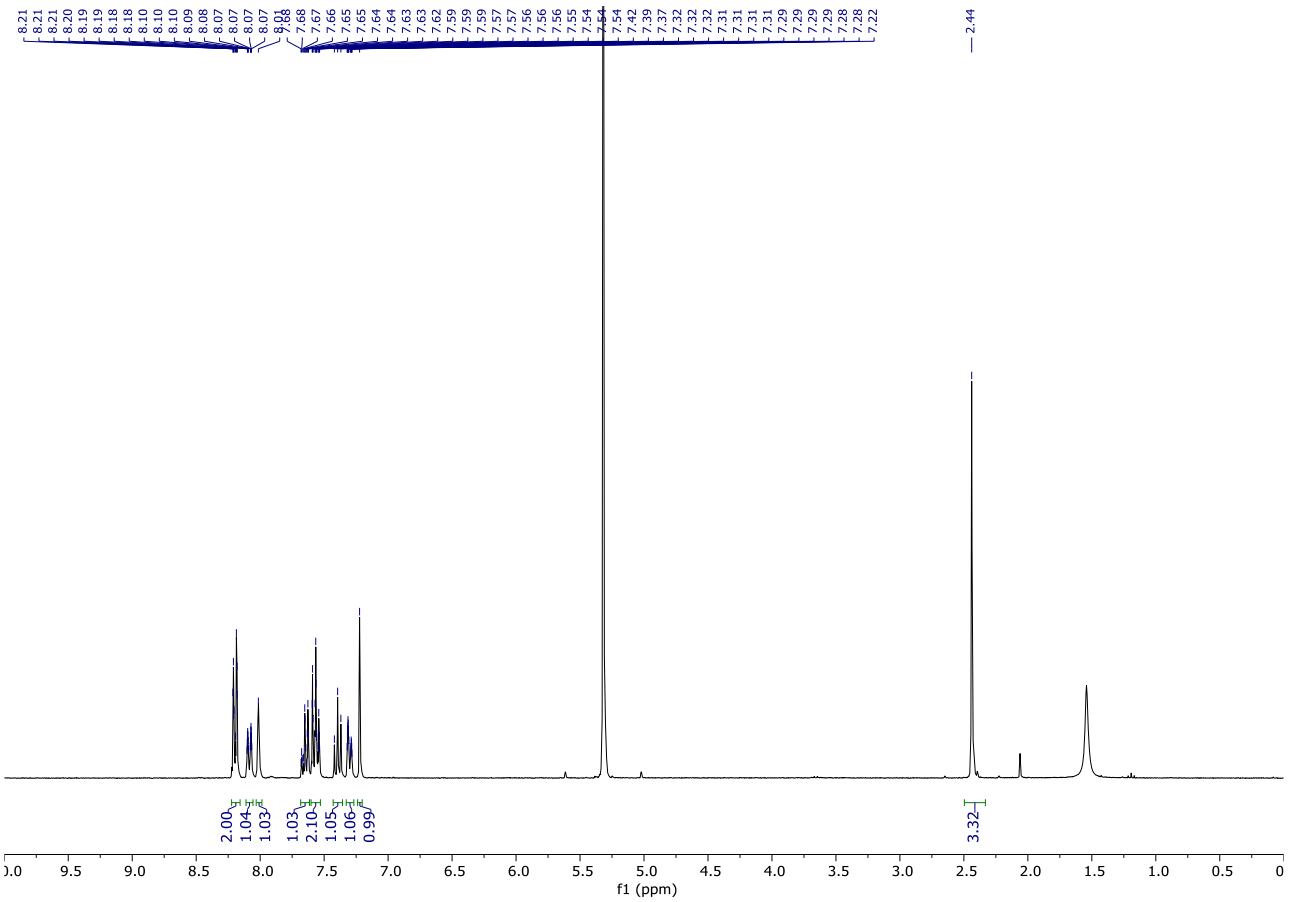
^{1}H NMR ($CDCl_3$, 300.13 MHz) spectrum of oxazolone **1f**



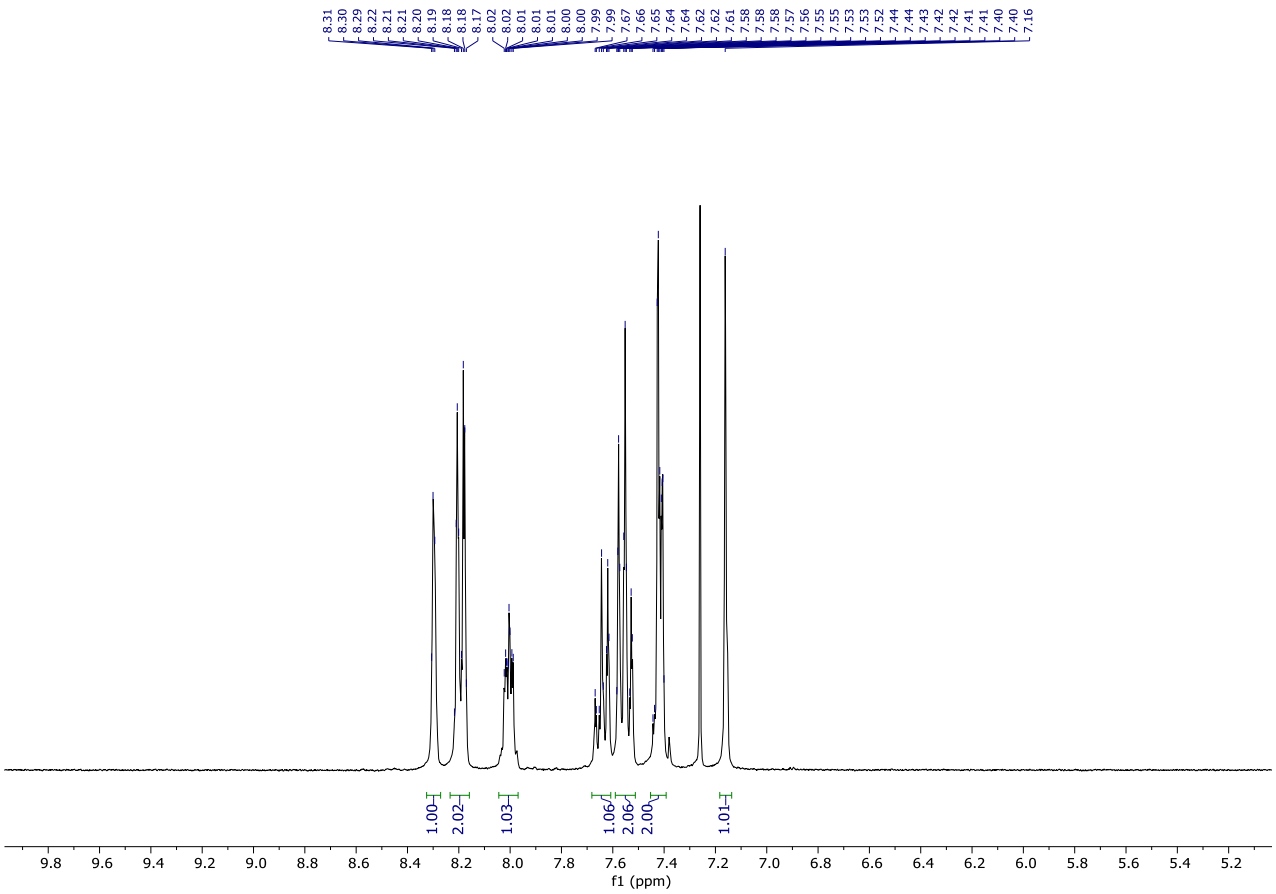
^{1}H NMR ($CDCl_3$, 300.13 MHz) spectrum of oxazolone **1g**



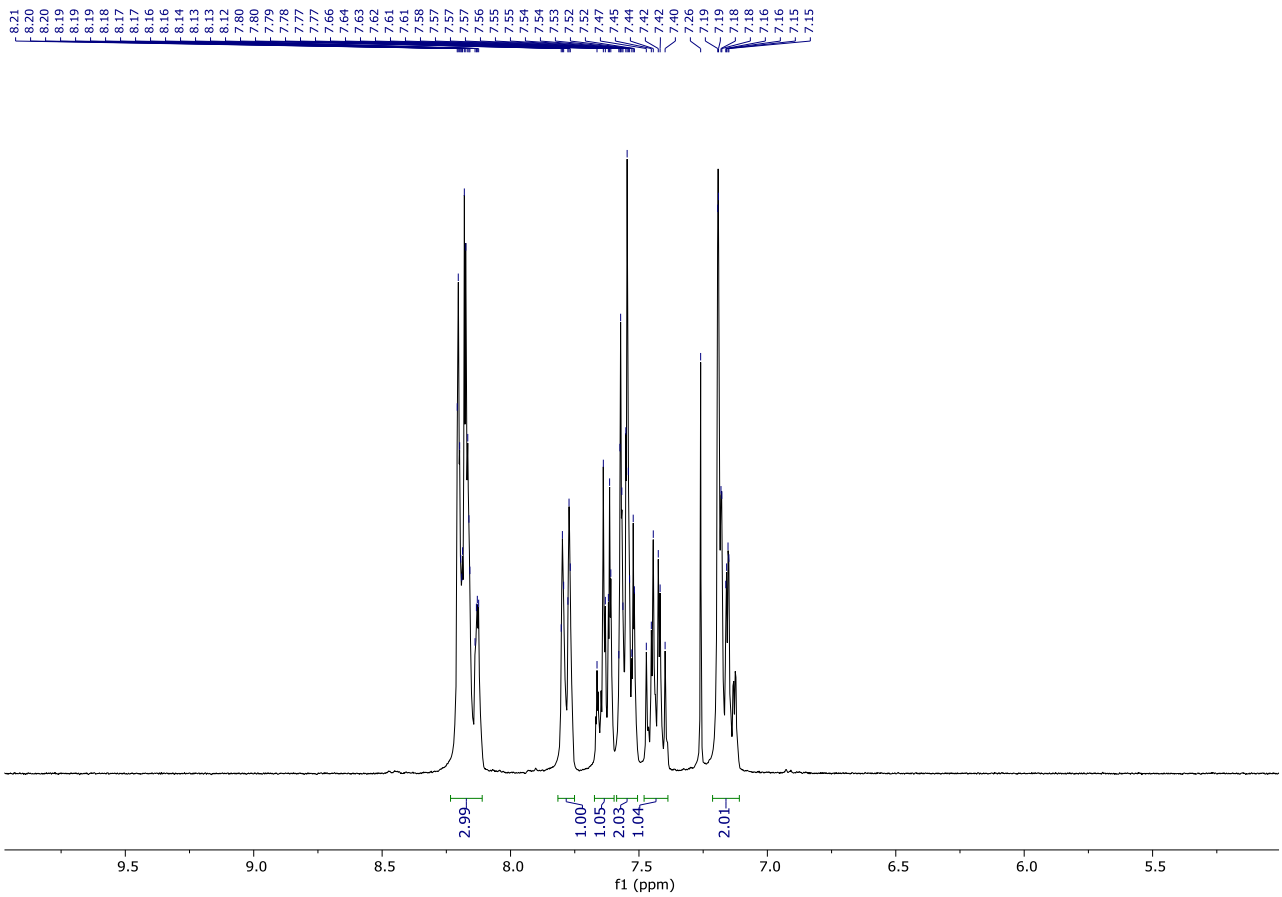
^{1}H NMR ($CDCl_3$, 300.13 MHz) spectrum of oxazolone **1h**



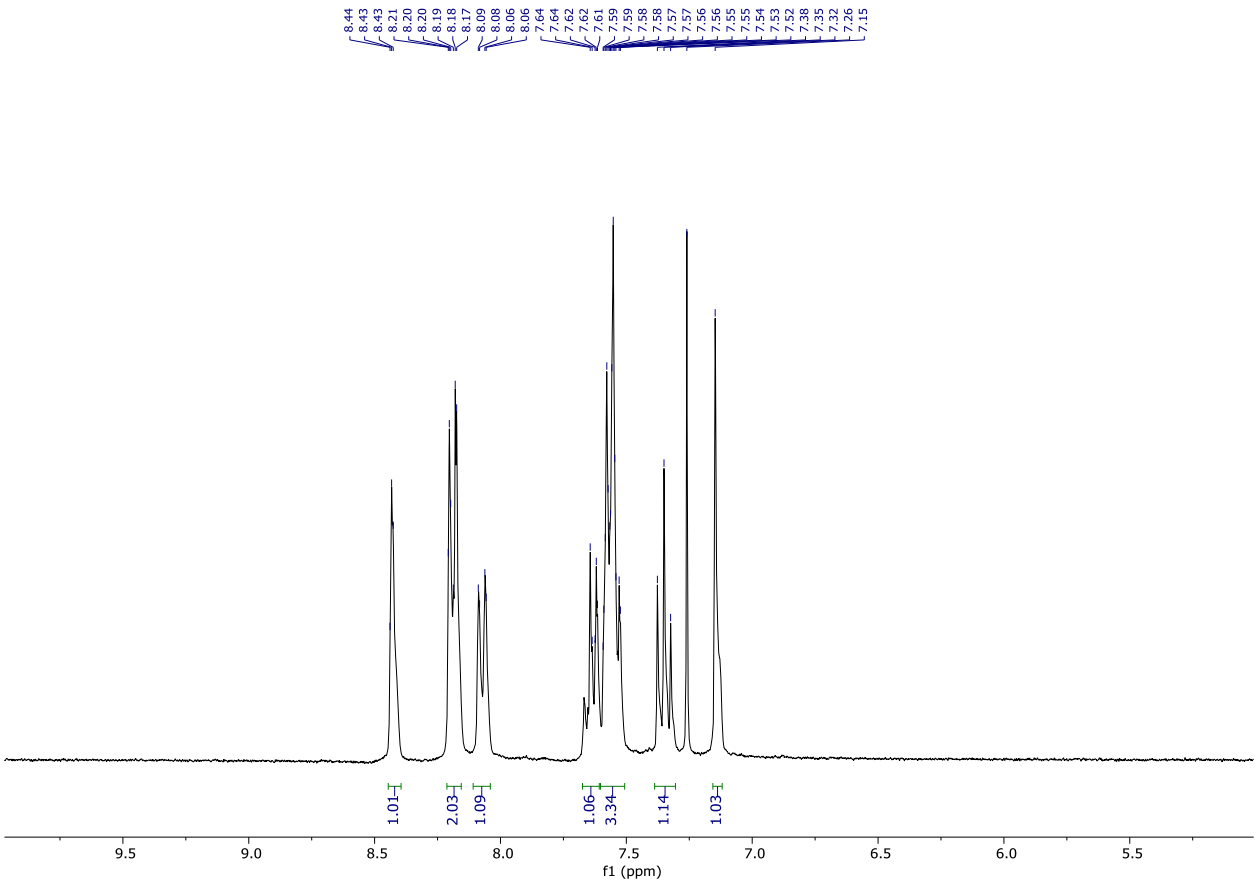
^{1}H NMR ($CDCl_3$, 300.13 MHz) spectrum of oxazolone **1i**



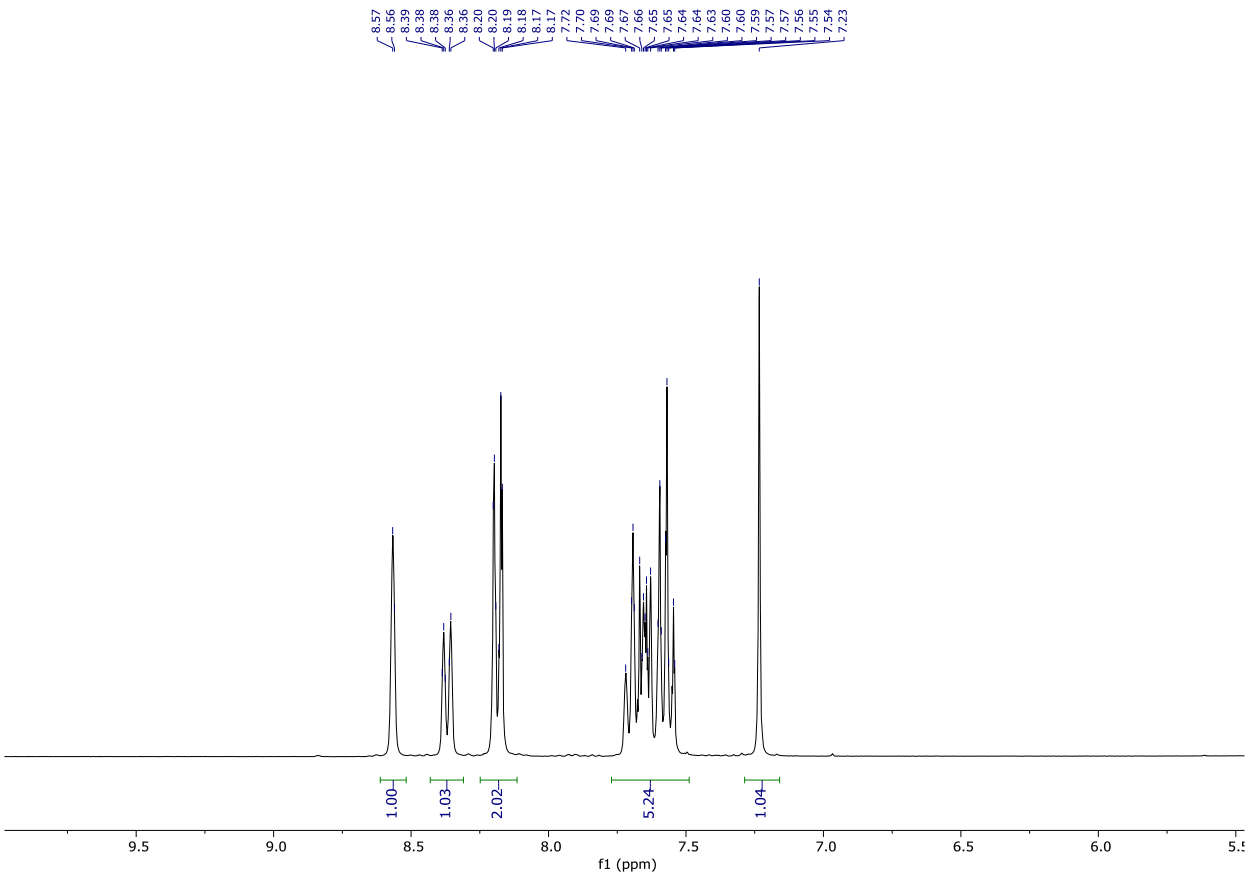
^{1}H NMR ($CDCl_3$, 300.13 MHz) spectrum of oxazolone **1j**



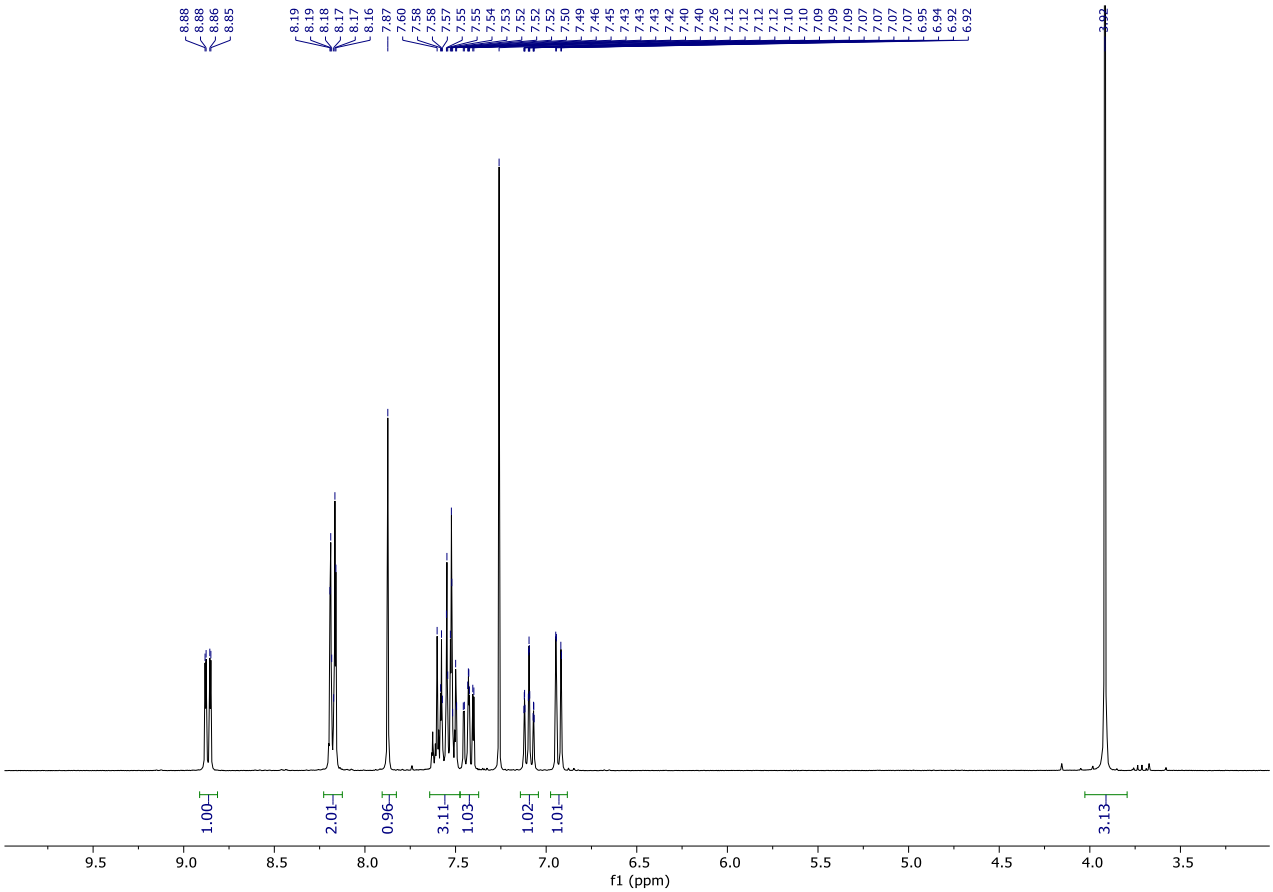
^{1}H NMR ($CDCl_3$, 300.13 MHz) spectrum of oxazolone **1k**



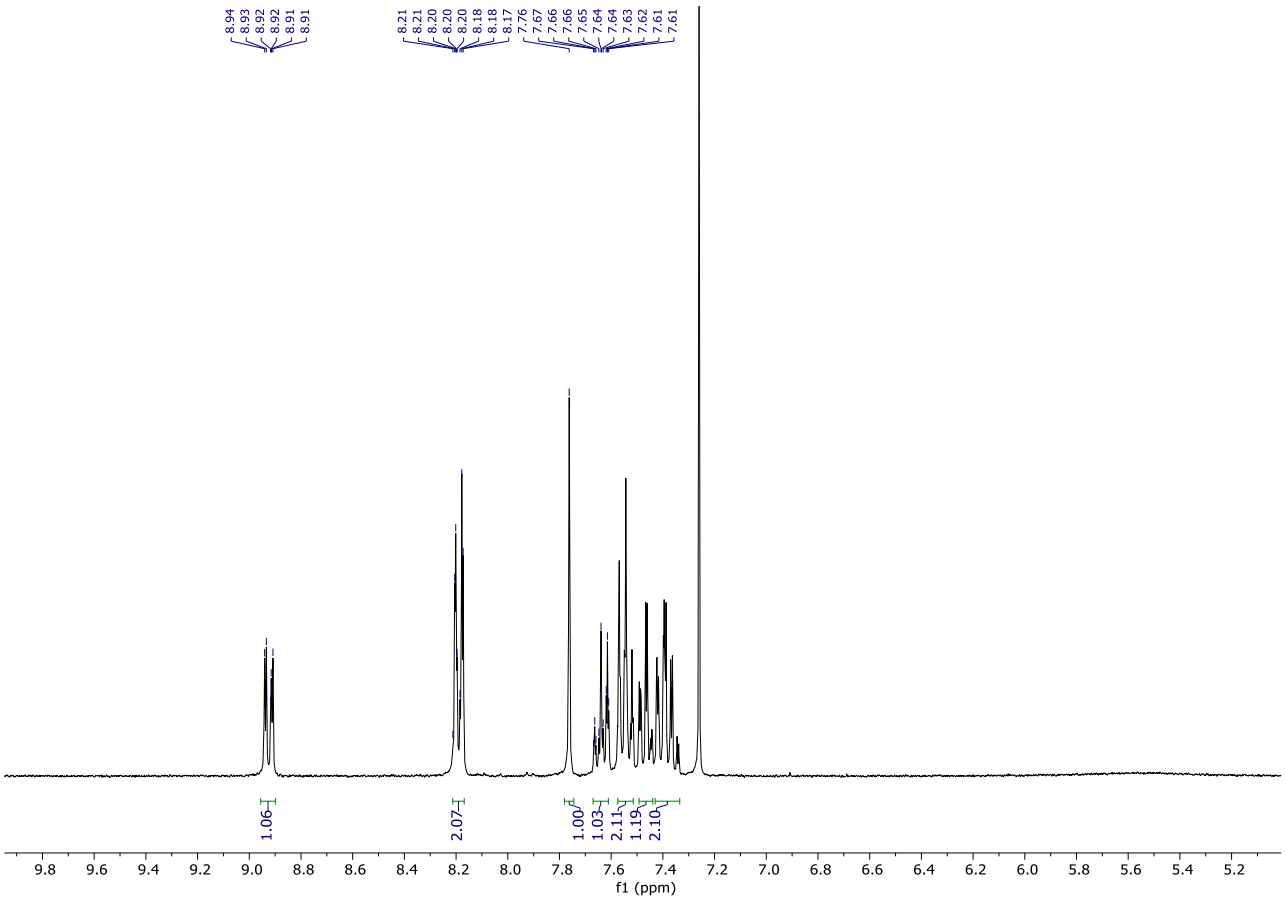
^{1}H NMR ($CDCl_3$, 300.13 MHz) spectrum of oxazolone **1l**



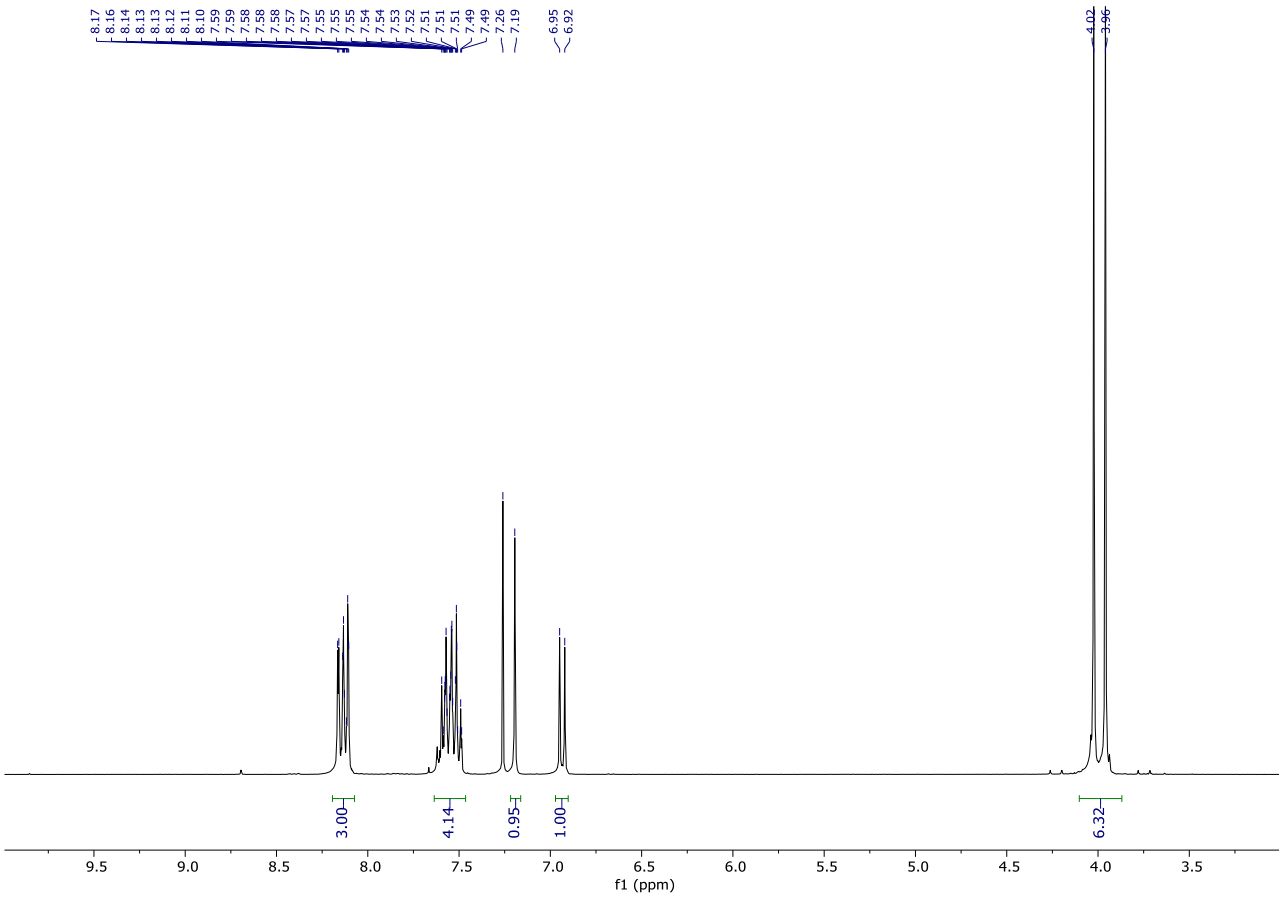
^{1}H NMR (CD_2Cl_2, 300.13 MHz) spectrum of oxazolone **1m**



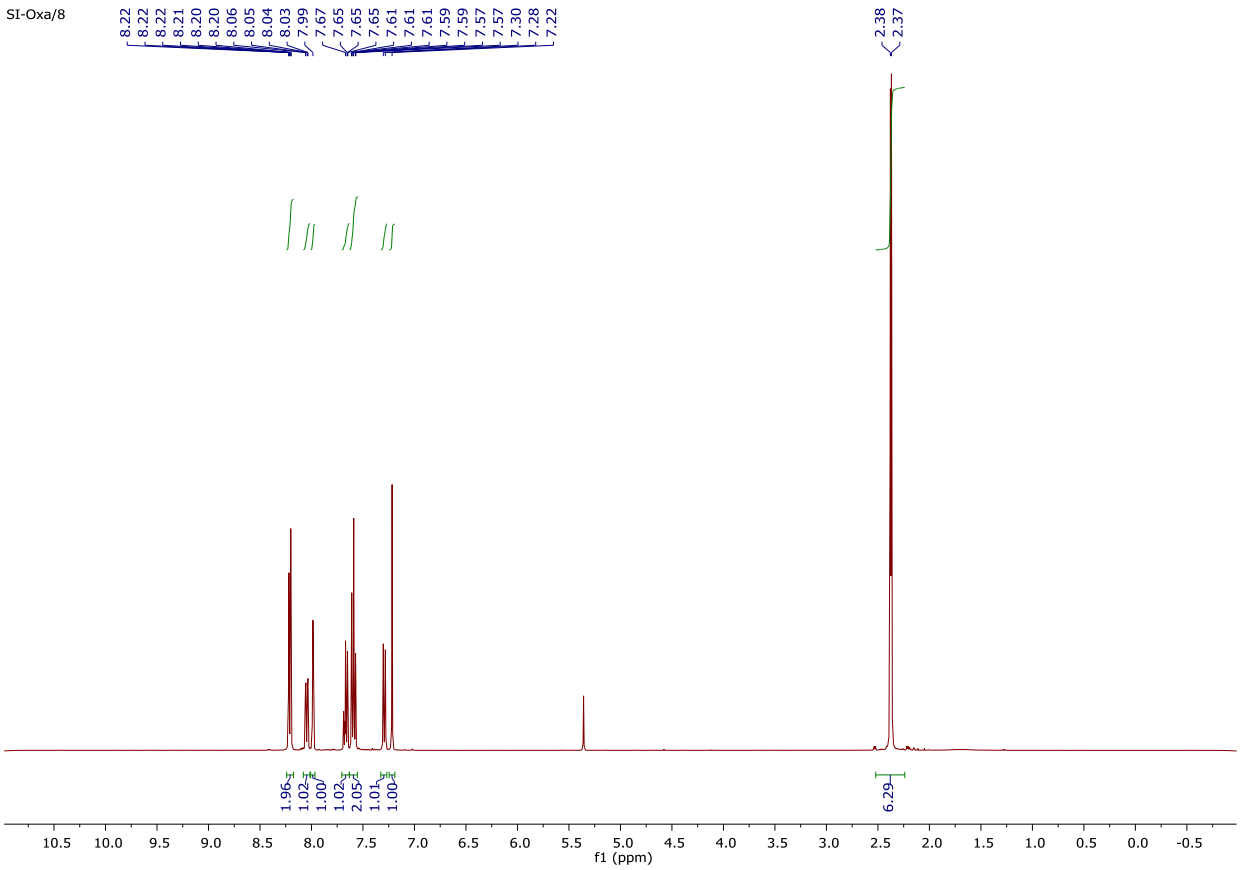
^{1}H NMR ($CDCl_3$, 300.13 MHz) spectrum of oxazolone **1n**



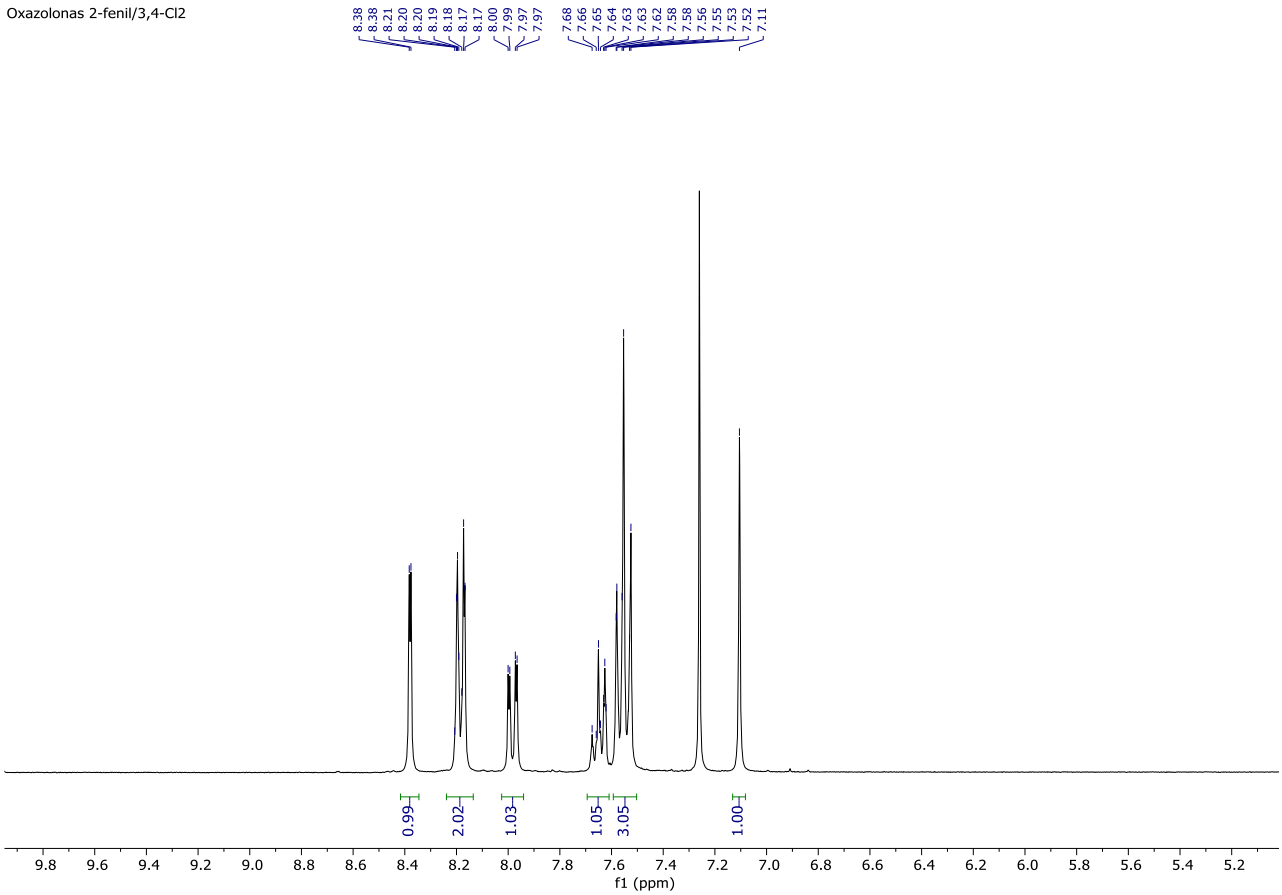
^{1}H NMR ($CDCl_3$, 300.13 MHz) spectrum of oxazolone **1o**



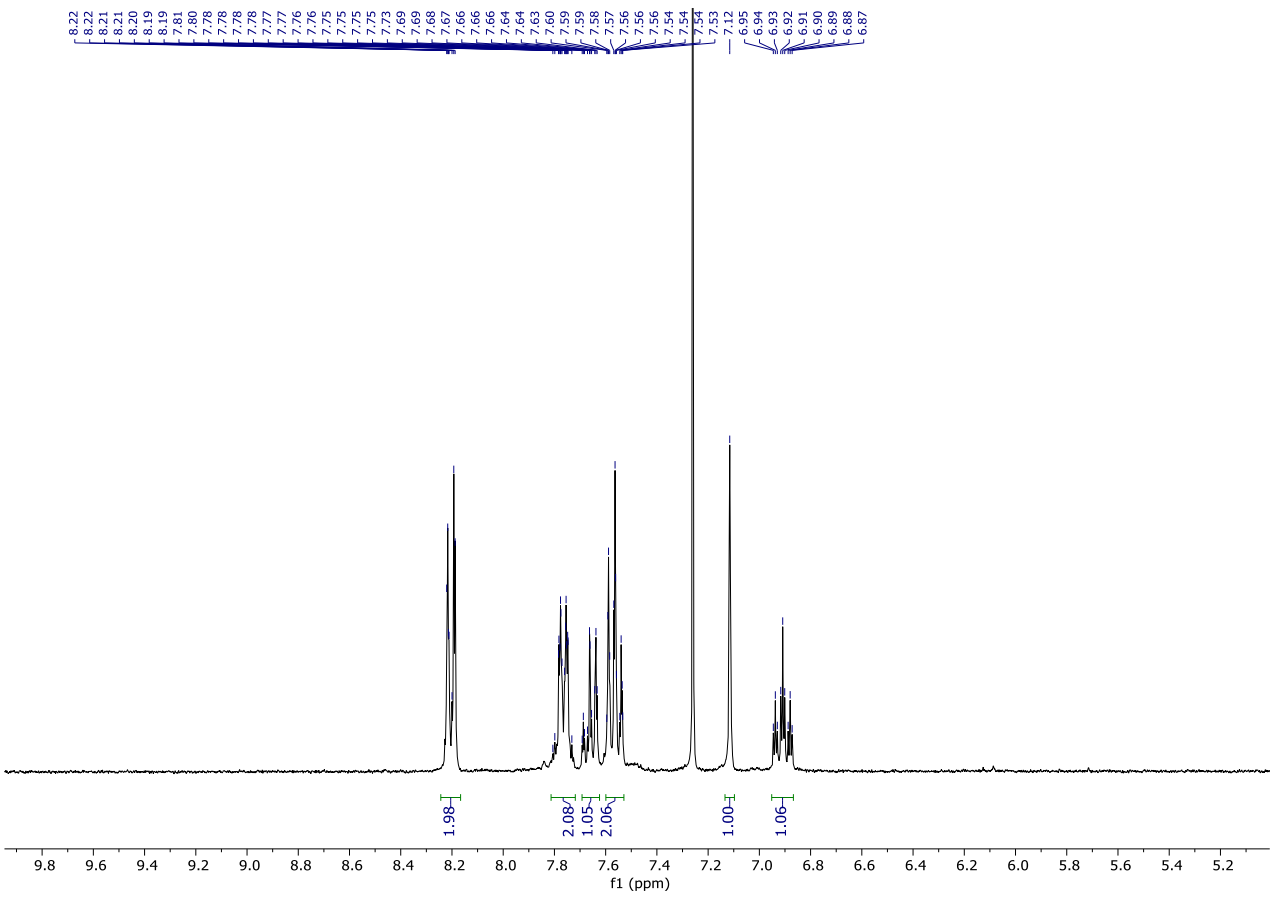
^{1}H NMR ($CDCl_3$, 300.13 MHz) spectrum of oxazolone **1p**



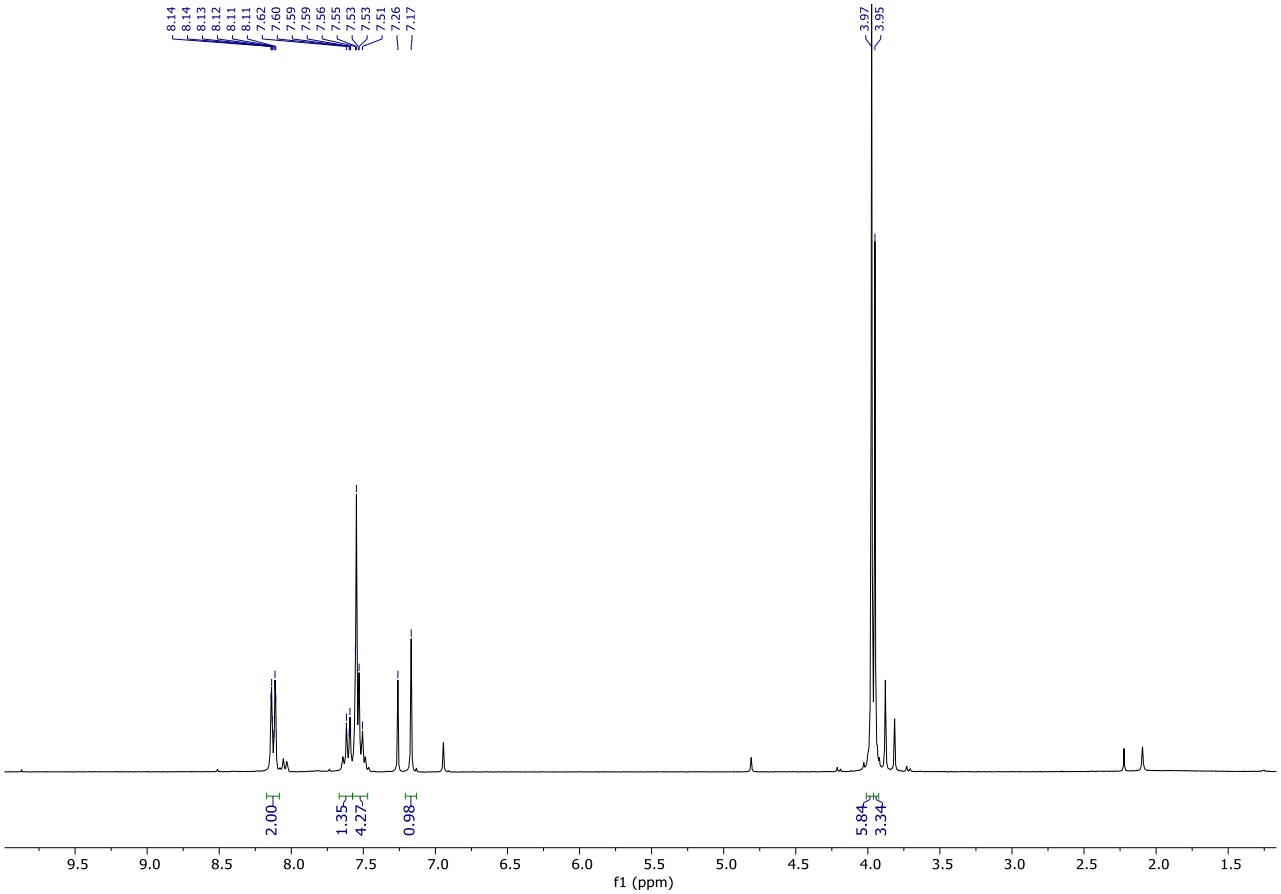
^{1}H NMR (CD_2Cl_2, 300.13 MHz) spectrum of oxazolone **1q**



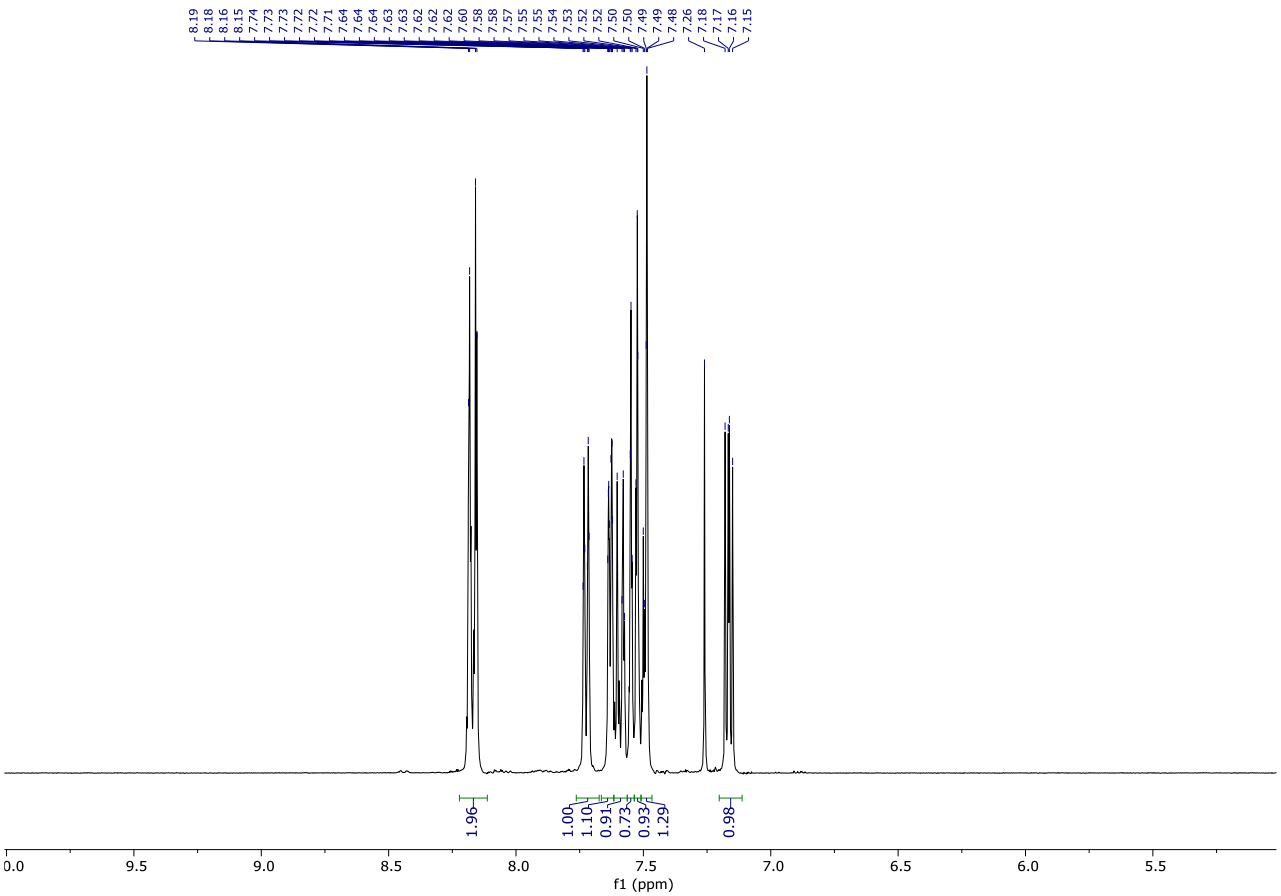
^{1}H NMR ($CDCl_3$, 300.13 MHz) spectrum of oxazolone **1r**



^{1}H NMR ($CDCl_3$, 300.13 MHz) spectrum of oxazolone **1s**

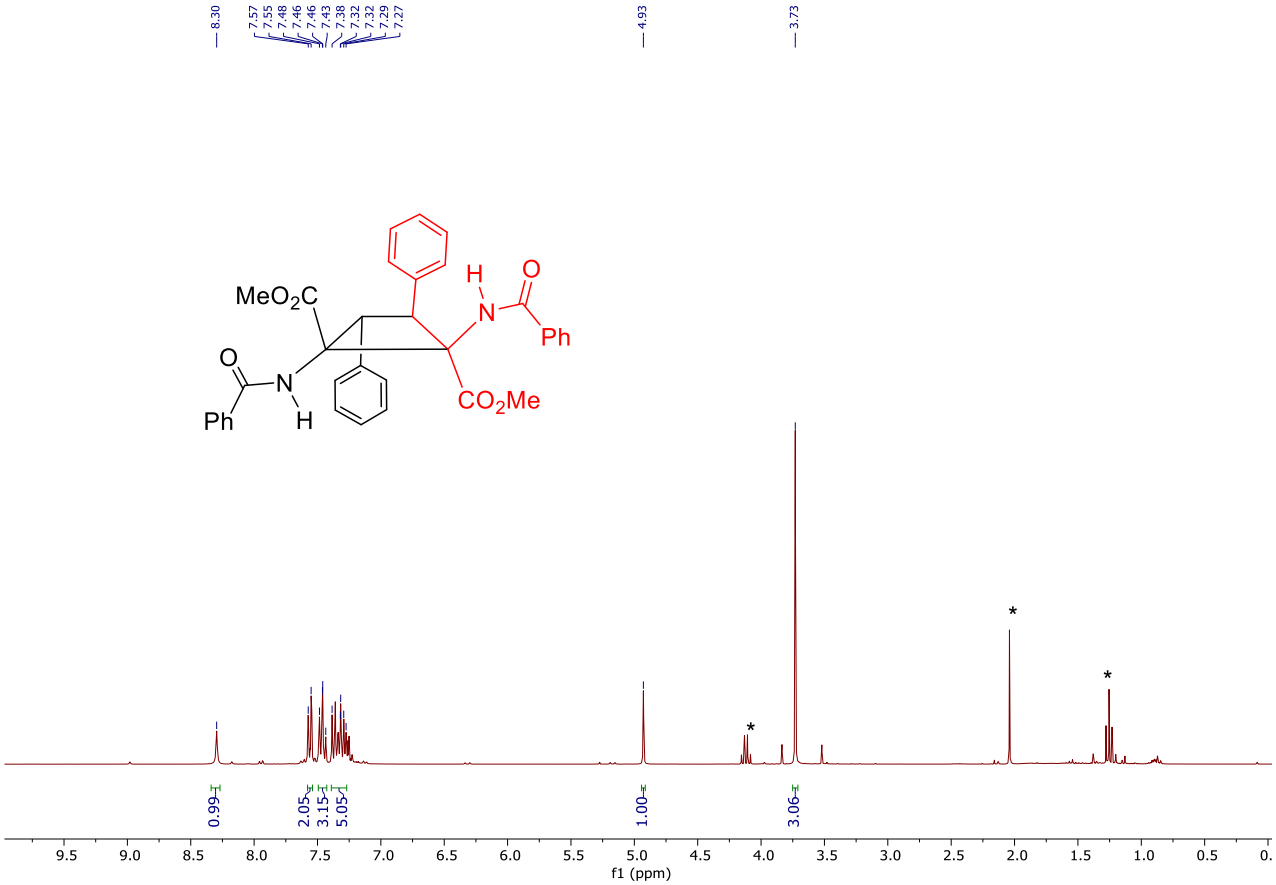


^{1}H NMR ($CDCl_3$, 300.13 MHz) spectrum of oxazolone **1t**

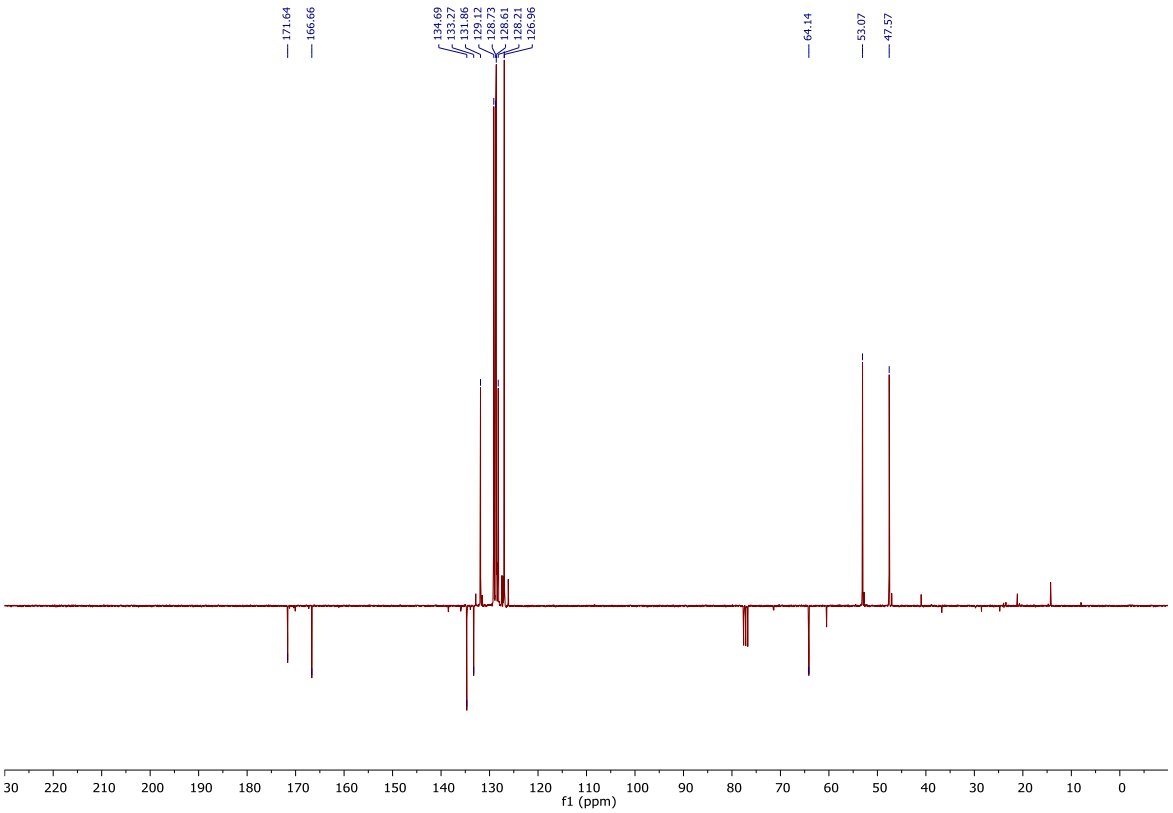


^{1}H NMR ($CDCl_3$, 300.13 MHz) spectrum of oxazolone **1u**

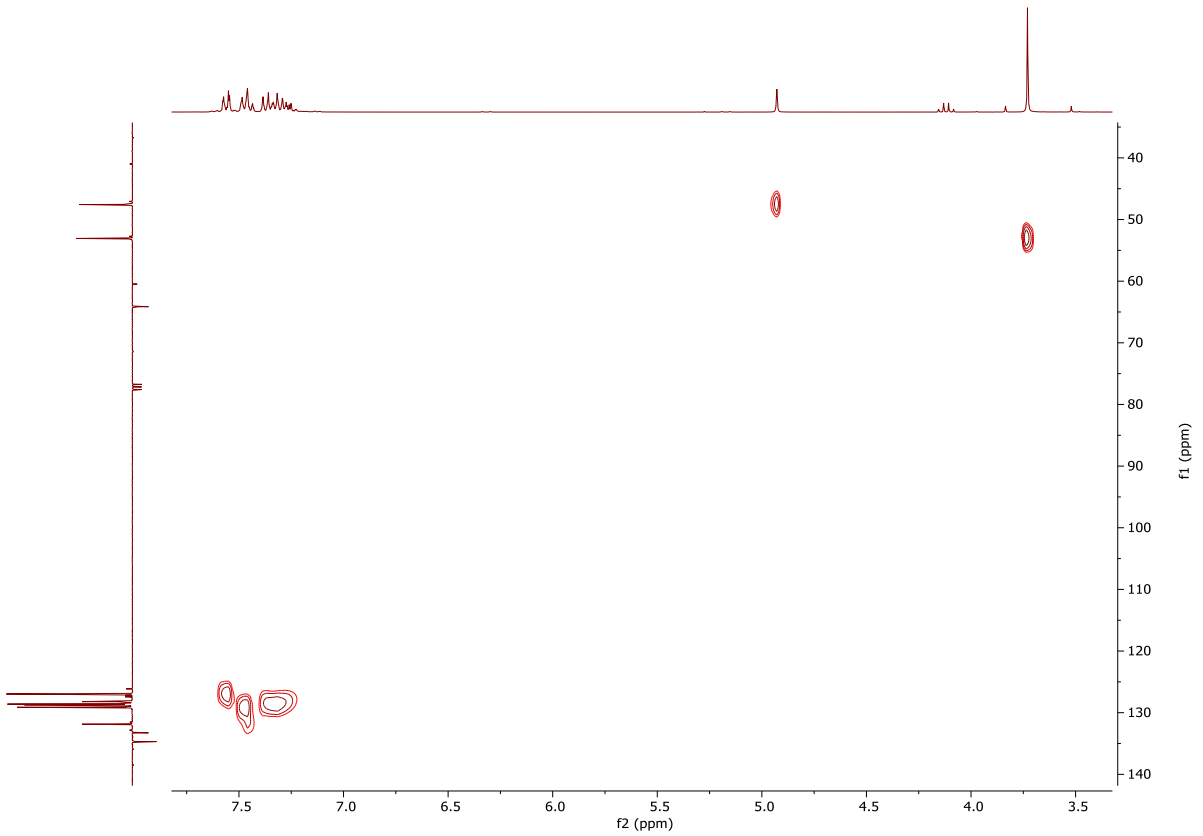
4.- Copies of NMR spectra of delta-1,2-diaminotruxinic derivatives 2a-2u



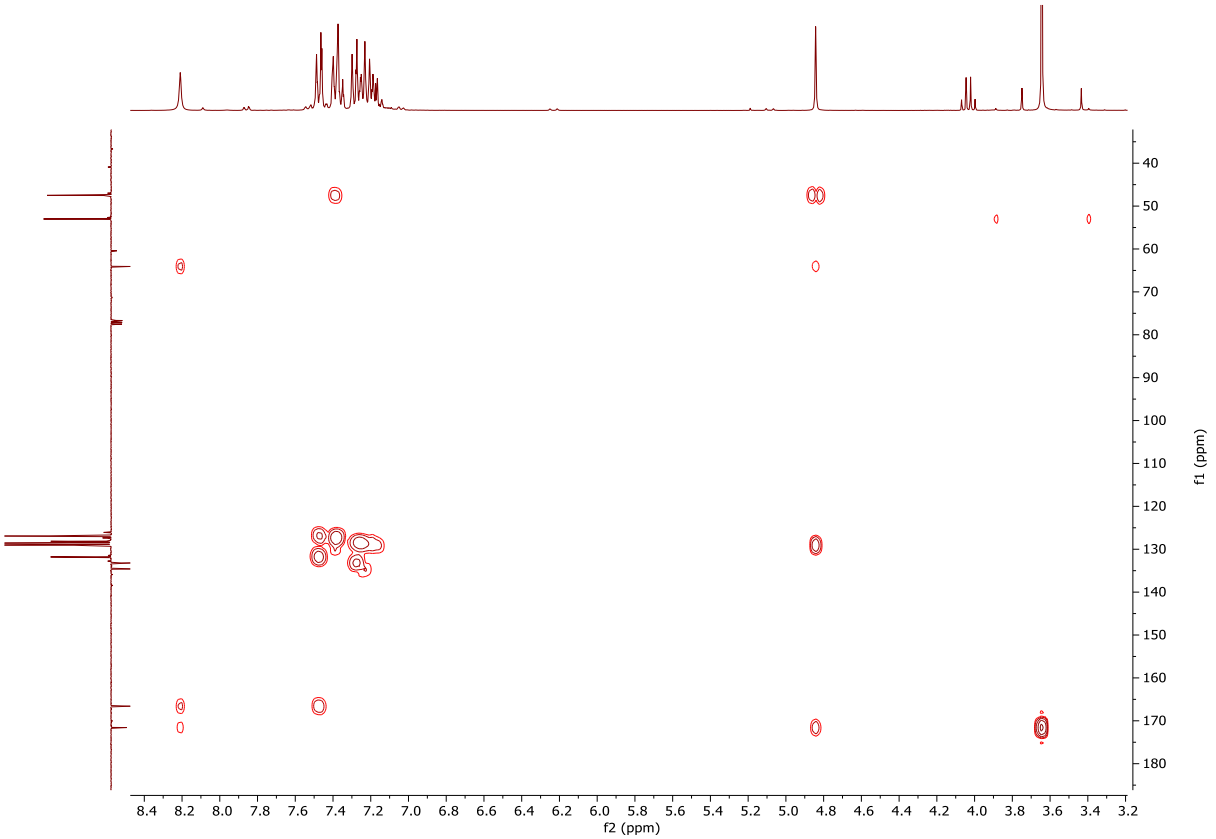
^{1}H NMR spectrum ($CDCl_3$, 300.13 MHz) of **2a** (* = ethyl acetate).



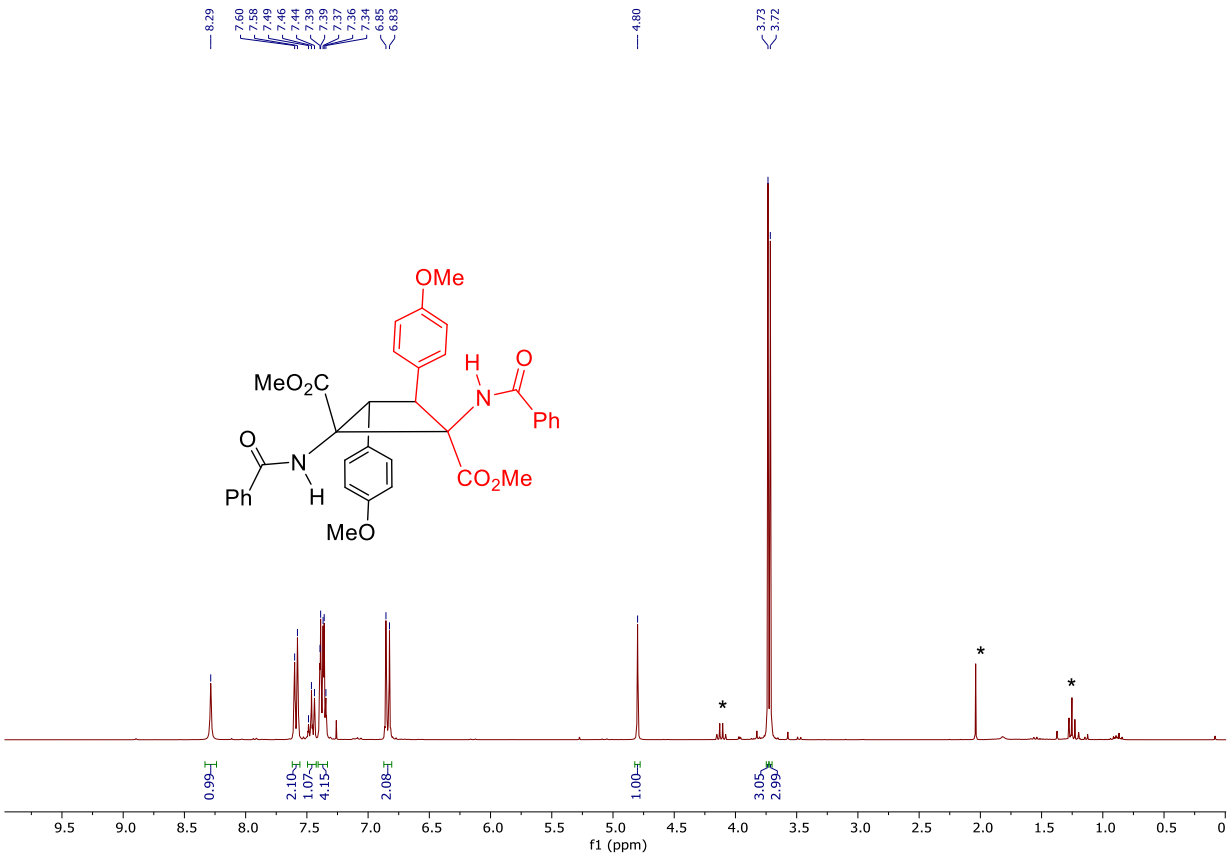
^{13}C{^{1}H} (APT) NMR spectrum ($CDCl_3$, 75.5 MHz) of **2a**



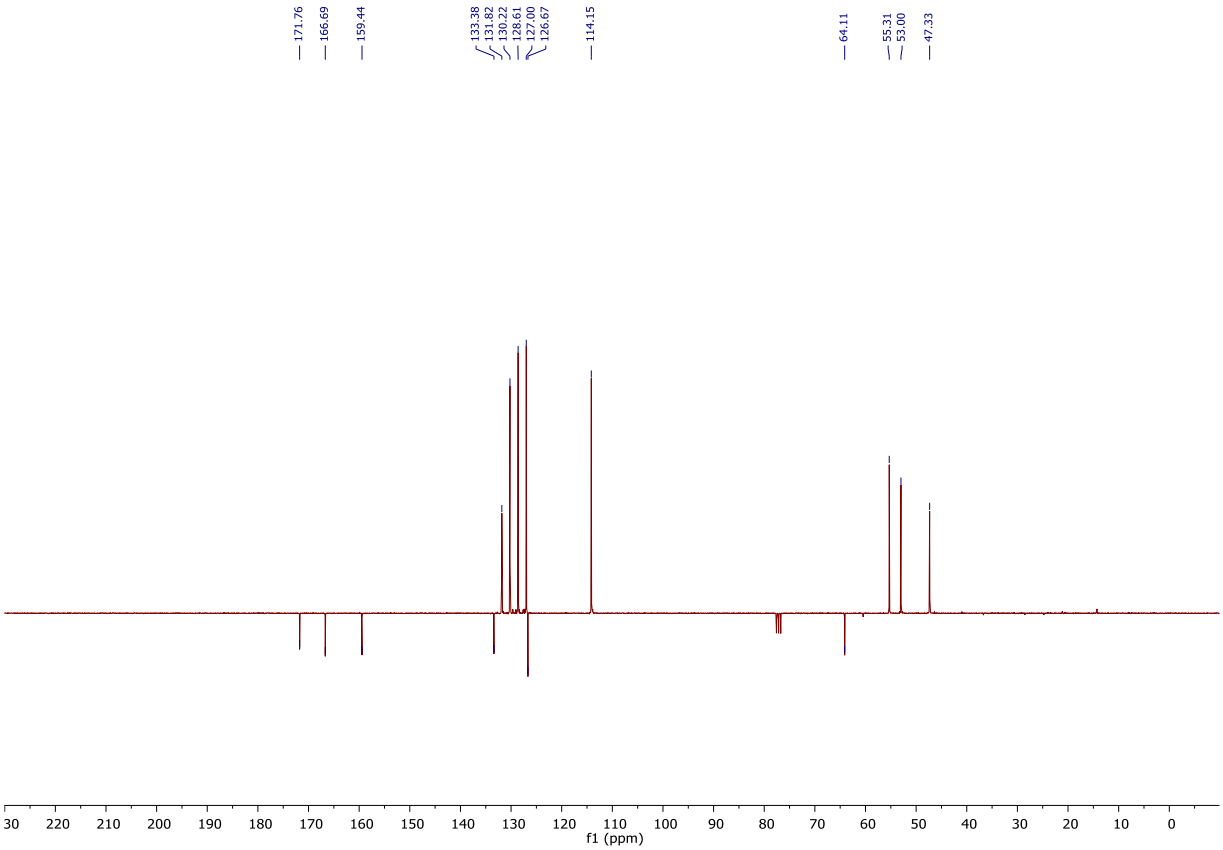
^{1}H-^{13}C HSQC ($CDCl_3$) correlation spectrum of **2a**



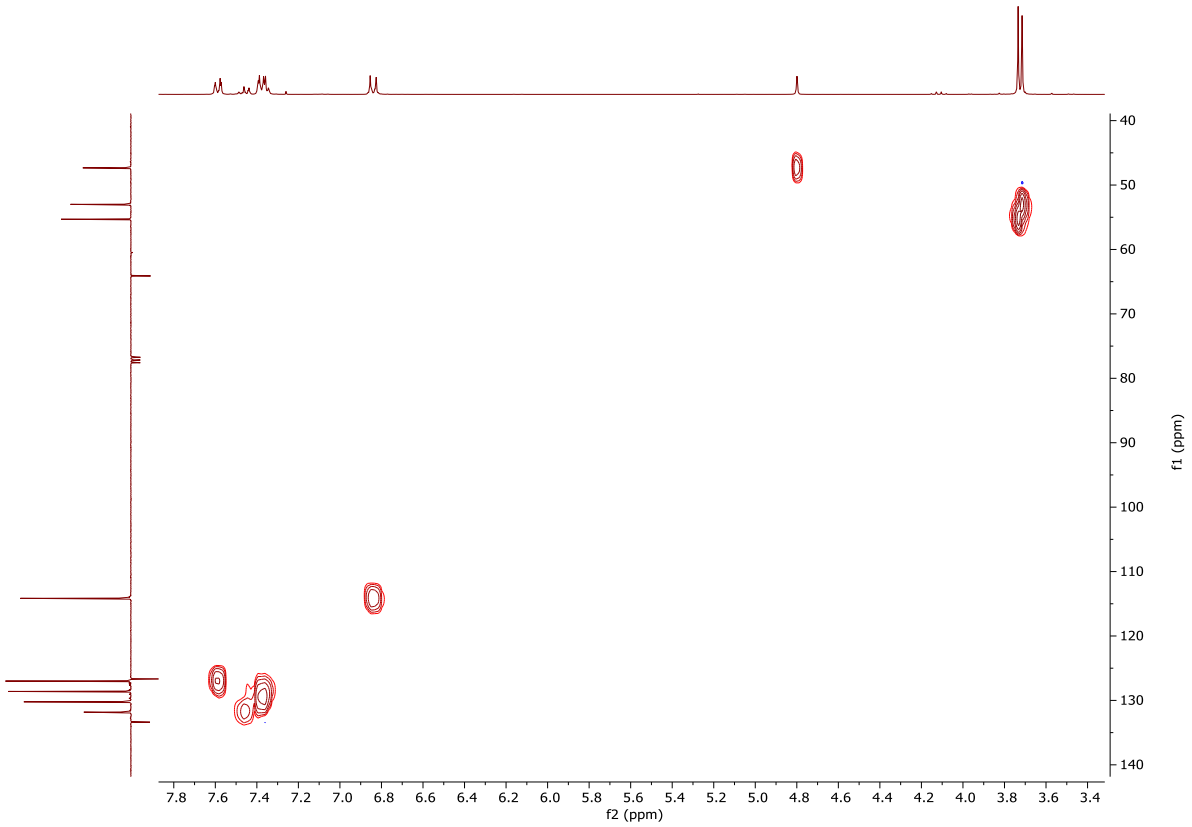
^{1}H-^{13}C HMBC ($CDCl_3$) correlation spectrum of **2a**



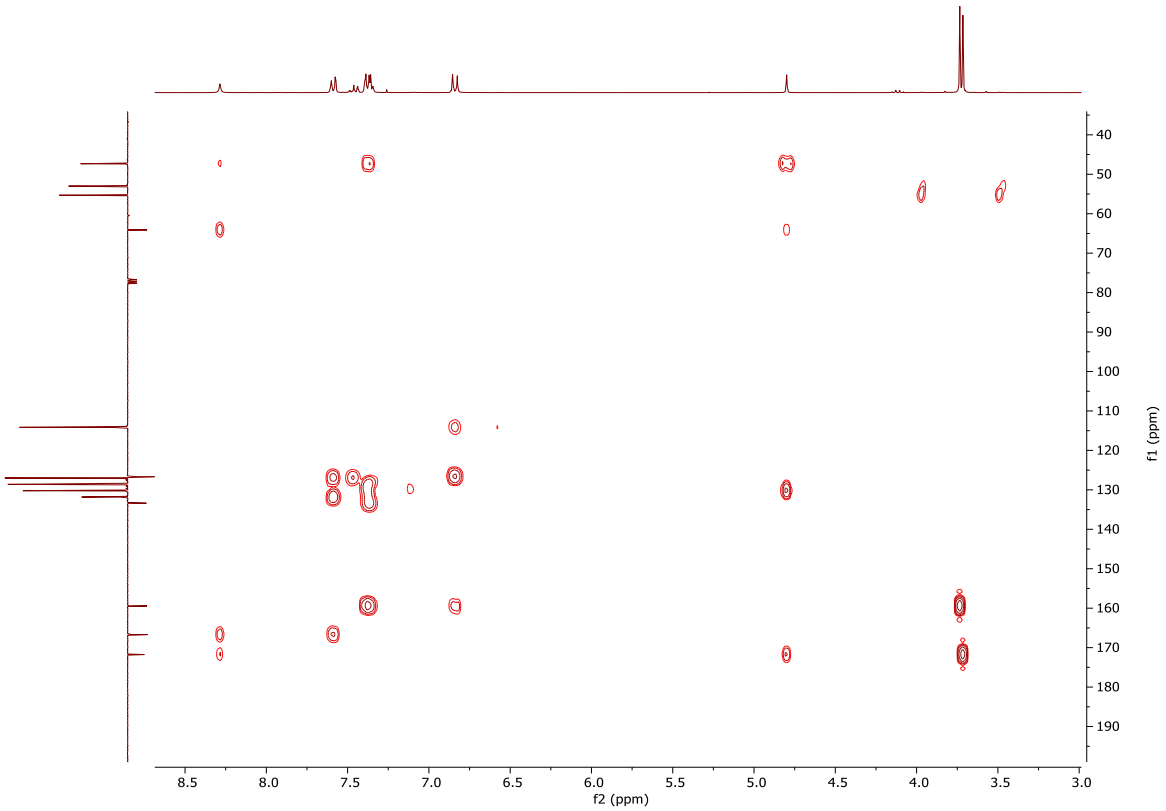
^{1}H NMR spectrum ($CDCl_3$, 300.13 MHz) of **2b** (* = ethyl acetate)



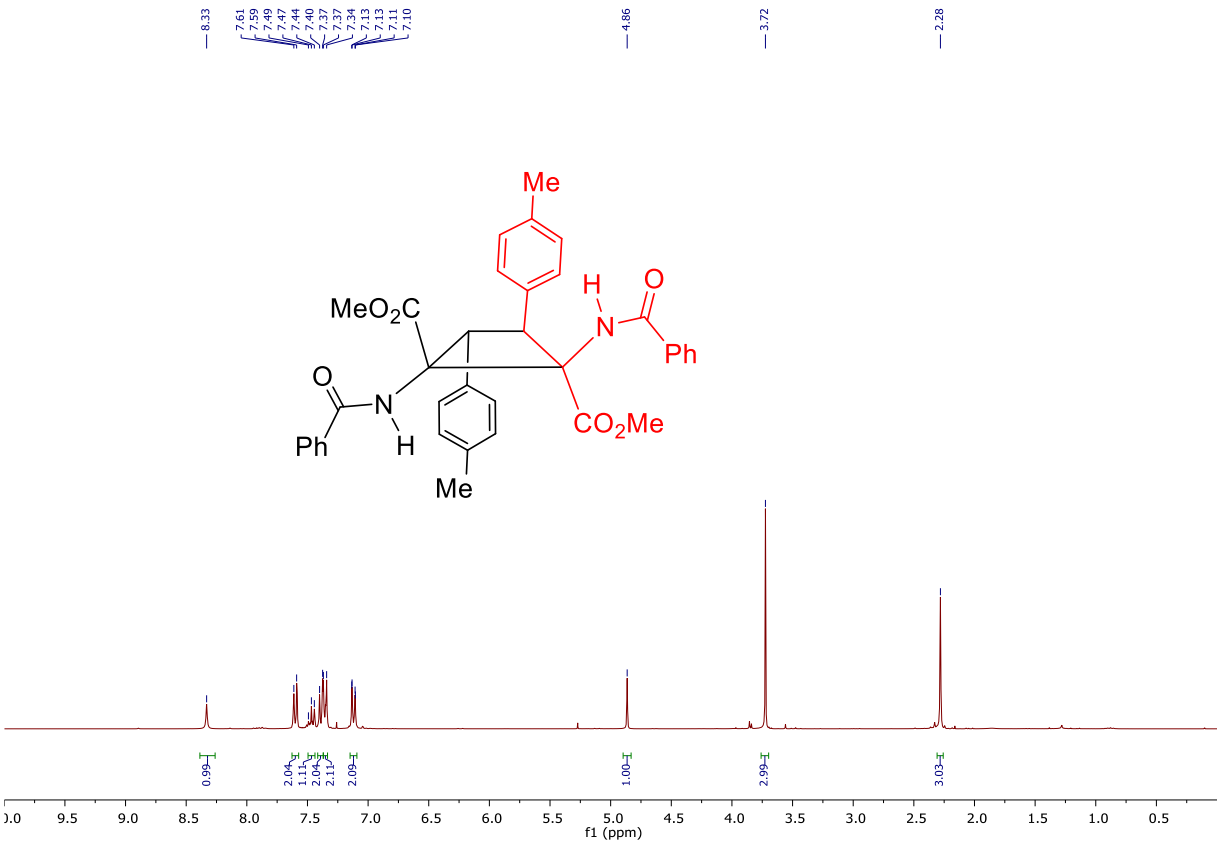
^{13}C{^{1}H} (APT) NMR spectrum ($CDCl_3$, 75.5 MHz) of **2b**



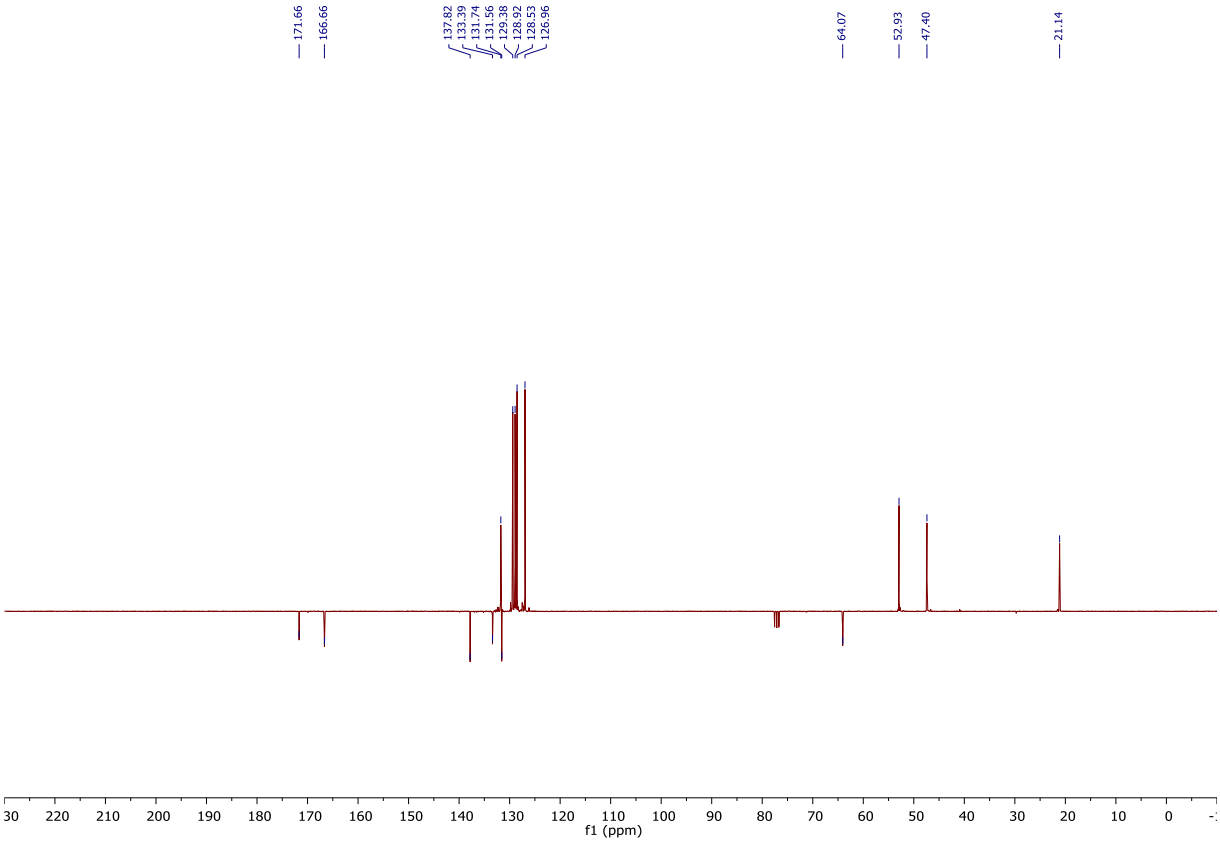
^{1}H-^{13}C HSQC ($CDCl_3$) correlation spectrum of **2b**



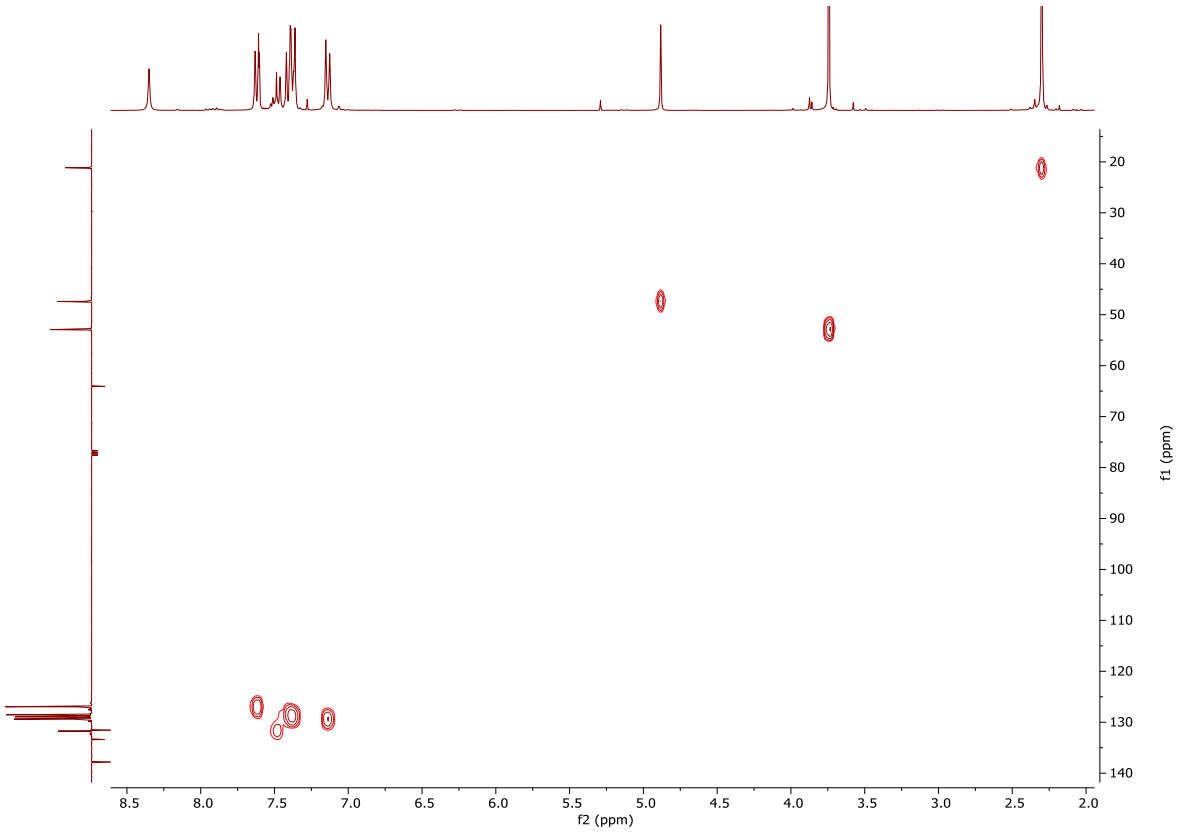
^{1}H-^{13}C HMBC ($CDCl_3$) correlation spectrum of **2b**



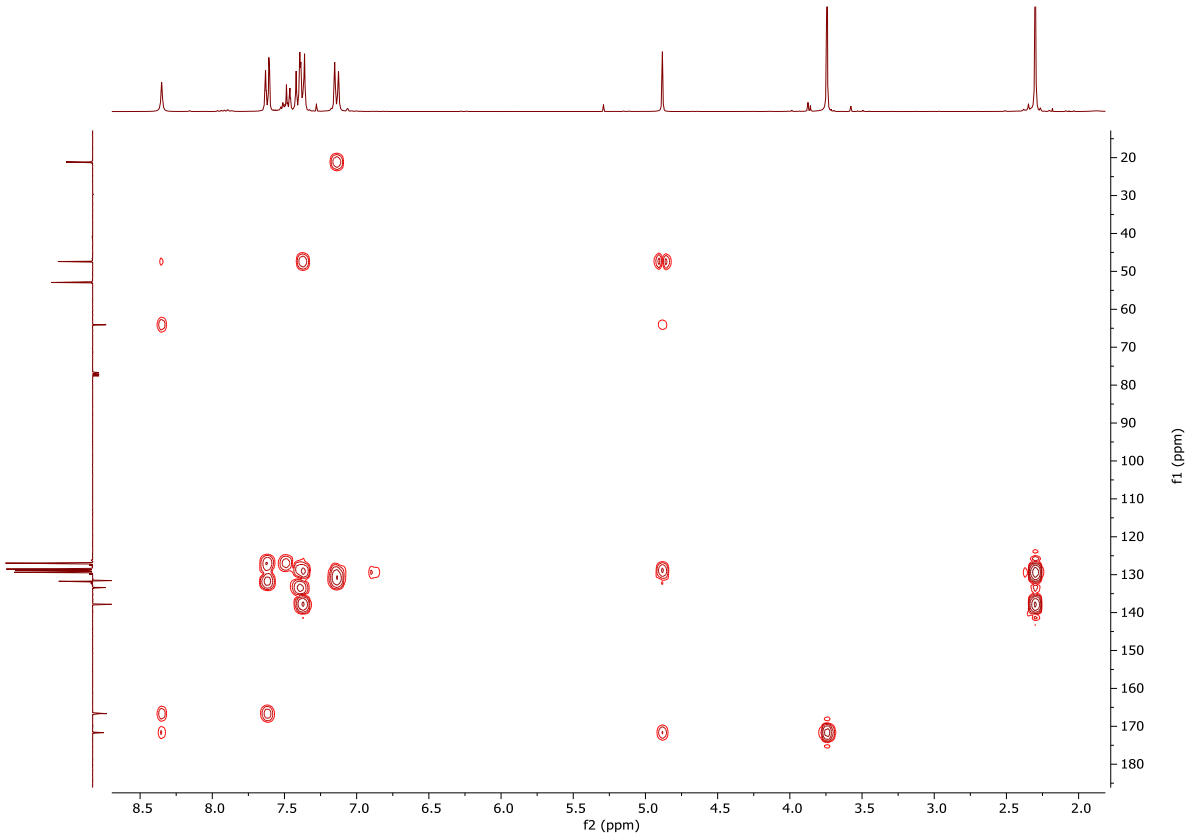
^{1}H NMR spectrum ($CDCl_3$, 300.13 MHz) of **2c**



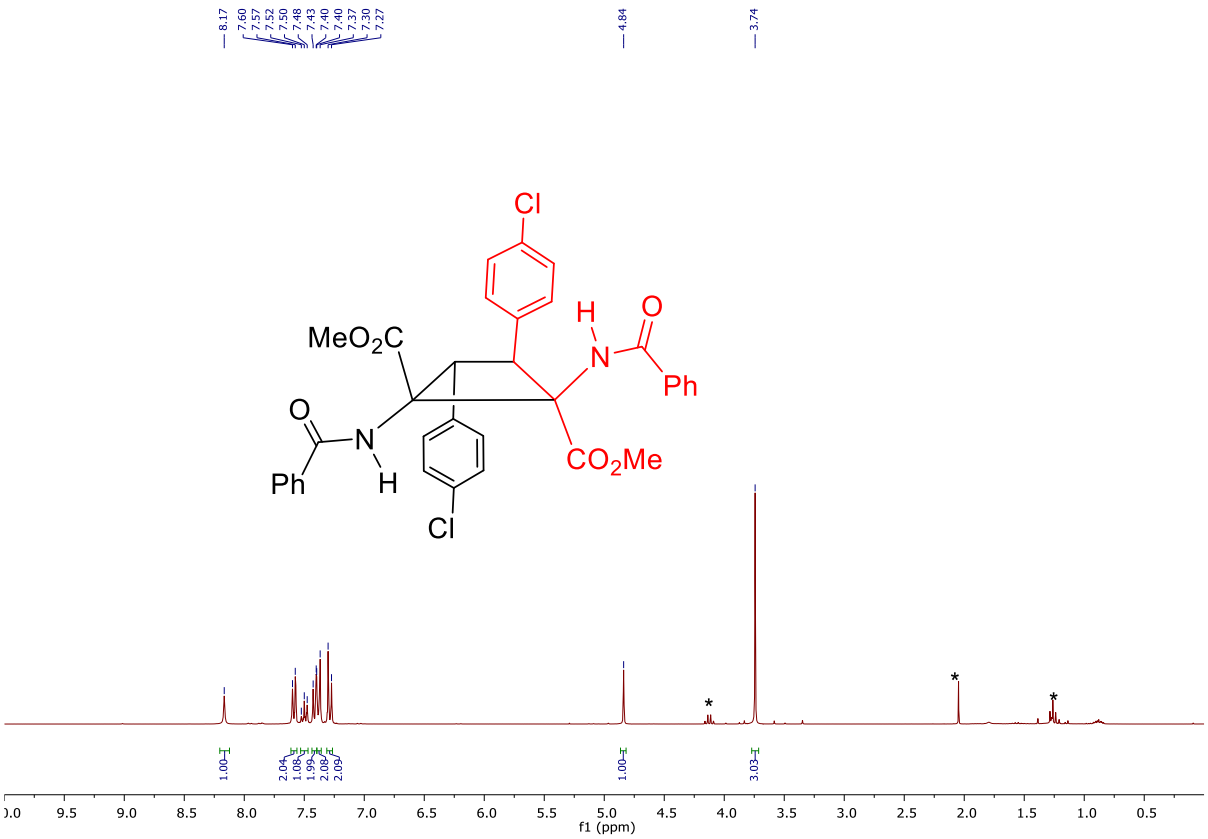
^{13}C{^{1}H} (APT) NMR spectrum ($CDCl_3$, 75.5 MHz) of **2c**



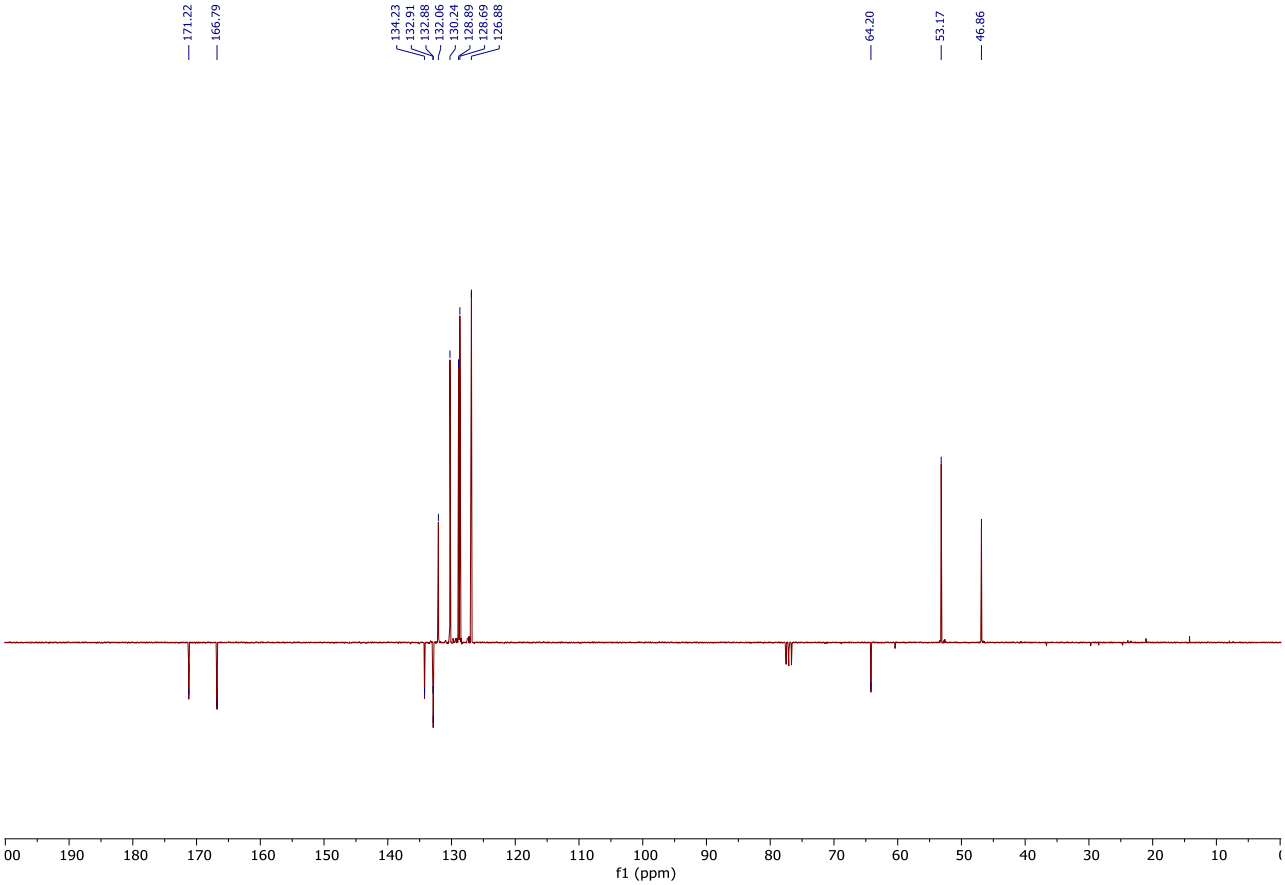
^{1}H-^{13}C HSQC ($CDCl_3$) correlation spectrum of **2c**



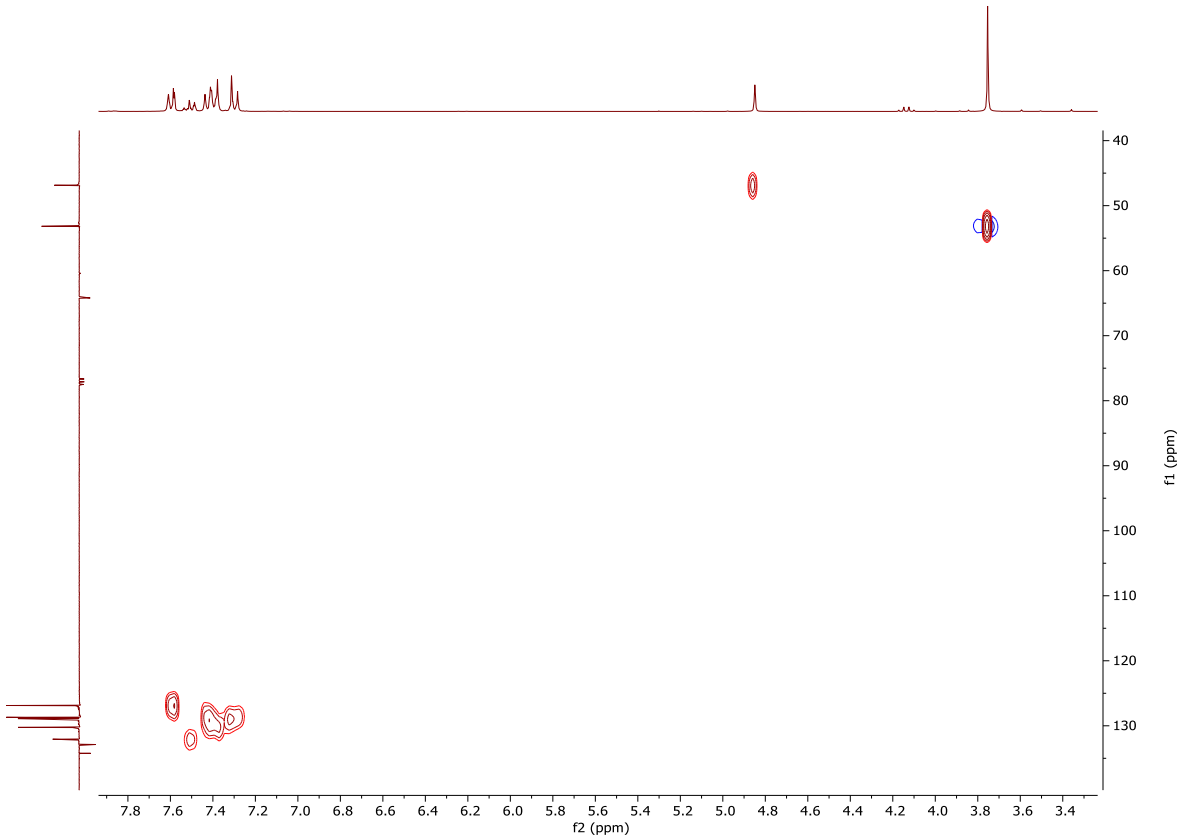
^{1}H-^{13}C HMBC ($CDCl_3$) correlation spectrum of **2c**



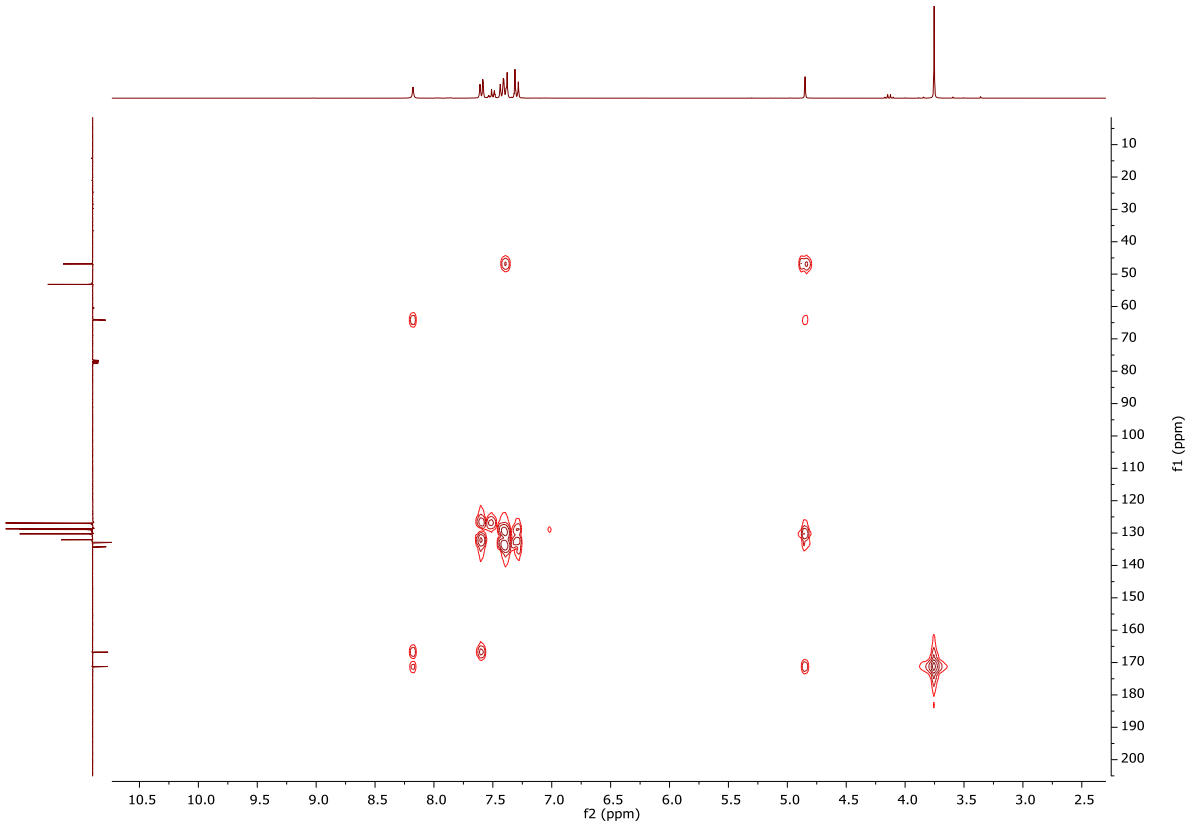
^{1}H NMR spectrum ($CDCl_3$, 300.13 MHz) of **2d** (* = ethyl acetate)



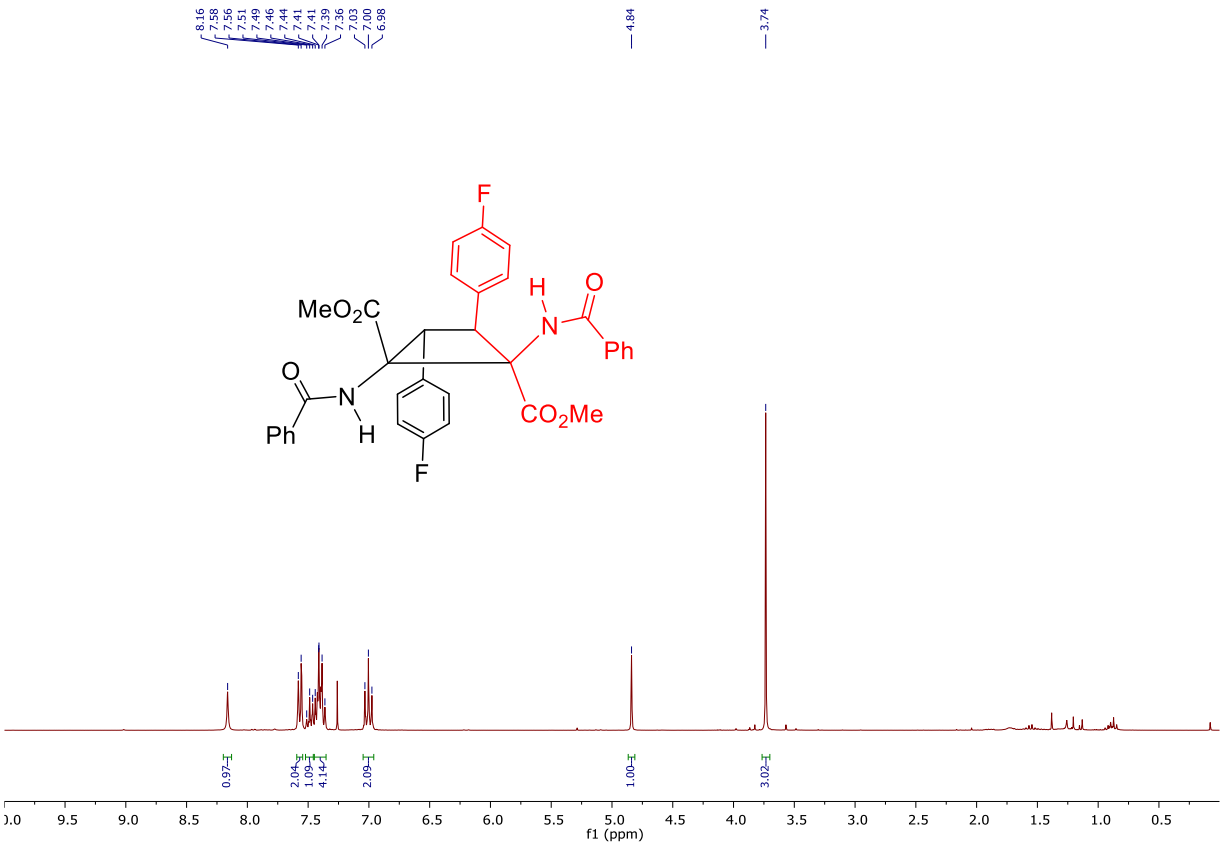
^{13}C{^{1}H} (APT) NMR spectrum ($CDCl_3$, 75.5 MHz) of **2d**



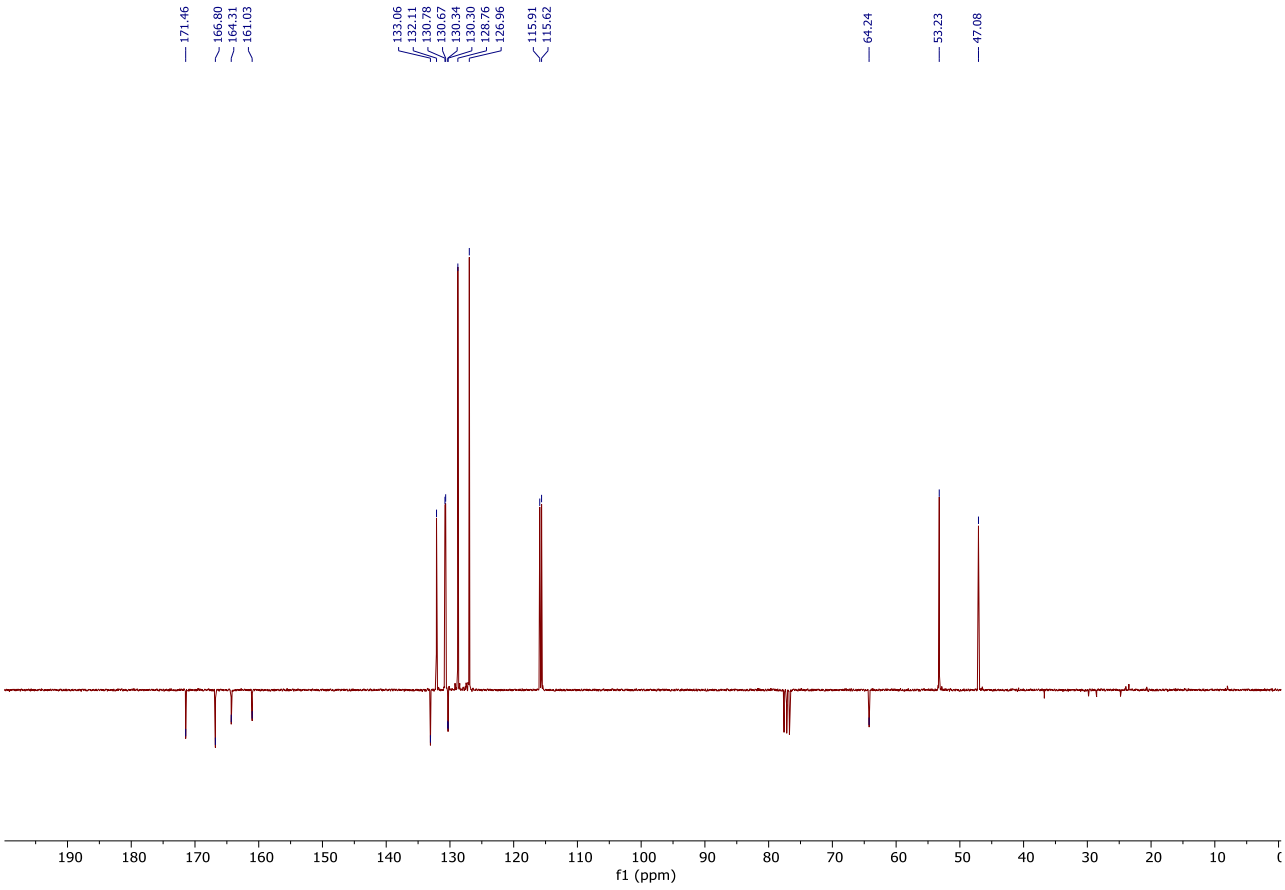
^{1}H-^{13}C HSQC ($CDCl_3$) correlation spectrum of **2d**



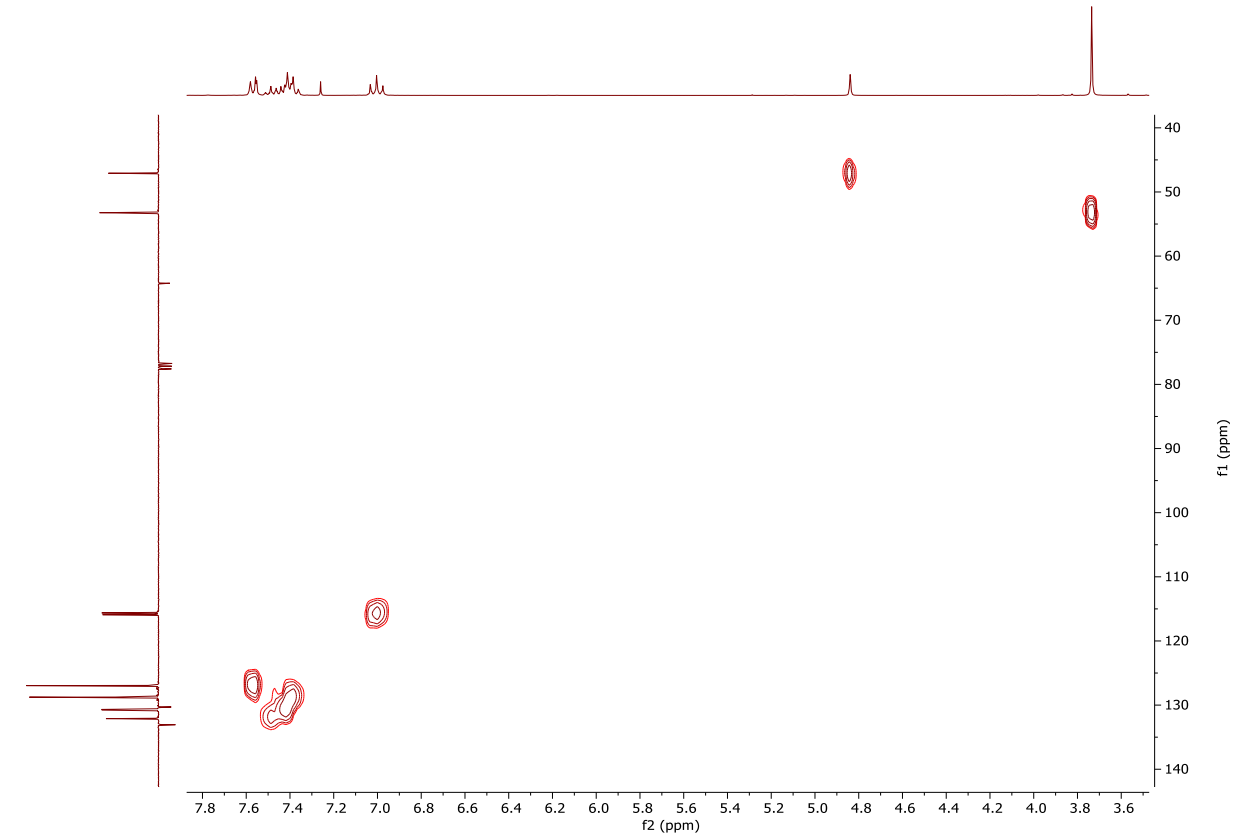
^{1}H-^{13}C HMBC ($CDCl_3$) correlation spectrum of **2d**



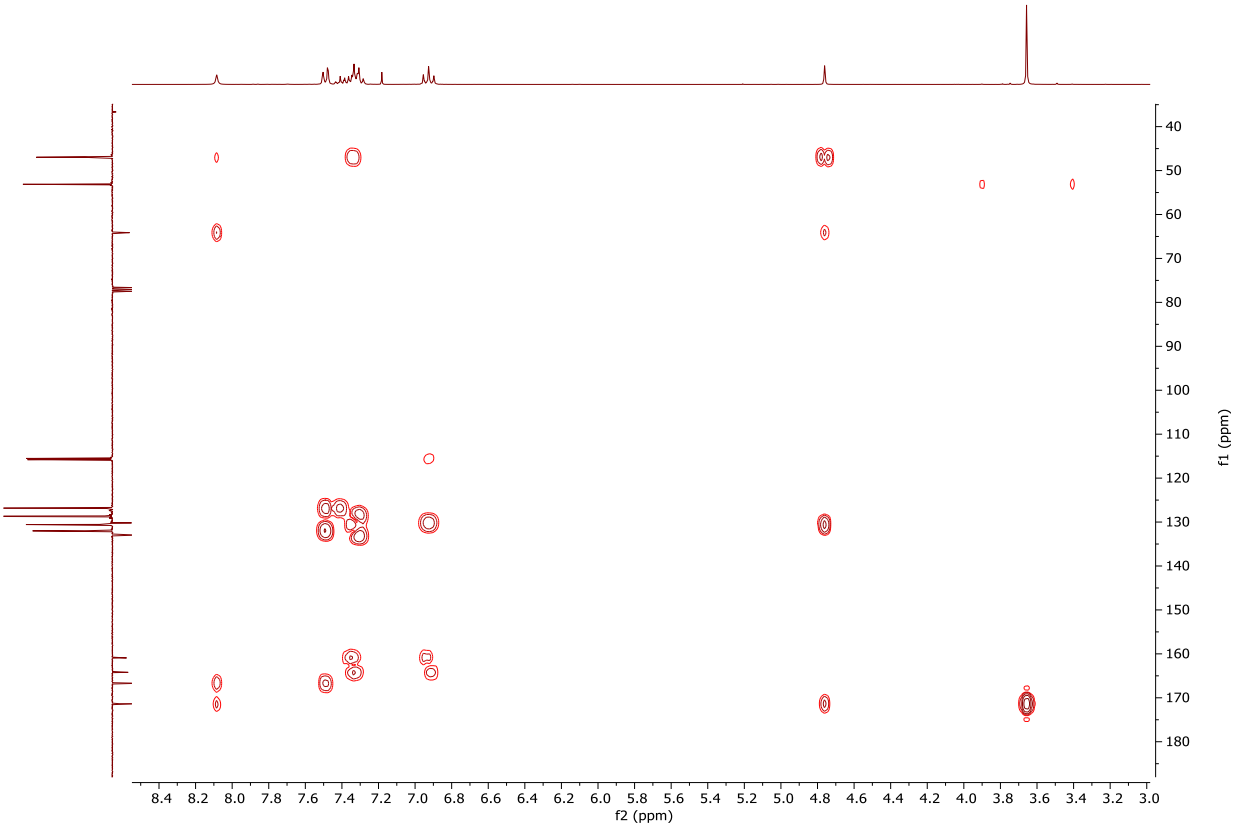
^{1}H NMR spectrum ($CDCl_3$, 300.13 MHz) of **2e**



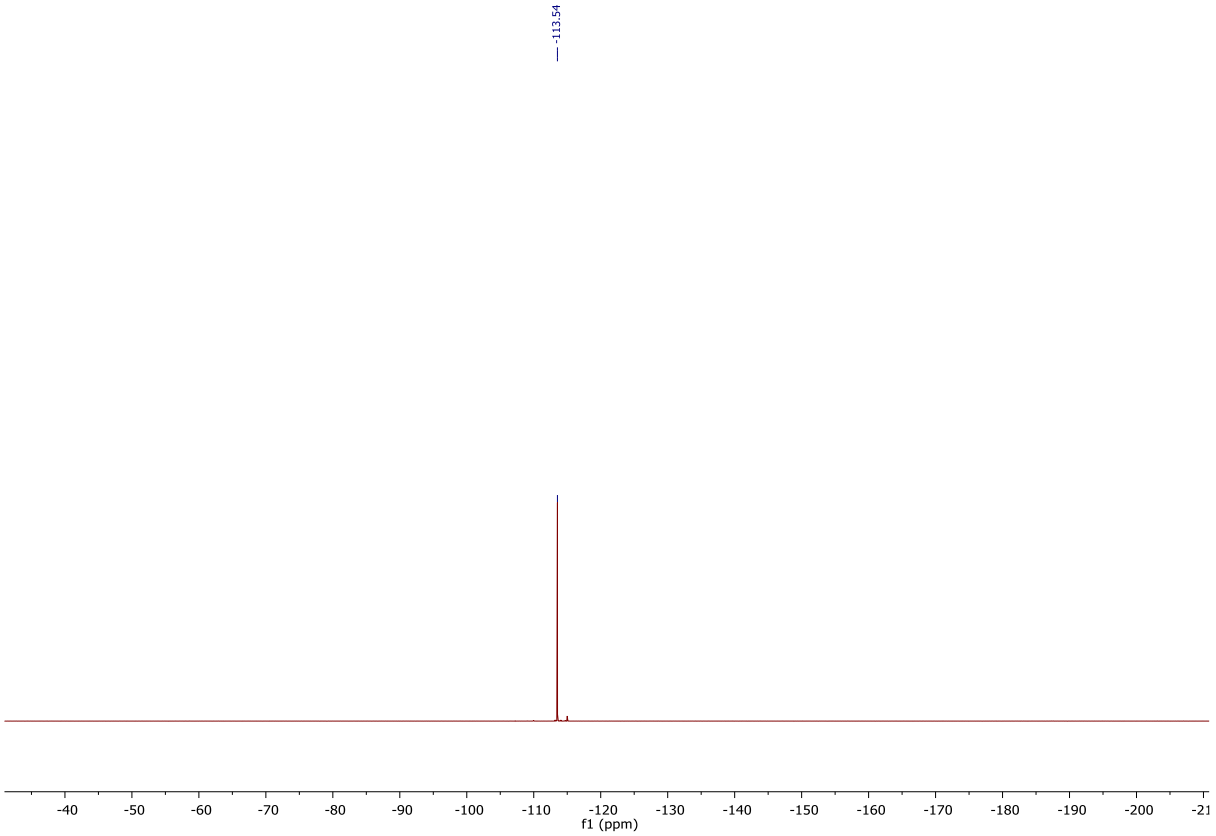
^{13}C{^{1}H} (APT) NMR spectrum ($CDCl_3$, 75.5 MHz) of **2e**



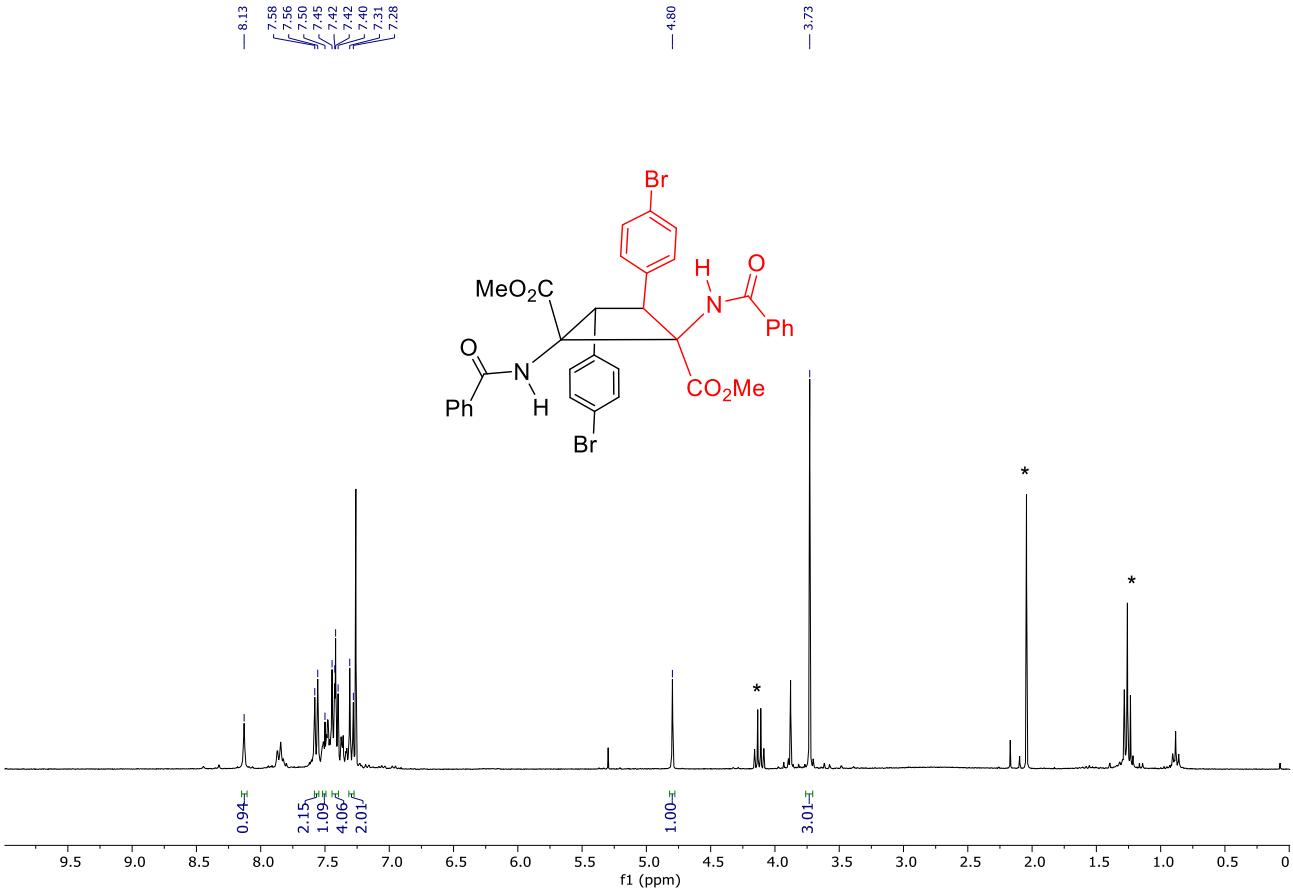
^{1}H-^{13}C HSQC ($CDCl_3$) correlation spectrum of **2e**



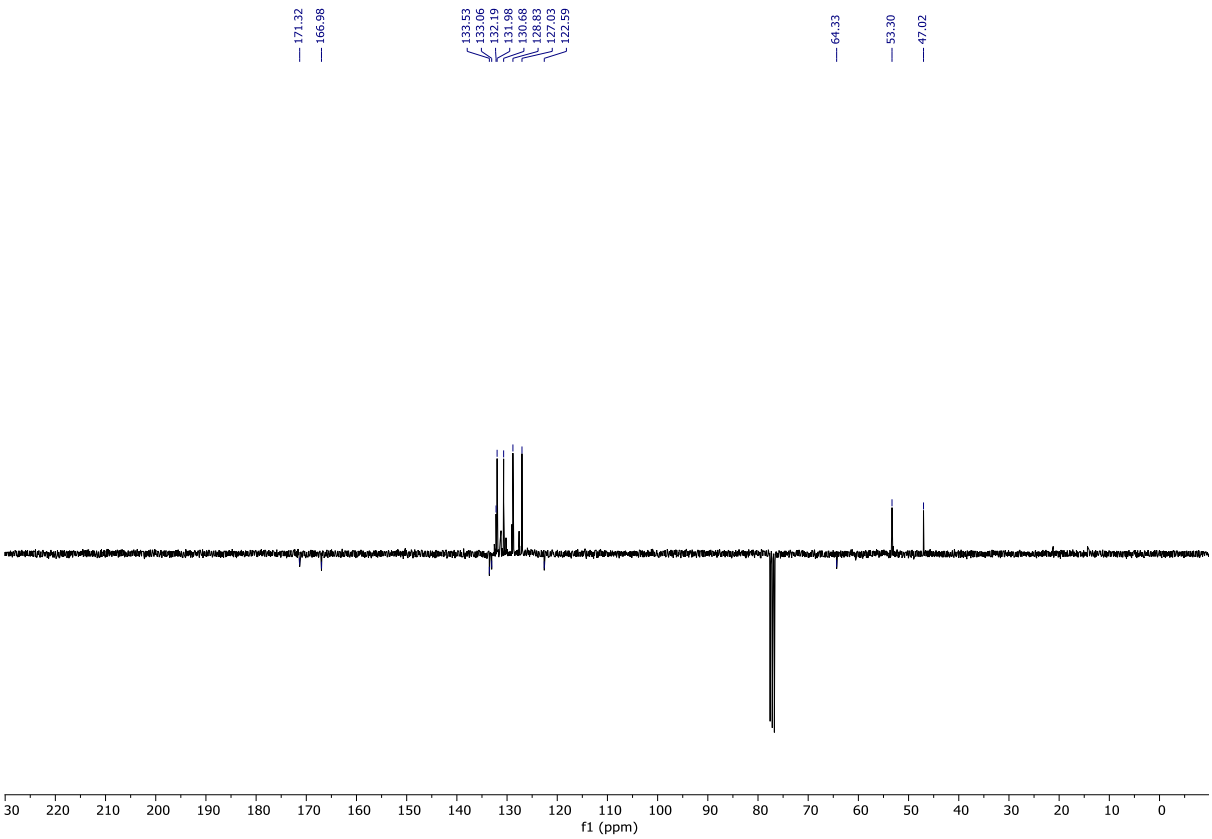
^{1}H-^{13}C HMBC ($CDCl_3$) correlation spectrum of **2e**



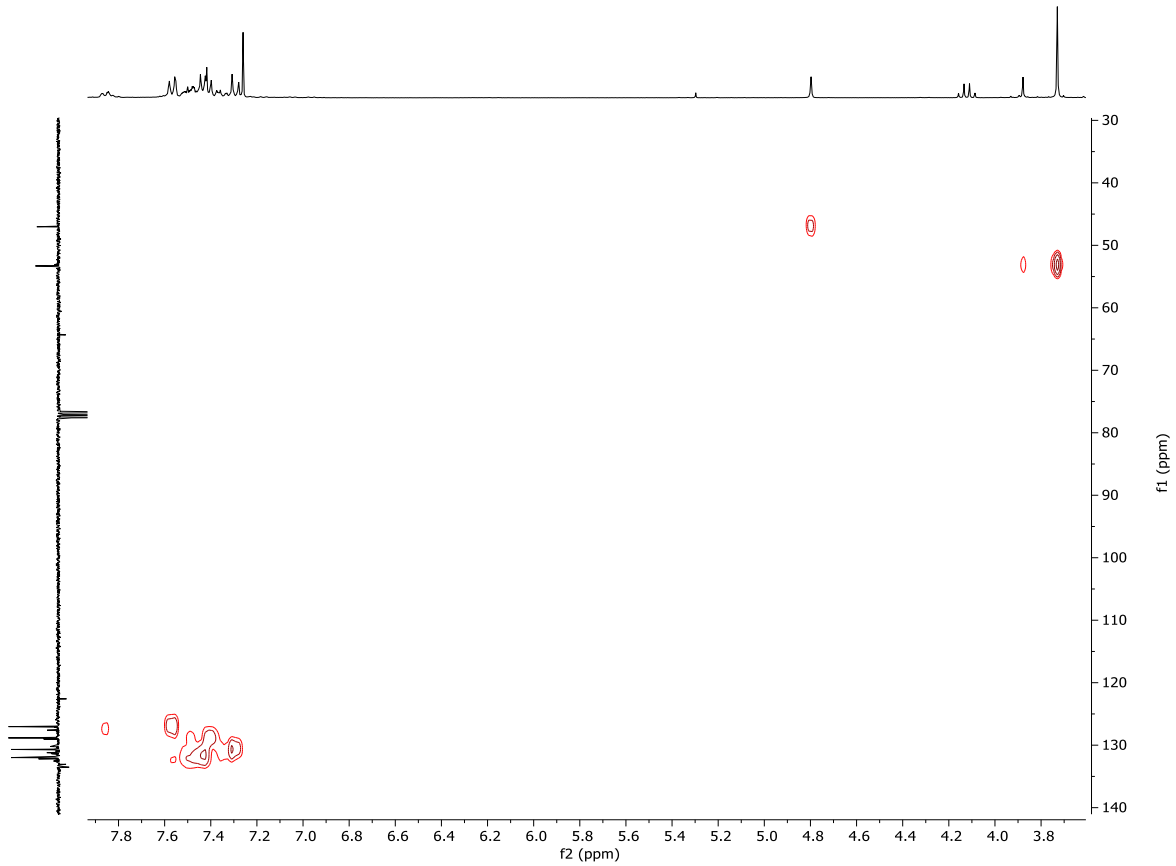
^{19}F NMR spectrum ($CDCl_3$, 282.40 MHz) of **2e**



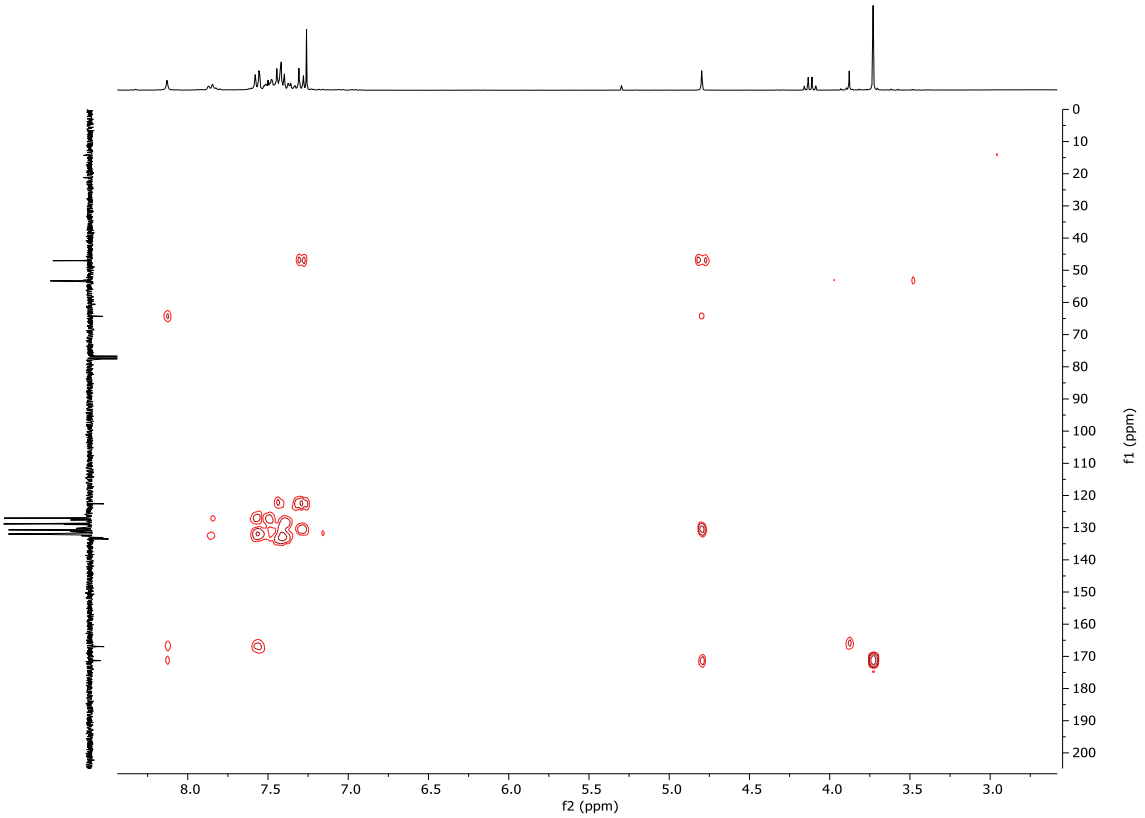
^{1}H NMR spectrum ($CDCl_3$, 300.13 MHz) of **2f** (* = ethyl acetate).



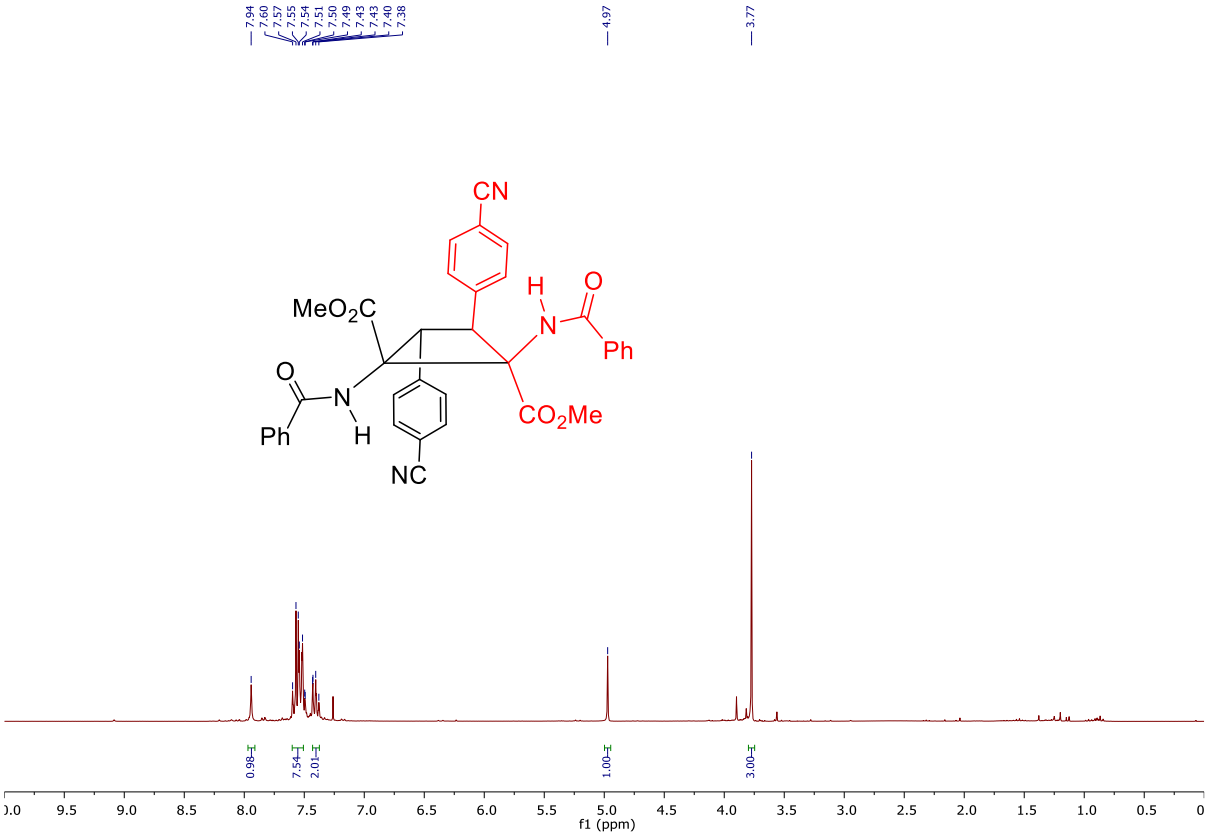
$^{13}C\{^{1}H\}$ (APT) NMR spectrum ($CDCl_3$, 75.5 MHz) of **2f**



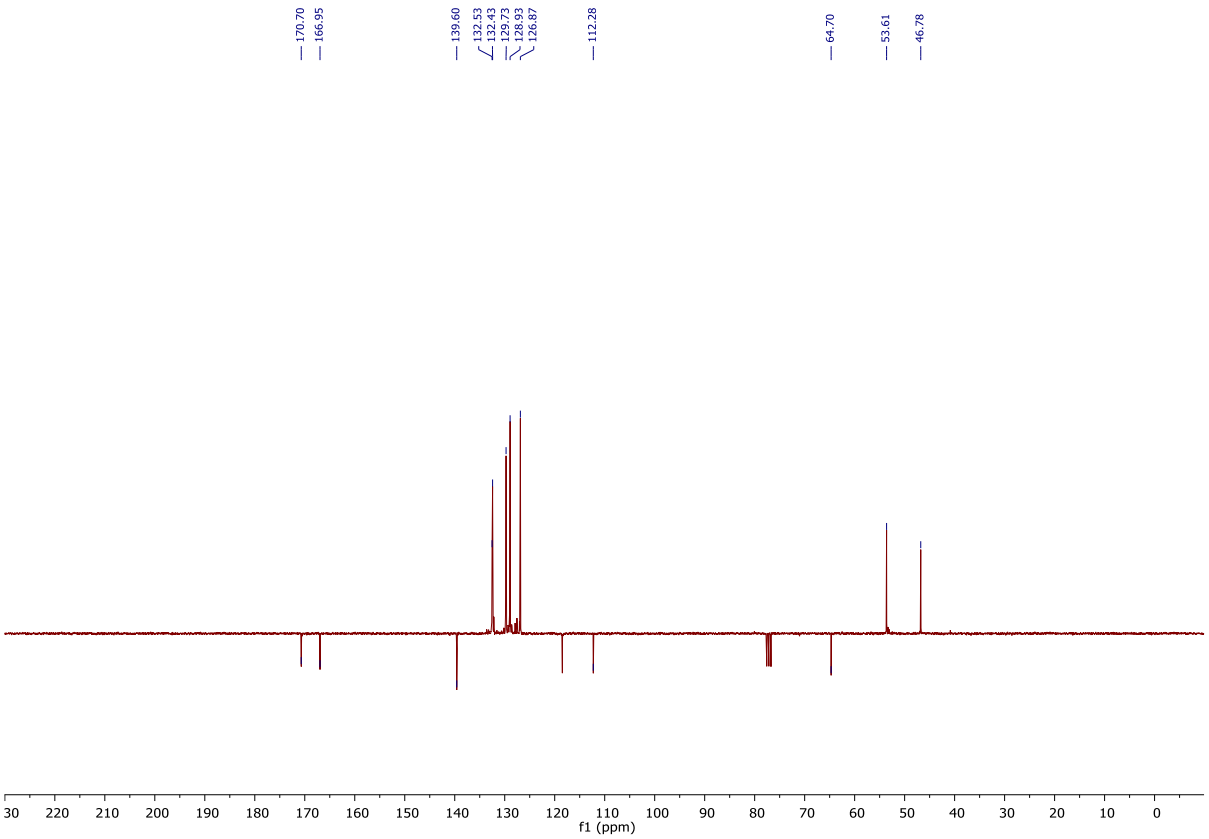
^{1}H-^{13}C HSQC ($CDCl_3$) correlation spectrum of **2f**



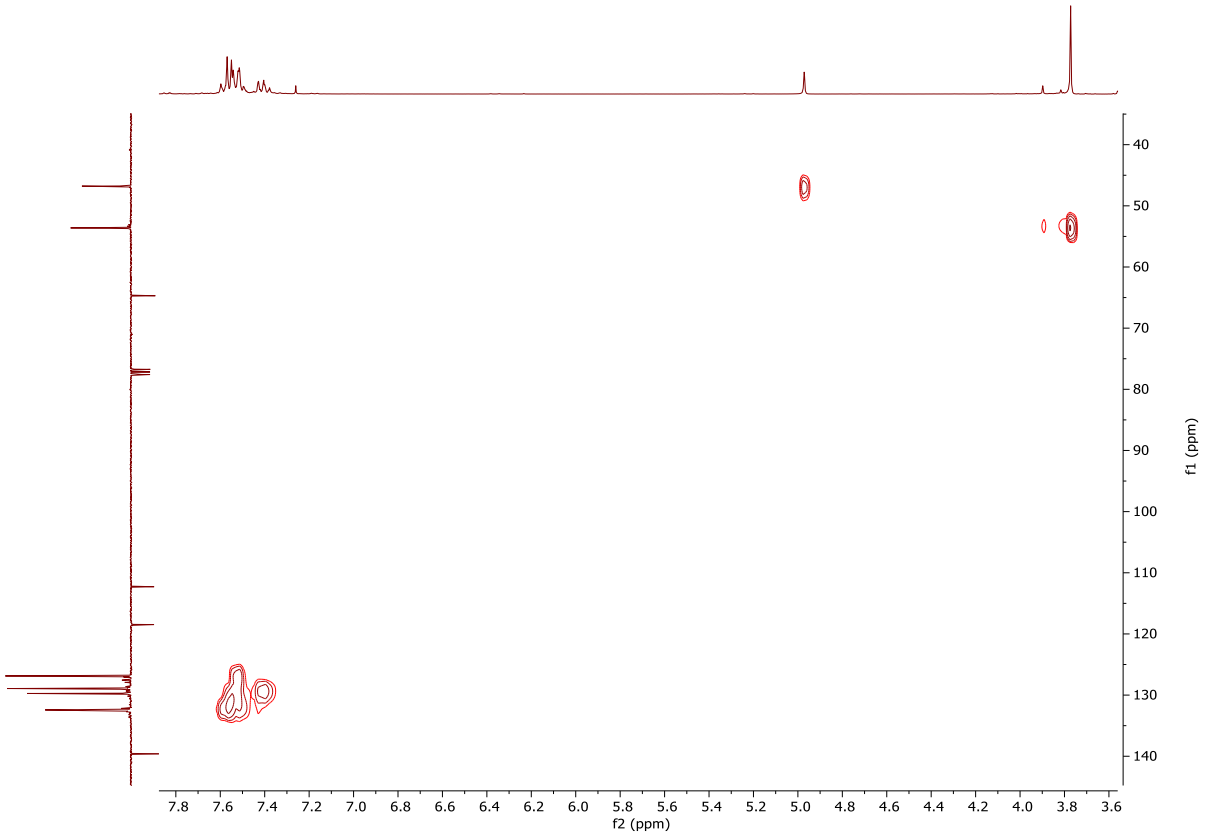
^{1}H-^{13}C HMBC ($CDCl_3$) correlation spectrum of **2f**



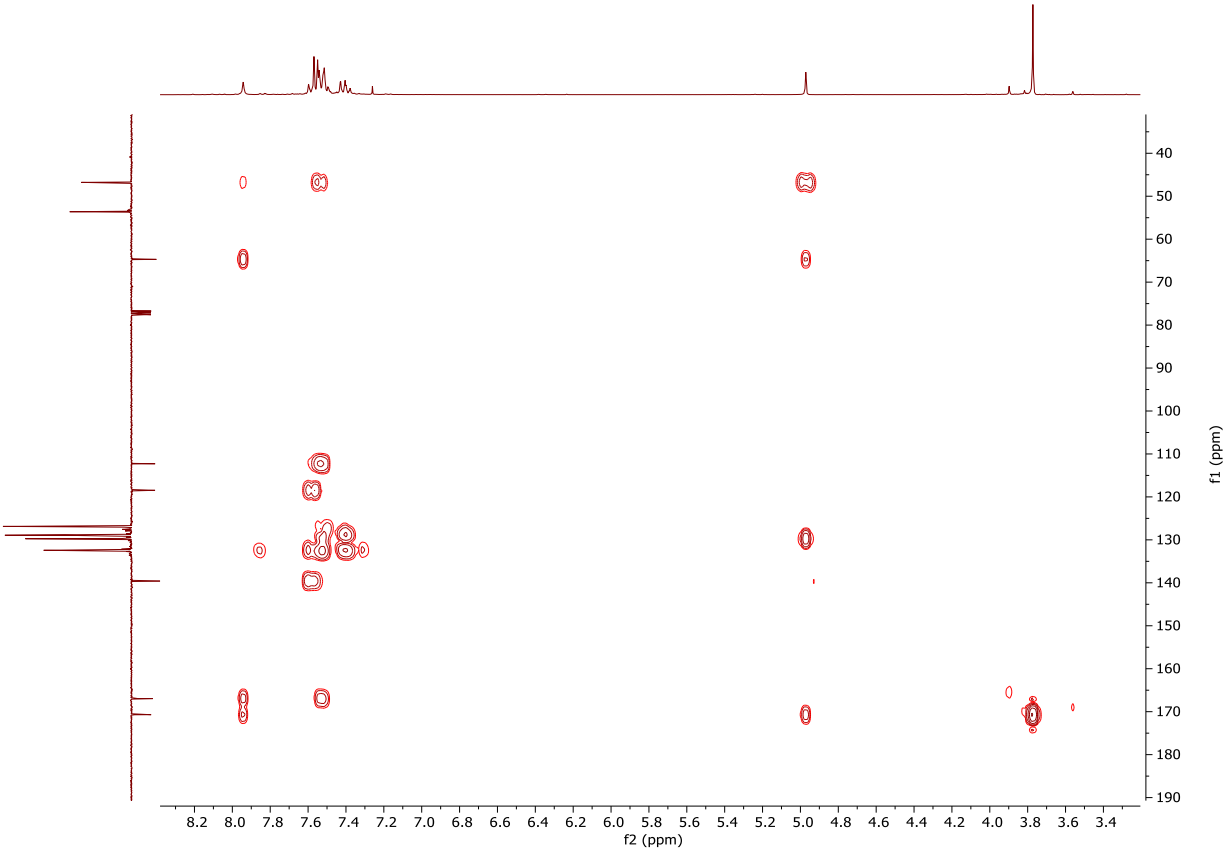
^{1}H NMR spectrum ($CDCl_3$, 300.13 MHz) of **2g**



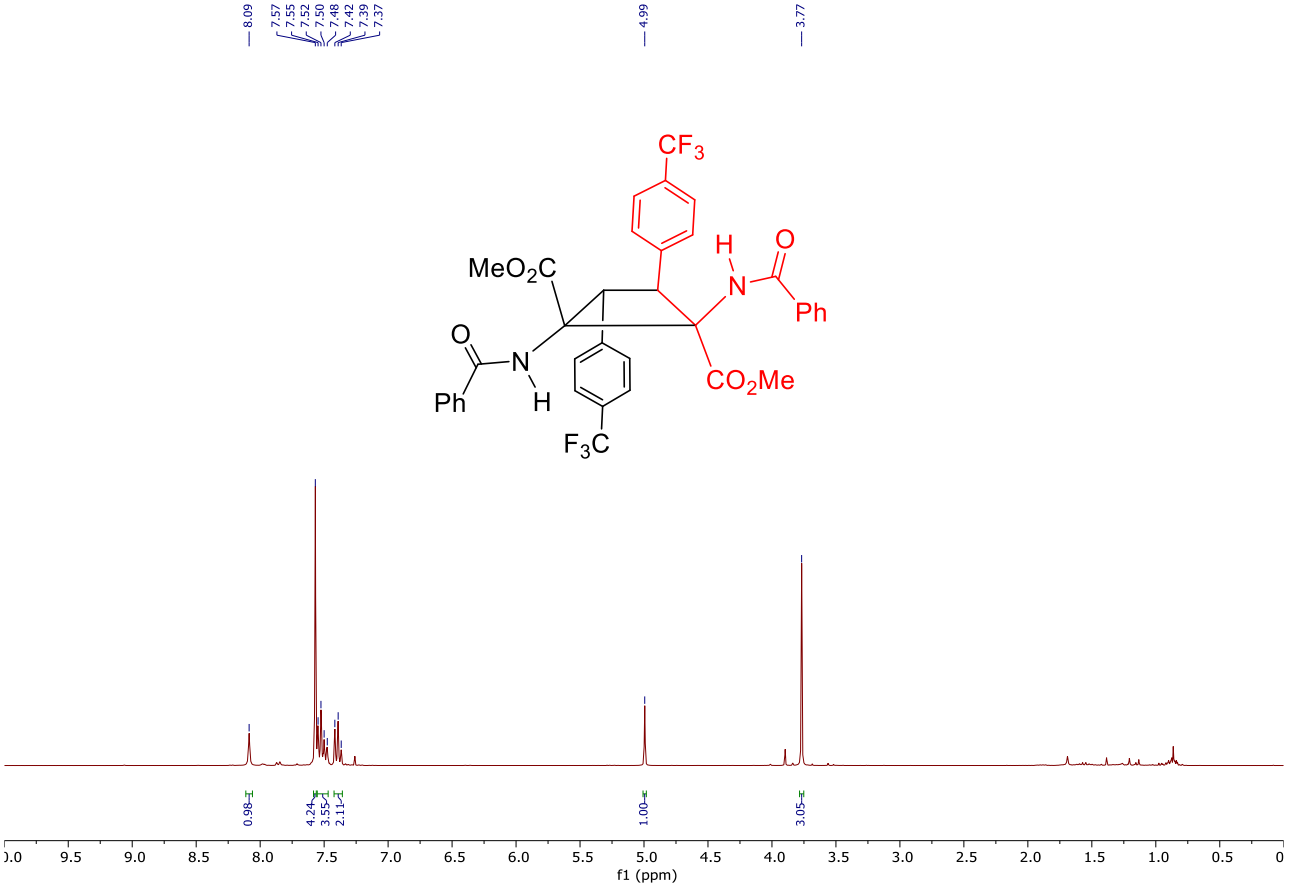
$^{13}C\{^{1}H\}$ (APT) NMR spectrum ($CDCl_3$, 75.5 MHz) of **2g**



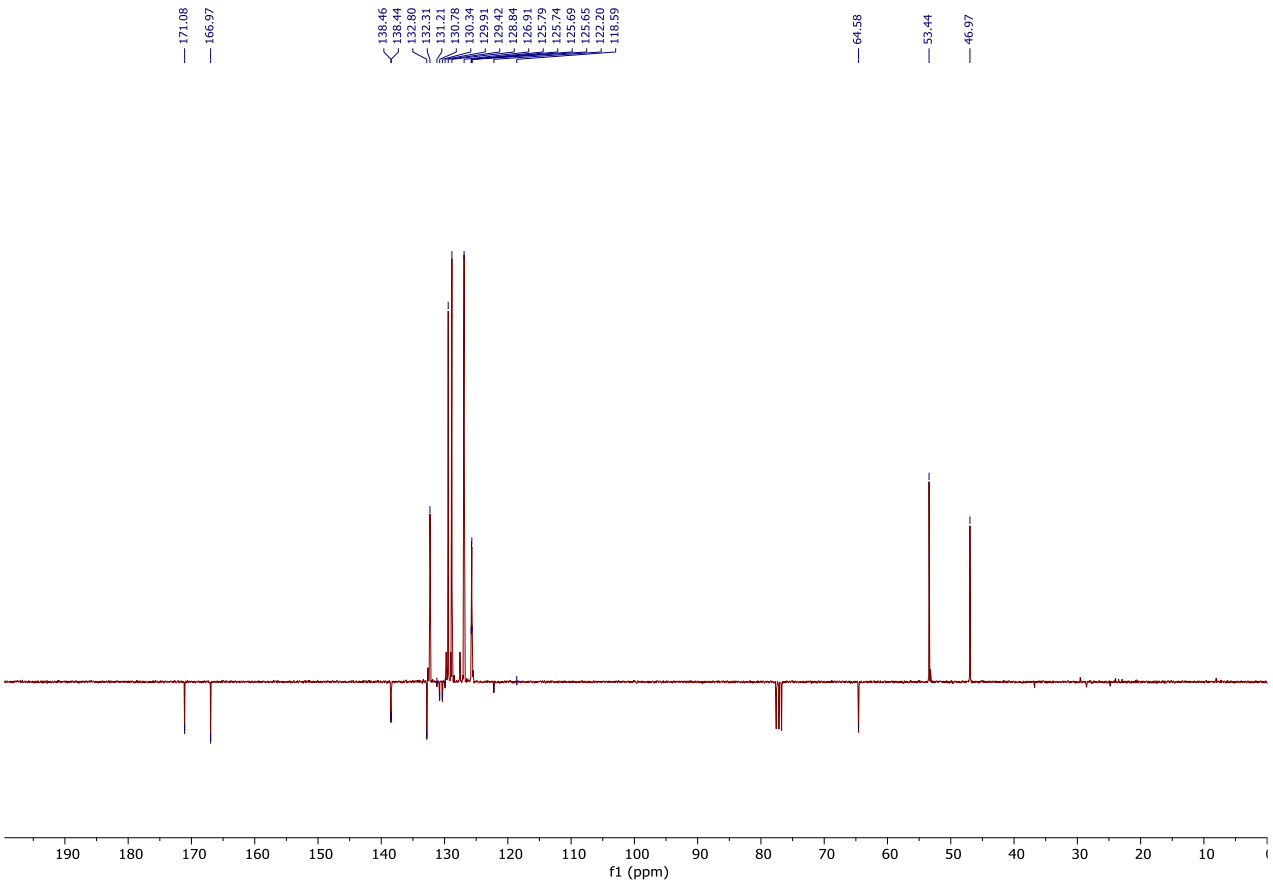
^{1}H-^{13}C HSQC ($CDCl_3$) correlation spectrum of **2g**



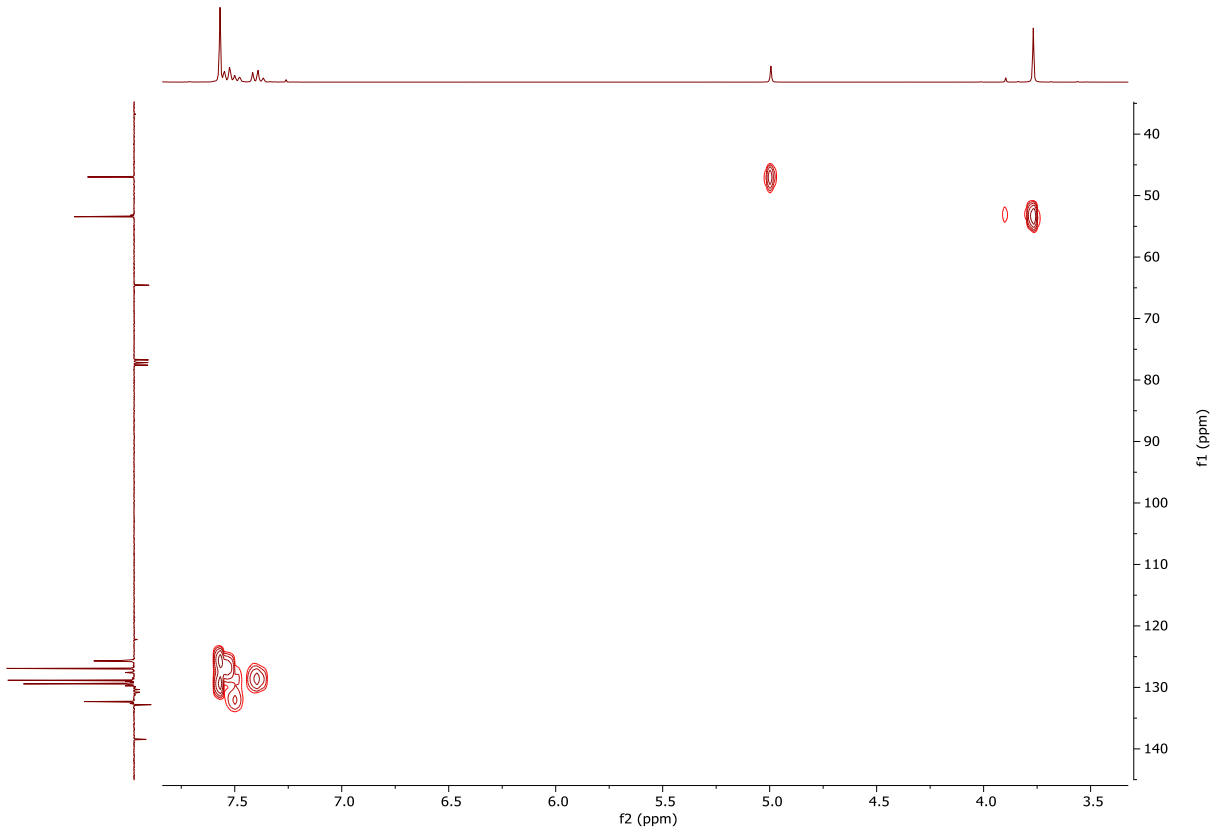
^{1}H-^{13}C HMBC ($CDCl_3$) correlation spectrum of **2g**



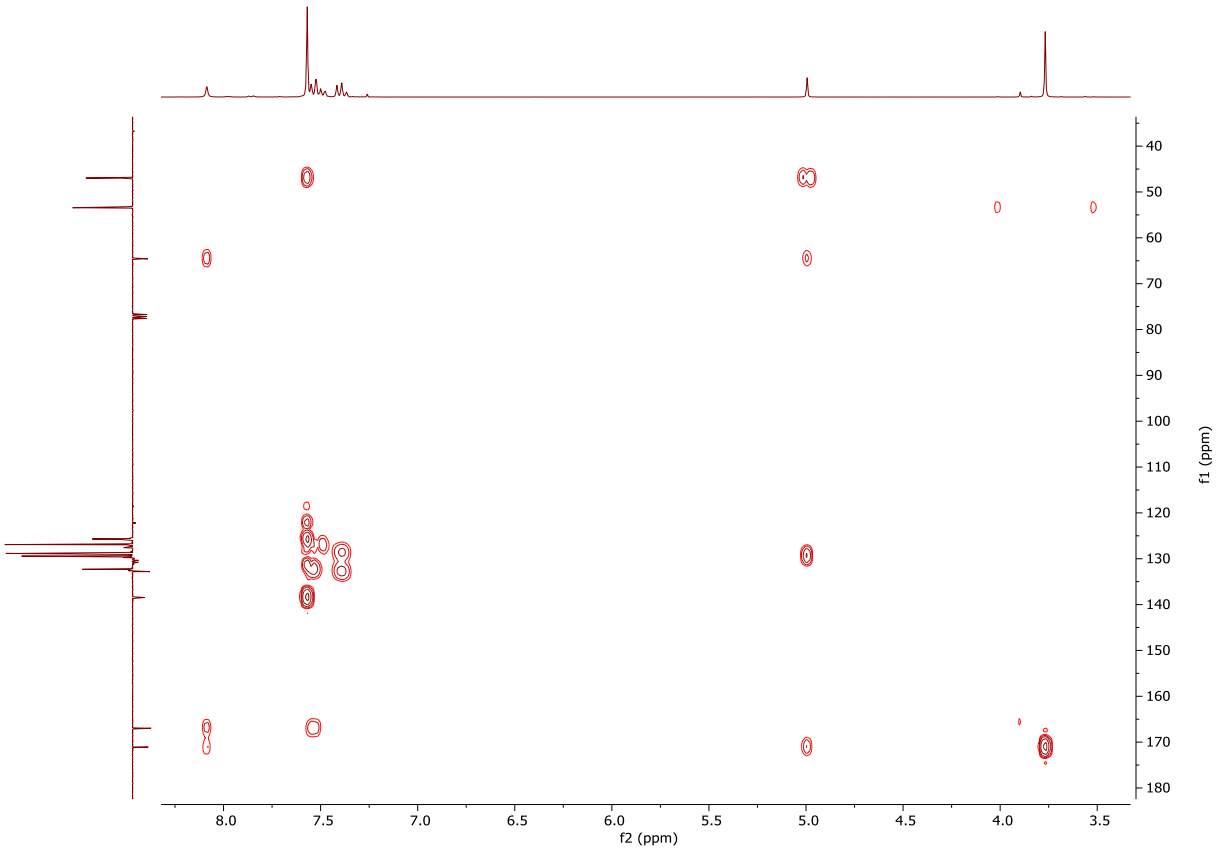
^{1}H NMR spectrum ($CDCl_3$, 300.13 MHz) of **2h**



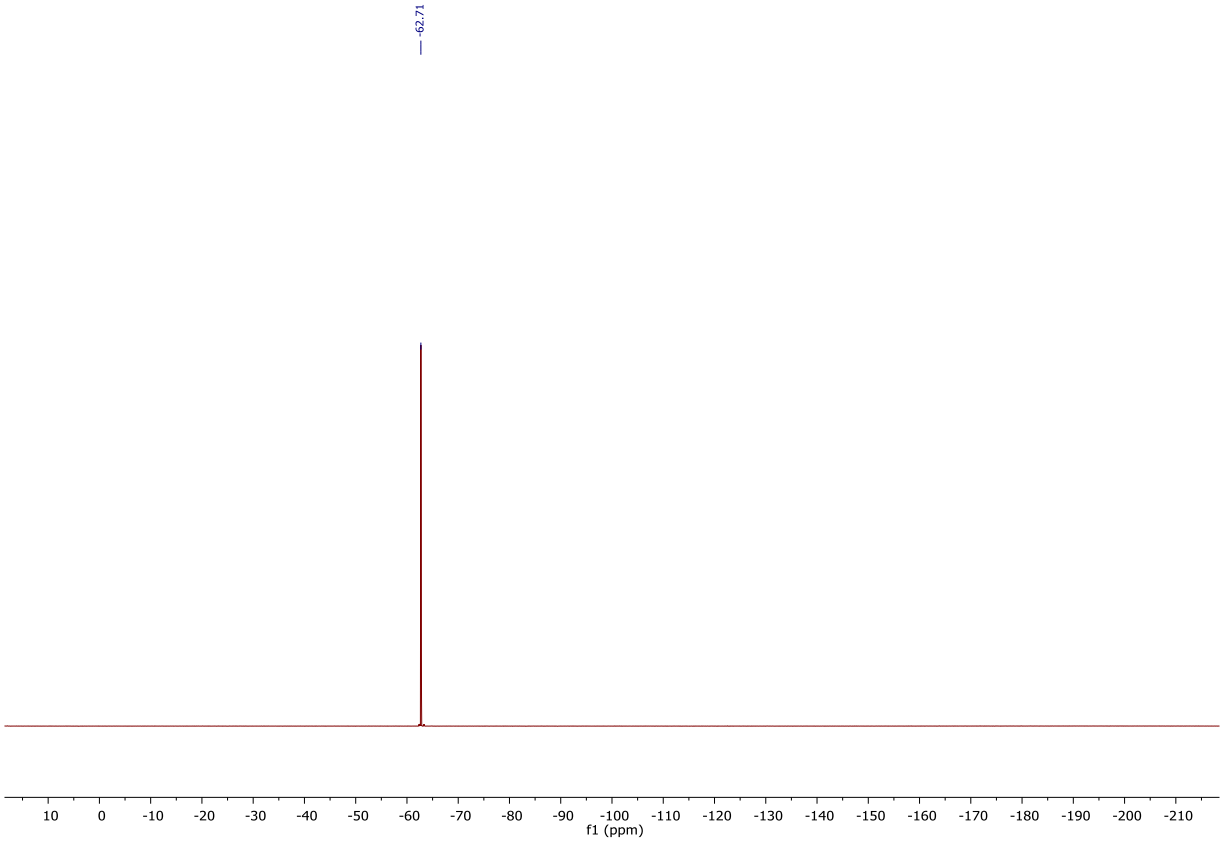
$^{13}C\{^{1}H\}$ (APT) NMR spectrum ($CDCl_3$, 75.5 MHz) of **2h**



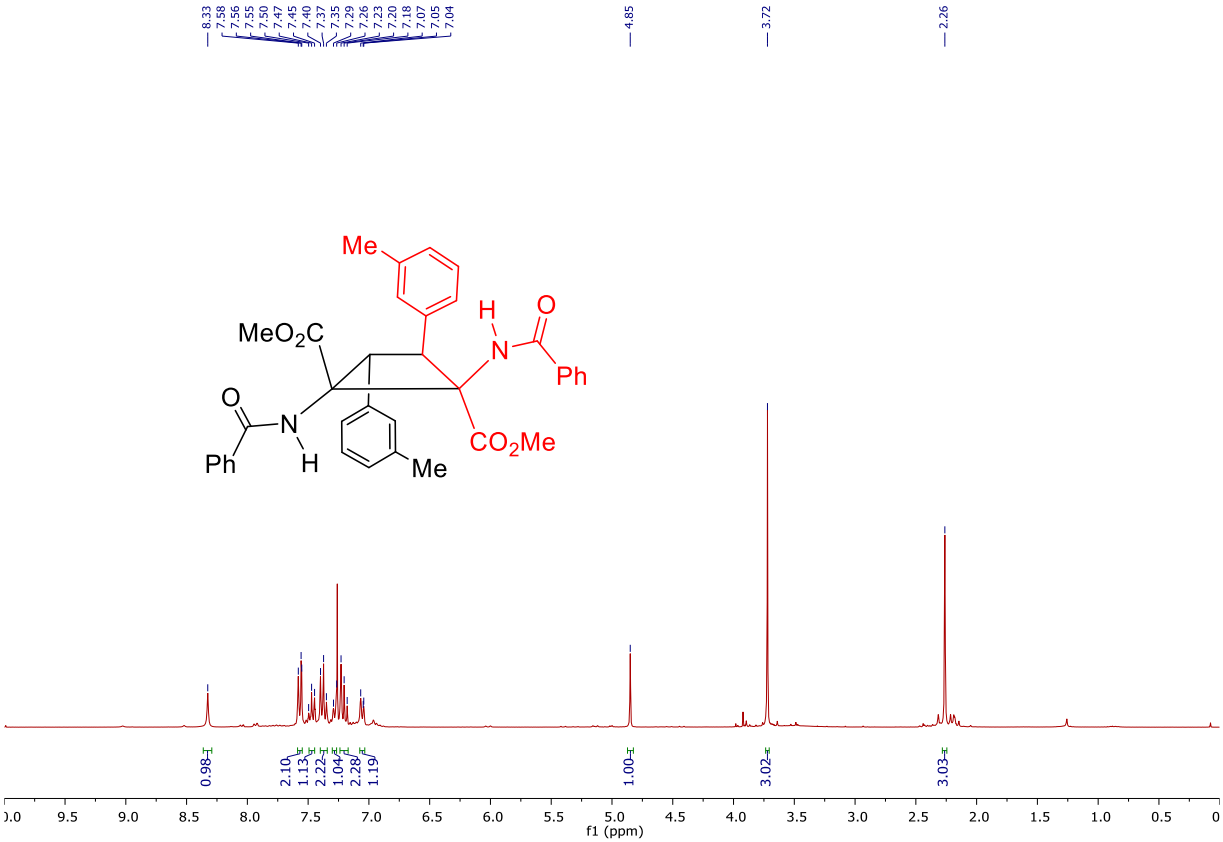
^{1}H-^{13}C HSQC ($CDCl_3$) correlation spectrum of **2h**



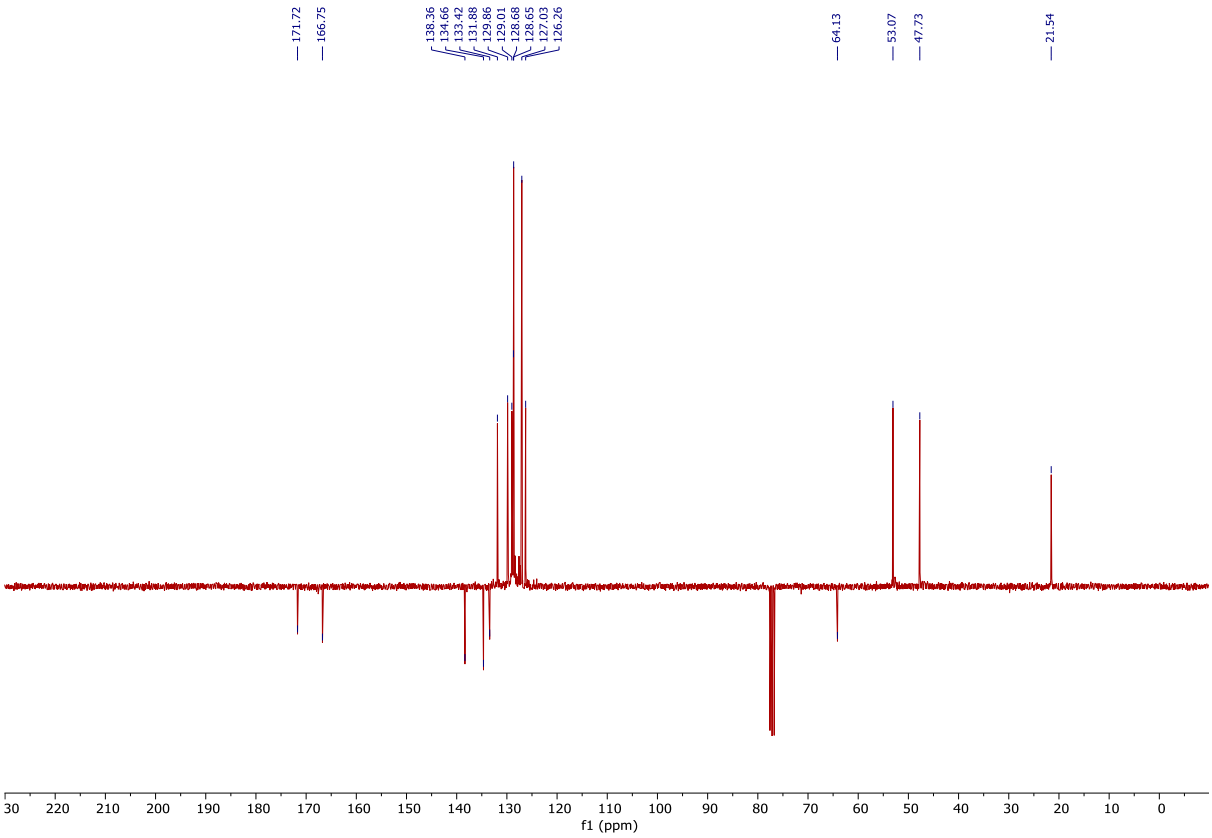
^{1}H-^{13}C HMBC ($CDCl_3$) correlation spectrum of **2h**



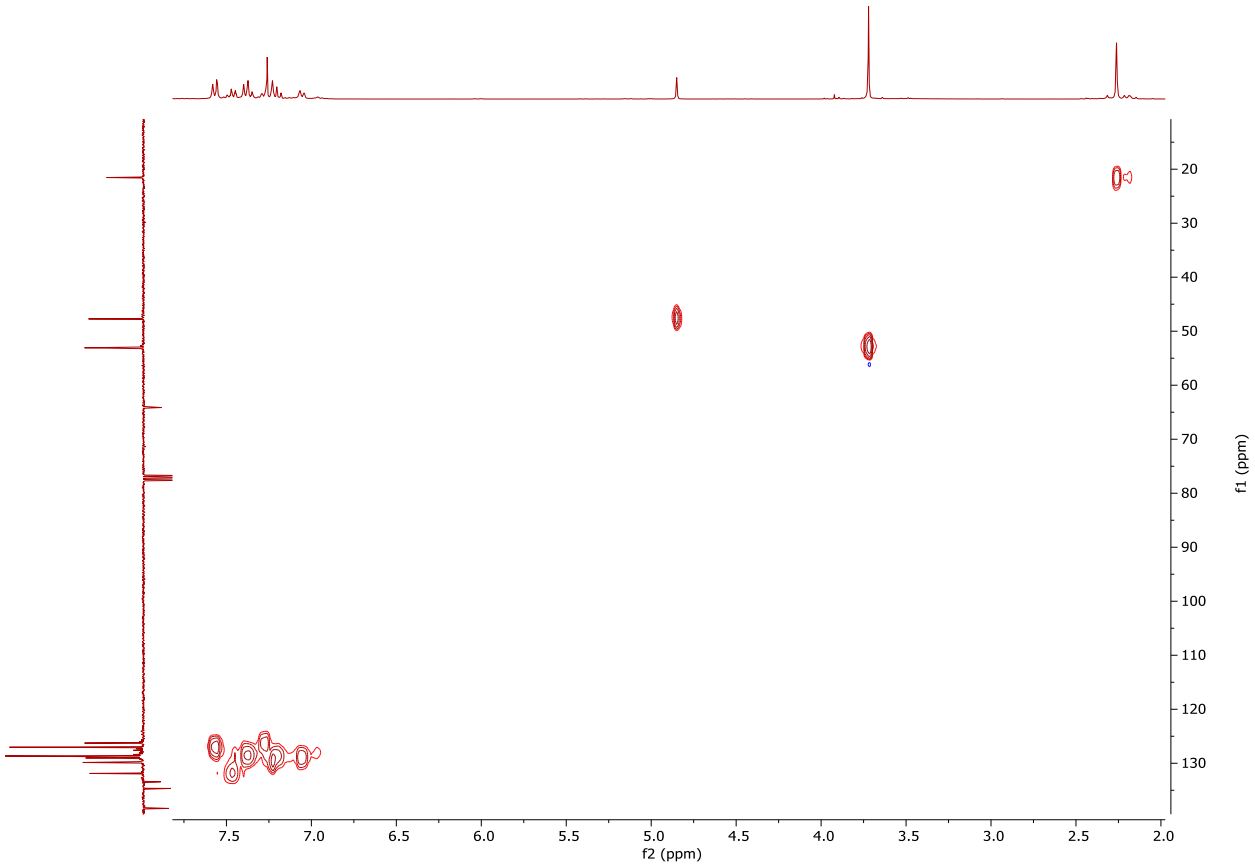
^{19}F NMR spectrum ($CDCl_3$, 282.40 MHz) of **2h**



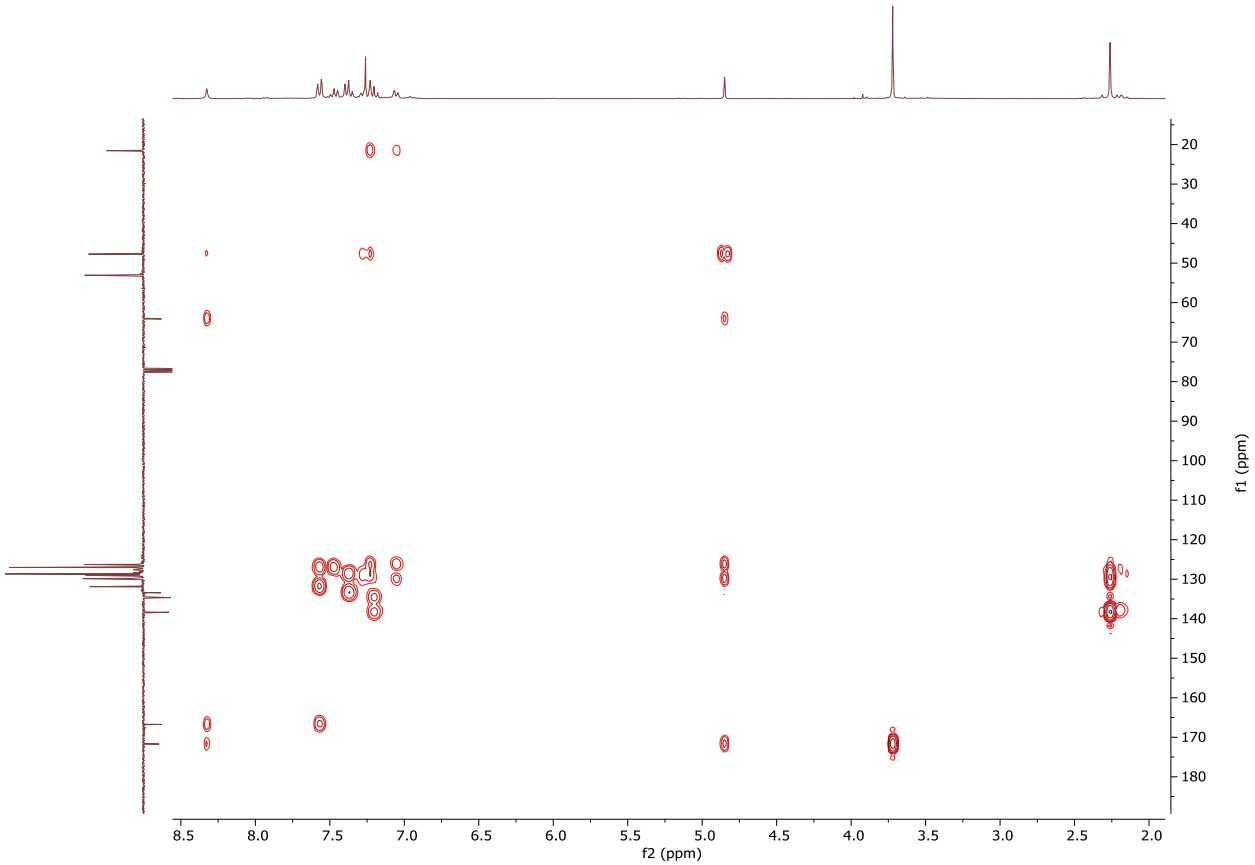
^{1}H NMR spectrum ($CDCl_3$, 300.13 MHz) of **2i**



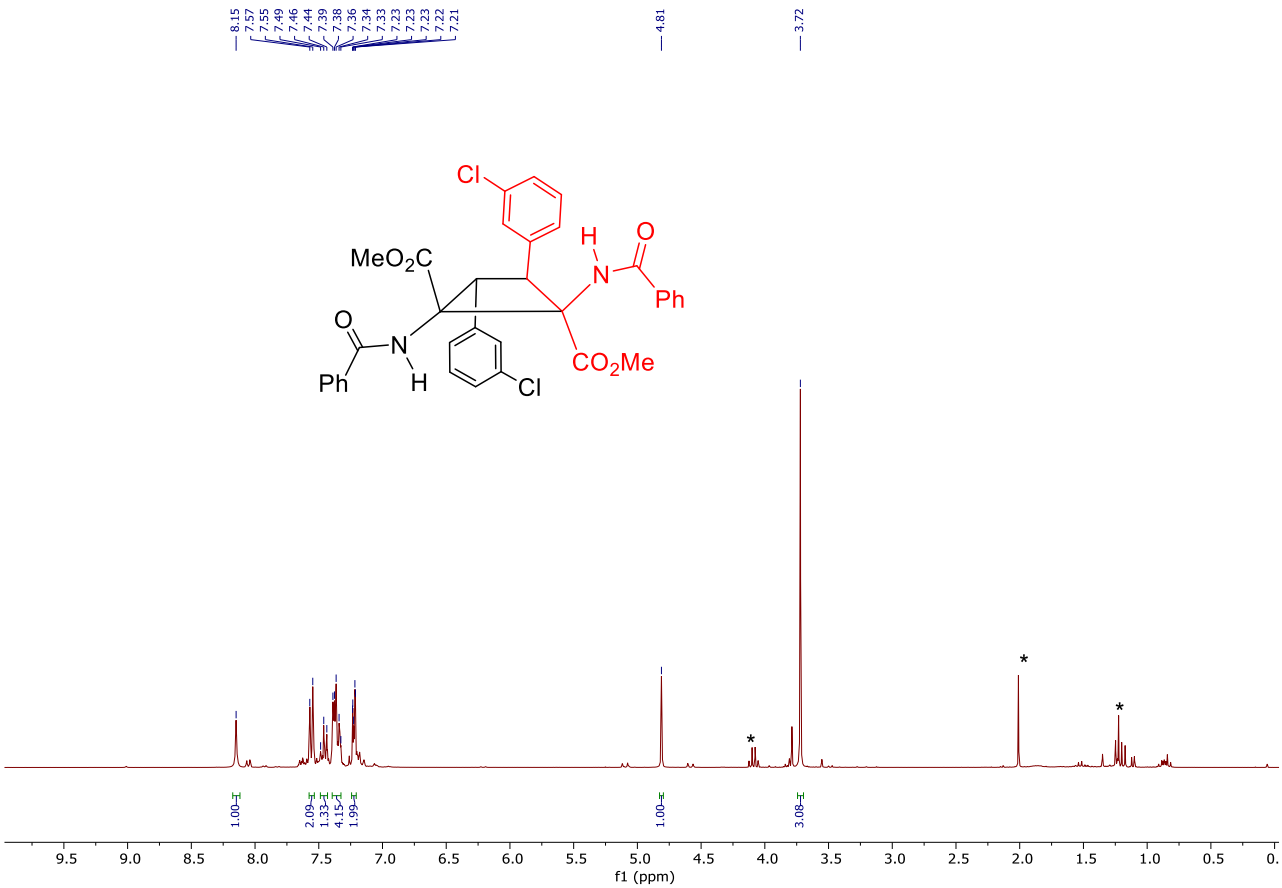
^{13}C{^{1}H} (APT) NMR spectrum ($CDCl_3$, 75.5 MHz) of **2i**



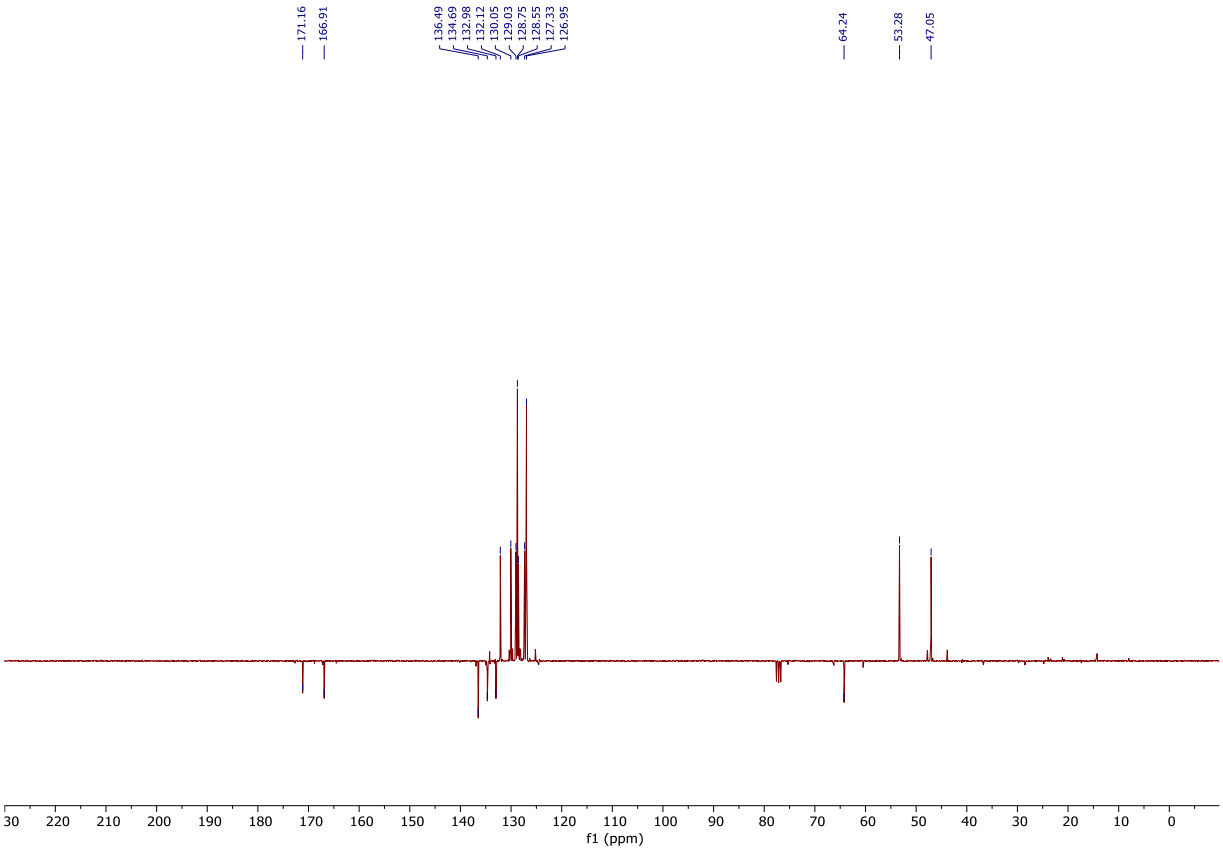
^{1}H-^{13}C HSQC ($CDCl_3$) correlation spectrum of **2i**



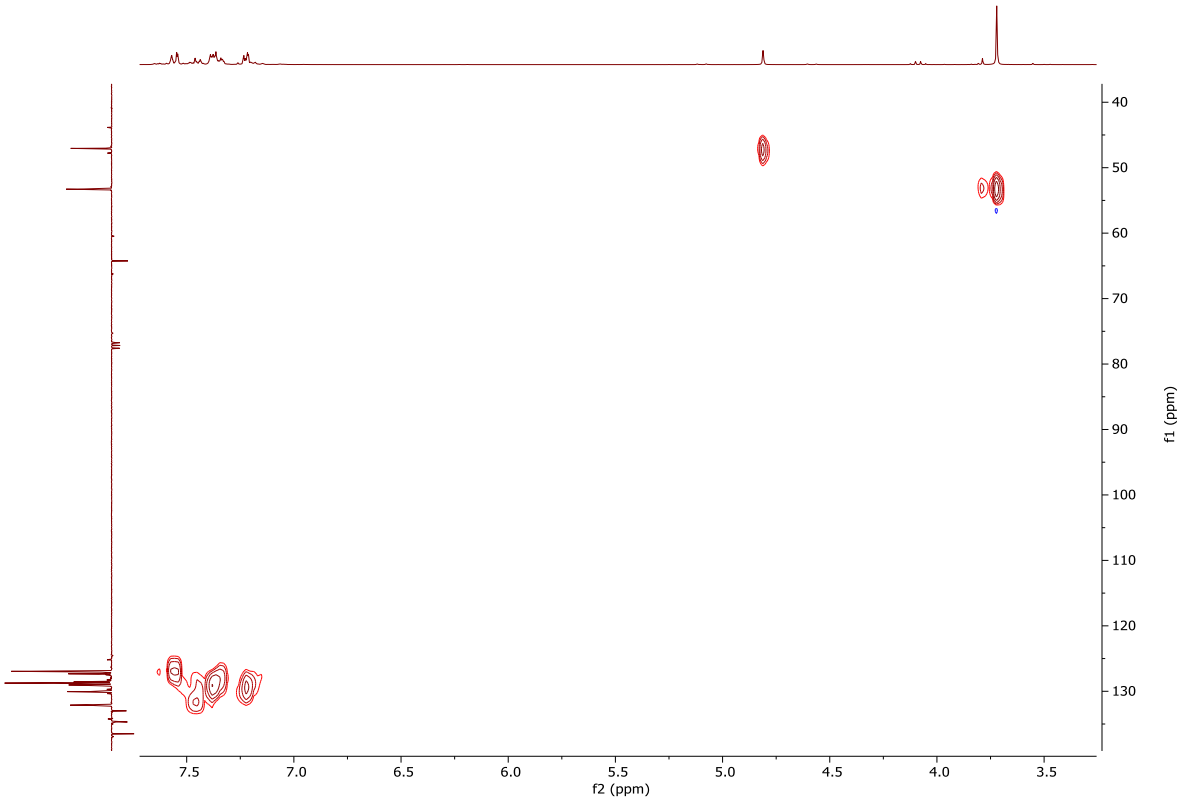
^{1}H-^{13}C HMBC ($CDCl_3$) correlation spectrum of **2i**



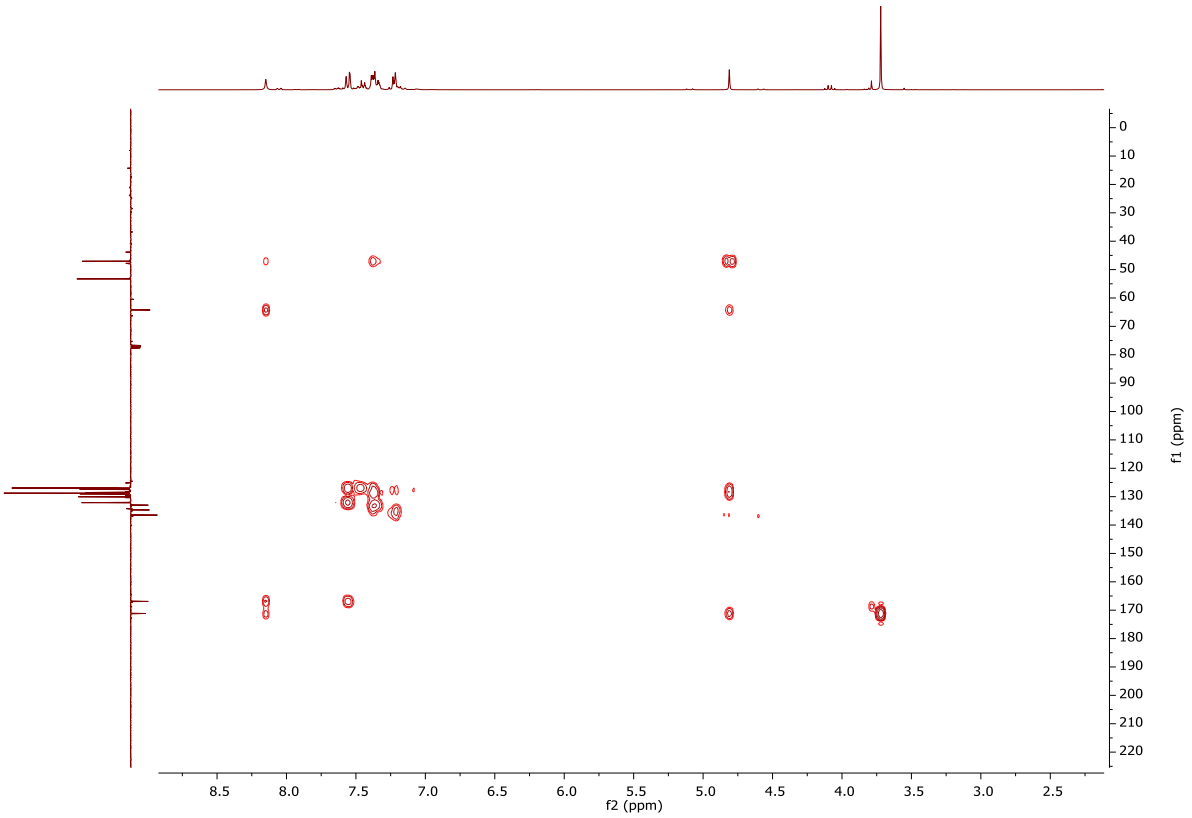
^{1}H NMR spectrum ($CDCl_3$, 300.13 MHz) of **2j** (* = ethyl acetate).



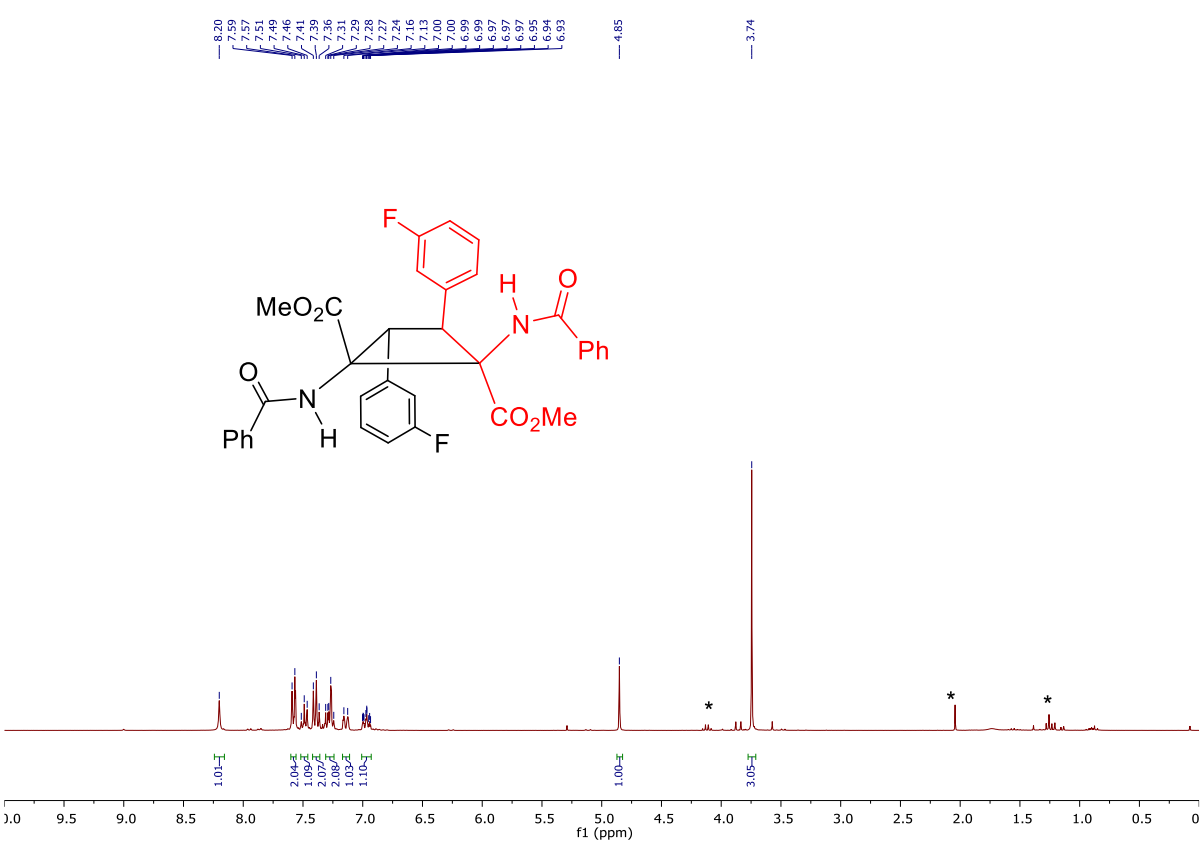
^{13}C{^{1}H} (APT) NMR spectrum ($CDCl_3$, 75.5 MHz) of **2j**



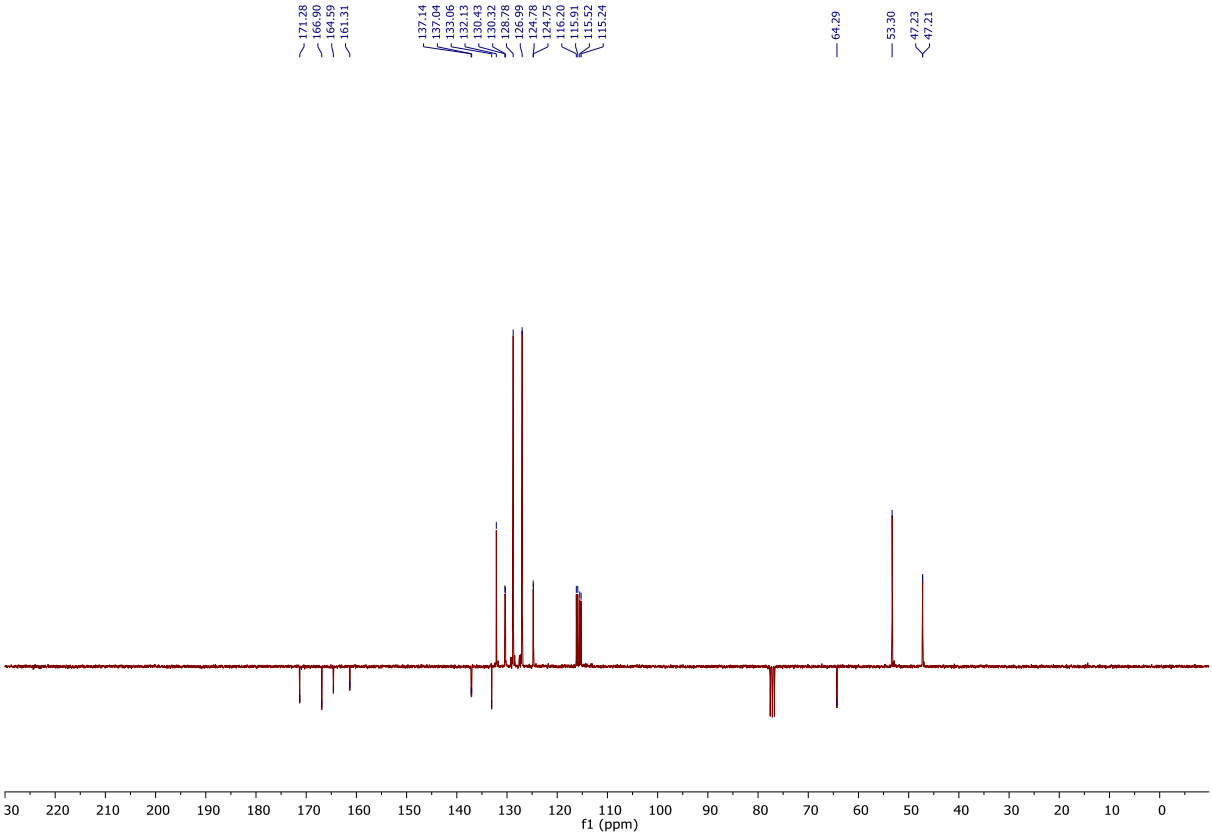
^{1}H-^{13}C HSQC ($CDCl_3$) correlation spectrum of **2j**



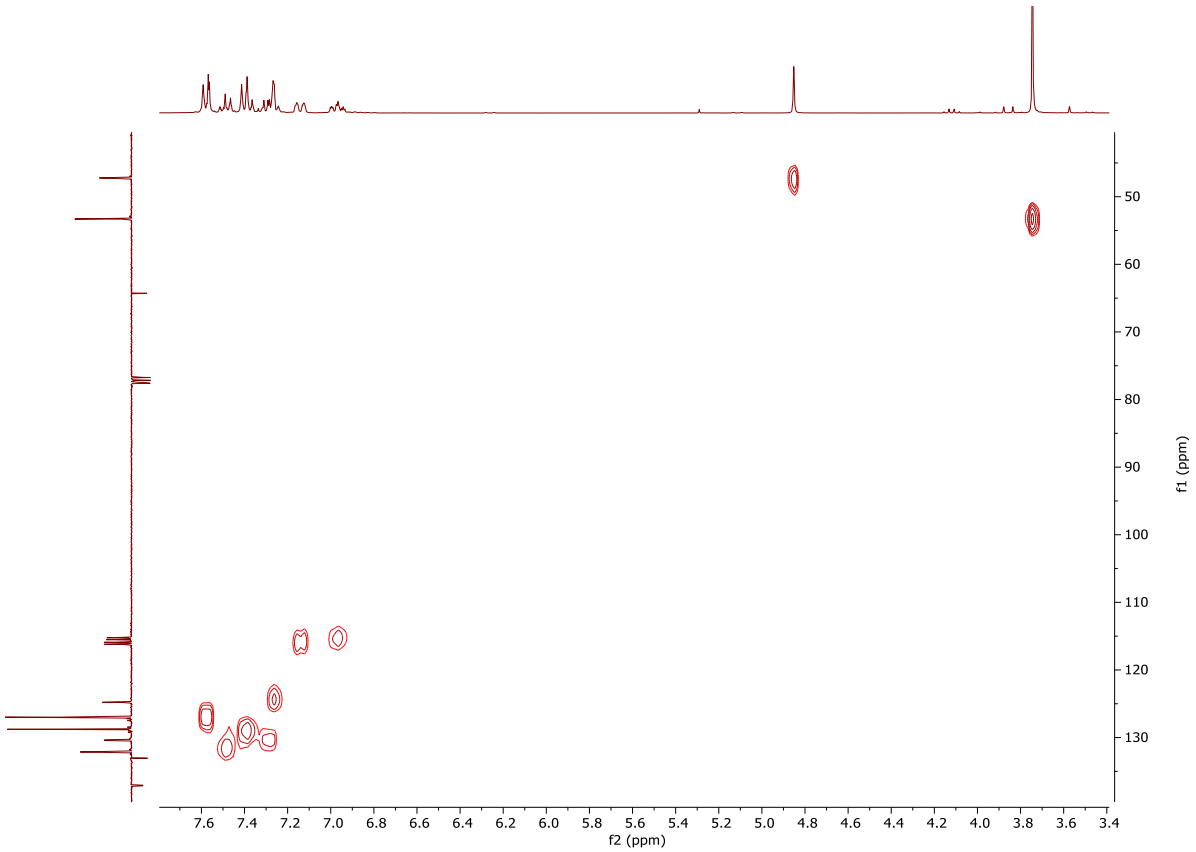
^{1}H-^{13}C HMBC ($CDCl_3$) correlation spectrum of **2j**



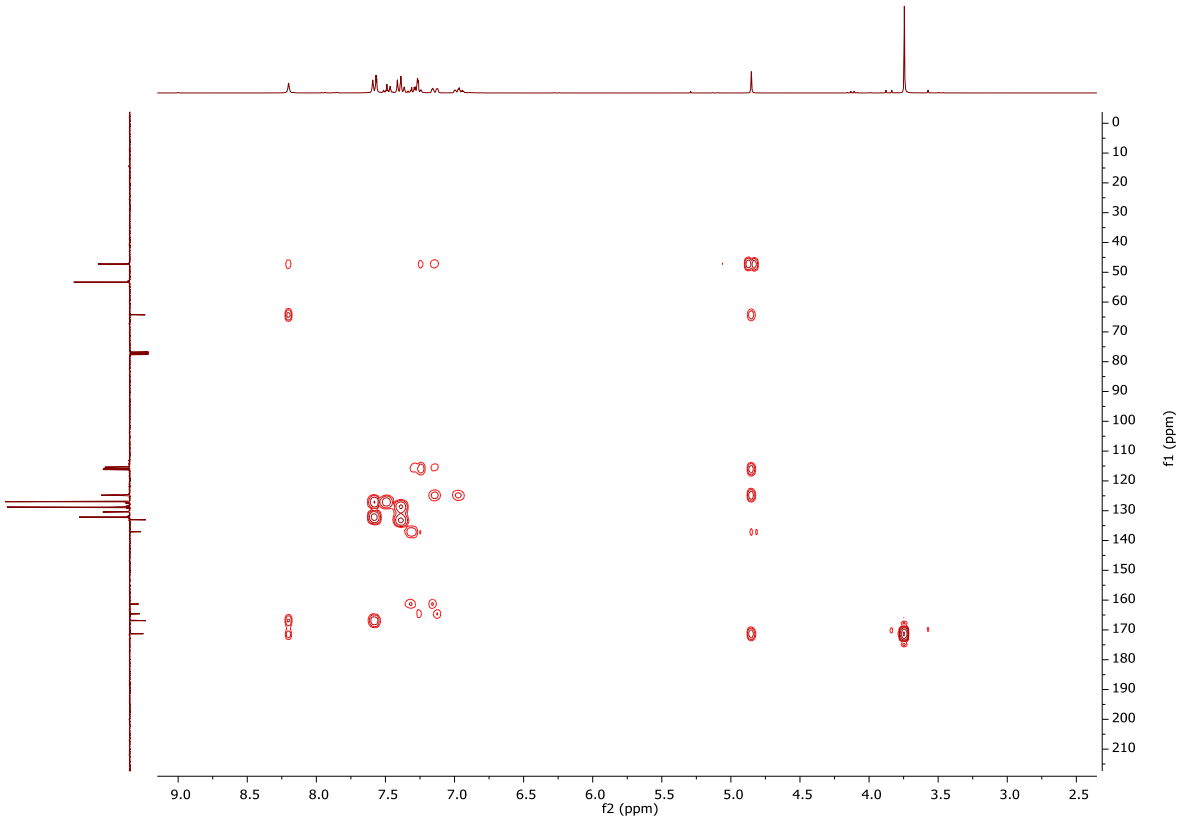
^{1}H NMR spectrum ($CDCl_3$, 300.13 MHz) of **2k** (* = ethyl acetate)



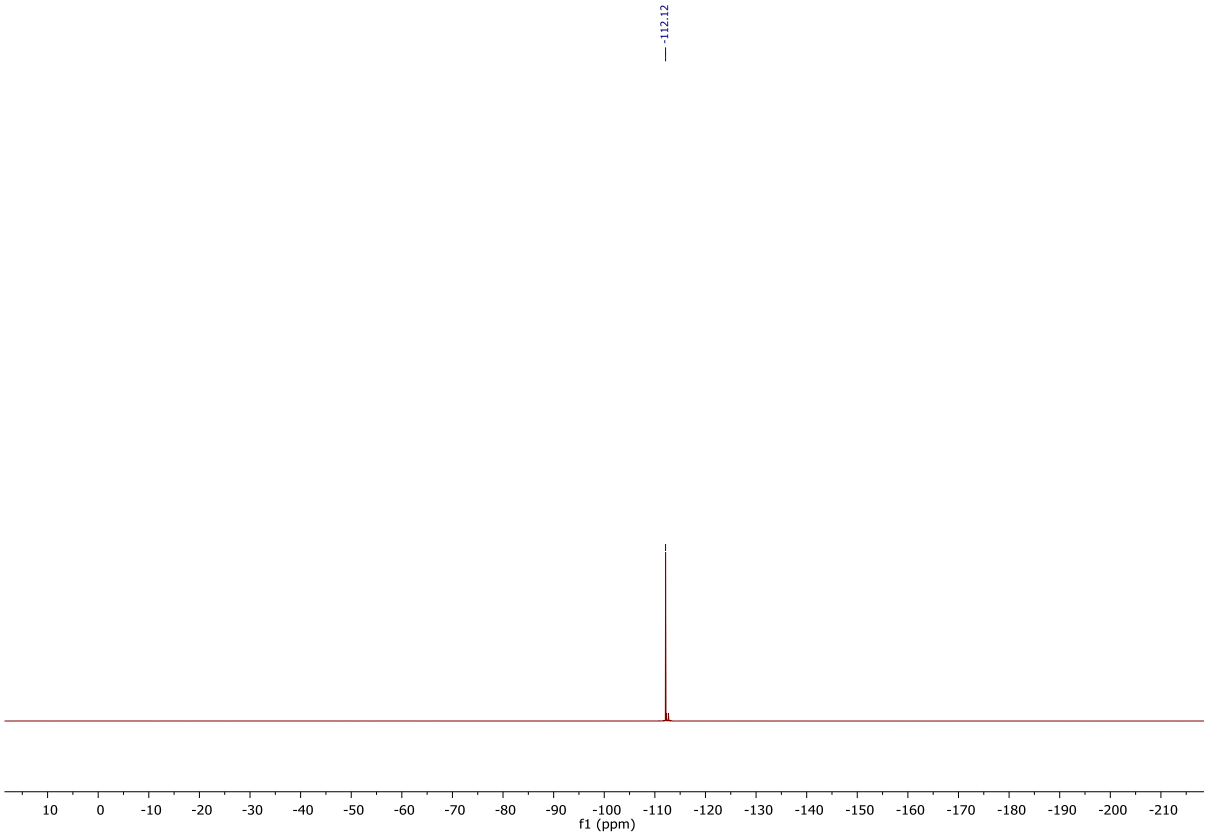
^{13}C{^{1}H} (APT) NMR spectrum ($CDCl_3$, 75.5 MHz) of **2k**



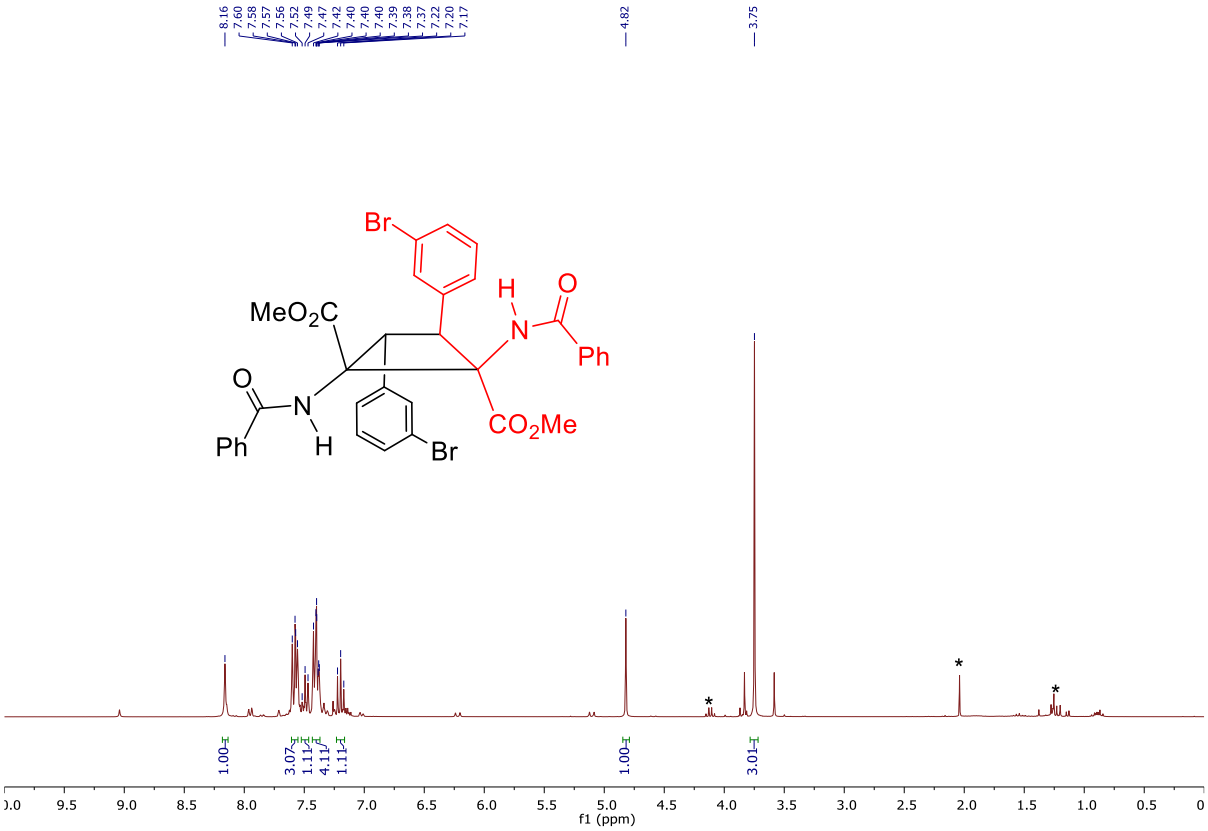
^{1}H-^{13}C HSQC ($CDCl_3$) correlation spectrum of **2k**



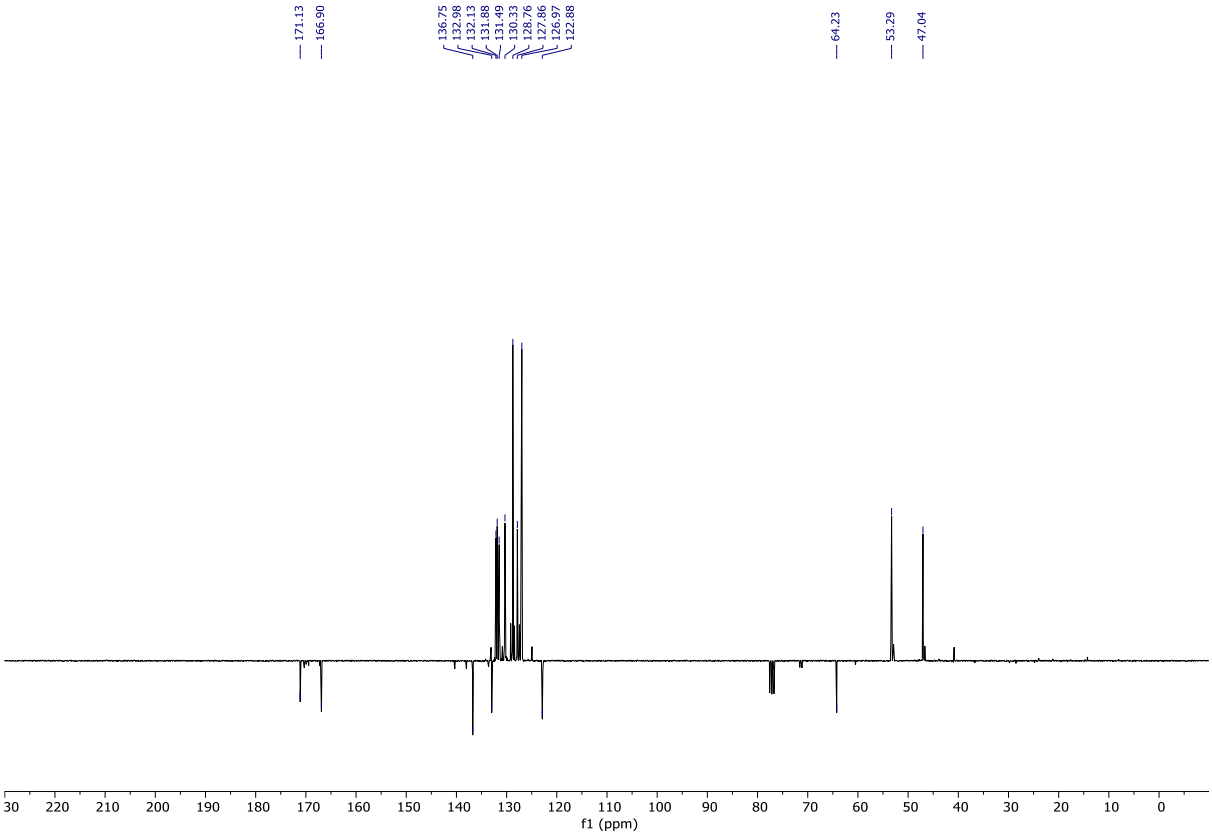
^{1}H-^{13}C HMBC ($CDCl_3$) correlation spectrum of **2k**



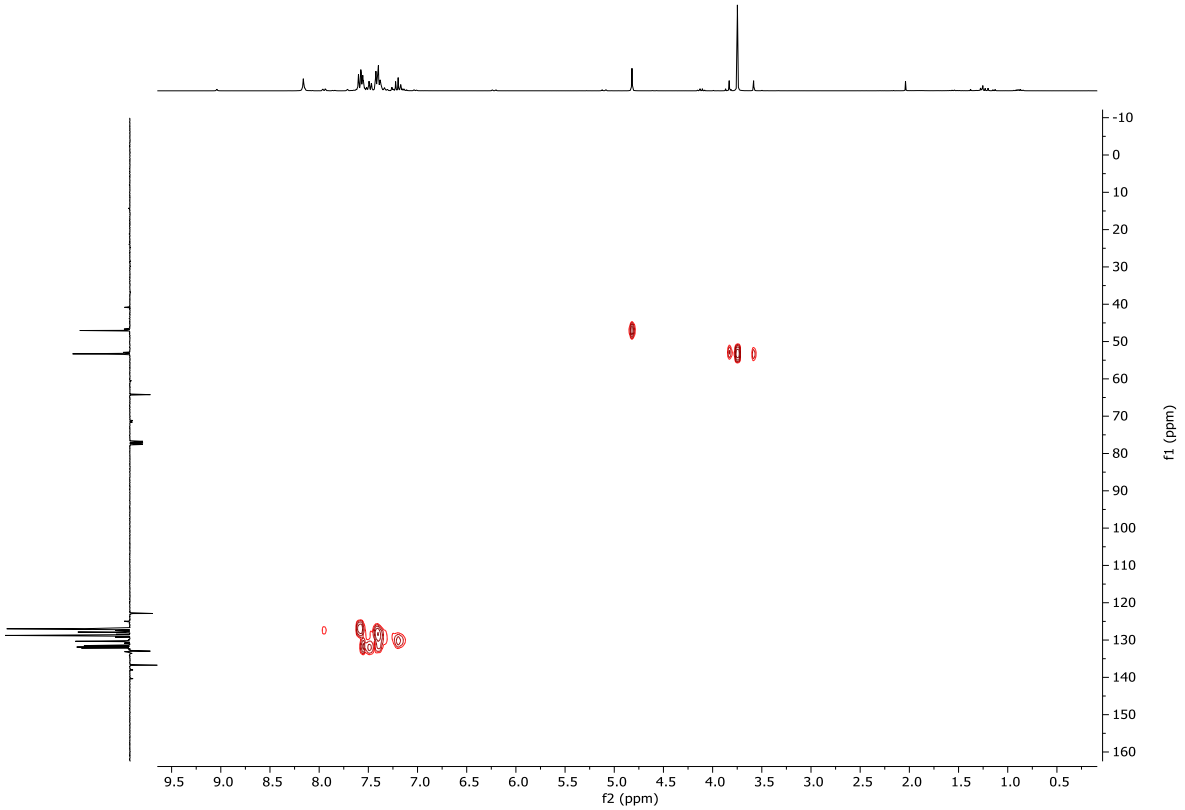
^{19}F {^{1}H} NMR spectrum ($CDCl_3$, 282.40 MHz) of **2k**



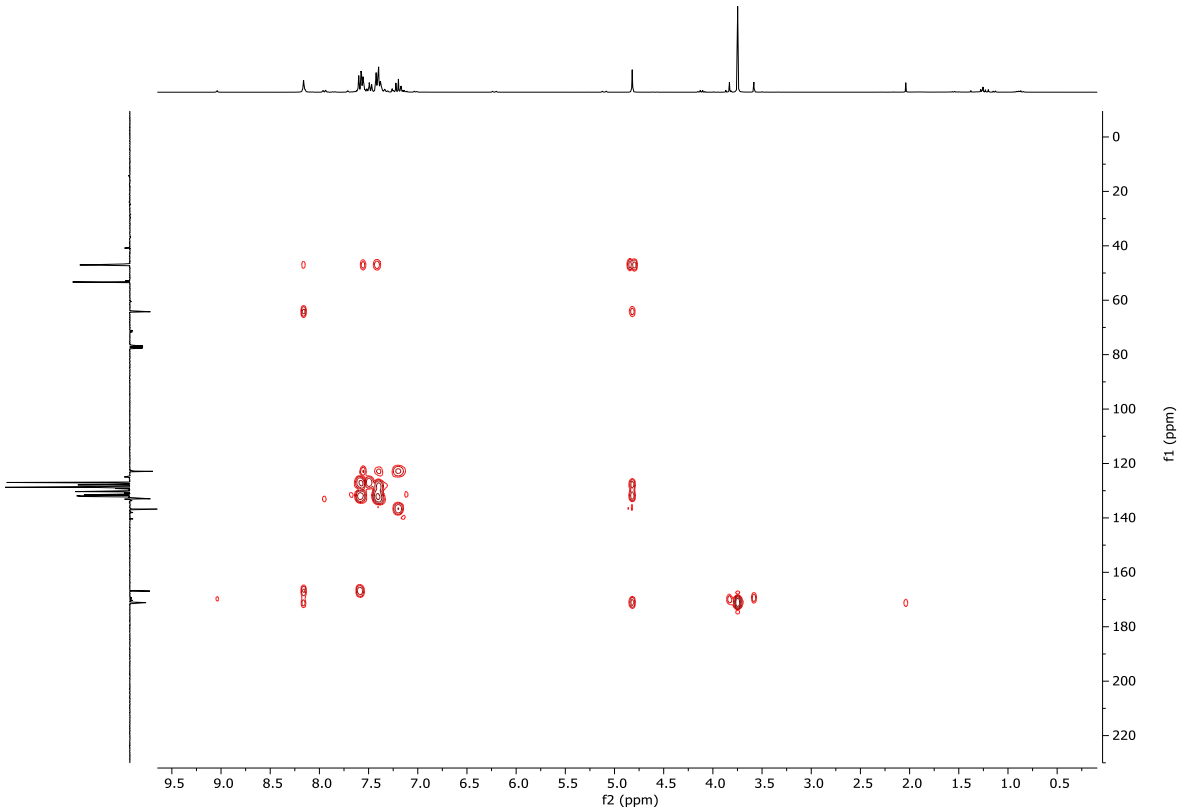
^{1}H NMR spectrum ($CDCl_3$, 300.13 MHz) of **2l** (* = ethyl acetate)



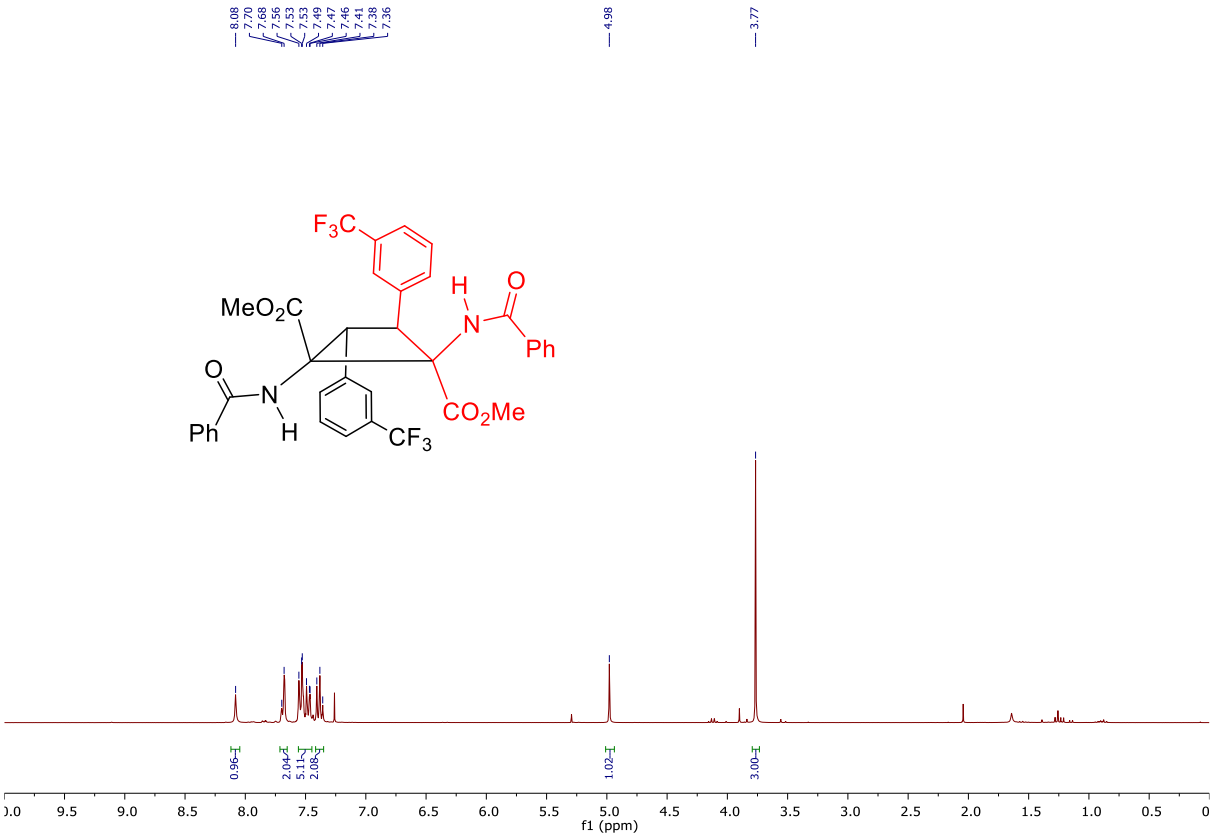
$^{13}C\{^{1}H\}$ (APT) NMR spectrum ($CDCl_3$, 75.5 MHz) of **2l**



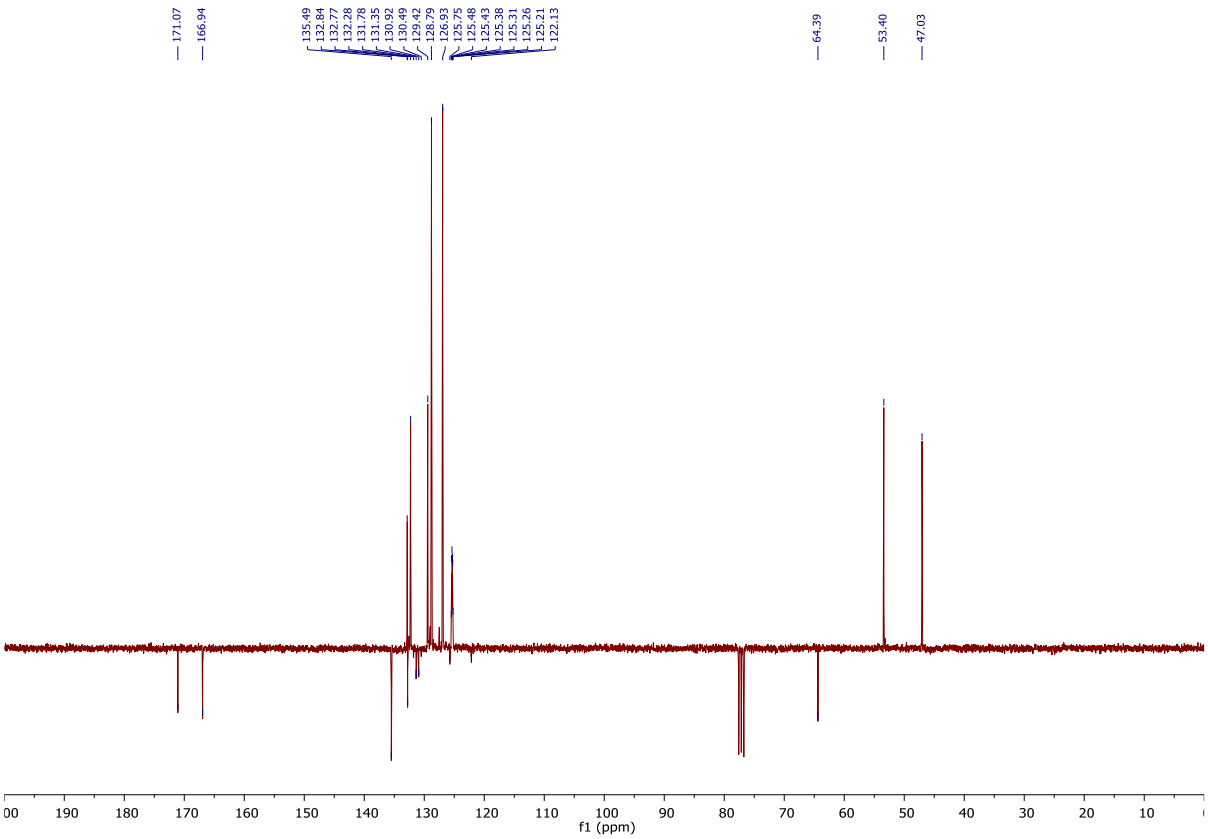
^{1}H-^{13}C HSQC ($CDCl_3$) correlation spectrum of **2l**



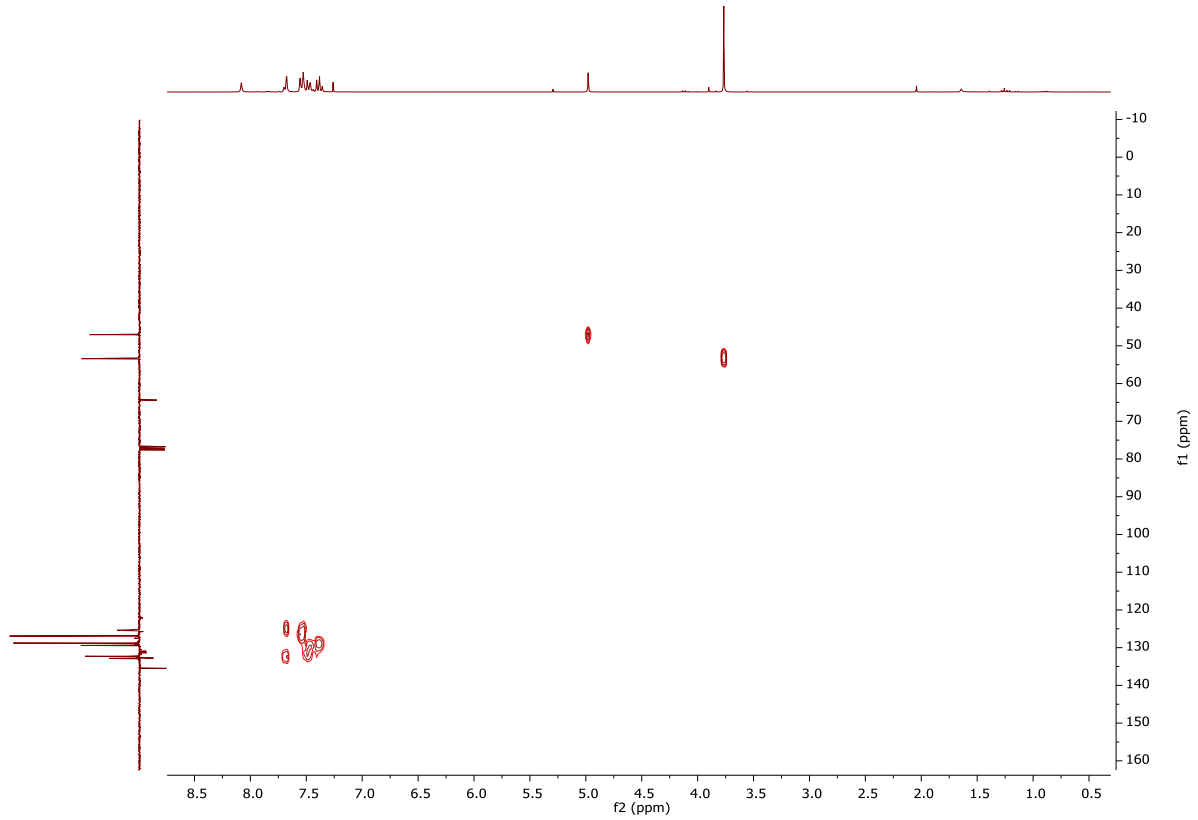
^{1}H-^{13}C HMBC ($CDCl_3$) correlation spectrum of **2l**



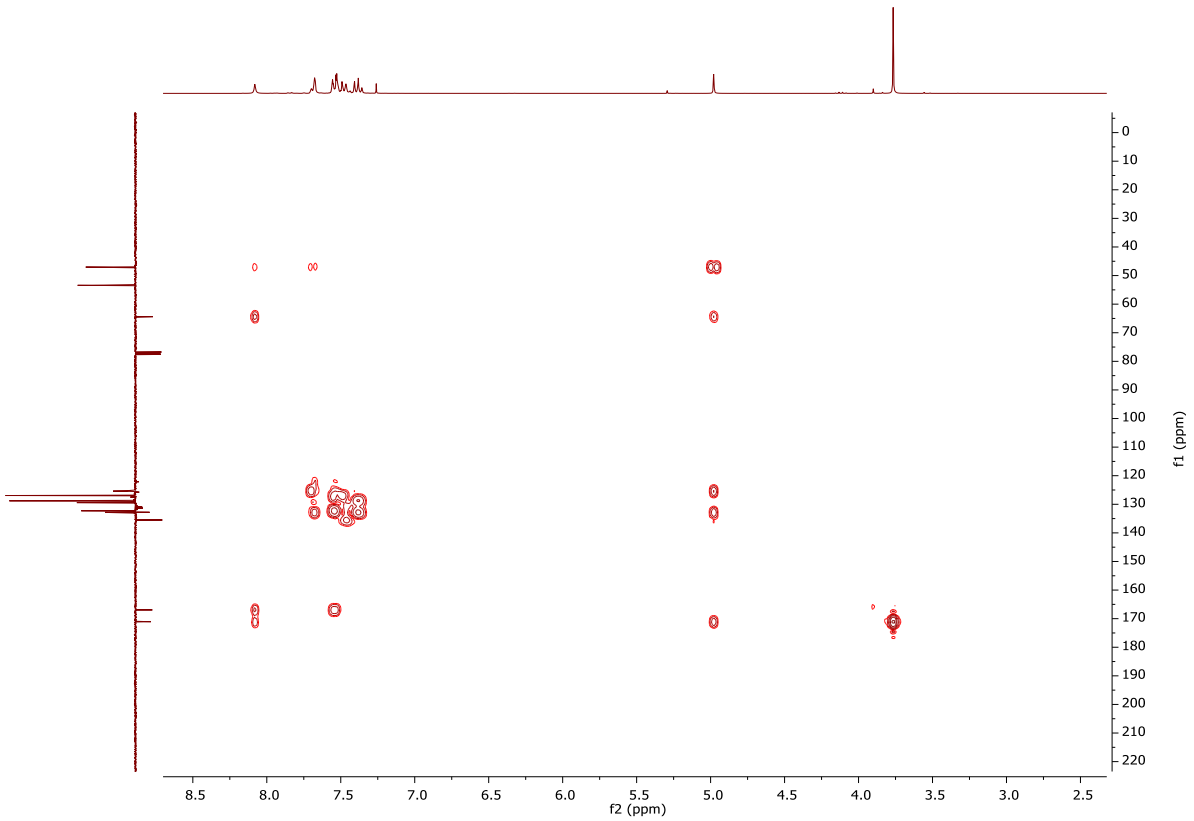
^{1}H NMR spectrum ($CDCl_3$, 300.13 MHz) of **2m**



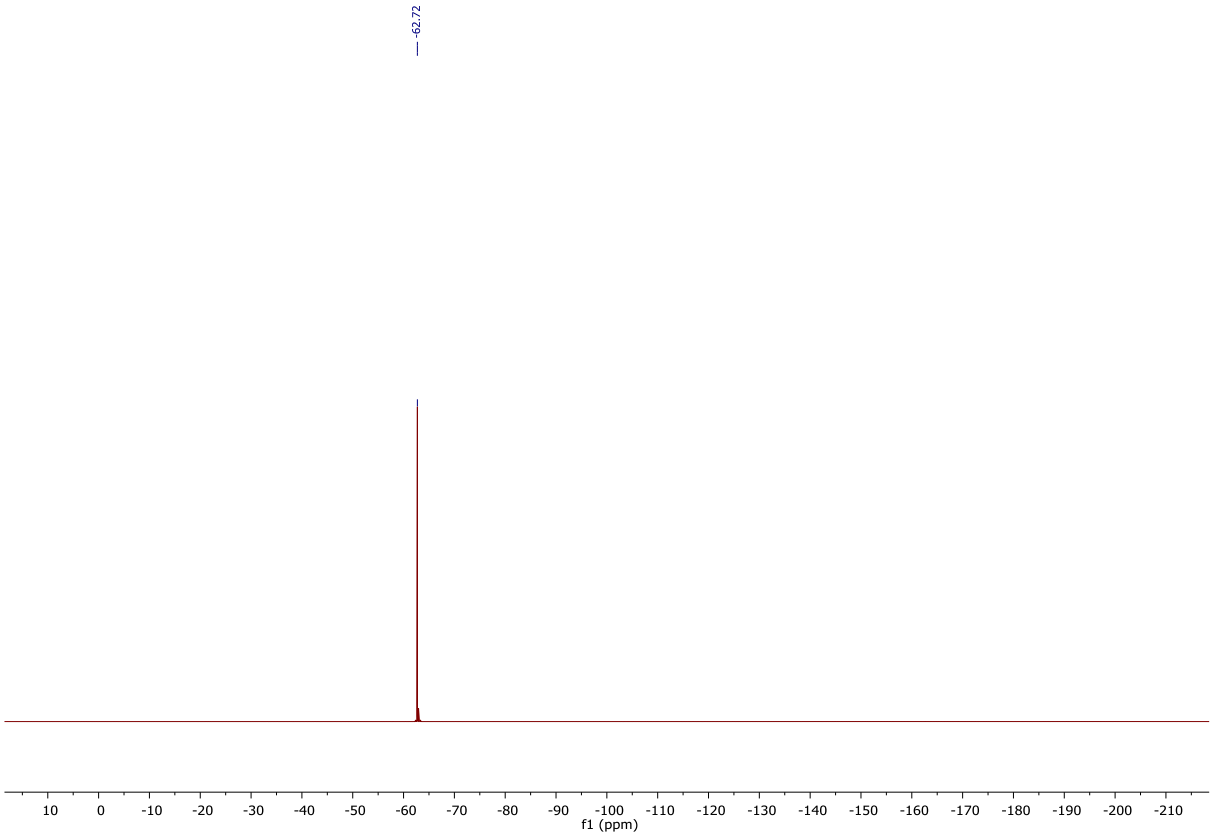
$^{13}C\{^{1}H\}$ (APT) NMR spectrum ($CDCl_3$, 75.5 MHz) of **2m**



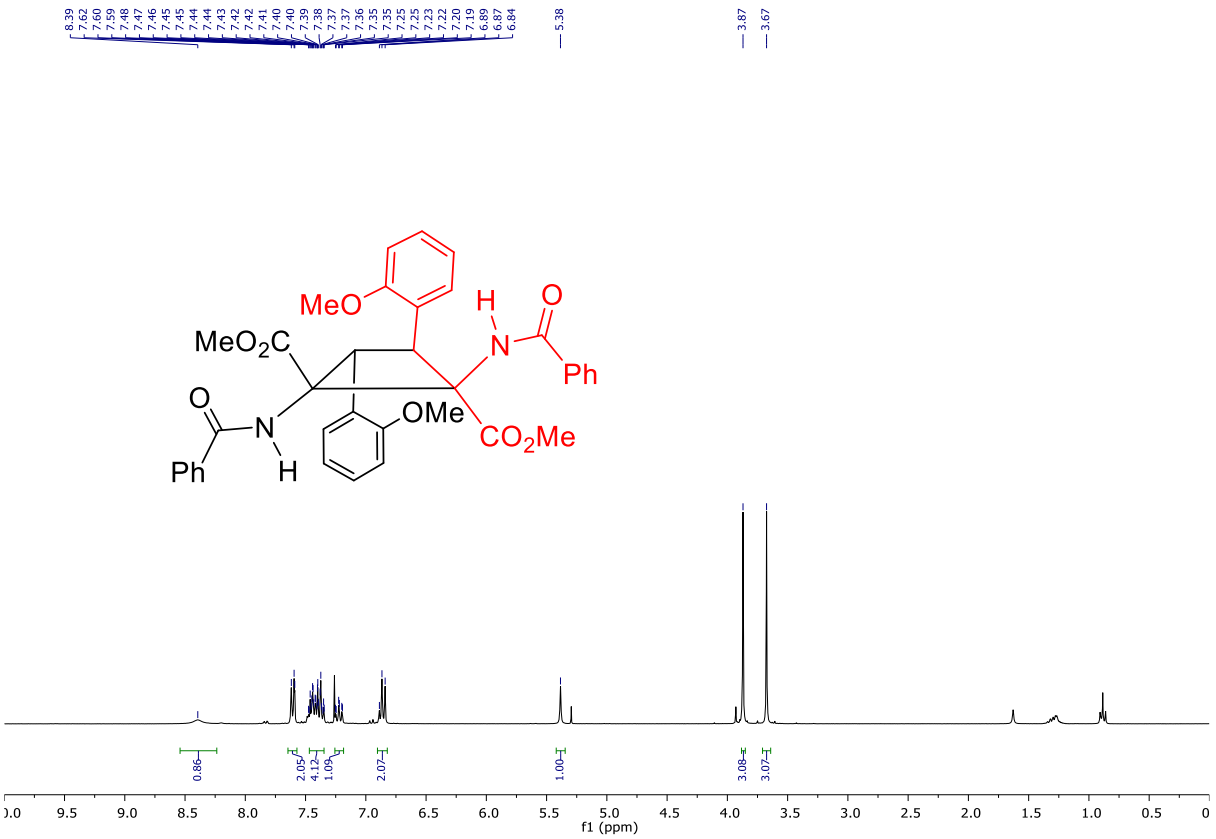
^{1}H-^{13}C HSQC ($CDCl_3$) correlation spectrum of **2m**



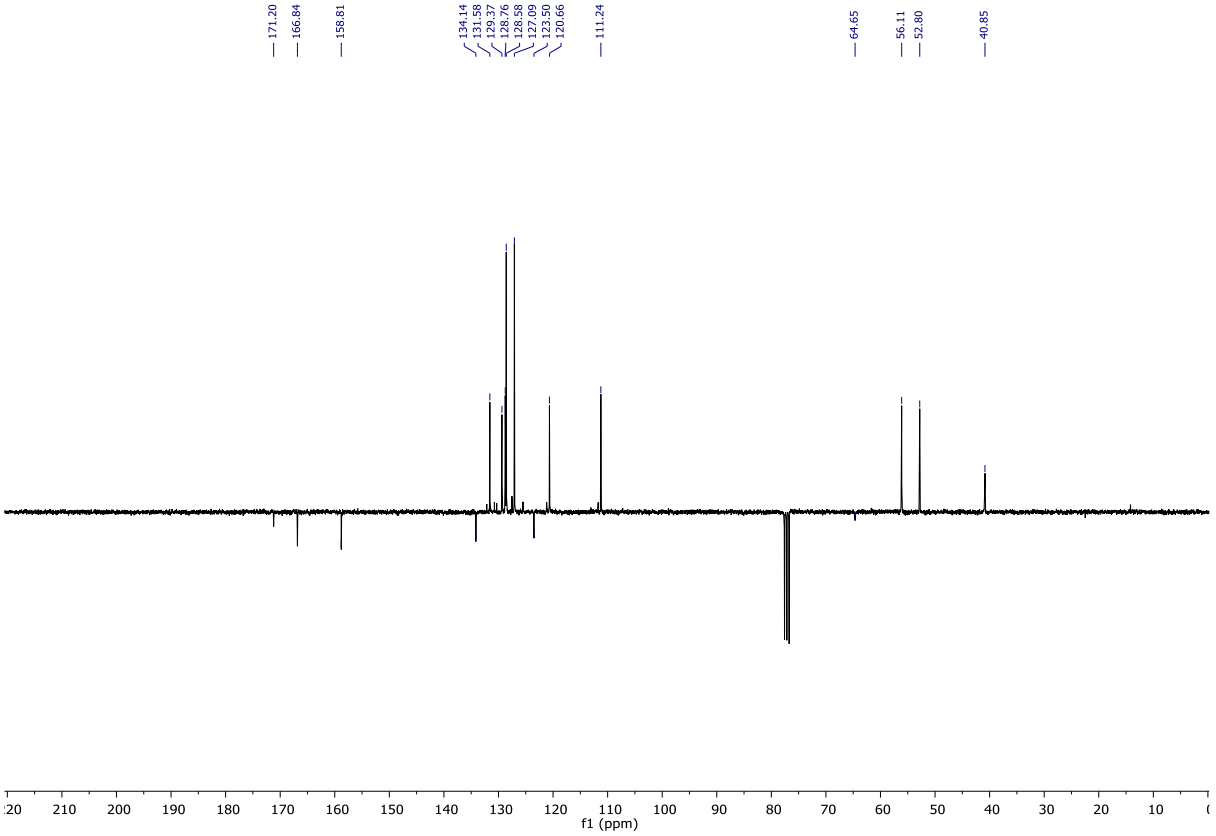
^{1}H-^{13}C HMBC ($CDCl_3$) correlation spectrum of **2m**



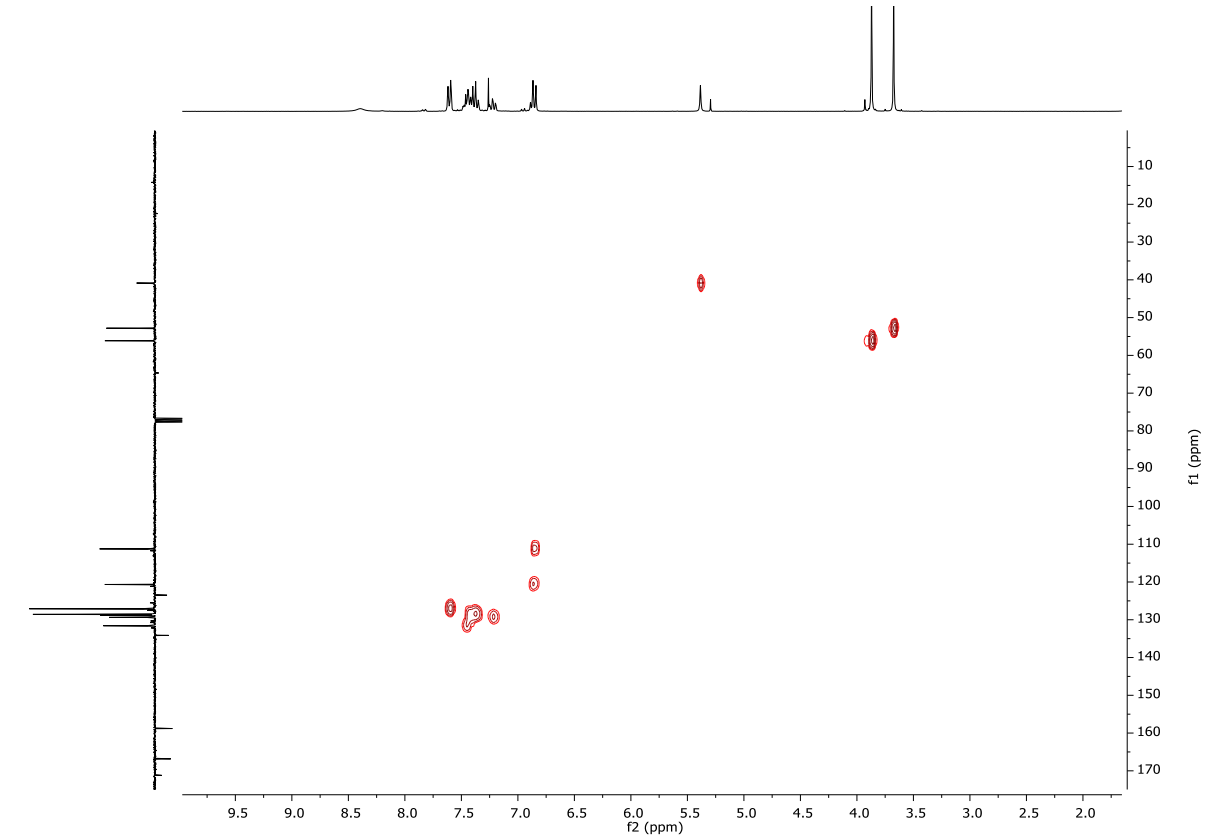
^{19}F NMR spectrum ($CDCl_3$, 282.40 MHz) of **2m**



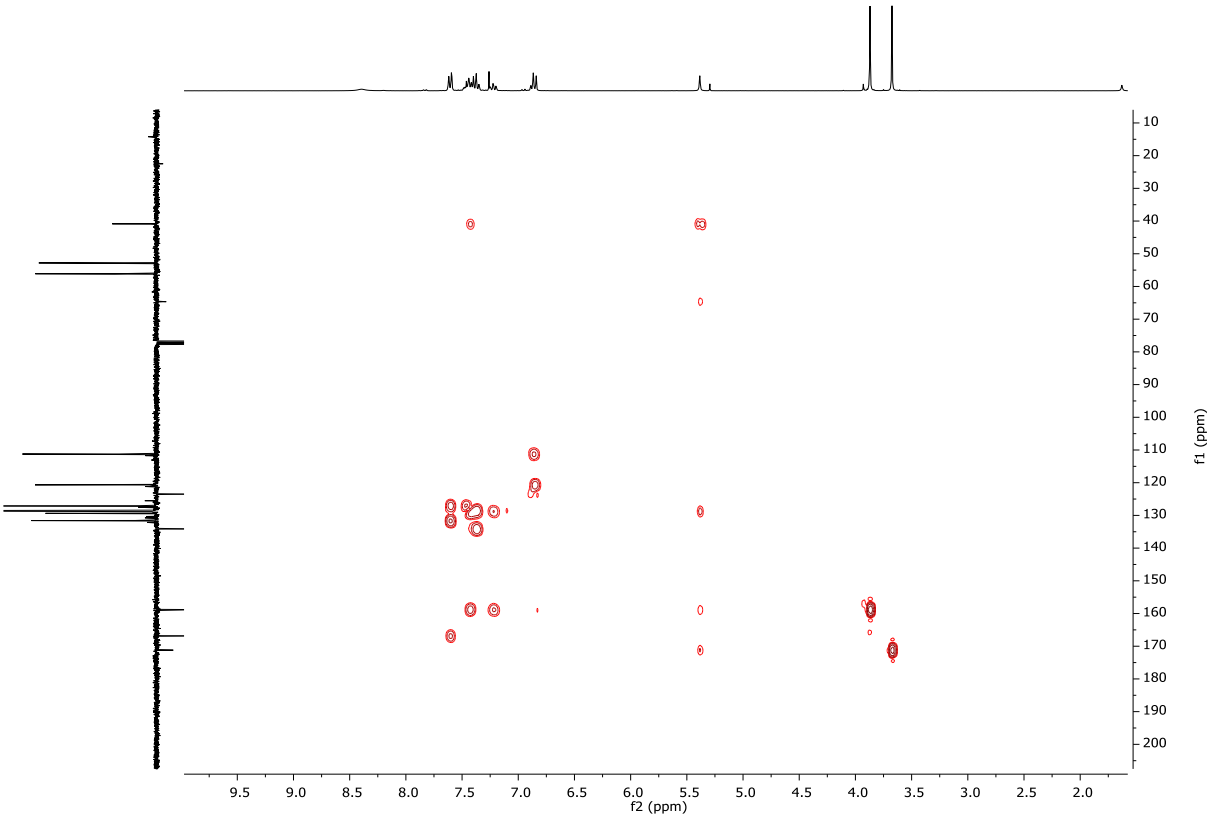
^{1}H NMR spectrum ($CDCl_3$, 300.13 MHz) of **2n**



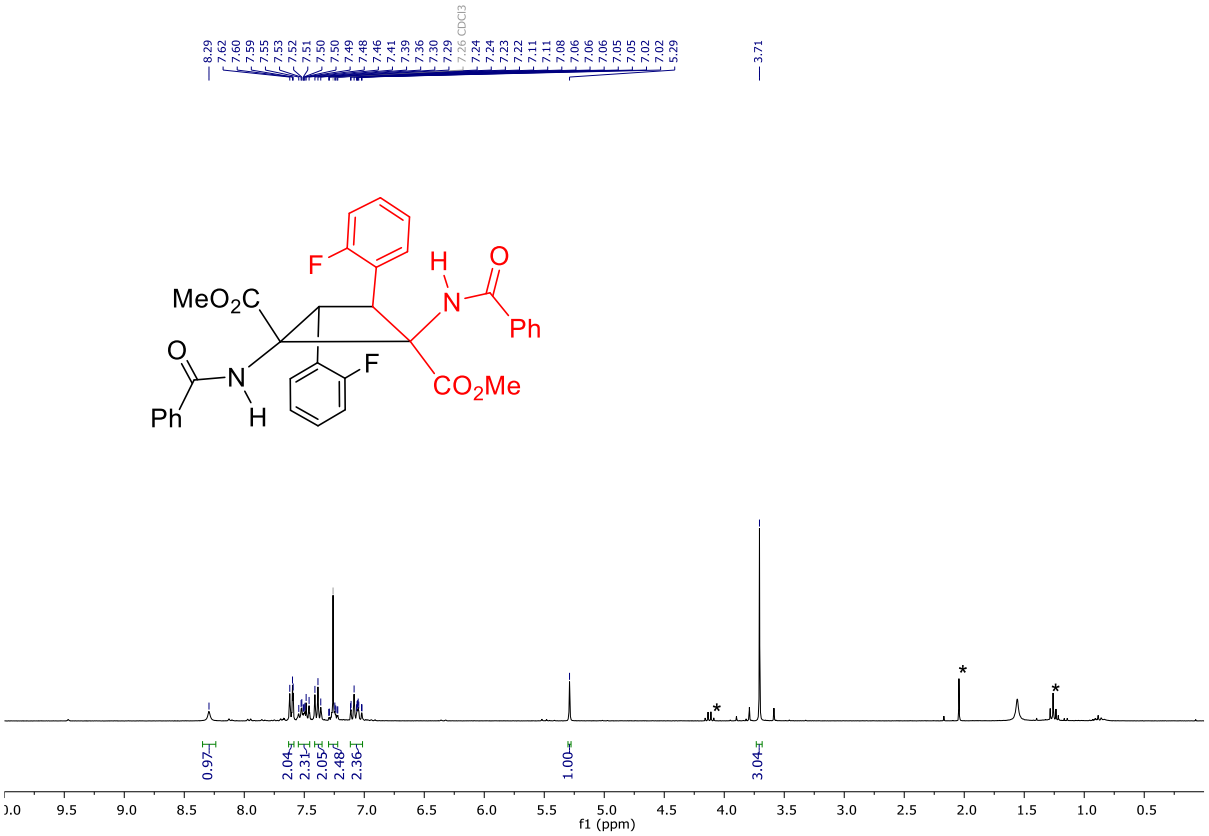
$^{13}C\{^{1}H\}$ (APT) NMR spectrum ($CDCl_3$, 75.5 MHz) of **2n**



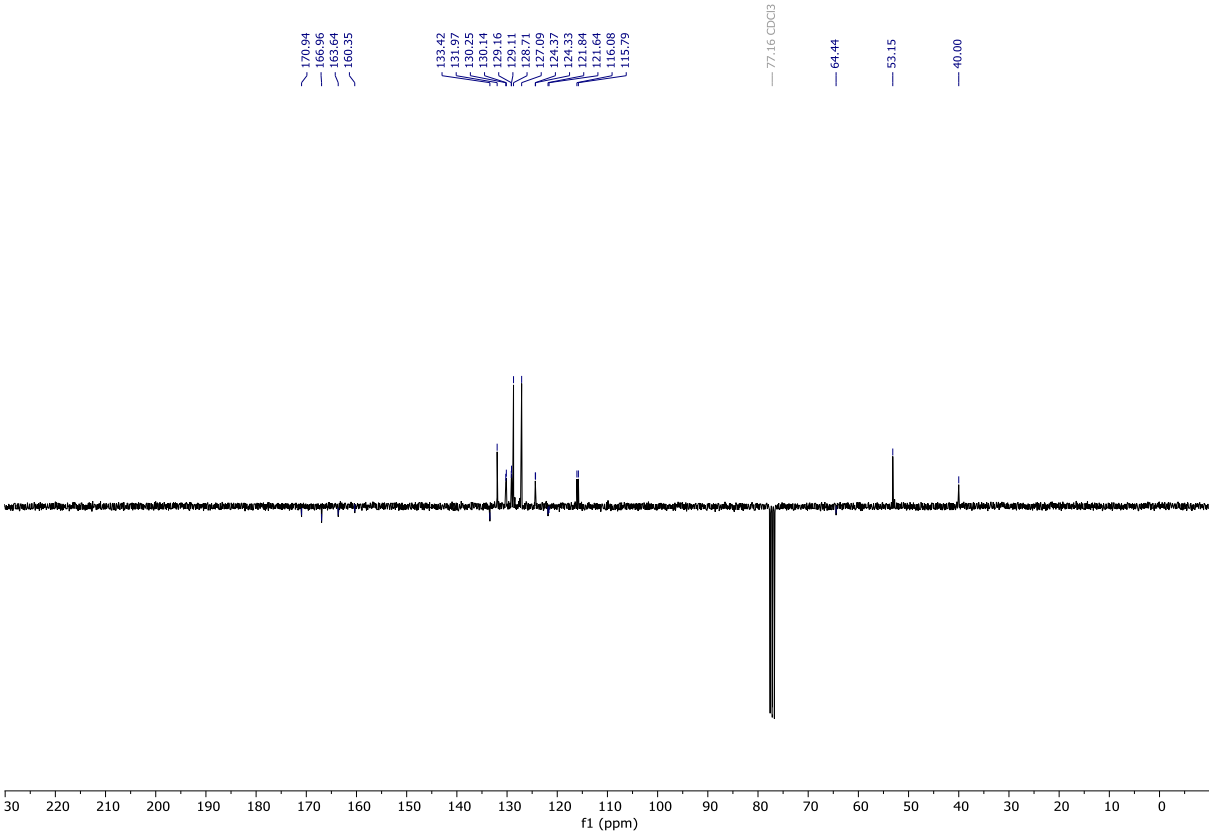
^{1}H-^{13}C HSQC ($CDCl_3$) correlation spectrum of **2n**



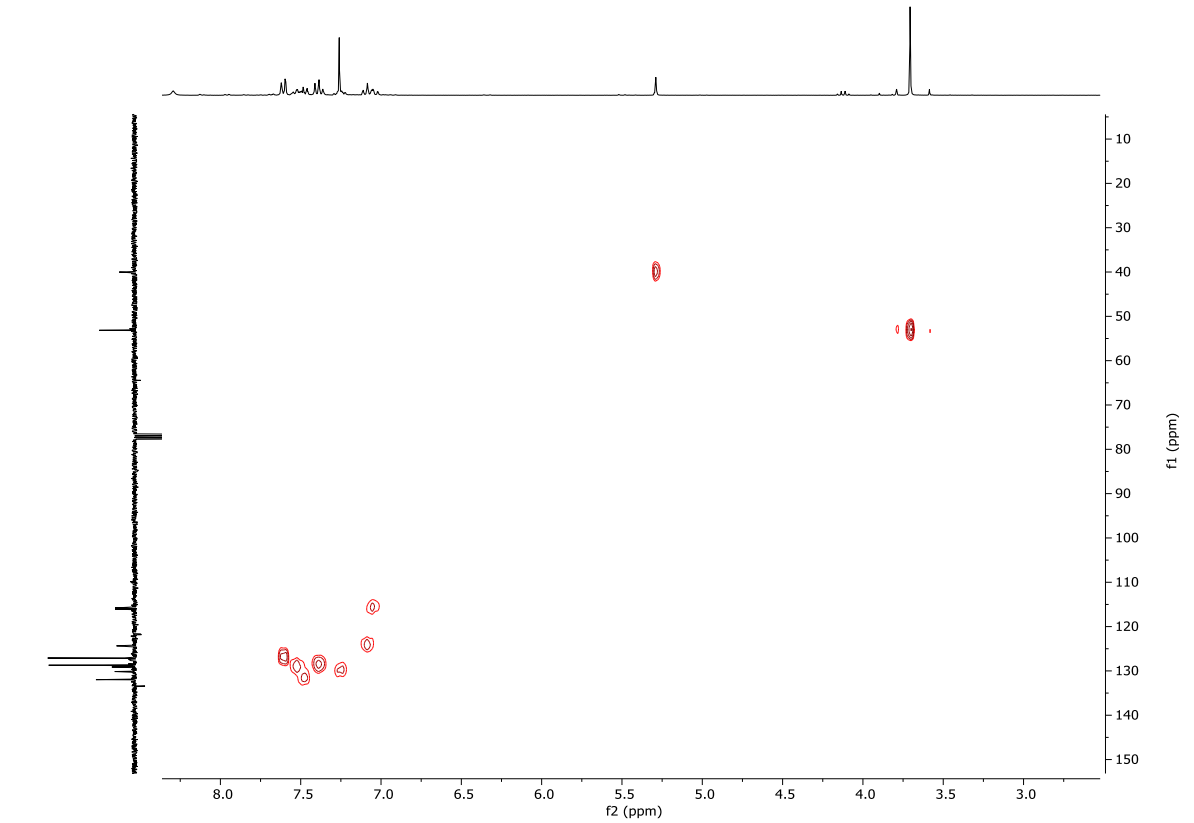
^{1}H-^{13}C HMBC ($CDCl_3$) correlation spectrum of **2n**



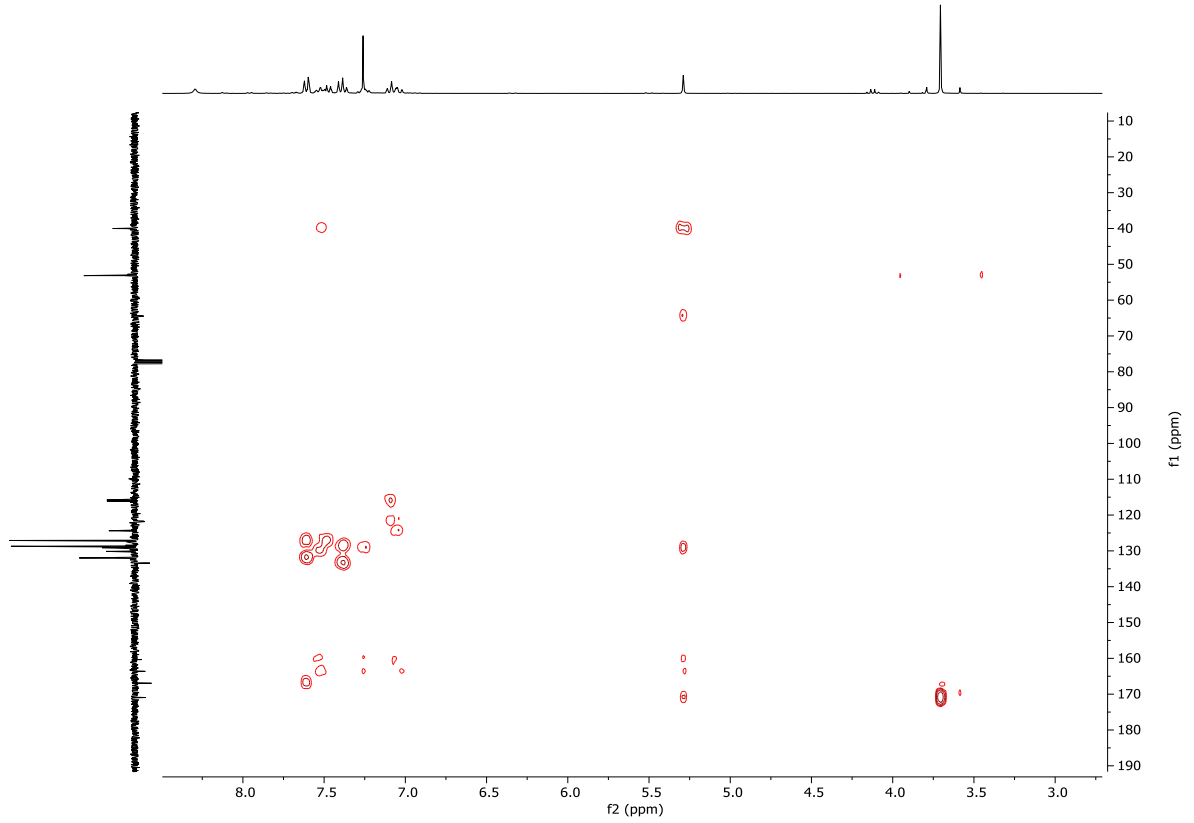
^{1}H NMR spectrum ($CDCl_3$, 300.13 MHz) of **2o** (* = ethyl acetate)



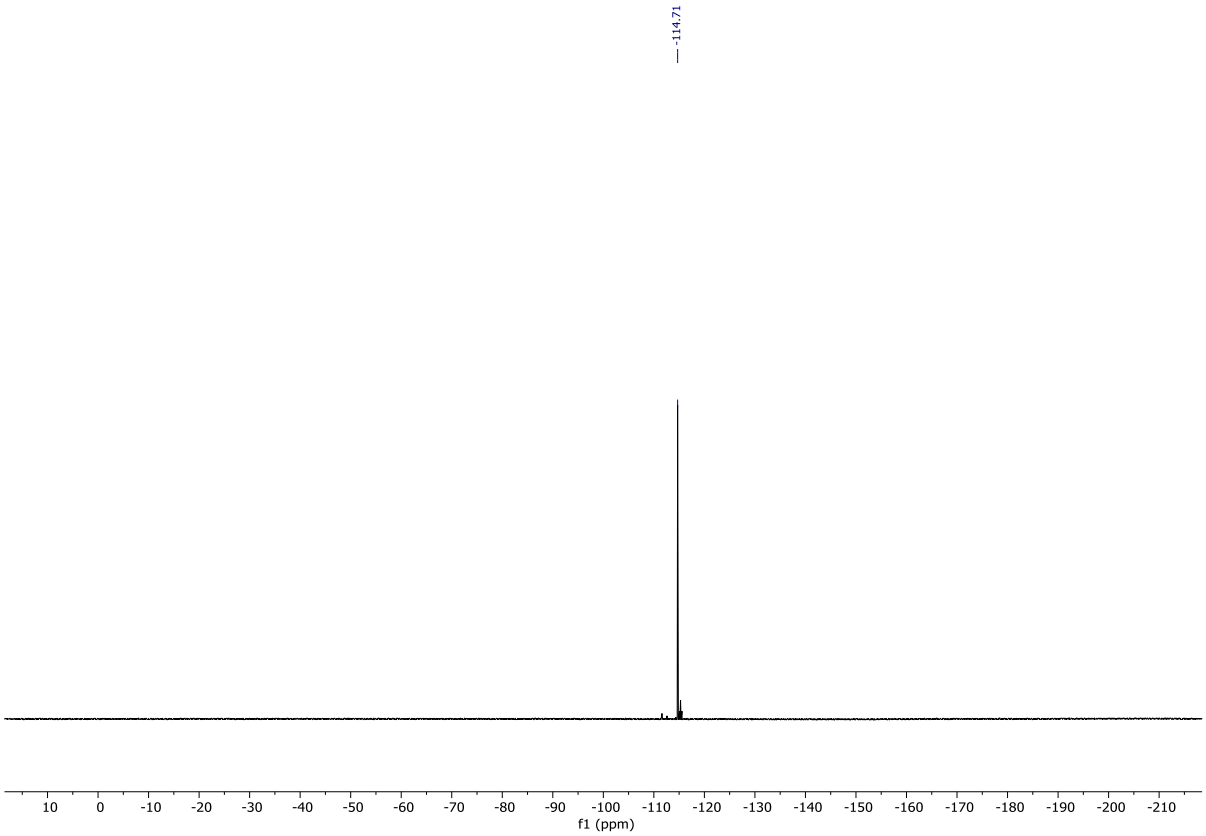
^{13}C{^{1}H} (APT) NMR spectrum ($CDCl_3$, 75.5 MHz) of **2o**



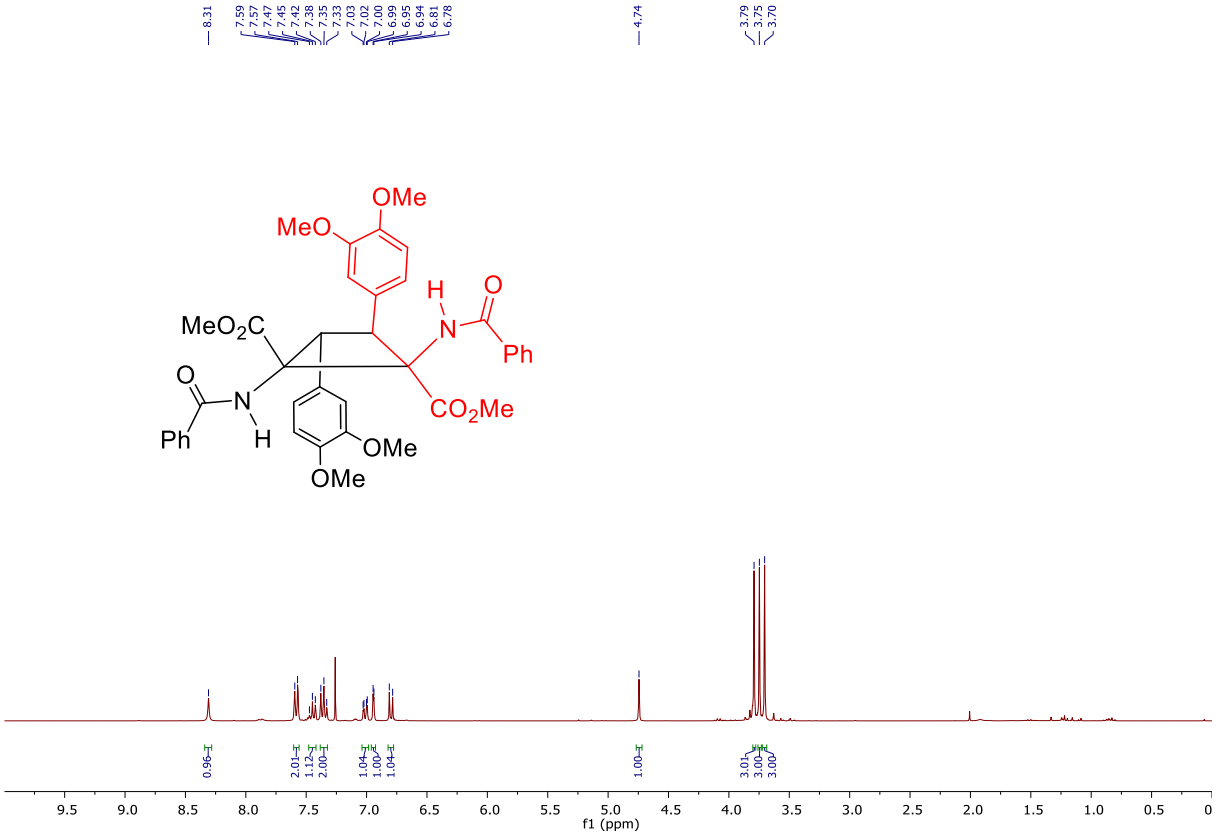
^{1}H-^{13}C HSQC ($CDCl_3$) correlation spectrum of **2o**



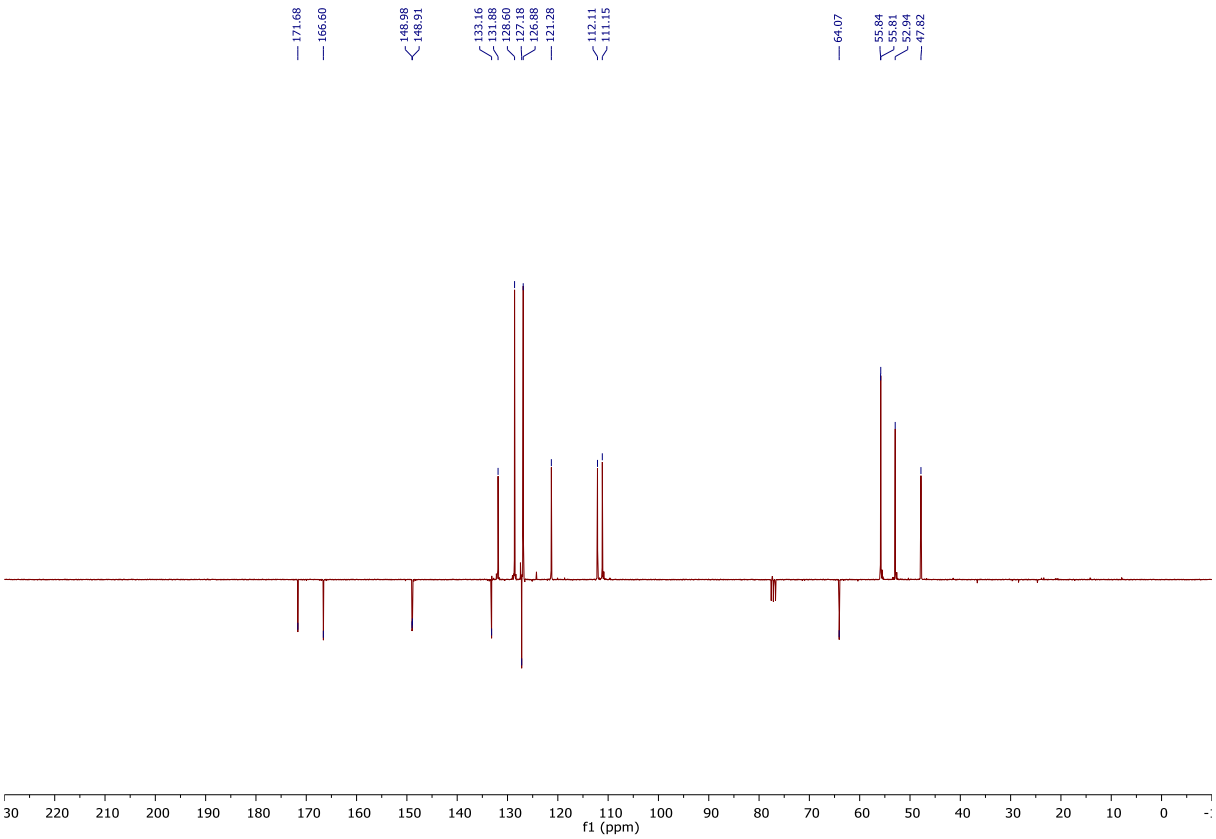
^{1}H-^{13}C HMBC ($CDCl_3$) correlation spectrum of **2o**



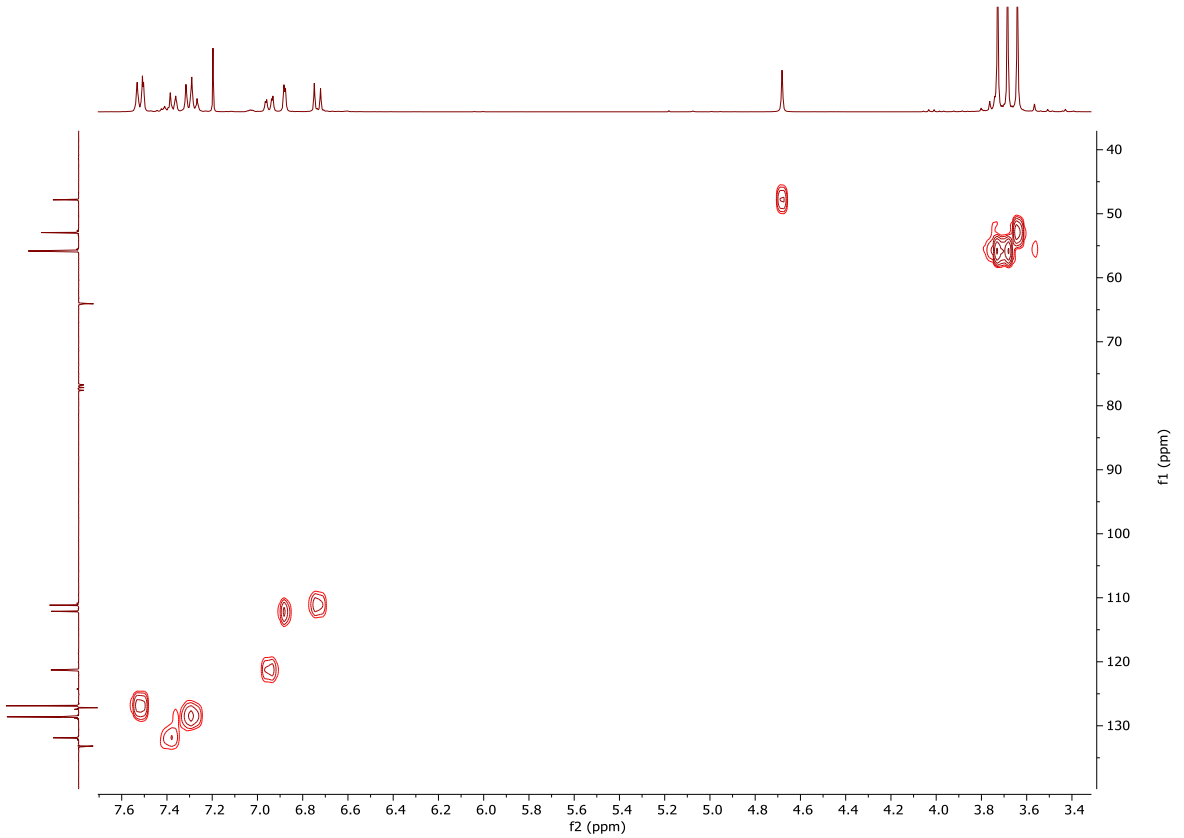
^{19}F {^{1}H} NMR spectrum ($CDCl_3$, 282.40 MHz) of **2o**



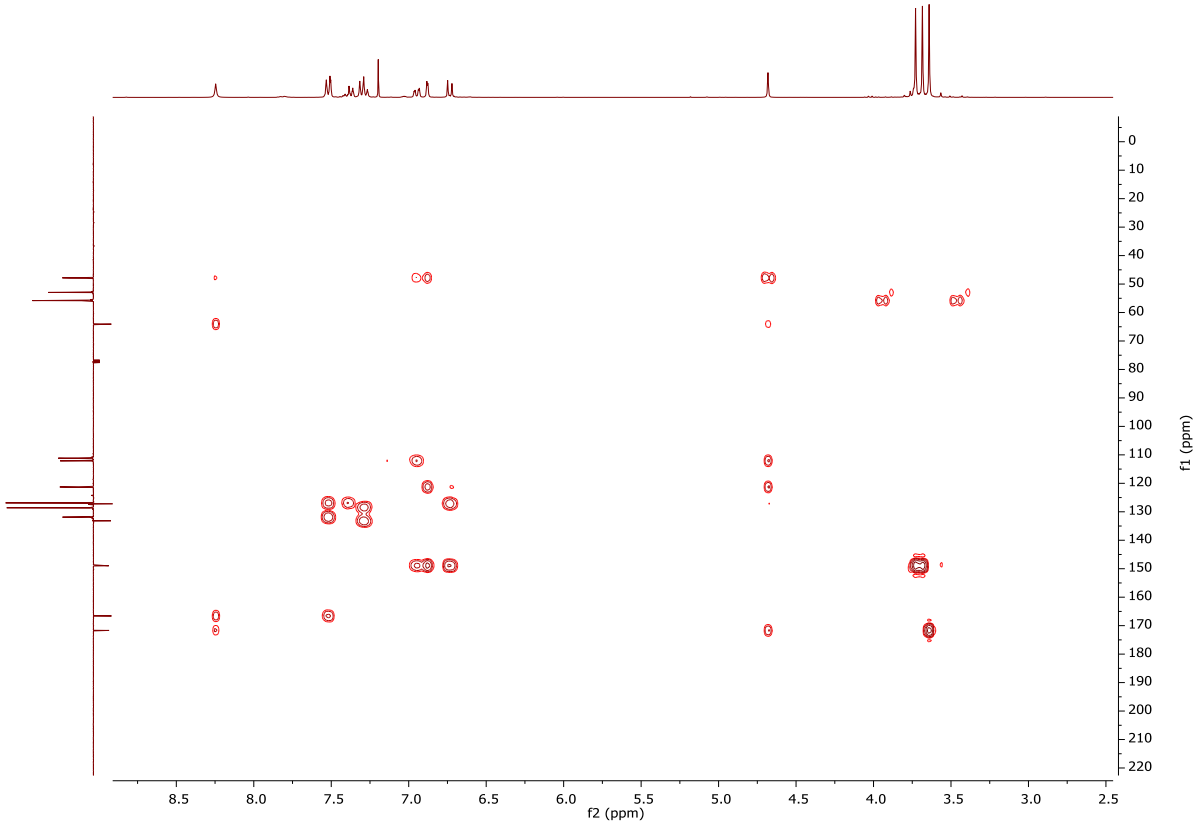
^{1}H NMR spectrum ($CDCl_3$, 300.13 MHz) of **2p**



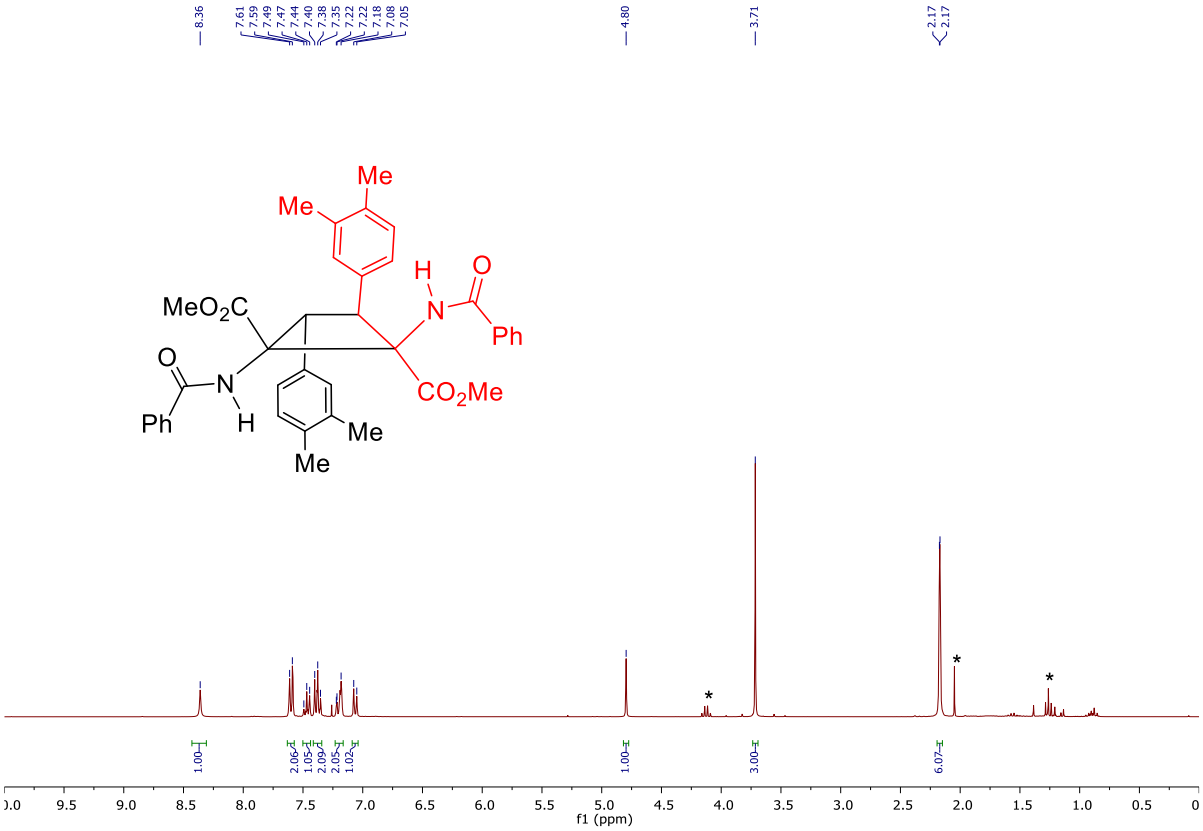
$^{13}C\{^{1}H\}$ (APT) NMR spectrum ($CDCl_3$, 75.5 MHz) of **2p**



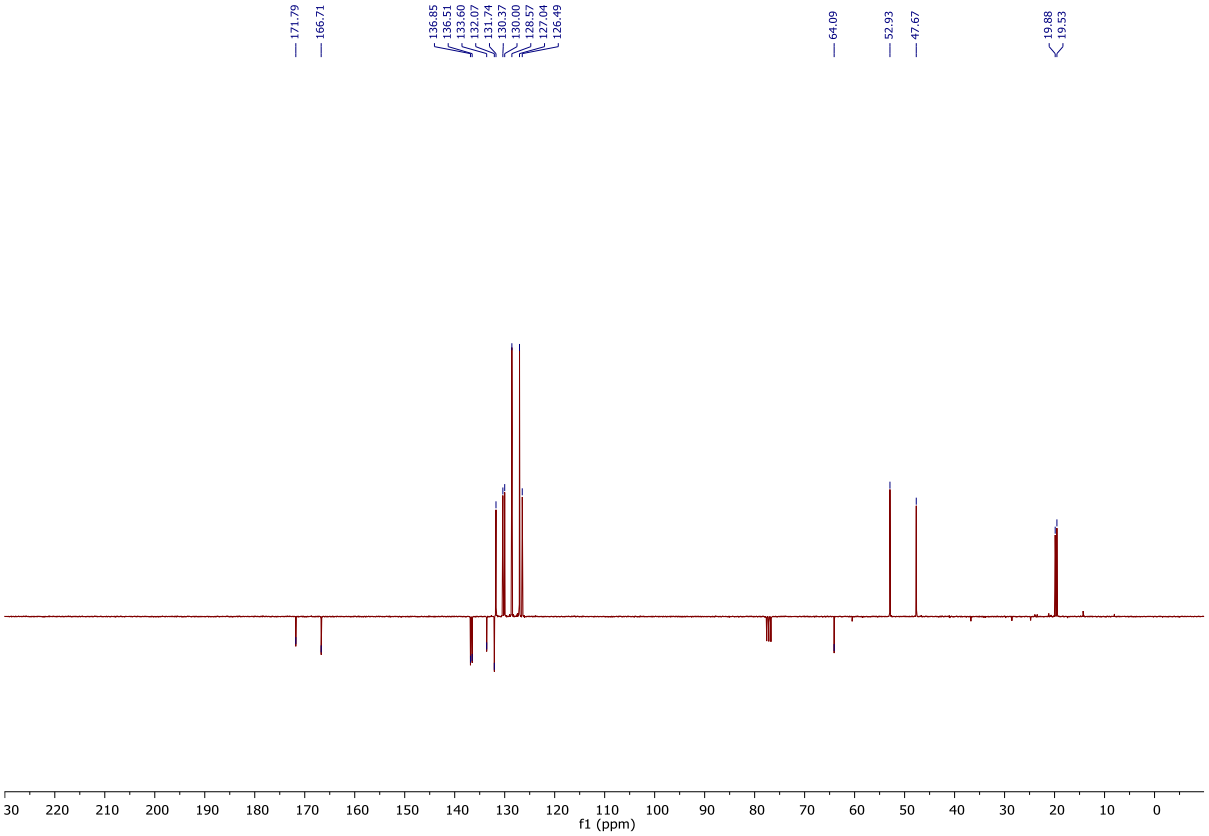
^{1}H-^{13}C HSQC ($CDCl_3$) correlation spectrum of **2p**



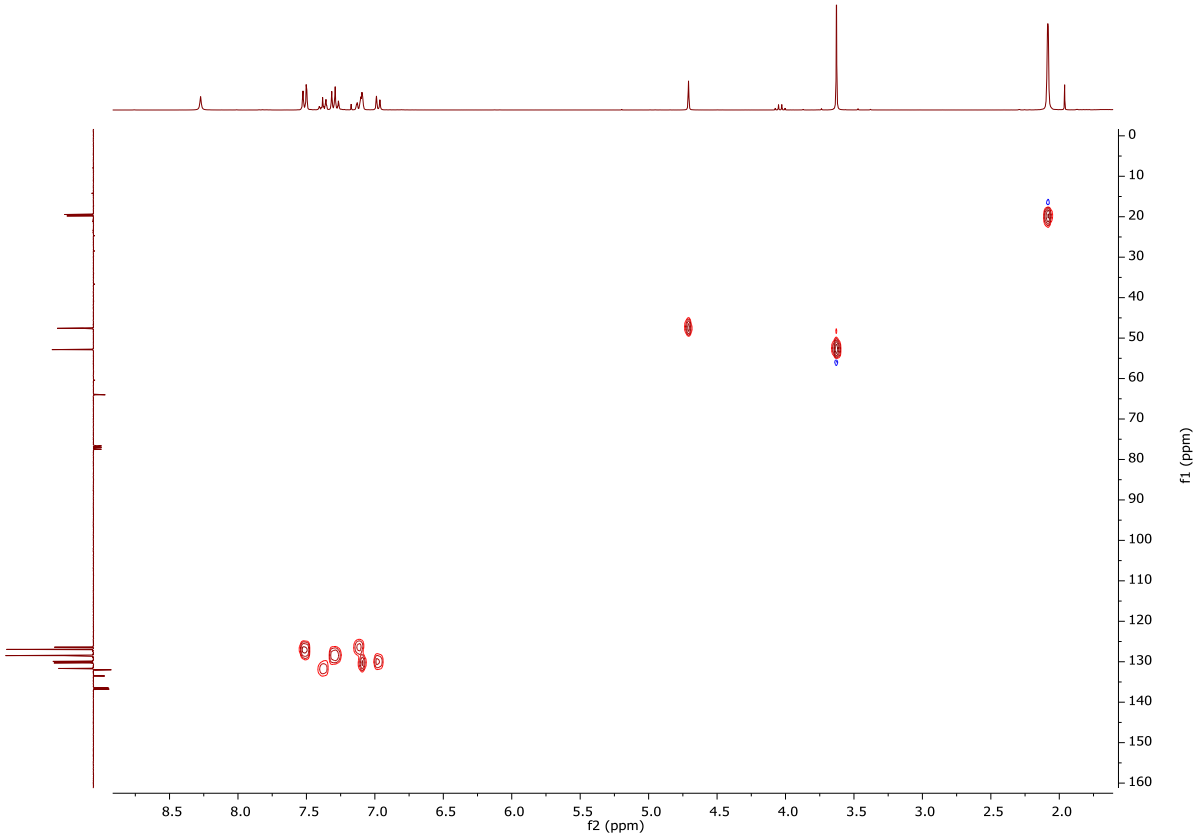
^{1}H-^{13}C HMBC ($CDCl_3$) correlation spectrum of **2p**



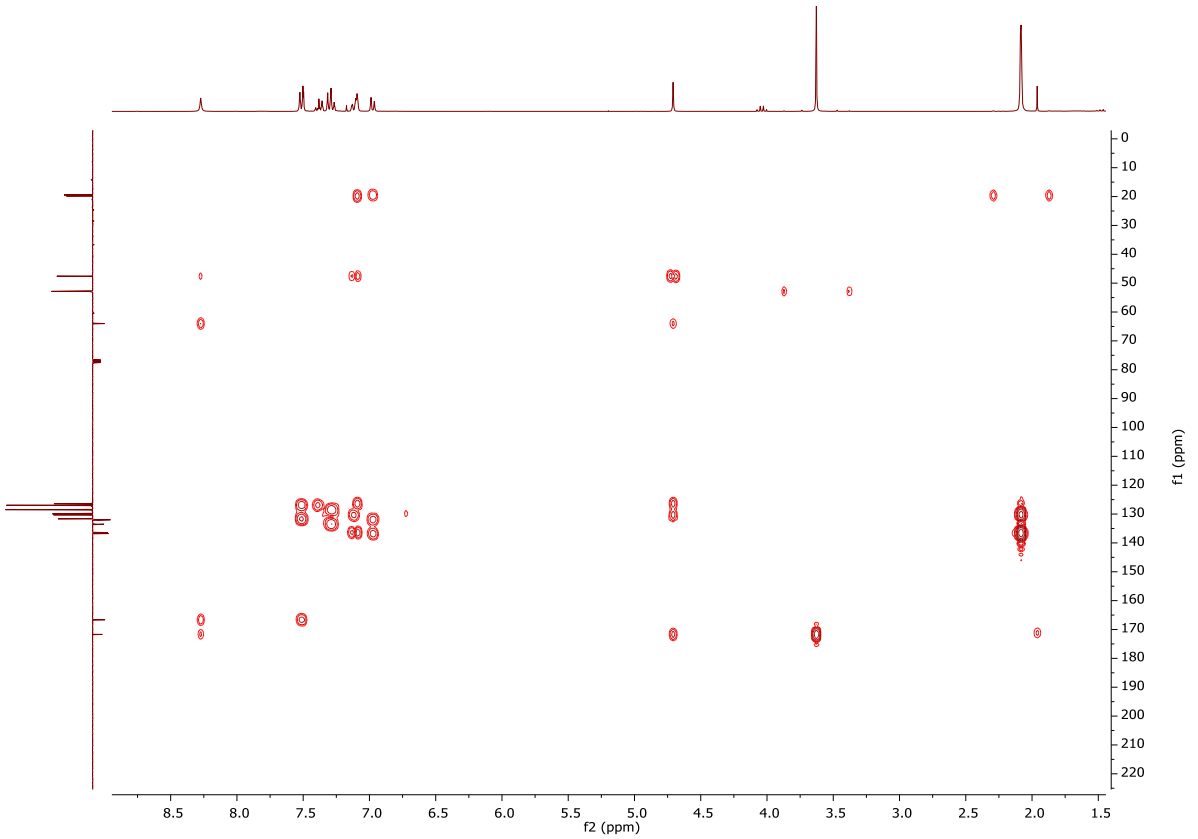
^{1}H NMR spectrum ($CDCl_3$, 300.13 MHz) of **2q** (* = ethyl acetate)



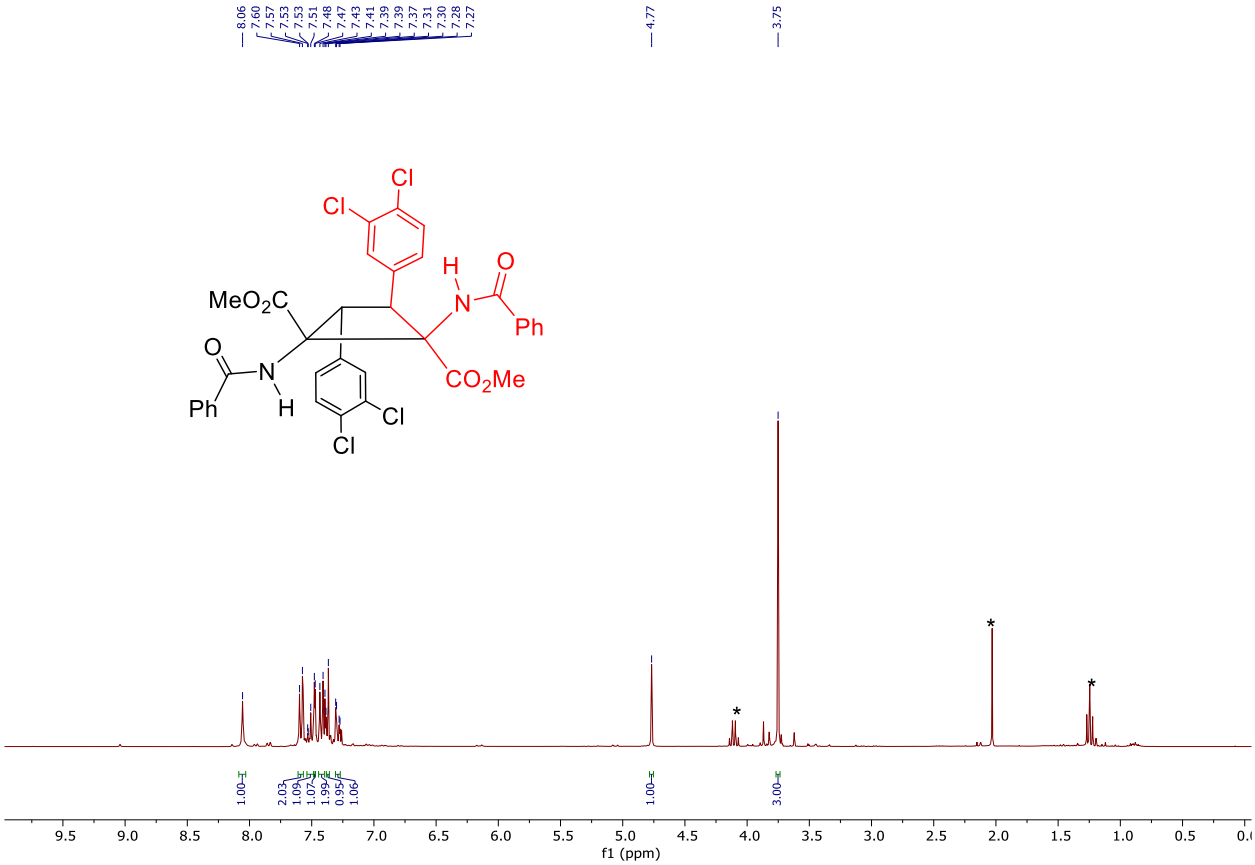
$^{13}C\{^{1}H\}$ (APT) NMR spectrum ($CDCl_3$, 75.5 MHz) of **2q**



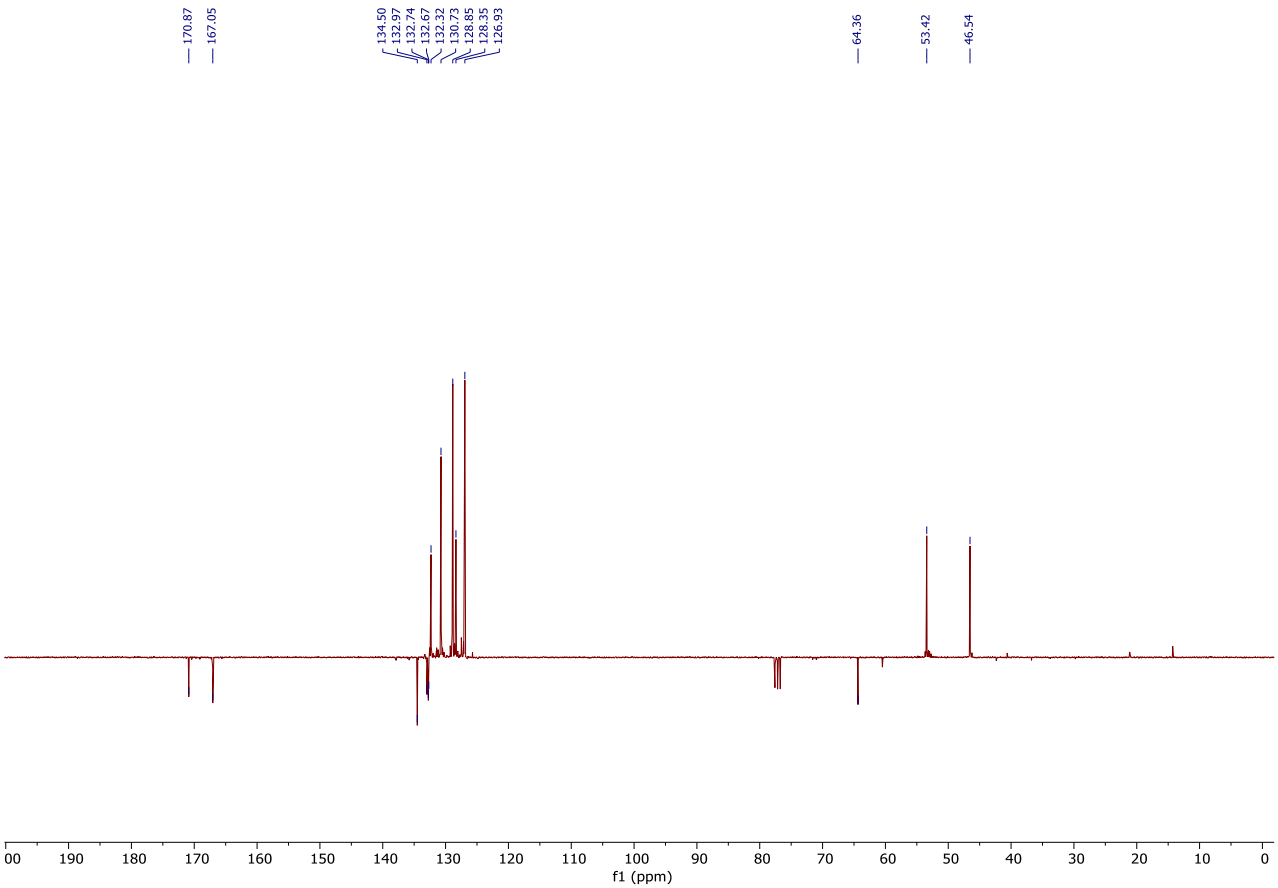
^{1}H-^{13}C HSQC ($CDCl_3$) correlation spectrum of **2q**



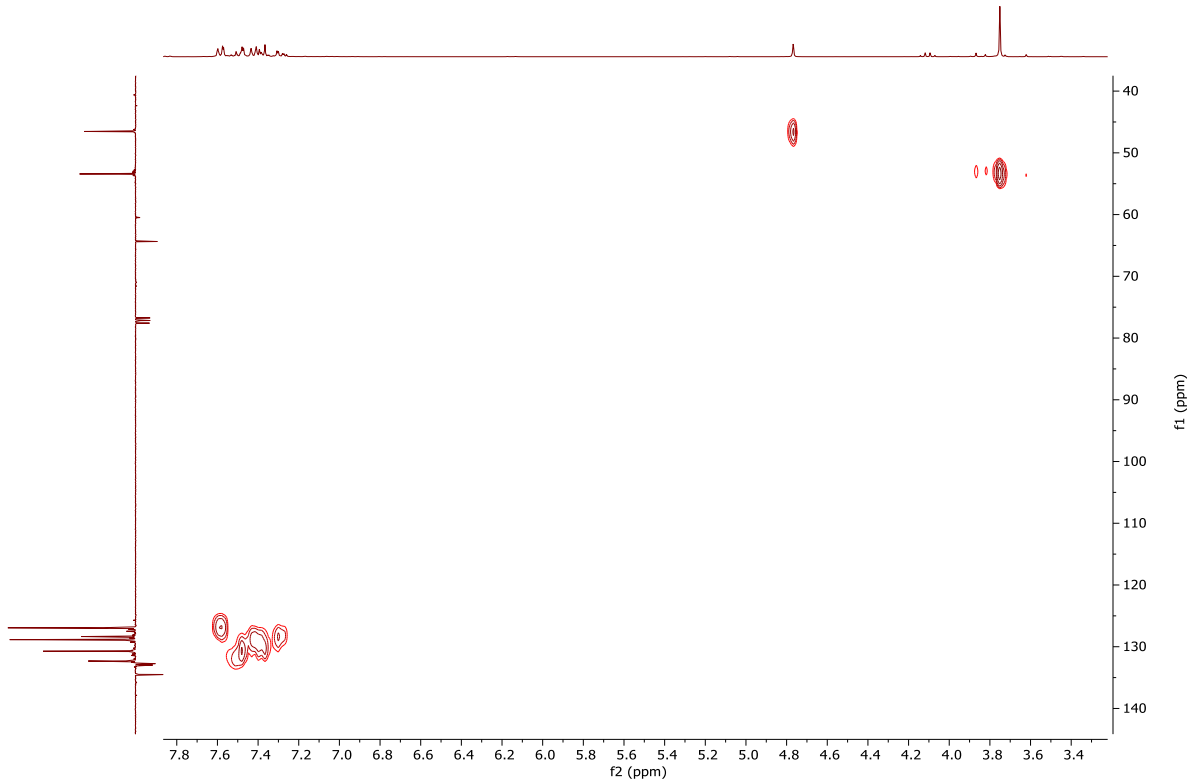
^{1}H-^{13}C HMBC ($CDCl_3$) correlation spectrum of **2q**



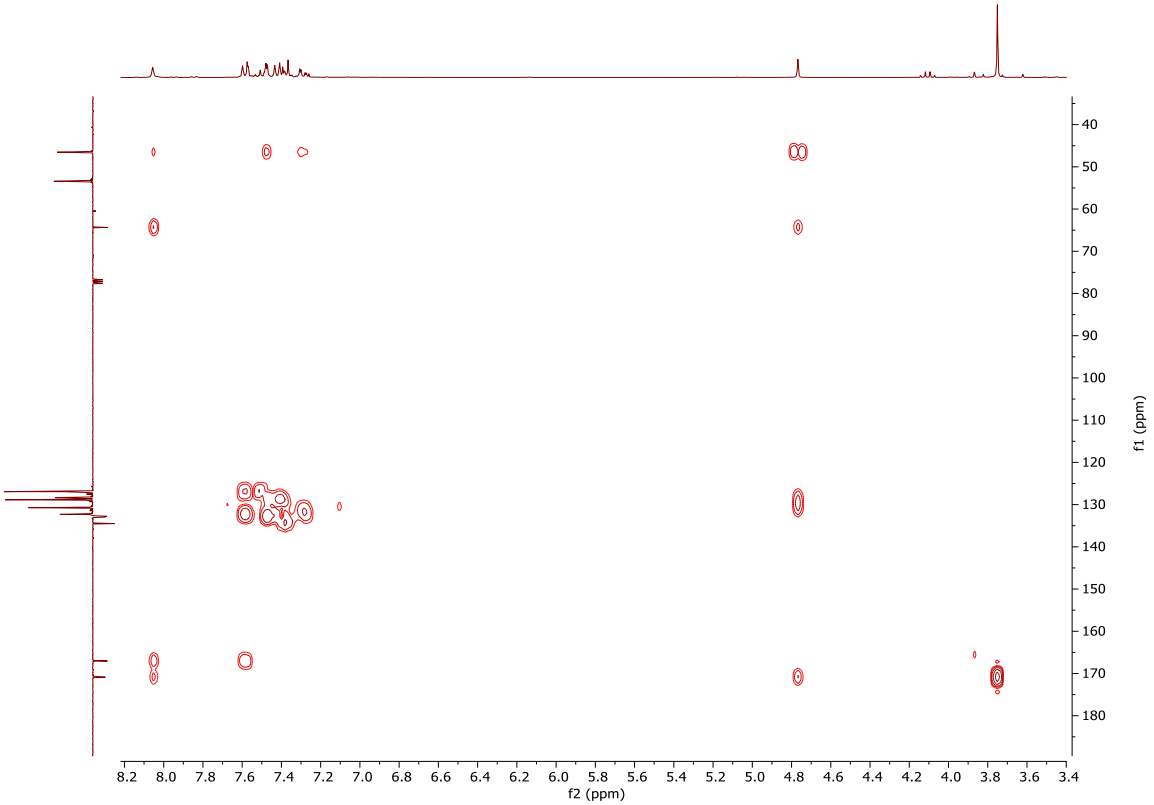
^{1}H NMR spectrum ($CDCl_3$, 300.13 MHz) of **2r** (* = ethyl acetate)



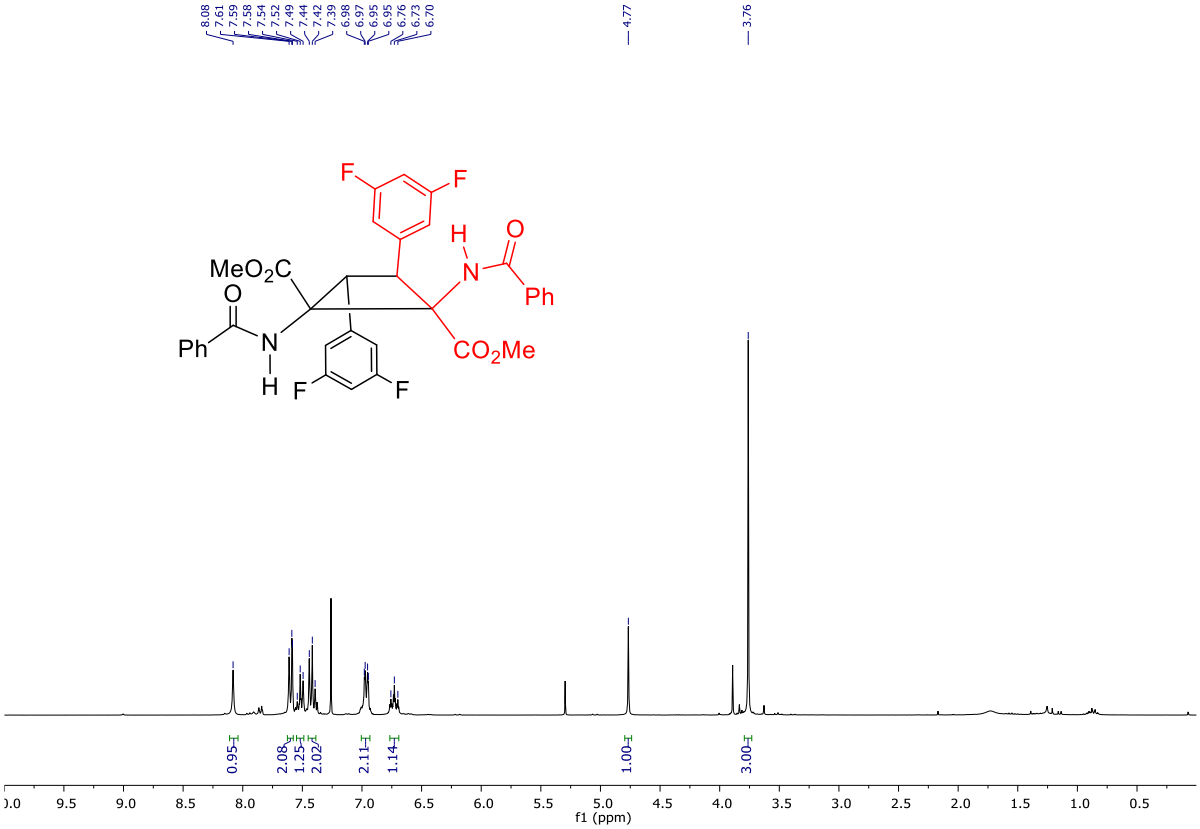
$^{13}C\{^{1}H\}$ (APT) NMR spectrum ($CDCl_3$, 75.5 MHz) of **2r**



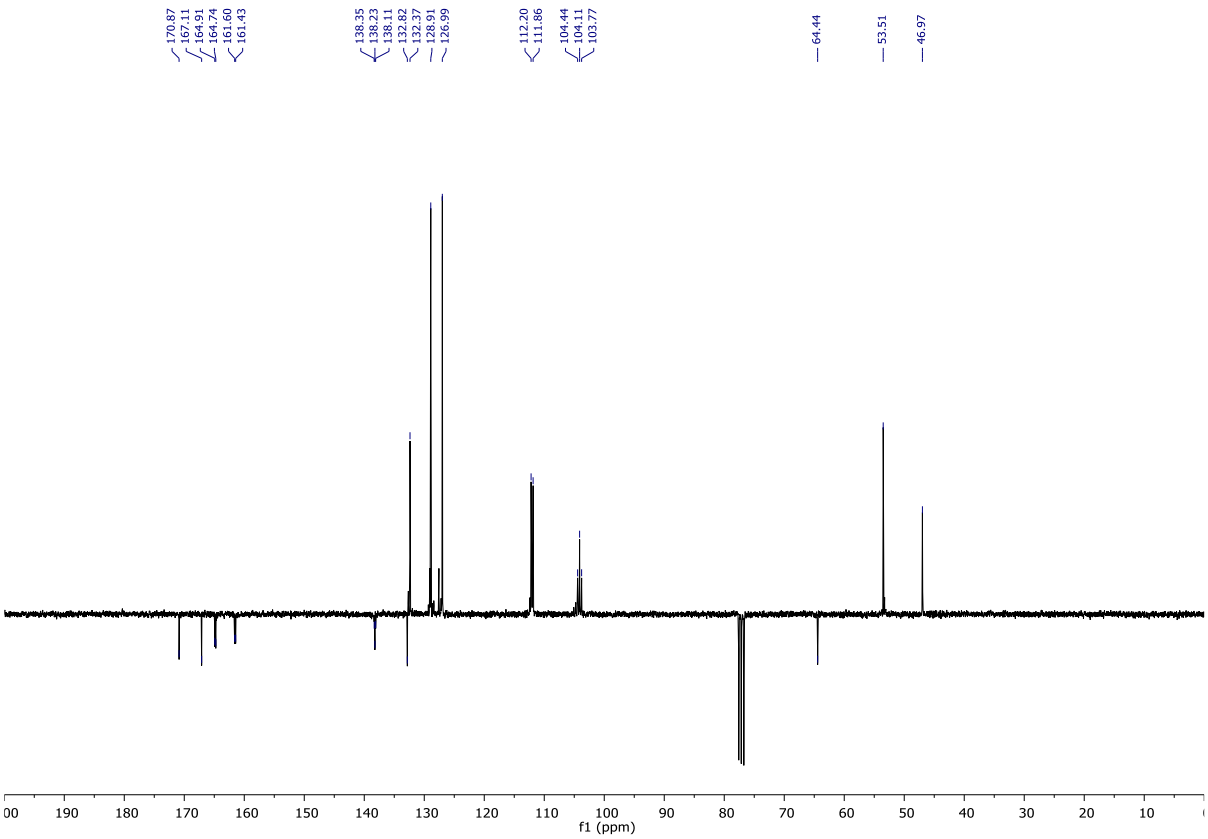
^{1}H-^{13}C HSQC ($CDCl_3$) correlation spectrum of **2r**



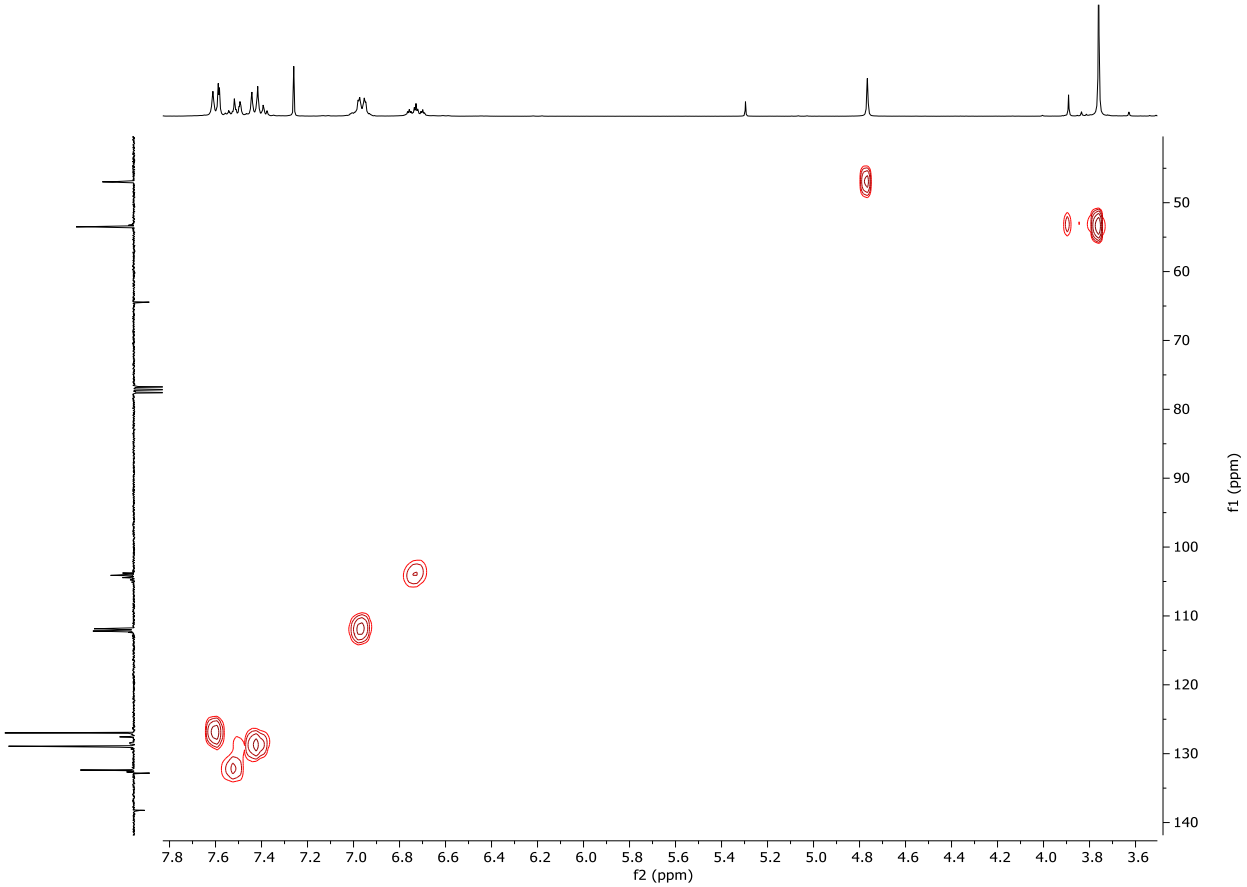
^{1}H-^{13}C HMBC ($CDCl_3$) correlation spectrum of **2r**



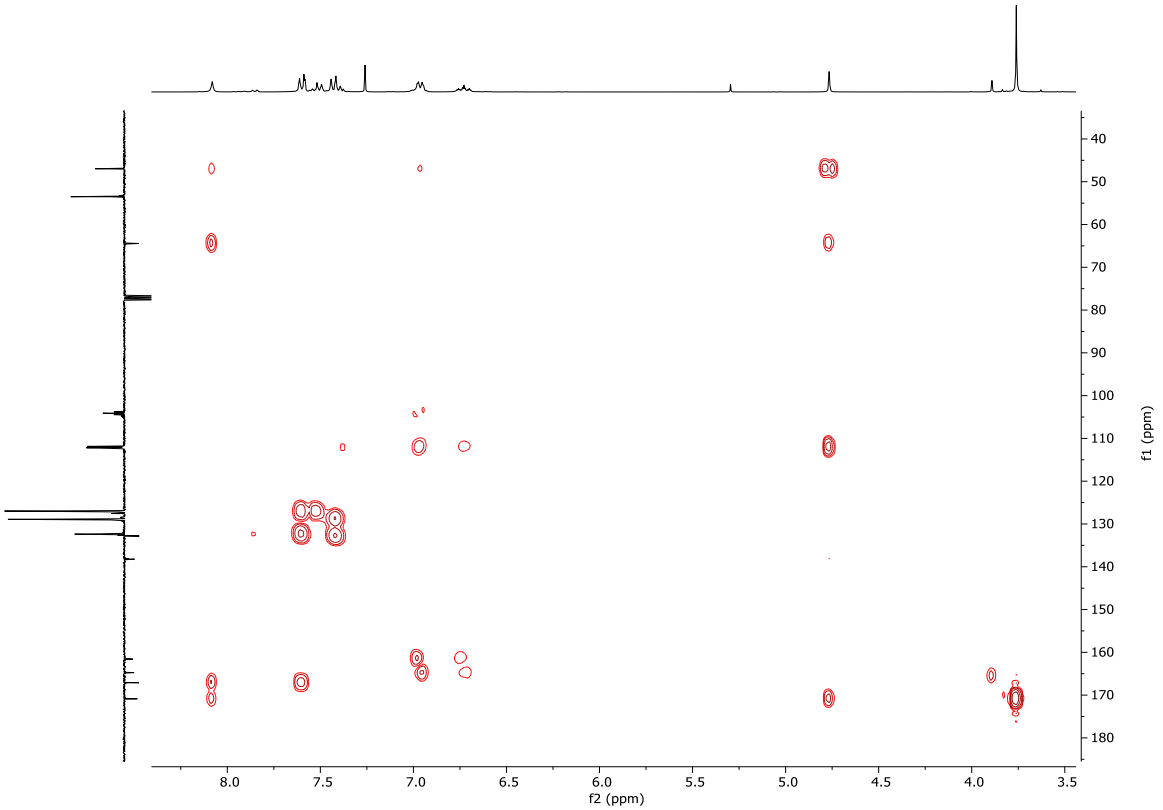
^{1}H NMR spectrum ($CDCl_3$, 300.13 MHz) of **2s**



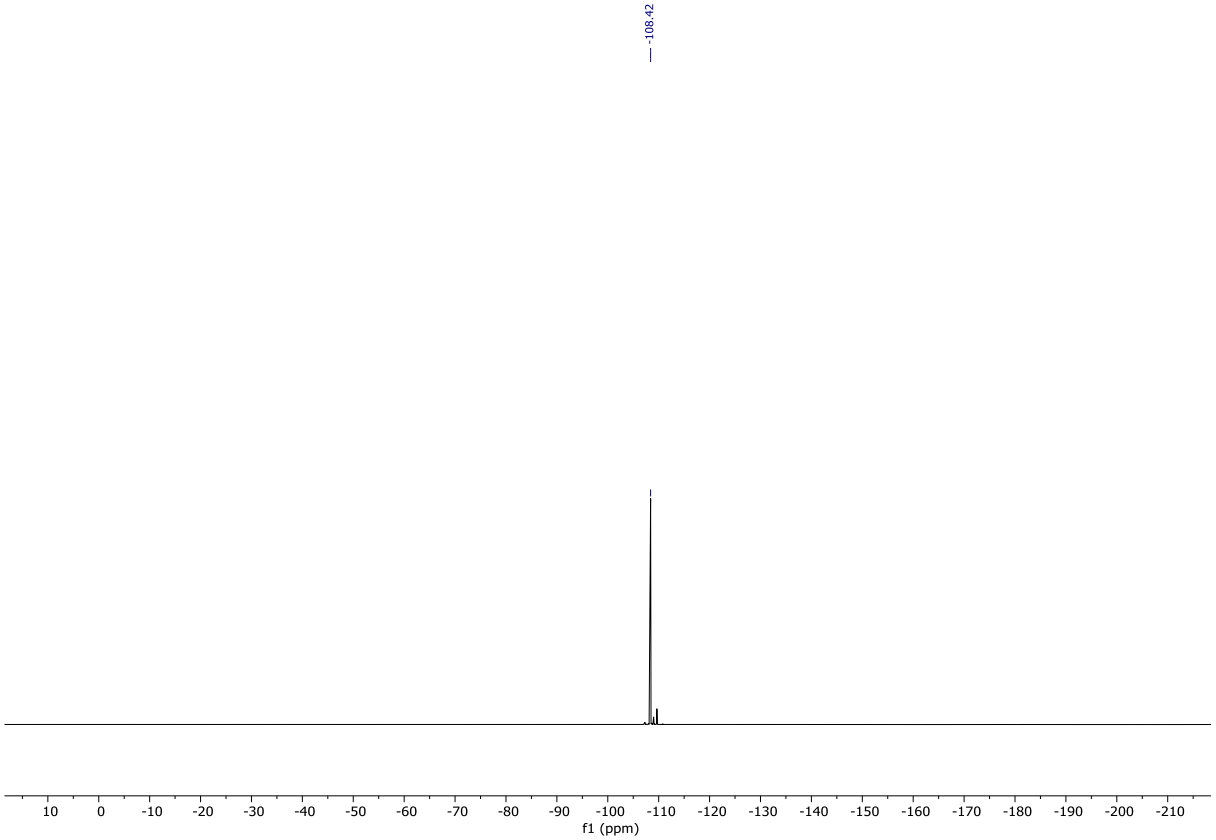
$^{13}C\{^{1}H\}$ (APT) NMR spectrum ($CDCl_3$, 75.5 MHz) of **2s**



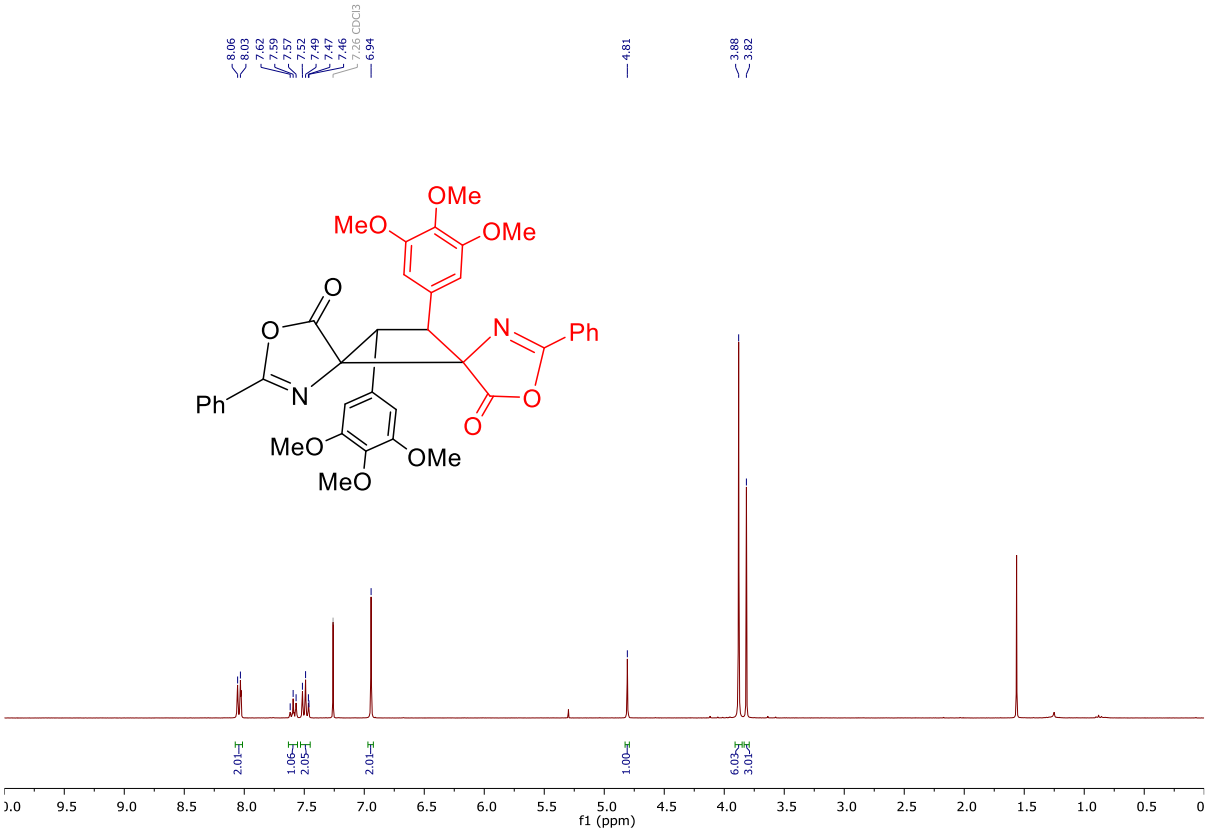
^{1}H-^{13}C HSQC ($CDCl_3$) correlation spectrum of **2s**



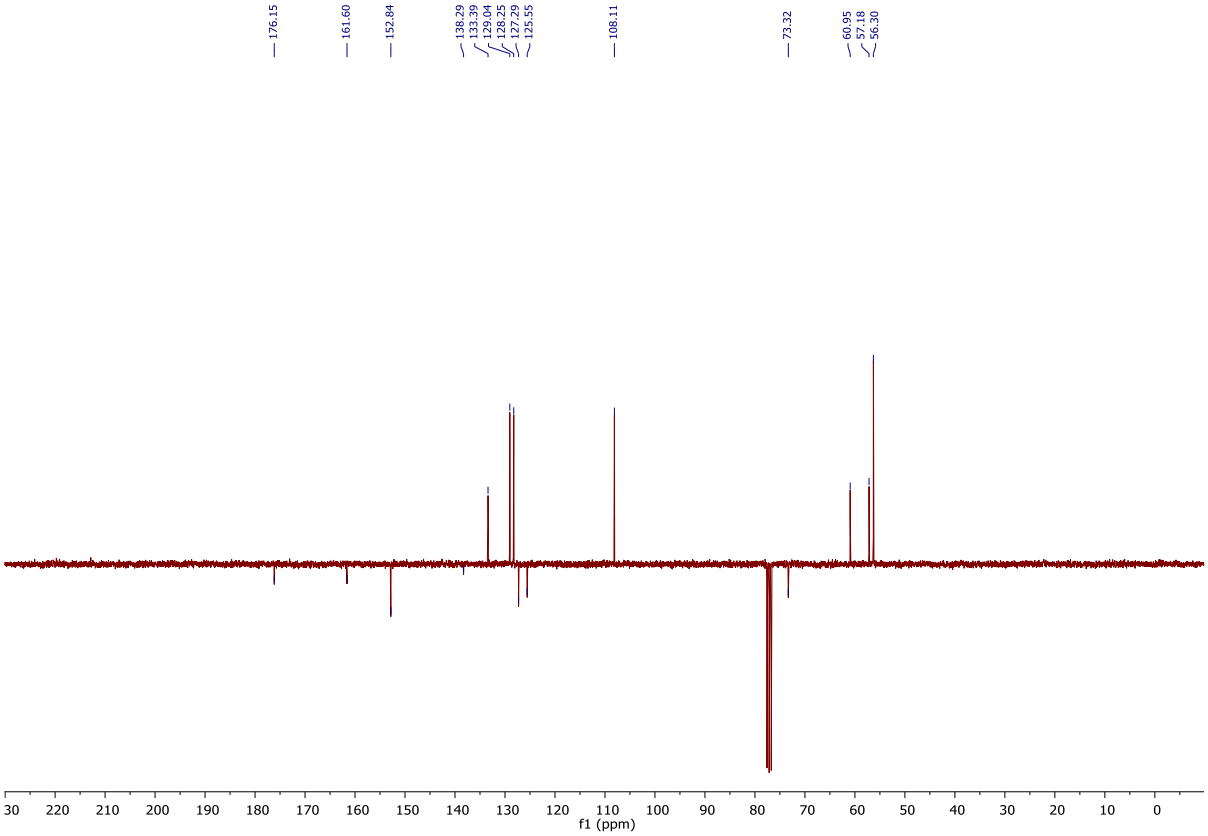
^{1}H-^{13}C HMBC ($CDCl_3$) correlation spectrum of **2s**



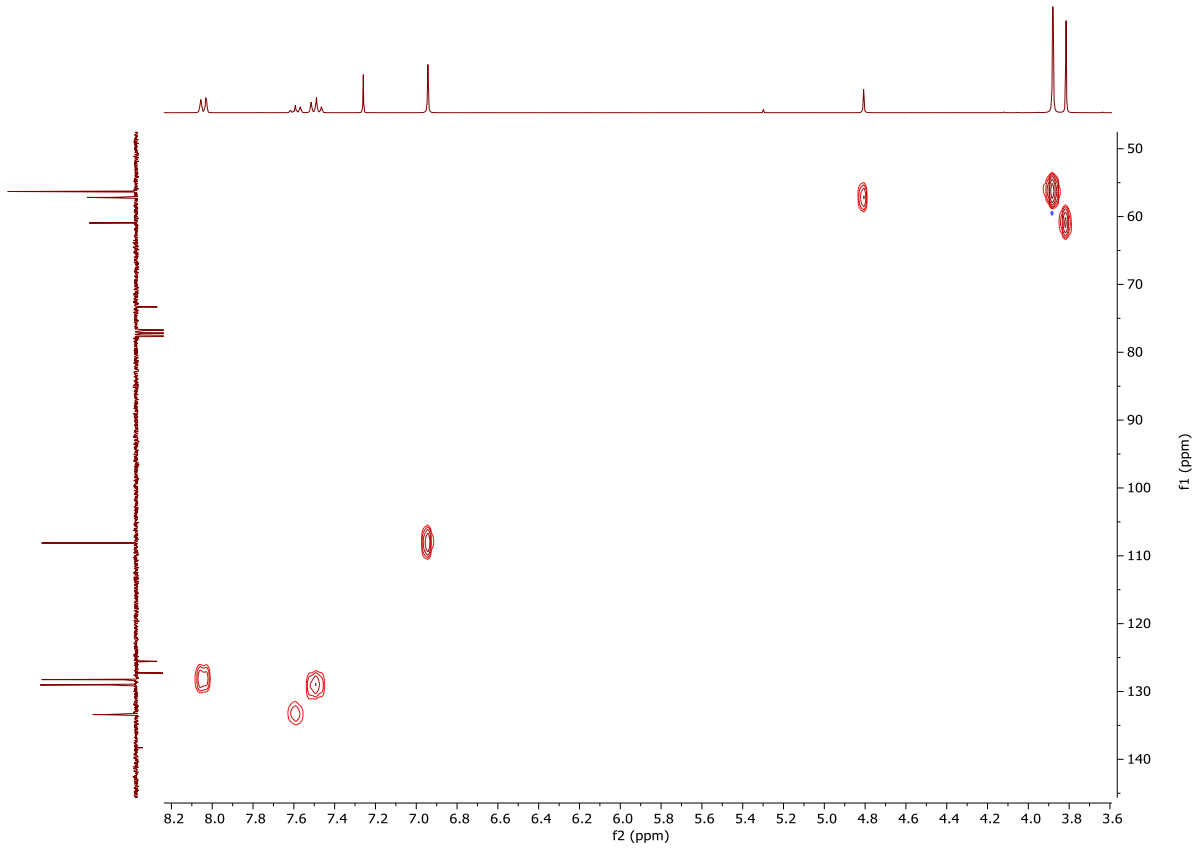
$^{19}F\{^{1}H\}$ NMR spectrum ($CDCl_3$, 282.40 MHz) of **2s**



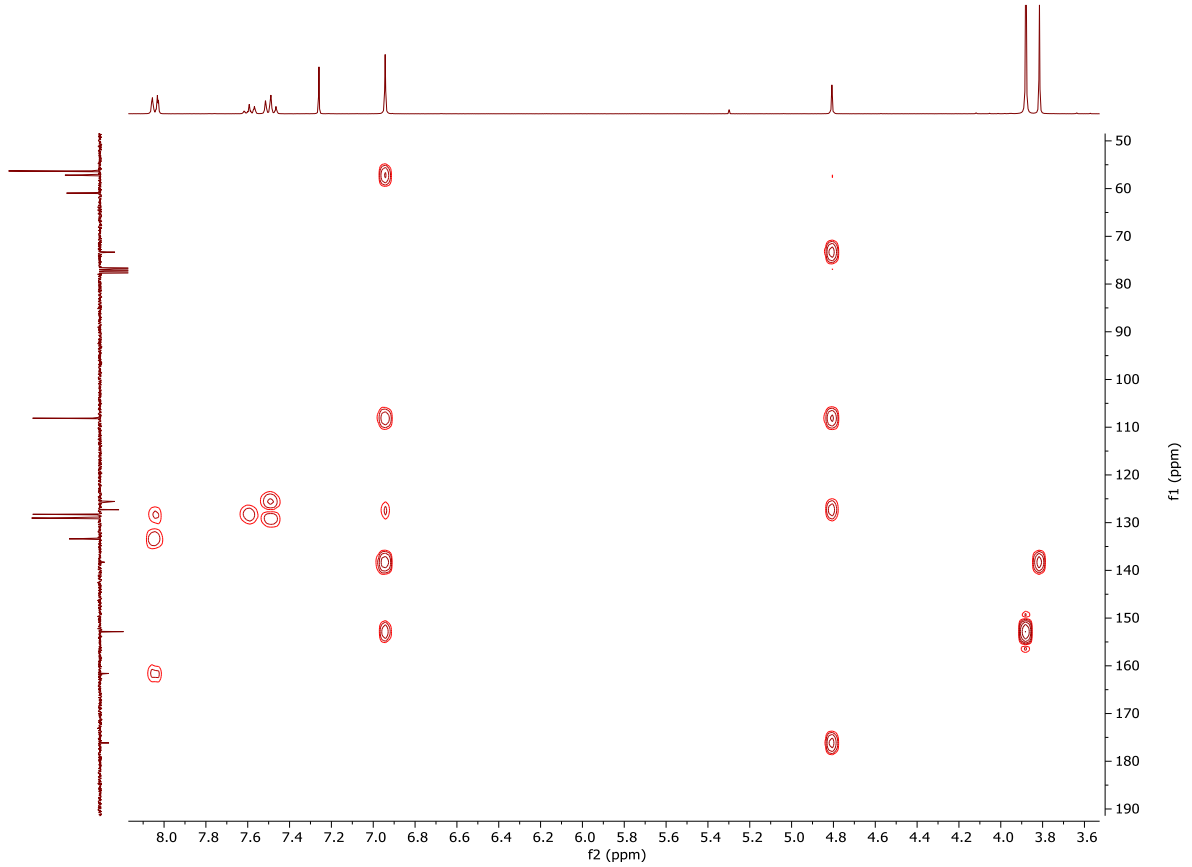
^{1}H NMR spectrum ($CDCl_3$, 300.13 MHz) of **2t***



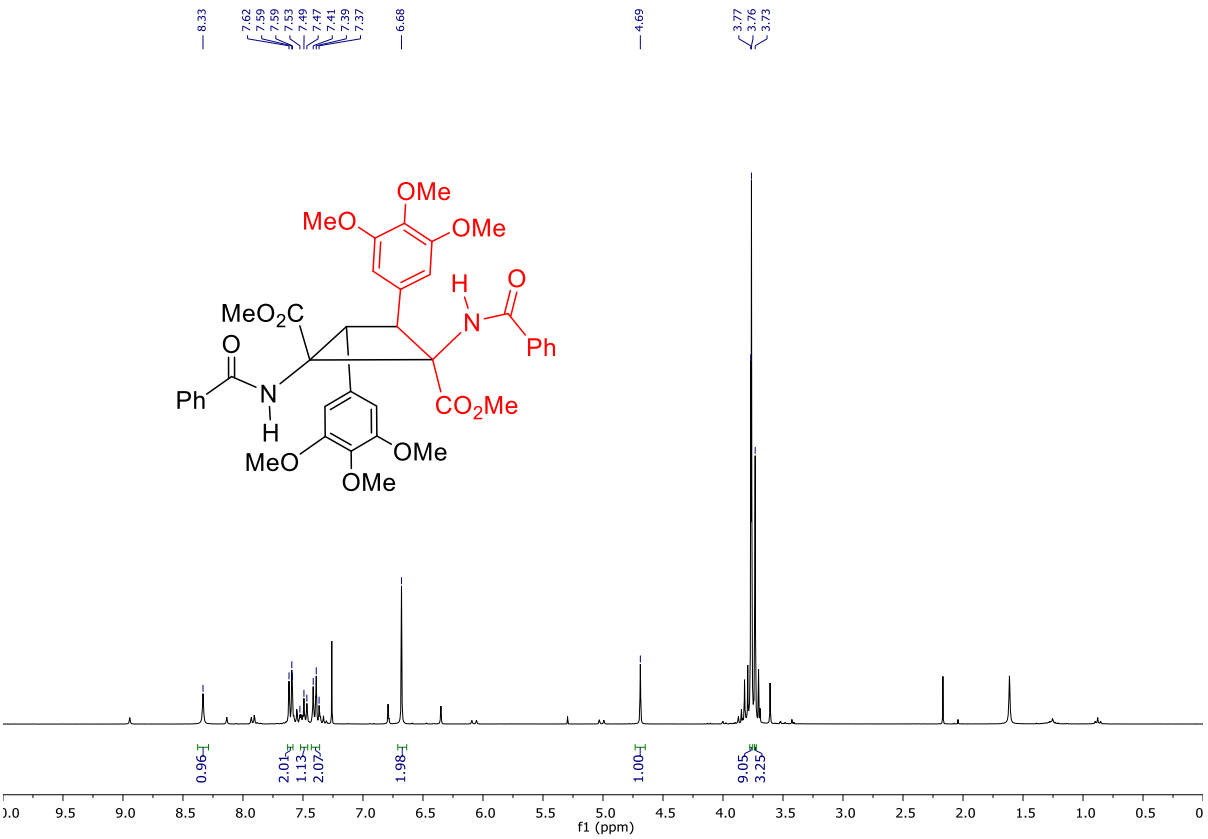
^{13}C{^{1}H} (APT) NMR spectrum ($CDCl_3$, 75.5 MHz) of **2t***



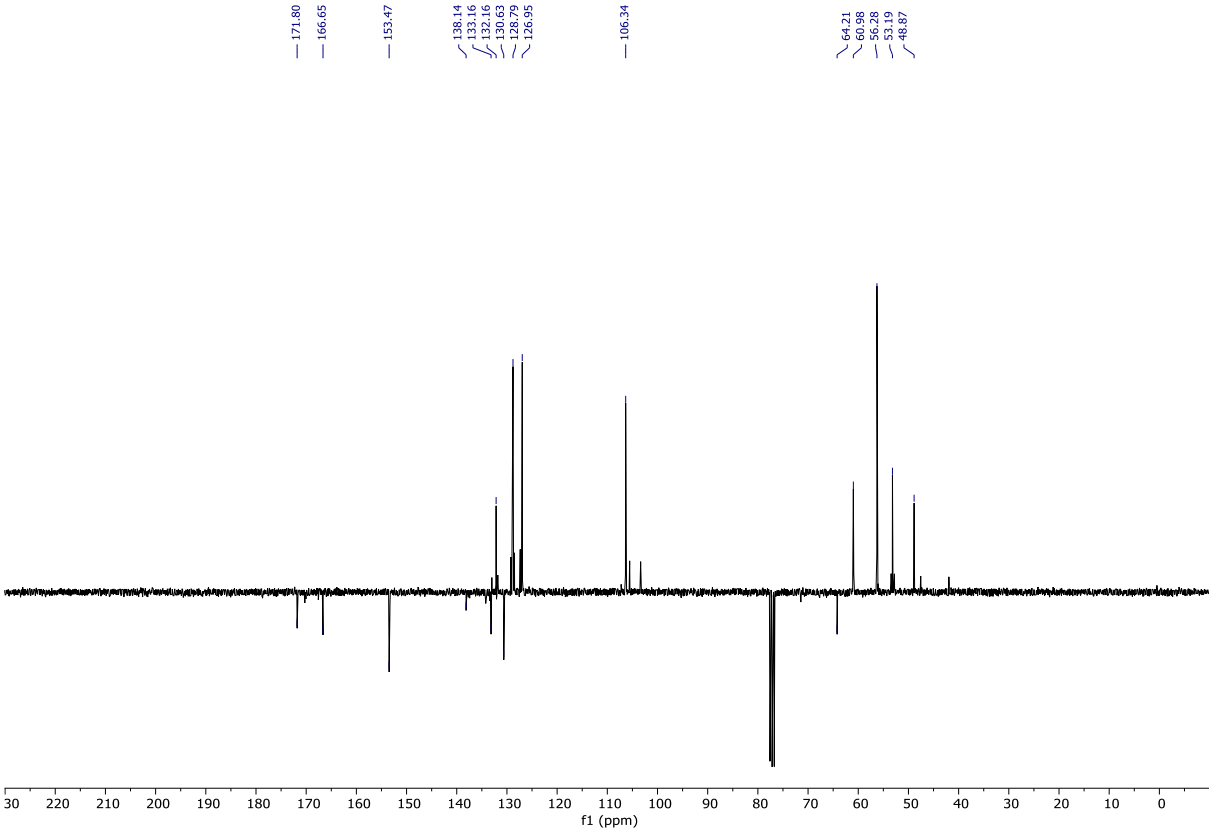
^{1}H-^{13}C HSQC ($CDCl_3$) correlation spectrum of **2t***



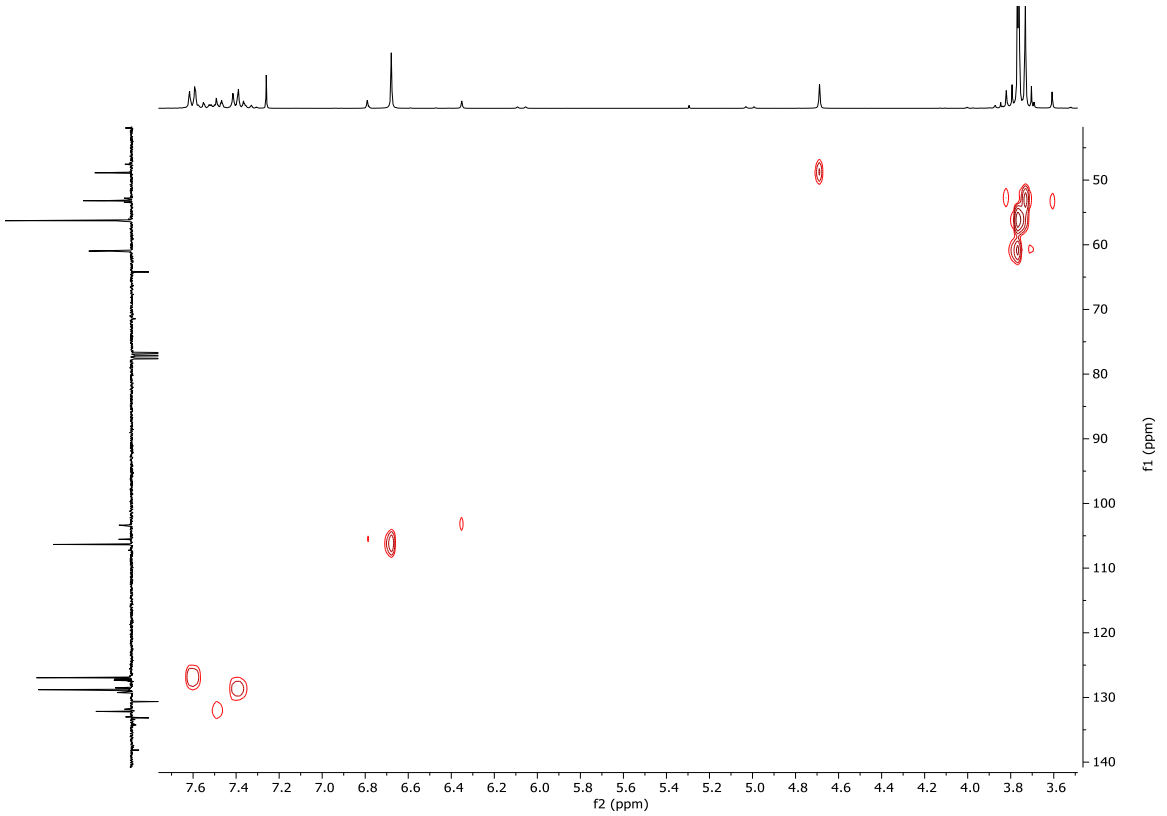
^{1}H-^{13}C HMBC ($CDCl_3$) correlation spectrum of **2t***



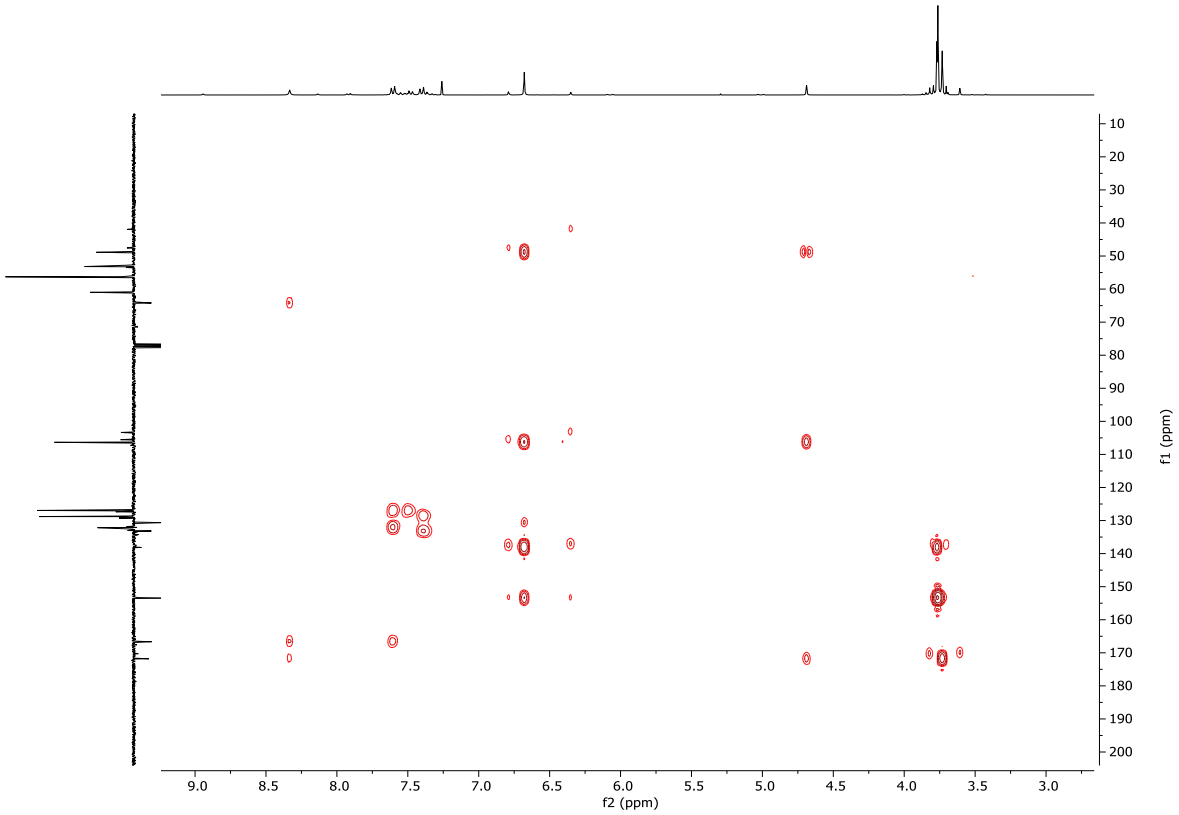
^{1}H NMR spectrum ($CDCl_3$, 300.13 MHz) of **2t**



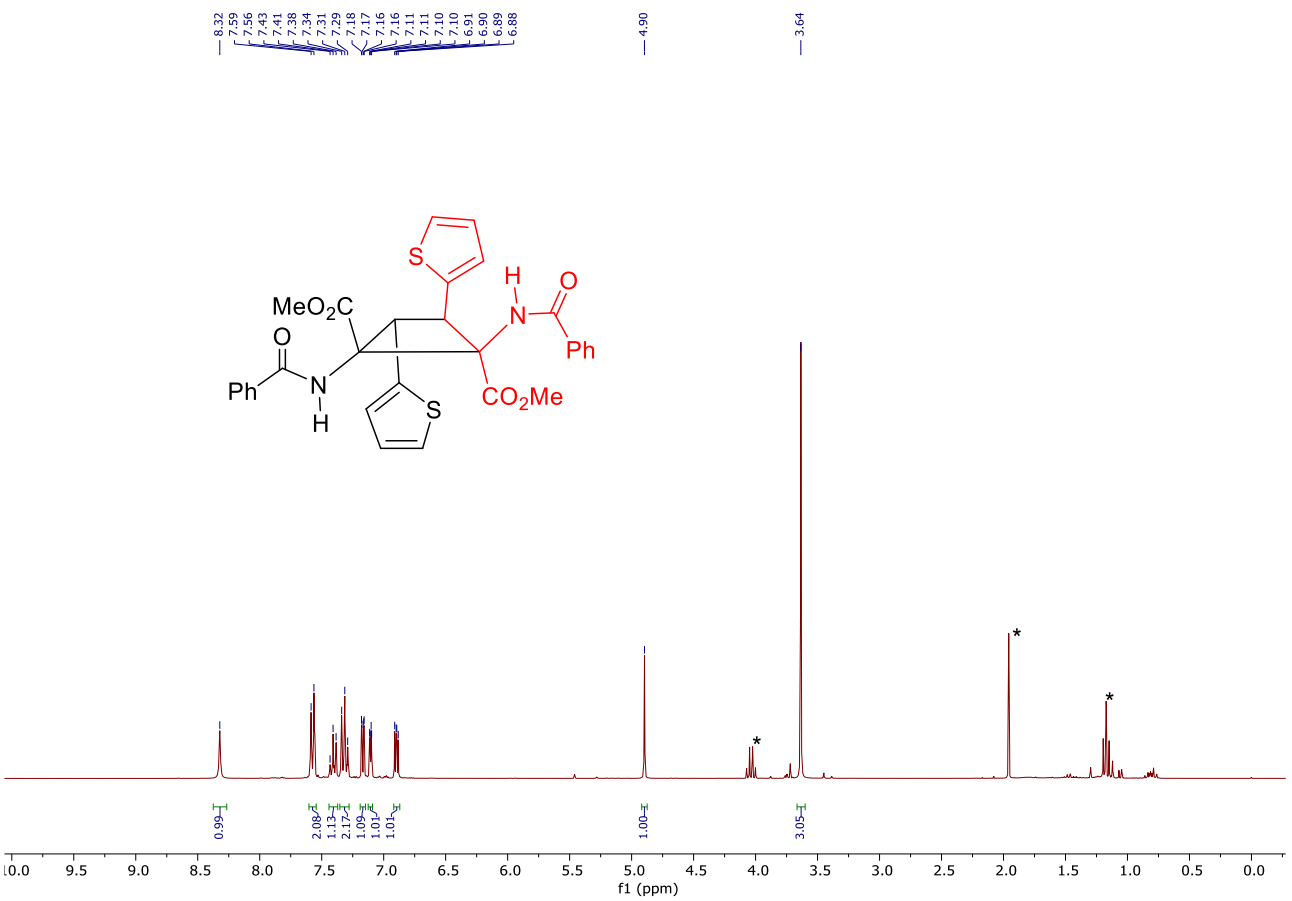
^{13}C{^{1}H} (APT) NMR spectrum ($CDCl_3$, 75.5 MHz) of **2t**



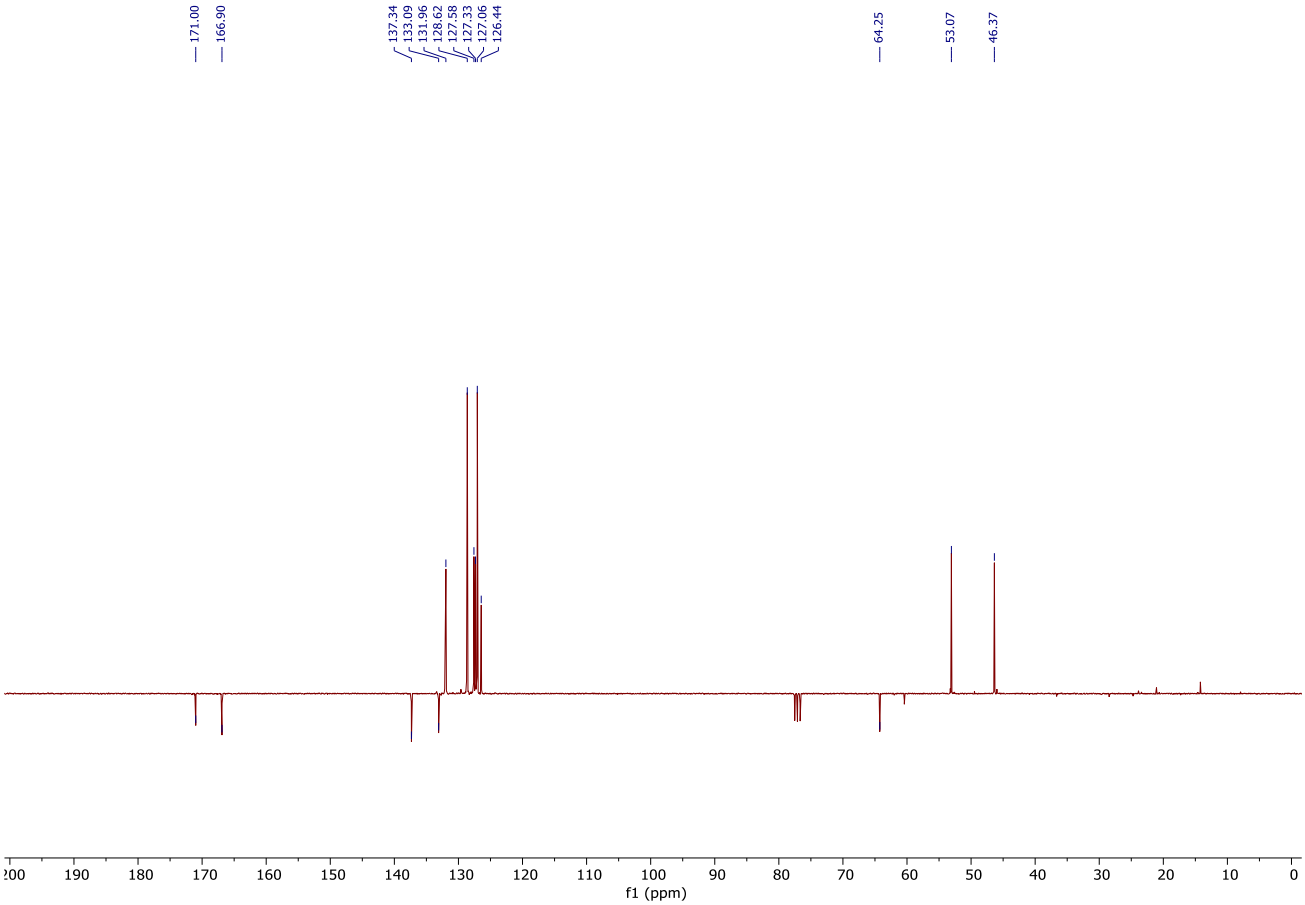
^{1}H-^{13}C HSQC ($CDCl_3$) correlation spectrum of **2t**



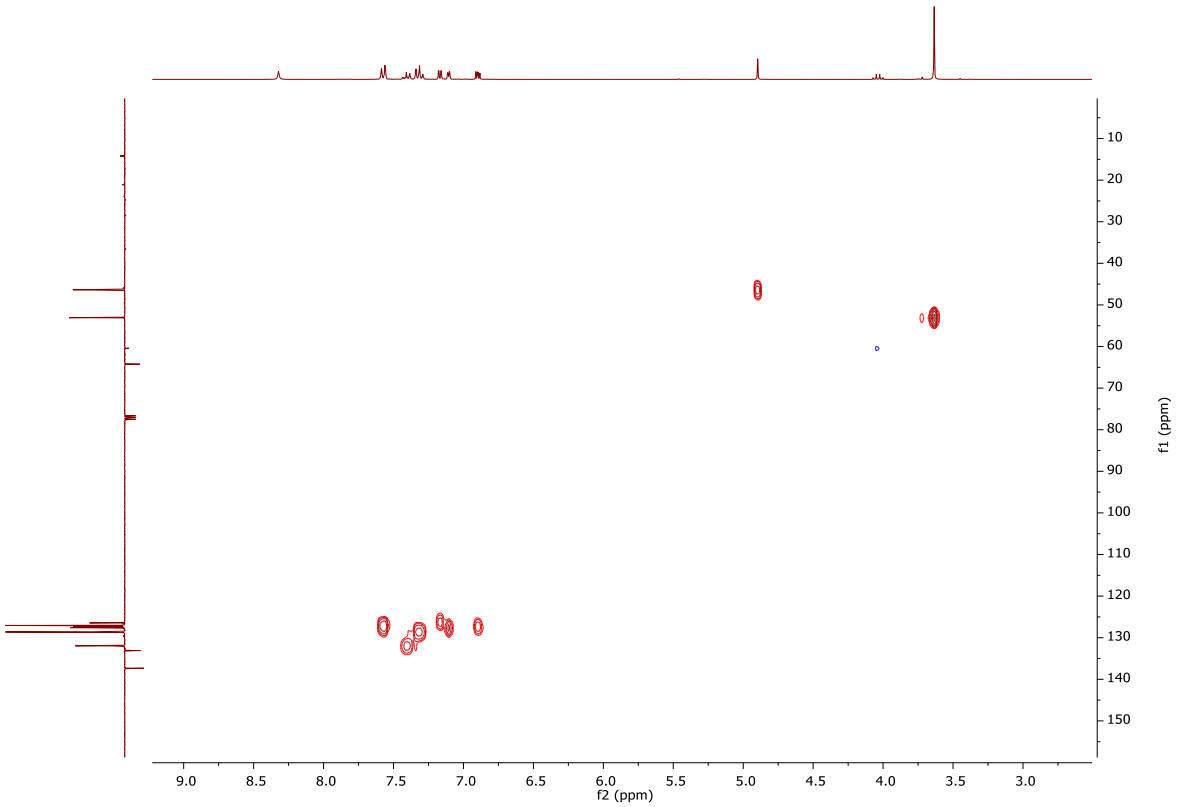
^{1}H-^{13}C HMBC ($CDCl_3$) correlation spectrum of **2t**



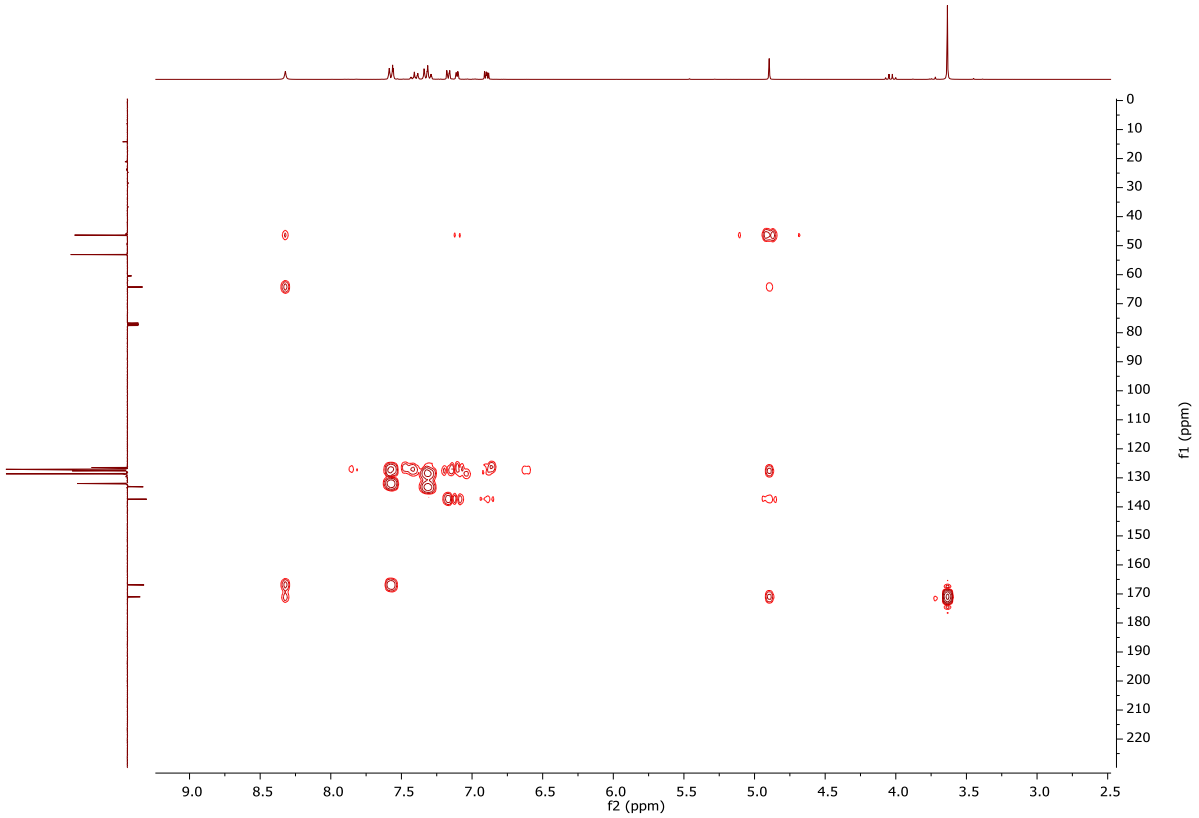
^{1}H NMR spectrum ($CDCl_3$, 300.13 MHz) of **2u** (* = ethyl acetate)



$^{13}C\{^{1}H\}$ (APT) NMR spectrum ($CDCl_3$, 75.5 MHz) of **2u**

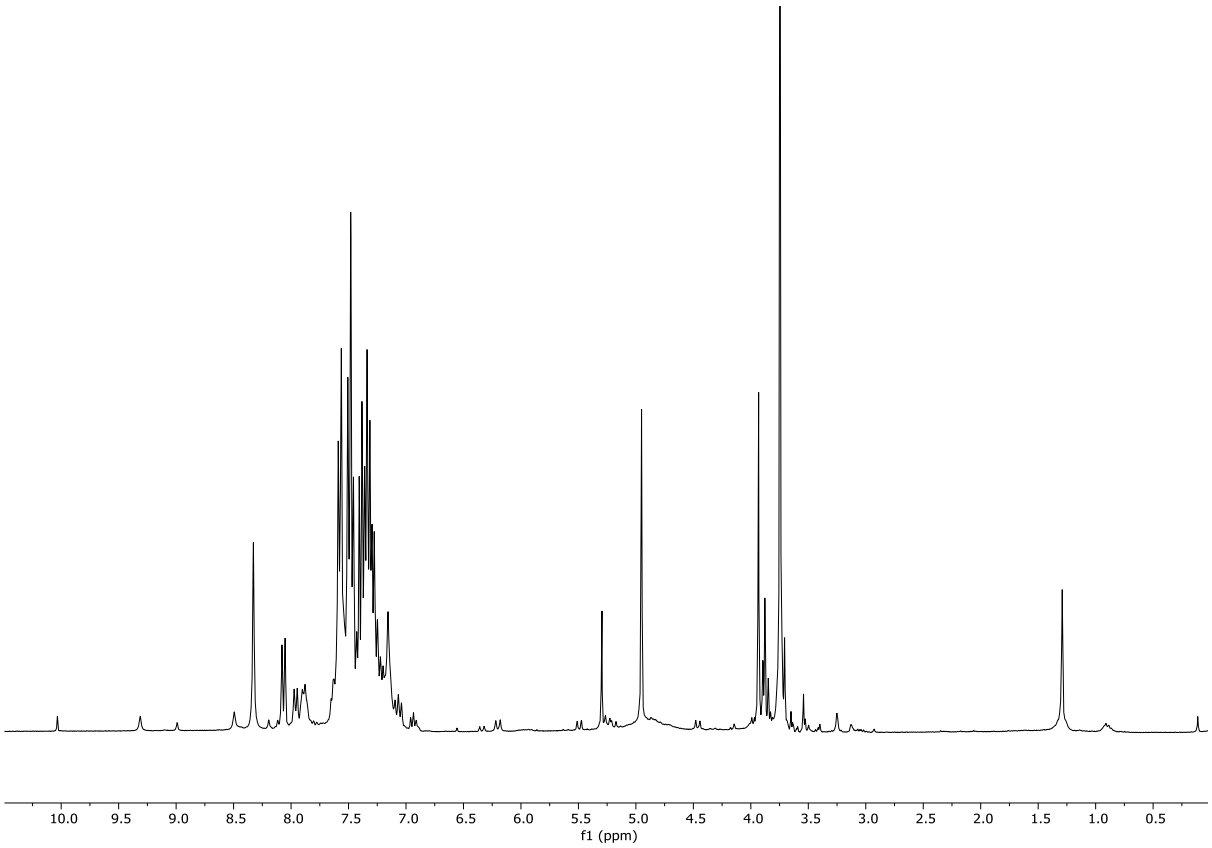


^{1}H-^{13}C HSQC ($CDCl_3$) correlation spectrum of **2u**

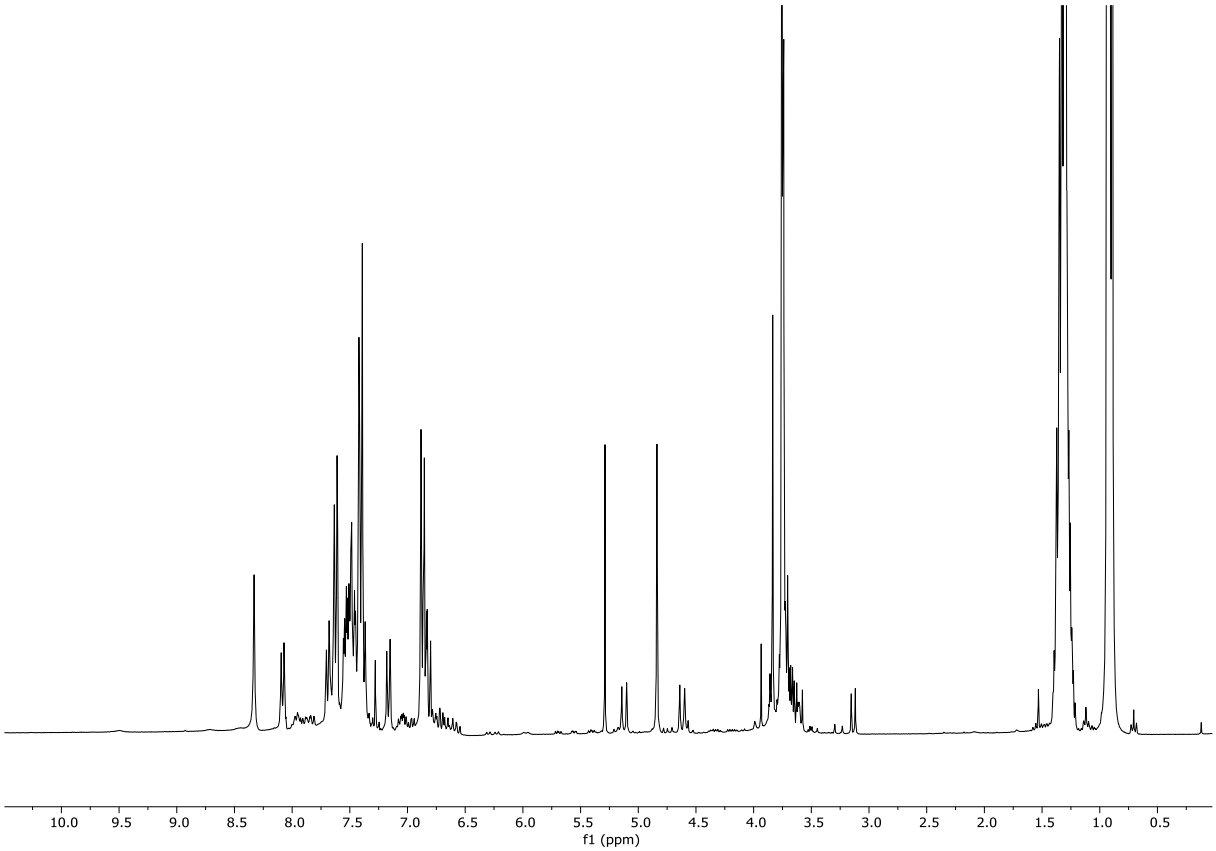


^{1}H-^{13}C HMBC ($CDCl_3$) correlation spectrum of **2u**

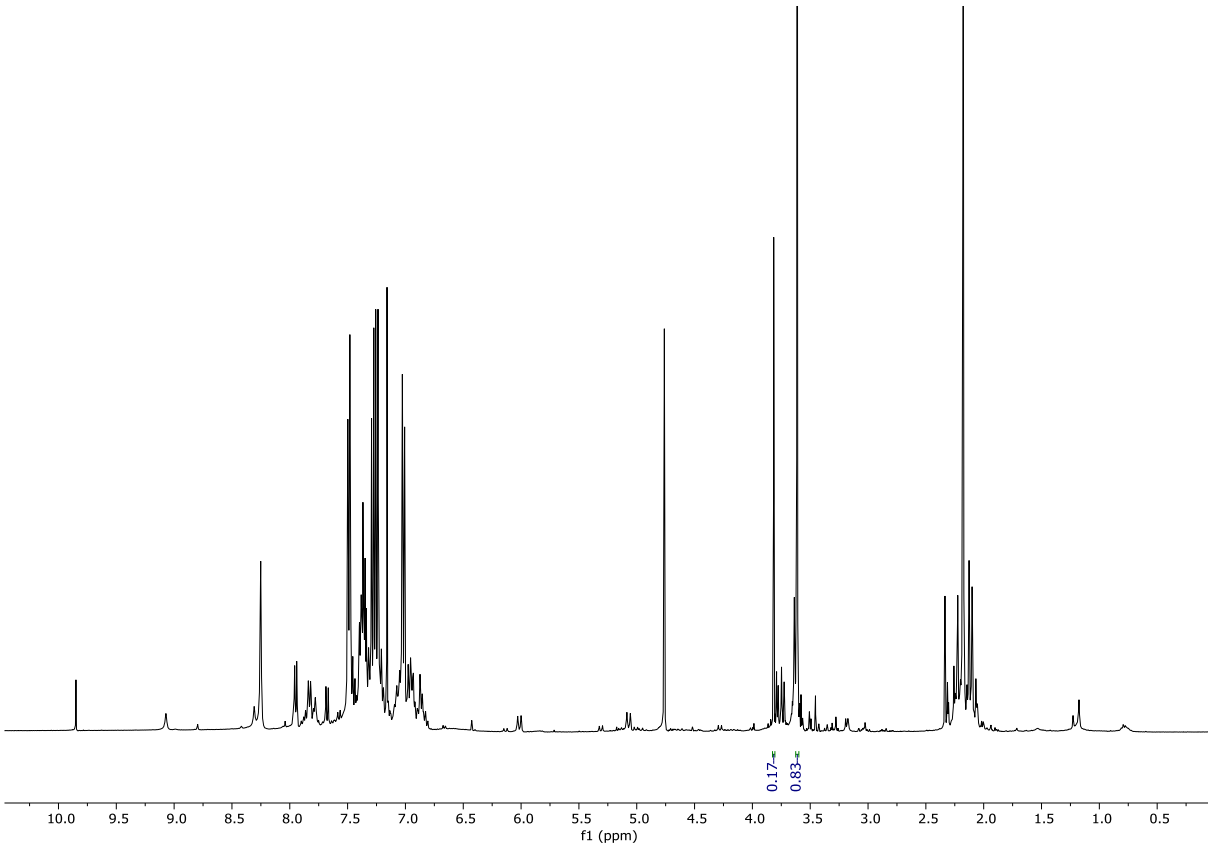
5.- ^{1}H NMR spectra of crudes during the synthesis of cyclobutanes 2a-2u (after washing with water, before column chromatography)



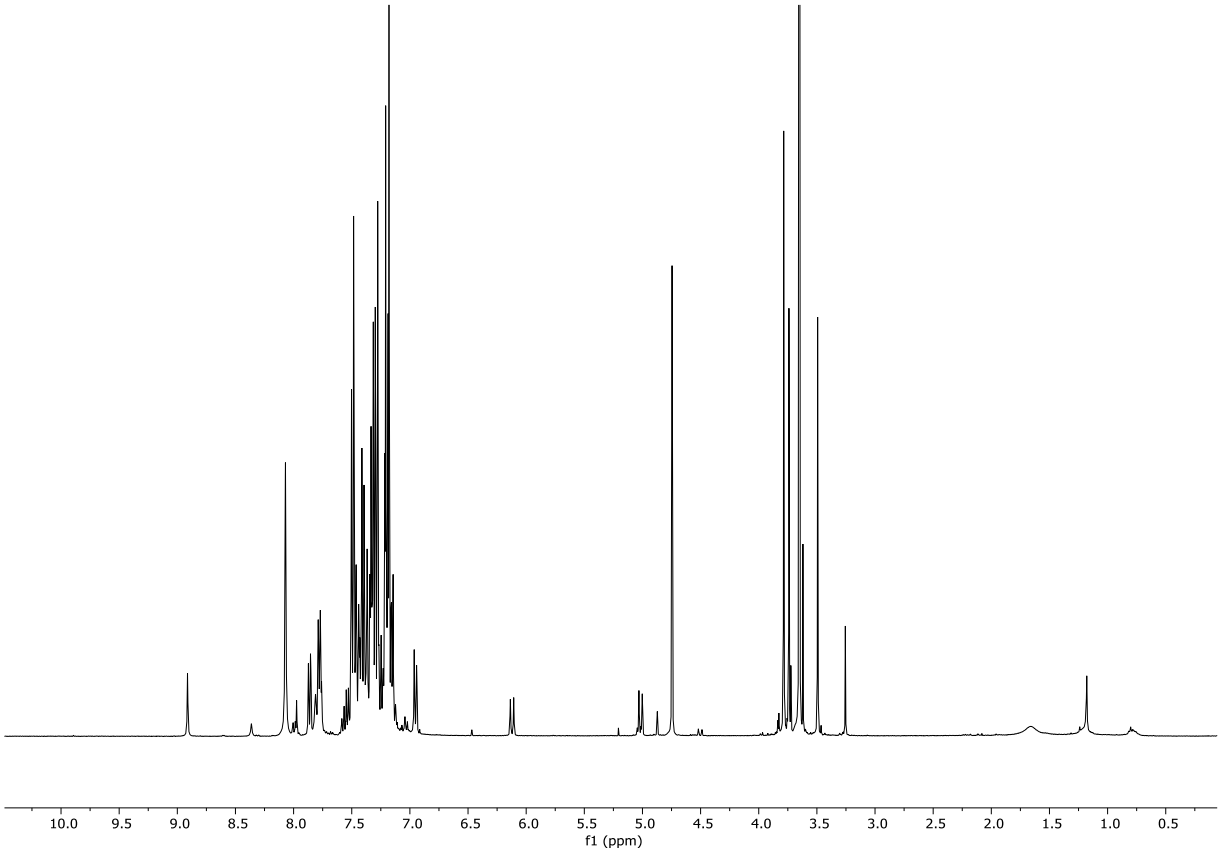
^{1}H NMR spectrum ($CDCl_3$, 300.13 MHz) of crude of **2a**



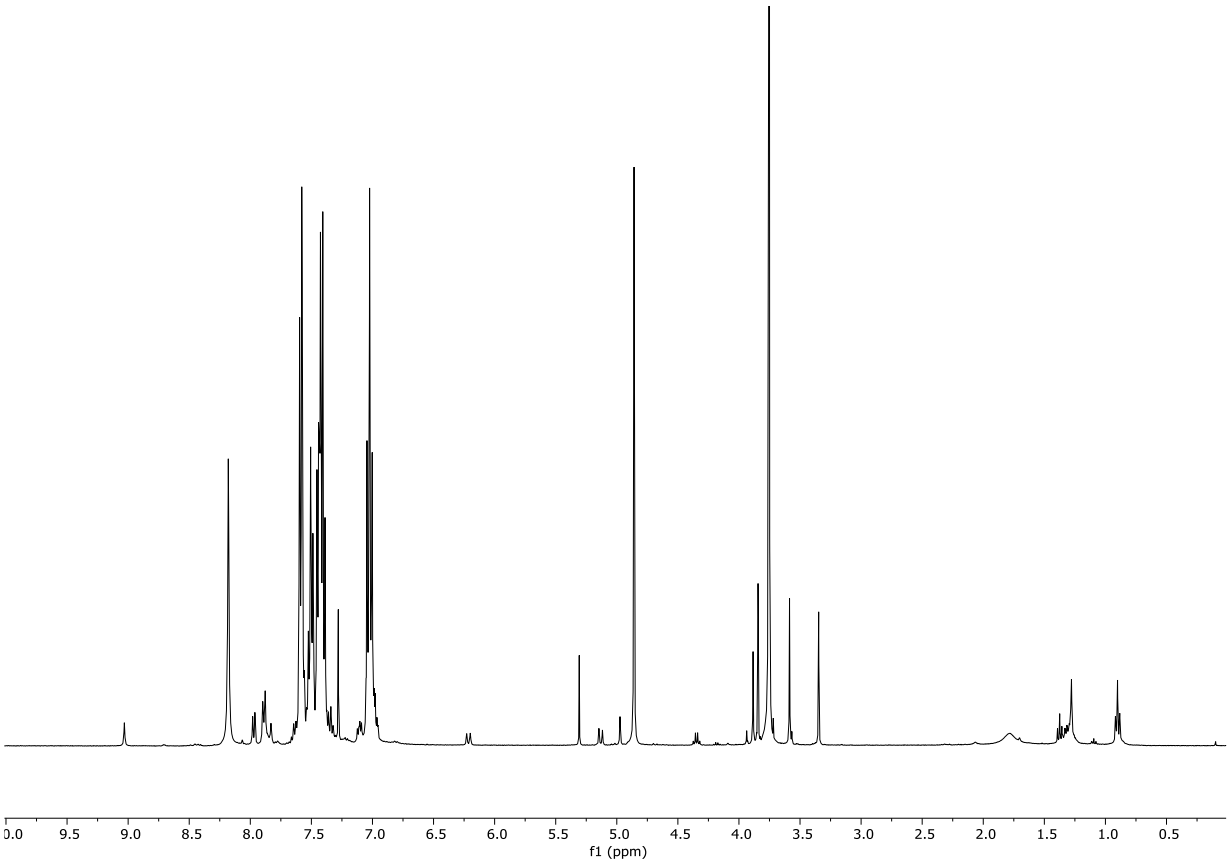
^{1}H NMR spectrum ($CDCl_3$, 300.13 MHz) of crude of **2b**



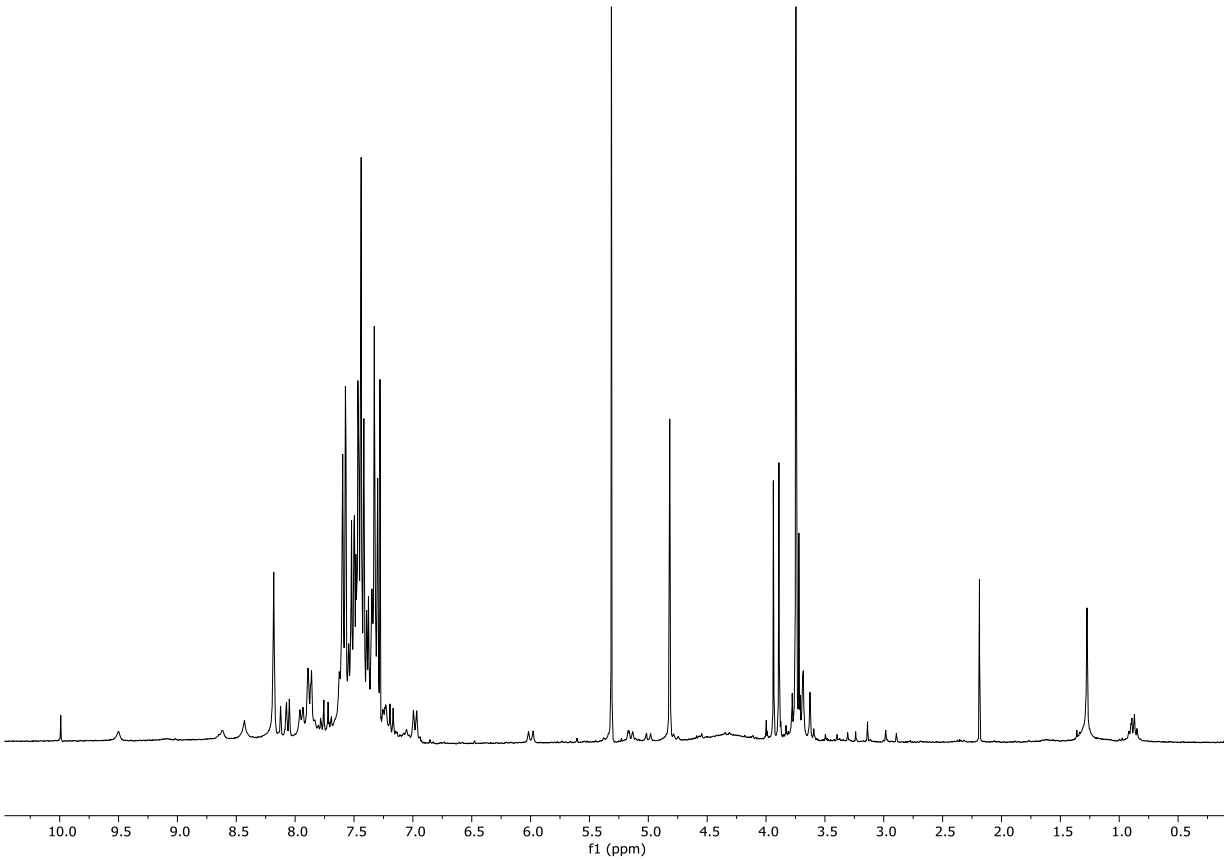
^{1}H NMR spectrum ($CDCl_3$, 300.13 MHz) of crude of **2c**



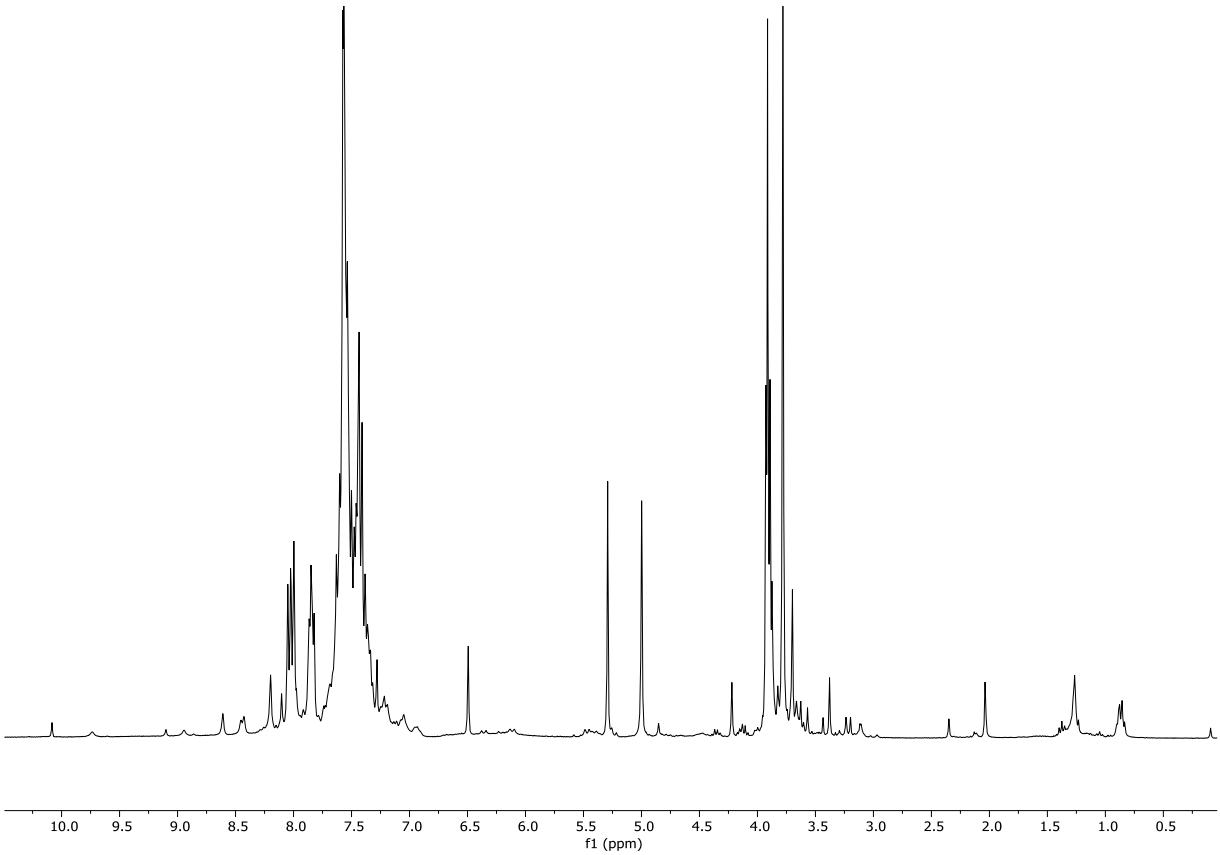
^{1}H NMR spectrum ($CDCl_3$, 300.13 MHz) of crude of **2d**



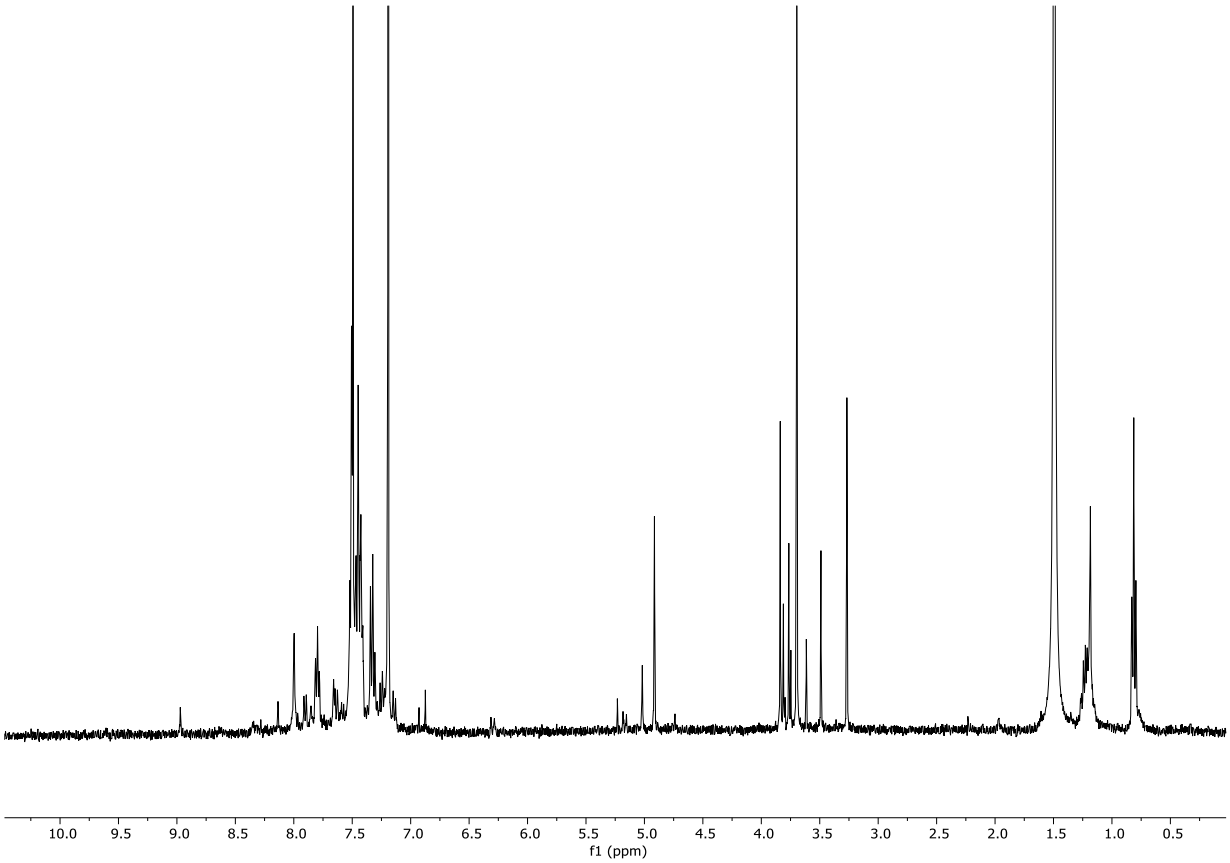
^{1}H NMR spectrum ($CDCl_3$, 300.13 MHz) of crude of **2e**



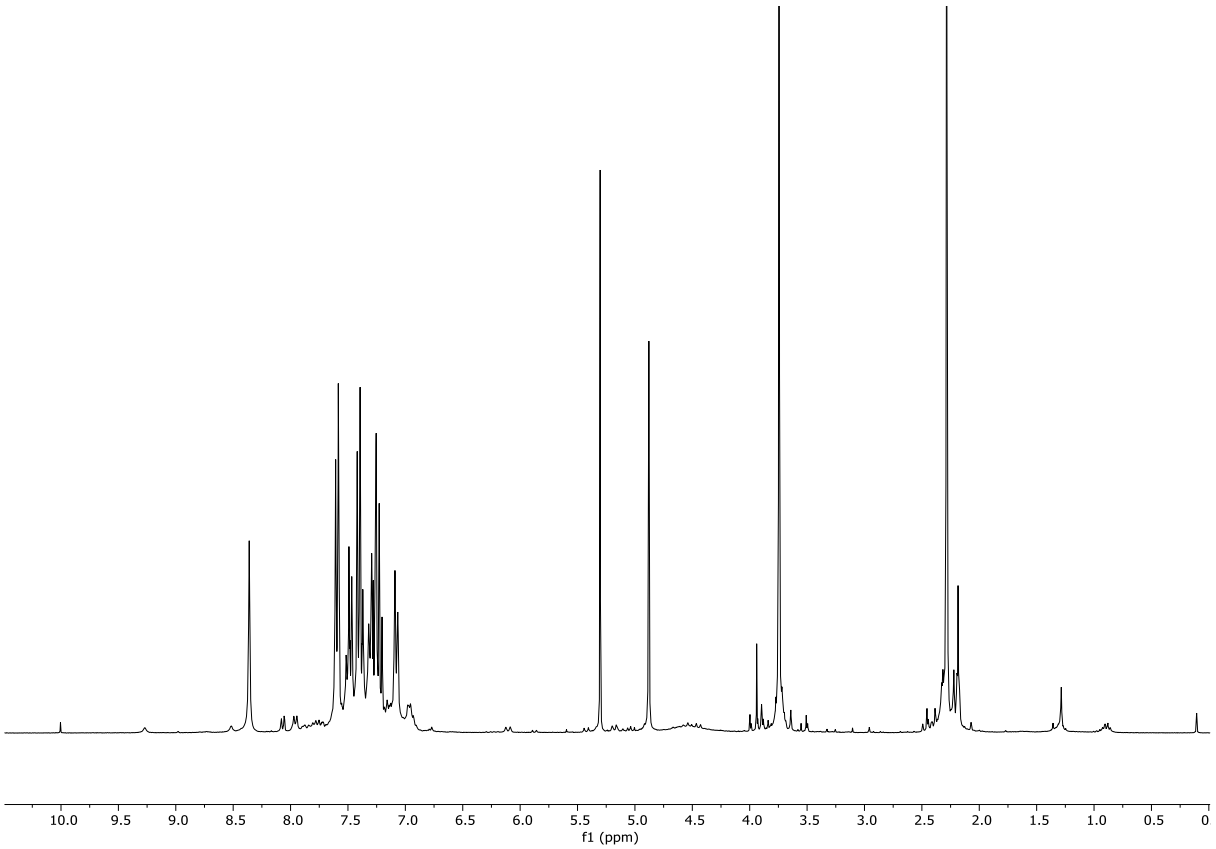
^{1}H NMR spectrum ($CDCl_3$, 300.13 MHz) of crude of **2f**



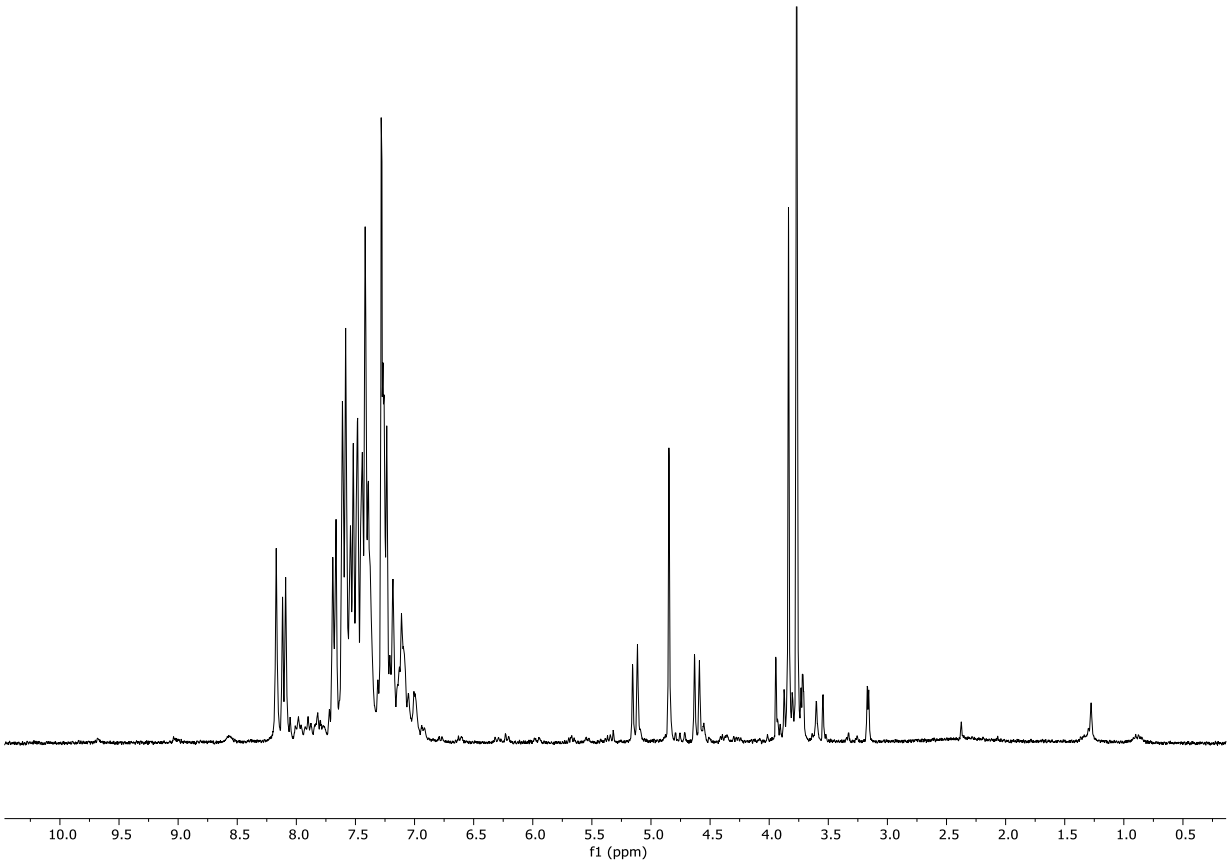
^{1}H NMR spectrum ($CDCl_3$, 300.13 MHz) of crude of **2g**



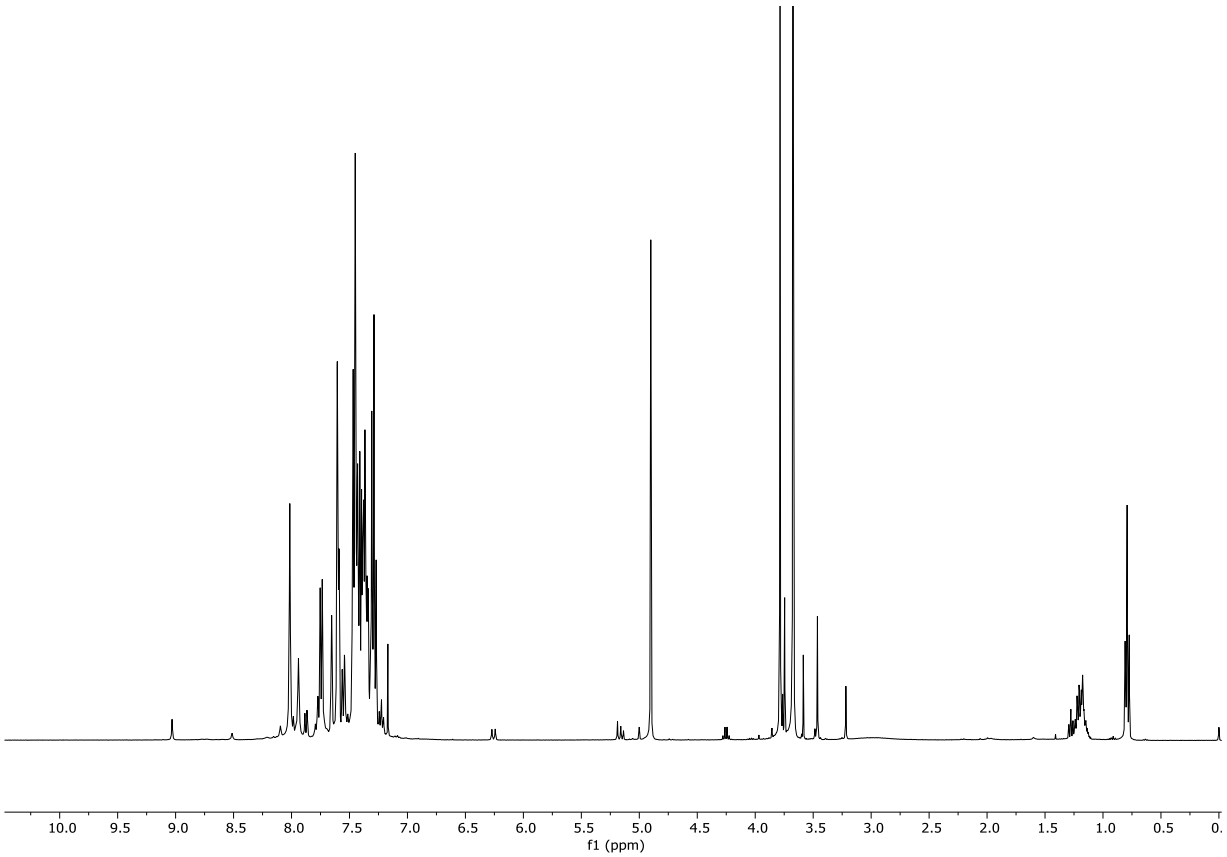
^{1}H NMR spectrum ($CDCl_3$, 300.13 MHz) of crude of **2h**



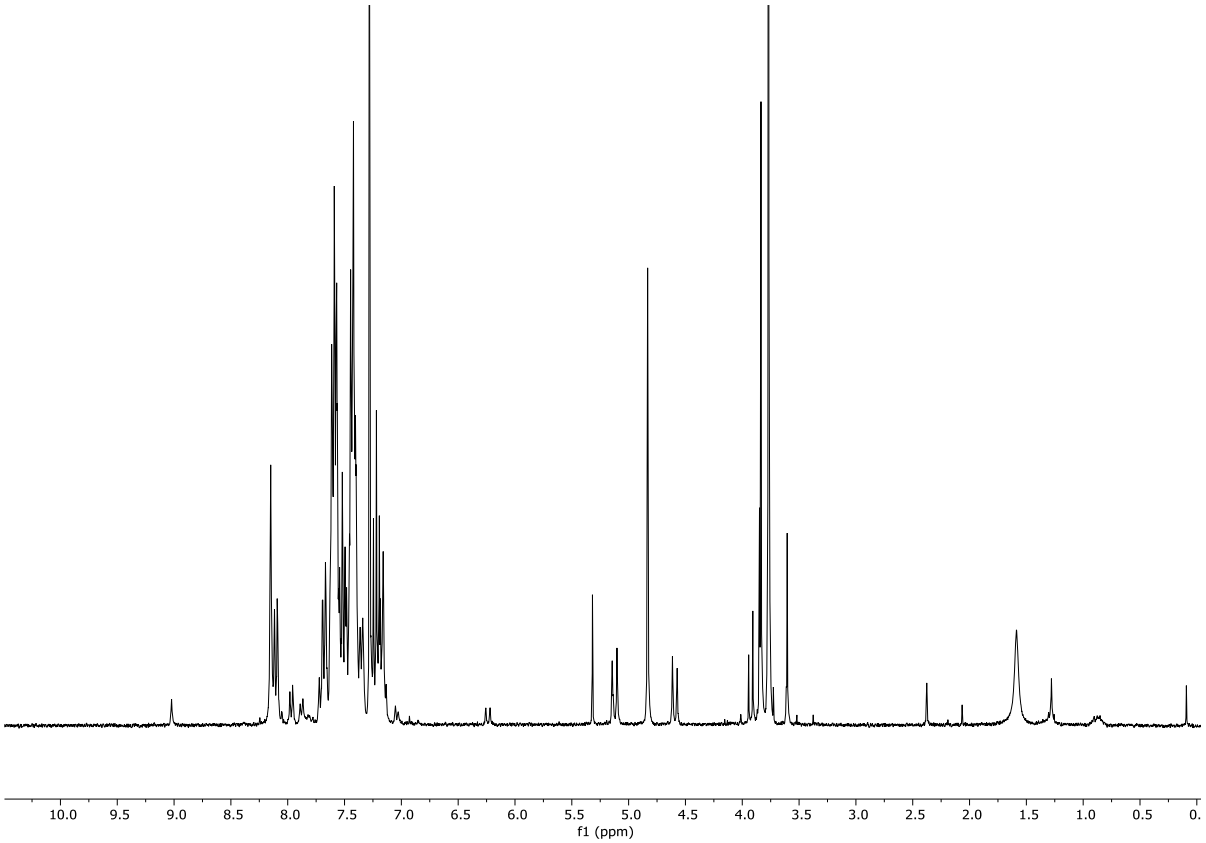
^{1}H NMR spectrum ($CDCl_3$, 300.13 MHz) of crude of **2i**



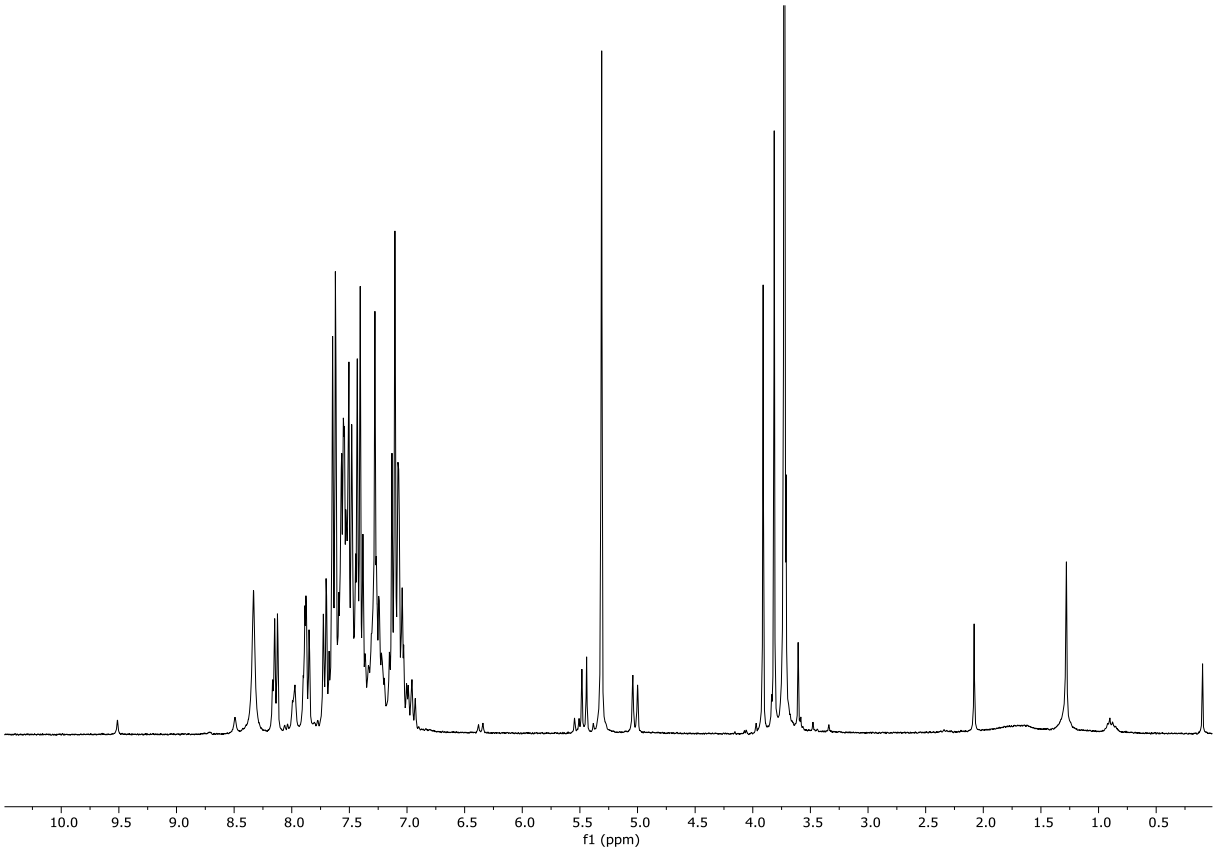
^{1}H NMR spectrum ($CDCl_3$, 300.13 MHz) of crude of **2j**



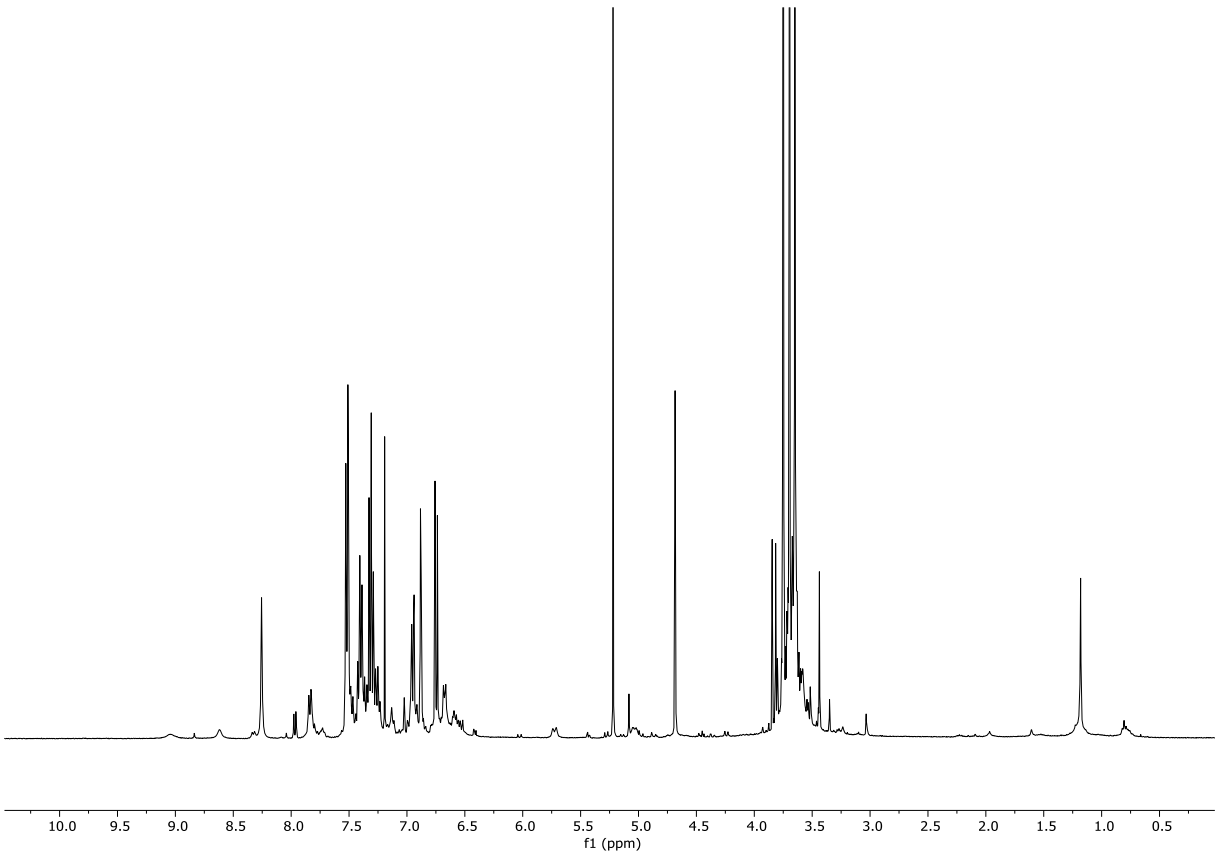
^{1}H NMR spectrum ($CDCl_3$, 300.13 MHz) of crude of **2k**



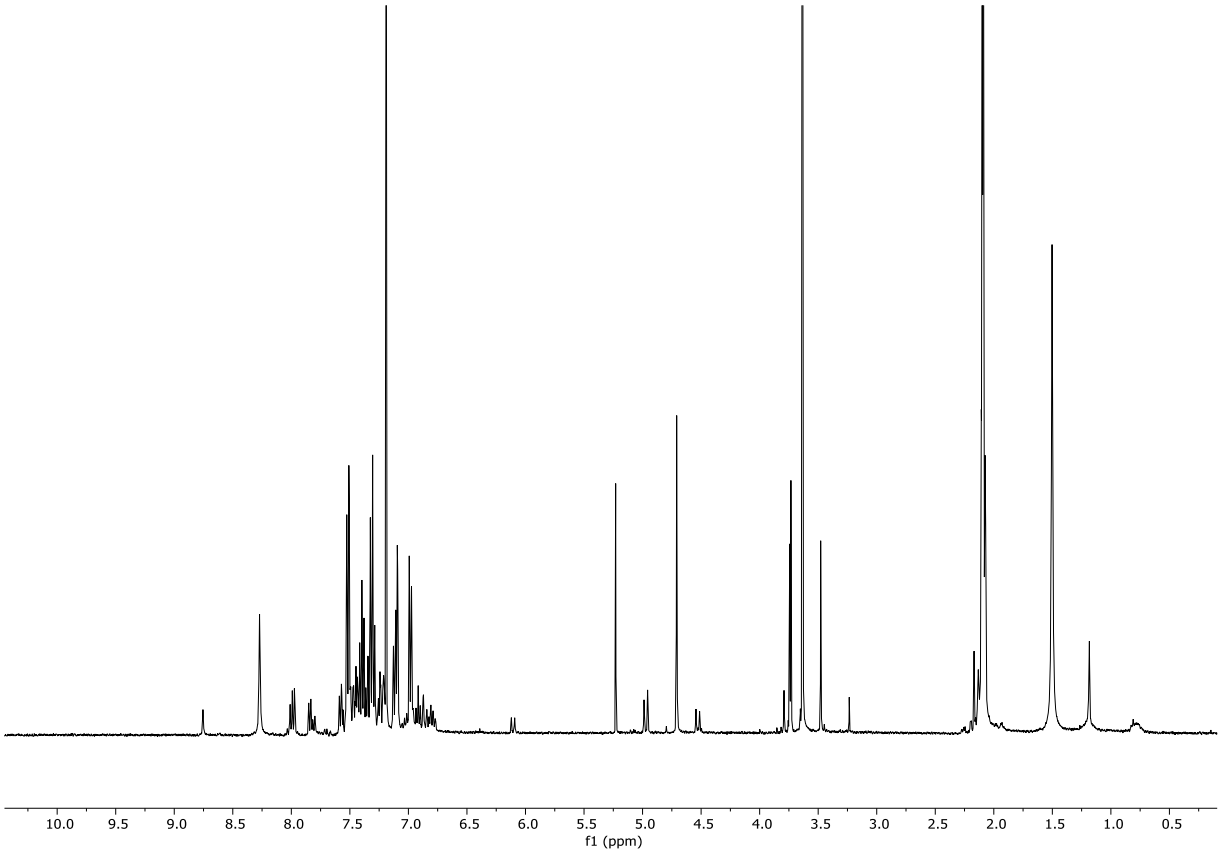
^{1}H NMR spectrum ($CDCl_3$, 300.13 MHz) of crude of **2l**



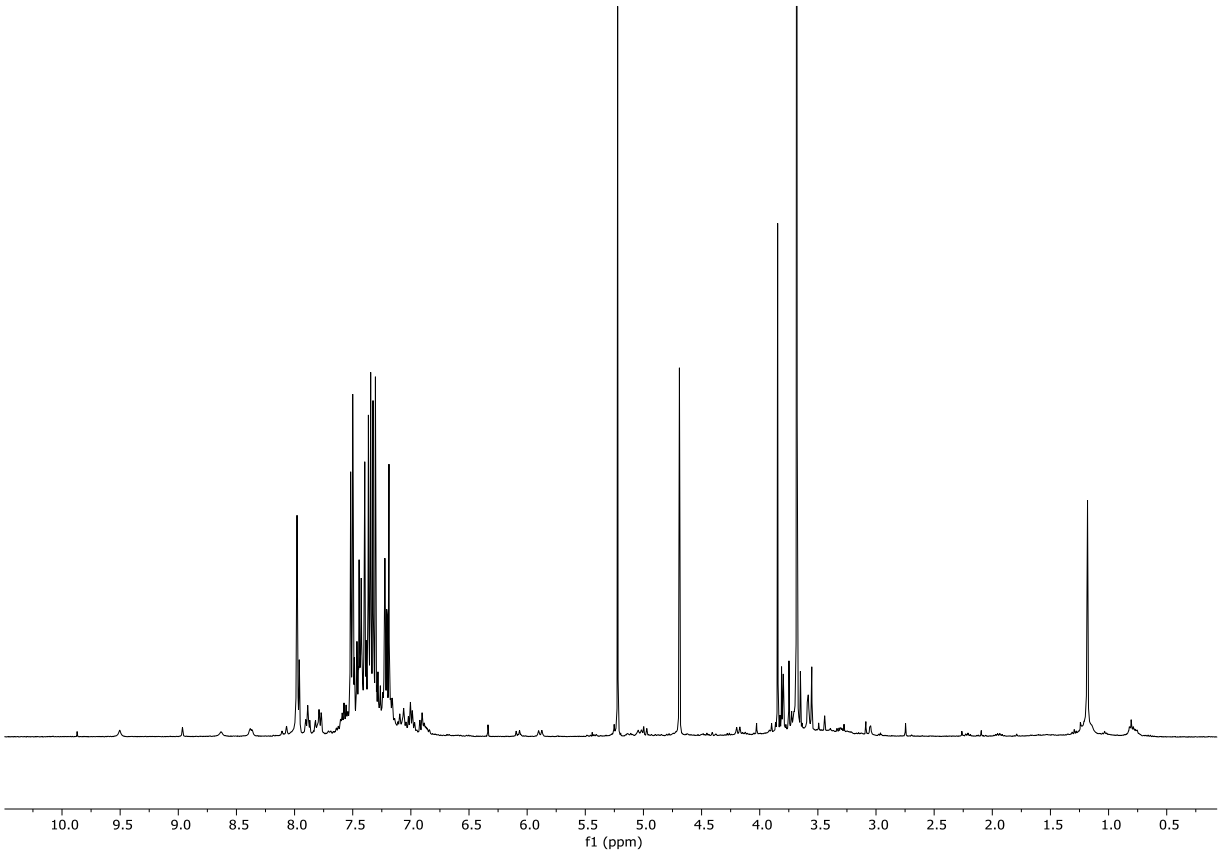
^{1}H NMR spectrum ($CDCl_3$, 300.13 MHz) of crude of **2o**



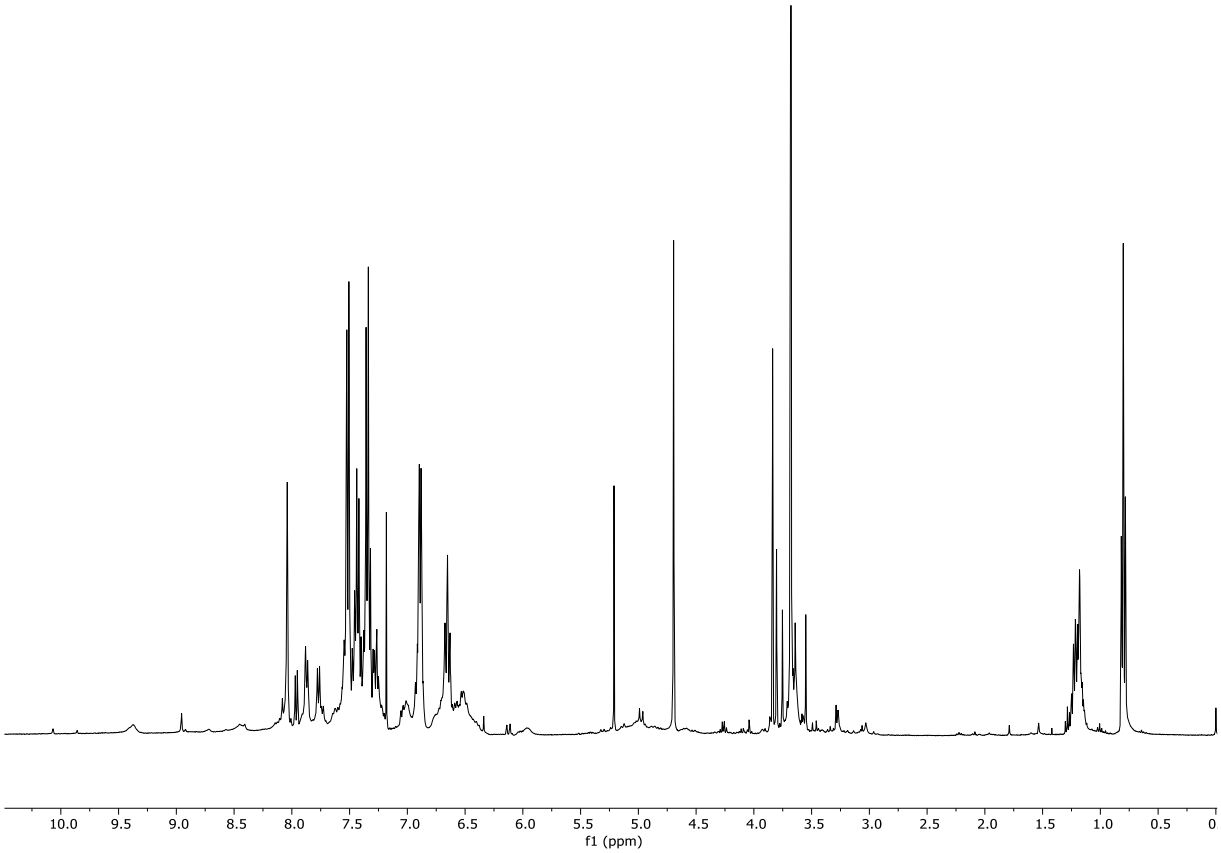
^{1}H NMR spectrum ($CDCl_3$, 300.13 MHz) of crude of **2p**



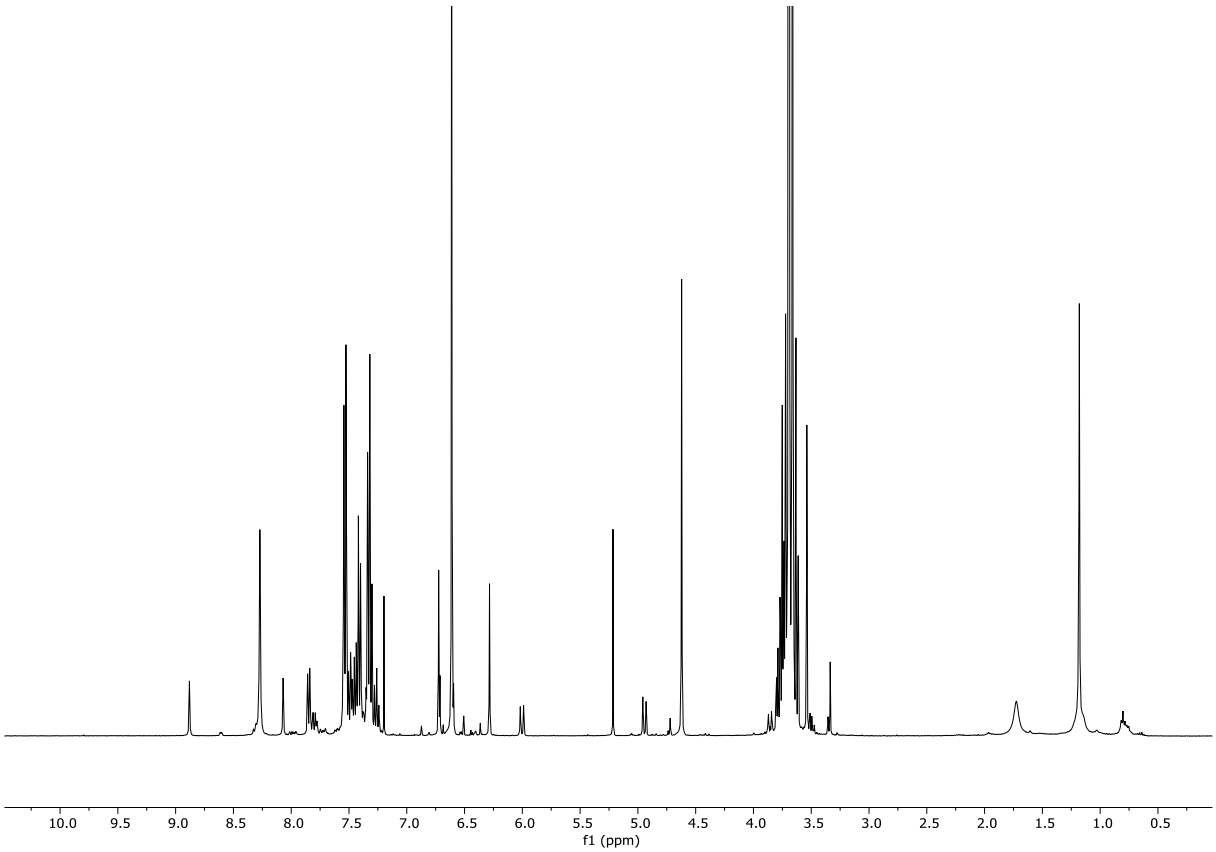
^{1}H NMR spectrum ($CDCl_3$, 300.13 MHz) of crude of **2q**



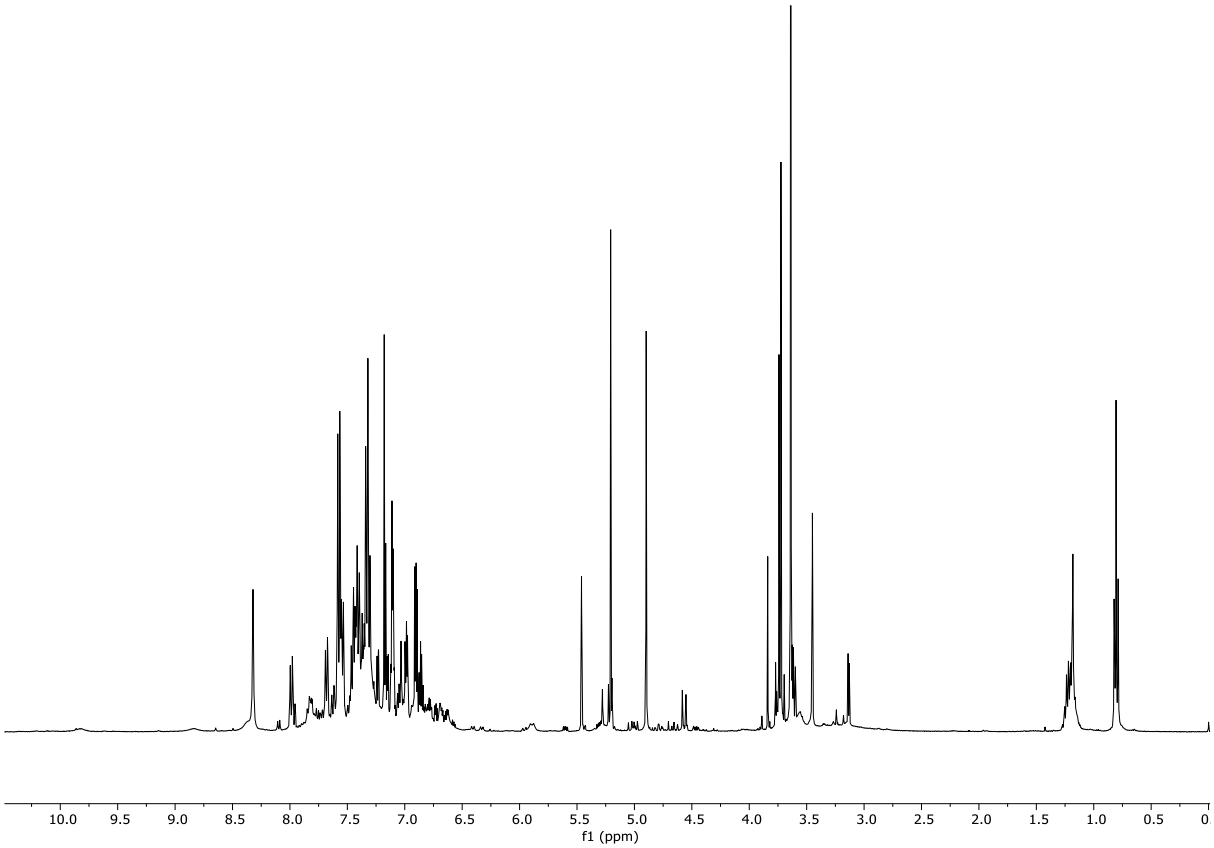
^{1}H NMR spectrum ($CDCl_3$, 300.13 MHz) of crude of **2r**



^{1}H NMR spectrum ($CDCl_3$, 300.13 MHz) of crude of **2s**

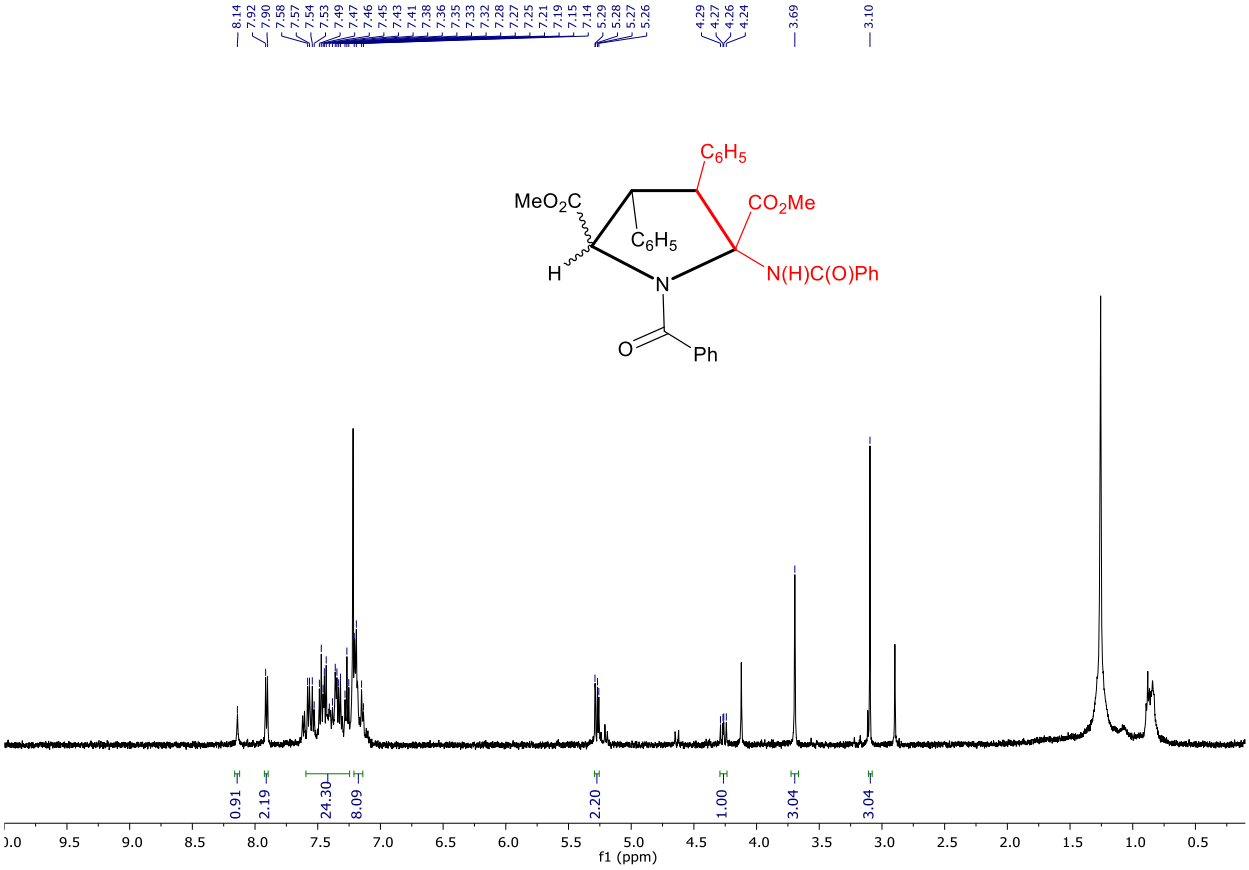


^{1}H NMR spectrum ($CDCl_3$, 300.13 MHz) of crude of **2t**

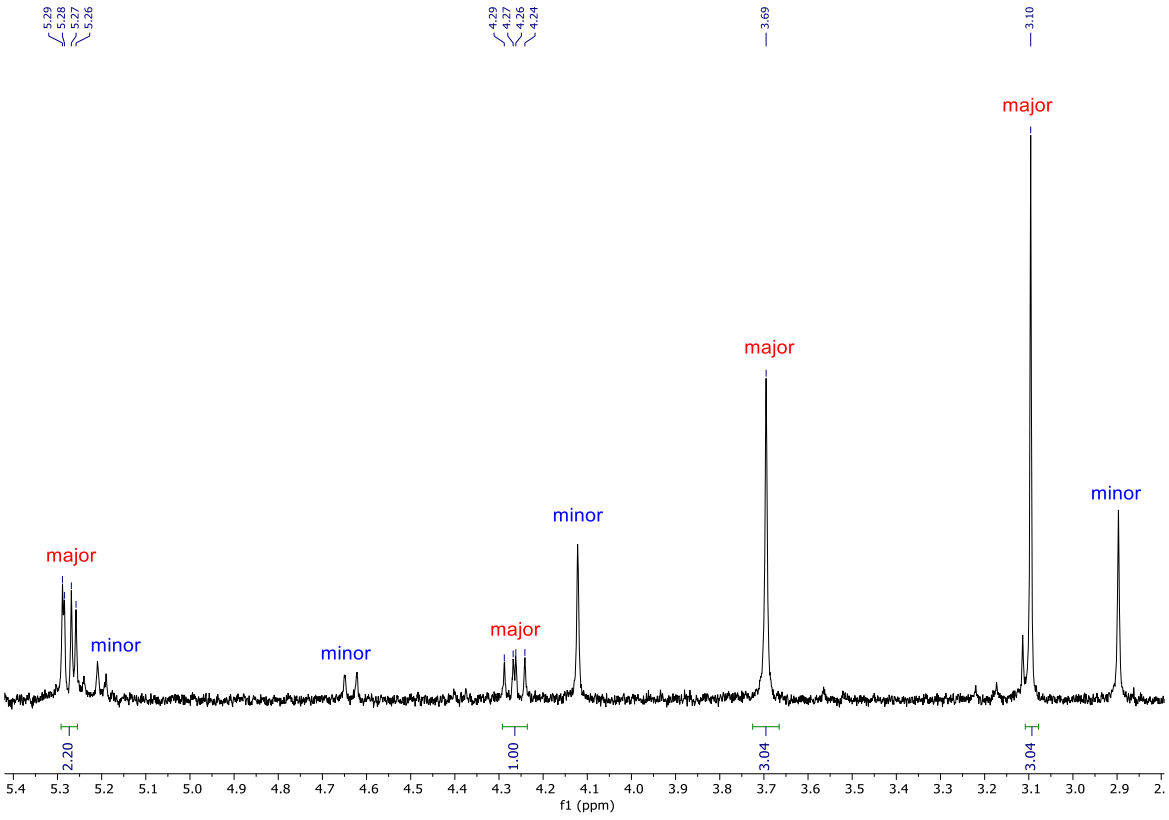


^{1}H NMR spectrum ($CDCl_3$, 300.13 MHz) of crude of **2u**

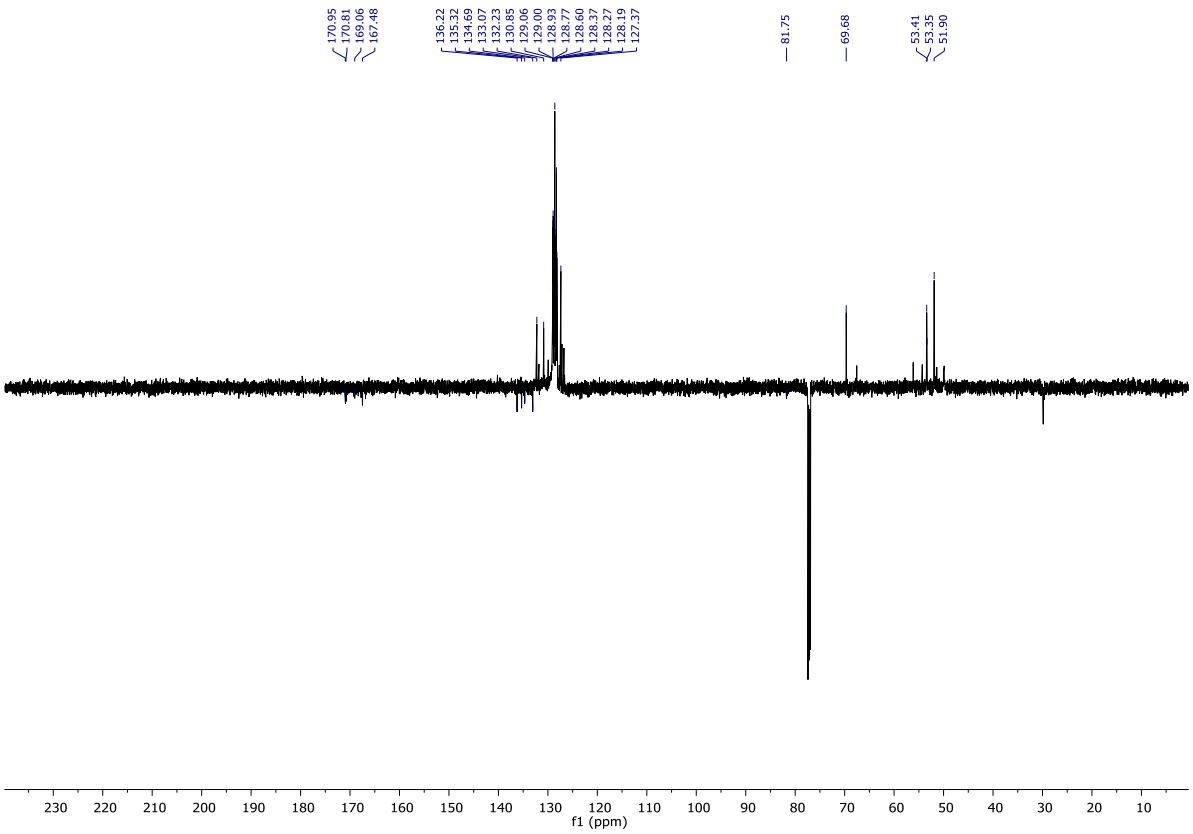
6.- Copies of NMR spectra of the pyrrolidine derivatives 3a-3r



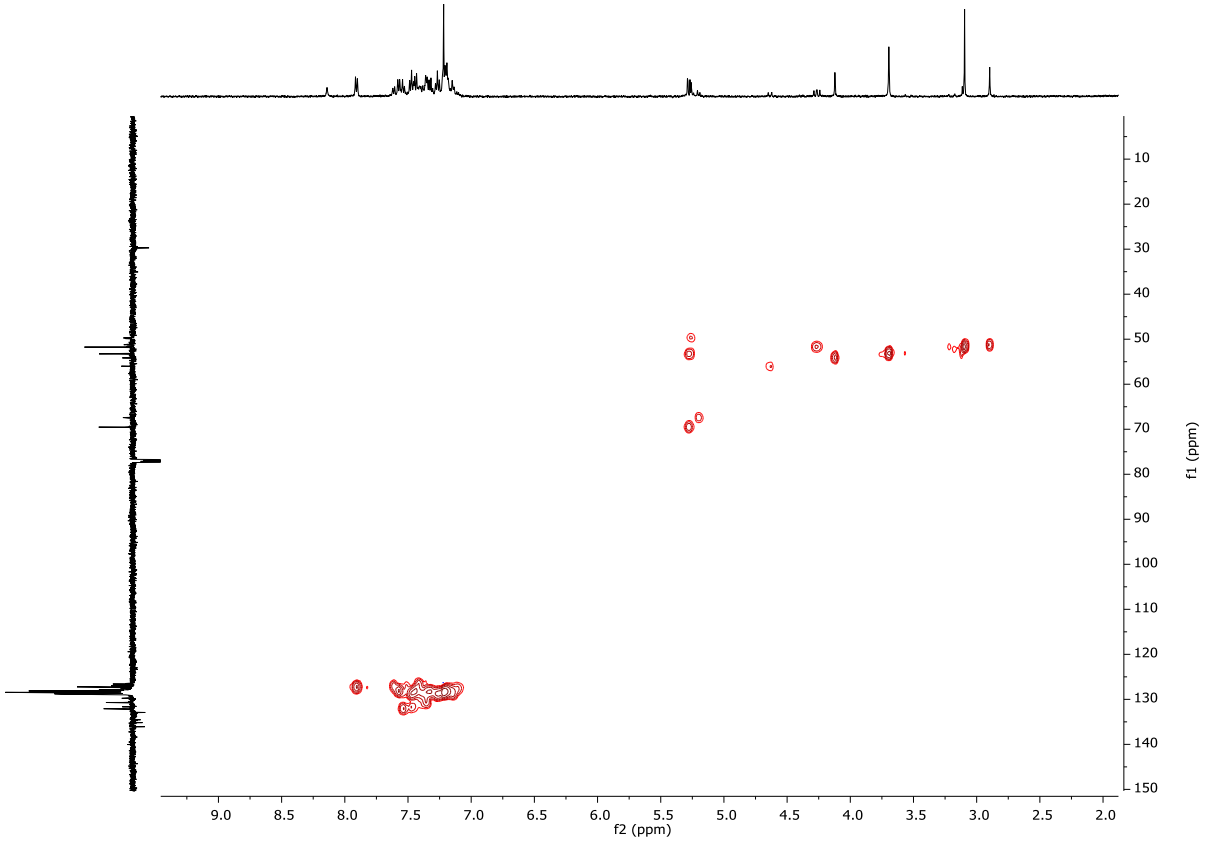
^{1}H NMR spectrum ($CDCl_3$, 300.13 MHz) of **3a** (mixture of diastereomers)



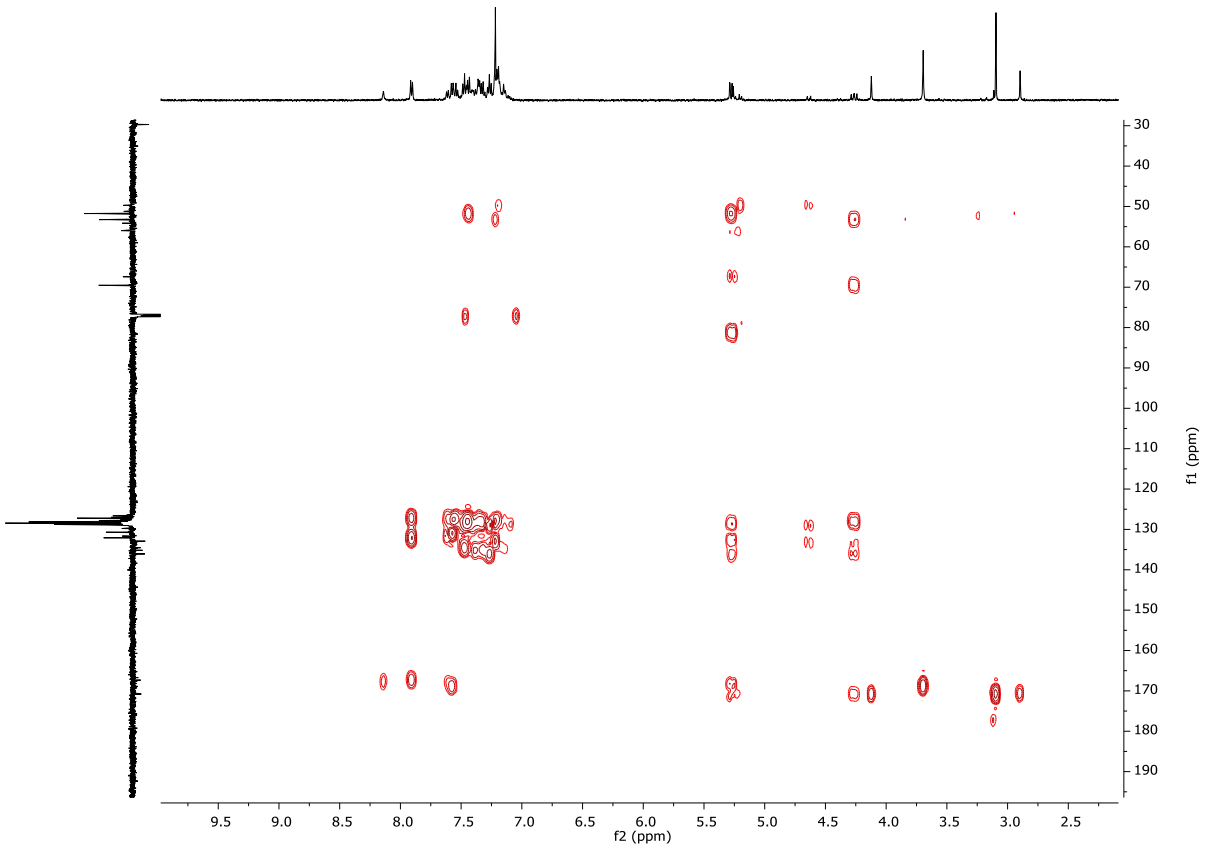
^{1}H NMR spectrum ($CDCl_3$, 300.13 MHz) of **3a** (mixture of diastereomers, zoom aliphatic part)



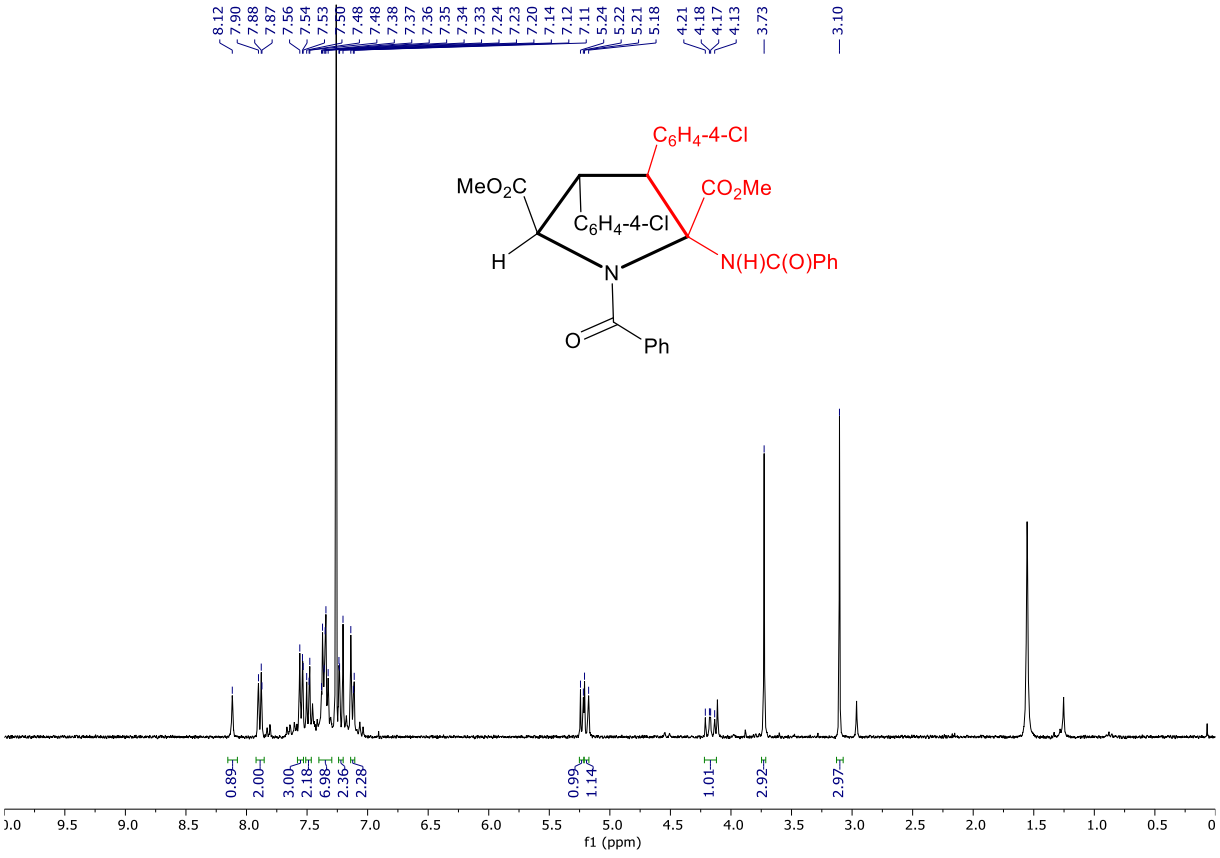
$^{13}C\{^{1}H\}$ (APT) NMR spectrum ($CDCl_3$, 75.5 MHz) of **3a** (mixture of diastereomers)



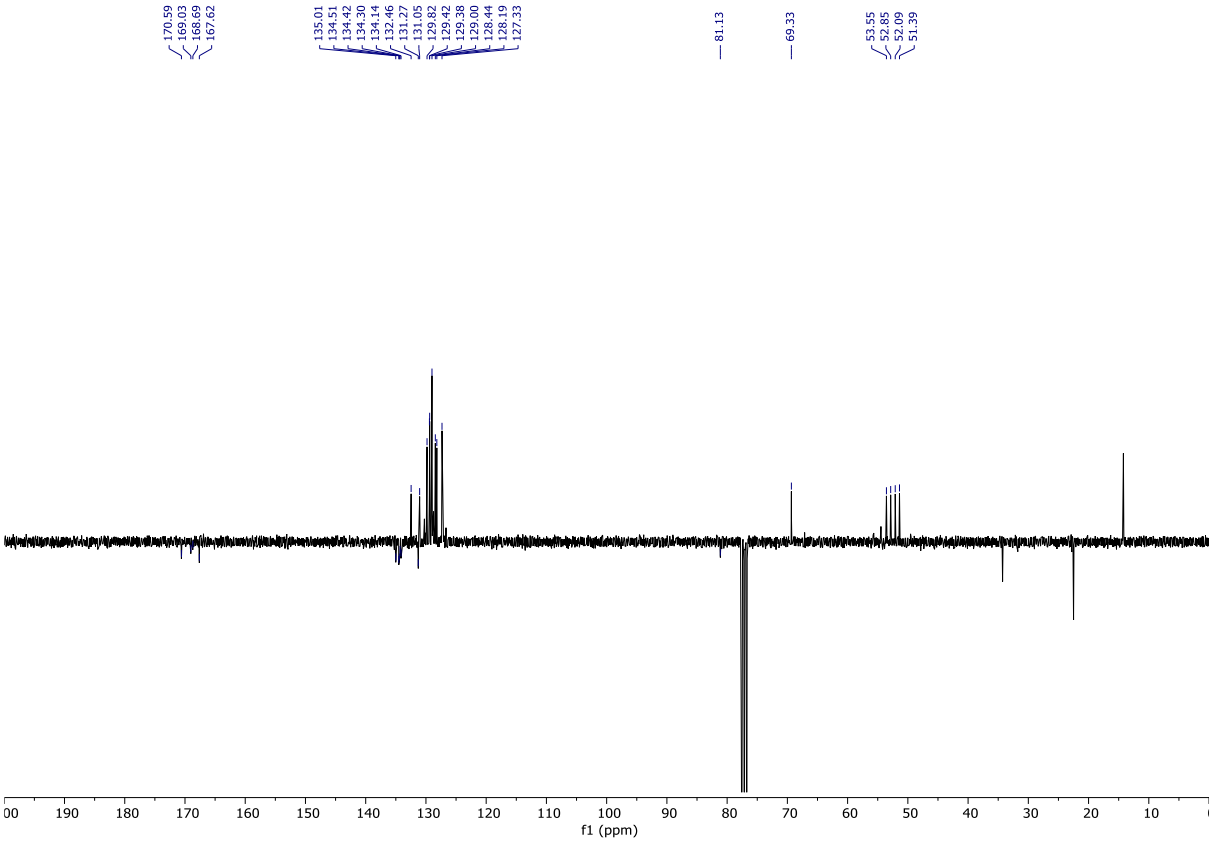
^{1}H-^{13}C HSQC ($CDCl_3$) correlation spectrum of **3a** (mixture of diastereomers)



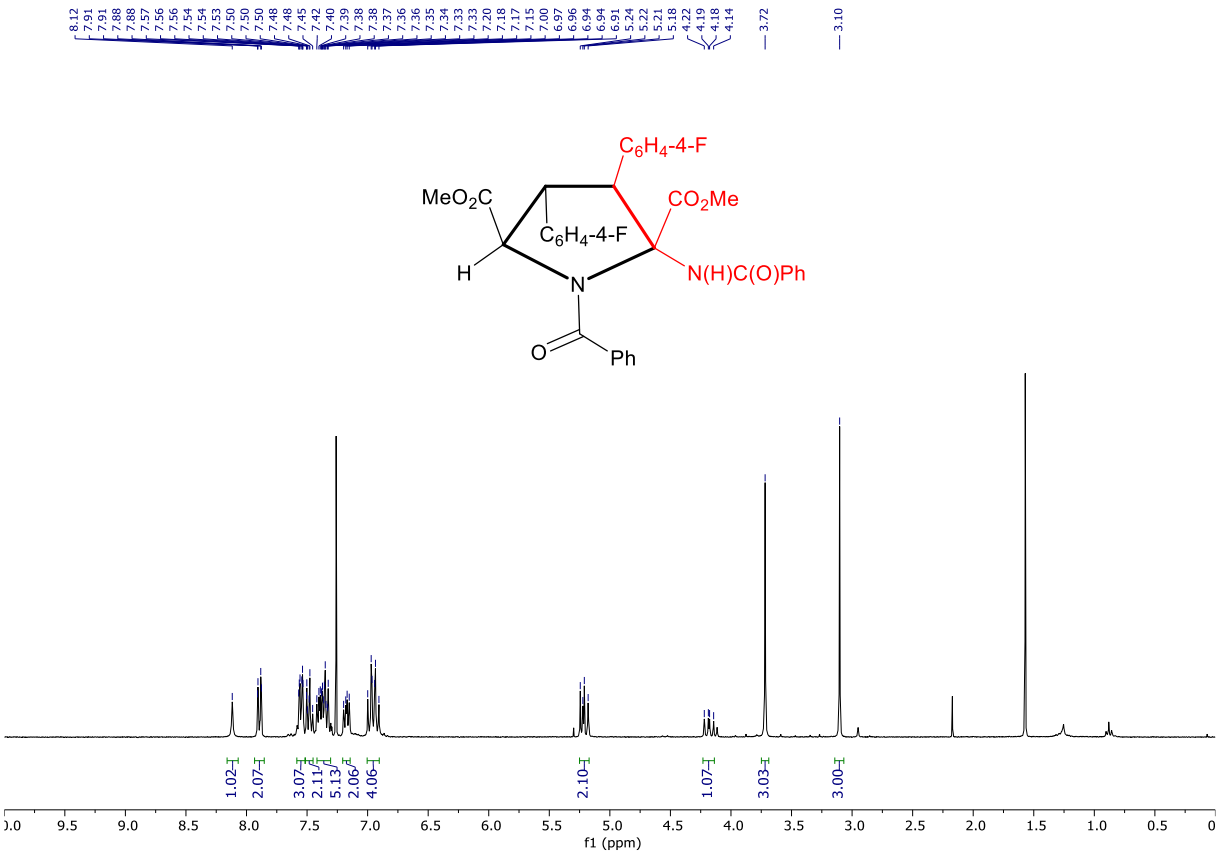
^{1}H-^{13}C HMBC ($CDCl_3$) correlation spectrum of **3a** (mixture of diastereomers)



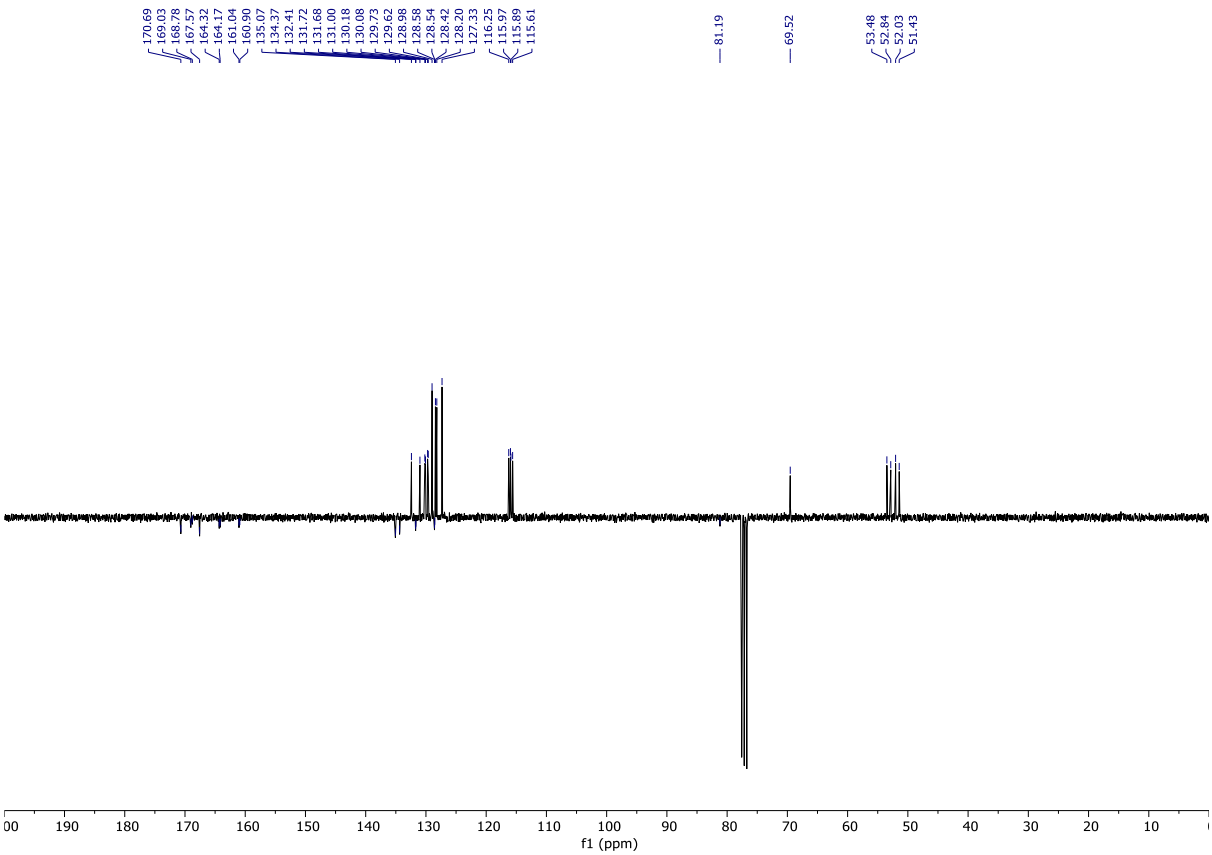
^{1}H NMR spectrum ($CDCl_3$, 300.13 MHz) of **3d**



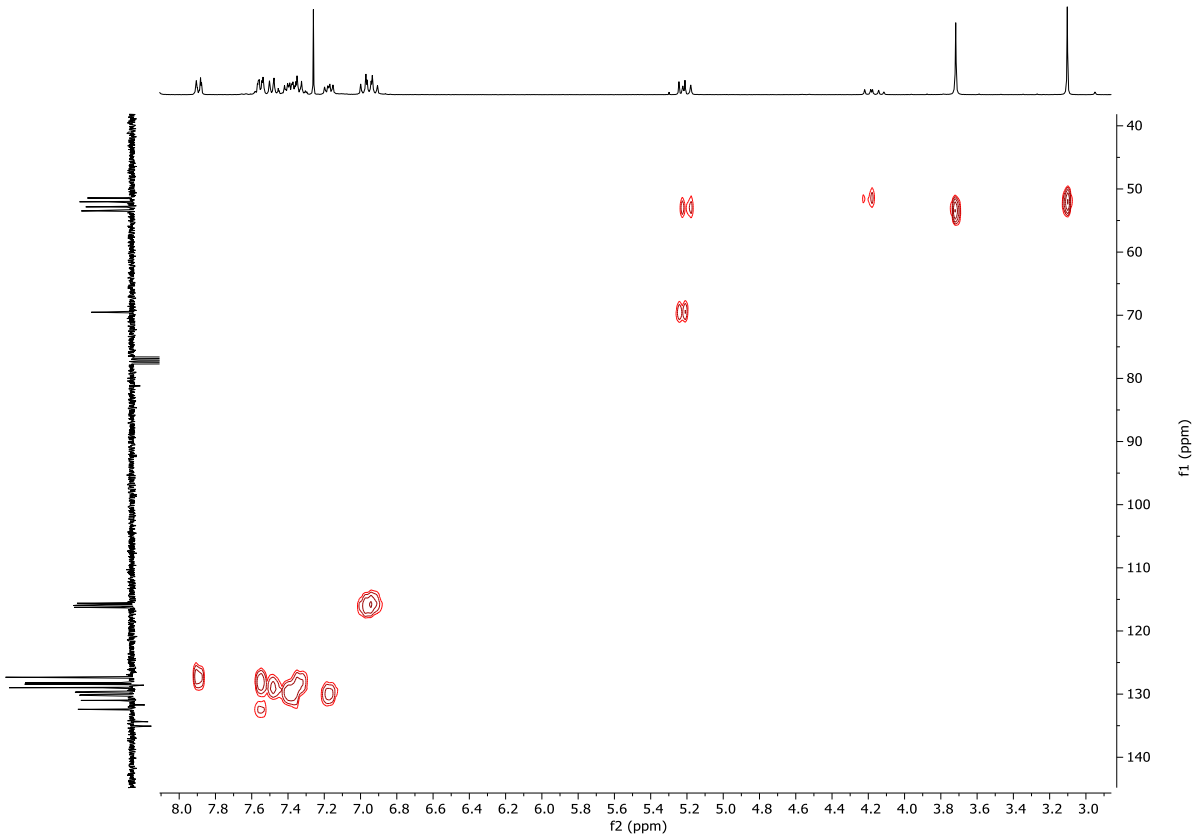
$^{13}C\{^{1}H\}$ (APT) NMR spectrum ($CDCl_3$, 75.5 MHz) of **3d**



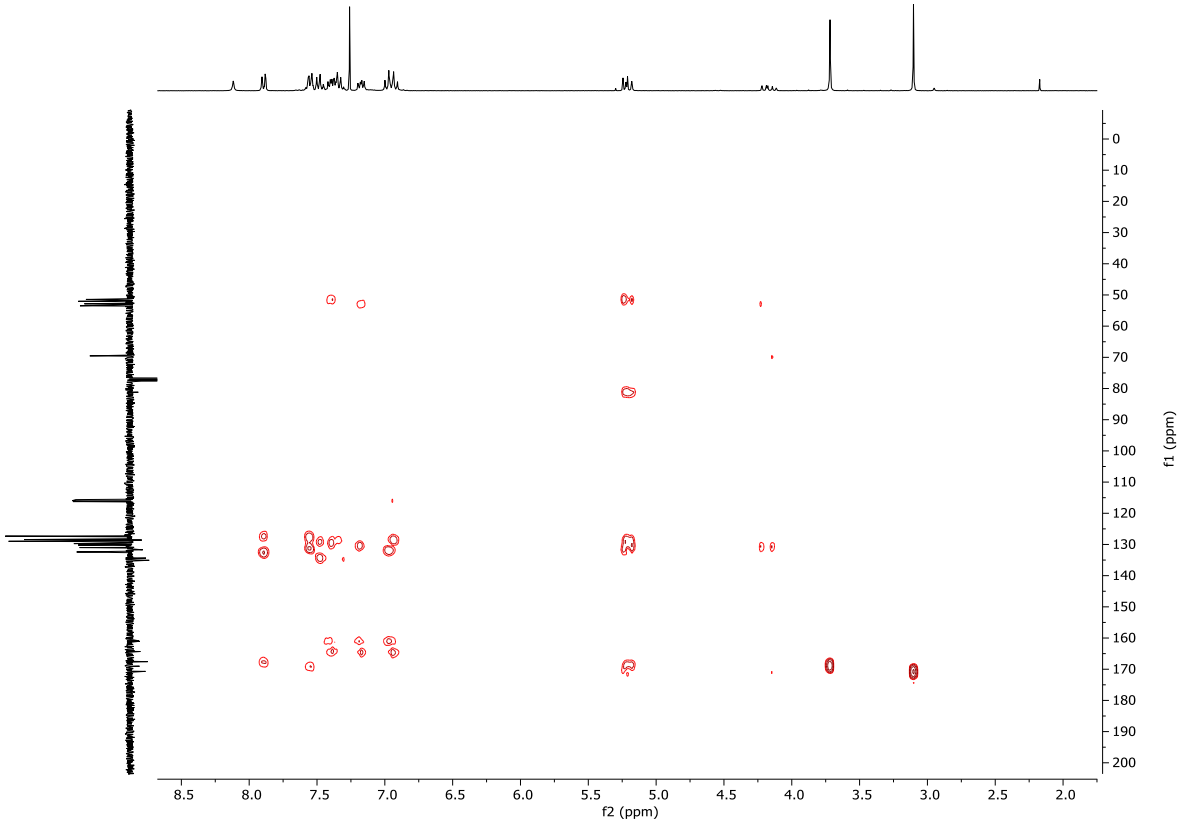
^{1}H NMR spectrum ($CDCl_3$, 300.13 MHz) of **3e**



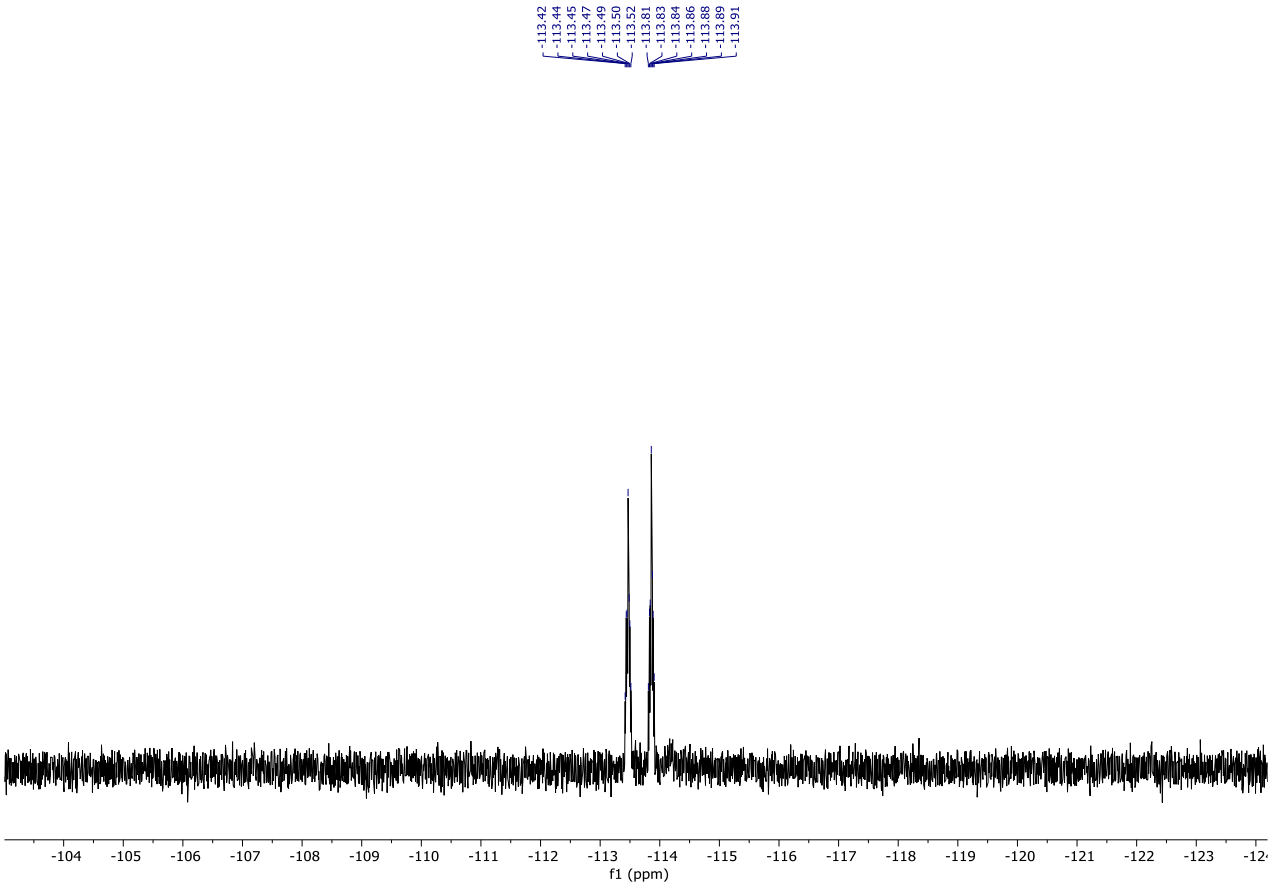
$^{13}C\{^{1}H\}$ (APT) NMR spectrum ($CDCl_3$, 75.5 MHz) of **3e**



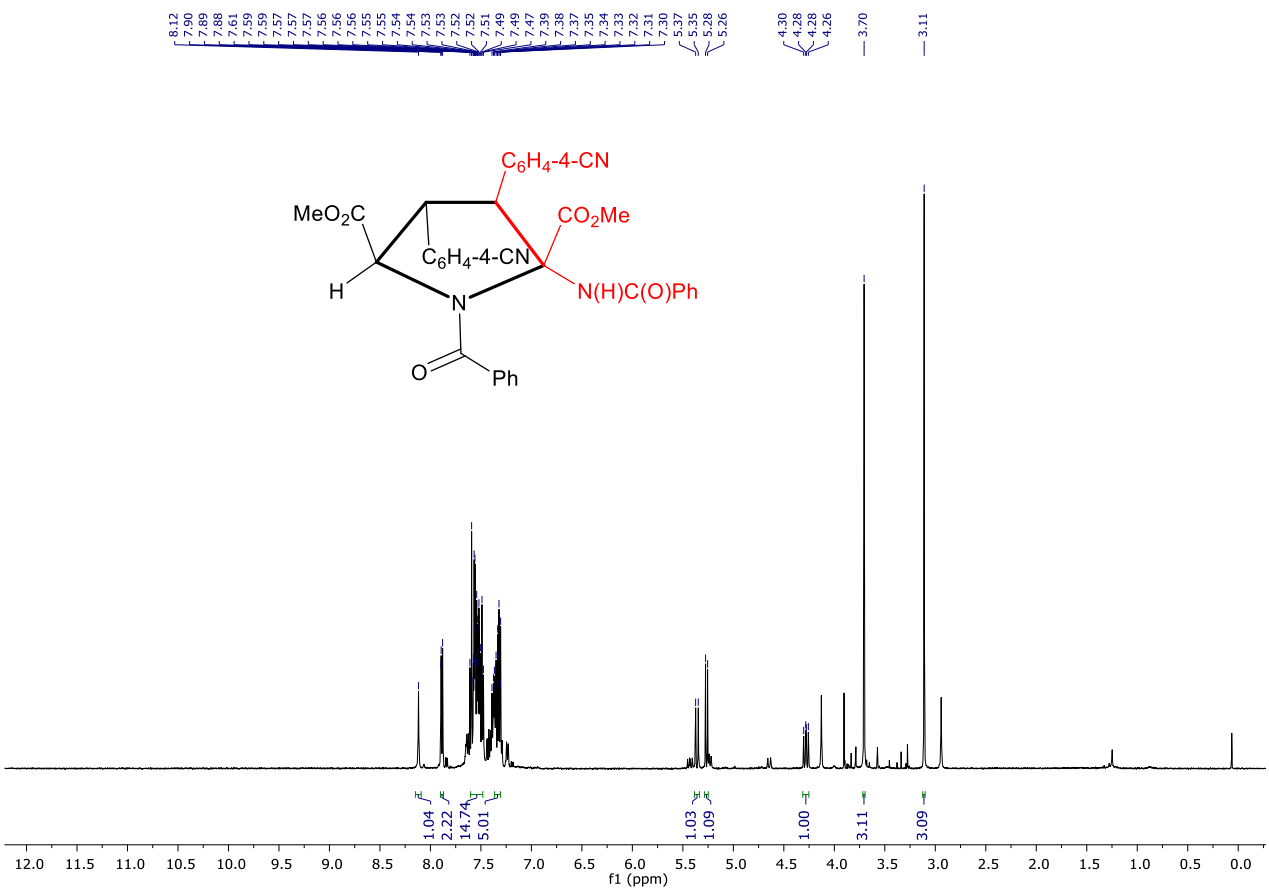
^{1}H-^{13}C HSQC ($CDCl_3$) correlation spectrum of **3e**



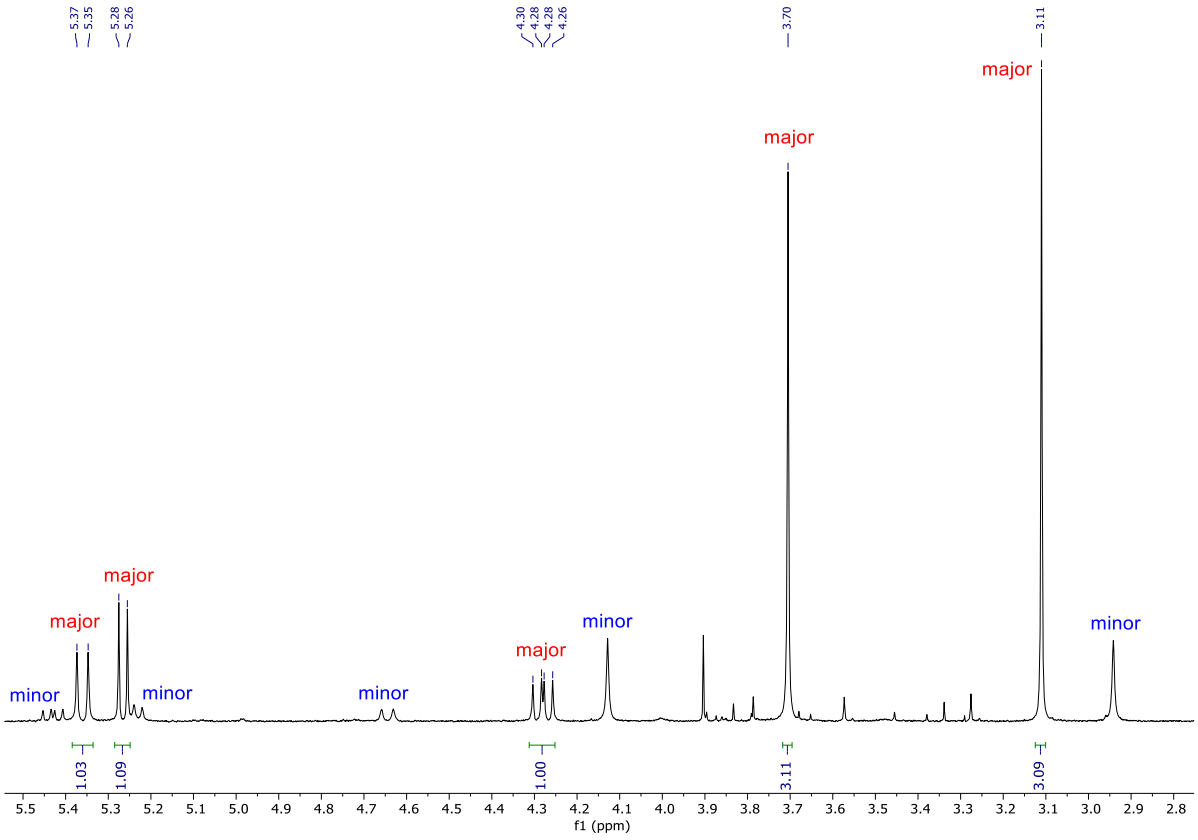
^{1}H-^{13}C HMBC ($CDCl_3$) correlation spectrum of **3e**



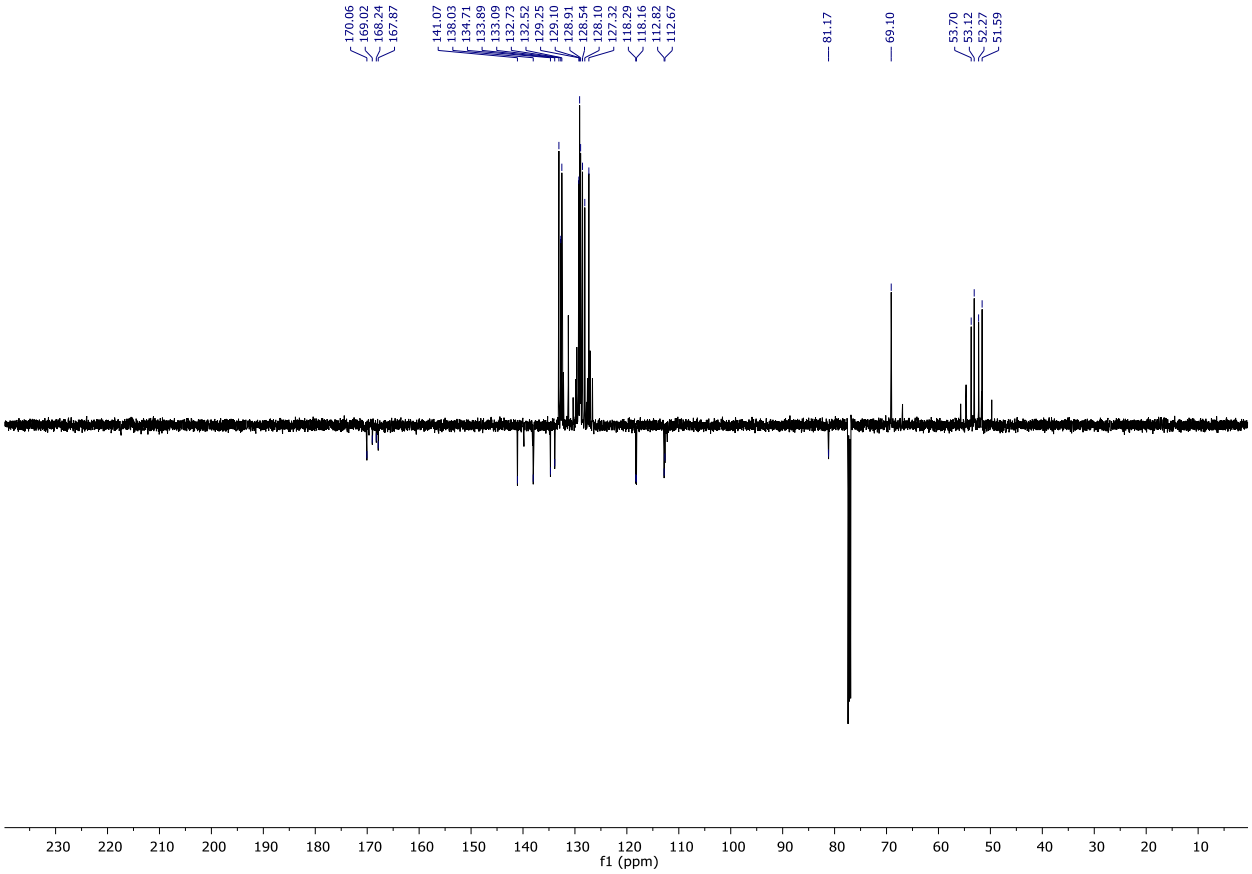
^{19}F NMR spectrum ($CDCl_3$, 282.4 MHz) of **3e**



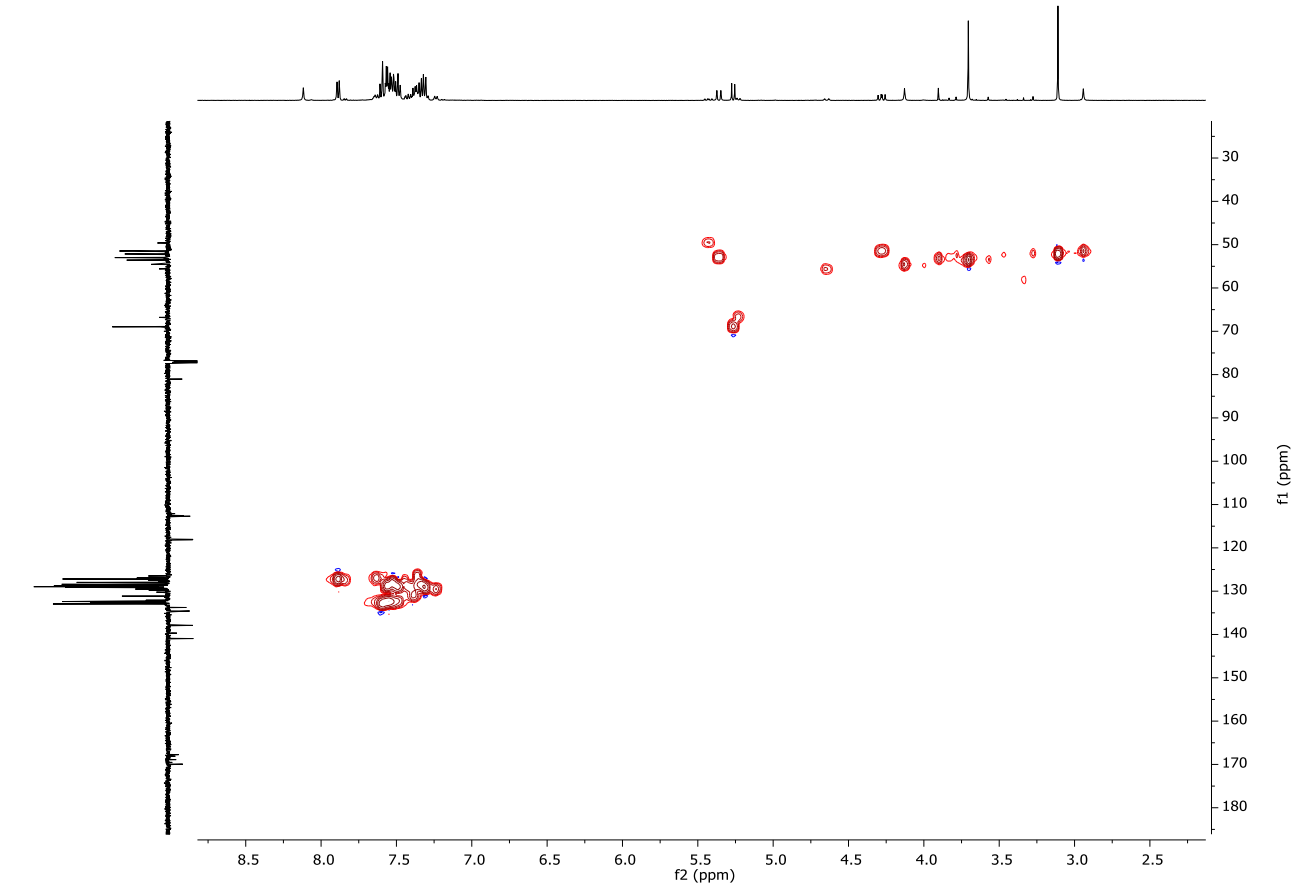
^{1}H NMR spectrum ($CDCl_3$, 400.13 MHz) of **3g** (mixture of diastereomers)



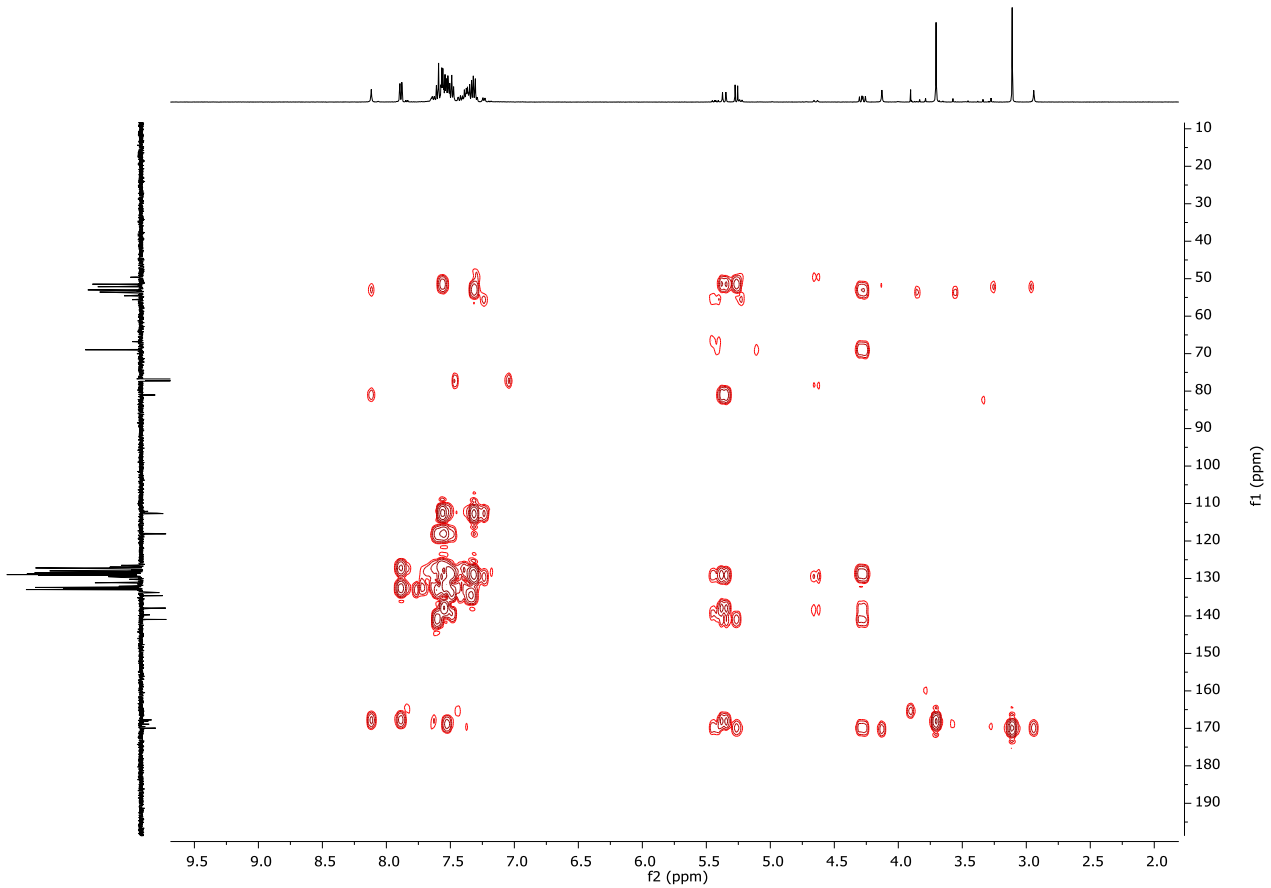
^{1}H NMR spectrum ($CDCl_3$, 400.13 MHz) of **3g** (mixture of diastereomers, zoom of the aliphatic part)



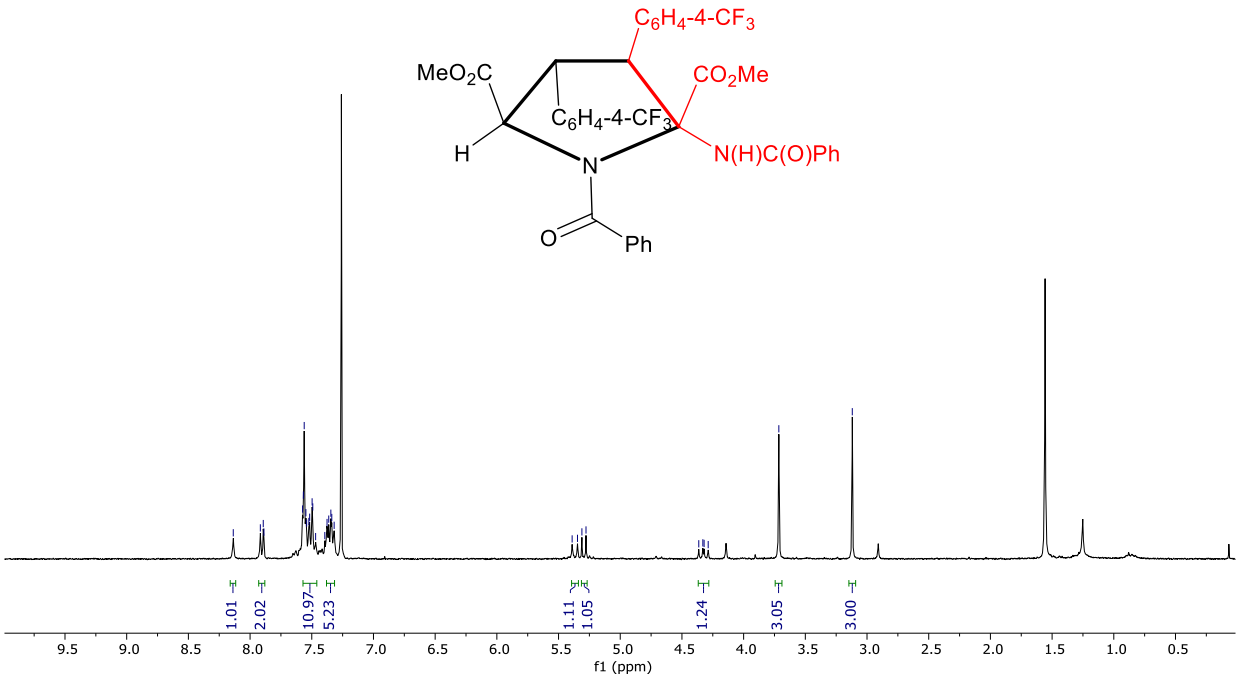
$^{13}C\{^{1}H\}$ (APT) NMR spectrum ($CDCl_3$, 100.6 MHz) of **3g** (mixture of diastereomers)



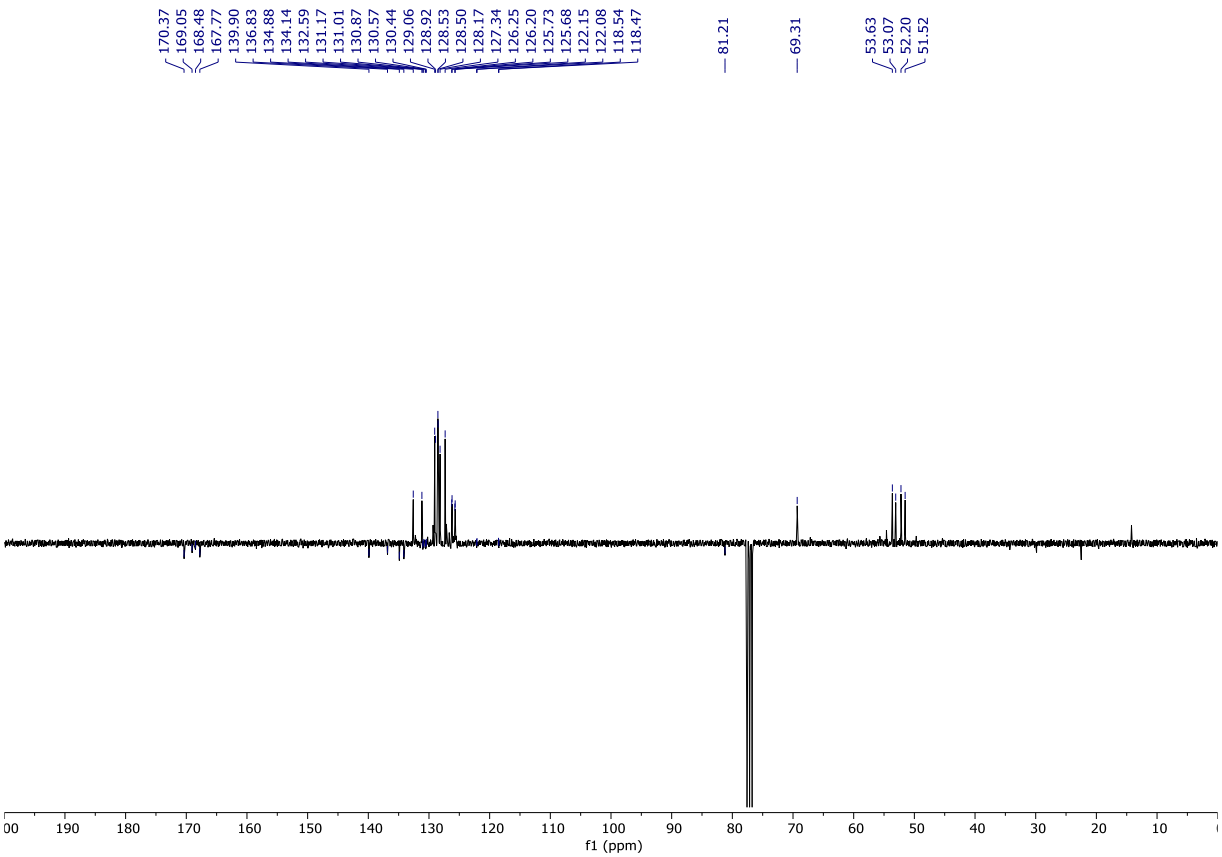
^{1}H-^{13}C HSQC ($CDCl_3$) correlation spectrum of **3g** (mixture of diastereomers)



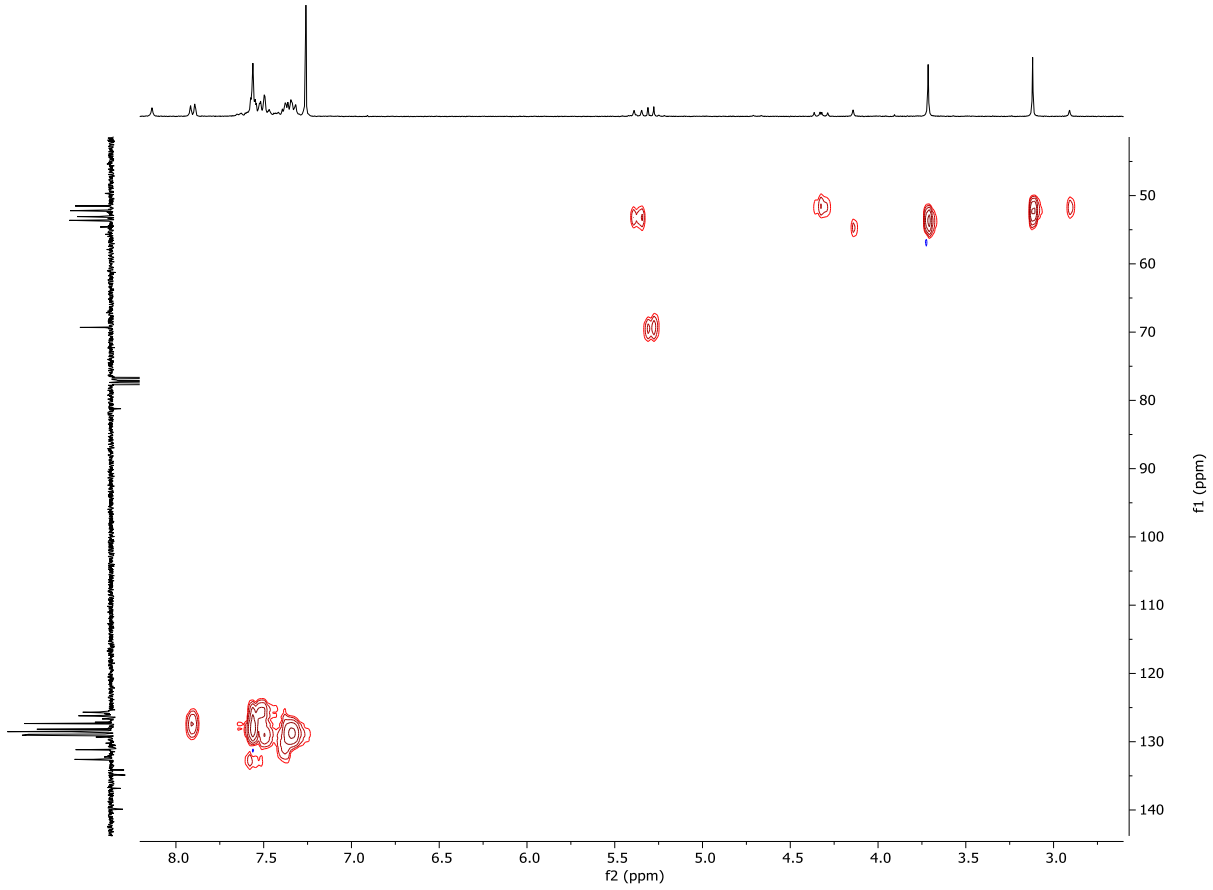
^{1}H-^{13}C HMBC ($CDCl_3$) correlation spectrum of **3g** (mixture of diastereomers)



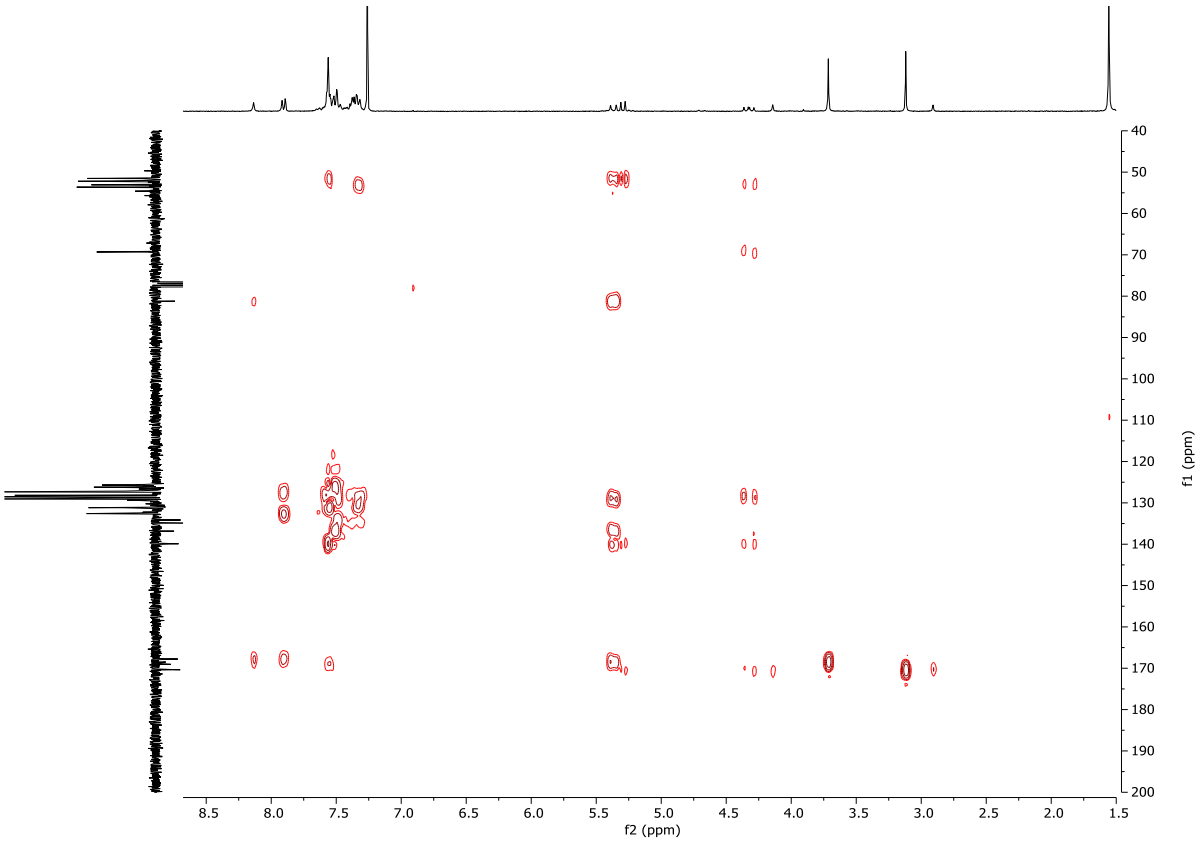
^{1}H NMR spectrum ($CDCl_3$, 300.13 MHz) of **3h**



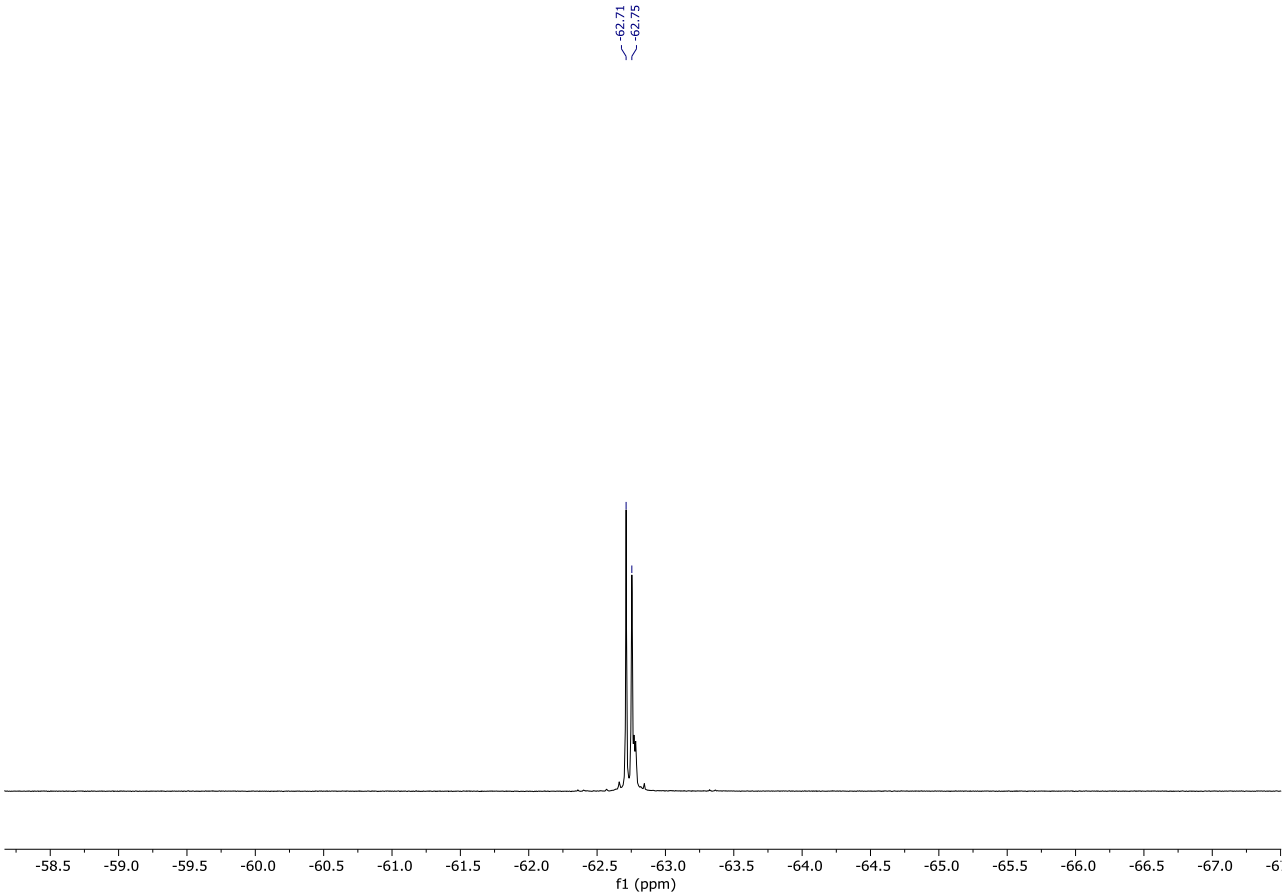
$^{13}C\{^{1}H\}$ (APT) NMR spectrum ($CDCl_3$, 75.5 MHz) of **3h**



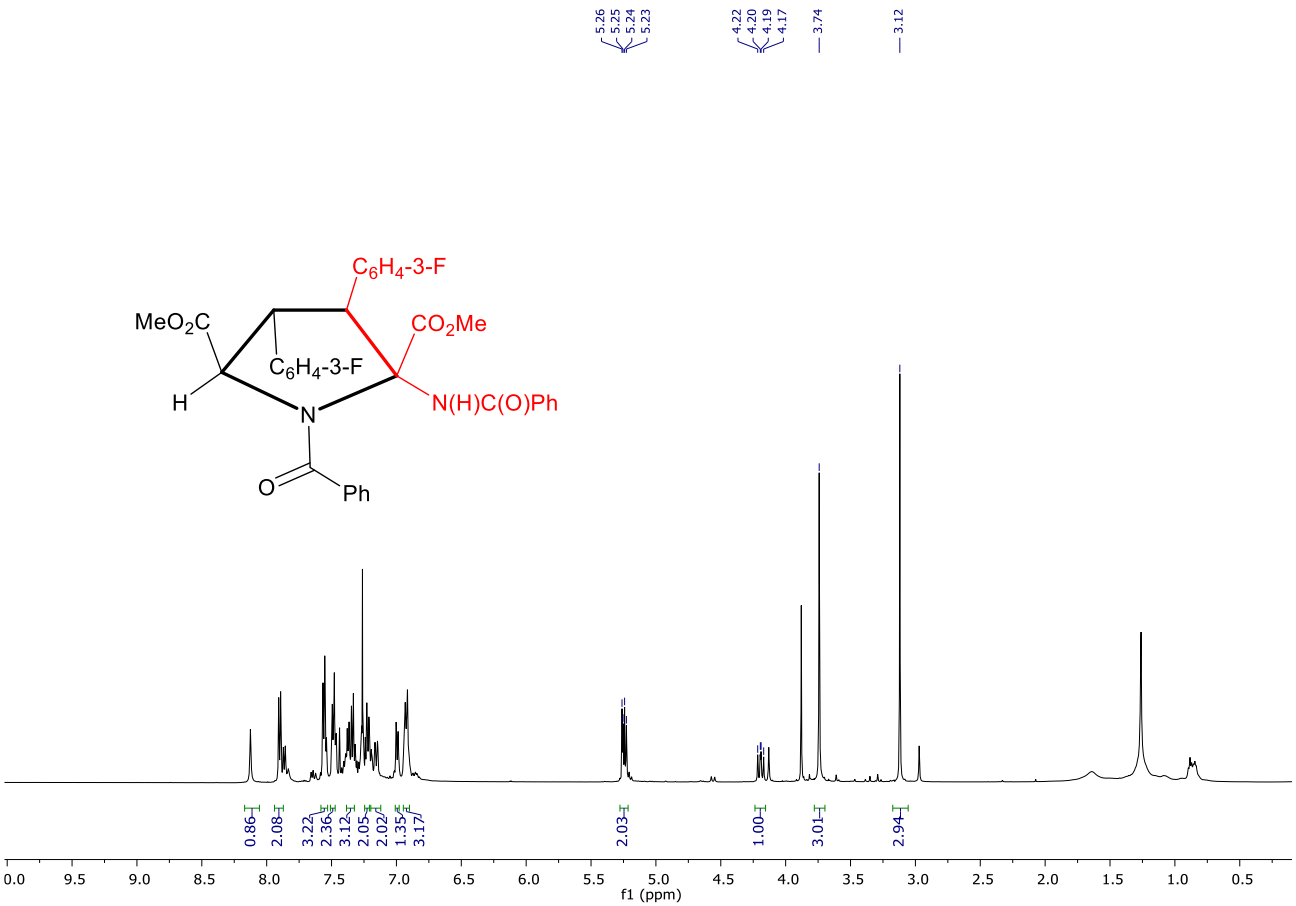
^{1}H-^{13}C HSQC ($CDCl_3$) correlation spectrum of **3h**



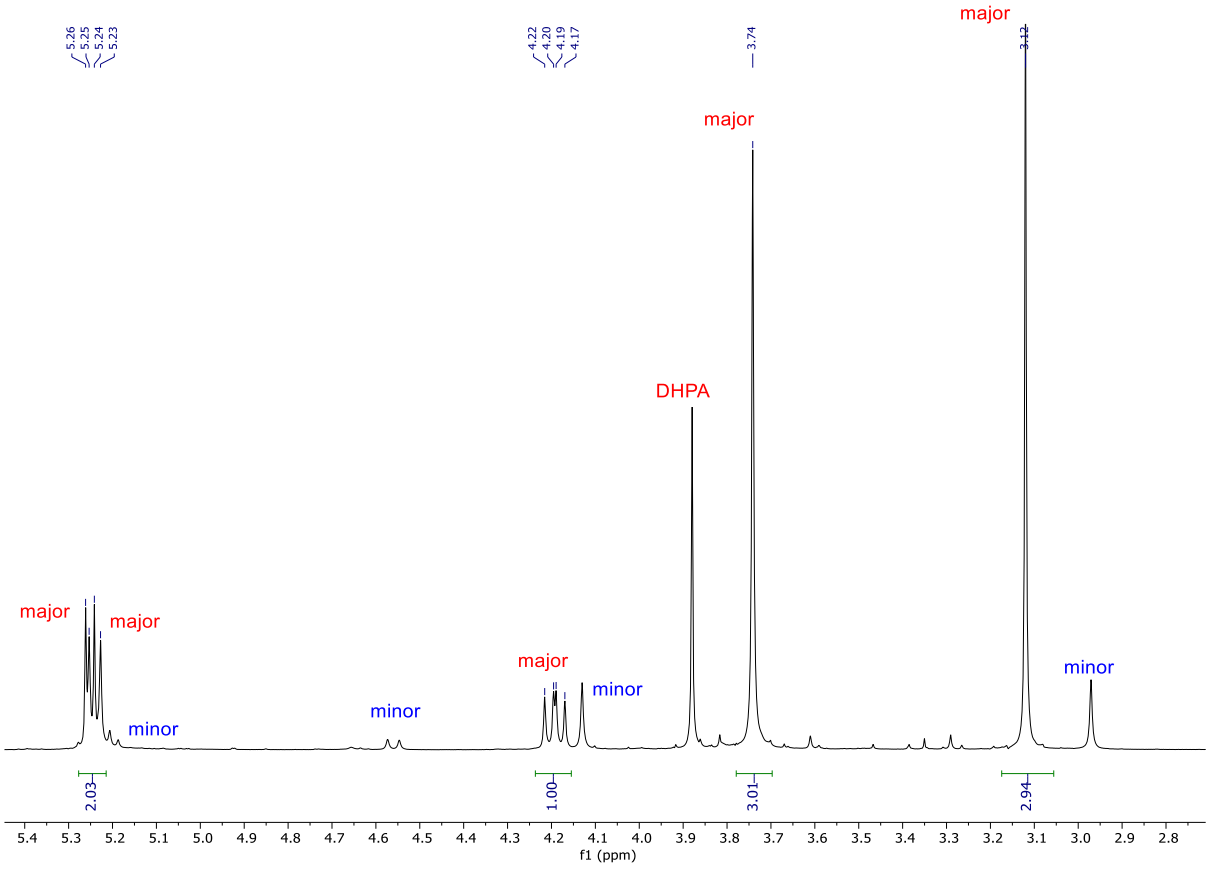
^{1}H-^{13}C HMBC ($CDCl_3$) correlation spectrum of **3h**



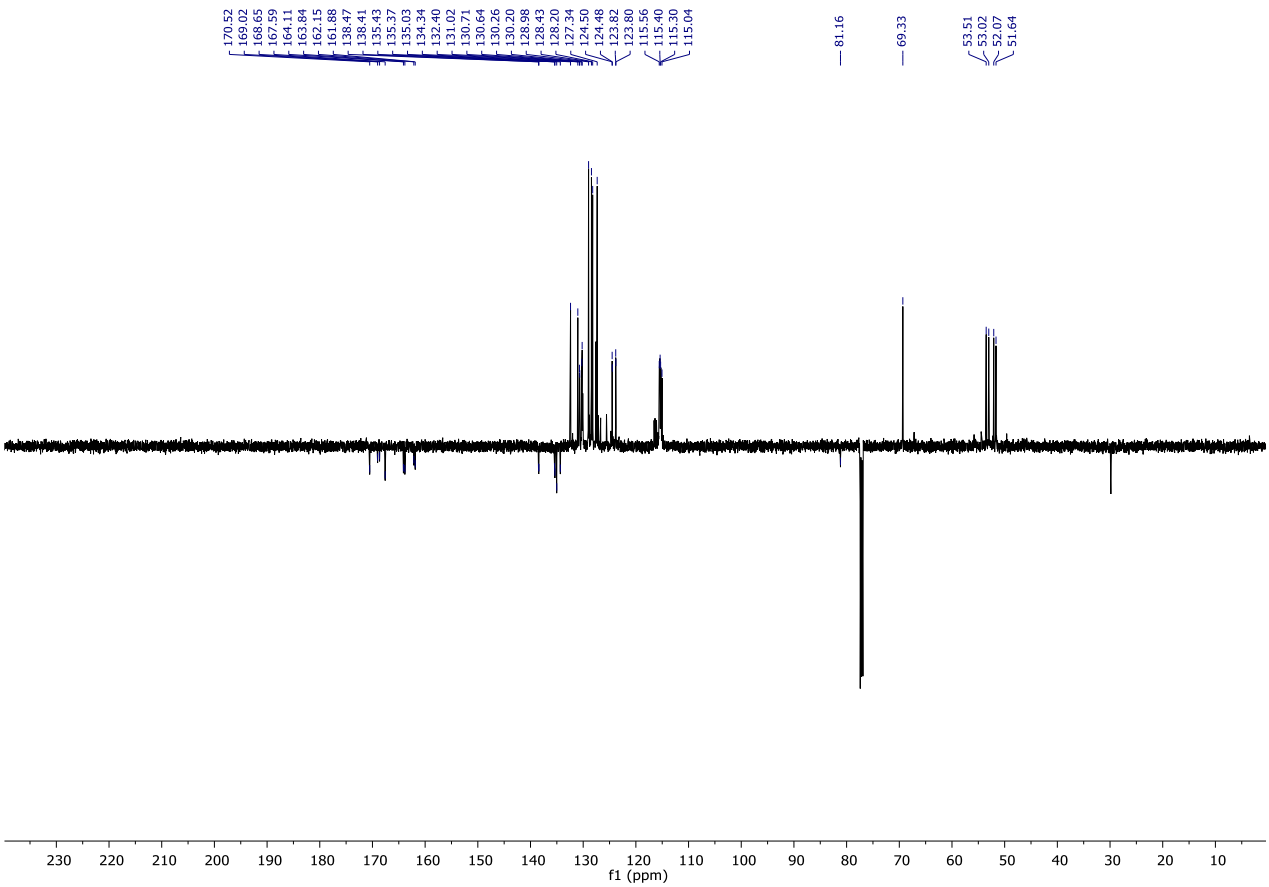
^{19}F NMR spectrum ($CDCl_3$, 282.4 MHz) of **3h**



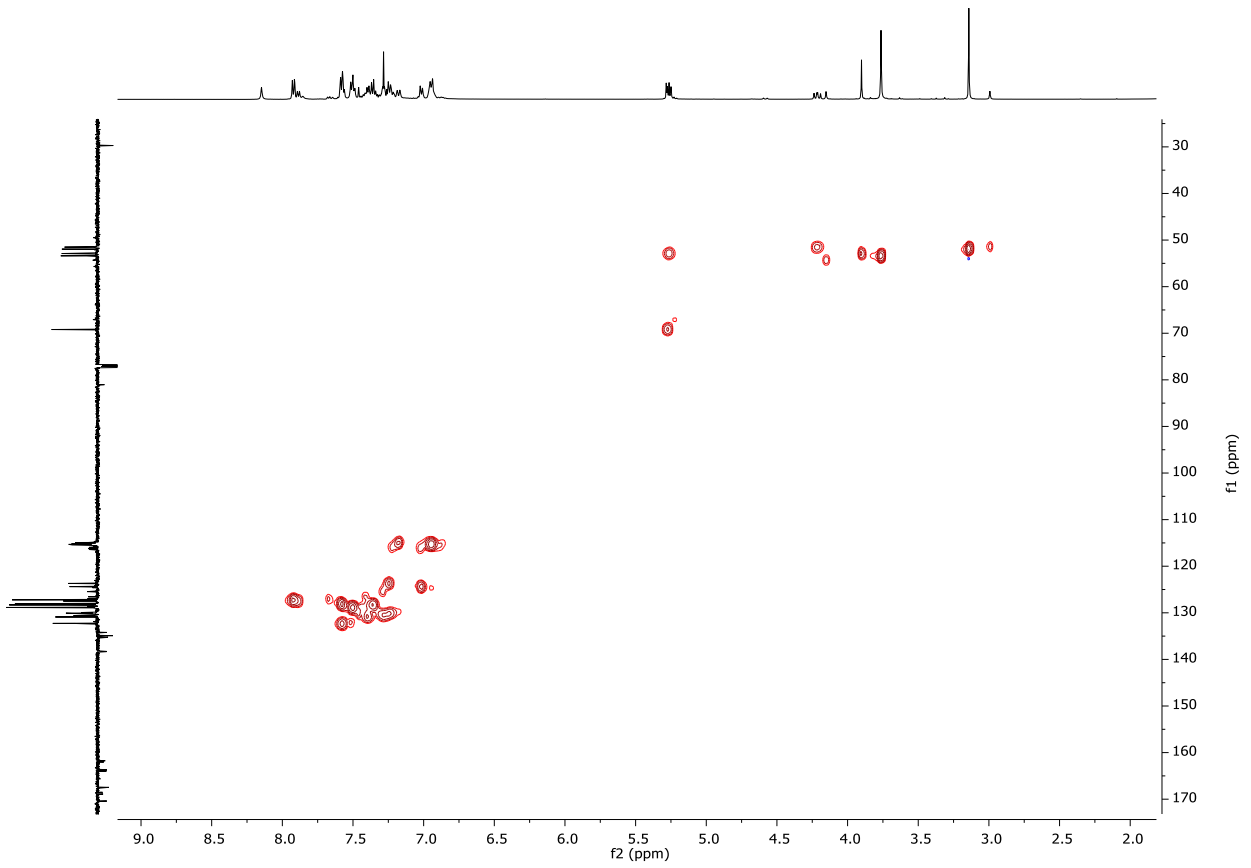
^{1}H NMR spectrum ($CDCl_3$, 300.13 MHz) of **3k** (mixture of isomers)



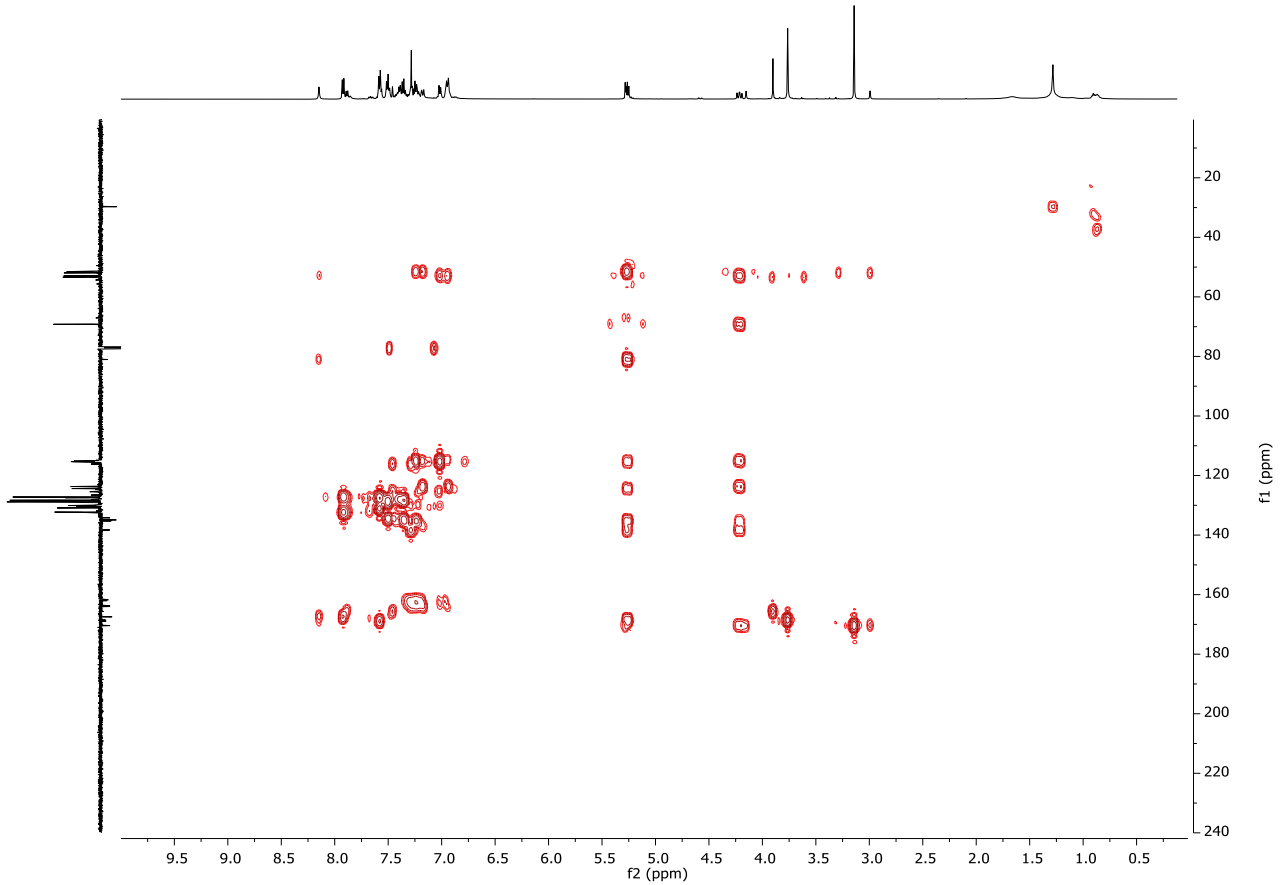
^{1}H NMR spectrum ($CDCl_3$, 300.13 MHz) of **3k** (mixture of isomers, zoom of the aliphatic part)



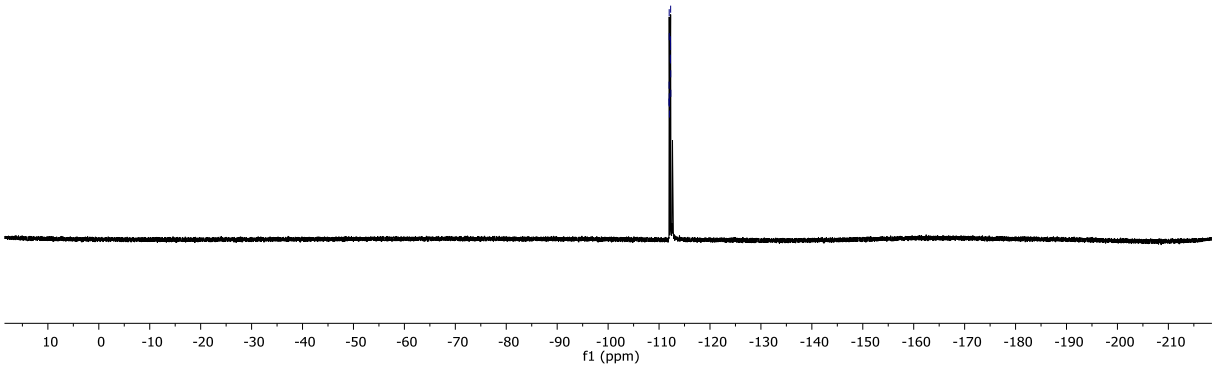
$^{13}C\{^{1}H\}$ (APT) NMR spectrum ($CDCl_3$, 75.5 MHz) of **3k** (mixture of isomers)



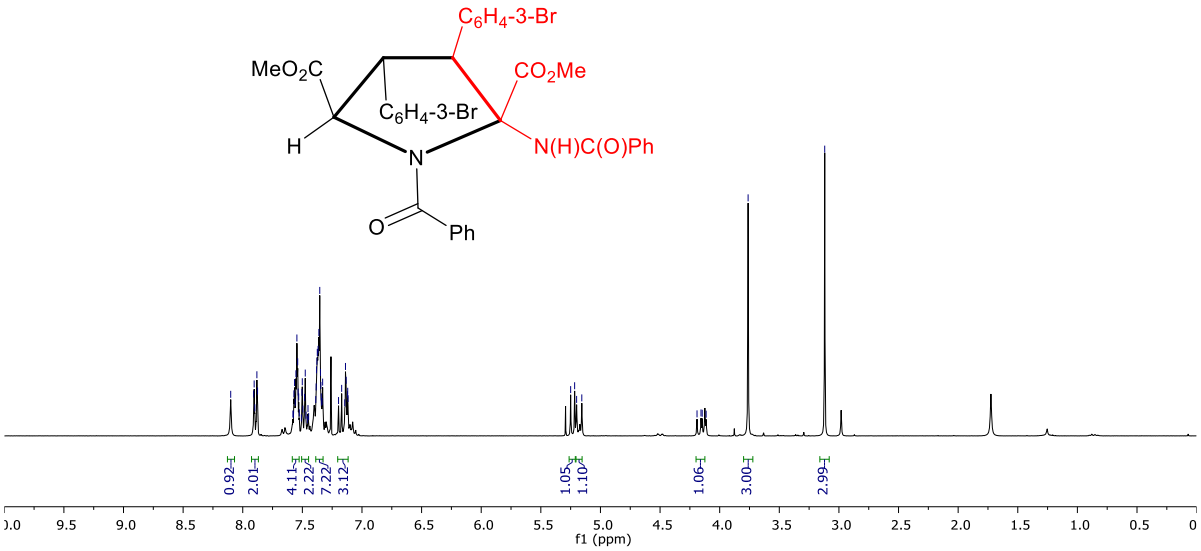
^{1}H-^{13}C HSQC ($CDCl_3$) correlation spectrum of **3k** (mixture of isomers)



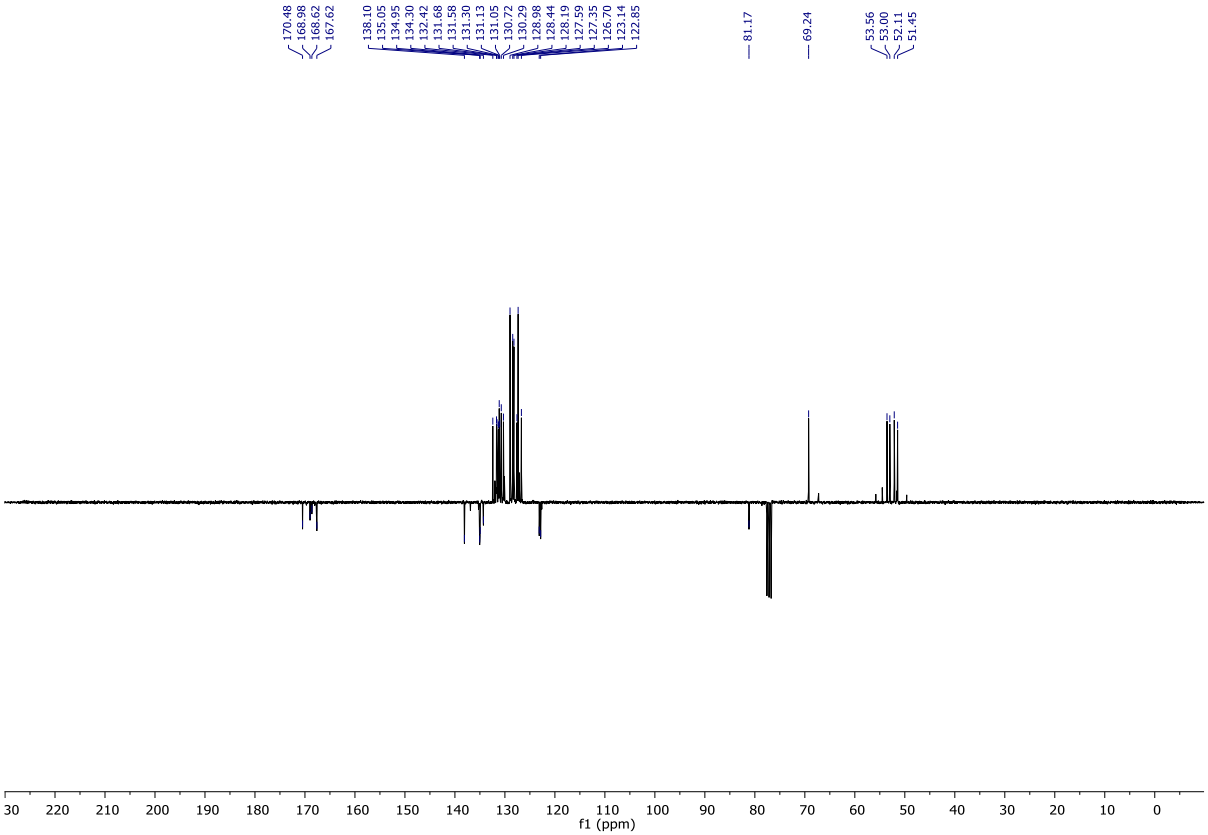
^{1}H-^{13}C HMBC ($CDCl_3$) correlation spectrum of **3k** (mixture of isomers)



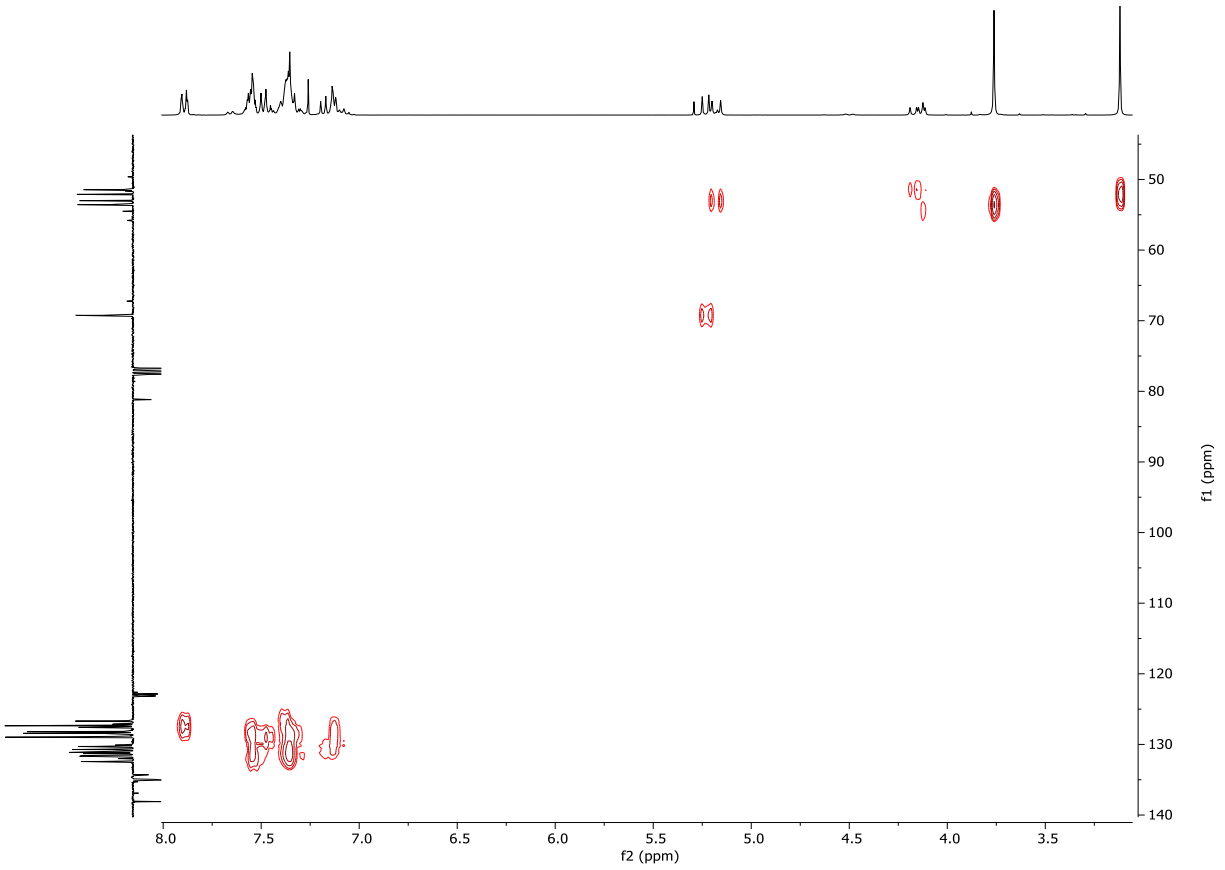
^{19}F NMR spectrum ($CDCl_3$, 282.4 MHz) of **3k** (mixture of isomers)



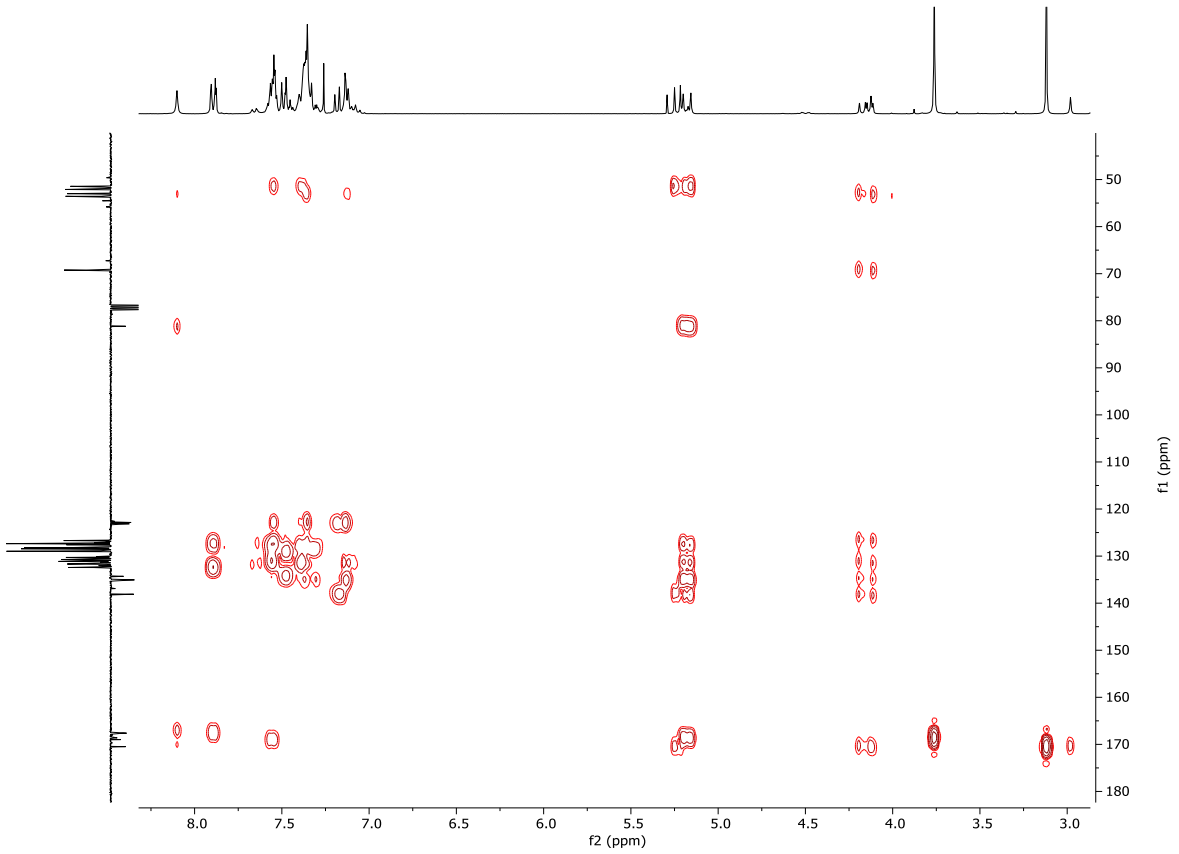
^{1}H NMR spectrum ($CDCl_3$, 300.13 MHz) of **3l**



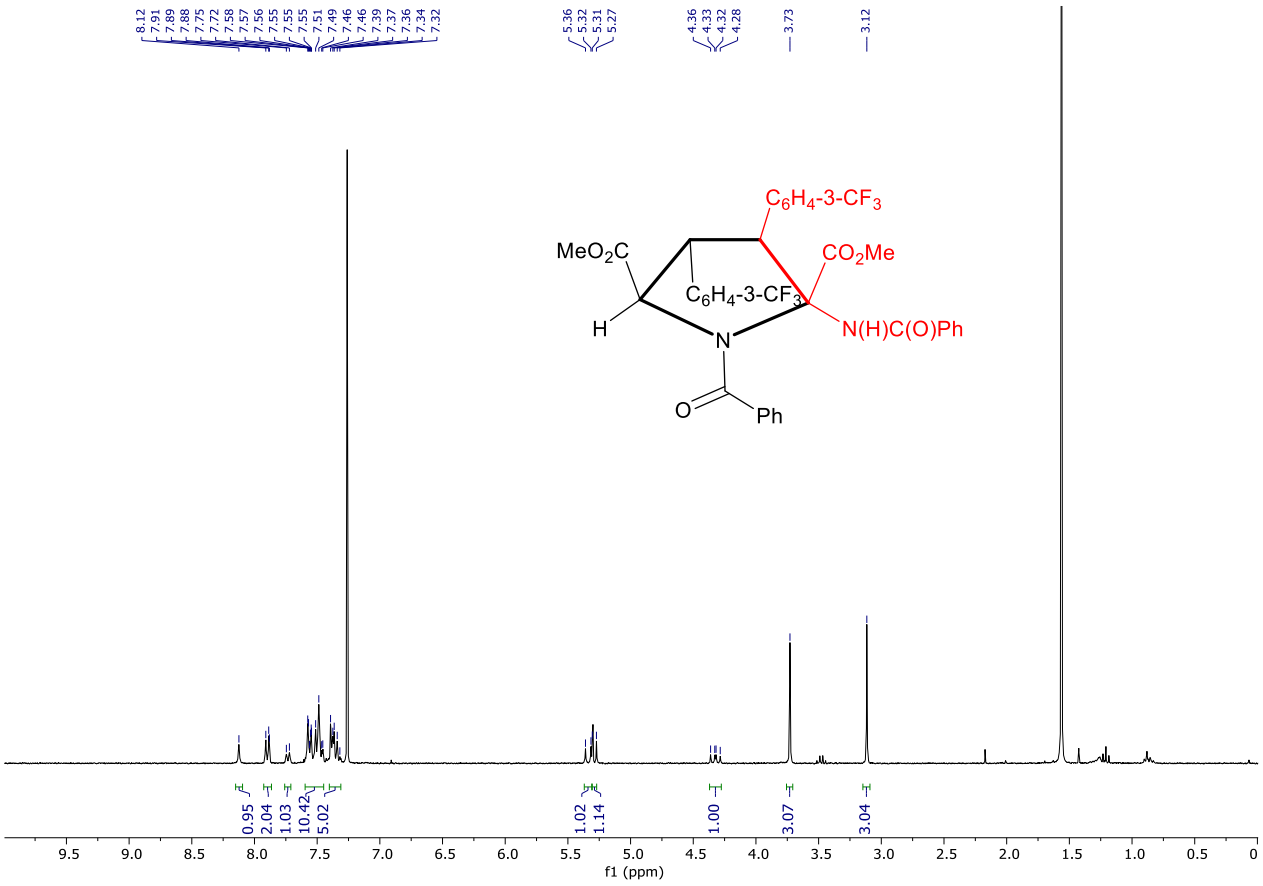
$^{13}C\{^{1}H\}$ (APT) NMR spectrum ($CDCl_3$, 75.5 MHz) of **3l**



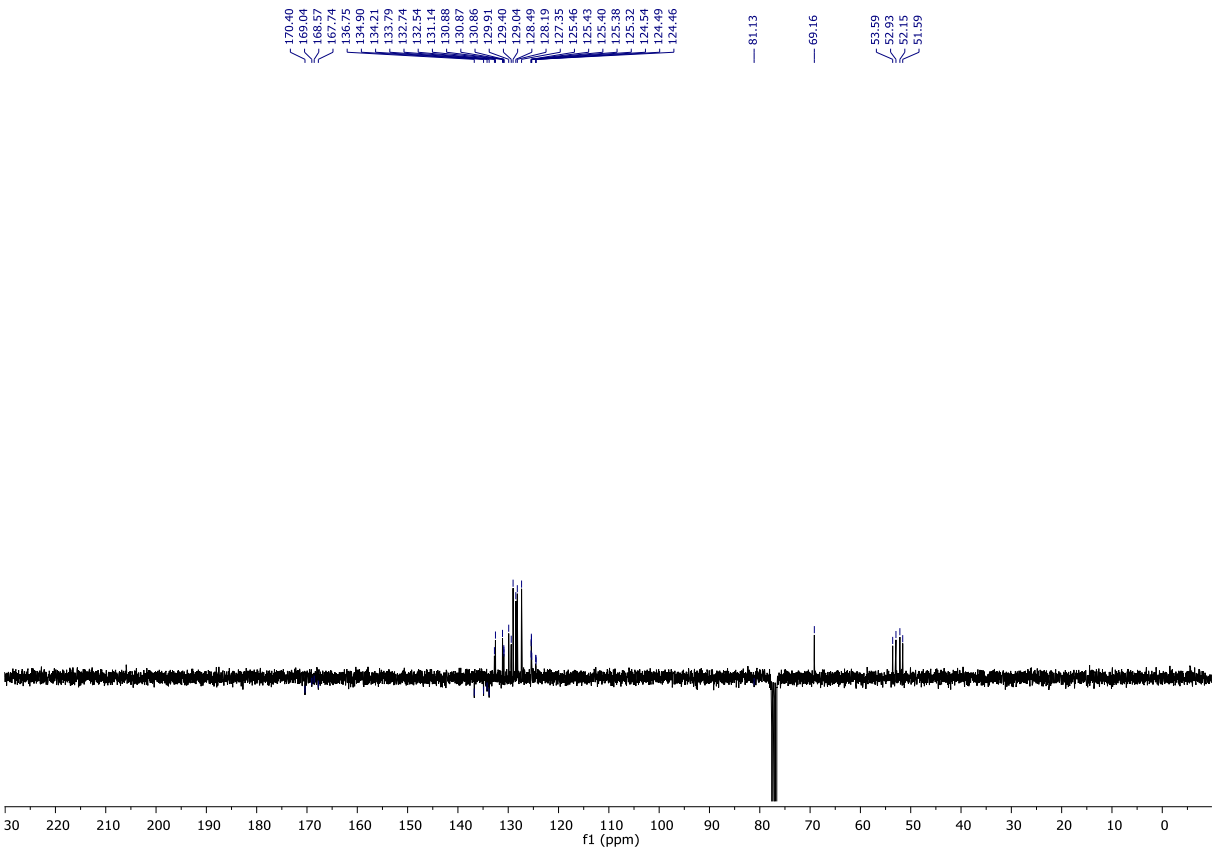
^{1}H-^{13}C HSQC ($CDCl_3$) correlation spectrum of **3l**



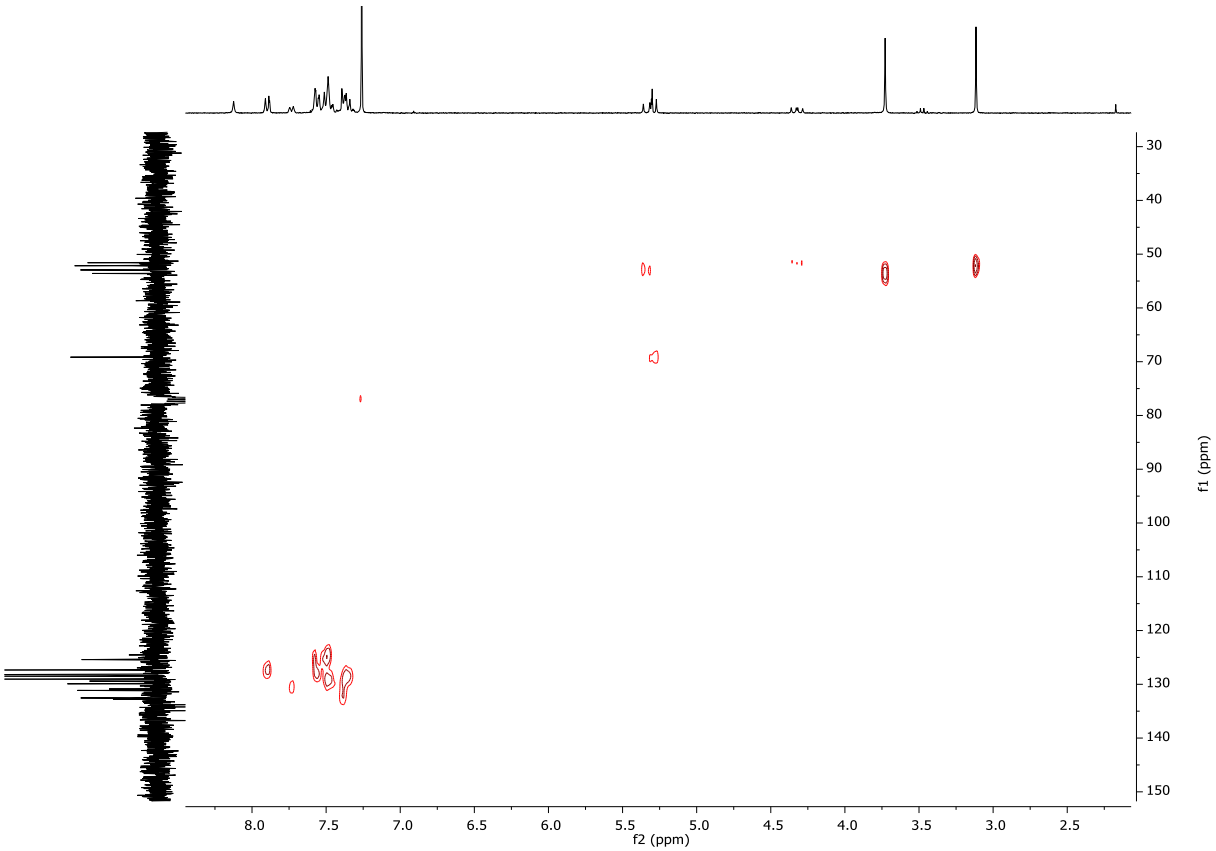
^{1}H-^{13}C HMBC ($CDCl_3$) correlation spectrum of **3l**



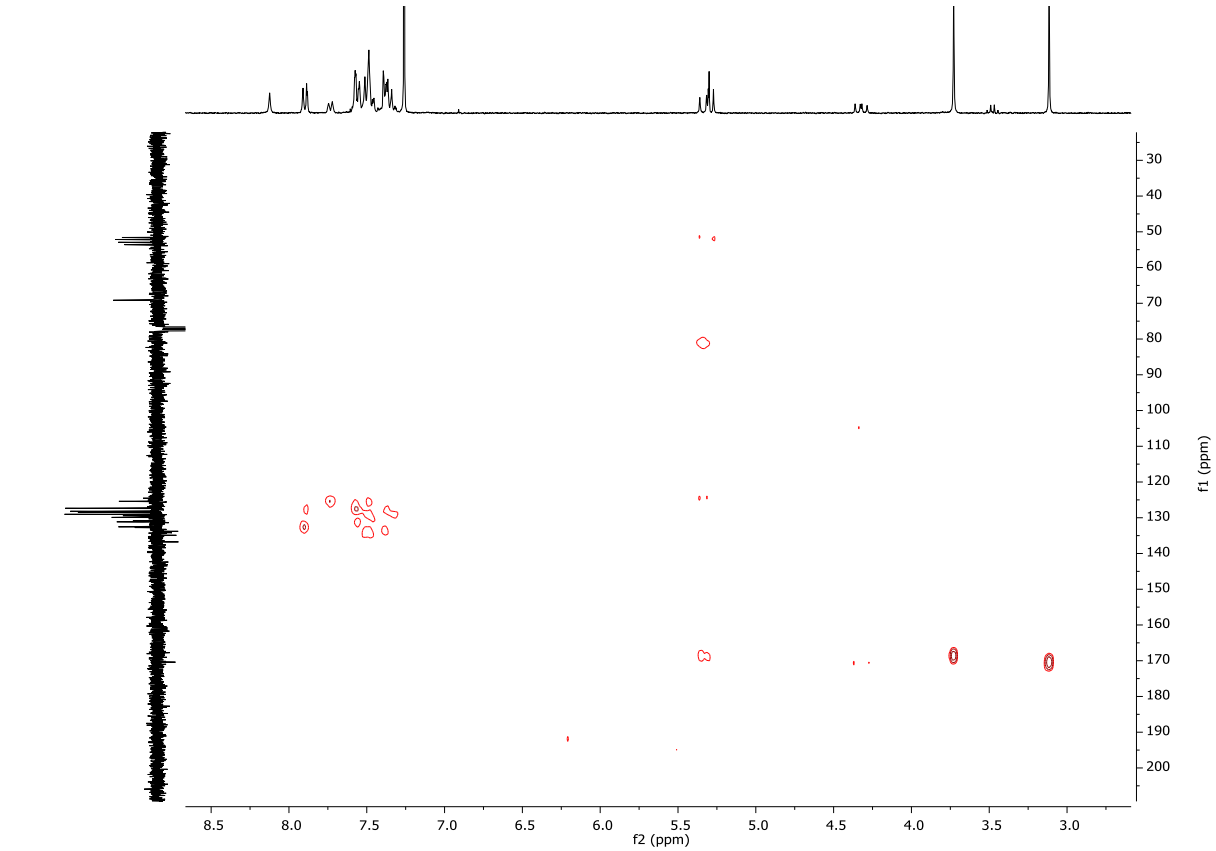
^{1}H NMR spectrum ($CDCl_3$, 300.13 MHz) of **3m**



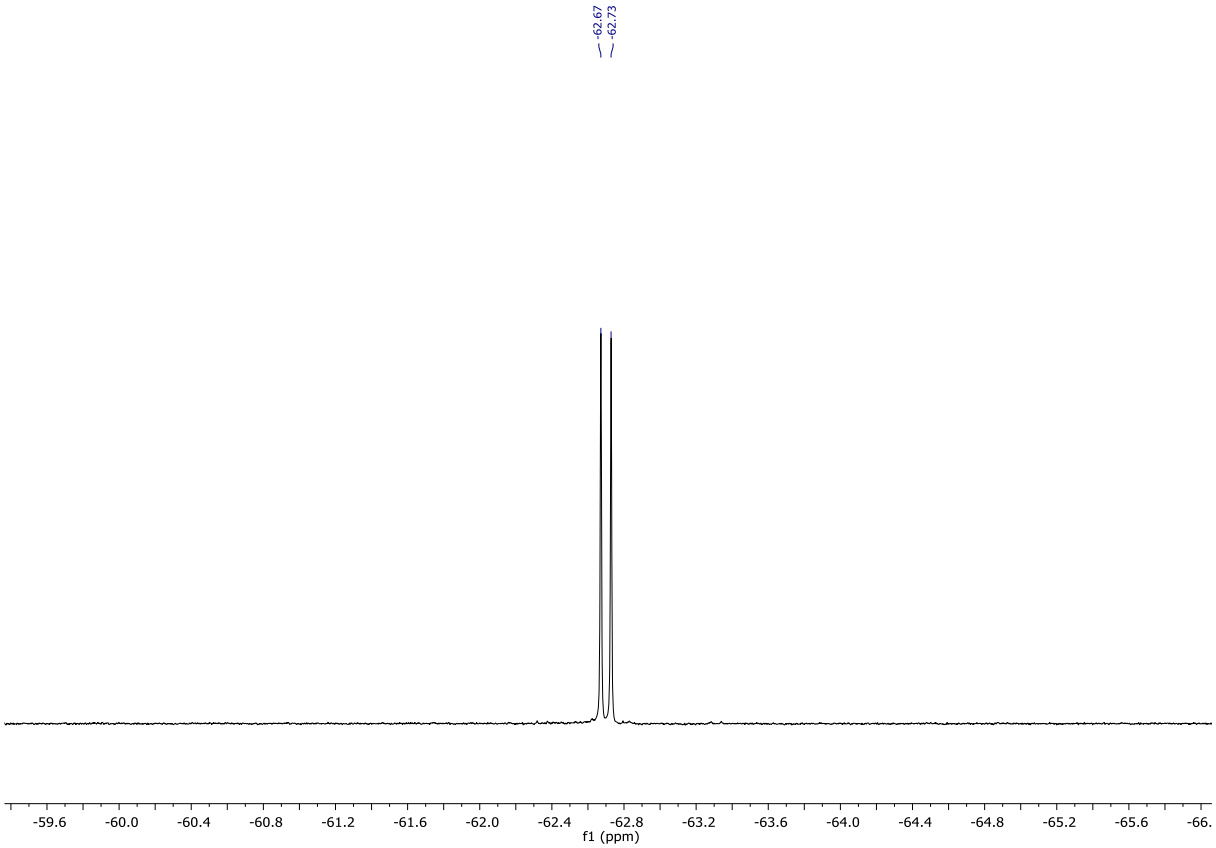
^{13}C{^{1}H} (APT) NMR spectrum ($CDCl_3$, 75.5 MHz) of **3m**



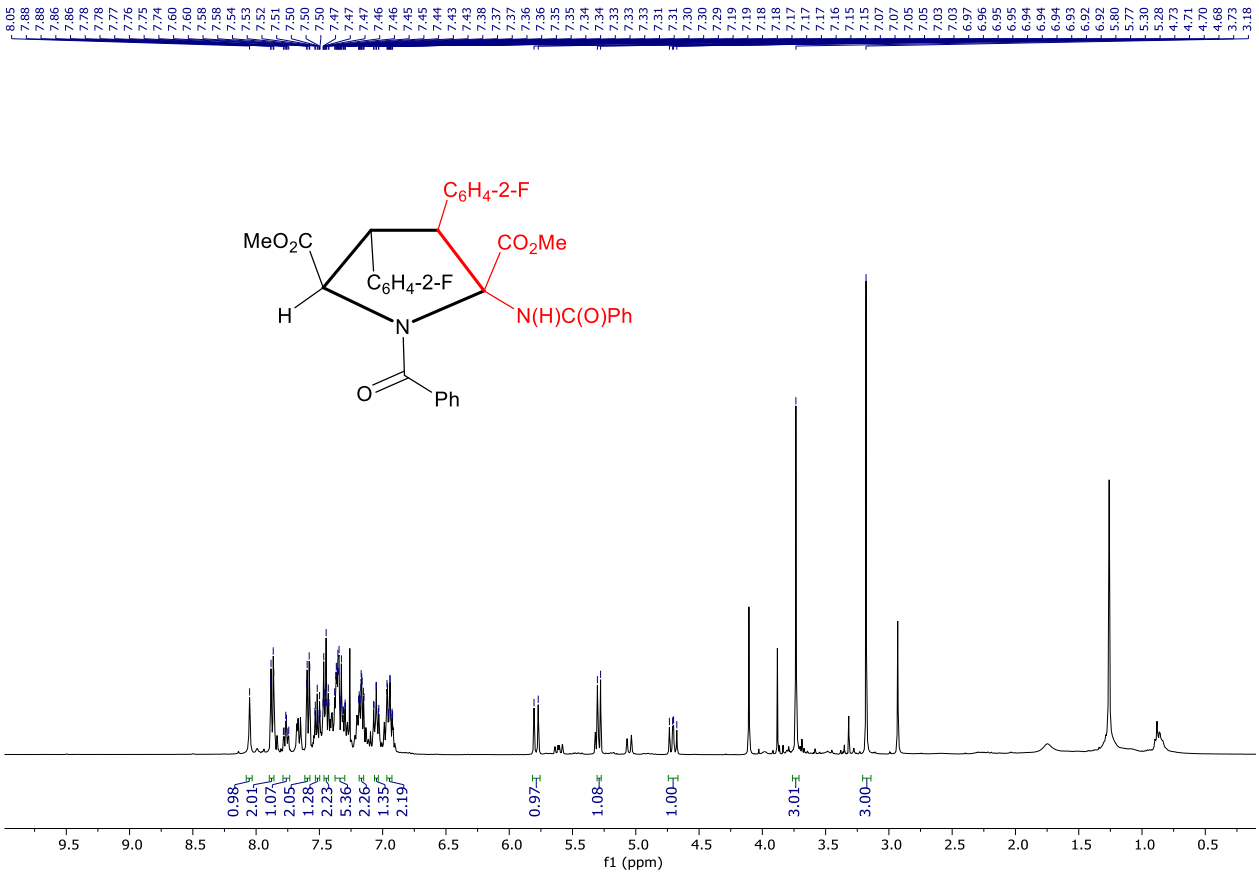
^{1}H-^{13}C HSQC ($CDCl_3$) correlation spectrum of **3m**



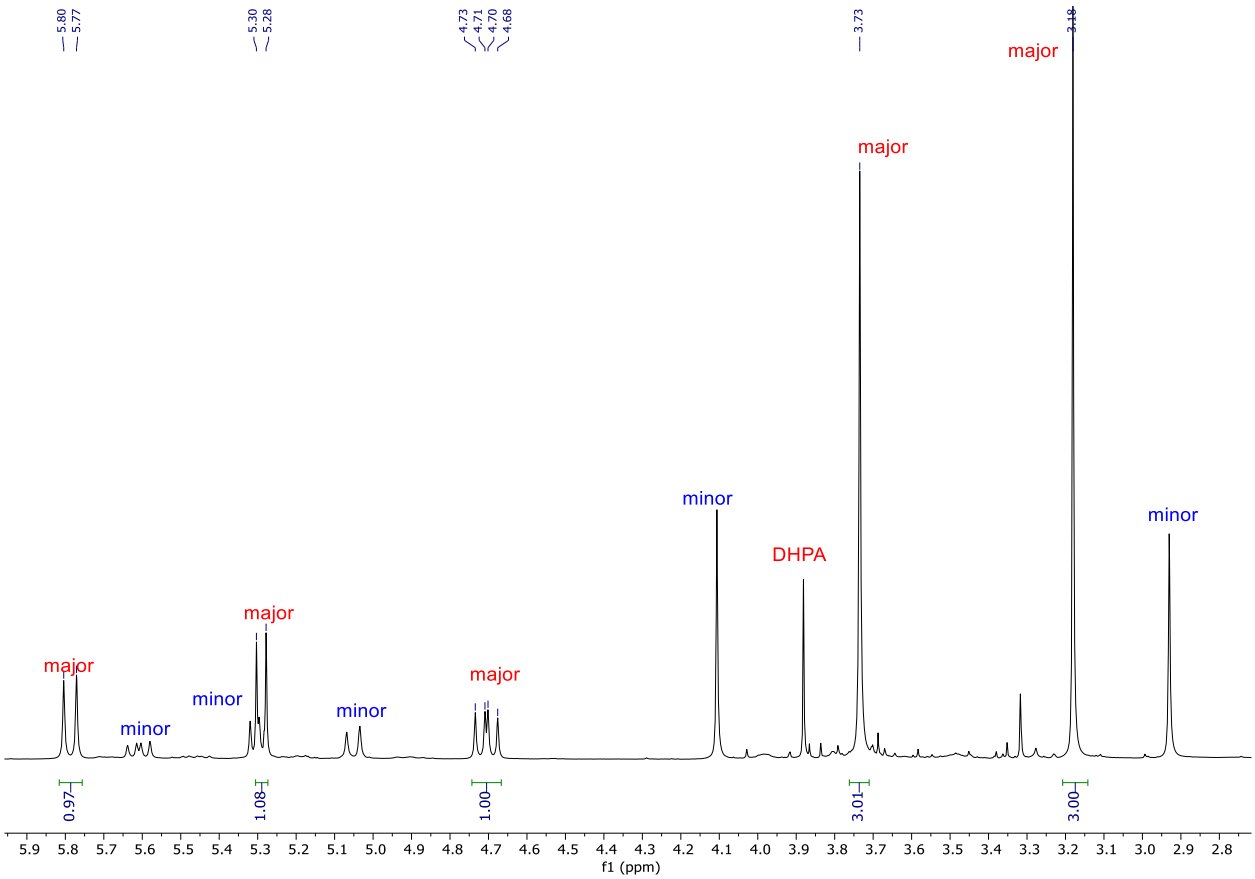
^{1}H-^{13}C HMBC ($CDCl_3$) correlation spectrum of **3m**



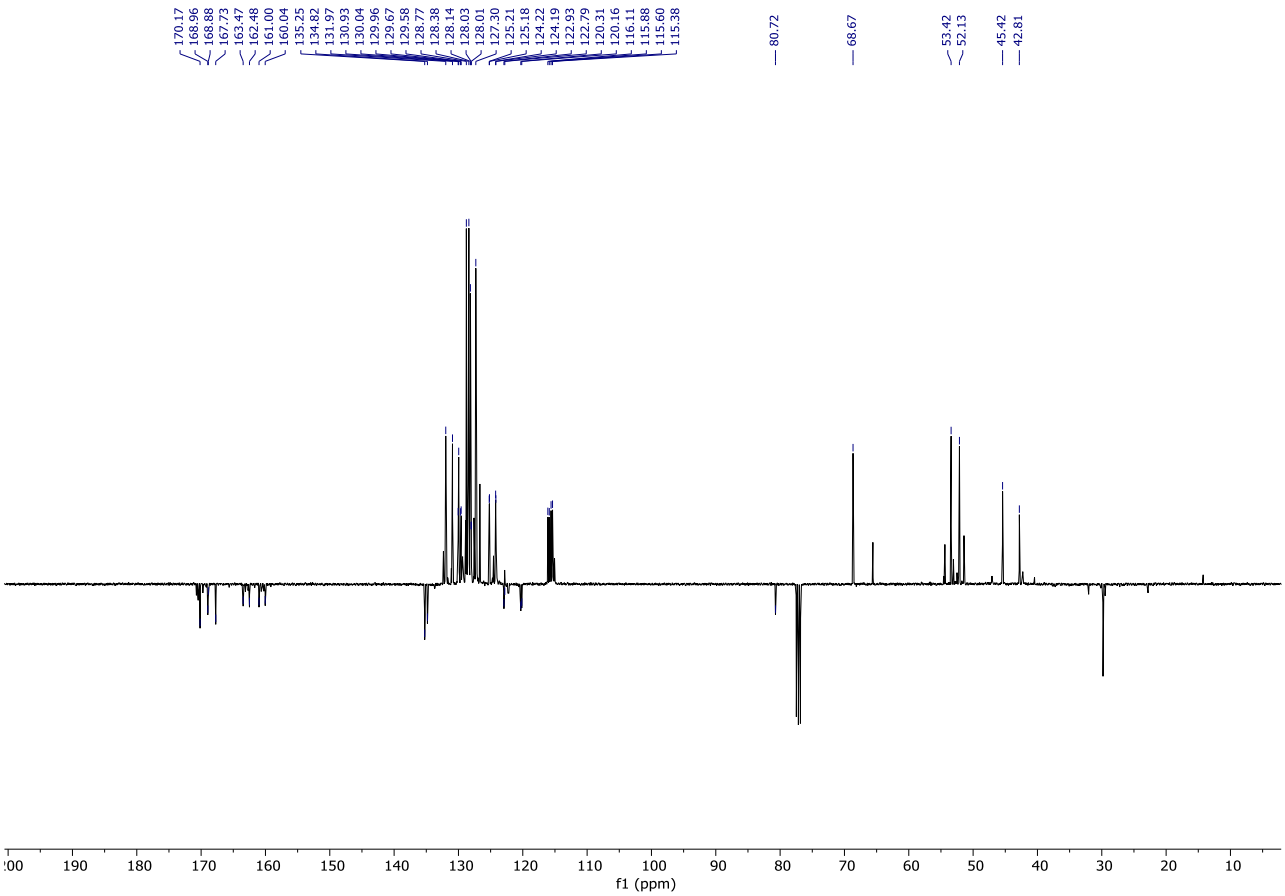
^{19}F NMR spectrum ($CDCl_3$, 282.4 MHz) of **3m**



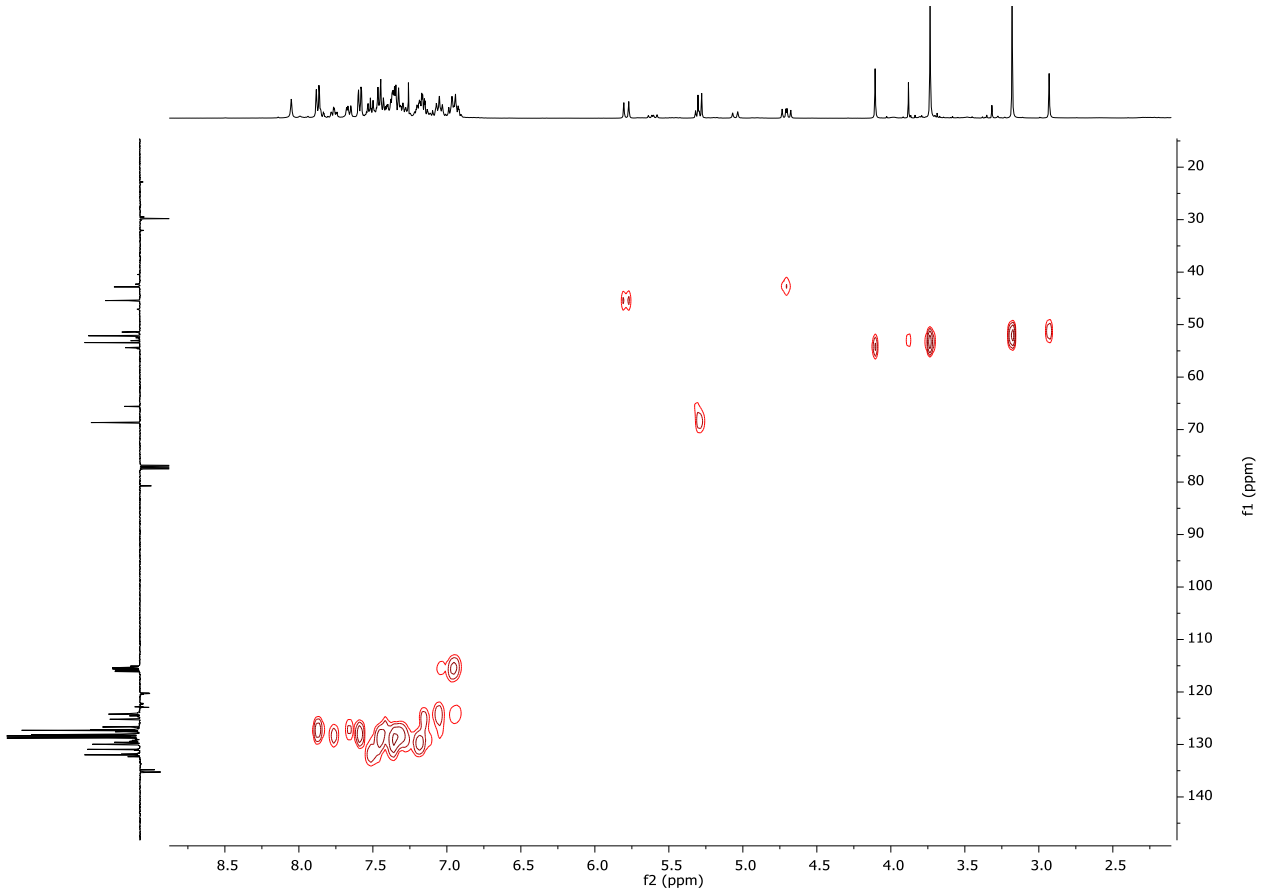
^{1}H NMR spectrum ($CDCl_3$, 400.13 MHz) of **3o** (mixture of isomers)



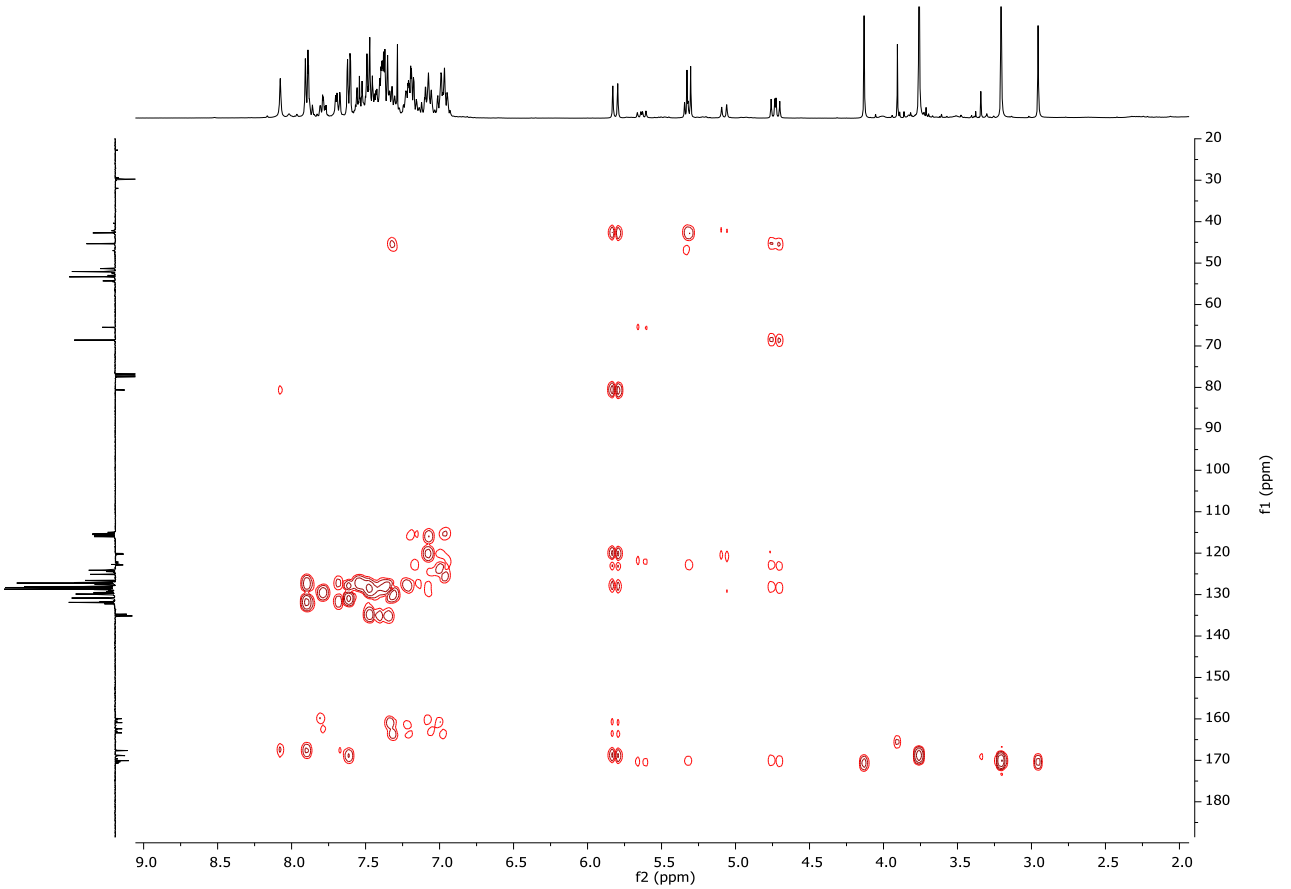
^{1}H NMR spectrum ($CDCl_3$, 400.13 MHz) of **3o** (mixture of isomers, zoom of the aliphatic part)



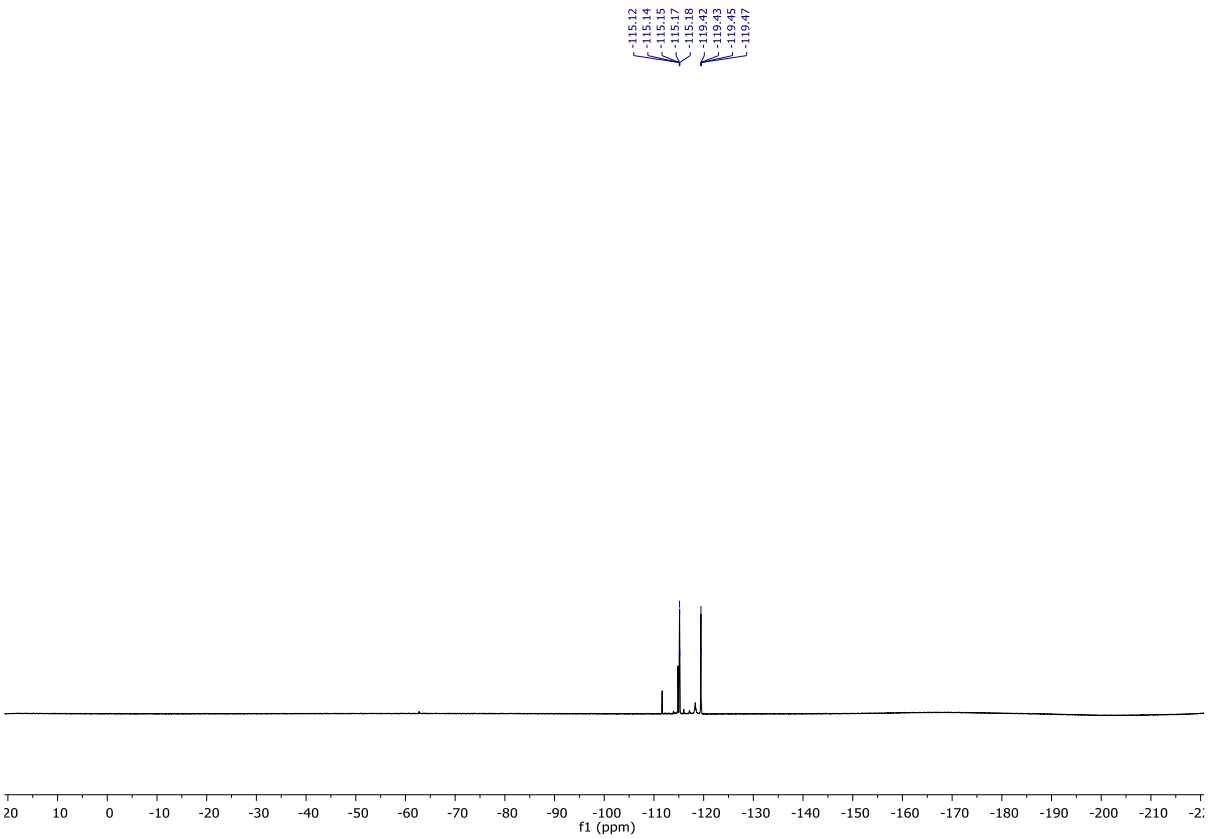
^{13}C{^{1}H} (APT) NMR spectrum ($CDCl_3$, 100.6 MHz) of **3o** (mixture of isomers)



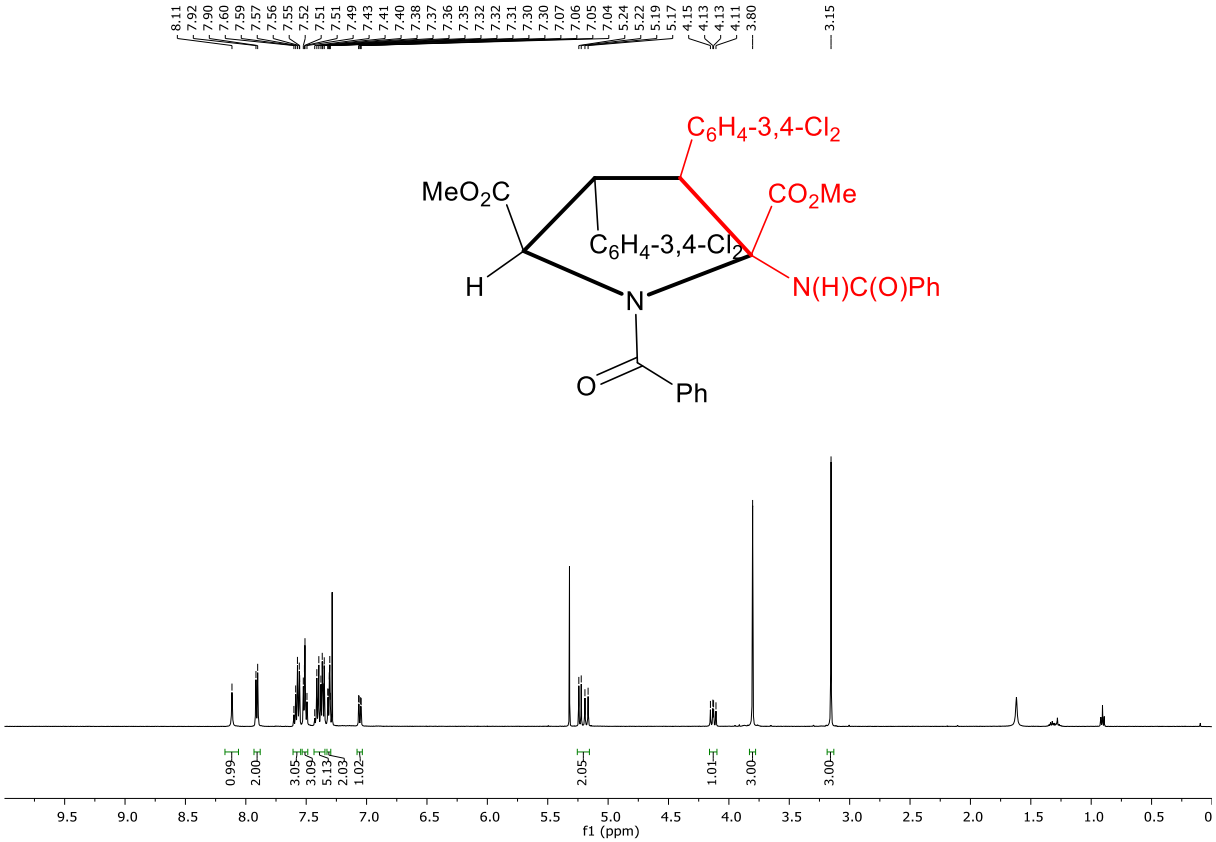
^{1}H-^{13}C HSQC ($CDCl_3$) correlation spectrum of **3o** (mixture of isomers)



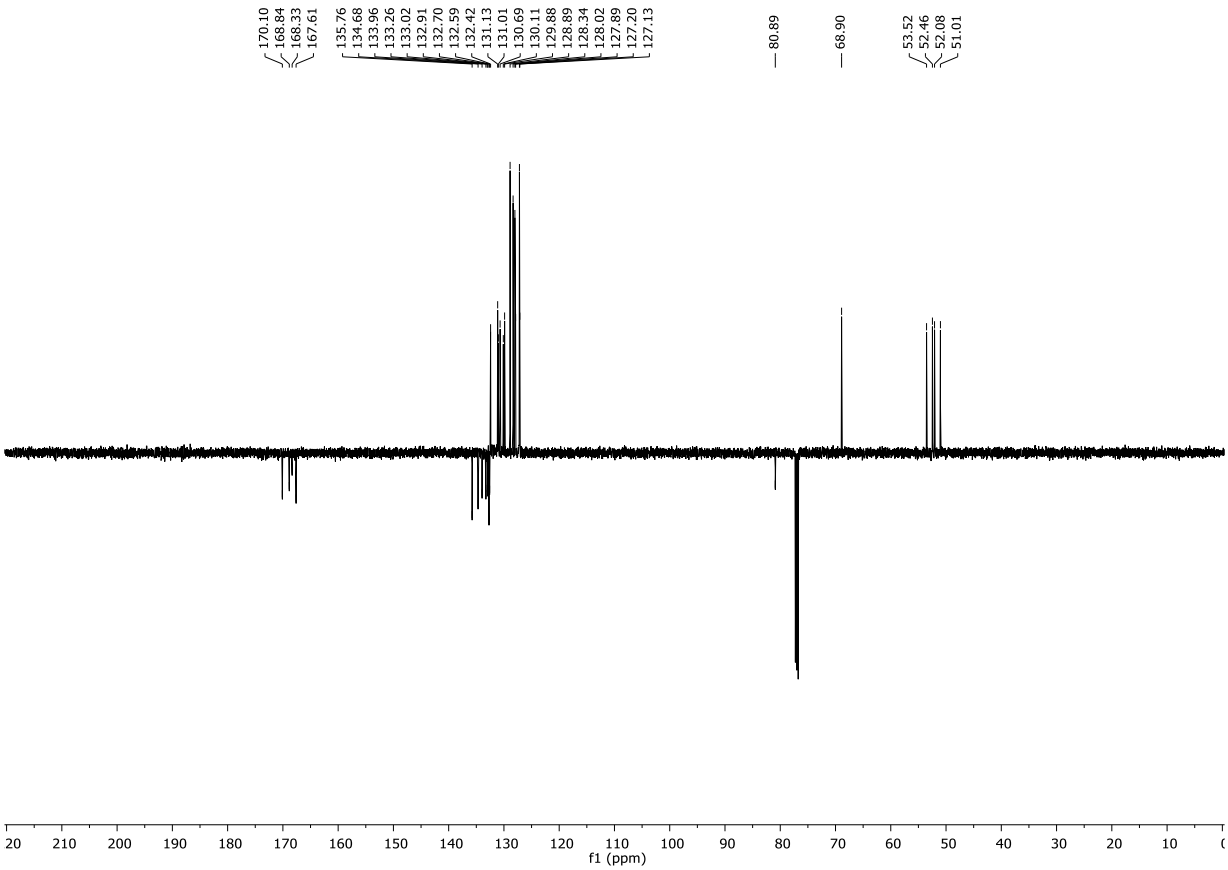
^{1}H-^{13}C HMBC ($CDCl_3$) correlation spectrum of **3o** (mixture of isomers)



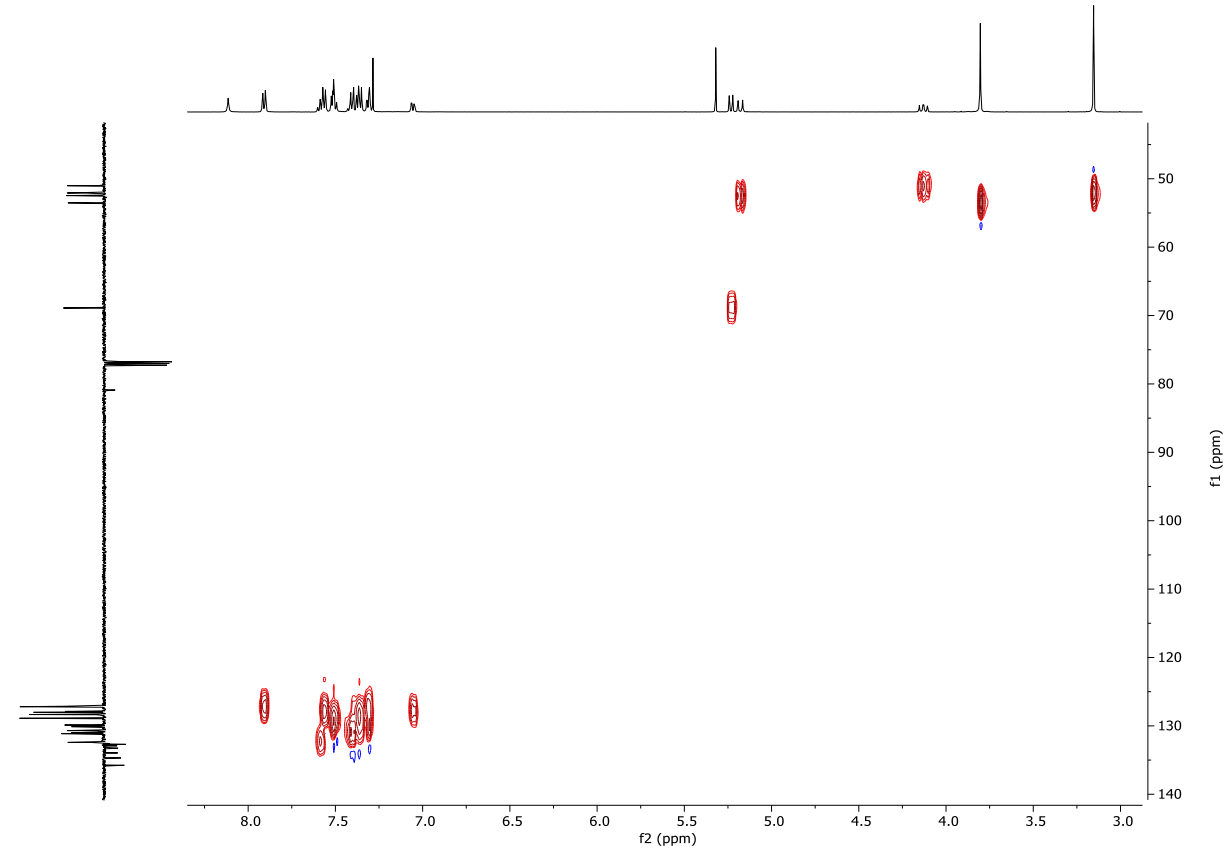
^{19}F NMR spectrum ($CDCl_3$, 376.5 MHz) of **3o** (mixture of isomers)



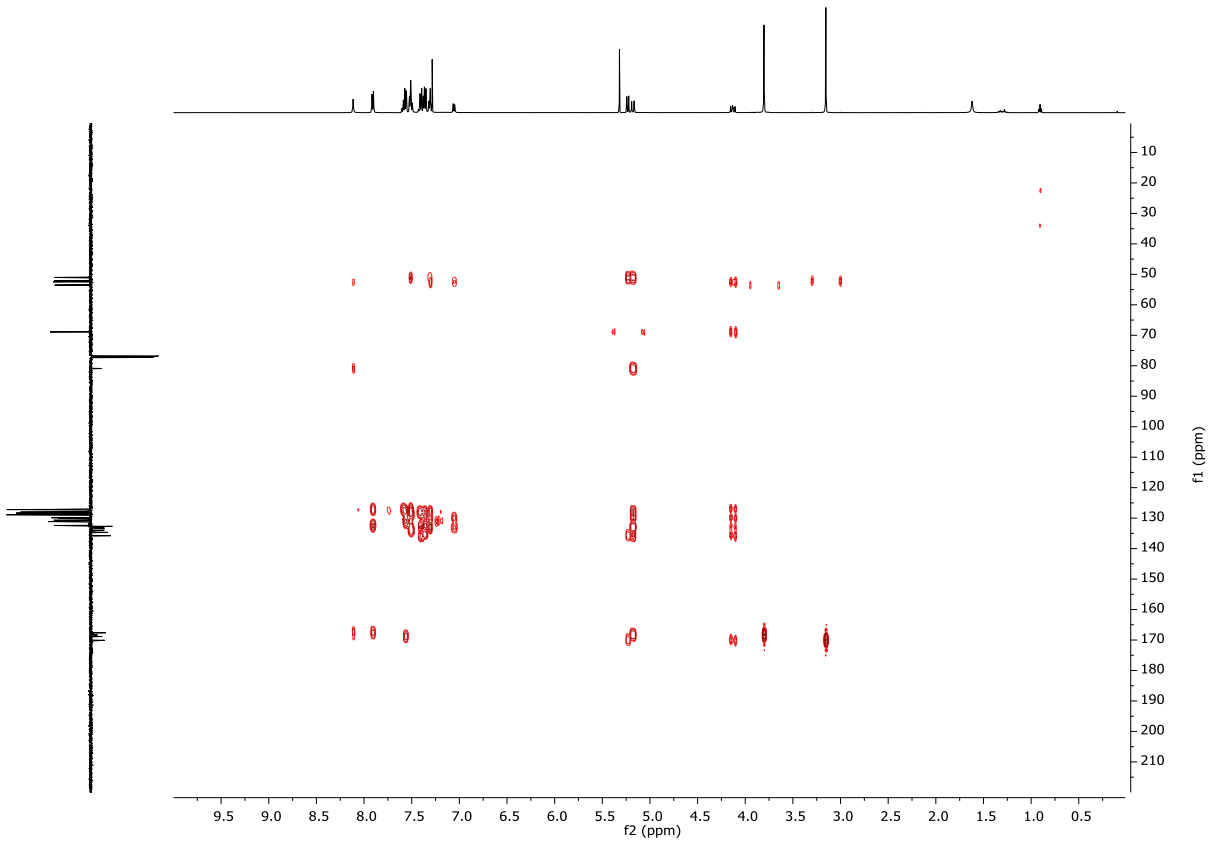
^{1}H NMR spectrum ($CDCl_3$, 500.13 MHz) of **3r**



$^{13}C\{^{1}H\}$ (APT) NMR spectrum ($CDCl_3$, 125.7 MHz) of **3r**



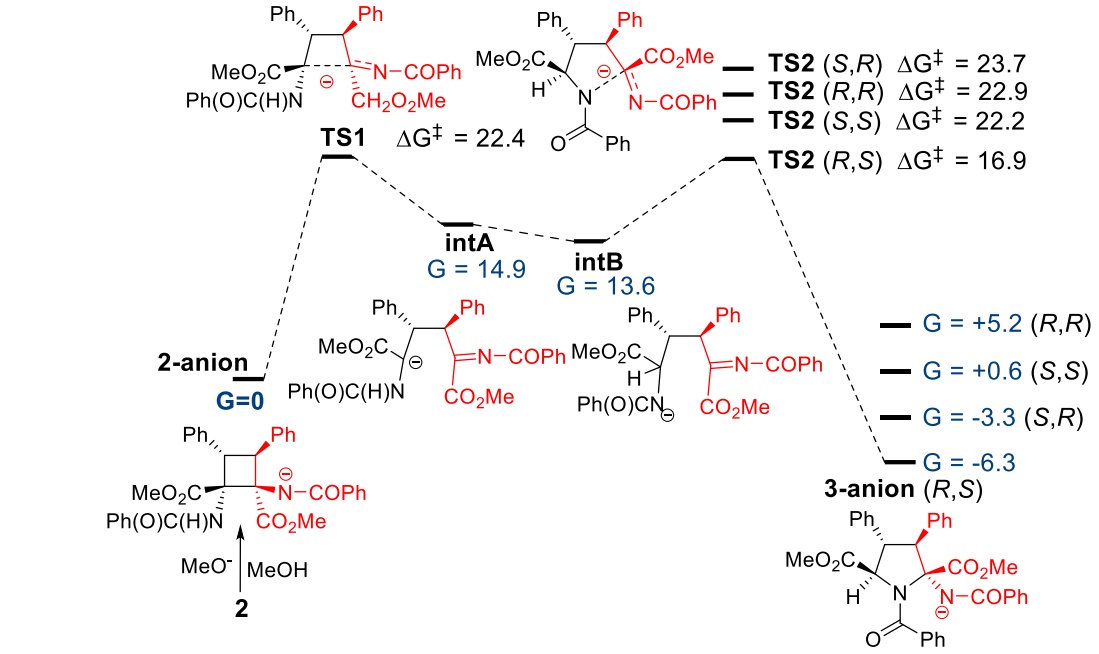
^{1}H-^{13}C HSQC ($CDCl_3$) correlation spectrum of **3r**

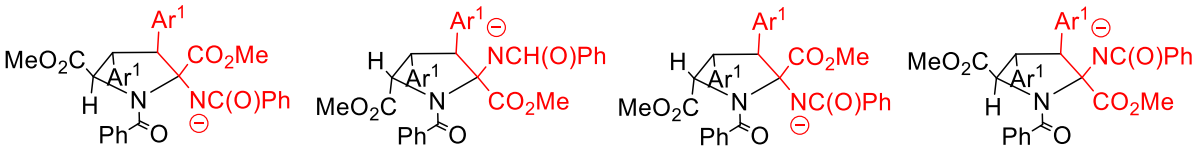


^{1}H-^{13}C HMBC ($CDCl_3$) correlation spectrum of **3r**

7.- Cartesian coordinates and energies of the anionic species calculated by DFT methods

Table S1. Energies of the computed structures in Figure 12 of the manuscript





3a-anion major
ΔG = -6.3 kcal/mol

3a-anion minor
ΔG = -3.3 kcal/mol

3a-anion-III
ΔG = 0.6 kcal/mol

3a-anion-IV
ΔG = 5.2 kcal/mol

Compound	G (M06-2X)	ΔG (kcal/mol)	Imaginary Frequency
2a anion	-1873.390565	0	--
TS1	-1873.354863	22.4	-141.0
int A	-1873.366774	14.9	--
int B	-1873.368873	13.6	--
TS2 *R,S*	-1873.363580	16.9	-42.0
TS2 *S,S*	-1873.355178	22.2	-70.1
TS2 *R,R*	-1873.354083	22.9	-145.8
TS2 *S,R*	-1873.352851	23.7	-59.6
3a anion *R,S*	-1873.400640	-6.3	--
3a anion *S,R*	-1873.395850	-3.3	--
3a anion *S,S*	-1873.389642	0.6	--
3a anion *R,R*	-1873.382201	5.2	--

Cartesian coordinates of the optimized structures are shown below:

2a Anion

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.654666	-0.434501	-0.426514
2	6	0	0.353527	1.085837	-0.726792
3	6	0	-0.338979	1.170072	0.652360
4	6	0	-0.553301	-0.372823	0.591299
5	1	0	0.411320	1.343035	1.424141
6	6	0	-1.520172	2.069186	0.870341
7	6	0	-2.481781	2.286257	-0.120695
8	6	0	-1.700885	2.677951	2.116032
9	6	0	-3.603927	3.070882	0.134896
10	1	0	-2.365887	1.840980	-1.102694
11	6	0	-2.817214	3.465869	2.373874
12	1	0	-0.959958	2.518245	2.892602
13	6	0	-3.777517	3.660310	1.383422
14	1	0	-4.341889	3.221631	-0.644731
15	1	0	-2.939079	3.927223	3.347081
16	1	0	-4.650163	4.271522	1.581661
17	6	0	0.379453	-1.373692	-1.597498
18	8	0	-0.223921	-1.051820	-2.599438
19	8	0	0.744248	-2.626277	-1.347601
20	6	0	0.487721	-3.569629	-2.391882
21	1	0	1.030878	-3.284011	-3.293068
22	1	0	0.844232	-4.526277	-2.020659
23	1	0	-0.579708	-3.617393	-2.607985
24	6	0	-0.319931	-1.122616	1.891808
25	8	0	0.055362	-0.609627	2.913860
26	8	0	-0.542307	-2.428060	1.753647
27	6	0	-0.329037	-3.219783	2.927114
28	1	0	-0.994434	-2.890677	3.725433
29	1	0	-0.555475	-4.242569	2.639969
30	1	0	0.706853	-3.135177	3.255178
31	6	0	1.464535	2.038393	-1.048078
32	6	0	1.503120	2.658598	-2.300025
33	6	0	2.476854	2.331546	-0.128185
34	6	0	2.531661	3.533150	-2.637474
35	1	0	0.720460	2.444045	-3.020978
36	6	0	3.509921	3.201605	-0.464379
37	1	0	2.470395	1.856384	0.845474
38	6	0	3.543243	3.804010	-1.719969
39	1	0	2.543418	4.001443	-3.615044
40	1	0	4.291817	3.410188	0.257299
41	1	0	4.348164	4.482082	-1.978804
42	1	0	-0.391195	1.124683	-1.523726
43	7	0	-1.794915	-0.765486	-0.039001
44	7	0	1.875859	-0.668469	0.274130
45	1	0	-1.835932	-0.744077	-1.050007
46	6	0	2.921247	-0.752478	-0.525926
47	6	0	-2.965286	-0.780078	0.650138
48	8	0	-3.010063	-0.619182	1.861462
49	8	0	2.912109	-0.730689	-1.785837
50	6	0	-4.199486	-1.009889	-0.169203
51	6	0	-5.397930	-0.473489	0.302622
52	6	0	-4.183619	-1.730428	-1.364904
53	6	0	-6.570451	-0.641660	-0.423786
54	1	0	-5.393790	0.079574	1.234379
55	6	0	-5.361424	-1.907978	-2.083958

56	1	0	-3.265740	-2.180954	-1.727585
57	6	0	-6.552975	-1.359784	-1.617610
58	1	0	-7.497334	-0.214503	-0.060389
59	1	0	-5.348329	-2.478069	-3.004891
60	1	0	-7.468068	-1.495337	-2.181755
61	6	0	4.258386	-0.888079	0.175595
62	6	0	5.401680	-1.157907	-0.577260
63	6	0	4.384144	-0.720551	1.557539
64	6	0	6.647015	-1.271583	0.035933
65	1	0	5.297498	-1.276217	-1.648953
66	6	0	5.627467	-0.827657	2.172525
67	1	0	3.495172	-0.503528	2.137276
68	6	0	6.763475	-1.105747	1.413432
69	1	0	7.526449	-1.486473	-0.560605
70	1	0	5.713185	-0.692640	3.244904
71	1	0	7.731904	-1.190093	1.893091

TS1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.111935	-0.305994	1.106107
2	6	0	0.722587	0.825845	0.155659
3	6	0	-0.718905	1.321443	0.348150
4	6	0	-1.624003	0.074555	0.241488
5	1	0	-0.838455	1.713515	1.359344
6	6	0	-1.118419	2.392183	-0.643647
7	6	0	-1.813774	3.518756	-0.200886
8	6	0	-0.866244	2.259803	-2.012050
9	6	0	-2.248983	4.491308	-1.097929
10	1	0	-2.017022	3.633184	0.859551
11	6	0	-1.295055	3.230778	-2.911266
12	1	0	-0.336981	1.390258	-2.387916
13	6	0	-1.989210	4.350225	-2.457406
14	1	0	-2.787177	5.358646	-0.733488
15	1	0	-1.089092	3.112321	-3.968761
16	1	0	-2.323146	5.105777	-3.158721
17	6	0	1.004580	-0.021881	2.593893
18	8	0	0.677149	1.048613	3.045162
19	8	0	1.357915	-1.057696	3.340928
20	6	0	1.226546	-0.871055	4.753802
21	1	0	0.189220	-0.650290	5.006189
22	1	0	1.536757	-1.809191	5.204572
23	1	0	1.865869	-0.054884	5.089581
24	6	0	-3.068489	0.508613	0.465476
25	8	0	-3.548235	0.797465	1.535169
26	8	0	-3.755059	0.565582	-0.679508
27	6	0	-5.122705	0.970973	-0.567490
28	1	0	-5.185976	1.973717	-0.144012
29	1	0	-5.520046	0.958003	-1.578618
30	1	0	-5.667402	0.268974	0.065062
31	6	0	1.791111	1.911446	0.217624
32	6	0	2.966065	1.730918	-0.516454
33	6	0	1.647278	3.075279	0.974506
34	6	0	3.980716	2.682941	-0.491036
35	1	0	3.088180	0.836187	-1.120104
36	6	0	2.657397	4.032861	0.996401
37	1	0	0.748449	3.233040	1.556997
38	6	0	3.828034	3.839773	0.267542
39	1	0	4.883784	2.523519	-1.068785
40	1	0	2.529068	4.932593	1.587014

41	1	0	4.612654	4.586936	0.287710
42	1	0	0.777821	0.385447	-0.841929
43	7	0	-1.149113	-0.865057	1.230385
44	7	0	1.834883	-1.305083	0.757429
45	6	0	1.926476	-1.765264	-0.539721
46	6	0	-1.587079	-2.113870	1.186058
47	8	0	-1.188891	-3.028593	1.941013
48	8	0	0.950022	-2.015799	-1.229227
49	6	0	-2.676740	-2.482599	0.193251
50	6	0	-4.011570	-2.486005	0.600396
51	6	0	-2.358804	-2.829222	-1.120853
52	6	0	-5.020486	-2.826237	-0.297314
53	1	0	-4.260777	-2.212964	1.620960
54	6	0	-3.367851	-3.175758	-2.015838
55	1	0	-1.320134	-2.810468	-1.434955
56	6	0	-4.700469	-3.171234	-1.608012
57	1	0	-6.055367	-2.821448	0.026194
58	1	0	-3.115182	-3.445294	-3.035209
59	1	0	-5.484526	-3.435738	-2.307964
60	6	0	3.318134	-2.032042	-1.027263
61	6	0	3.493033	-2.515491	-2.325290
62	6	0	4.432574	-1.768225	-0.228102
63	6	0	4.772265	-2.738041	-2.819688
64	1	0	2.619229	-2.710181	-2.935148
65	6	0	5.712407	-1.989623	-0.725131
66	1	0	4.289182	-1.393656	0.778192
67	6	0	5.882780	-2.475045	-2.019580
68	1	0	4.905790	-3.114024	-3.826912
69	1	0	6.575938	-1.786228	-0.103385
70	1	0	6.880574	-2.648607	-2.405261
71	1	0	-1.555640	-0.305433	-0.785574

Int A

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.796142	0.084938	-0.795724
2	6	0	0.731932	-1.201244	0.114936
3	6	0	-0.745640	-1.608122	0.100921
4	6	0	-1.445258	-0.231355	0.135226
5	1	0	-0.993062	-2.064722	-0.861171
6	6	0	-1.152073	-2.530431	1.221329
7	6	0	-1.735119	-3.766121	0.941292
8	6	0	-0.952332	-2.165629	2.556915
9	6	0	-2.111624	-4.625635	1.971581
10	1	0	-1.894836	-4.057783	-0.091841
11	6	0	-1.328199	-3.020820	3.586393
12	1	0	-0.502629	-1.205226	2.791771
13	6	0	-1.908707	-4.254692	3.296365
14	1	0	-2.562250	-5.582951	1.737144
15	1	0	-1.168760	-2.725465	4.616874
16	1	0	-2.200594	-4.920711	4.099722
17	6	0	1.069285	-0.384585	-2.236722
18	8	0	0.229546	-0.901875	-2.934475
19	8	0	2.341773	-0.272843	-2.599678
20	6	0	2.675098	-0.867811	-3.858415
21	1	0	2.108444	-0.399347	-4.662725
22	1	0	3.739646	-0.696950	-3.992229
23	1	0	2.458866	-1.936798	-3.831863
24	6	0	-2.880608	-0.382498	-0.336987
25	8	0	-3.226031	-0.585572	-1.472909

26	8	0	-3.721915	-0.322439	0.693304
27	6	0	-5.112492	-0.457170	0.370447
28	1	0	-5.300482	-1.424931	-0.093557
29	1	0	-5.643438	-0.375215	1.314157
30	1	0	-5.409822	0.342904	-0.308309
31	6	0	1.732793	-2.275012	-0.231089
32	6	0	2.983907	-2.251218	0.392384
33	6	0	1.477559	-3.275086	-1.173730
34	6	0	3.962003	-3.187441	0.073062
35	1	0	3.188877	-1.482219	1.130303
36	6	0	2.453176	-4.216672	-1.492253
37	1	0	0.518180	-3.320208	-1.675919
38	6	0	3.699334	-4.174103	-0.873864
39	1	0	4.926659	-3.148856	0.565694
40	1	0	2.237158	-4.984952	-2.225773
41	1	0	4.457479	-4.907102	-1.123373
42	1	0	0.962557	-0.828977	1.113530
43	7	0	-0.608119	0.564314	-0.747566
44	7	0	1.775511	1.028090	-0.358416
45	6	0	1.568885	1.588097	0.817244
46	6	0	-0.965082	1.685541	-1.416007
47	8	0	-0.270451	2.168378	-2.304822
48	8	0	0.604151	1.415789	1.613189
49	6	0	-2.239663	2.355868	-0.991450
50	6	0	-3.177836	2.736680	-1.950388
51	6	0	-2.445987	2.660297	0.353738
52	6	0	-4.338020	3.393516	-1.559259
53	1	0	-2.998799	2.502600	-2.993526
54	6	0	-3.599997	3.338315	0.739305
55	1	0	-1.691214	2.377715	1.082205
56	6	0	-4.549420	3.694561	-0.213698
57	1	0	-5.076877	3.674057	-2.300489
58	1	0	-3.757377	3.585578	1.782468
59	1	0	-5.452551	4.211754	0.088545
60	6	0	2.653251	2.567144	1.244616
61	6	0	2.536359	3.219051	2.472800
62	6	0	3.767983	2.834179	0.445169
63	6	0	3.510370	4.119651	2.897755
64	1	0	1.669652	3.007578	3.086949
65	6	0	4.743605	3.732075	0.866310
66	1	0	3.852108	2.327738	-0.507964
67	6	0	4.618115	4.378706	2.095214
68	1	0	3.405176	4.619018	3.854401
69	1	0	5.603415	3.930382	0.236191
70	1	0	5.377782	5.079112	2.422957
71	1	0	-1.432058	0.167798	1.150345

Int B

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.237332	0.289552	0.351005
2	6	0	-1.089634	-0.525207	0.544453
3	6	0	-1.847991	-0.258236	-0.756515
4	6	0	-1.632827	1.257257	-0.939371
5	1	0	-1.314708	-0.738390	-1.580781
6	6	0	-3.293703	-0.694933	-0.796045
7	6	0	-4.120506	-0.634902	0.329253
8	6	0	-3.841558	-1.127860	-2.005043
9	6	0	-5.464858	-0.985736	0.240691
10	1	0	-3.721679	-0.309414	1.283788

11	6	0	-5.184737	-1.480487	-2.096632
12	1	0	-3.207647	-1.184520	-2.884273
13	6	0	-6.002349	-1.406885	-0.972482
14	1	0	-6.091884	-0.932634	1.123191
15	1	0	-5.591071	-1.813847	-3.044426
16	1	0	-7.048427	-1.681409	-1.039482
17	6	0	0.704287	0.781699	1.751211
18	8	0	0.036073	0.718026	2.754930
19	8	0	1.896437	1.360407	1.709542
20	6	0	2.397477	1.869379	2.945072
21	1	0	2.528016	1.054964	3.658895
22	1	0	3.353841	2.327700	2.706149
23	1	0	1.712981	2.611384	3.357592
24	6	0	-2.669931	2.069429	-0.177552
25	8	0	-2.609309	2.351480	0.992149
26	8	0	-3.699251	2.379835	-0.964334
27	6	0	-4.814466	3.004838	-0.317014
28	1	0	-4.508287	3.946536	0.137176
29	1	0	-5.550151	3.177627	-1.097038
30	1	0	-5.216608	2.338838	0.447419
31	6	0	-0.935445	-1.983344	0.885950
32	6	0	-1.213856	-2.417868	2.182619
33	6	0	-0.542177	-2.928040	-0.065736
34	6	0	-1.073583	-3.756740	2.535063
35	1	0	-1.523070	-1.689689	2.925335
36	6	0	-0.395477	-4.267297	0.283653
37	1	0	-0.323099	-2.614330	-1.079320
38	6	0	-0.656184	-4.686334	1.586203
39	1	0	-1.288042	-4.073611	3.549382
40	1	0	-0.078398	-4.986010	-0.463674
41	1	0	-0.542263	-5.729704	1.856881
42	1	0	-1.620947	-0.035490	1.361447
43	7	0	-0.287370	1.469490	-0.424311
44	7	0	1.224486	-0.395264	-0.416508
45	6	0	2.010096	-1.212336	0.256218
46	6	0	0.249823	2.690355	-0.704121
47	8	0	-0.471569	3.575516	-1.165605
48	8	0	2.004313	-1.440420	1.493848
49	6	0	1.708108	2.975553	-0.513981
50	6	0	2.061568	4.130289	0.183753
51	6	0	2.691527	2.184250	-1.102641
52	6	0	3.401146	4.468342	0.335662
53	1	0	1.284643	4.749534	0.617882
54	6	0	4.030578	2.540749	-0.971176
55	1	0	2.405835	1.281608	-1.626317
56	6	0	4.388274	3.672313	-0.242648
57	1	0	3.675385	5.352948	0.898395
58	1	0	4.796665	1.928390	-1.433074
59	1	0	5.433096	3.938333	-0.131186
60	6	0	3.037317	-1.939603	-0.593876
61	6	0	3.919562	-2.830640	0.018661
62	6	0	3.128117	-1.745739	-1.975101
63	6	0	4.875932	-3.513648	-0.728767
64	1	0	3.842245	-2.976502	1.089148
65	6	0	4.082576	-2.425722	-2.725310
66	1	0	2.438525	-1.058574	-2.449370
67	6	0	4.960656	-3.312594	-2.103958
68	1	0	5.554813	-4.202716	-0.239043
69	1	0	4.142472	-2.265906	-3.796054
70	1	0	5.703964	-3.842909	-2.688183
71	1	0	-1.690139	1.550335	-1.987945

TS2 *R,S*

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.111935	-0.305994	1.106107
2	6	0	0.722587	0.825845	0.155659
3	6	0	-0.718905	1.321443	0.348150
4	6	0	-1.624003	0.074555	0.241488
5	1	0	-0.838455	1.713515	1.359344
6	6	0	-1.118419	2.392183	-0.643647
7	6	0	-1.813774	3.518756	-0.200886
8	6	0	-0.866244	2.259803	-2.012050
9	6	0	-2.248983	4.491308	-1.097929
10	1	0	-2.017022	3.633184	0.859551
11	6	0	-1.295055	3.230778	-2.911266
12	1	0	-0.336981	1.390258	-2.387916
13	6	0	-1.989210	4.350225	-2.457406
14	1	0	-2.787177	5.358646	-0.733488
15	1	0	-1.089092	3.112321	-3.968761
16	1	0	-2.323146	5.105777	-3.158721
17	6	0	1.004580	-0.021881	2.593893
18	8	0	0.677149	1.048613	3.045162
19	8	0	1.357915	-1.057696	3.340928
20	6	0	1.226546	-0.871055	4.753802
21	1	0	0.189220	-0.650290	5.006189
22	1	0	1.536757	-1.809191	5.204572
23	1	0	1.865869	-0.054884	5.089581
24	6	0	-3.068489	0.508613	0.465476
25	8	0	-3.548235	0.797465	1.535169
26	8	0	-3.755059	0.565582	-0.679508
27	6	0	-5.122705	0.970973	-0.567490
28	1	0	-5.185976	1.973717	-0.144012
29	1	0	-5.520046	0.958003	-1.578618
30	1	0	-5.667402	0.268974	0.065062
31	6	0	1.791111	1.911446	0.217624
32	6	0	2.966065	1.730918	-0.516454
33	6	0	1.647278	3.075279	0.974506
34	6	0	3.980716	2.682941	-0.491036
35	1	0	3.088180	0.836187	-1.120104
36	6	0	2.657397	4.032861	0.996401
37	1	0	0.748449	3.233040	1.556997
38	6	0	3.828034	3.839773	0.267542
39	1	0	4.883784	2.523519	-1.068785
40	1	0	2.529068	4.932593	1.587014
41	1	0	4.612654	4.586936	0.287710
42	1	0	0.777821	0.385447	-0.841929
43	7	0	-1.149113	-0.865057	1.230385
44	7	0	1.834883	-1.305083	0.757429
45	6	0	1.926476	-1.765264	-0.539721
46	6	0	-1.587079	-2.113870	1.186058
47	8	0	-1.188891	-3.028593	1.941013
48	8	0	0.950022	-2.015799	-1.229227
49	6	0	-2.676740	-2.482599	0.193251
50	6	0	-4.011570	-2.486005	0.600396
51	6	0	-2.358804	-2.829222	-1.120853
52	6	0	-5.020486	-2.826237	-0.297314
53	1	0	-4.260777	-2.212964	1.620960
54	6	0	-3.367851	-3.175758	-2.015838
55	1	0	-1.320134	-2.810468	-1.434955
56	6	0	-4.700469	-3.171234	-1.608012
57	1	0	-6.055367	-2.821448	0.026194
58	1	0	-3.115182	-3.445294	-3.035209
59	1	0	-5.484526	-3.435738	-2.307964

60	6	0	3.318134	-2.032042	-1.027263
61	6	0	3.493033	-2.515491	-2.325290
62	6	0	4.432574	-1.768225	-0.228102
63	6	0	4.772265	-2.738041	-2.819688
64	1	0	2.619229	-2.710181	-2.935148
65	6	0	5.712407	-1.989623	-0.725131
66	1	0	4.289182	-1.393656	0.778192
67	6	0	5.882780	-2.475045	-2.019580
68	1	0	4.905790	-3.114024	-3.826912
69	1	0	6.575938	-1.786228	-0.103385
70	1	0	6.880574	-2.648607	-2.405261
71	1	0	-1.555640	-0.305433	-0.785574

TS2 *S,S*

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.527964	-1.111680	-0.131364
2	6	0	-0.551349	0.419081	-0.263795
3	6	0	0.797408	1.016543	-0.677079
4	6	0	1.892977	0.408683	0.260327
5	1	0	1.044833	0.661074	-1.676365
6	6	0	0.832553	2.530518	-0.702757
7	6	0	1.696588	3.166137	-1.598475
8	6	0	0.085307	3.323312	0.173303
9	6	0	1.822301	4.551772	-1.616277
10	1	0	2.279201	2.563426	-2.288452
11	6	0	0.206214	4.710537	0.157260
12	1	0	-0.597734	2.863274	0.878507
13	6	0	1.076997	5.329907	-0.734727
14	1	0	2.499413	5.022809	-2.319387
15	1	0	-0.383511	5.307692	0.843308
16	1	0	1.170274	6.409433	-0.745896
17	6	0	-0.043438	-1.946852	-1.324381
18	8	0	0.712869	-1.549305	-2.178663
19	8	0	-0.601318	-3.149679	-1.361563
20	6	0	-0.099392	-4.021614	-2.377801
21	1	0	0.973240	-4.161905	-2.240947
22	1	0	-0.627876	-4.961725	-2.246856
23	1	0	-0.295045	-3.607939	-3.366884
24	6	0	-1.702557	0.835855	-1.160155
25	6	0	-2.866180	1.352302	-0.586400
26	6	0	-1.646829	0.694079	-2.550052
27	6	0	-3.955551	1.711070	-1.375112
28	1	0	-2.920303	1.473602	0.491383
29	6	0	-2.735246	1.051275	-3.341017
30	1	0	-0.750974	0.300502	-3.016913
31	6	0	-3.893943	1.557841	-2.756867
32	1	0	-4.849665	2.109737	-0.909498
33	1	0	-2.677425	0.934618	-4.417096
34	1	0	-4.739403	1.835594	-3.375226
35	1	0	-0.772881	0.756921	0.750732
36	7	0	1.472296	-0.933520	0.578300
37	7	0	-1.412712	-1.707858	0.603371
38	6	0	-2.133609	-1.162488	1.625278
39	6	0	2.286599	-1.972919	0.426224
40	8	0	1.880731	-3.151620	0.388215
41	8	0	-1.663876	-0.685855	2.651291
42	6	0	3.781039	-1.764034	0.281463
43	6	0	4.439348	-2.345597	-0.802855
44	6	0	4.518430	-1.051612	1.226687

45	6	0	5.815075	-2.199954	-0.951345
46	1	0	3.864008	-2.910037	-1.528479
47	6	0	5.898649	-0.924933	1.092432
48	1	0	4.014901	-0.602521	2.075936
49	6	0	6.548130	-1.492295	-0.000732
50	1	0	6.316731	-2.642711	-1.804075
51	1	0	6.465489	-0.381006	1.839104
52	1	0	7.621023	-1.386122	-0.110488
53	6	0	-3.628934	-1.265318	1.452610
54	6	0	-4.457822	-0.713817	2.430237
55	6	0	-4.194256	-1.840320	0.312801
56	6	0	-5.839086	-0.733866	2.270732
57	1	0	-4.006304	-0.264460	3.306528
58	6	0	-5.575765	-1.862266	0.154035
59	1	0	-3.542717	-2.261199	-0.443914
60	6	0	-6.399575	-1.307621	1.131233
61	1	0	-6.478560	-0.301054	3.031010
62	1	0	-6.010870	-2.308963	-0.732229
63	1	0	-7.475975	-1.322180	1.005188
64	6	0	2.082856	1.295356	1.485567
65	8	0	3.049633	1.998487	1.667682
66	8	0	1.050968	1.247434	2.325583
67	6	0	1.111174	2.130116	3.450426
68	1	0	1.158866	3.165060	3.108014
69	1	0	0.197600	1.955143	4.011833
70	1	0	1.984873	1.906225	4.061965
71	1	0	2.848752	0.457470	-0.269397

TS2 *R,R*

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.415207	-1.445818	-0.938484
2	6	0	-0.812465	-1.032571	0.494408
3	6	0	-0.533281	0.468871	0.668306
4	6	0	0.952353	0.619210	0.272259
5	1	0	-1.138789	1.044051	-0.034770
6	6	0	-0.842505	0.958897	2.066773
7	6	0	-1.738840	2.009558	2.264778
8	6	0	-0.254065	0.365018	3.186089
9	6	0	-2.046658	2.456433	3.546238
10	1	0	-2.191878	2.487240	1.401401
11	6	0	-0.557536	0.808190	4.470304
12	1	0	0.449375	-0.452957	3.061887
13	6	0	-1.456984	1.854902	4.654887
14	1	0	-2.745516	3.274250	3.678886
15	1	0	-0.091612	0.334802	5.326775
16	1	0	-1.694757	2.199700	5.654301
17	6	0	0.348259	-2.777859	-0.991939
18	8	0	0.865815	-3.284506	-0.024460
19	8	0	0.343990	-3.331648	-2.192631
20	6	0	1.151975	-4.504705	-2.326982
21	1	0	0.791775	-5.291756	-1.664839
22	1	0	1.058904	-4.809272	-3.365657
23	1	0	2.186282	-4.258509	-2.087777
24	6	0	-2.218847	-1.480338	0.832134
25	6	0	-2.413278	-2.780348	1.306668
26	6	0	-3.331518	-0.653559	0.674260
27	6	0	-3.688593	-3.248482	1.607748
28	1	0	-1.551906	-3.427432	1.441356
29	6	0	-4.608445	-1.116315	0.978391

30	1	0	-3.211745	0.359790	0.307460
31	6	0	-4.792013	-2.415312	1.444067
32	1	0	-3.819486	-4.259832	1.974830
33	1	0	-5.461585	-0.460089	0.850333
34	1	0	-5.786709	-2.773804	1.681596
35	1	0	-0.128106	-1.569800	1.155257
36	7	0	1.223232	-0.351421	-0.757987
37	7	0	-1.187418	-1.238512	-1.969939
38	6	0	-2.097257	-0.288593	-2.279567
39	6	0	2.443003	-0.859270	-0.943563
40	8	0	2.723205	-1.608706	-1.894683
41	8	0	-3.276338	-0.552626	-2.514983
42	6	0	3.528532	-0.614302	0.083179
43	6	0	4.638914	0.179299	-0.195446
44	6	0	3.445185	-1.281511	1.306527
45	6	0	5.655358	0.311698	0.746607
46	1	0	4.697664	0.700157	-1.143884
47	6	0	4.465610	-1.154942	2.245274
48	1	0	2.580459	-1.907153	1.509525
49	6	0	5.571210	-0.354825	1.967347
50	1	0	6.514576	0.935454	0.528441
51	1	0	4.398118	-1.680100	3.191055
52	1	0	6.364671	-0.251630	2.698234
53	6	0	-1.625436	1.127281	-2.506490
54	6	0	-2.545279	2.167342	-2.350848
55	6	0	-0.315856	1.412311	-2.891745
56	6	0	-2.157463	3.483815	-2.569272
57	1	0	-3.561255	1.929006	-2.058046
58	6	0	0.063445	2.730028	-3.136380
59	1	0	0.397690	0.603471	-2.992870
60	6	0	-0.853215	3.764805	-2.973567
61	1	0	-2.870617	4.288780	-2.435293
62	1	0	1.079962	2.948238	-3.442178
63	1	0	-0.552606	4.790063	-3.158041
64	1	0	1.559775	0.456932	1.175092
65	6	0	1.345908	2.023357	-0.185601
66	8	0	2.317634	2.263074	-0.856824
67	8	0	0.537062	2.967665	0.298475
68	6	0	0.922798	4.322374	0.036981
69	1	0	0.123092	4.939353	0.437950
70	1	0	1.864874	4.543098	0.539618
71	1	0	1.030852	4.483628	-1.034348

TS2 *S,R*

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.712882	-1.648271	-0.518734
2	6	0	1.406674	-0.290909	-0.683307
3	6	0	0.670985	0.742337	0.183770
4	6	0	-0.828276	0.756554	-0.294910
5	1	0	0.645158	0.387882	1.214941
6	6	0	1.298686	2.118758	0.210299
7	6	0	1.168914	2.898464	1.360830
8	6	0	1.961282	2.659466	-0.894291
9	6	0	1.676039	4.193492	1.408155
10	1	0	0.662100	2.482708	2.227441
11	6	0	2.470977	3.954074	-0.850684
12	1	0	2.085270	2.068372	-1.795664
13	6	0	2.327374	4.726448	0.299136
14	1	0	1.565368	4.784065	2.310175
15	1	0	2.984323	4.358632	-1.715425
16	1	0	2.725752	5.733623	0.332300

17	6	0	0.496778	-2.424738	-1.818217
18	8	0	0.655271	-1.949978	-2.917060
19	8	0	0.194040	-3.697587	-1.609895
20	6	0	-0.149730	-4.443206	-2.779116
21	1	0	0.684410	-4.462136	-3.480271
22	1	0	-0.379132	-5.447278	-2.433344
23	1	0	-1.022470	-3.993591	-3.253319
24	6	0	2.896026	-0.420747	-0.420097
25	6	0	3.713807	-0.893779	-1.449933
26	6	0	3.481251	-0.105003	0.806669
27	6	0	5.082646	-1.056398	-1.258963
28	1	0	3.267362	-1.131915	-2.410636
29	6	0	4.850324	-0.263495	1.000616
30	1	0	2.872353	0.269214	1.622726
31	6	0	5.655607	-0.740773	-0.030005
32	1	0	5.700745	-1.423273	-2.070192
33	1	0	5.288916	-0.011784	1.959311
34	1	0	6.721803	-0.860739	0.122243
35	1	0	1.268589	-0.020275	-1.731508
36	7	0	-1.085516	-0.551427	-0.833544
37	7	0	0.736943	-2.360440	0.553775
38	6	0	1.059532	-2.098209	1.850546
39	6	0	-2.279502	-1.111288	-0.920393
40	8	0	-2.444081	-2.301493	-1.266622
41	8	0	2.096421	-2.501018	2.363143
42	6	0	-3.530590	-0.323670	-0.584682
43	6	0	-4.379328	-0.802994	0.414904
44	6	0	-3.896789	0.818095	-1.296039
45	6	0	-5.551757	-0.125538	0.731801
46	1	0	-4.118712	-1.717954	0.936505
47	6	0	-5.081129	1.487091	-0.995321
48	1	0	-3.273651	1.171350	-2.110436
49	6	0	-5.903634	1.024709	0.027681
50	1	0	-6.195719	-0.498379	1.520080
51	1	0	-5.361000	2.367405	-1.562222
52	1	0	-6.820279	1.550339	0.267968
53	6	0	0.030481	-1.405945	2.706127
54	6	0	0.473298	-0.750595	3.857126
55	6	0	-1.321217	-1.369788	2.360776
56	6	0	-0.423945	-0.042980	4.647899
57	1	0	1.525838	-0.792401	4.111303
58	6	0	-2.220649	-0.675668	3.165772
59	1	0	-1.655522	-1.888225	1.468491
60	6	0	-1.772894	-0.005601	4.301741
61	1	0	-0.074127	0.477749	5.531399
62	1	0	-3.271792	-0.649453	2.906023
63	1	0	-2.475957	0.542585	4.917866
64	6	0	-1.011023	1.909992	-1.277485
65	8	0	-1.462435	2.988108	-0.974472
66	8	0	-0.579333	1.621869	-2.506867
67	6	0	-0.623342	2.698941	-3.450560
68	1	0	0.004115	3.521311	-3.103979
69	1	0	-0.241445	2.291683	-4.382327
70	1	0	-1.647886	3.048881	-3.577089
71	1	0	-1.462016	1.012511	0.563534

3a Anion *R,S*

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.698575	-0.066110	0.732813
2	6	0	-0.123490	-1.324262	-0.017987
3	6	0	1.369937	-1.312368	0.313575
4	6	0	1.700498	0.205843	0.232925
5	1	0	1.509354	-1.577565	1.362205
6	6	0	2.262070	-2.196891	-0.526673
7	6	0	1.973036	-2.510519	-1.856878

8	6	0	3.444118	-2.687527	0.034245
9	6	0	2.852346	-3.286006	-2.609065
10	1	0	1.060375	-2.150407	-2.317431
11	6	0	4.324682	-3.460910	-0.714523
12	1	0	3.675159	-2.455798	1.069356
13	6	0	4.031435	-3.760409	-2.042668
14	1	0	2.612030	-3.521009	-3.639440
15	1	0	5.236650	-3.831565	-0.261300
16	1	0	4.713671	-4.364287	-2.629214
17	6	0	-0.920164	-0.490227	2.209279
18	8	0	-0.008249	-0.692453	2.977758
19	8	0	-2.189849	-0.709234	2.526919
20	6	0	-2.411658	-1.240397	3.837622
21	1	0	-2.038010	-0.551521	4.594842
22	1	0	-3.487559	-1.360331	3.928575
23	1	0	-1.909257	-2.203280	3.939346
24	6	0	2.063290	0.564964	-1.202858
25	8	0	1.286739	0.692089	-2.113731
26	8	0	3.387850	0.644953	-1.341435
27	6	0	3.862716	0.842676	-2.678877
28	1	0	3.479402	1.782389	-3.076700
29	1	0	4.946001	0.871200	-2.607289
30	1	0	3.540972	0.014906	-3.311725
31	6	0	-0.866823	-2.607410	0.251734
32	6	0	-1.962184	-2.935037	-0.552176
33	6	0	-0.527279	-3.467014	1.299992
34	6	0	-2.710047	-4.082296	-0.309295
35	1	0	-2.230814	-2.271992	-1.367390
36	6	0	-1.273866	-4.617377	1.544975
37	1	0	0.319813	-3.242227	1.938233
38	6	0	-2.368789	-4.927425	0.744011
39	1	0	-3.557491	-4.318026	-0.942693
40	1	0	-0.996152	-5.272444	2.362732
41	1	0	-2.948090	-5.823112	0.935210
42	1	0	-0.259313	-1.060530	-1.068888
43	7	0	0.478011	0.826966	0.718408
44	7	0	-1.904070	0.360352	0.116533
45	6	0	-2.051782	1.508073	-0.509170
46	6	0	0.442279	1.975009	1.443234
47	8	0	-0.460160	2.225506	2.230295
48	8	0	-1.264337	2.477760	-0.660731
49	6	0	1.572014	2.933377	1.214794
50	6	0	2.320052	3.403561	2.292580
51	6	0	1.831651	3.390974	-0.077201
52	6	0	3.351685	4.311050	2.072982
53	1	0	2.096698	3.052460	3.293810
54	6	0	2.853482	4.311638	-0.289845
55	1	0	1.199657	3.042571	-0.887695
56	6	0	3.619071	4.763898	0.782544
57	1	0	3.944497	4.667779	2.906886
58	1	0	3.049765	4.679382	-1.290308
59	1	0	4.419662	5.474740	0.614672
60	6	0	-3.435734	1.655506	-1.148310
61	6	0	-3.802111	2.883308	-1.701381
62	6	0	-4.346192	0.596713	-1.209400
63	6	0	-5.050035	3.056312	-2.296476
64	1	0	-3.090657	3.698849	-1.656640
65	6	0	-5.591203	0.762311	-1.808819
66	1	0	-4.057066	-0.354539	-0.779797
67	6	0	-5.949186	1.994836	-2.353562
68	1	0	-5.320218	4.018482	-2.717380
69	1	0	-6.285187	-0.069940	-1.851896
70	1	0	-6.919574	2.125090	-2.818979
71	1	0	2.550664	0.453345	0.868860

3a Anion *S,R*

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.569712	-0.174546	0.483007
2	6	0	-0.450470	1.320650	0.040929
3	6	0	1.033679	1.540233	-0.353603
4	6	0	1.727431	0.161725	-0.199255
5	1	0	1.049713	1.784160	-1.419270
6	6	0	1.711334	2.697501	0.358400
7	6	0	1.002073	3.894029	0.516194
8	6	0	3.033707	2.651206	0.802152
9	6	0	1.587089	5.001313	1.118751
10	1	0	-0.021118	3.961313	0.160557
11	6	0	3.621405	3.759893	1.410694
12	1	0	3.628768	1.755537	0.670998
13	6	0	2.901657	4.937108	1.575680
14	1	0	1.015270	5.914999	1.232545
15	1	0	4.647749	3.697618	1.753614
16	1	0	3.358935	5.797151	2.050226
17	6	0	-0.231030	-0.247670	1.996802
18	8	0	0.352623	0.613510	2.611777
19	8	0	-0.508554	-1.445989	2.510304
20	6	0	-0.178085	-1.619614	3.891593
21	1	0	-0.724286	-0.897717	4.499181
22	1	0	-0.479198	-2.632589	4.143211
23	1	0	0.892856	-1.490095	4.049072
24	6	0	2.619555	-0.086788	-1.410017
25	8	0	2.204048	-0.320715	-2.516431
26	8	0	3.906999	0.040757	-1.108359
27	6	0	4.826900	-0.144001	-2.194718
28	1	0	4.651222	0.606110	-2.965117
29	1	0	5.816860	-0.028114	-1.763728
30	1	0	4.703662	-1.143126	-2.612164
31	6	0	-1.410659	1.655648	-1.077816
32	6	0	-2.522917	2.456202	-0.824420
33	6	0	-1.225152	1.154242	-2.370412
34	6	0	-3.434075	2.754783	-1.837053
35	1	0	-2.683133	2.834568	0.179756
36	6	0	-2.132980	1.445768	-3.381483
37	1	0	-0.370796	0.516656	-2.580476
38	6	0	-3.242447	2.249279	-3.118254
39	1	0	-4.292440	3.381113	-1.622219
40	1	0	-1.978680	1.044037	-4.376508
41	1	0	-3.948902	2.478712	-3.907505
42	1	0	-0.702630	1.927564	0.907146
43	7	0	0.629711	-0.805818	-0.149305
44	7	0	-1.794126	-0.798911	0.128573
45	6	0	-2.800651	-0.382551	0.862230
46	6	0	0.855973	-2.162018	-0.217179
47	8	0	-0.012783	-3.010562	-0.277472
48	8	0	-2.744716	0.429140	1.831046
49	6	0	2.301264	-2.599178	-0.189649
50	6	0	2.854629	-3.273501	-1.276523
51	6	0	3.051143	-2.409270	0.970364
52	6	0	4.167277	-3.728959	-1.212416
53	1	0	2.261637	-3.424651	-2.171495
54	6	0	4.356436	-2.885017	1.040588
55	1	0	2.612251	-1.896892	1.821213
56	6	0	4.918457	-3.534662	-0.055093

57	1	0	4.603646	-4.237346	-2.064100
58	1	0	4.933991	-2.744970	1.946412
59	1	0	5.939496	-3.894045	-0.005988
60	6	0	-4.157824	-0.938539	0.478274
61	6	0	-5.291013	-0.510411	1.170939
62	6	0	-4.311994	-1.858943	-0.562448
63	6	0	-6.554917	-0.989782	0.834902
64	1	0	-5.163712	0.204340	1.974679
65	6	0	-5.572547	-2.341380	-0.899280
66	1	0	-3.431279	-2.189280	-1.099107
67	6	0	-6.699364	-1.907641	-0.201859
68	1	0	-7.426549	-0.647124	1.381142
69	1	0	-5.678603	-3.056706	-1.707149
70	1	0	-7.681560	-2.282776	-0.465723
71	1	0	2.331735	0.134865	0.708874

3a Anion *S,S*

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.698575	-0.066110	0.732813
2	6	0	-0.123490	-1.324262	-0.017987
3	6	0	1.369937	-1.312368	0.313575
4	6	0	1.700498	0.205843	0.232925
5	1	0	1.509354	-1.577565	1.362205
6	6	0	2.262070	-2.196891	-0.526673
7	6	0	1.973036	-2.510519	-1.856878
8	6	0	3.444118	-2.687527	0.034245
9	6	0	2.852346	-3.286006	-2.609065
10	1	0	1.060375	-2.150407	-2.317431
11	6	0	4.324682	-3.460910	-0.714523
12	1	0	3.675159	-2.455798	1.069356
13	6	0	4.031435	-3.760409	-2.042668
14	1	0	2.612030	-3.521009	-3.639440
15	1	0	5.236650	-3.831565	-0.261300
16	1	0	4.713671	-4.364287	-2.629214
17	6	0	-0.920164	-0.490227	2.209279
18	8	0	-0.008249	-0.692453	2.977758
19	8	0	-2.189849	-0.709234	2.526919
20	6	0	-2.411658	-1.240397	3.837622
21	1	0	-2.038010	-0.551521	4.594842
22	1	0	-3.487559	-1.360331	3.928575
23	1	0	-1.909257	-2.203280	3.939346
24	6	0	2.063290	0.564964	-1.202858
25	8	0	1.286739	0.692089	-2.113731
26	8	0	3.387850	0.644953	-1.341435
27	6	0	3.862716	0.842676	-2.678877
28	1	0	3.479402	1.782389	-3.076700
29	1	0	4.946001	0.871200	-2.607289
30	1	0	3.540972	0.014906	-3.311725
31	6	0	-0.866823	-2.607410	0.251734
32	6	0	-1.962184	-2.935037	-0.552176
33	6	0	-0.527279	-3.467014	1.299992
34	6	0	-2.710047	-4.082296	-0.309295
35	1	0	-2.230814	-2.271992	-1.367390
36	6	0	-1.273866	-4.617377	1.544975
37	1	0	0.319813	-3.242227	1.938233
38	6	0	-2.368789	-4.927425	0.744011
39	1	0	-3.557491	-4.318026	-0.942693
40	1	0	-0.996152	-5.272444	2.362732
41	1	0	-2.948090	-5.823112	0.935210

42	1	0	-0.259313	-1.060530	-1.068888
43	7	0	0.478011	0.826966	0.718408
44	7	0	-1.904070	0.360352	0.116533
45	6	0	-2.051782	1.508073	-0.509170
46	6	0	0.442279	1.975009	1.443234
47	8	0	-0.460160	2.225506	2.230295
48	8	0	-1.264337	2.477760	-0.660731
49	6	0	1.572014	2.933377	1.214794
50	6	0	2.320052	3.403561	2.292580
51	6	0	1.831651	3.390974	-0.077201
52	6	0	3.351685	4.311050	2.072982
53	1	0	2.096698	3.052460	3.293810
54	6	0	2.853482	4.311638	-0.289845
55	1	0	1.199657	3.042571	-0.887695
56	6	0	3.619071	4.763898	0.782544
57	1	0	3.944497	4.667779	2.906886
58	1	0	3.049765	4.679382	-1.290308
59	1	0	4.419662	5.474740	0.614672
60	6	0	-3.435734	1.655506	-1.148310
61	6	0	-3.802111	2.883308	-1.701381
62	6	0	-4.346192	0.596713	-1.209400
63	6	0	-5.050035	3.056312	-2.296476
64	1	0	-3.090657	3.698849	-1.656640
65	6	0	-5.591203	0.762311	-1.808819
66	1	0	-4.057066	-0.354539	-0.779797
67	6	0	-5.949186	1.994836	-2.353562
68	1	0	-5.320218	4.018482	-2.717380
69	1	0	-6.285187	-0.069940	-1.851896
70	1	0	-6.919574	2.125090	-2.818979
71	1	0	2.550664	0.453345	0.868860

3a Anion *R,R*

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.569712	-0.174546	0.483007
2	6	0	-0.450470	1.320650	0.040929
3	6	0	1.033679	1.540233	-0.353603
4	6	0	1.727431	0.161725	-0.199255
5	1	0	1.049713	1.784160	-1.419270
6	6	0	1.711334	2.697501	0.358400
7	6	0	1.002073	3.894029	0.516194
8	6	0	3.033707	2.651206	0.802152
9	6	0	1.587089	5.001313	1.118751
10	1	0	-0.021118	3.961313	0.160557
11	6	0	3.621405	3.759893	1.410694
12	1	0	3.628768	1.755537	0.670998
13	6	0	2.901657	4.937108	1.575680
14	1	0	1.015270	5.914999	1.232545
15	1	0	4.647749	3.697618	1.753614
16	1	0	3.358935	5.797151	2.050226
17	6	0	-0.231030	-0.247670	1.996802
18	8	0	0.352623	0.613510	2.611777
19	8	0	-0.508554	-1.445989	2.510304
20	6	0	-0.178085	-1.619614	3.891593
21	1	0	-0.724286	-0.897717	4.499181
22	1	0	-0.479198	-2.632589	4.143211
23	1	0	0.892856	-1.490095	4.049072
24	6	0	2.619555	-0.086788	-1.410017
25	8	0	2.204048	-0.320715	-2.516431
26	8	0	3.906999	0.040757	-1.108359

27	6	0	4.826900	-0.144001	-2.194718
28	1	0	4.651222	0.606110	-2.965117
29	1	0	5.816860	-0.028114	-1.763728
30	1	0	4.703662	-1.143126	-2.612164
31	6	0	-1.410659	1.655648	-1.077816
32	6	0	-2.522917	2.456202	-0.824420
33	6	0	-1.225152	1.154242	-2.370412
34	6	0	-3.434075	2.754783	-1.837053
35	1	0	-2.683133	2.834568	0.179756
36	6	0	-2.132980	1.445768	-3.381483
37	1	0	-0.370796	0.516656	-2.580476
38	6	0	-3.242447	2.249279	-3.118254
39	1	0	-4.292440	3.381113	-1.622219
40	1	0	-1.978680	1.044037	-4.376508
41	1	0	-3.948902	2.478712	-3.907505
42	1	0	-0.702630	1.927564	0.907146
43	7	0	0.629711	-0.805818	-0.149305
44	7	0	-1.794126	-0.798911	0.128573
45	6	0	-2.800651	-0.382551	0.862230
46	6	0	0.855973	-2.162018	-0.217179
47	8	0	-0.012783	-3.010562	-0.277472
48	8	0	-2.744716	0.429140	1.831046
49	6	0	2.301264	-2.599178	-0.189649
50	6	0	2.854629	-3.273501	-1.276523
51	6	0	3.051143	-2.409270	0.970364
52	6	0	4.167277	-3.728959	-1.212416
53	1	0	2.261637	-3.424651	-2.171495
54	6	0	4.356436	-2.885017	1.040588
55	1	0	2.612251	-1.896892	1.821213
56	6	0	4.918457	-3.534662	-0.055093
57	1	0	4.603646	-4.237346	-2.064100
58	1	0	4.933991	-2.744970	1.946412
59	1	0	5.939496	-3.894045	-0.005988
60	6	0	-4.157824	-0.938539	0.478274
61	6	0	-5.291013	-0.510411	1.170939
62	6	0	-4.311994	-1.858943	-0.562448
63	6	0	-6.554917	-0.989782	0.834902
64	1	0	-5.163712	0.204340	1.974679
65	6	0	-5.572547	-2.341380	-0.899280
66	1	0	-3.431279	-2.189280	-1.099107
67	6	0	-6.699364	-1.907641	-0.201859
68	1	0	-7.426549	-0.647124	1.381142
69	1	0	-5.678603	-3.056706	-1.707149
70	1	0	-7.681560	-2.282776	-0.465723
71	1	0	2.331735	0.134865	0.708874
