Supporting Information for

Stereospecific synthesis of pyrrolidines with varied configurations via 1,3-dipolar cycloadditions to sugar-derived enones

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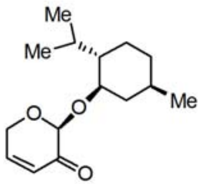
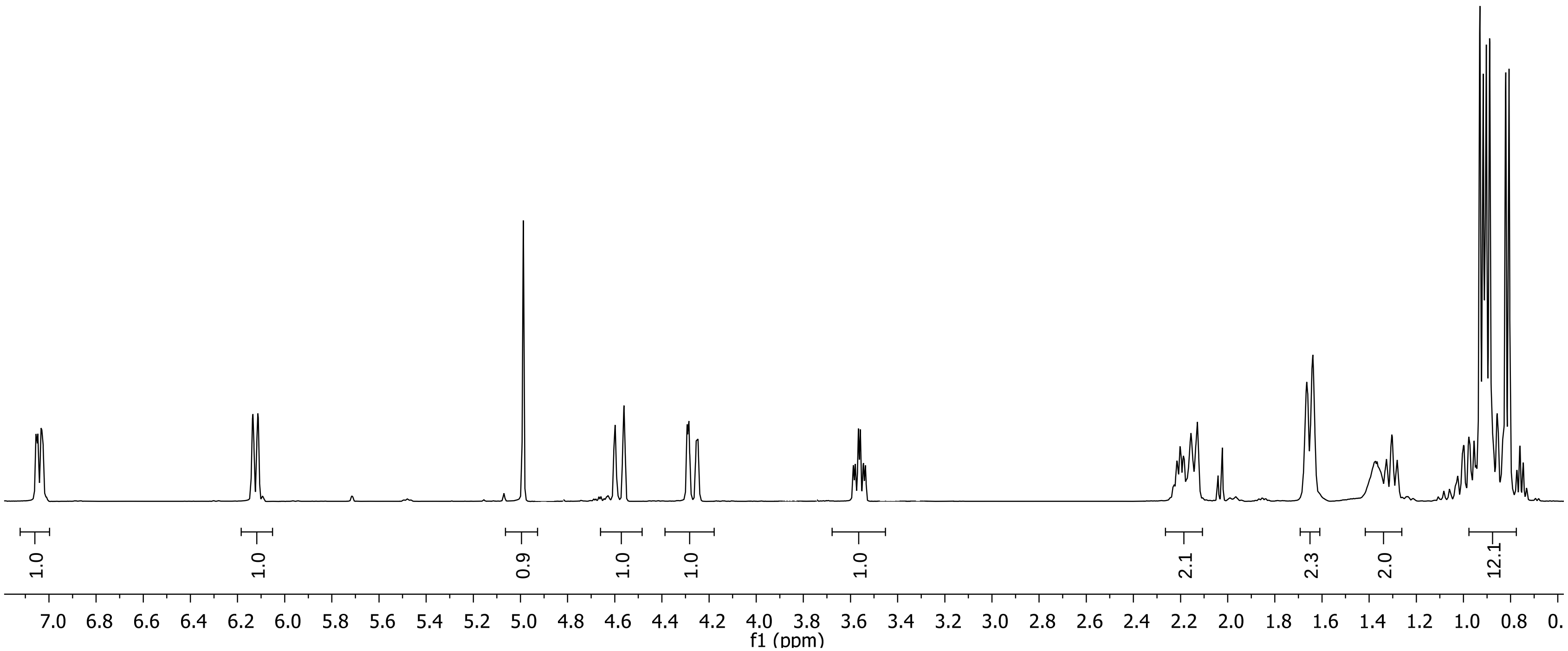
General Information

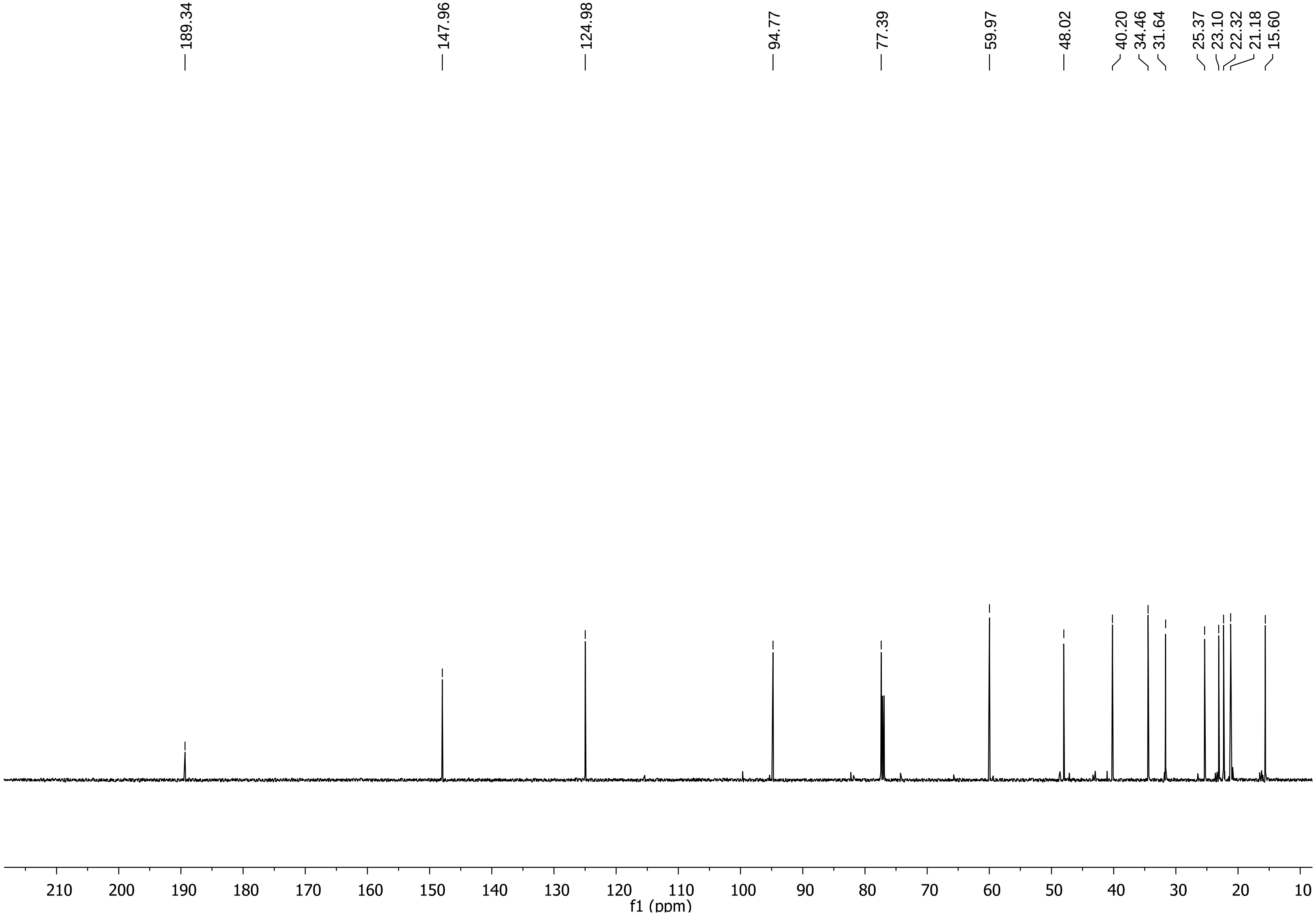
Melting points were determined with a Fisher–Johns apparatus. Column chromatography was carried out with silica gel 60 (230–400 mesh). Analytical thin-layer chromatography (TLC) was carried out on silica gel 60 F254 aluminum-supported plates (layer thickness 0.2 mm). The spots were visualized by exposure to UV light and by charring with sulfuric acid (5% v/v in EtOH, containing 0.5% *p*-anisaldehyde). Optical rotations were measured at 25 °C in a 1 dm cell in the solvent indicated. Nuclear magnetic resonance (NMR) spectra were recorded at 500 MHz (^{1}H) or 125.7 MHz (^{13}C). Chemical shifts were calibrated to tetramethylsilane or to a residual solvent peak ($CHCl_3$: ^{1}H: δ = 7.26 ppm, ^{13}C: δ = 77.2 ppm). Assignments of ^{1}H and ^{13}C NMR spectra were assisted by 2D ^{1}H–COSY and 2D ^{1}H–^{13}C HSQC and HMBC experiments. High-resolution mass spectra (HRMS) were obtained using the electrospray ionization (ESI) technique and Q-TOF detection. Molecular mechanics calculations (MM+) were carried out with Hyperchem Professional 8.0.3, the low-energy conformations were refined using the semiempirical AM1 method.

^{1}H NMR ($CDCl_3$, 500 MHz) of compound **2**

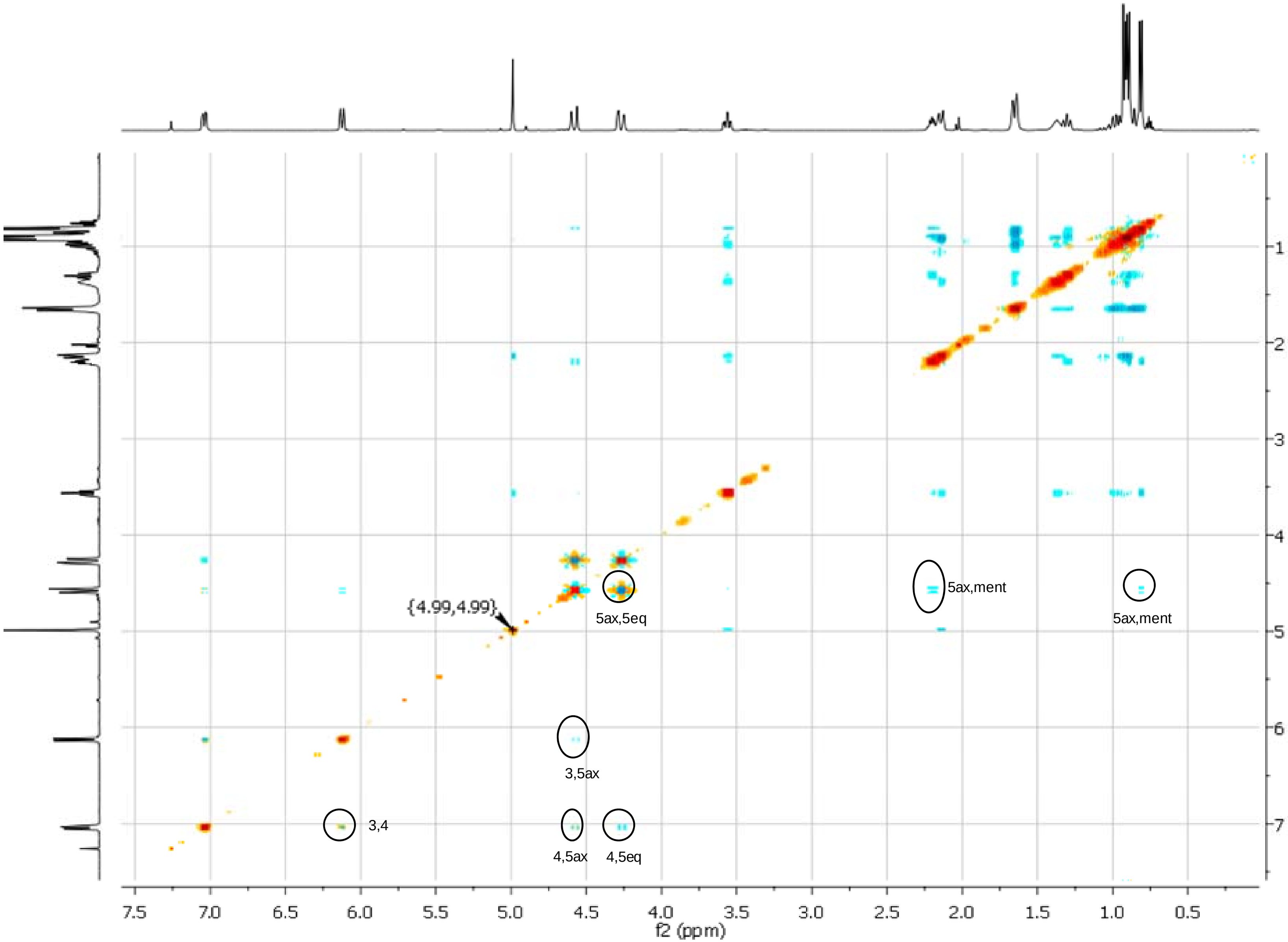




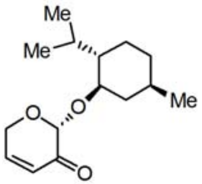
^{13}C NMR (CDCl$_3$, 125.7 MHz) of compound **2**

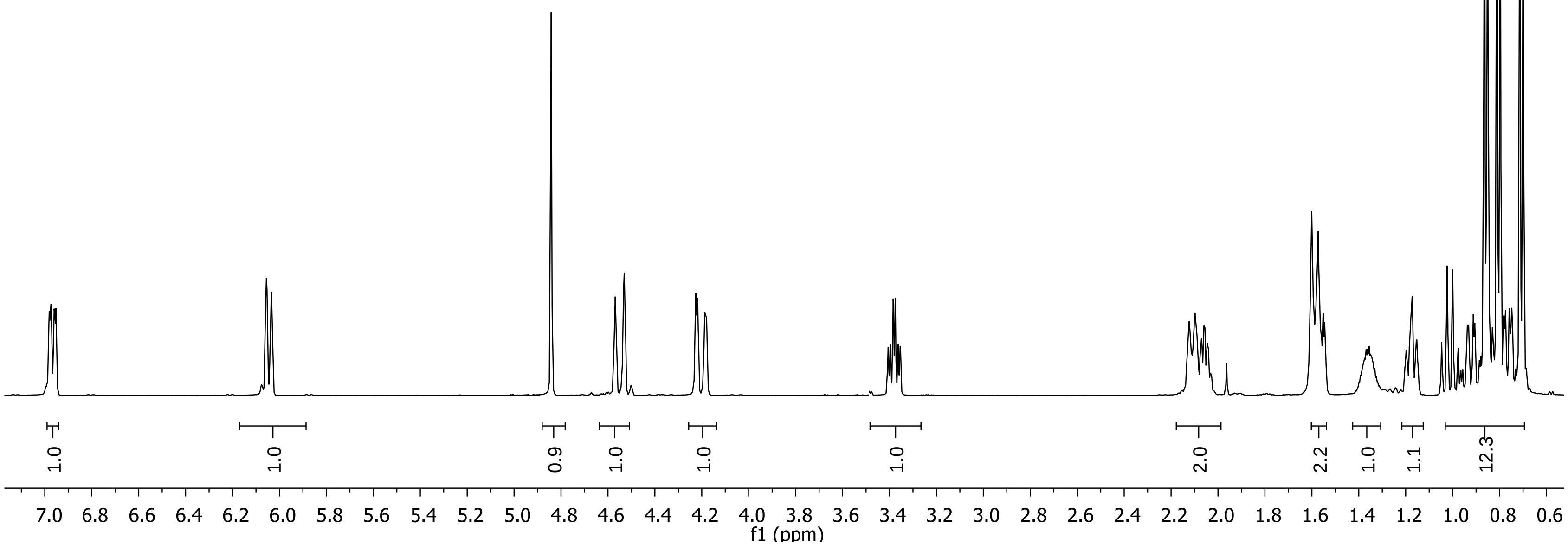


NOESY of compound **2**

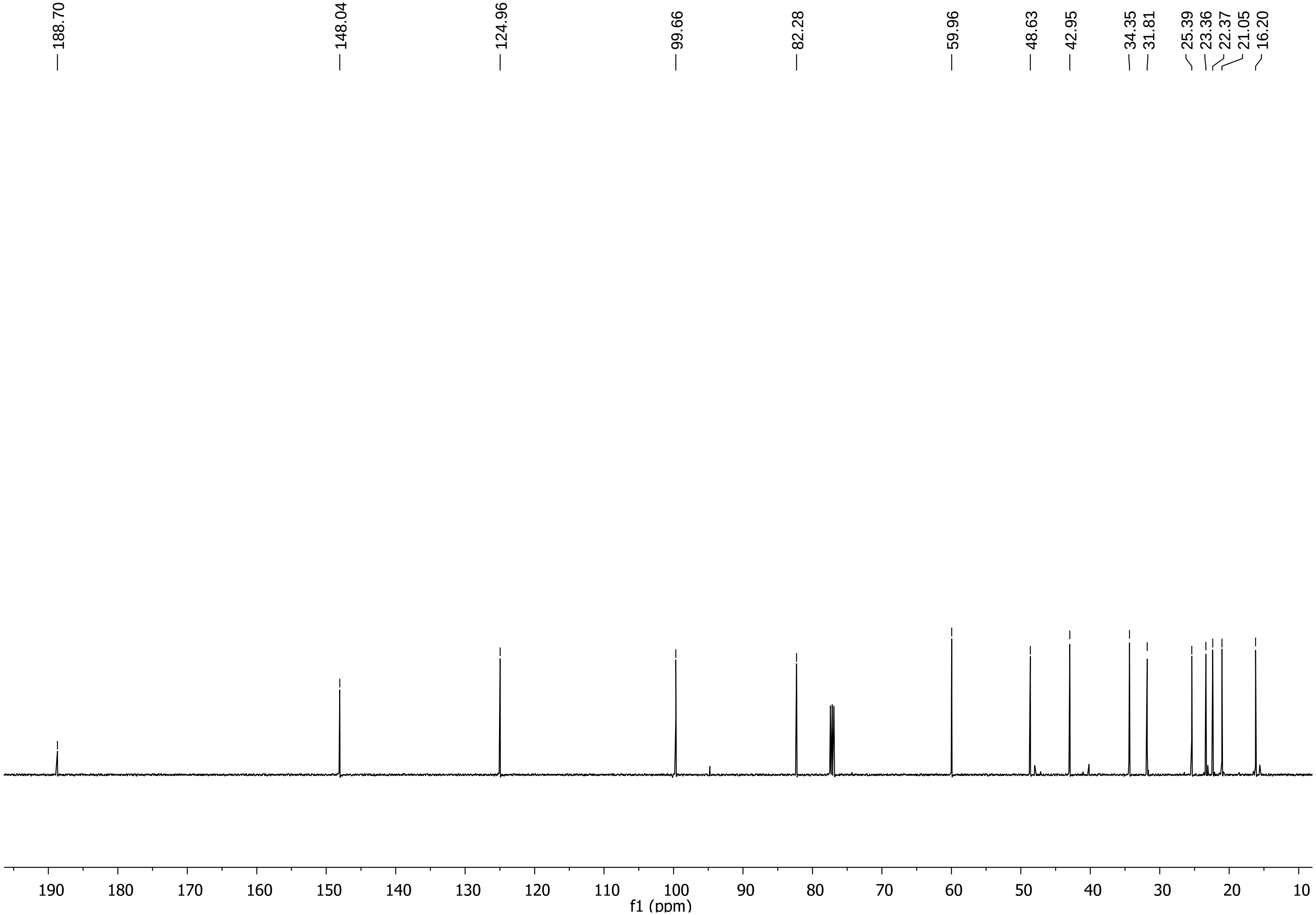


[1]H NMR ($CDCl_3$, 500 MHz) of compound **4**





^{13}C NMR ($CDCl_3$, 125.7 MHz) of compound **4**



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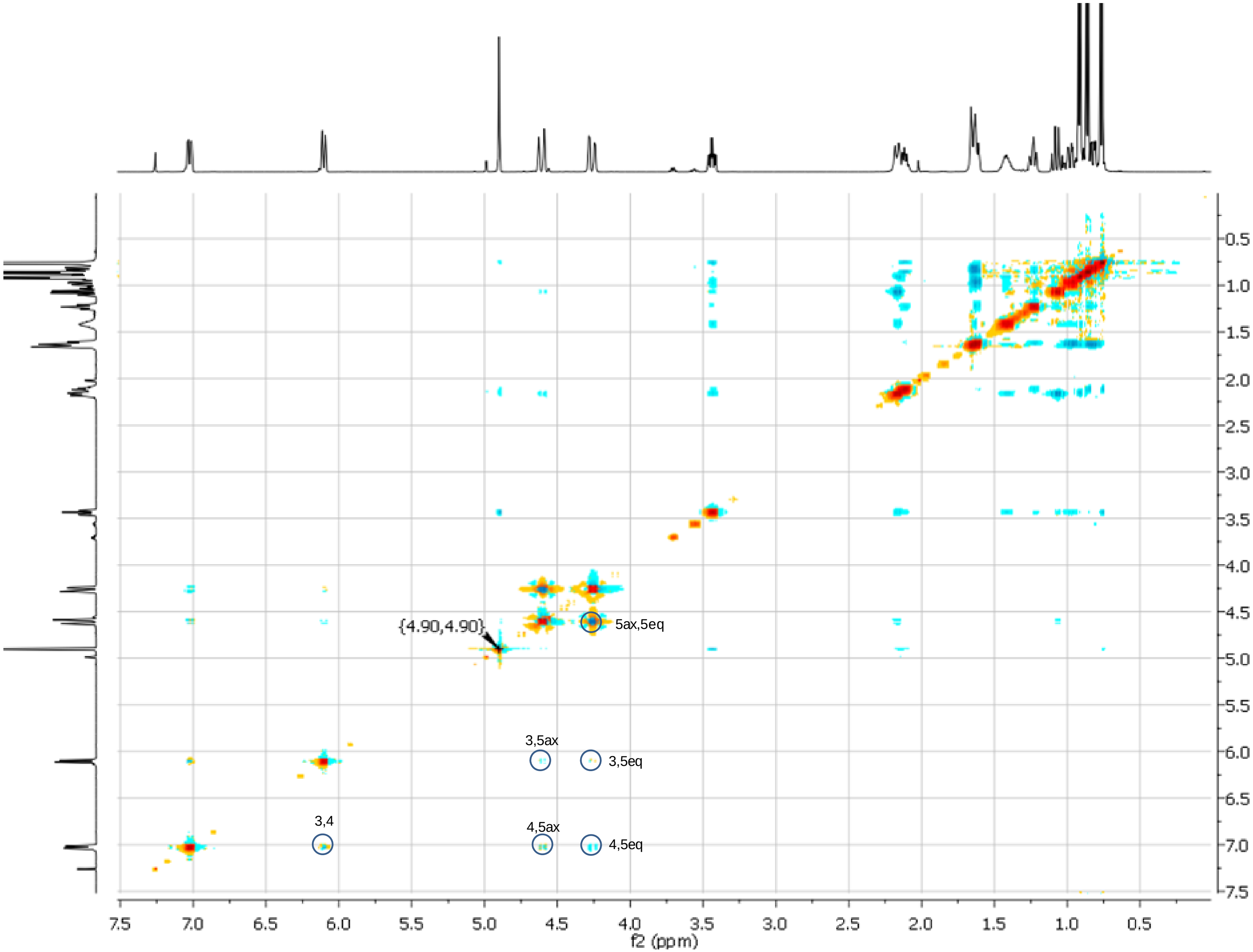

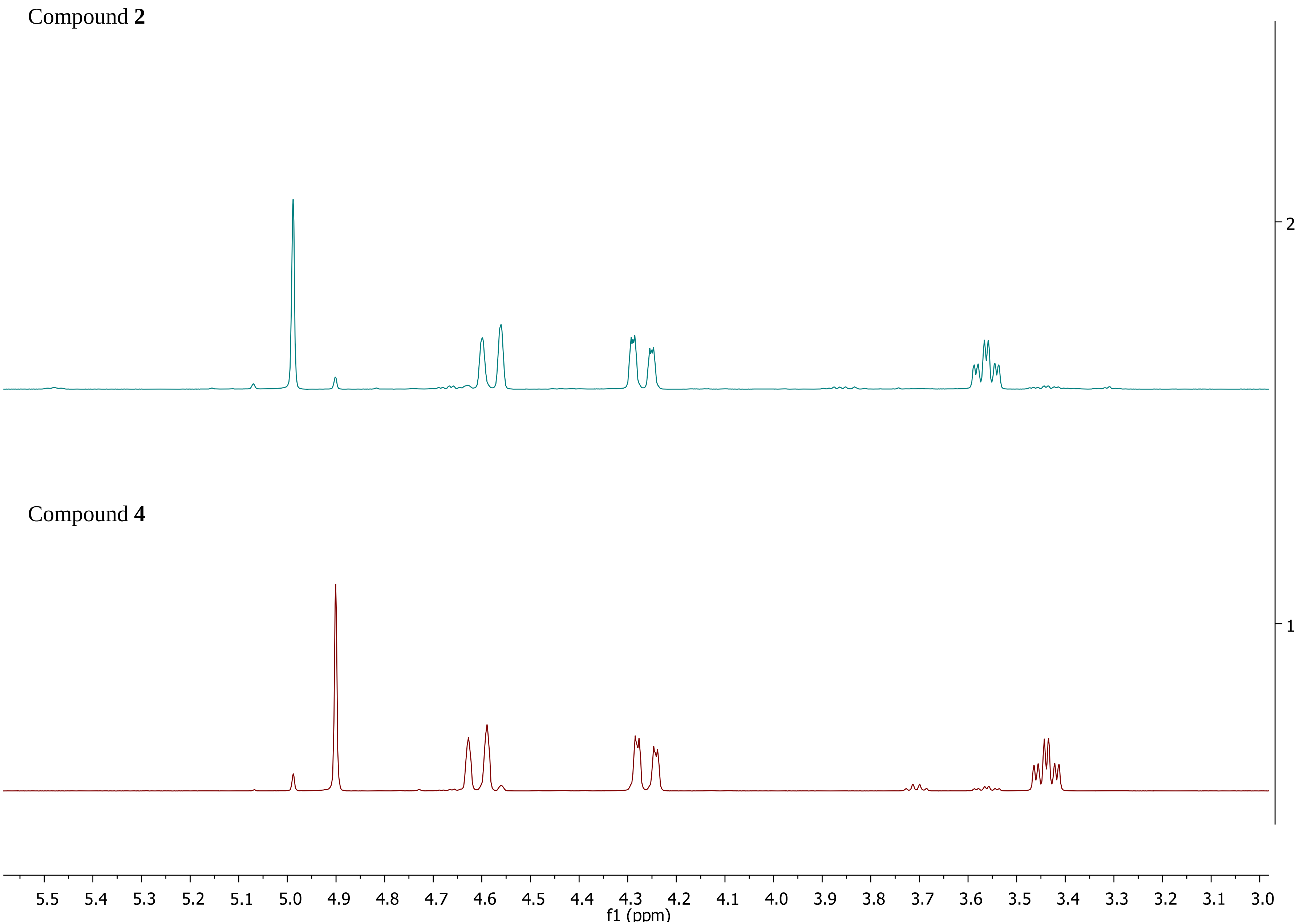
Compound **2**
Compound **4**
2
1
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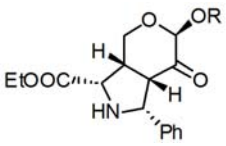
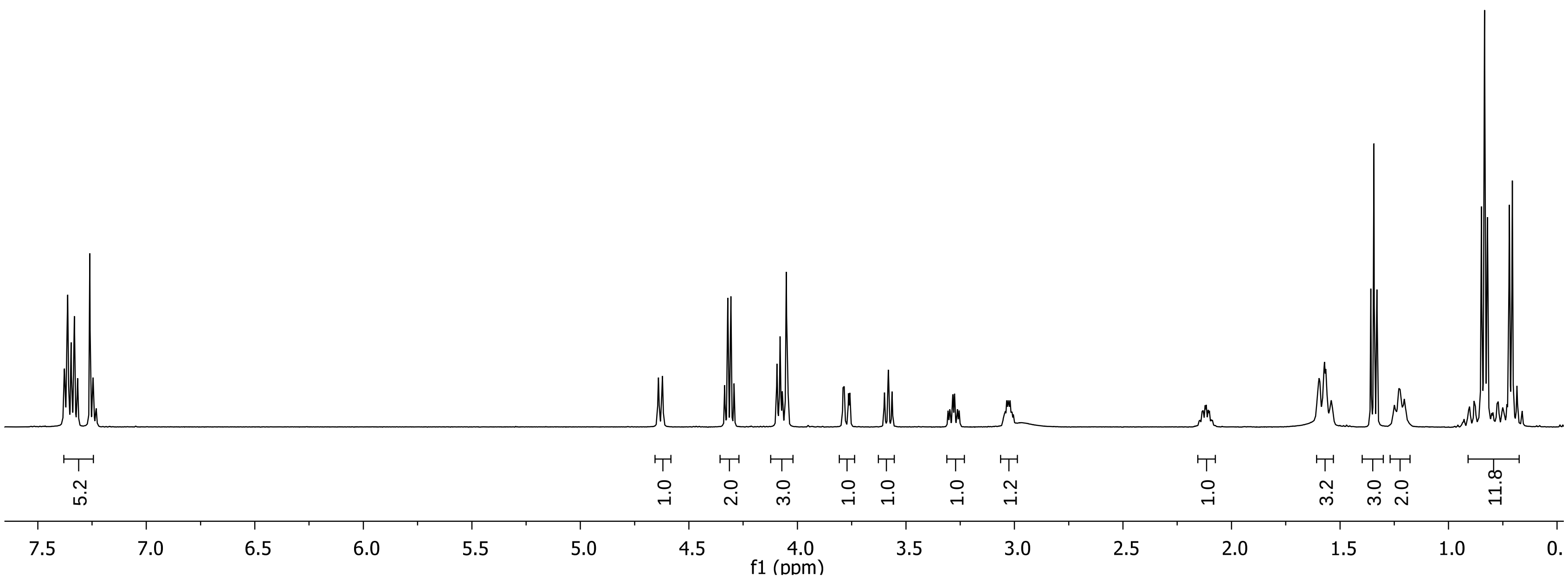
f1 (ppm)

^{1}H NMR ($CDCl_3$, 500 MHz) of compound **7**





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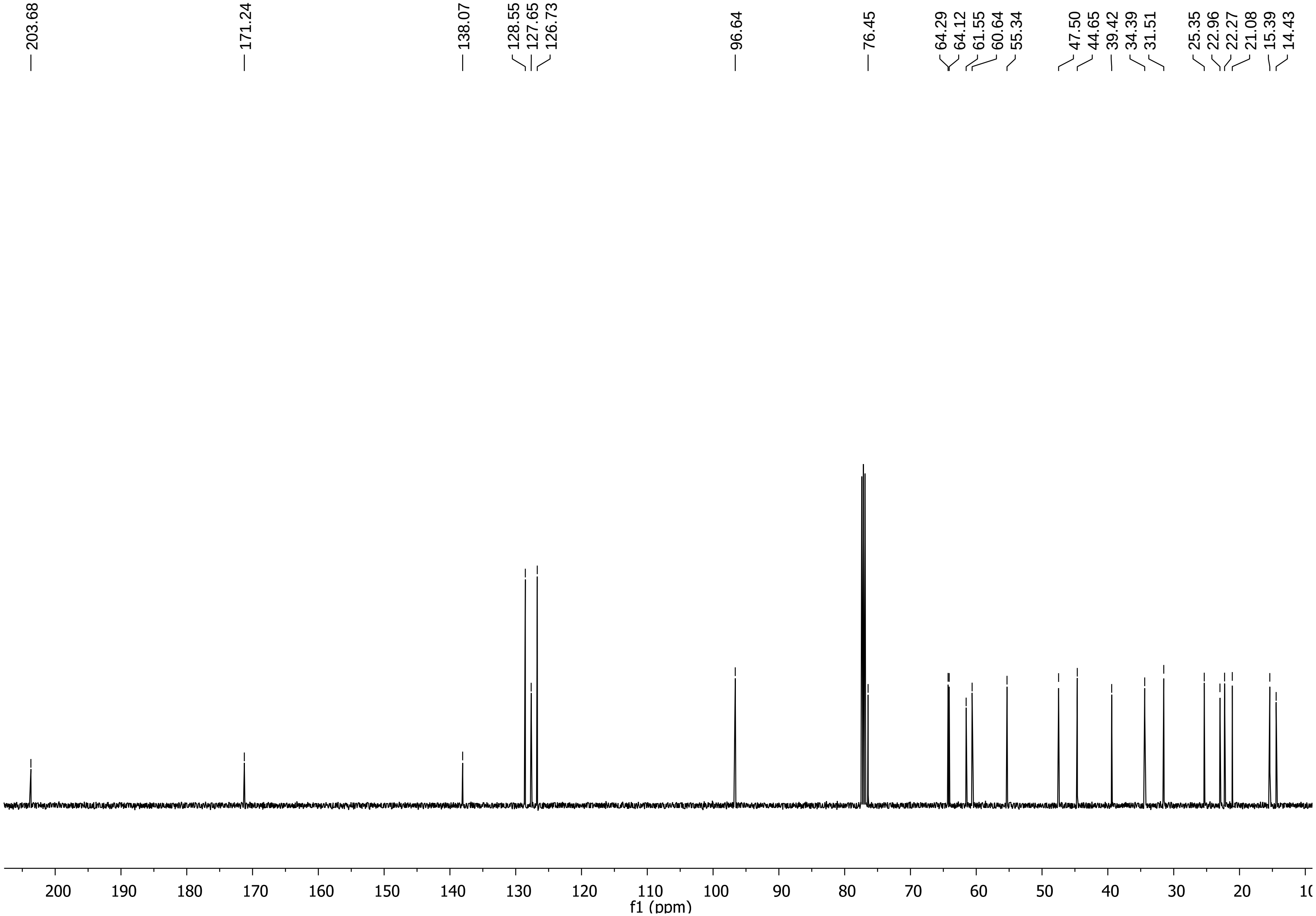

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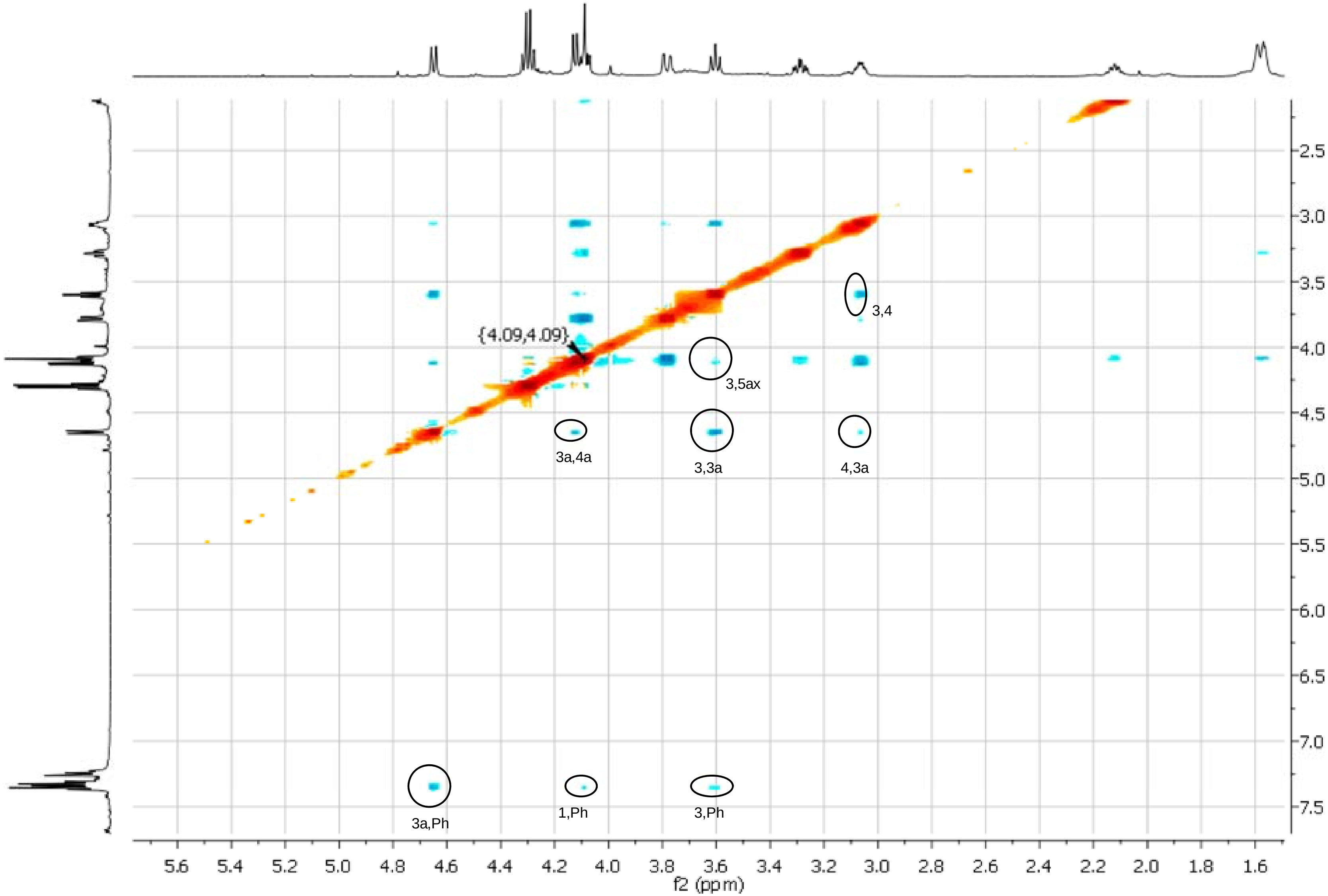

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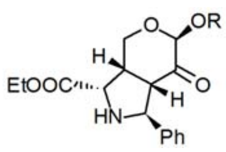
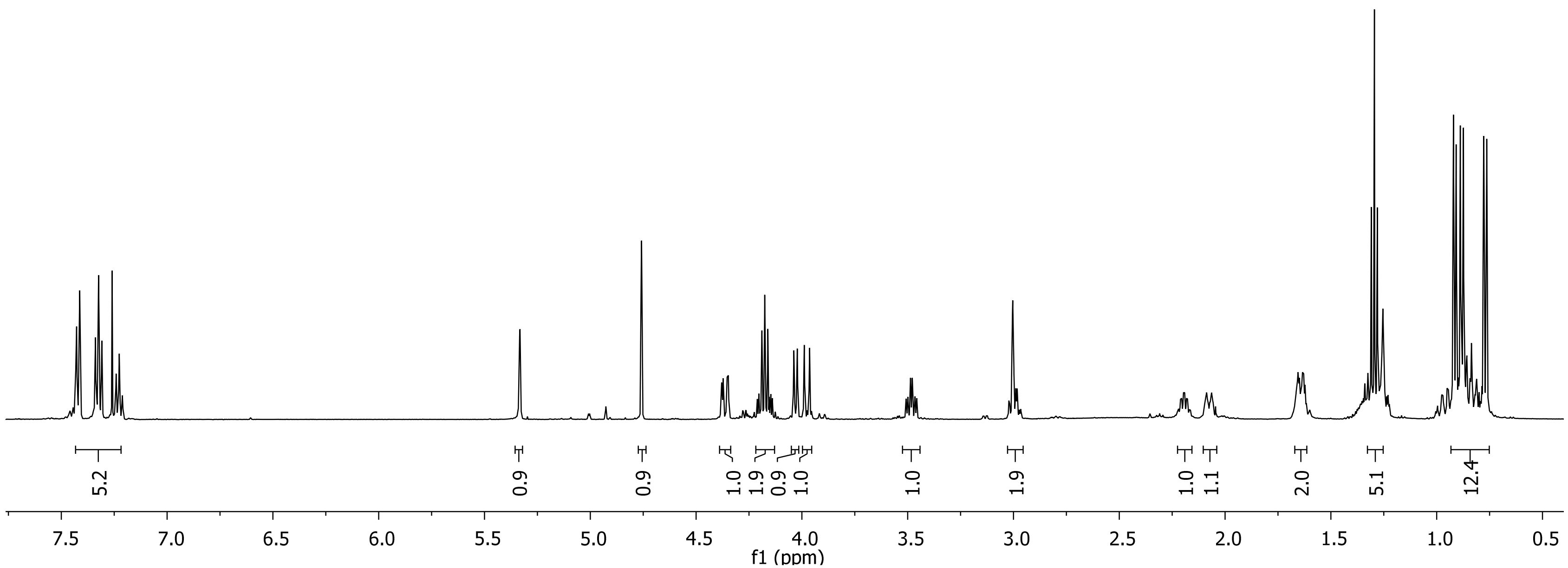
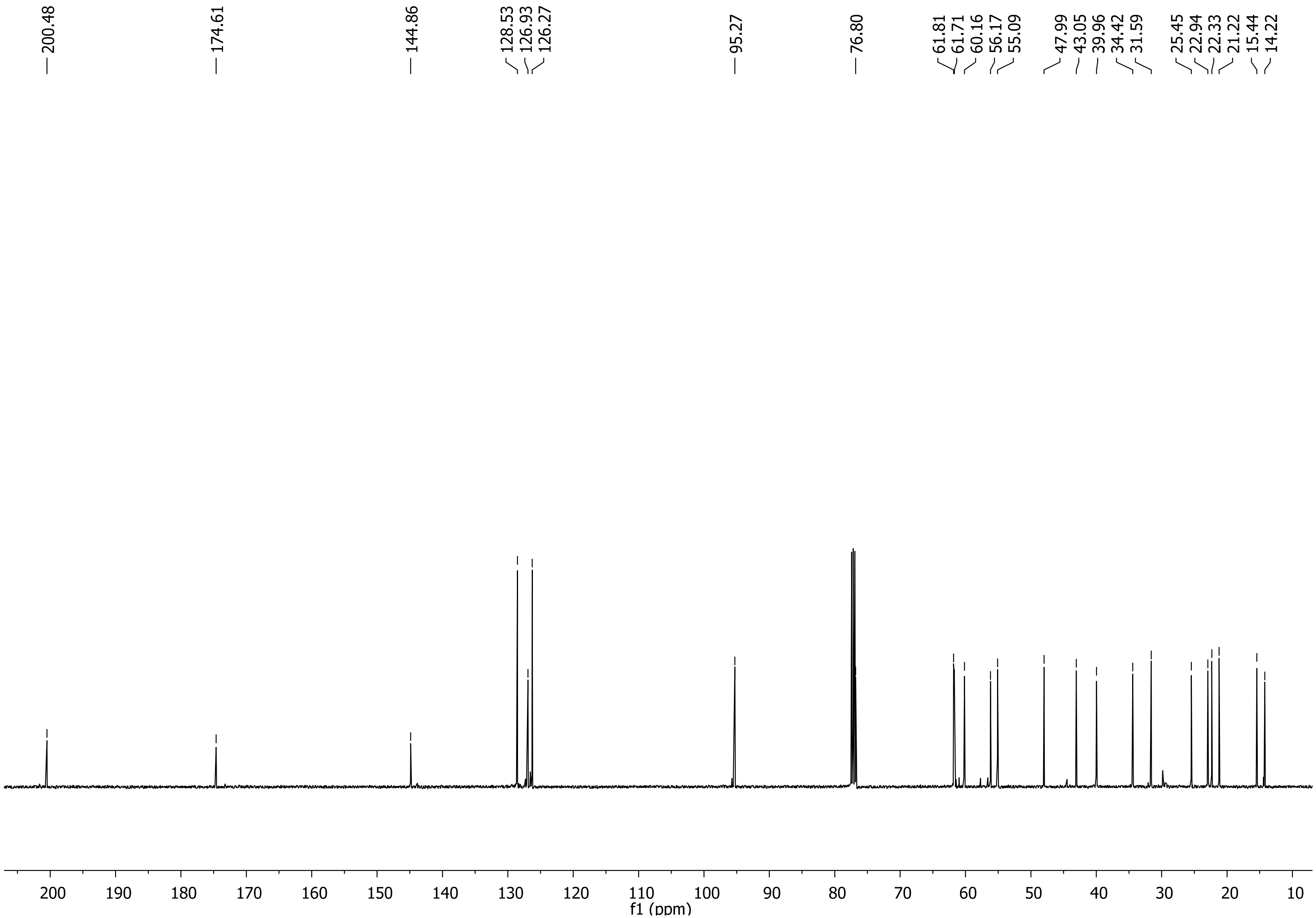




^{13}C NMR ($CDCl_3$, 125.7 MHz) of compound *epi*-**7**



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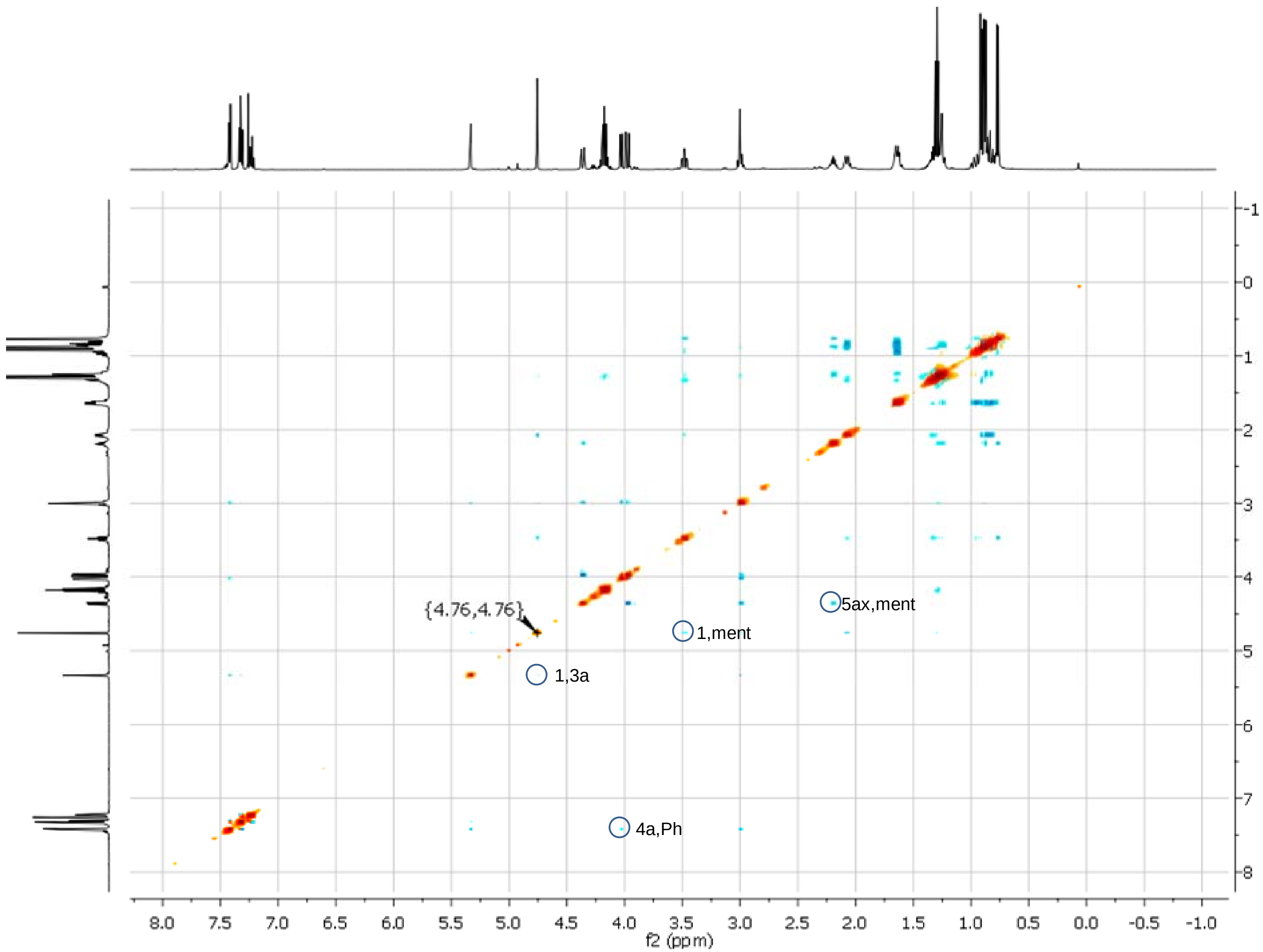

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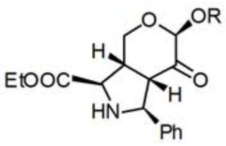

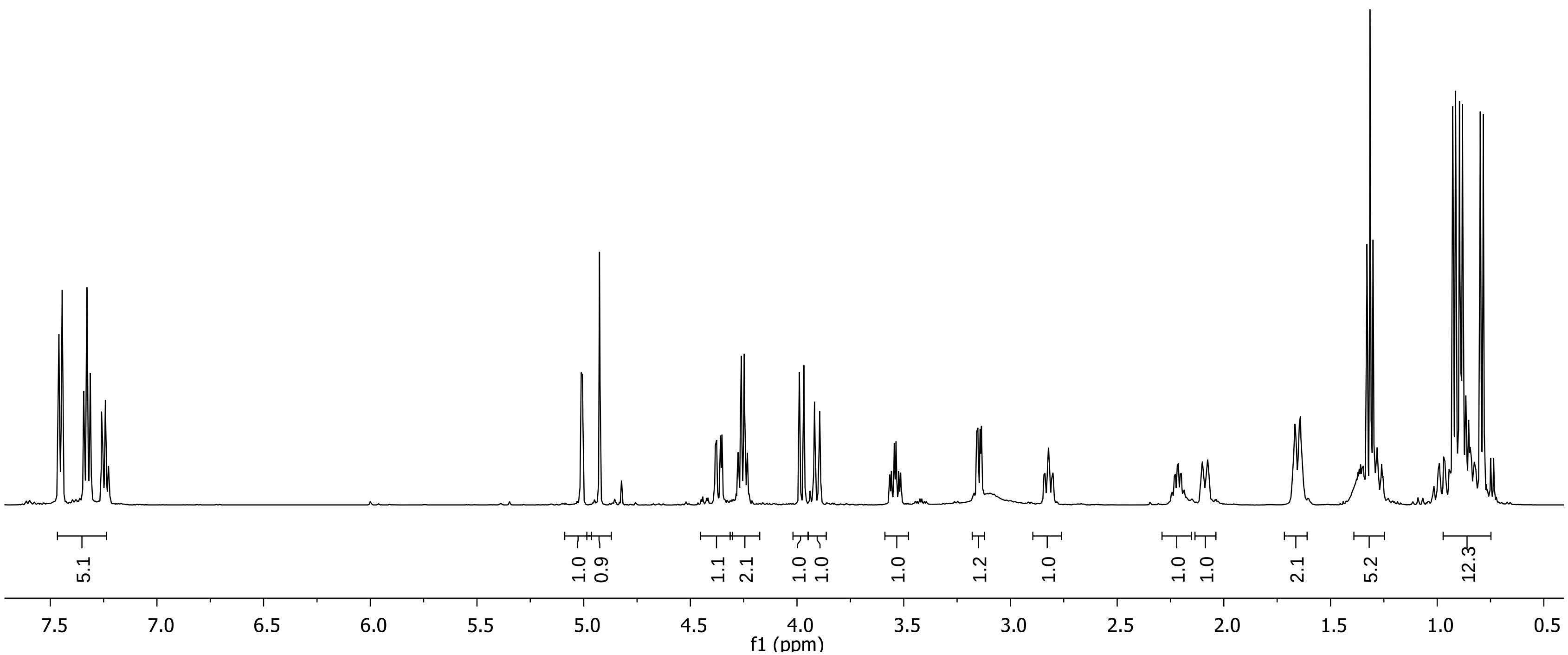

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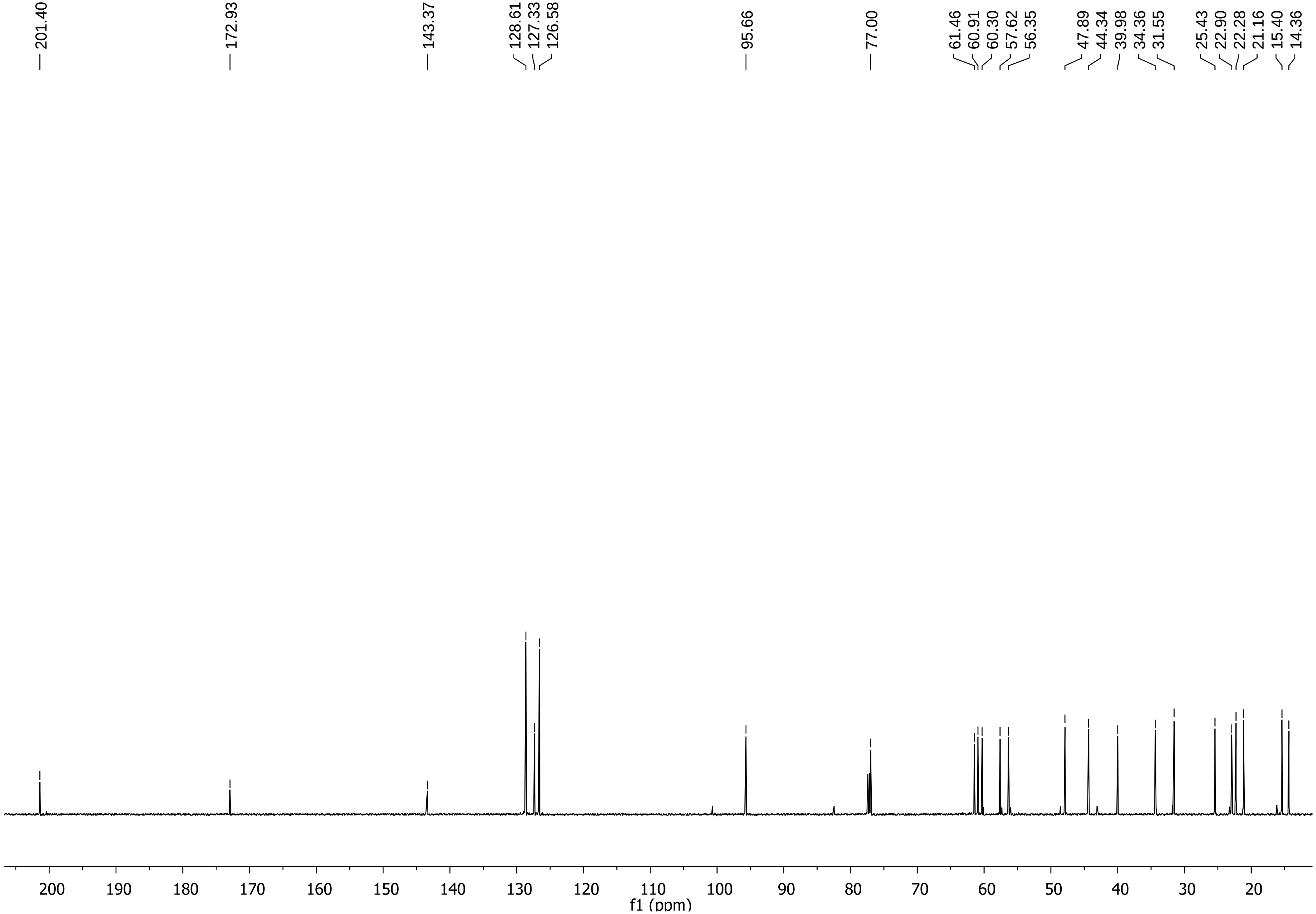

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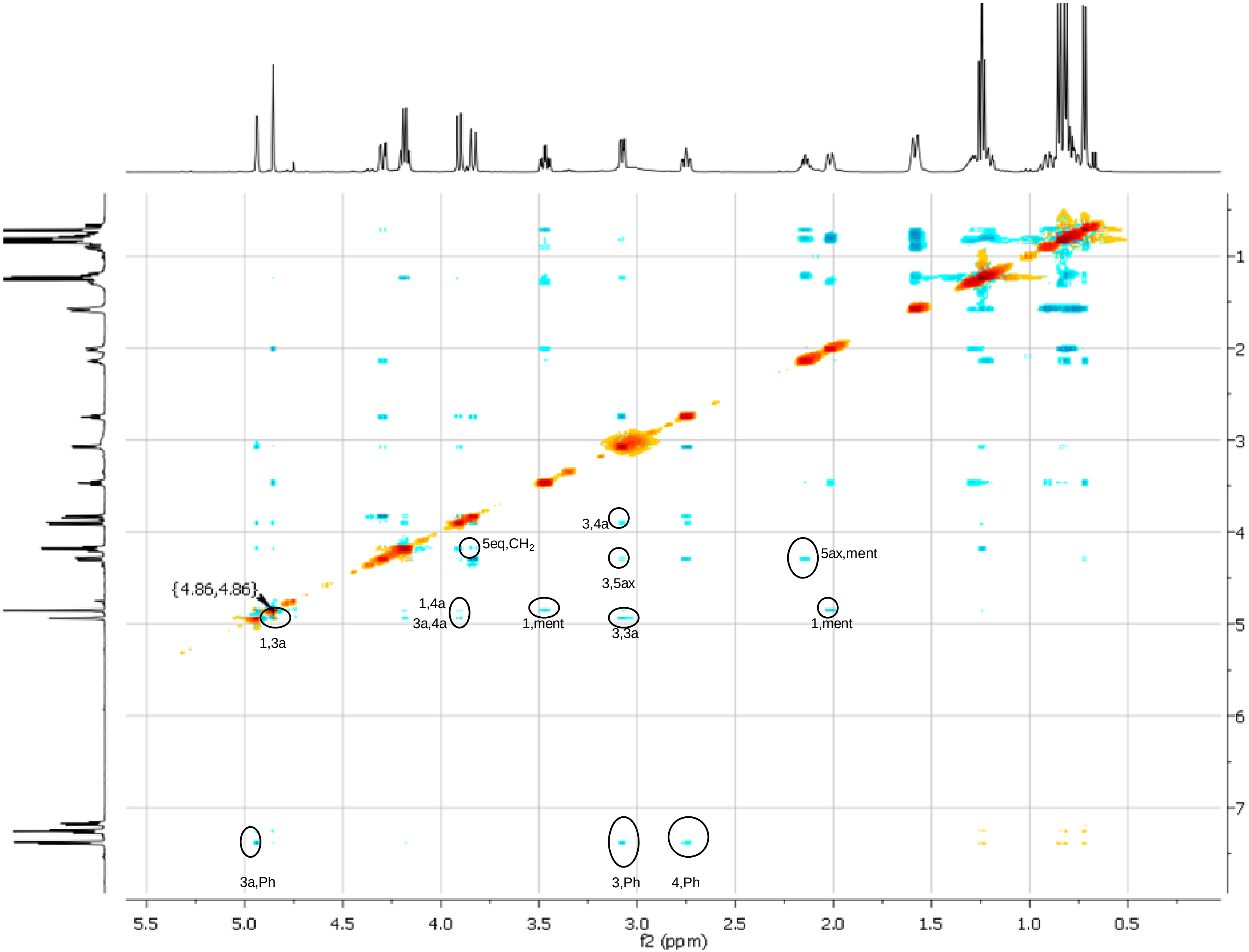

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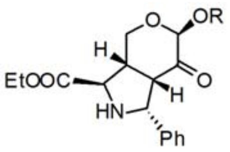

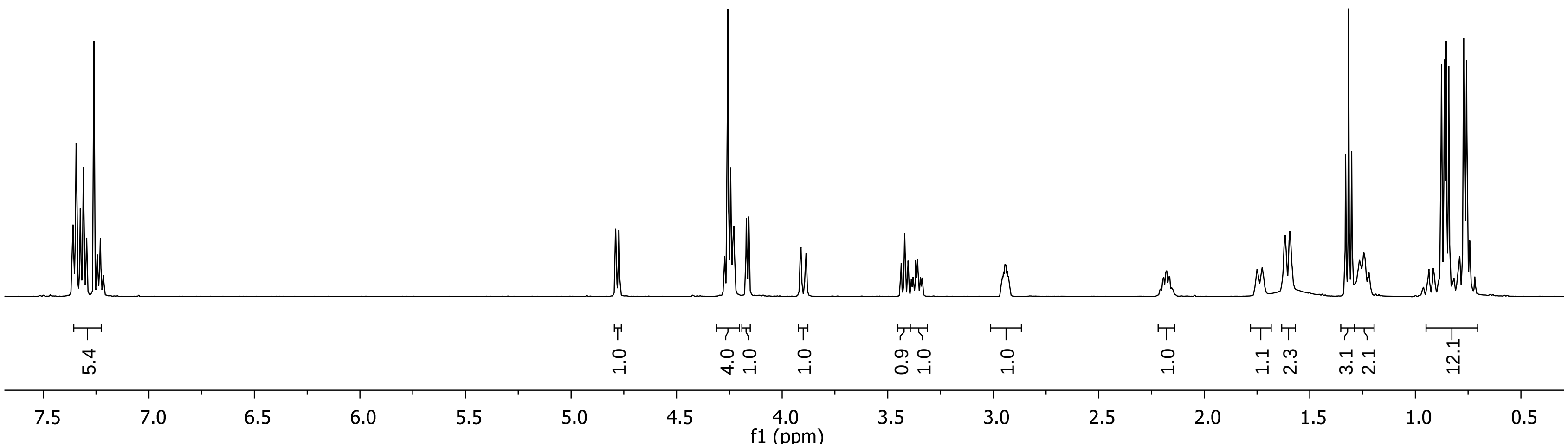

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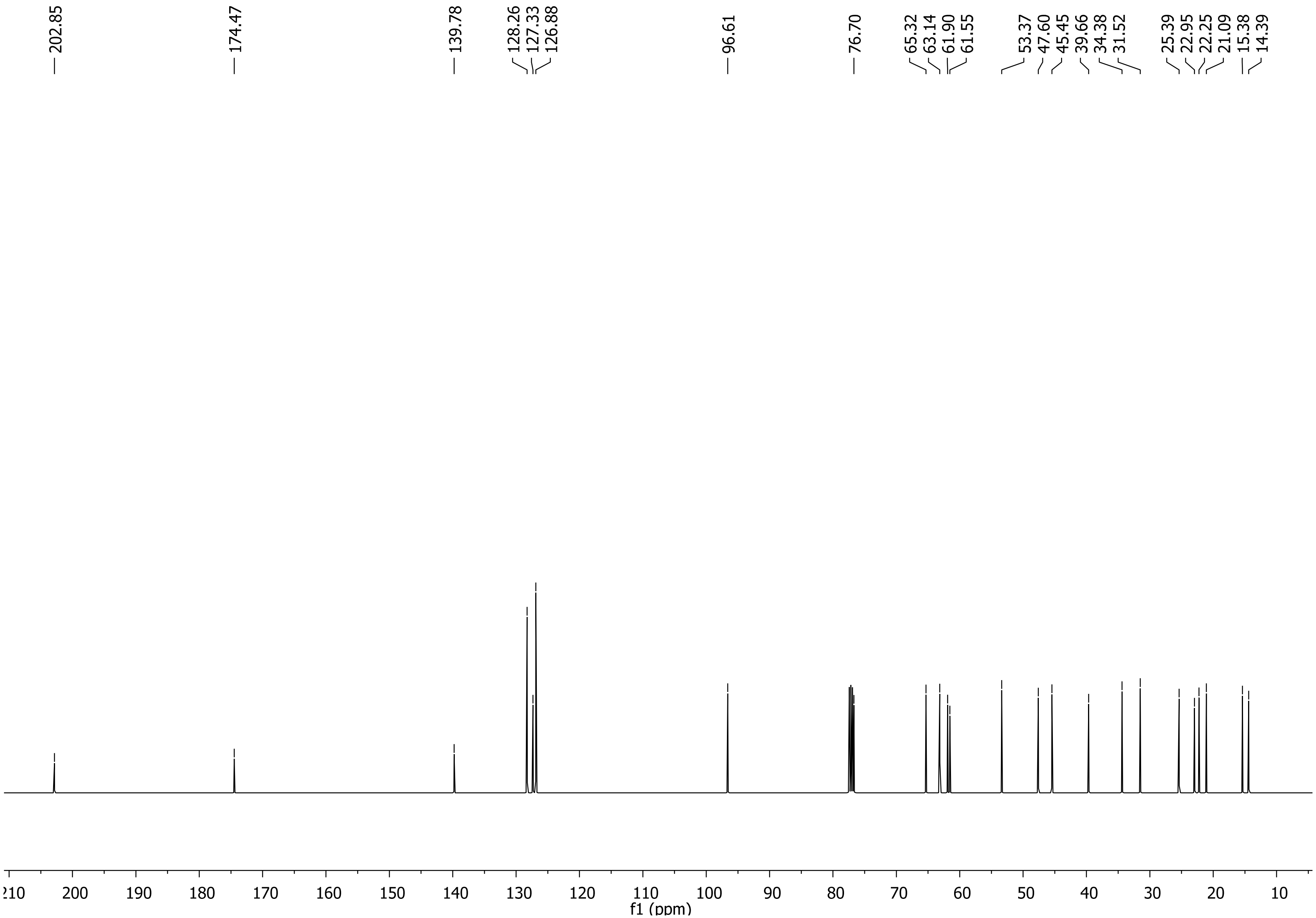

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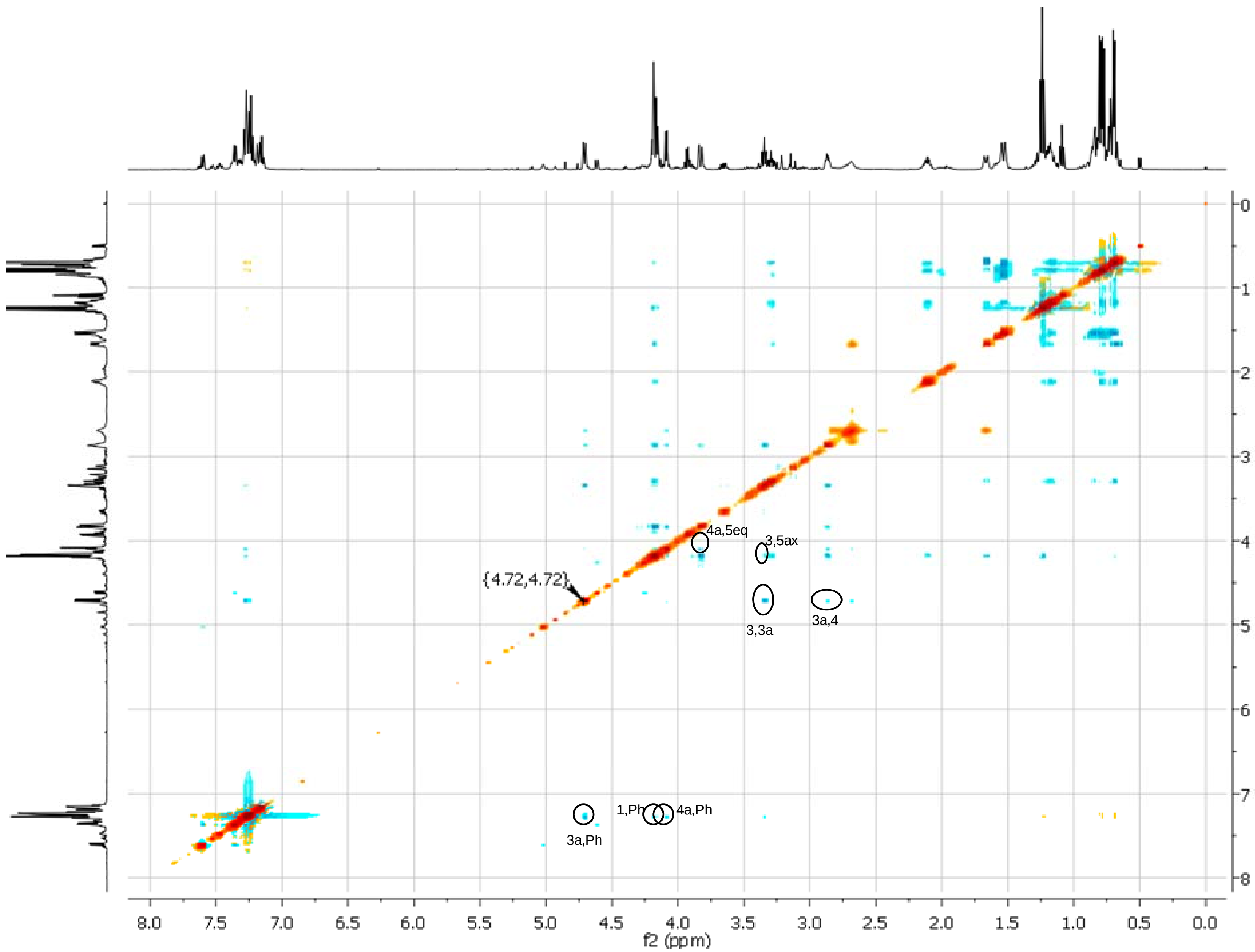

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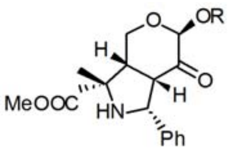

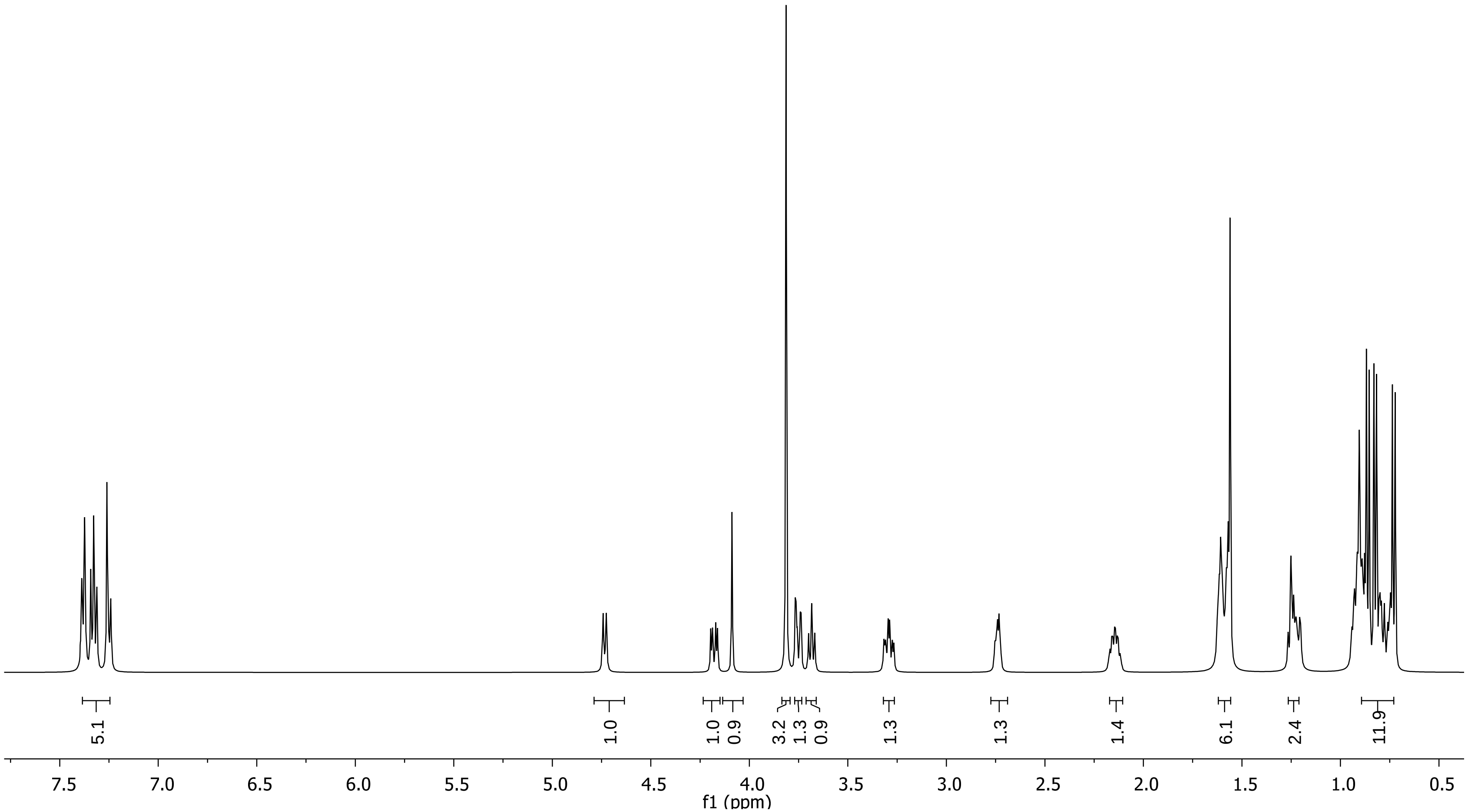

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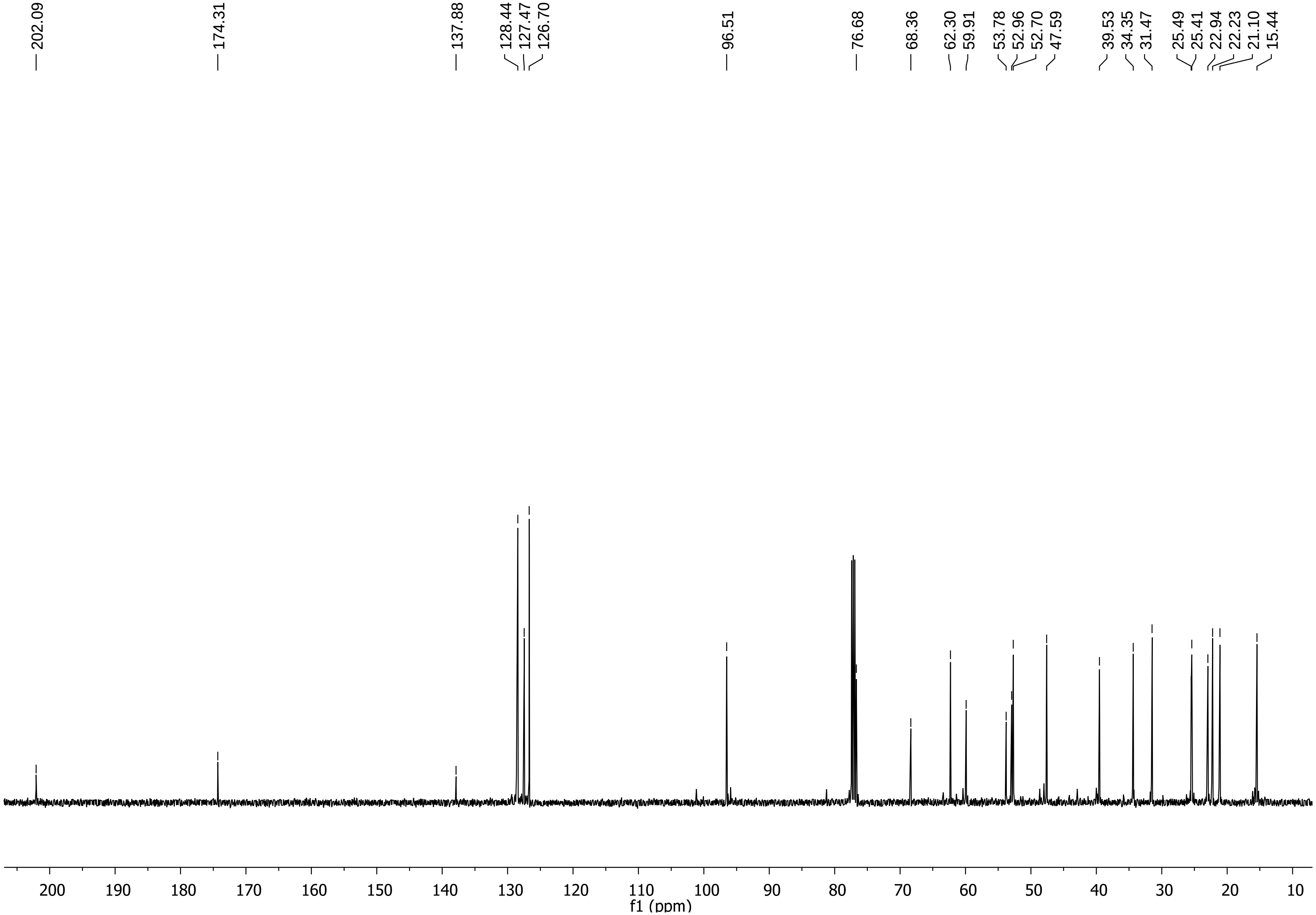

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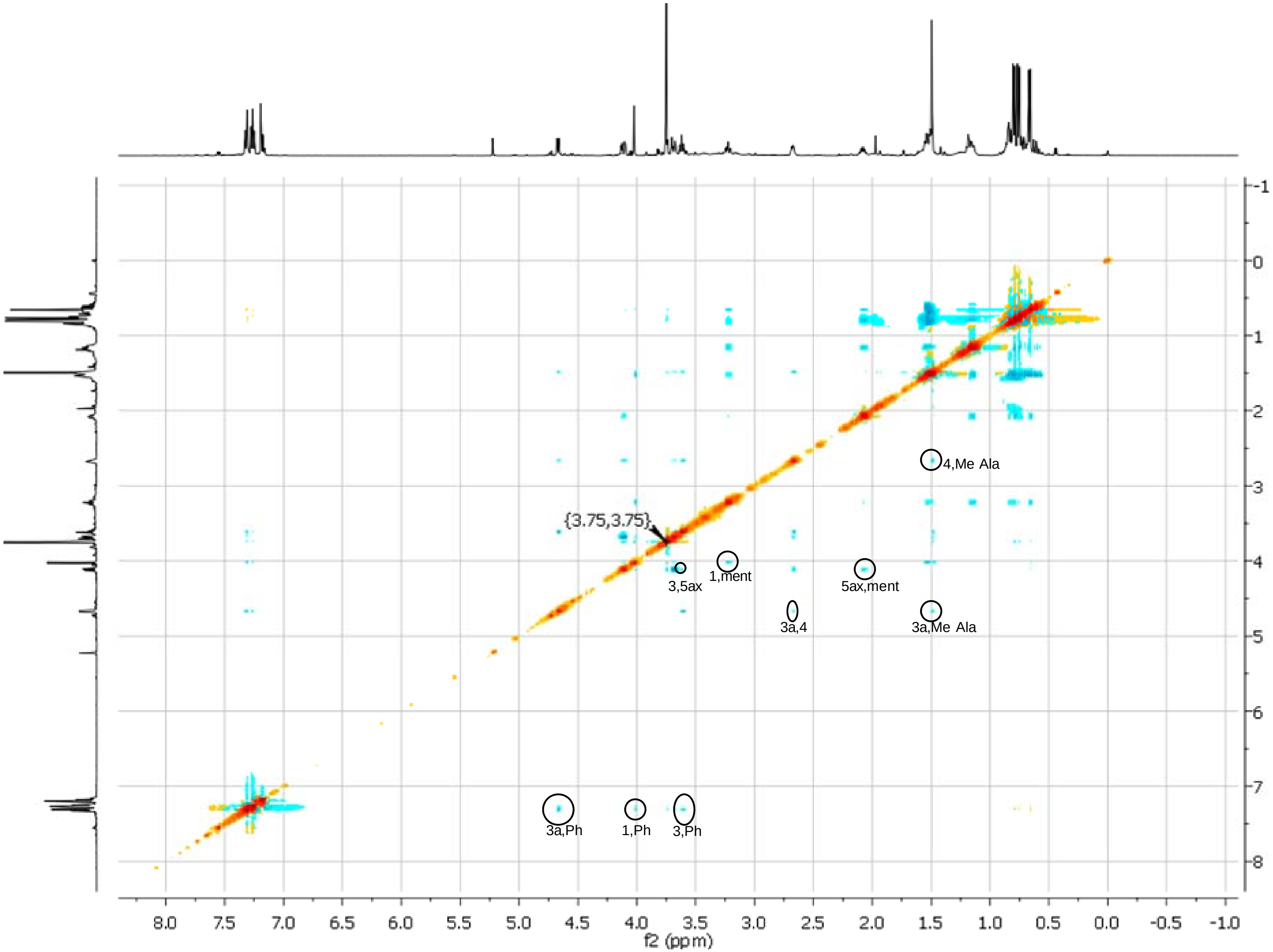

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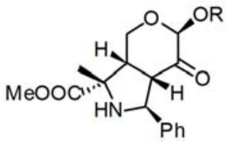

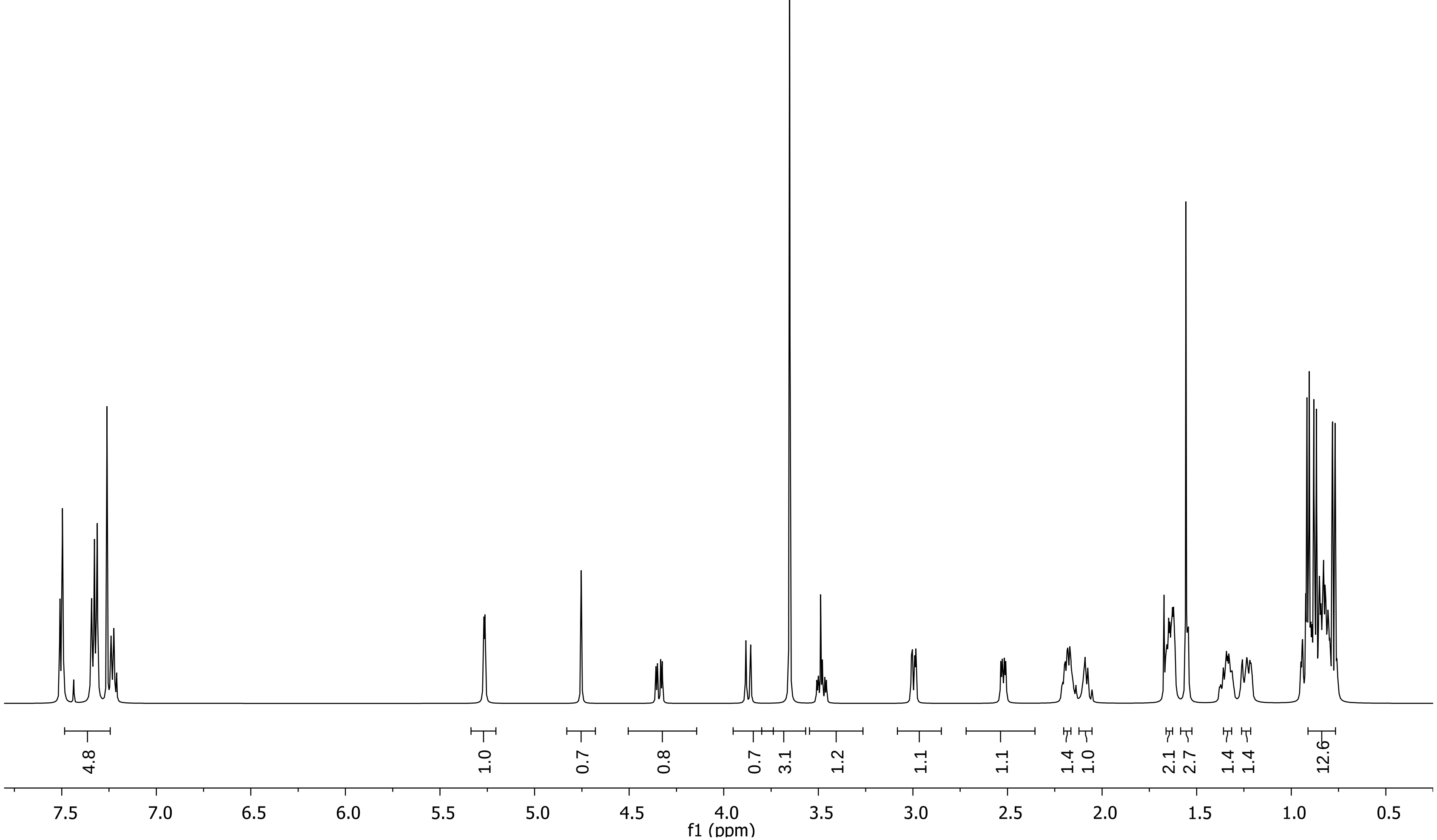

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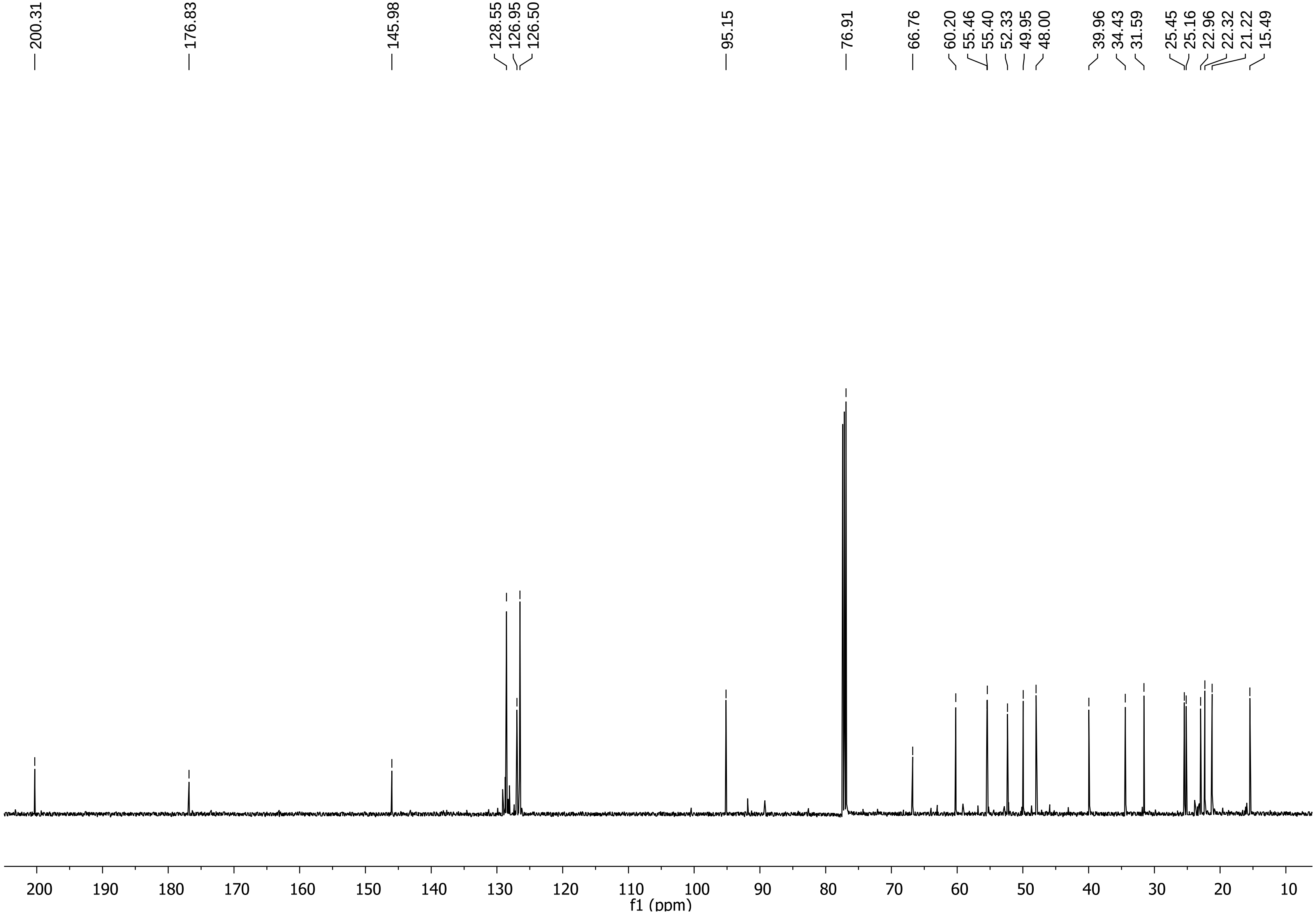

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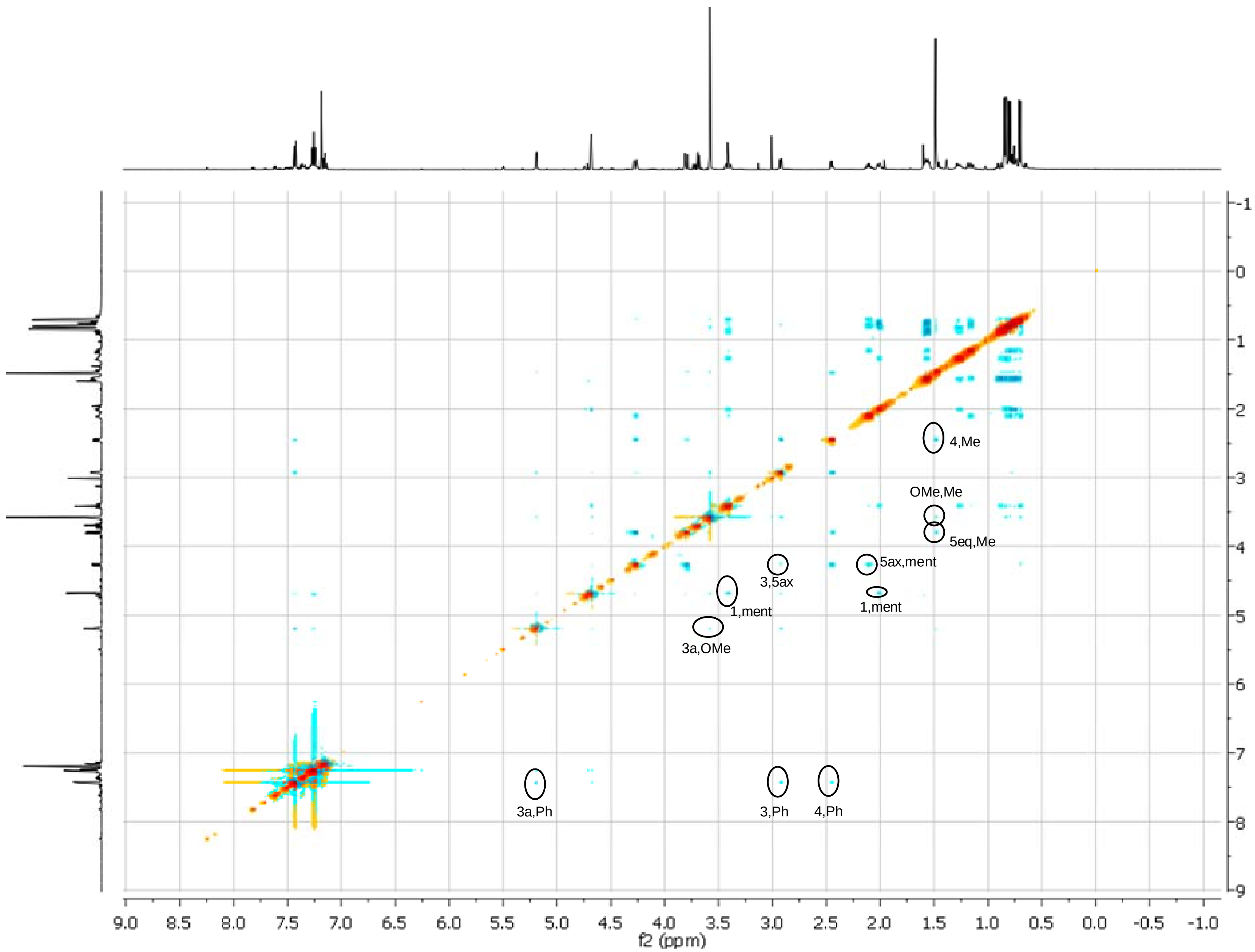

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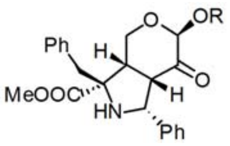
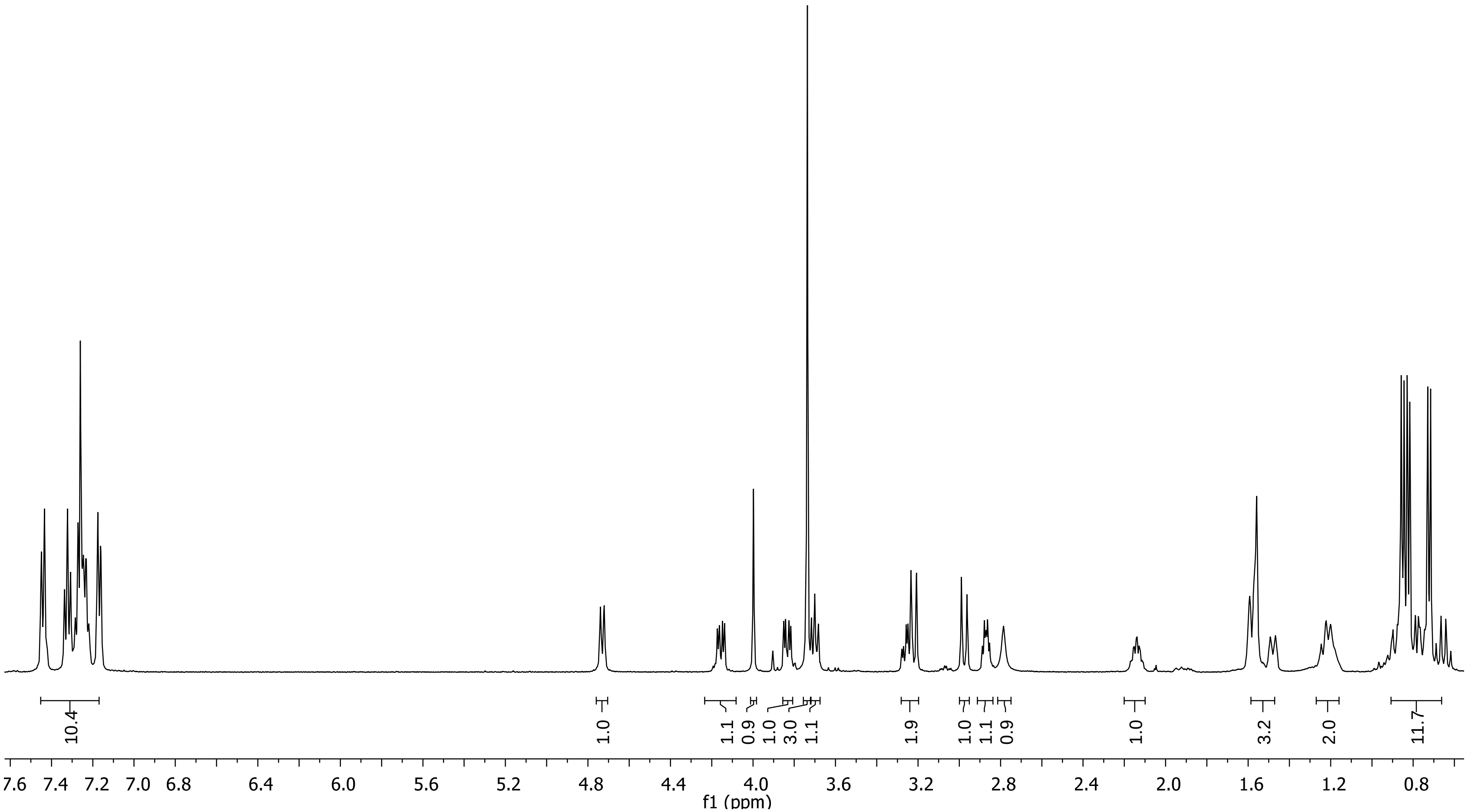
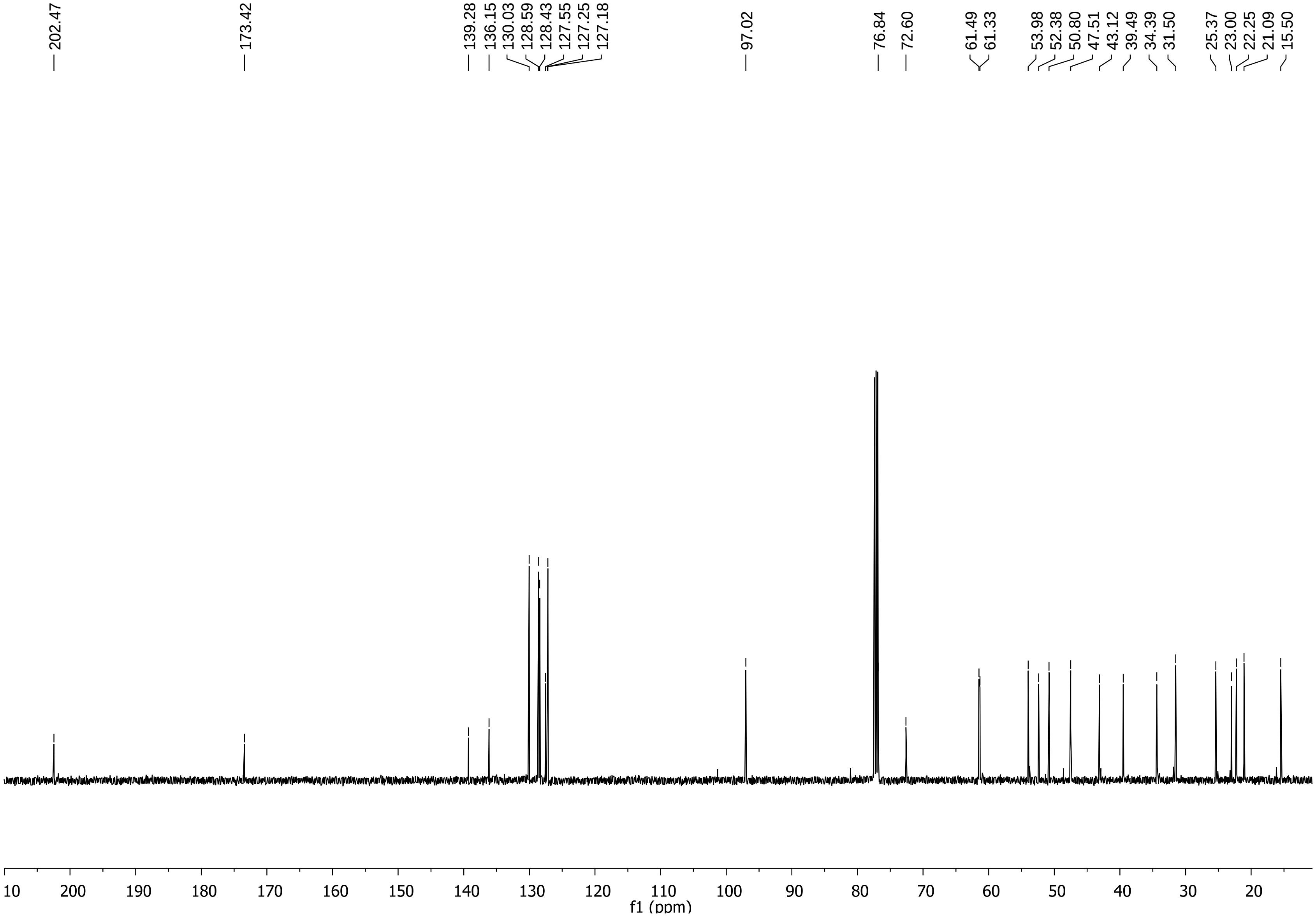




^{13}C NMR ($CDCl_3$, 125.7 MHz) of compound **11**



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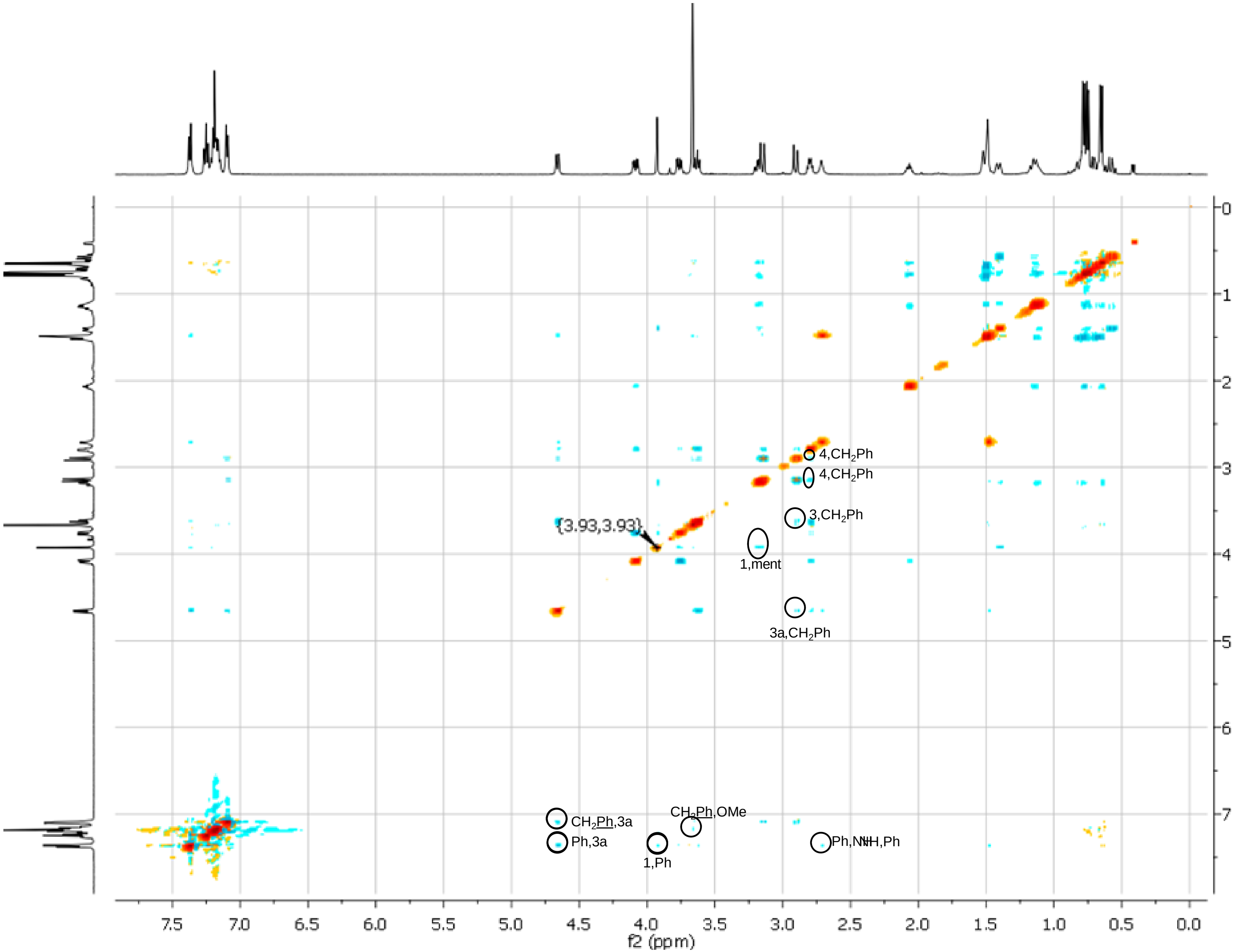

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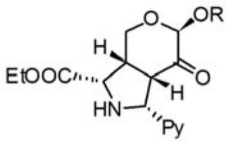

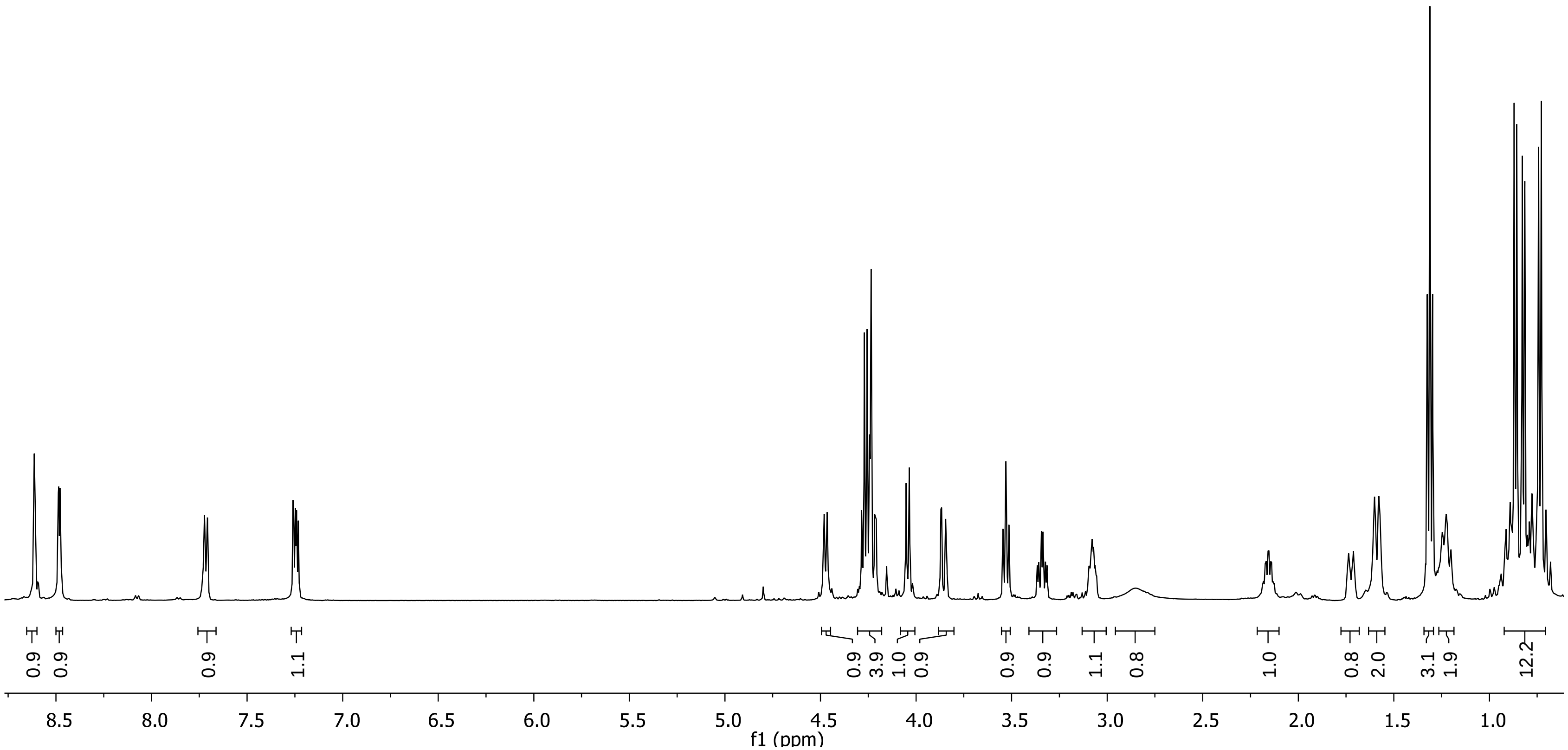

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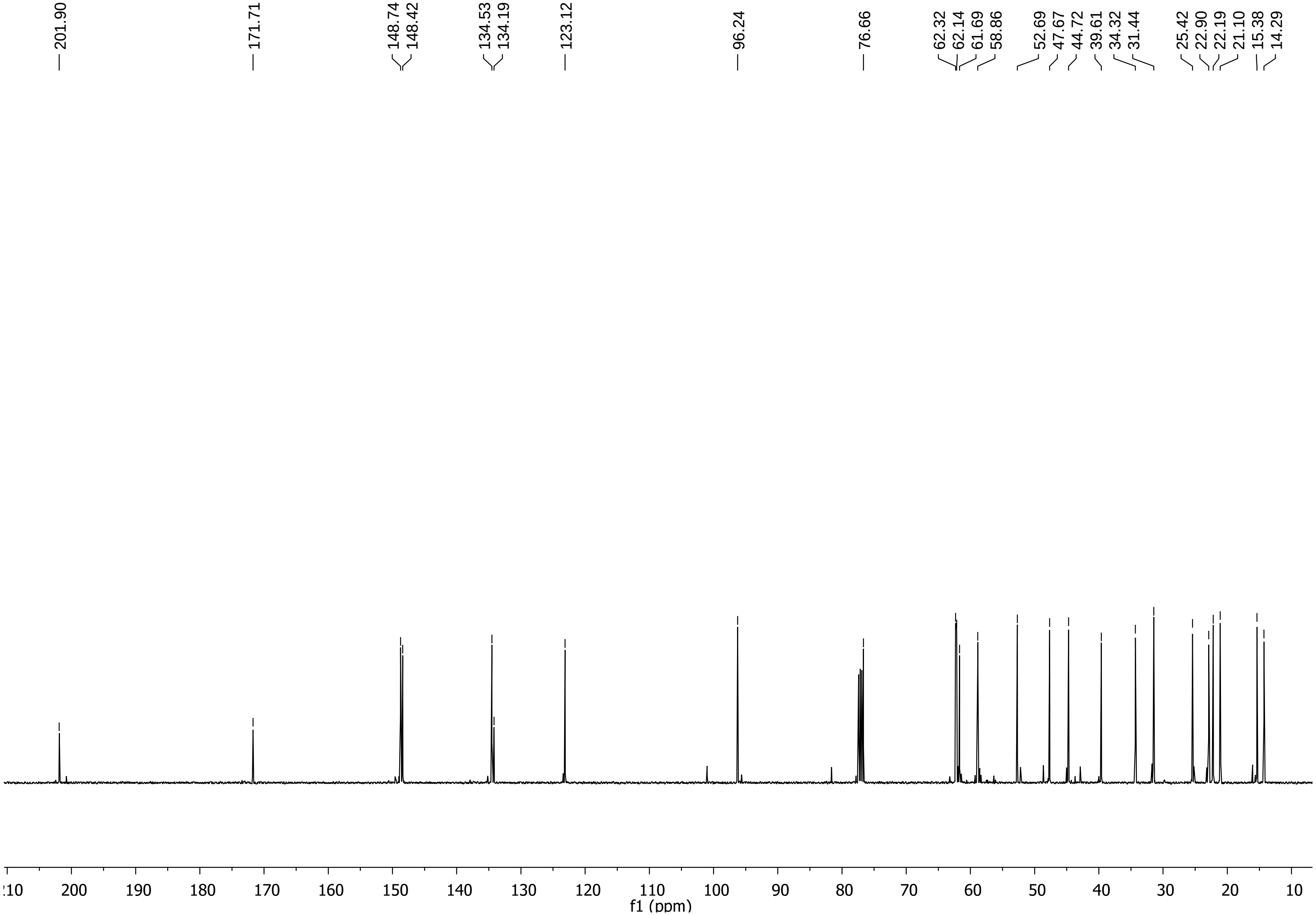

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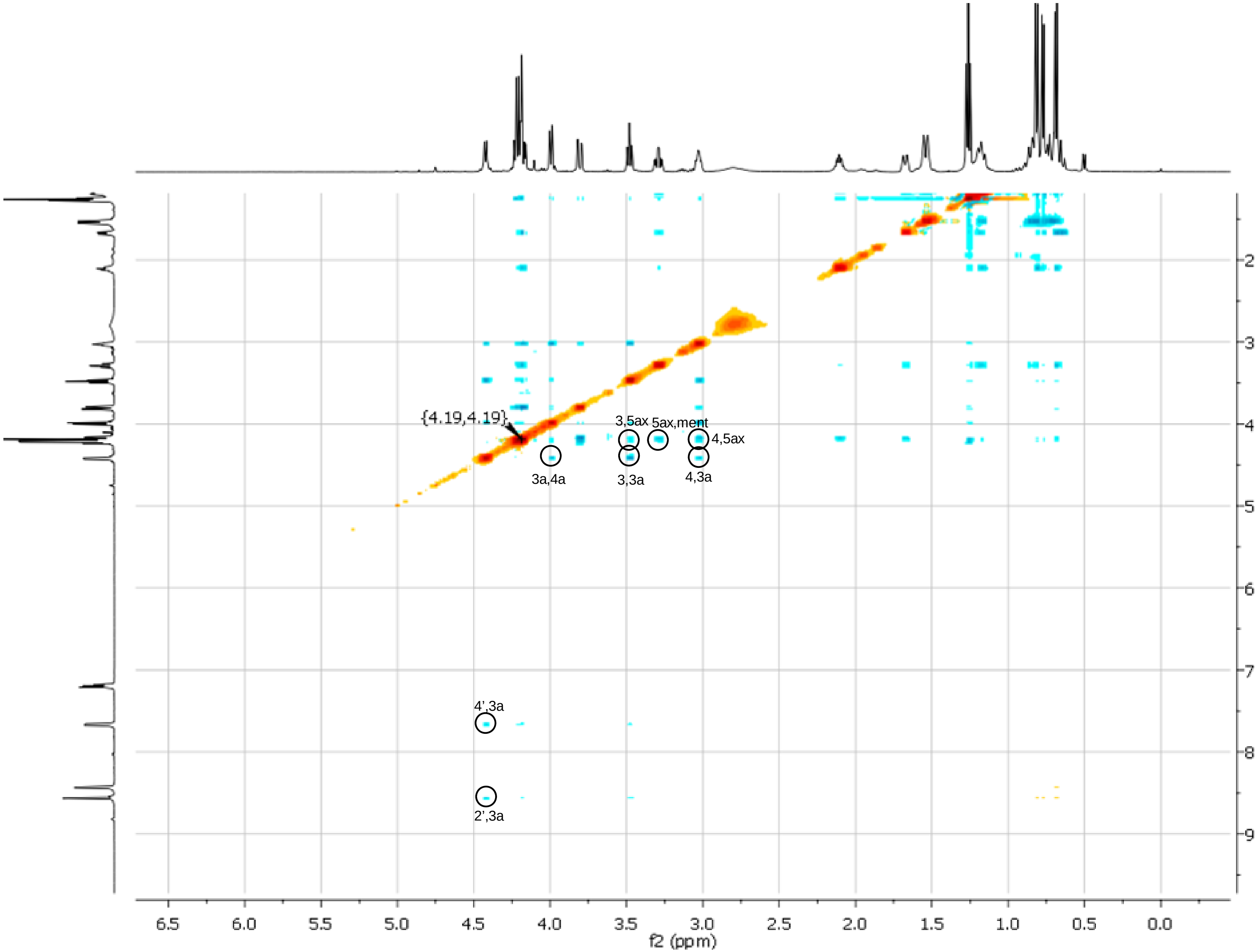

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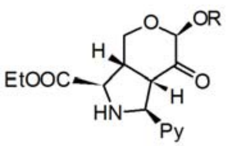

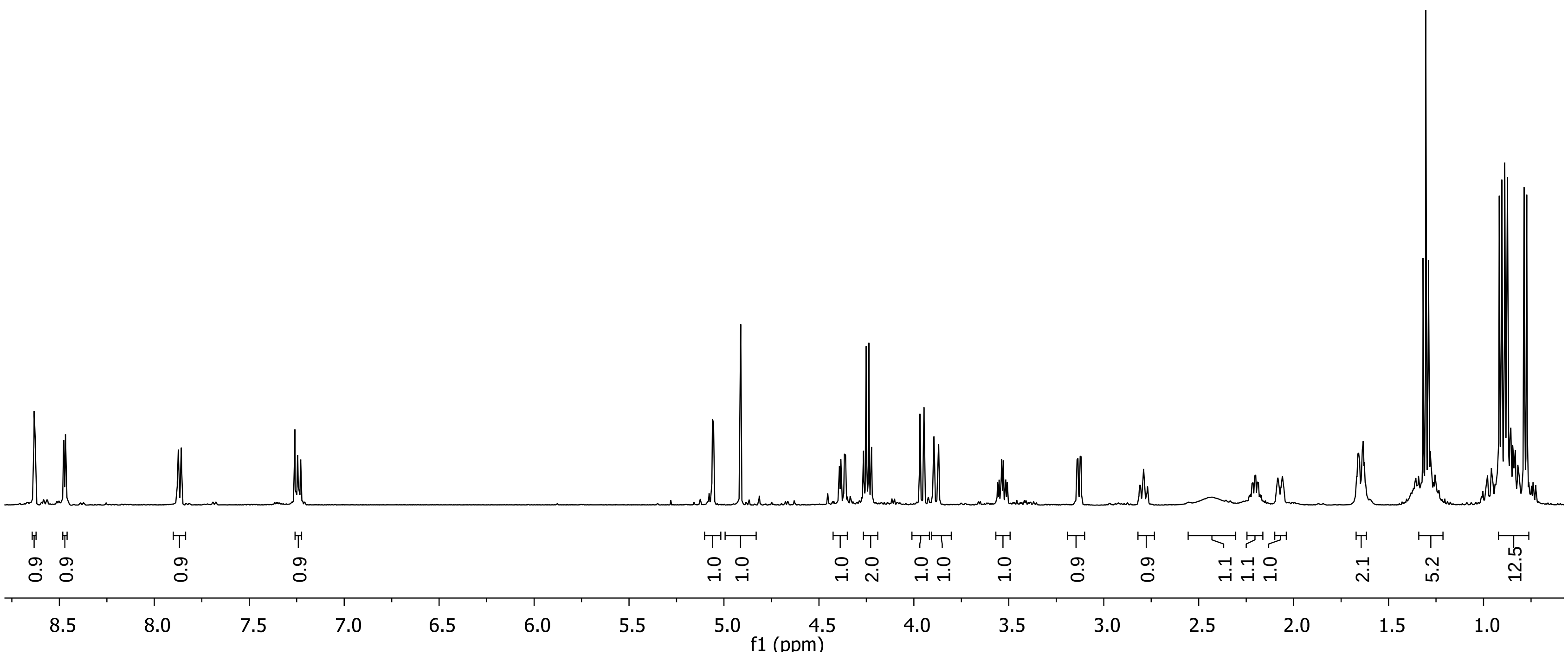

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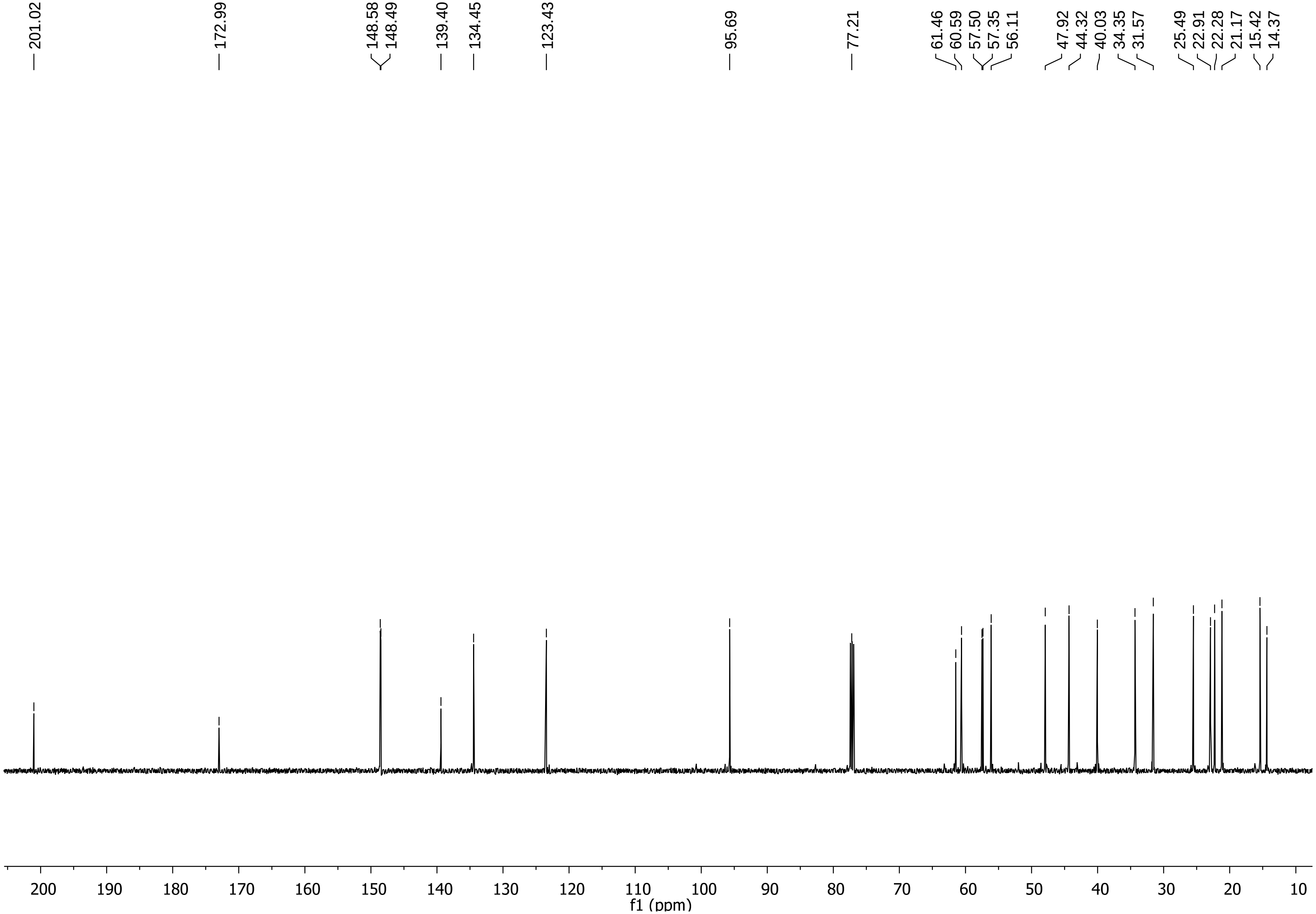

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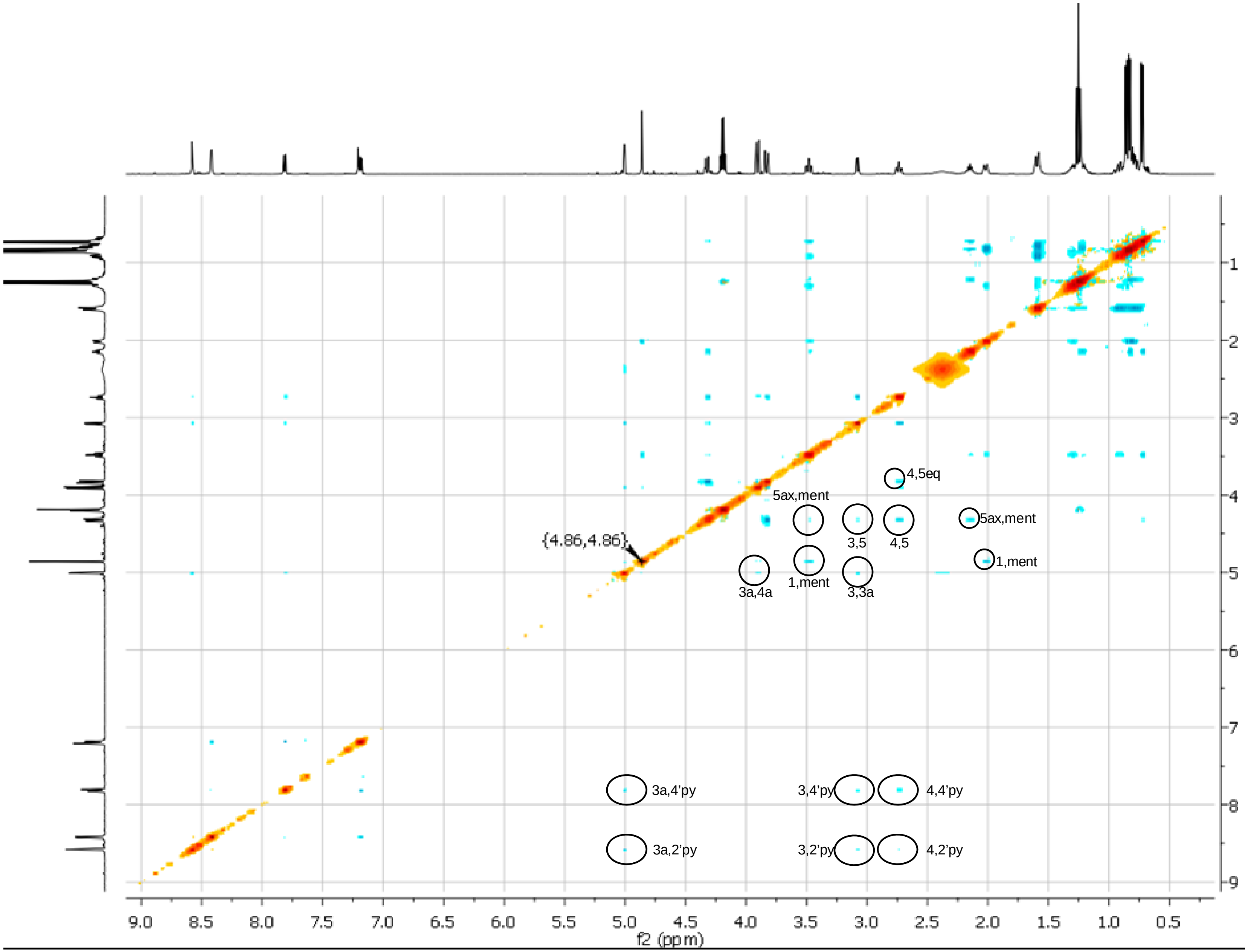

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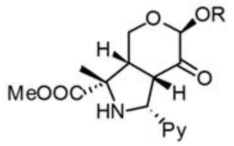

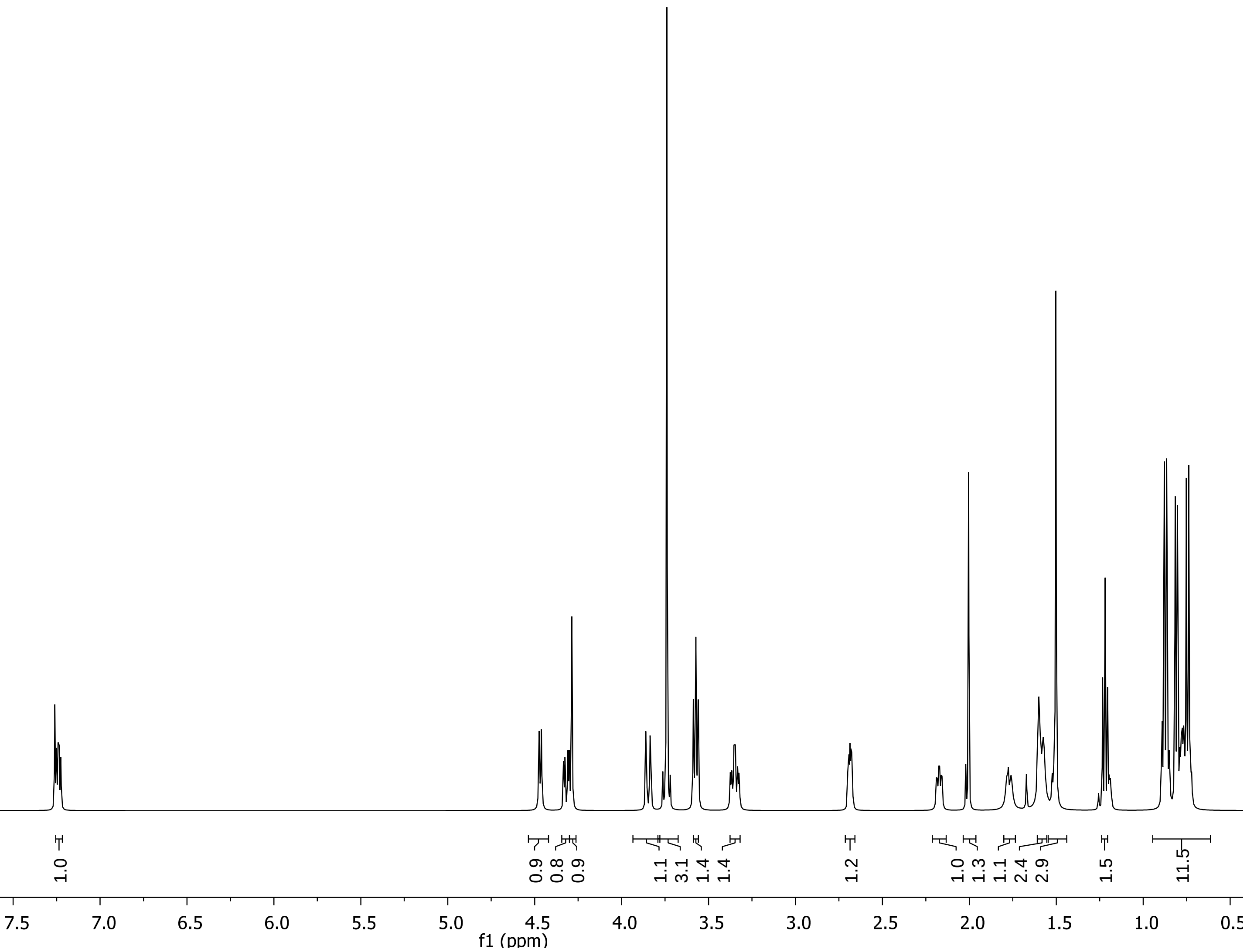

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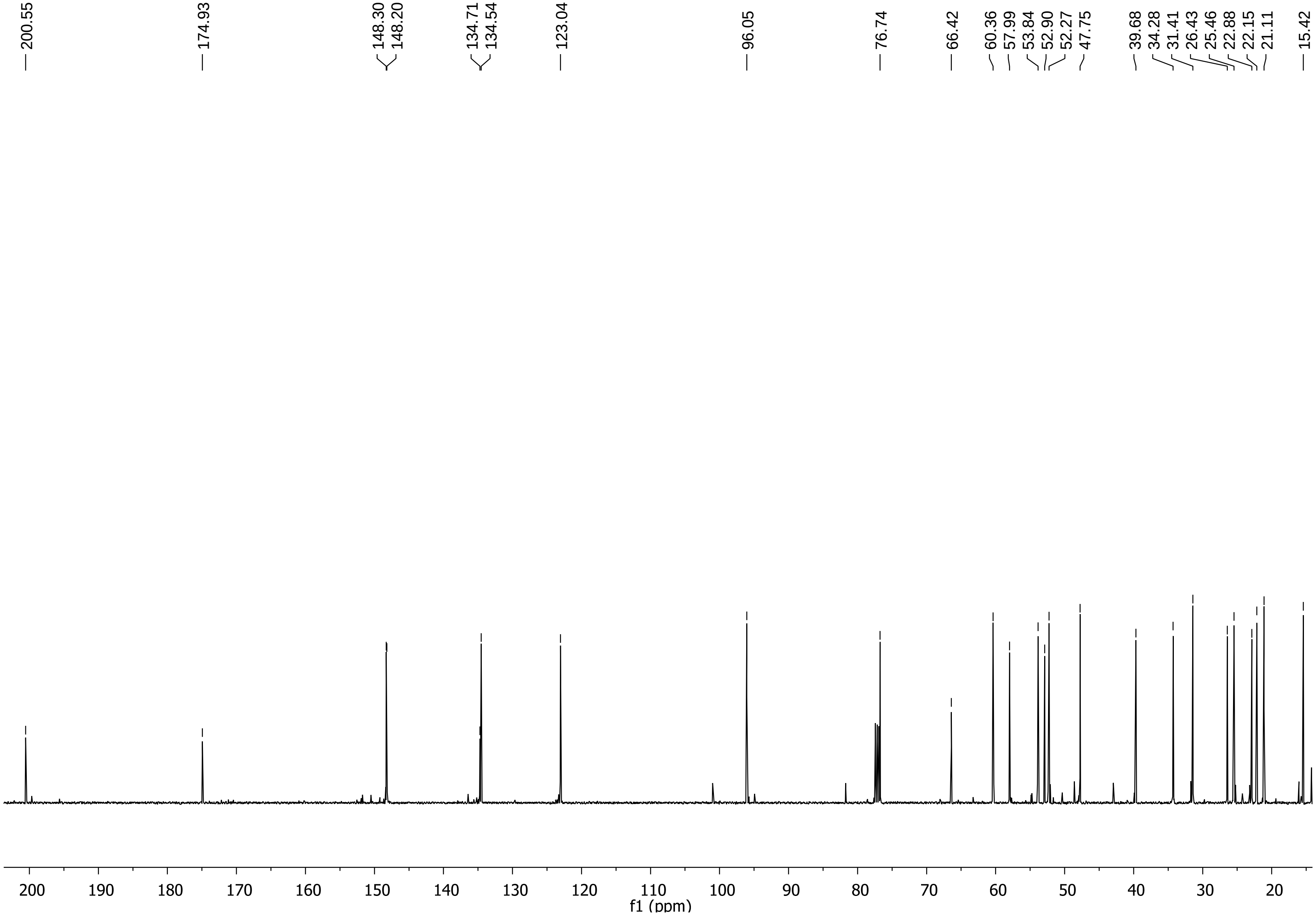

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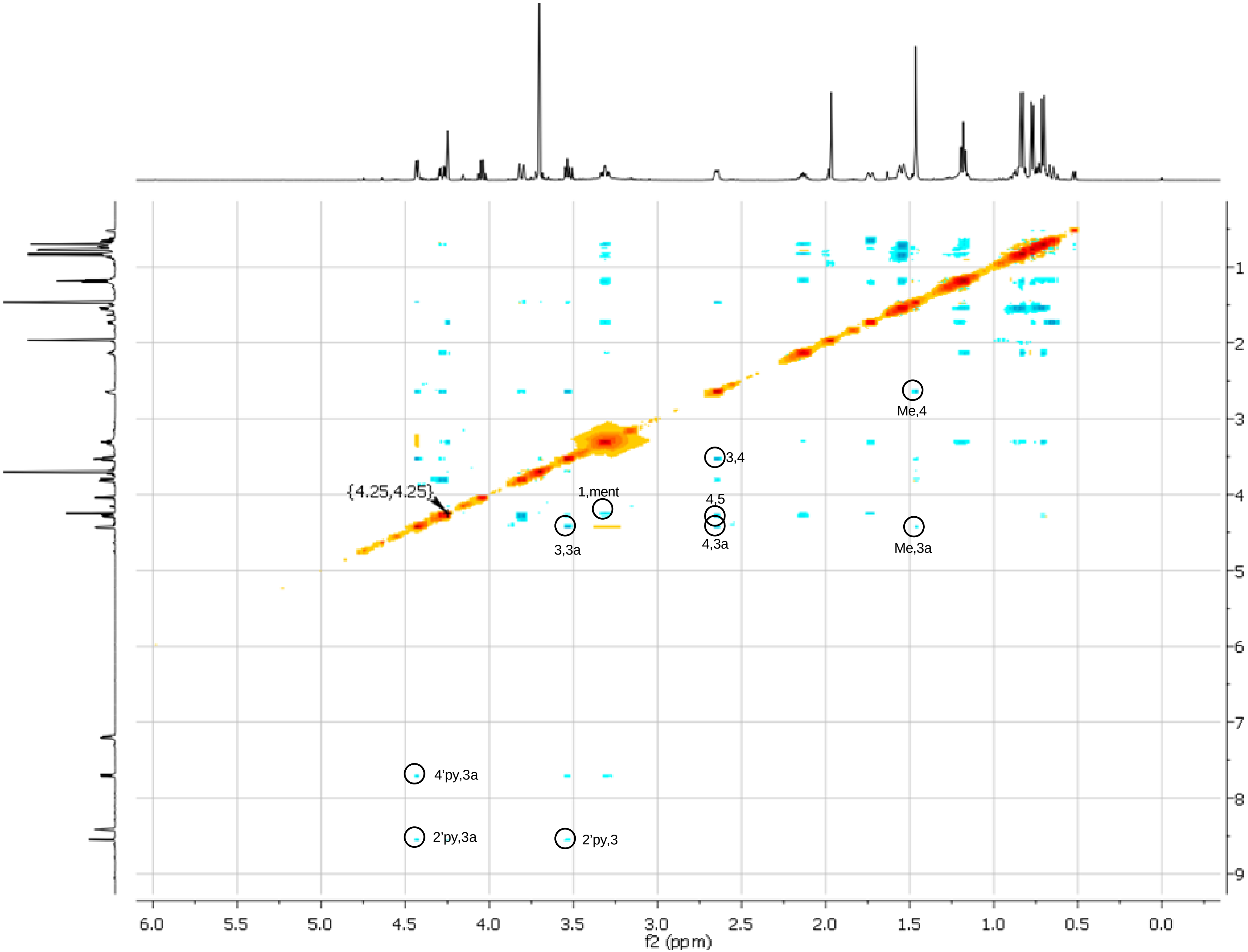

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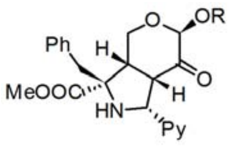

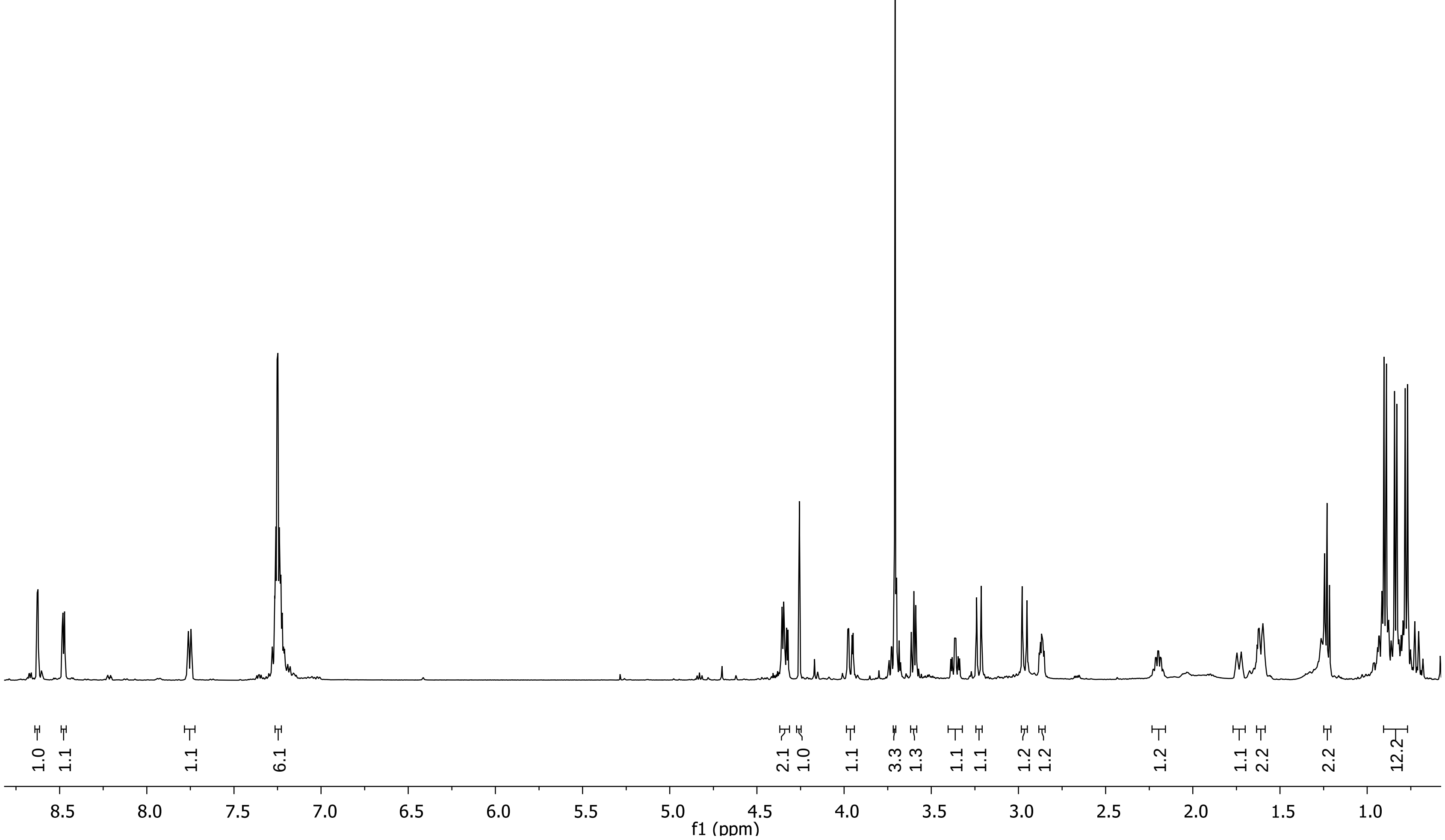

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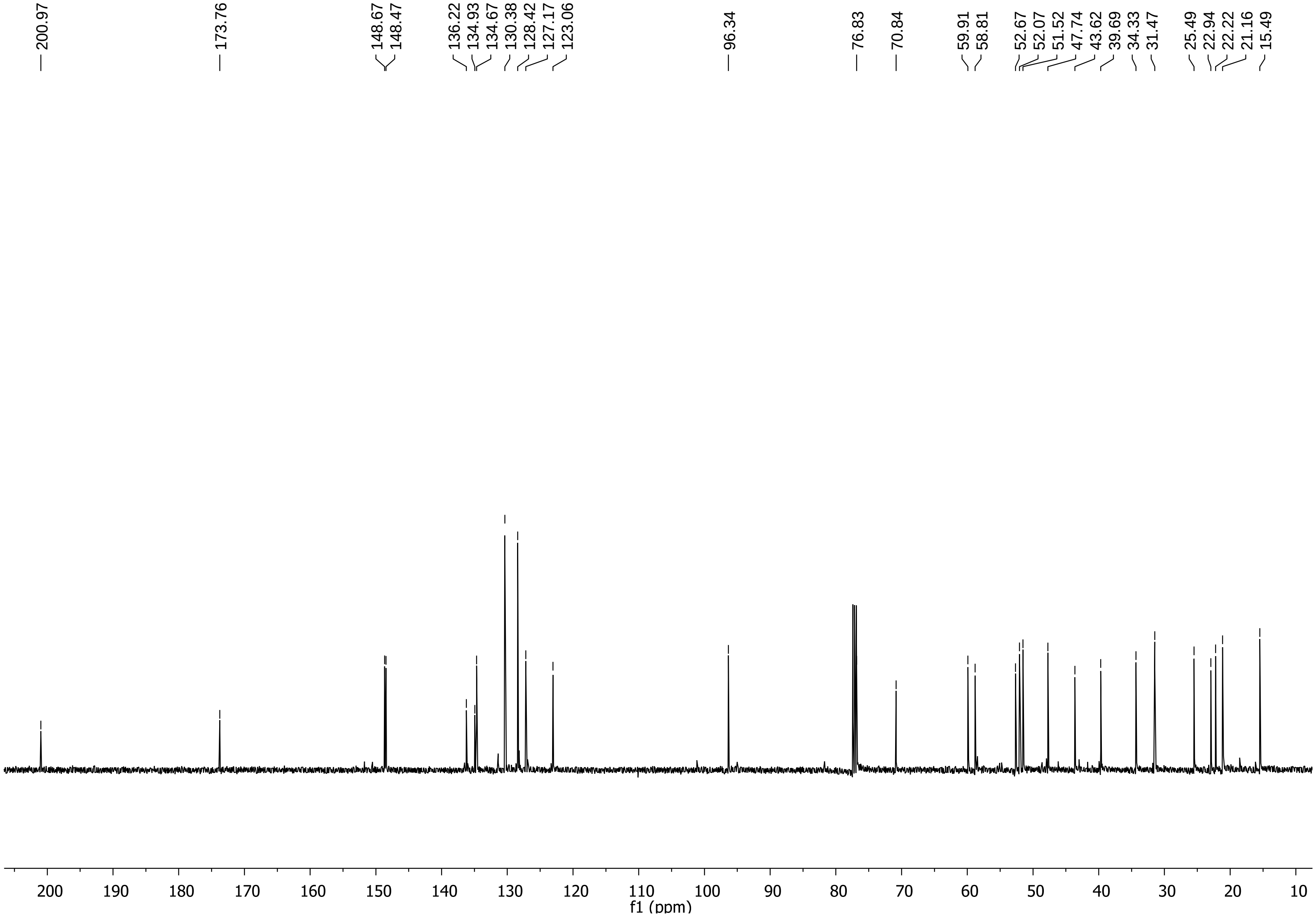

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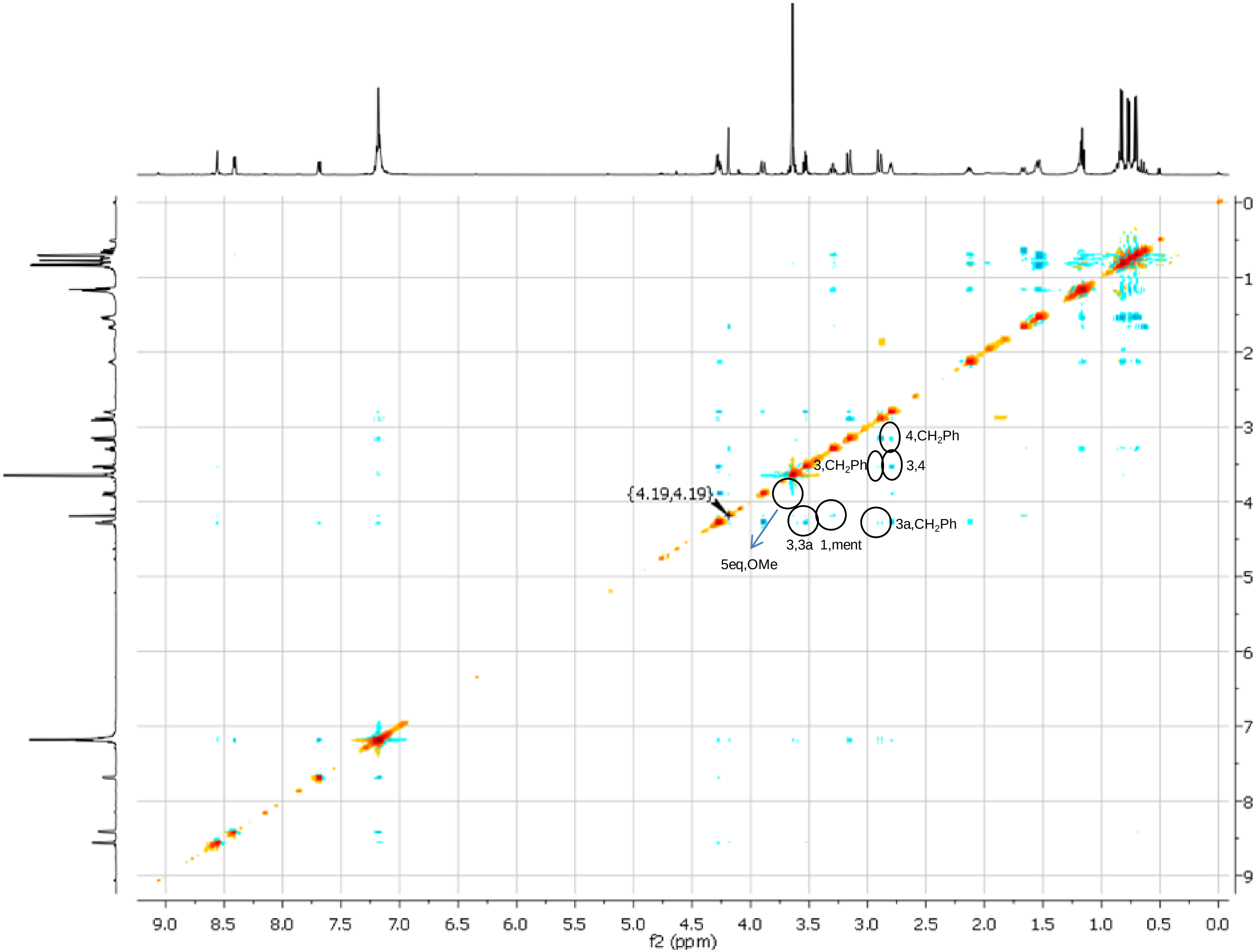

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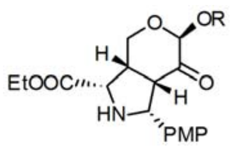

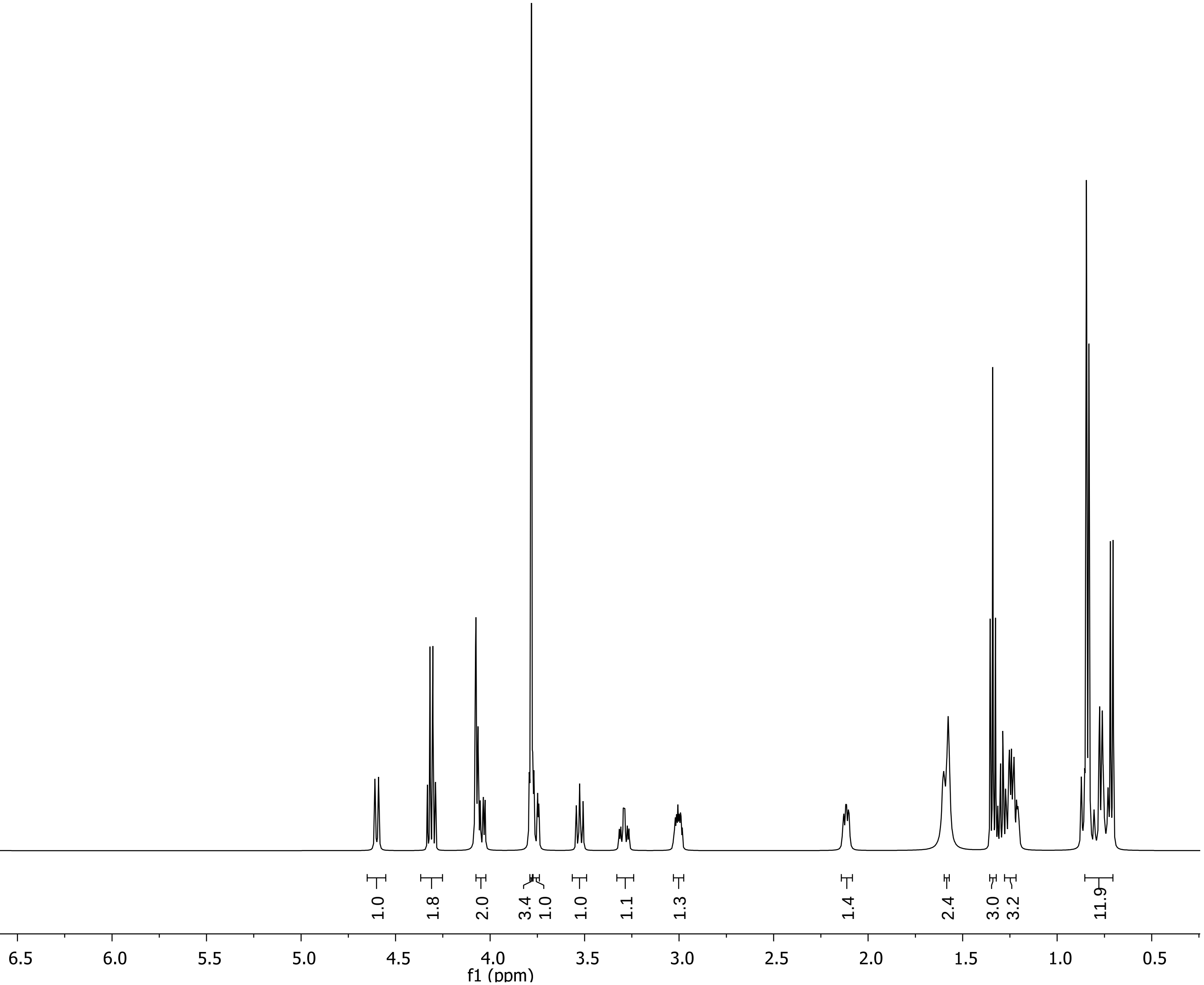

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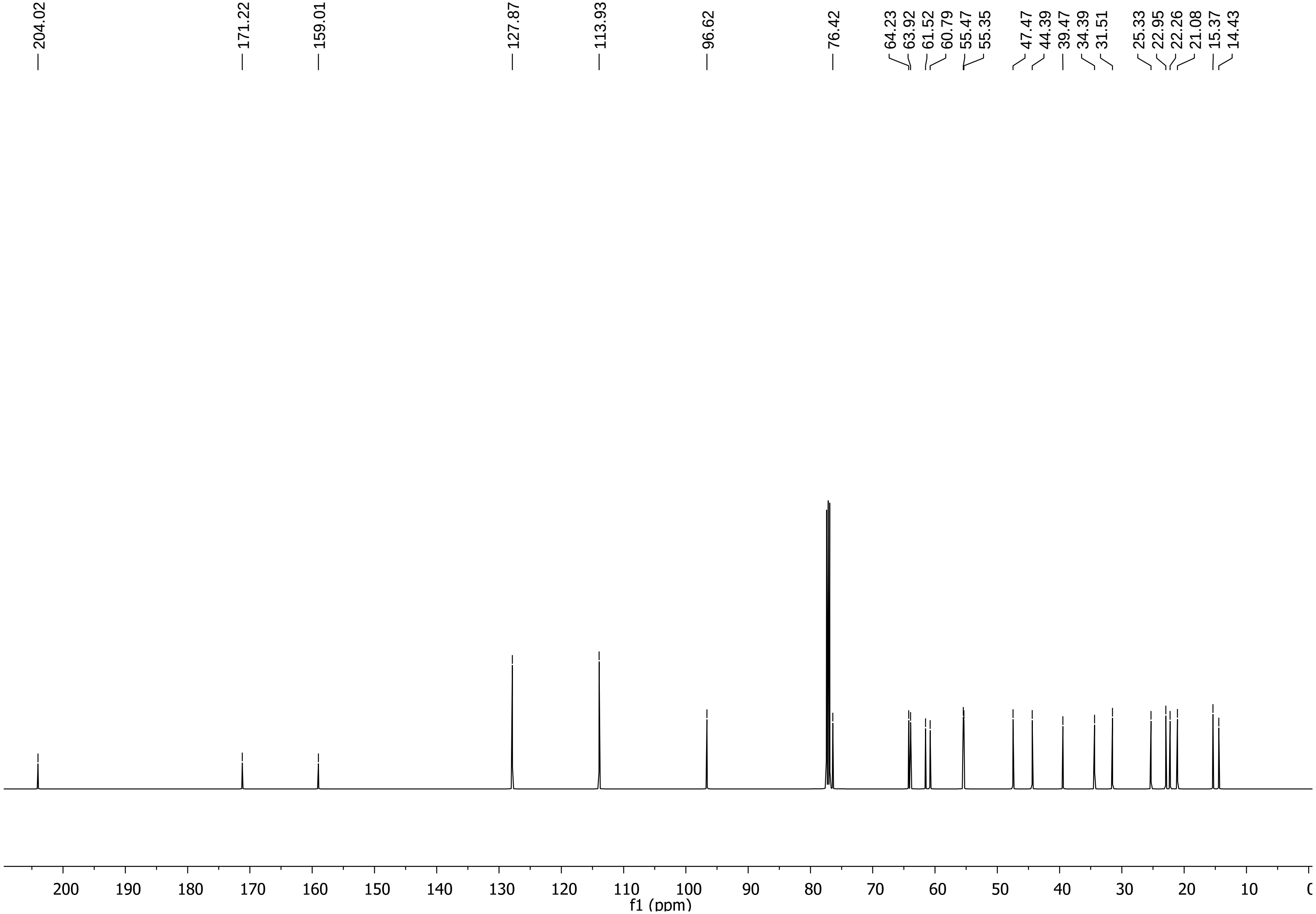

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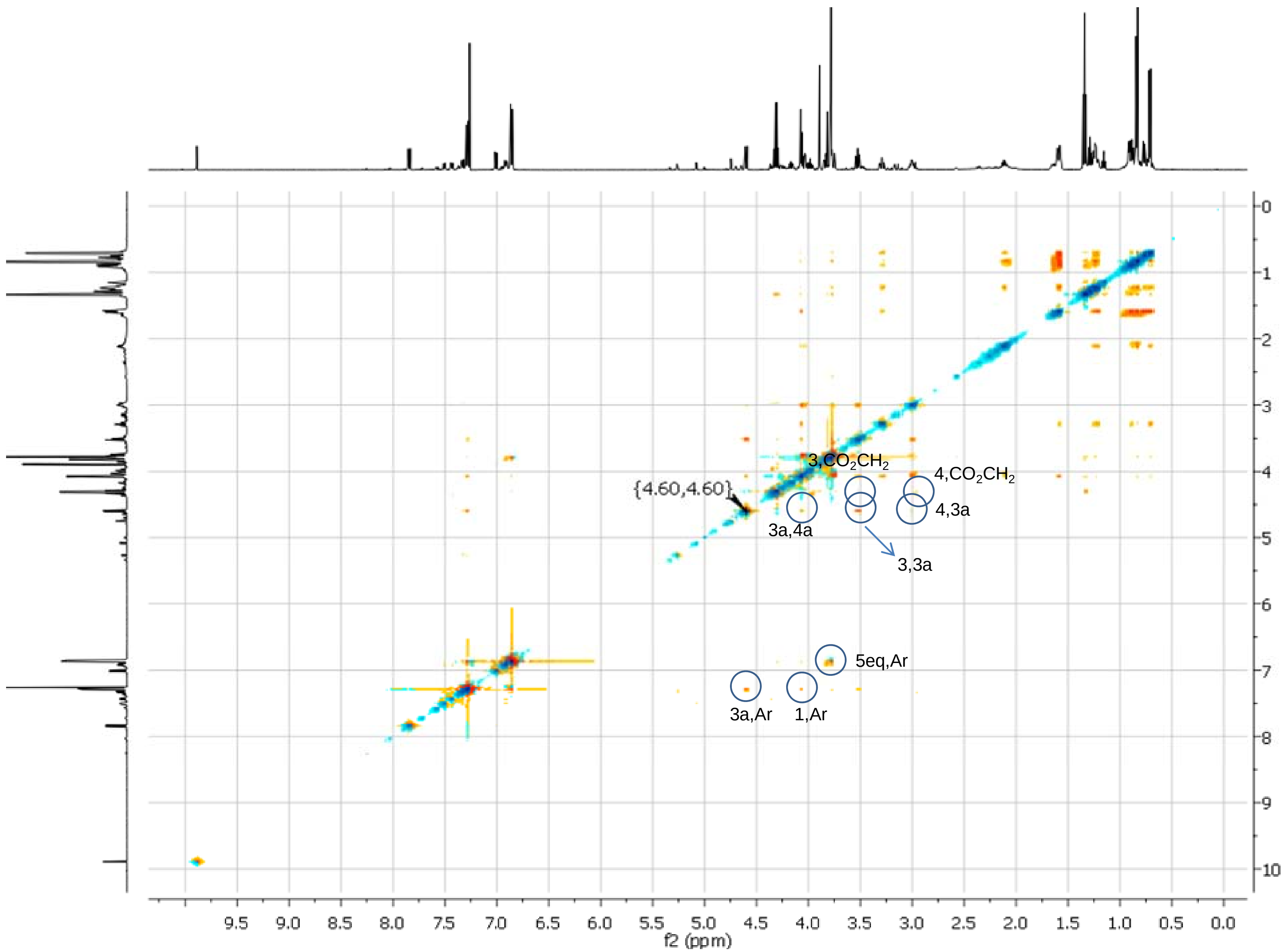

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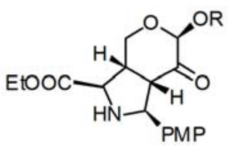

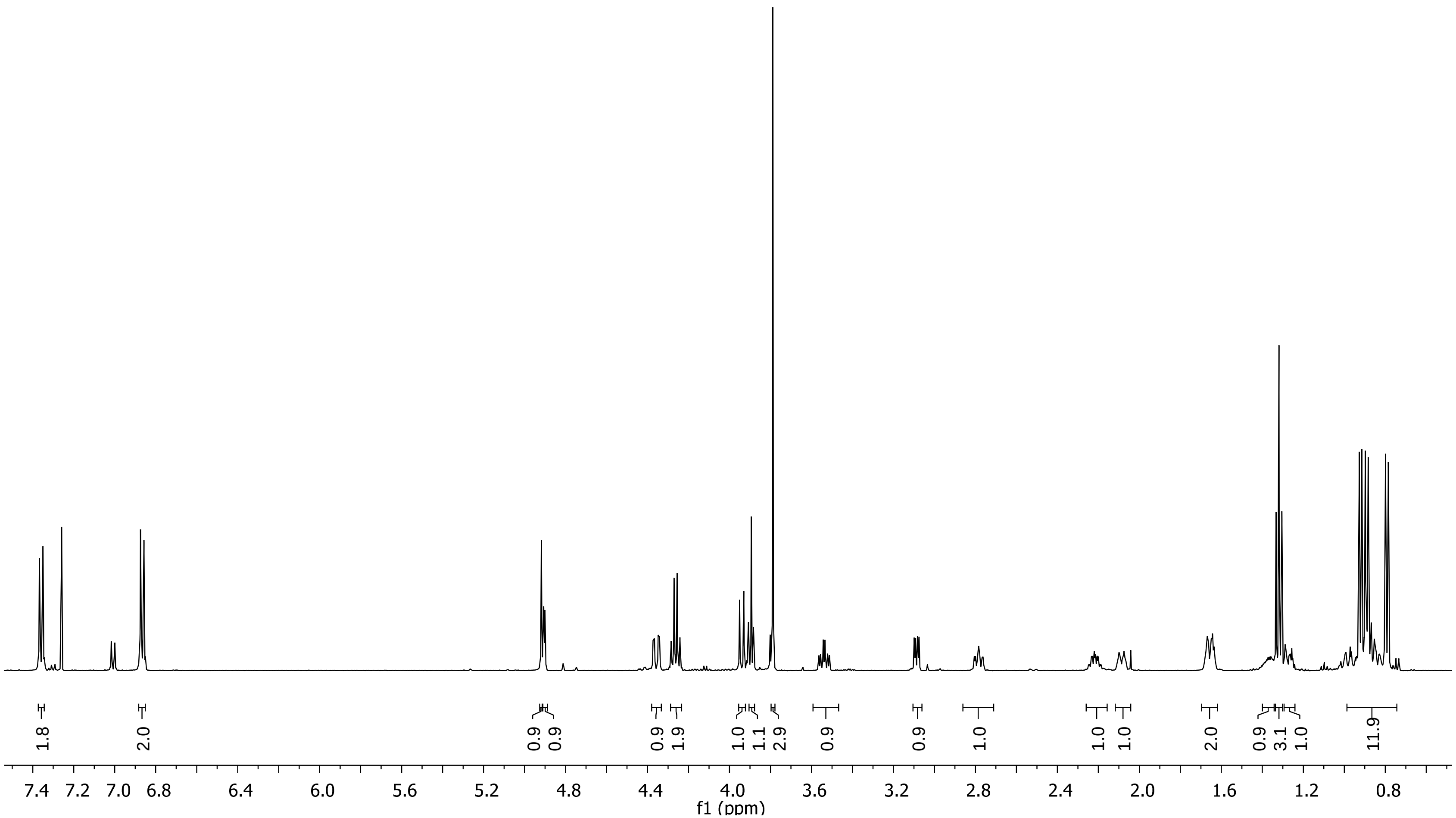

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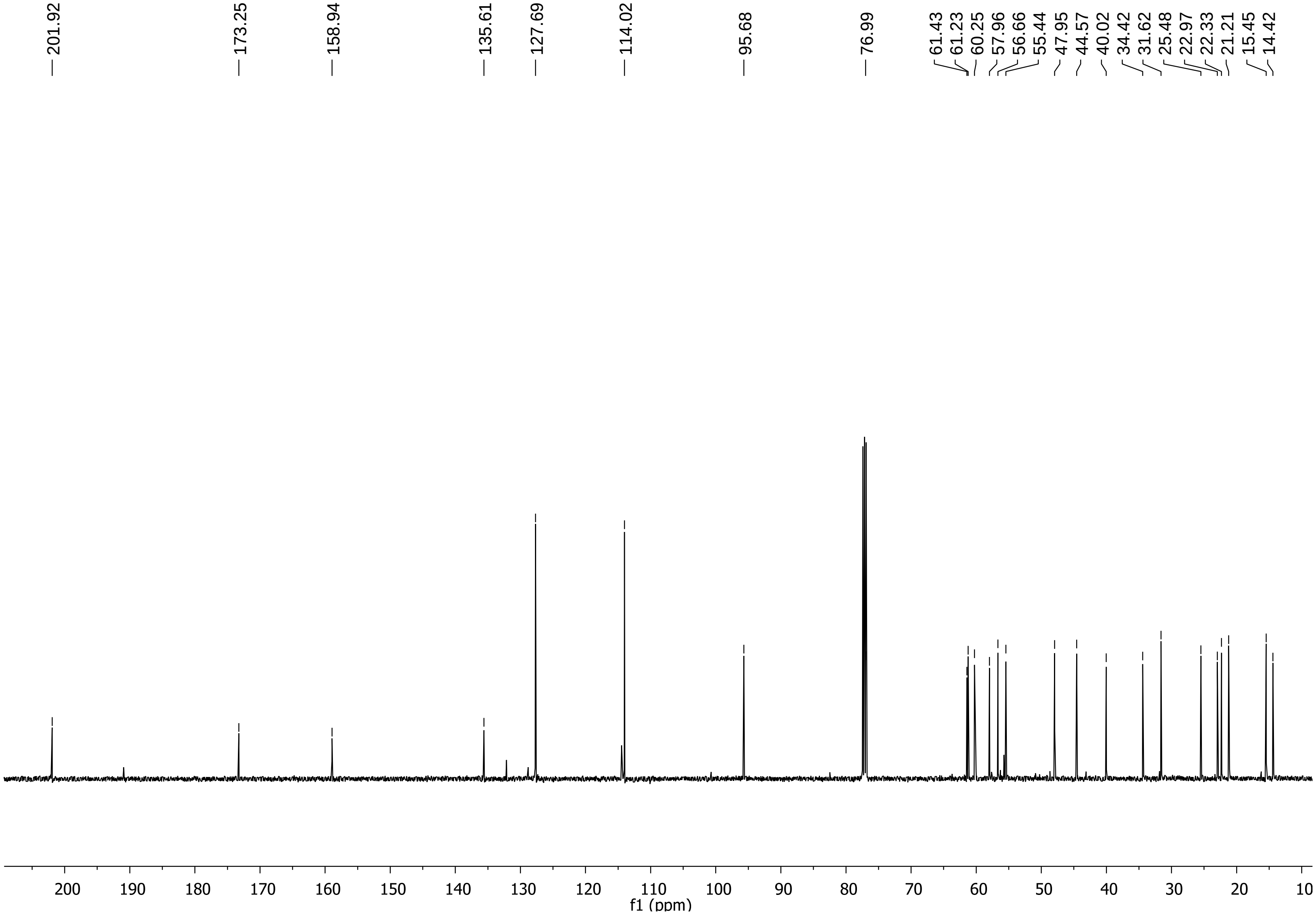
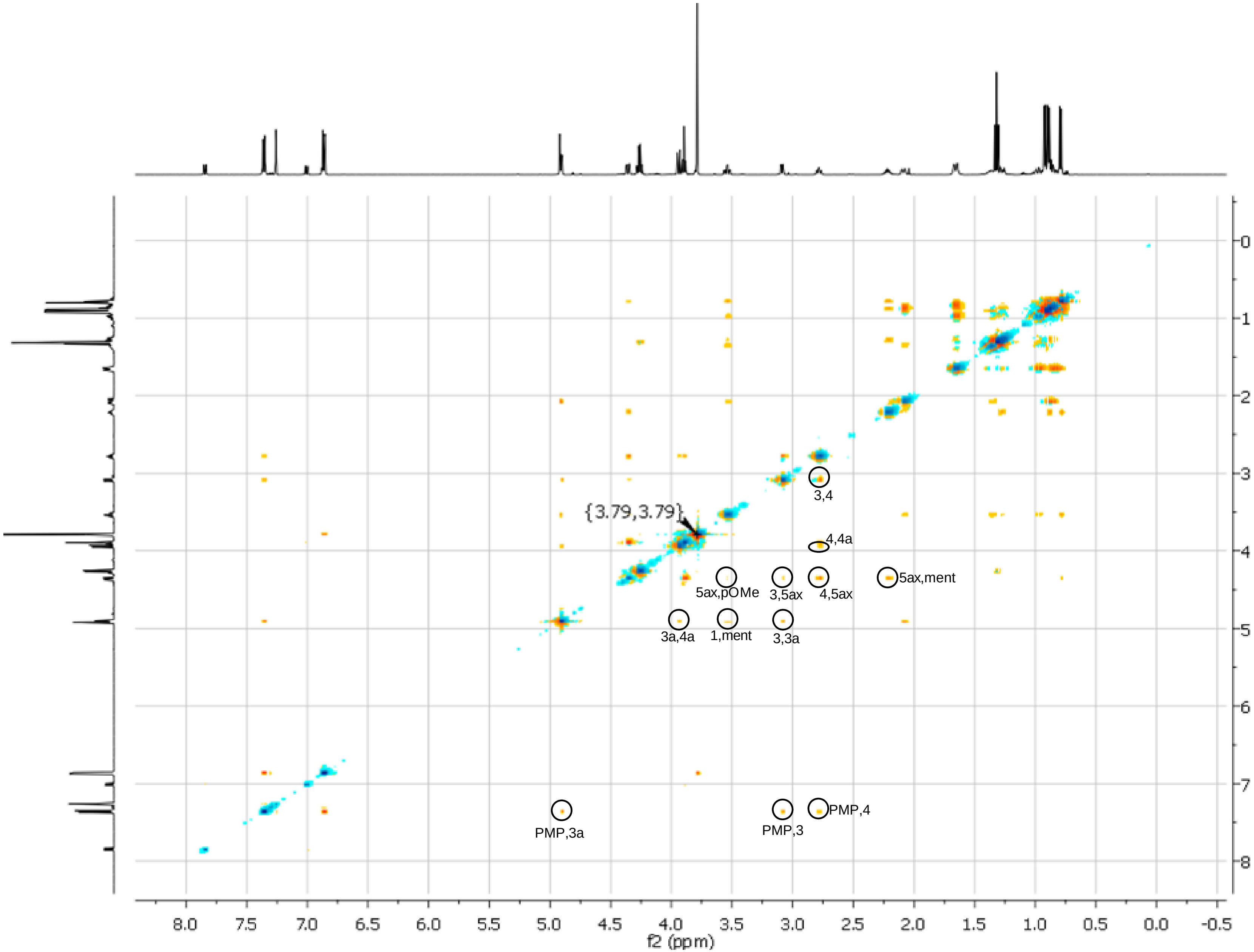


NOESY of compound **17**



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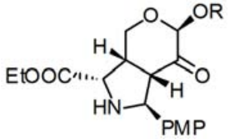

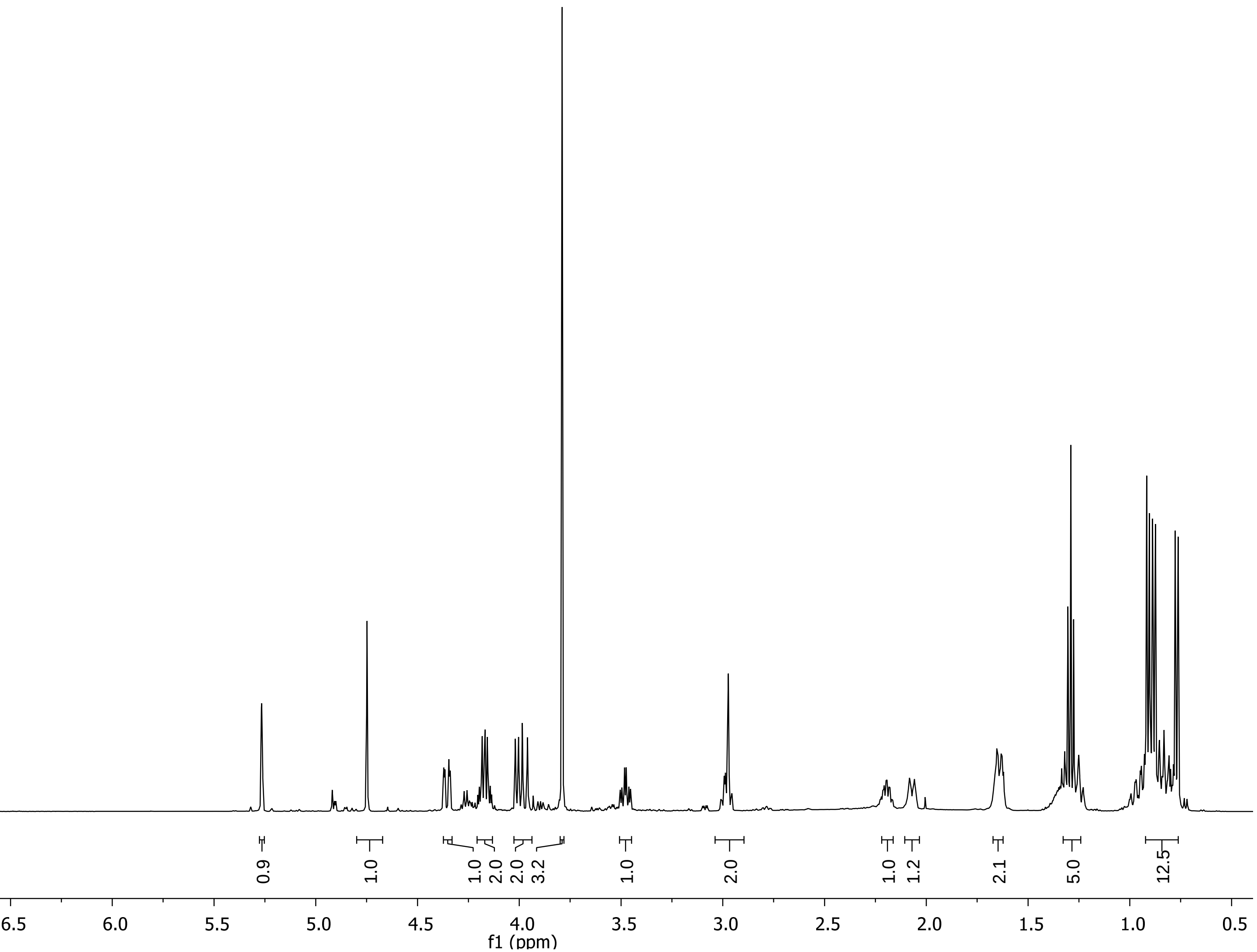

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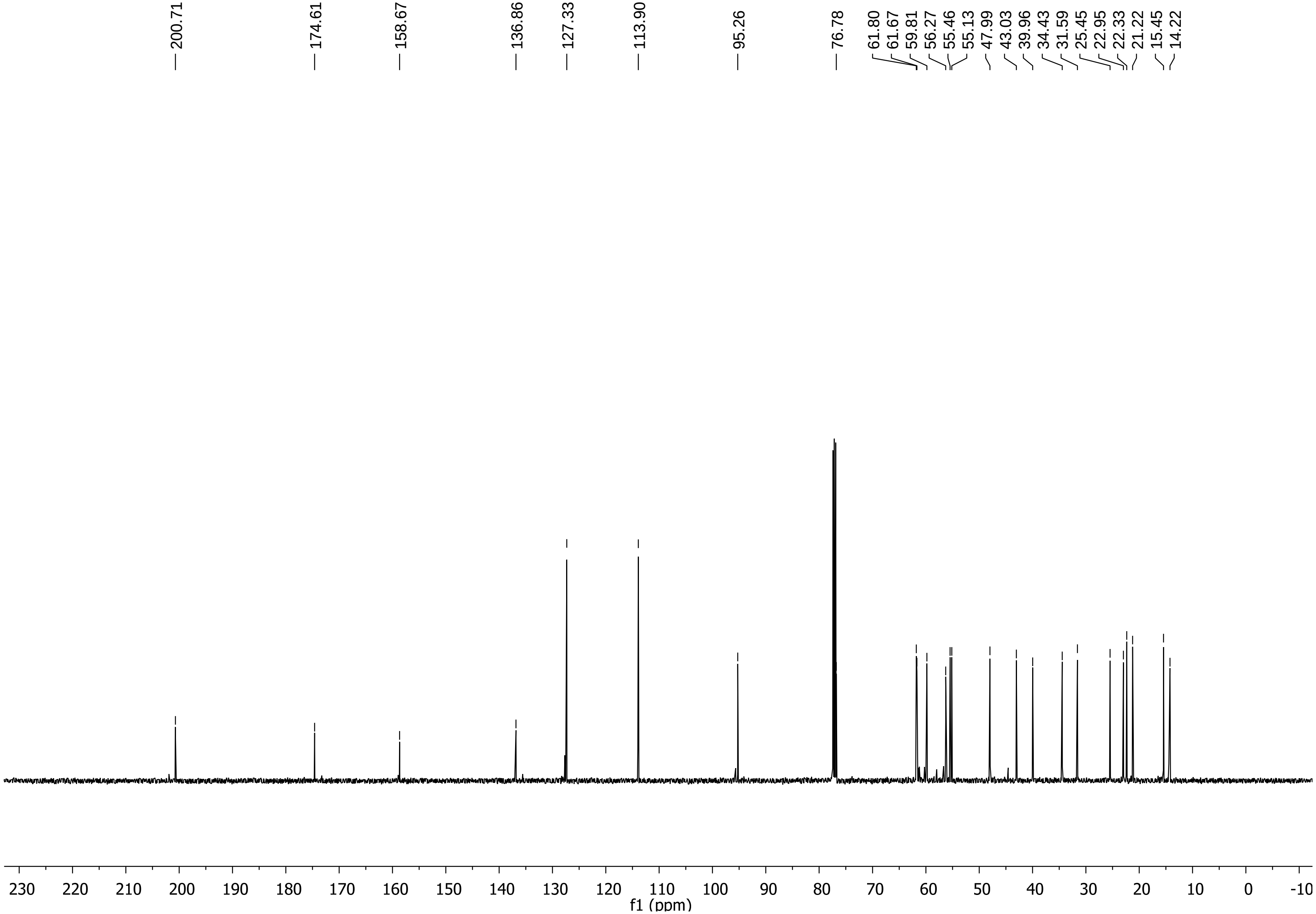
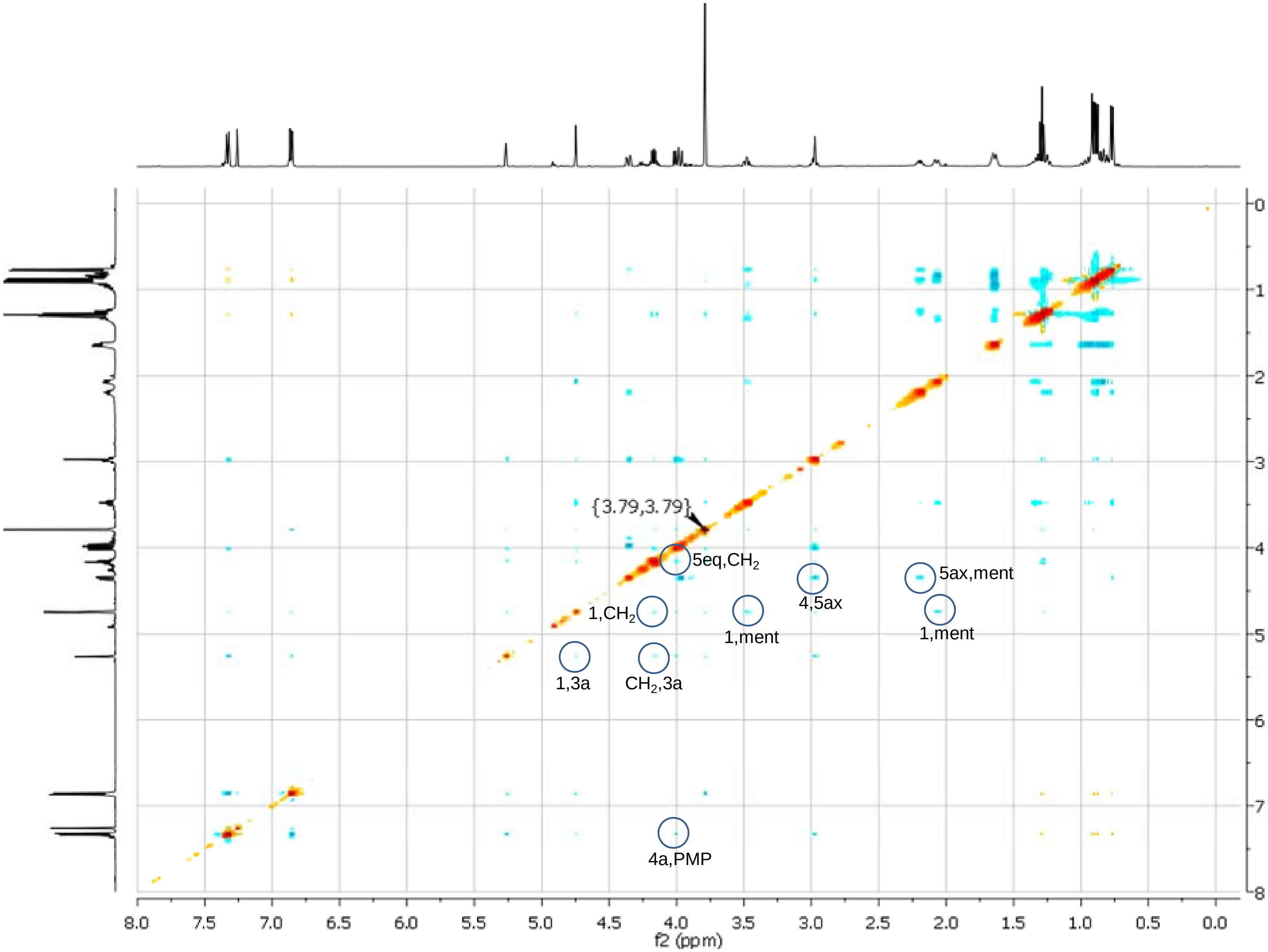
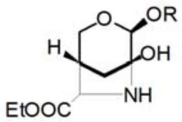
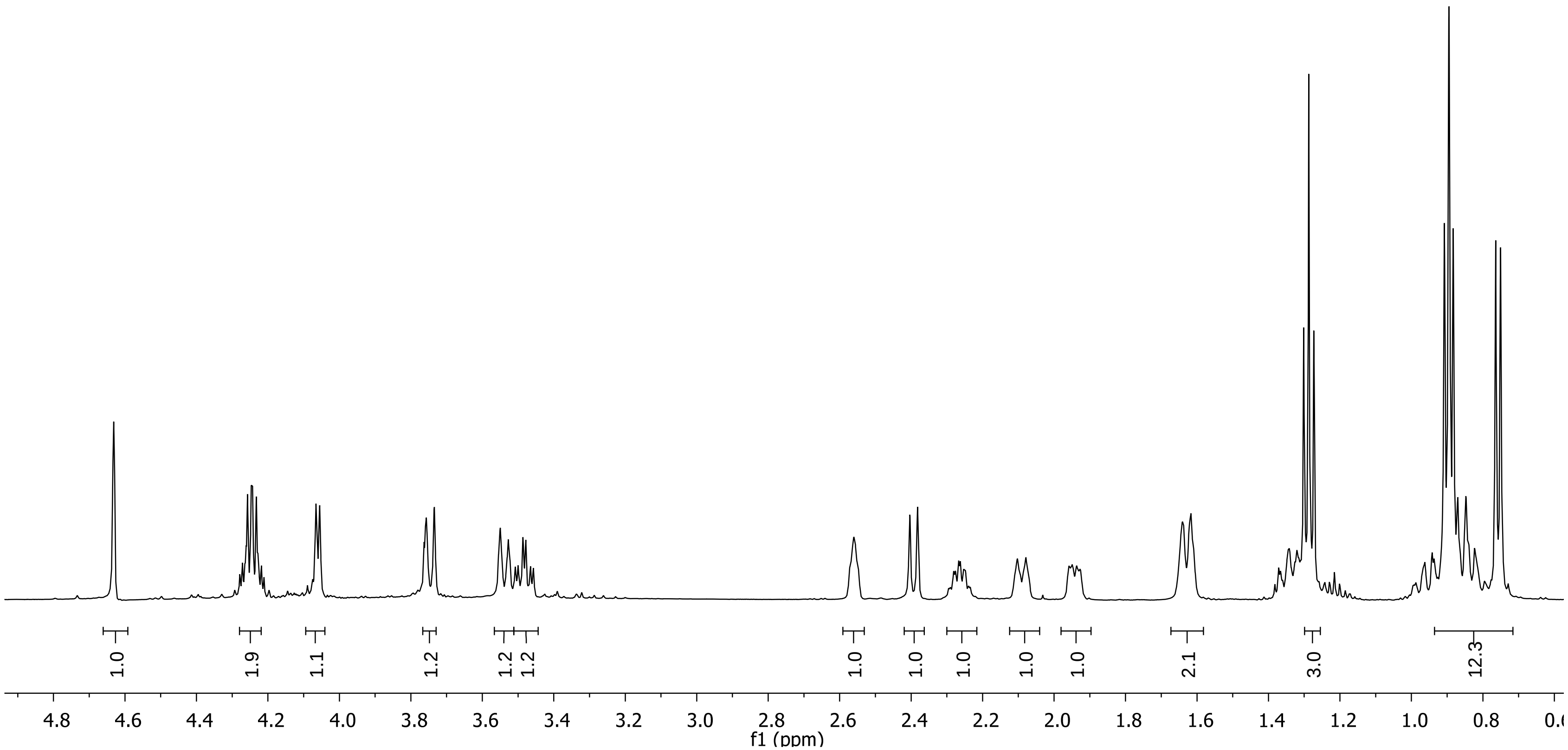


NOESY of compound **18**

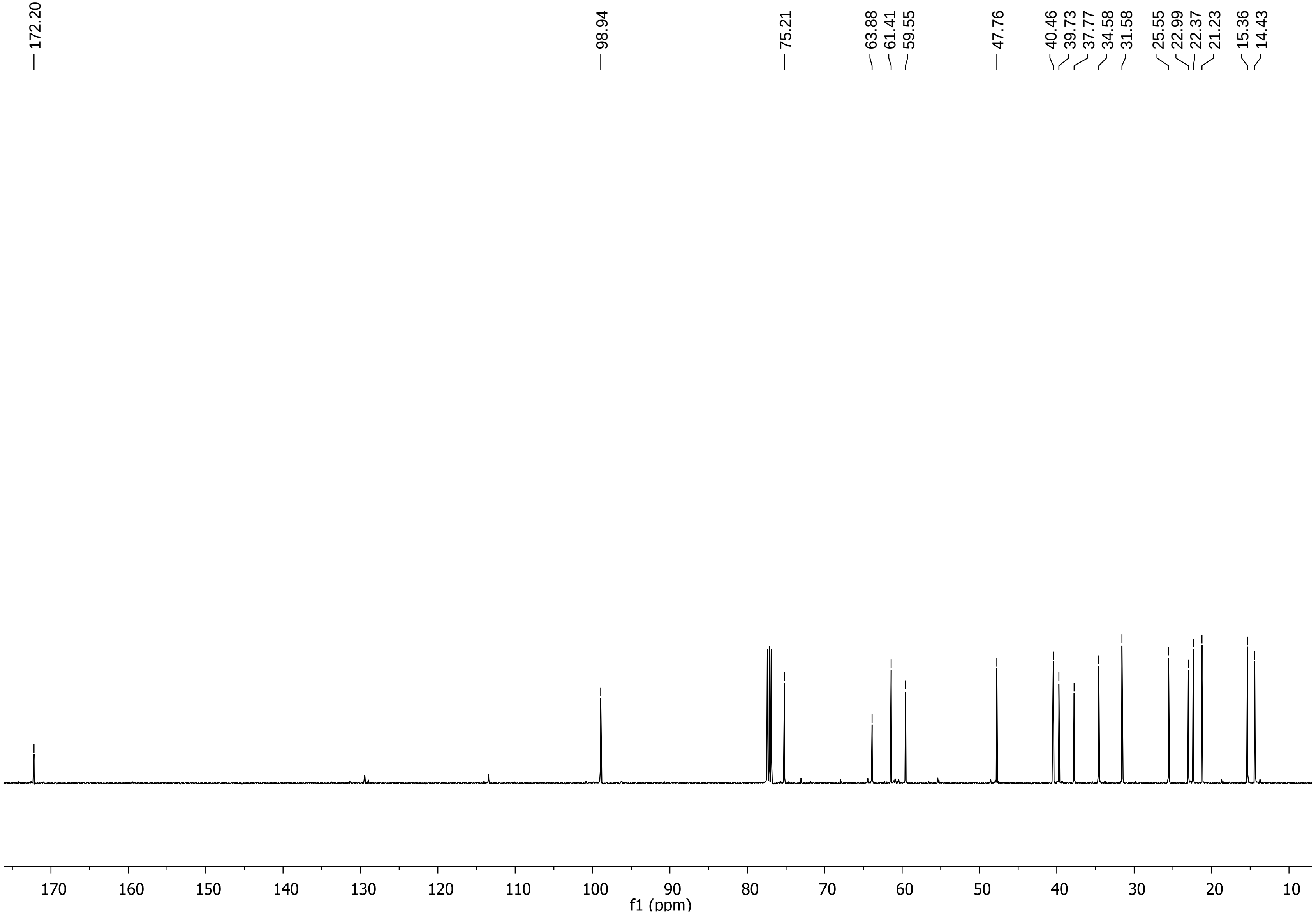


[1]H NMR ($CDCl_3$, 500 MHz) of compound **19**

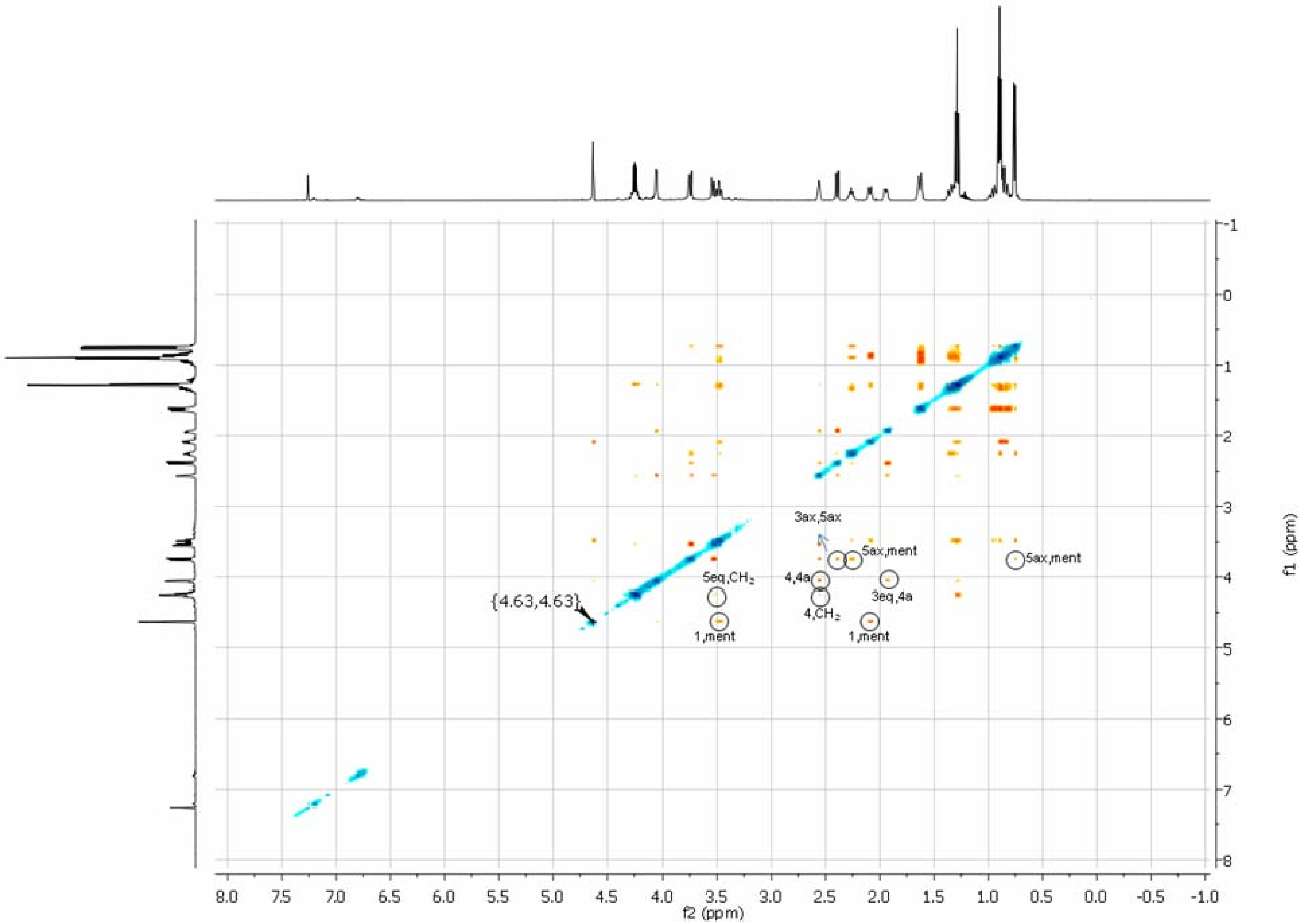




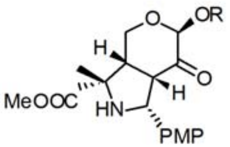
^{13}C NMR ($CDCl_3$, 125.7 MHz) of compound **19**

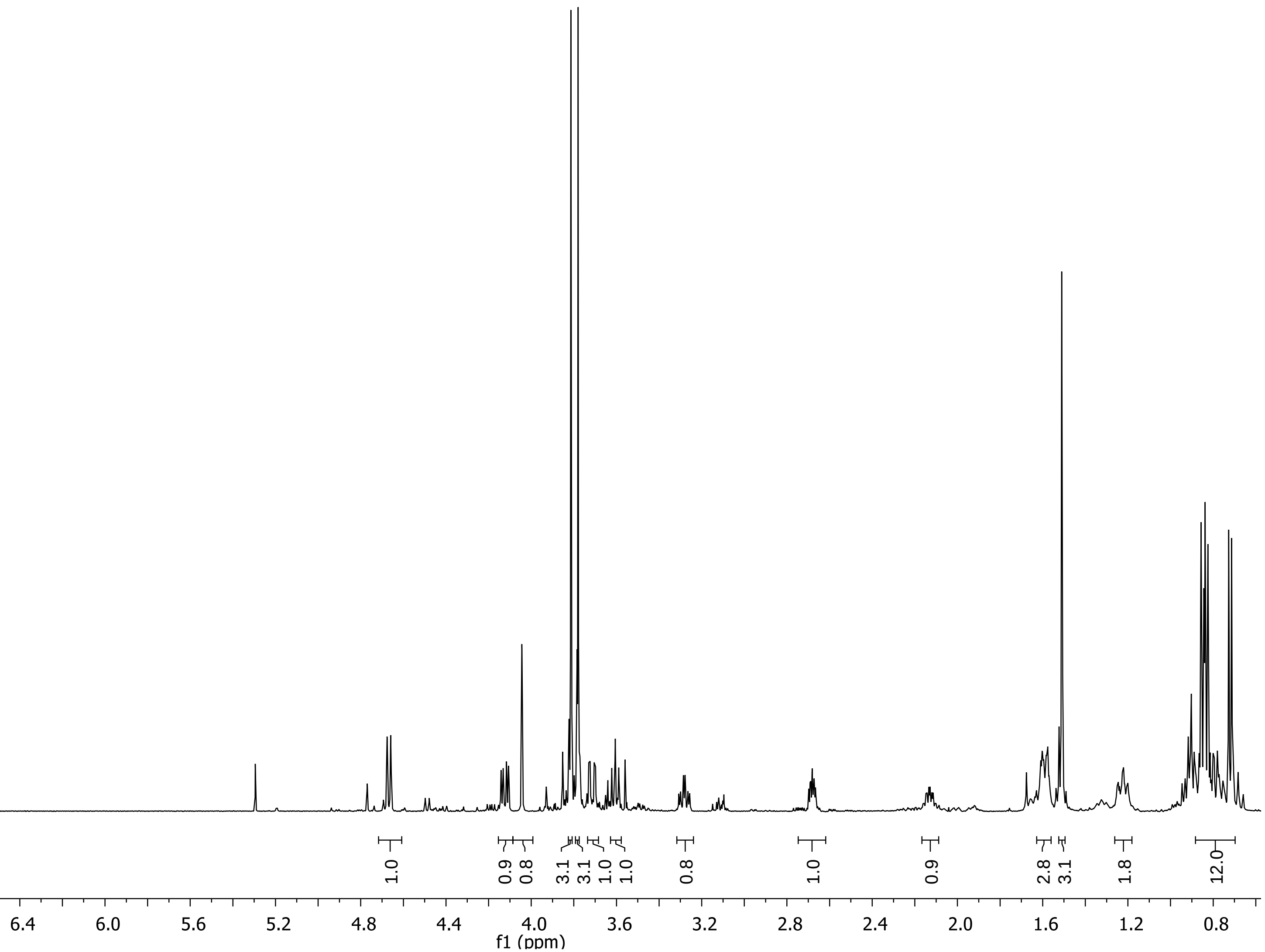


NOESY of compound **19**

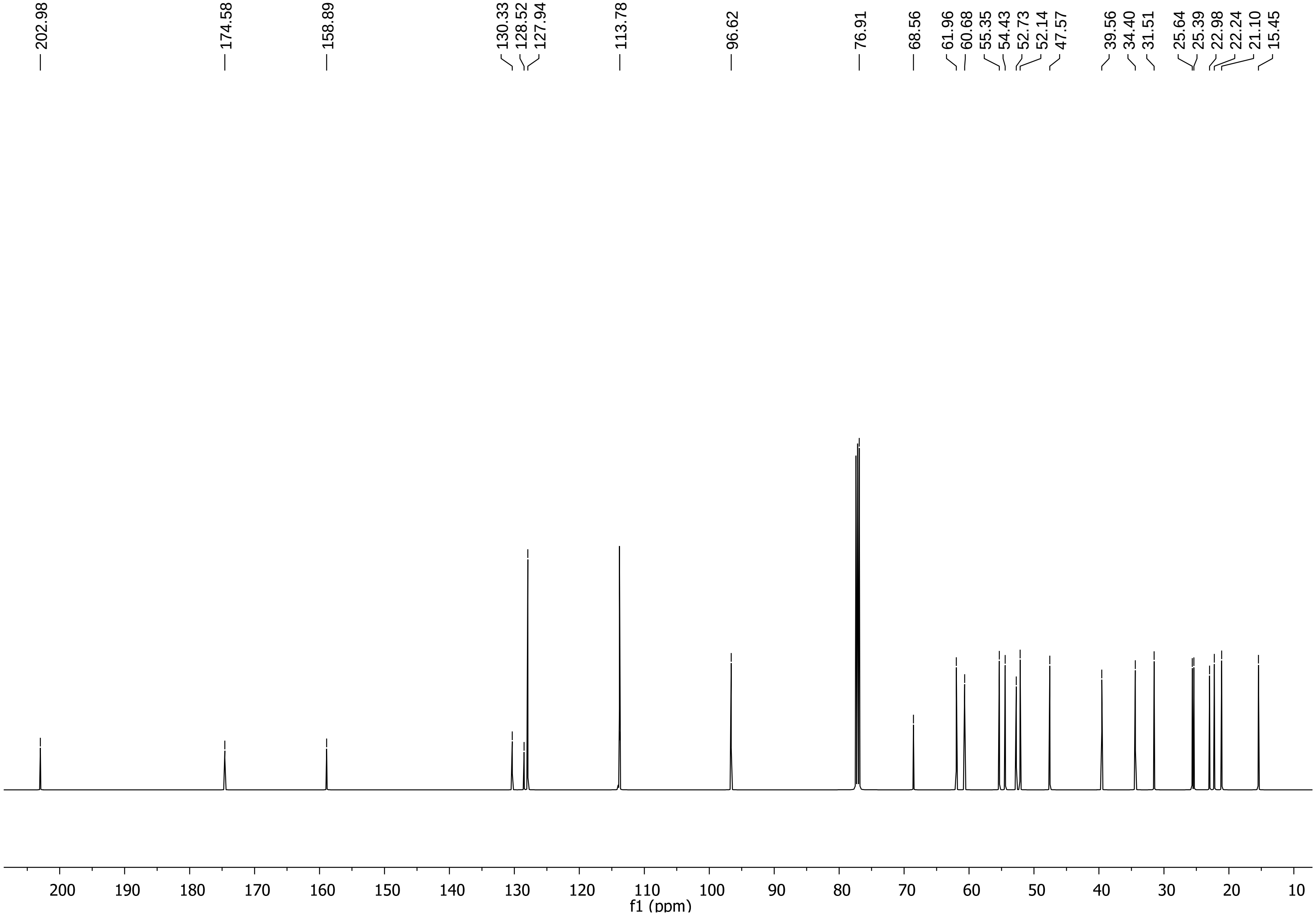


^{1}H NMR ($CDCl_3$, 500 MHz) of compound **20**

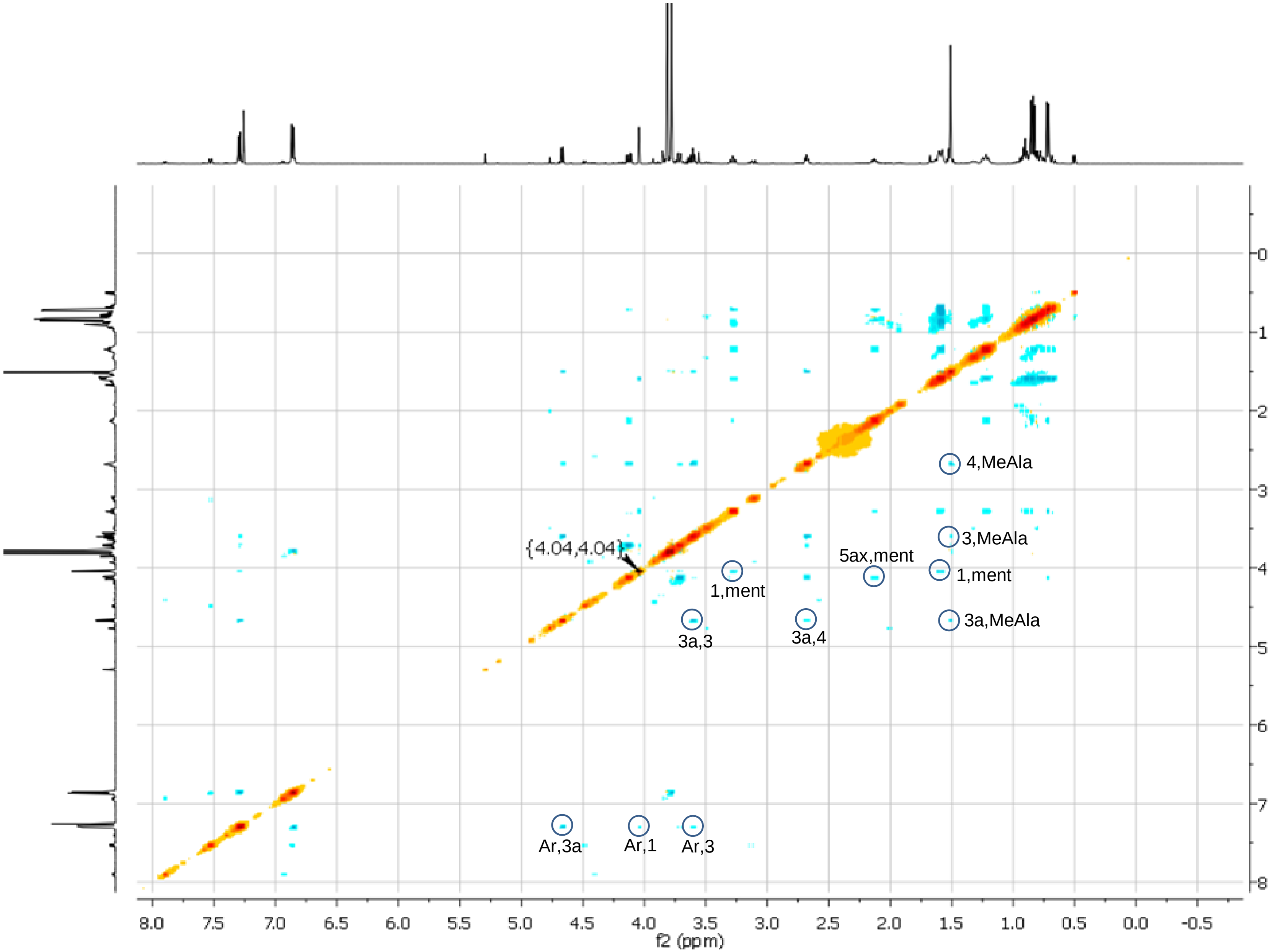




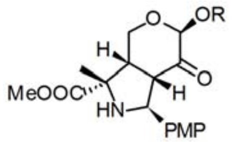
^{13}C NMR ($CDCl_3$, 125.7 MHz) of compound **20**

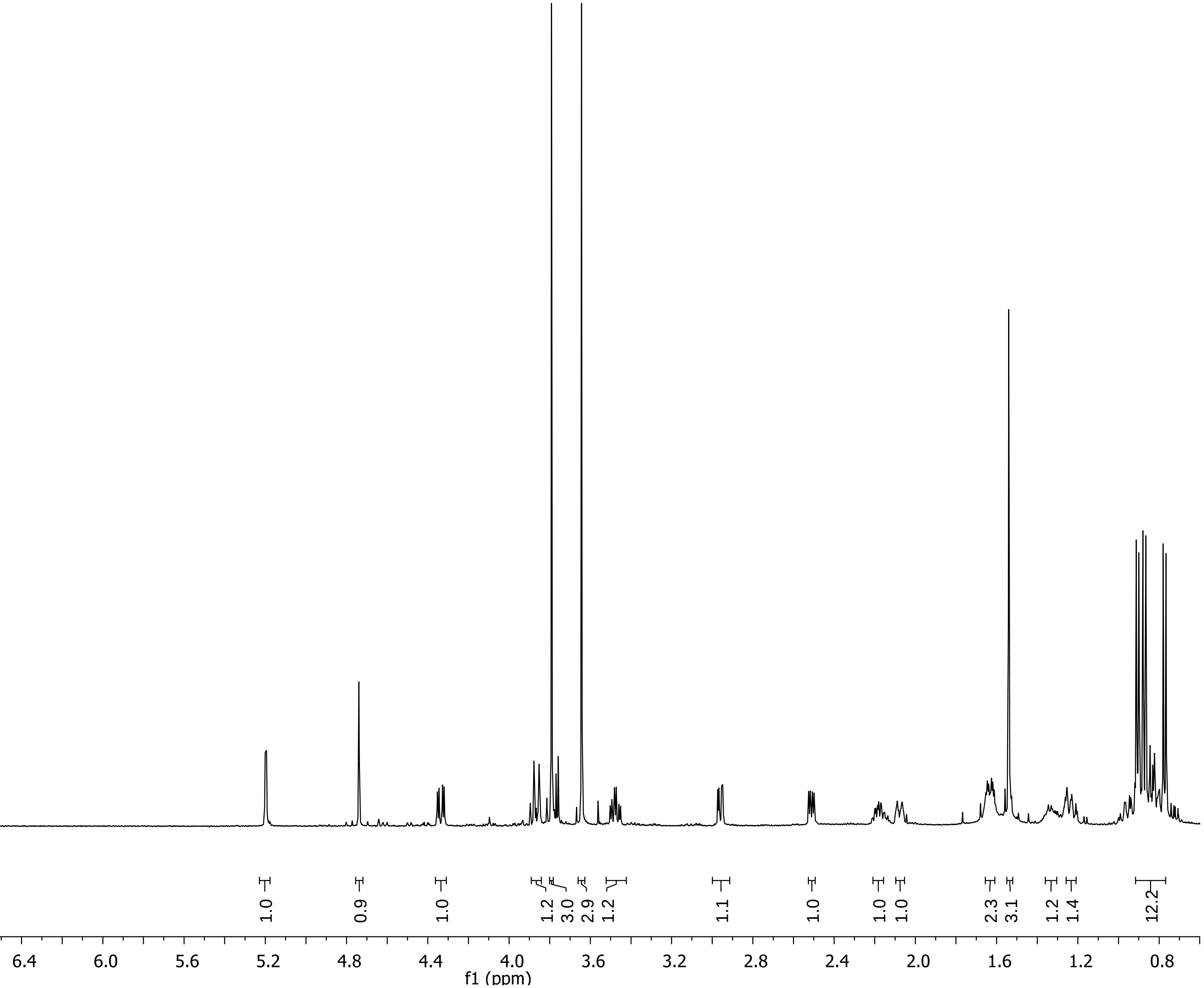


NOESY of compound **20**

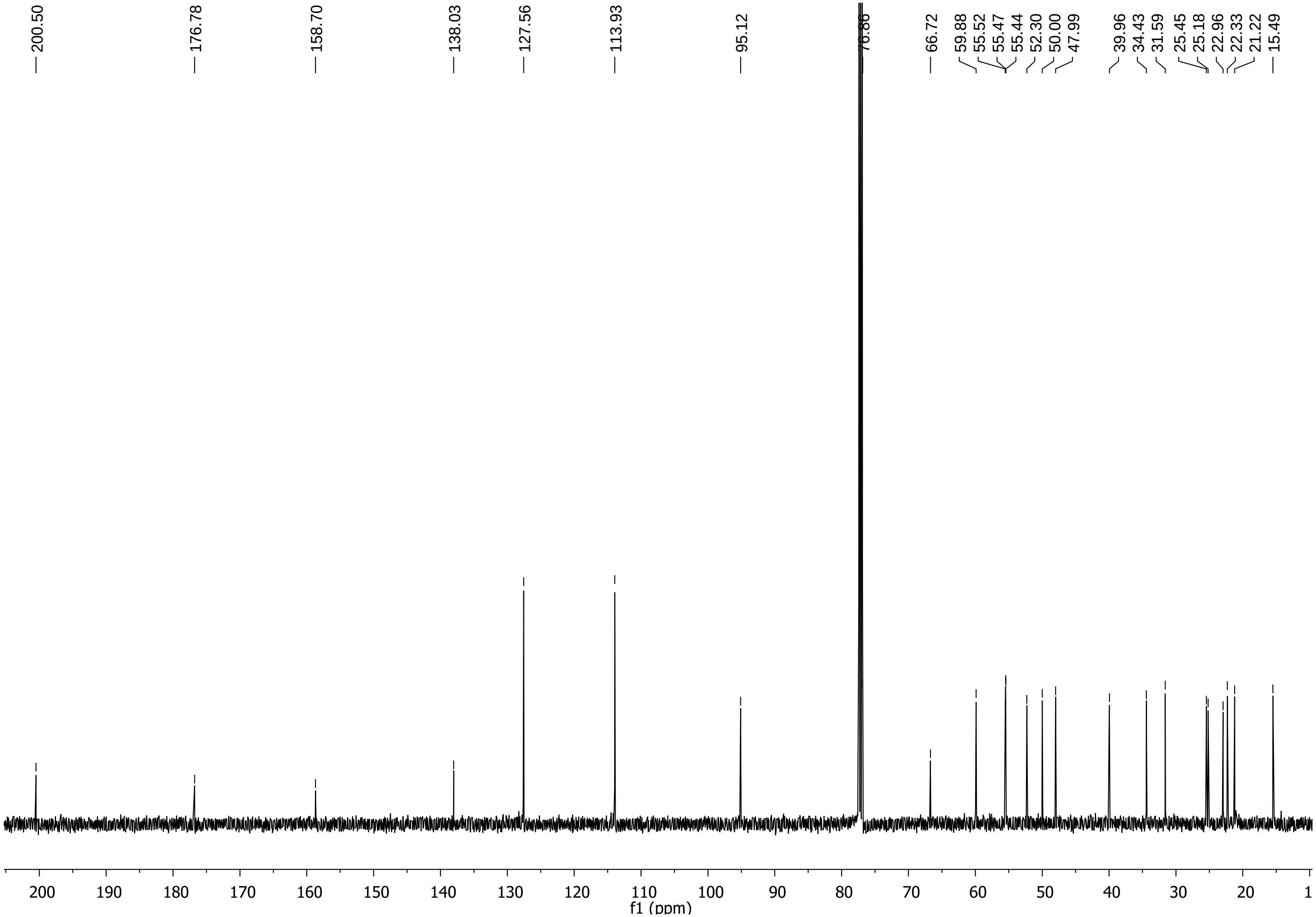


^{1}H NMR ($CDCl_3$, 500 MHz) of compound **21**

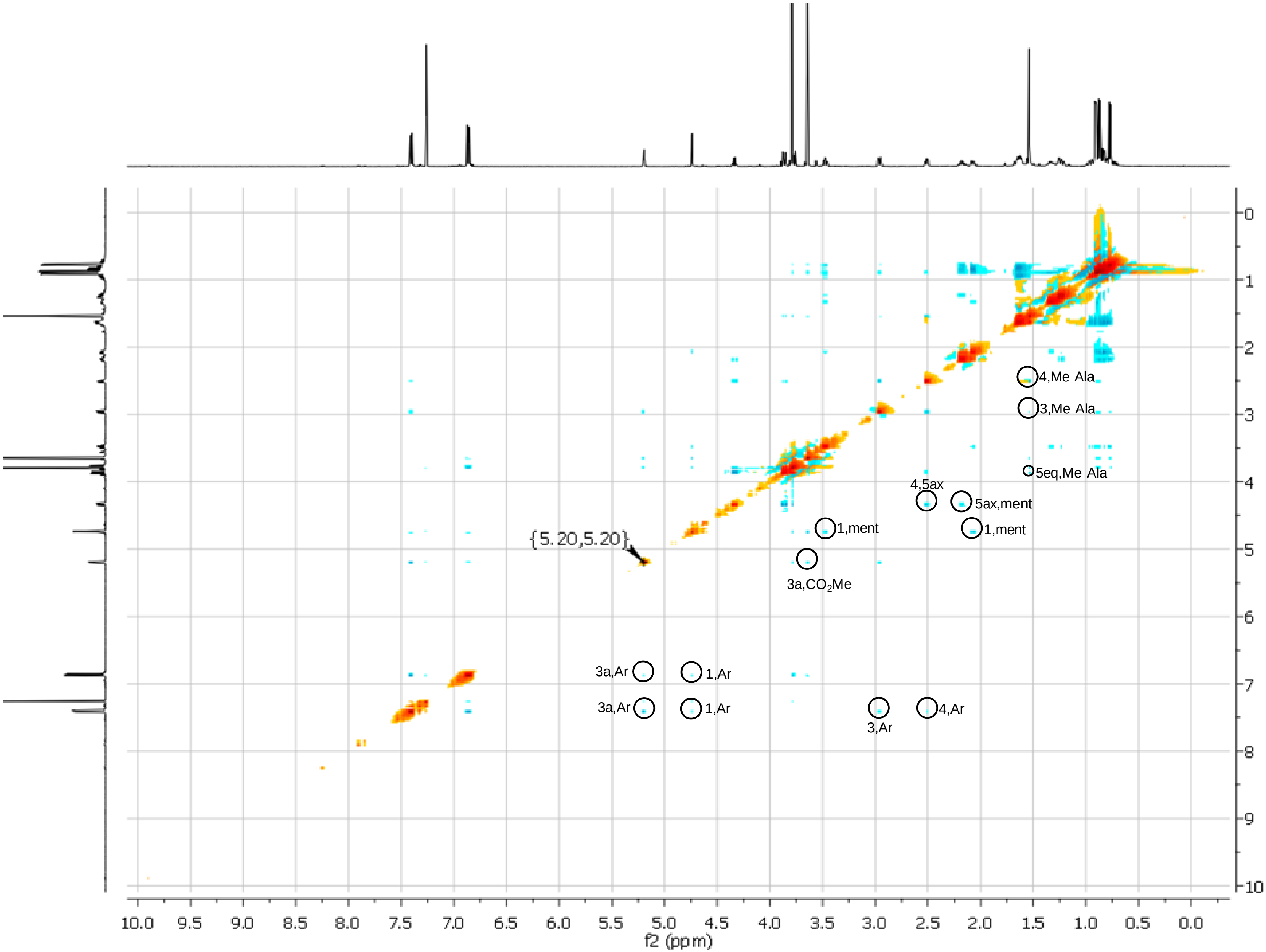




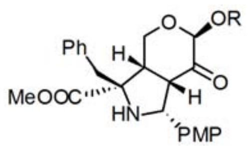
^{13}C NMR ($CDCl_3$, 125.7 MHz) of compound **21**

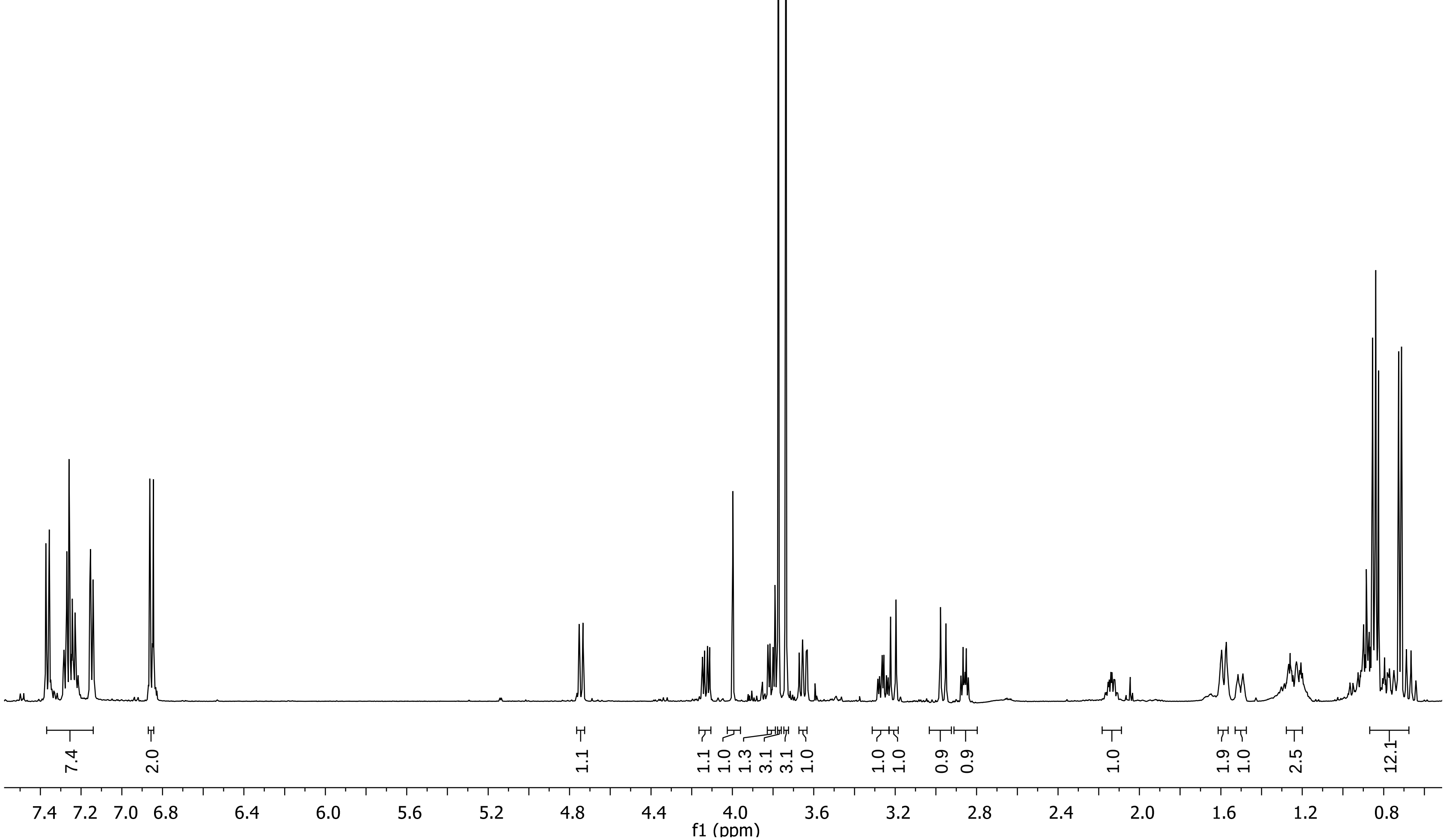


NOESY of compound **21**

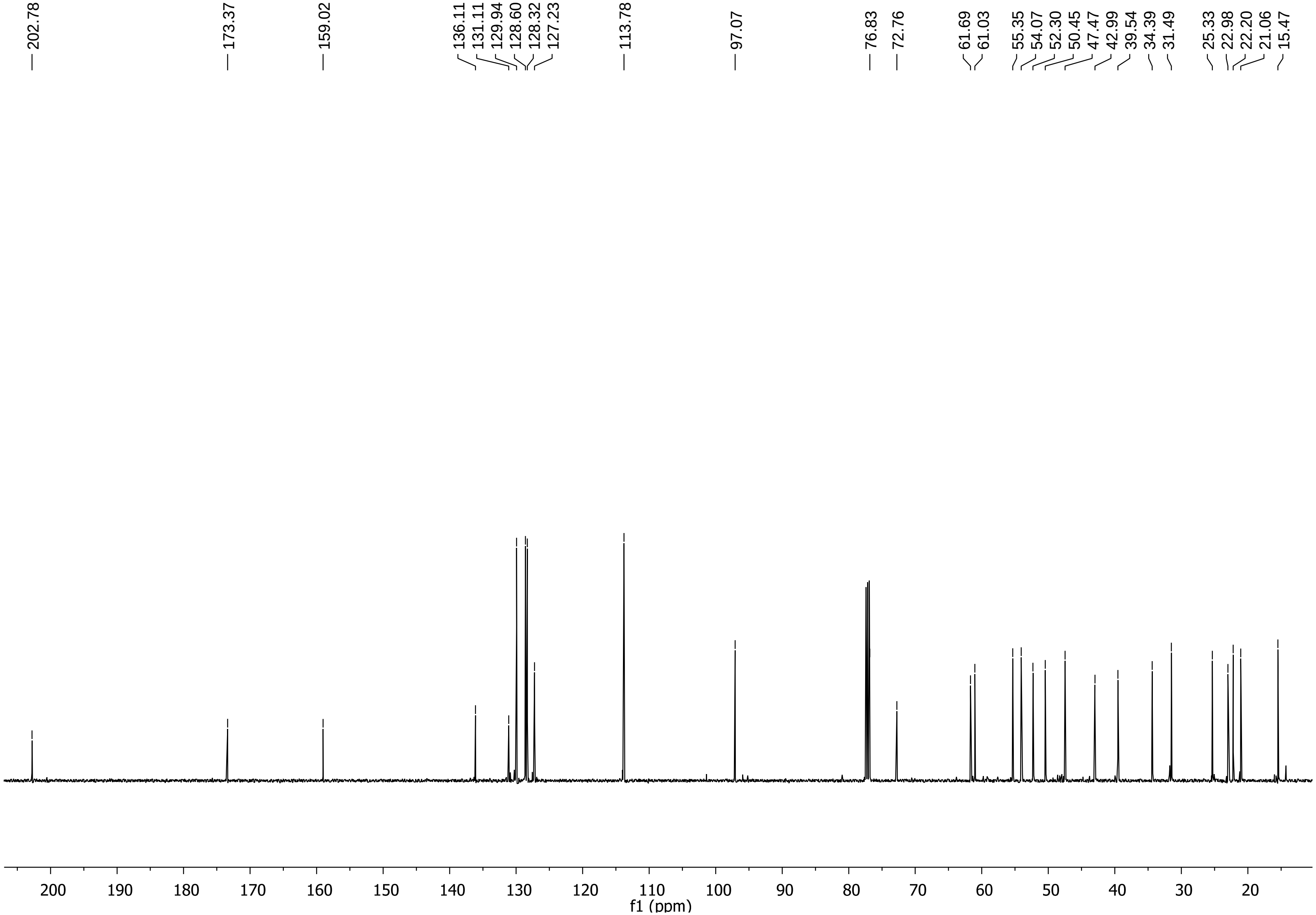


^{1}H NMR ($CDCl_3$, 500 MHz) of compound **22**

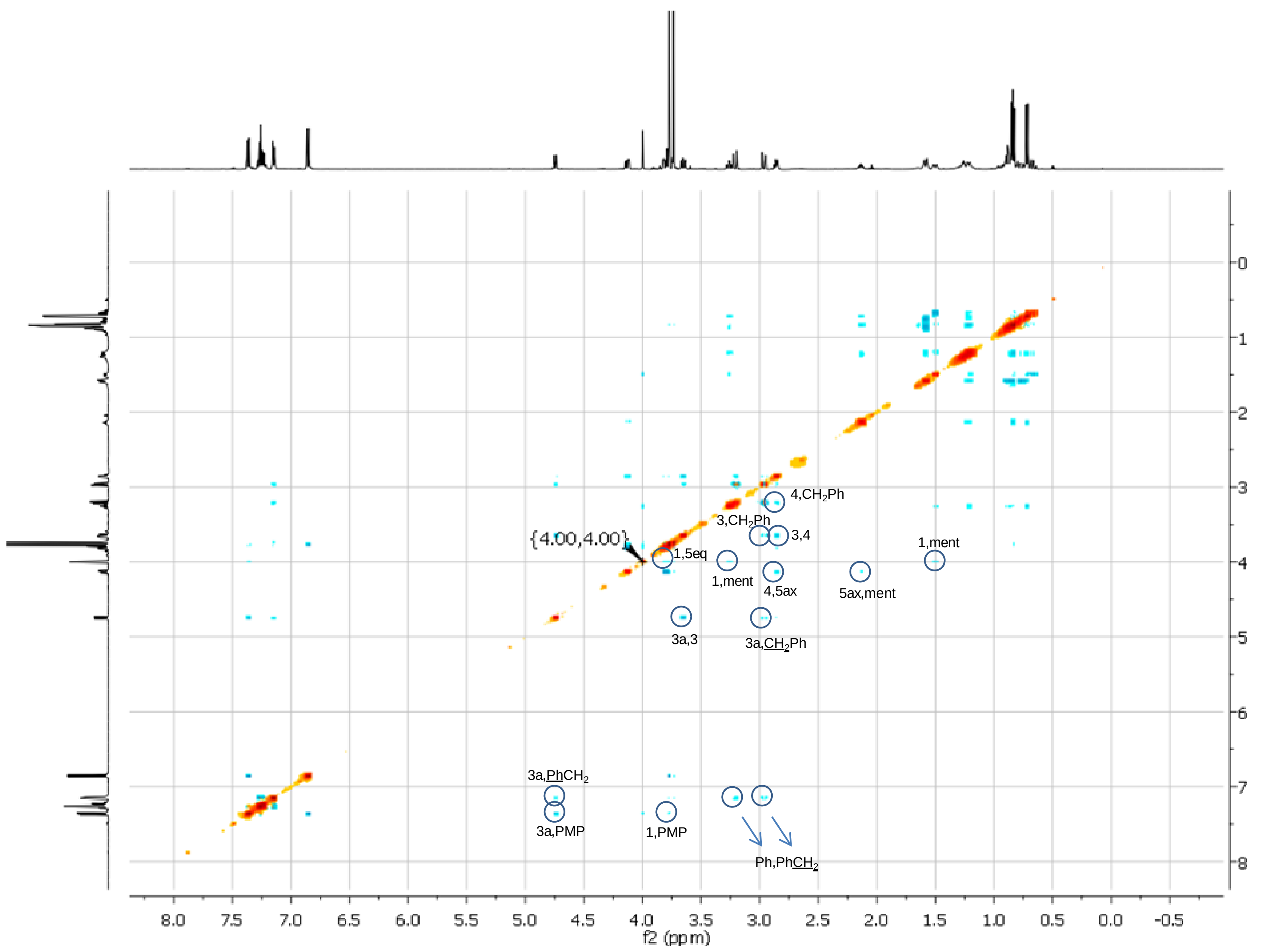




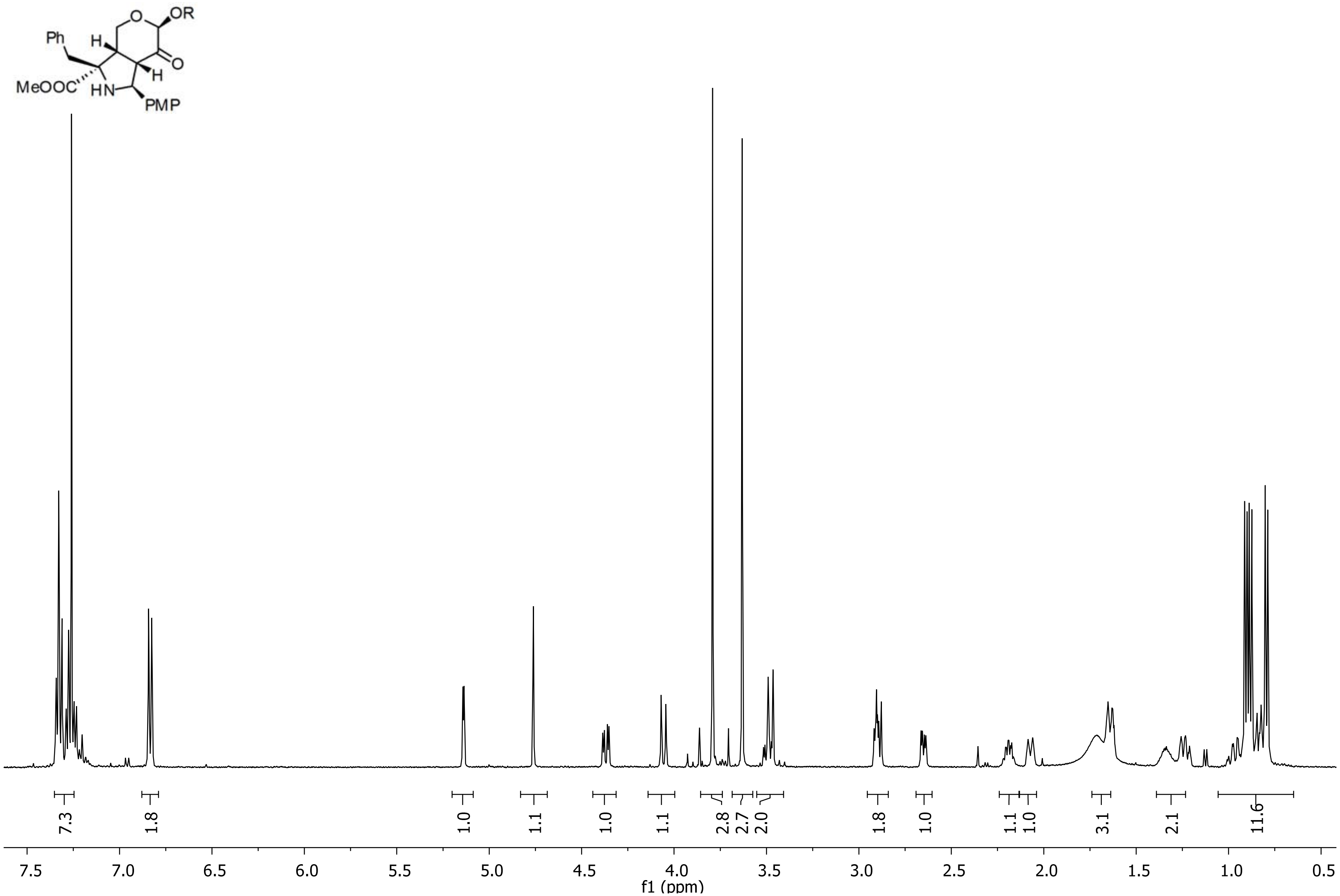
^{13}C NMR ($CDCl_3$, 125.7 MHz) of compound **22**



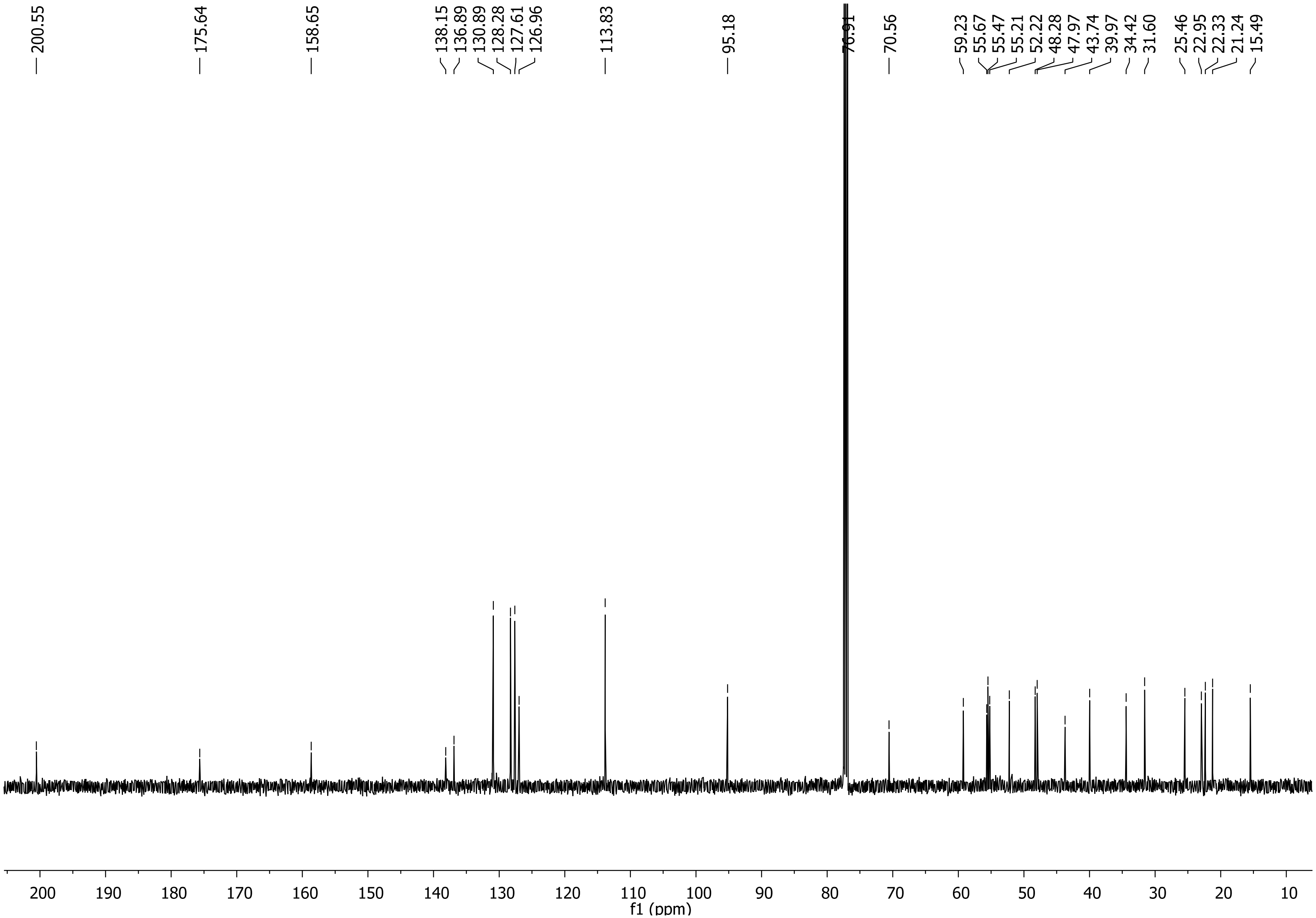
NOESY of compound **22**



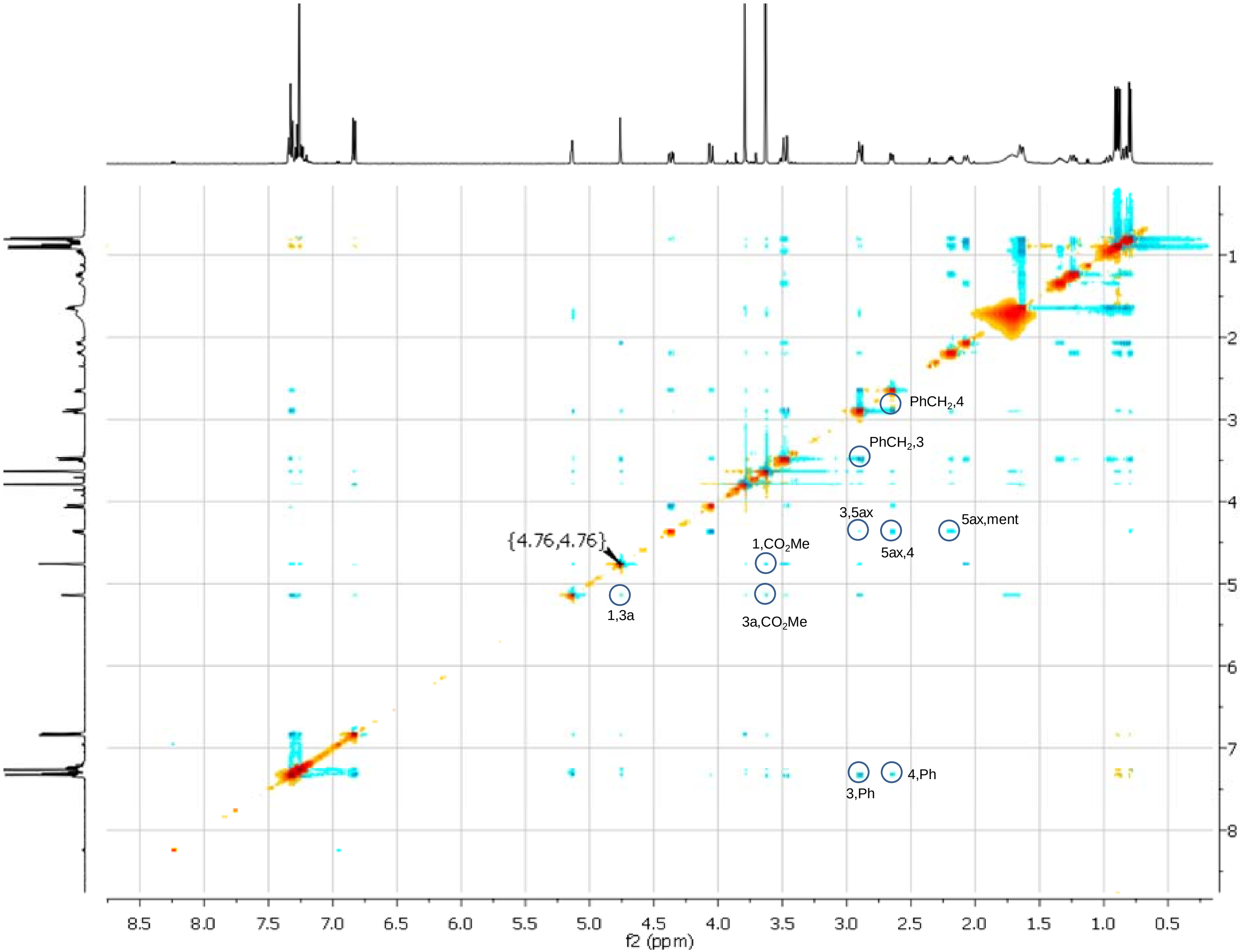
[1]H NMR ($CDCl_3$, 500 MHz) of compound **23**



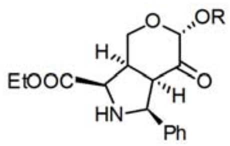
^{13}C NMR ($CDCl_3$, 125.7 MHz) of compound **23**

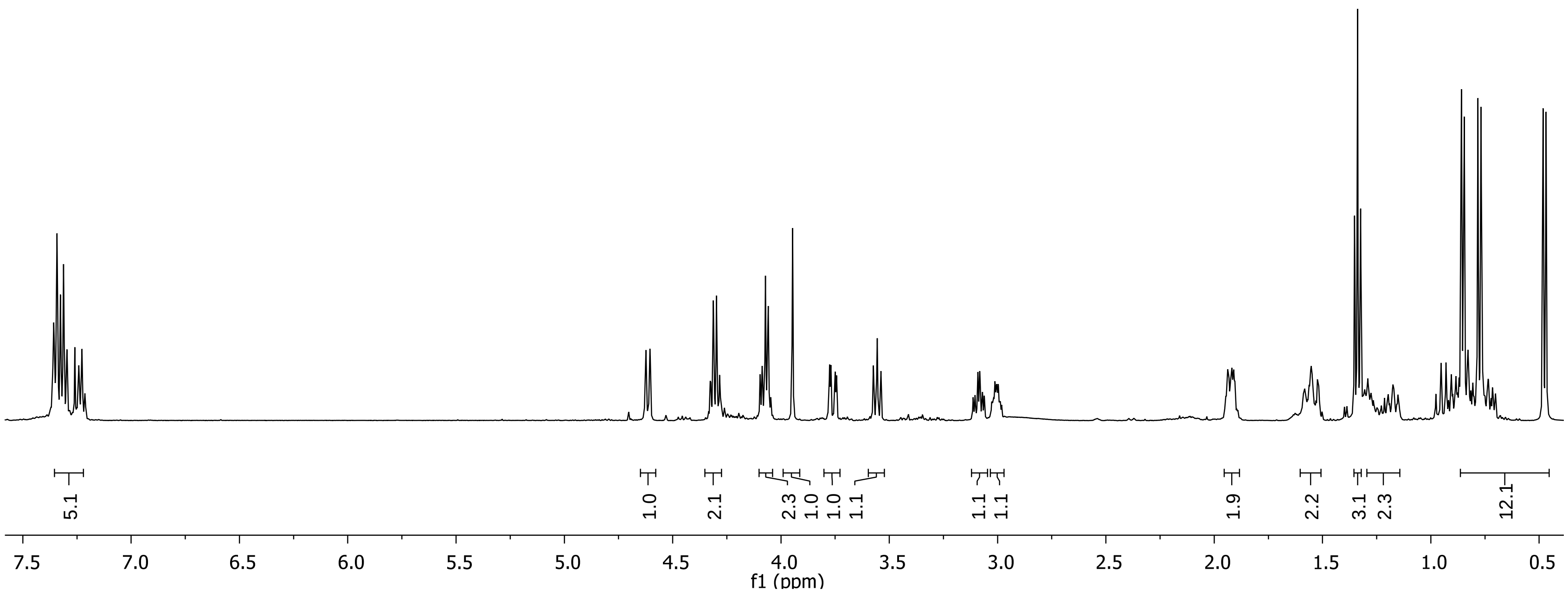


NOESY of compound **23**

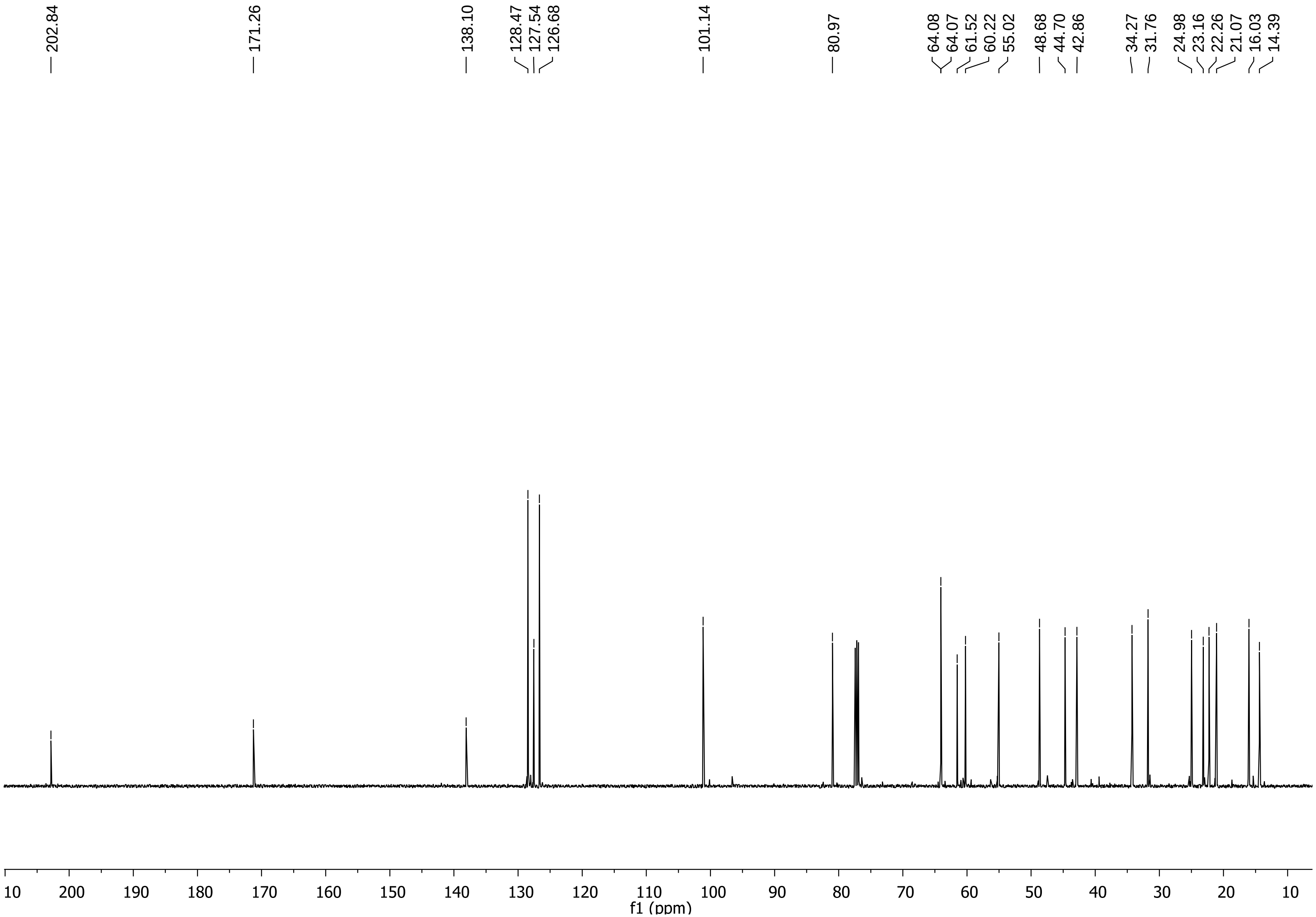


^{1}H NMR ($CDCl_3$, 500 MHz) of compound **24**

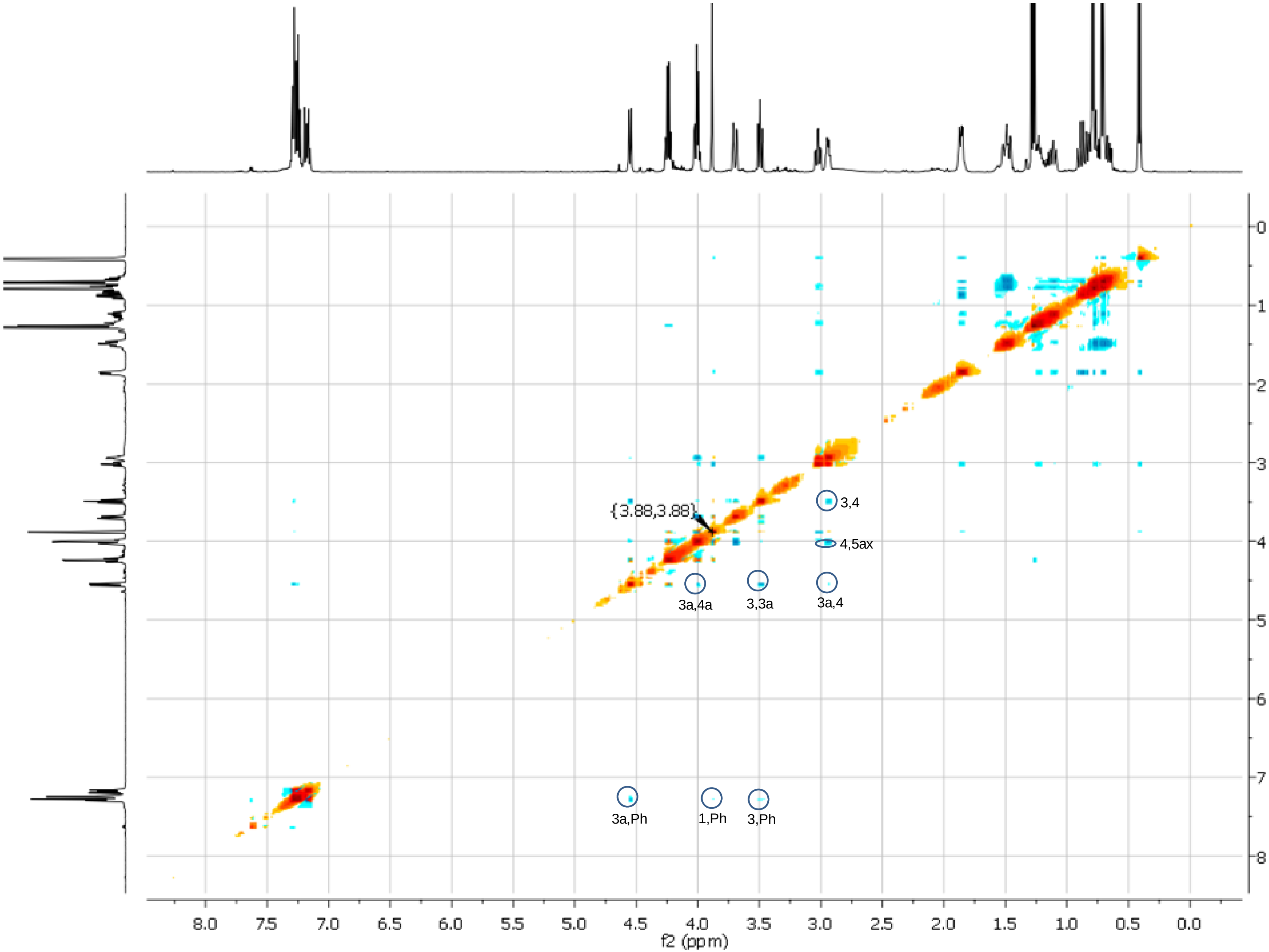




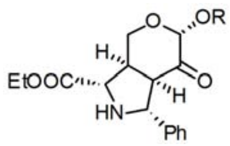
^{13}C NMR ($CDCl_3$, 125.7 MHz) of compound **24**

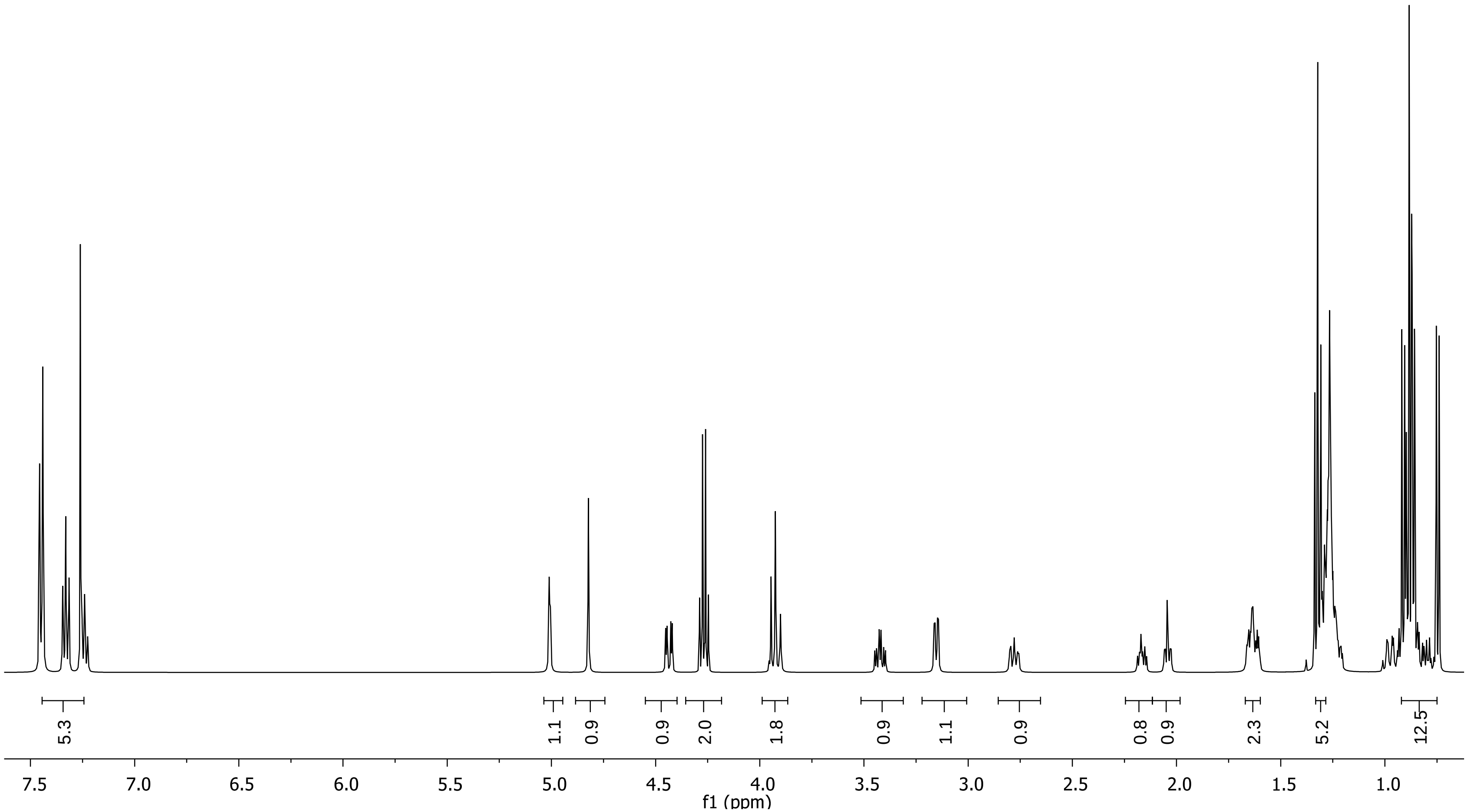


NOESY of compound **24**

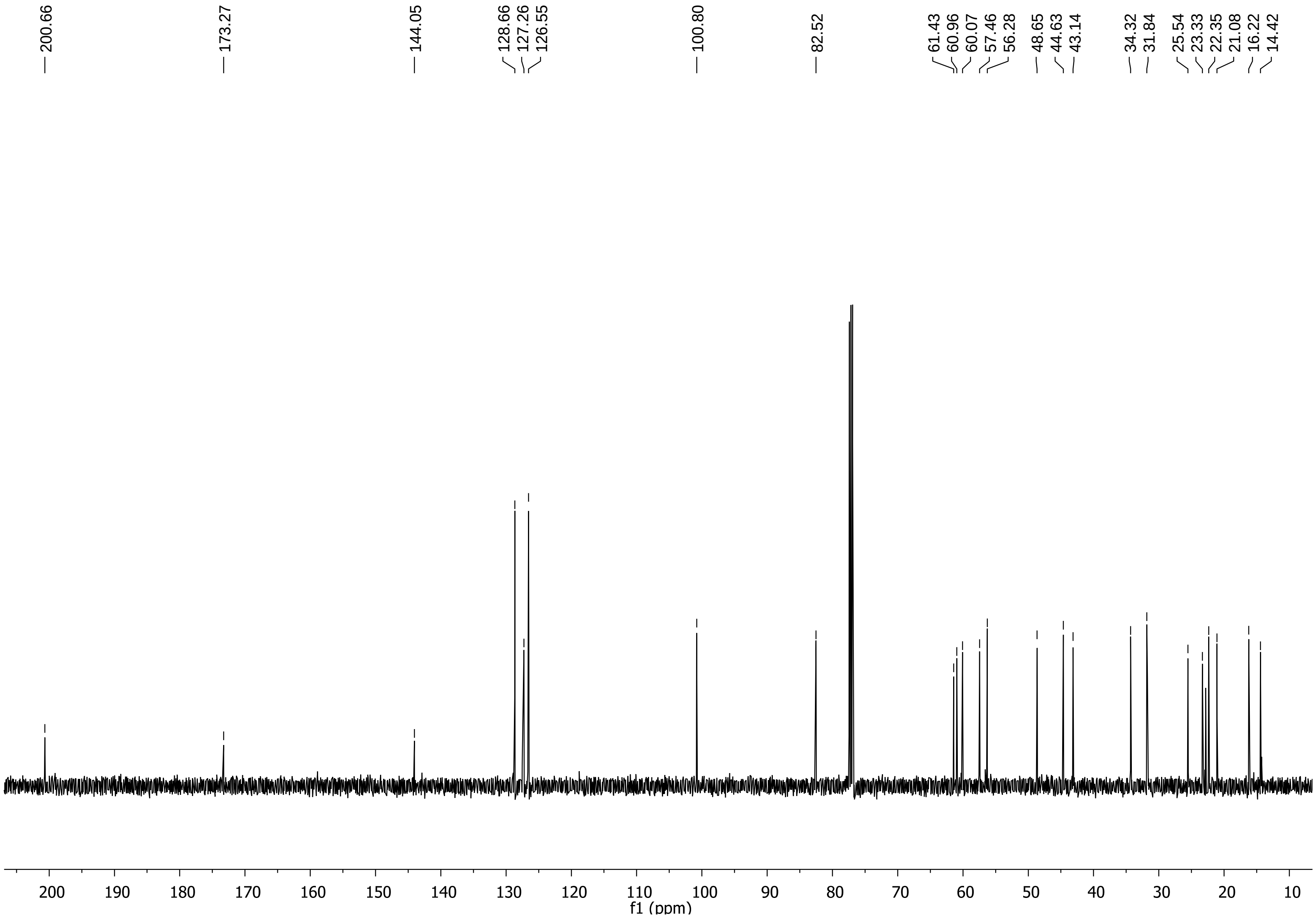


^{1}H NMR ($CDCl_3$, 500 MHz) of compound **25**

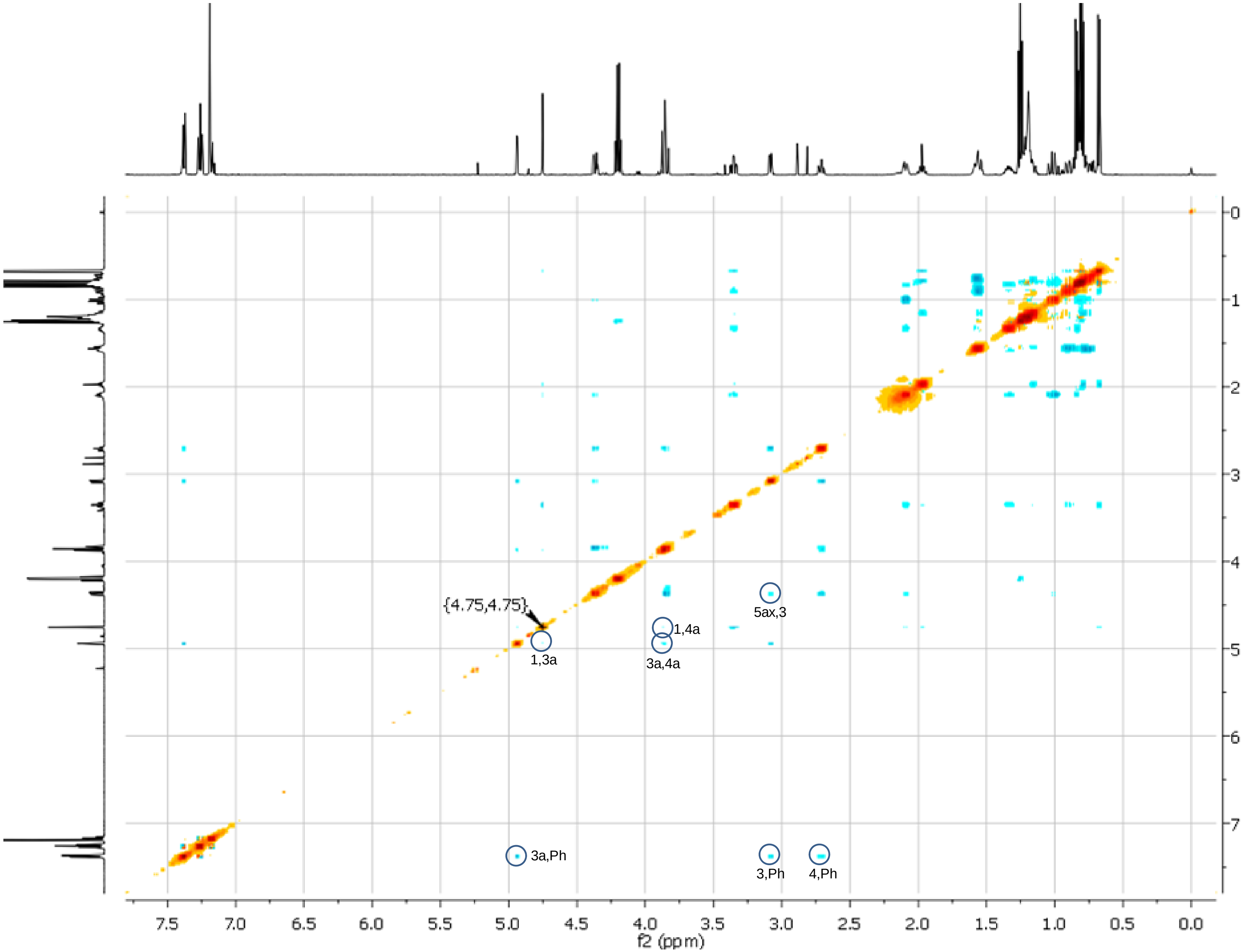




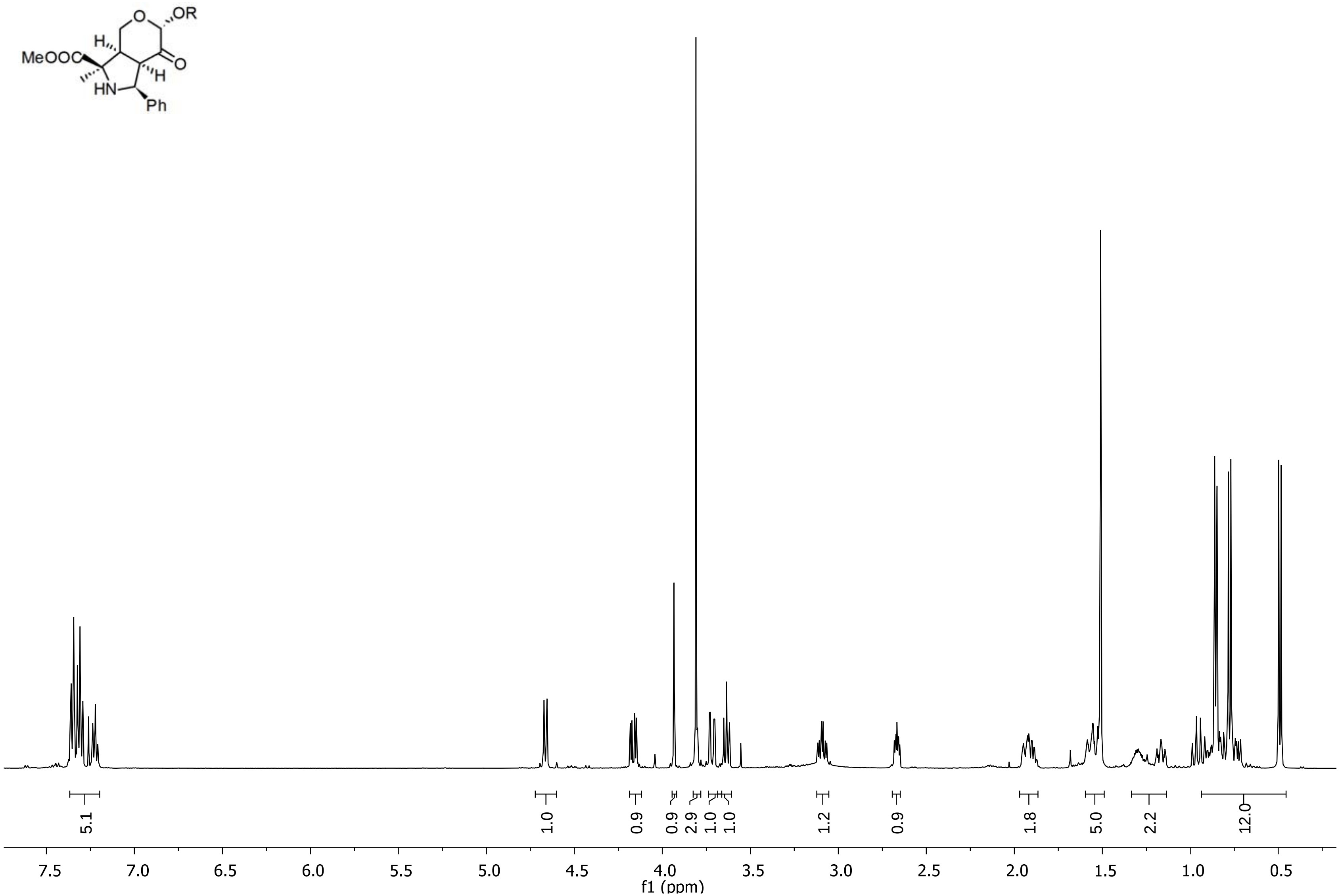
^{13}C NMR ($CDCl_3$, 125.7 MHz) of compound **25**



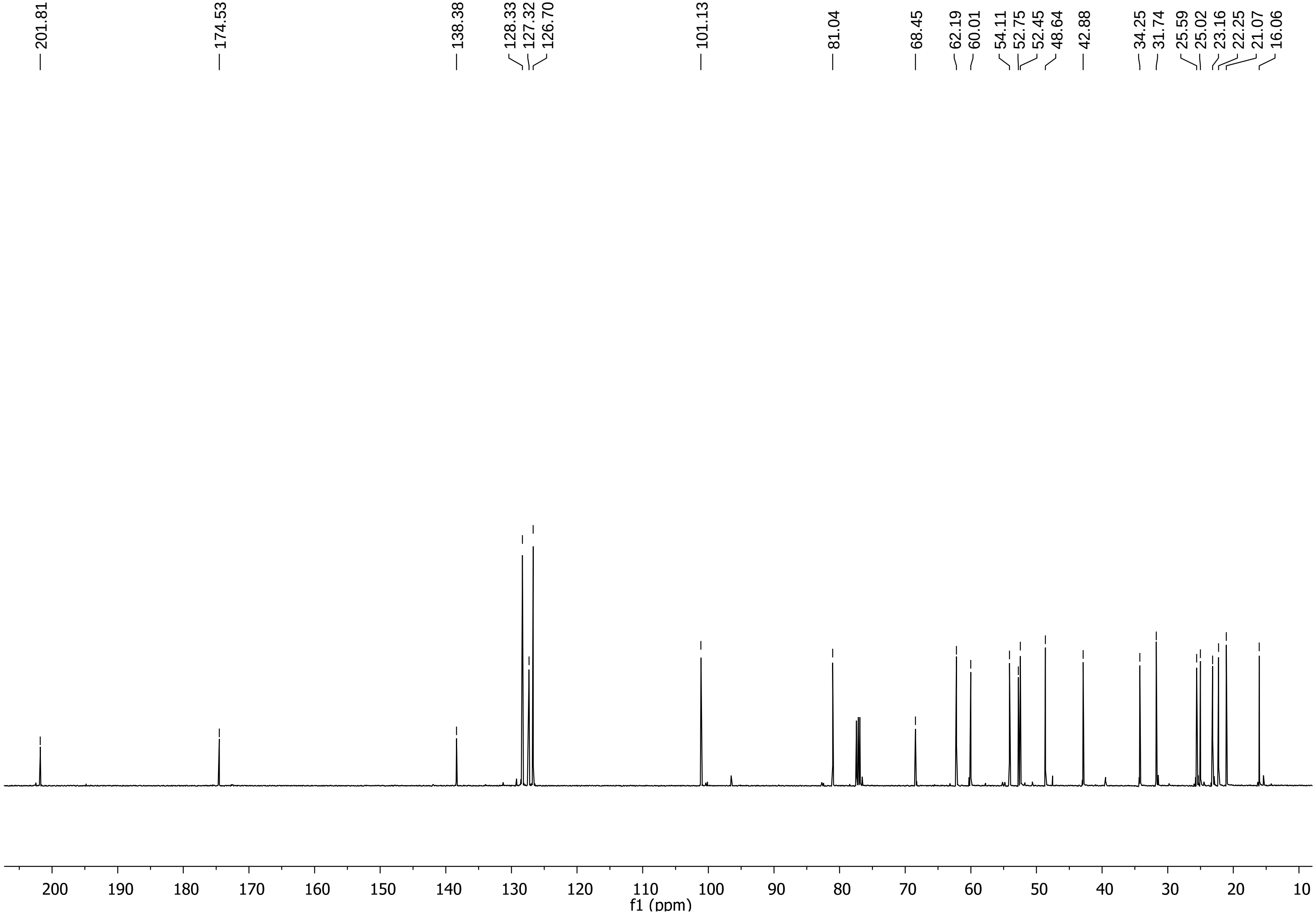
NOESY of compound **25**



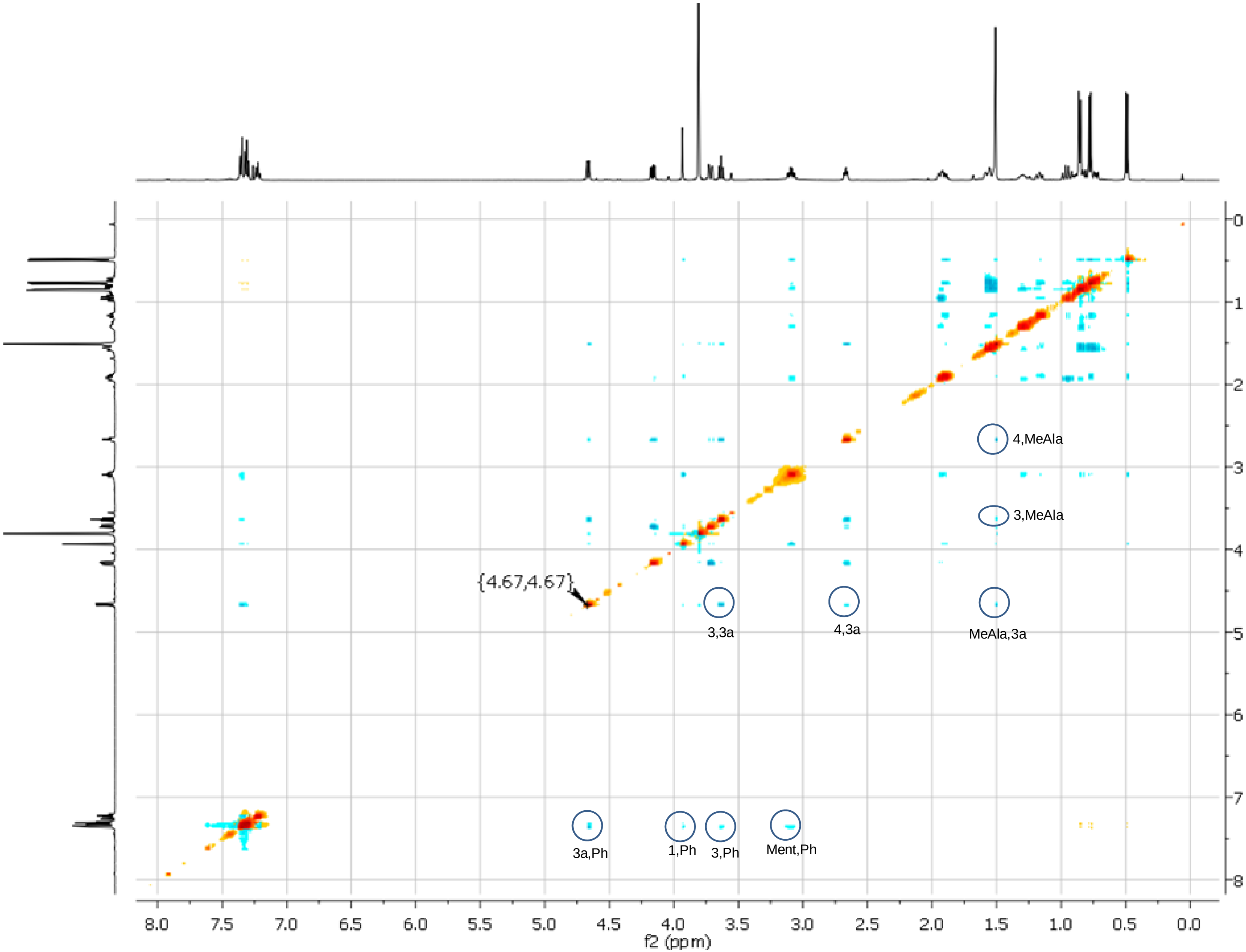
[1]H NMR ($CDCl_3$, 500 MHz) of compound **26**



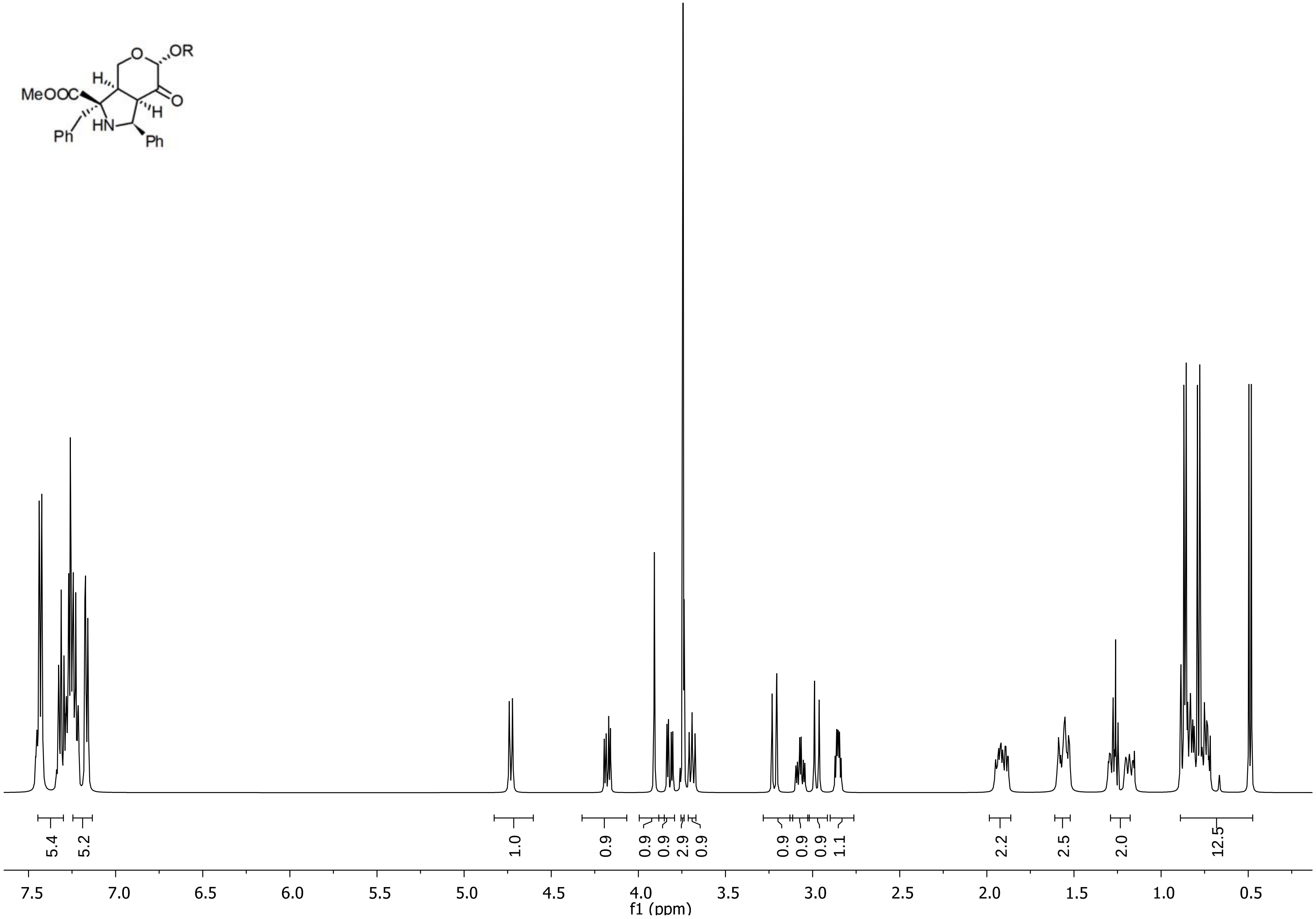
^{13}C NMR ($CDCl_3$, 125.7 MHz) of compound **26**



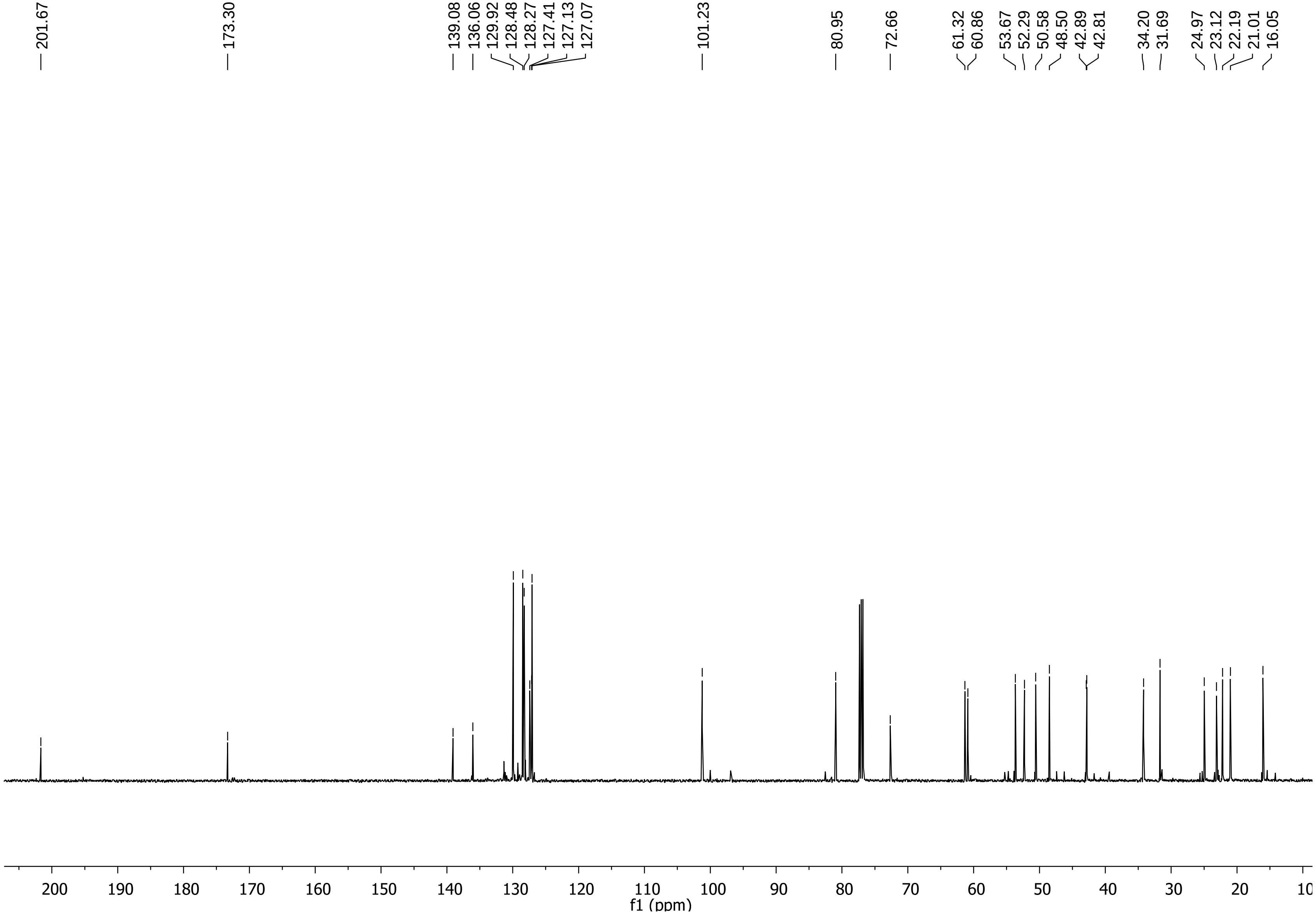
NOESY of compound **26**



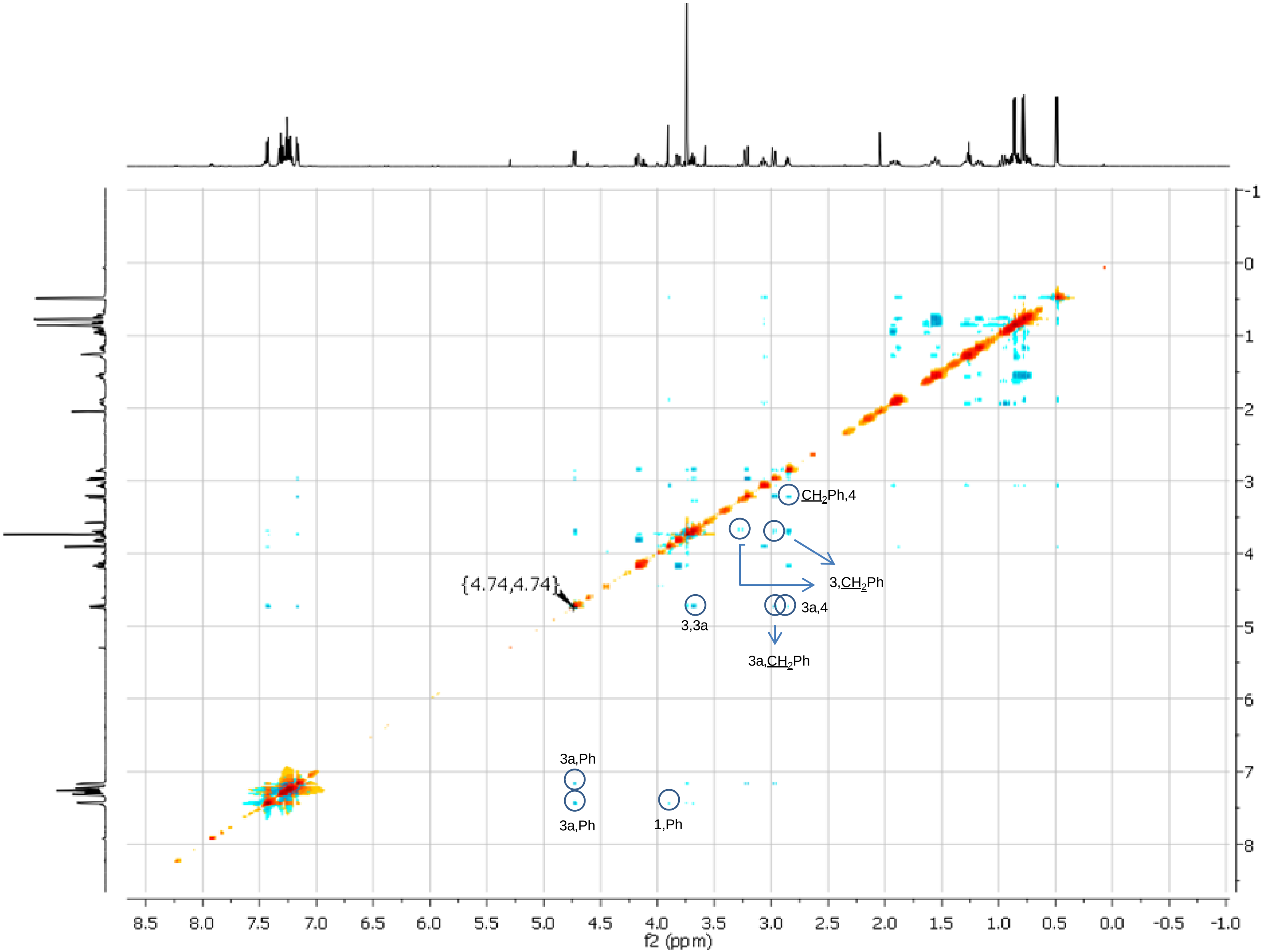
^{1}H NMR ($CDCl_3$, 500 MHz) of compound **27**



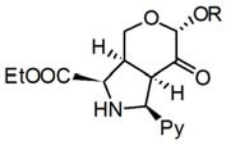
^{13}C NMR ($CDCl_3$, 125.7 MHz) of compound **27**

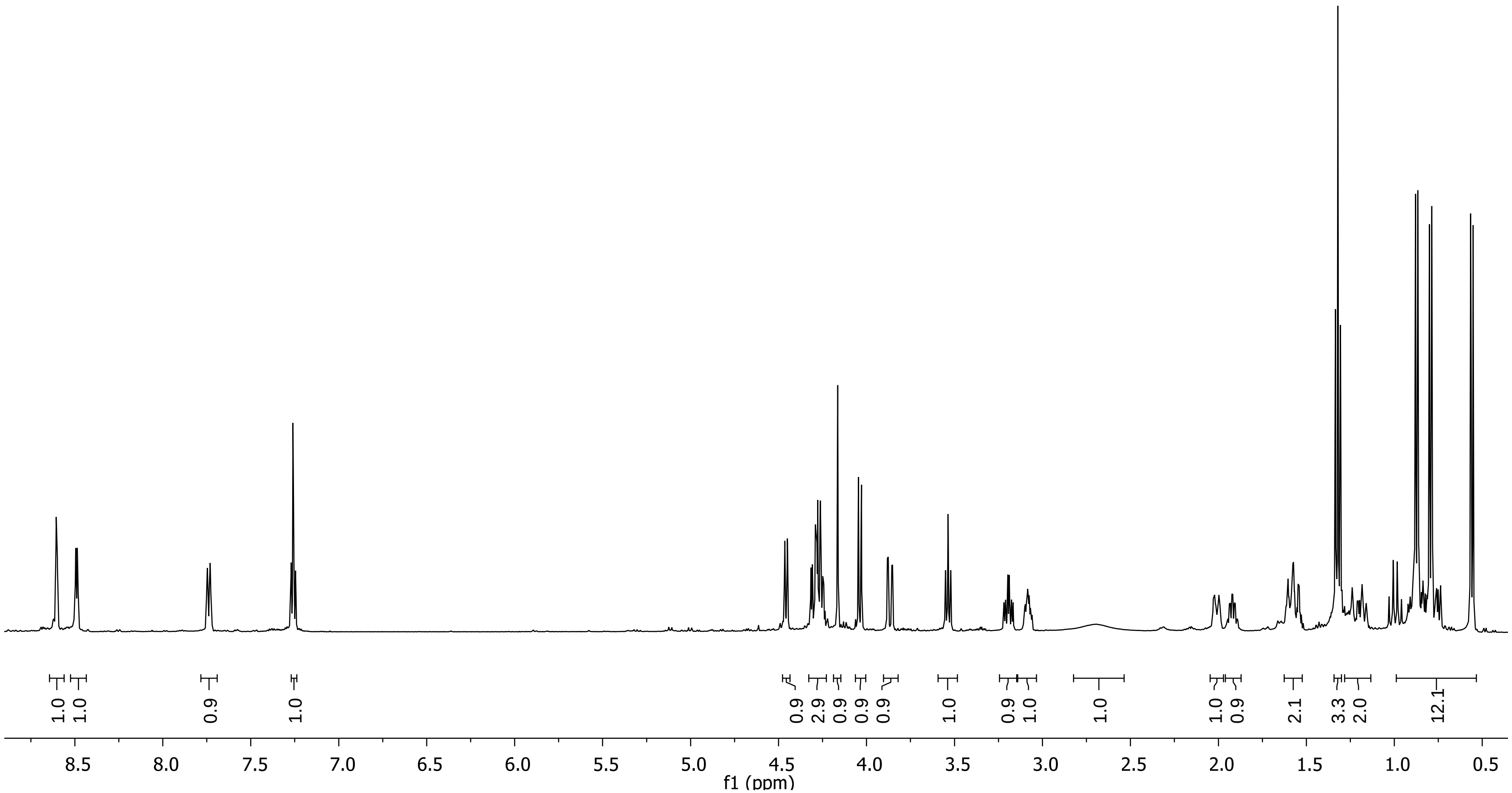


NOESY of compound **27**

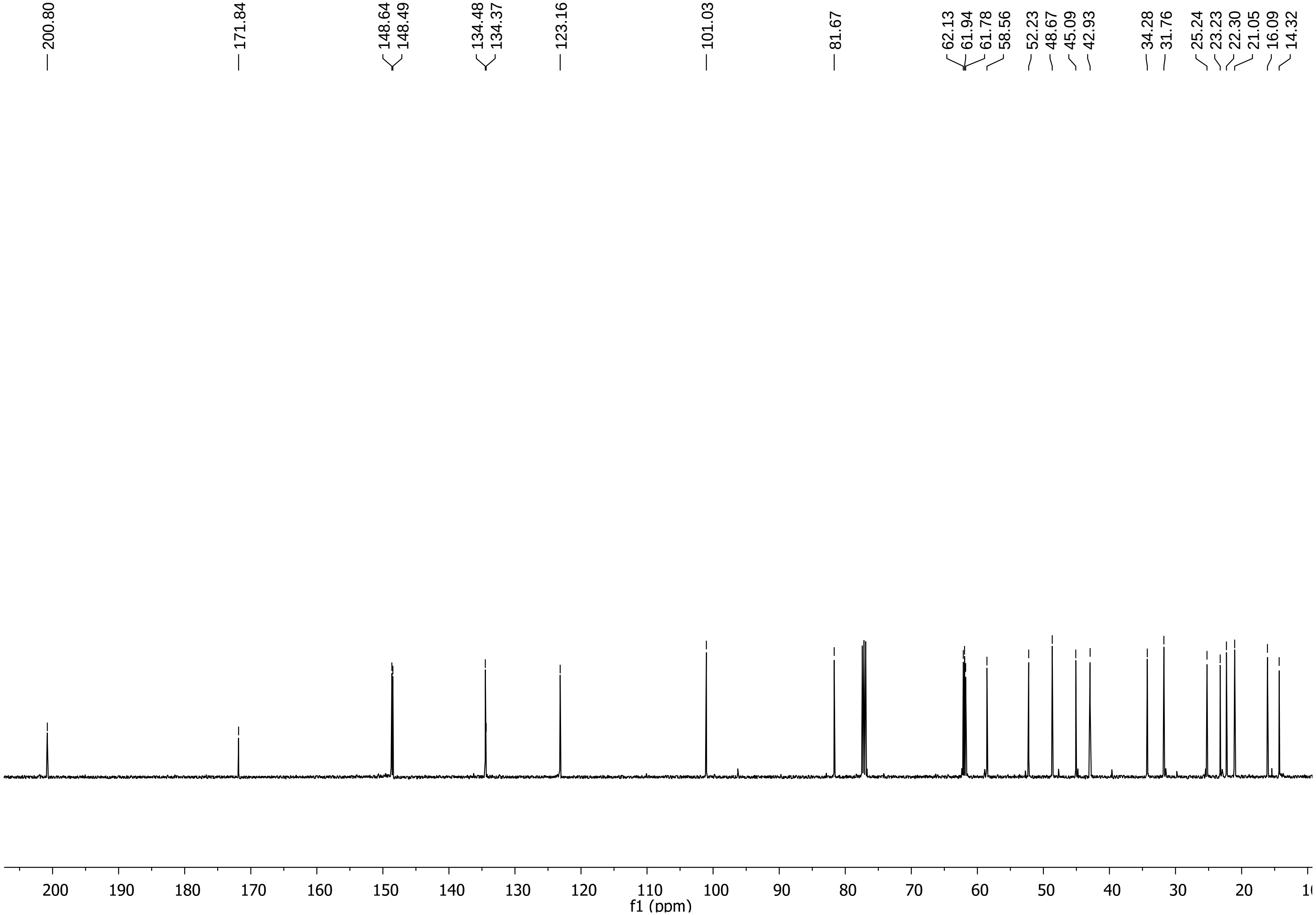


^{1}H NMR ($CDCl_3$, 500 MHz) of compound **28**

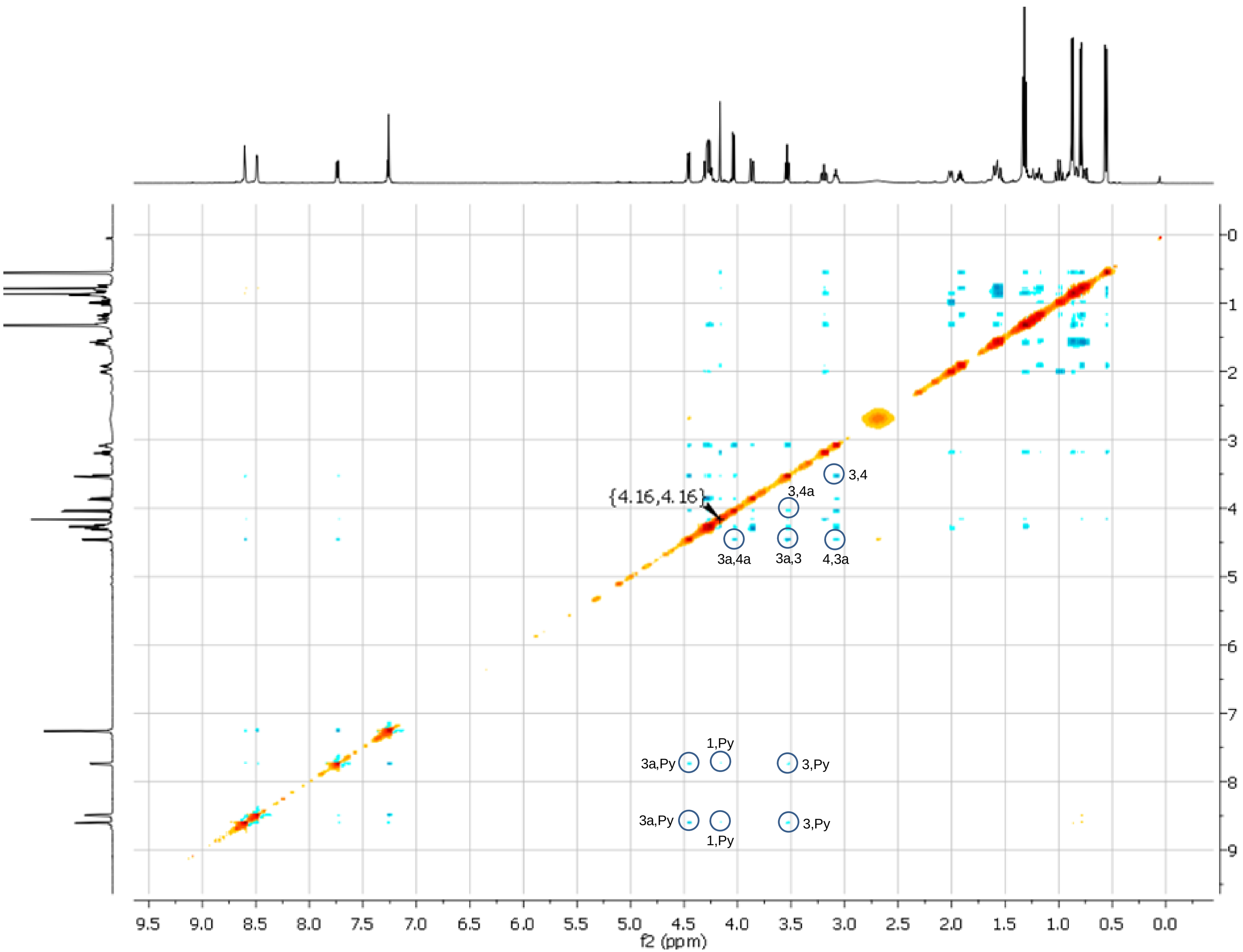




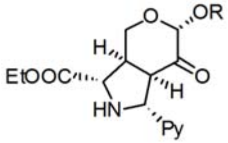
^{13}C NMR ($CDCl_3$, 125.7 MHz) of compound **28**

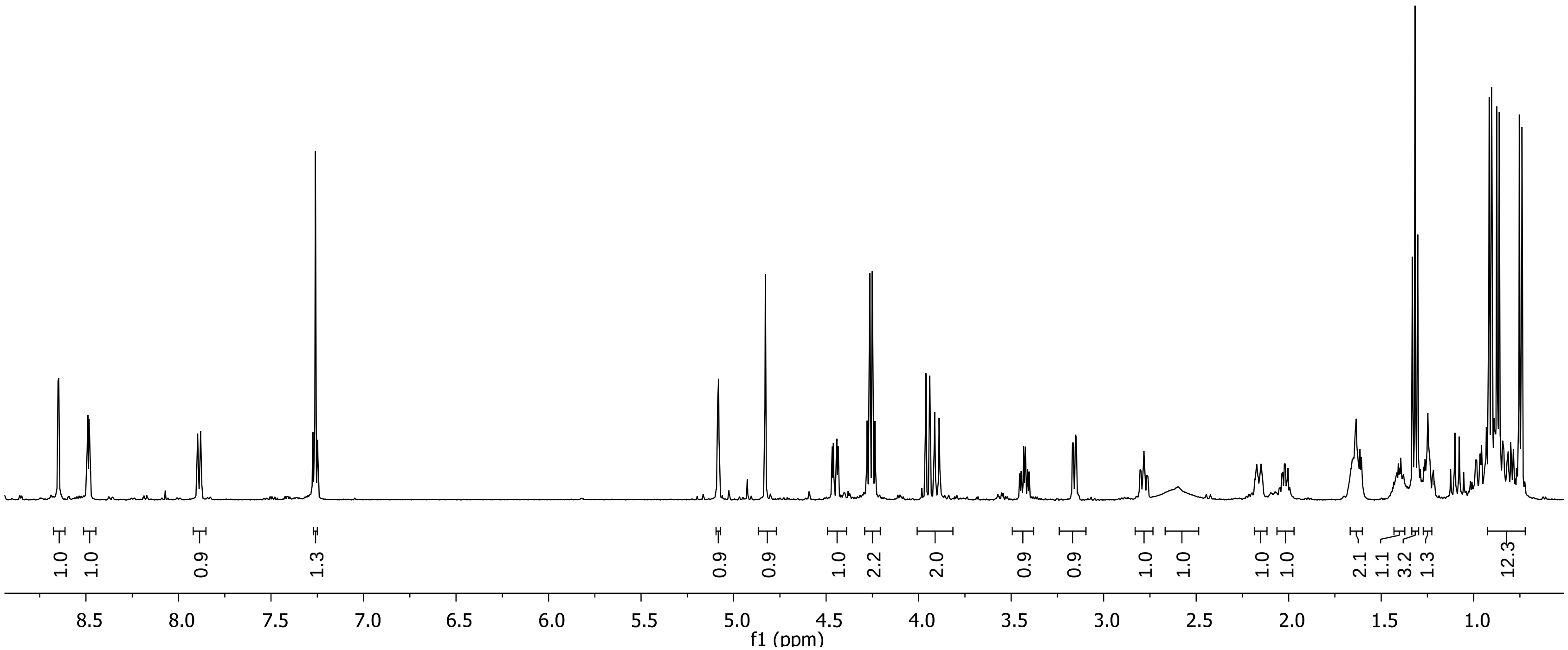


NOESY of compound **28**

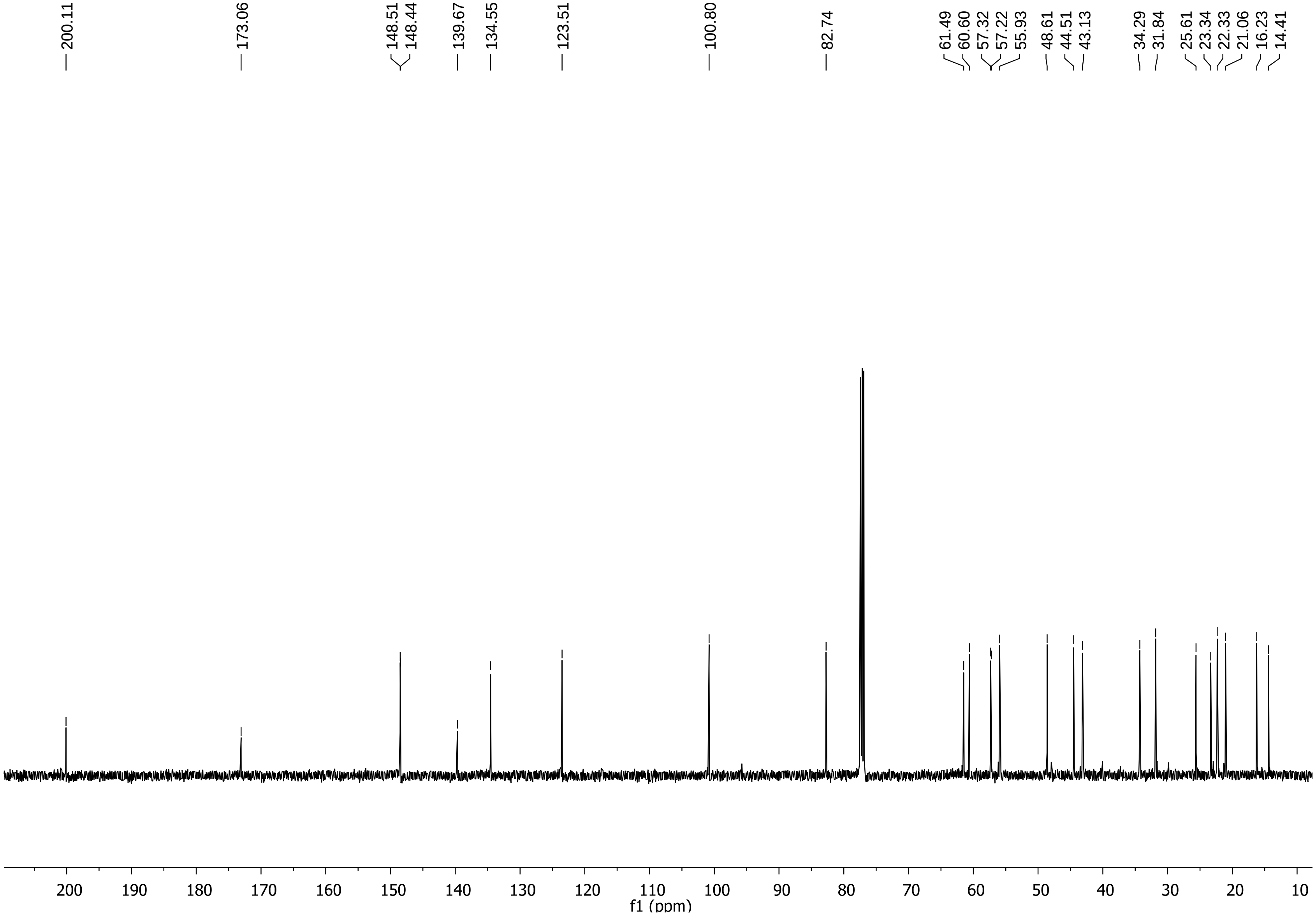


^1H NMR ($CDCl_3$, 500 MHz) of compound **29**

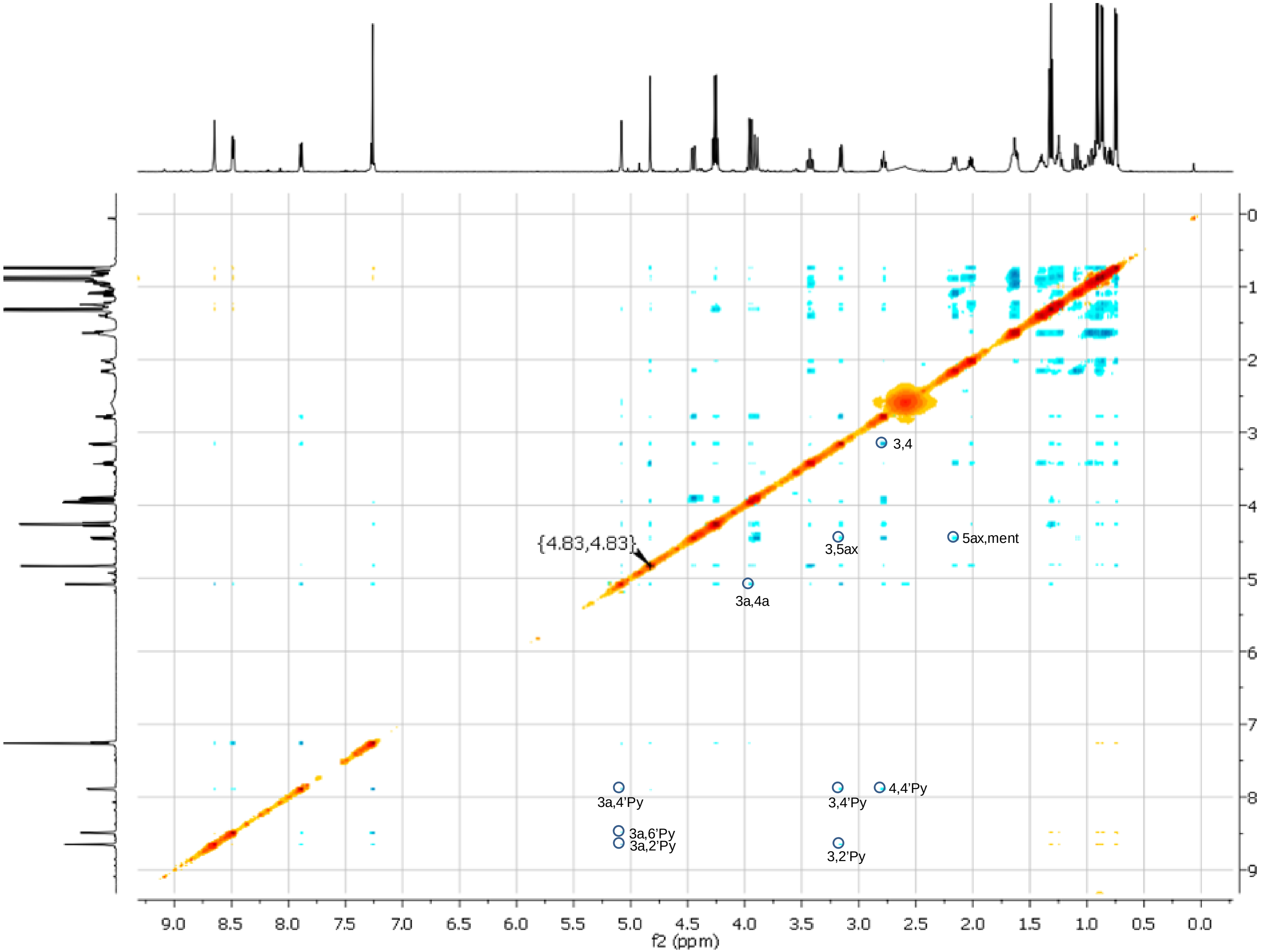




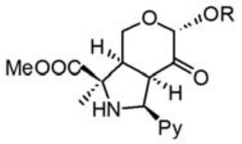
^{13}C NMR ($CDCl_3$, 125.7 MHz) of compound **29**

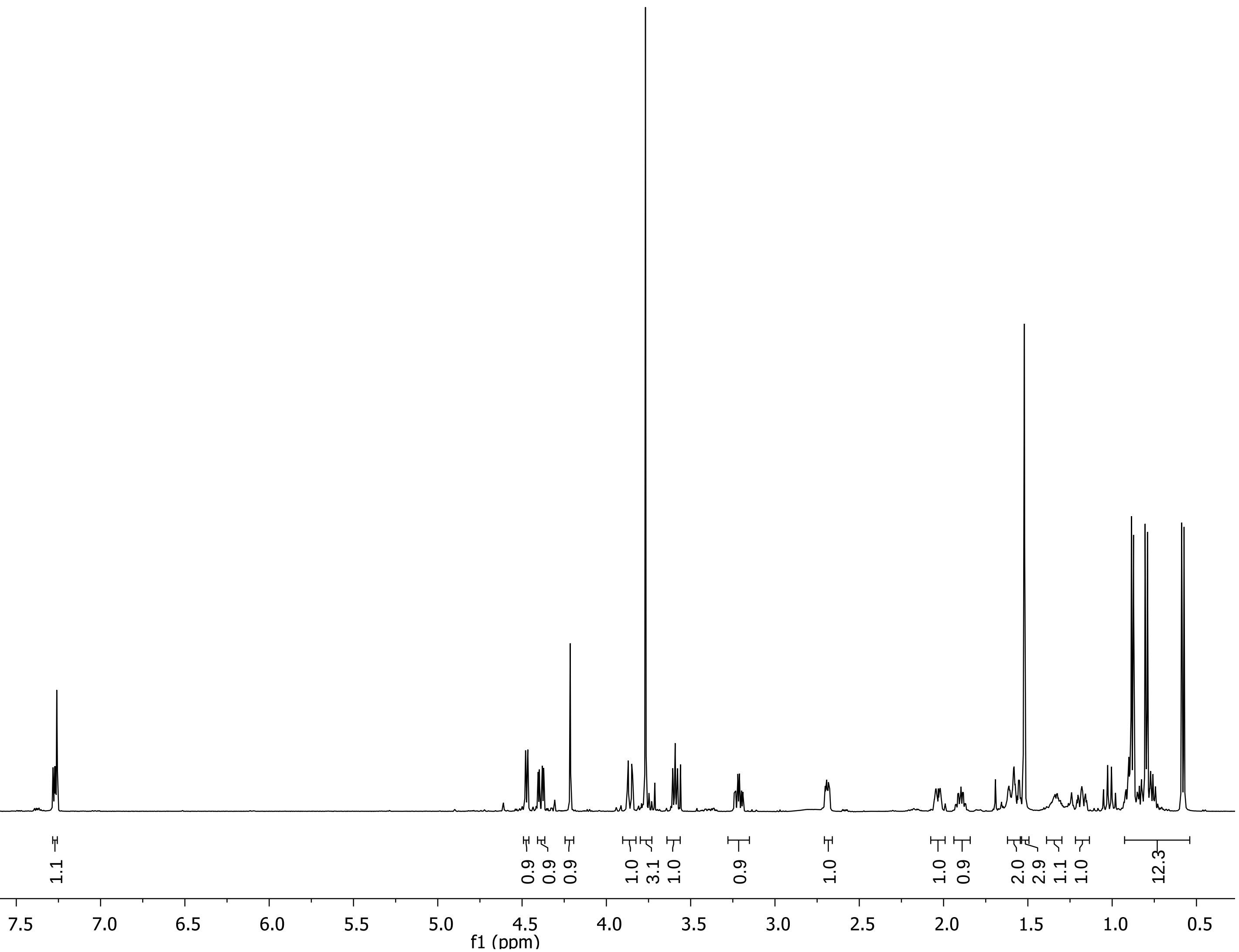


NOESY of compound **29**

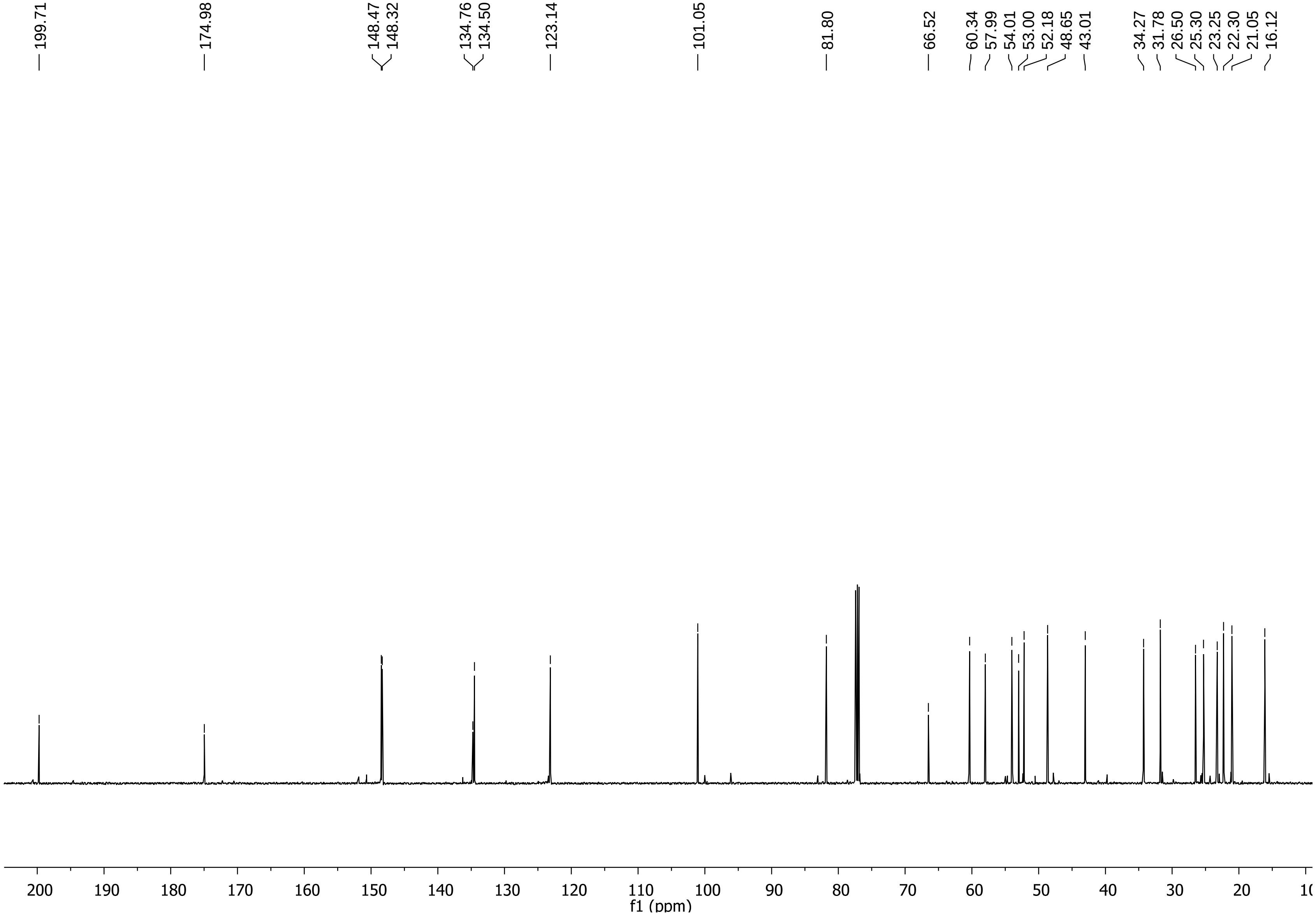


[1]H NMR ($CDCl_3$, 500 MHz) of compound **30**

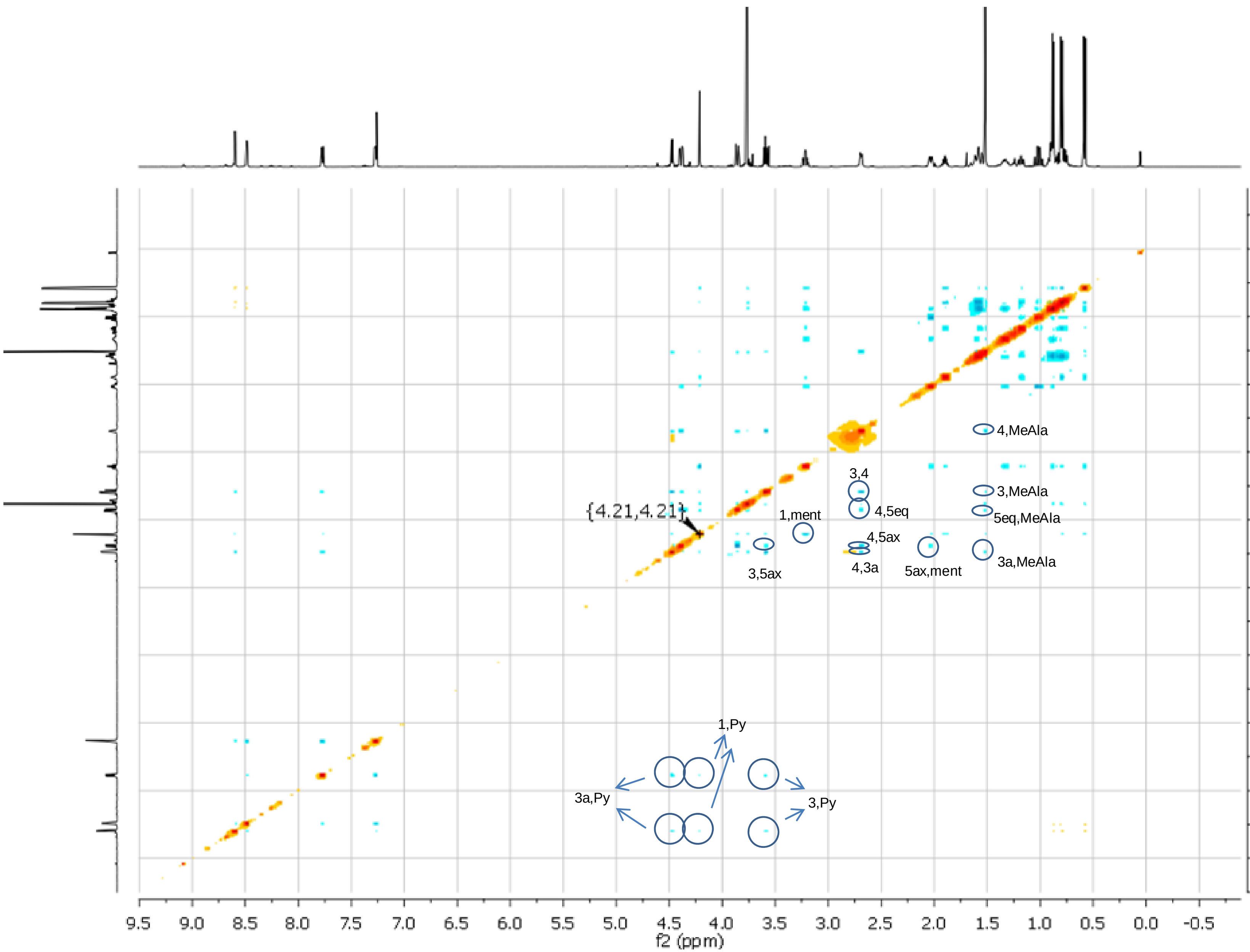




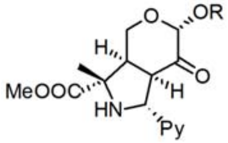
^{13}C NMR ($CDCl_3$, 125.7 MHz) of compound **30**

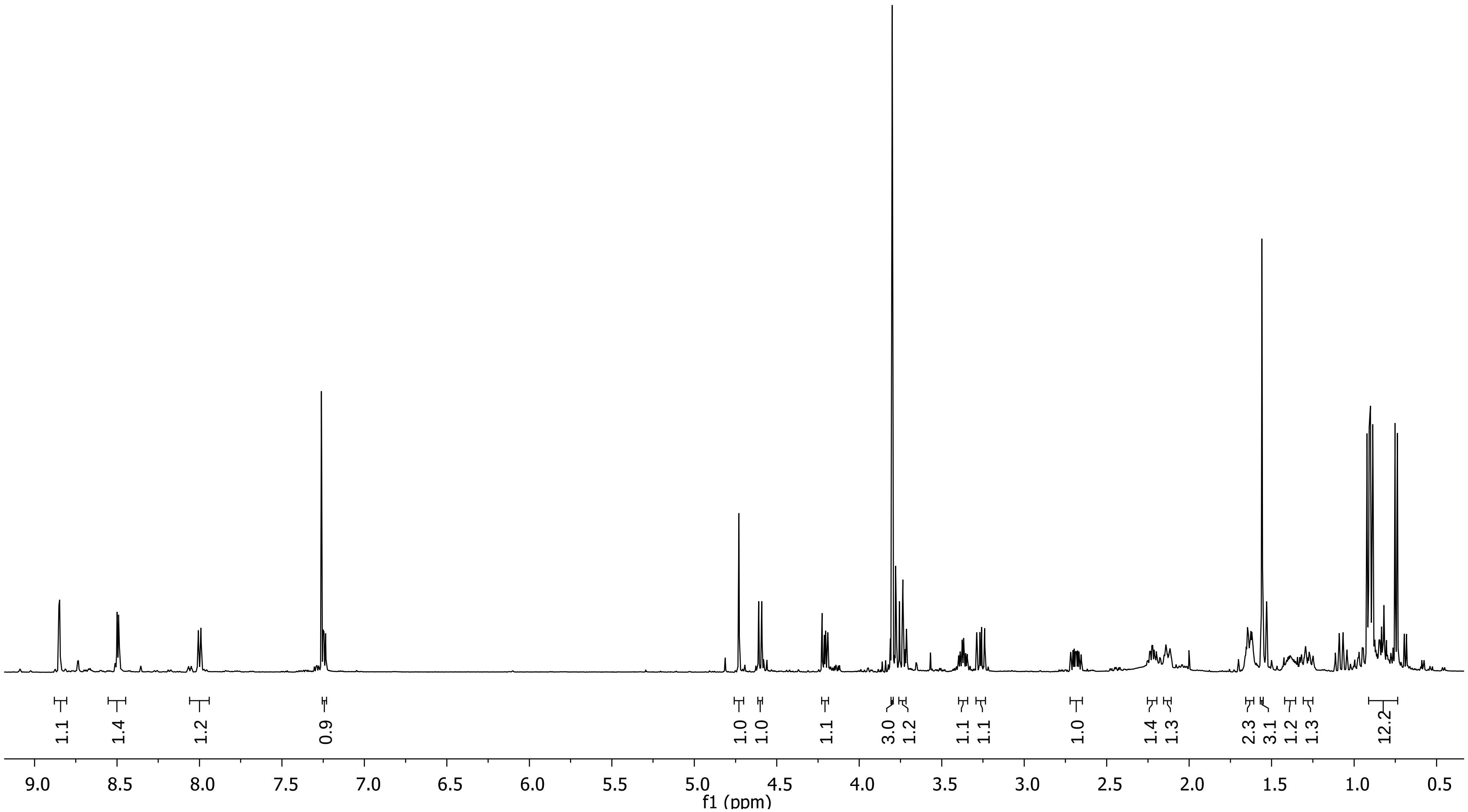


NOESY of compound **30**

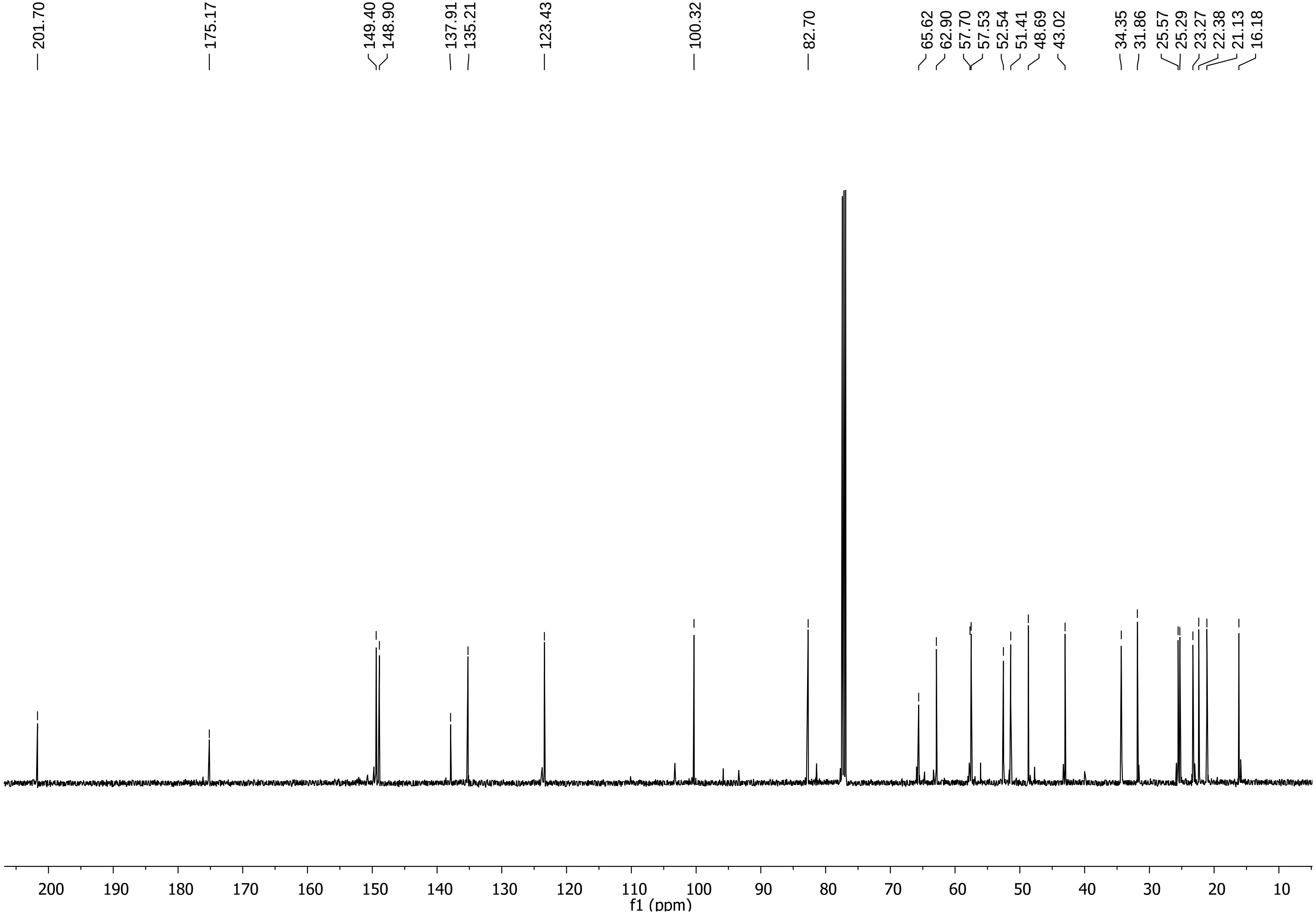


[1]H NMR ($CDCl_3$, 500 MHz) of compound **31**

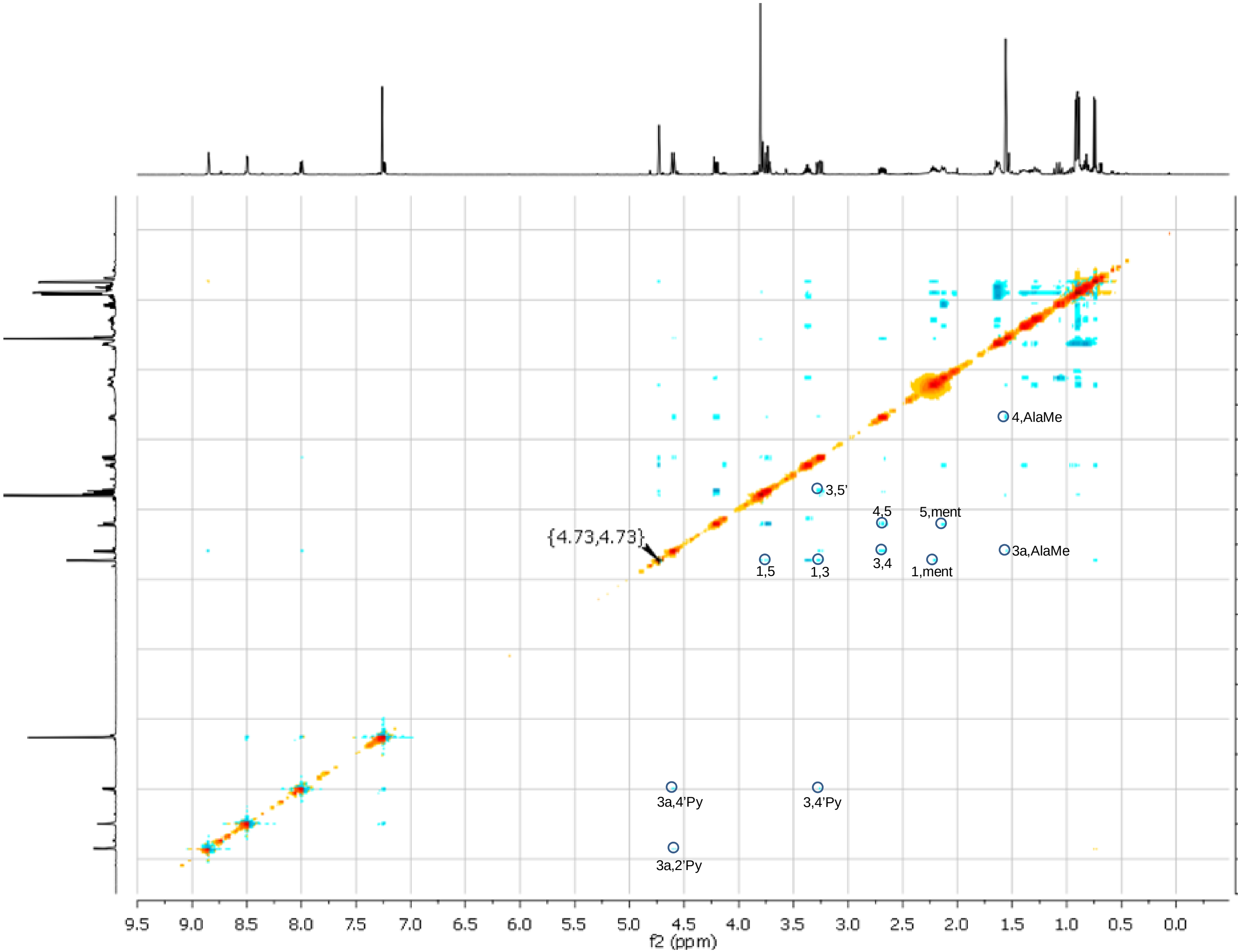




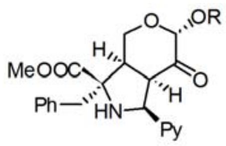
^{13}C NMR ($CDCl_3$, 125.7 MHz) of compound **31**

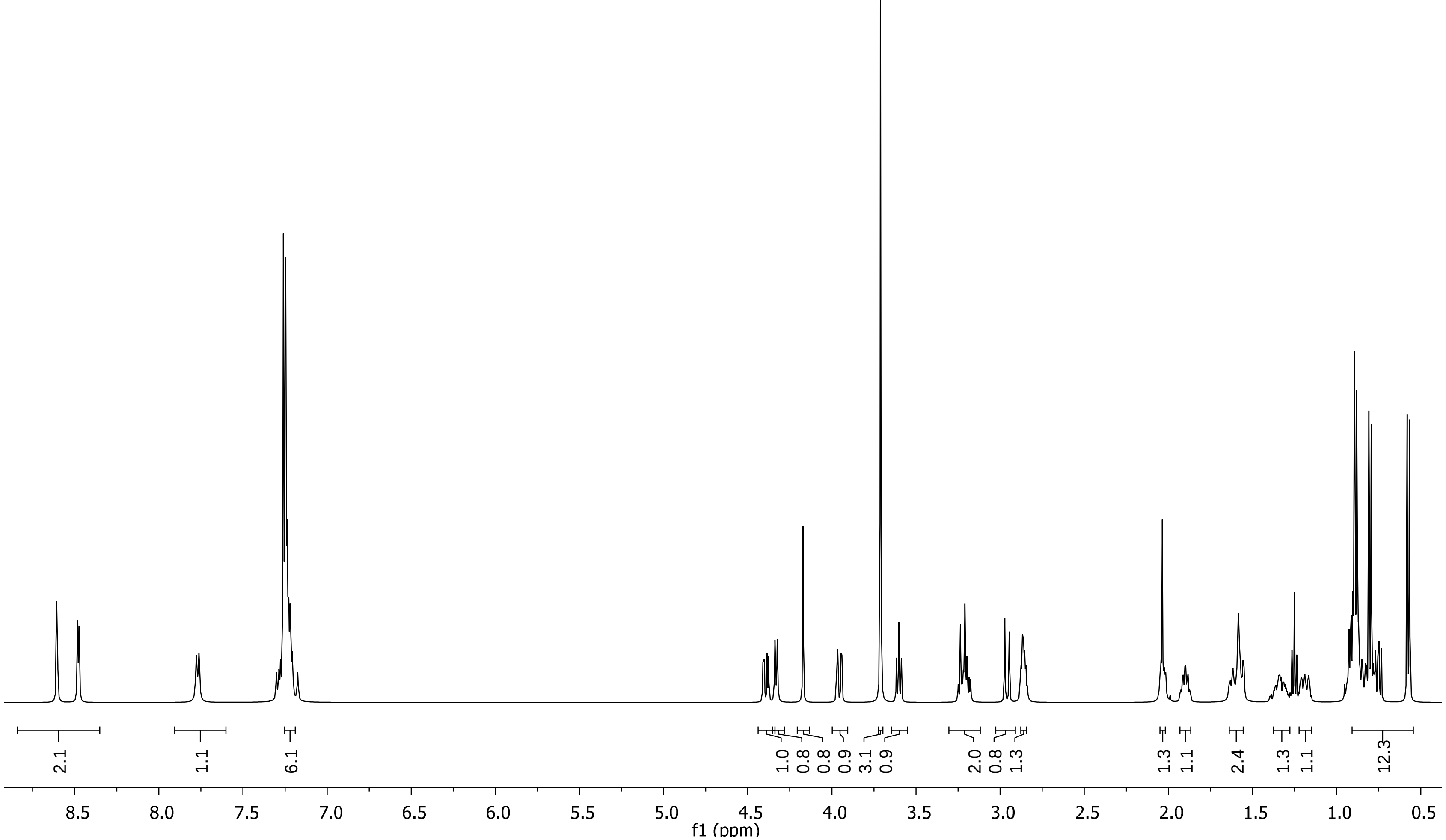


NOESY of compound **31**

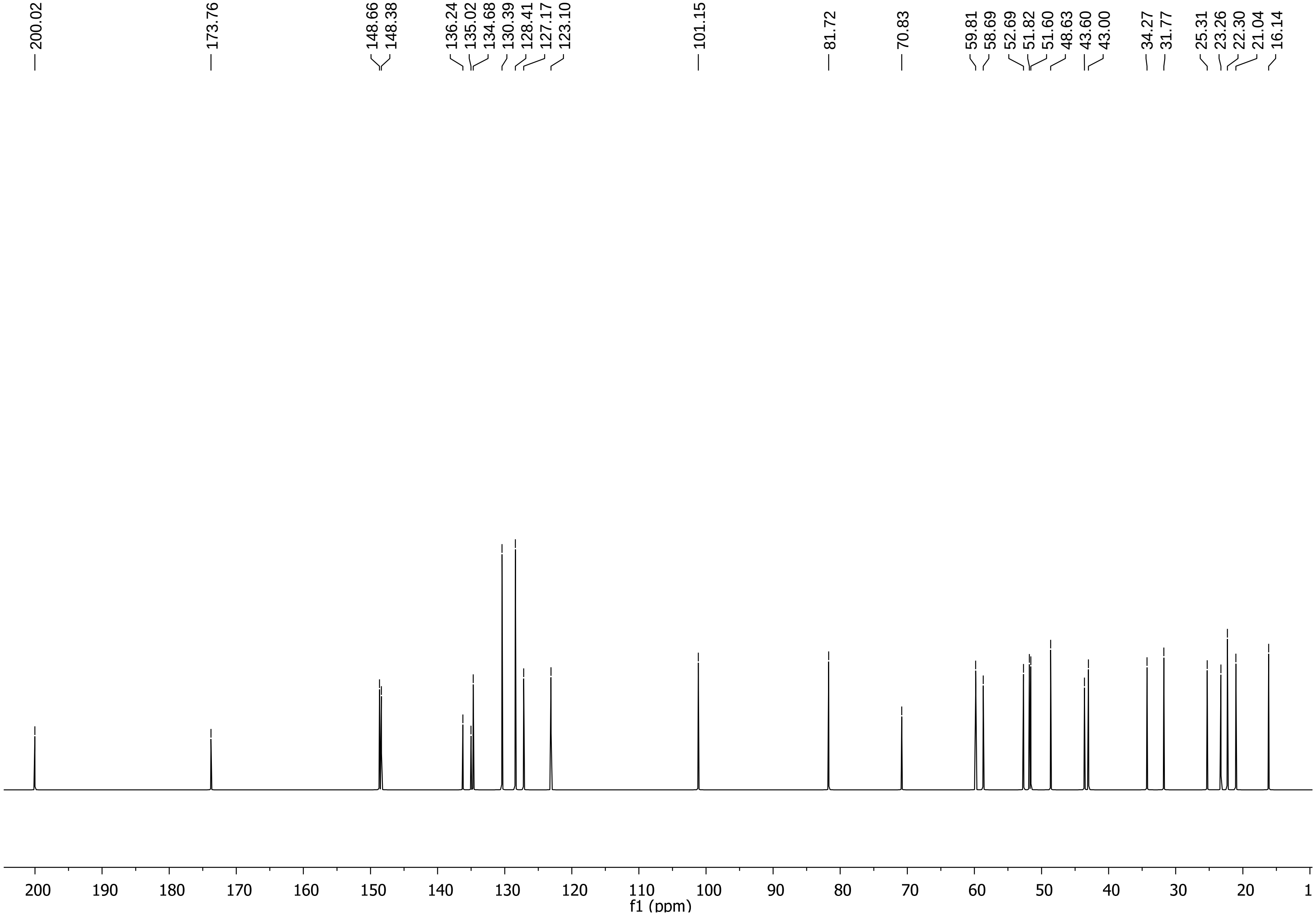


^{1}H NMR ($CDCl_3$, 500 MHz) of compound **32**

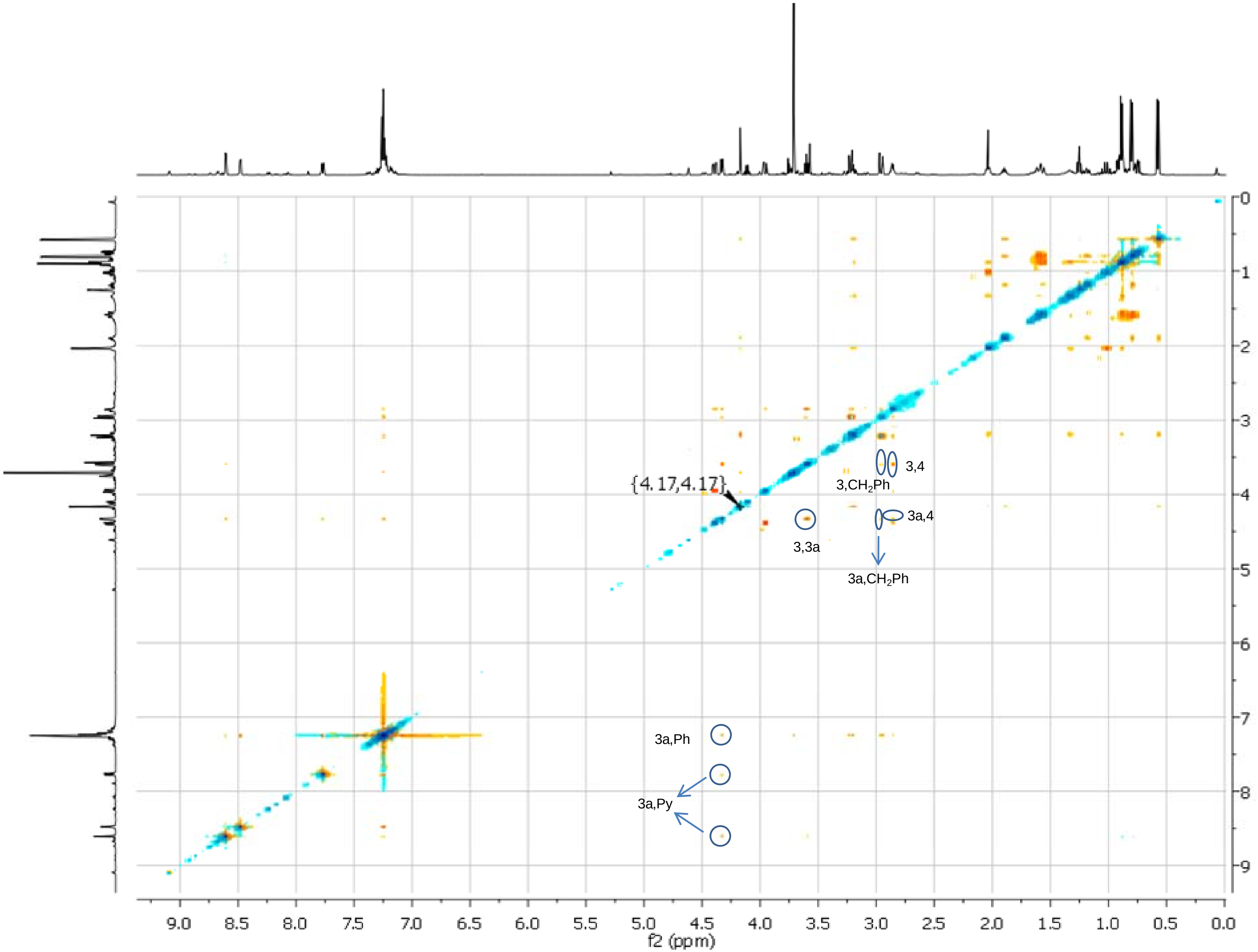




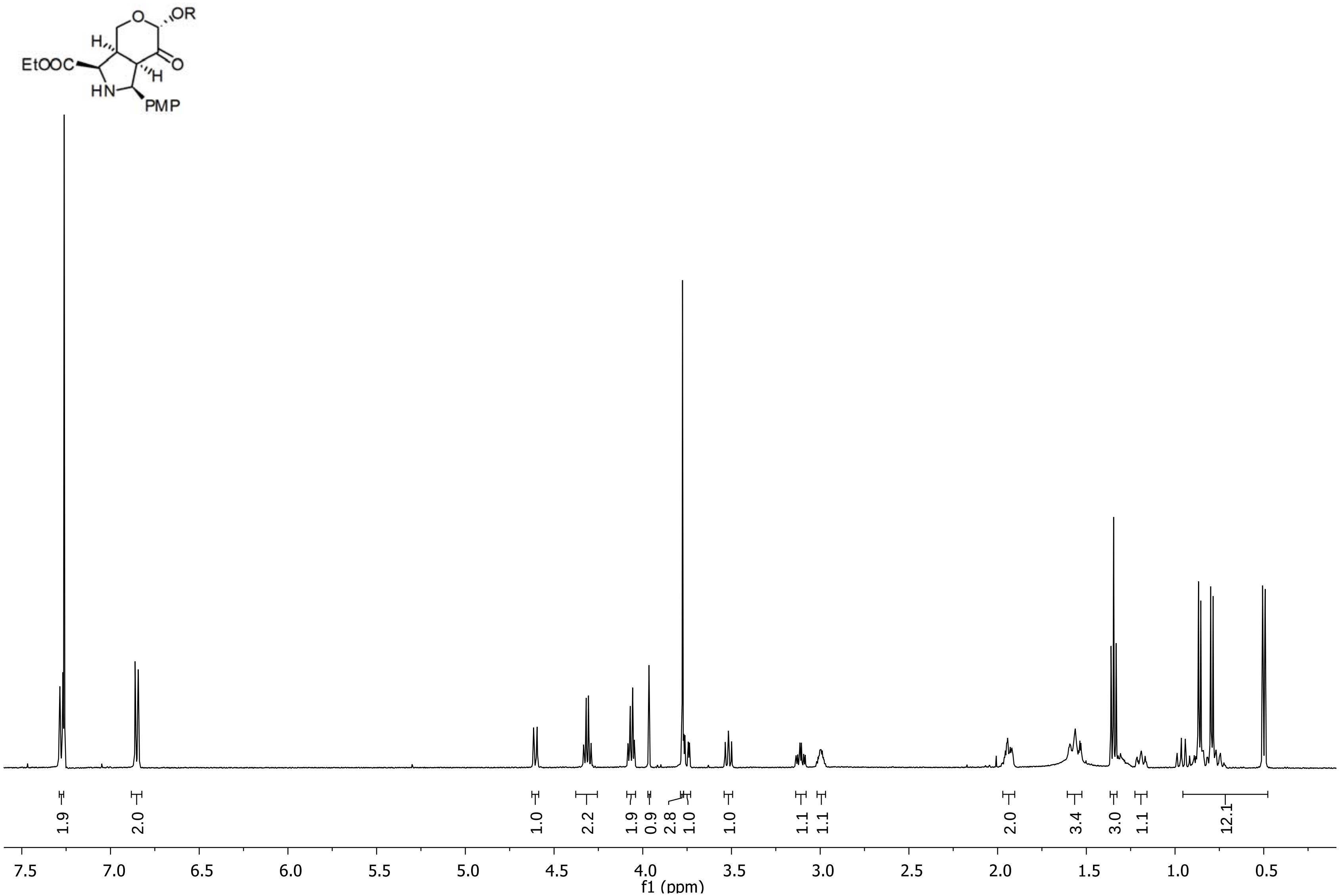
^{13}C NMR ($CDCl_3$, 125.7 MHz) of compound **32**



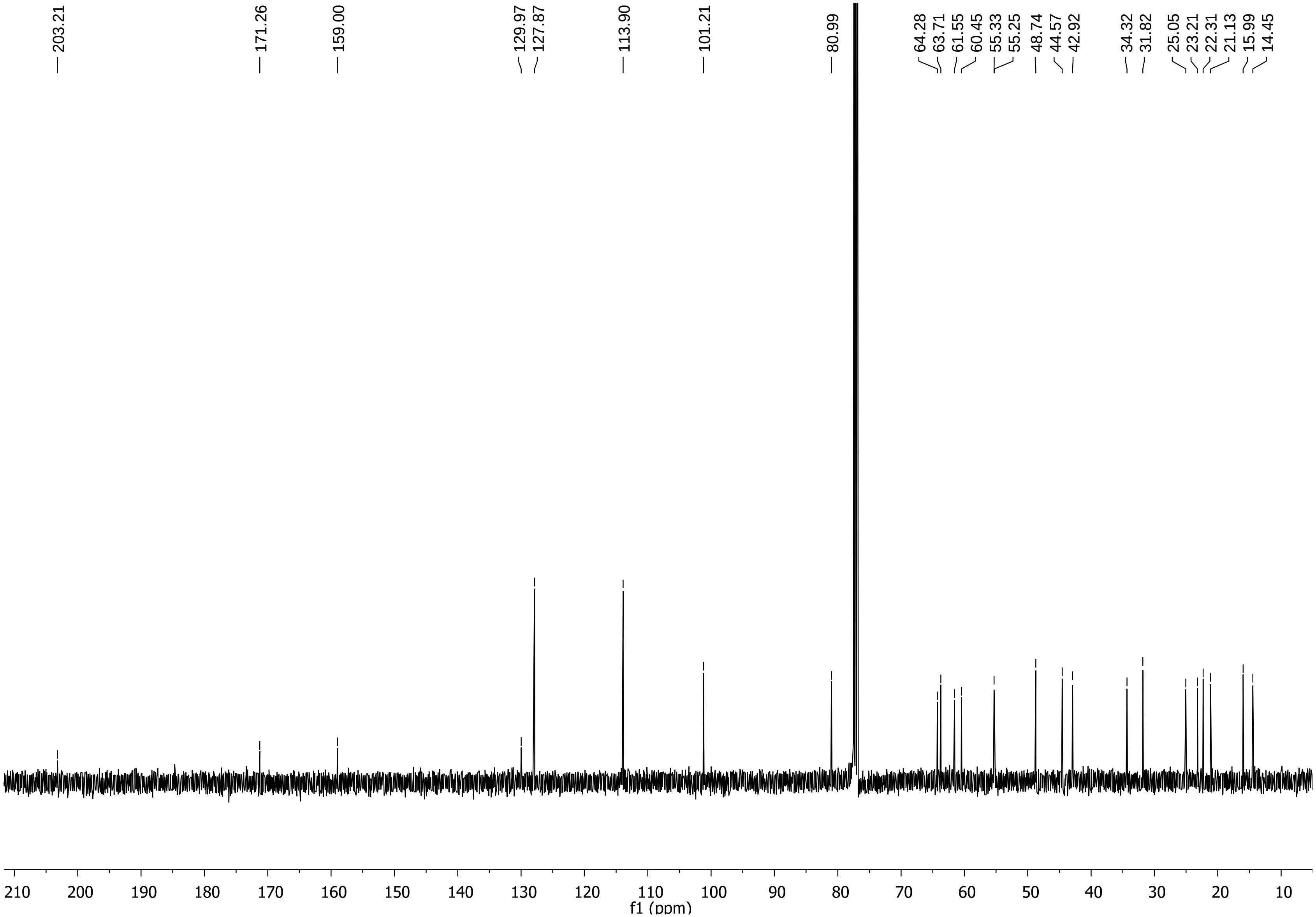
NOESY of compound **32**



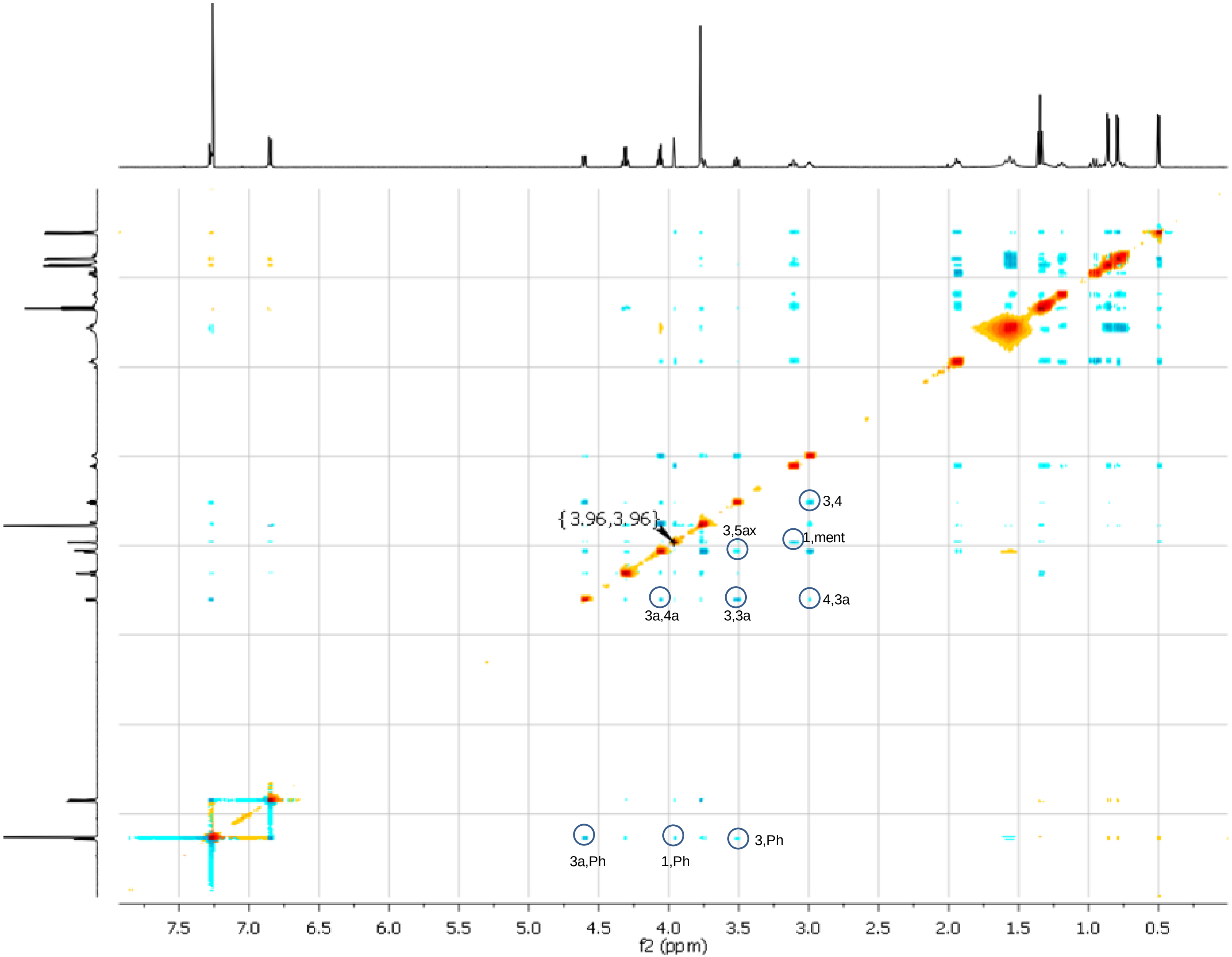
^{1}H NMR ($CDCl_3$, 500 MHz) of compound **33**



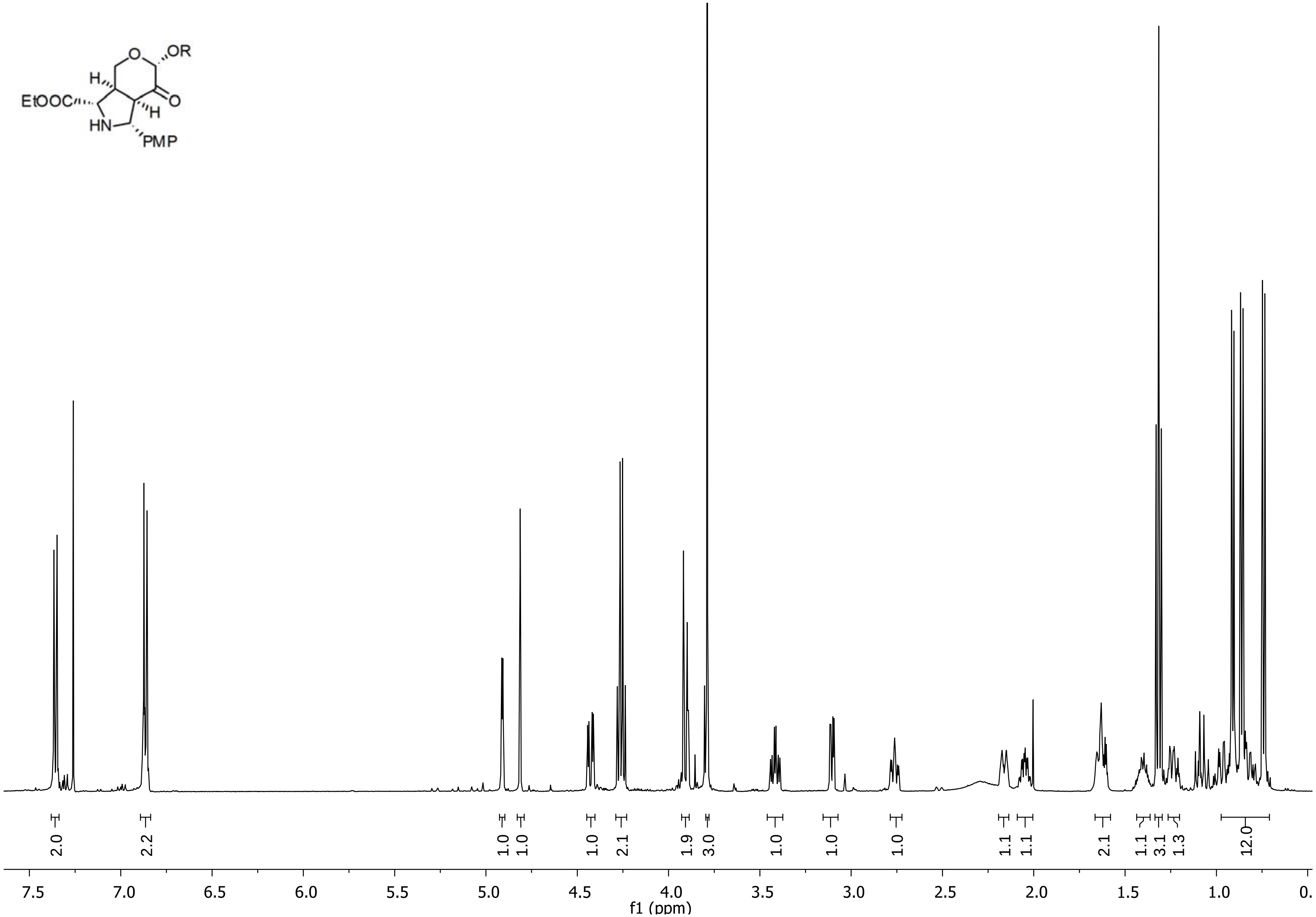
^{13}C NMR ($CDCl_3$, 125.7 MHz) of compound **33**



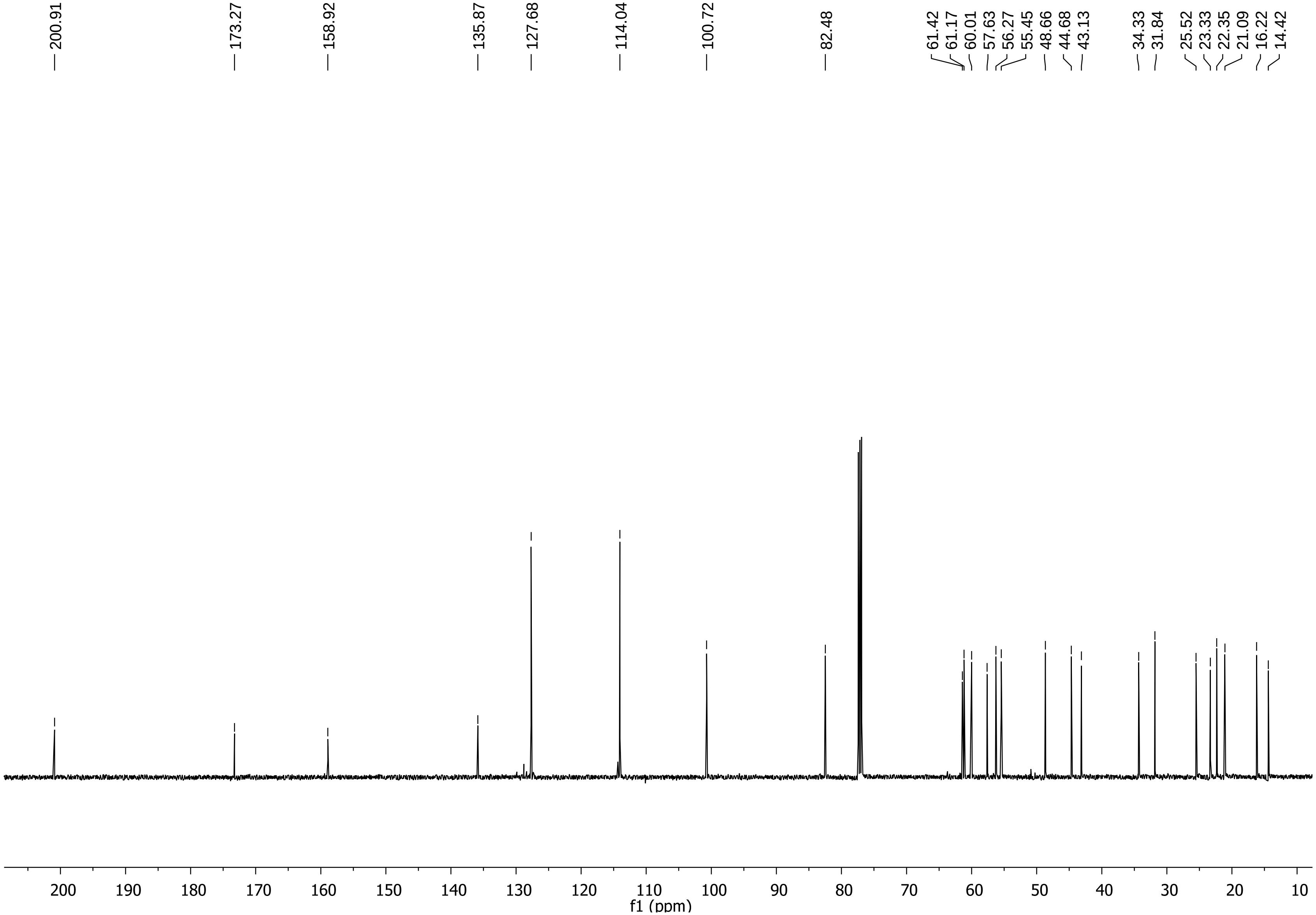
NOESY of compound **33**



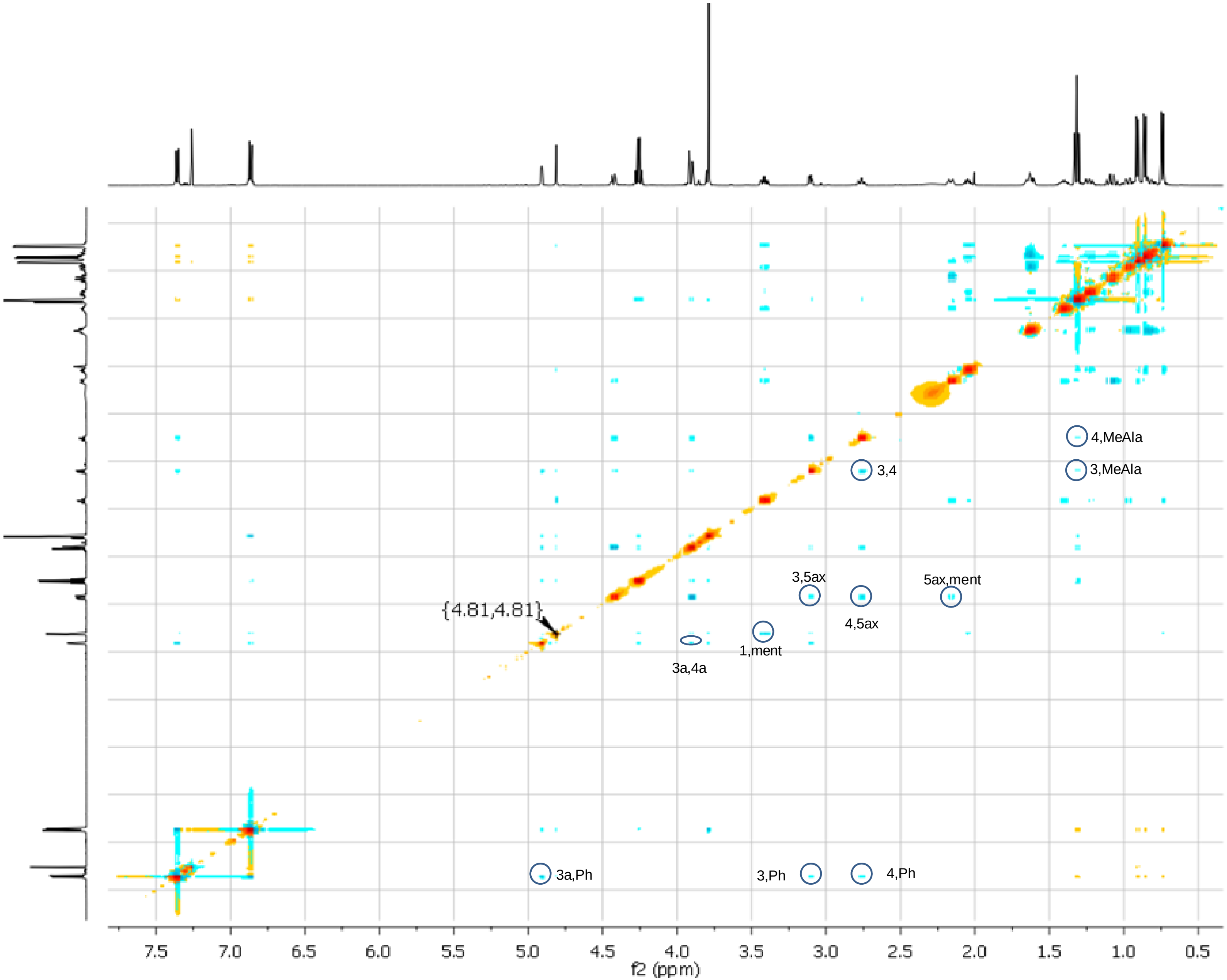
[1]H NMR ($CDCl_3$, 500 MHz) of compound **34**



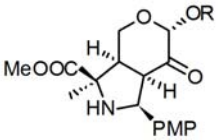
^{13}C NMR ($CDCl_3$, 125.7 MHz) of compound **34**

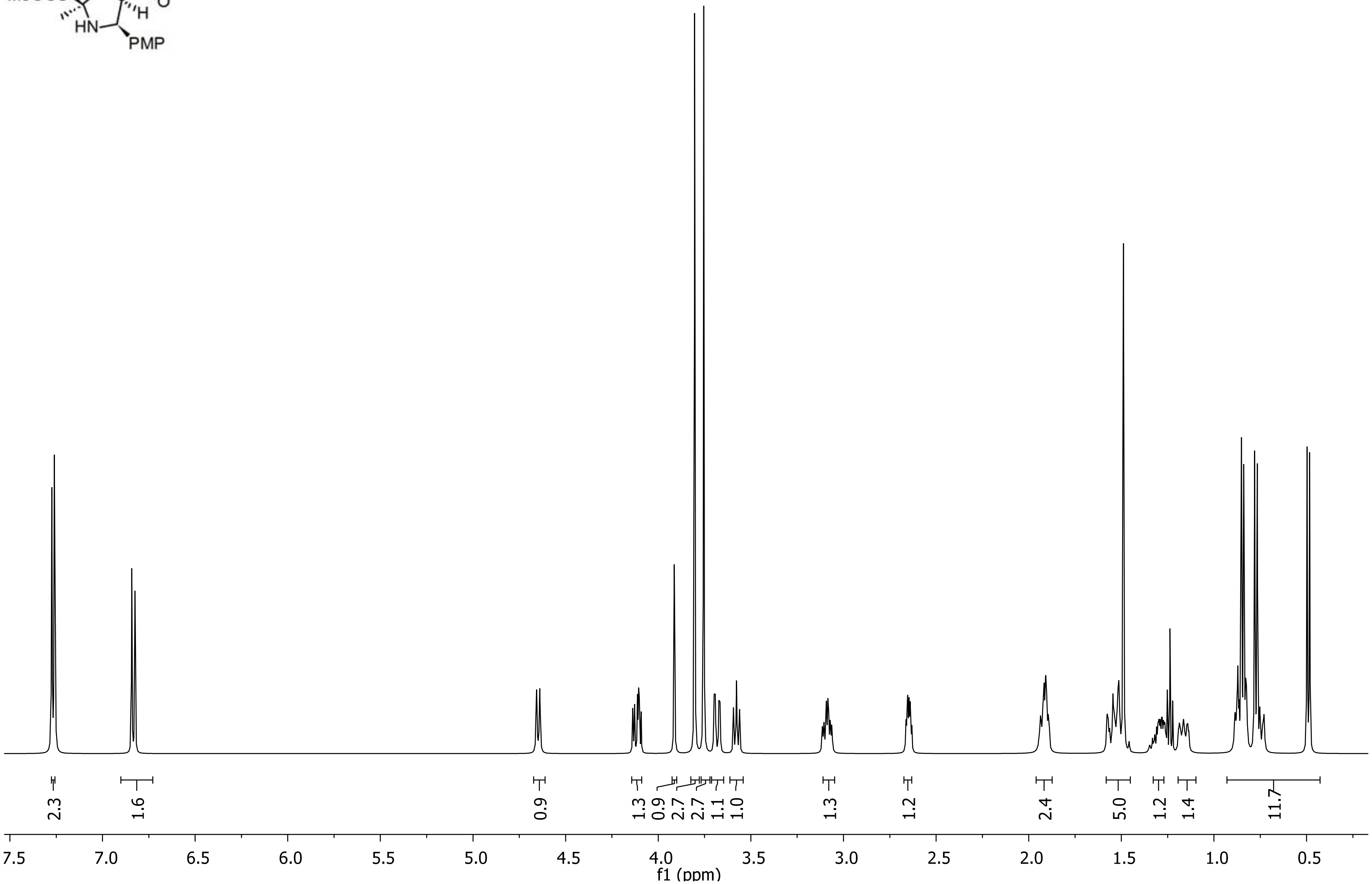


NOESY of compound **34**

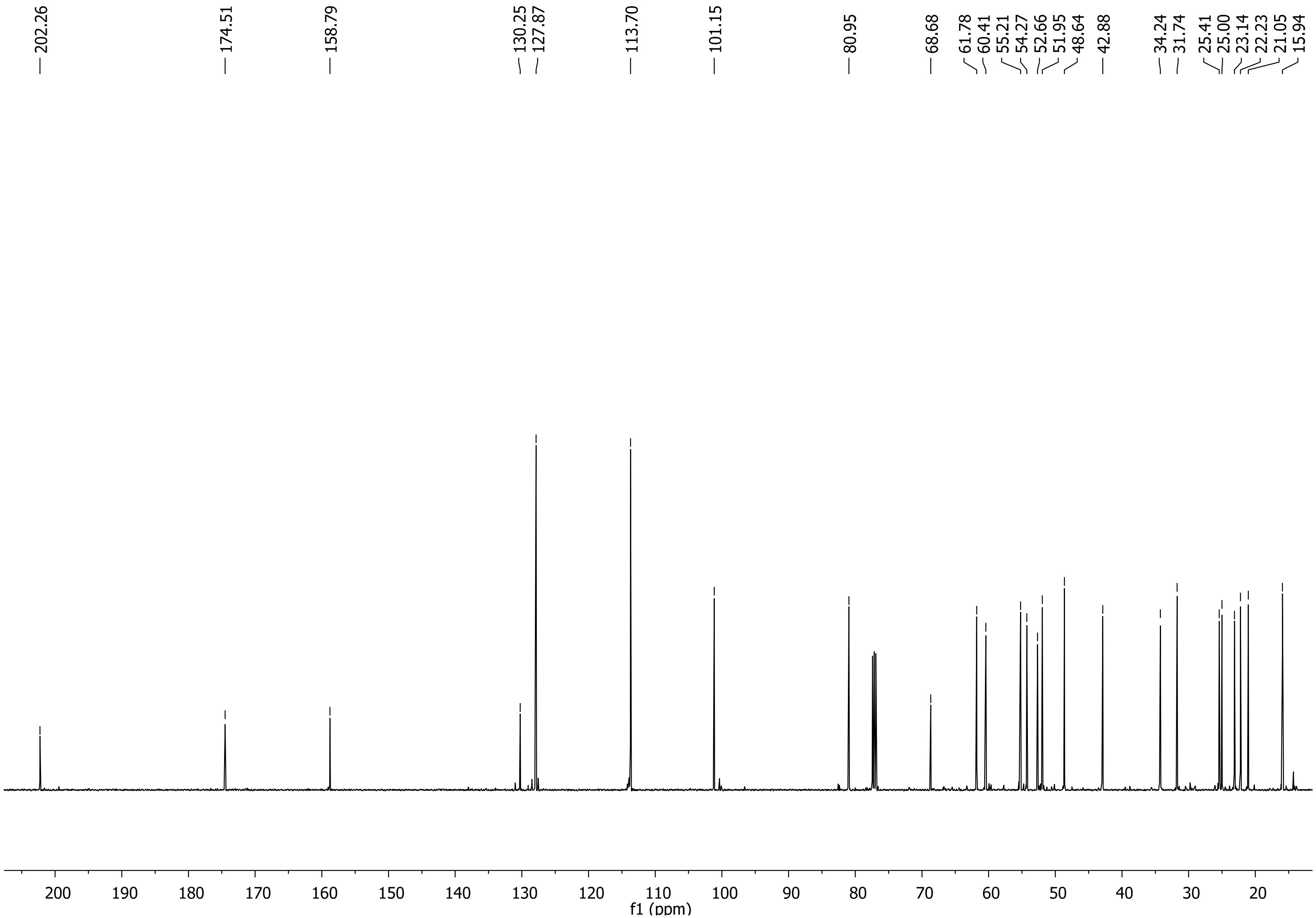


^{1}H NMR ($CDCl_3$, 500 MHz) of compound **35**

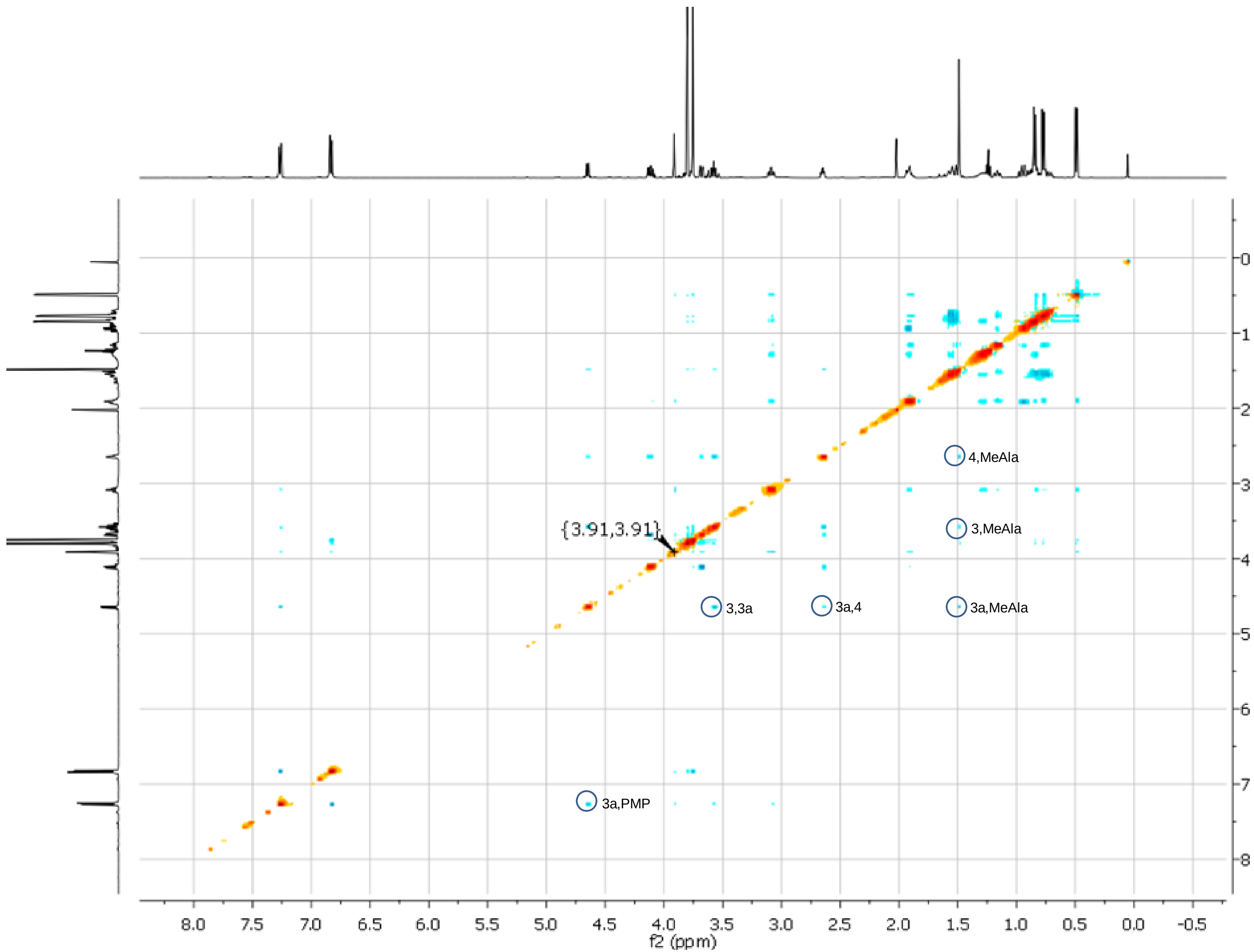




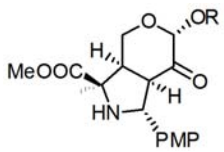
^{13}C NMR ($CDCl_3$, 125.7 MHz) of compound **35**

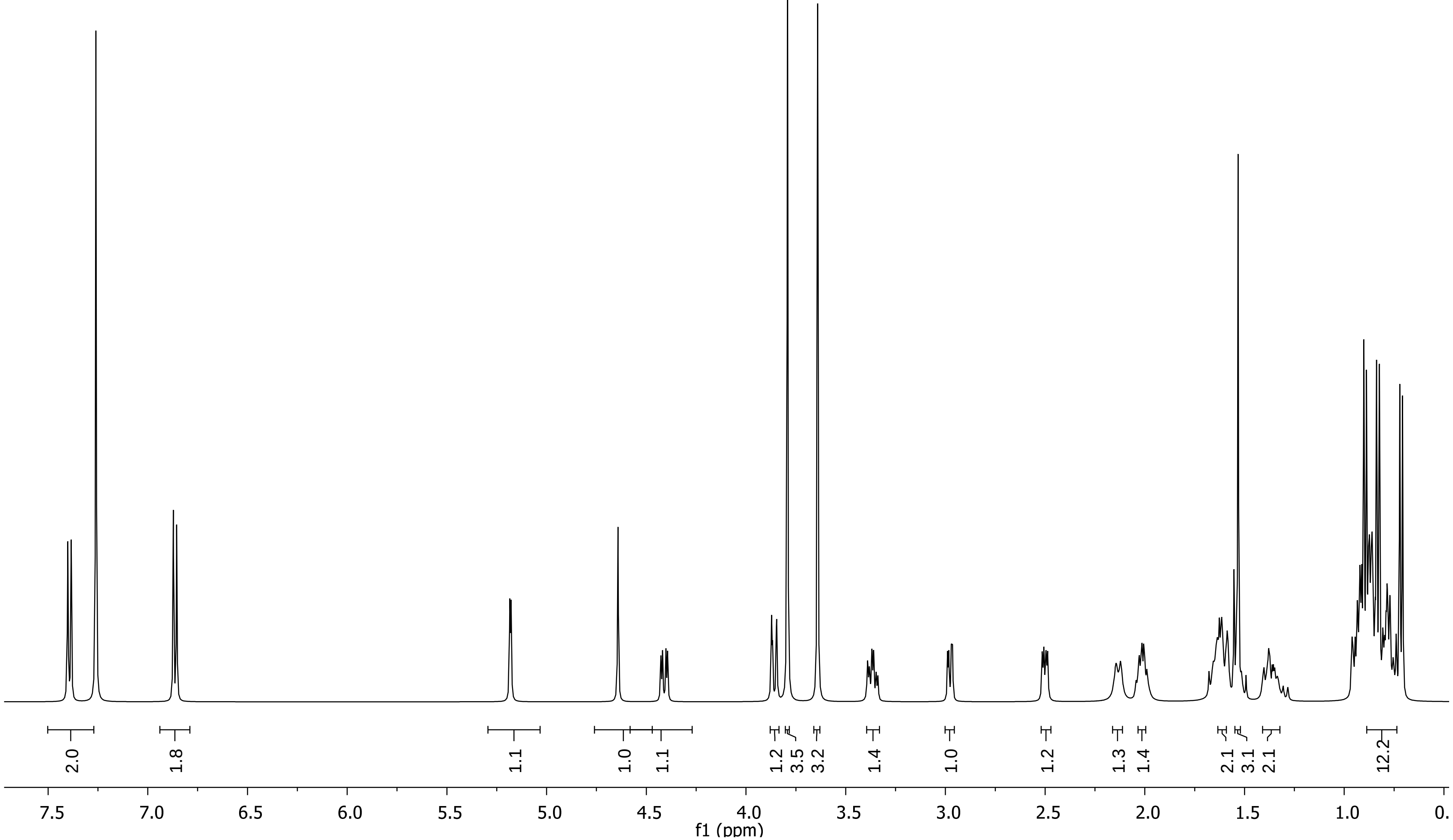


NOESY of compound **35**

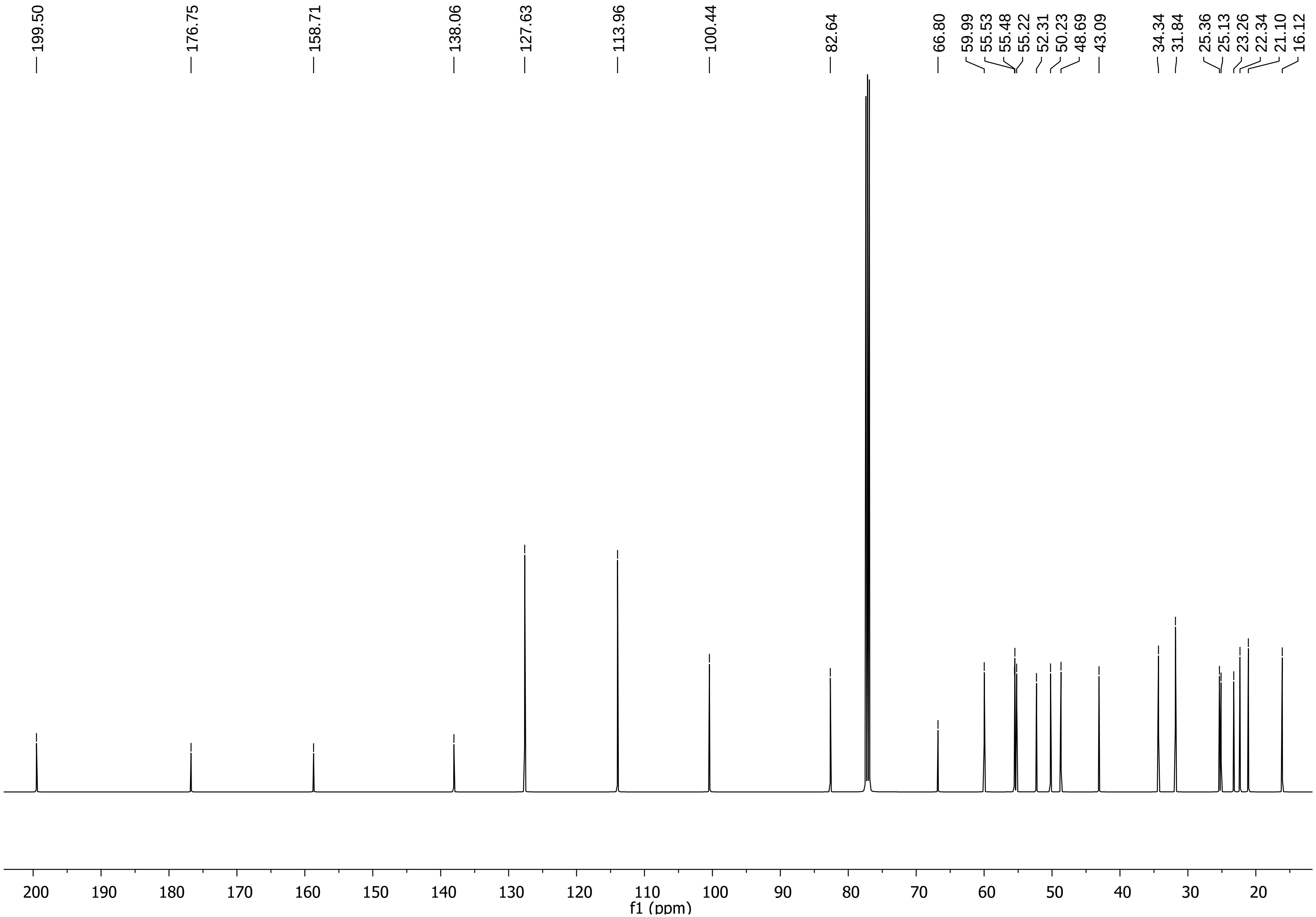


^{1}H NMR ($CDCl_3$, 500 MHz) of compound **36**

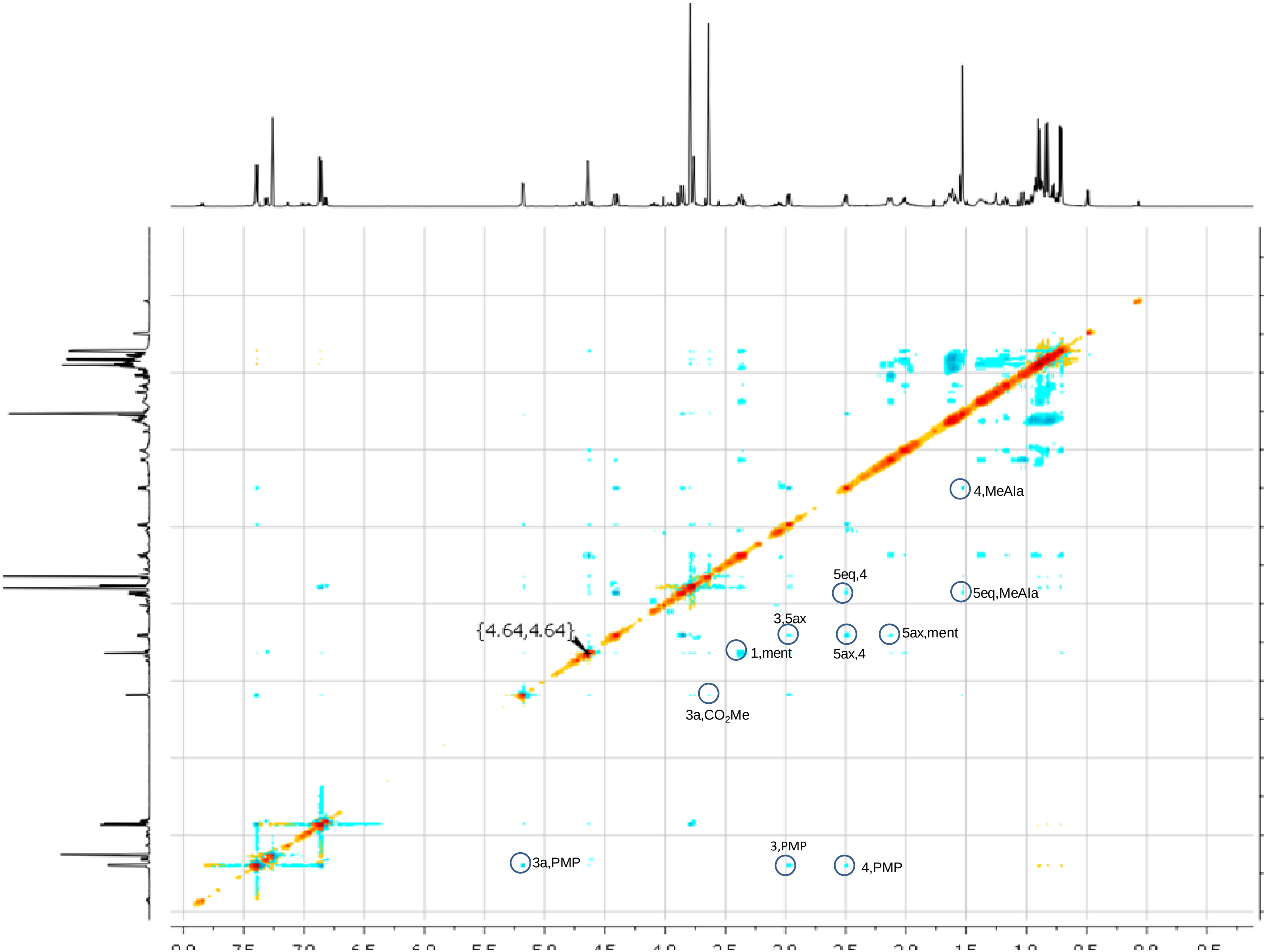




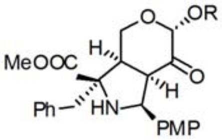
^{13}C NMR ($CDCl_3$, 125.7 MHz) of compound **36**

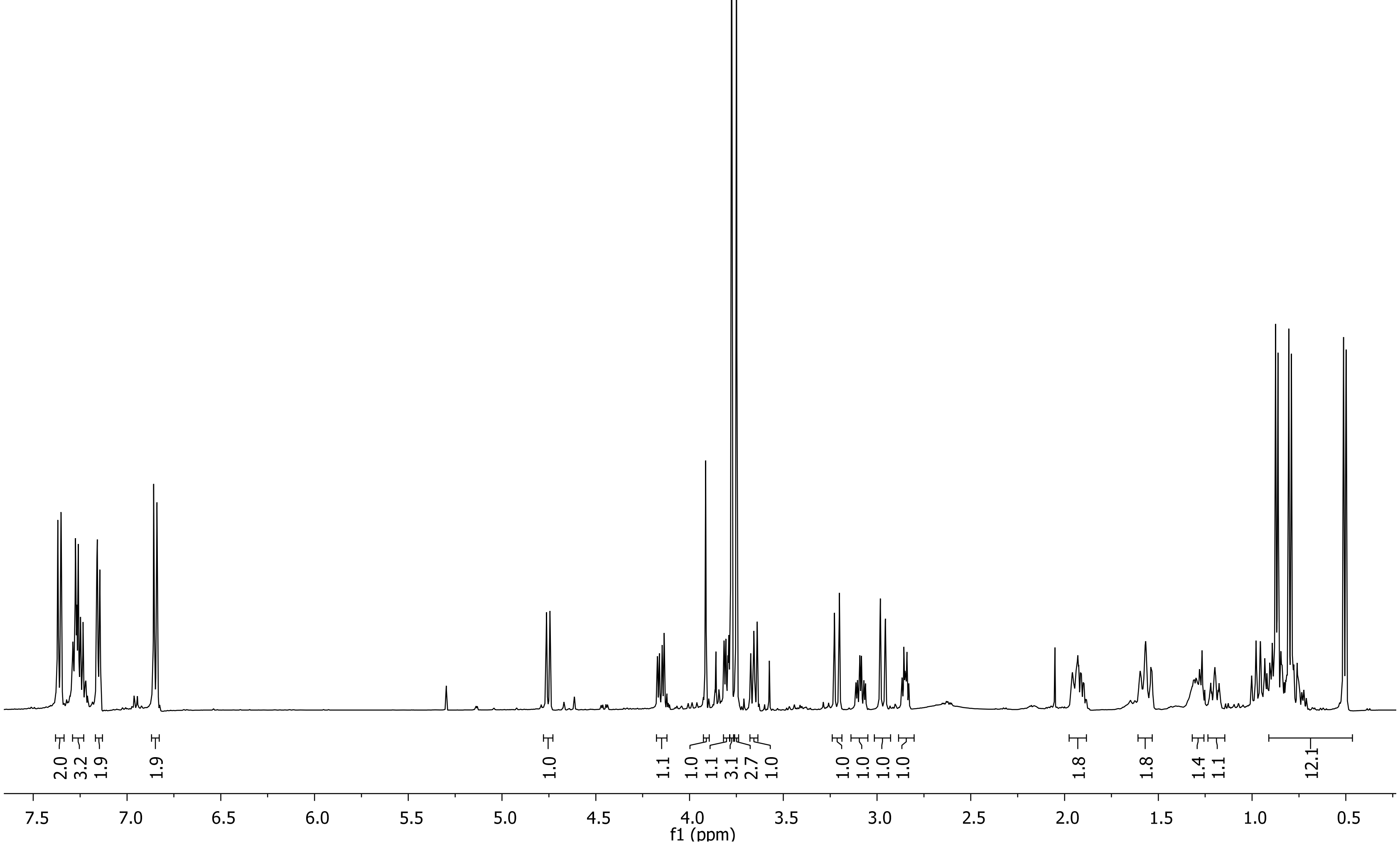


NOESY of compound **36**

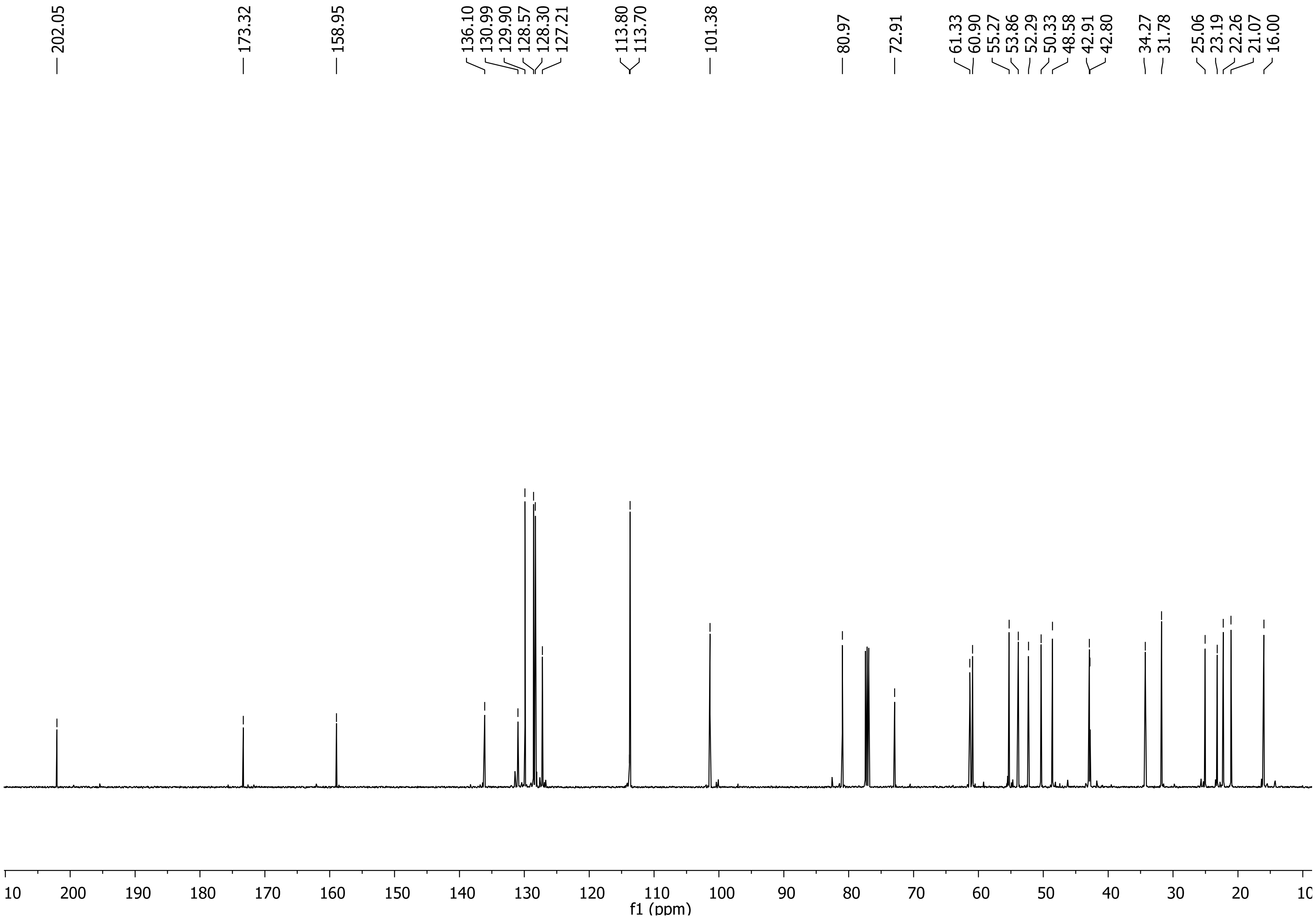


^{1}H NMR ($CDCl_3$, 500 MHz) of compound **37**

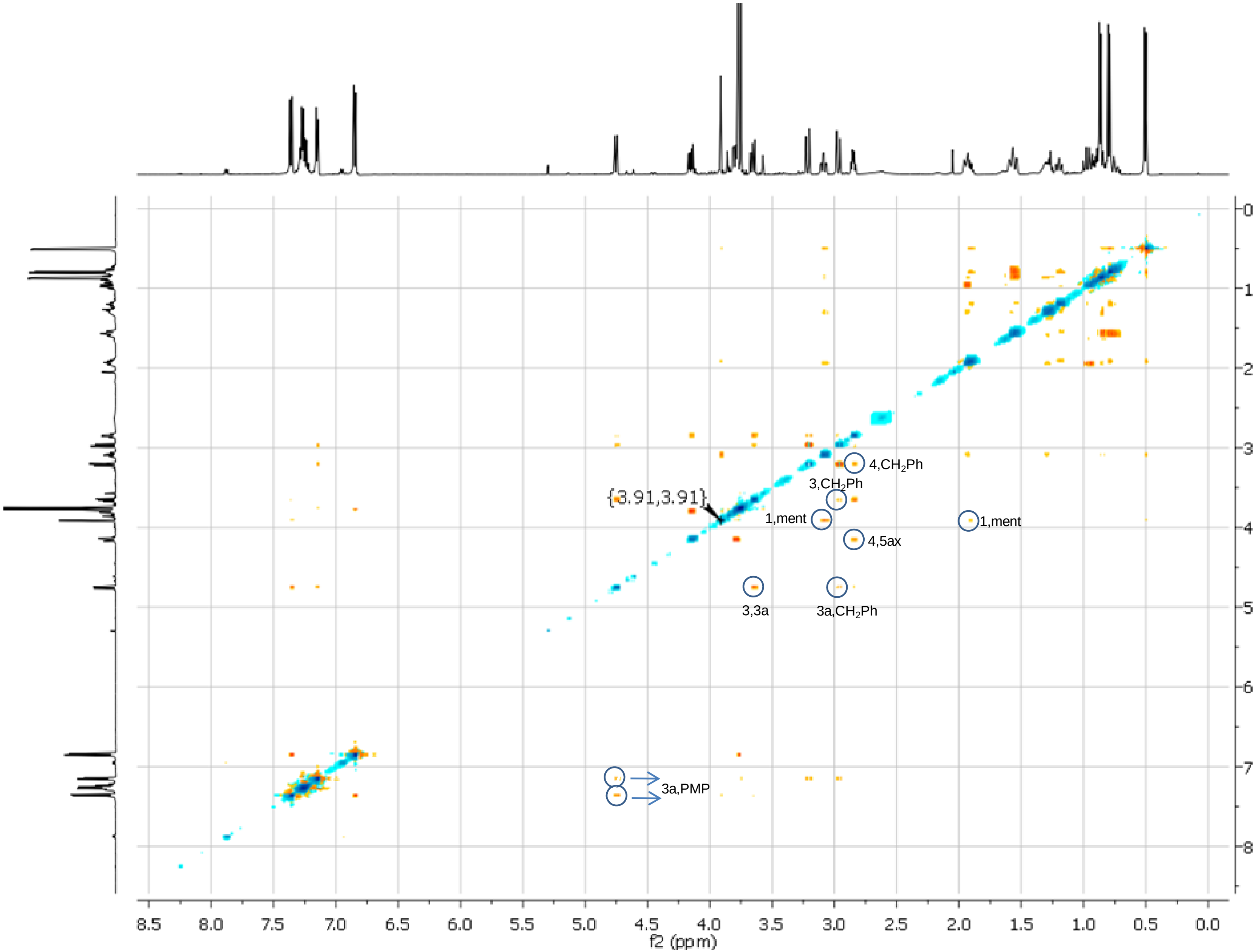




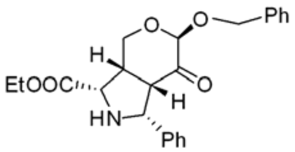
^{13}C NMR ($CDCl_3$, 125.7 MHz) of compound **37**

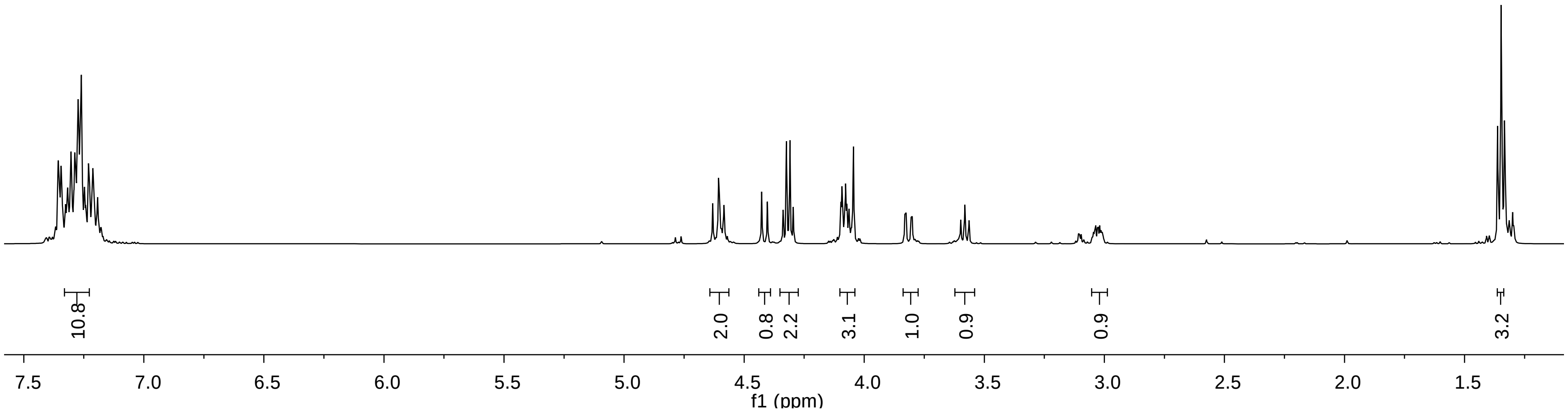


NOESY of compound **37**

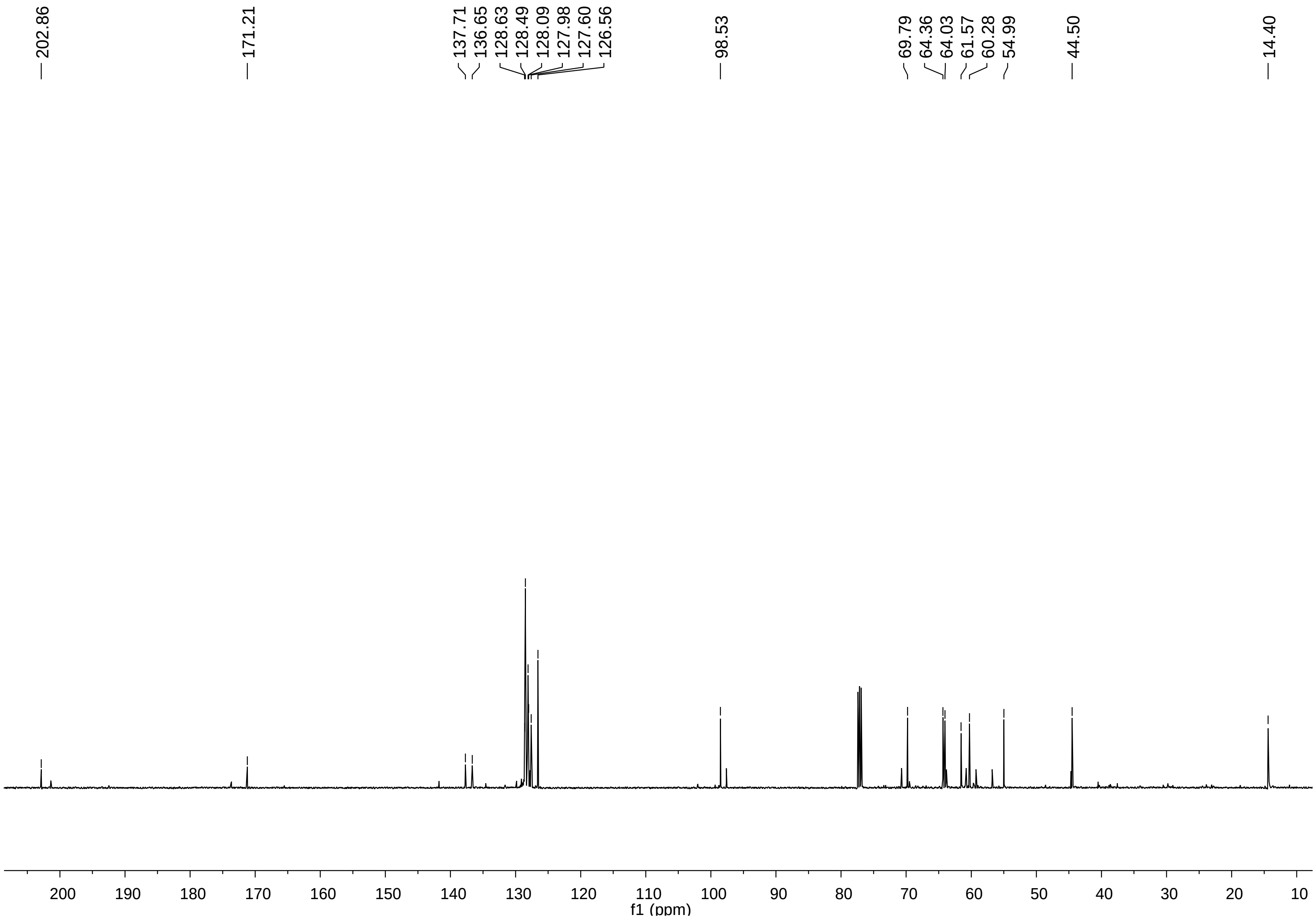


[1]H NMR ($CDCl_3$, 500 MHz) of compound **39**

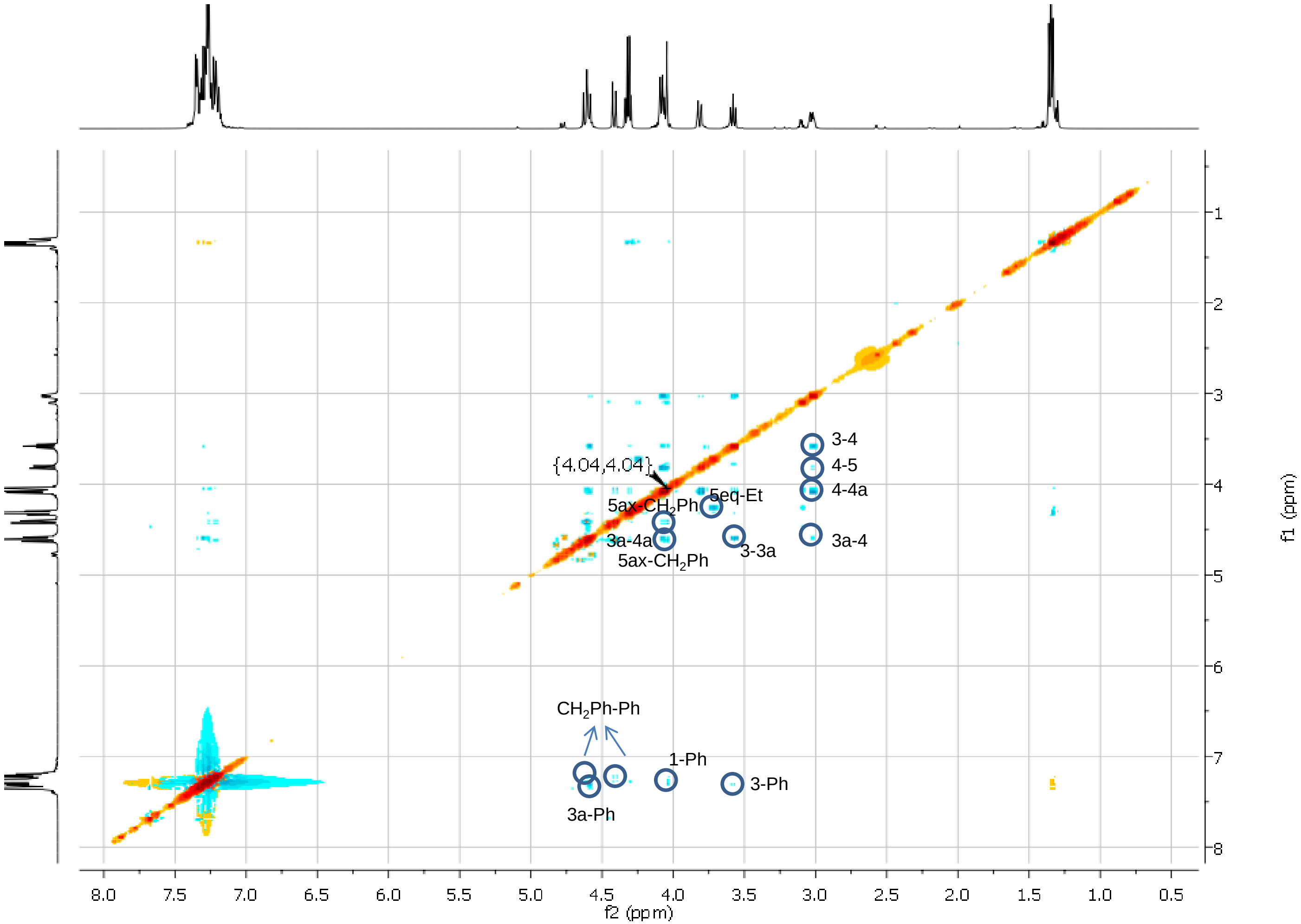




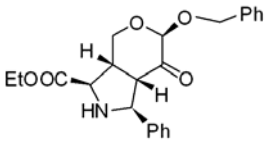
^{13}C NMR ($CDCl_3$, 125. MHz) of compound **39**

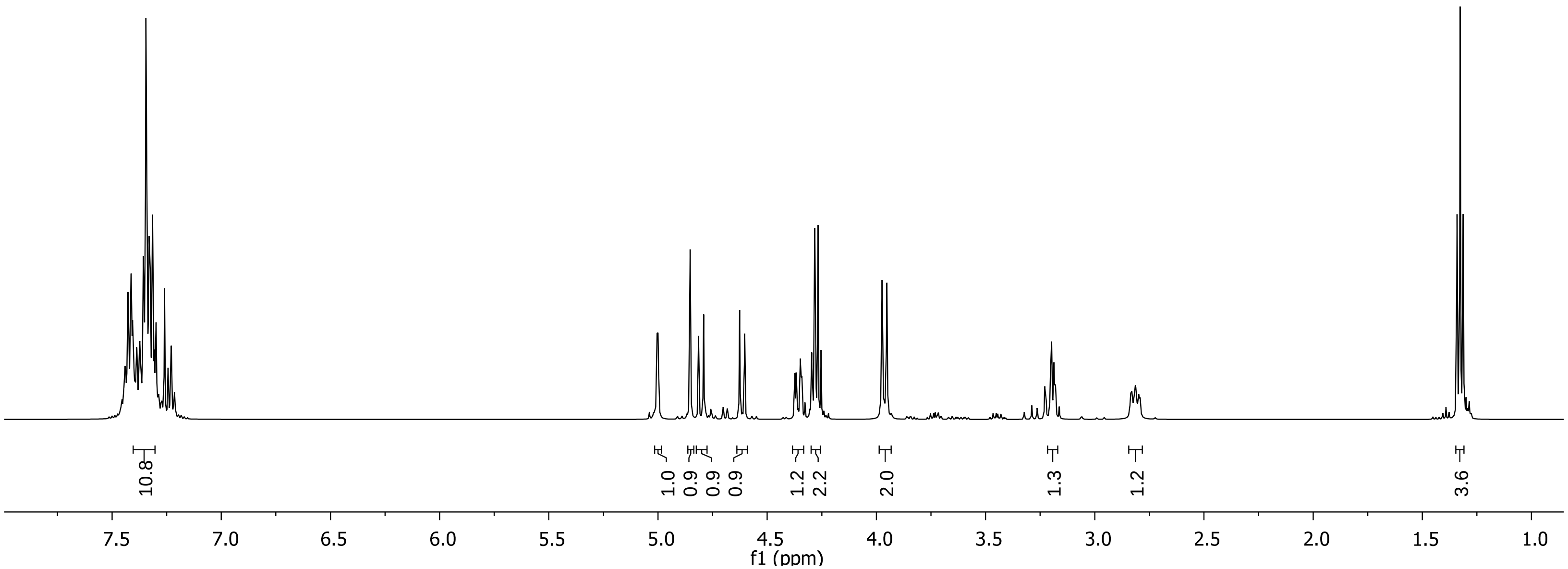


NOESY of compound **39**

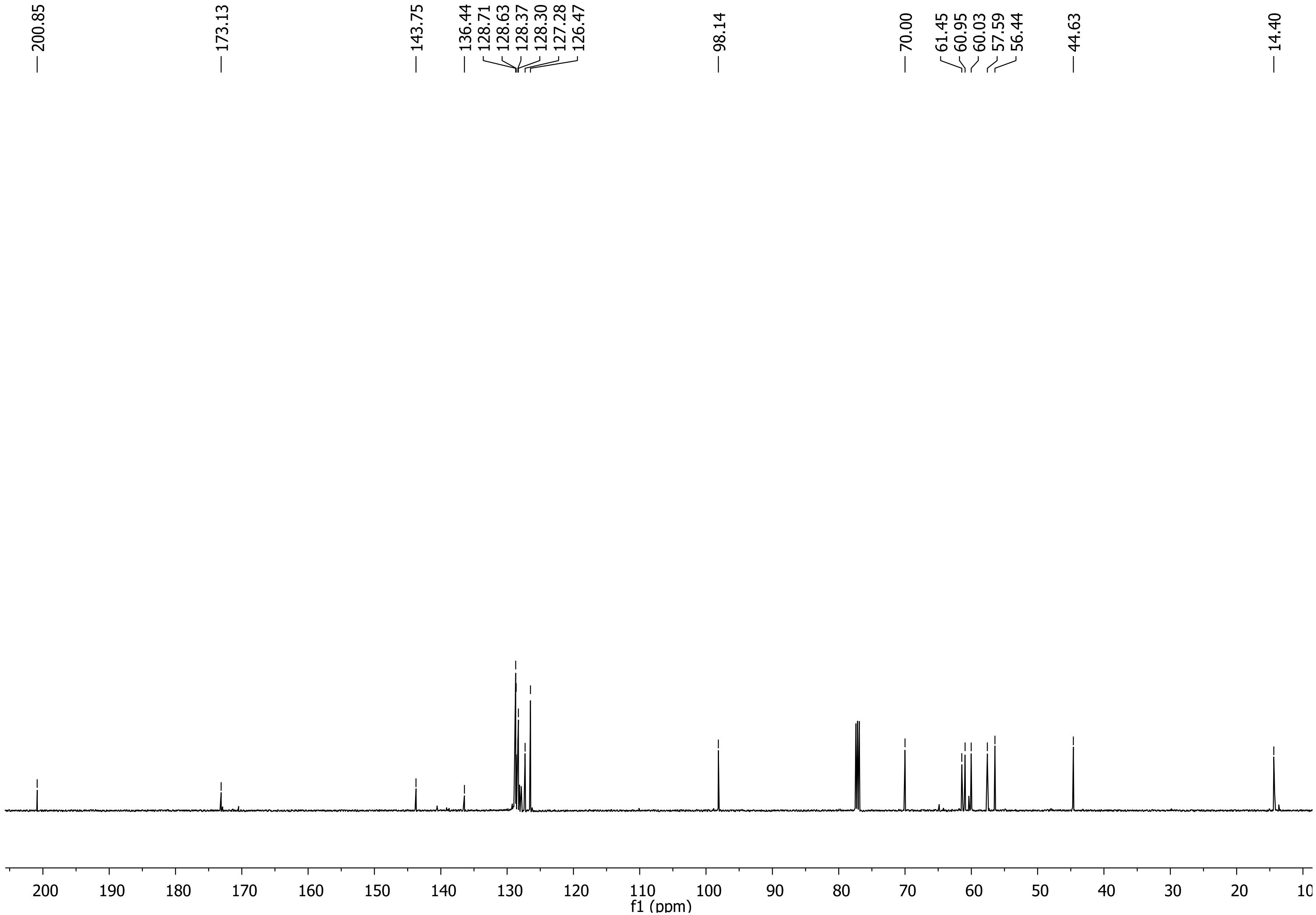


[1]H NMR ($CDCl_3$, 500 MHz) of compound **40**





^{13}C NMR ($CDCl_3$, 125.7 MHz) of compound **40**



NOESY of compound **40**

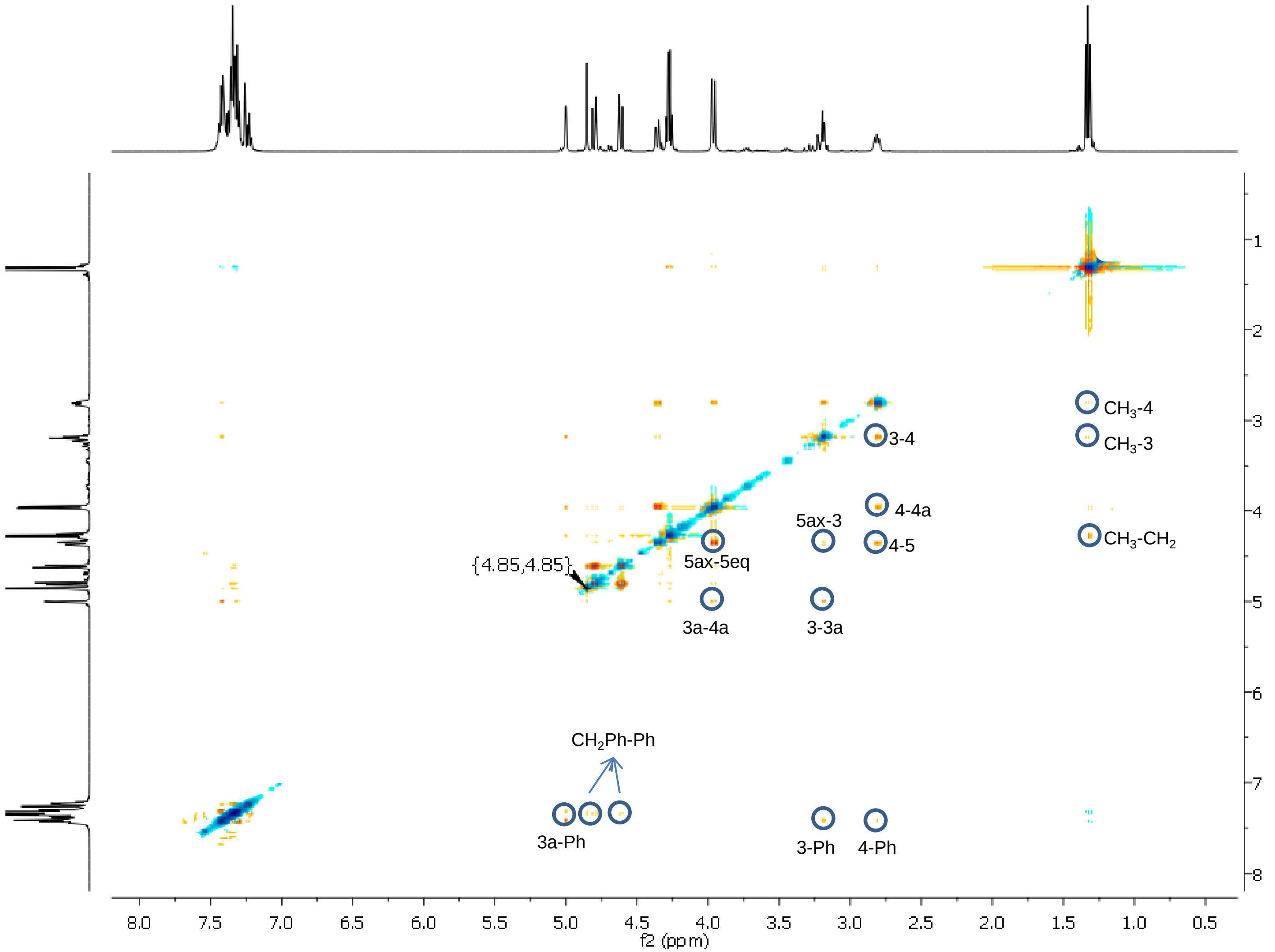


Table: Comparison of NMR data for each group of selected isomers.

Compound	δH-1	δH-3 ($J_{3,4}$ Hz)	δH-3a ($J_{3,3a}$ Hz)	δH-4 ($J_{4,5ax}$; $J_{4,5eq}$ Hz)	δH-4a ($J_{4,4a}$ Hz)
***Endo*-adducts**					
7	4.05	3.58 (8.2)	4.63 (9.3)	3.03 (4.6; 2.8)	4.09 (7.3)
12	4.23	3.53 (7.8)	4.47 (7.7)	3.08 (4.2; 2.0)	4.04 (8.3)
24	3.94	3.56 (8.4)	4.62 (9.3)	3.00 (4.7; 2.9)	4.06 (6.9)
***Exo*-adducts**					
8	4.92	3.15 (8.2)	5.01 (2.8)	2.82 (3,2; 0)	3.98 (10.4)
13	4.91	3.13 (8.1)	5.06 (2.4)	2.79 (3.0; 0)	3.96 (10.5)
25	4.82	3.15 (8.2)	5.01 (2.5)	2.78 (3.3; 0)	3.93 (10.5)
***Epi*-adducts**[a]					
18 (*epi*-**16**)	4.75	2.97 (9.0)	5.26 (<1)	2.99 (2.9; 0)	4.01 (7.9)
epi-**7**	4.76	3.00	5.33 (<1)	3.00 (3.0; 0)	4.03 (8.0)
epi-**10**	4.75	2.99 (9.3)	5.27 (3.0)	2.52 (4.1; 0)	

[a] *Epi* at C-3a of *endo*-adducts.