Supplementary Information

Cascade reactions initiated by radical addition of tetrahydrofuran to β-bromonitrostyrenes

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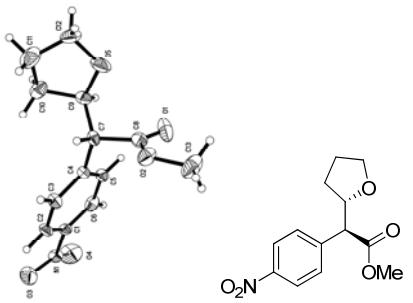
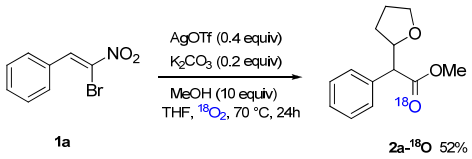
4. X-ray data of compound 2h-1



Crystal data and structure refinement for compound **2h-1**

Identification code	compound **2h-1**	
Empirical formula	C13 H15 N O5	
Formula weight	265.26	
Temperature	103(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.0104(6) Å	a= 102.106(2)°.
	b = 8.0179(8) Å	b= 109.539(3)°.
	c = 10.7954(7) Å	g = 95.818(2)°.
Volume	627.73(9) $Å^3$	
Z	2	
Density (calculated)	1.403 Mg/m^3	
Absorption coefficient	0.109 mm^{-1}	
F(000)	280	
Crystal size	0.40 x 0.24 x 0.20 mm^3	
Theta range for data collection	2.07 to 32.02°.	
Index ranges	-11<=h<=11, -11<=k<=11, -16<=l<=16	
Reflections collected	13070	
Independent reflections	4334 [R(int) = 0.0180]	
Completeness to theta = 32.02°	99.8 %	
Absorption correction	None	
Max. and min. transmission	0.9786 and 0.9578	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4334 / 915 / 346	
Goodness-of-fit on F^2	1.038	
Final R indices [I>2sigma(I)]	R1 = 0.0462, wR2 = 0.1126	
R indices (all data)	R1 = 0.0675, wR2 = 0.1230	
Largest diff. peak and hole	0.223 and -0.205 $e.Å^{-3}$	

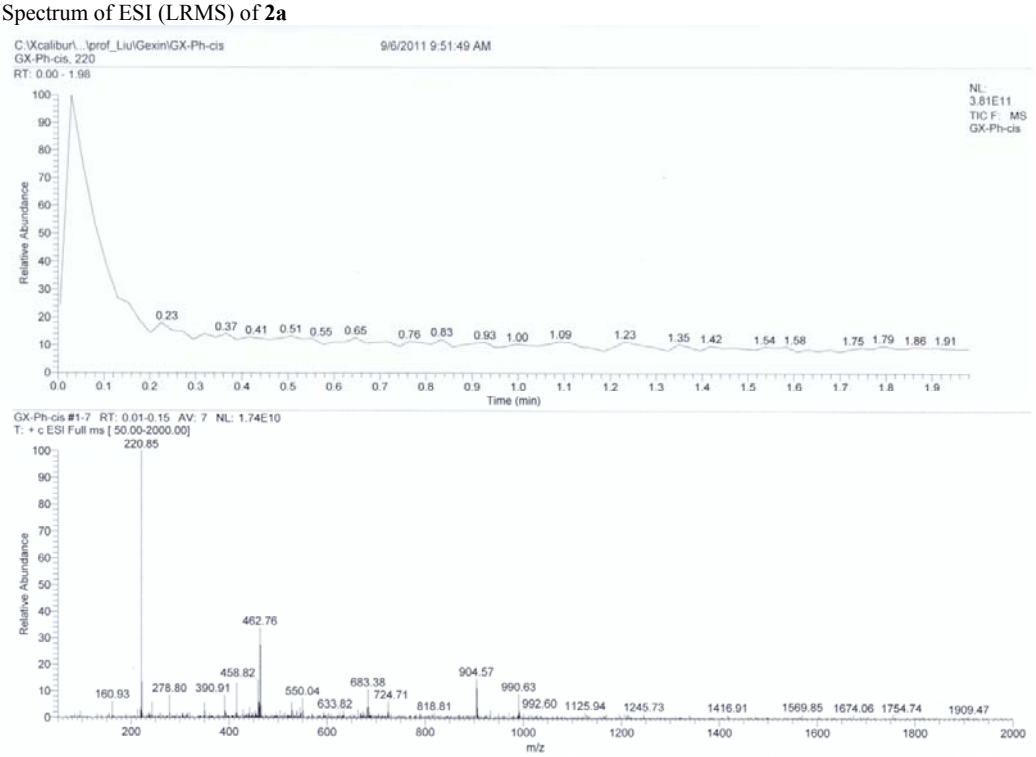
5. Isotope labeling experiments



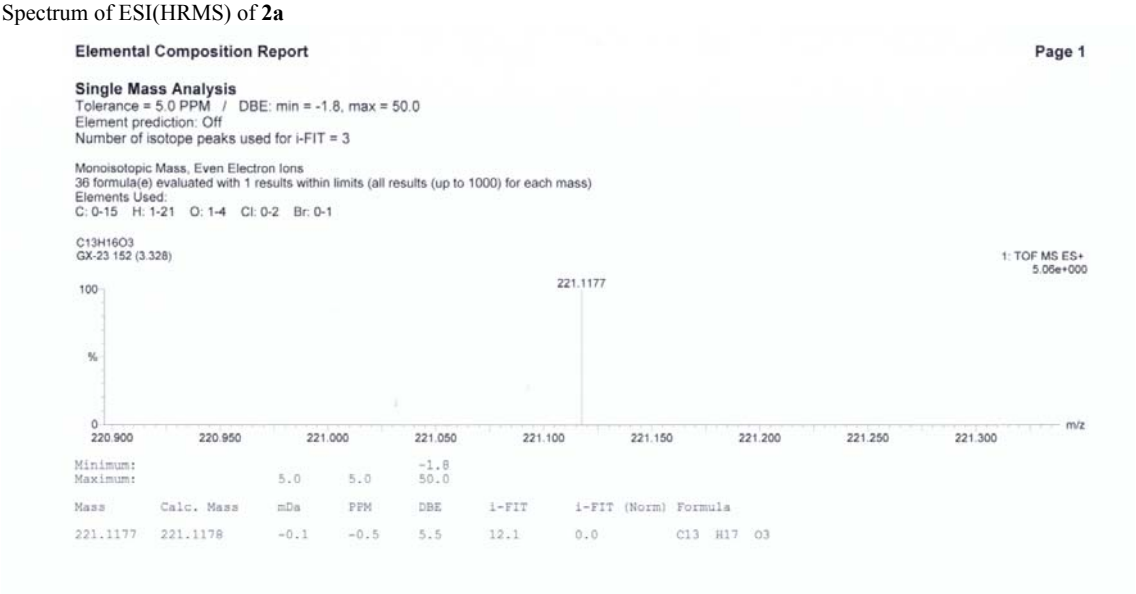
1a **2a-^{18}O** 52%

When the reaction was conducted under an $^{18}O_2$ atmosphere, the ester was obtained in 52% yield. The differences in mass spectroscopy showed that an ^{18}O atom was incorporated into the ester.

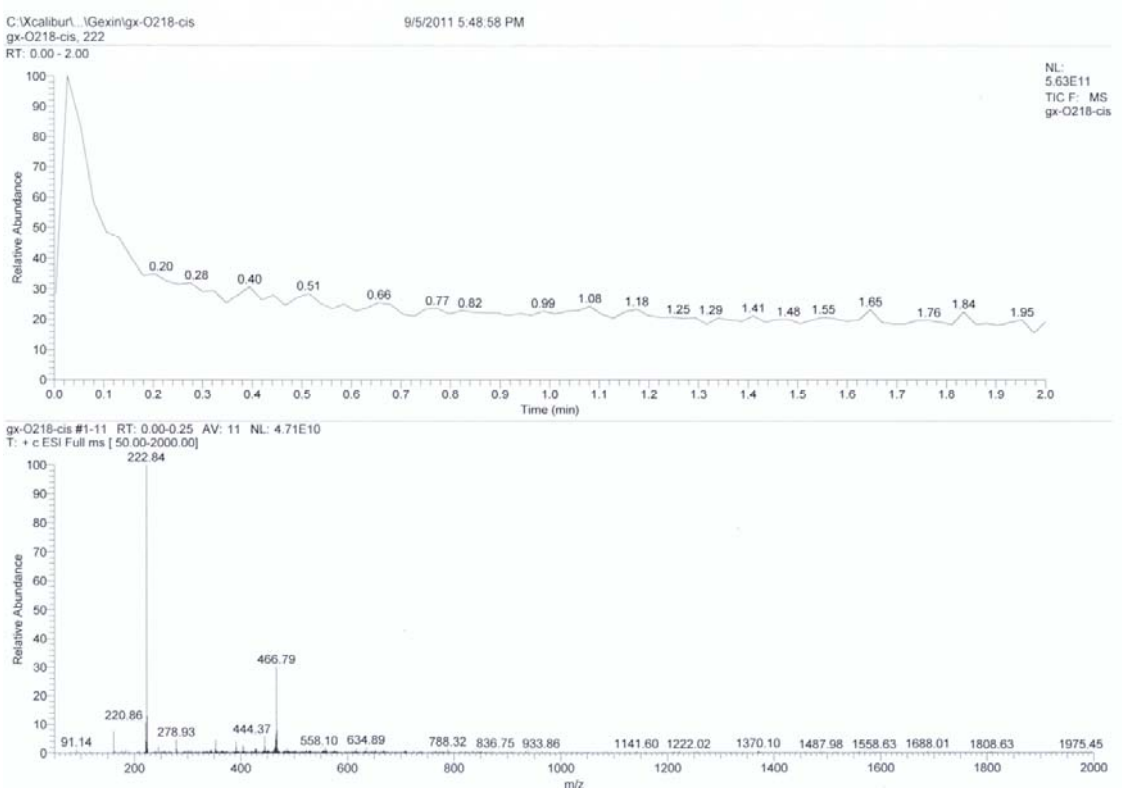
Spectrum of ESI (LRMS) of **2a**



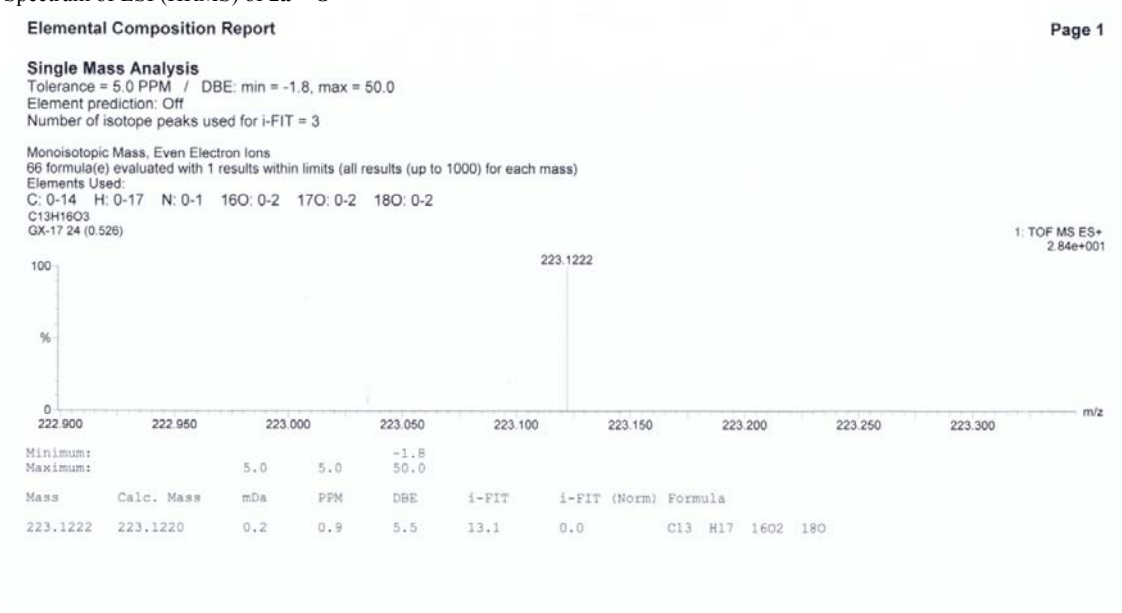
Spectrum of ESI(HRMS) of **2a**



Spectrum of ESI (LRMS) of **2a-^{18}O**

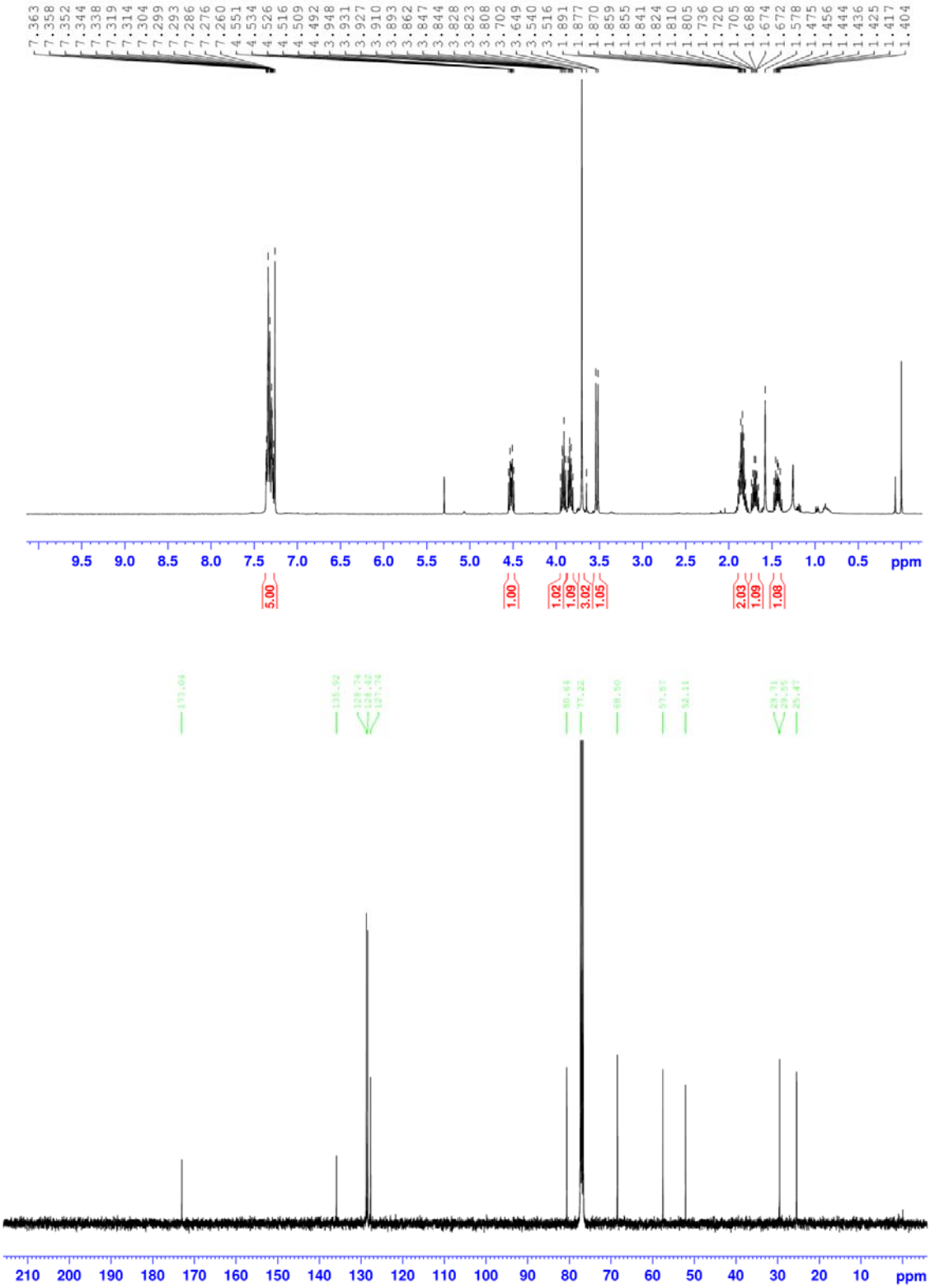


Spectrum of ESI (HRMS) of **2a-^{18}O**

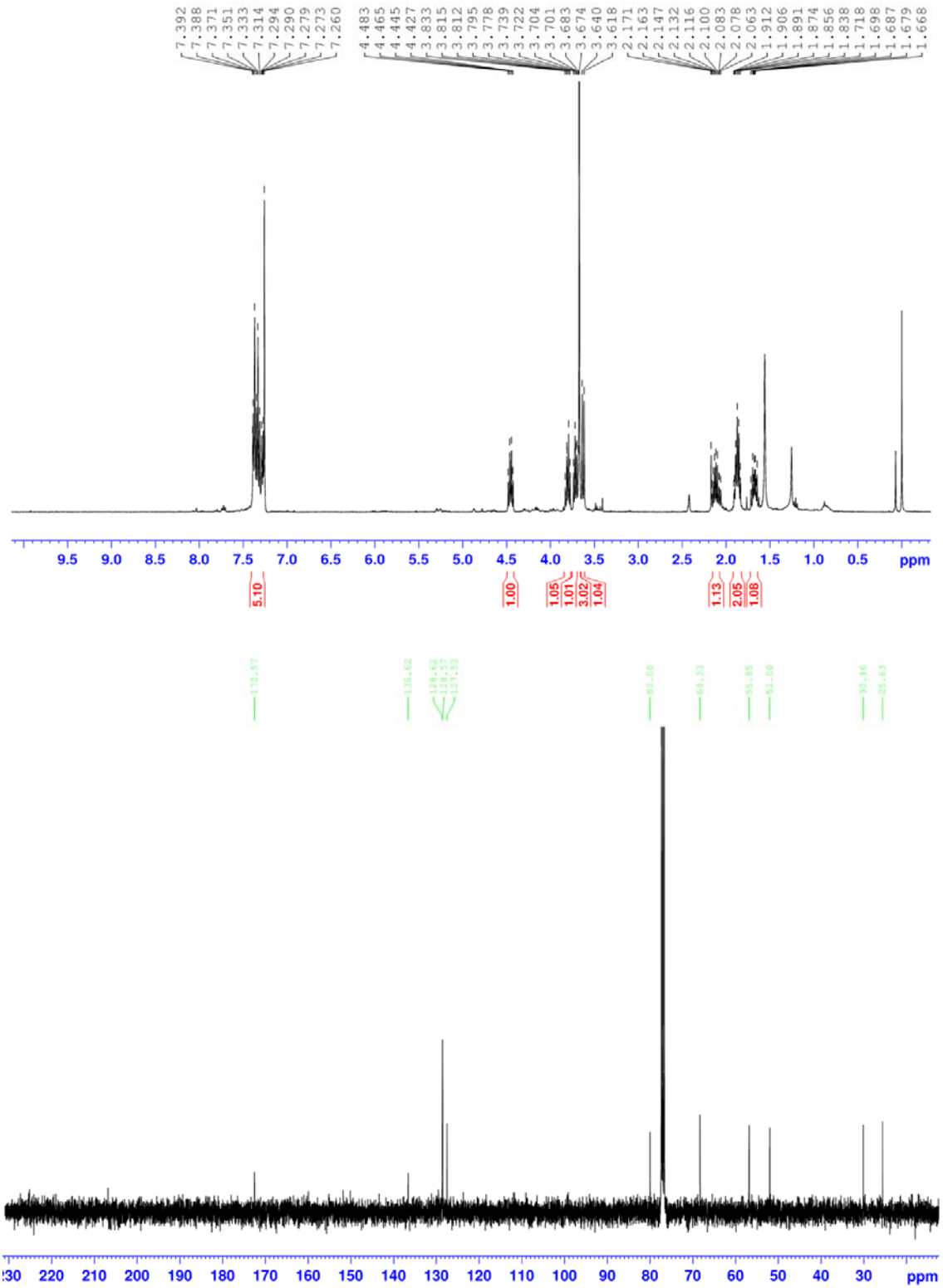


6. ^{1}H and ^{13}C NMR spectra of compounds 2a-2s

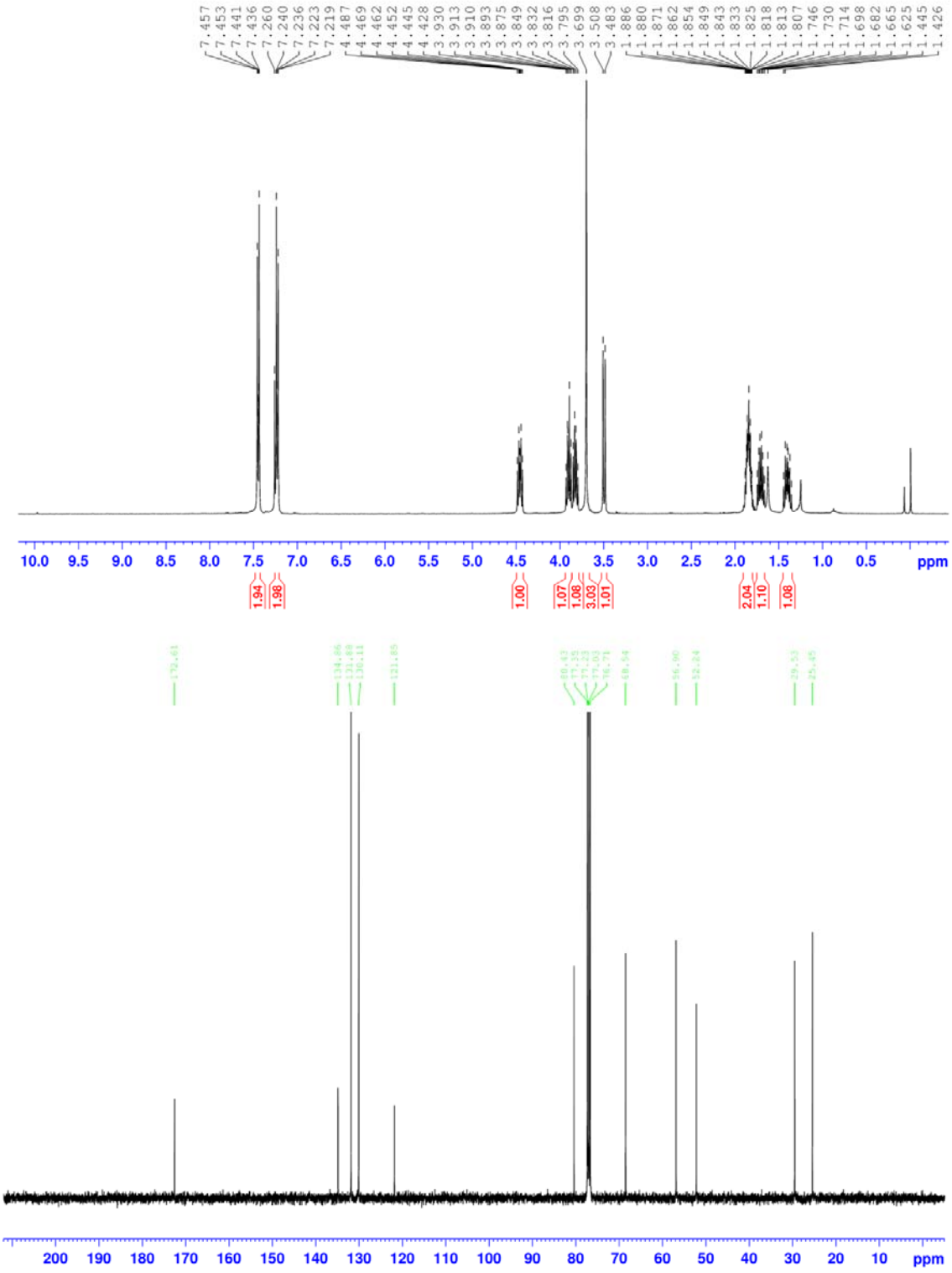
^{1}H and ^{13}C NMR spectra of compound 2a-1 (the *anti*-isomer)



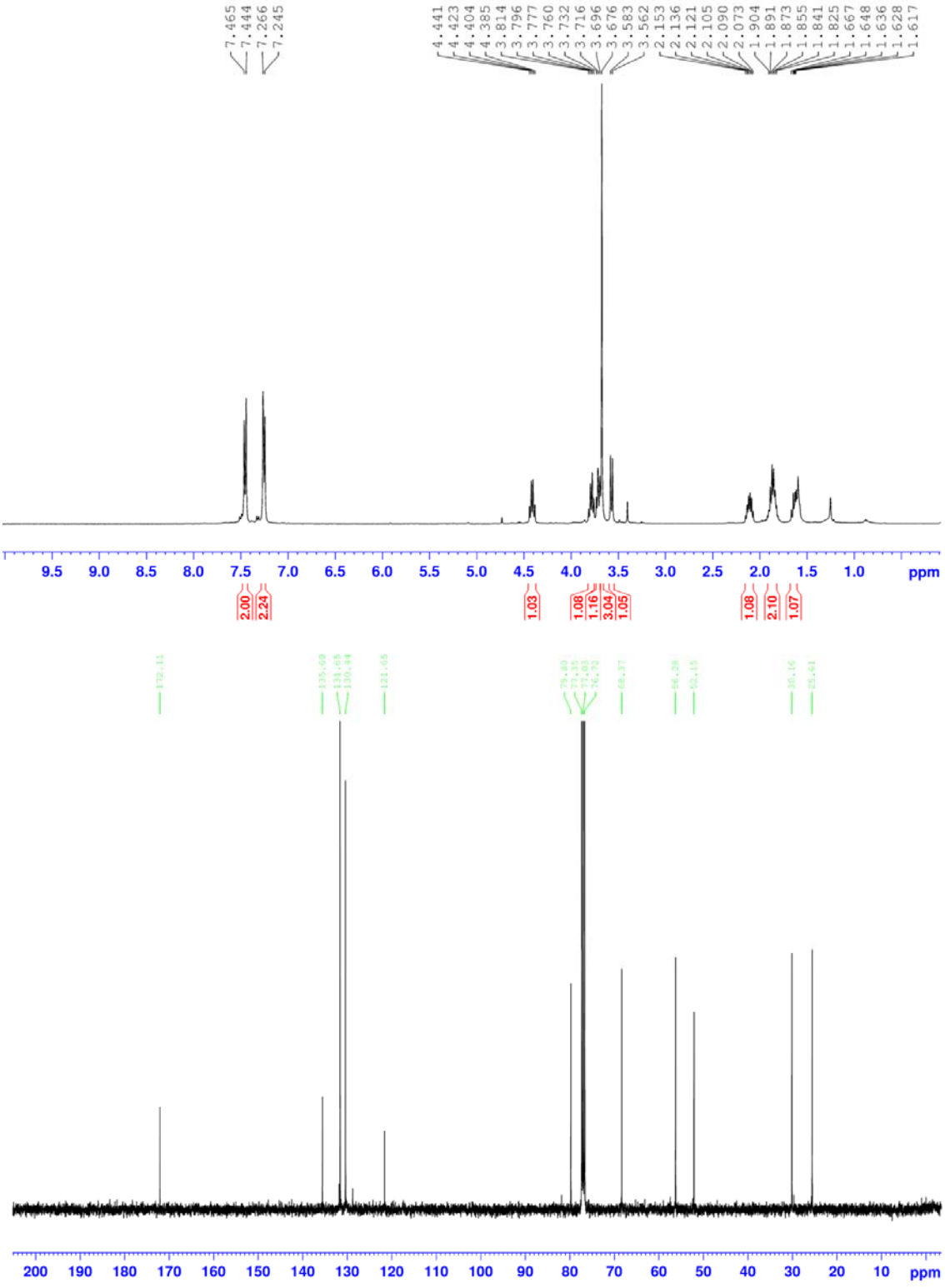
^{1}H and ^{13}C NMR spectra of compound 2a-2 (the *syn*-isomer)



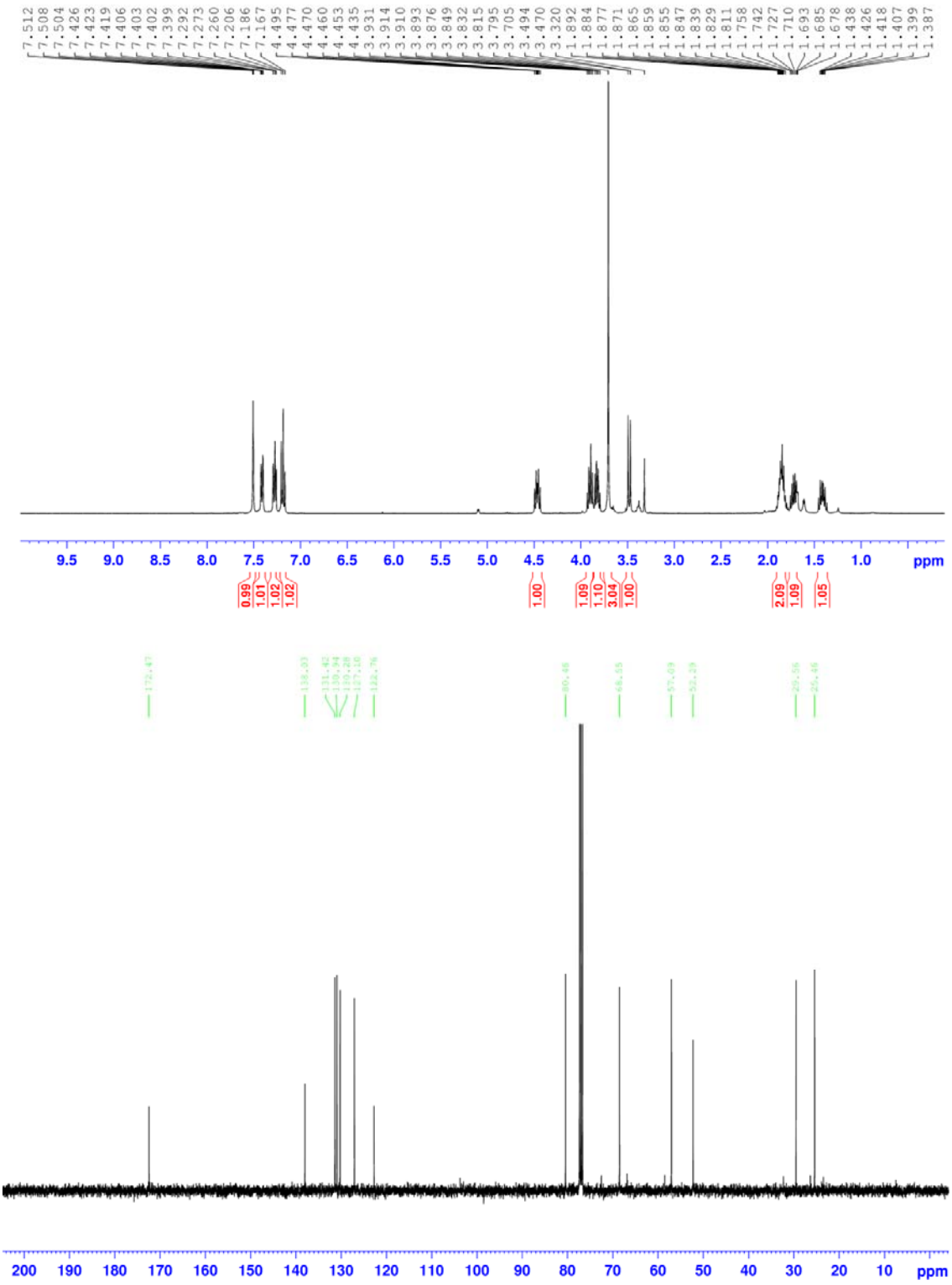
^{1}H and ^{13}C NMR spectra of compound 2b-1 (the *anti*-isomer)



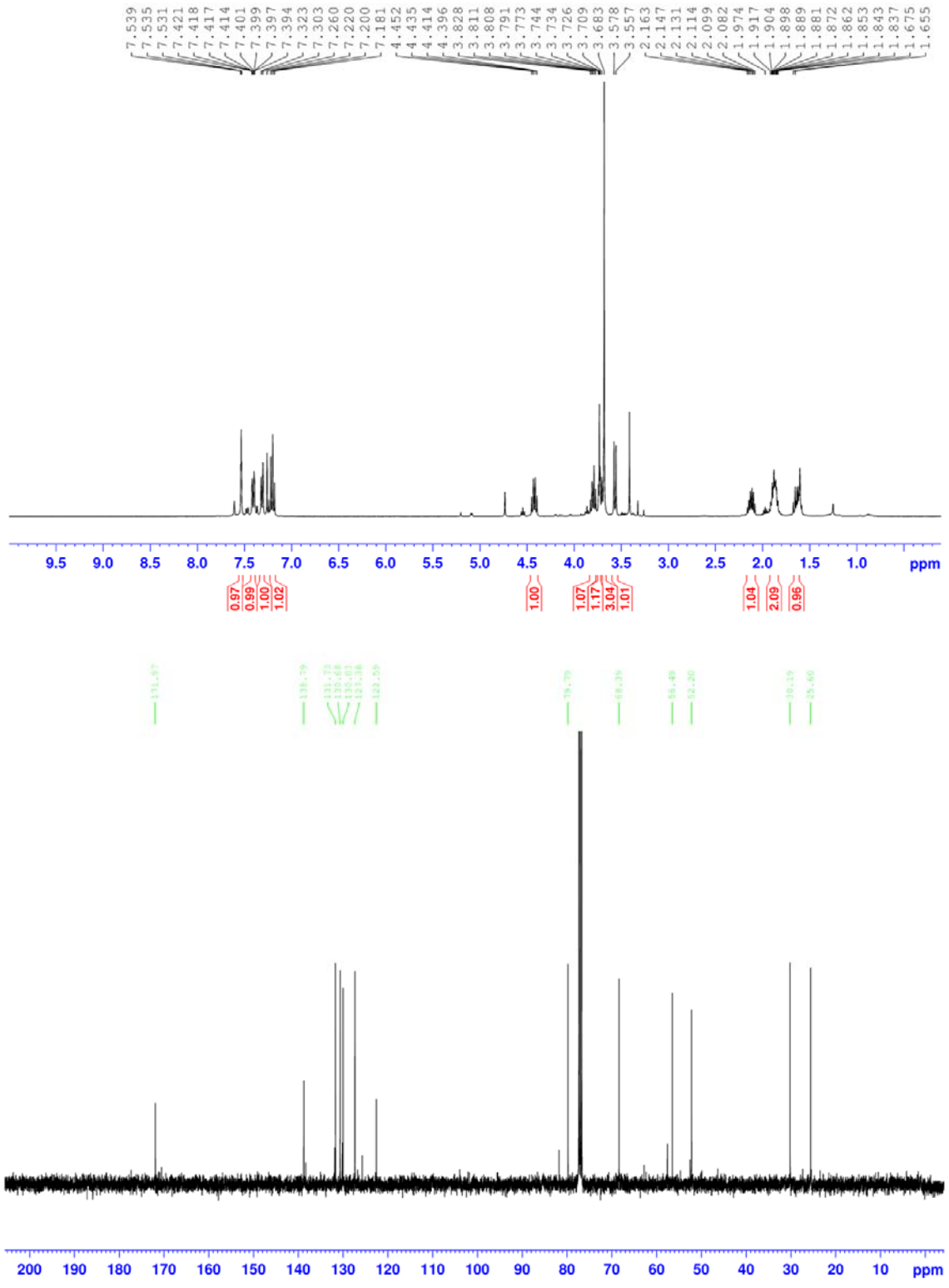
^{1}H and ^{13}C NMR spectra of compound 2b-2 (the *syn*-isomer)



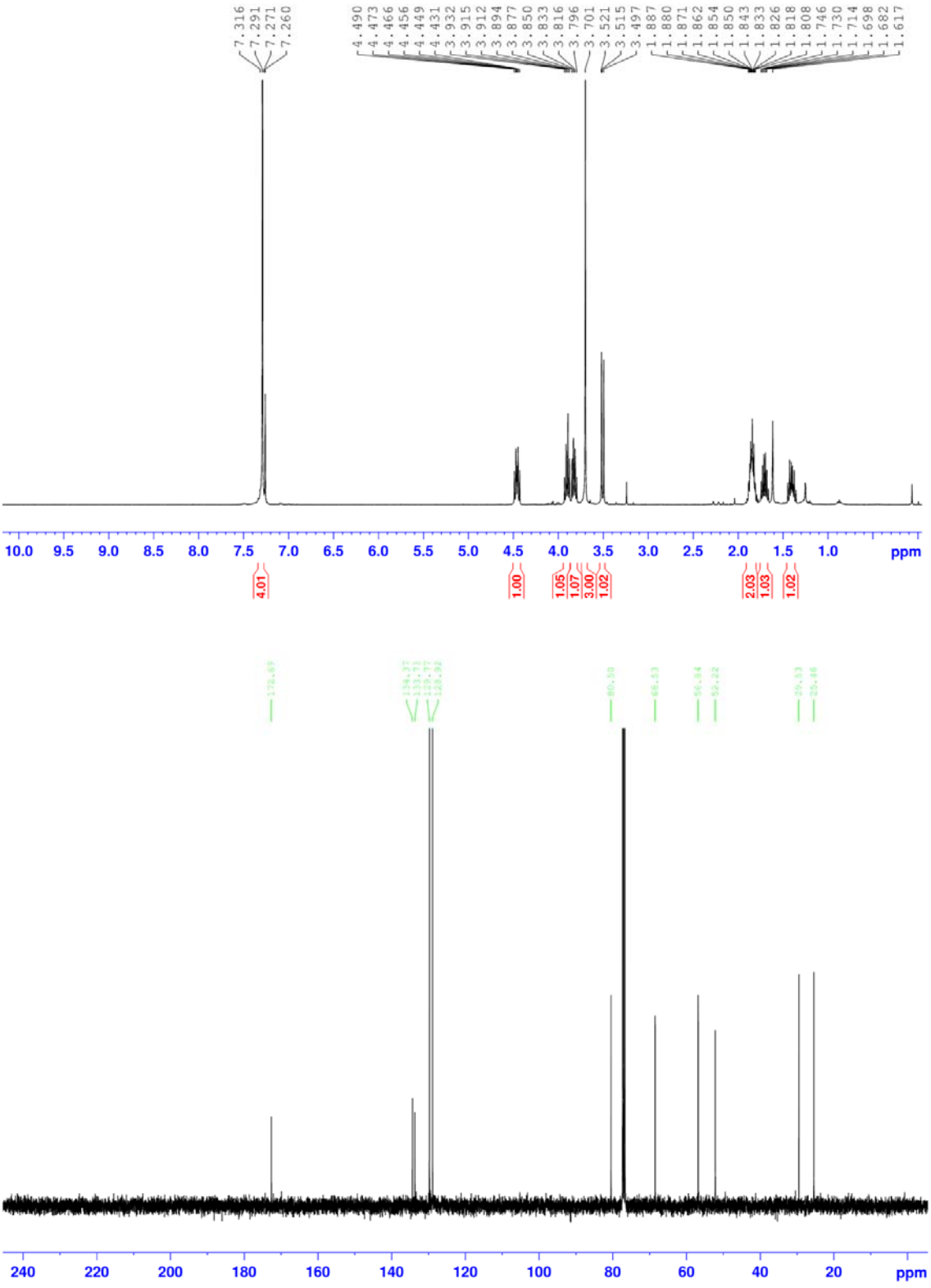
^{1}H and ^{13}C NMR spectra of compound 2c-1 (the *anti*-isomer)



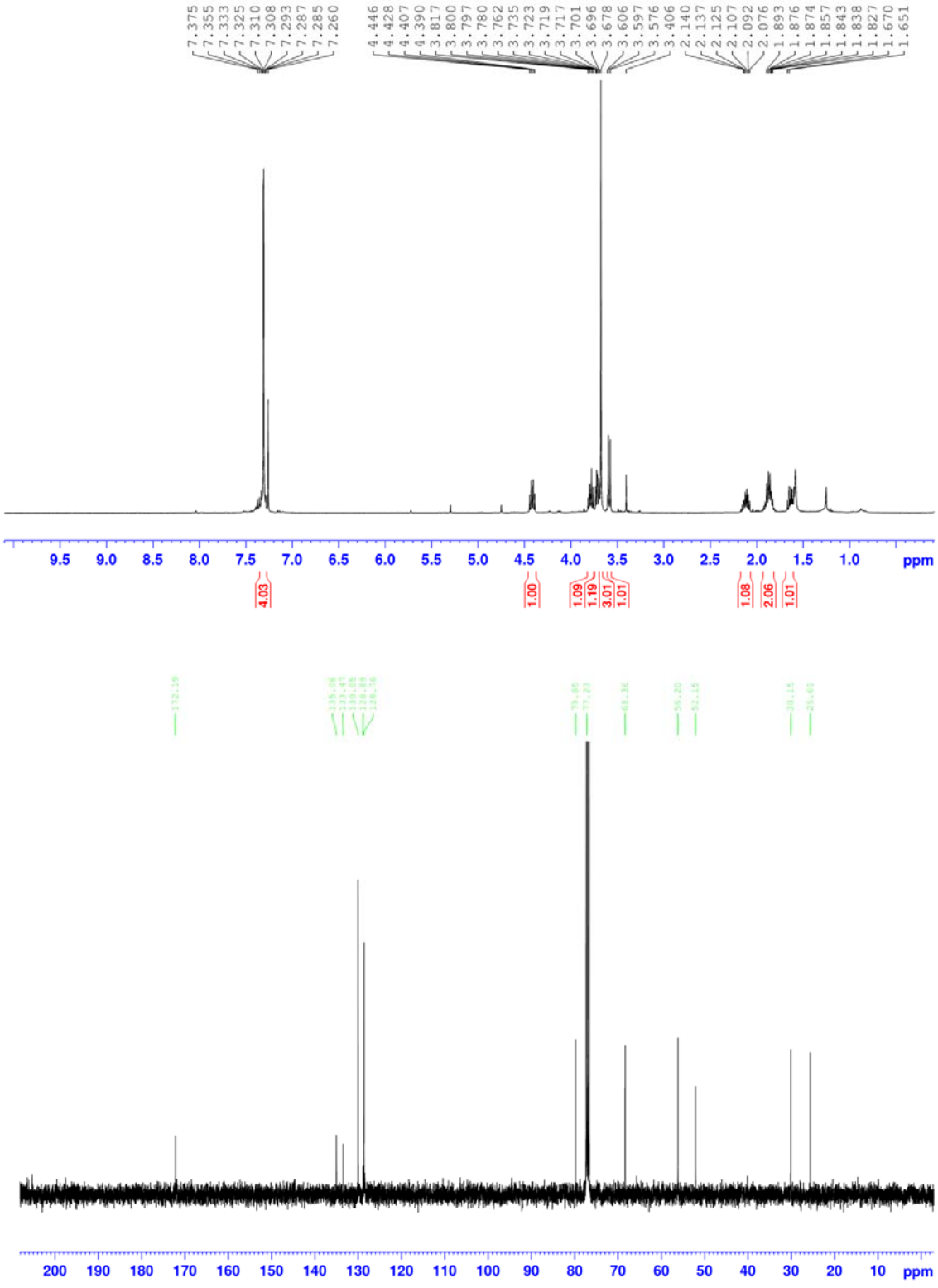
^{1}H and ^{13}C NMR spectra of compound 2c-2 (the *syn*-isomer)



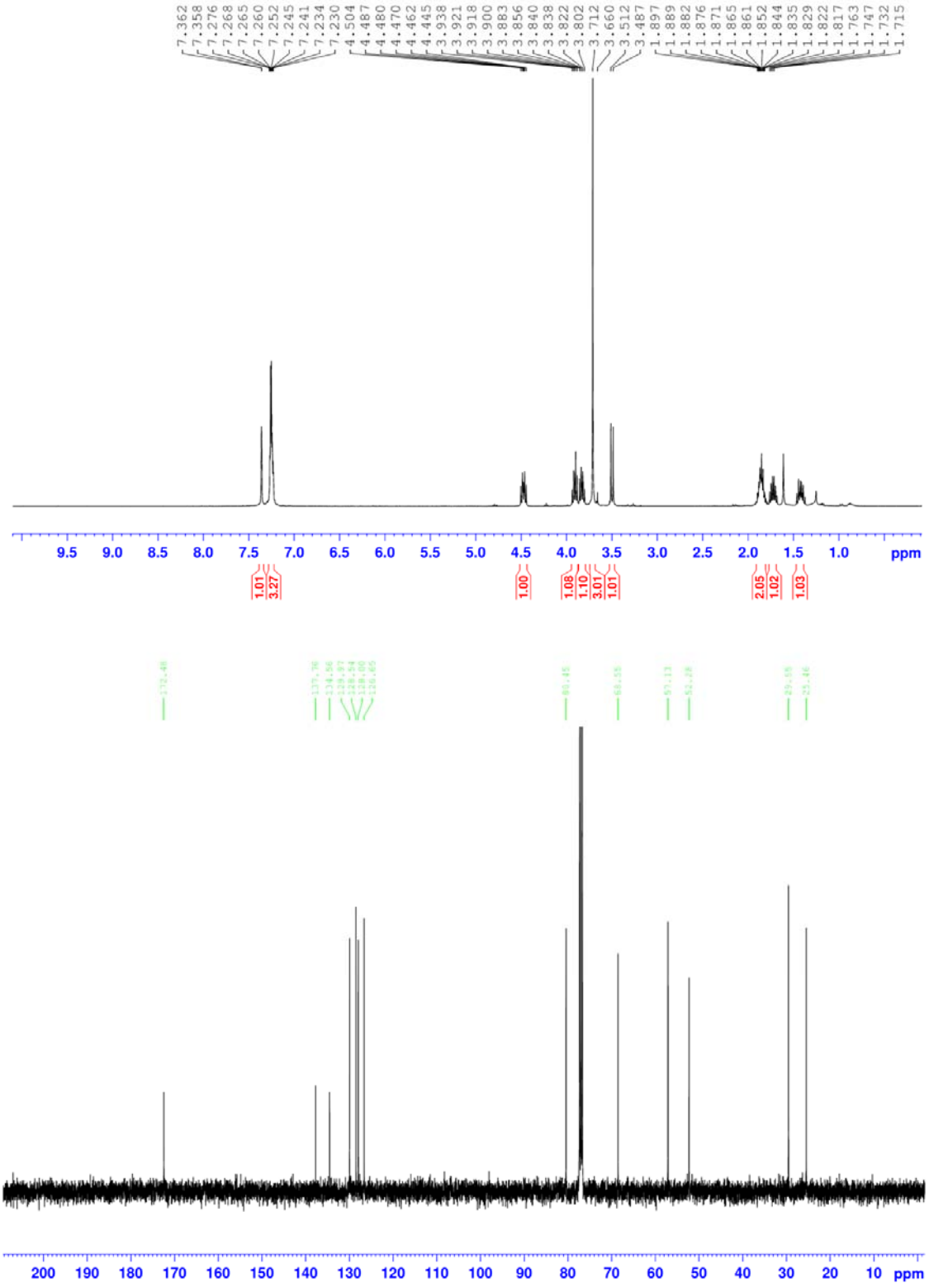
^{1}H and ^{13}C NMR spectra of compound 2d-1 (the *anti*-isomer)



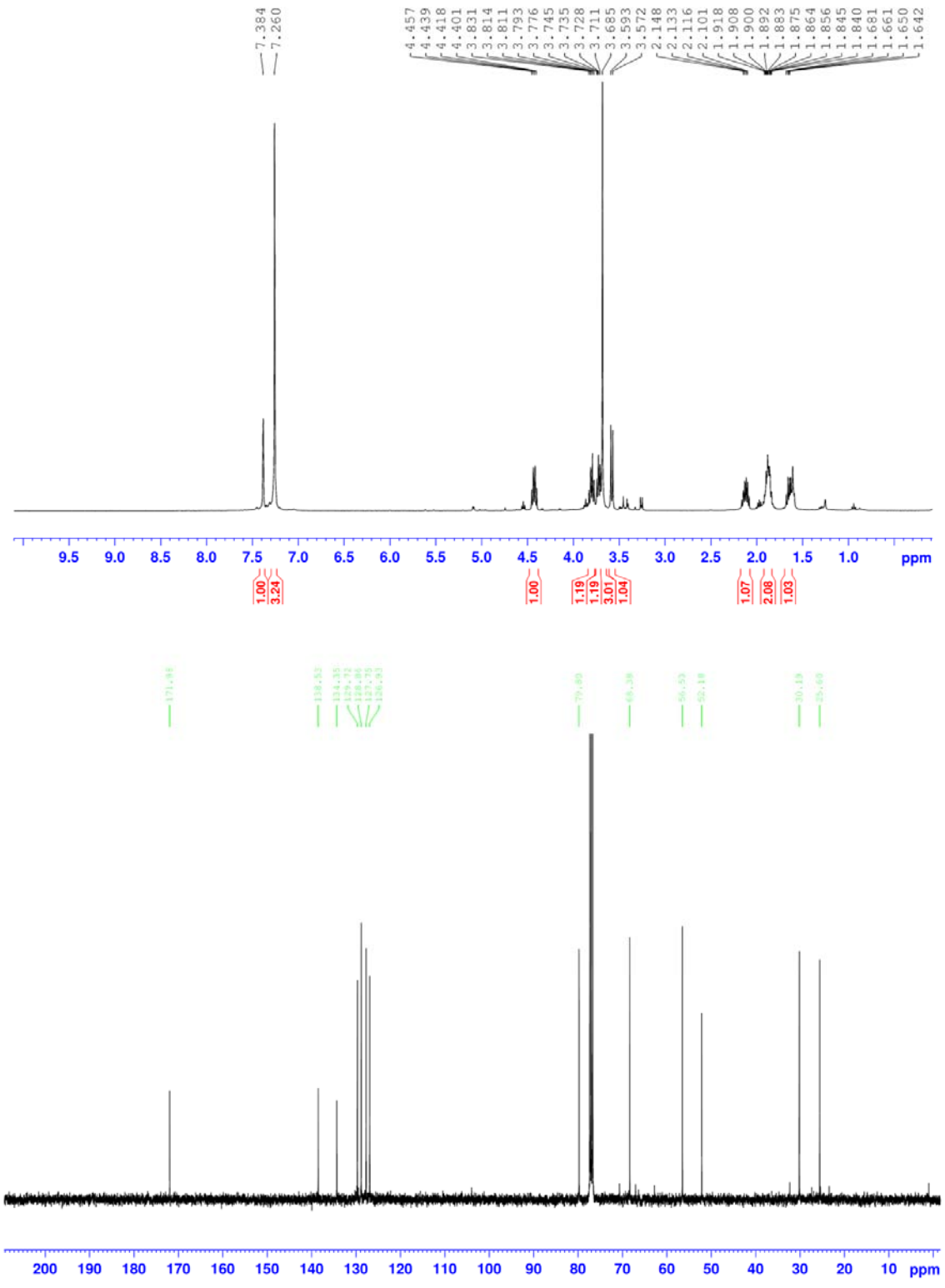
^{1}H and ^{13}C NMR spectra of compound 2d-2 (the *syn*-isomer)



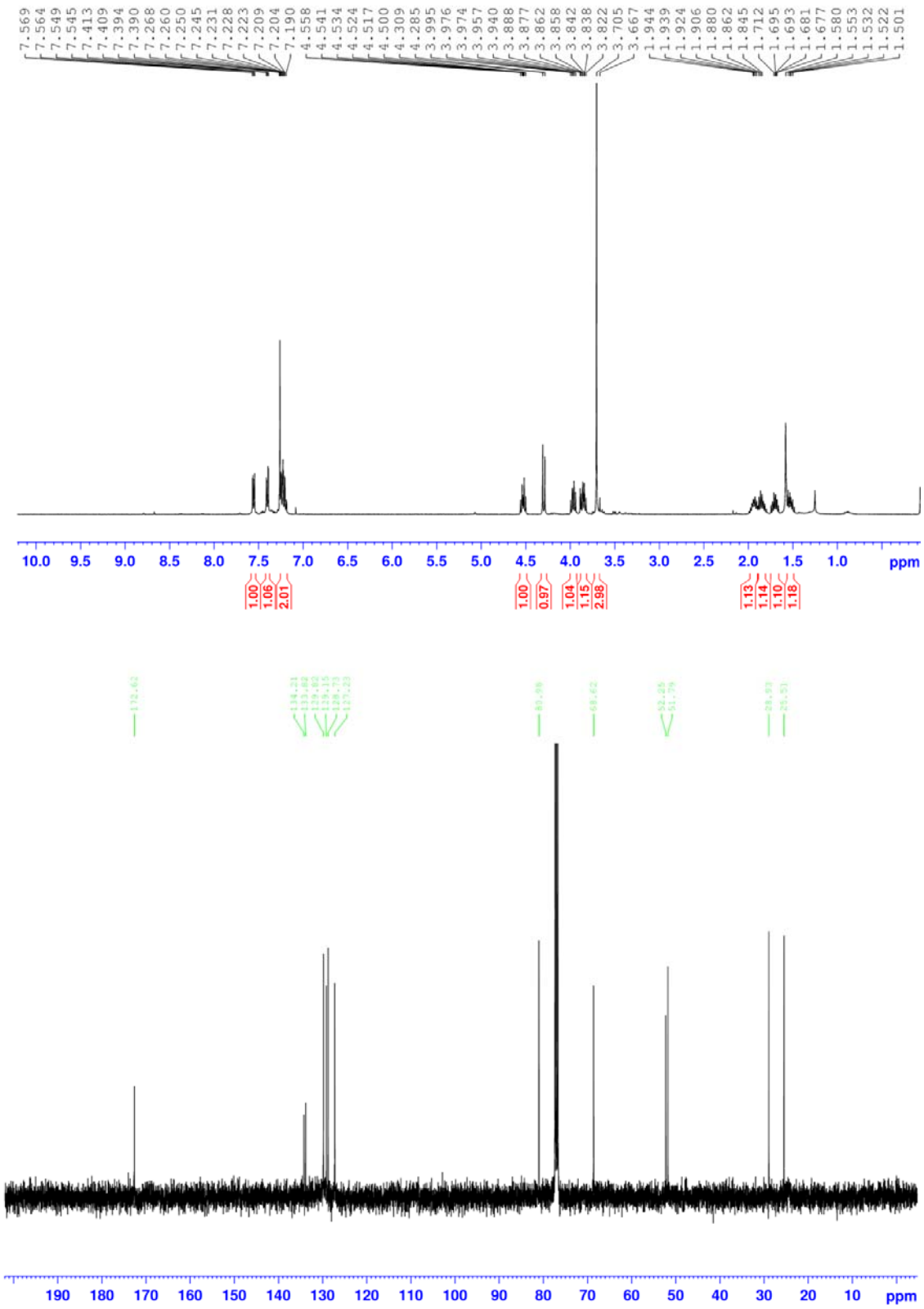
^{1}H and ^{13}C NMR spectra of compound 2e-1 (the *anti*-isomer)



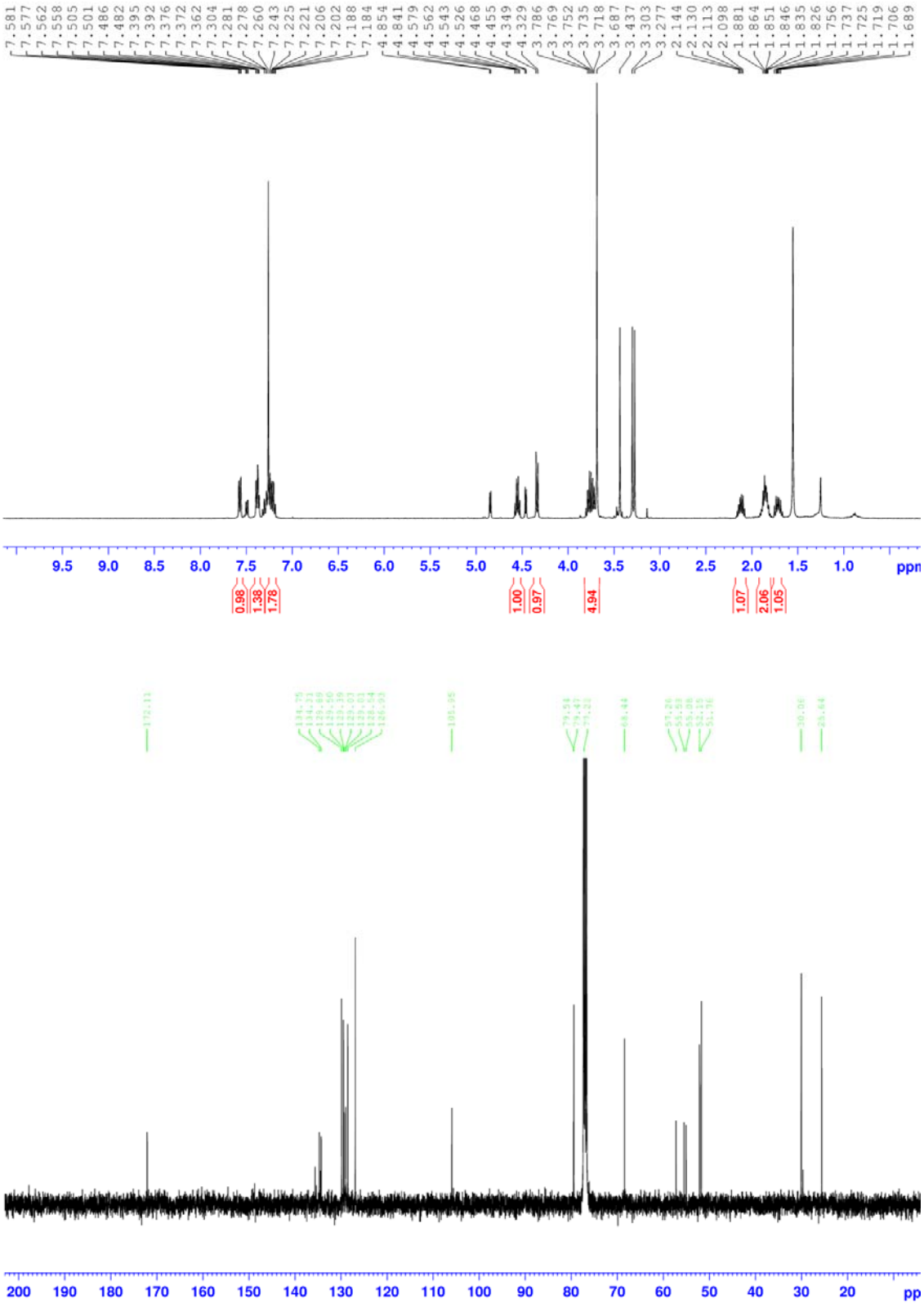
^{1}H and ^{13}C NMR spectra of compound 2e-2 (the *syn*-isomer)



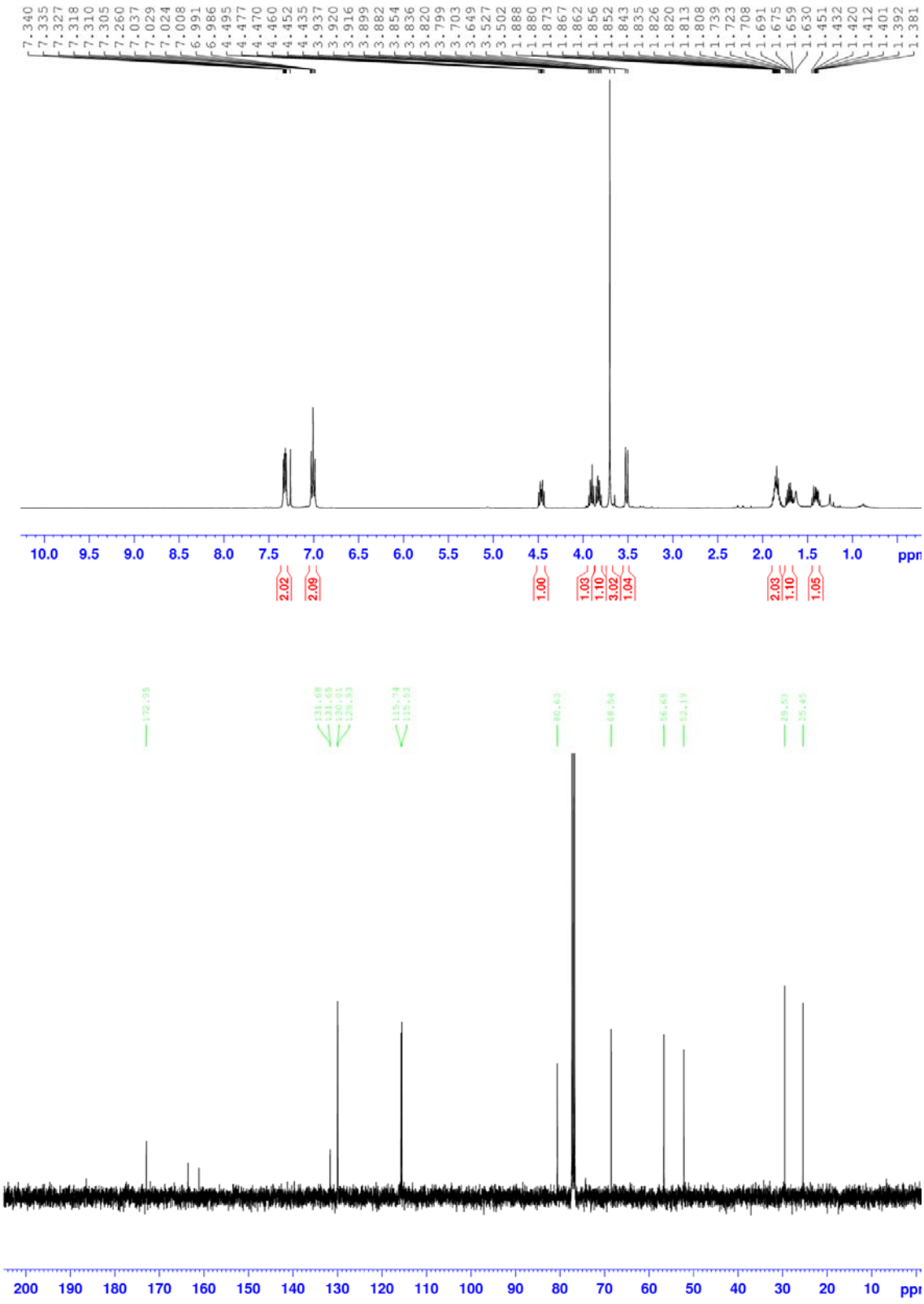
^{1}H and ^{13}C NMR spectra of compound 2f-1 (the *anti*-isomer)



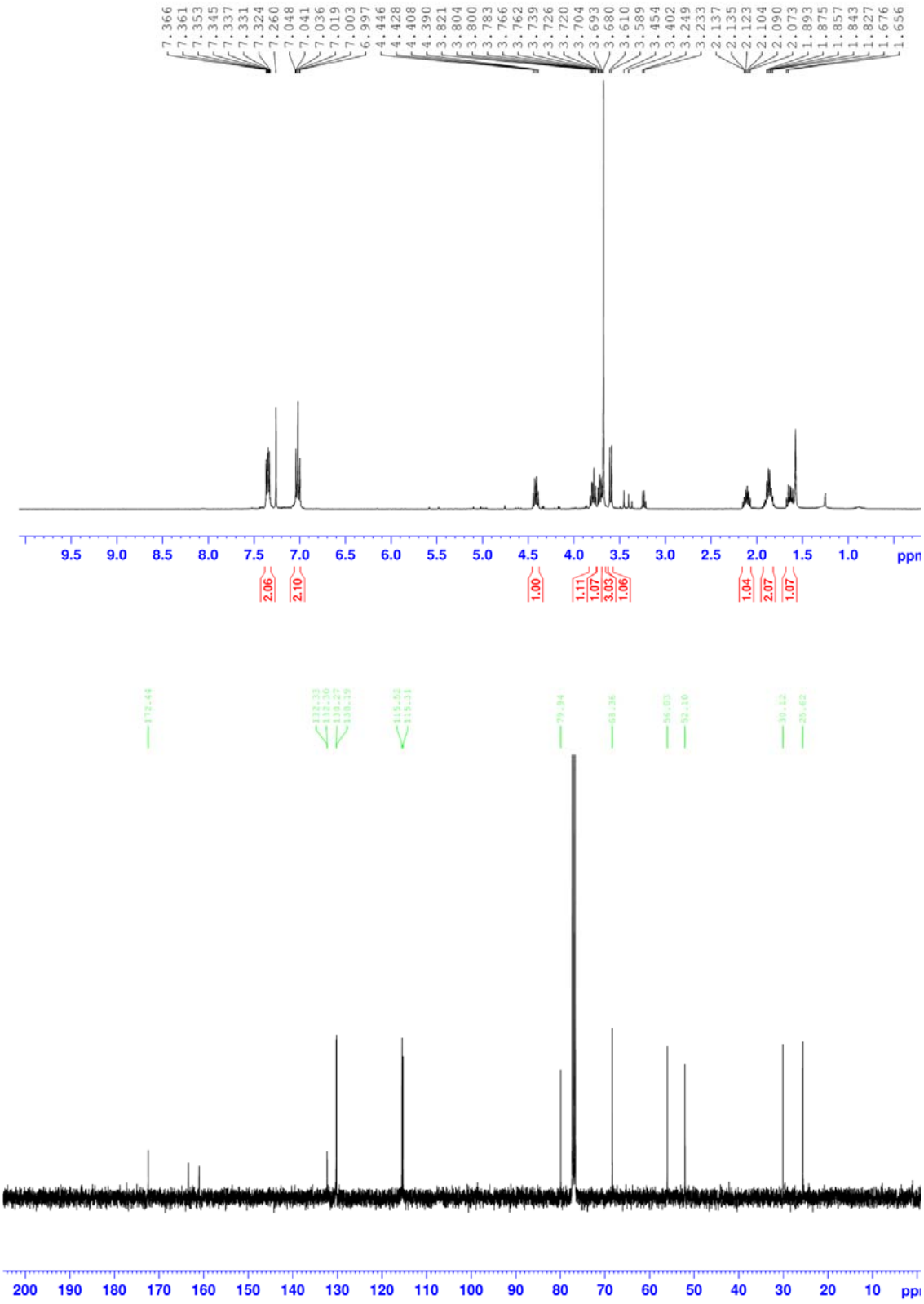
^{1}H and ^{13}C NMR spectra of compound 2f-2 (the *syn*-isomer)



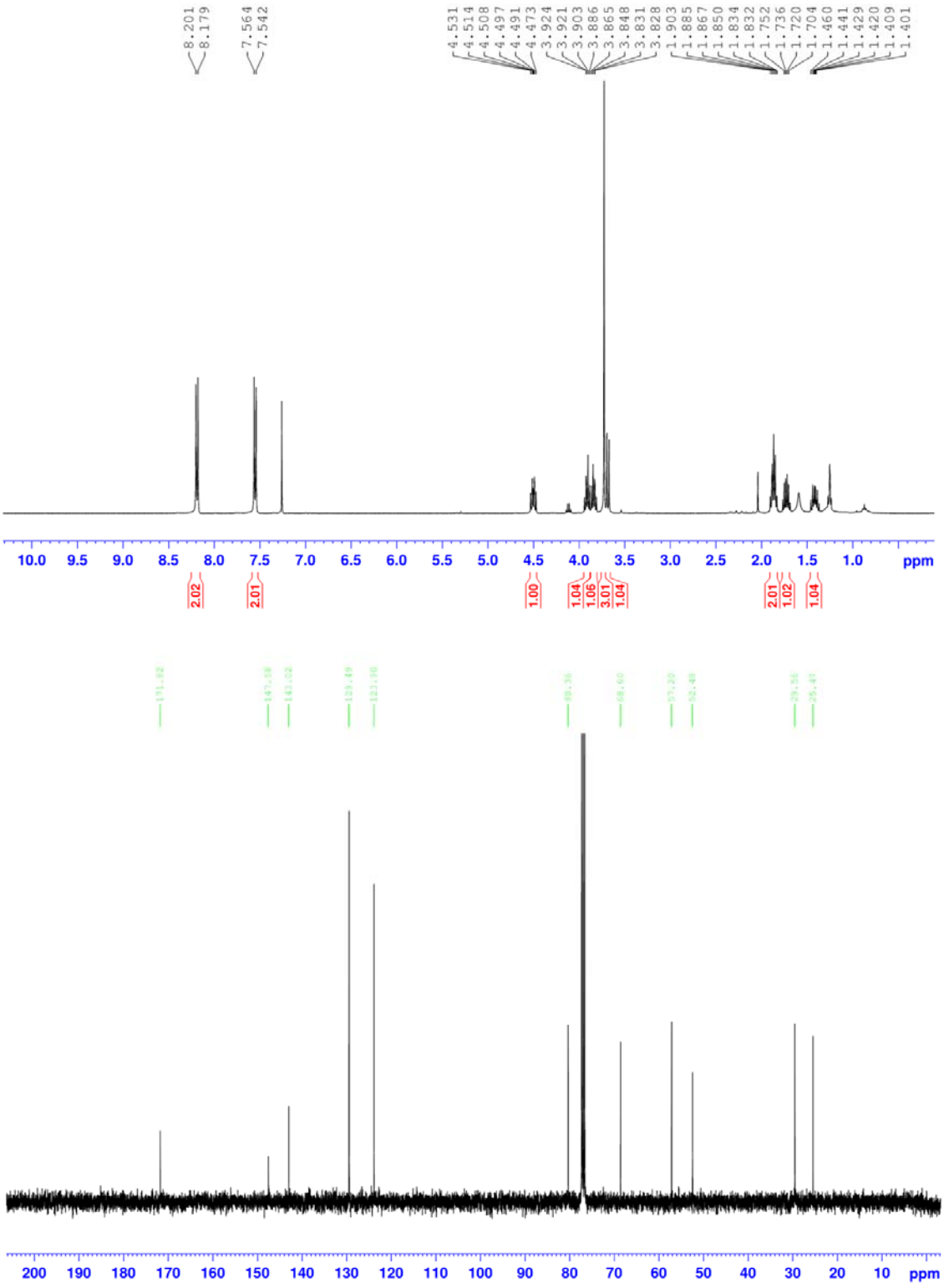
^{1}H and ^{13}C NMR spectra of compound 2g-1 (the *anti*-isomer)



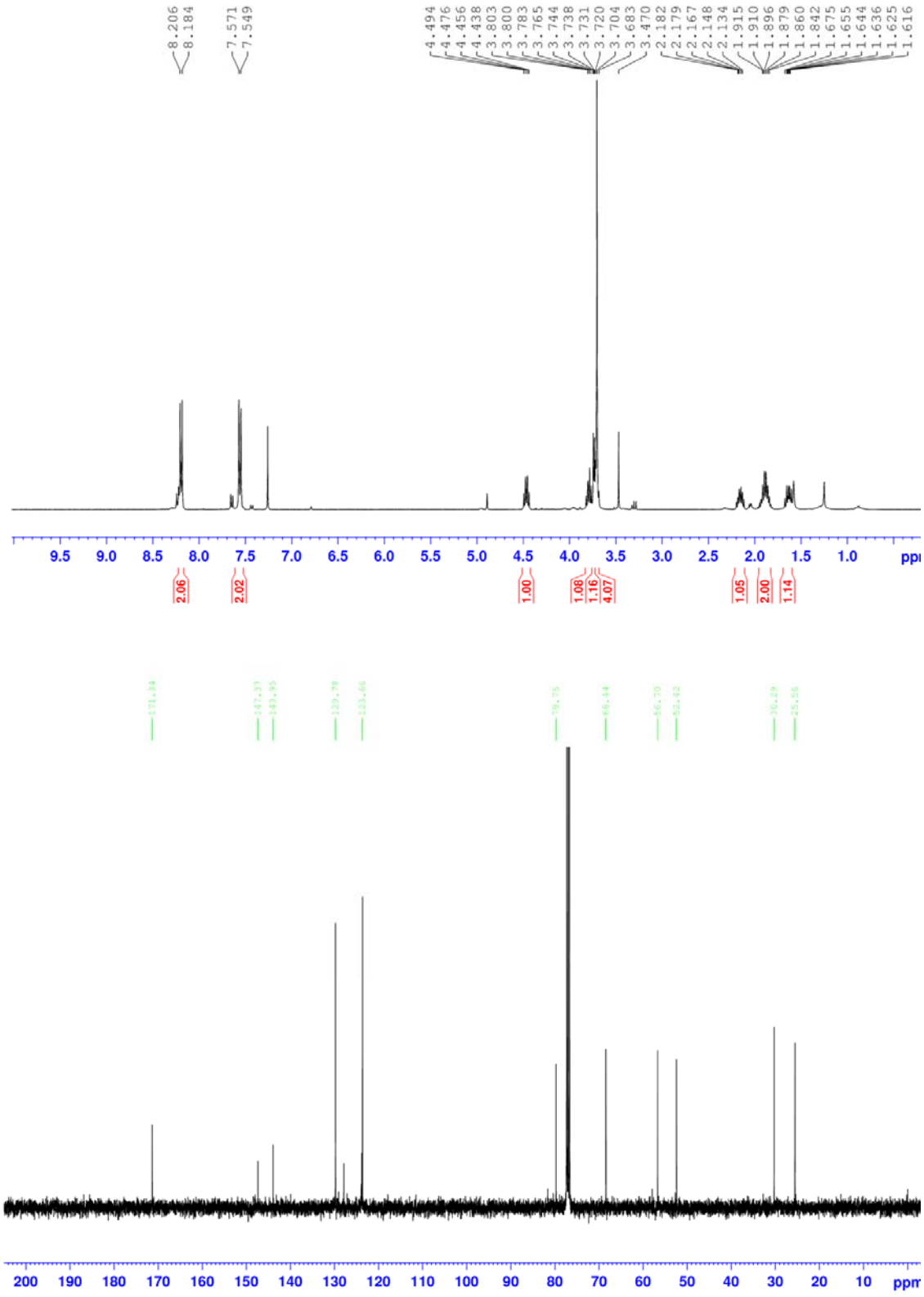
^{1}H and ^{13}C NMR spectra of compound 2g-2 (the *syn*-isomer)



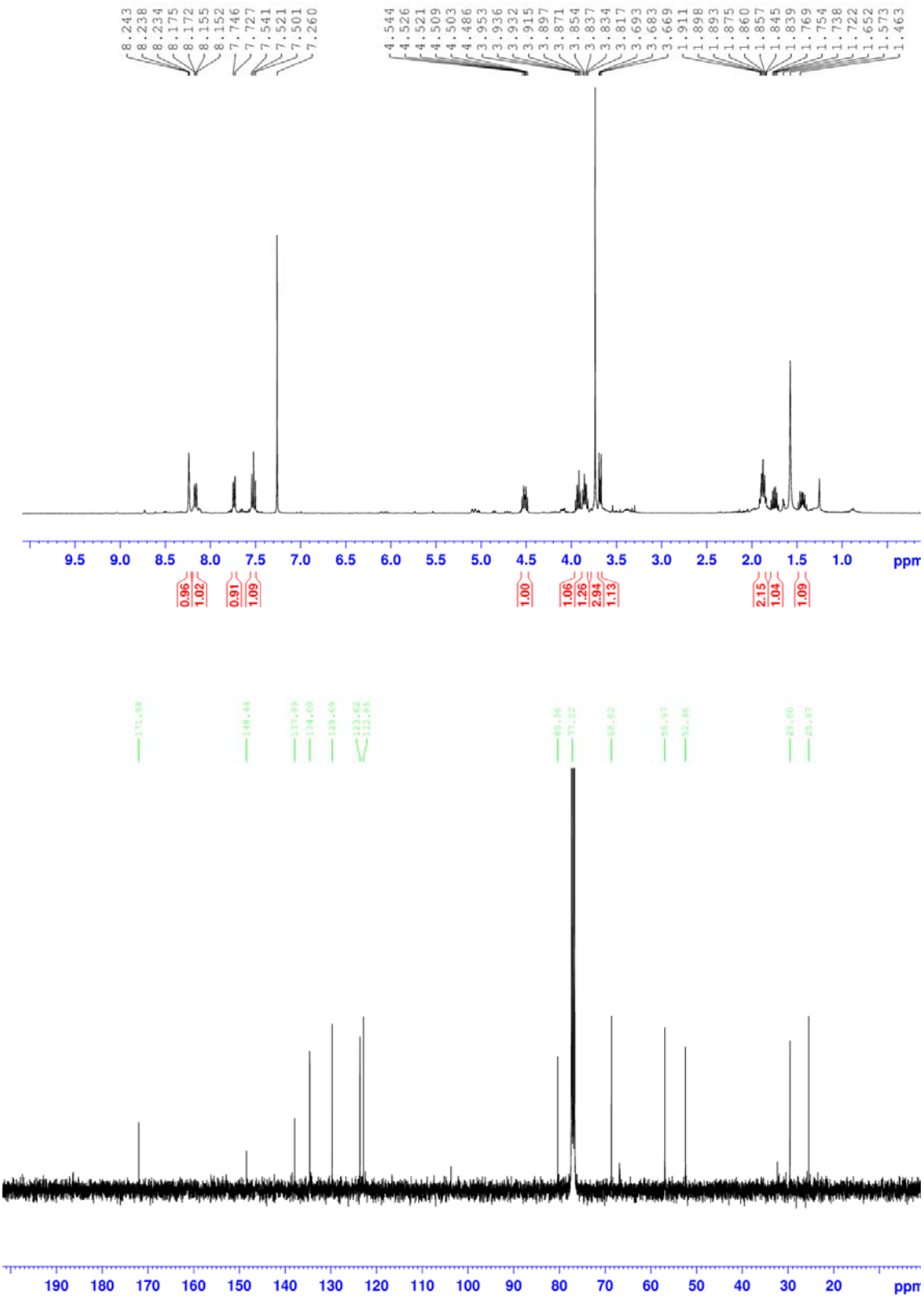
^{1}H and ^{13}C NMR spectra of compound 2h-1 (the *anti*-isomer)



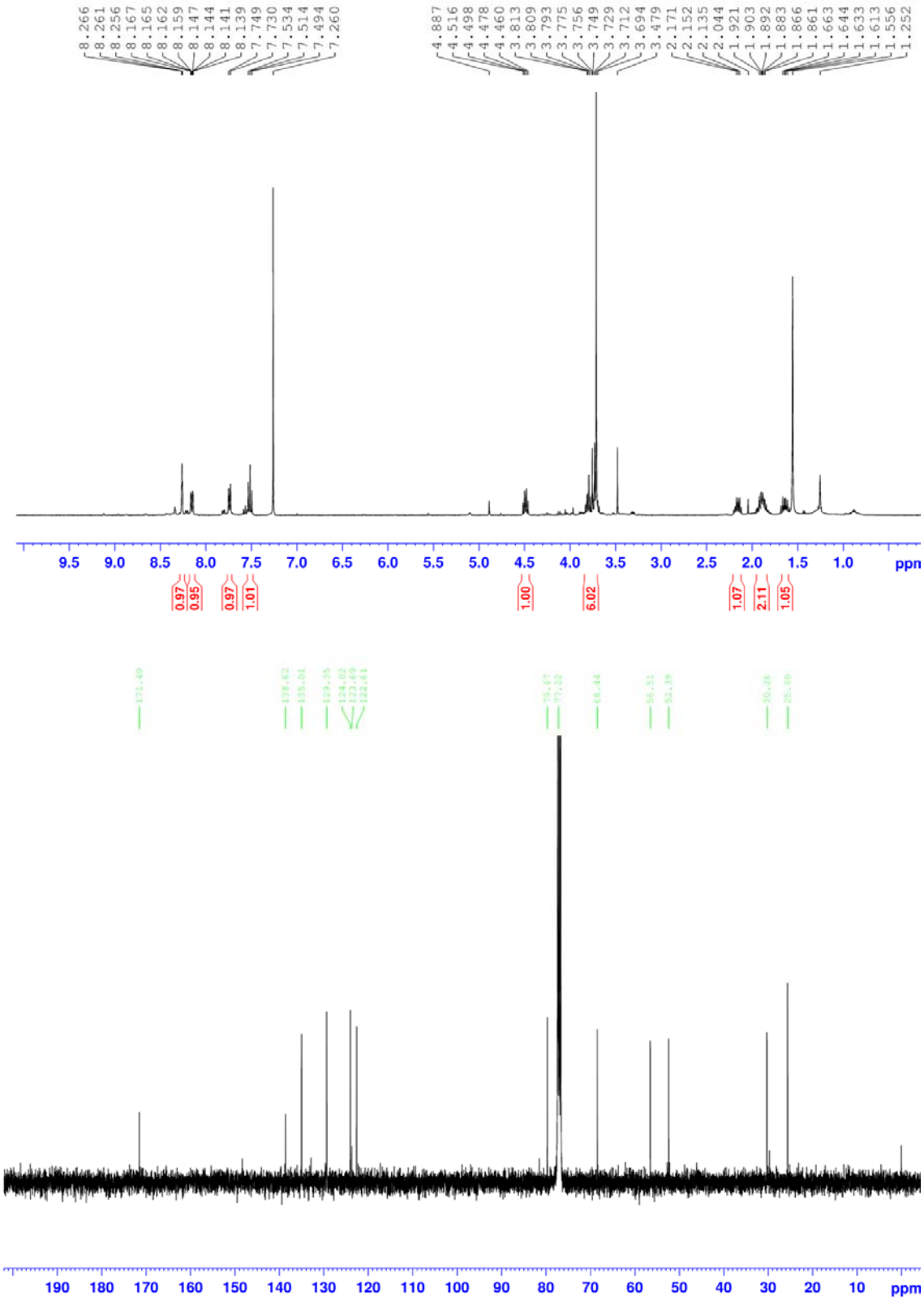
^{1}H and ^{13}C NMR spectra of compound 2h-2 (the *syn*-isomer)



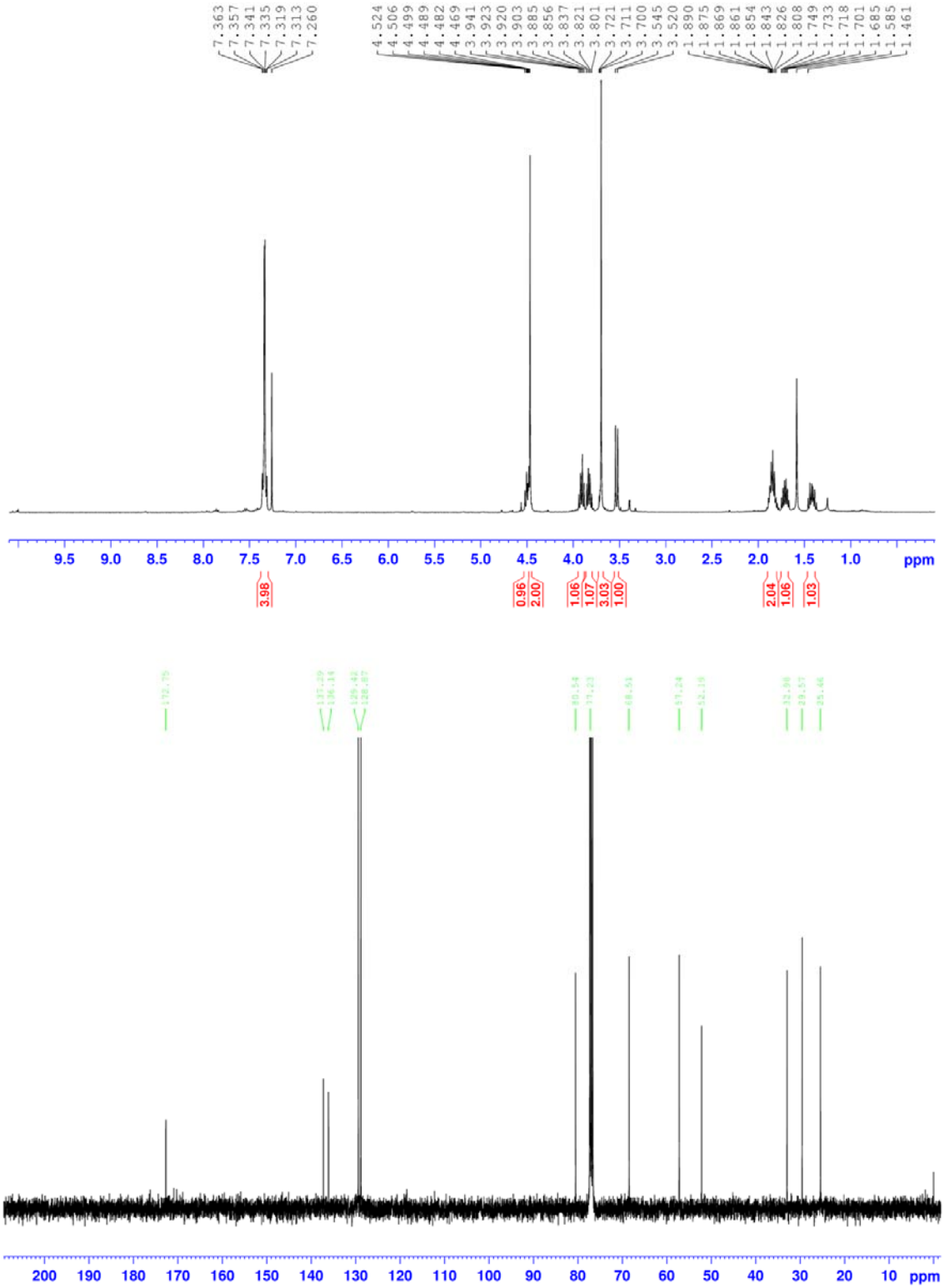
^{1}H and ^{13}C NMR spectra of compound 2i-1 (the *anti*-isomer)



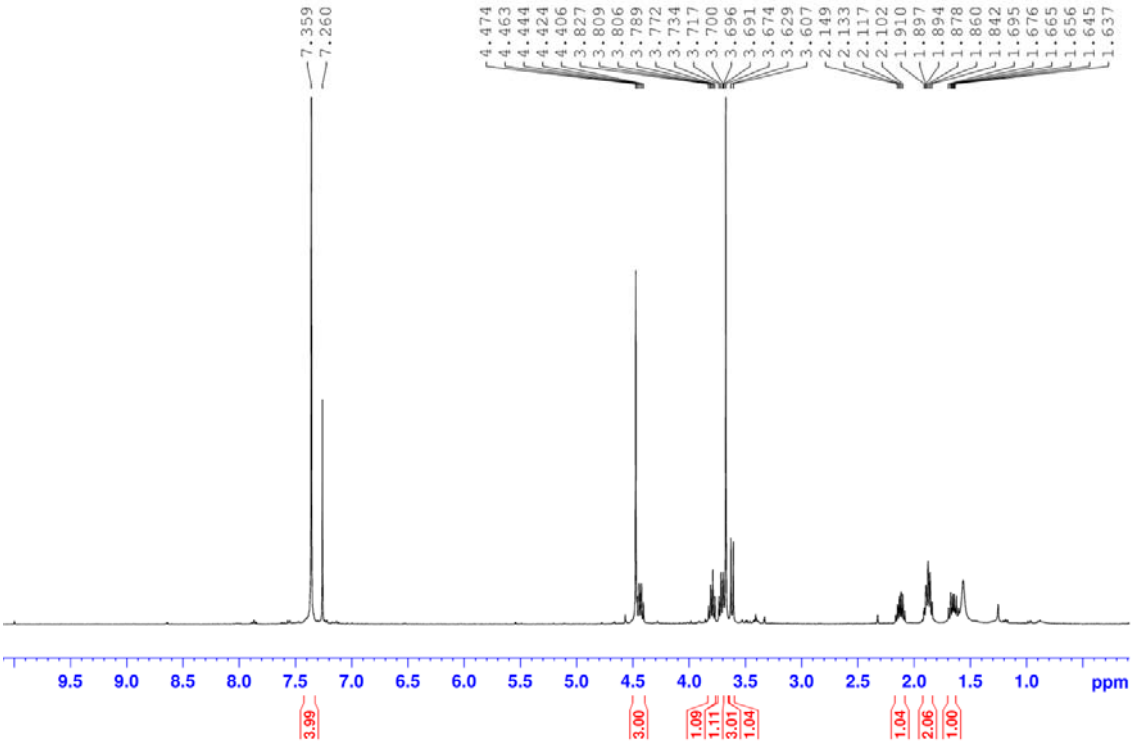
^{1}H and ^{13}C NMR spectra of compound 2i-2 (the *syn*-isomer)

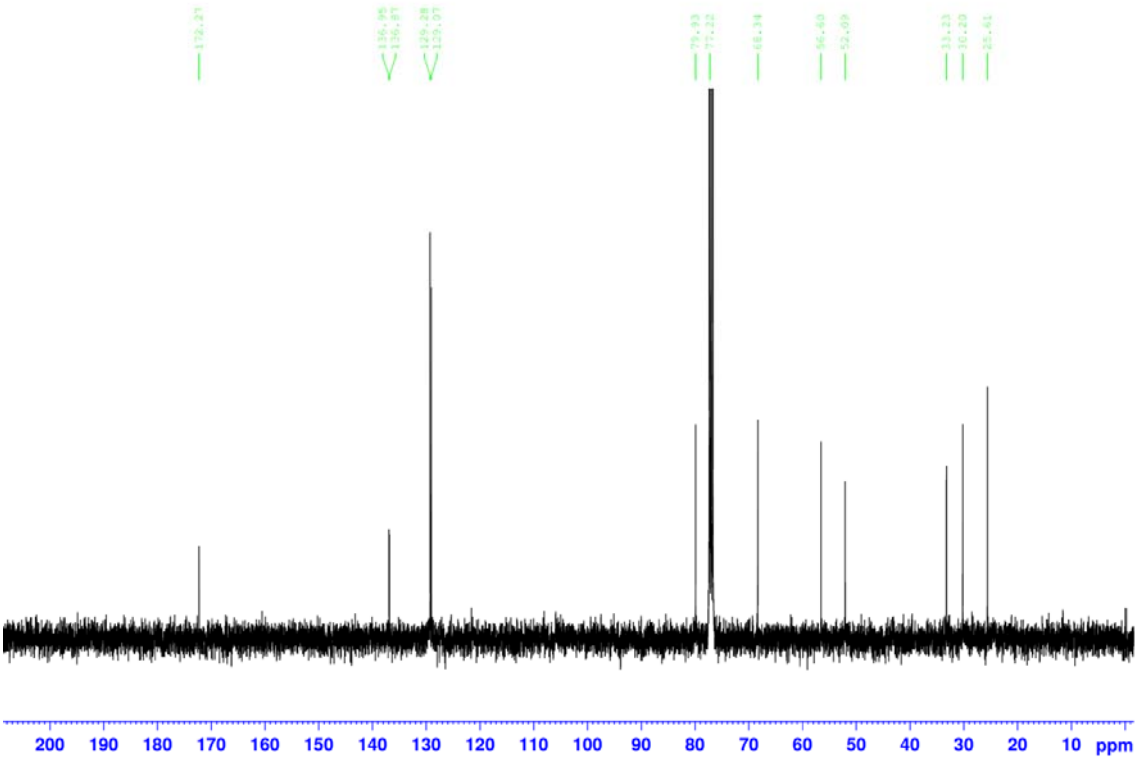


^{1}H and ^{13}C NMR spectra of compound 2j-1 (the *anti*-isomer)

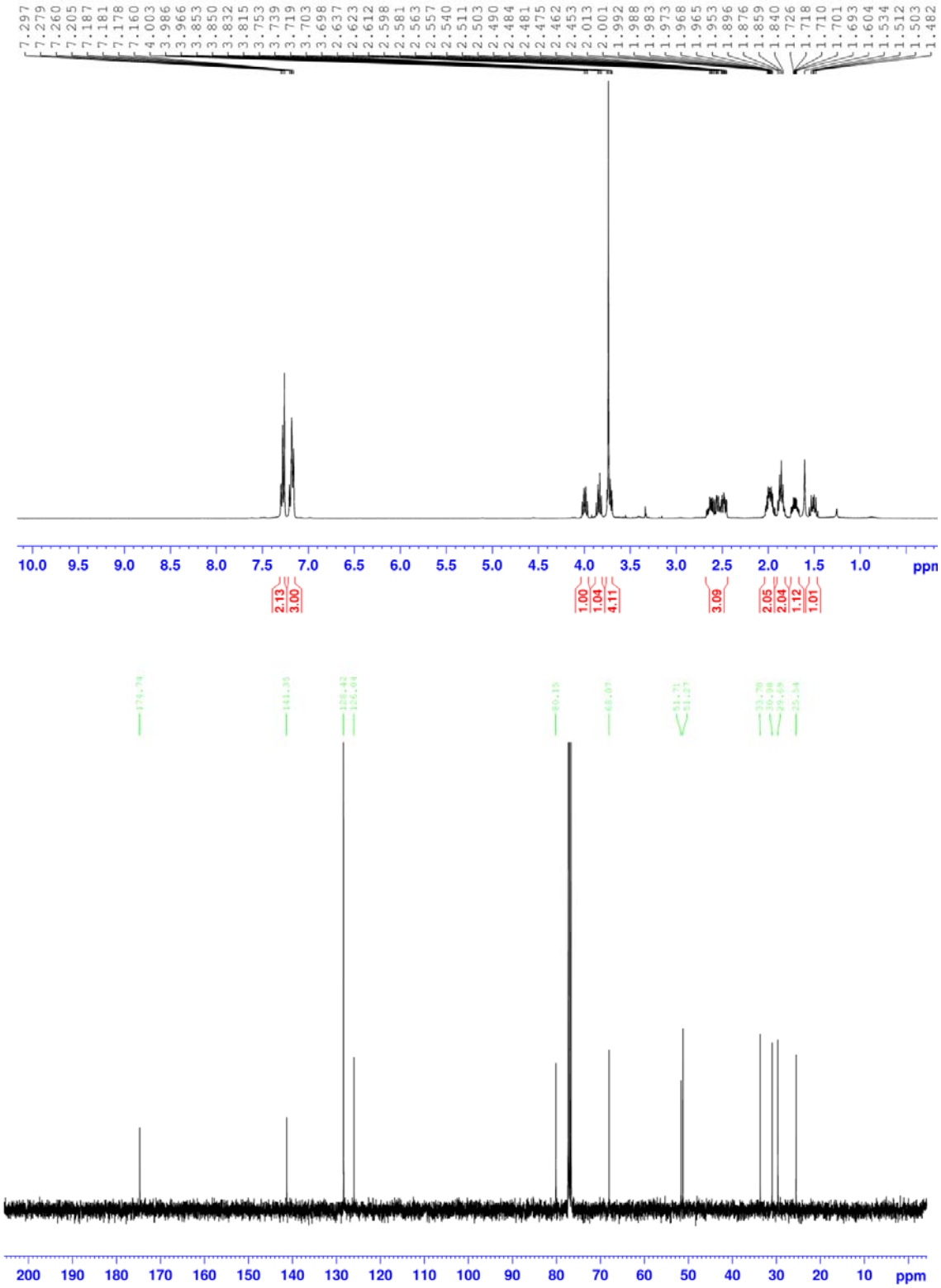


^{1}H and ^{13}C NMR spectra of compound 2j-2 (the *syn*-isomer)

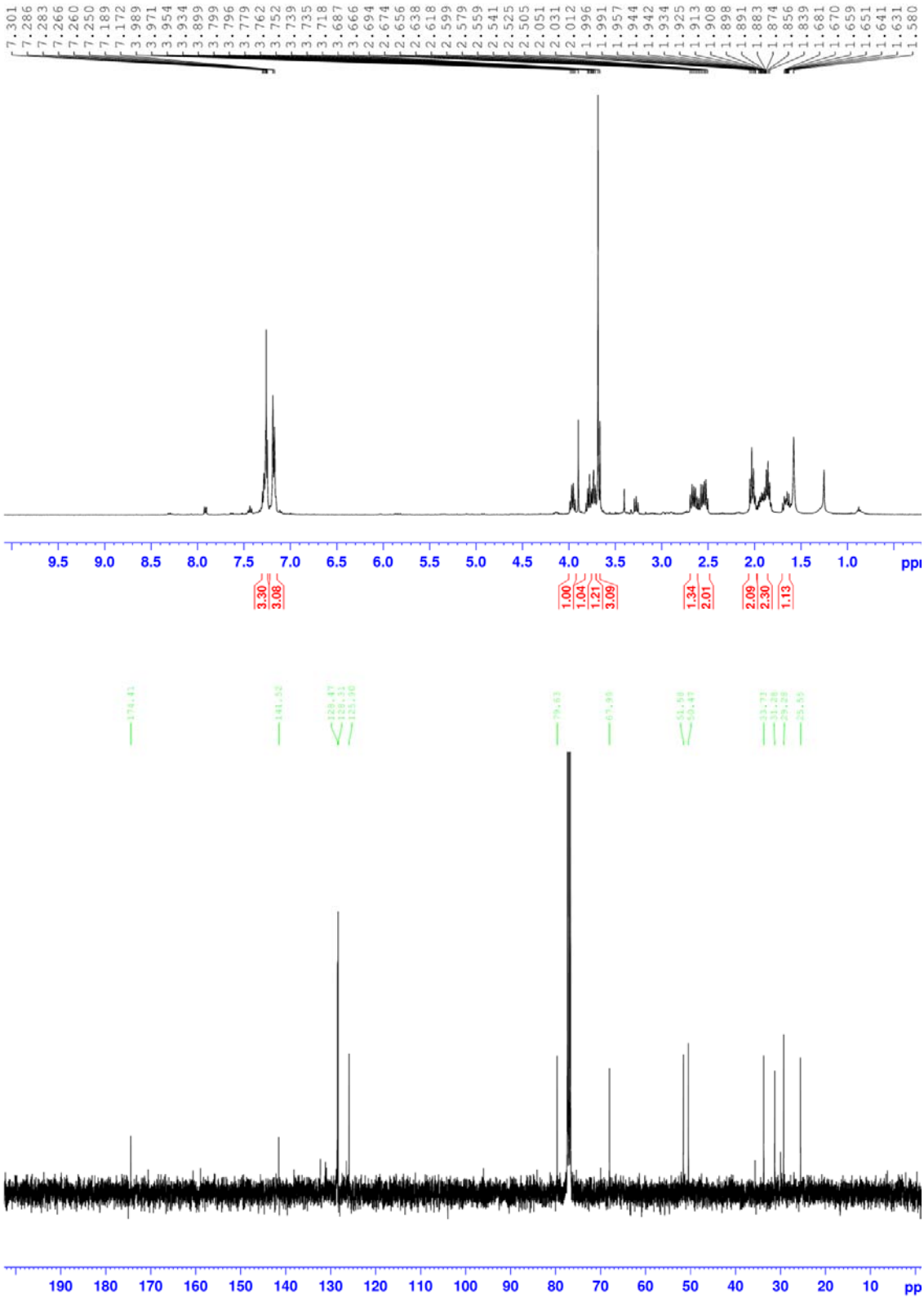




^{1}H and ^{13}C NMR spectra of compound 2m-1 (the *anti*-isomer)



^{1}H and ^{13}C NMR spectra of compound 2m-2 (the *syn*-isomer)



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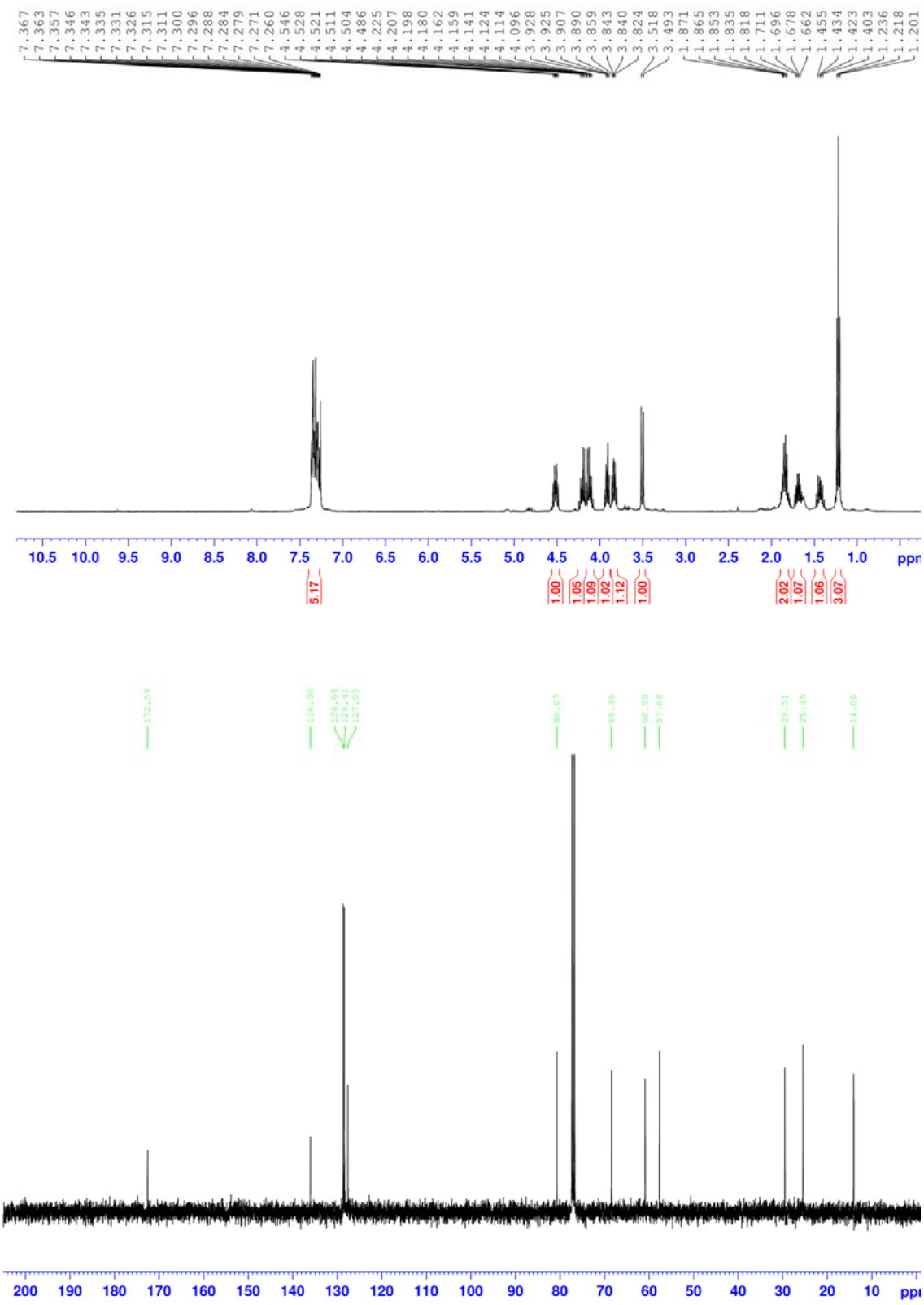
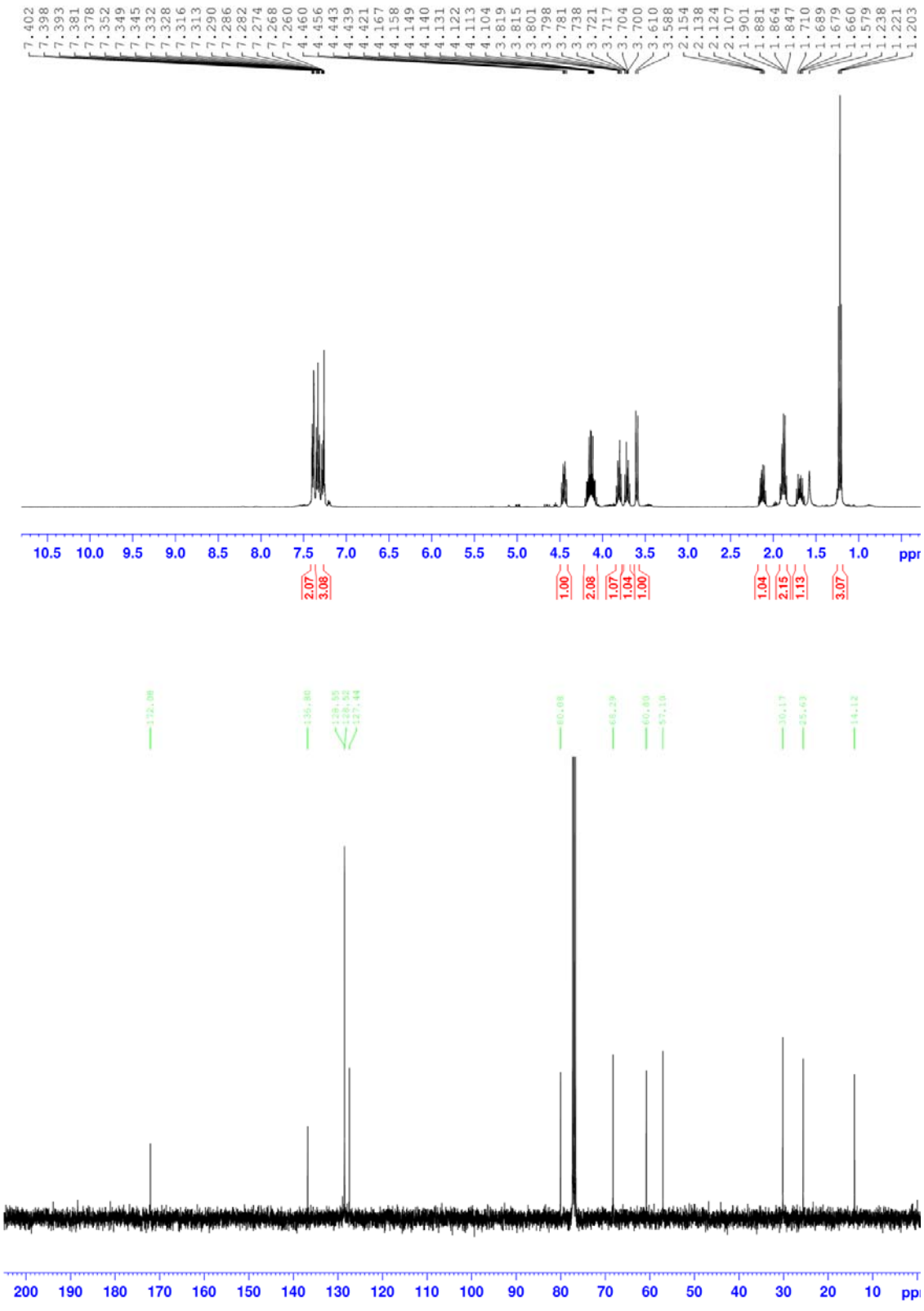


^{1}H and ^{13}C NMR spectra of compound 2o-2 (the *syn*-isomer)



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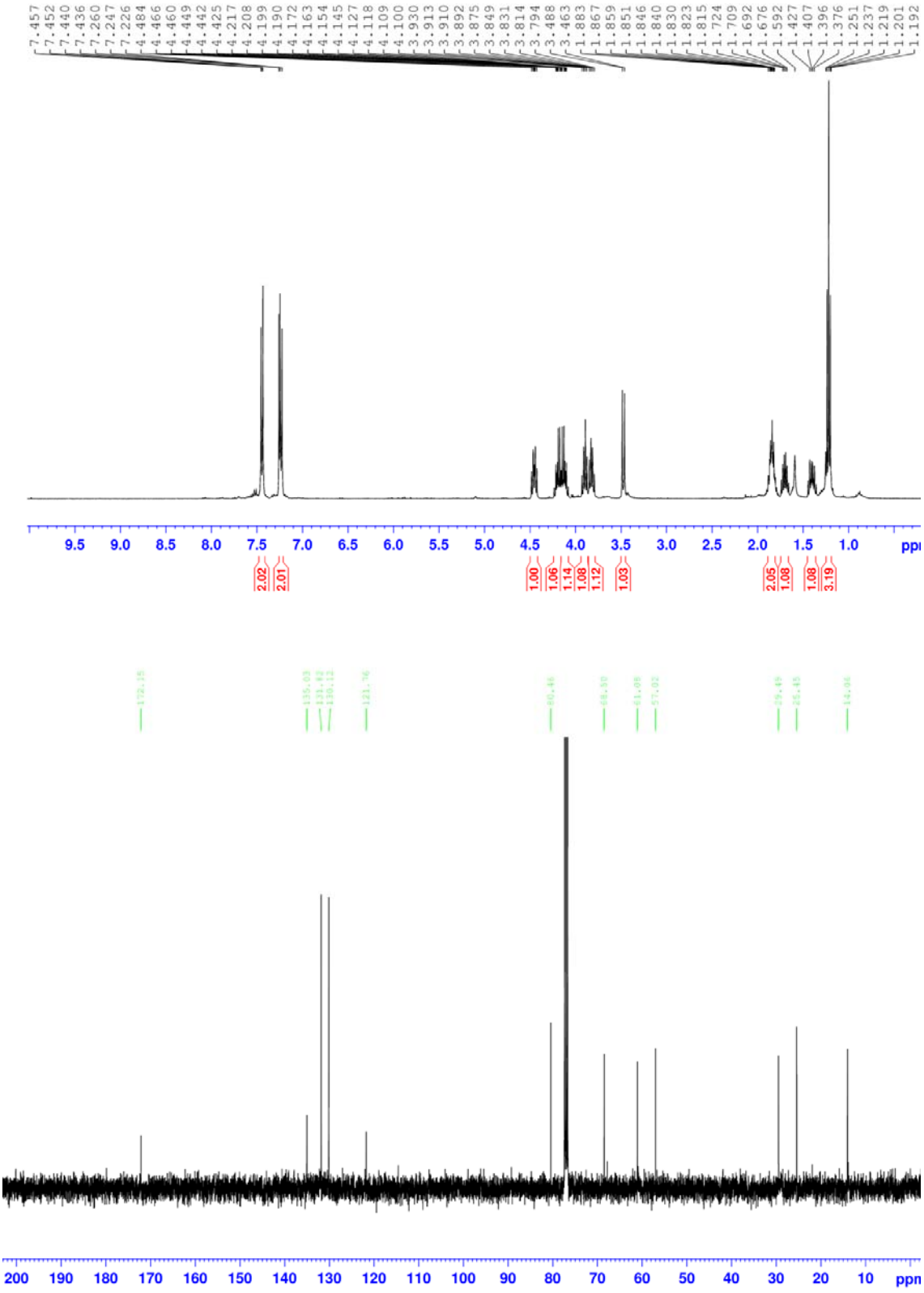
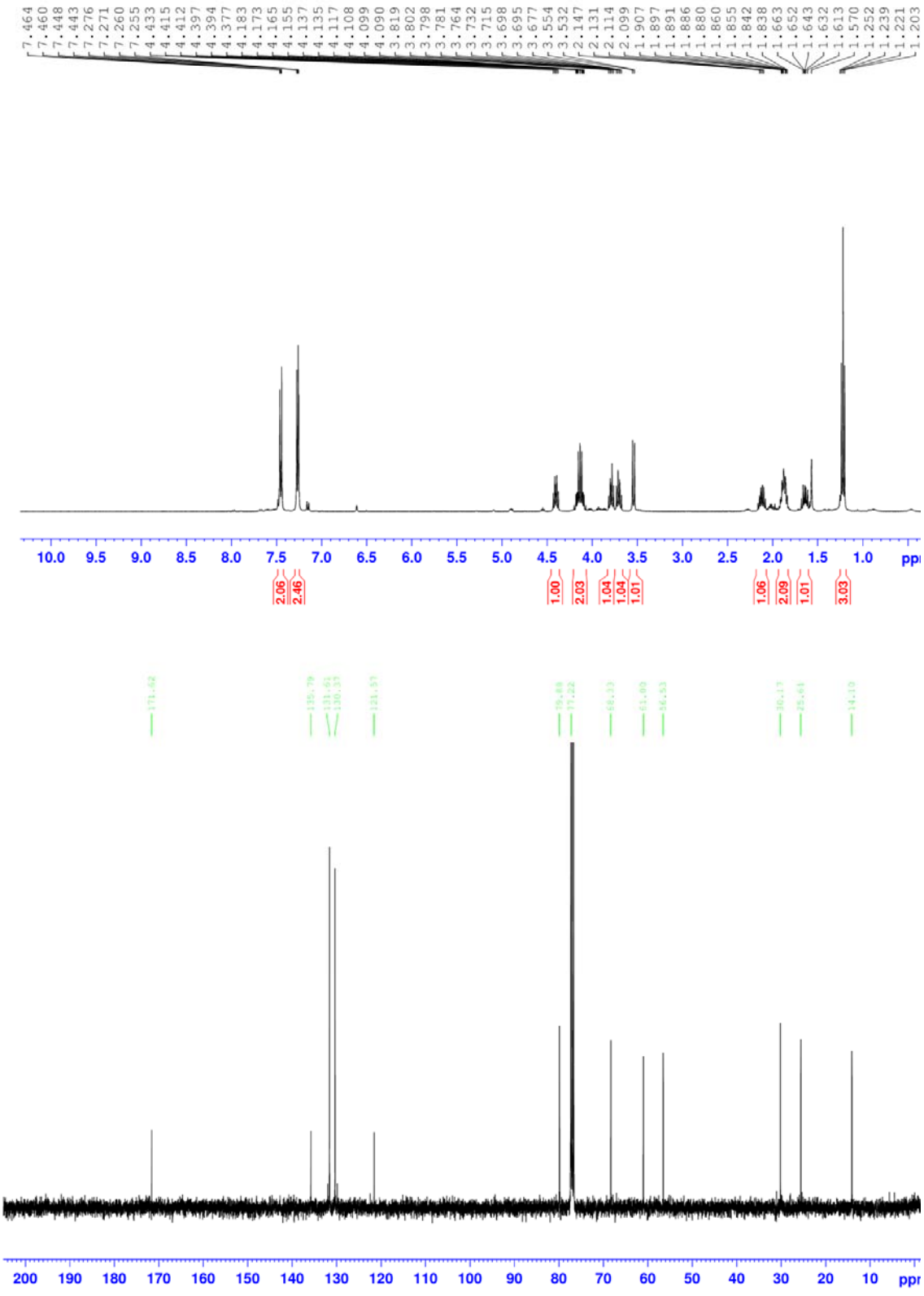
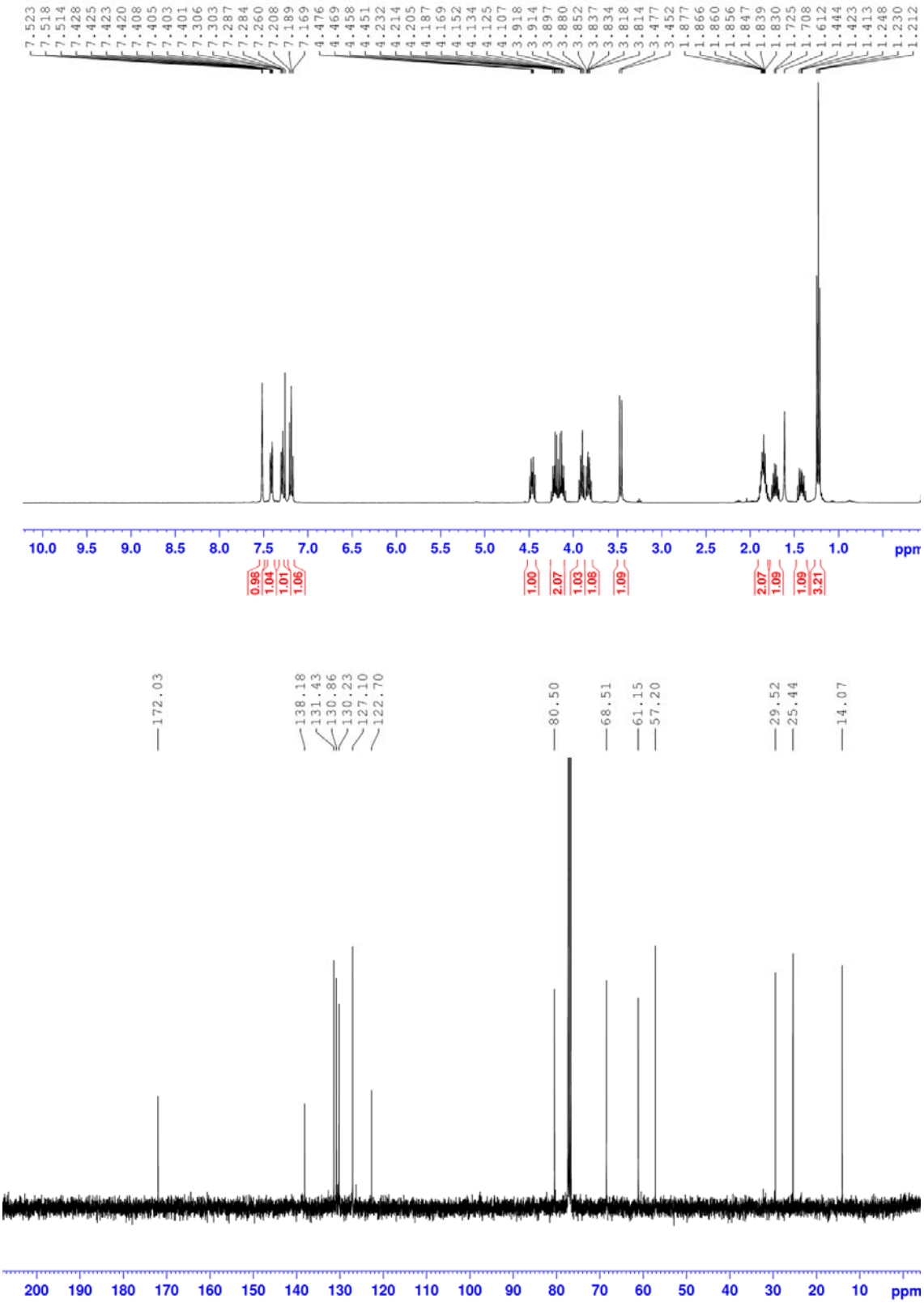


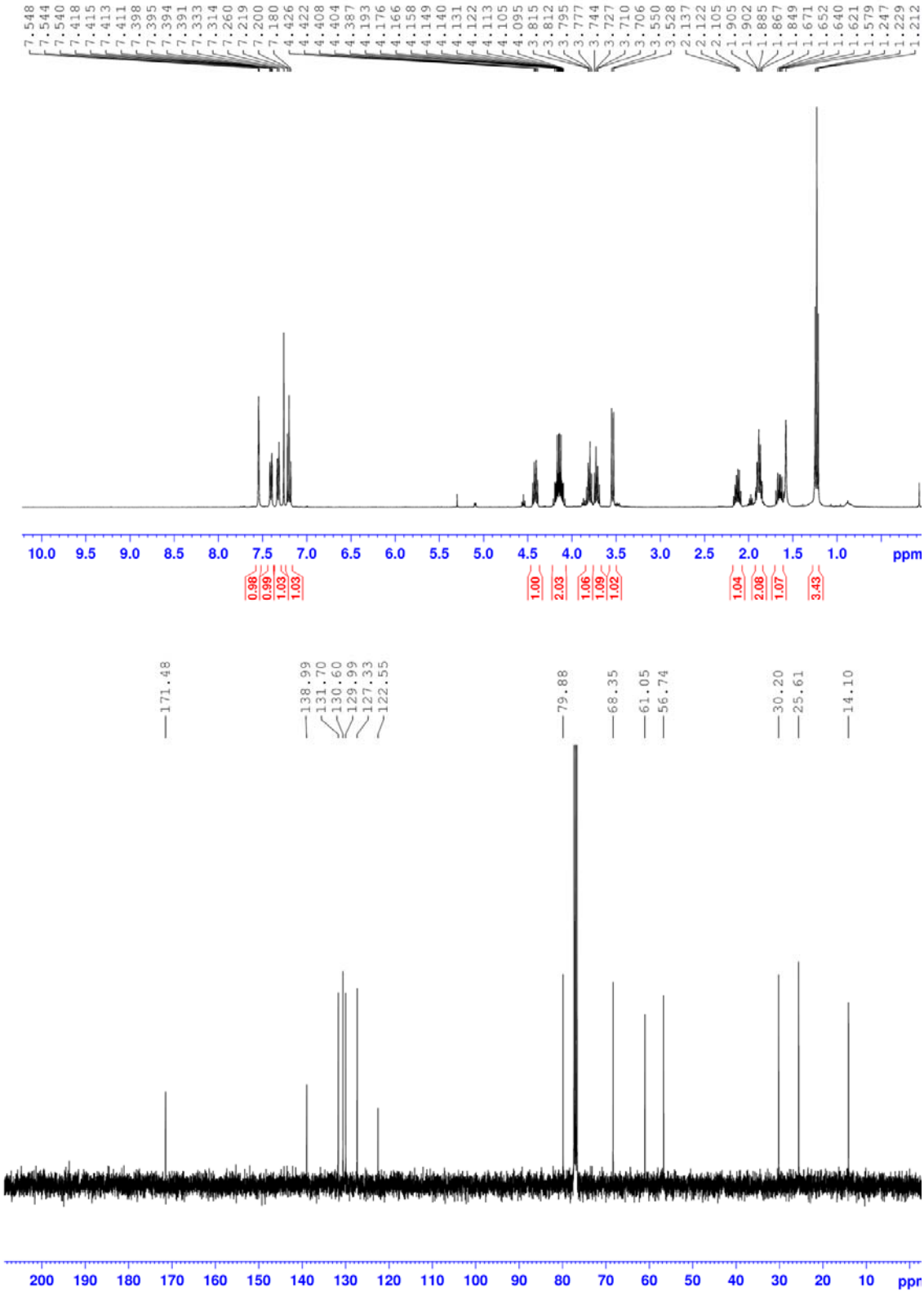
^{1}H and ^{13}C NMR spectra of compound 2p-2 (the *syn*-isomer)



^{1}H and ^{13}C NMR spectra of compound 2q-1 (the *anti*-isomer)



^{1}H and ^{13}C NMR spectra of compound 2q-2 (the *syn*-isomer)



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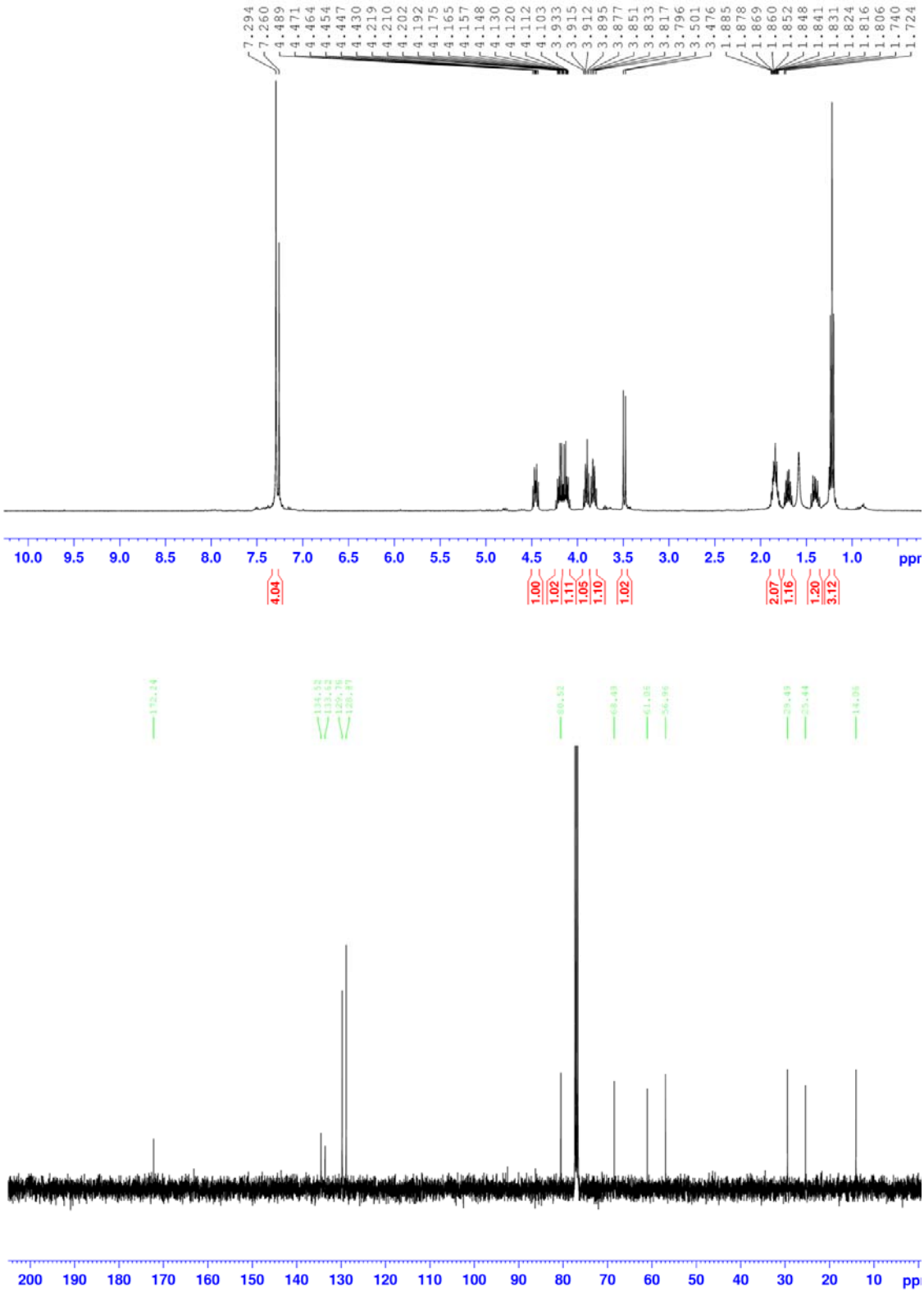
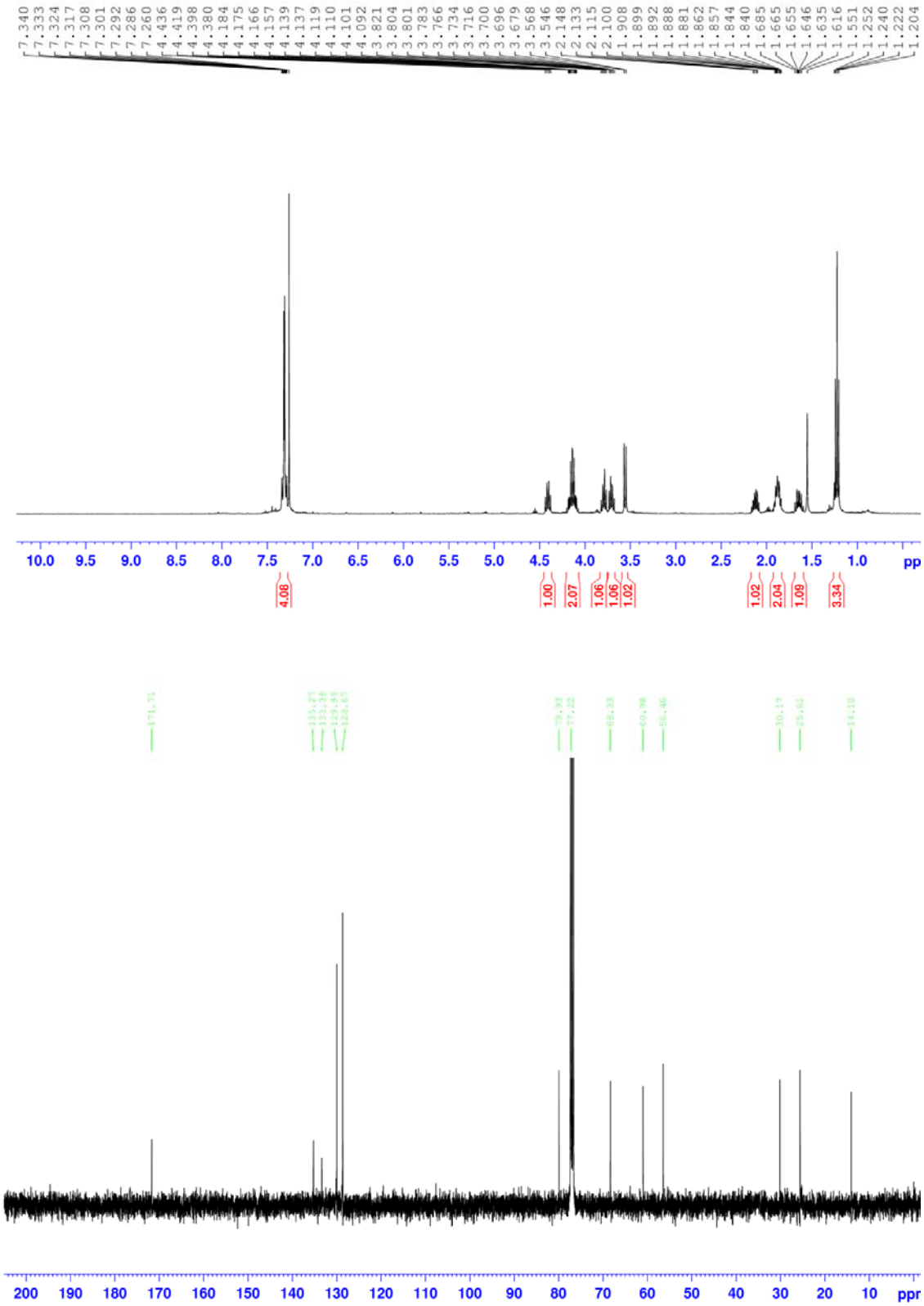
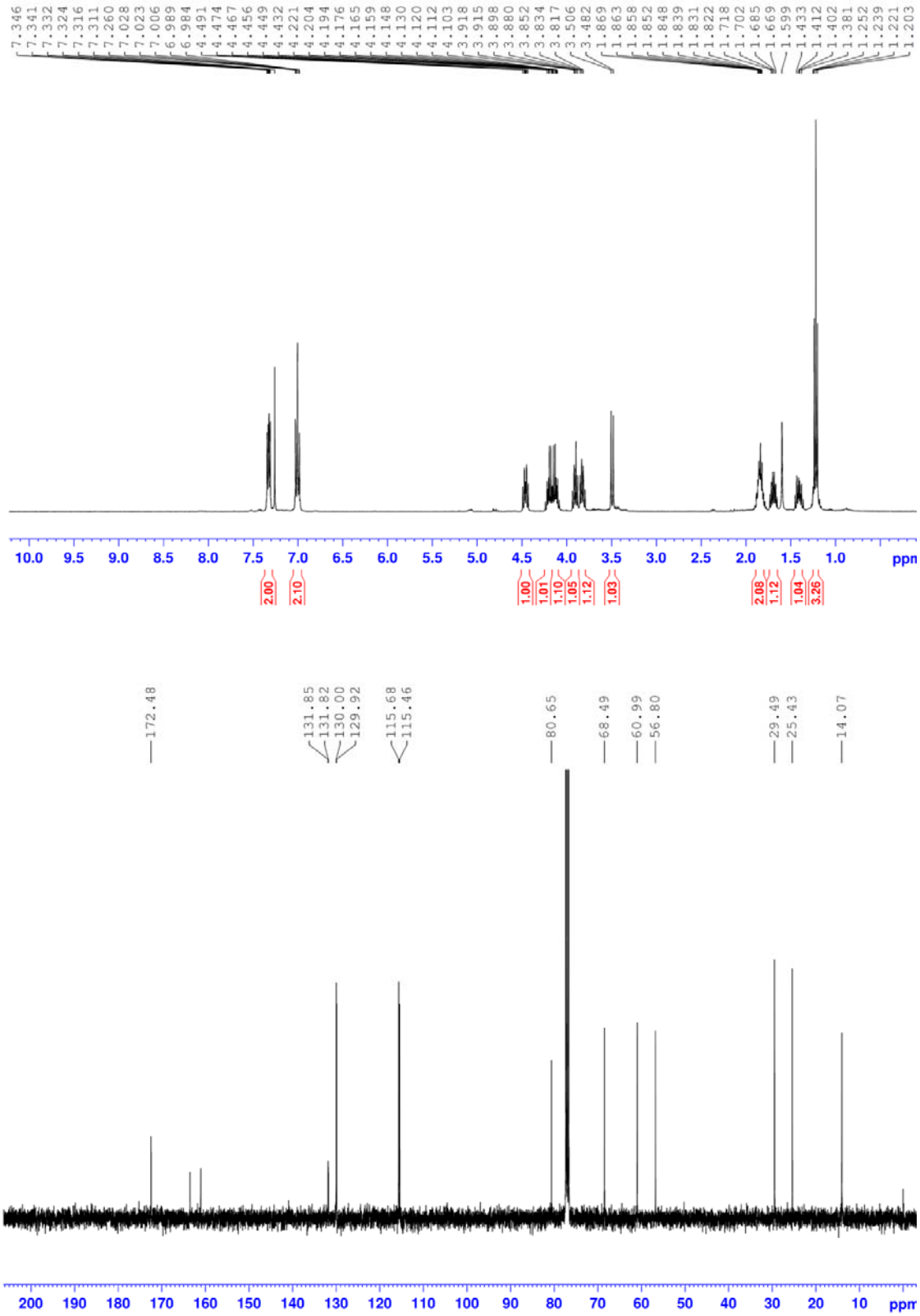


^{1}H and ^{13}C NMR spectra of compound 2r-2 (the *syn*-isomer)



^{1}H and ^{13}C NMR spectra of compound 2s-1 (the *anti*-isomer)



^{1}H and ^{13}C NMR spectra of compound 2s-2 (the *syn*-isomer)