Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Materials for

Synthesis of 1,2-disubstituted Benzimidazoles using an Aza-Wittig-Equivalent Process

*Yuan Chen, Fanghui Xu and Zhihua Sun**

College of Chemistry and Chemical Engineering, Shanghai University of Engineering Science, 333 Longteng Road, Shanghai 201620, China

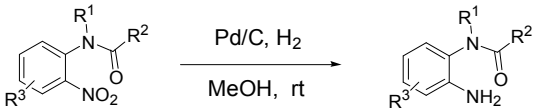
** Corresponding author: Zhihua Sun*

E-mail address: sungaris@gmail.com

1. Experimental

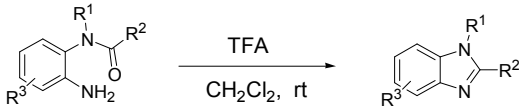
1.1 Preparation of Substrates

General procedure for the preparation of **1a-1o**



A MeOH solution of ortho-nitroaniline derivatives (0.5 mmol) was added Pd/C (200 mg). The reaction was filled up with H_2 and stirred for 10 h. The mixture was filtered to recycle the catalyst and solvent was evaporated in vacuo. The residue was purified by silica-gel column chromatography with CH_2Cl_2 as an eluent. Recrystallization from CH_2Cl_2/Hexane gave the white solid **1**.

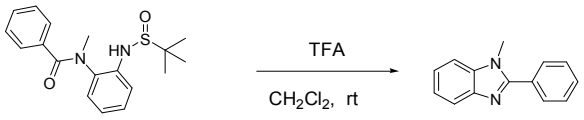
1.2 Additional synthesis of 2k, 2l and 2n



1k **2k**
1l **2l**
1n **2n**

In a 25 mL vial along with a stirring bar, to a mixture of **1** (1.0 mmol) in CH_2Cl_2 (50 mL) under N_2. TFA (0.5 mmol) was added to the mixture and the reaction was stirred at RT for additional 1 h. The reaction mixture was washed with water; dried over anhydrous Na_2SO_4 and evaporated in vacuo. The residue was purified by silica-gel column chromatography with CH_2Cl_2/PE as an eluent. Recrystallization from CH_2Cl_2/Hexane gave the white solid **2**.(**2k**, 25%; **2l**, 34%; **2n**, 23%)

1.3 Additional synthesis of 2h



4 **2h**

In a 25 mL vial along with a stirring bar, to a mixture of **4** (1.0 mmol) in CH_2Cl_2 (50 mL) under N_2. TFA (0.5 mmol) was added to the mixture and the reaction was stirred at RT for additional 1 h. The reaction mixture was washed with water; dried over anhydrous Na_2SO_4 and evaporated in vacuo. The residue was purified by silica-gel column chromatography with CH_2Cl_2/PE as an eluent. Recrystallization from CH_2Cl_2/Hexane gave the white solid **2h** (96%).

2. Spectra of compounds

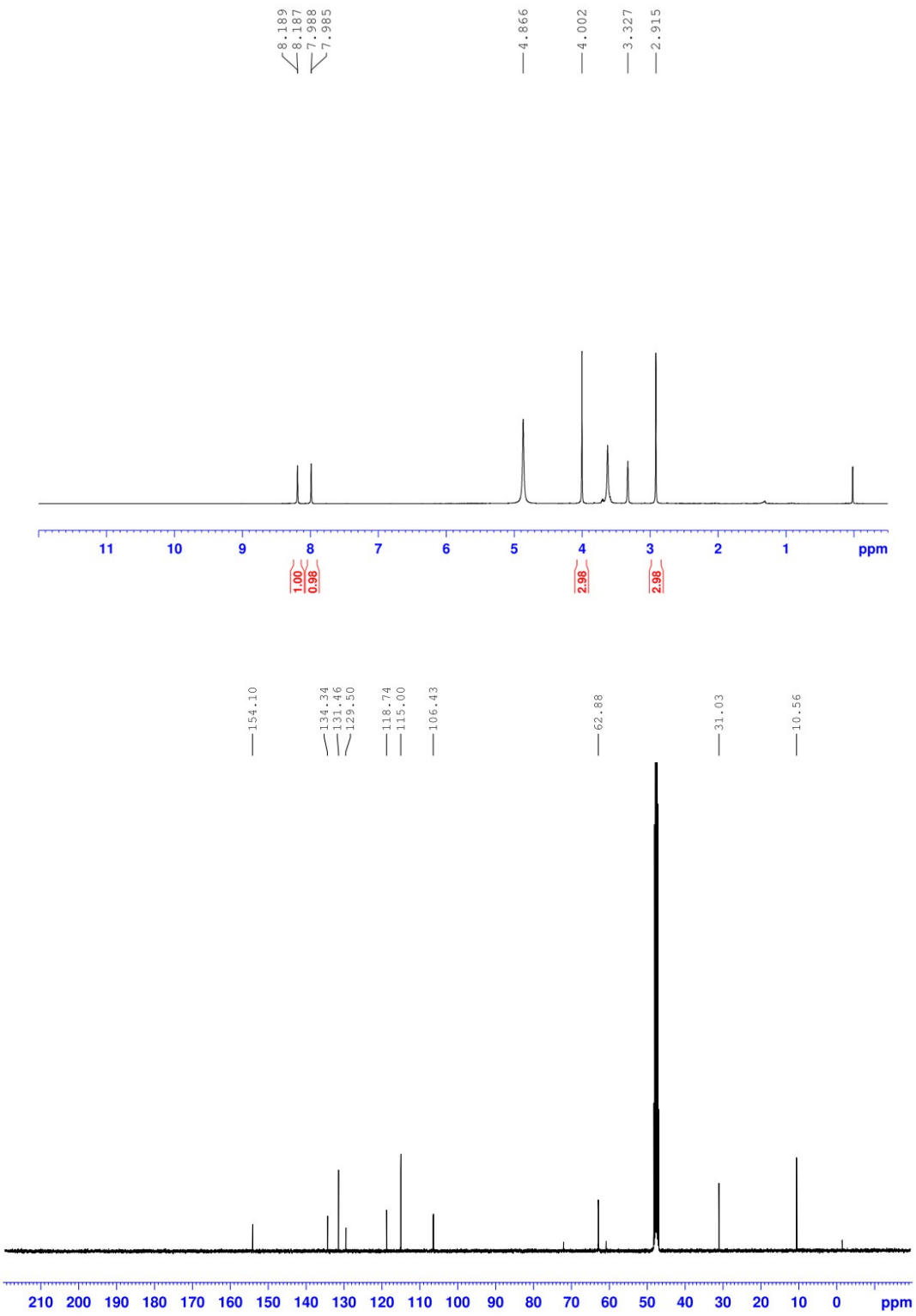


Figure S1. ^{1}H and ^{13}C NMR spectra of **2a** in MeOD.

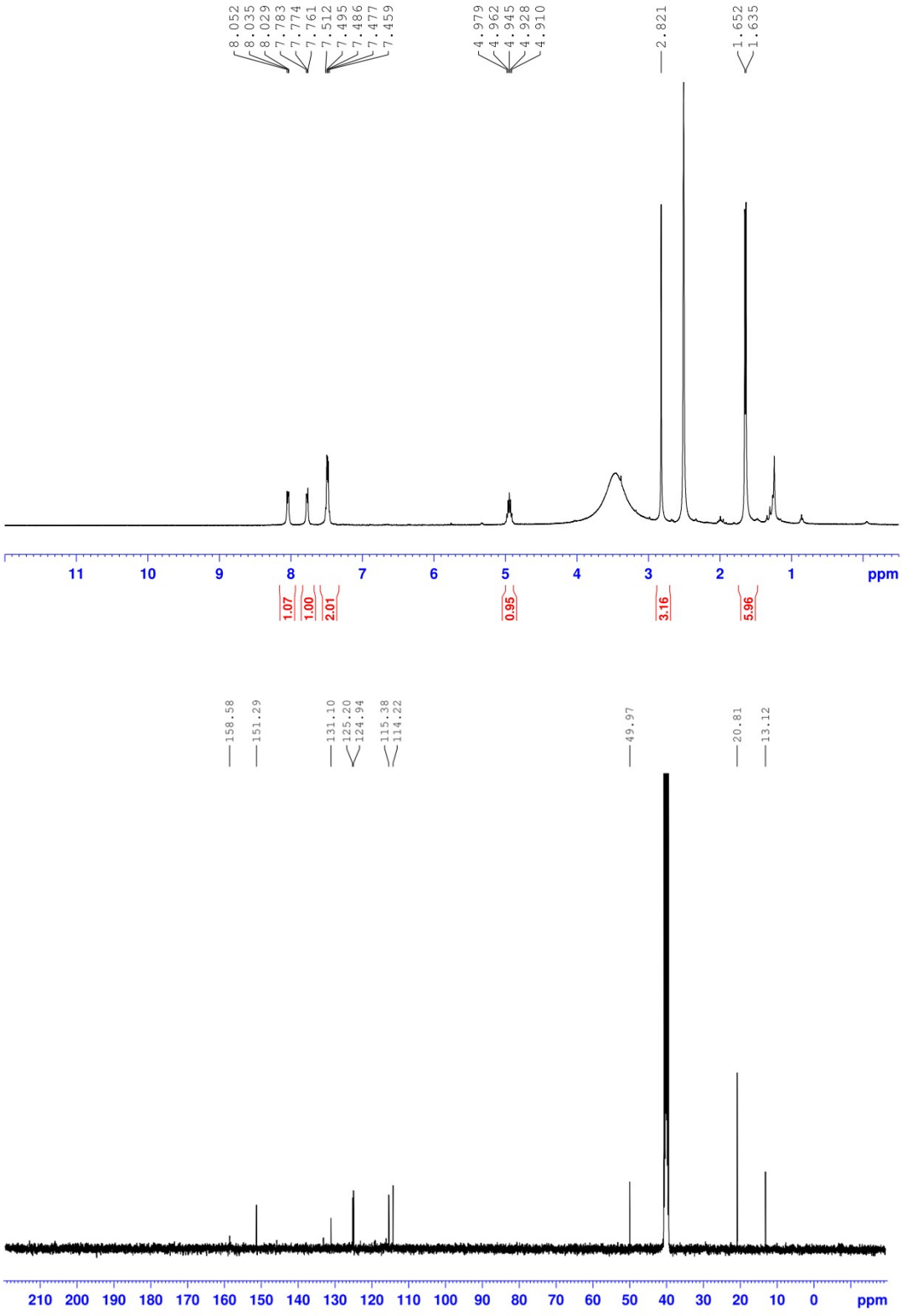


Figure S2. ^{1}H and ^{13}C NMR spectra of **2b** in DMSO-d_6.

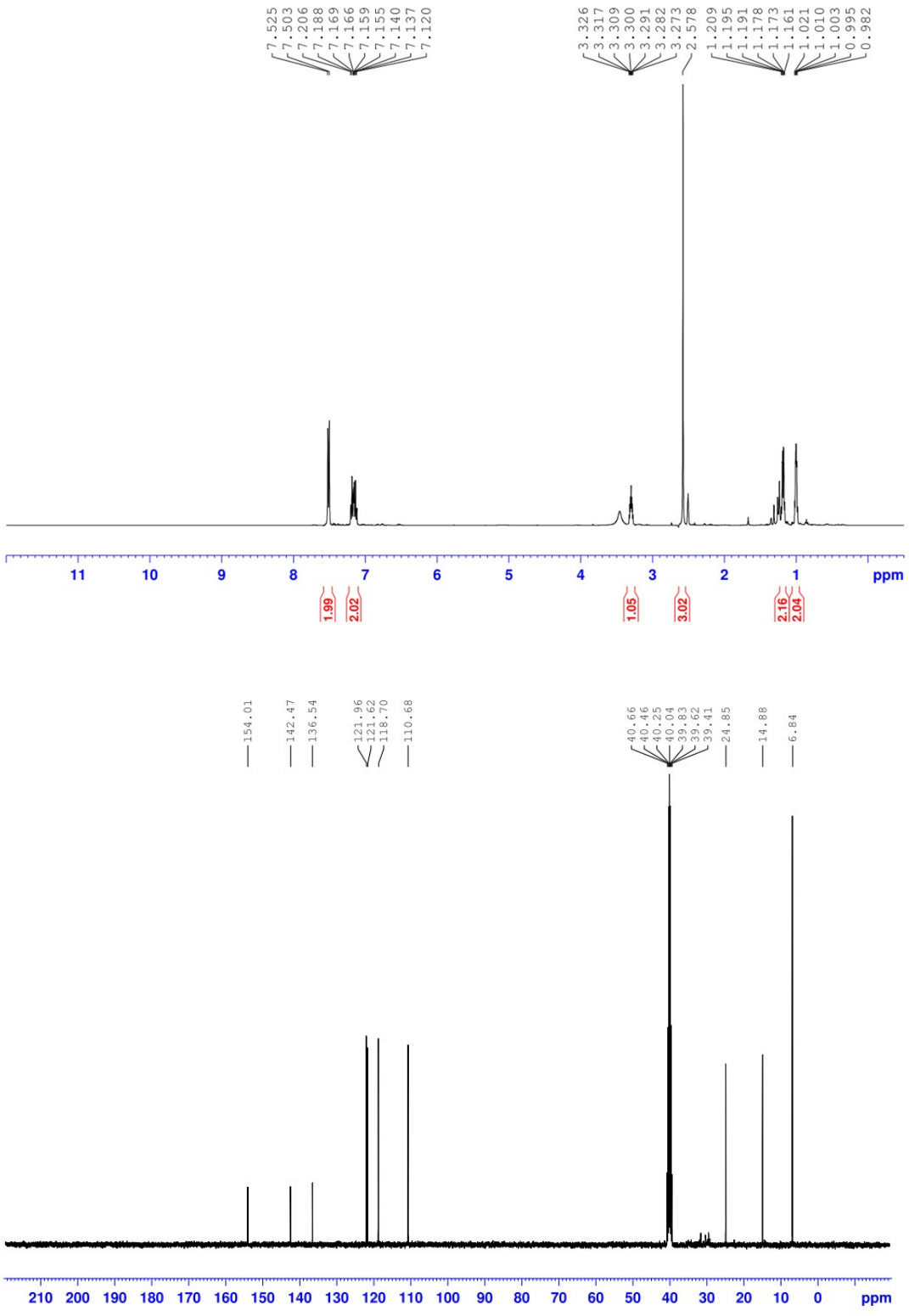


Figure S3. ^{1}H and ^{13}C NMR spectra of **2c** in DMSO-d_6.

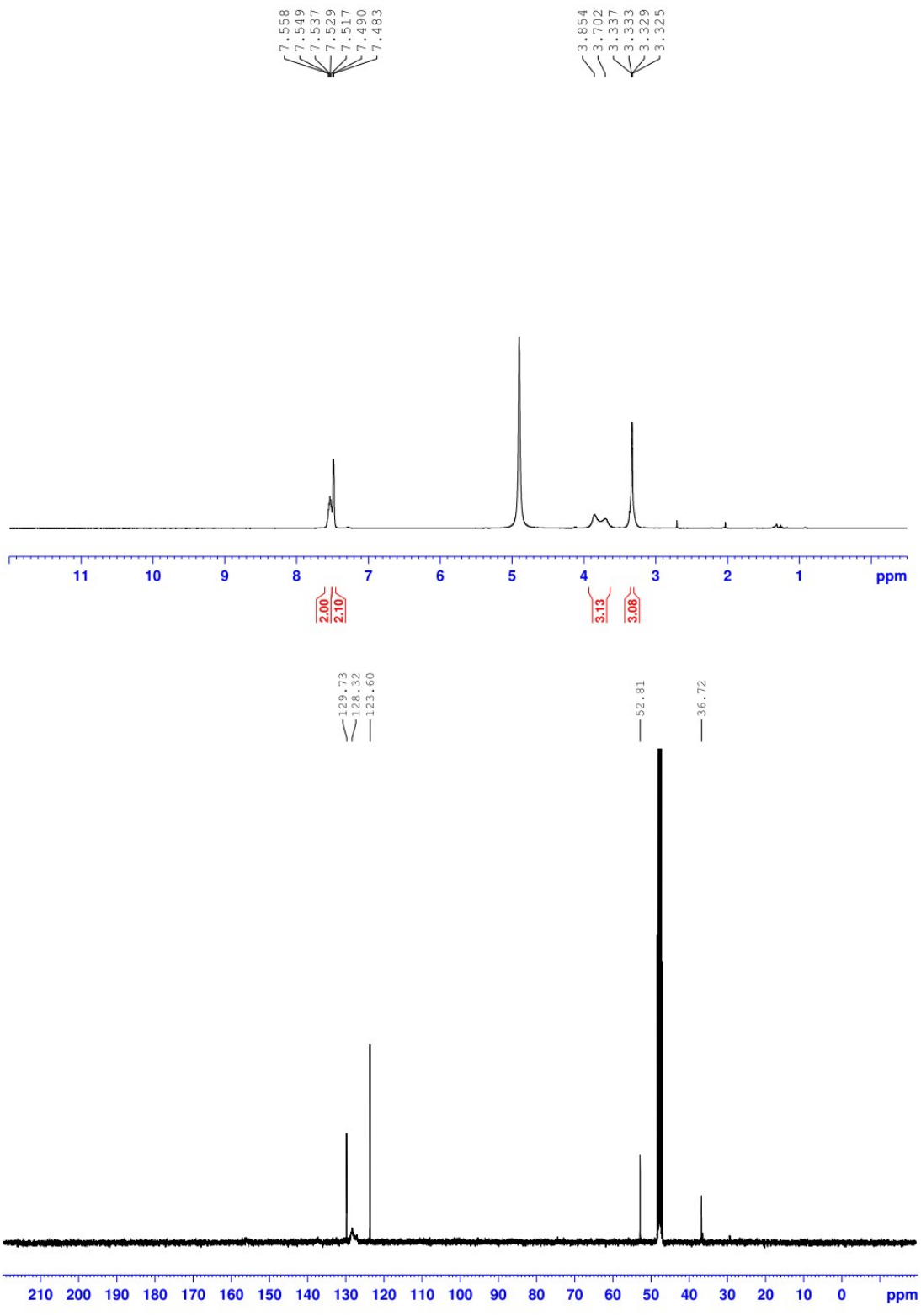


Figure S4. ^{1}H and ^{13}C NMR spectra of **2d** in MeOD.

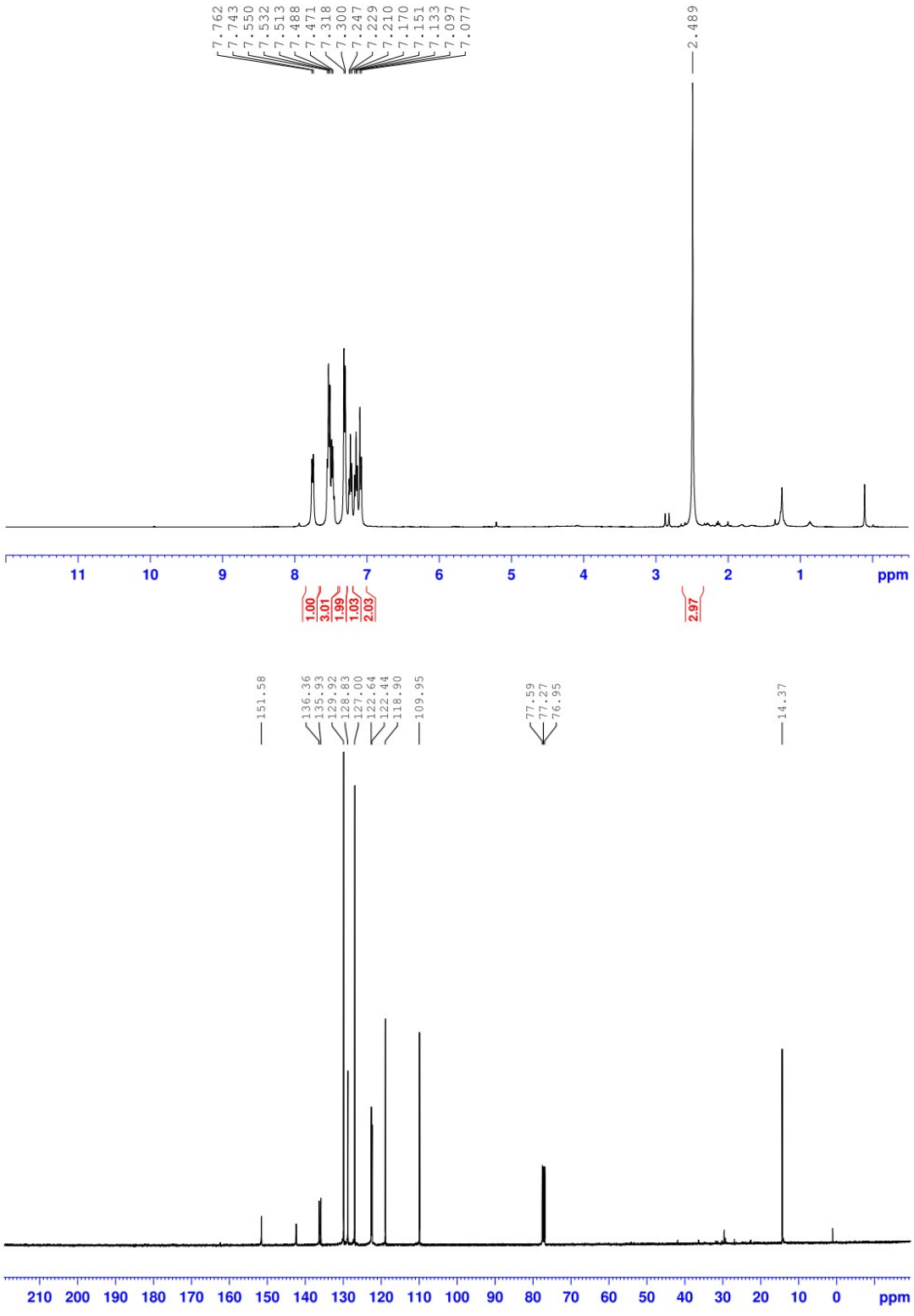


Figure S5. ^{1}H and ^{13}C NMR spectra of **2e** in $CDCl_3$.

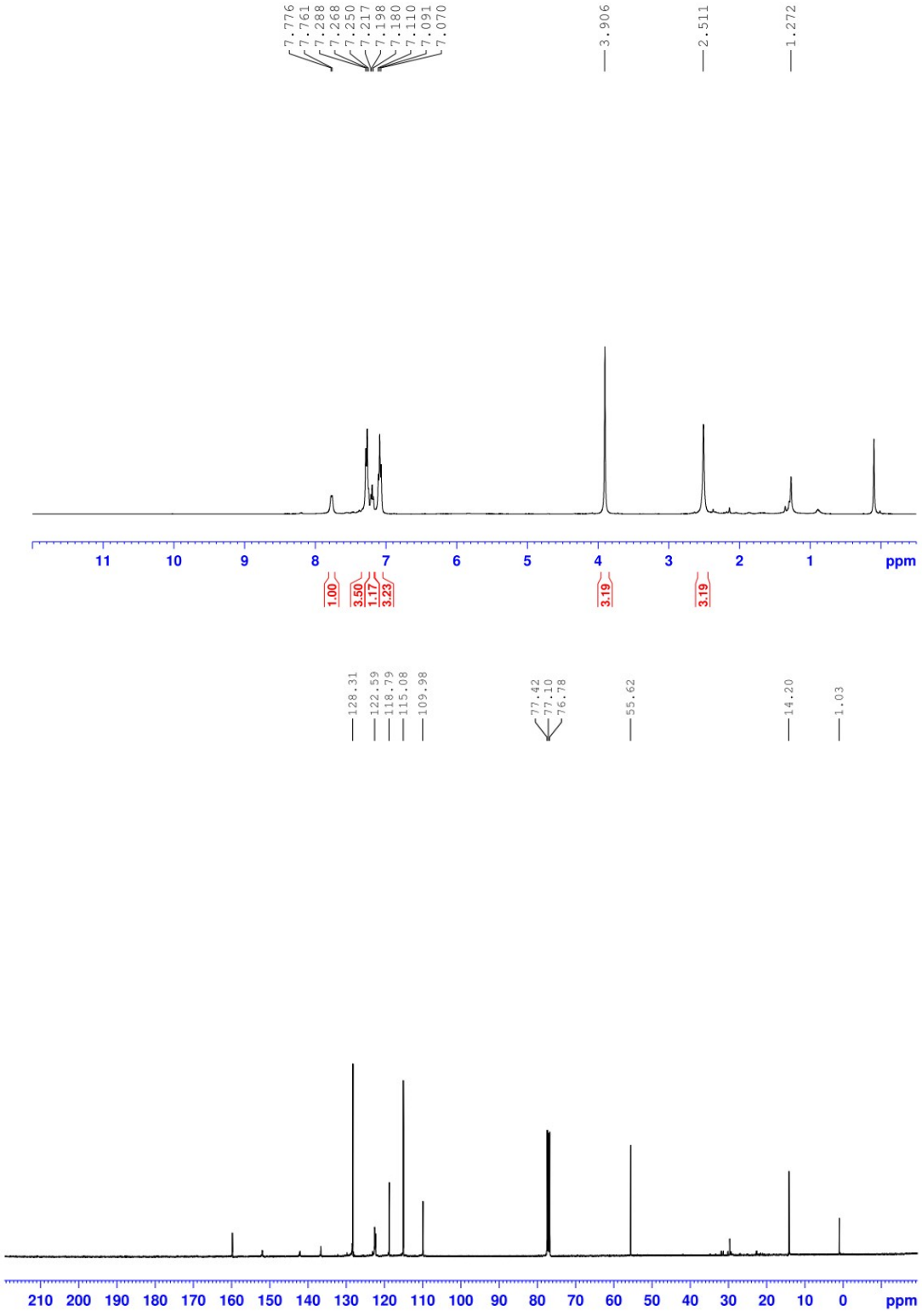


Figure S6. ^{1}H and ^{13}C NMR spectra of **2f** in $CDCl_3$.

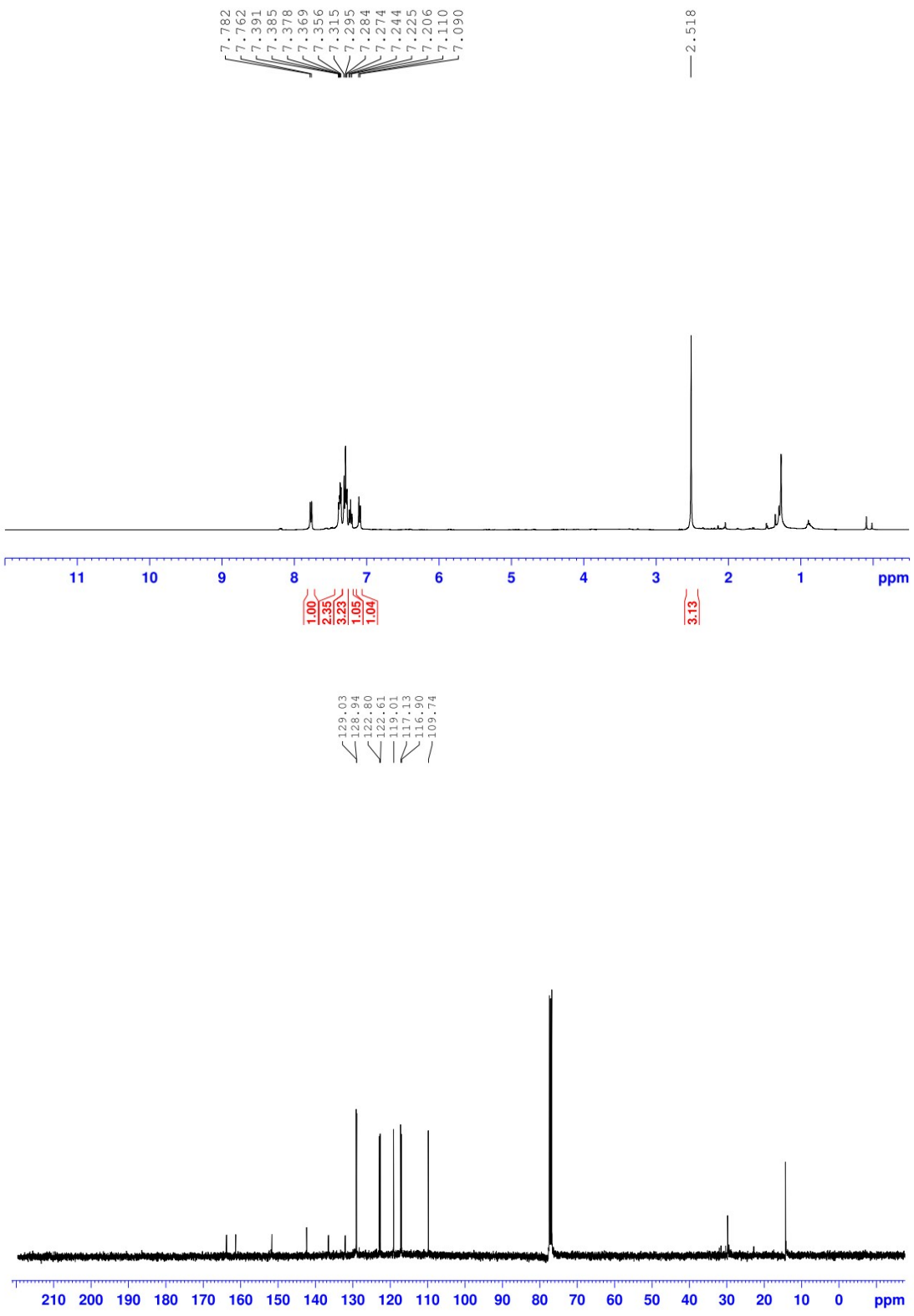


Figure S7. ^{1}H and ^{13}C NMR spectra of **2g** in $CDCl_3$.

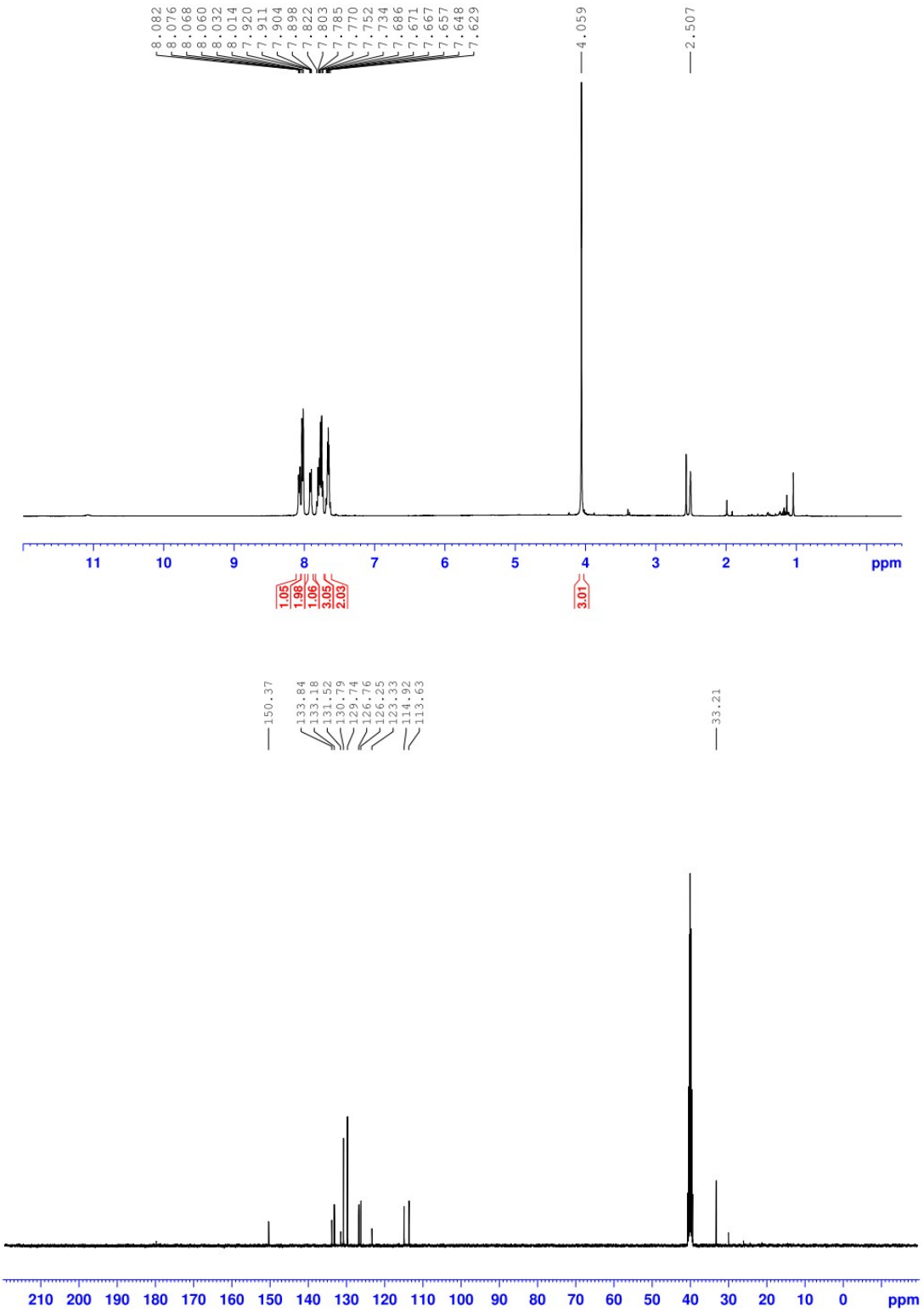


Figure S8. ^{1}H and ^{13}C NMR spectra of **2h** in DMSO-d_6.

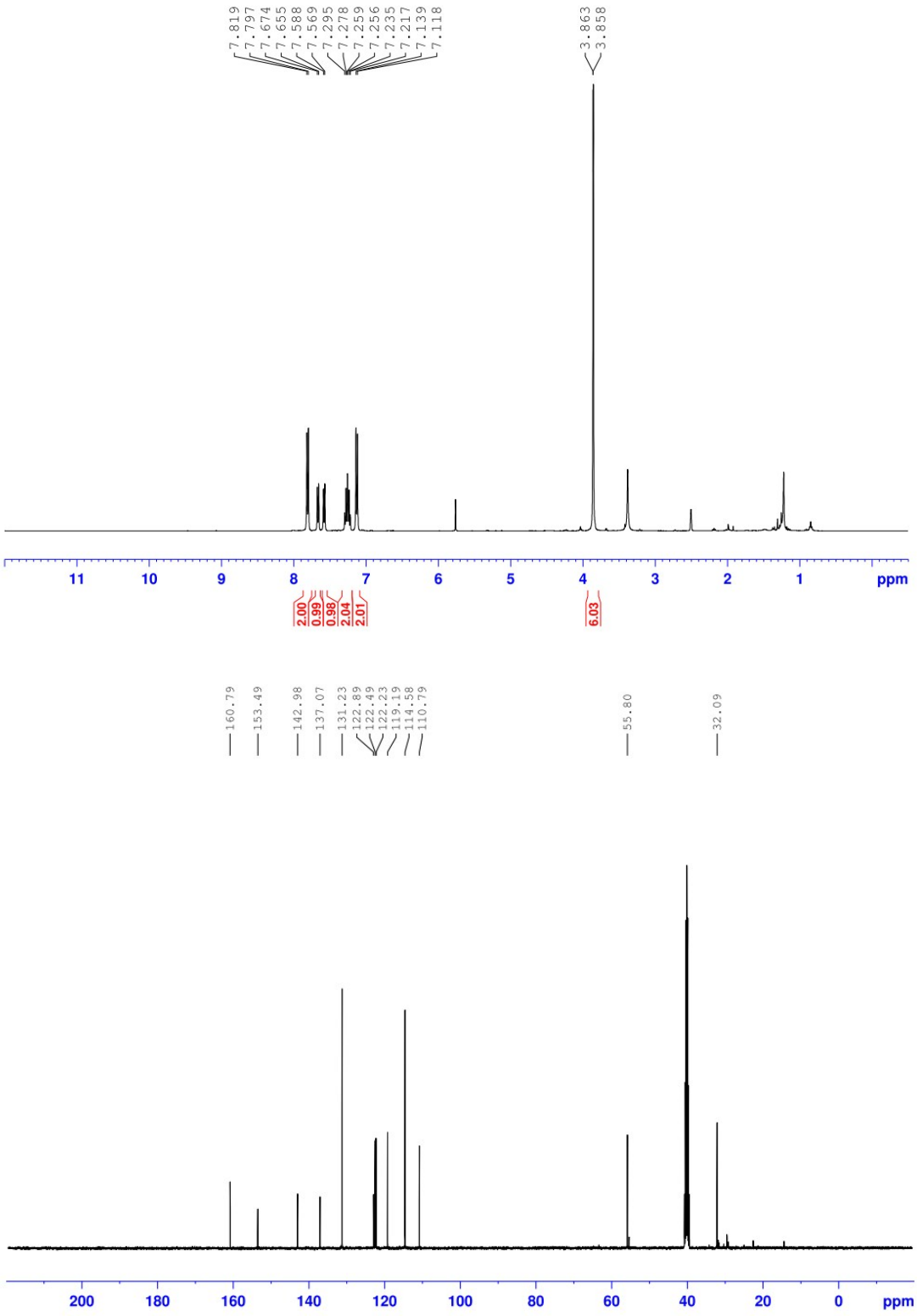


Figure S9. ^{1}H and ^{13}C NMR spectra of **2i** in DMSO-d_6.

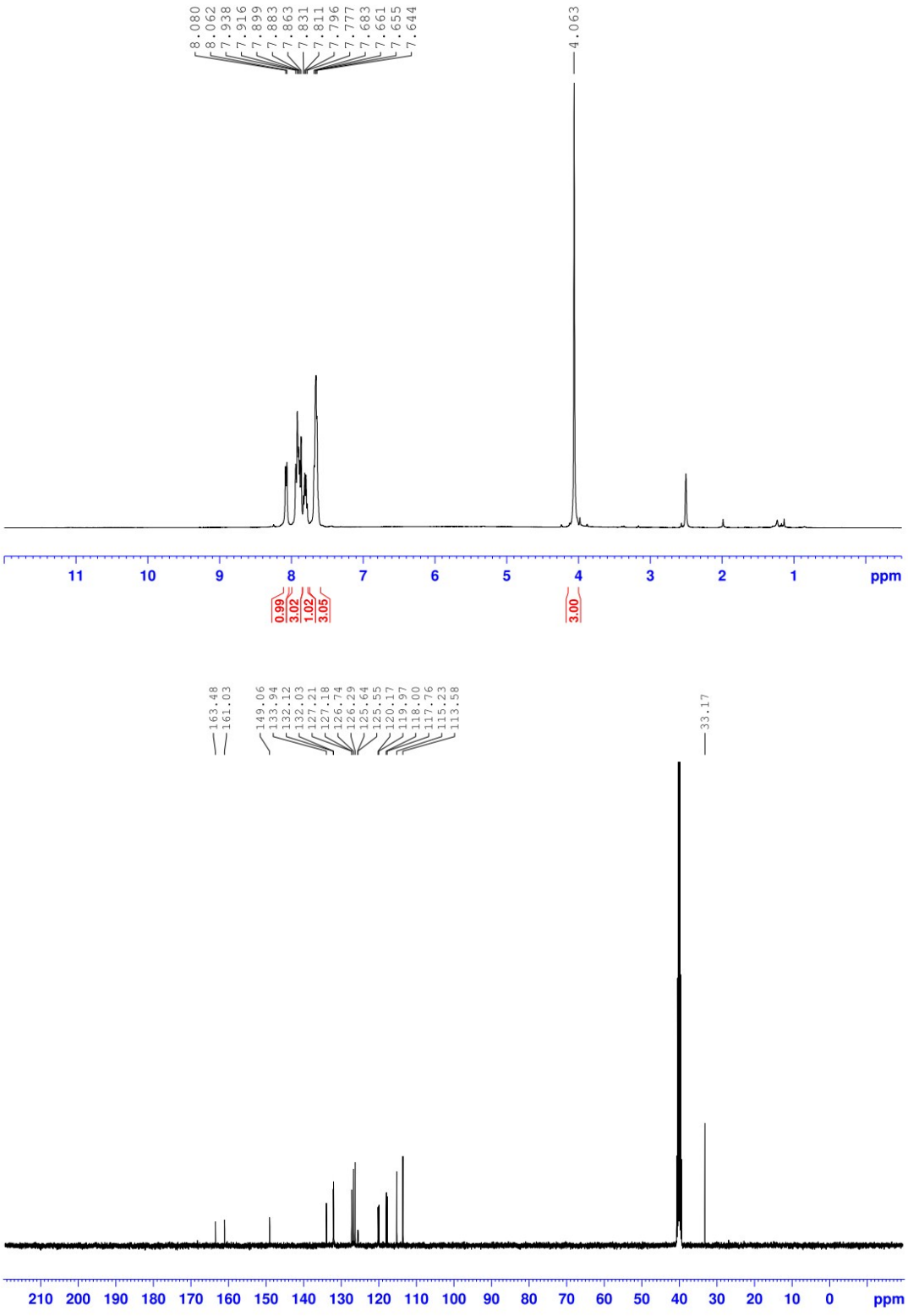


Figure S10. ^{1}H and ^{13}C NMR spectra of **2j** in DMSO-d_6.

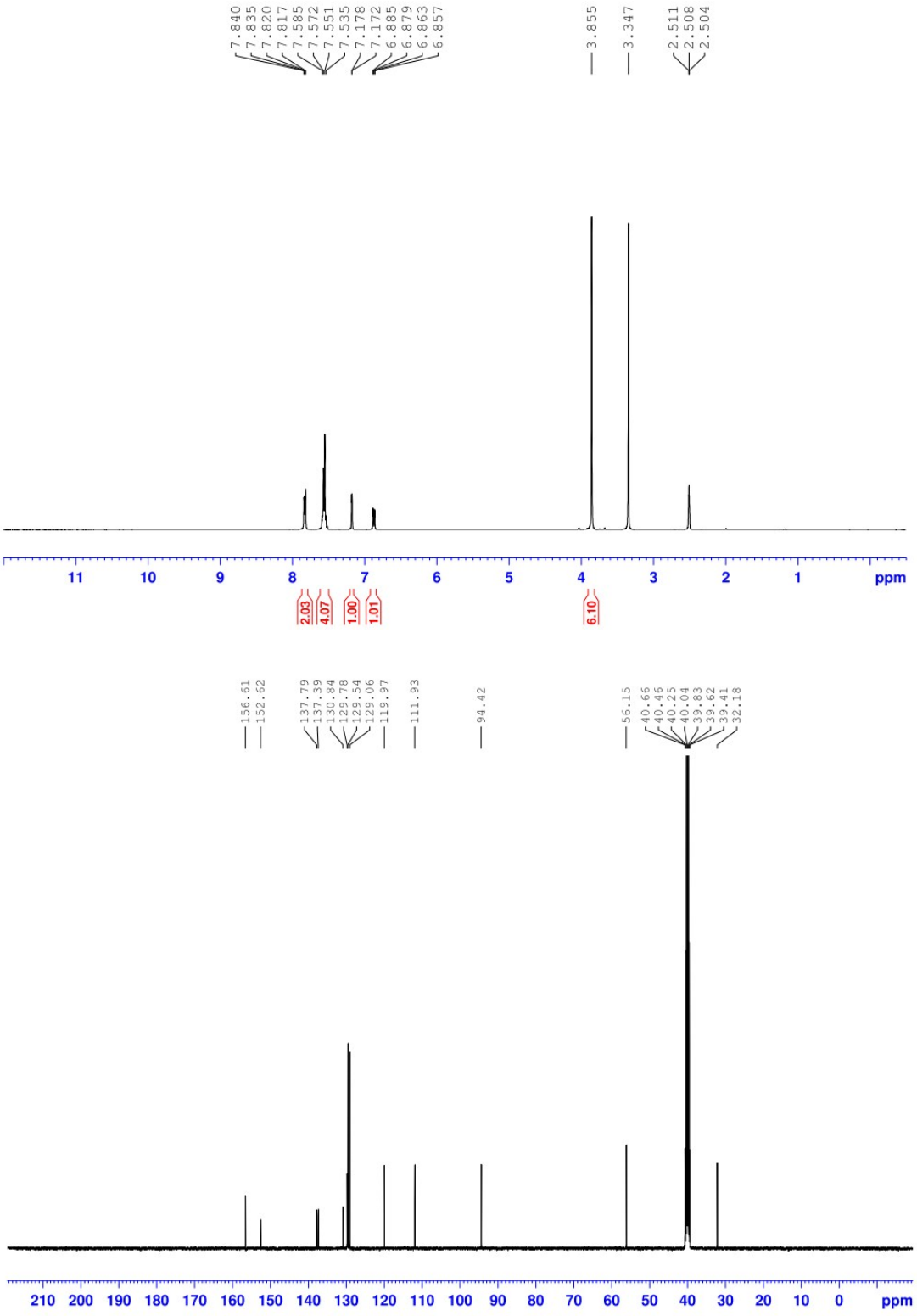


Figure S11. ^{1}H and ^{13}C NMR spectra of **2k** in DMSO-d_6.

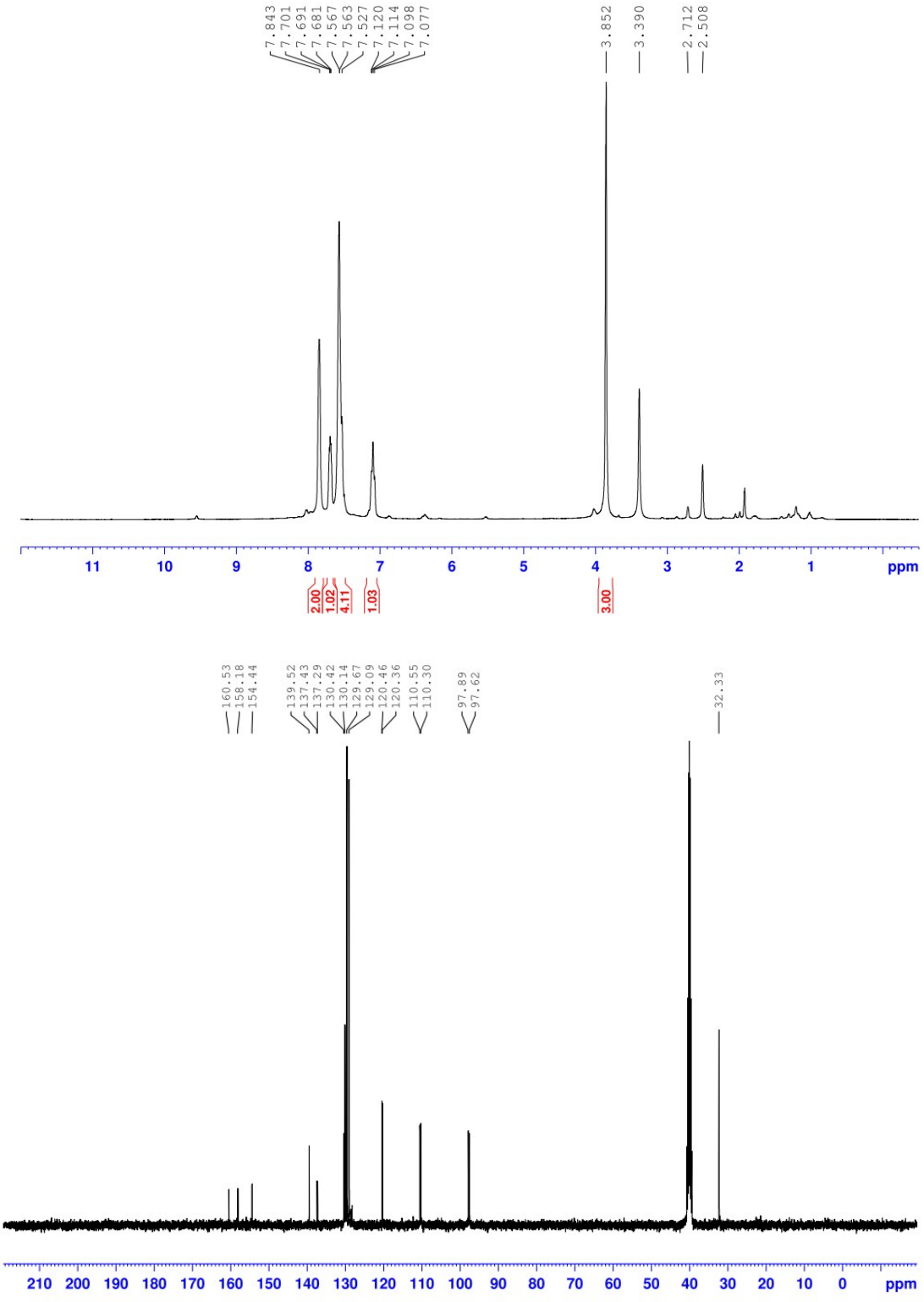


Figure S12. ^{1}H and ^{13}C NMR spectra of **2l** in DMSO-d_6.

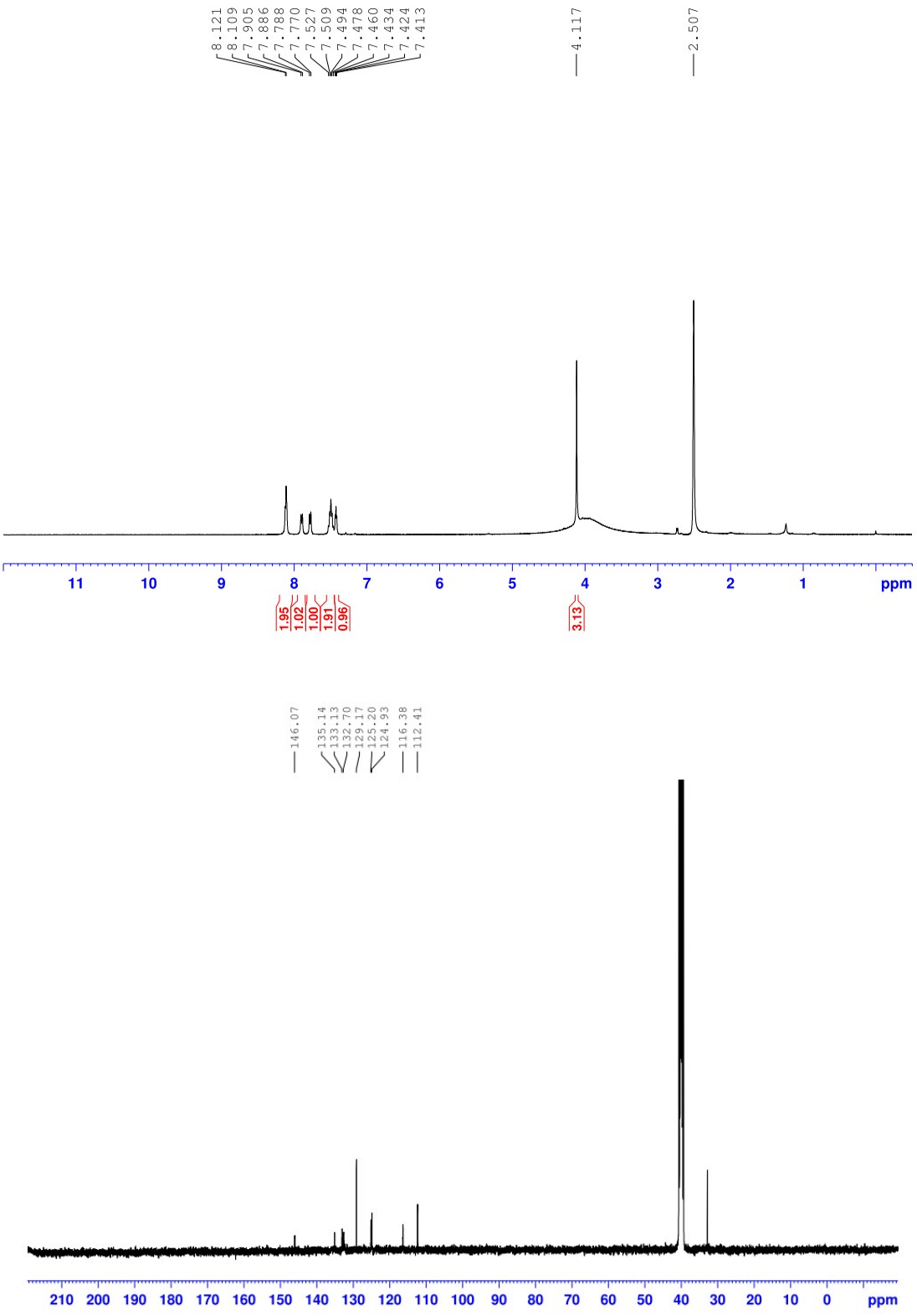


Figure S13. ^{1}H and ^{13}C NMR spectra of **2m** in DMSO-d_6.

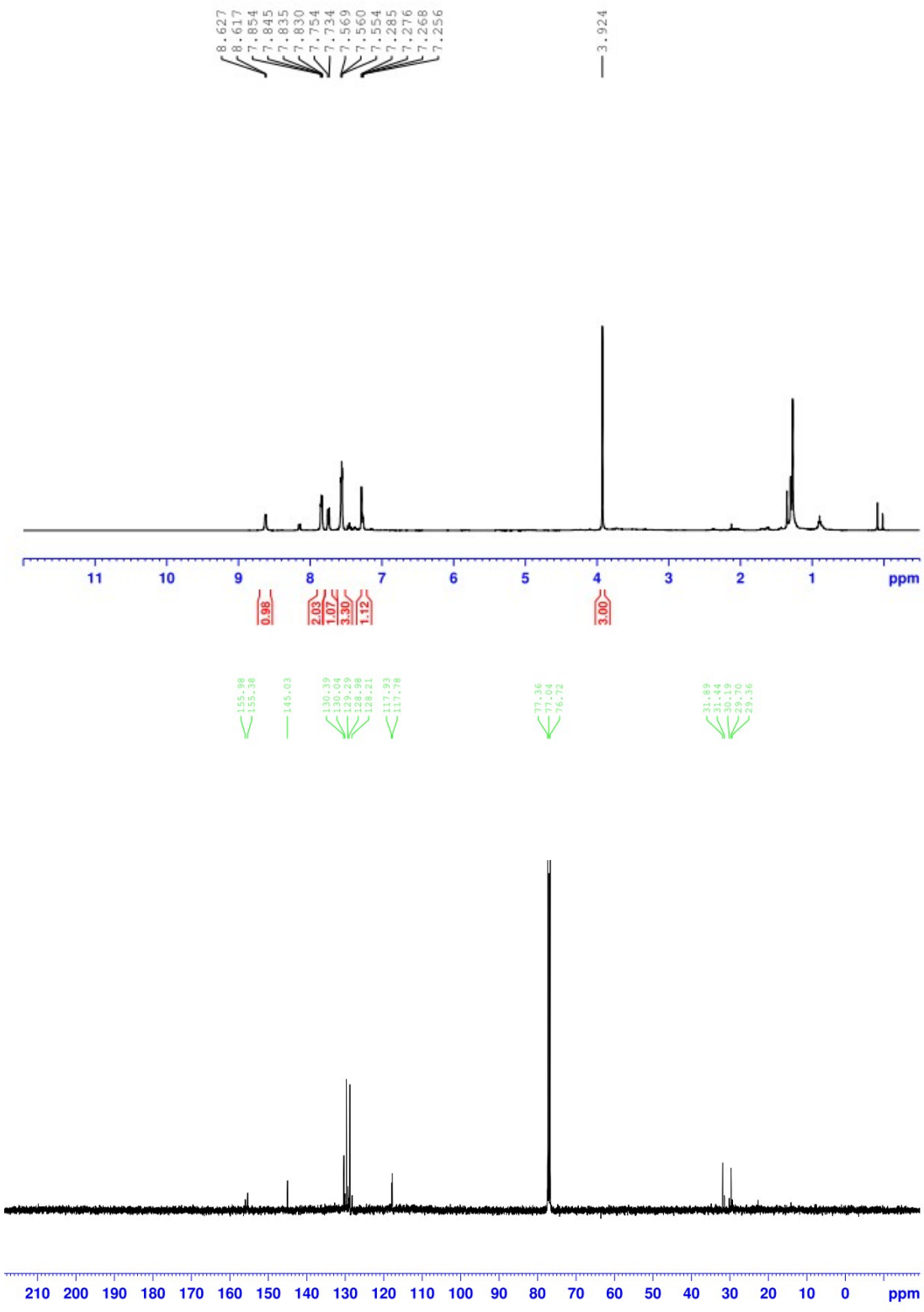


Figure S14. ^{1}H and ^{13}C NMR spectra of **2n** in $CDCl_3$.

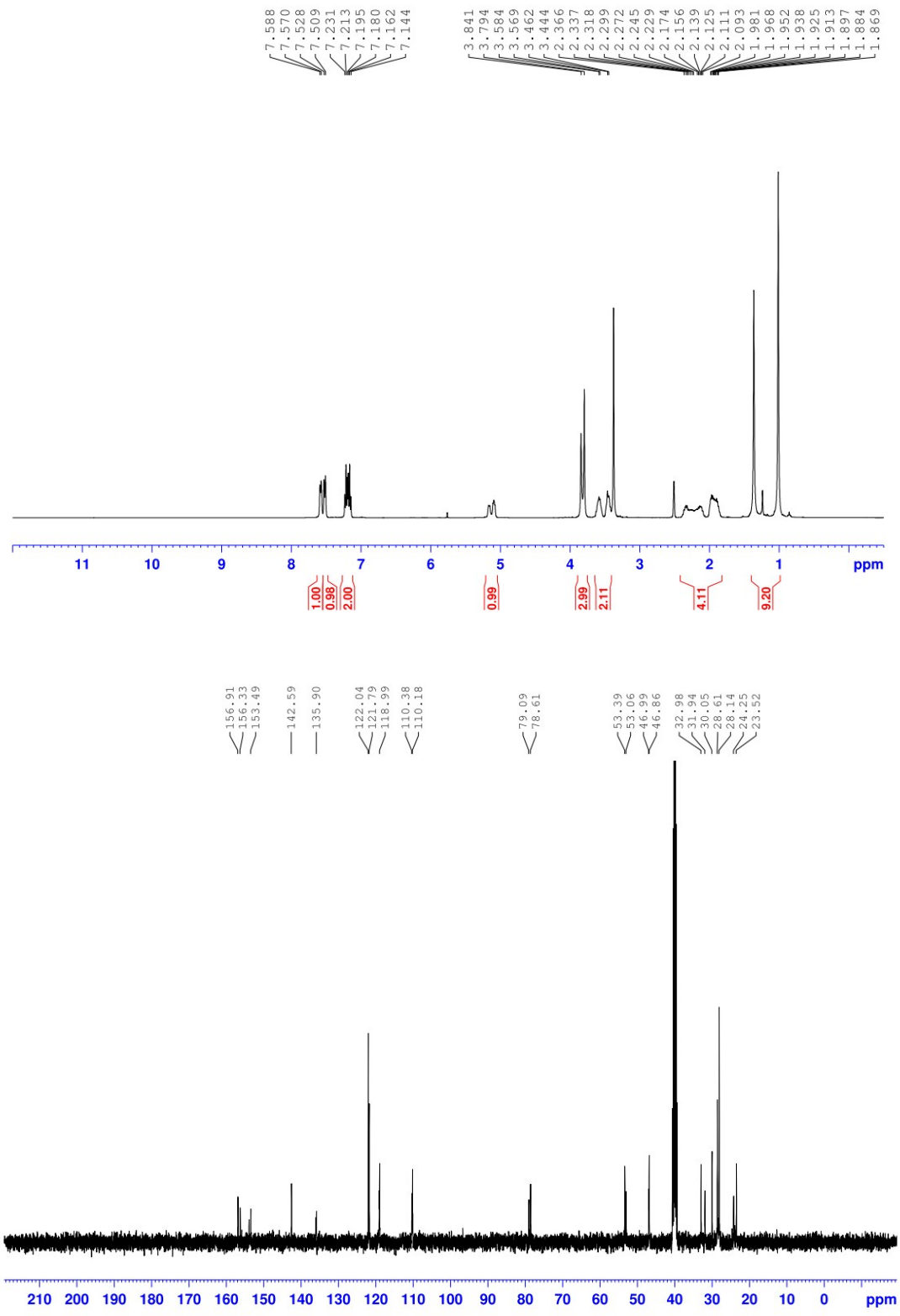


Figure S15. ^{1}H and ^{13}C NMR spectra of **2o** in DMSO-d_6.

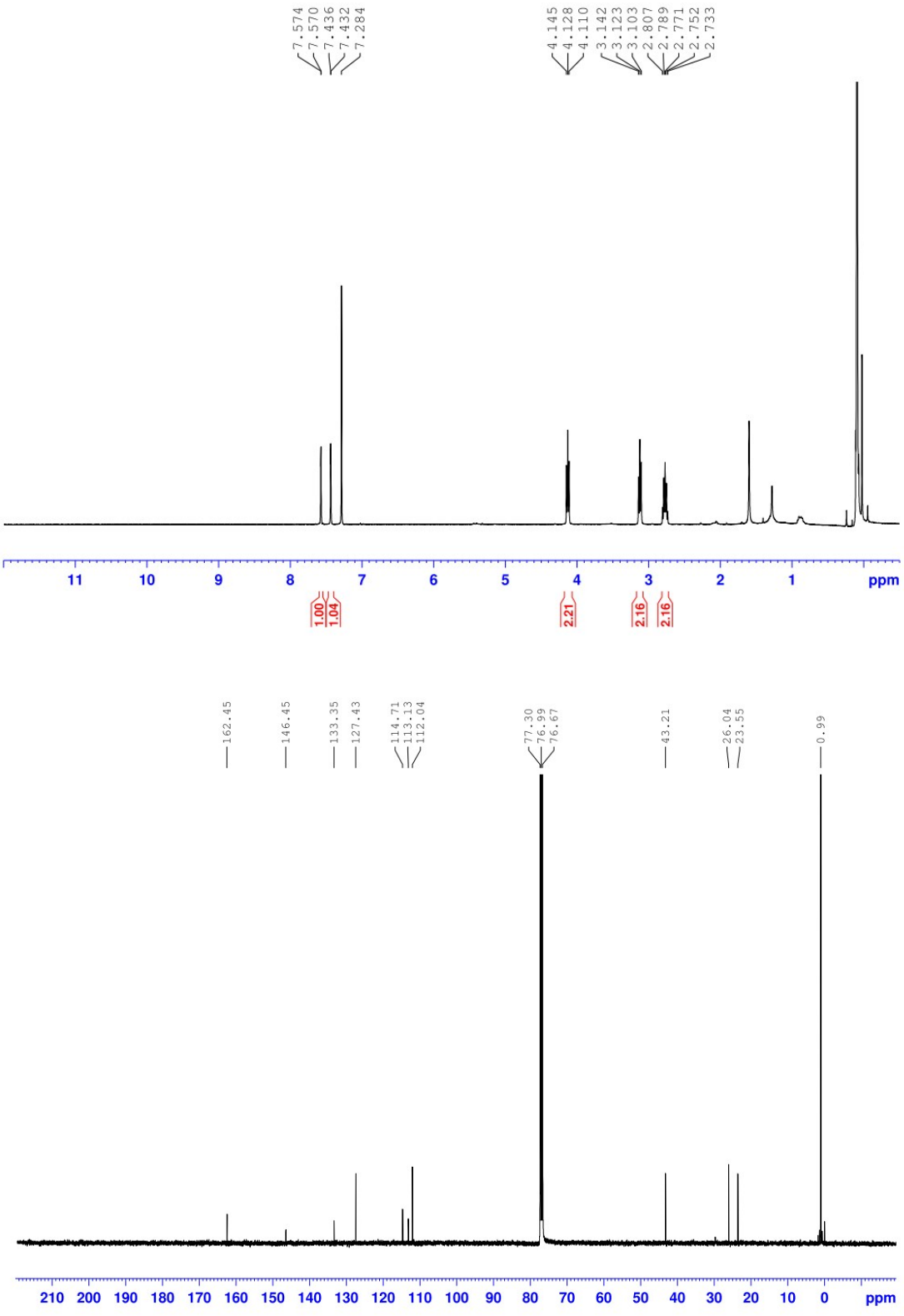


Figure S16. ^{1}H and ^{13}C NMR spectra of **2p** in $CDCl_3$.

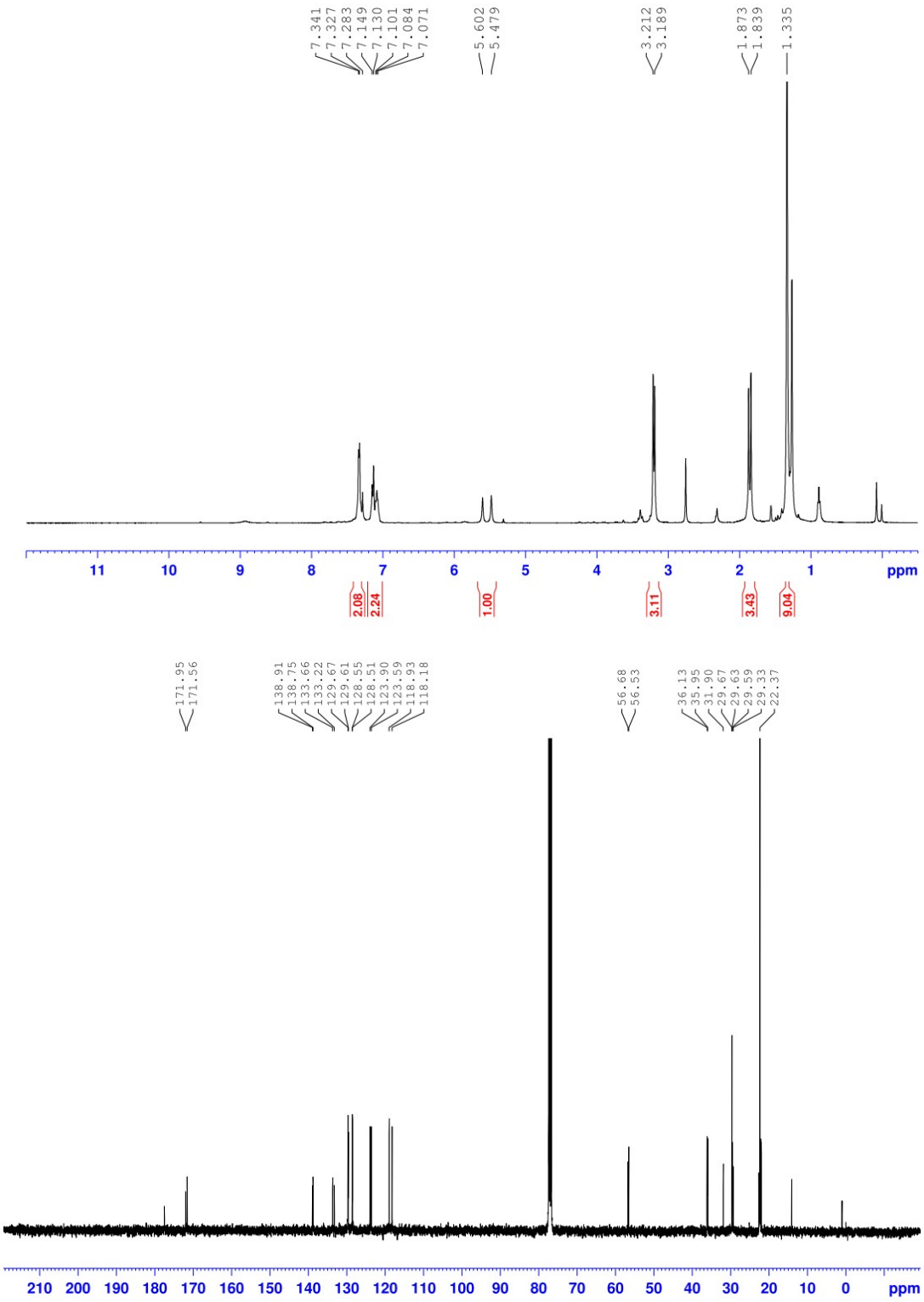


Figure S17. ^{1}H and ^{13}C NMR spectra of **4** in $CDCl_3$.