Supplementary Material

Cu-catalyzed solvent-free, pot-economic synthesis of 1,3-dynes from 1,1-dibromoalkenes in the presence of DBU·H_2O

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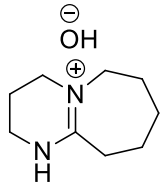
Table of Contents

1. General experimental Methods

All reactions were carried out in oven dried reaction flasks under nitrogen atmosphere and dry solvents and reagents were transferred by oven-dried syringes to ambient temperature. TLC was performed on Merck silica gel aluminium sheets and solvents were removed under reduced pressure. Columns were packed as slurry of silica gel in hexane and ethyl acetate solvent mixture. The elution was assisted by applying pressure with an air pump. ^{13}C NMR spectra were recorded on 101 MHz spectrometers. ^{1}HNMR spectra were recorded on 400 and 500 MHz spectrometers in appropriate solvents using TMS as internal standard. The following abbreviations were used to explain multiplicities: s = singlet, d = doublet, dd = double doublet, t = triplet, m = multiplet. All reactions were performed at room temperature. Reagents were obtained from Aldrich, Alfa Aesar, and TCI used without further purification. All compounds are characterized by ^{1}HNMR and ^{13}CNMR. Additionally, unknown compounds are characterized by HRMS analysis. All known compounds data are in consistent with the given literature report.

2. General procedure for the preparation of DBU·H_2O

The DBU [with 0.2% water content (KF)] was purchased from commercial source (spectrochem) and used as such without further purification. Freshly prepared hydrated DBU (DBU.H_2O) was used in all reactions. About 1 equivalent of H_2O was mixed with DBU to get hydrated DBU (DBU.H_2O). Water (HPLC grade) purchased from commercial sources were directly used without any further purification.



5. ^{1}H, ^{13}C NMR spectra

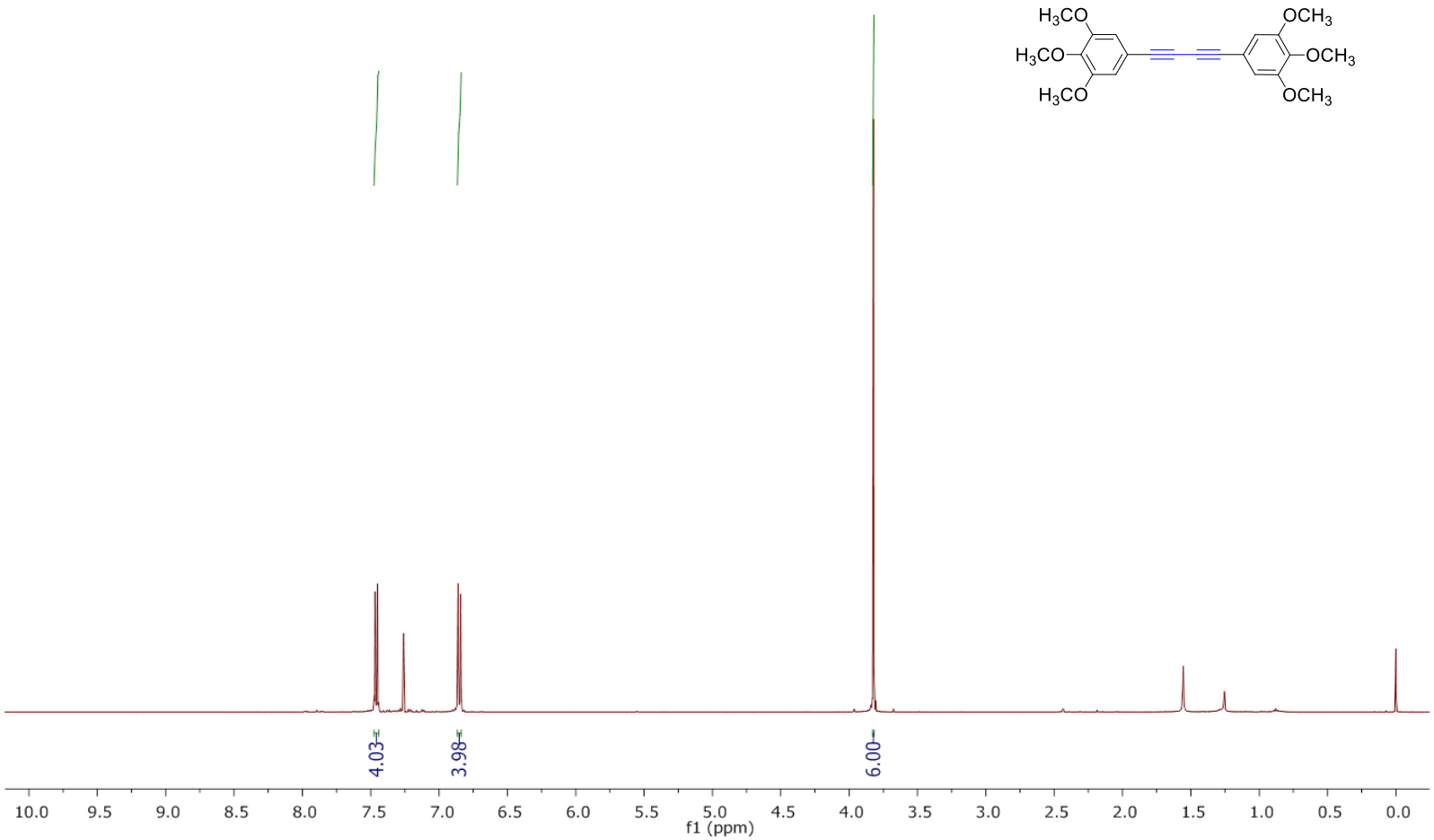


Fig. 1. ^{1}H-NMR-spectrum of compound **2a**[1] (400 MHz, $CDCl_3$, 298K)

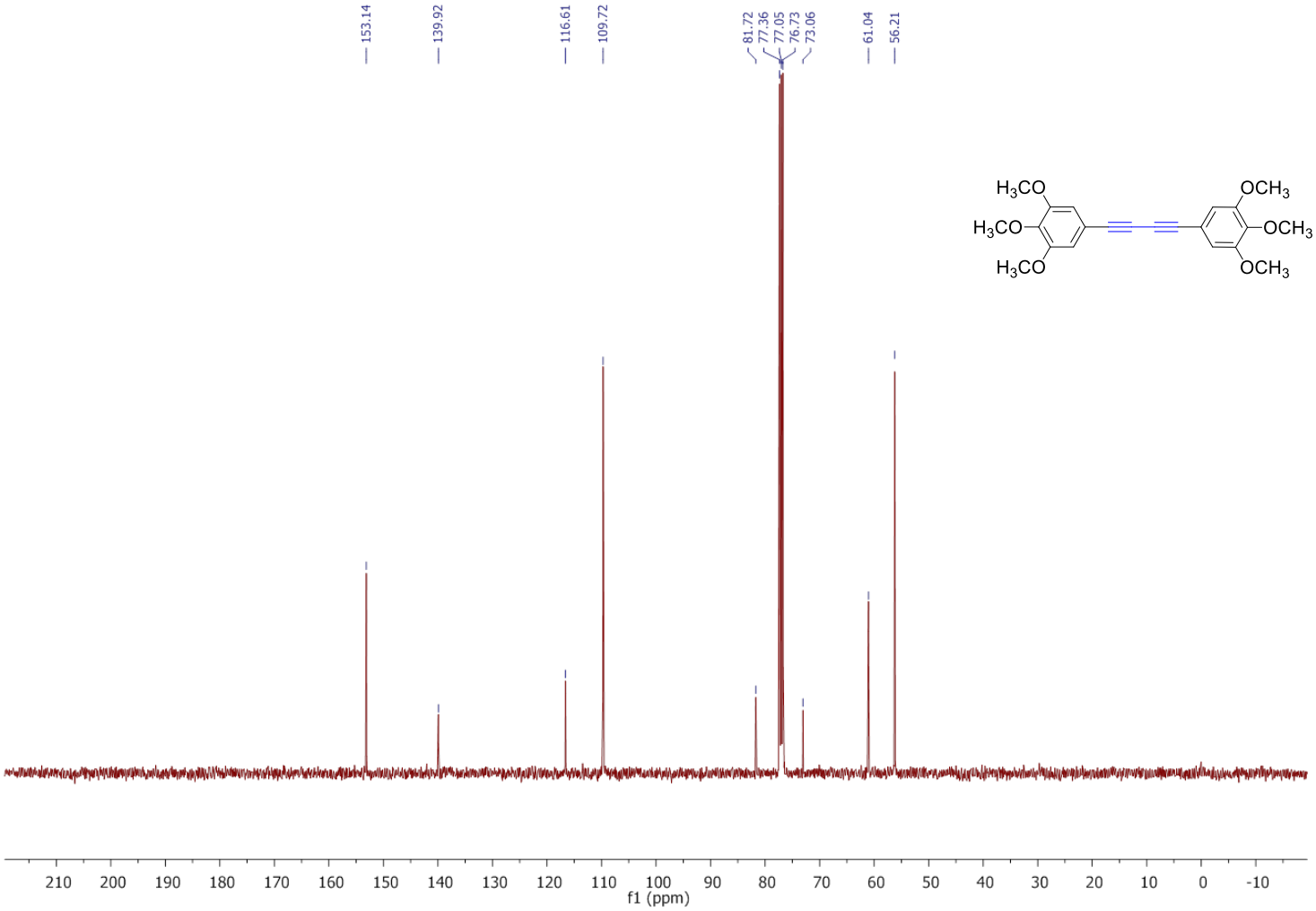


Fig. 2. ^{13}C-NMR-spectrum of compound **2a**[1](101 MHz, $CDCl_3$, 298K)

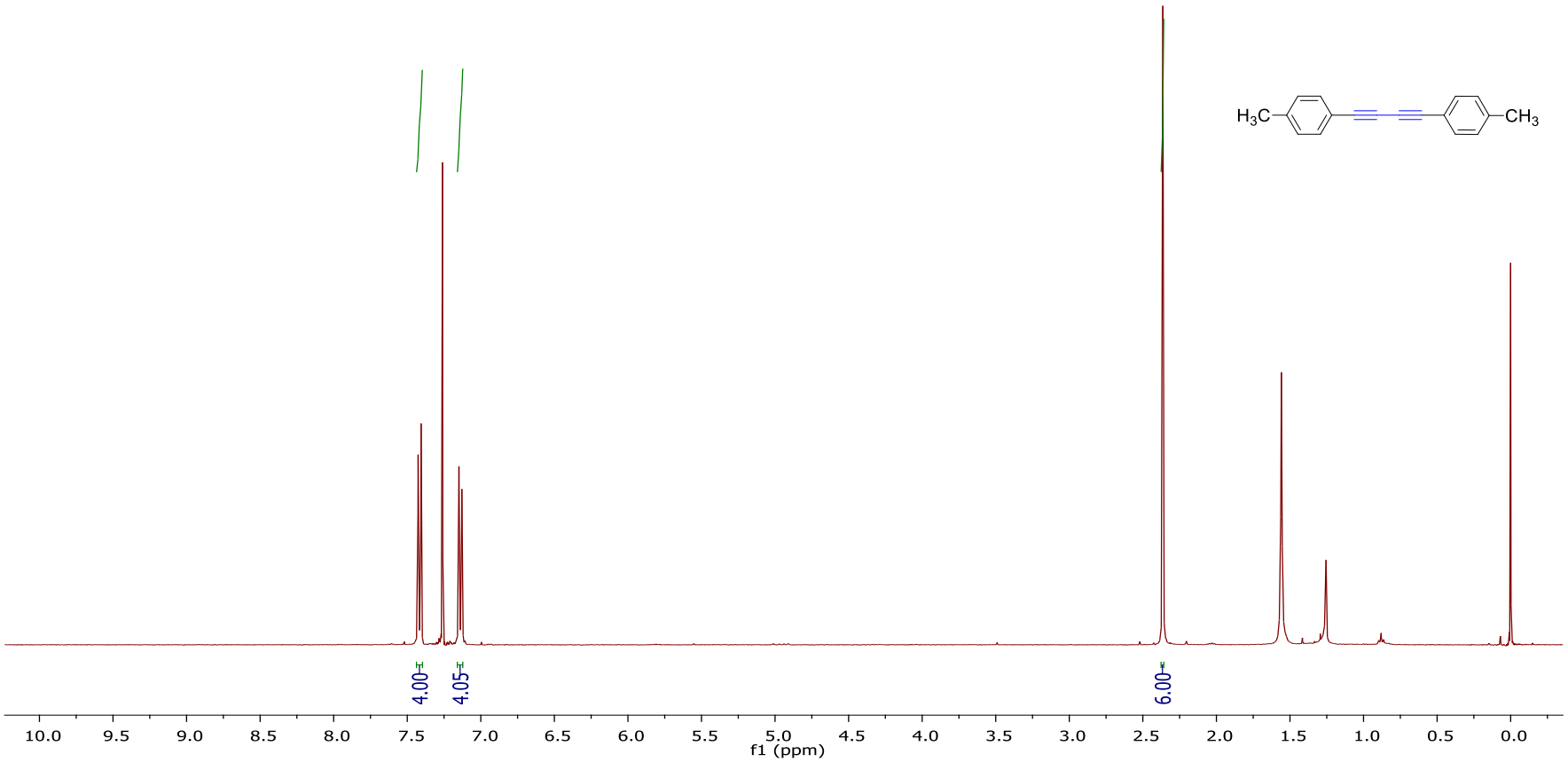


Fig. 3. ^{1}H-NMR-spectrum of compound **2b**[1] (400 MHz, $CDCl_3$, 298K)

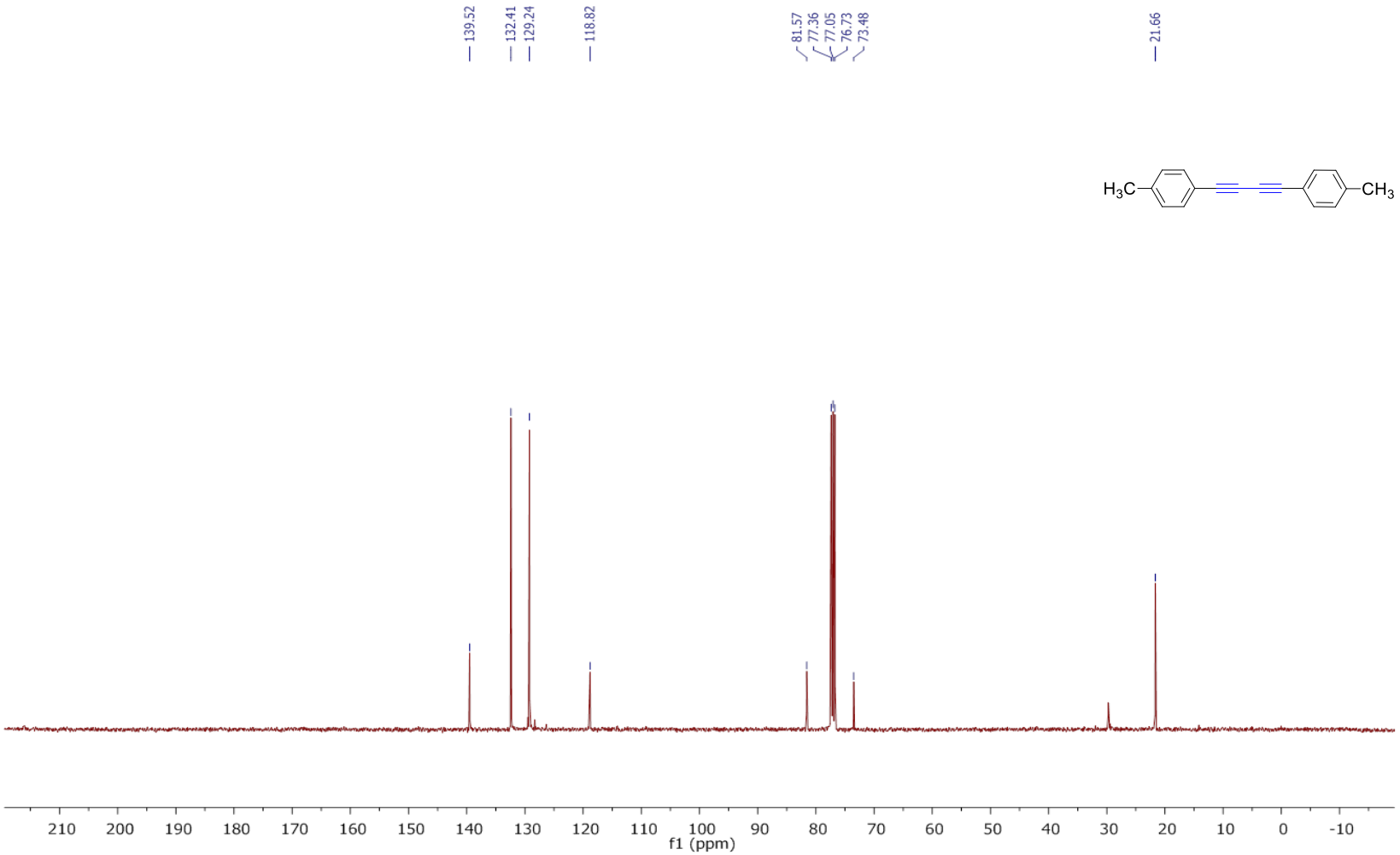
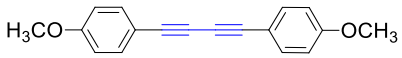


Fig. 4. ^{13}C-NMR-spectrum of compound **2b**[1] (101 MHz, $CDCl_3$, 298K)



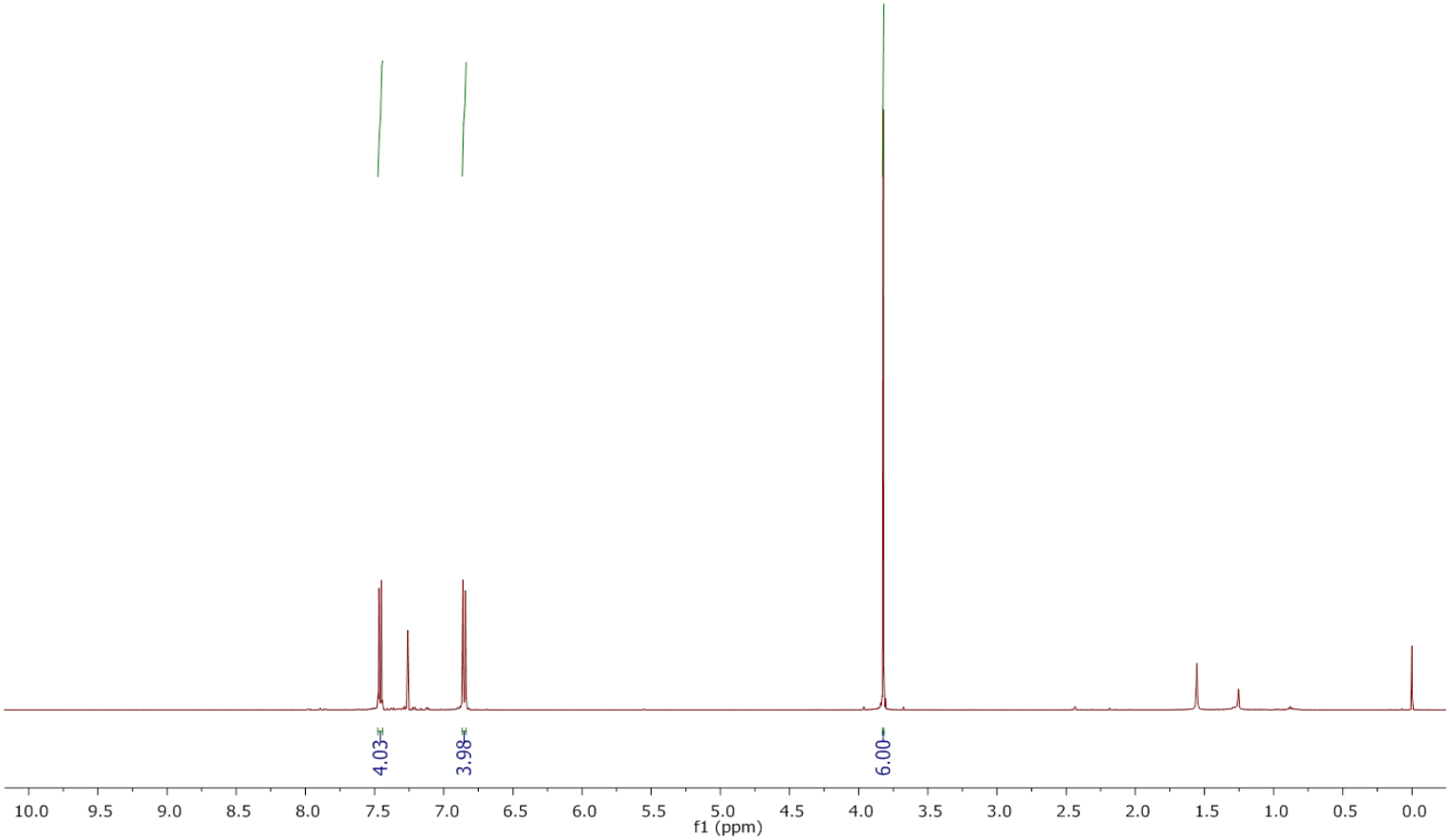


Fig. 5. ^{1}H-NMR-spectrum of compound **2c**[1](500 MHz, $CDCl_3$, 298K)

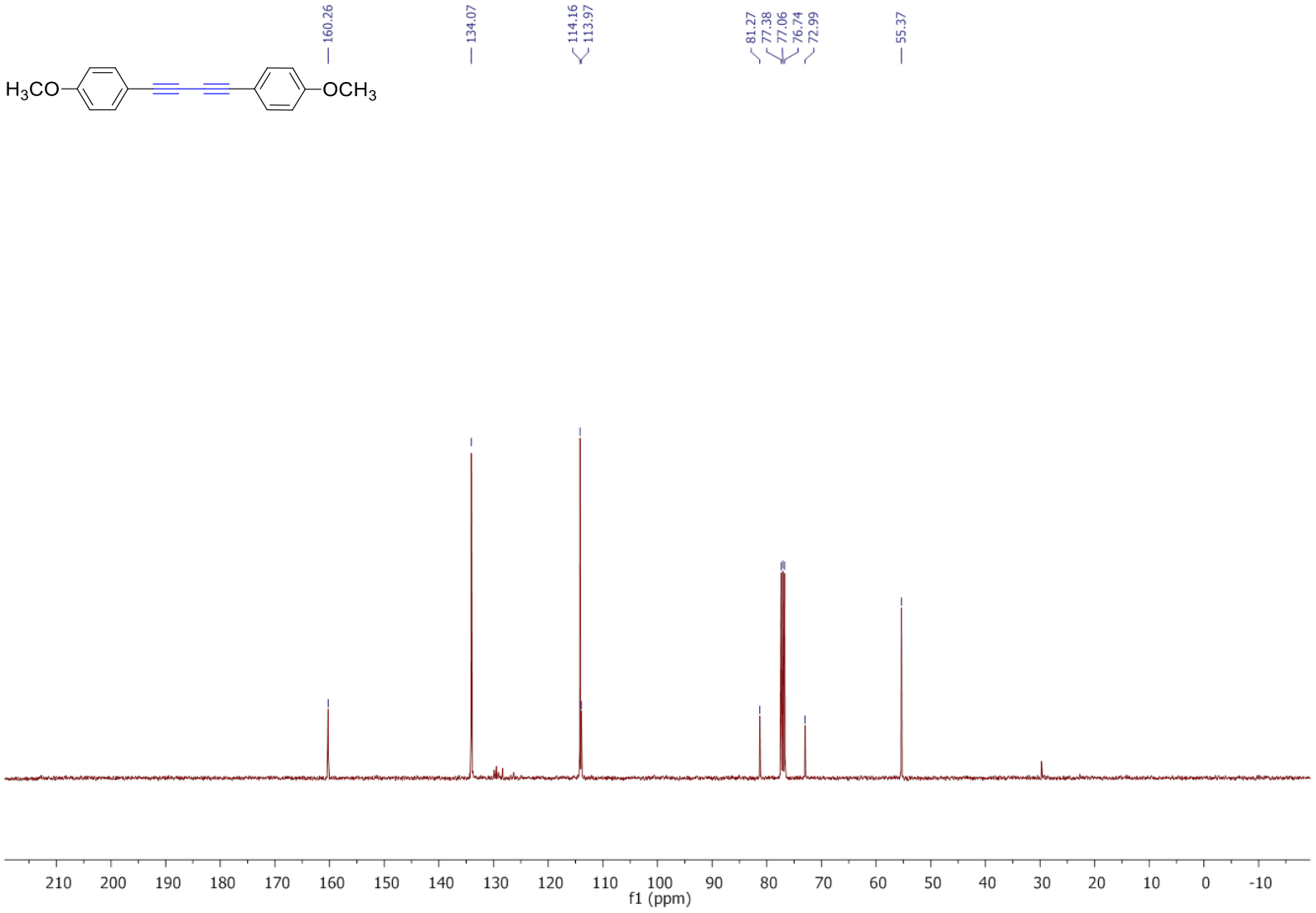


Fig. 6. ^{13}C-NMR-spectrum of compound **2c**[1] (101 MHz, $CDCl_3$, 298K)

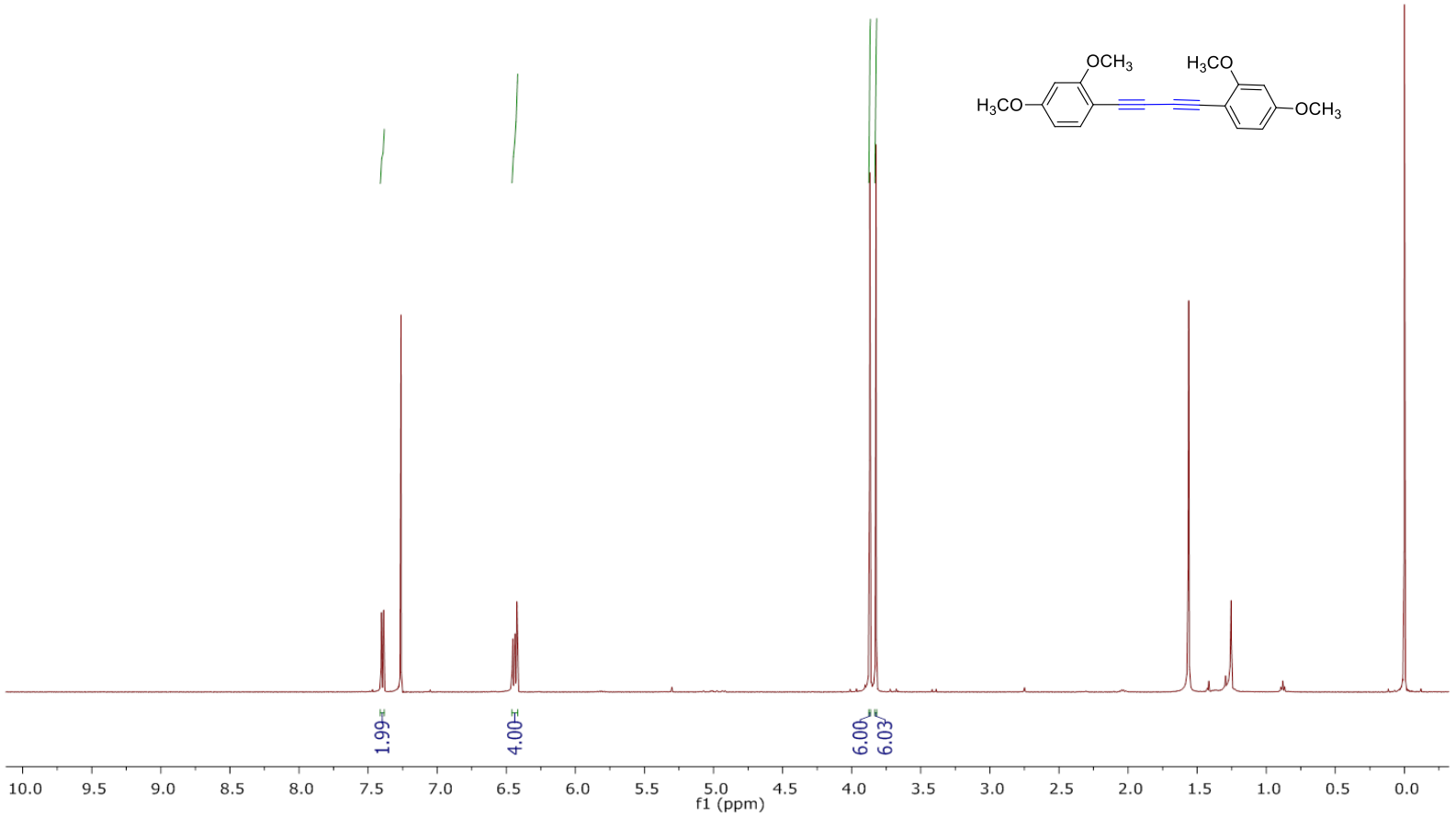


Fig. 7. ^{1}H-NMR-spectrum of compound **2d** (400 MHz, $CDCl_3$, 298K)

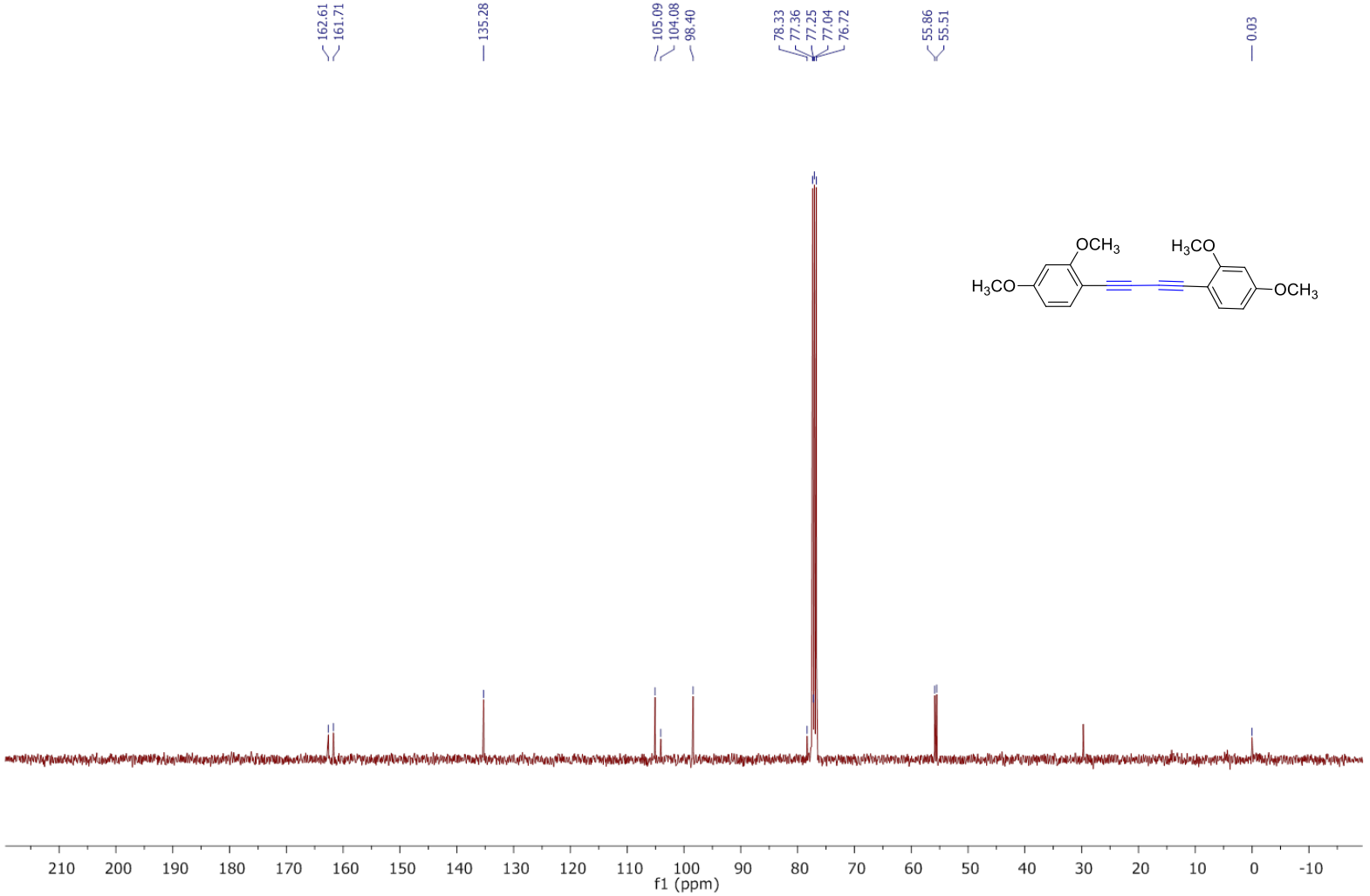


Fig. 8. ^{13}C-NMR-spectrum of compound **2d** (101 MHz, $CDCl_3$, 298K)

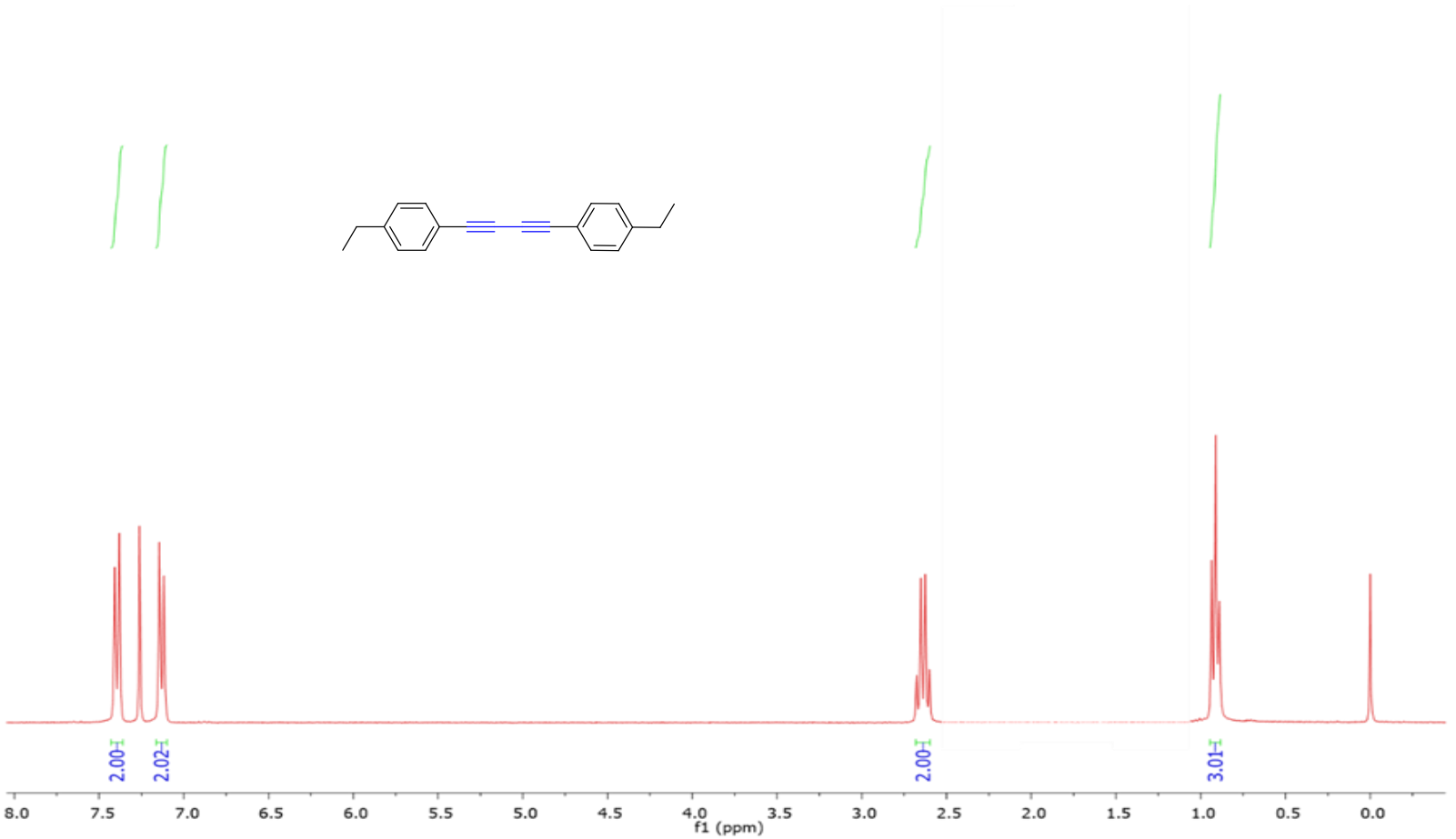


Fig. 9. ^{1}H-NMR-spectrum of compound **2e** (500 MHz, $CDCl_3$, 298K)

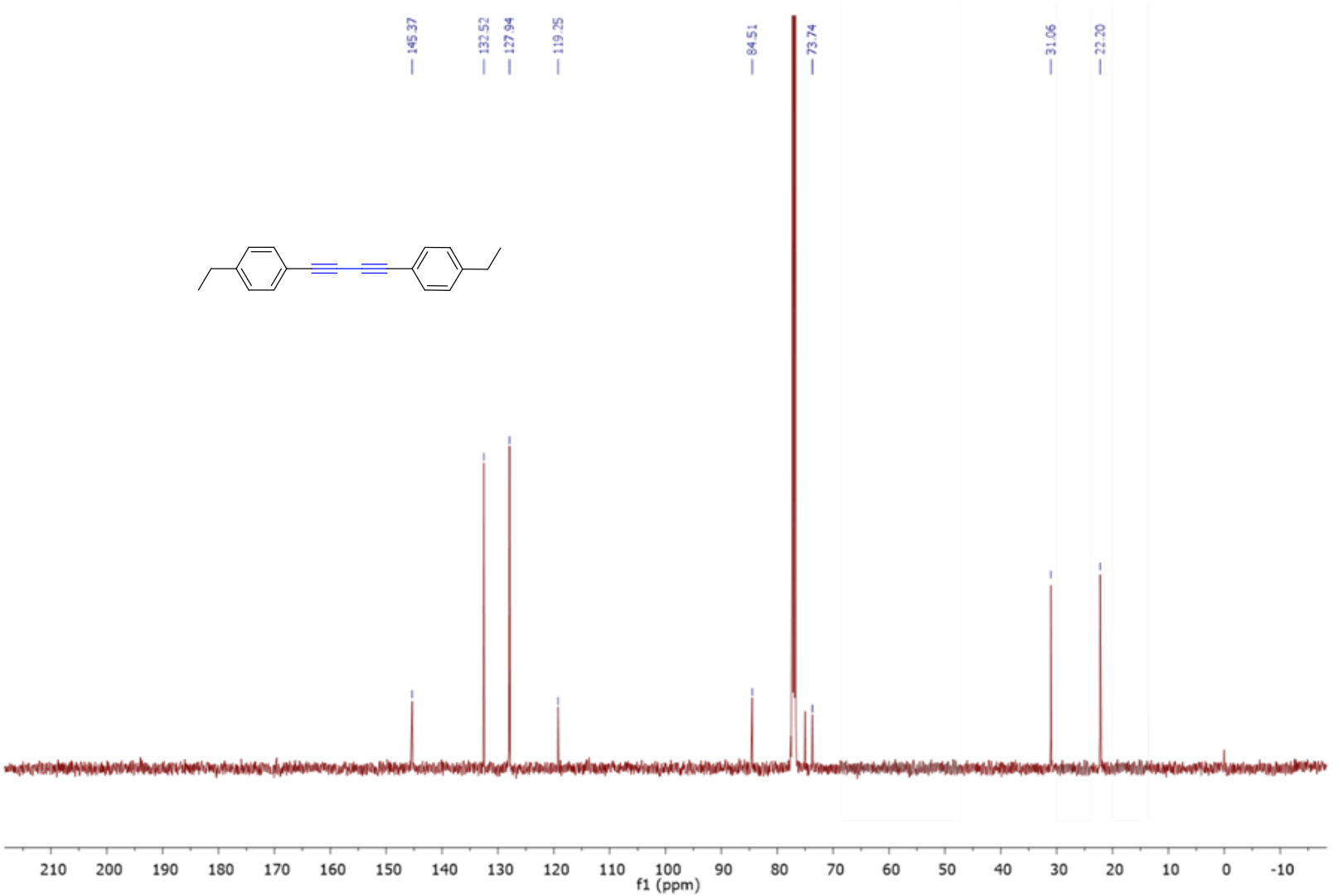


Fig. 10. ^{13}C-NMR-spectrum of compound **2e** (101 MHz, $CDCl_3$, 298K)

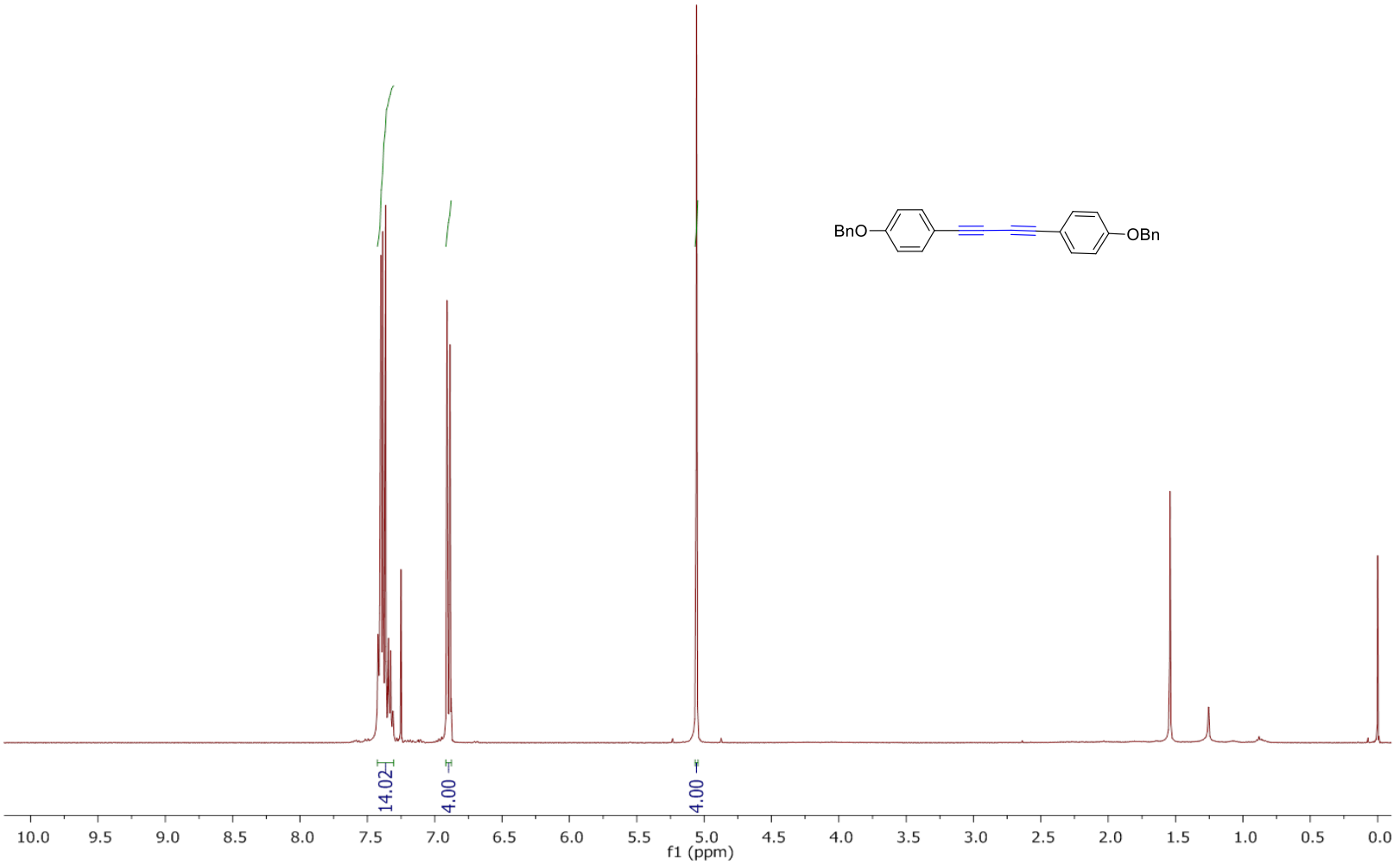


Fig. 11. ^{1}H-NMR-spectrum of compound **2f**[1](400 MHz, $CDCl_3$, 298K)

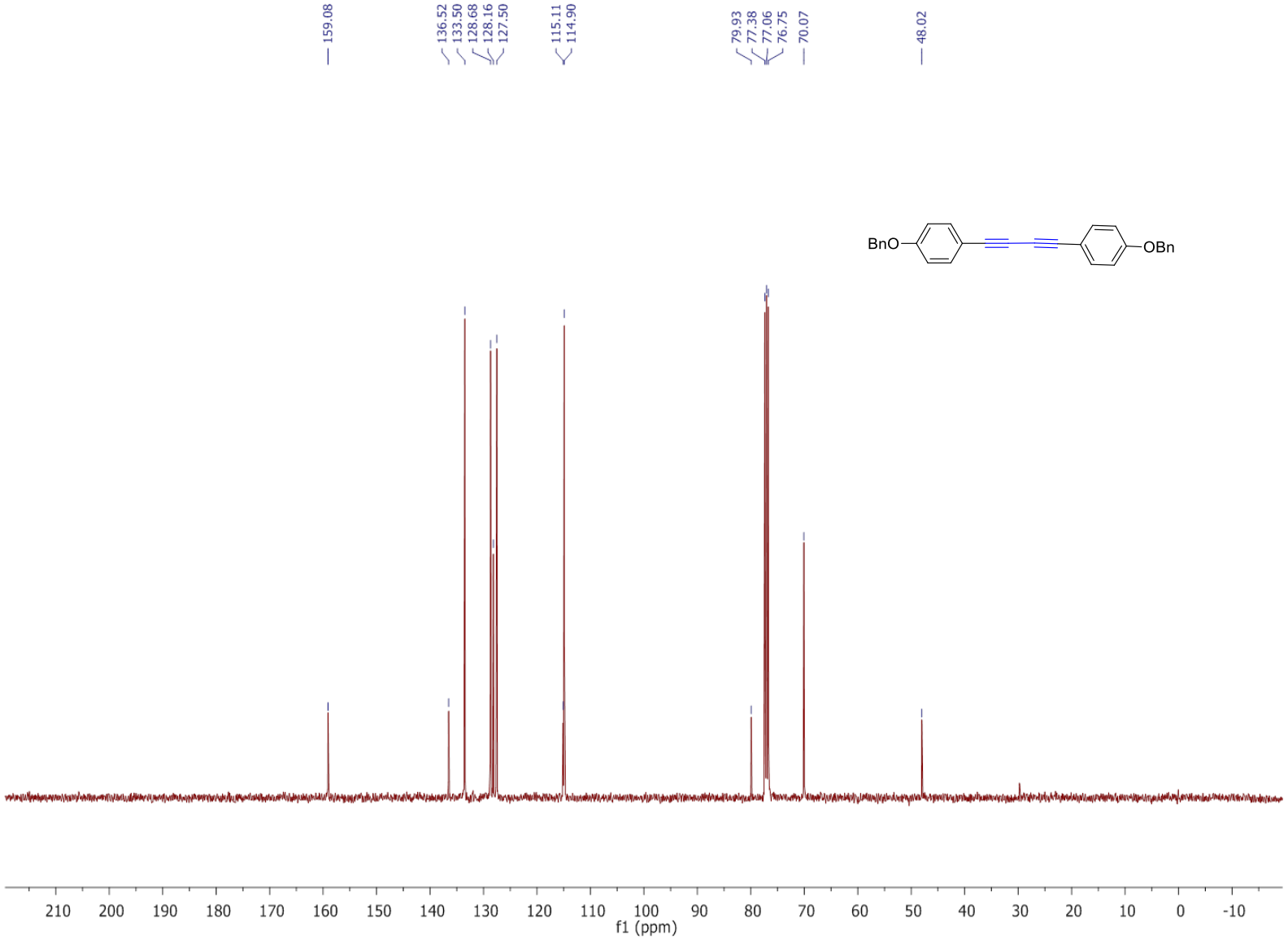


Fig. 12. ^{13}C-NMR-spectrum of compound **2f**[1](101 MHz, $CDCl_3$, 298K)

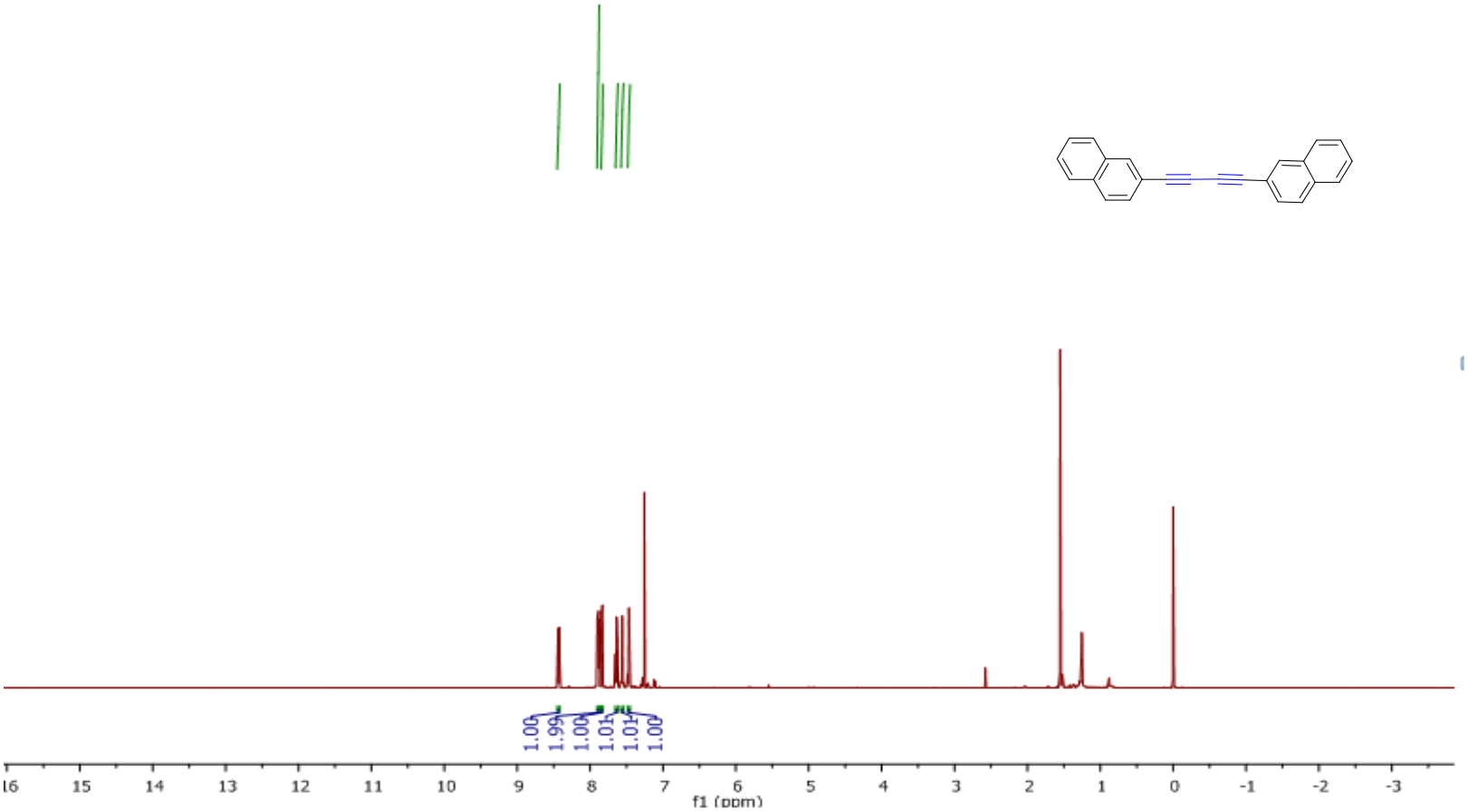


Fig. 13. ^{1}H-NMR-spectrum of compound **2g**[1] (500 MHz, $CDCl_3$, 298K)

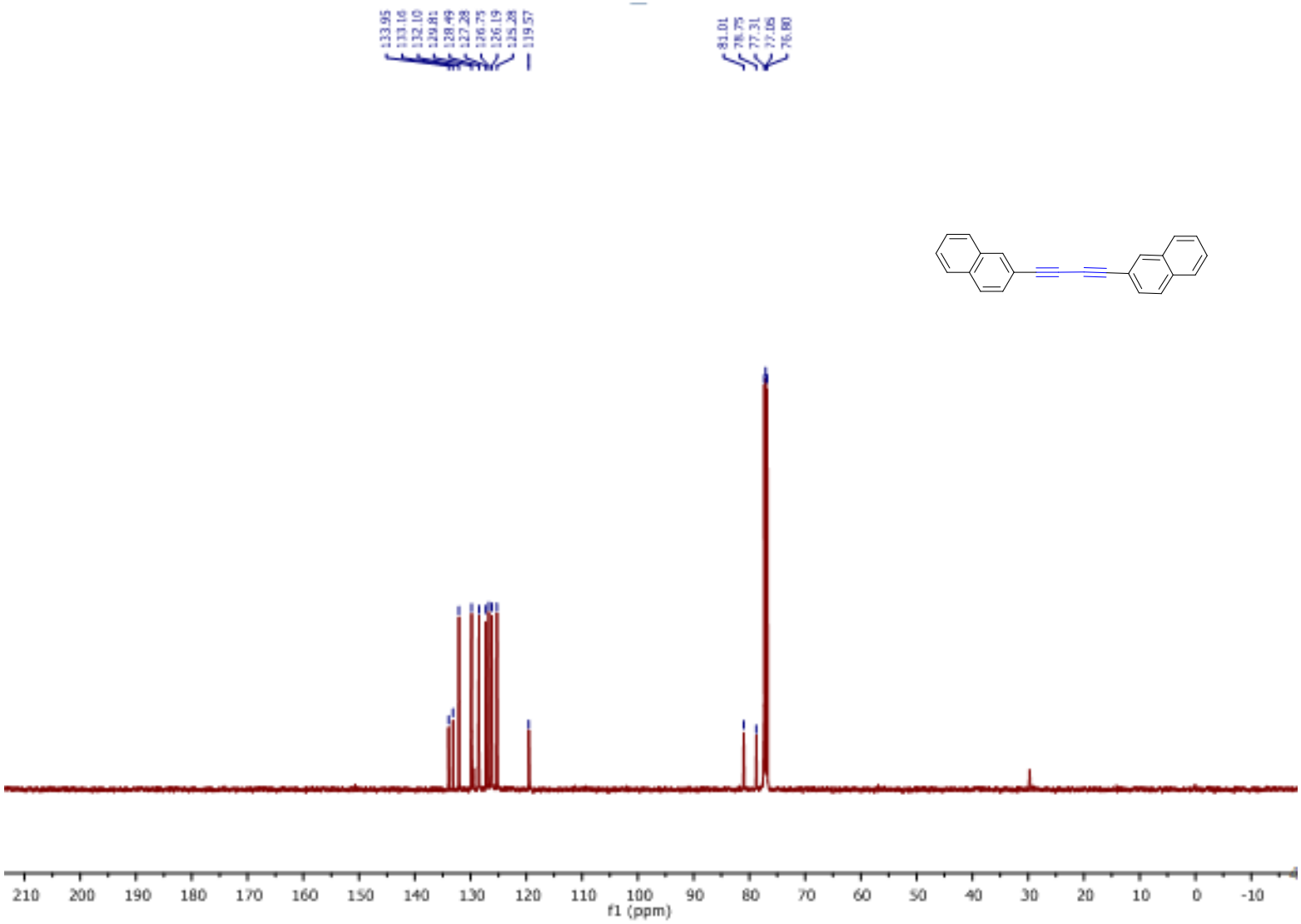


Fig. 14. ^{13}C-NMR-spectrum of compound **2g**[1] (101 MHz, $CDCl_3$, 298K)

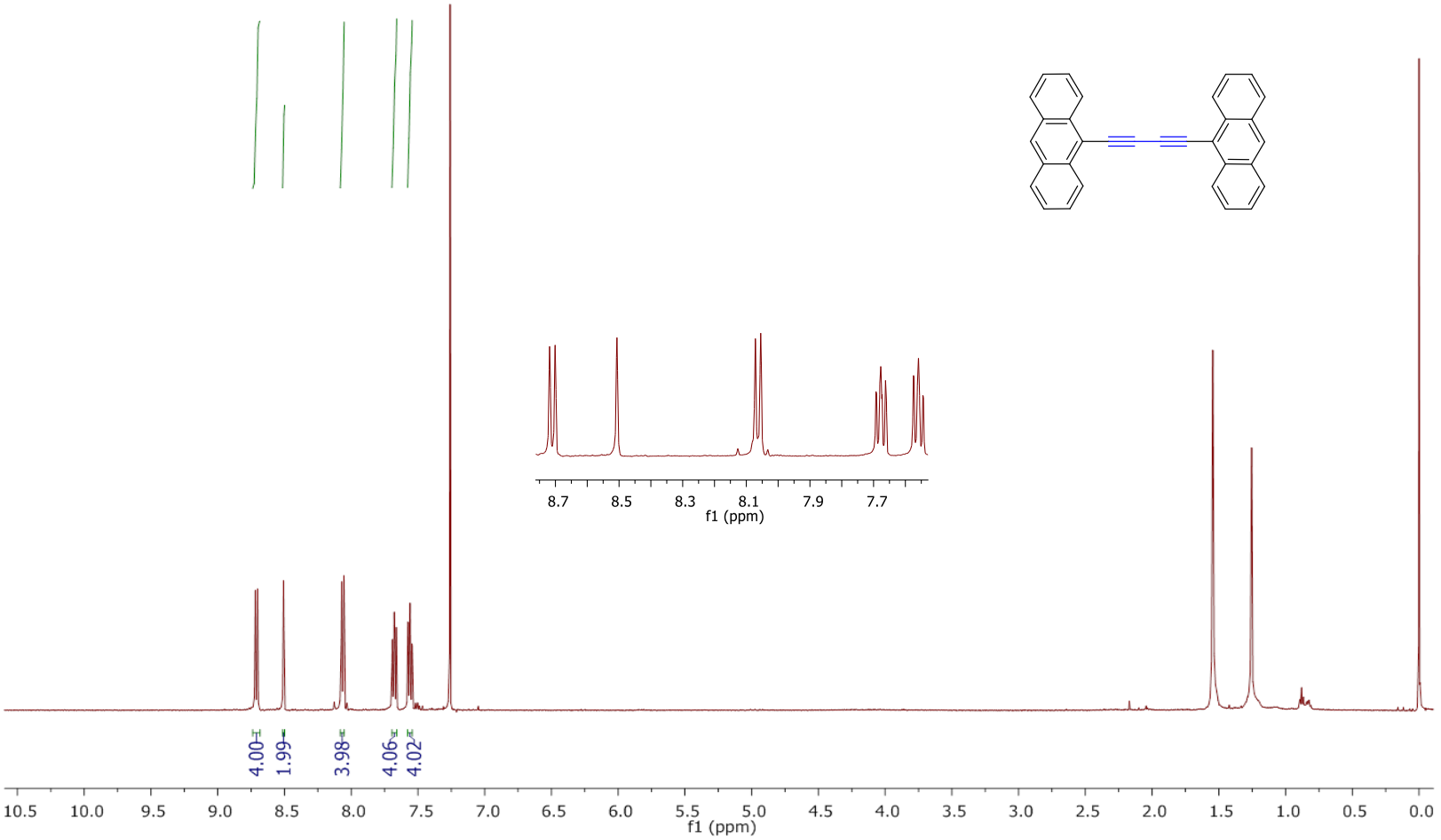


Fig. 15. ^{1}H-NMR-spectrum of compound **2h** (500 MHz, $CDCl_3$, 298K)

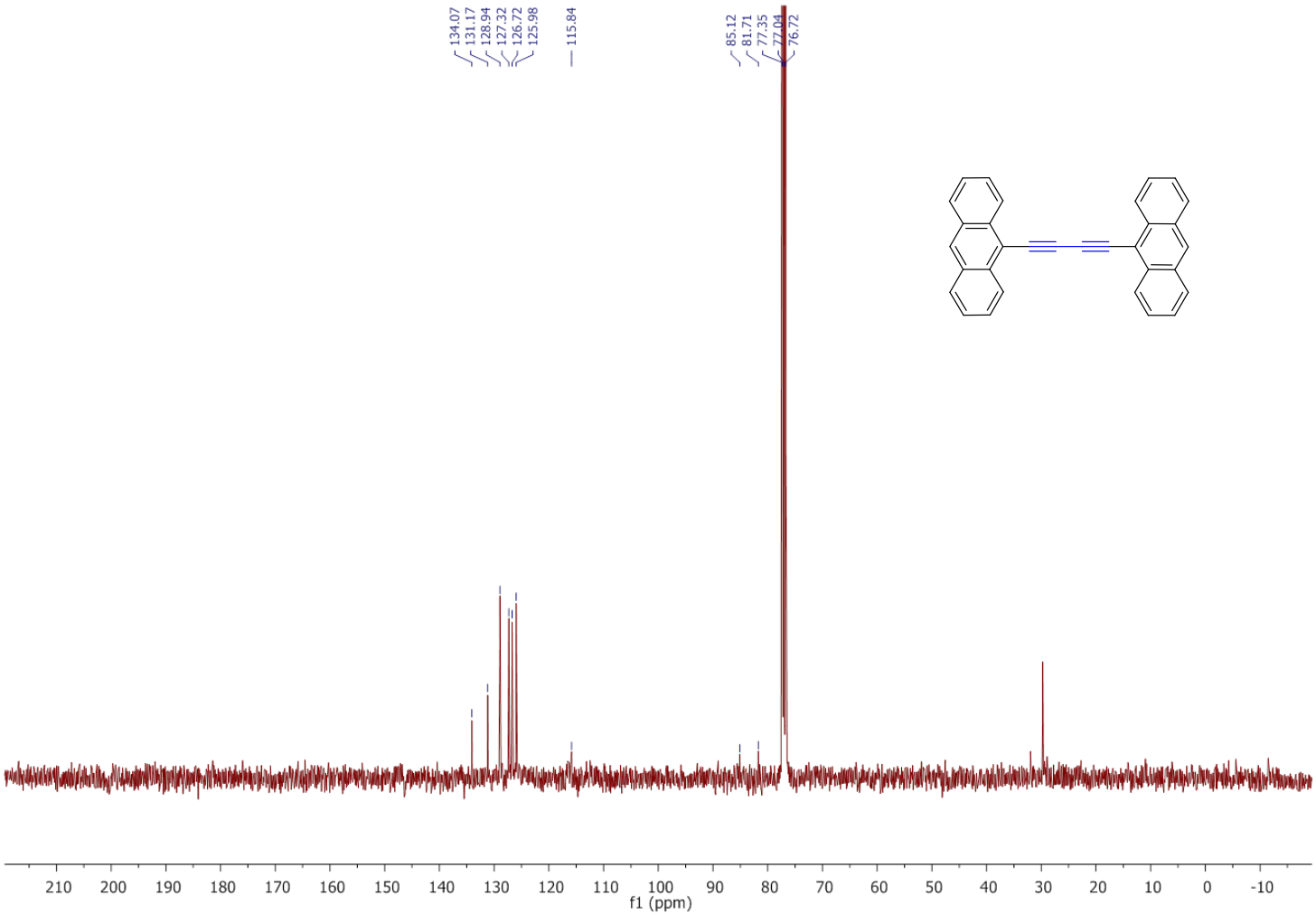


Fig. 16. ^{13}C-NMR-spectrum of compound **2h** (101 MHz, $CDCl_3$, 298K)

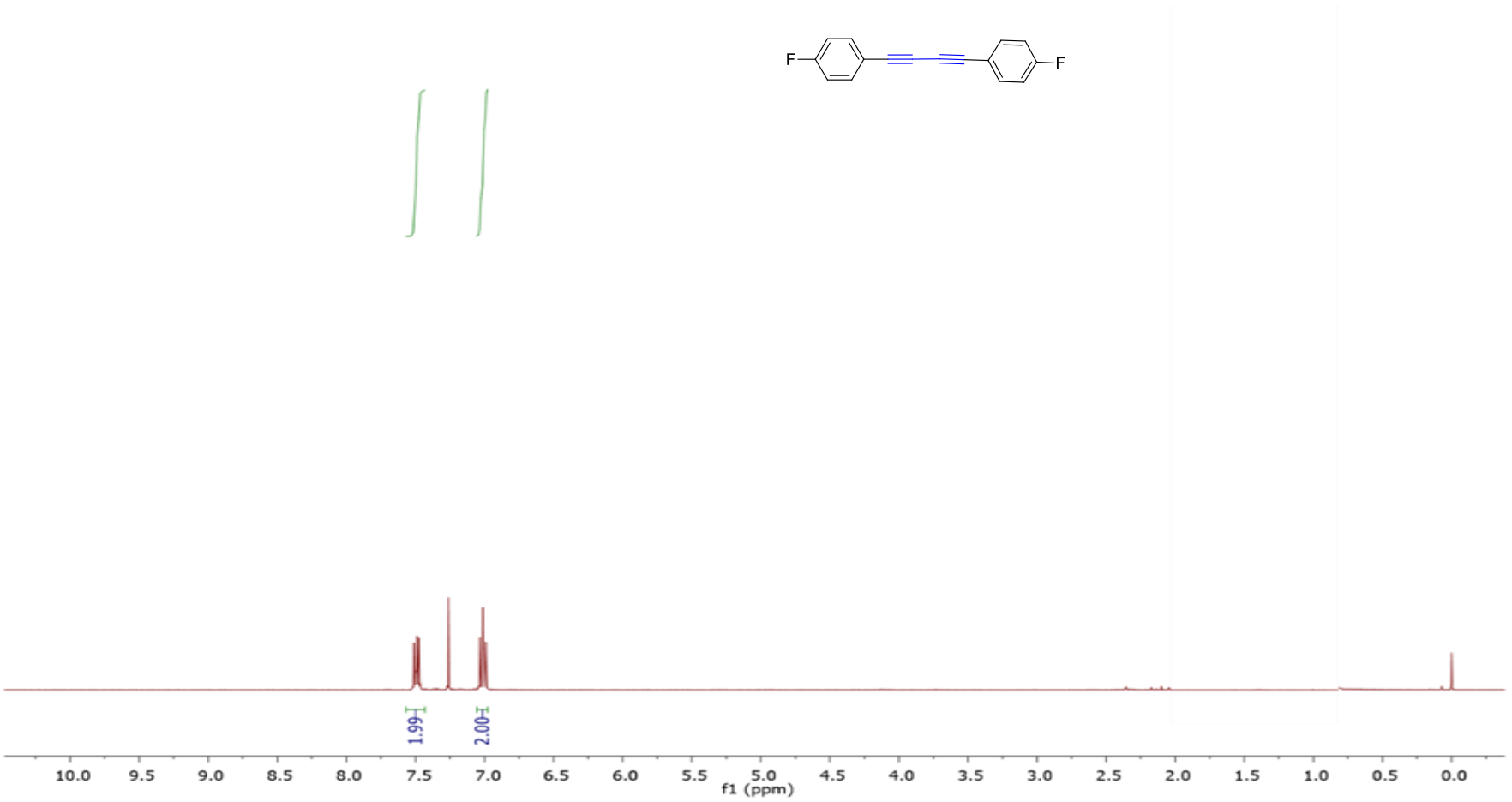


Fig. 17. ^{1}H-NMR-spectrum of compound **2i** (500 MHz, $CDCl_3$, 298K)

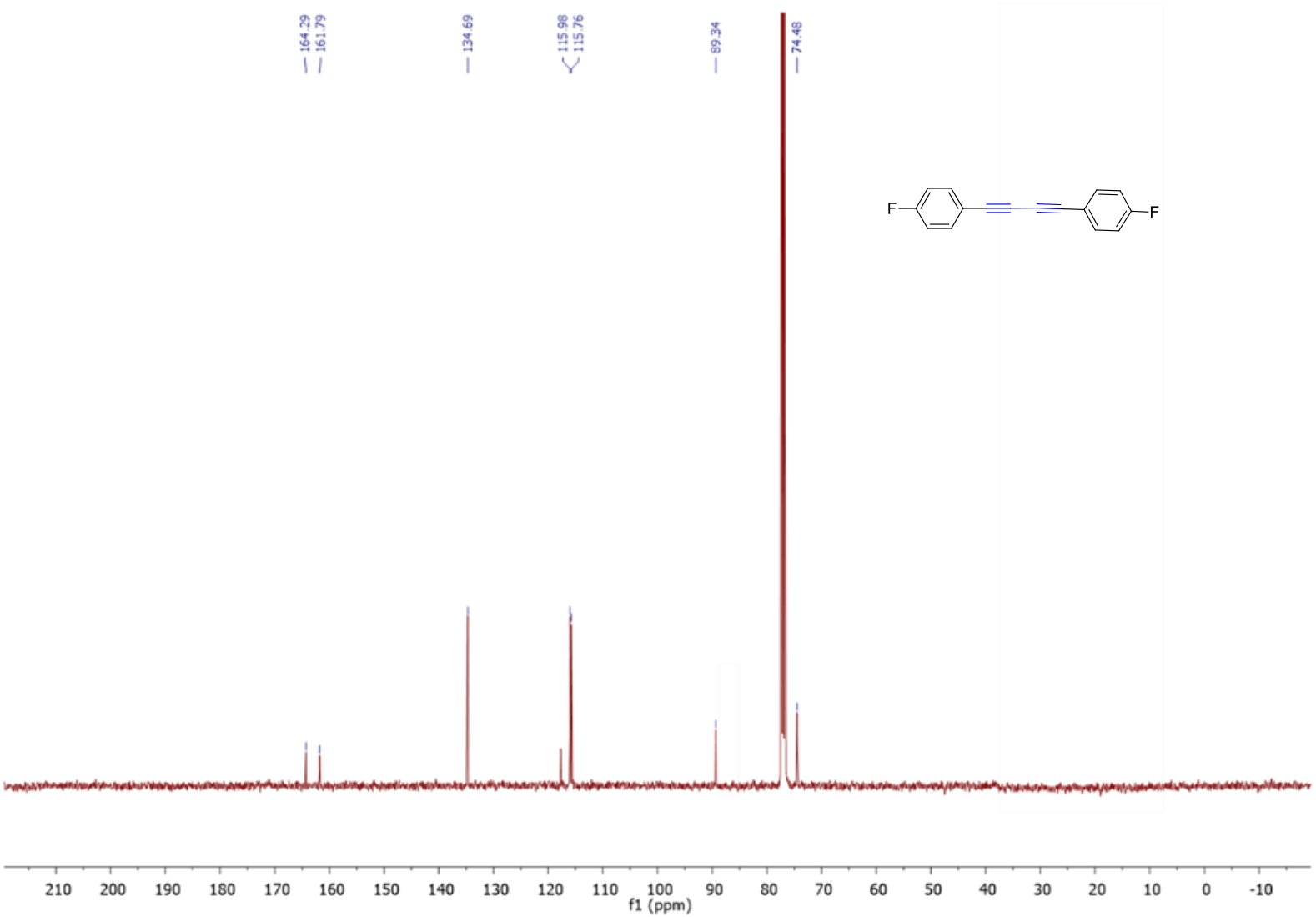


Fig. 18. ^{13}C-NMR-spectrum of compound **2i** (101 MHz, $CDCl_3$, 298K)

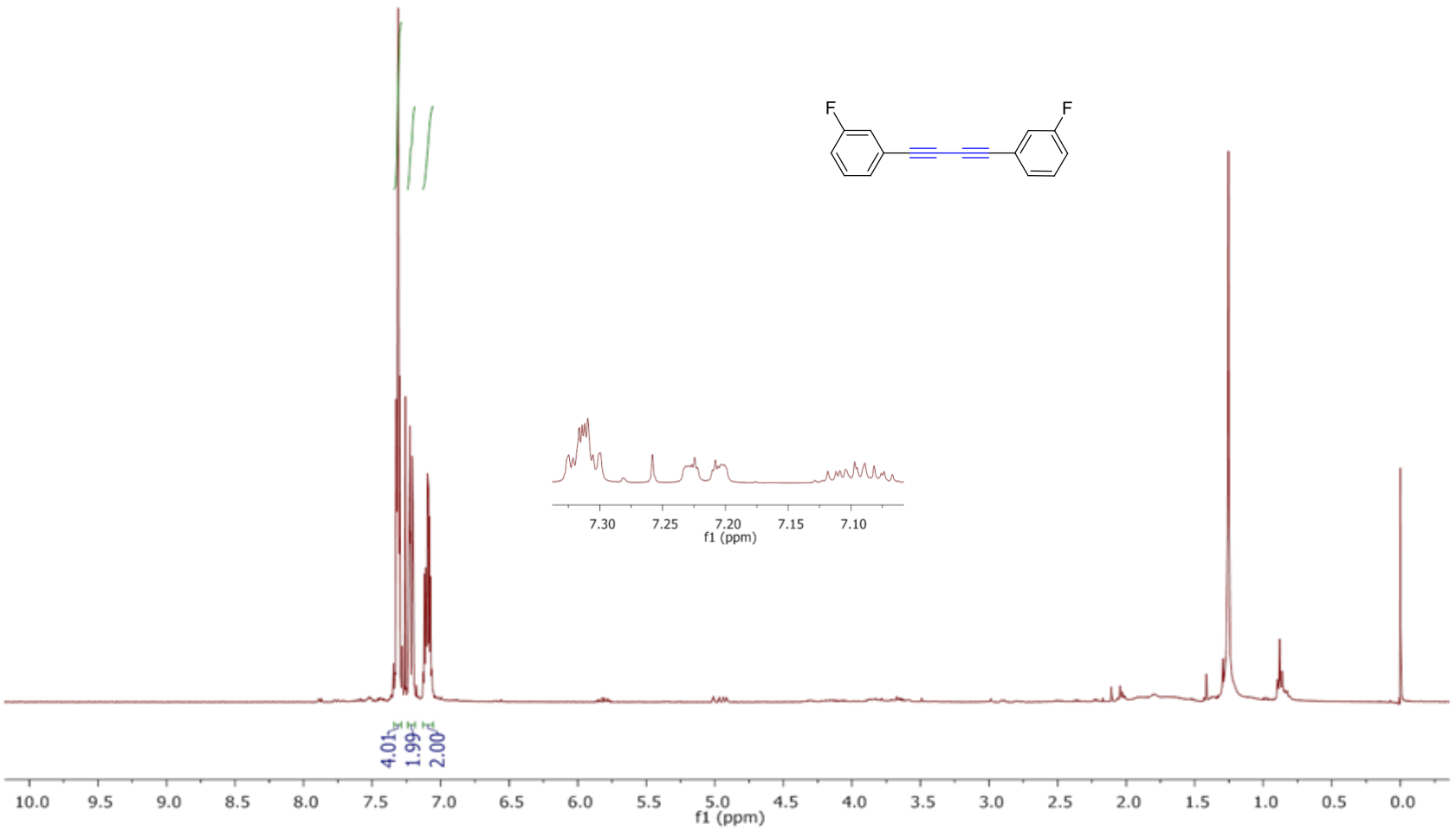


Fig. 19. ^{1}H-NMR-spectrum of compound **2j** (400 MHz, $CDCl_3$, 298K)

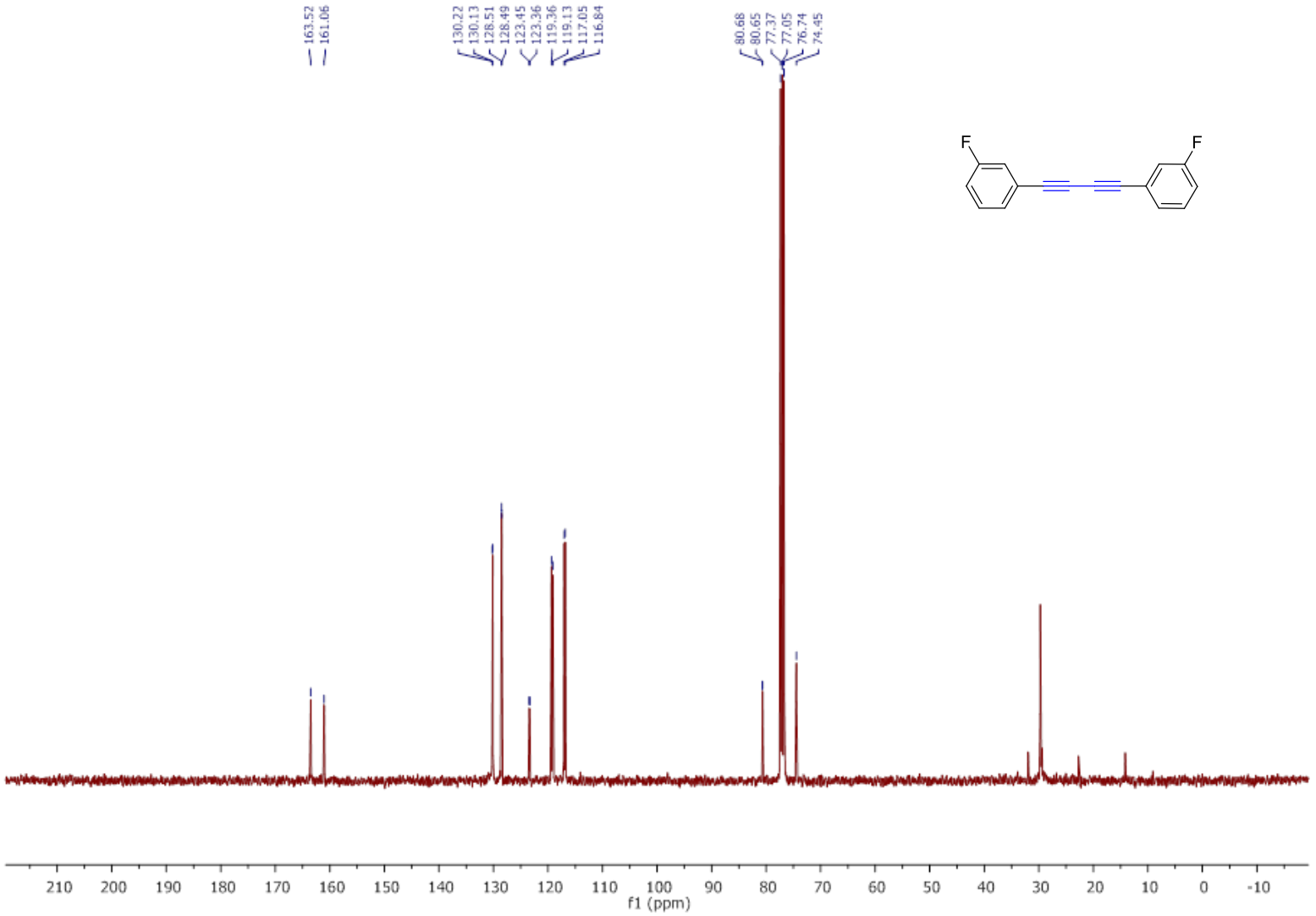


Fig. 20. ^{13}C-NMR-spectrum of compound **2j** (101 MHz, $CDCl_3$, 298K)

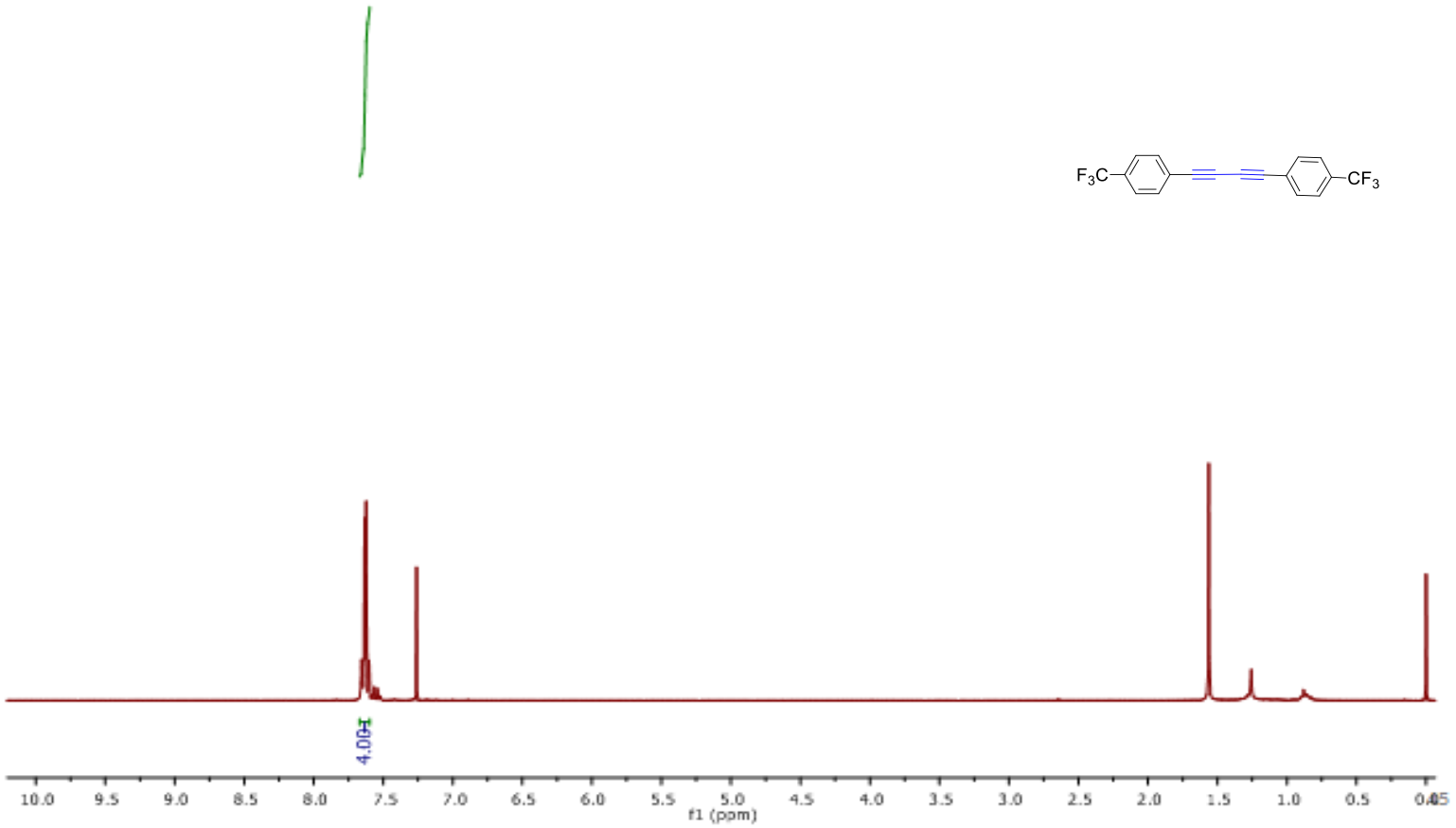


Fig. 21. ^{1}H-NMR-spectrum of compound **2k** (400 MHz, $CDCl_3$, 298K)

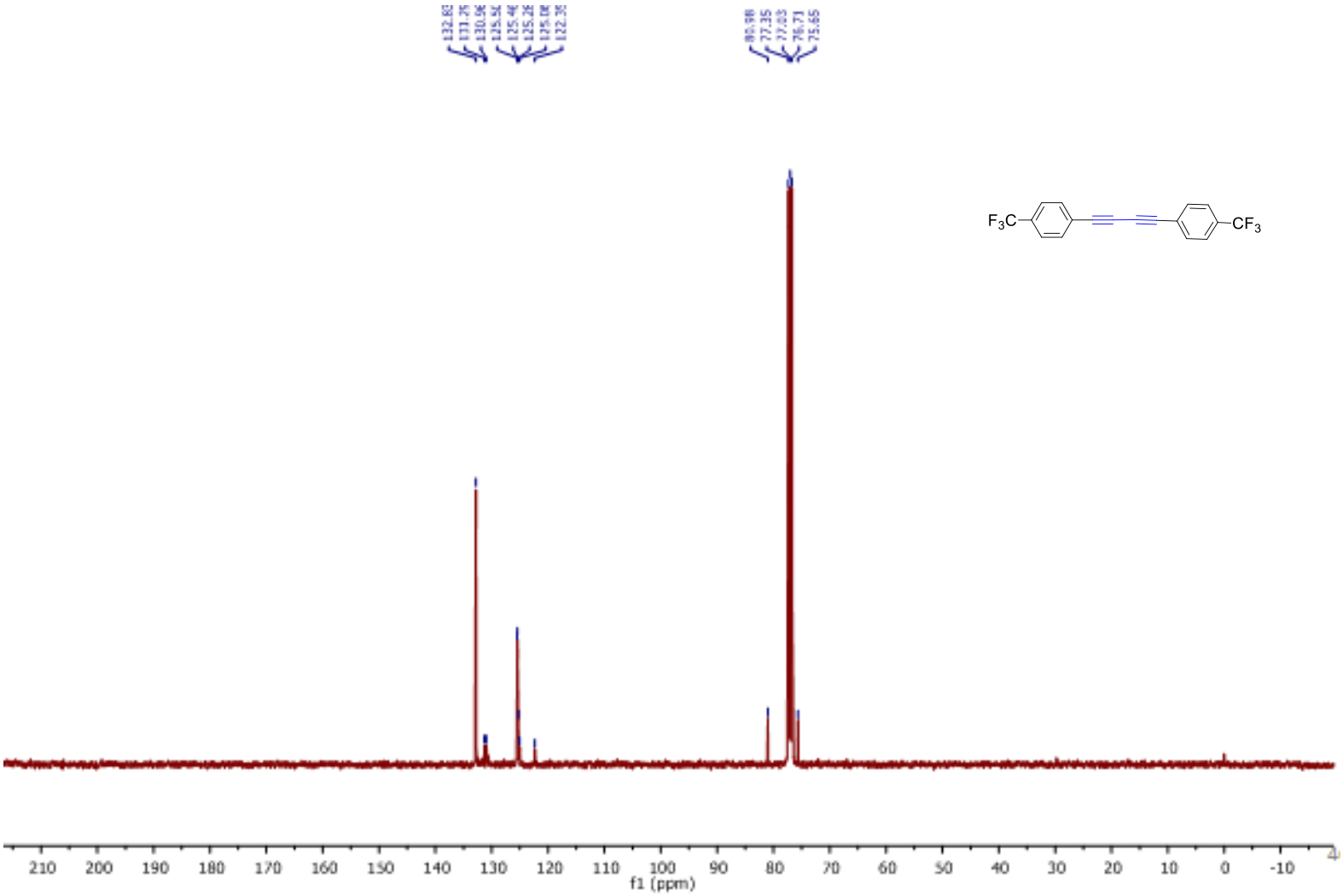


Fig. 22. ^{13}C-NMR-spectrum of compound **2k** (101 MHz, $CDCl_3$, 298K)

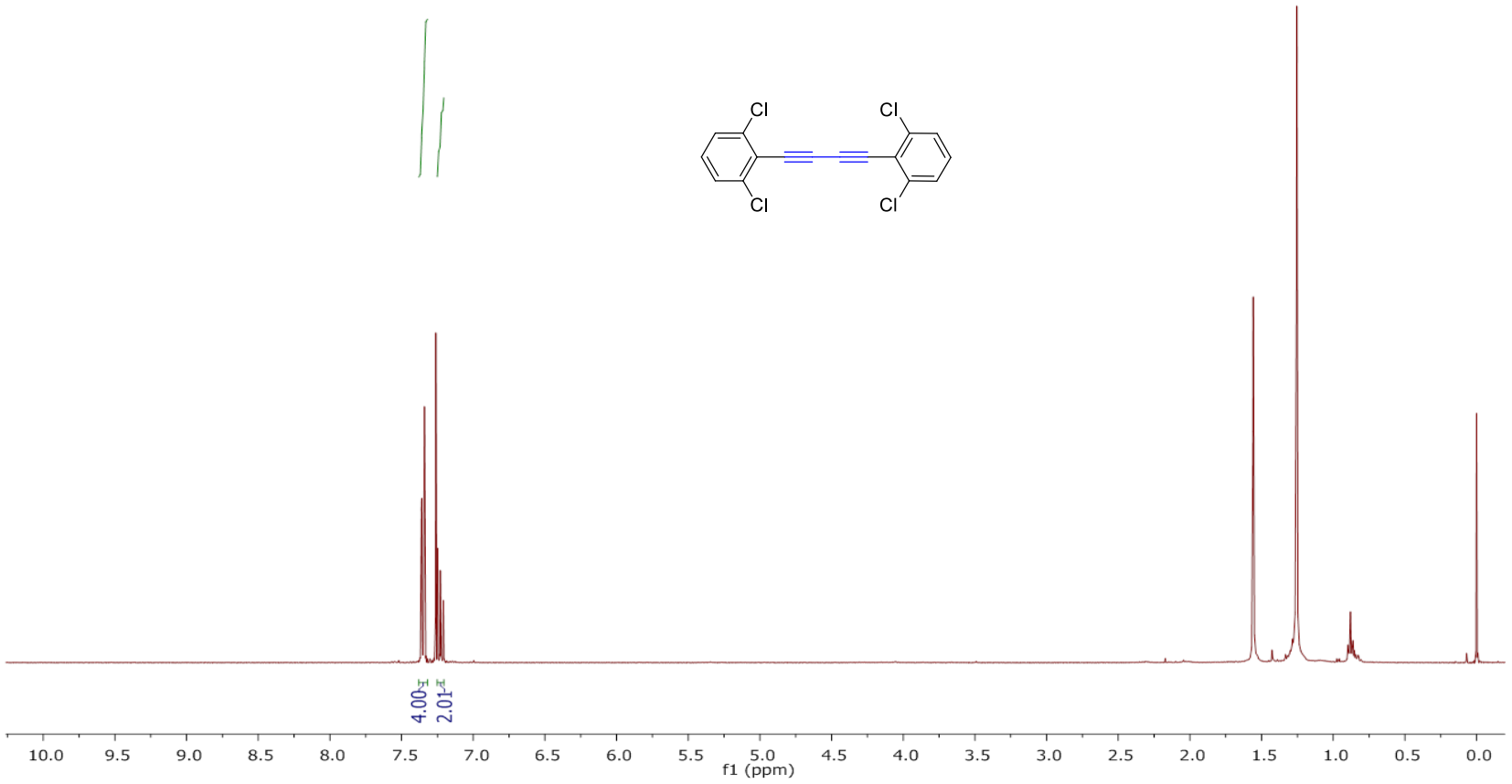


Fig. 23. ^{1}H-NMR-spectrum of compound **2l** (400 MHz, $CDCl_3$, 298K)

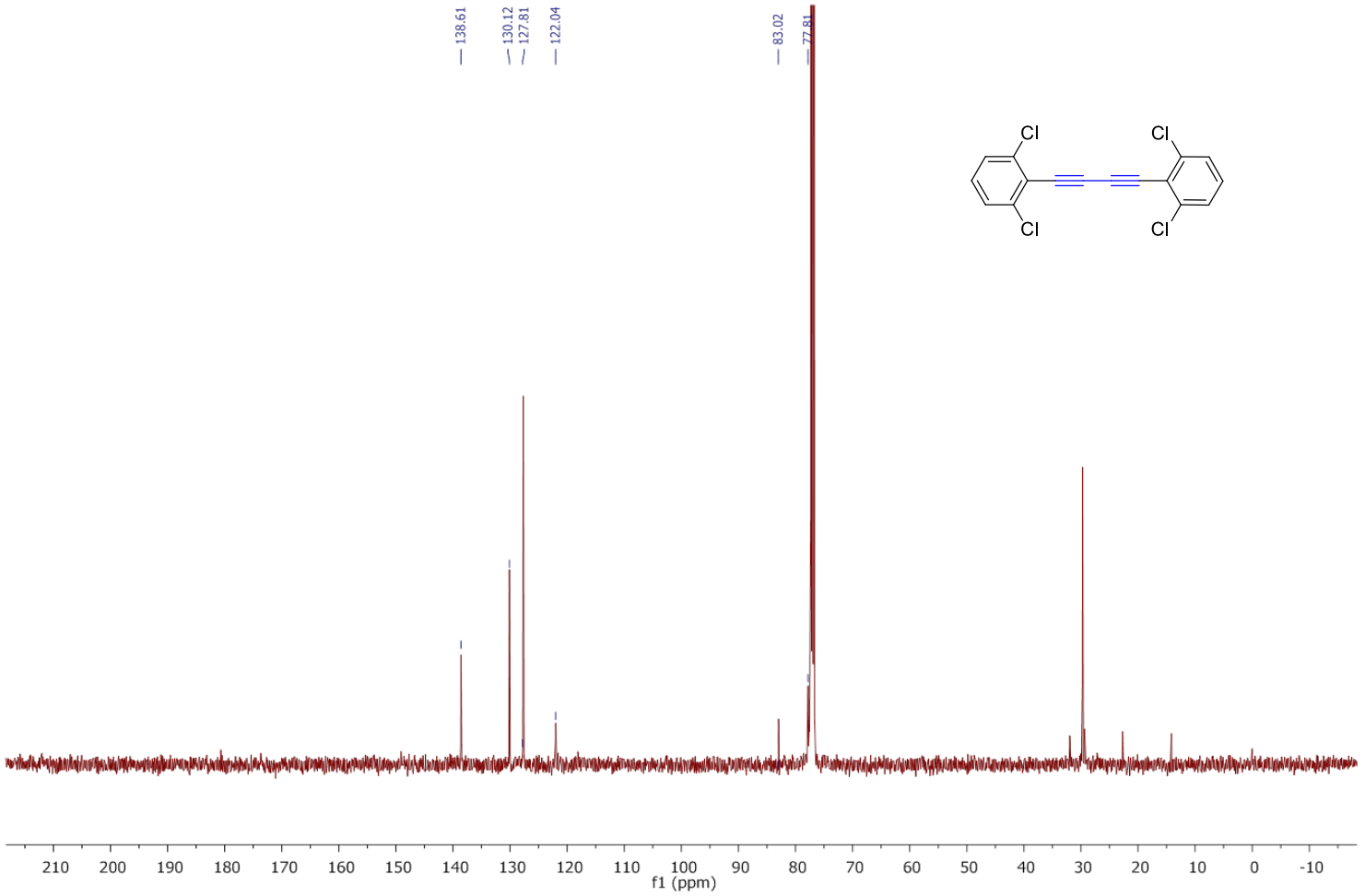


Fig. 24. ^{13}C-NMR-spectrum of compound **2l** (101 MHz, $CDCl_3$, 298K)

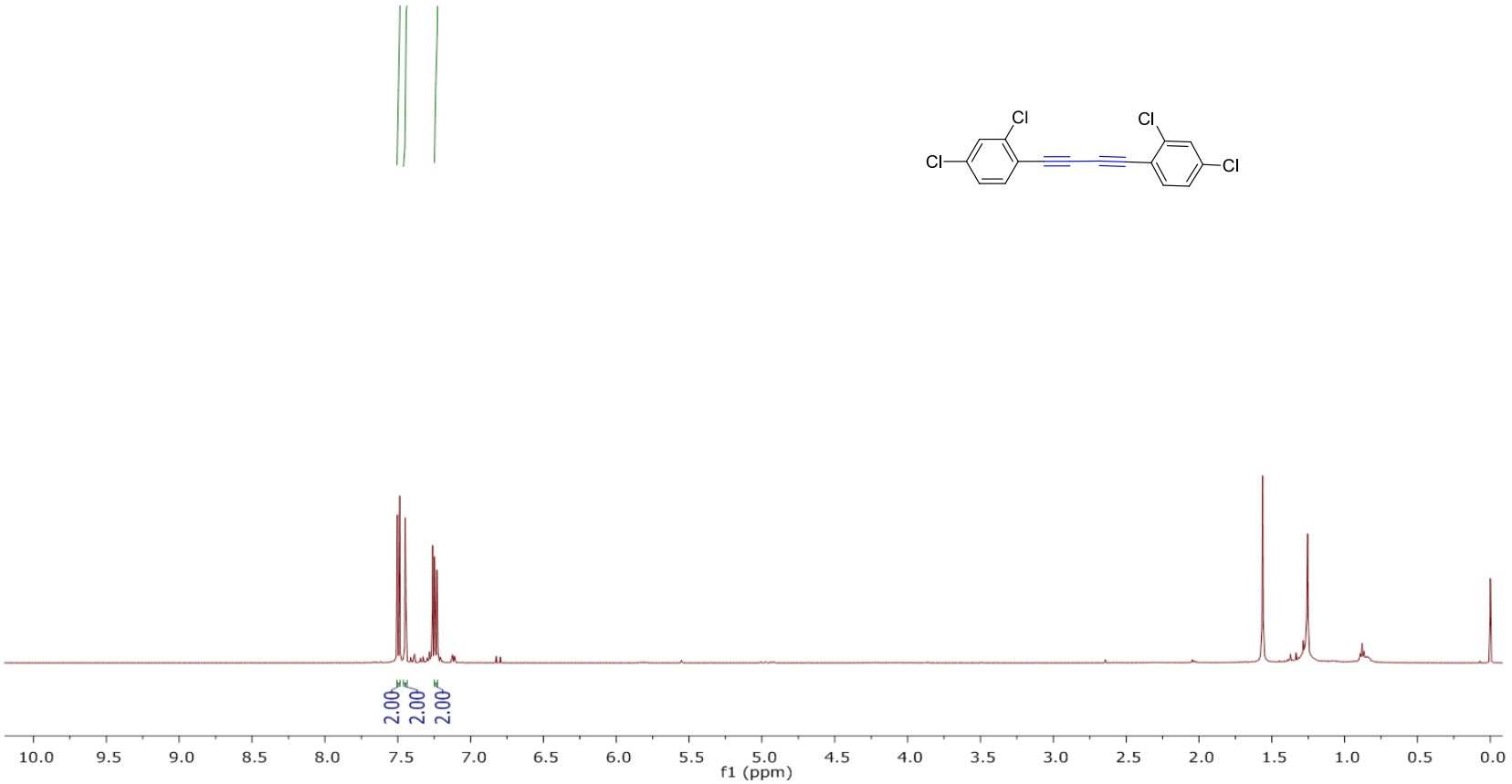


Fig. 25. ^{1}H-NMR-spectrum of compound **2m** (500 MHz, $CDCl_3$, 298K)

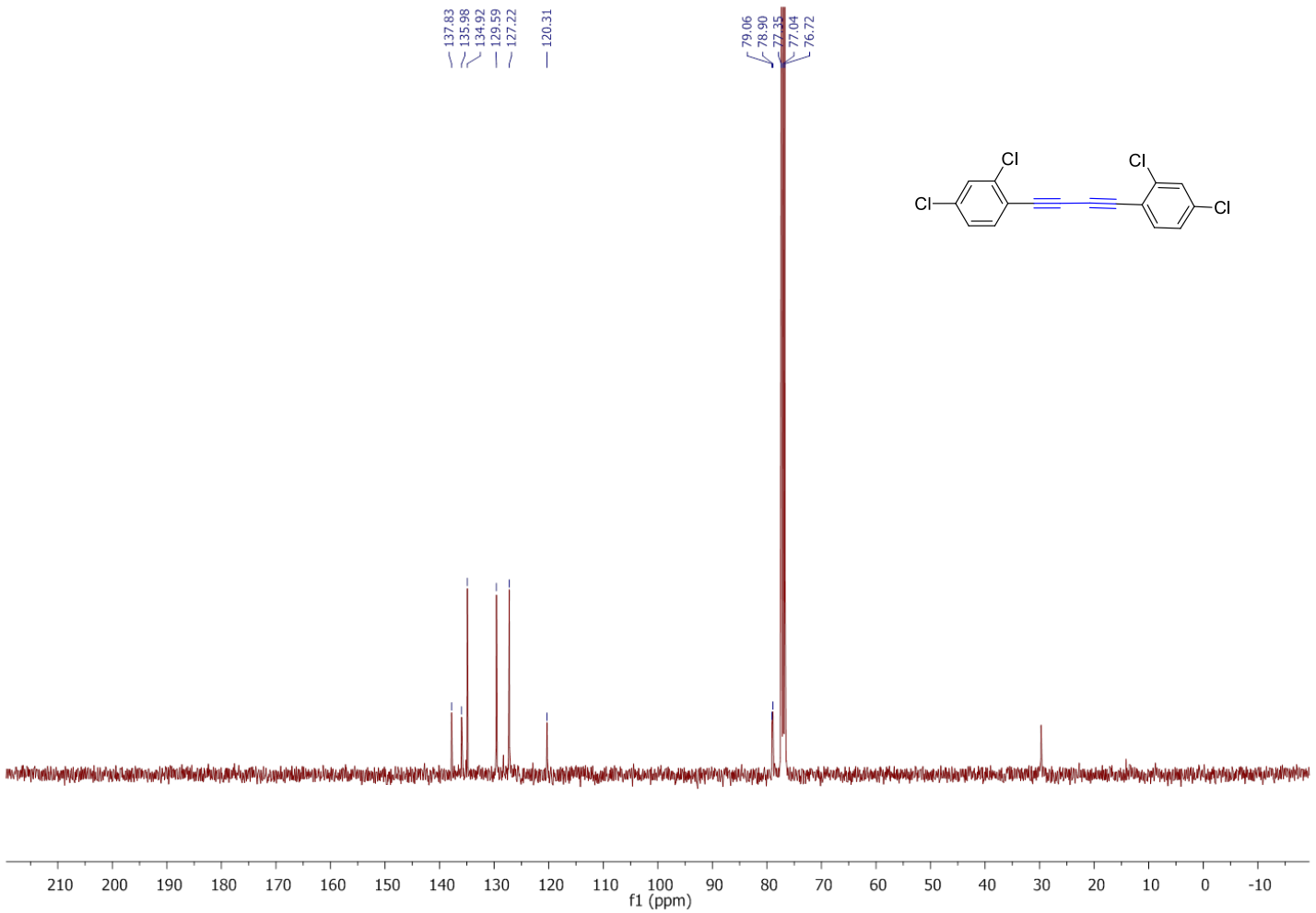


Fig. 26. ^{13}C-NMR-spectrum of compound **2m** (101 MHz, $CDCl_3$, 298K)

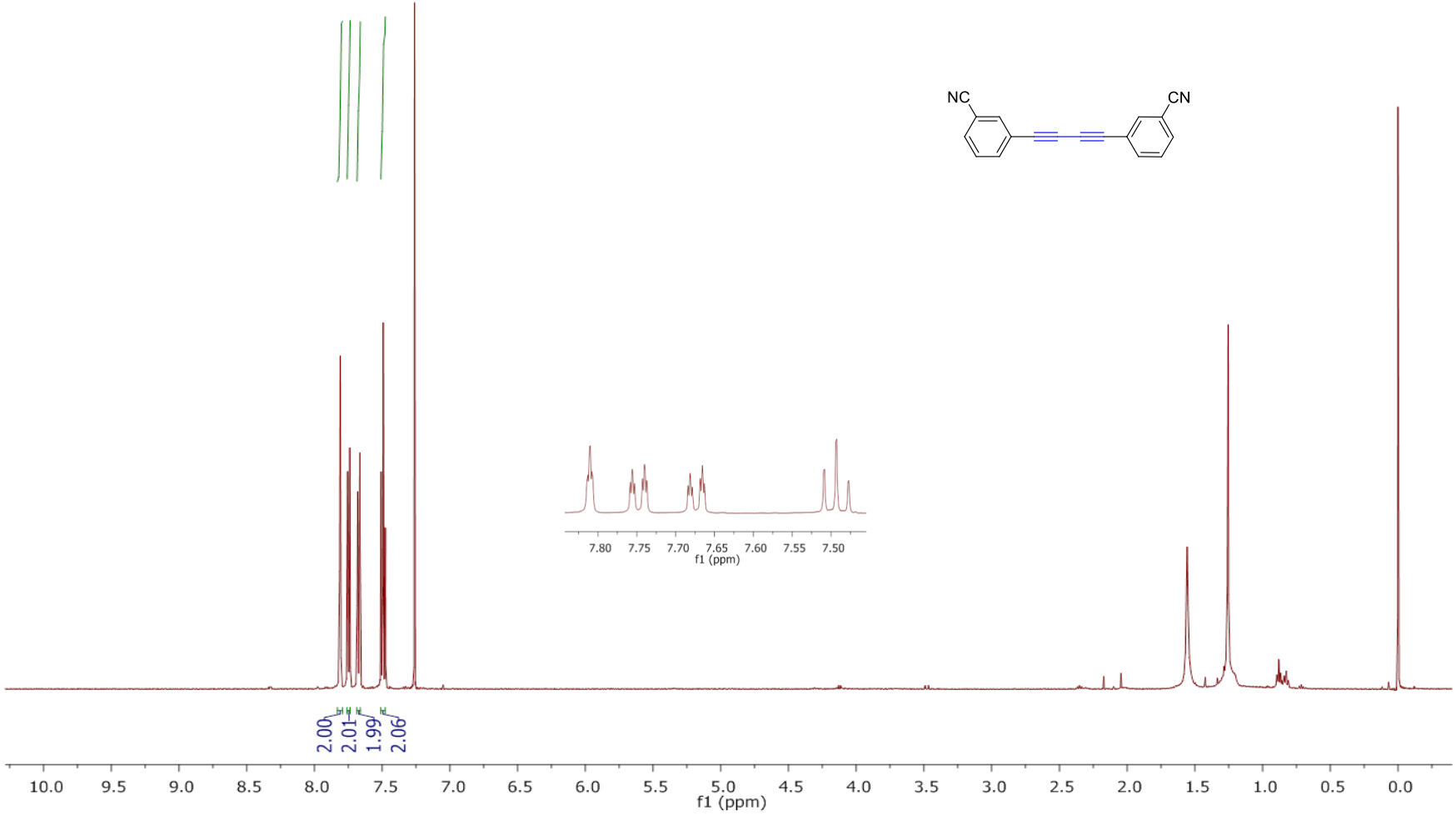


Fig. 27. ^{1}H-NMR-spectrum of compound **2n** (500 MHz, $CDCl_3$, 298K)

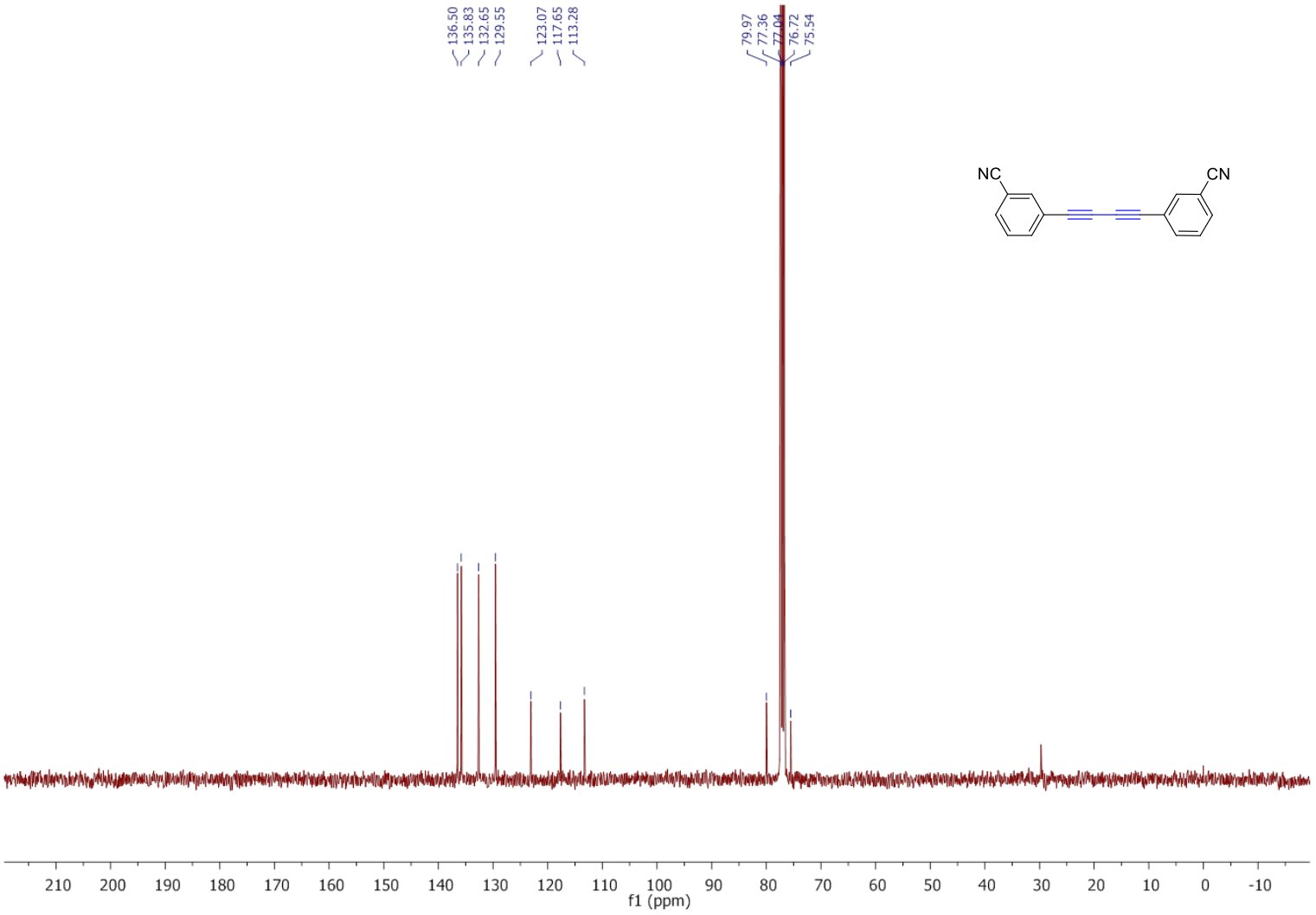


Fig. 28. ^{13}C-NMR-spectrum of compound **2n** (101 MHz, $CDCl_3$, 298K)

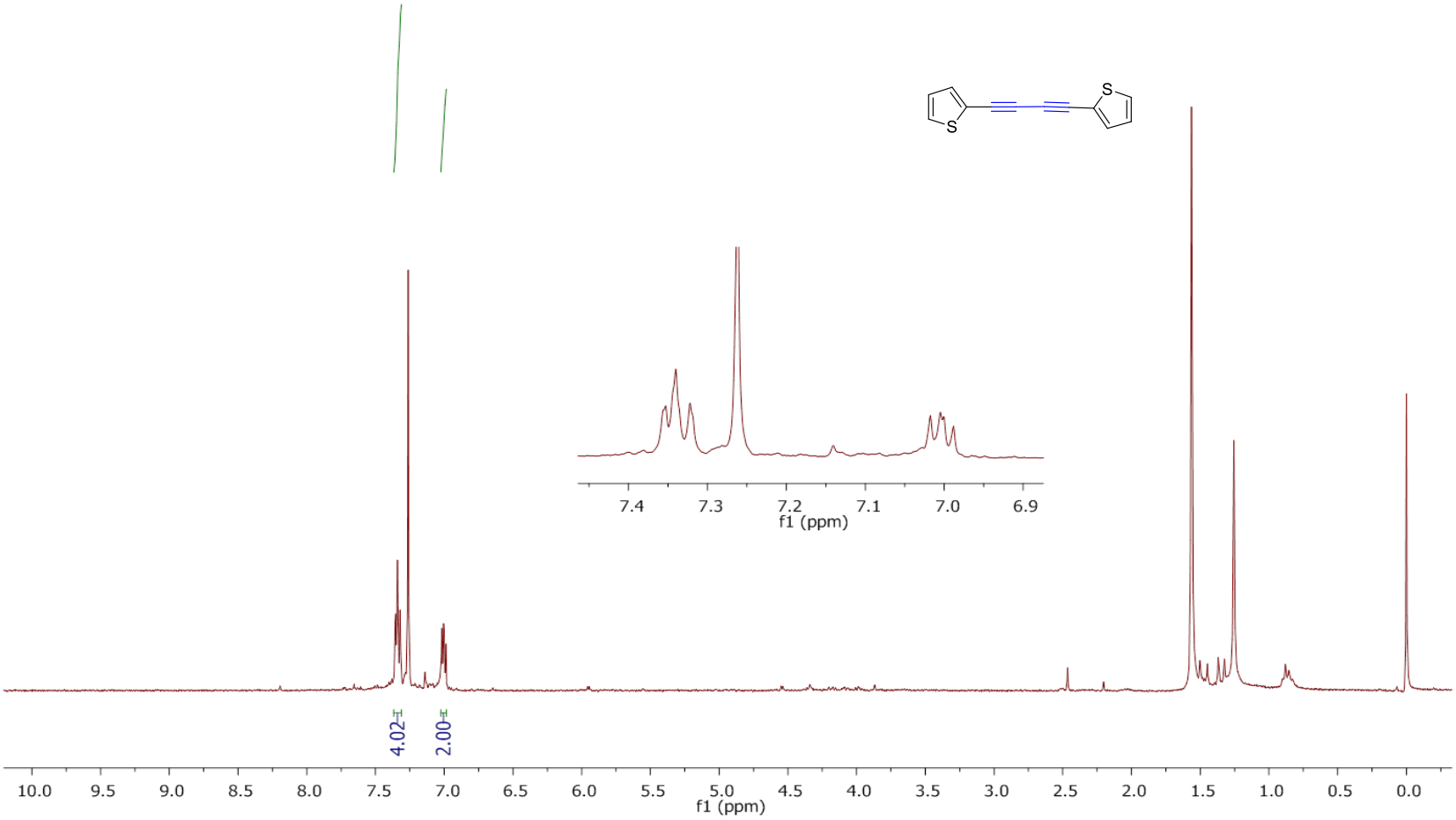


Fig. 29. ^{1}H-NMR-spectrum of compound **2o**[1] (400 MHz, $CDCl_3$, 298K)

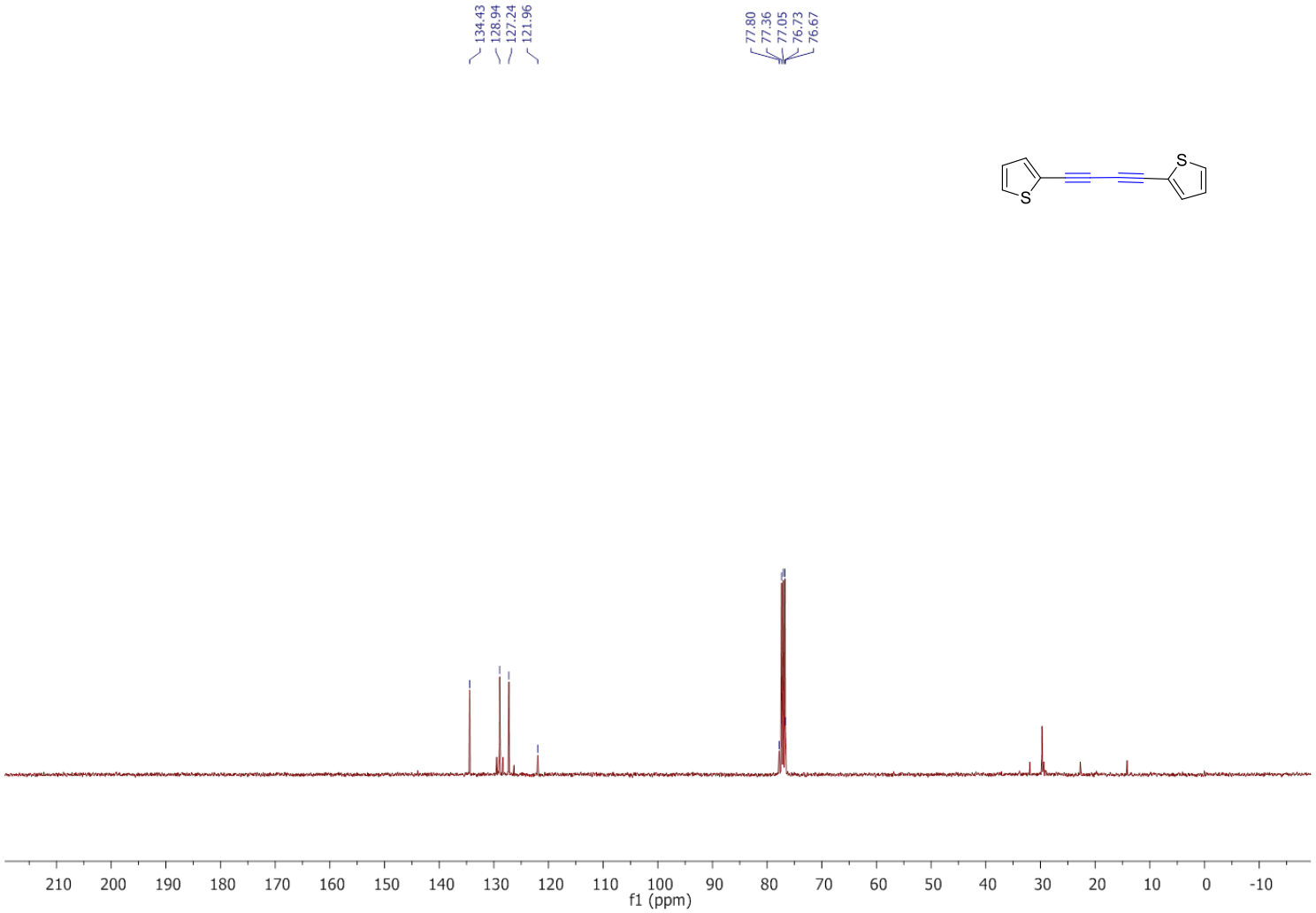


Fig. 30. ^{13}C-NMR-spectrum of compound **2o**[1] (101 MHz, $CDCl_3$, 298K)

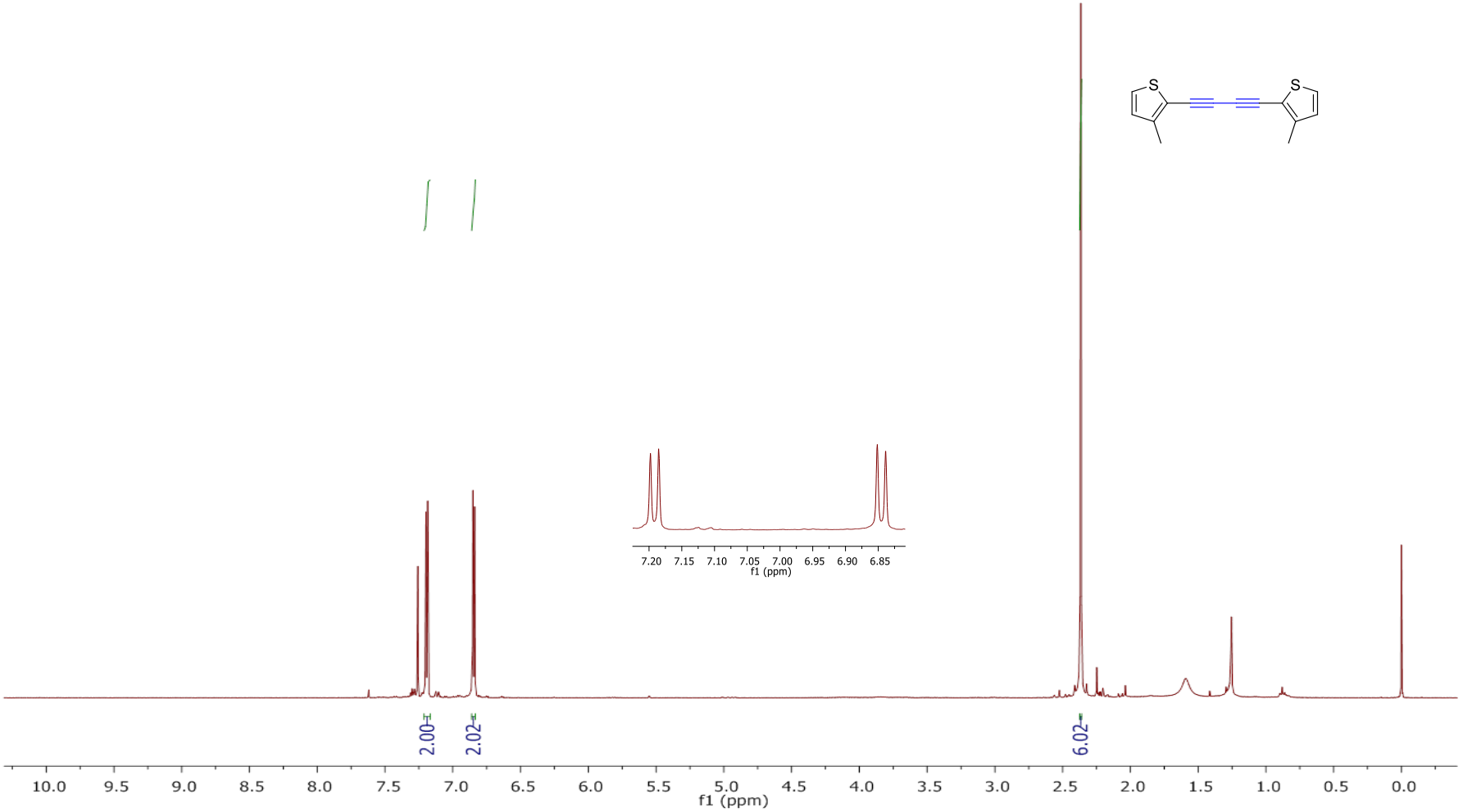


Fig. 31. ^{1}H-NMR-spectrum of compound **2p** (400 MHz, $CDCl_3$, 298K)

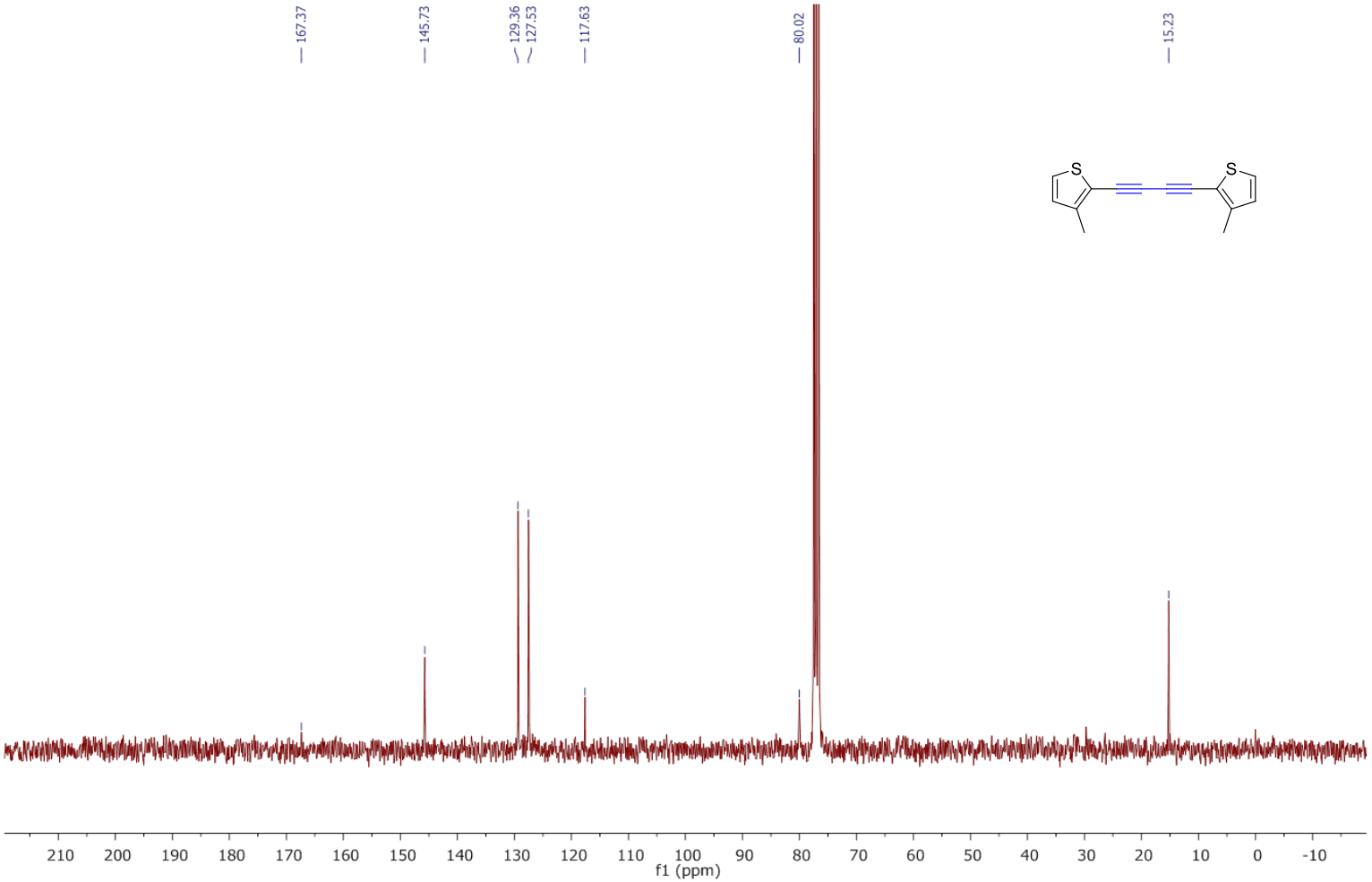


Fig. 32. ^{13}C-NMR-spectrum of compound **2p** (101 MHz, $CDCl_3$, 298K)

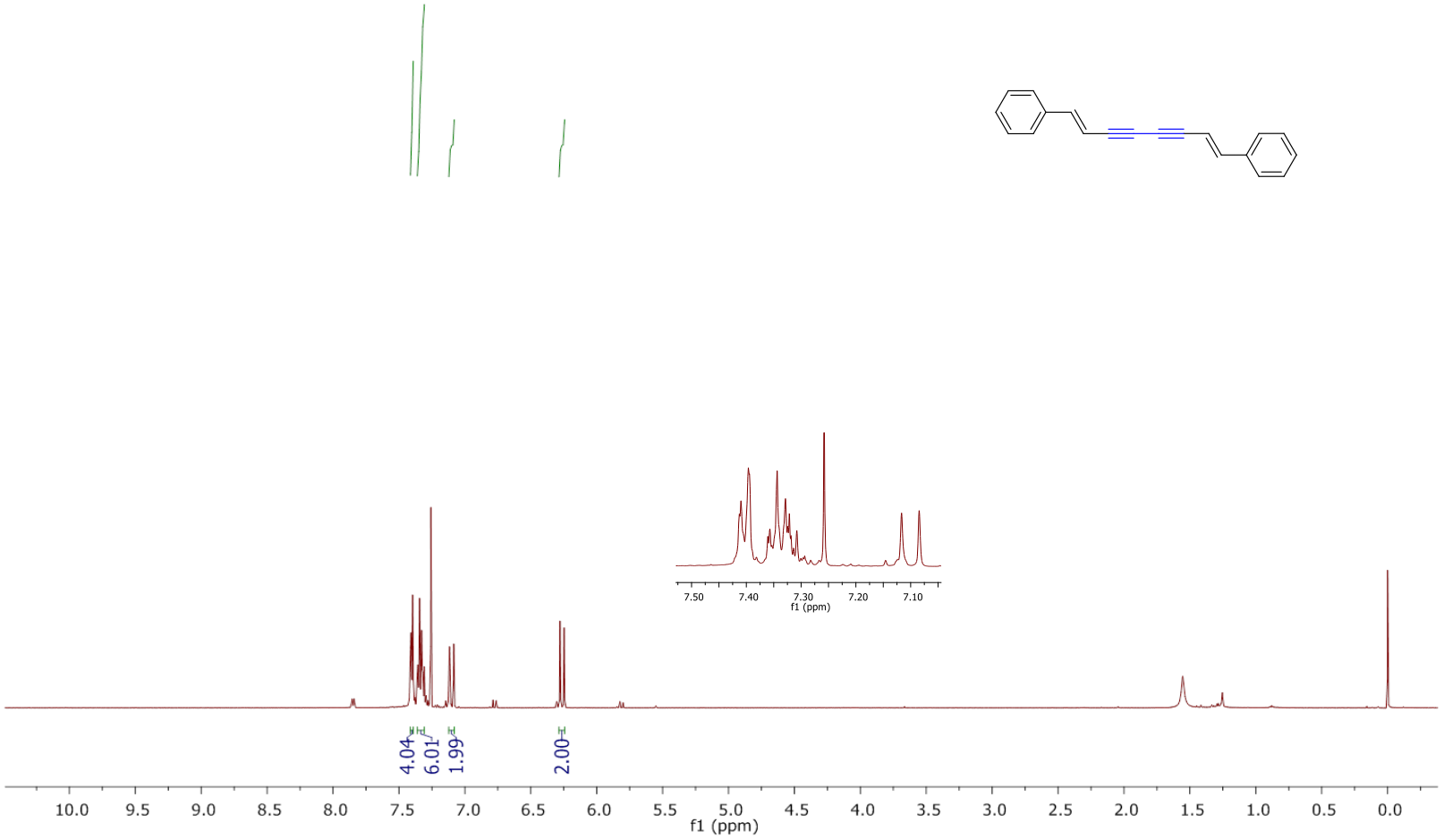


Fig. 33. ^{1}H-NMR-spectrum of compound **2q** (500 MHz, $CDCl_3$, 298K)

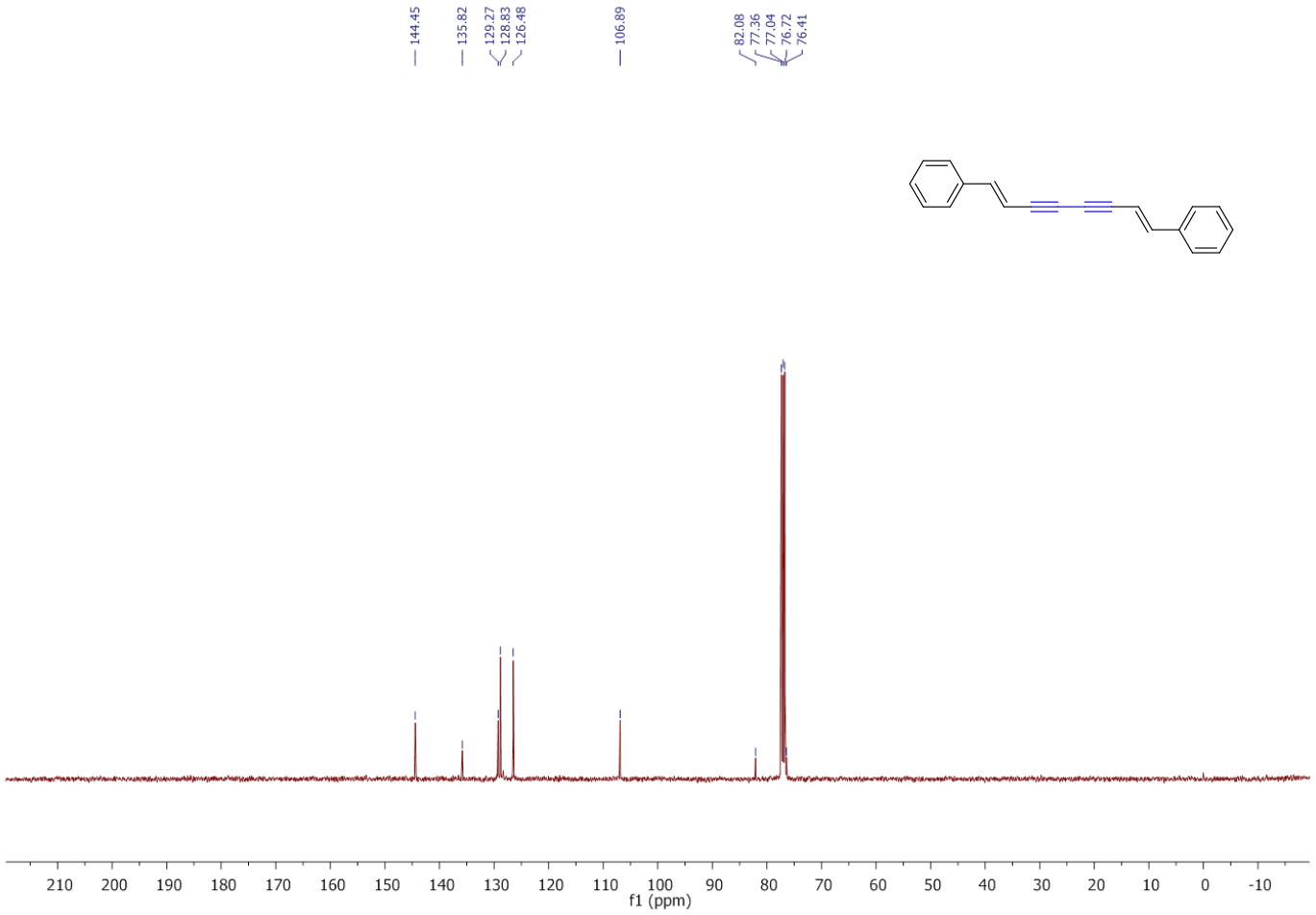


Fig. 34. ^{13}C-NMR-spectrum of compound **2q** (101 MHz, $CDCl_3$, 298K)

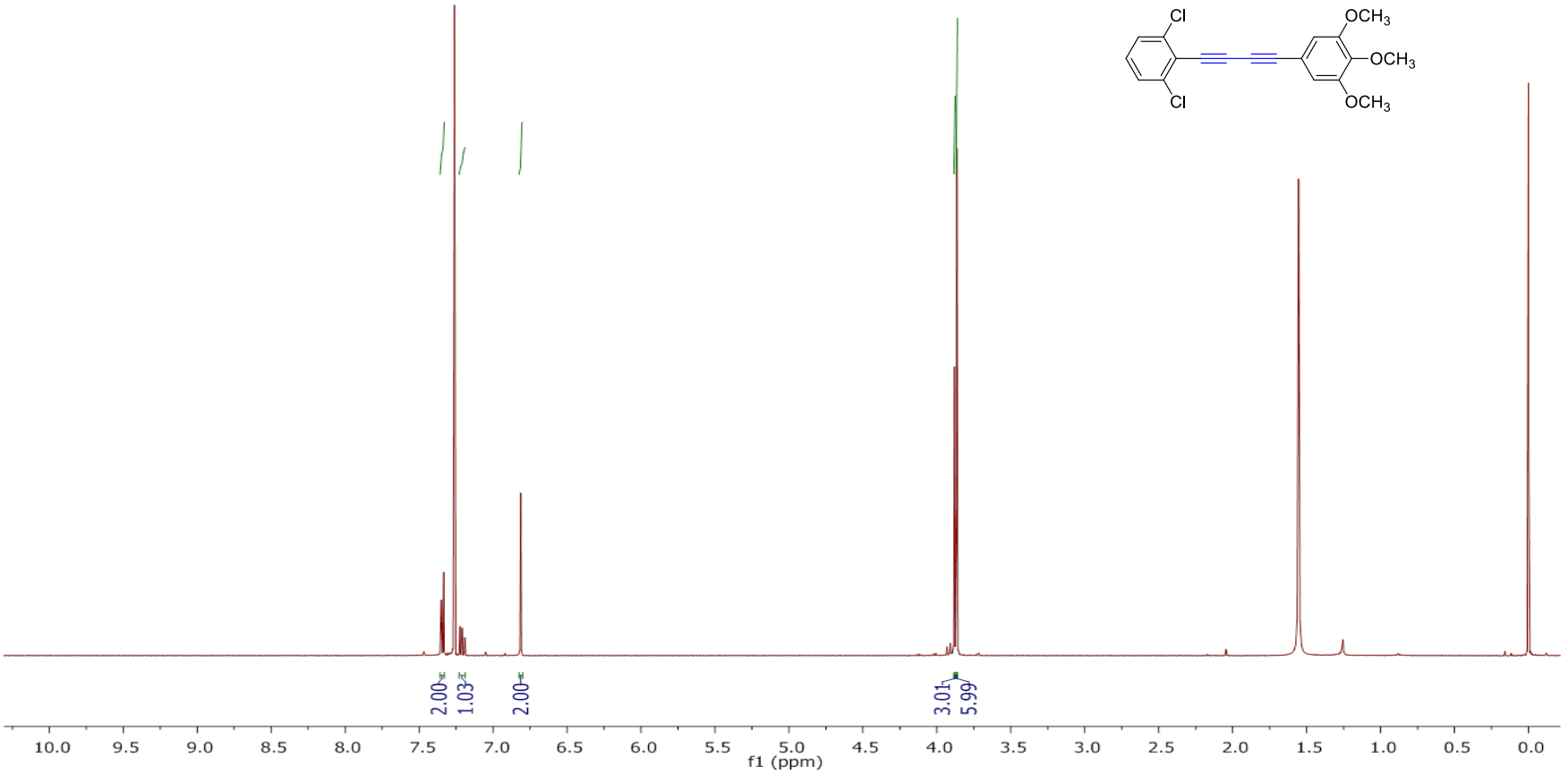


Fig. 35. ^{1}H-NMR-spectrum of compound **2r** (500 MHz, $CDCl_3$, 298K)

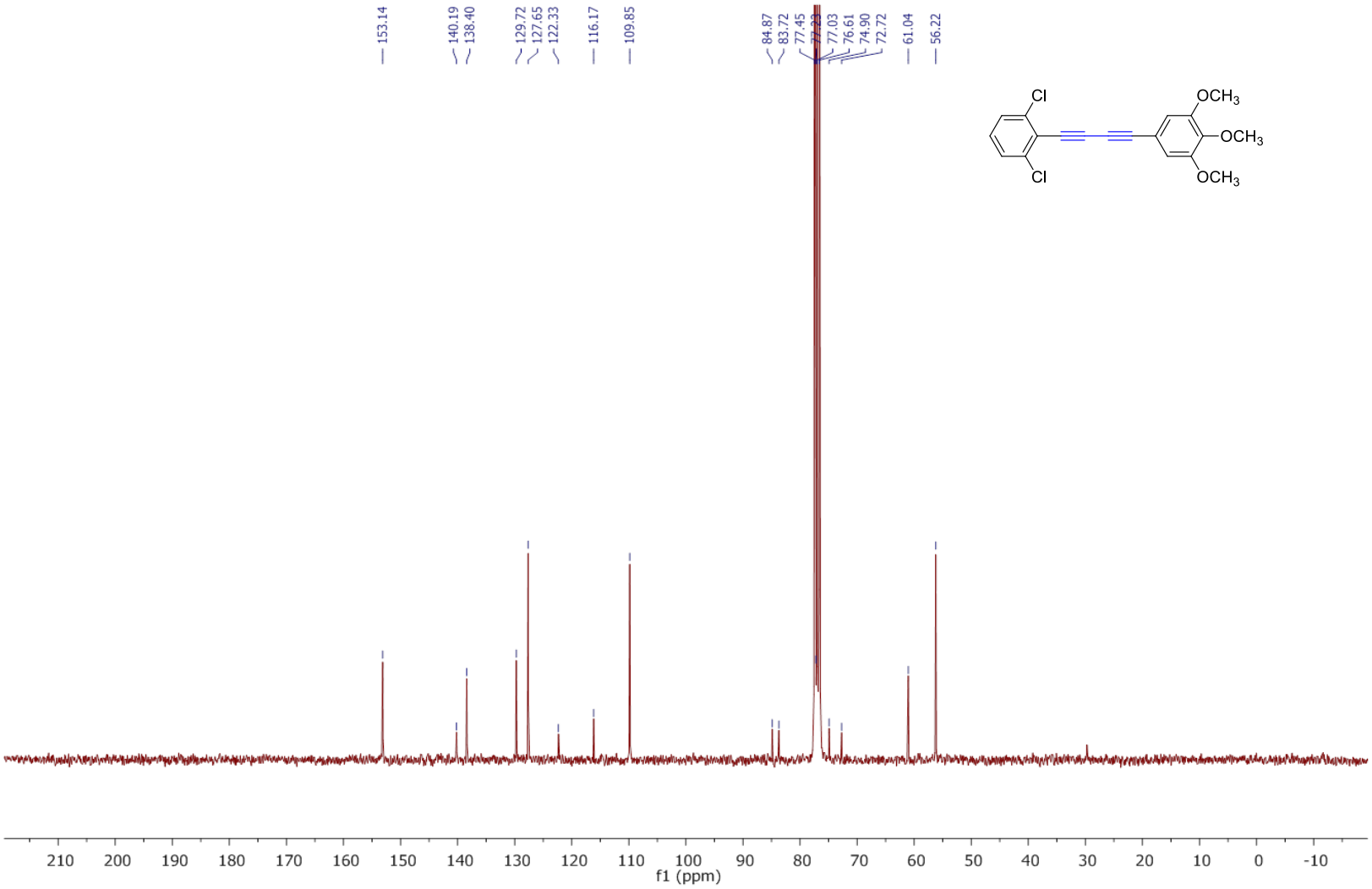


Fig. 36. ^{13}C-NMR-spectrum of compound **2r** (101 MHz, $CDCl_3$, 298K)

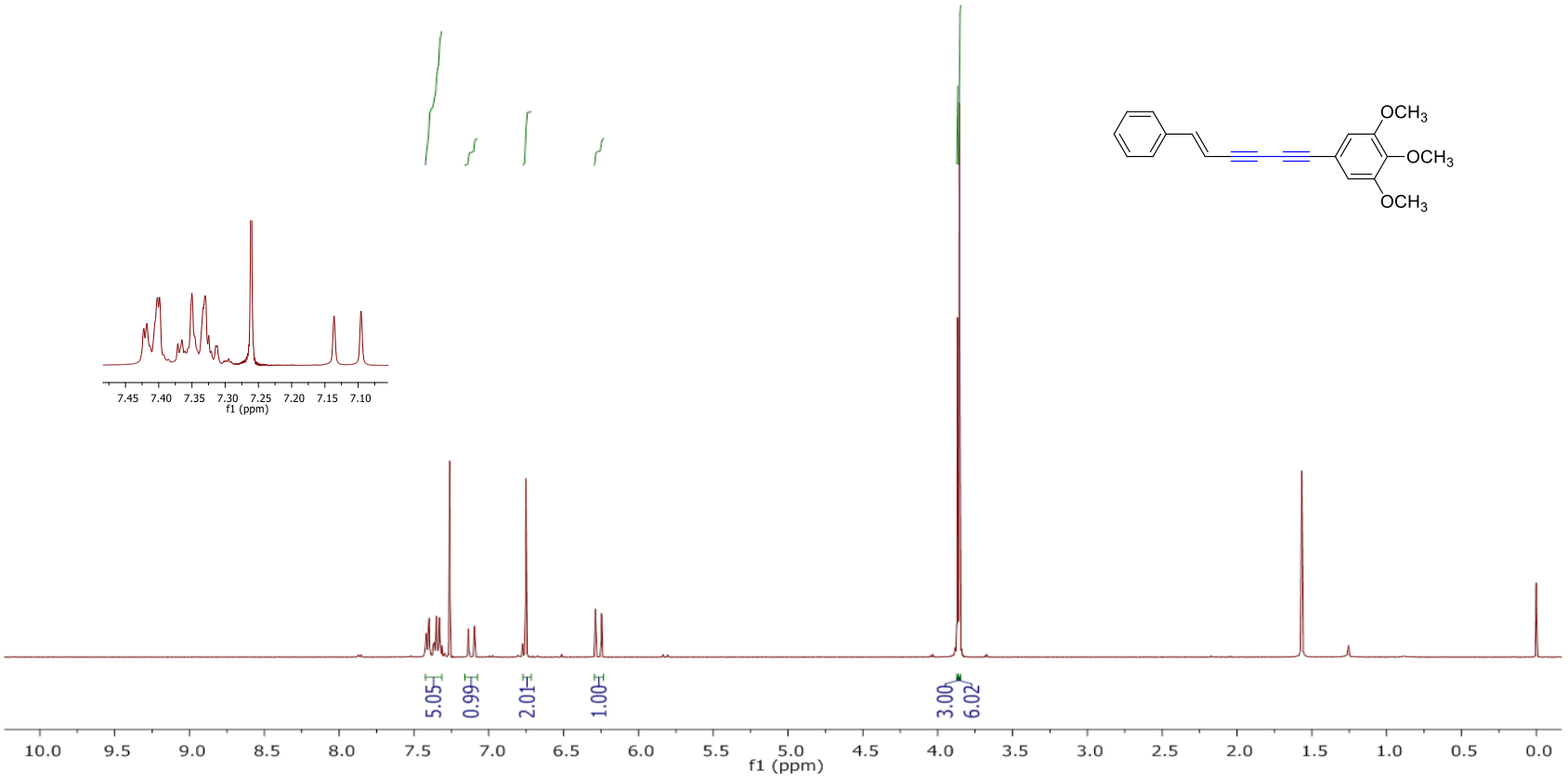


Fig. 37. ^{1}H-NMR-spectrum of compound **2s** (500 MHz, $CDCl_3$, 298K)

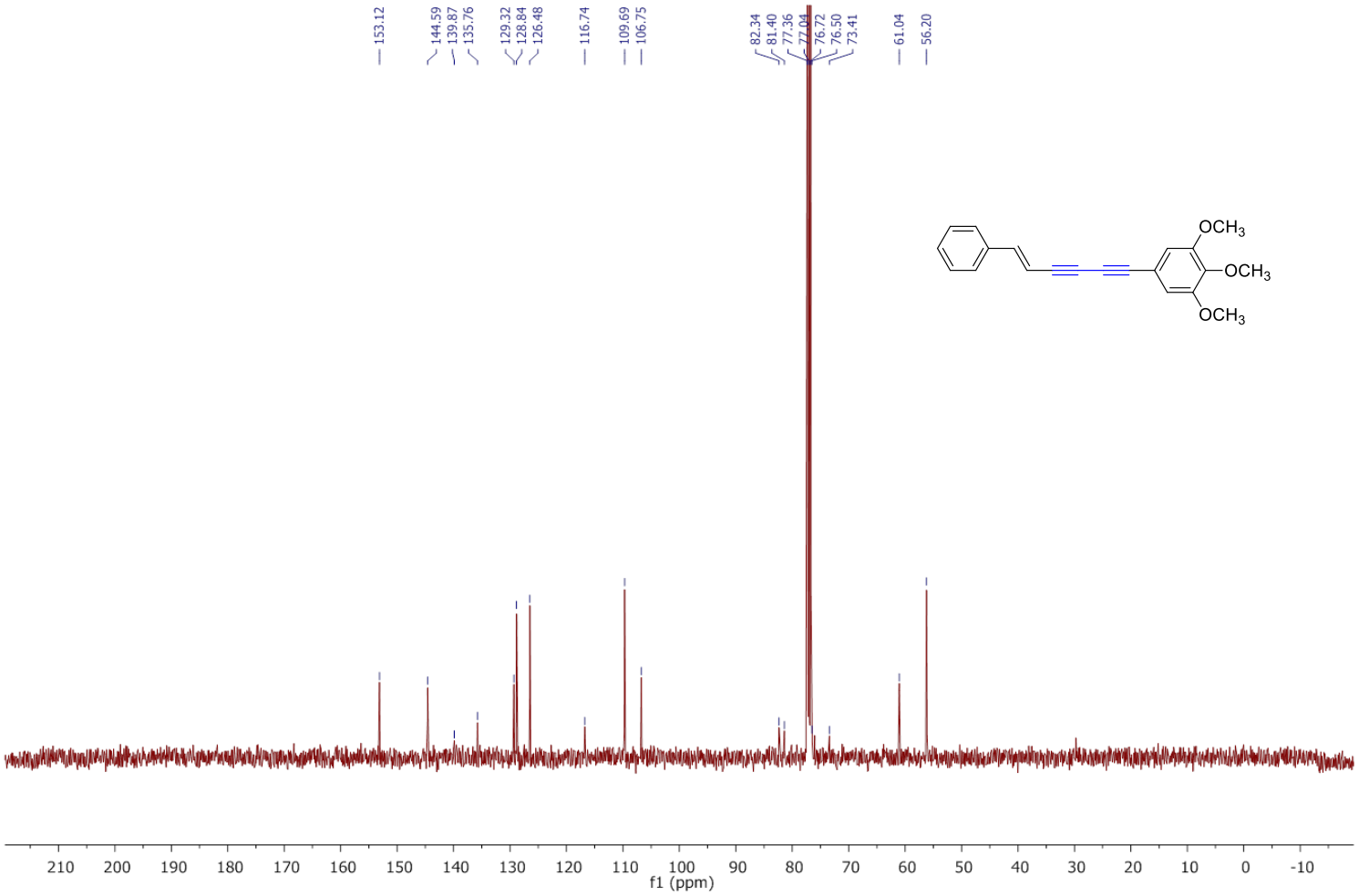


Fig. 38. ^{13}C-NMR-spectrum of compound **2s** (101 MHz, $CDCl_3$, 298K)

References

1. Rao, M. L. N.; Priyabrata, D.; Ramakrishna, B. S.; Murty, V. N. *Tetrahedron Lett*. **2014,** *55*, 3529–3533. doi: 10.1016/j.tetlet.2014.04.092

