

Uncovering A Solvent-free Eco-friendly Cyanosilylation of Aldehydes Through A Well-defined Gold(I)-NHC Heterogeneous Catalyst

Saurabh Kumar Tiwari^{†1}, Ankit Kumar^{†2}, Ankit Verma³, I. R. Siddiqui³

¹Department of Chemistry, KBPG College, Mirjapur, Uttar Pradesh-231001

²Department of Chemistry, University of Delhi, New Delhi, India.

³Department of Chemistry, University of Allahabad, Prayagraj, Uttar Pradesh, India.

† Authors contributed equally to the study.

*E-mail: saurabht2016@gmail.com, sktiwari@allduniv.ac.in

Electronic Supplementary Information

Experimental Section:

Unless otherwise mentioned, all reactions were carried out under open atmosphere. All the chemicals were purchased from Spectrochem Chemicals and Sigma Aldrich Chemicals were used without any further purification. ^1H NMR and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra were recorded on Bruker 400 MHz and Bruker 500 MHz NMR spectrometer. ^1H NMR peaks are labeled as singlet (s), doublet (d), triplet (t), quartet (q), doublet of doublet (dd), doublet of triplets (dt), triplets of triplets (tt), multiplet (m).

$^1\text{H-NMR}$ and $^{13}\text{C-NMR}$ data for all the catalysis products:

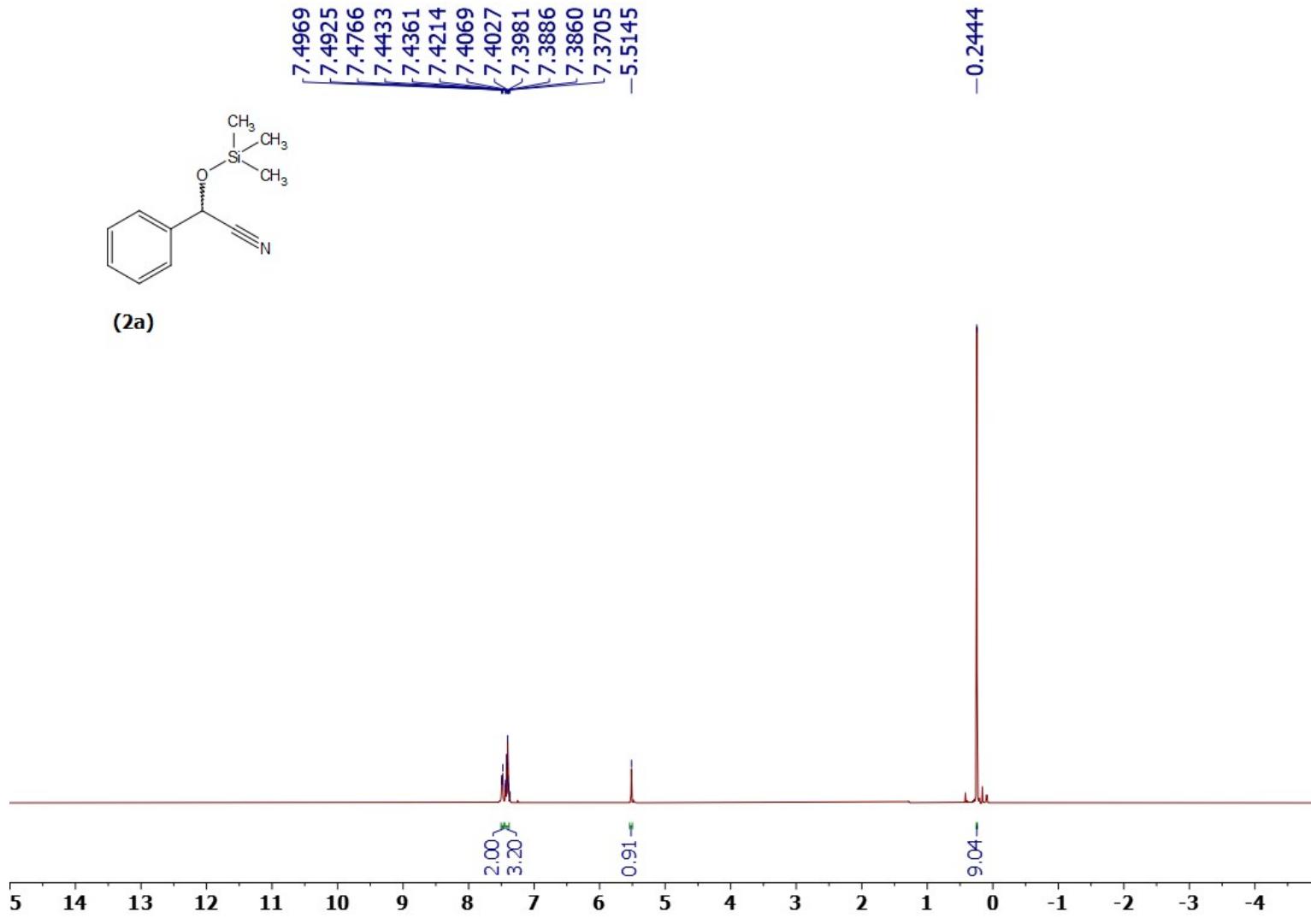
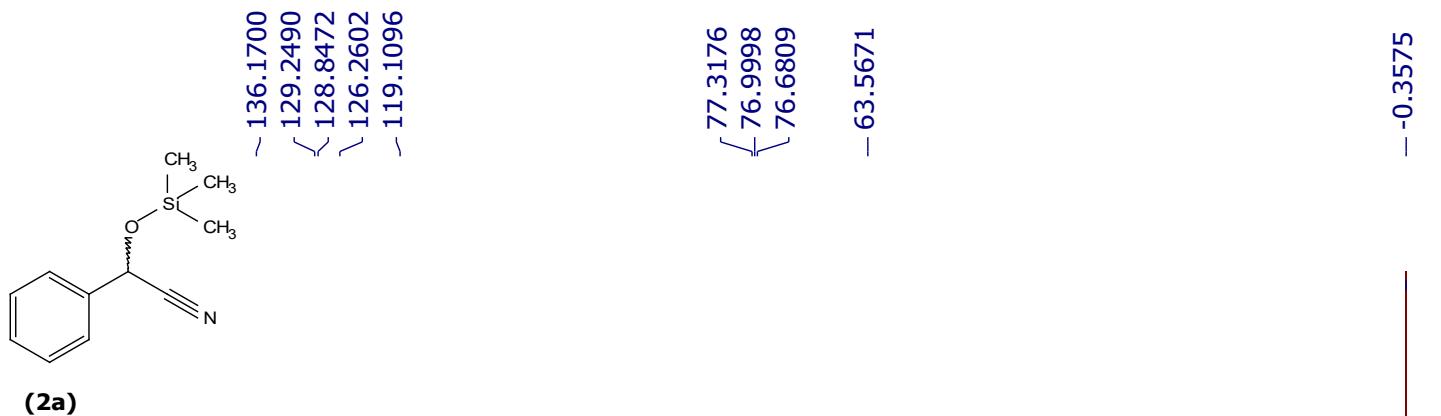


Figure S1. ^1H NMR spectrum of **2a** in CDCl_3 .



(2a)

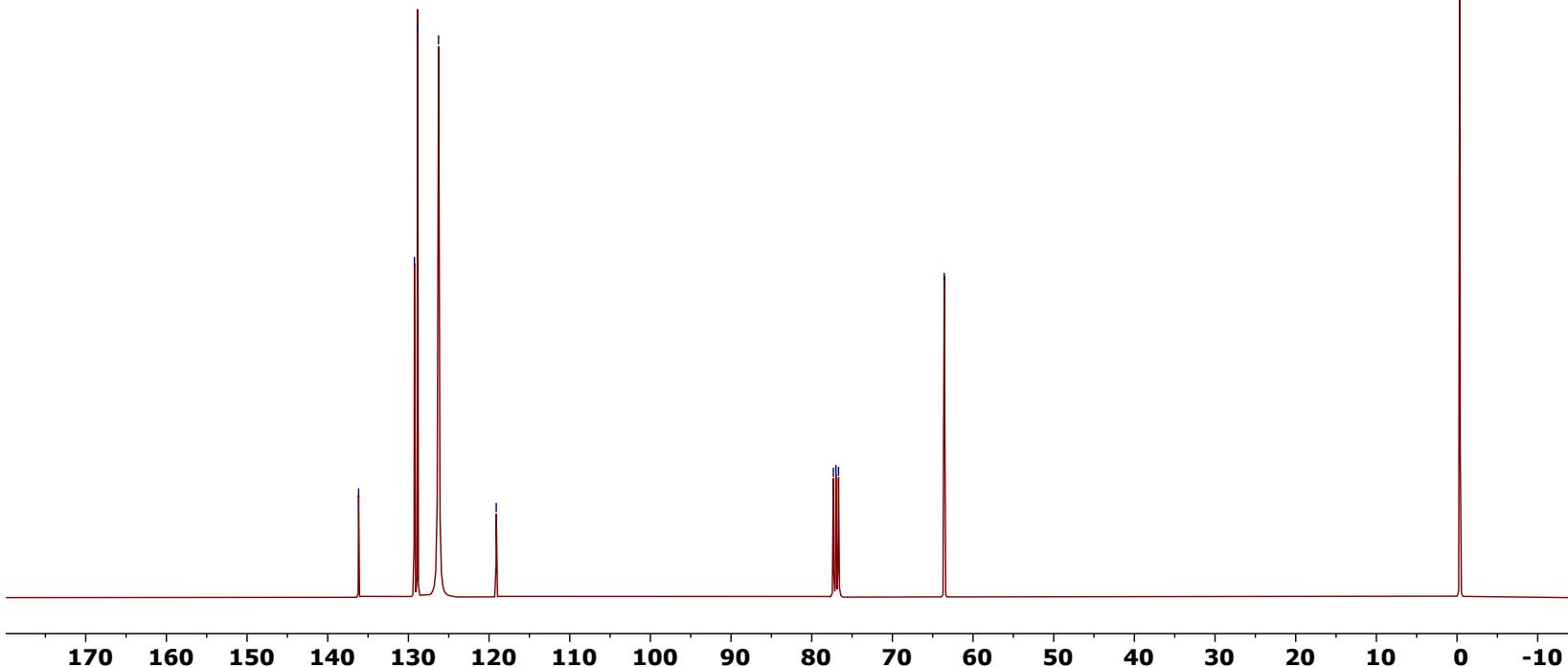
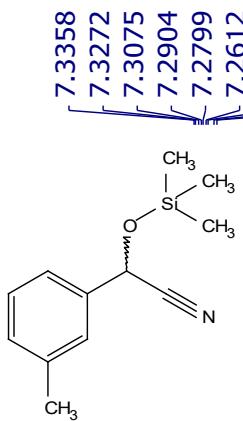


Figure S2. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **2a** in CDCl_3 .



(2b)

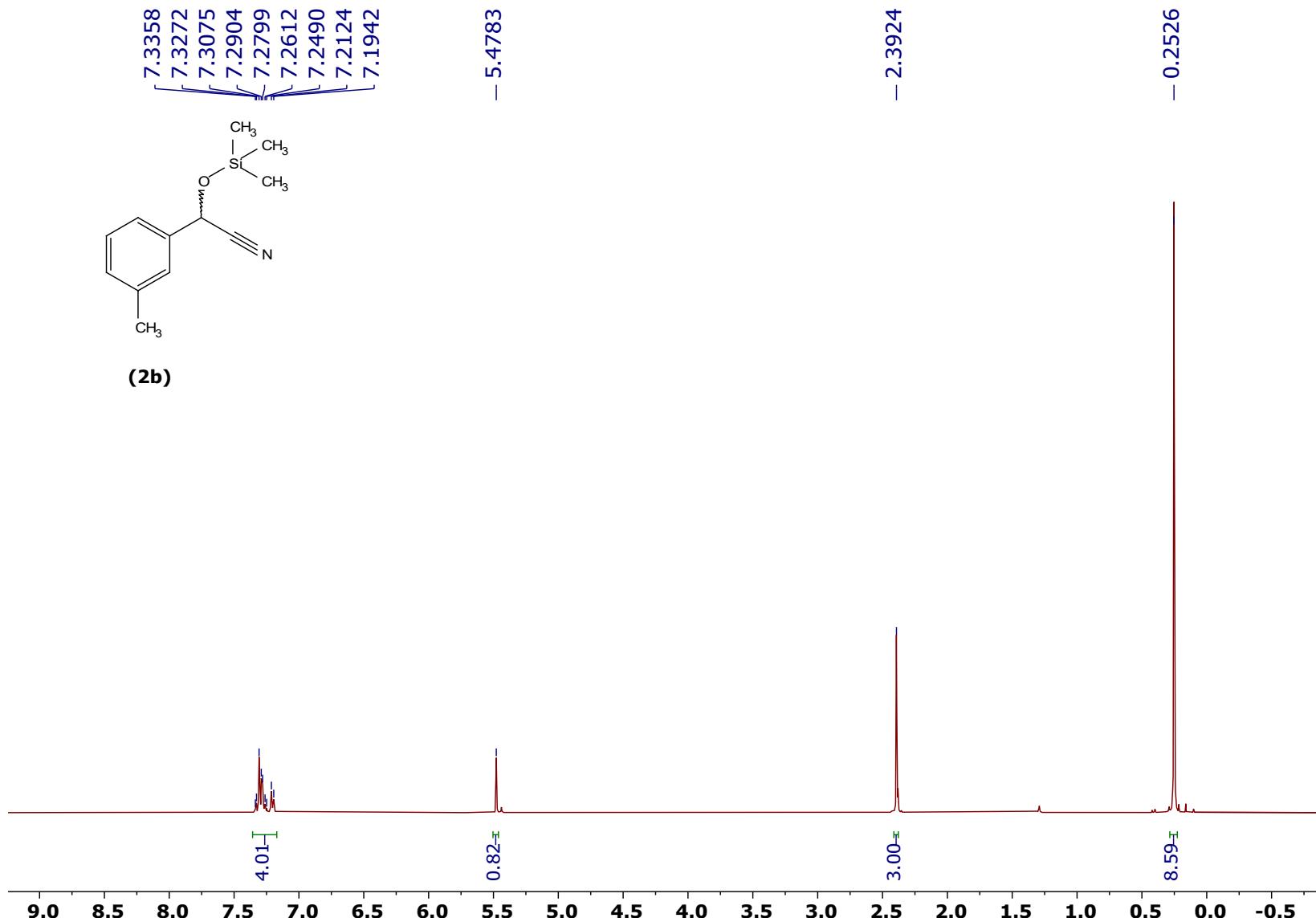


Figure S3. ^1H NMR spectrum of **2b** in CDCl_3 .

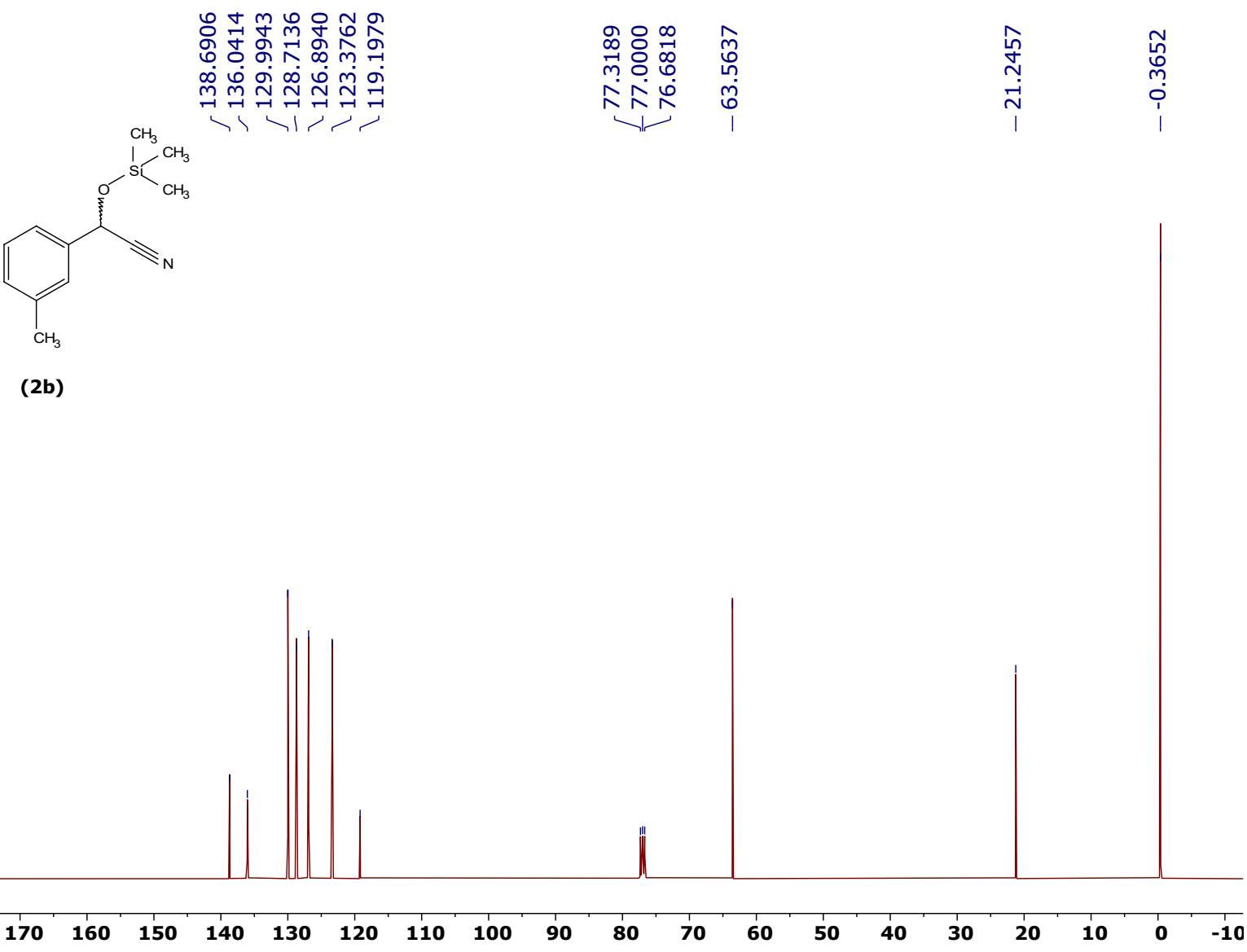


Figure S4. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **2b** in CDCl_3 .

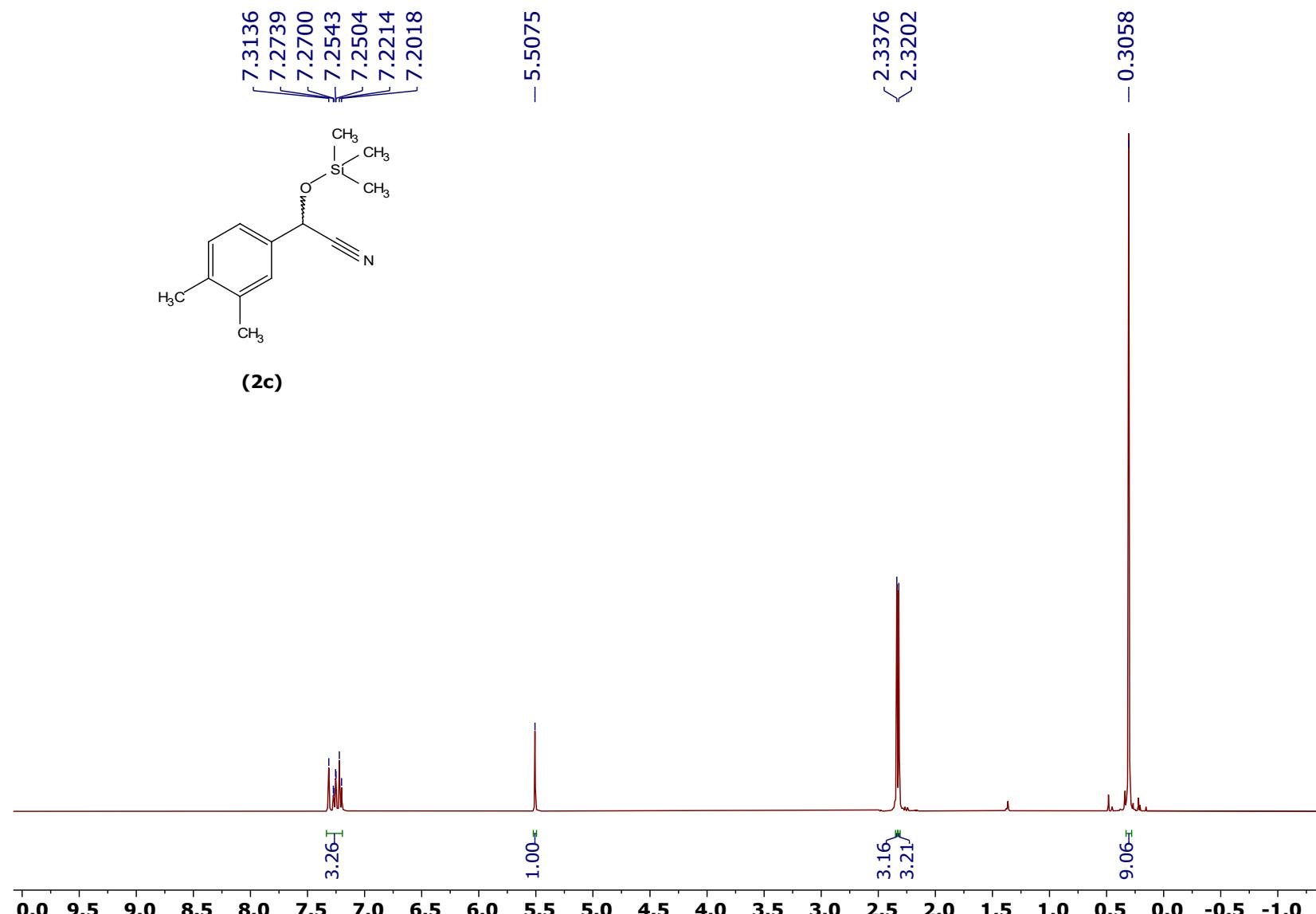
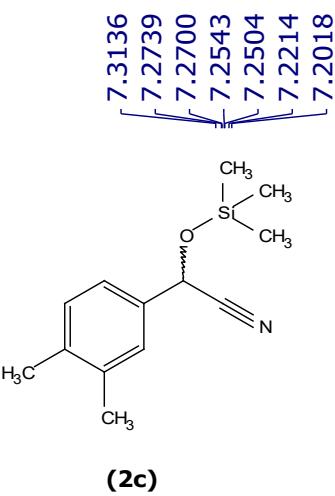


Figure S5. ^1H NMR spectrum of **2c** in CDCl_3 .

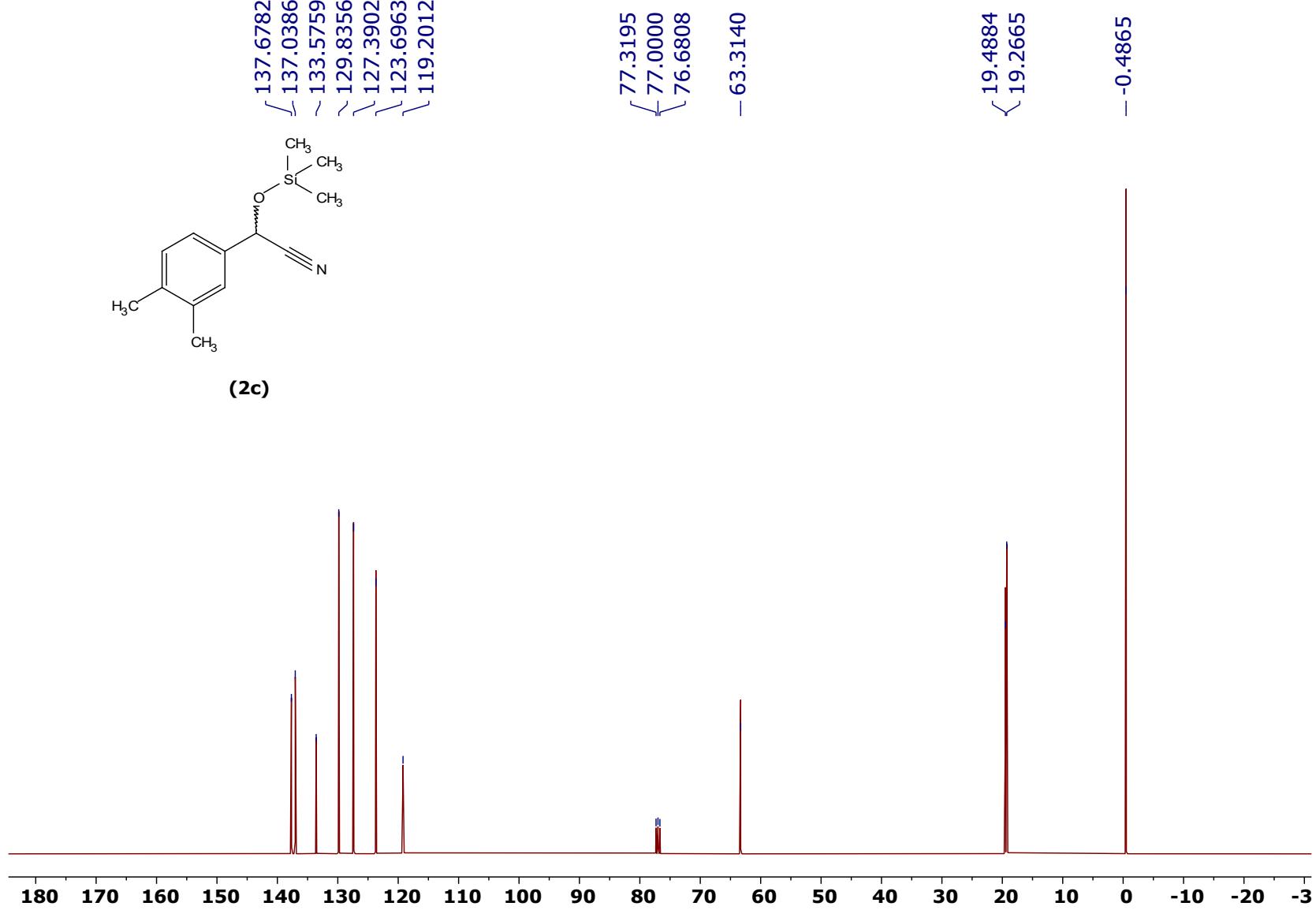
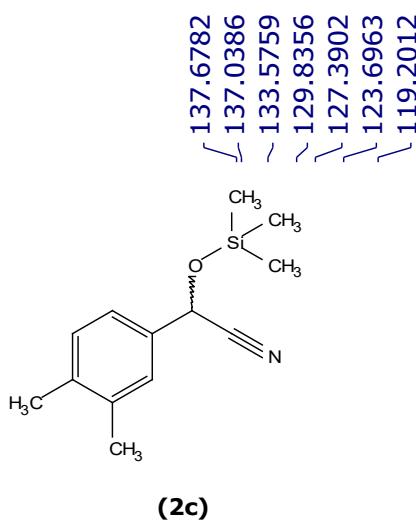


Figure S6. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **2c** in CDCl_3 .

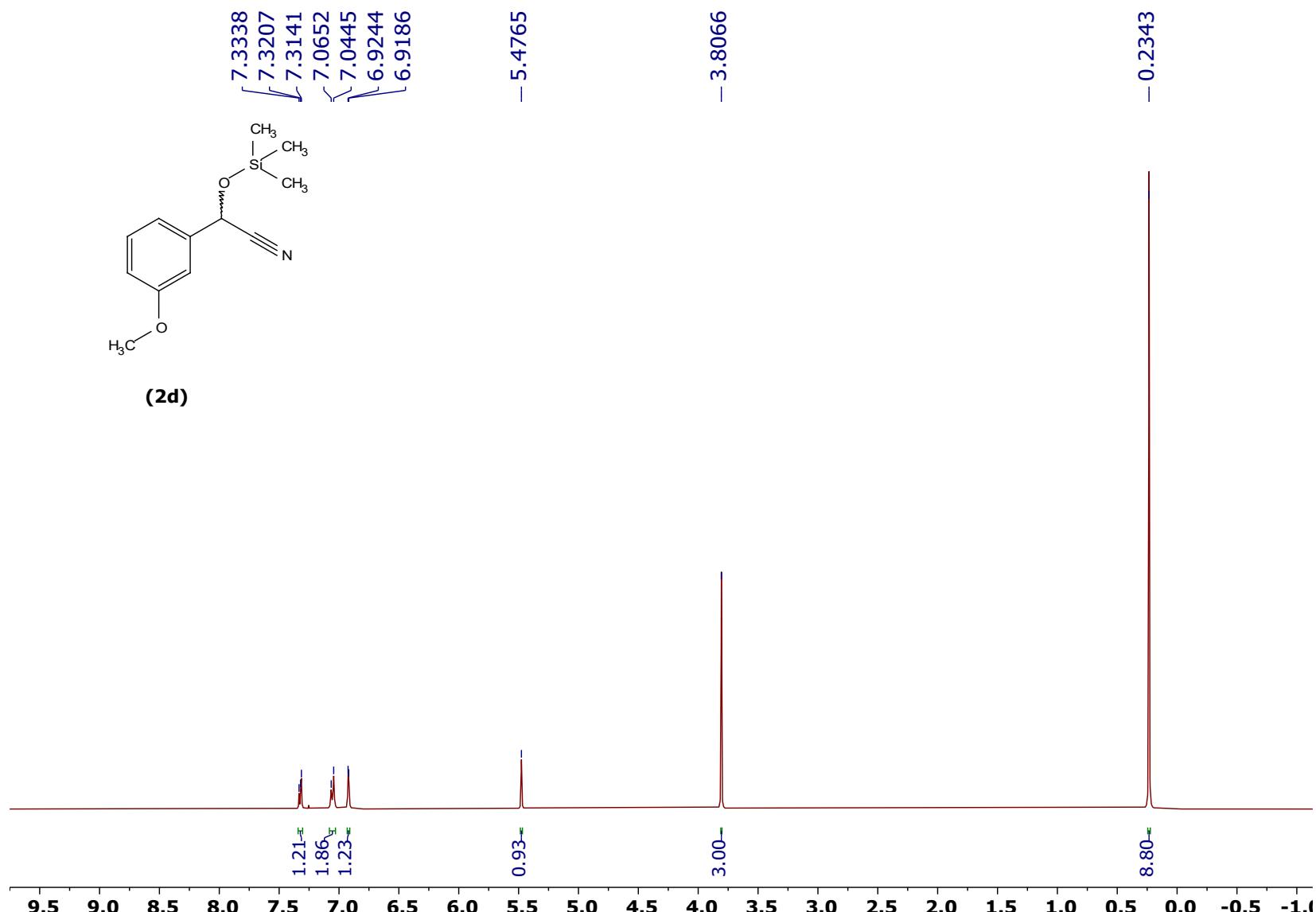
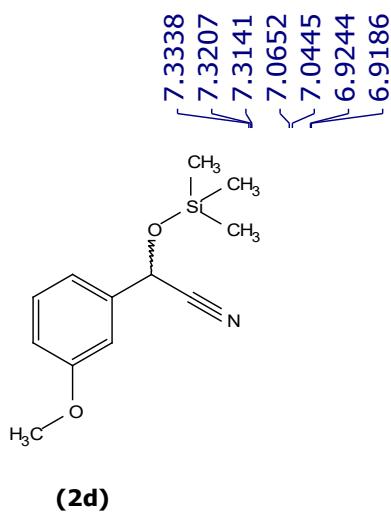


Figure S7. ^1H NMR spectrum of **2d** in CDCl_3 .

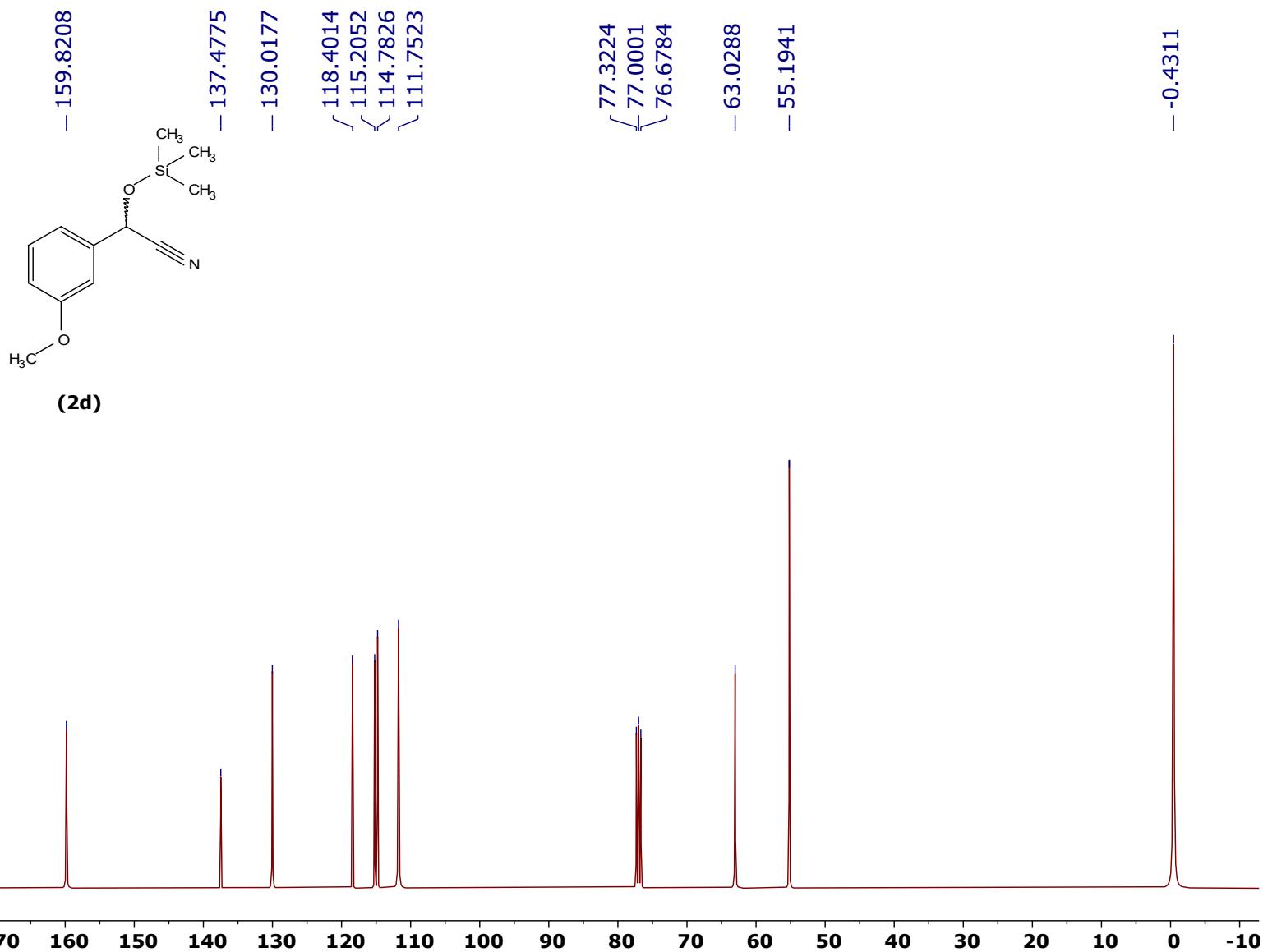


Figure S8. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **2d** in CDCl_3 .

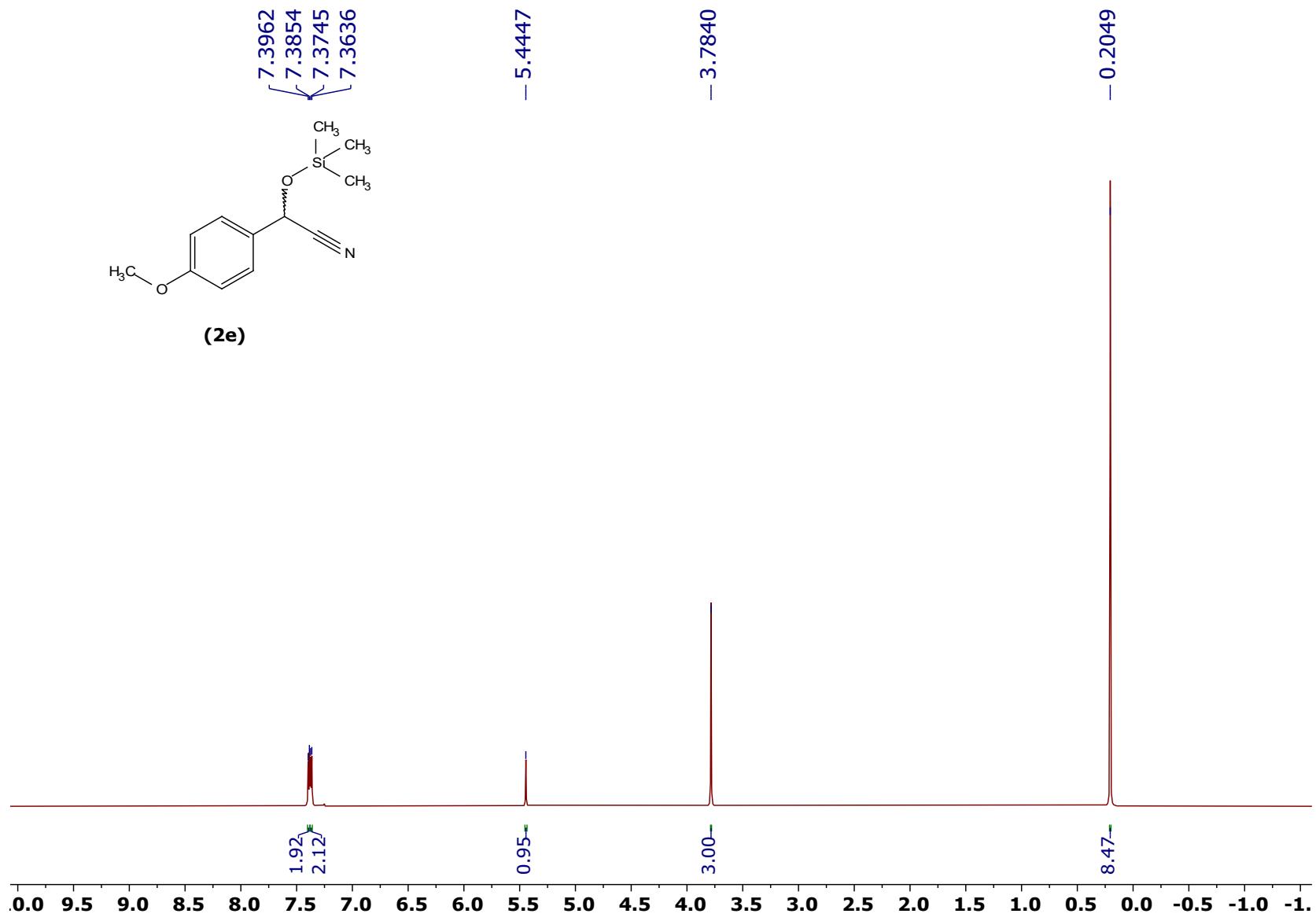
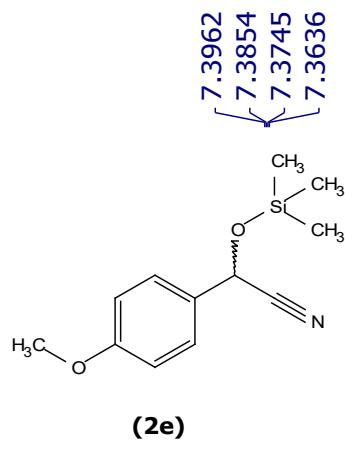


Figure S9. ^1H NMR spectrum of **2e** in CDCl_3 .

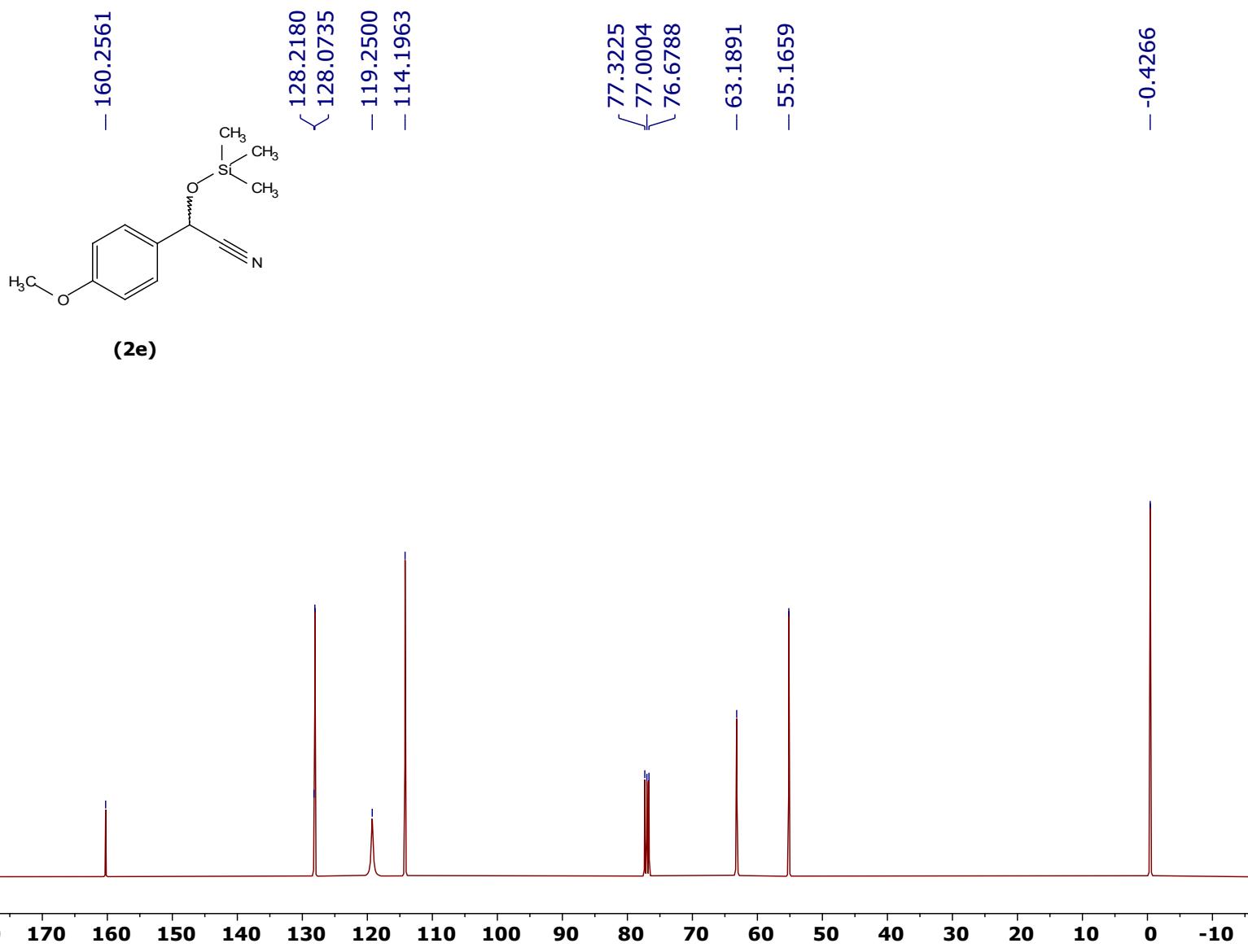


Figure S10. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **2e** in CDCl_3 .

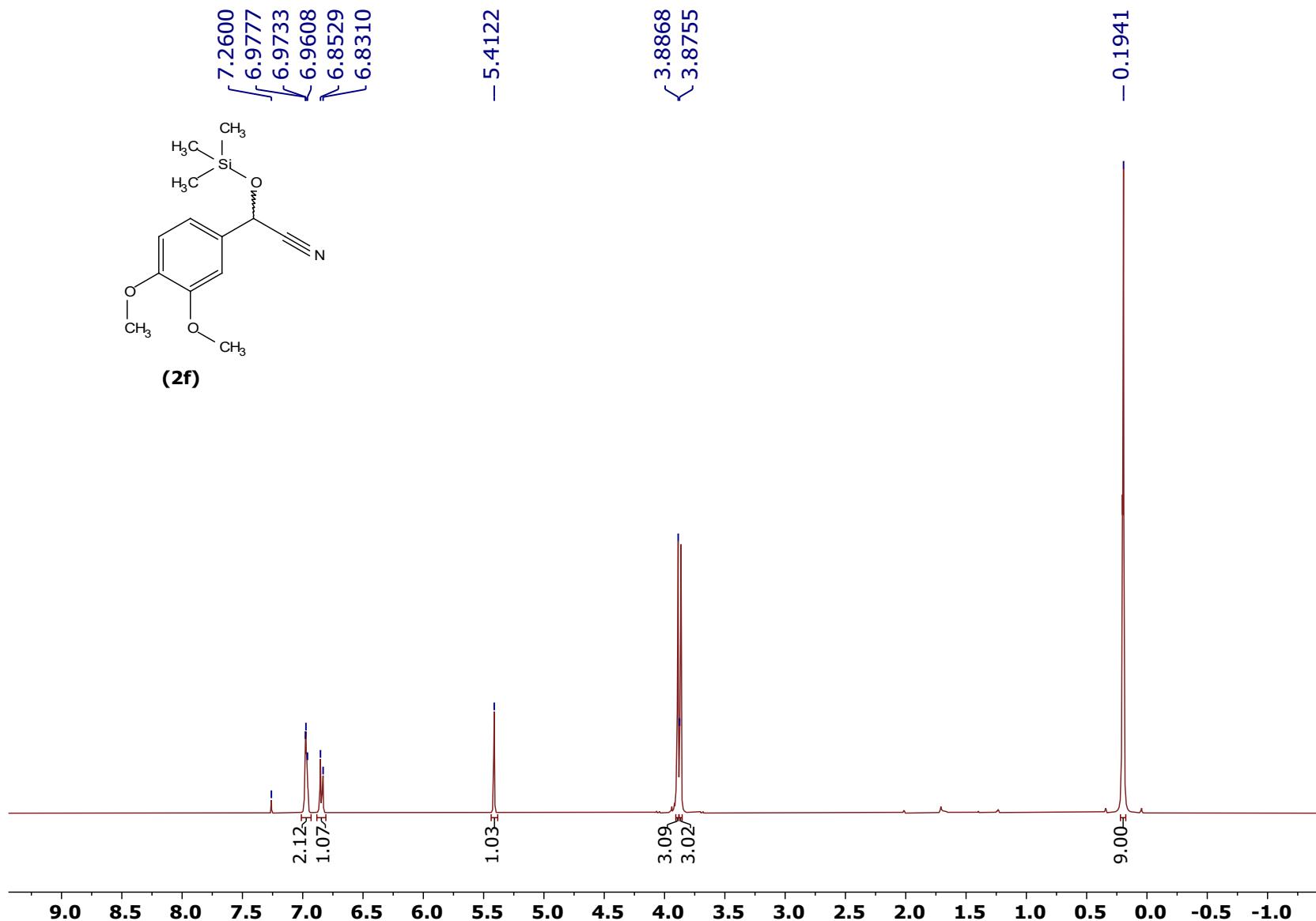
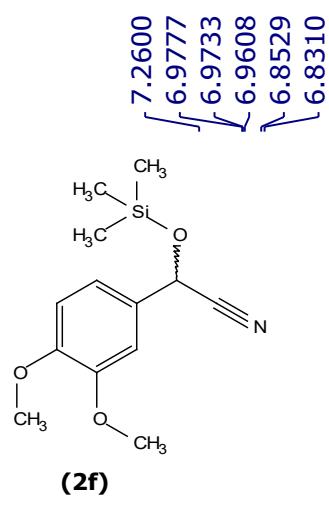


Figure S11. ^1H NMR spectrum of **2f** in CDCl_3 .

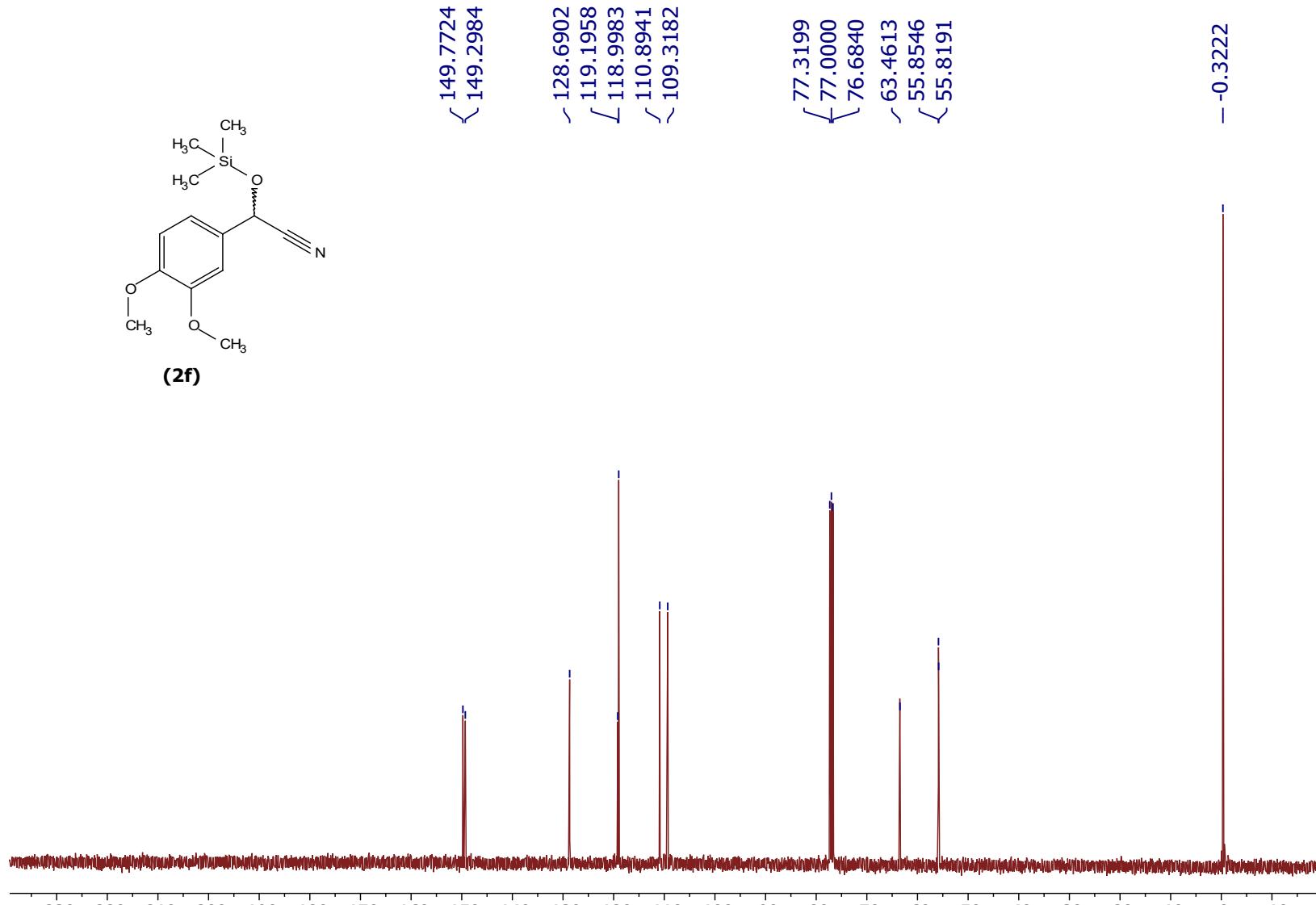
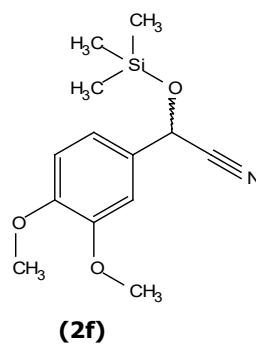
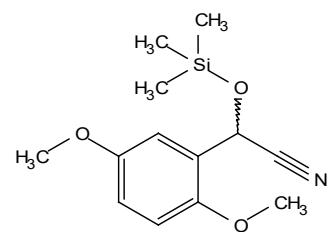


Figure S12. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **2f** in CDCl_3 .



(2g)

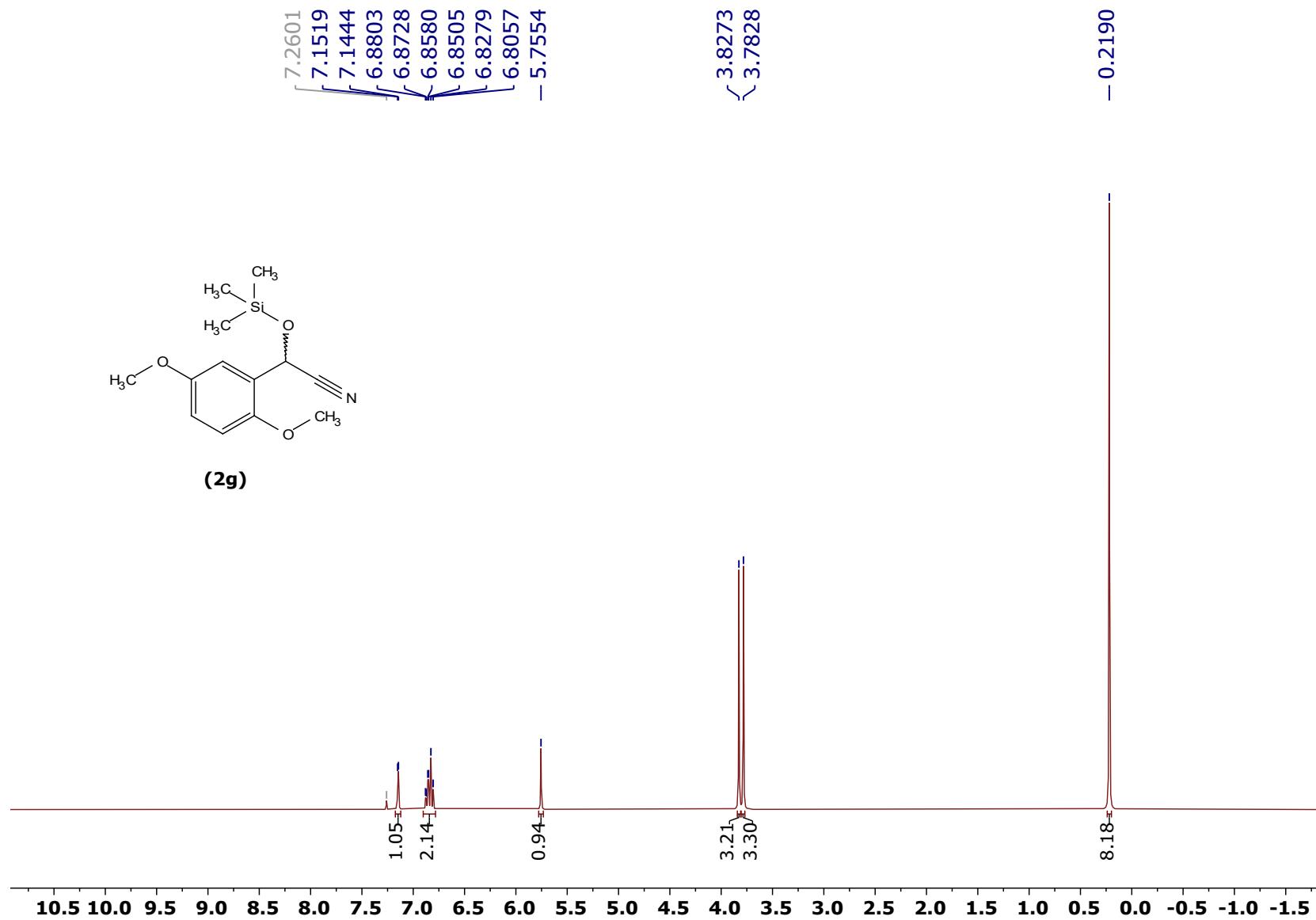
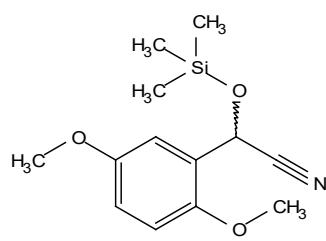


Figure S13. ^1H NMR spectrum of **2g** in CDCl_3 .



(2g)

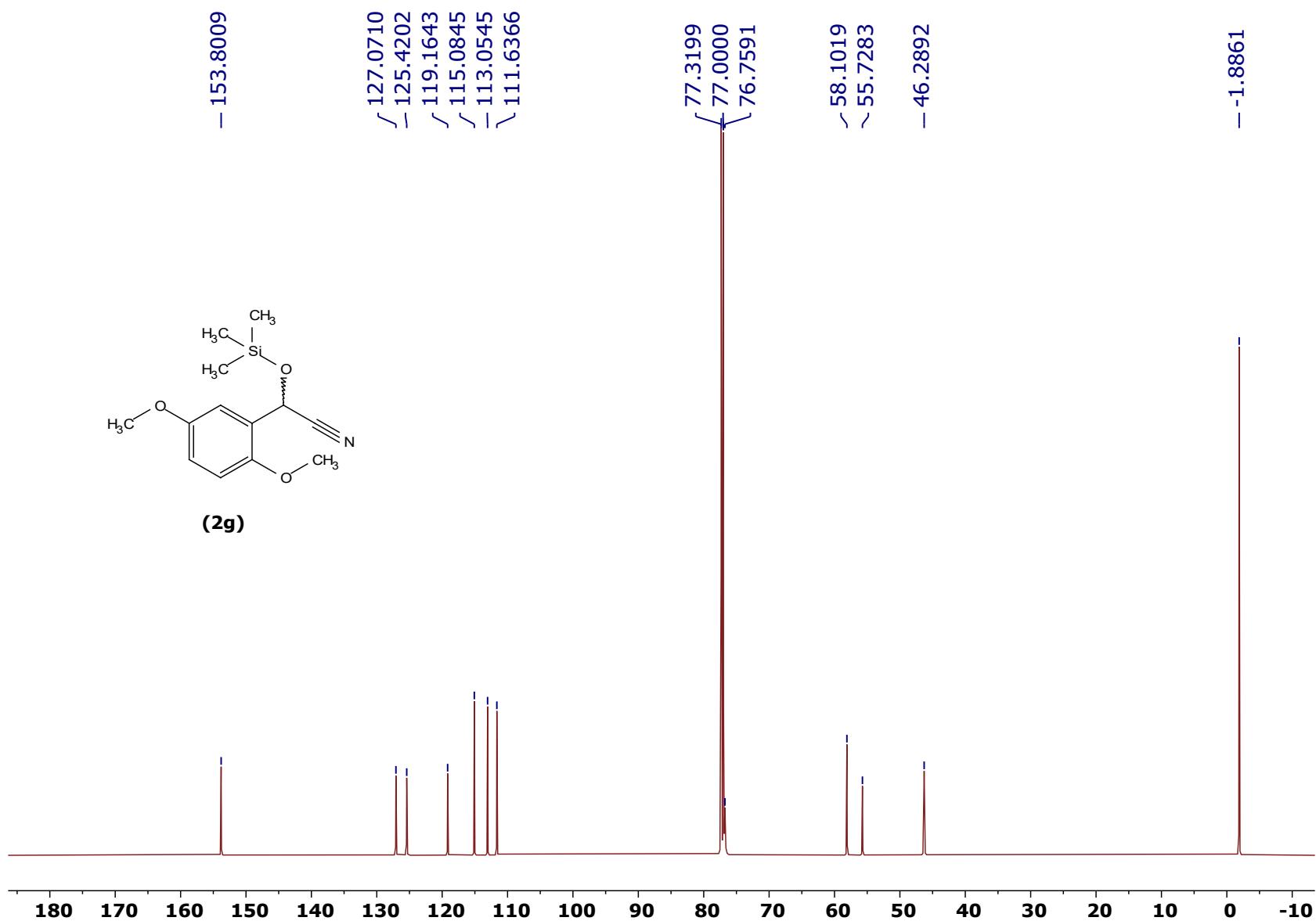


Figure S14. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **2g** in CDCl_3 .

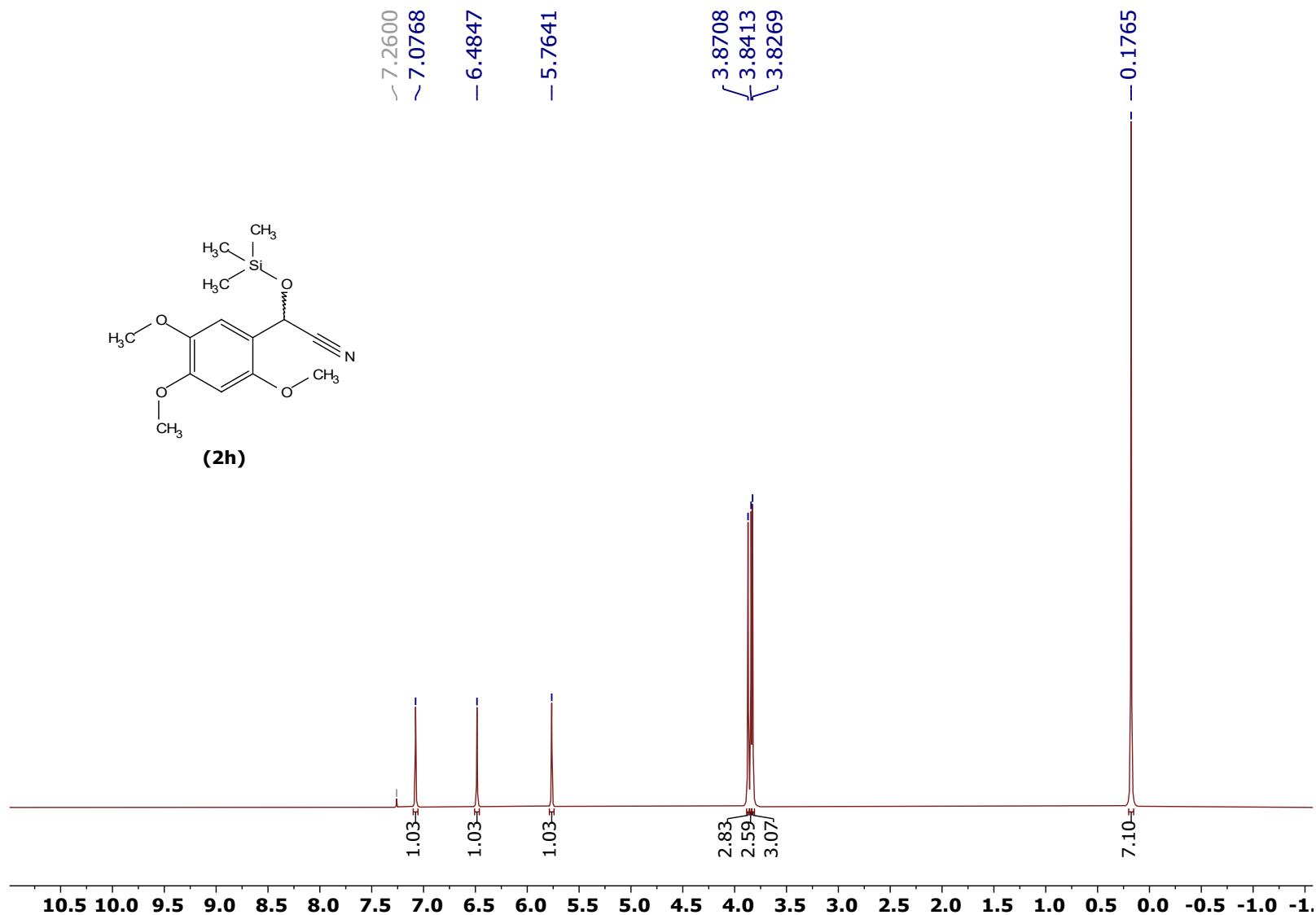
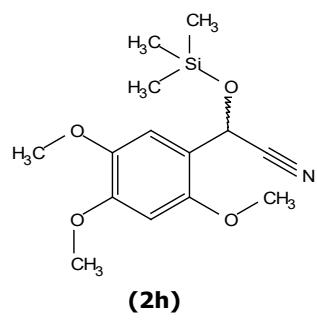


Figure S15. ^1H NMR spectrum of **2h** in CDCl_3 .

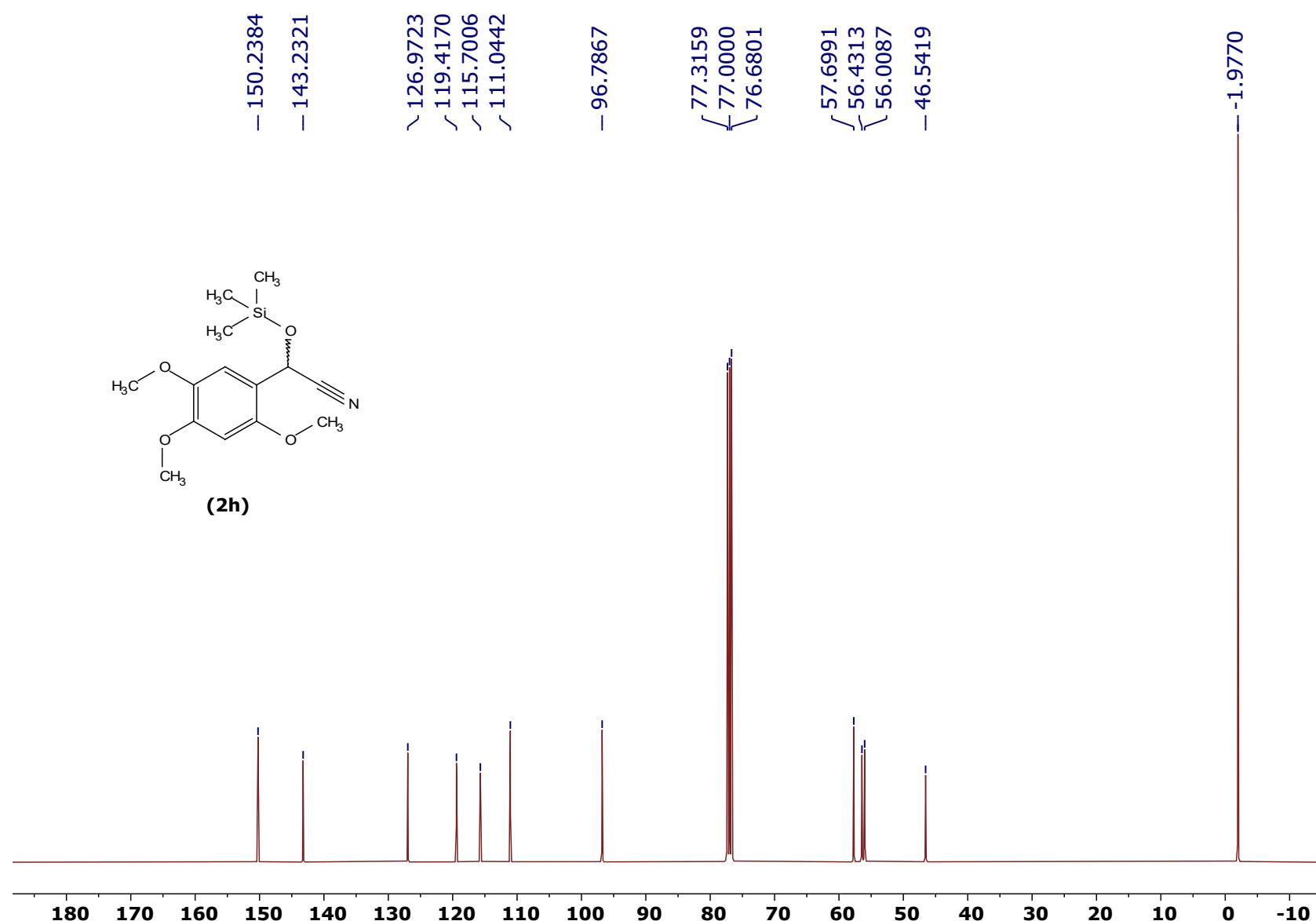


Figure S16. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **2h** in CDCl_3 .

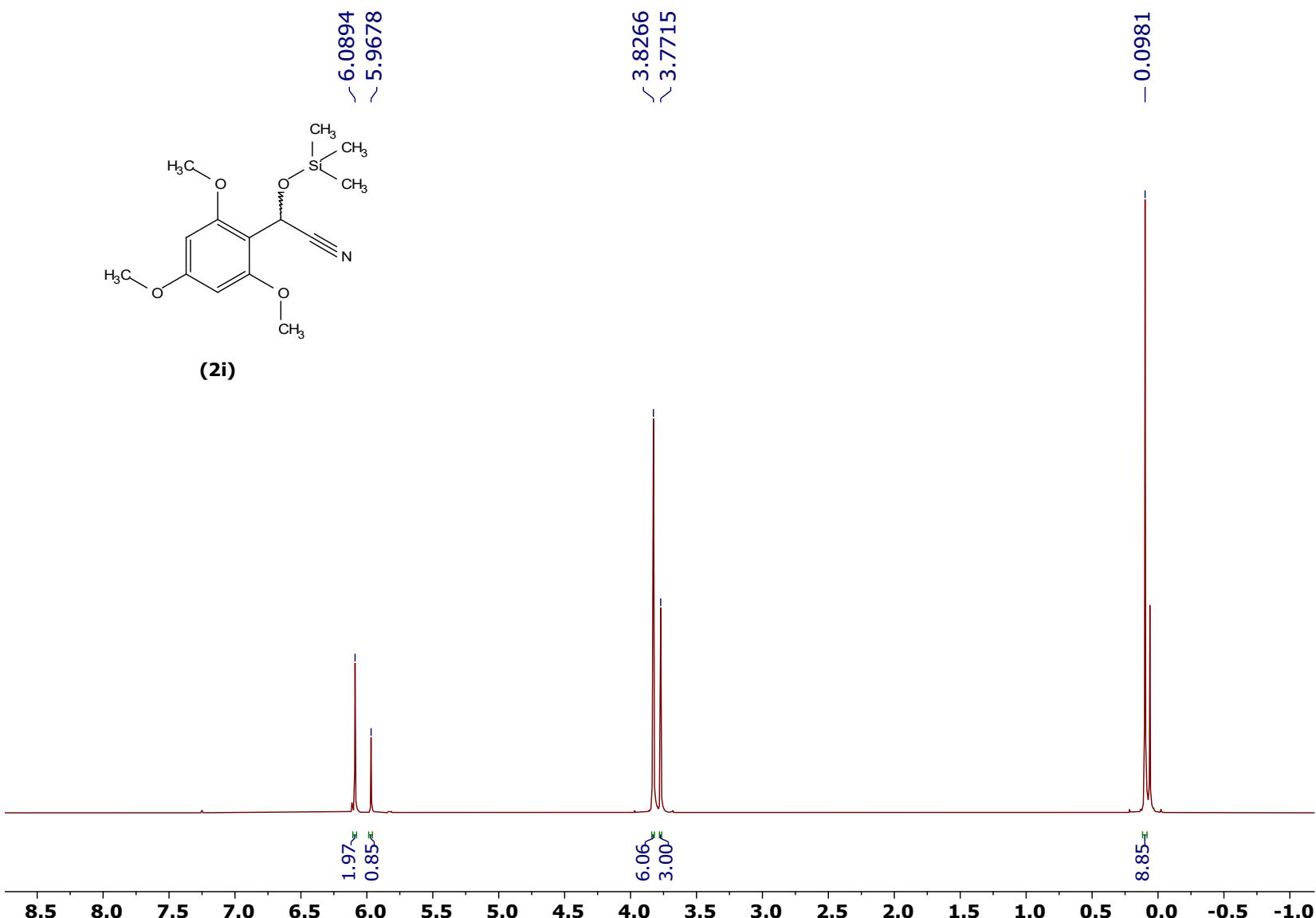
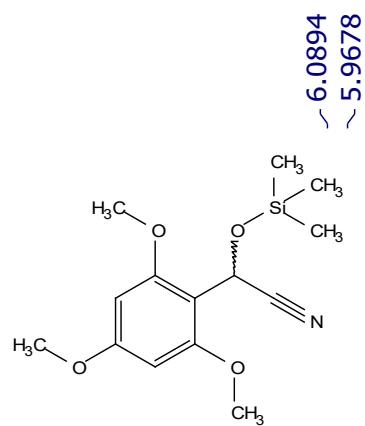


Figure S17. ^1H NMR spectrum of **2i** in CDCl_3 .

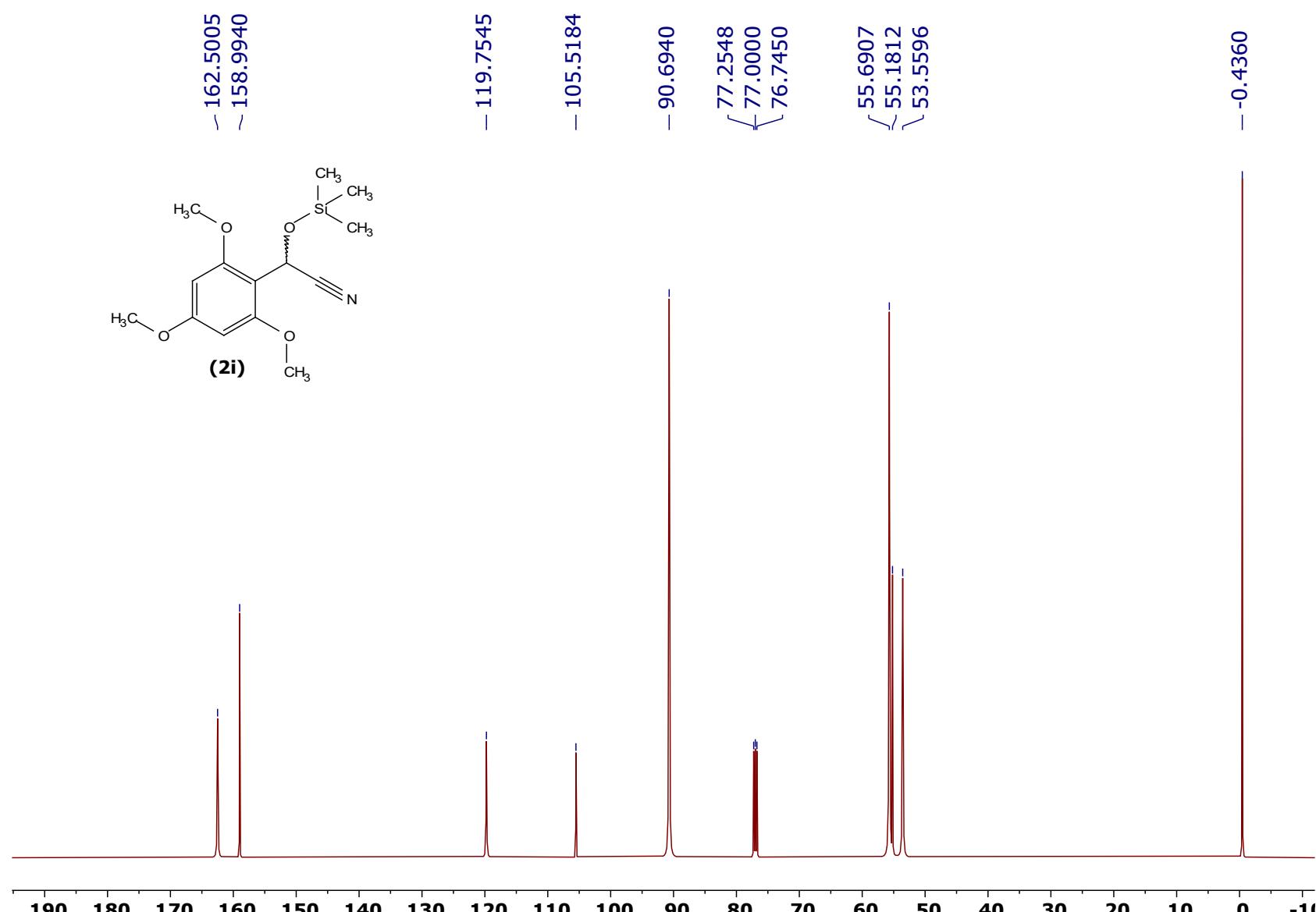


Figure S18. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **2i** in CDCl_3 .

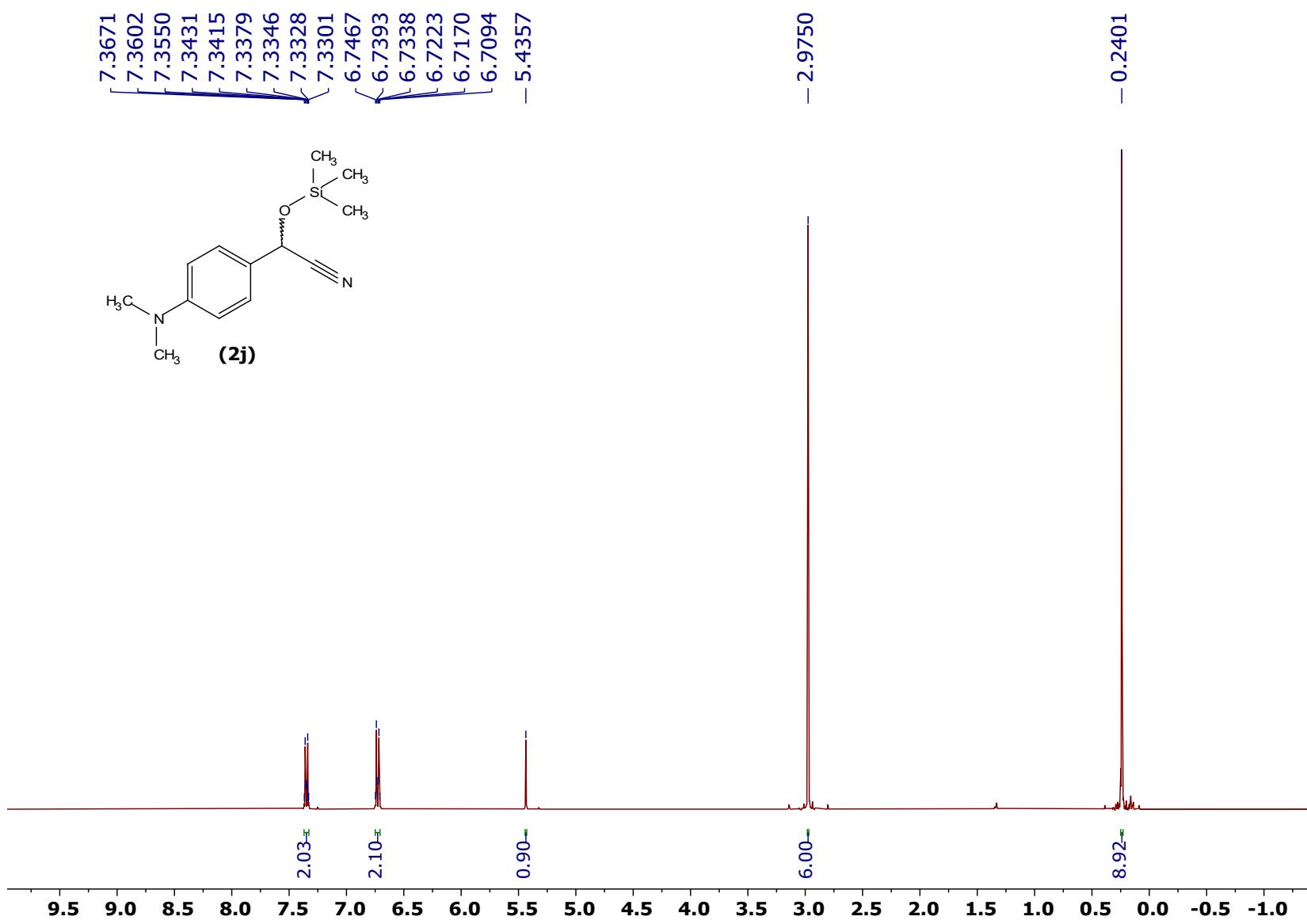


Figure S19. ^1H NMR spectrum of **2j** in CDCl_3 .

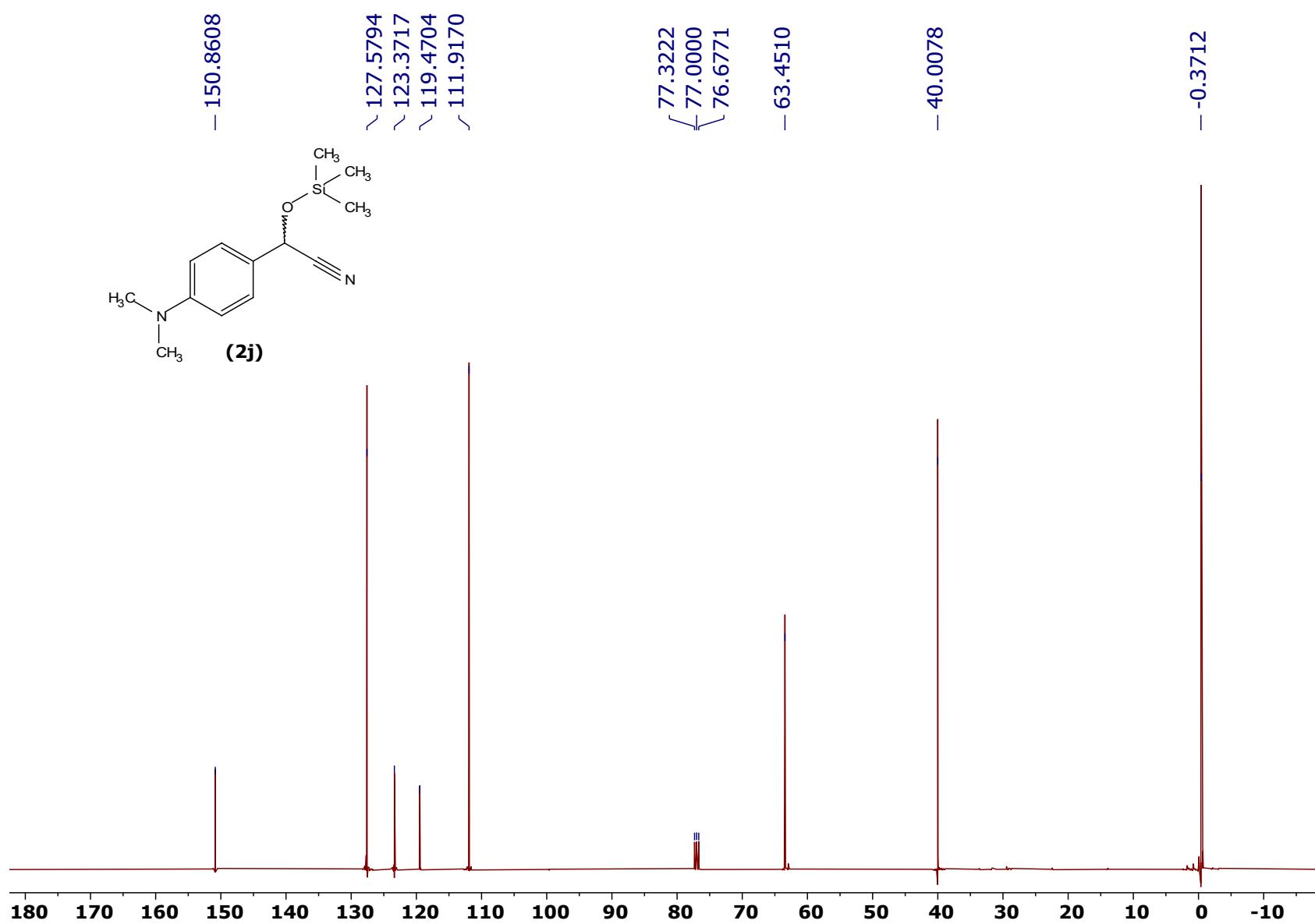


Figure S20. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **2j** in CDCl_3 .

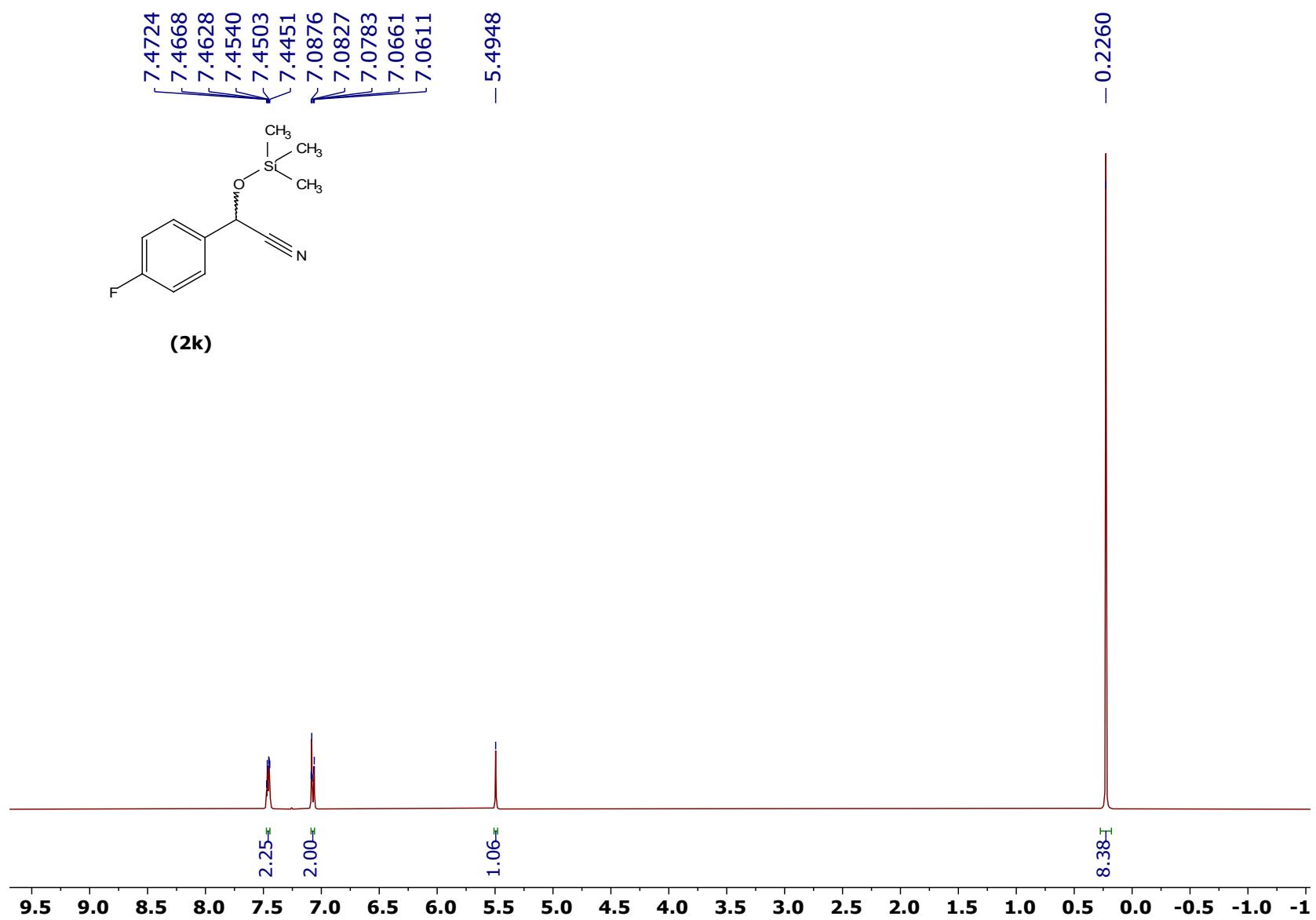


Figure S21. ¹H NMR spectrum of **2k** in CDCl₃.

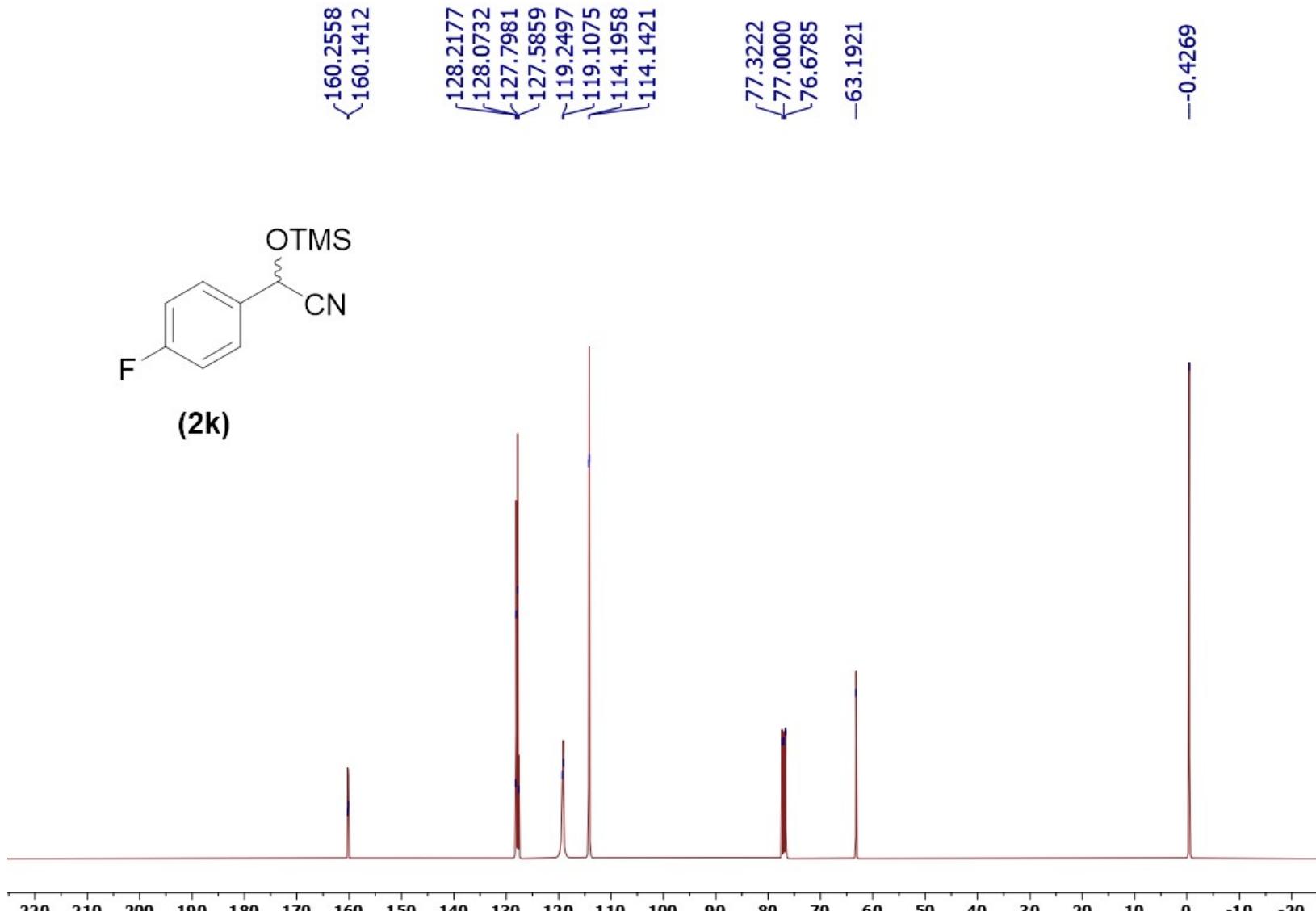


Figure S22. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **2k** in CDCl_3 .

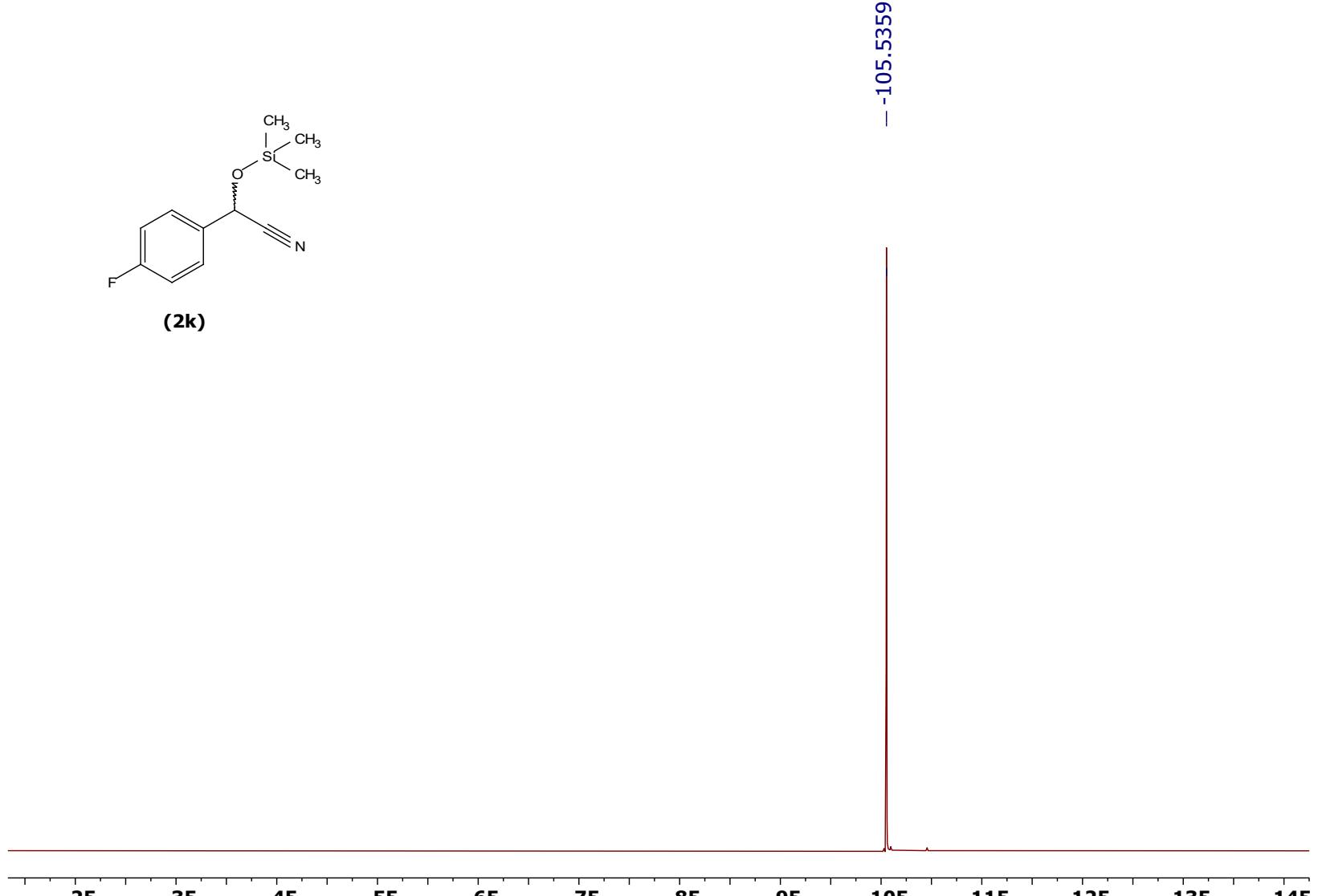
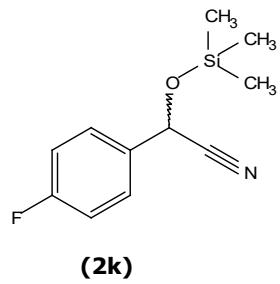


Figure S23. ^{19}F NMR spectrum of **2k** in CDCl_3 .

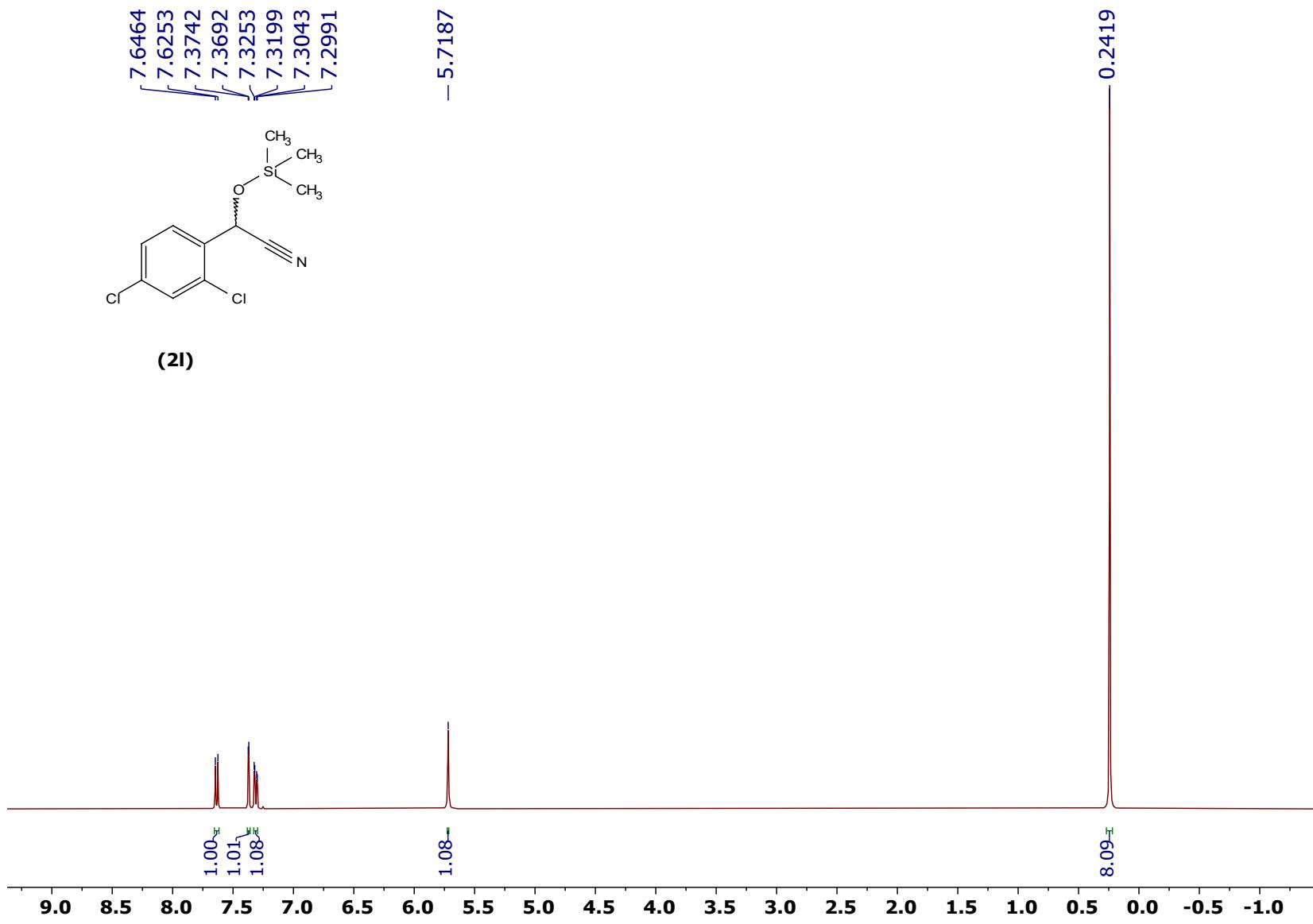
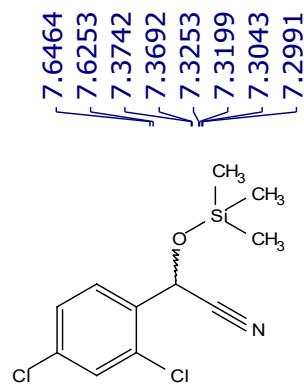


Figure S24. ^1H NMR spectrum of **2l** in CDCl_3 .

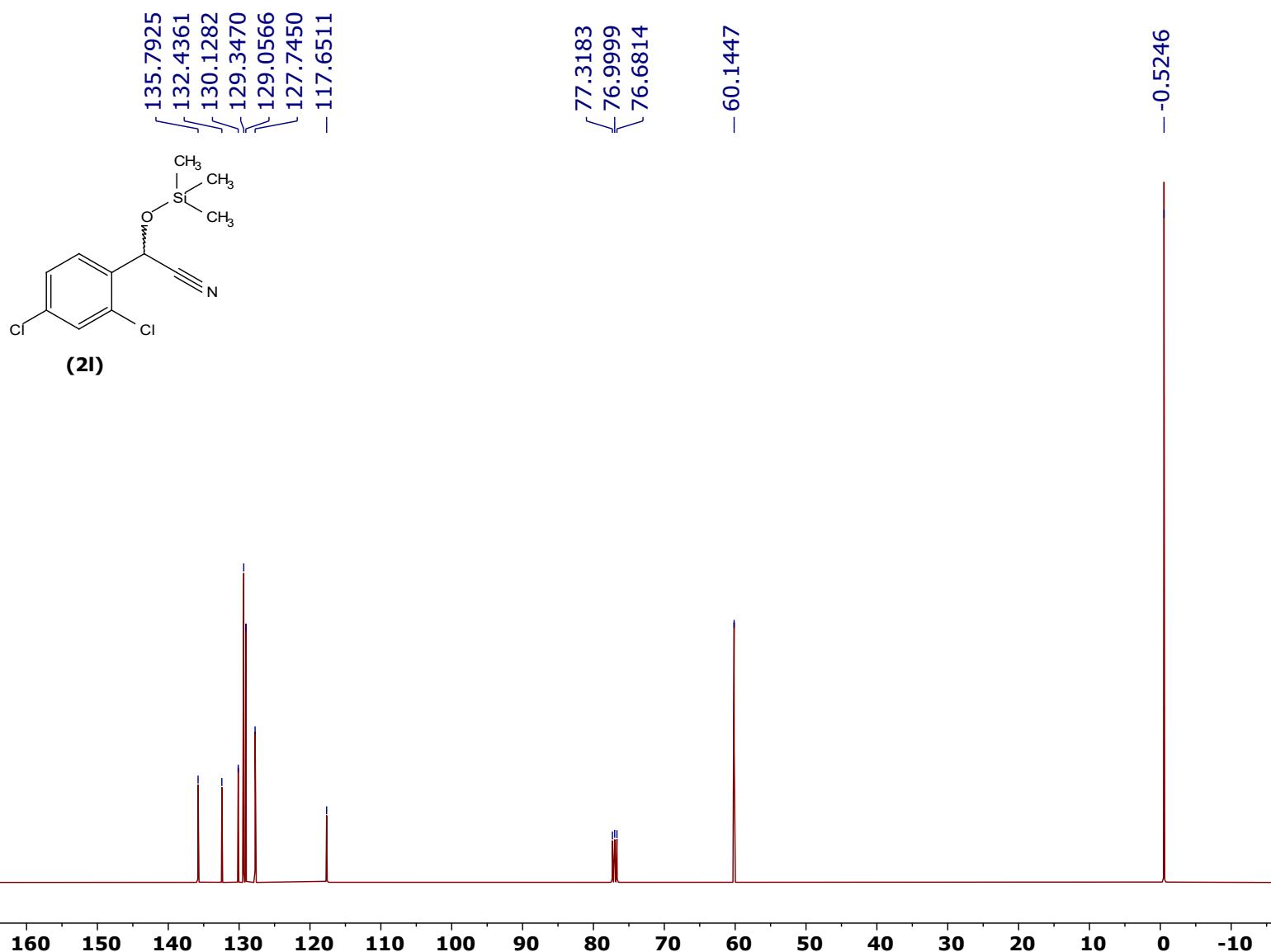
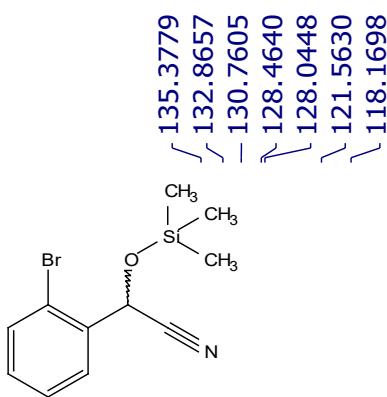


Figure S25. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **2I** in CDCl_3 .



Figure S26. ^1H NMR spectrum of **2m** in CDCl_3 .



(2m)

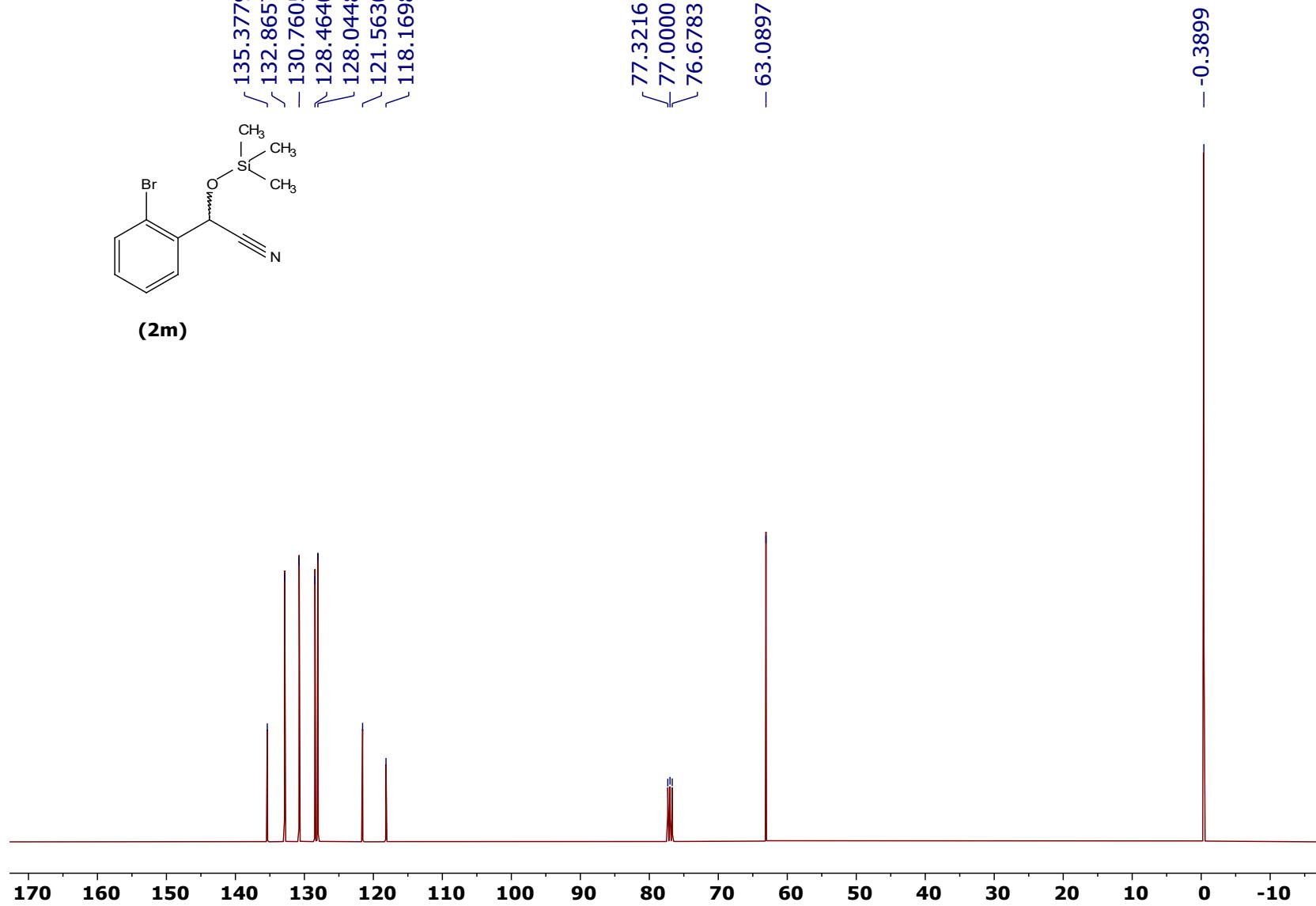


Figure S27. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **2m** in CDCl_3 .

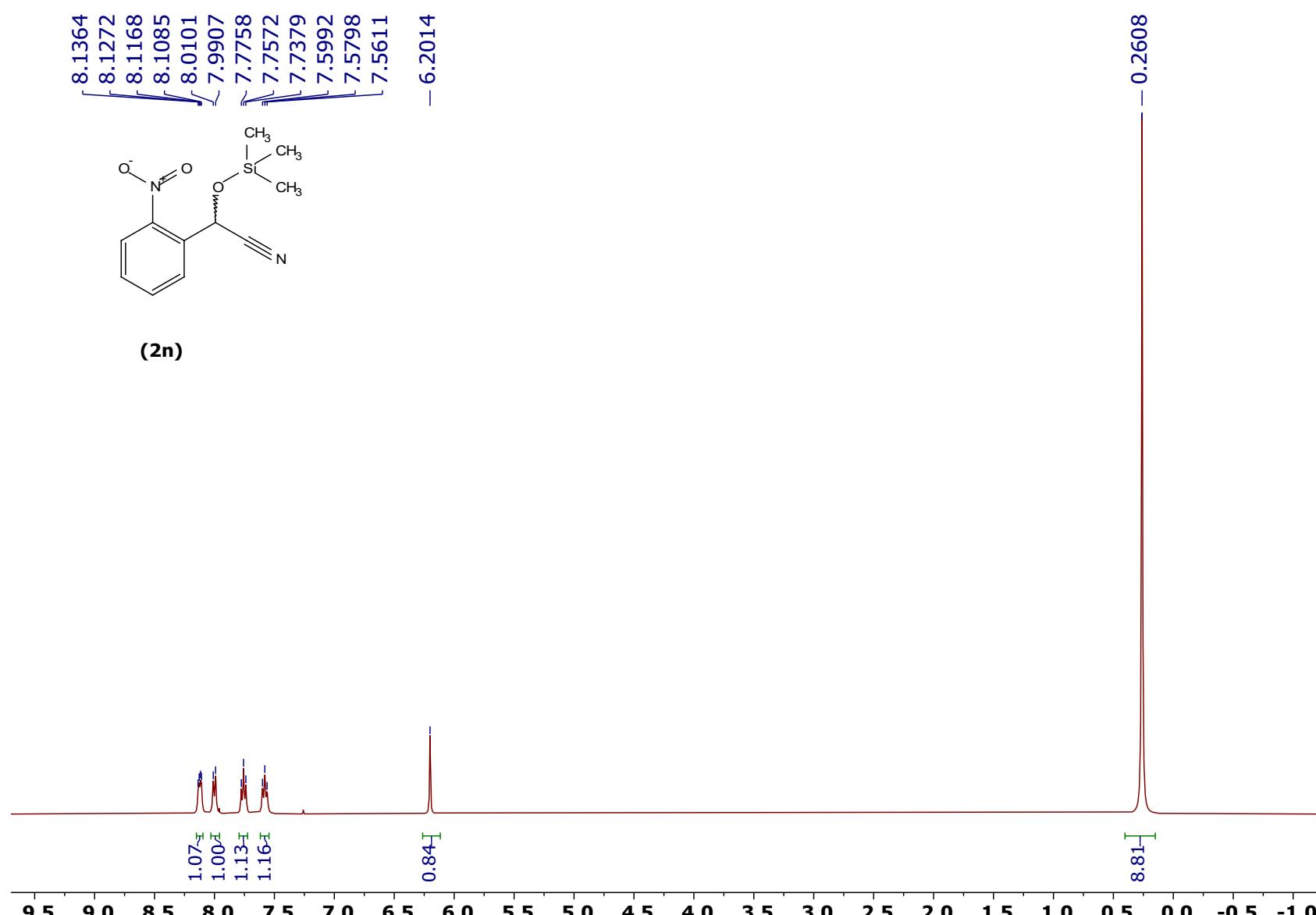


Figure S28. ^1H NMR spectrum of **2n** in CDCl_3 .

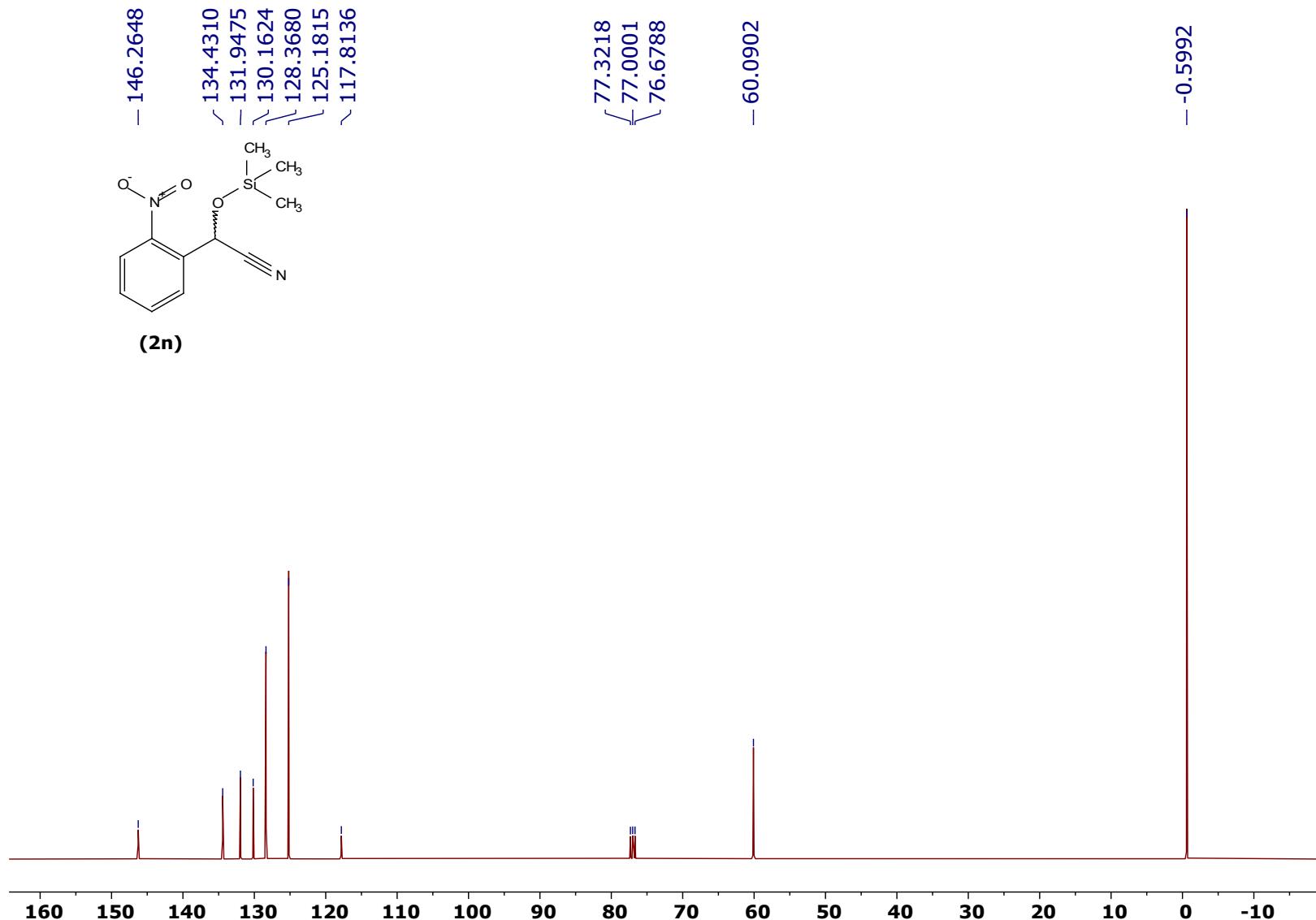


Figure S29. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **2n** in CDCl_3 .

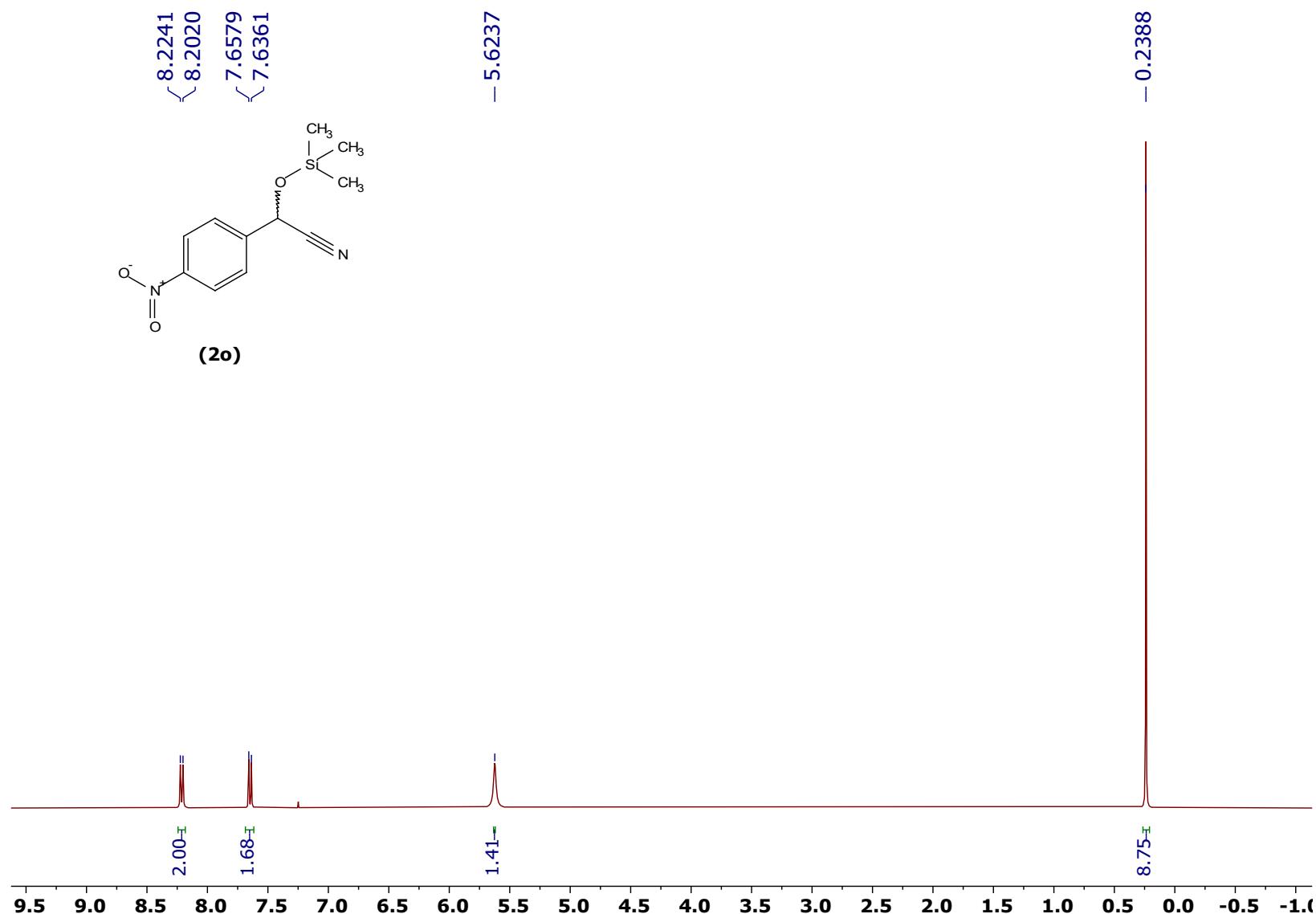


Figure S30. ^1H NMR spectrum of **2o** in CDCl_3 .

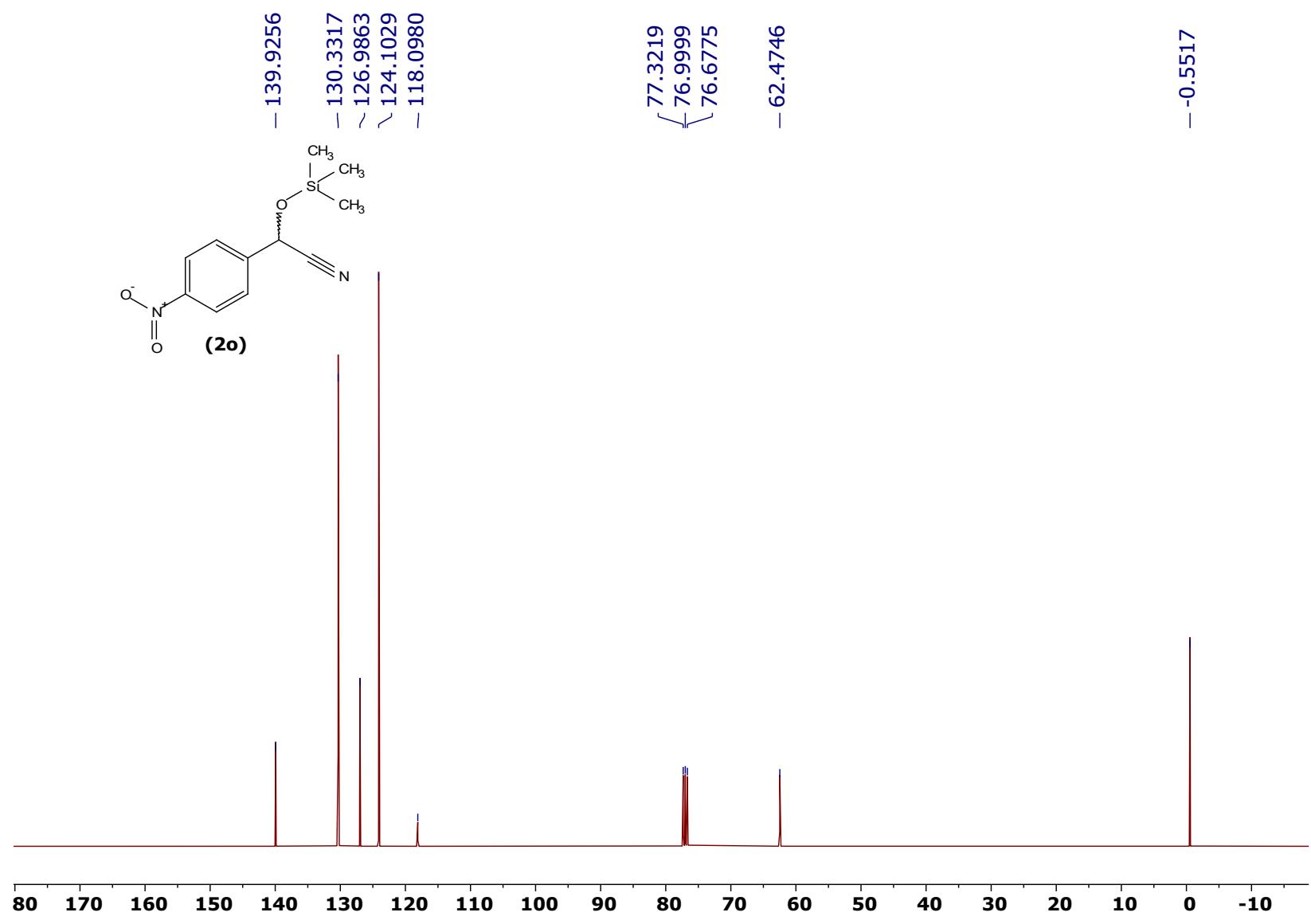


Figure S31. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **2o** in CDCl₃.

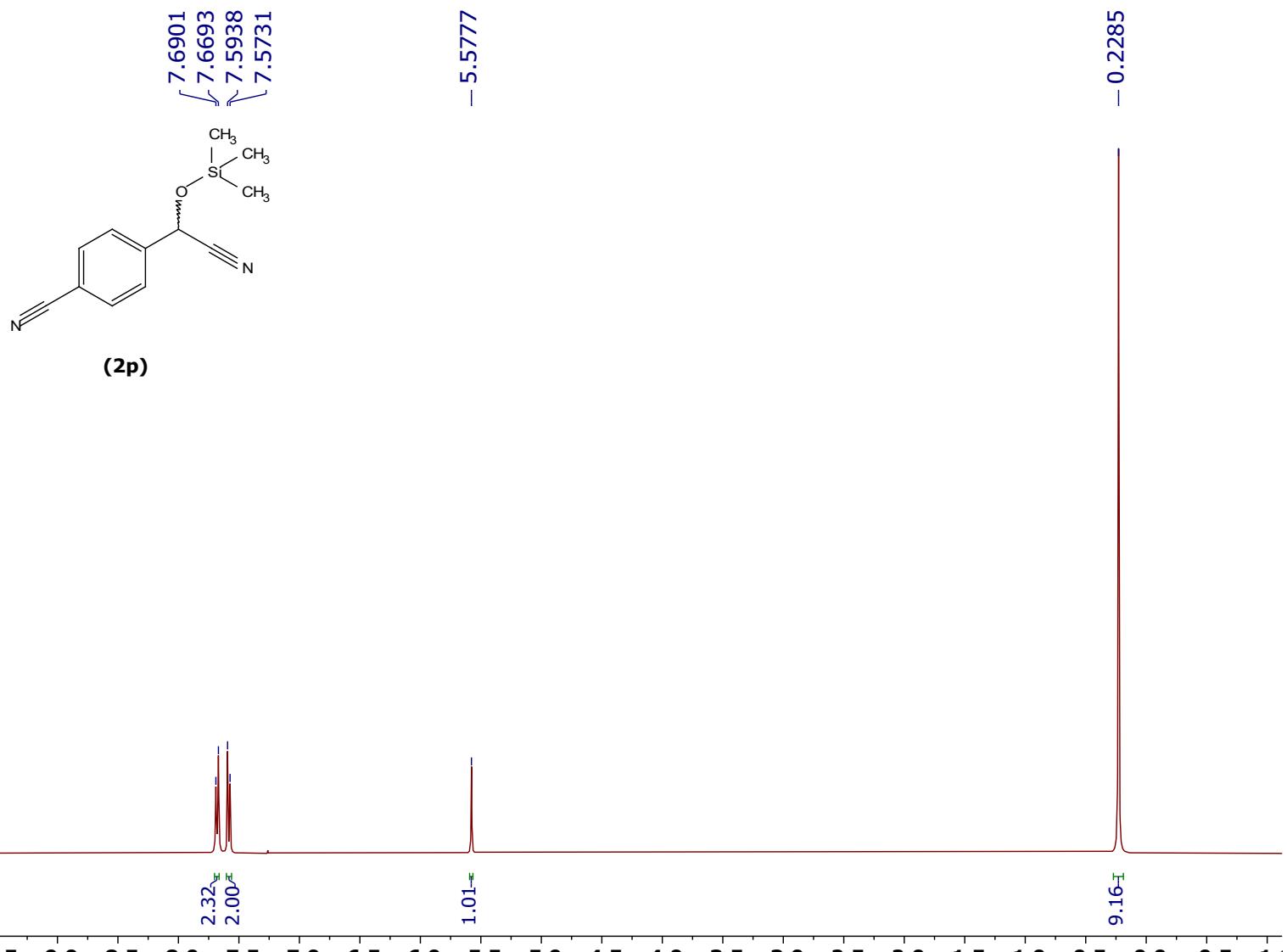


Figure S32. ^1H NMR spectrum of **2p** in CDCl_3 .

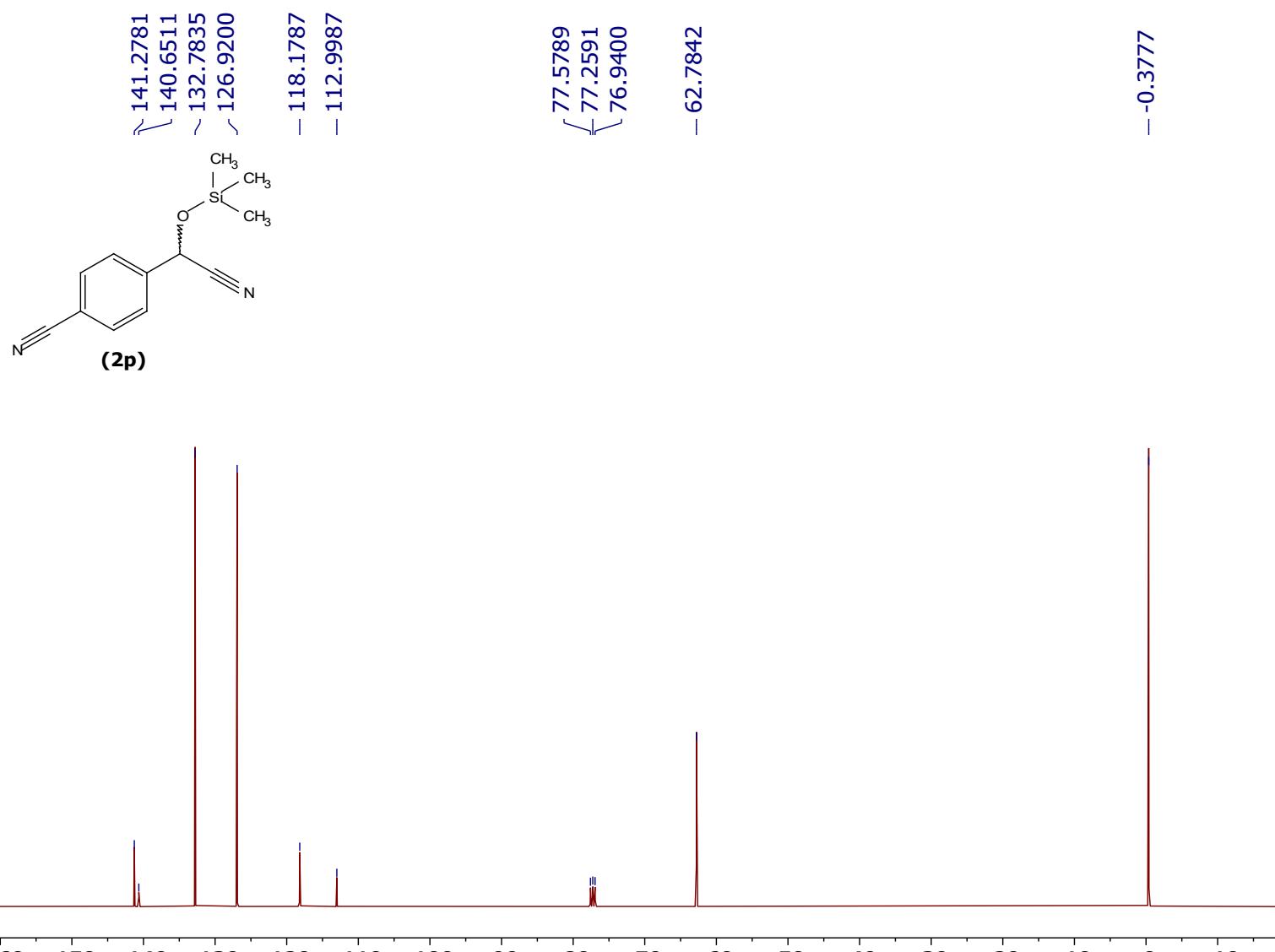


Figure S33. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **2p** in CDCl_3 .

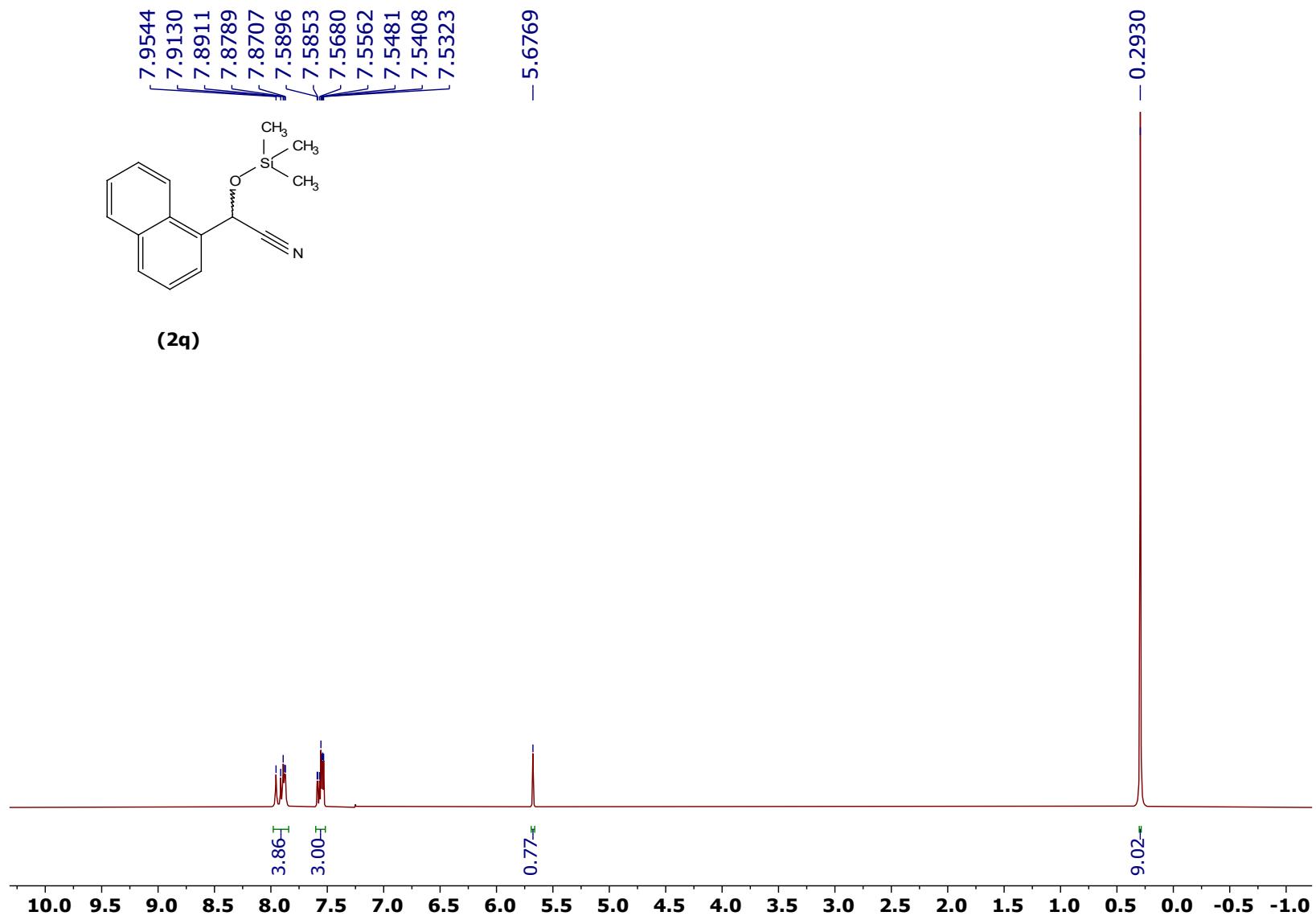
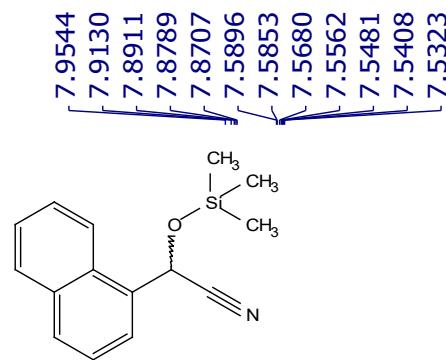


Figure S34. ^1H NMR spectrum of **2q** in CDCl_3 .

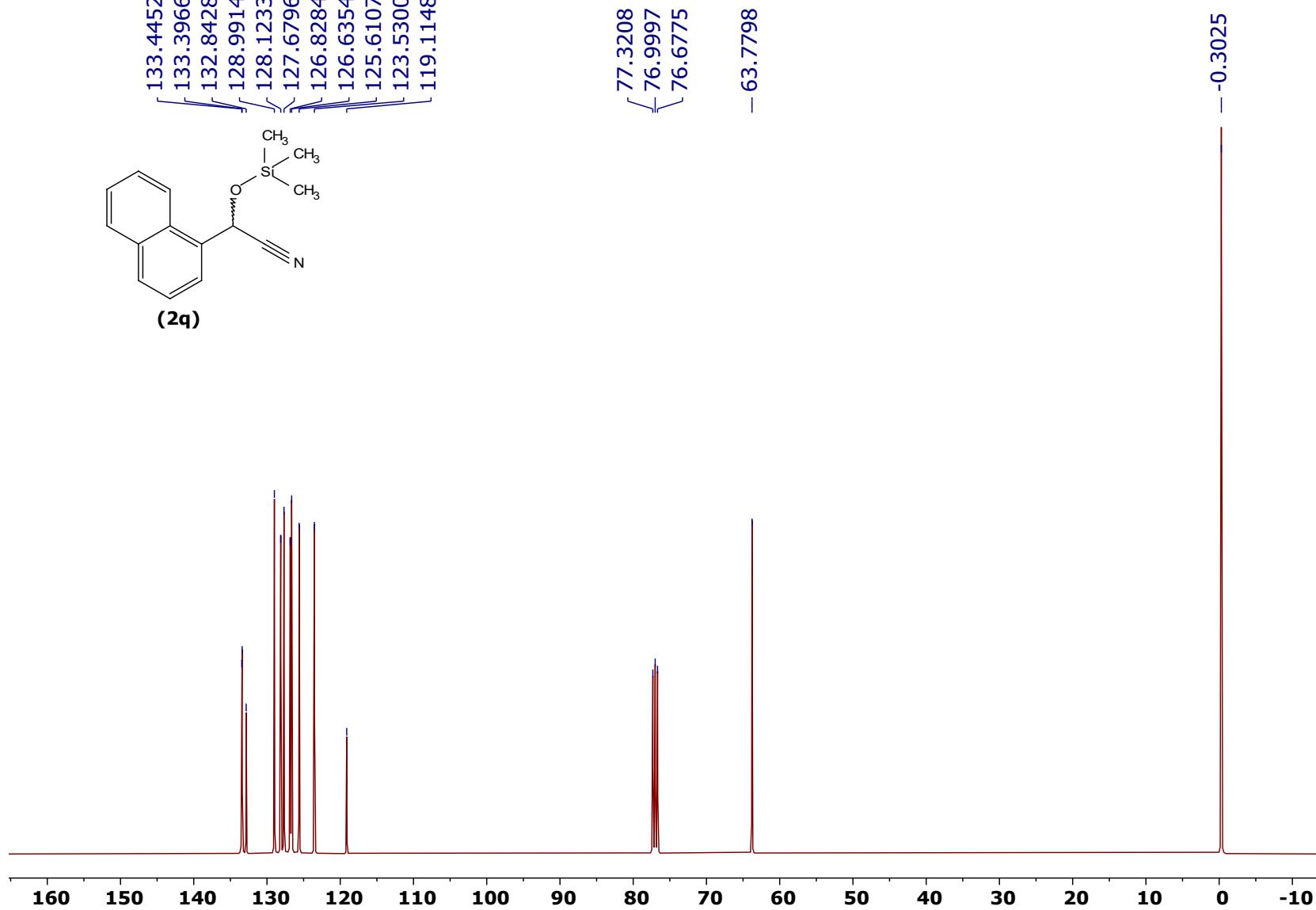
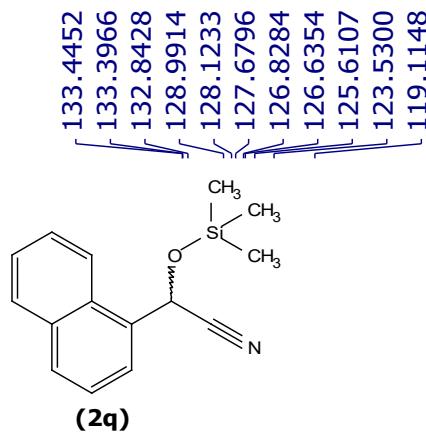


Figure S35. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **2q** in CDCl_3 .

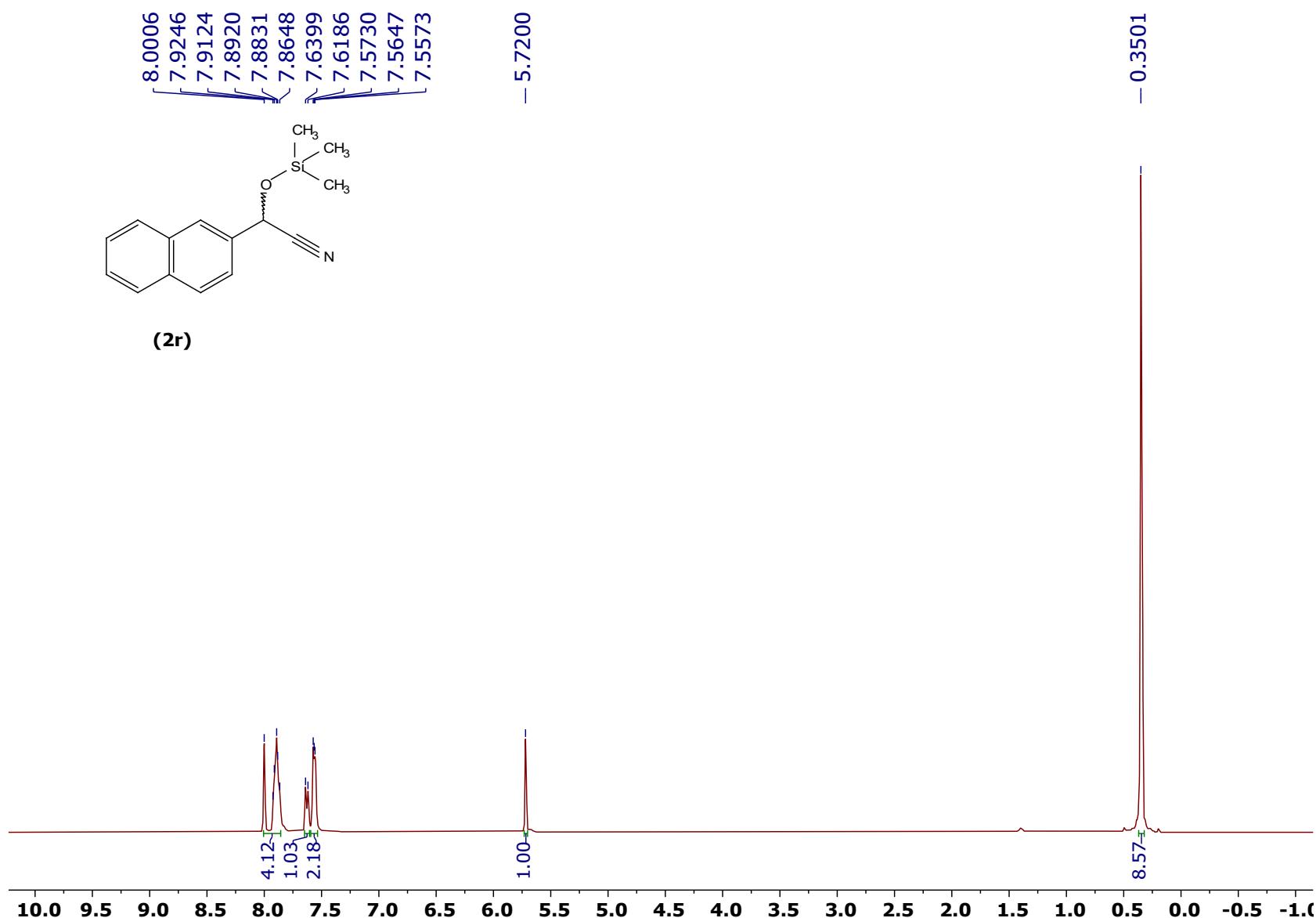


Figure S36. ^1H NMR spectrum of **2r** in CDCl_3 .

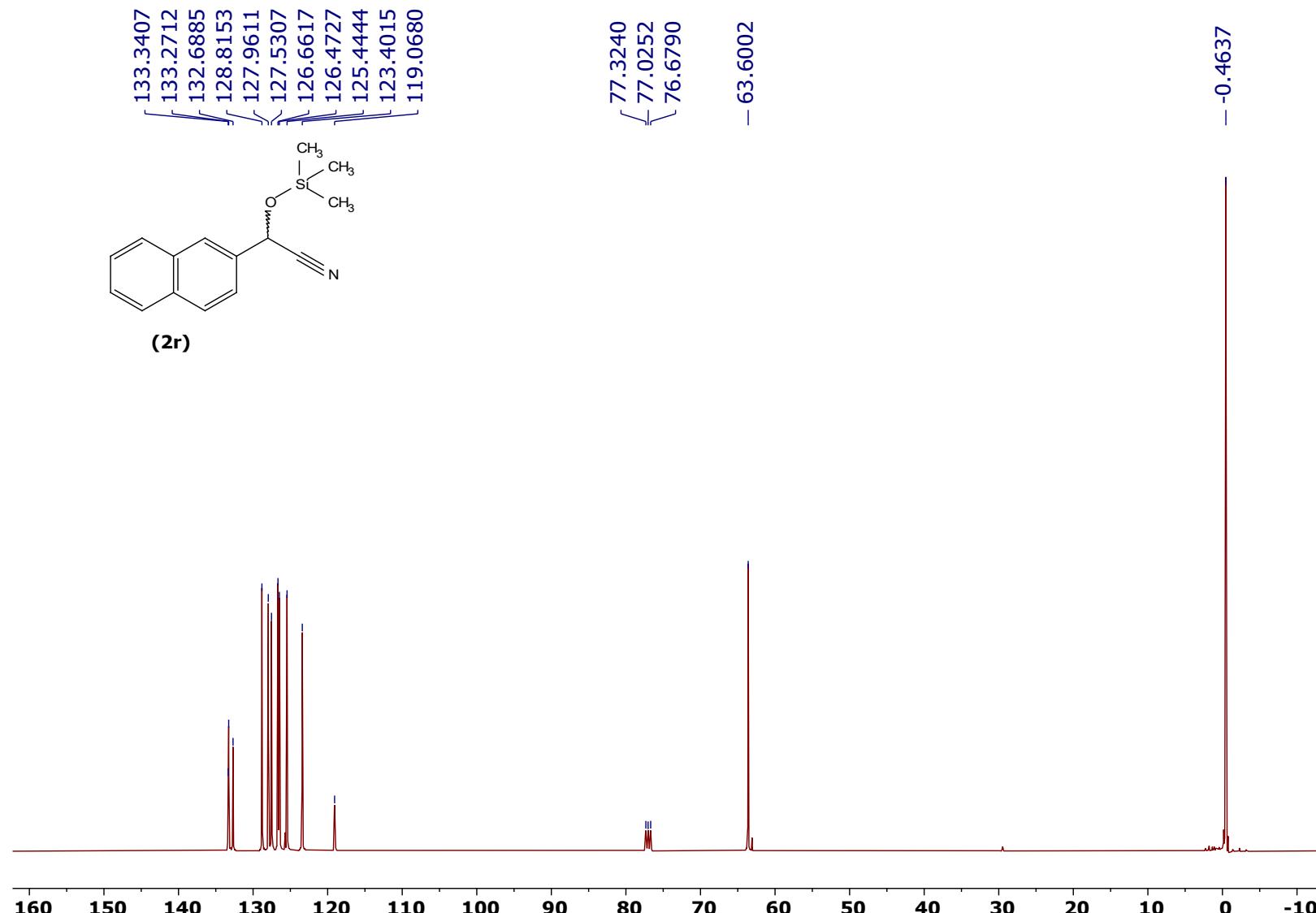
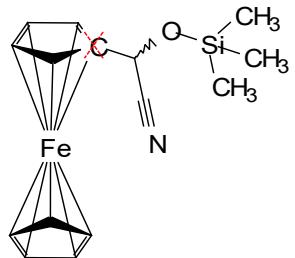


Figure S37. $^{13}\text{C}\{\text{H}\}$ NMR spectrum of **2r** in CDCl_3 .



(2s)

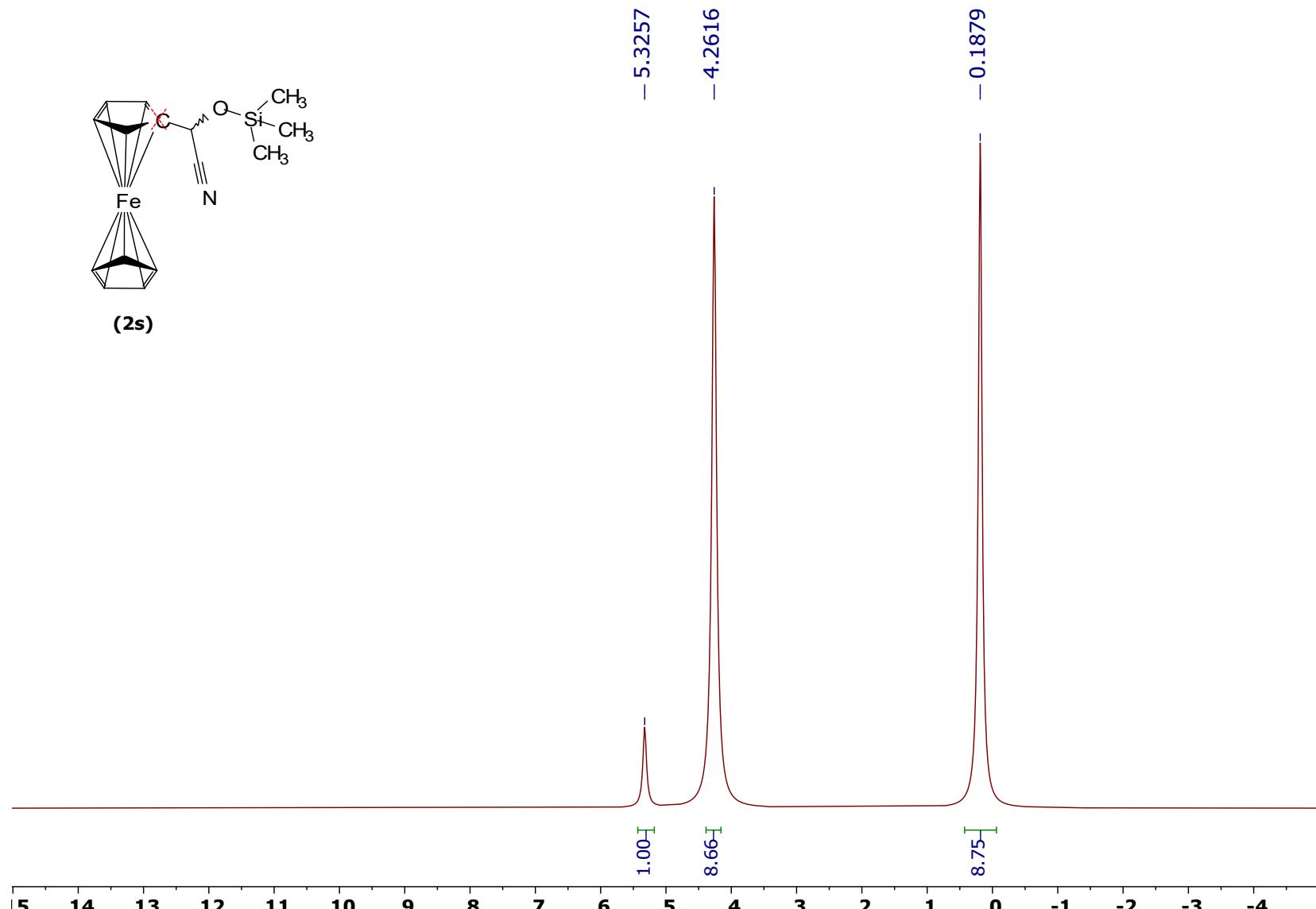


Figure S38. ^1H NMR spectrum of **2s** in CDCl_3 .

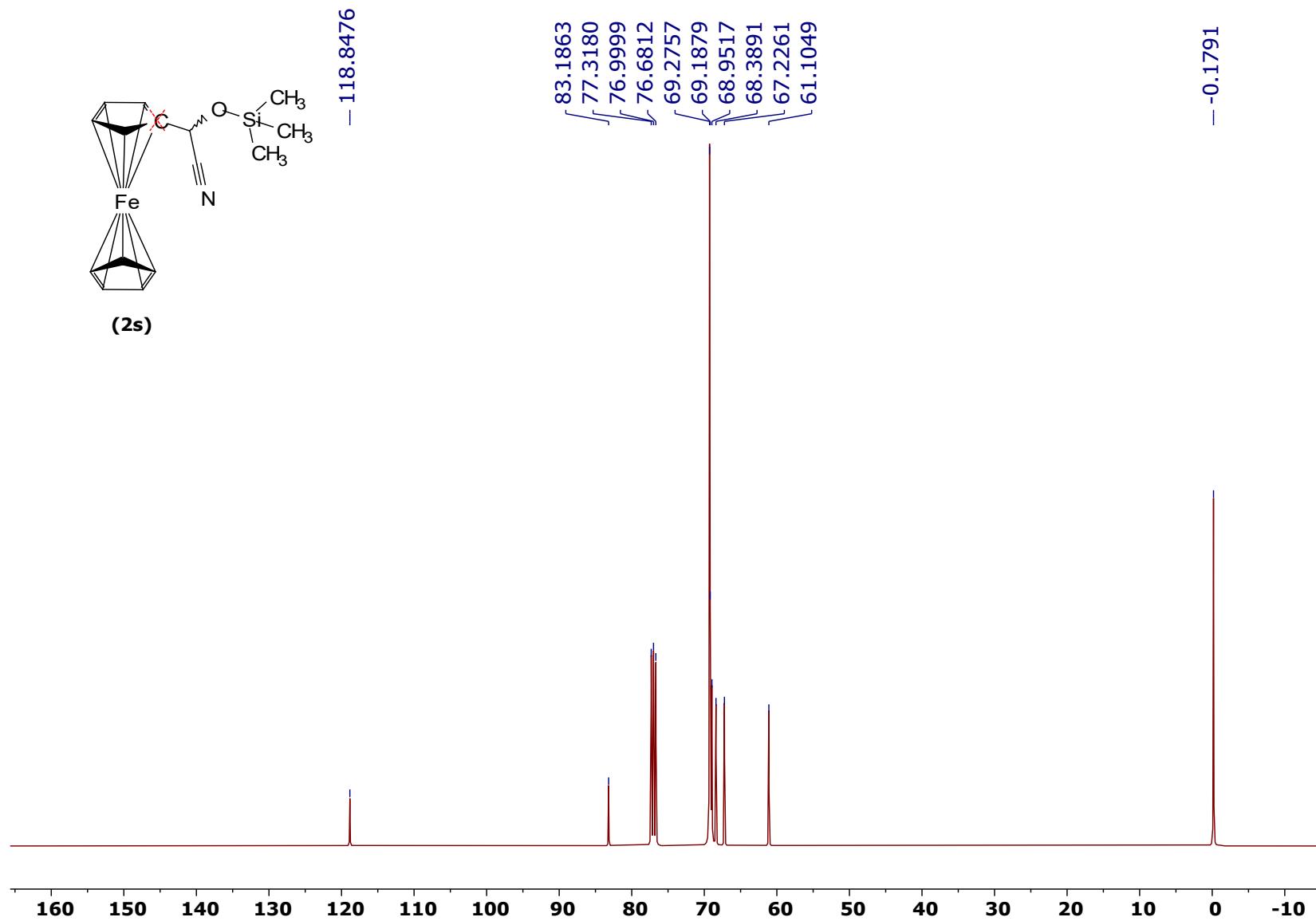


Figure S39. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **2s** in CDCl_3 .

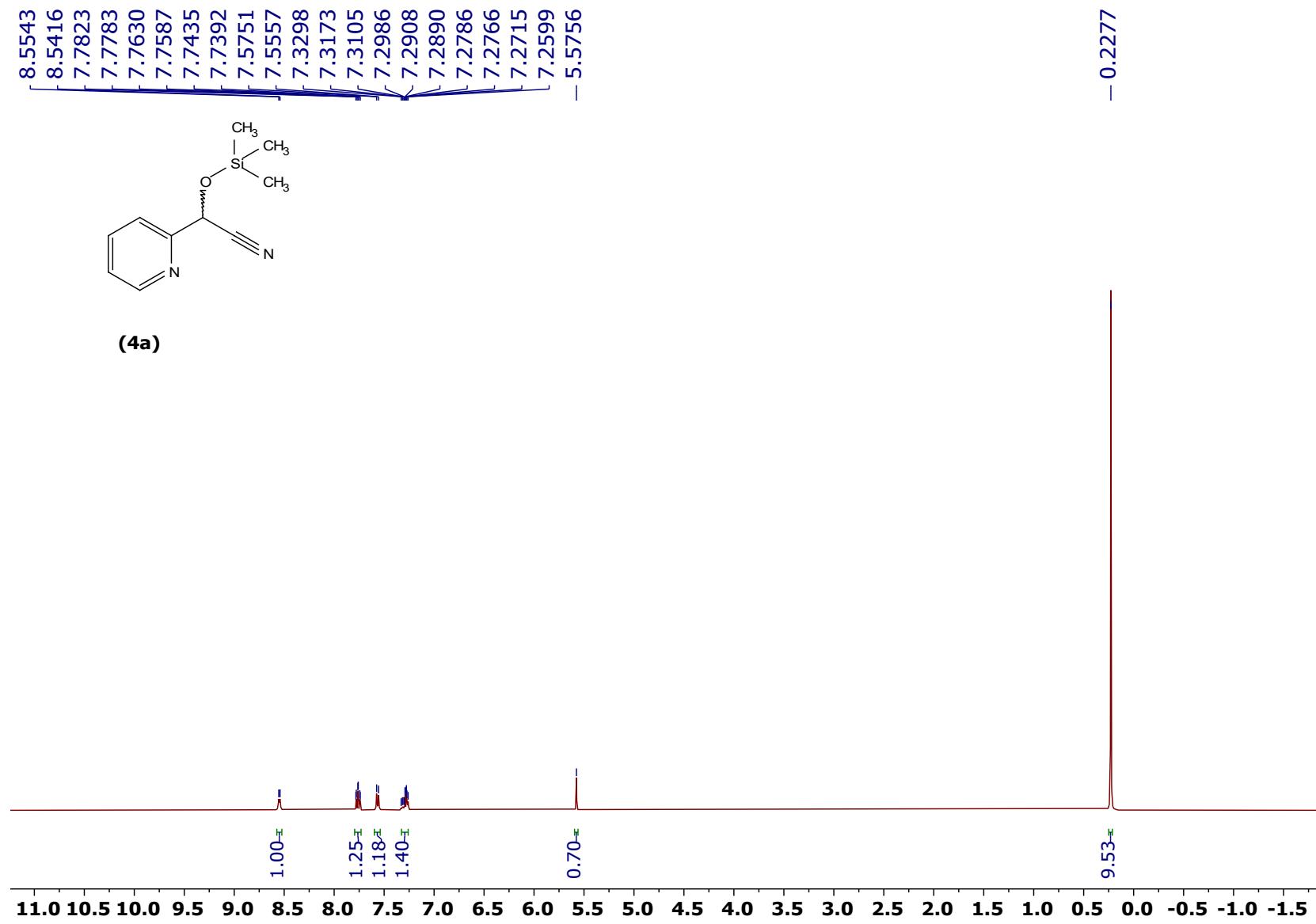


Figure S40. ^1H NMR spectrum of **4a** in CDCl_3 .

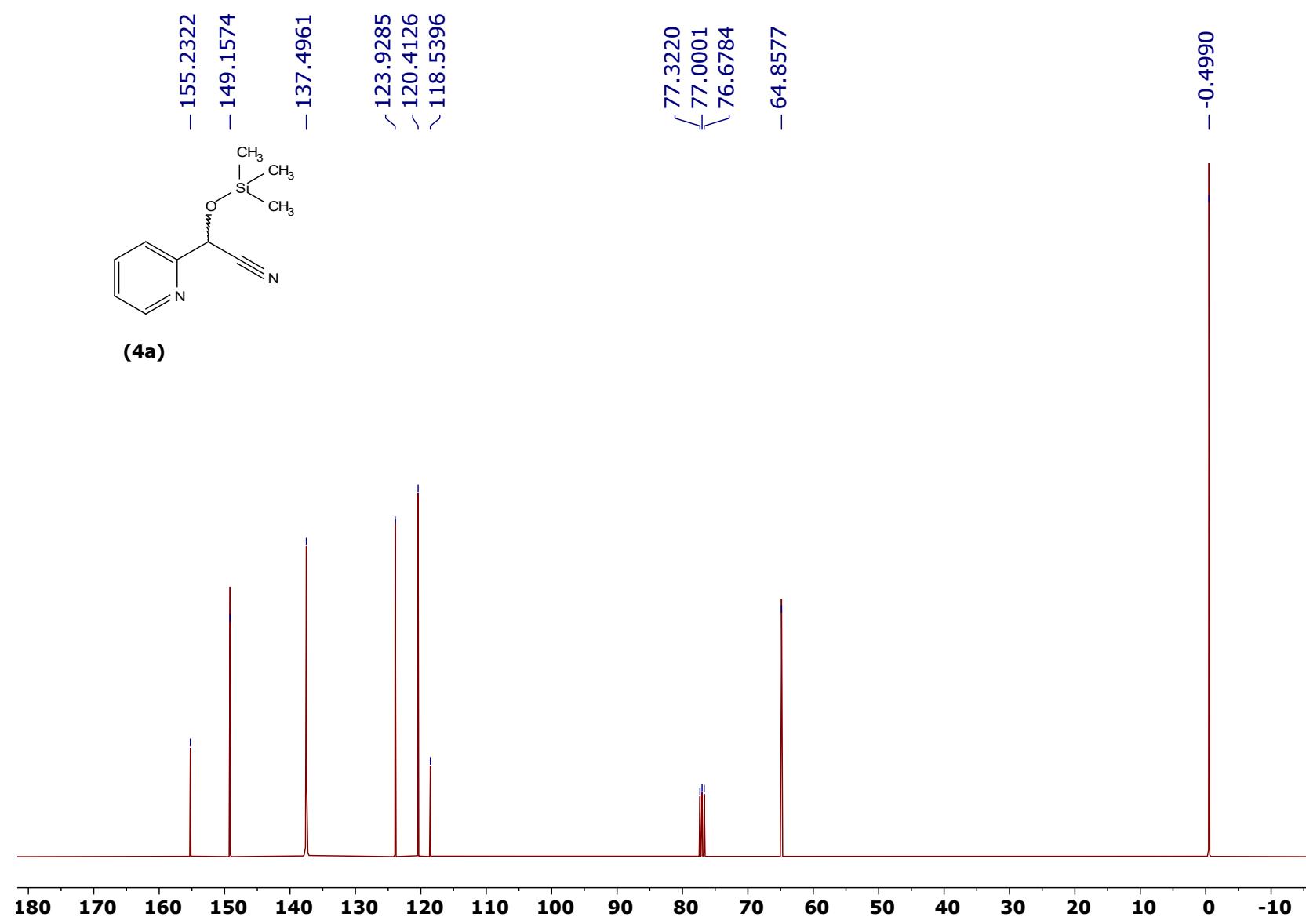


Figure S41. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **4a** in CDCl_3 .

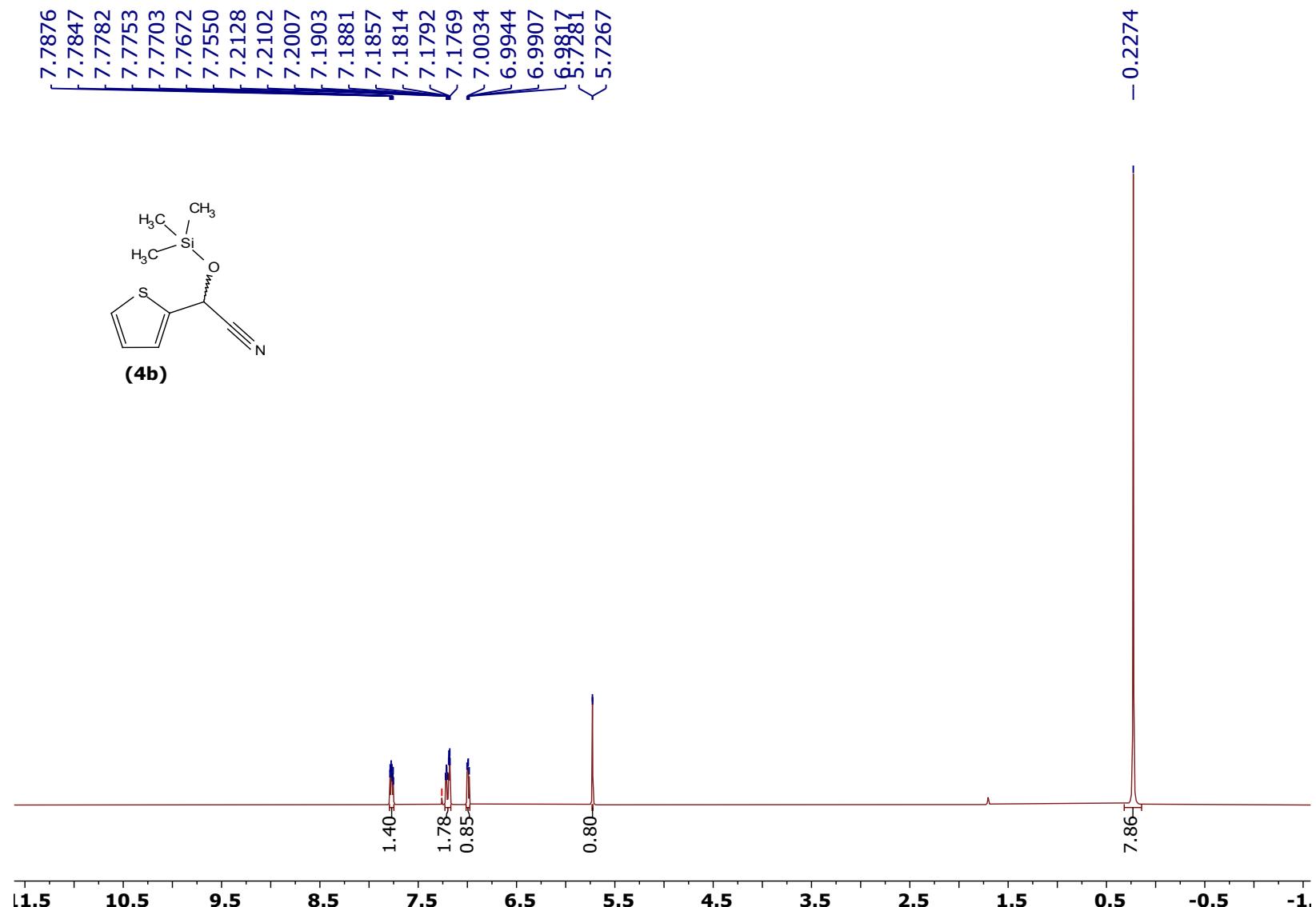


Figure S42. ^1H NMR spectrum of **4b** in CDCl_3 .

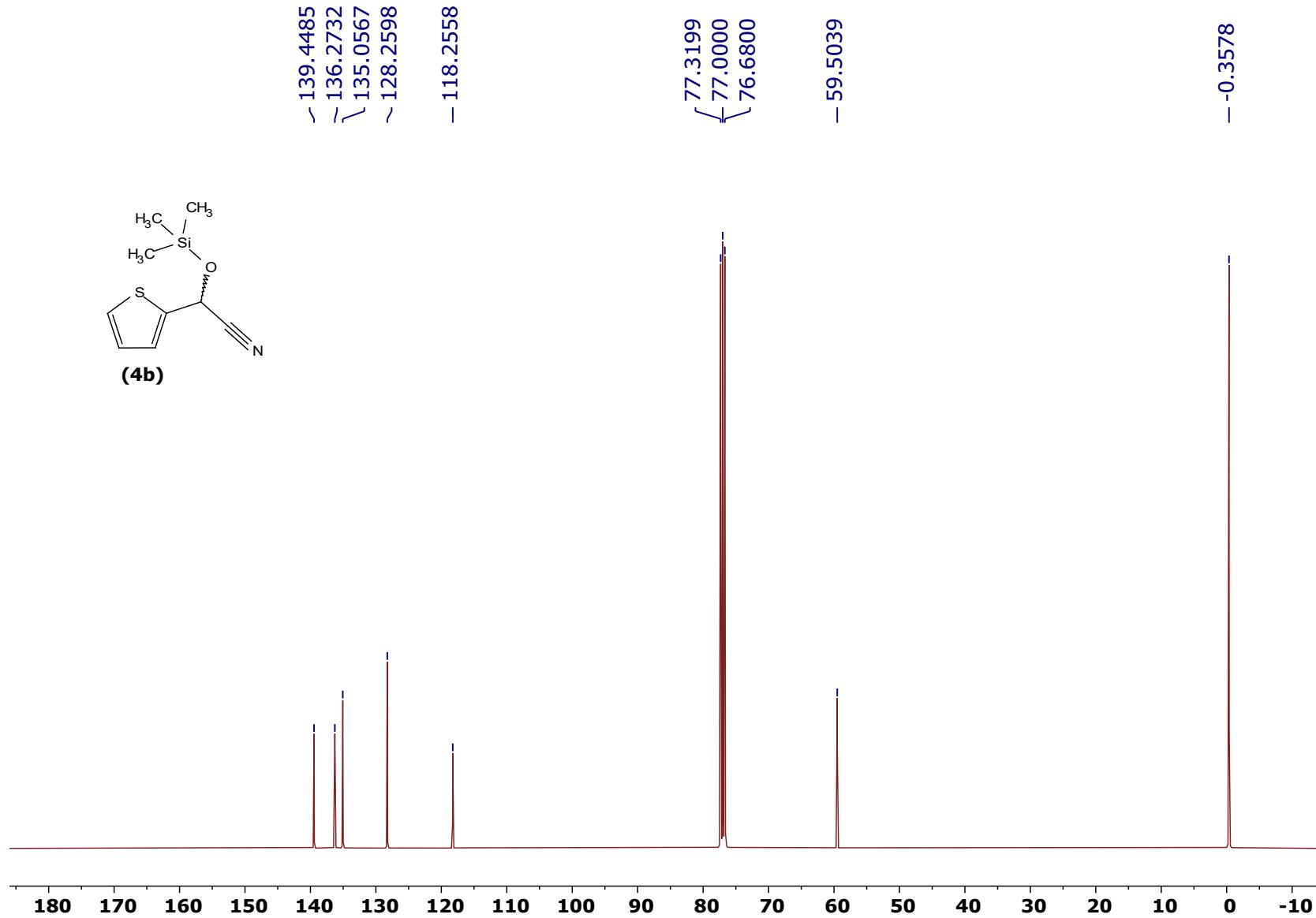
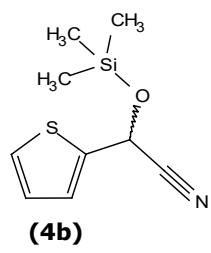


Figure S43. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **4b** in CDCl_3 .

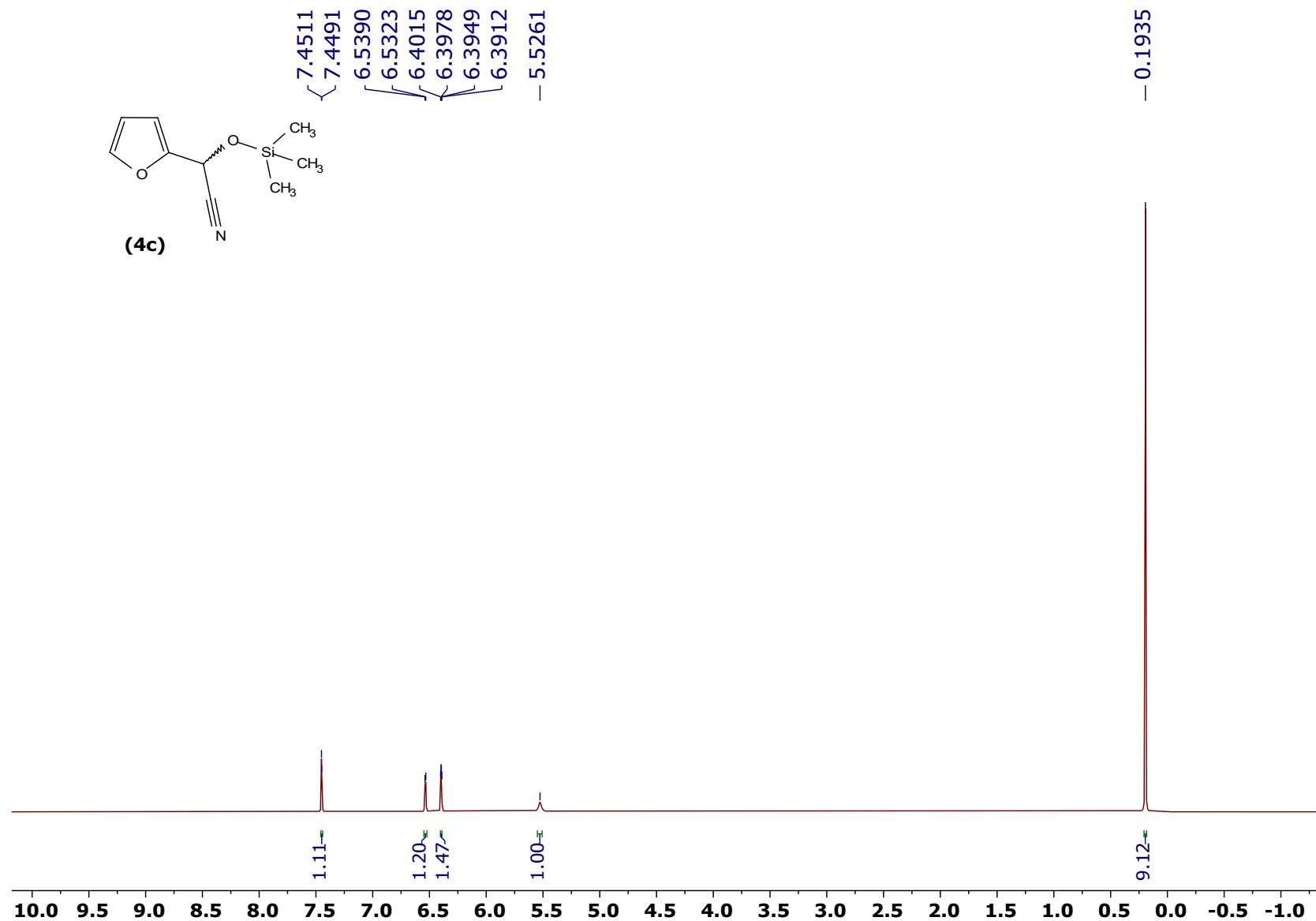


Figure S44. ¹H NMR spectrum of **4c** in CDCl₃.

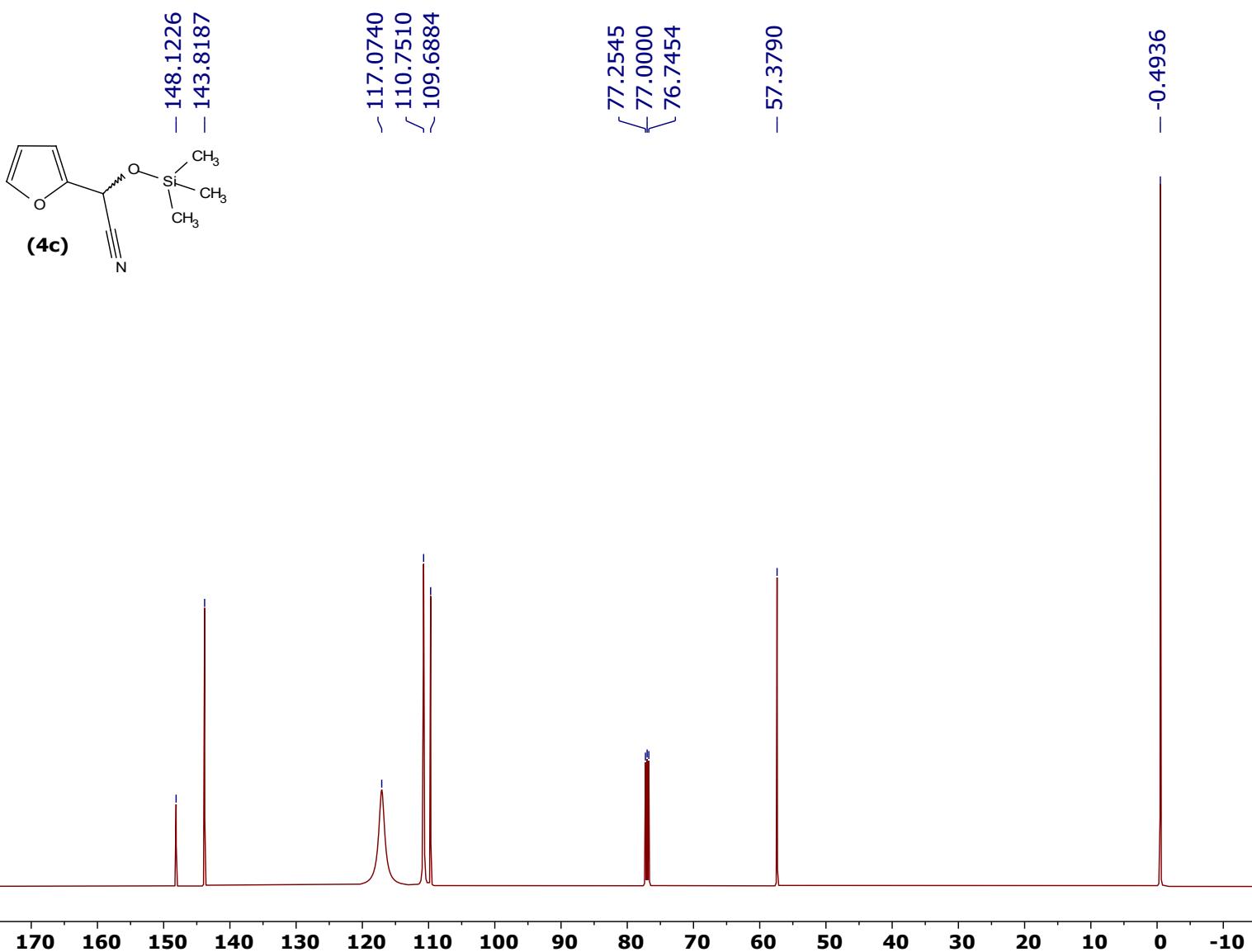


Figure S45. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **4c** in CDCl_3 .

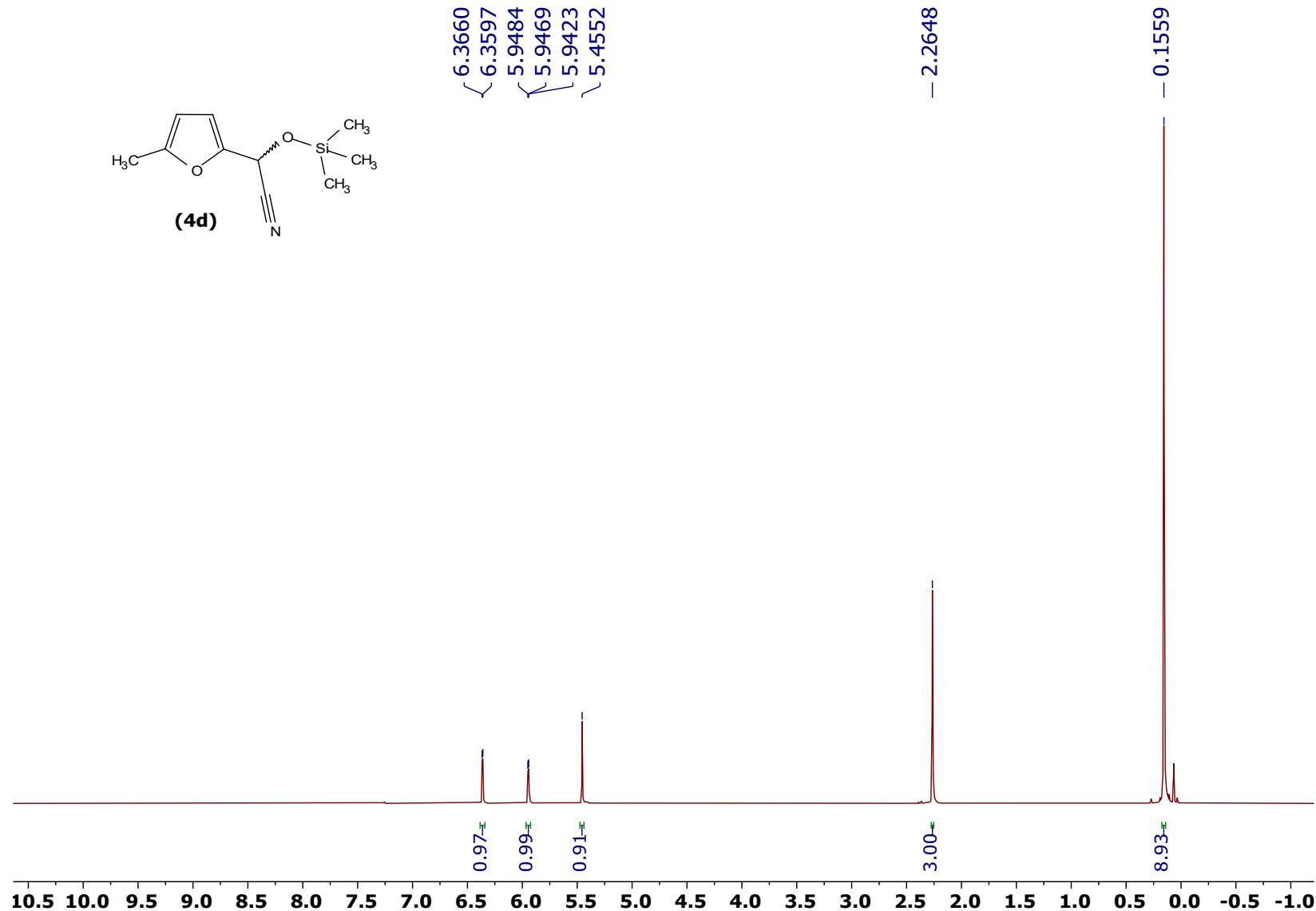
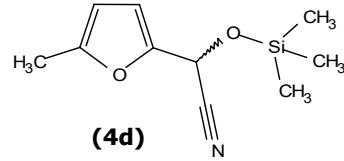


Figure S46. ^1H NMR spectrum of **4d** in CDCl_3 .

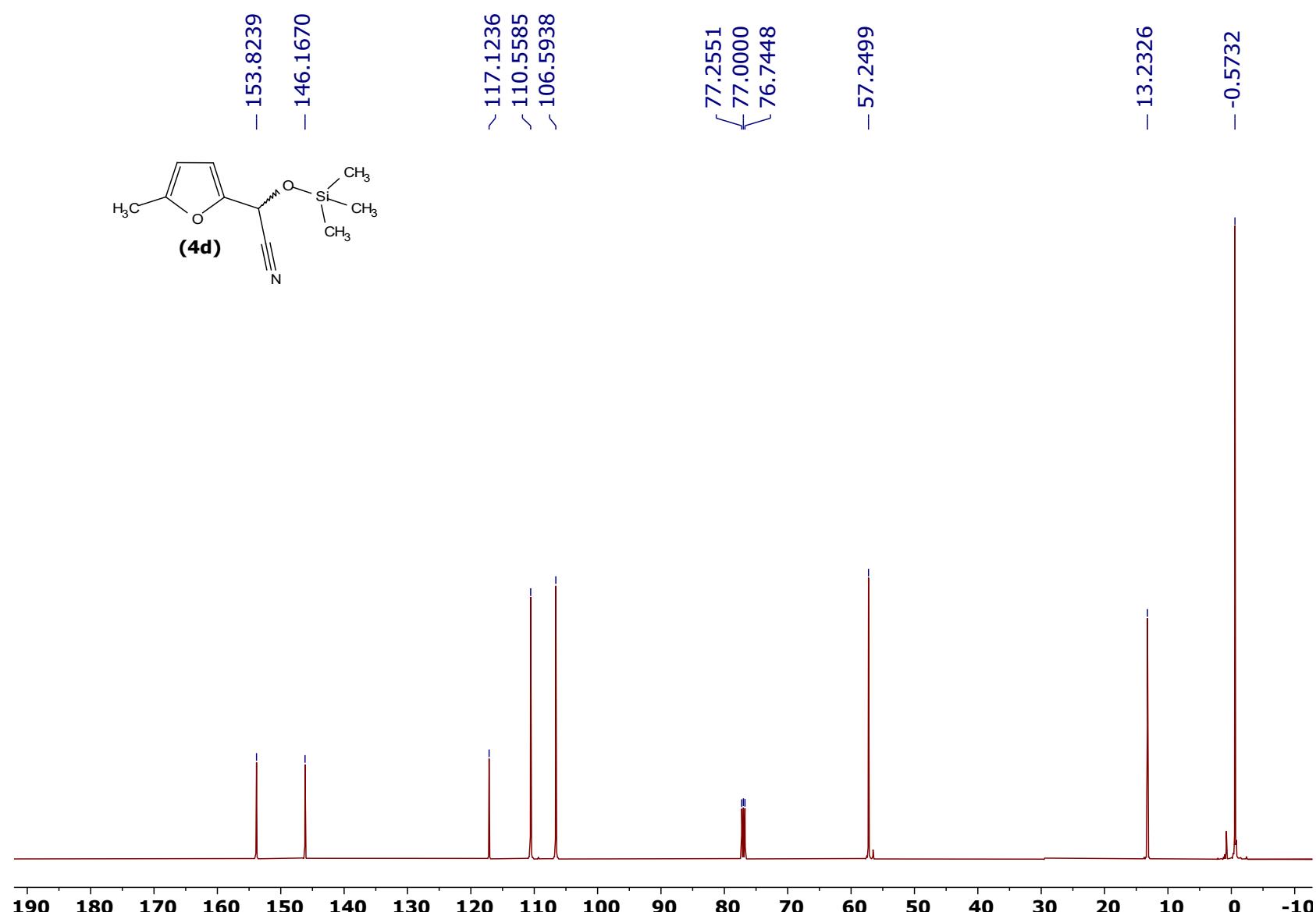


Figure S47. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **4d** in CDCl_3 .

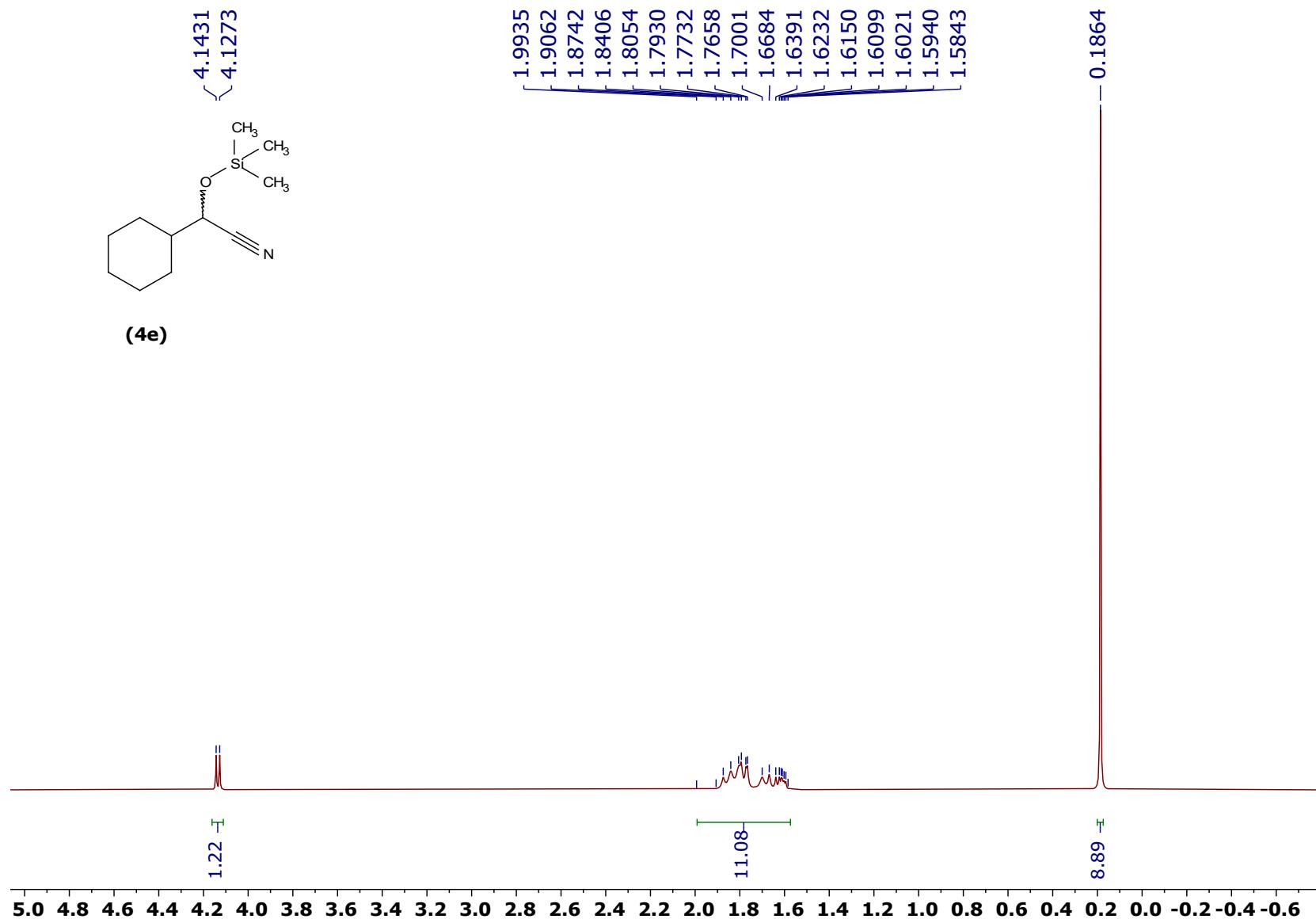
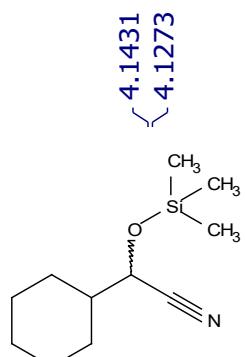


Figure S48. ^1H NMR spectrum of **4e** in CDCl_3 .

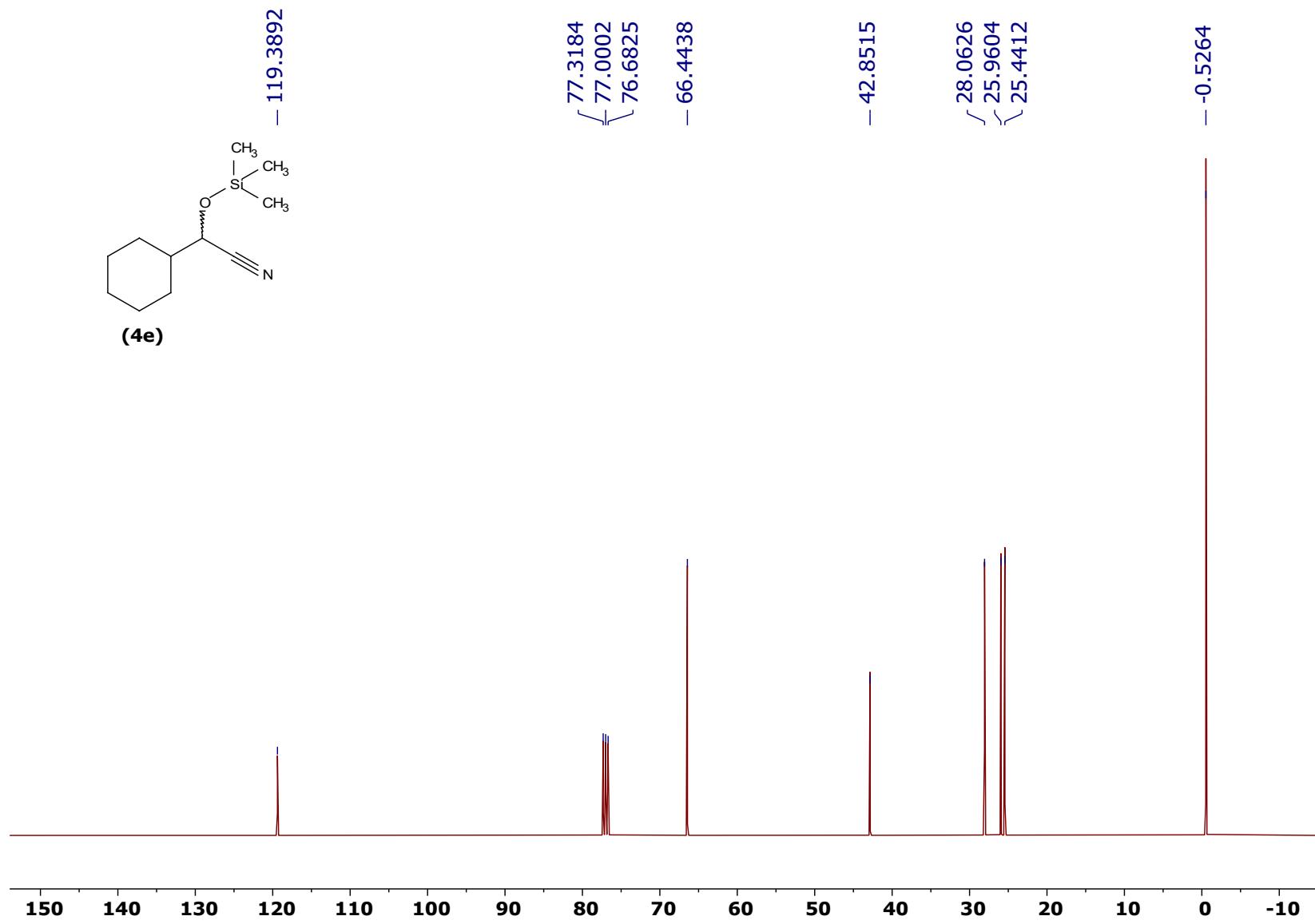
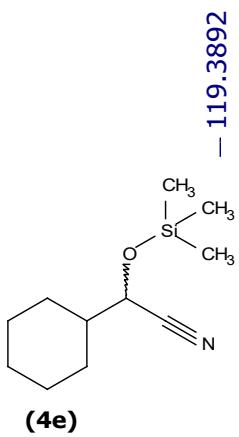


Figure S49. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **4e** in CDCl_3 .

