Supporting Information for

Inherent chirality through a simple dialkylation of 2,14-dithiacalix[4]arene

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1. SPECTRAL CHARACTERISATION

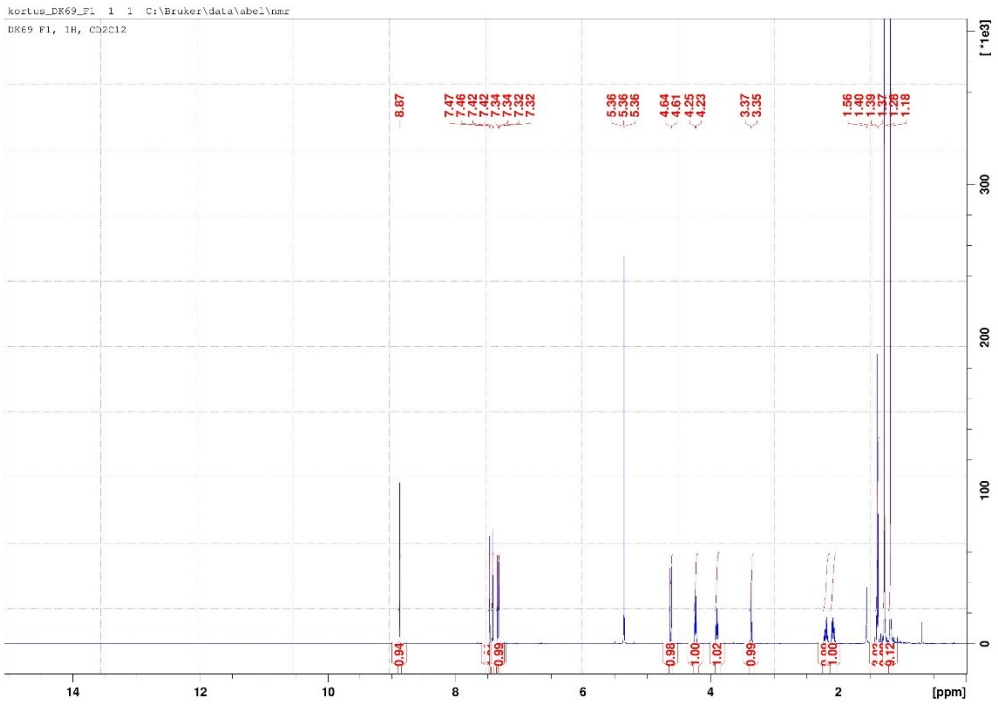

Figure 1. ^{1}H NMR of compound **4** (CD_2Cl_2, 600 MHz).

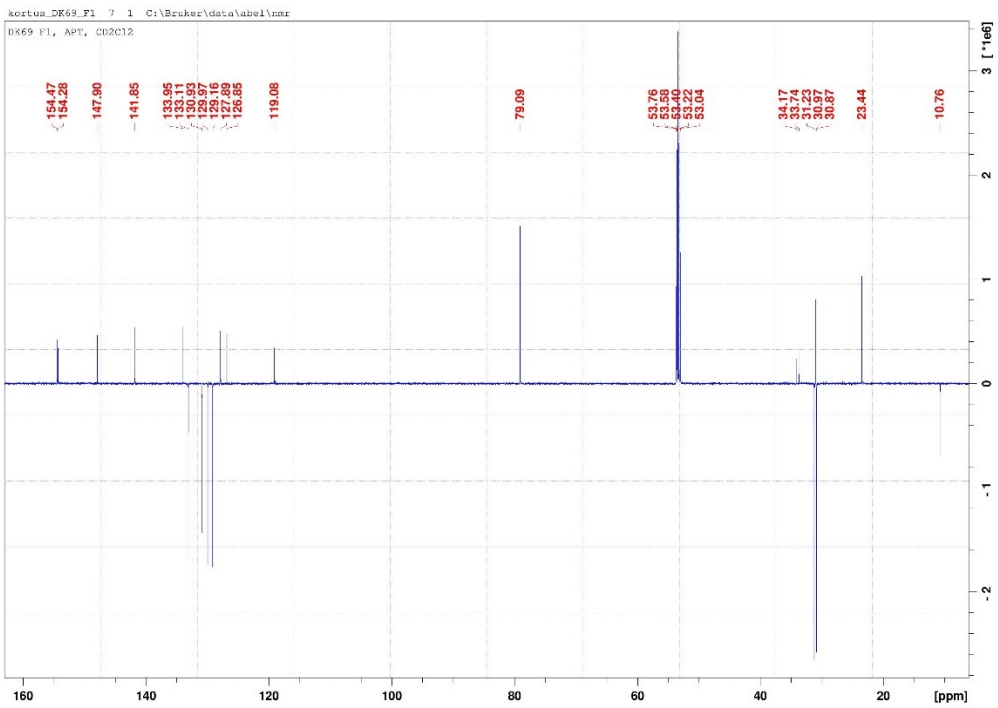

Figure 2. ^{13}C NMR of compound **4** (CD_2Cl_2, 151 MHz).

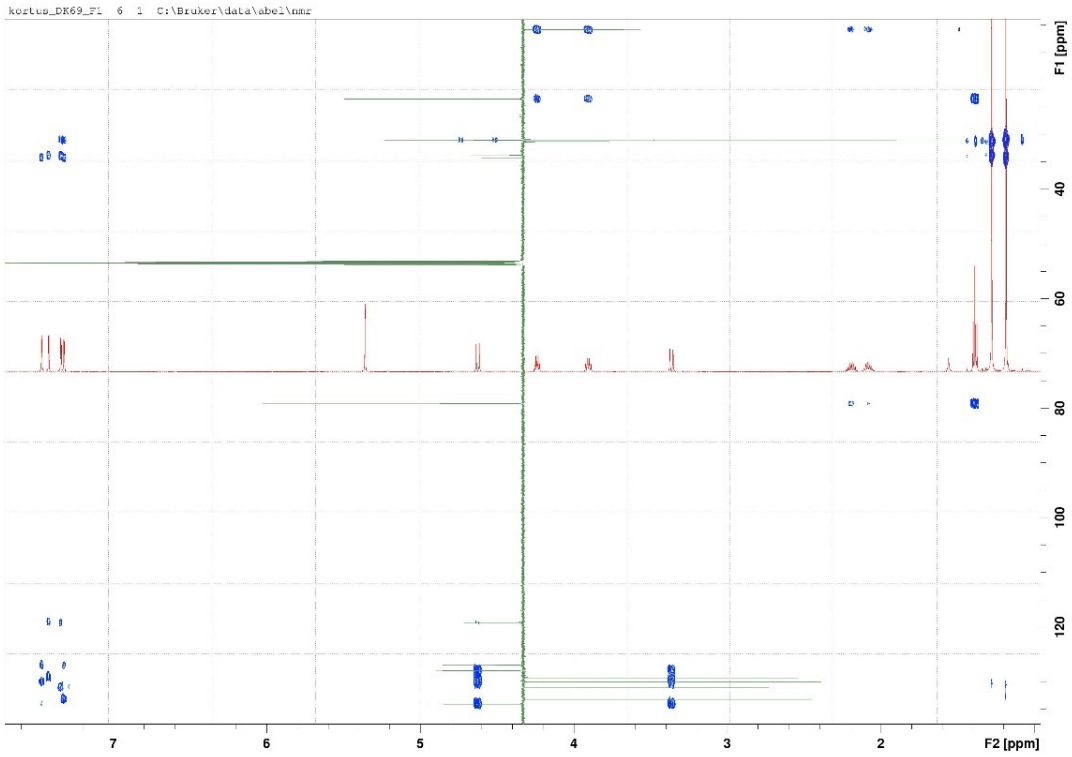

Figure 3. HMBC NMR of compound **4 (**CD_2Cl_2).

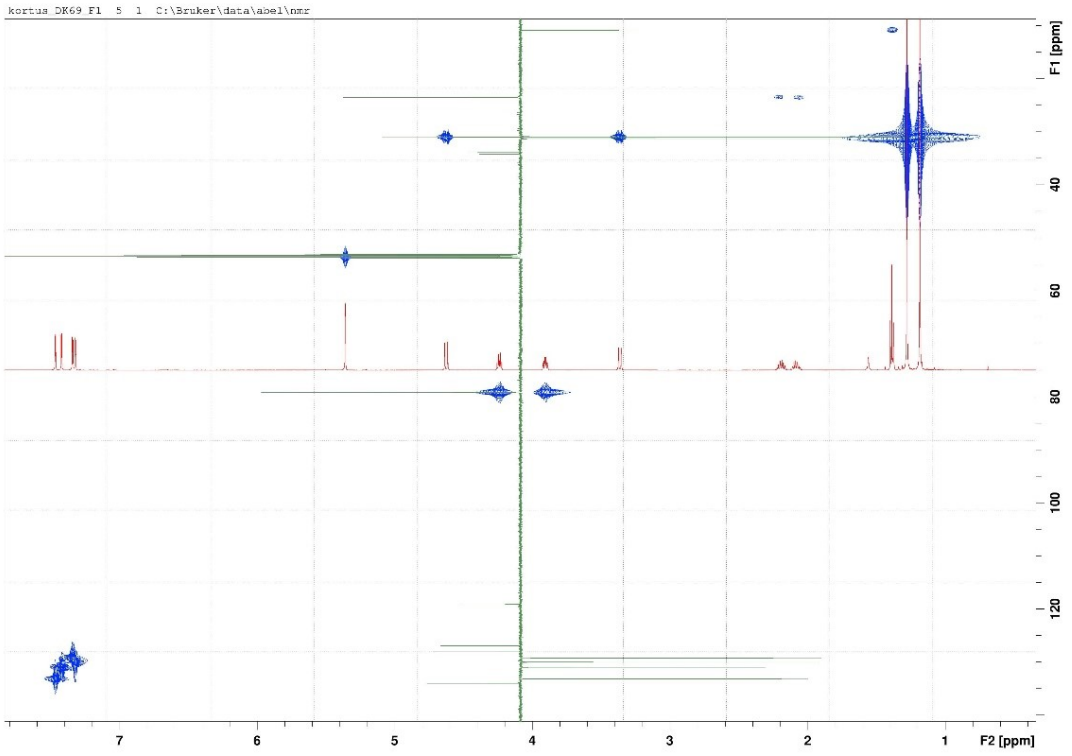

Figure 4. HMQC NMR of compound **4 (**CD_2Cl_2).

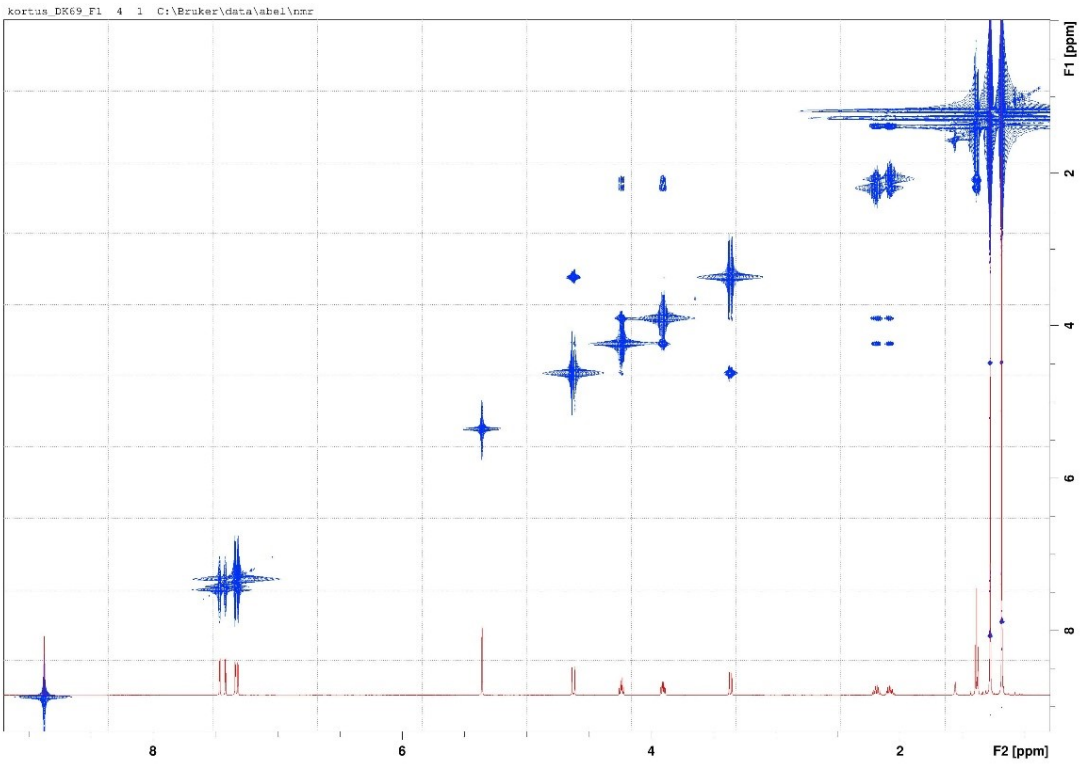

Figure 5. COSY NMR of compound **4 (**CD_2Cl_2).

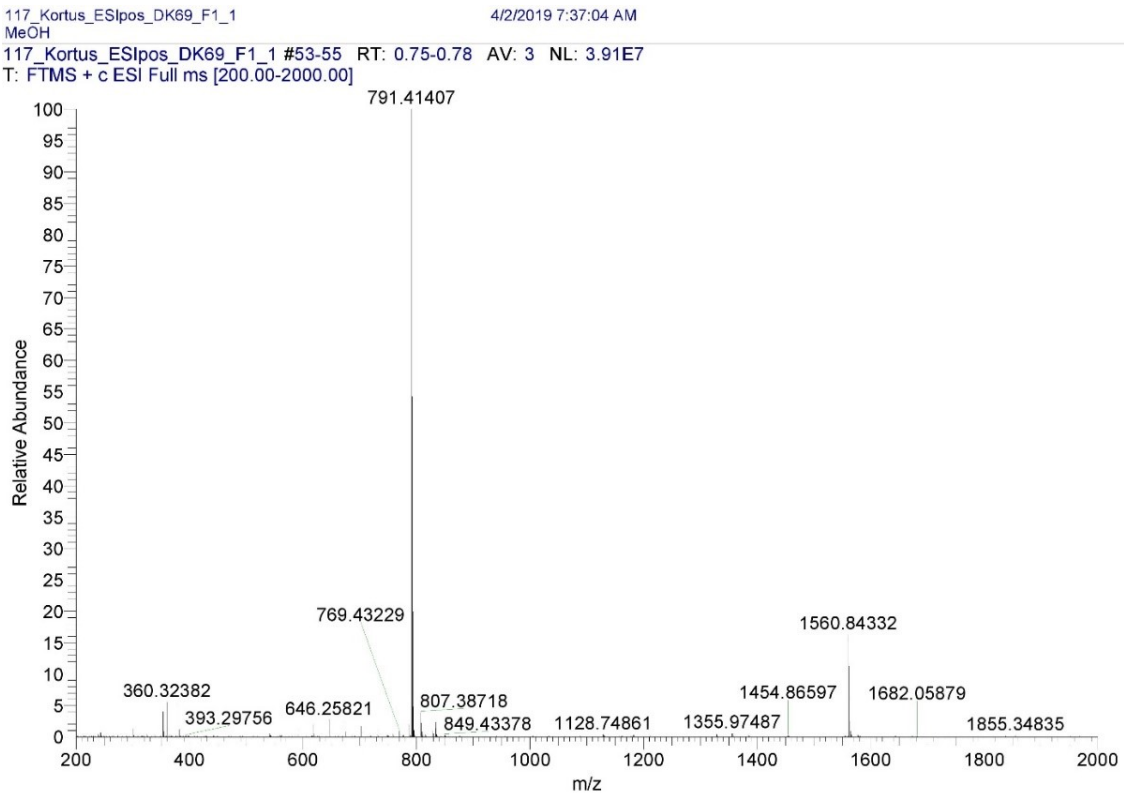

Figure 6. HRMS of compound **4** (ESI^+).

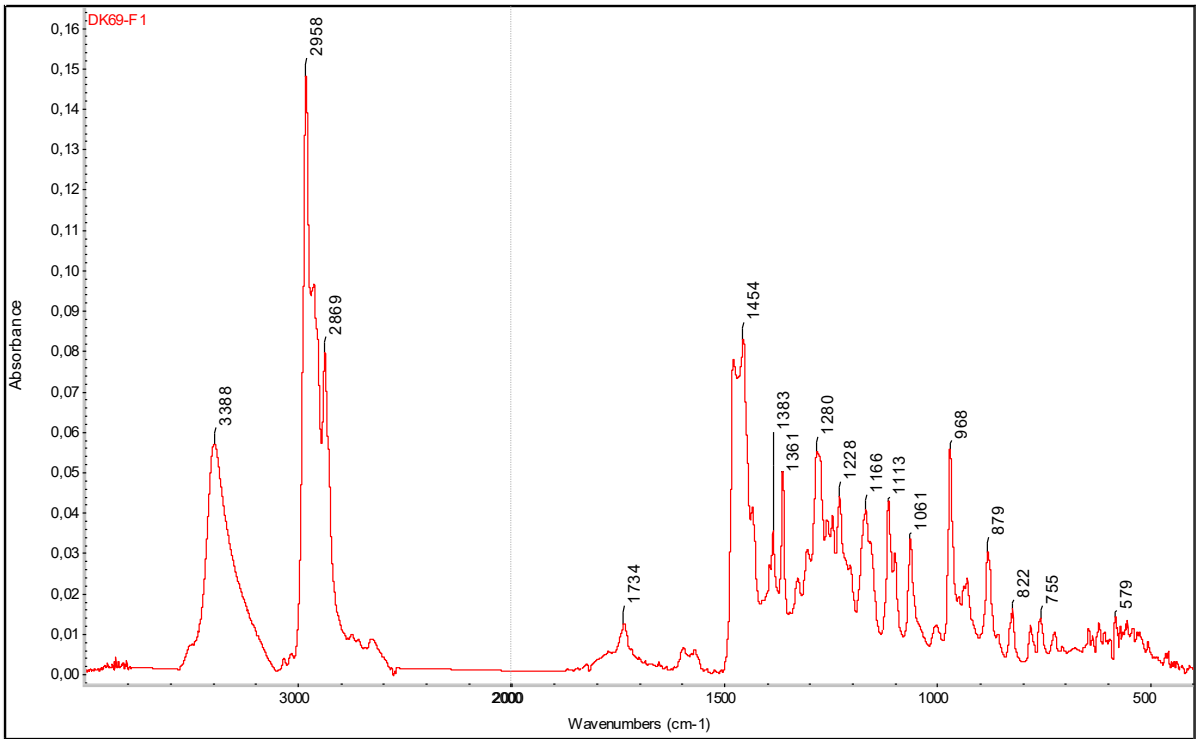

Figure 7. IR of compound **4** (KBr).

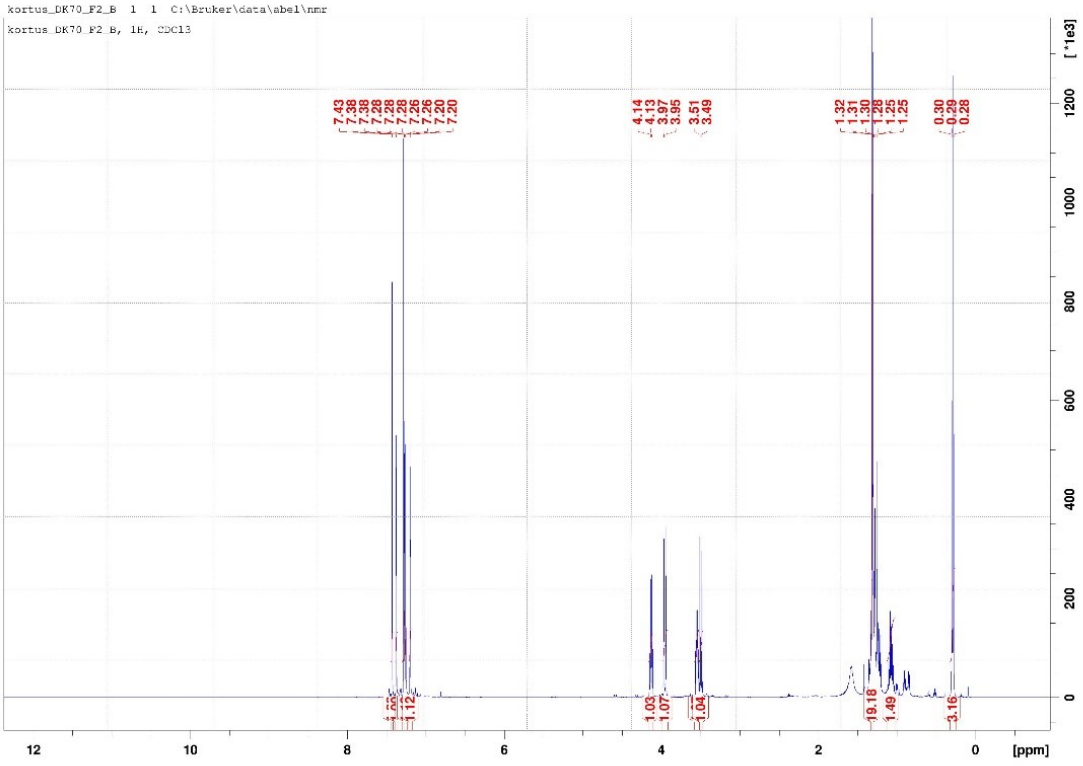

Figure 8. ^{1}H NMR of compound **5** ($CDCl_3$, 600 MHz).

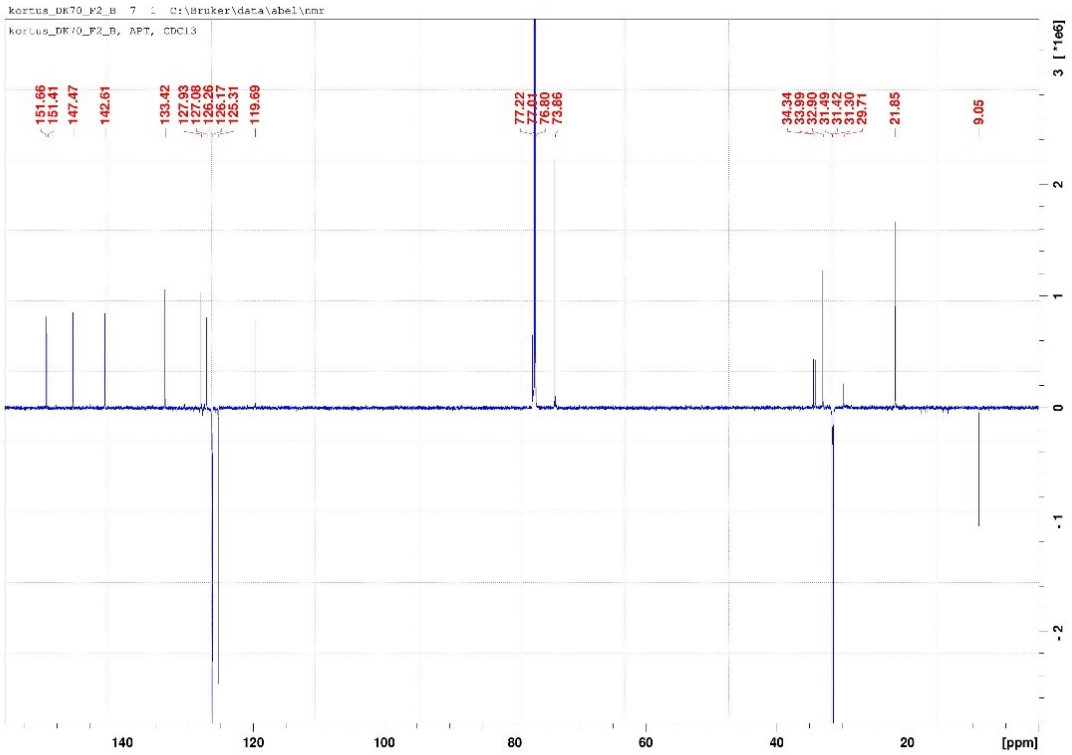

Figure 9. ^{13}C NMR of compound **5** ($CDCl_3$, 151 MHz).

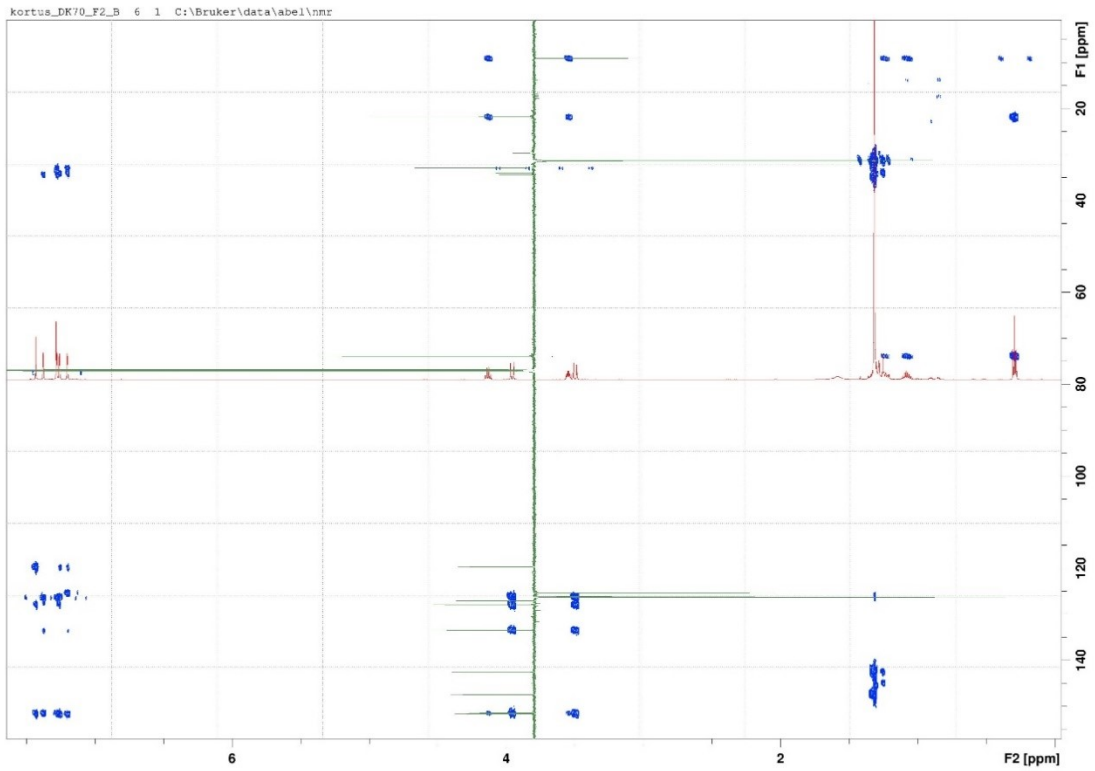

Figure 10. HMBC NMR of compound **5 (**$CDCl_3$).

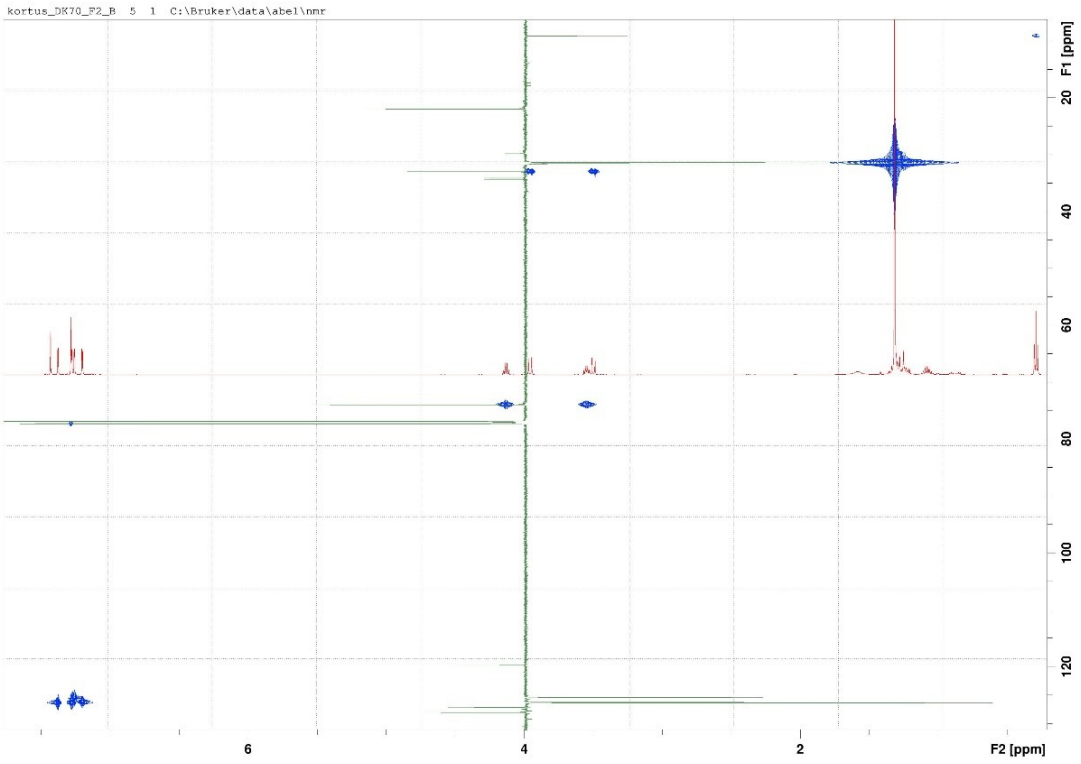

Figure 11. HMQC NMR of compound **5 (**$CDCl_3$).

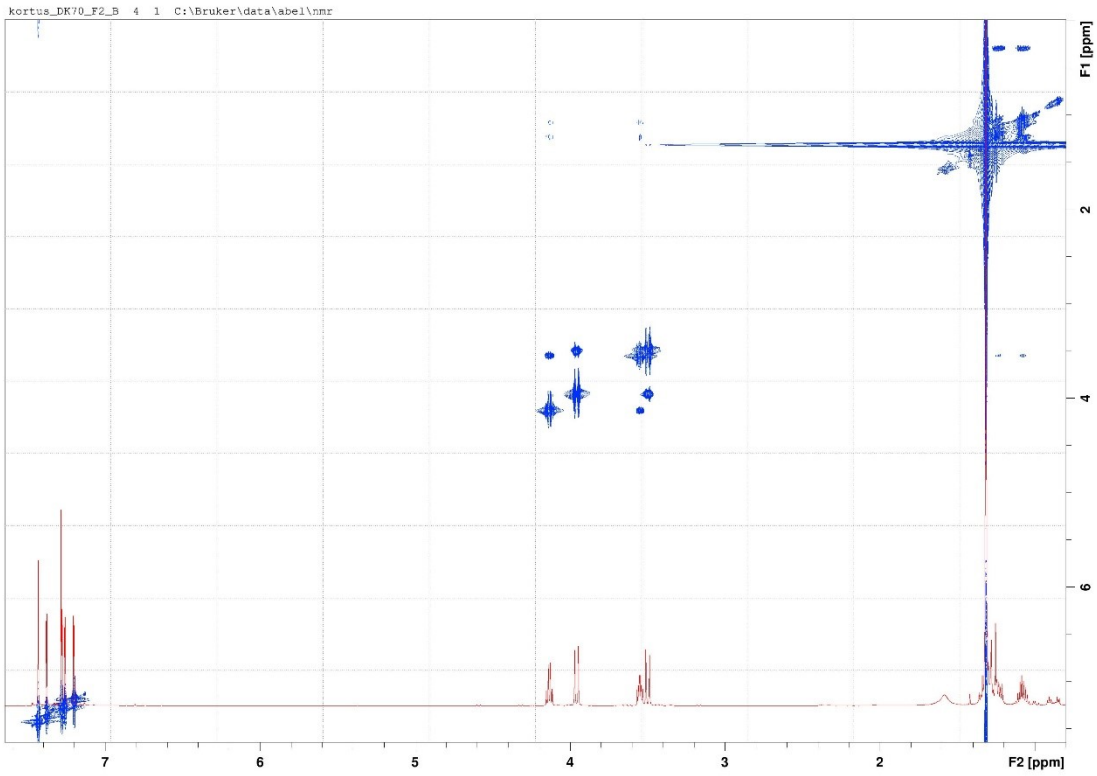

Figure 12. COSY NMR of compound **5**.

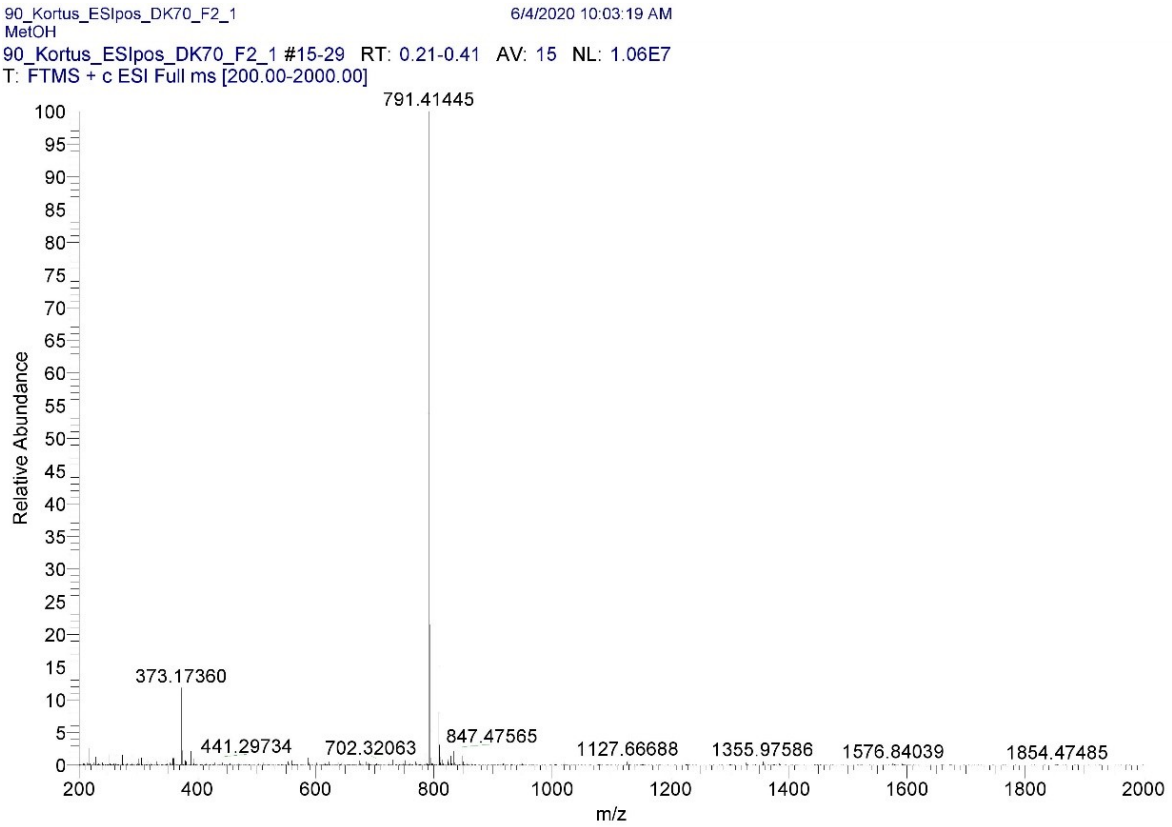

Figure 13. HRMS of compound **5** (ESI^+).

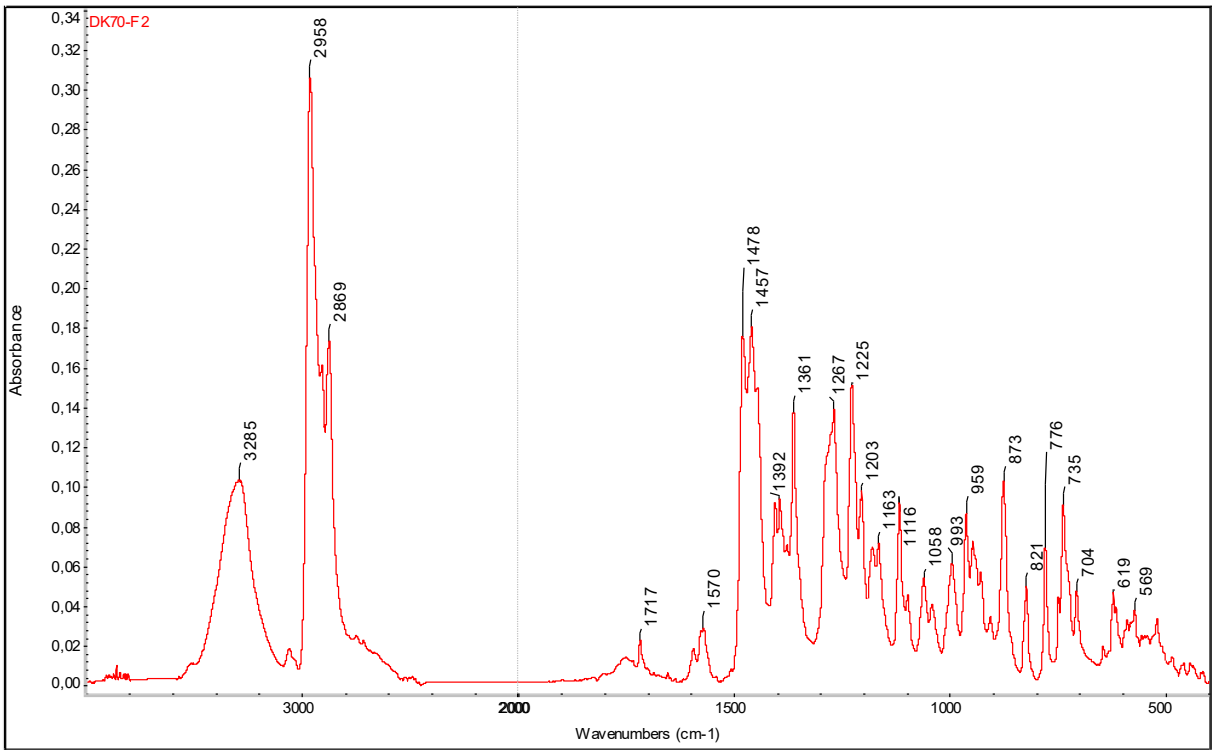

Figure 14. IR of compound **5** (KBr).

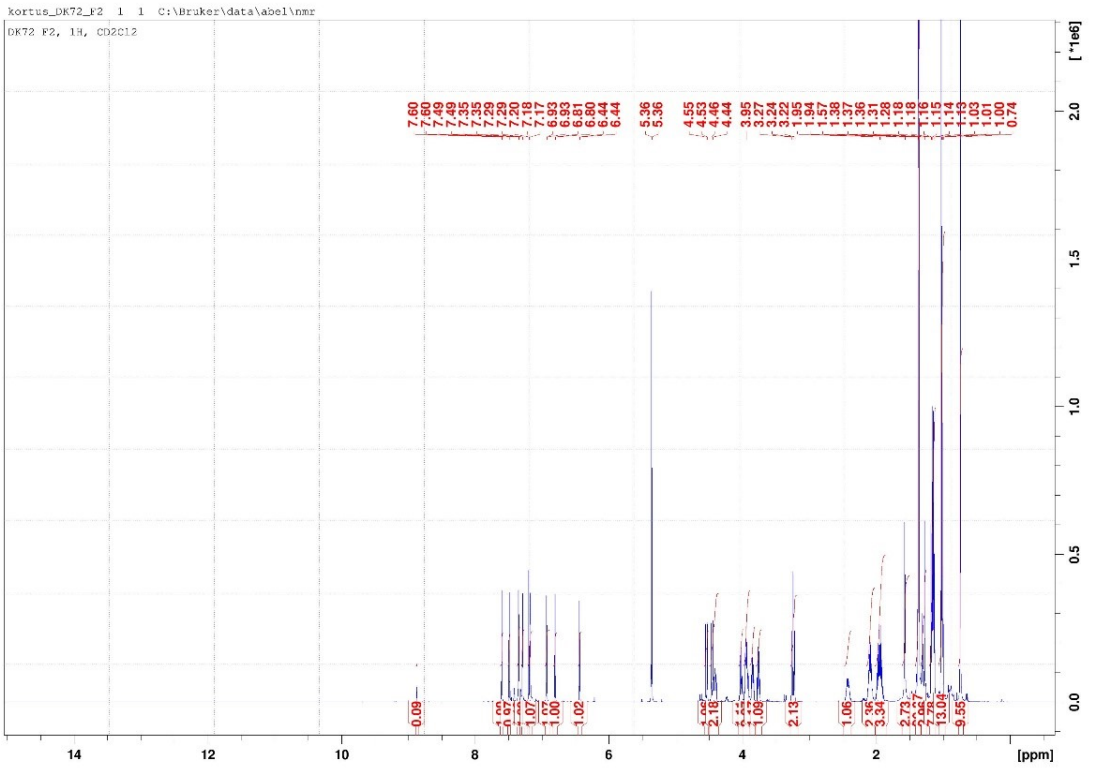

Figure 15. ^{1}H NMR of compound **6** (CD_2Cl_2, 600 MHz).

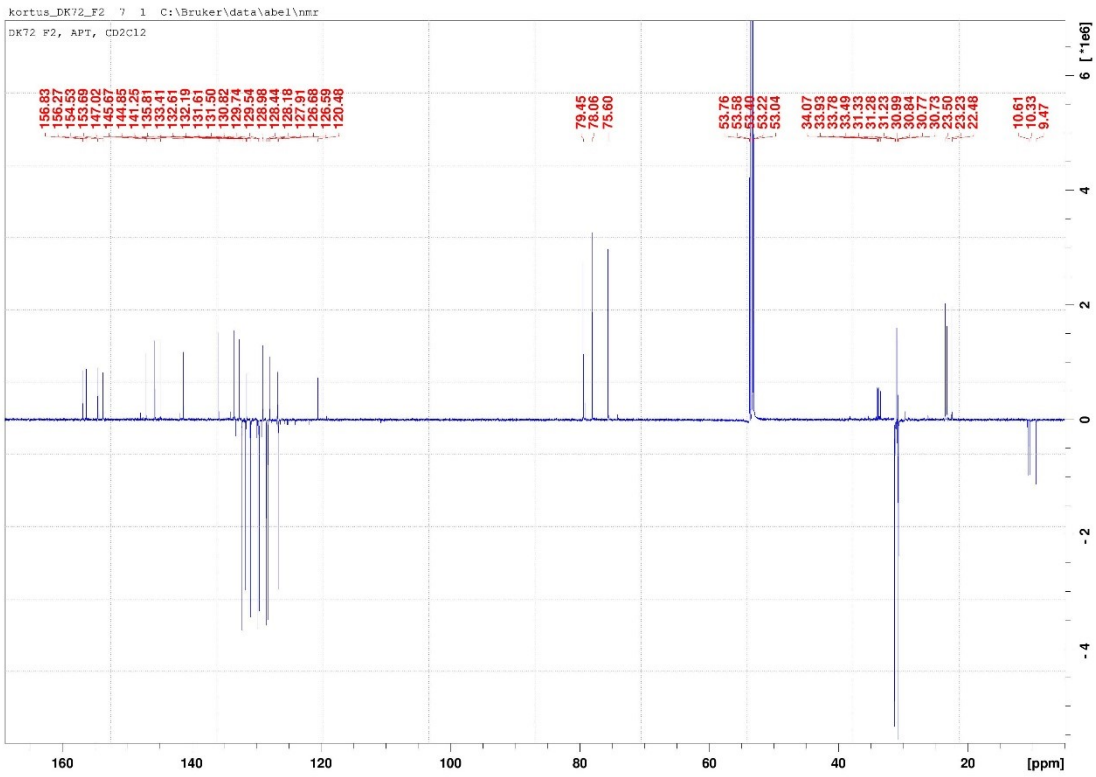

Figure 16. ^{13}C NMR of compound **6** (CD_2Cl_2, 151 MHz).

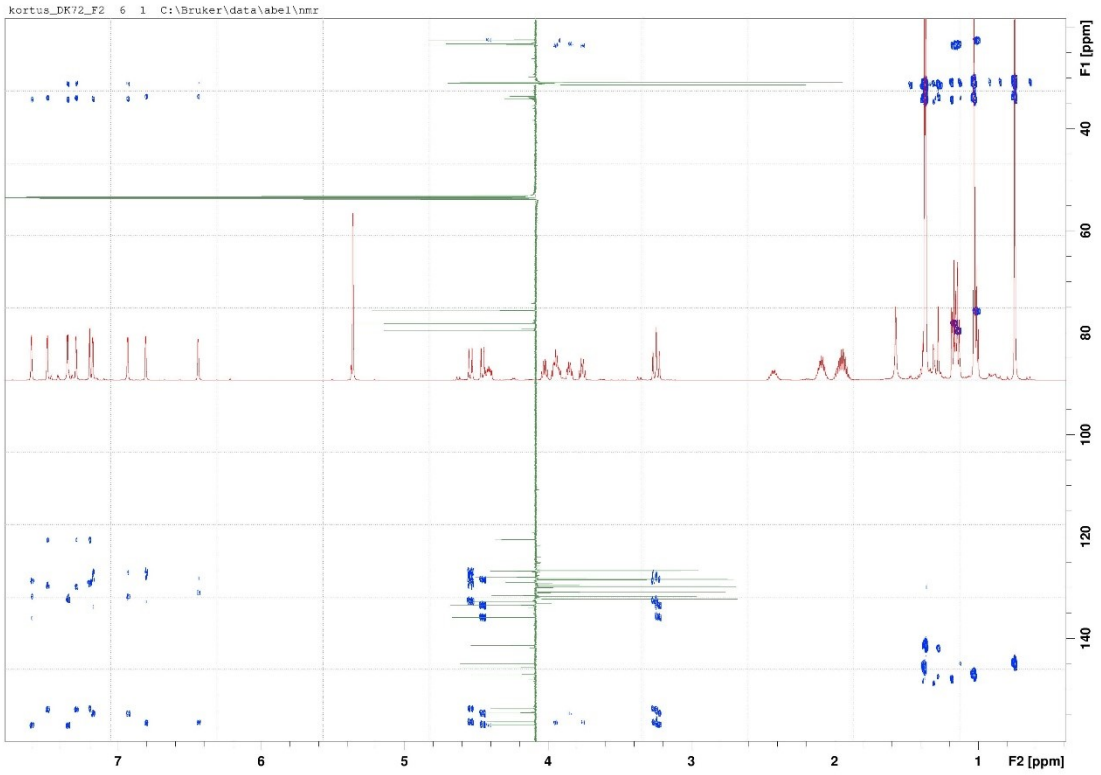

Figure 17. HMBC NMR of compound **6 (**CD_2Cl_2).

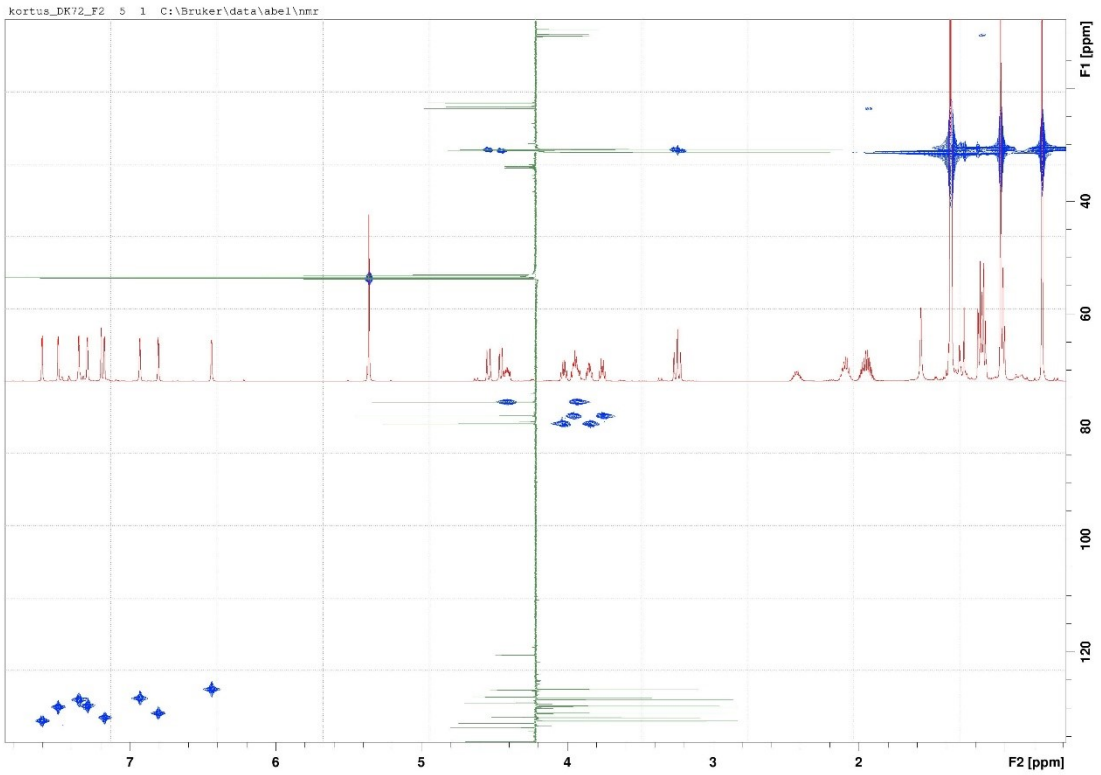

Figure 18. HMQC NMR of compound **6 (**CD_2Cl_2).

Figure 19. COSY NMR of compound **6** (CD_2Cl_2).

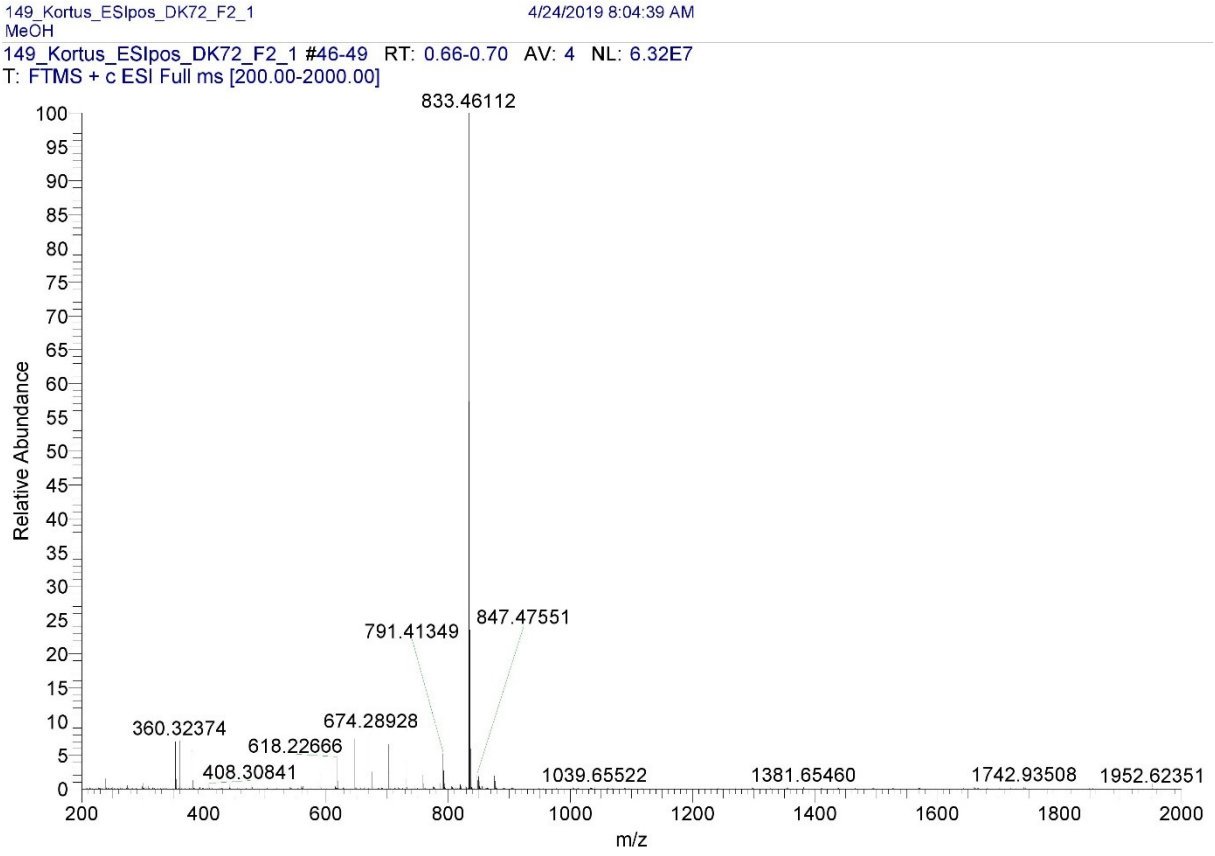

Figure 20. HRMS of compound **6** (ESI^+).

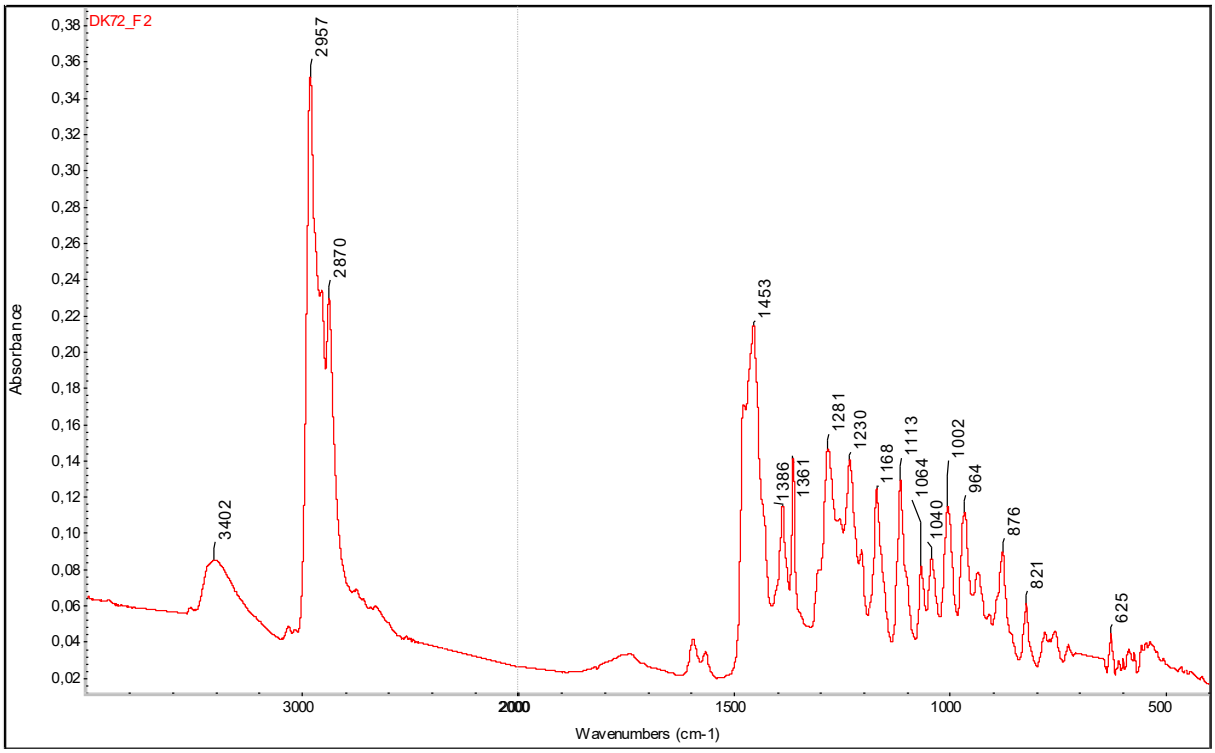

Figure 21. IR of compound **6** (KBr).

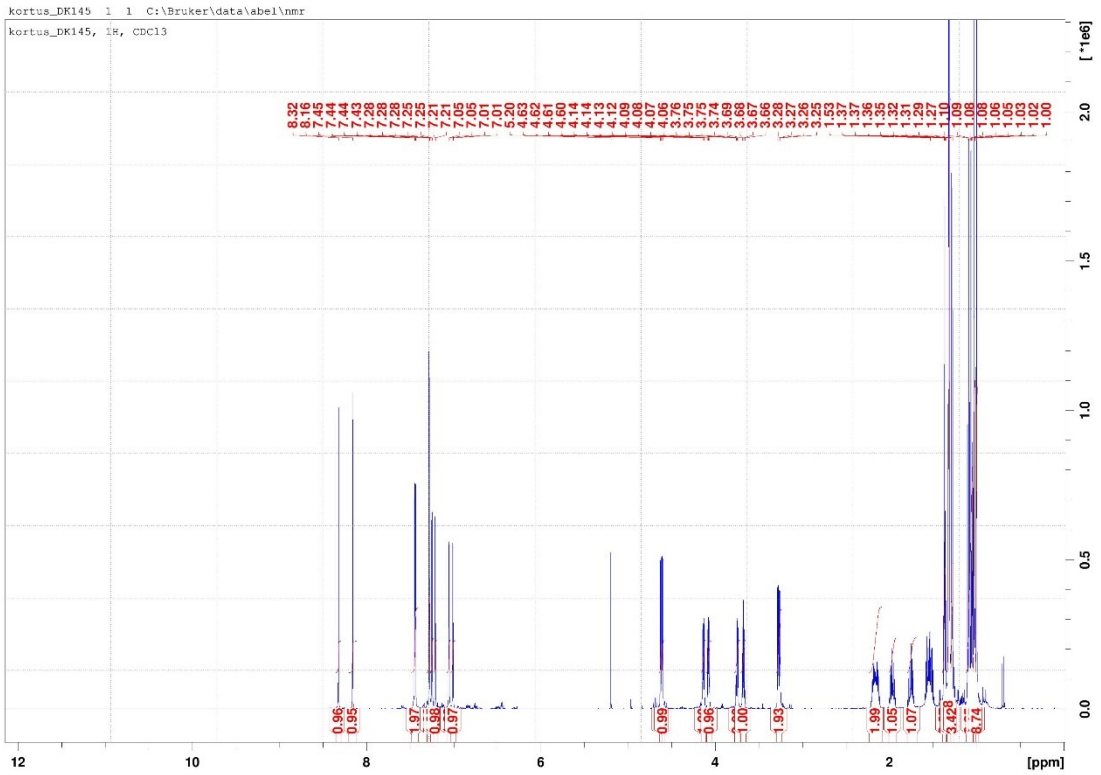

Figure 22. ^{1}H NMR of compound **8** ($CDCl_3$, 600 MHz).

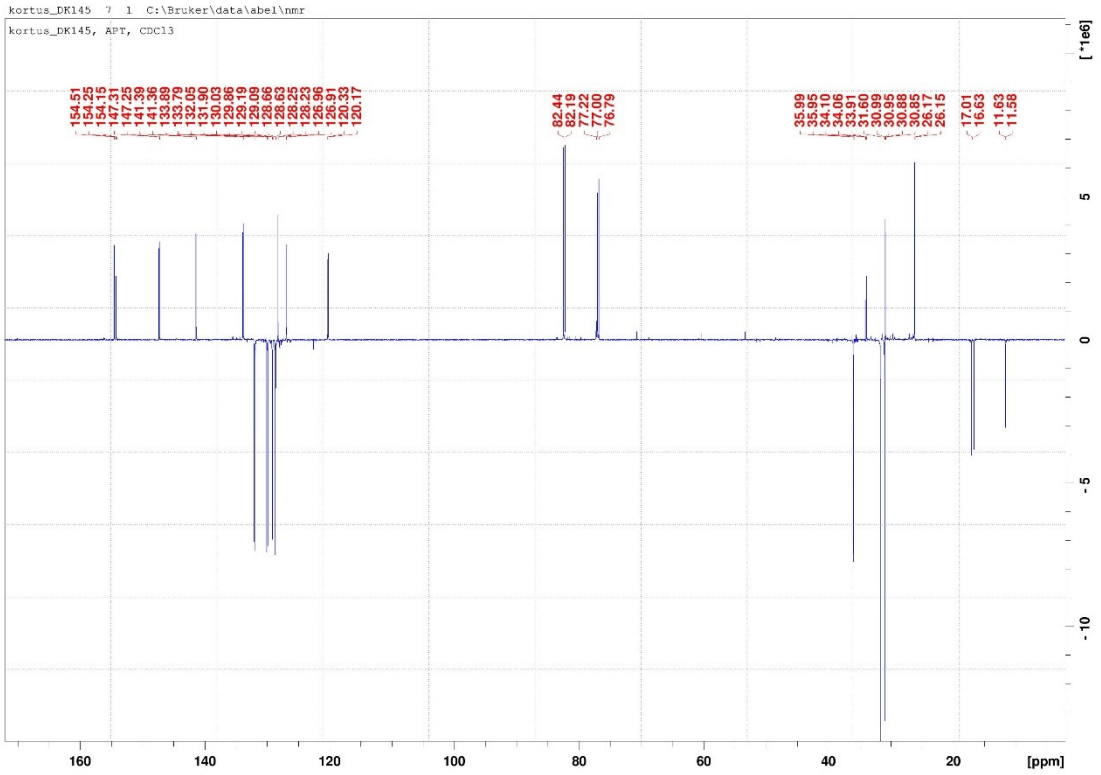

Figure 23. ^{13}C NMR of compound **8** ($CDCl_3$, 151 MHz).

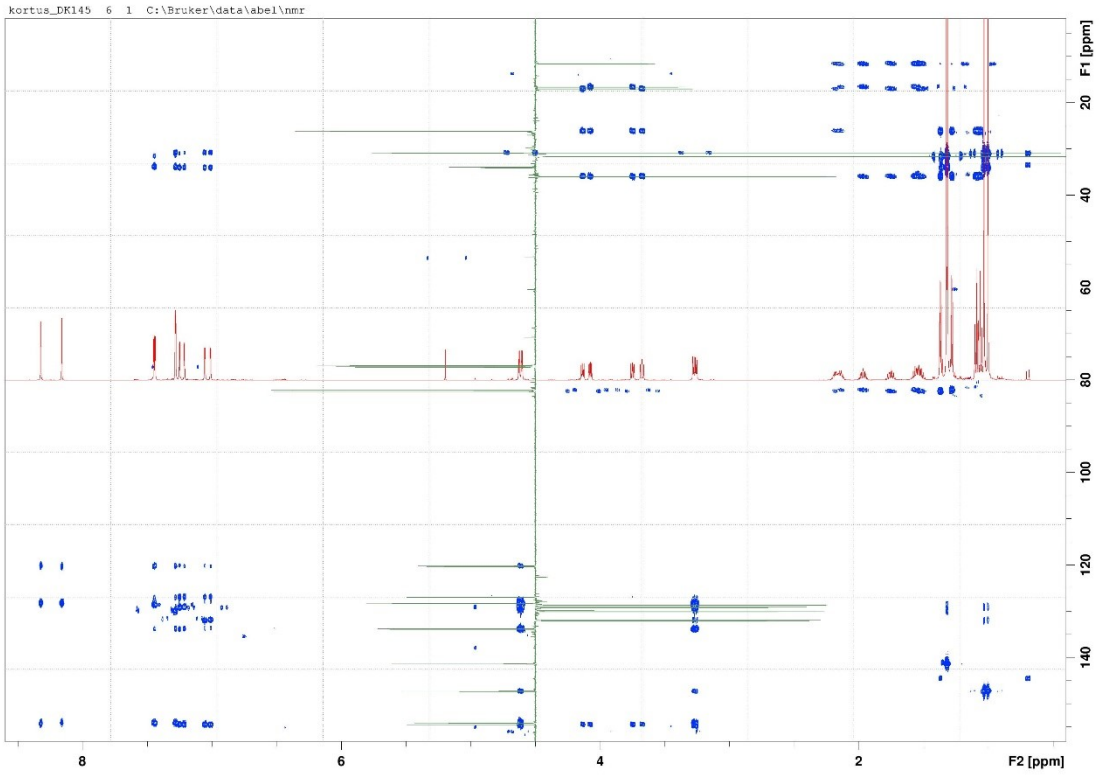

Figure 24. HMBC NMR of compound **8** ($CDCl_3$).

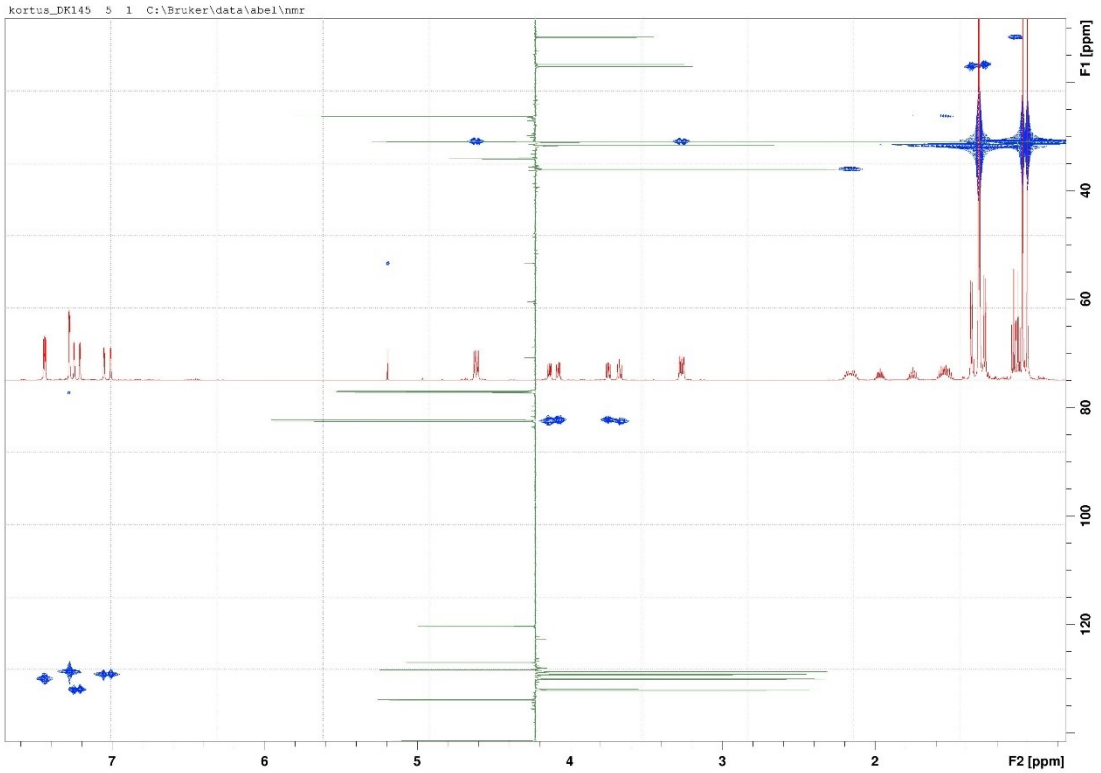

Figure 25. HMQC NMR of compound **8** ($CDCl_3$).

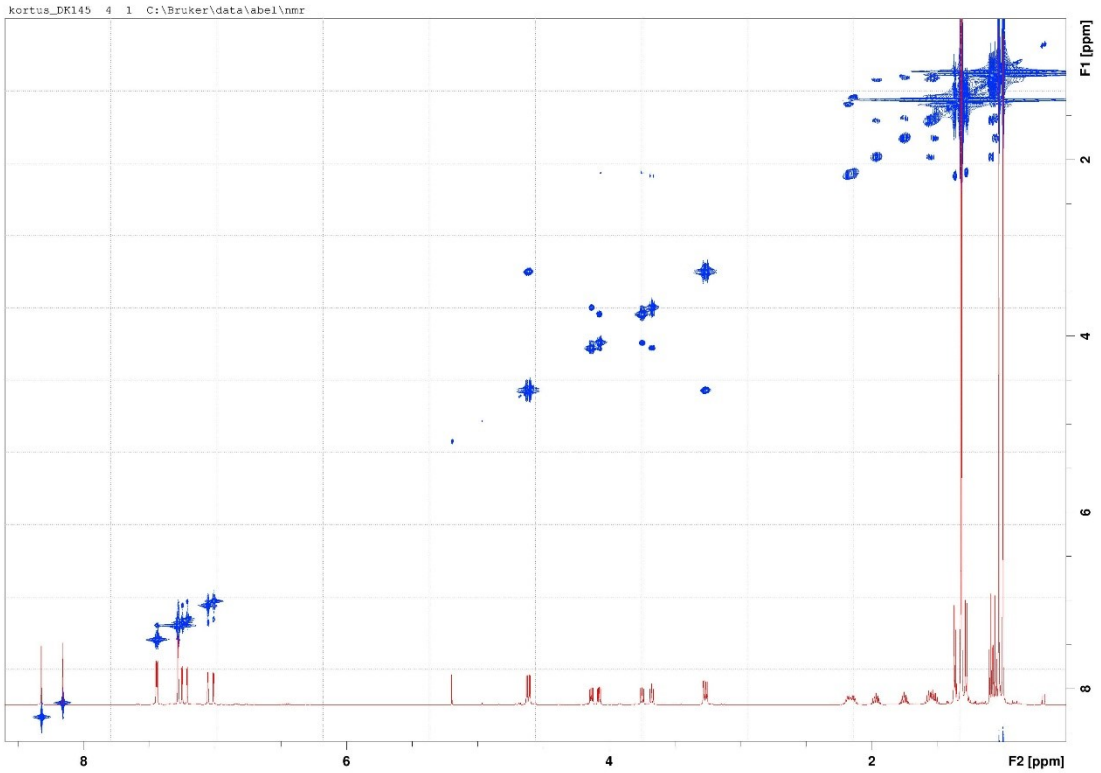

Figure 26. COSY NMR of compound **8** ($CDCl_3$).

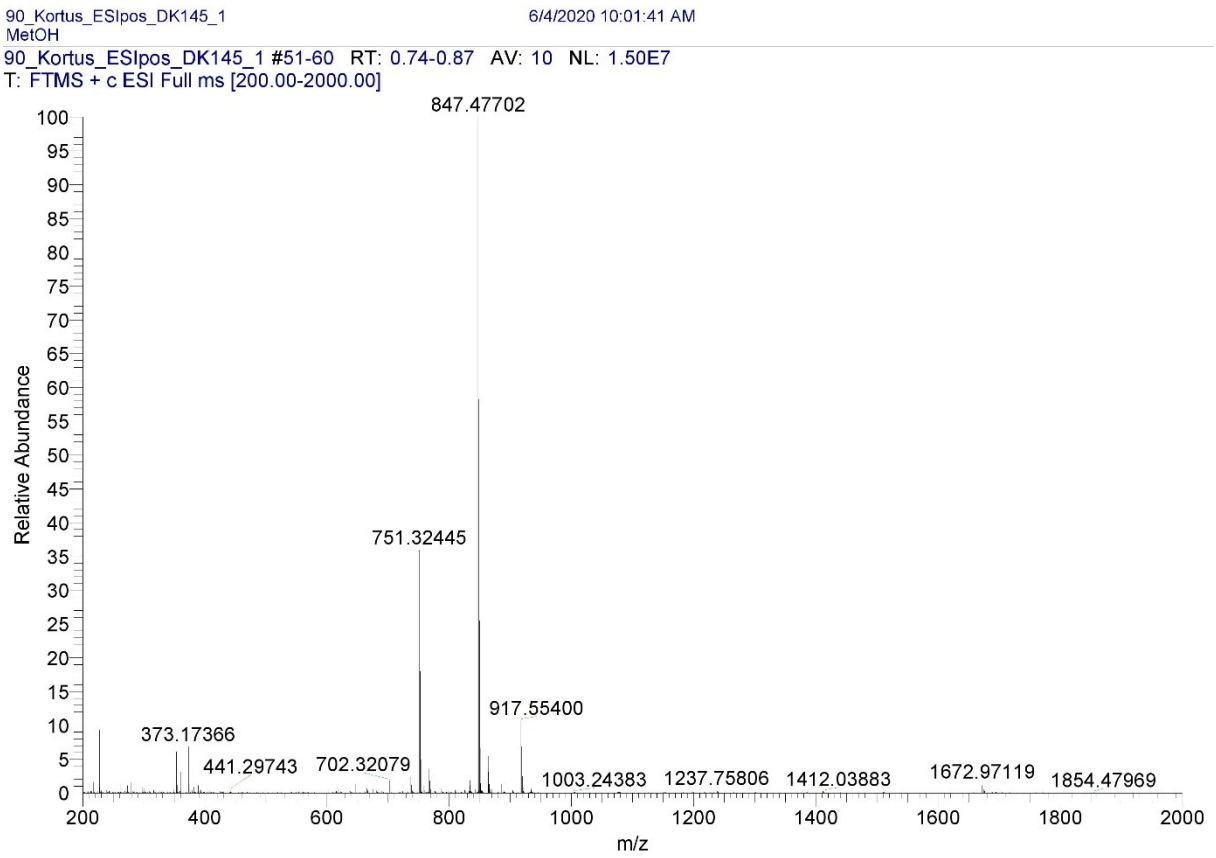

Figure 27. HRMS of compound **8** (ESI^+).

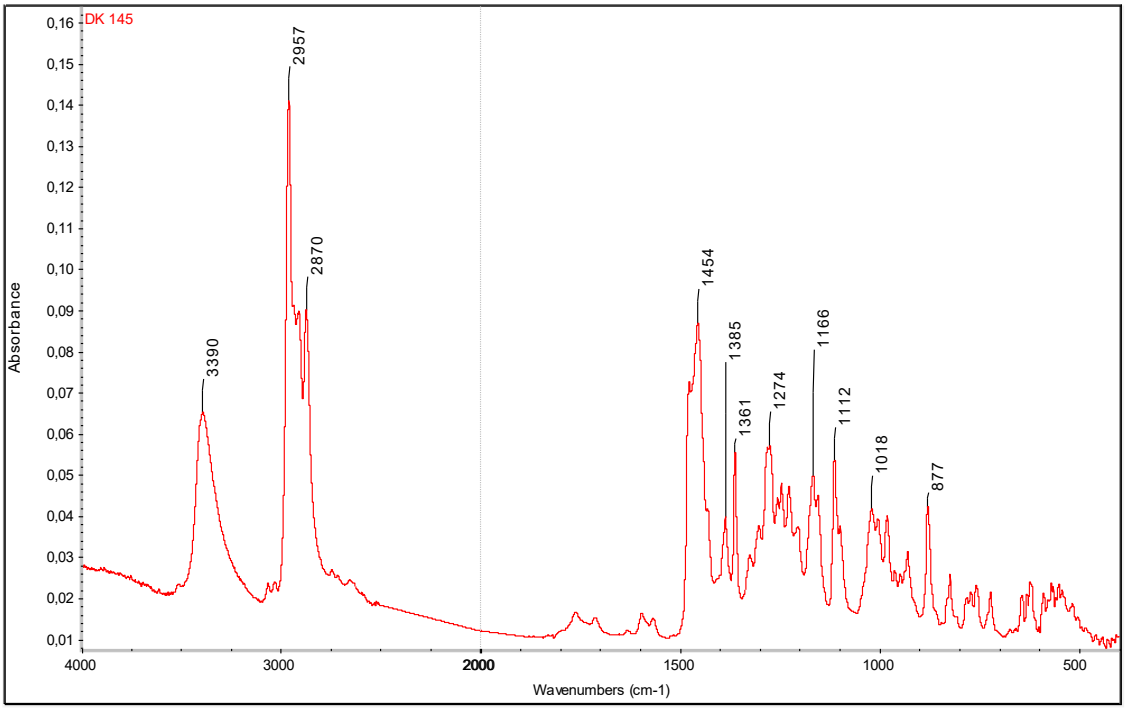

Figure 28. IR of compound **8** (KBr).

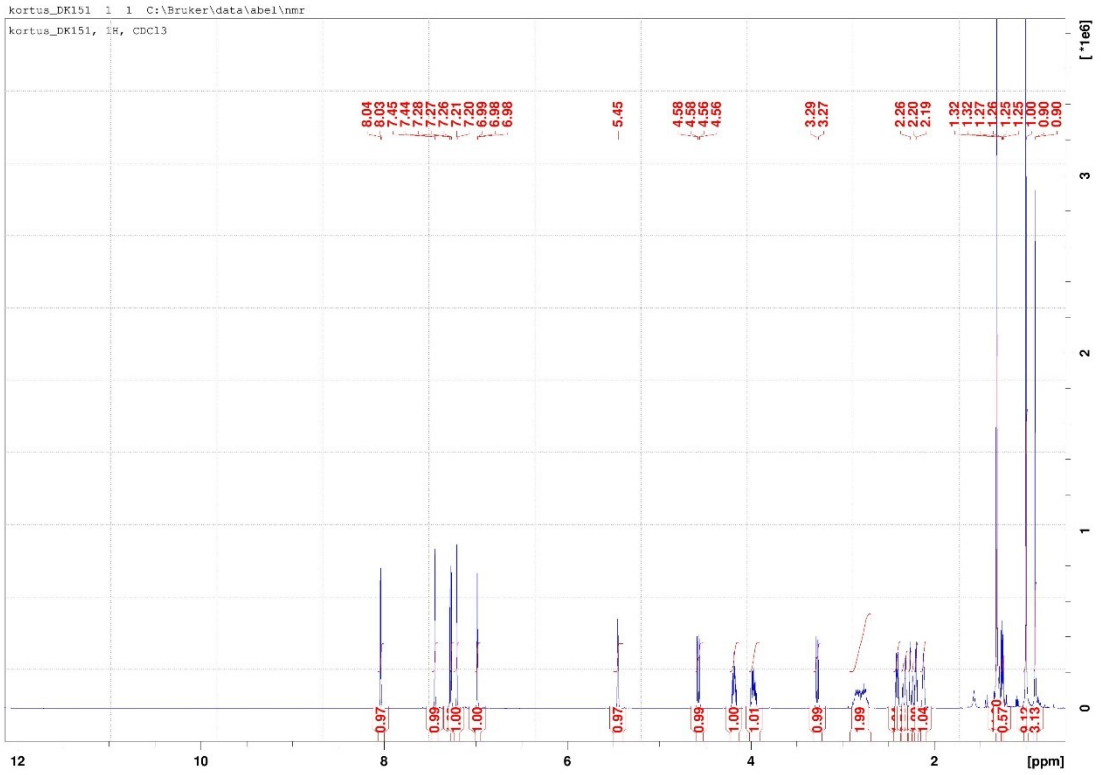

Figure 29. ^{1}H NMR of compound **9** ($CDCl_3$, 600 MHz).

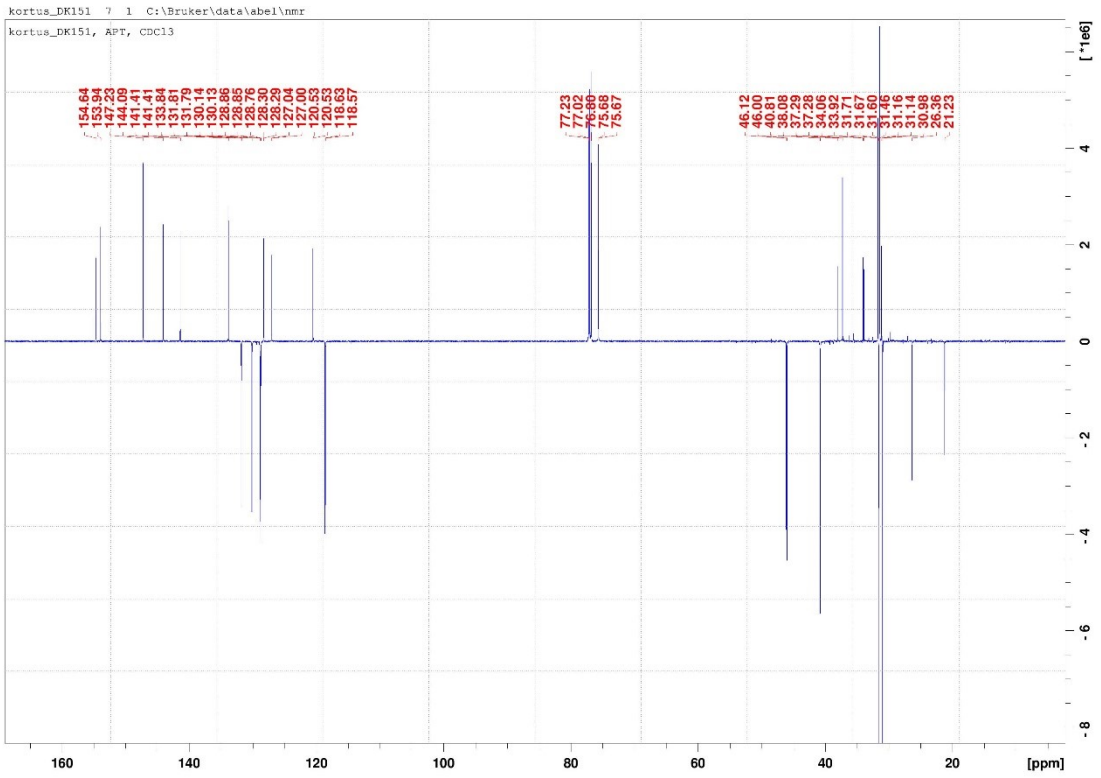

Figure 30. ^{13}C NMR of compound **9** ($CDCl_3$, 151 MHz).

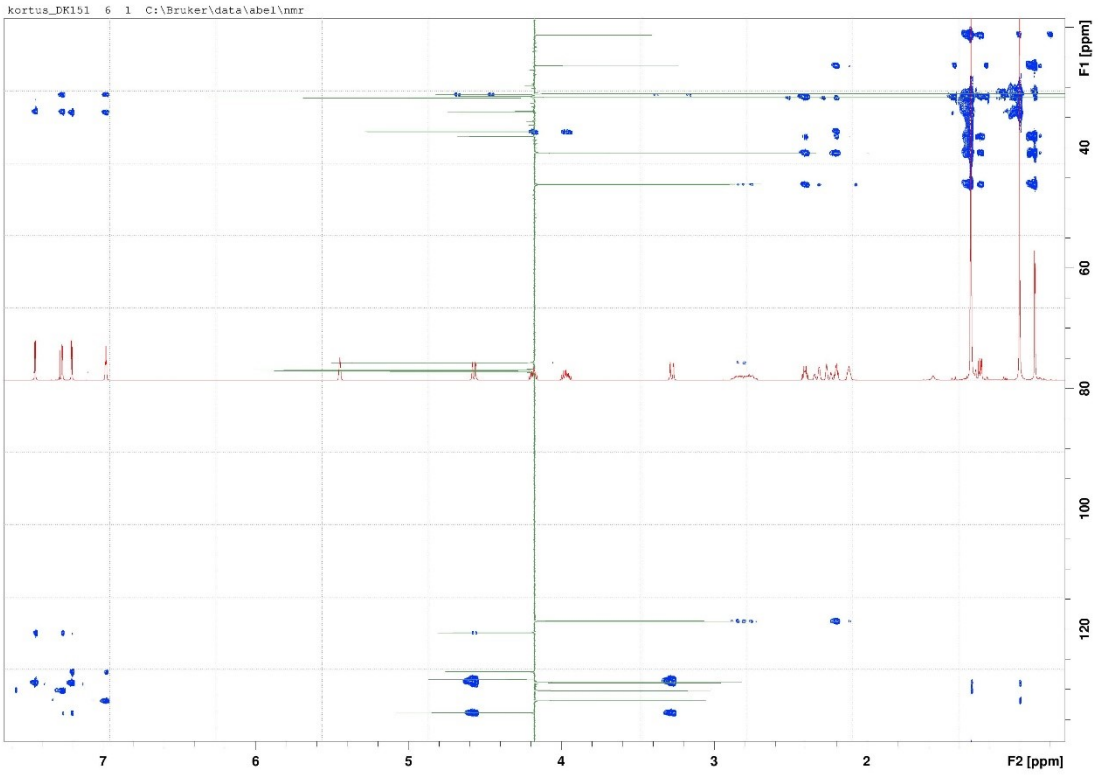

Figure 31. HMBC NMR of compound **9** ($CDCl_3$).

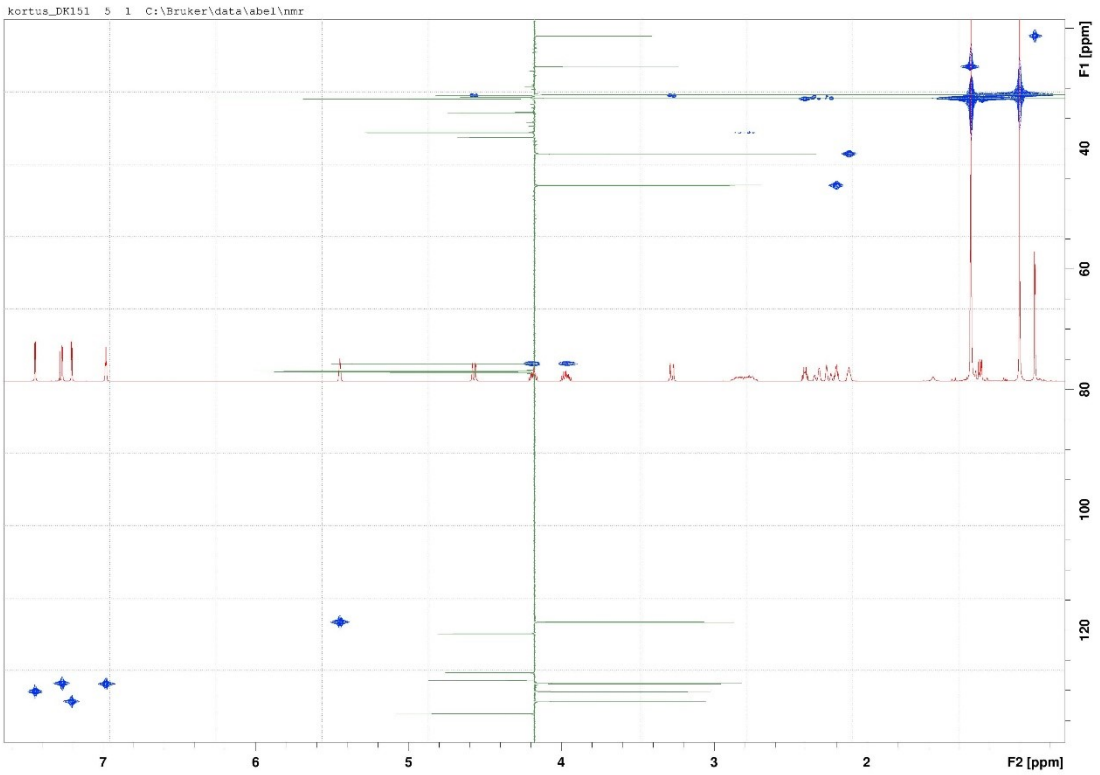

Figure 32. HMQC NMR of compound **9** ($CDCl_3$).

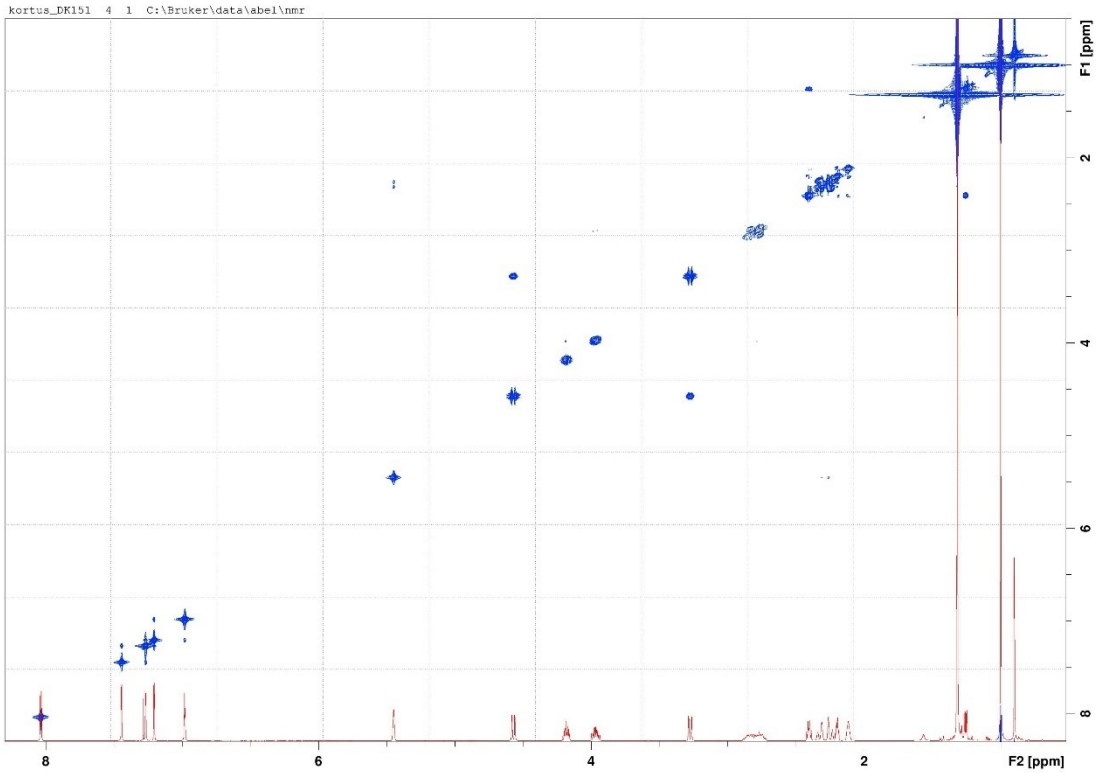

Figure 33. COSY NMR of compound **9** ($CDCl_3$).

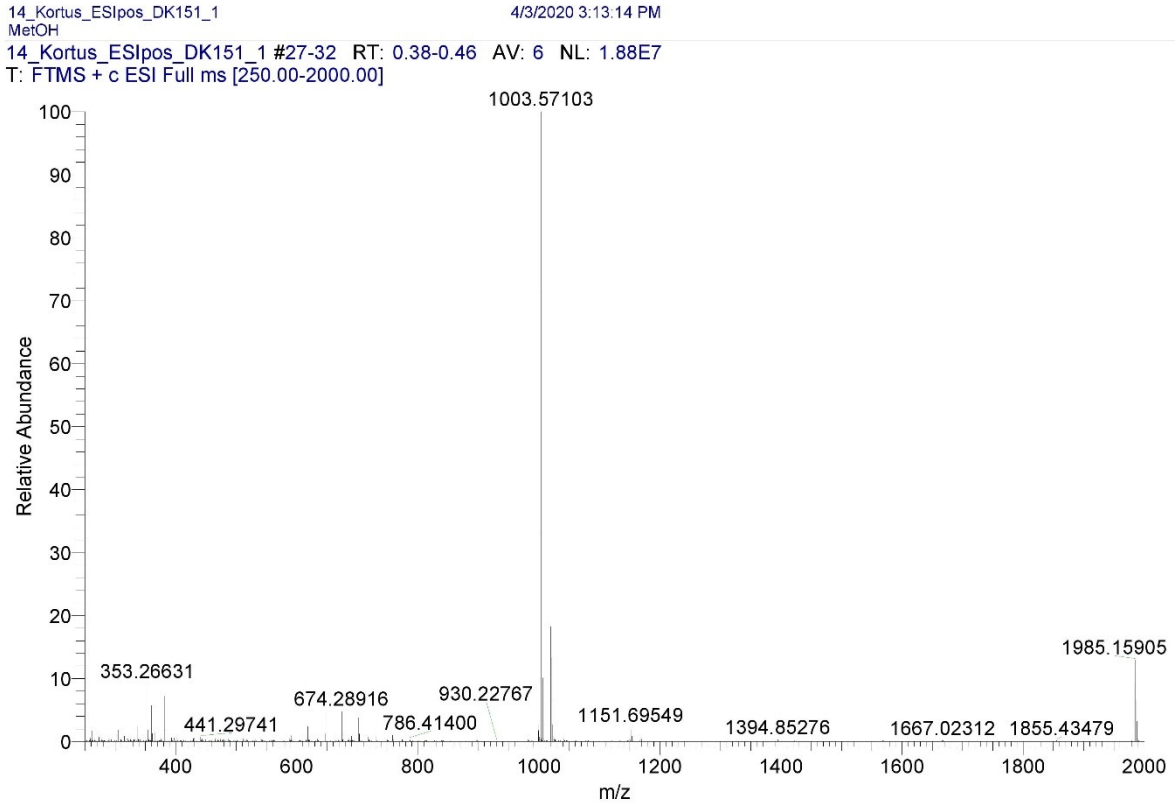

Figure 34. HRMS of compound **9** (ESI^+).

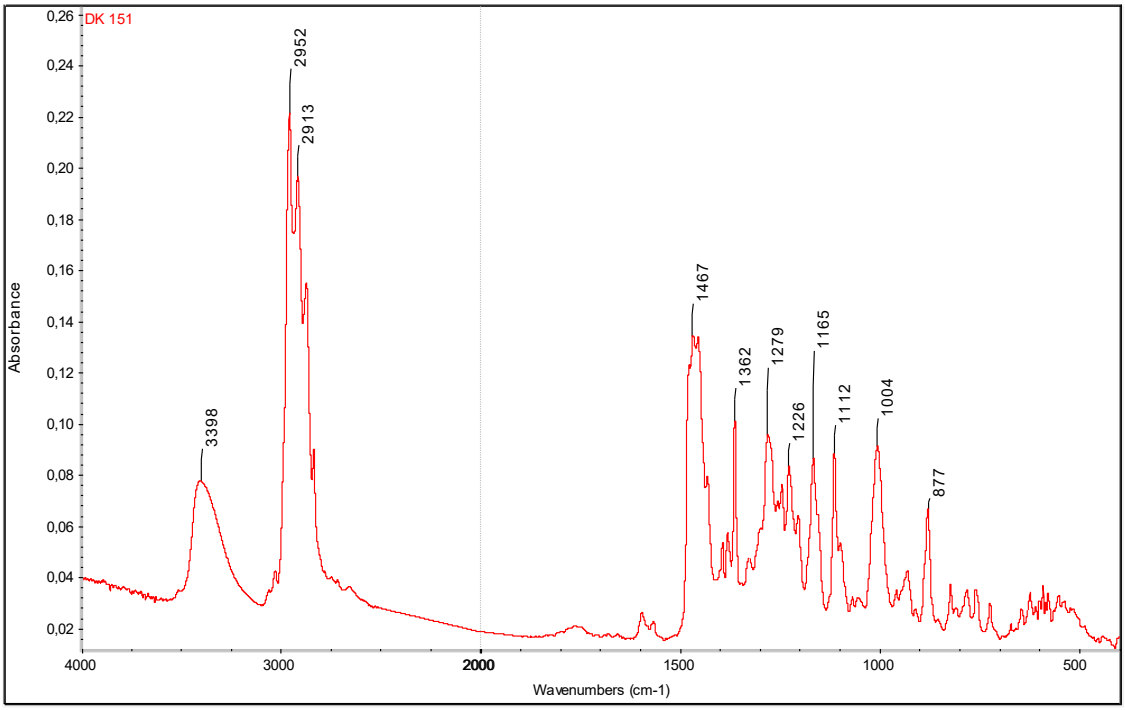

Figure 35. IR of compound **9** (KBr).

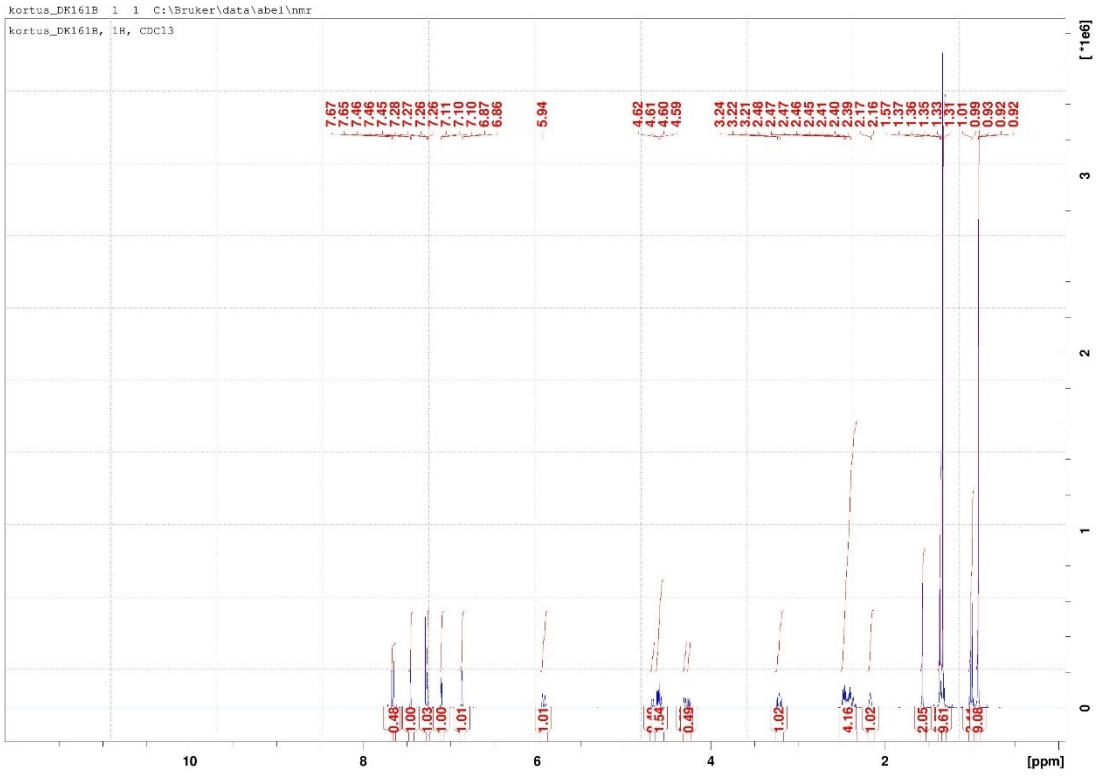

Figure 36. ^{1}H NMR of compound **10** ($CDCl_3$, 600 MHz).

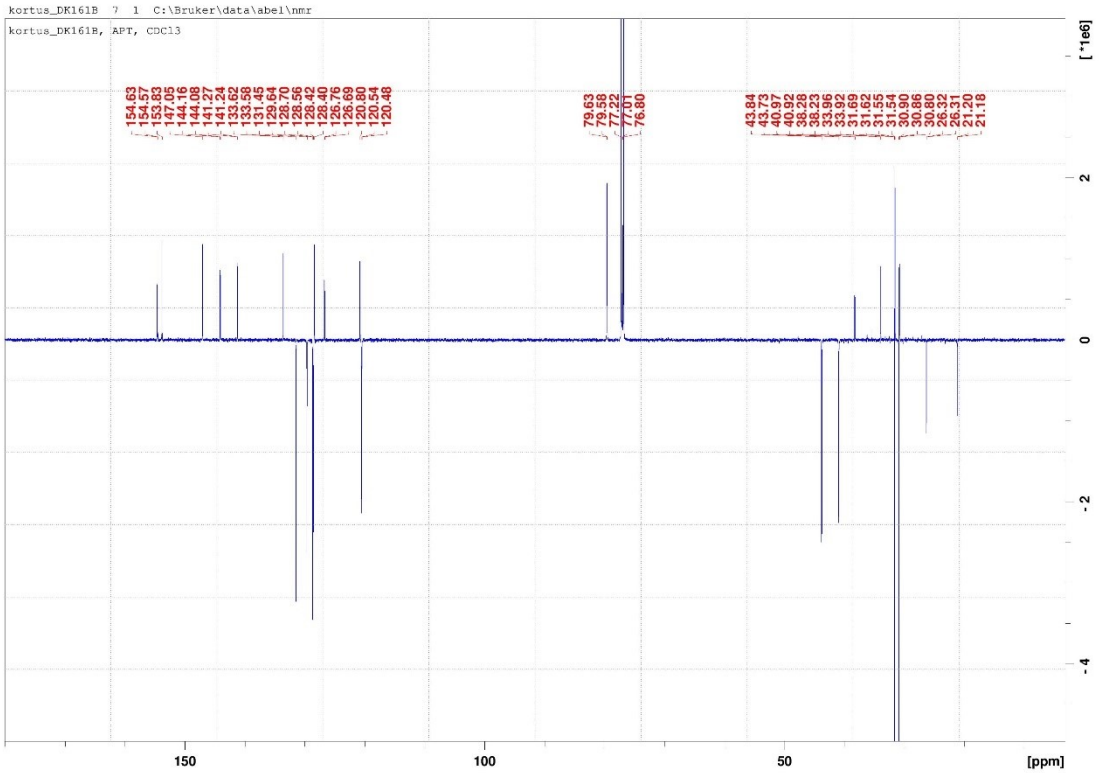

Figure 37. ^{13}C NMR of compound **10** ($CDCl_3$, 151 MHz).

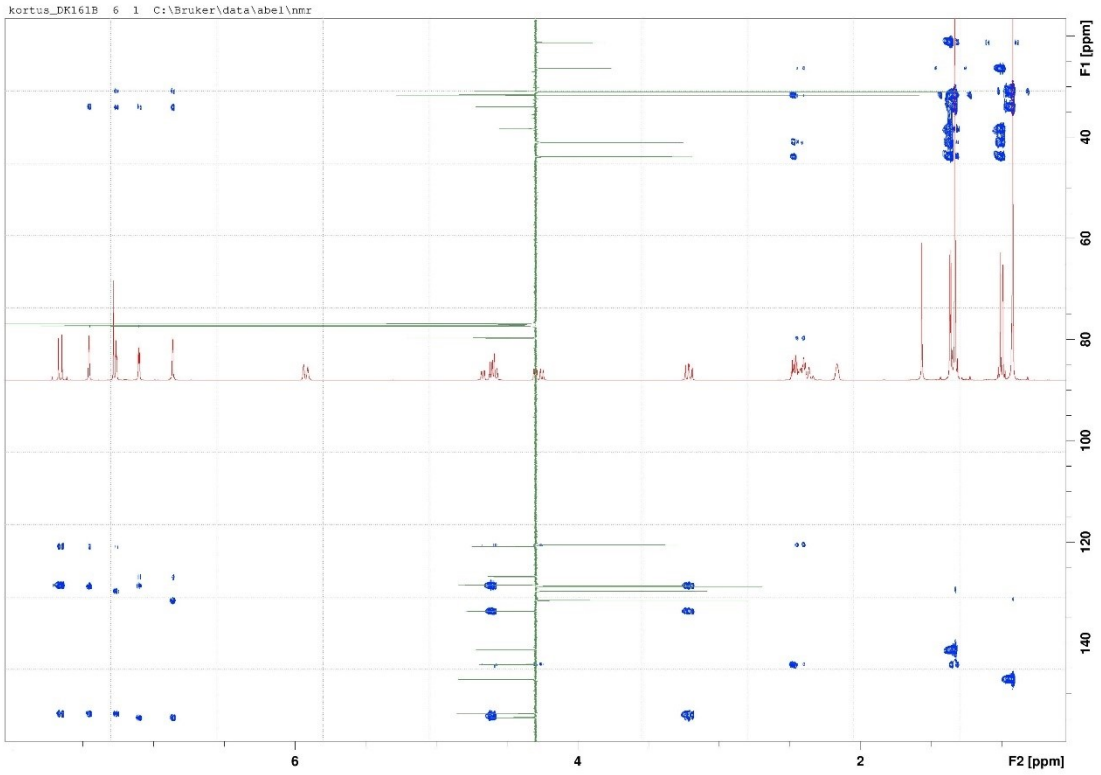

Figure 38. HMBC NMR of compound **10** ($CDCl_3$).

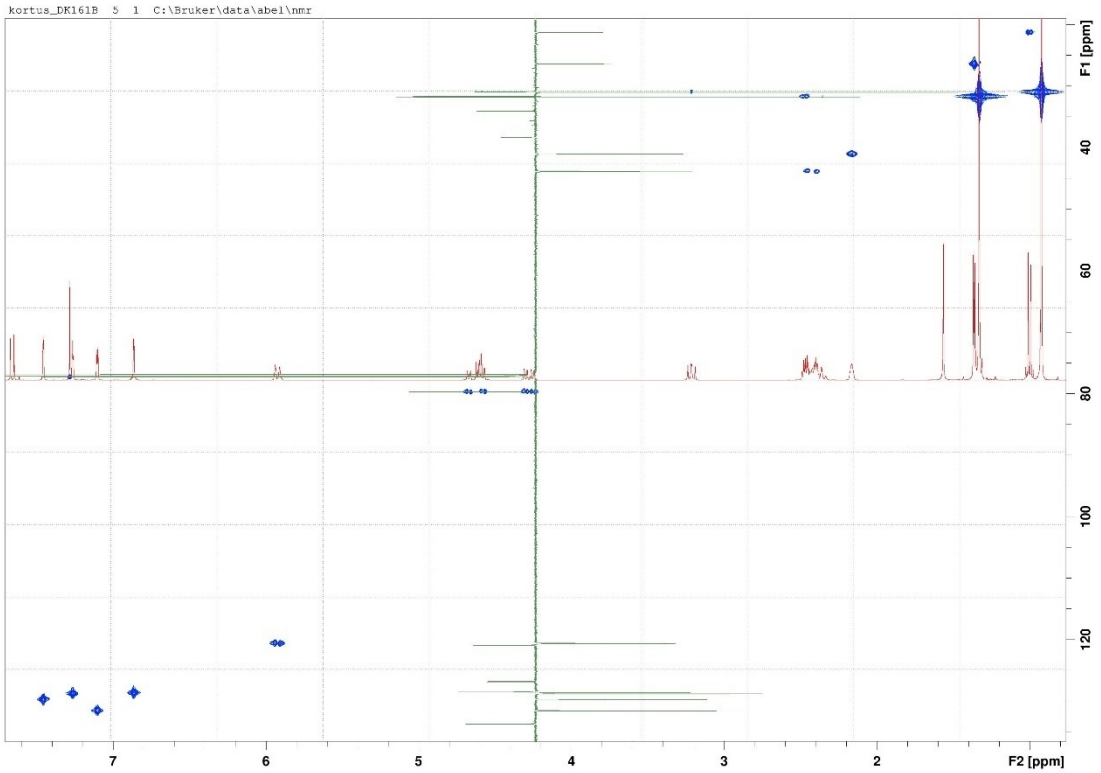

Figure 39. HMBC NMR of compound **10** ($CDCl_3$).

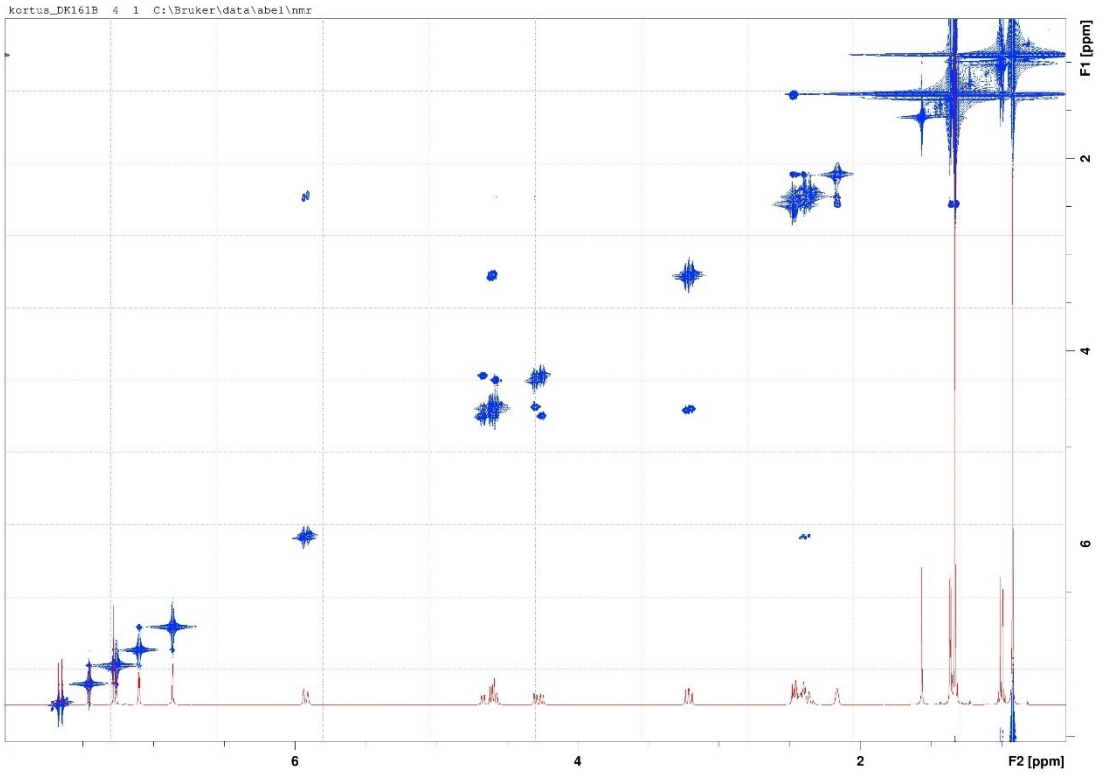

Figure 40. COSY NMR of compound **10** ($CDCl_3$).

Figure 41. HRMS of compound **10** (ESI^+).

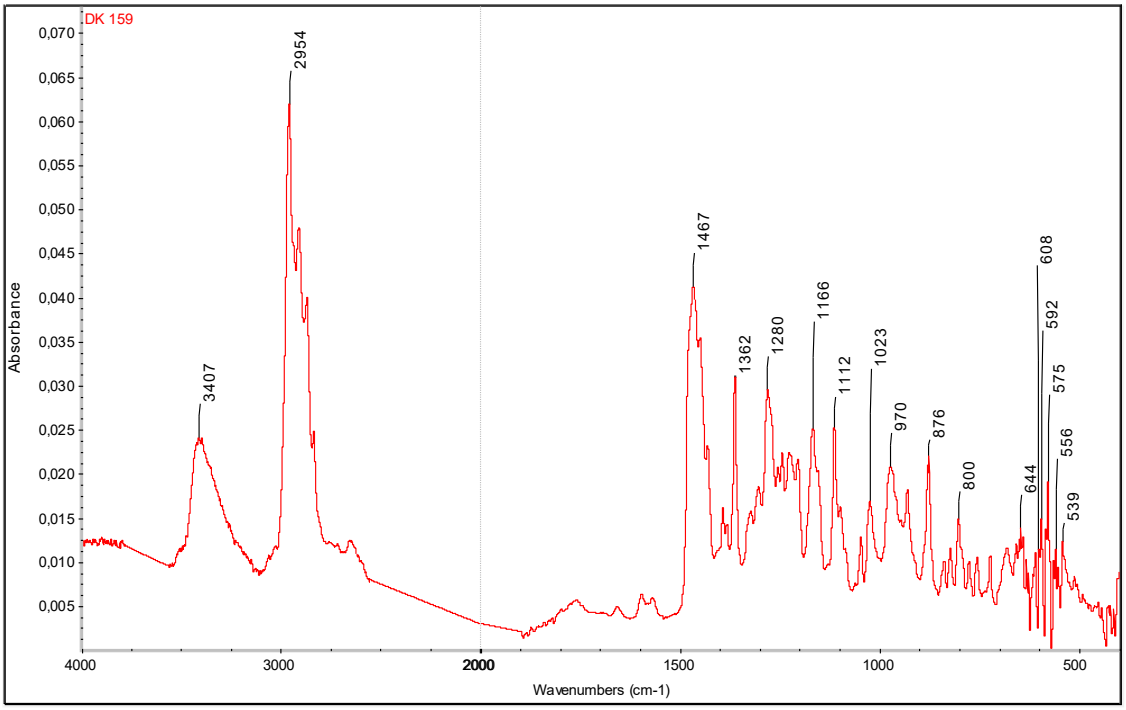

Figure 42. IR of compound **10** (KBr).

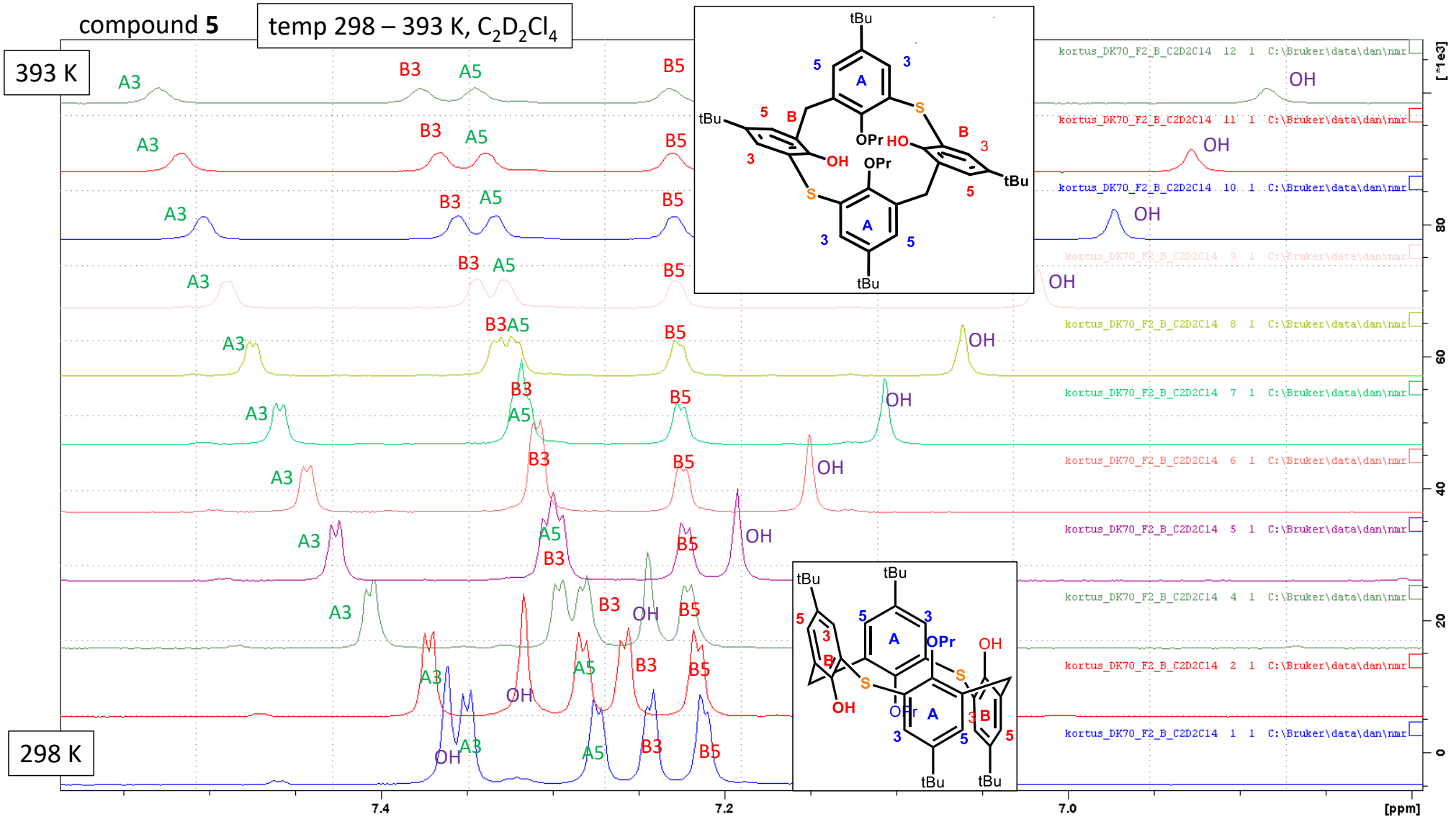

Fig. 43. Variable temperature ^{1}H NMR spectra of **5** in the range of 298 - 413 K ($C_2D_2Cl_4$, 500 MHz)

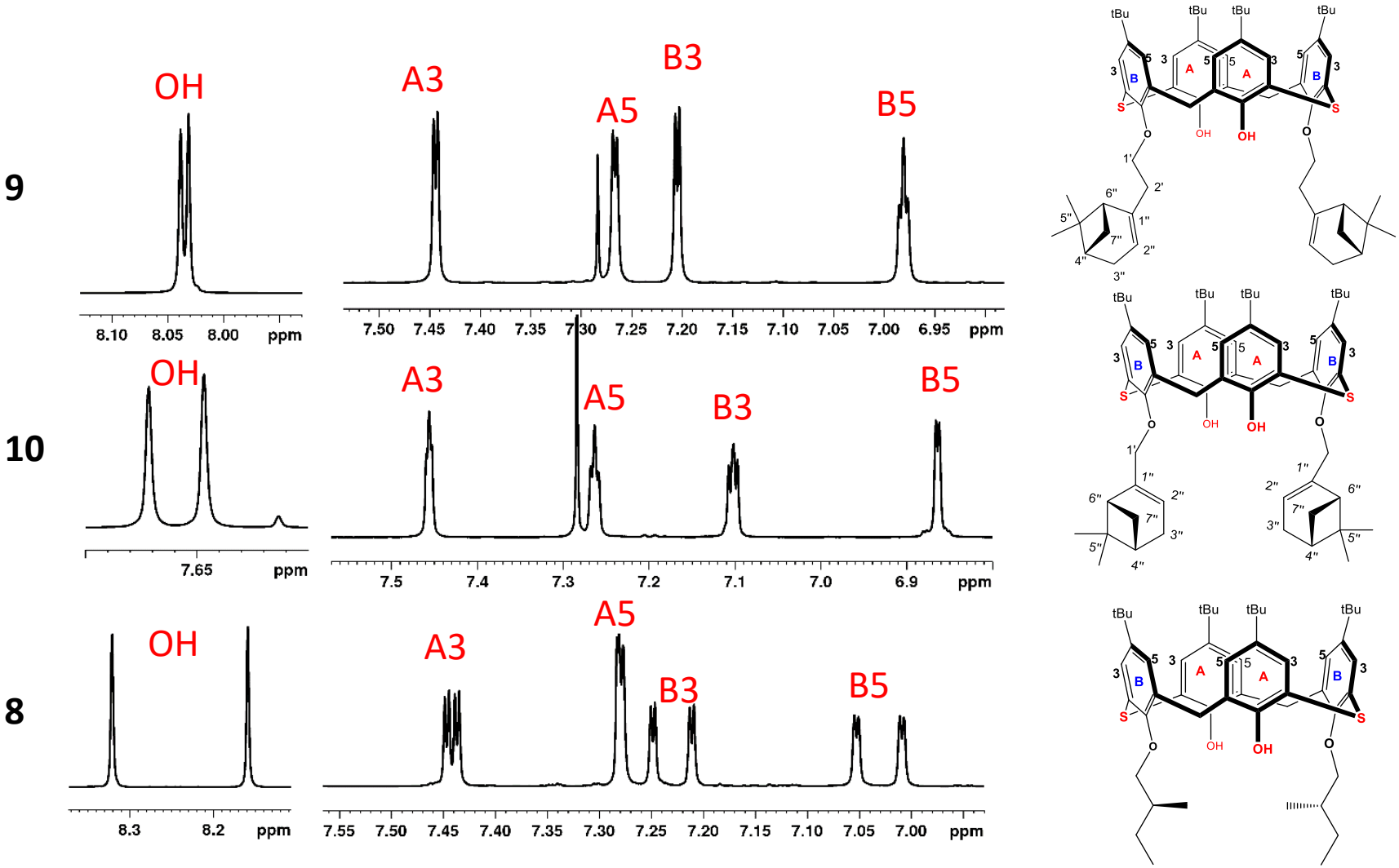

Fig. 44. Comparison of partial ^{1}H NMR spectra (aromatic region) of **8, 9** and **10** (298 K, $CDCl_3$, 600 MHz).

2. CRYSTALOGRAPHIC STRUCTURES

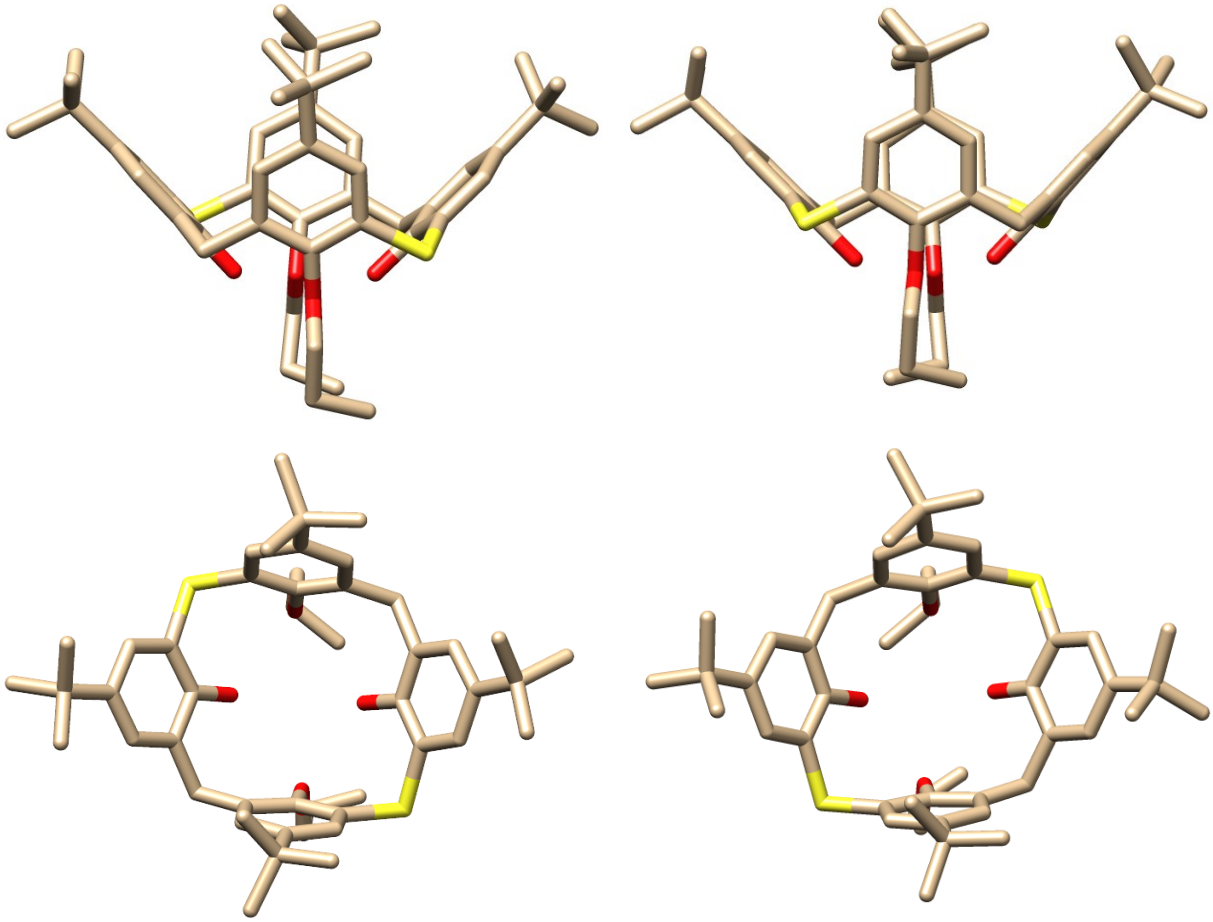

Figure 45. Crystalographic structures of two enantiomers of compound **4**.

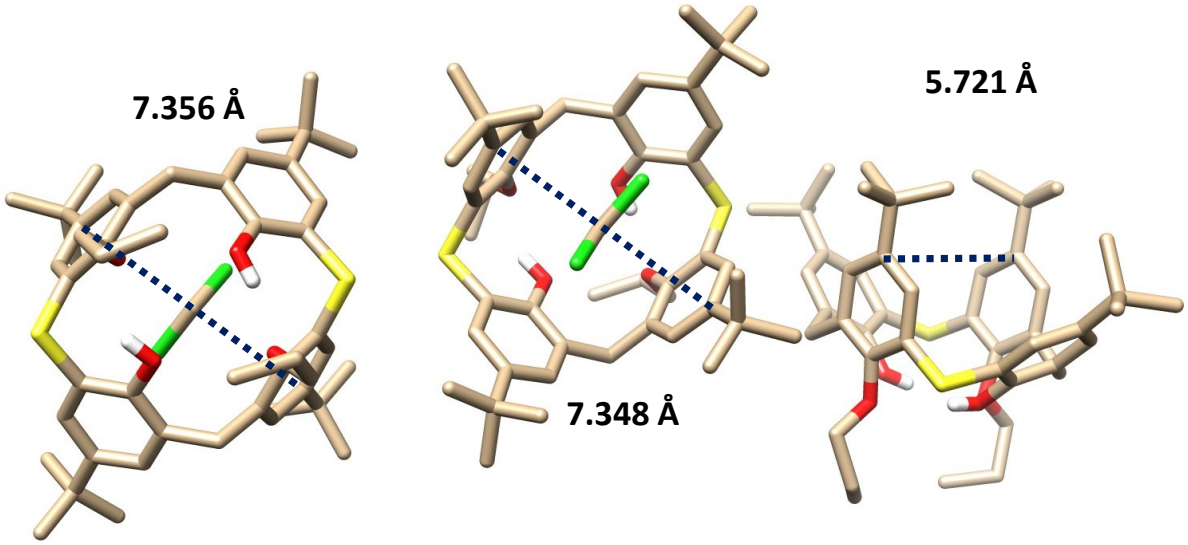

Figure 46. Crystalographic structure of compound **4** - three symmetrically independent molecules in the unit cell, two of them containing solvent molecule (DCM).

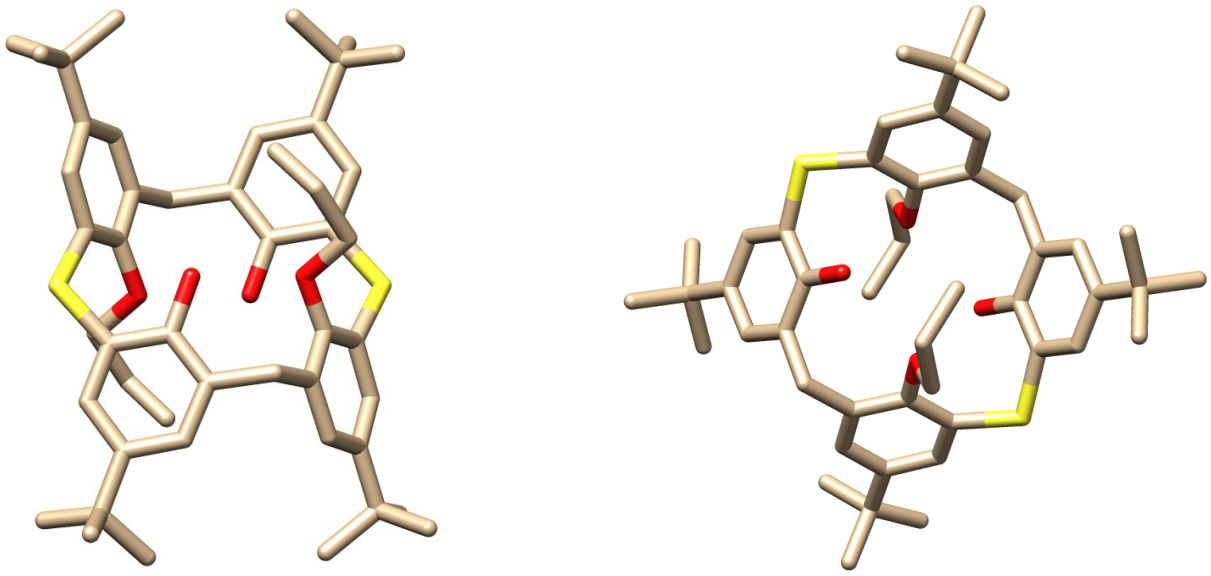

Figure 47. Crystalographic structure of compound **5**.

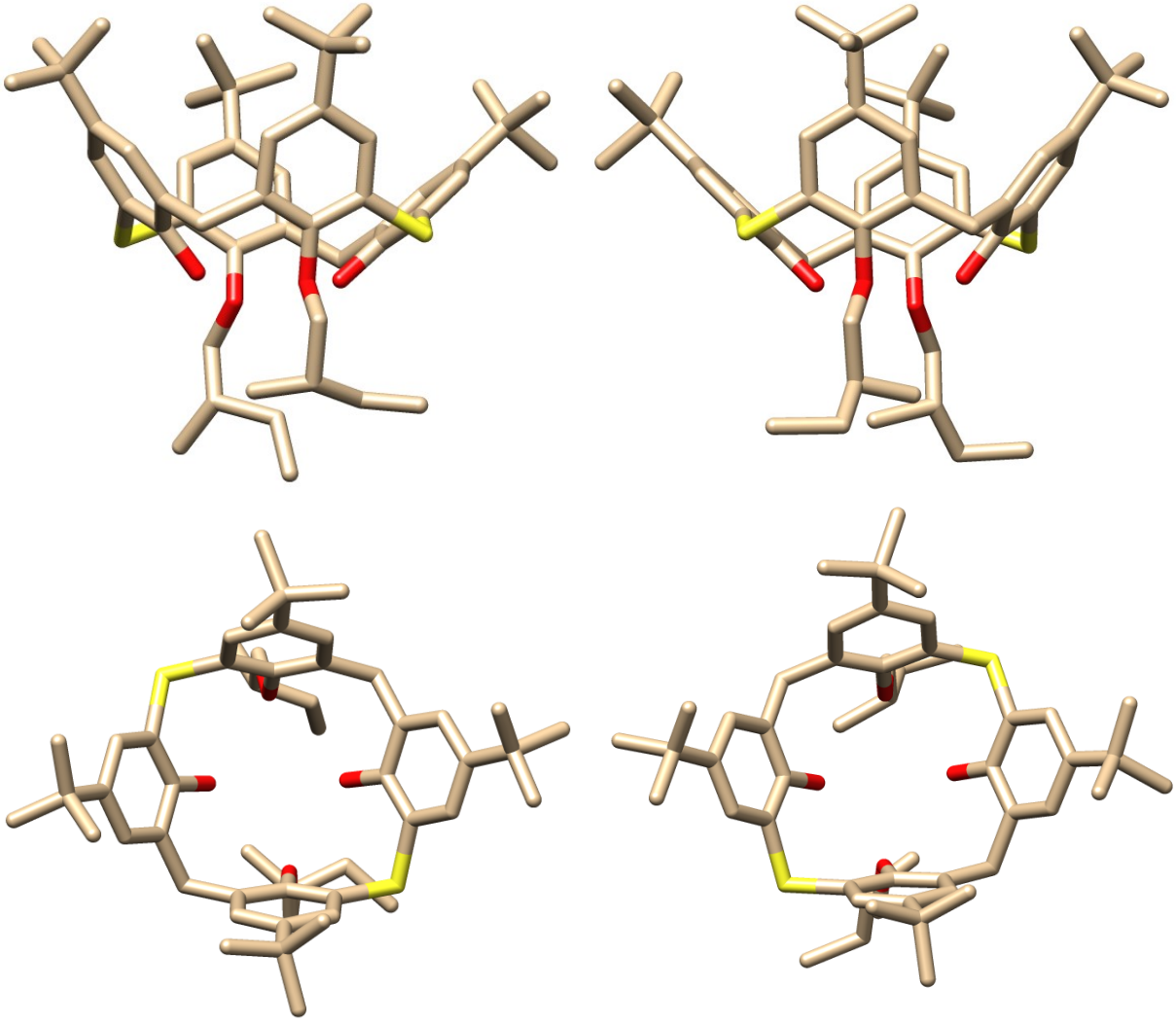

Figure 48. Crystalographic structures of two diastereomers of compound **8**.

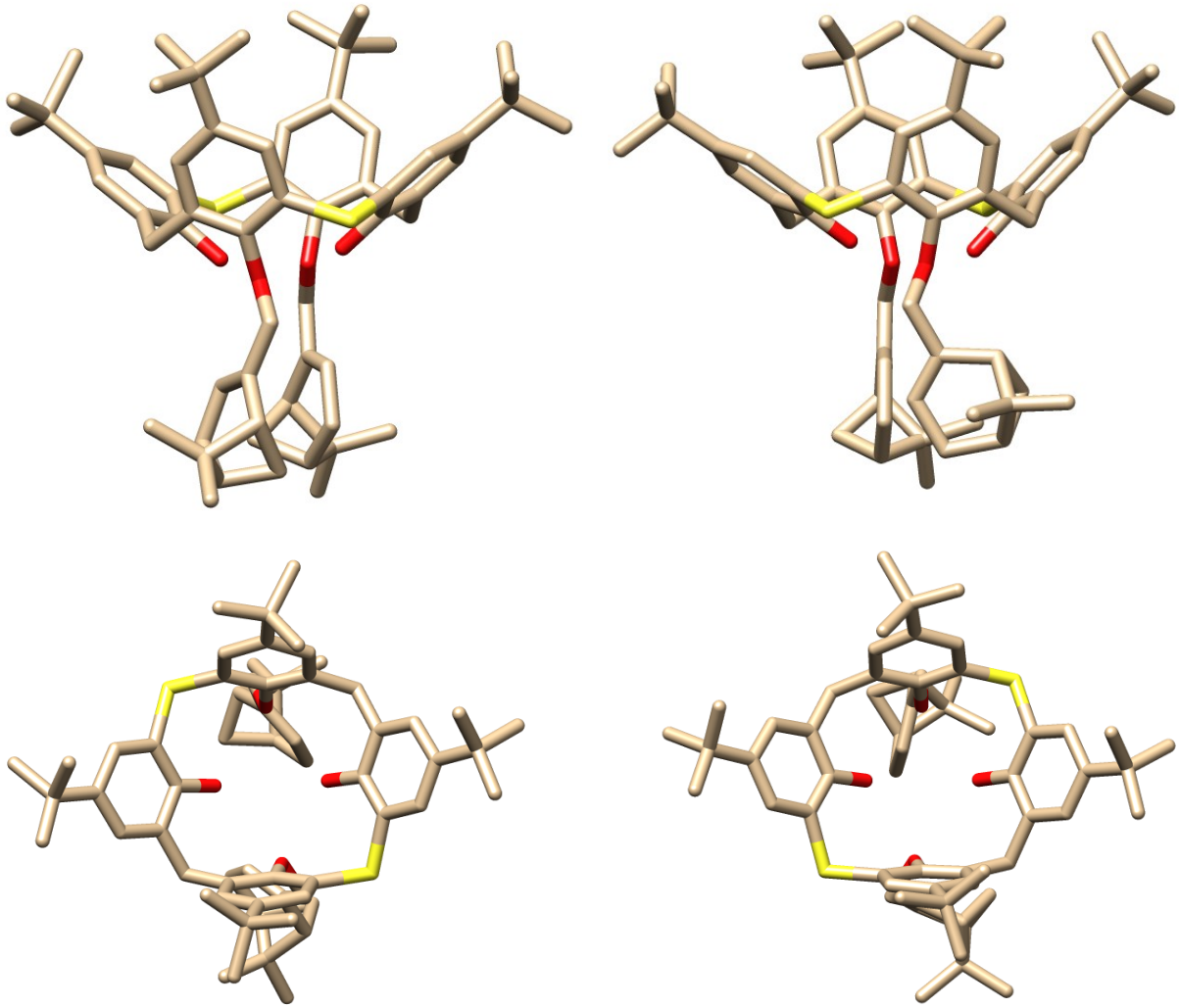

Figure 49. Crystalographic structures of two diastereomers of compound **10**.

3. HPLC MEASUREMENTS

Compounds **4, 8** and **9** were subjected to HPLC on a chiral column Chiralpak IA (250 × 4.6 mm ID, 10 μm) using heptane:CH_2Cl_2 = 90:10 or 95:5 v/v as a mobile phase. Flow rate was 0.7 mL min^{-1}, column temperature 298 K and detection wavelength 254 nm. These conditions have led to a base-line separation of two peaks.

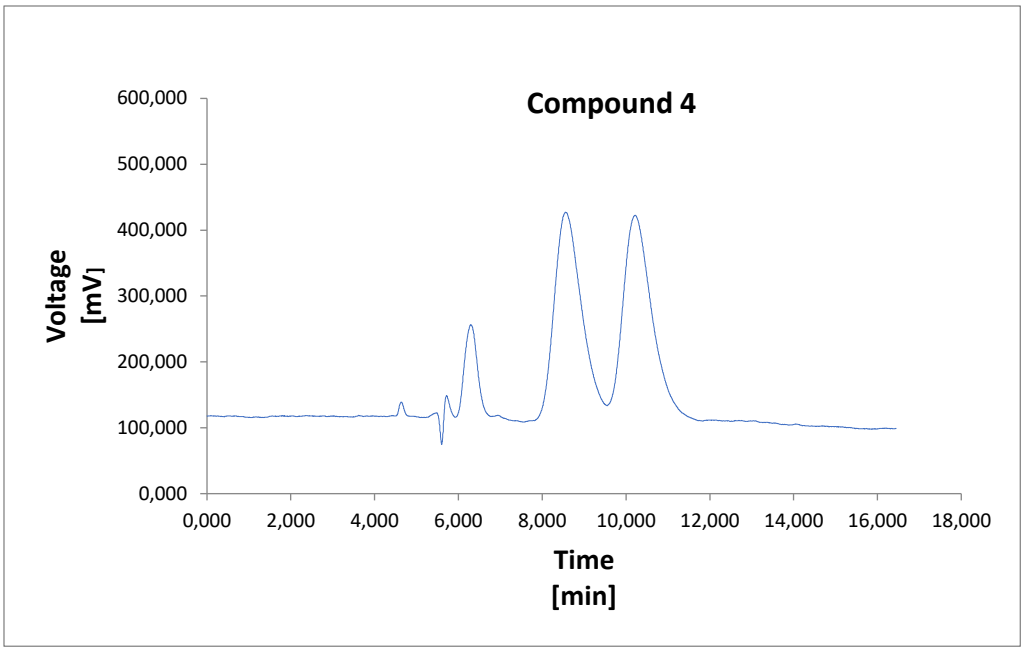

Figure 50. HPLC measurement of compound **4**, mobile phase: heptane:CH_2Cl_2 = 90:10, retention times: 8.55 and 10.22 min.

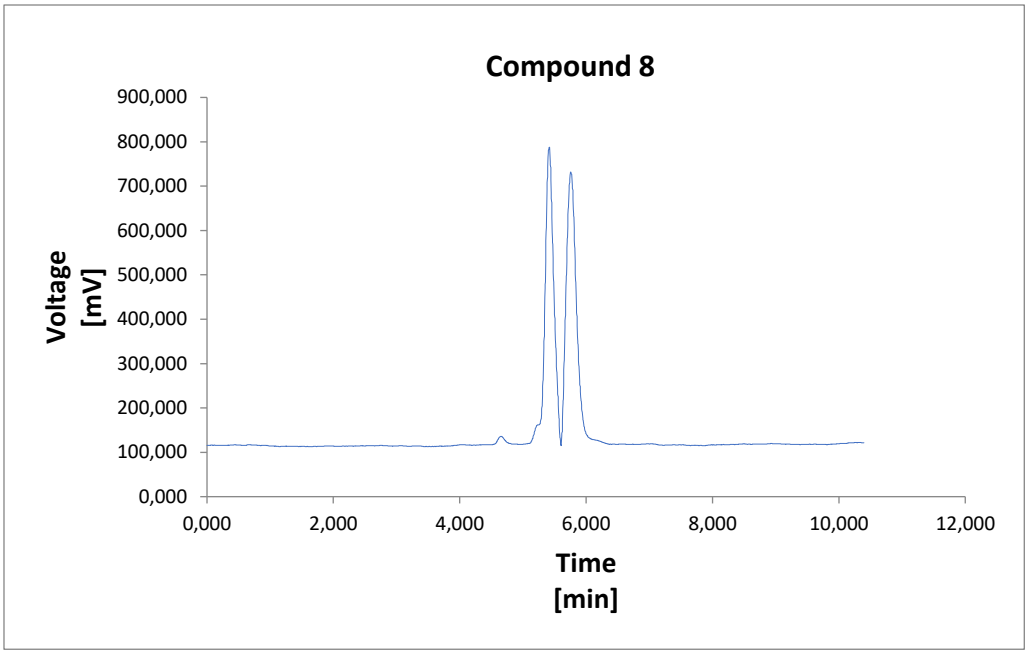

Figure 51. HPLC measurement of compound **8**, mobile phase: heptane:CH_2Cl_2 = 95:5, retention times: 5.42 and 5.76 min.

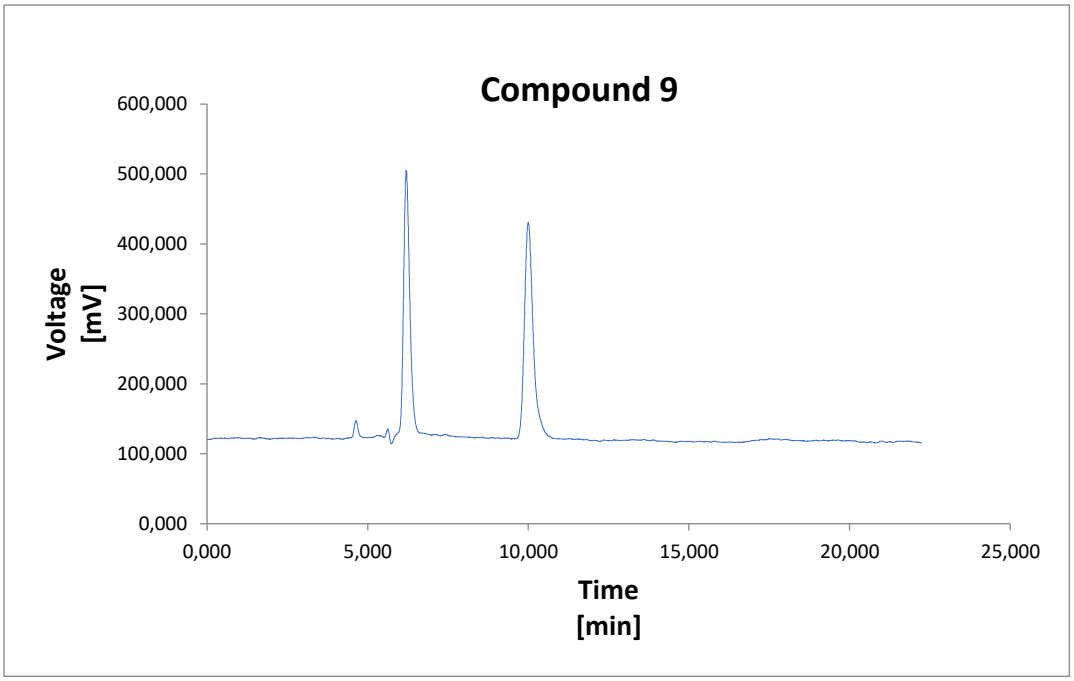

Figure 52. HPLC measurement of compound **9**, mobile phase: heptane:CH_2Cl_2 = 95:5, retention times: 6.20 and 10.22 min.