Supplementary materials for

^{13}C CPMAS NMR as a tool for full structural description of 2-phenyl substituted imidazoles that overcomes the effects of fast tautomerization

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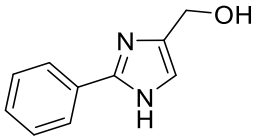
Spectra of (2-phenyl-1H-imidazol-4-yl)methanol (1a).



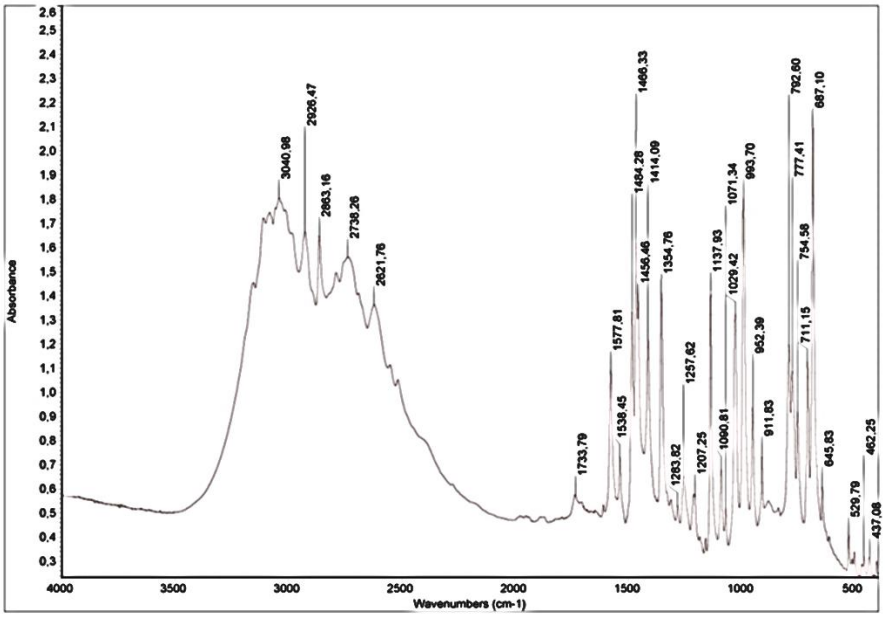


Figure 1. IR spectrum of **1a** in KBr pellets.

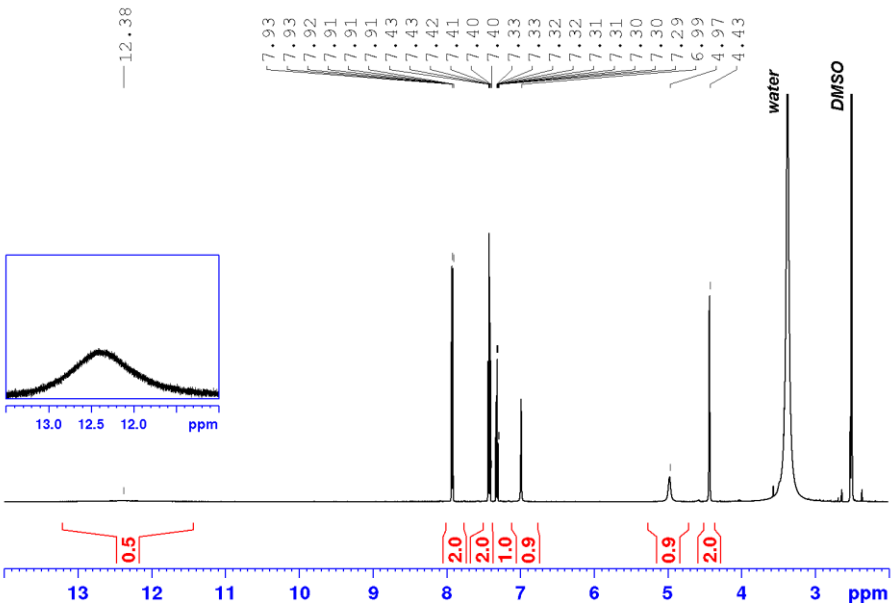


Figure 2. ^{1}H NMR (DMSO-d_6) of **1a** at 298 K.

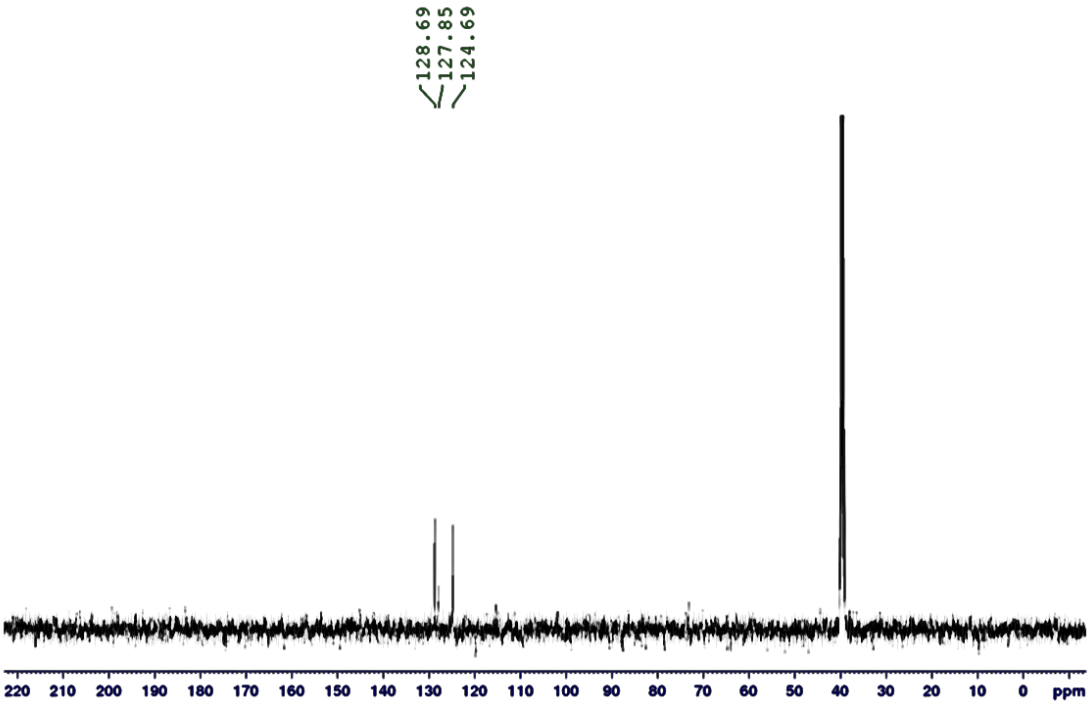


Figure 3. ^{13}C NMR (DMSO-d_6) of **1a**.

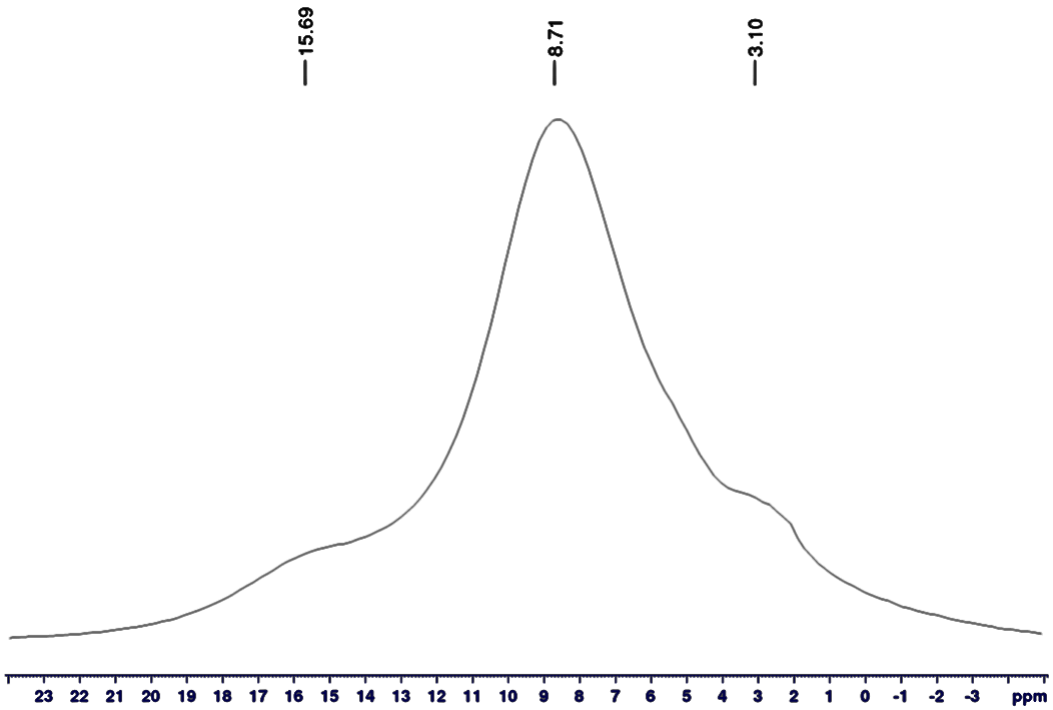


Figure 4. ^{1}H-MAS NMR (solid state 500MHz, 15kHz) of **1a**.

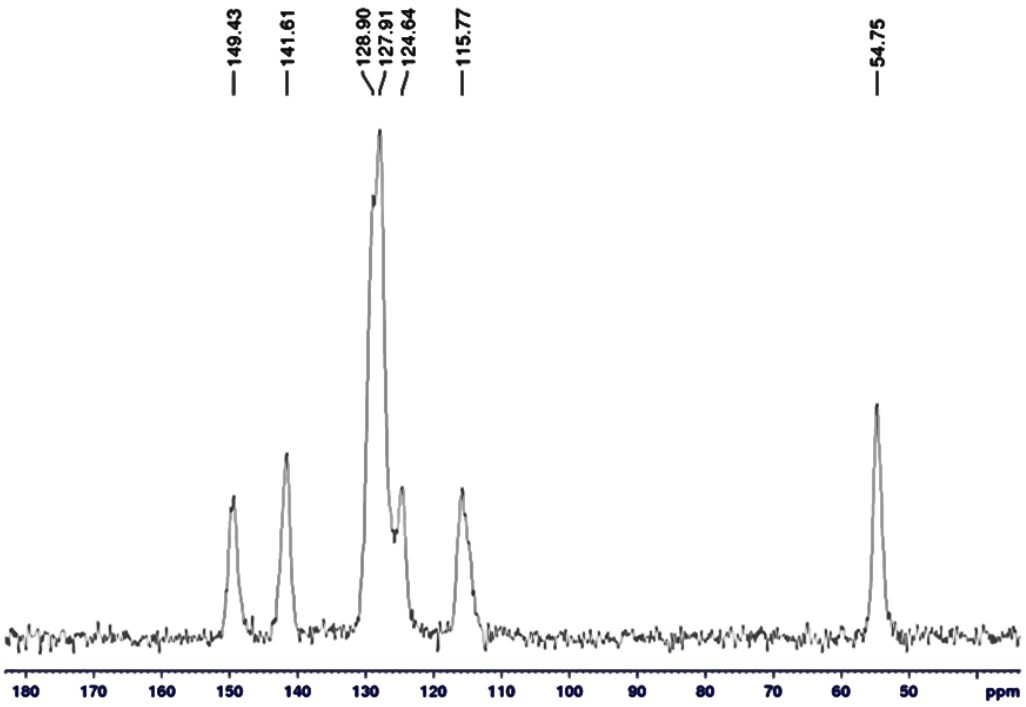


Figure 5. ^{13}C CP-MAS (solid state 125MHz, 15kHz) of **1a**.

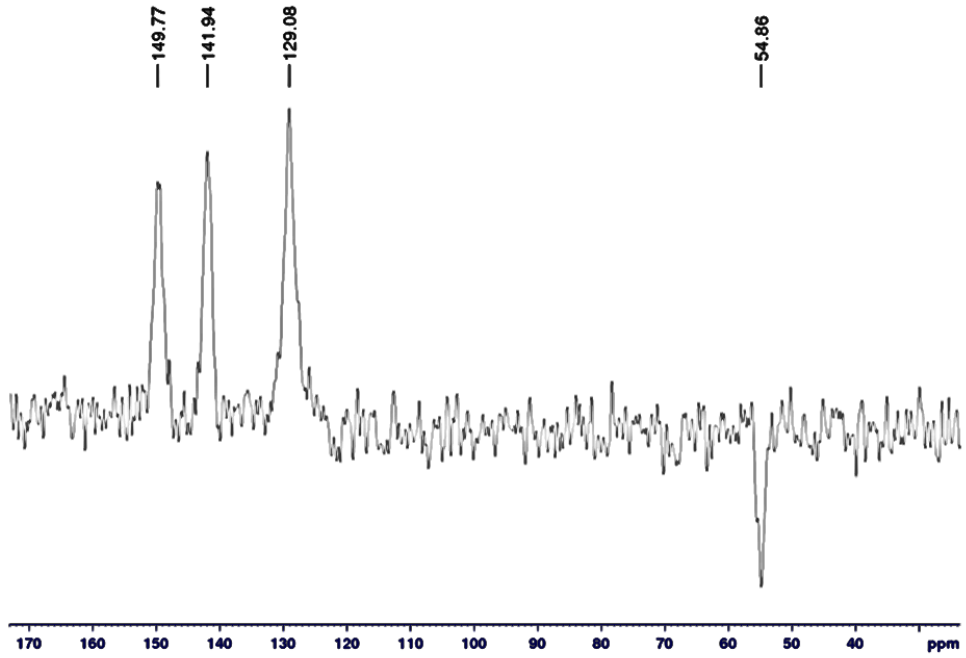
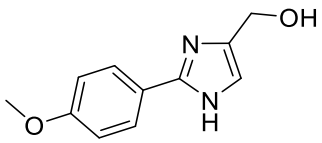


Figure 6. ^{13}C CPPI spectrum of **1a**; null signal for CH, negative signal for CH_2, and positive signal for C and CH_3.

Spectra of (2-(4-methoxyphenyl)-1H-imidazol-4-yl)methanol (1b)



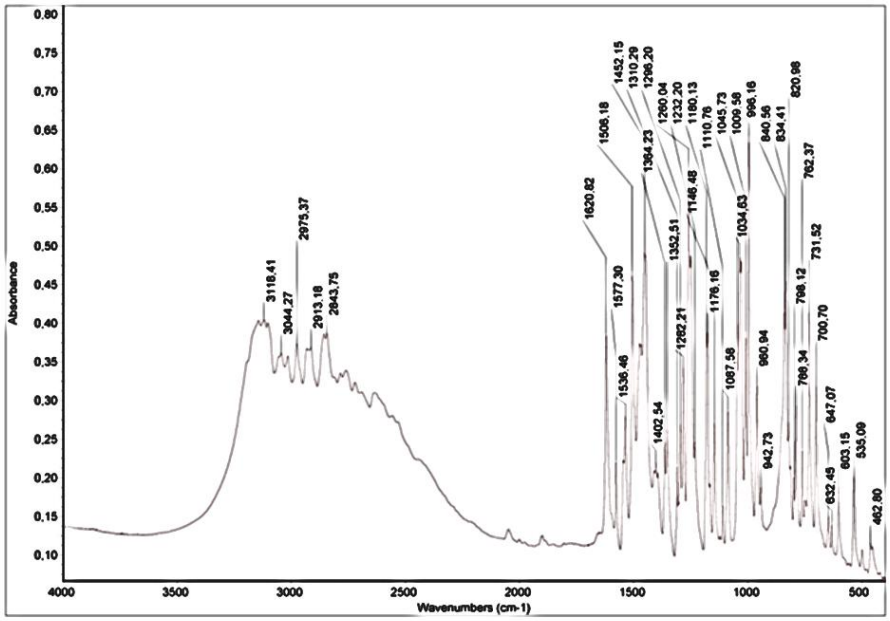


Figure 7. IR spectrum of **1b** in KBr pellets.

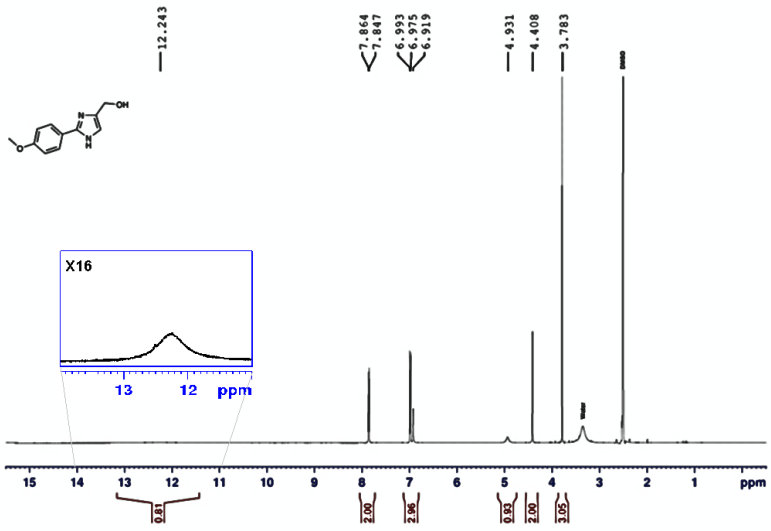


Figure 8. ^{1}H NMR (DMSO-d_6) of **1b**.

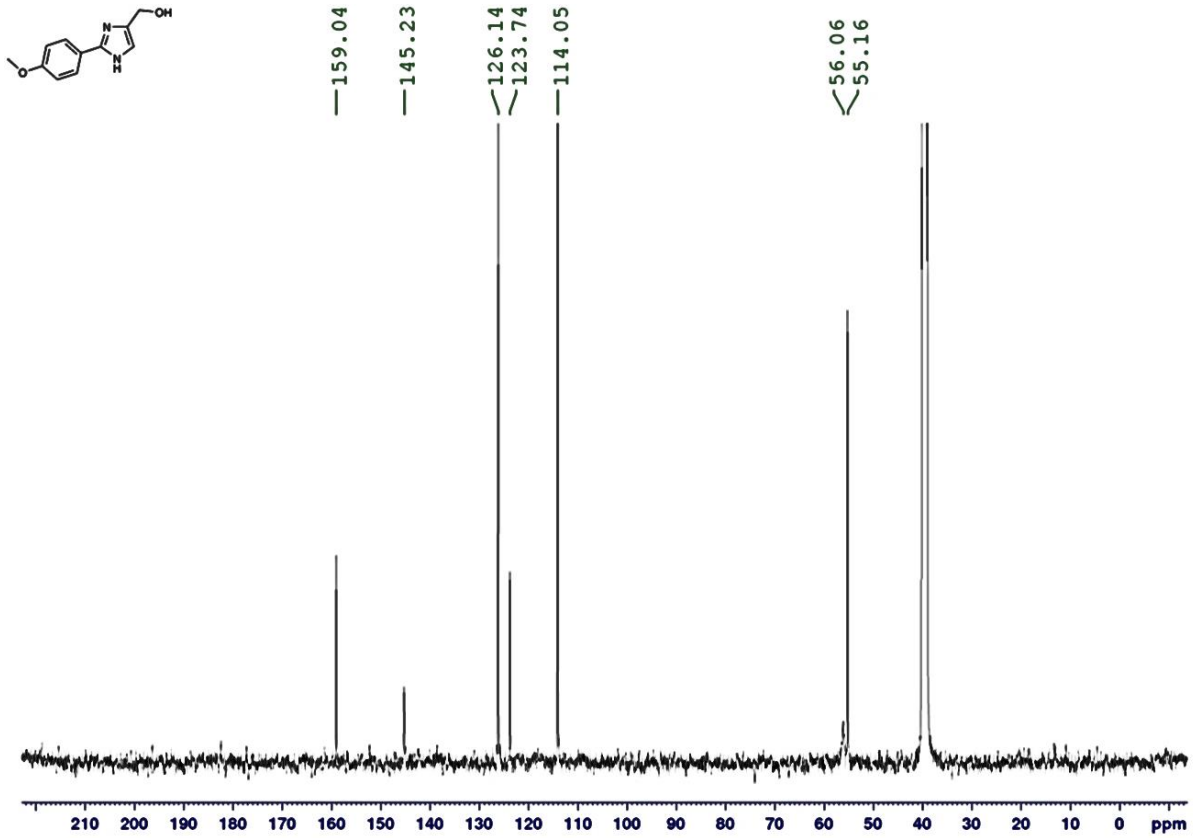


Figure 9. ^{13}C NMR (DMSO-d_6) of **1b**.

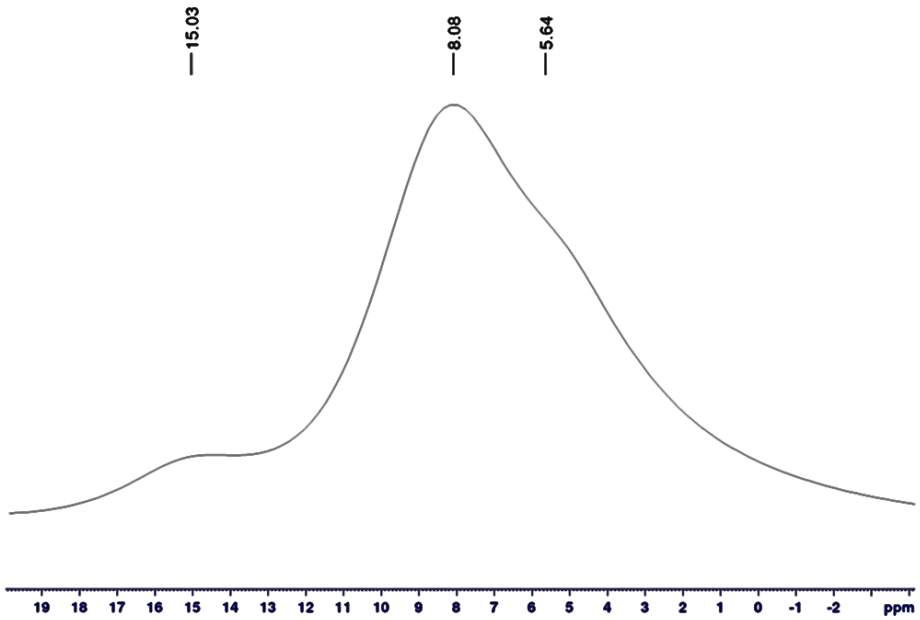


Figure 10. ^{1}H-MAS NMR (solid state 500MHz, 15kHz) of **1b**.

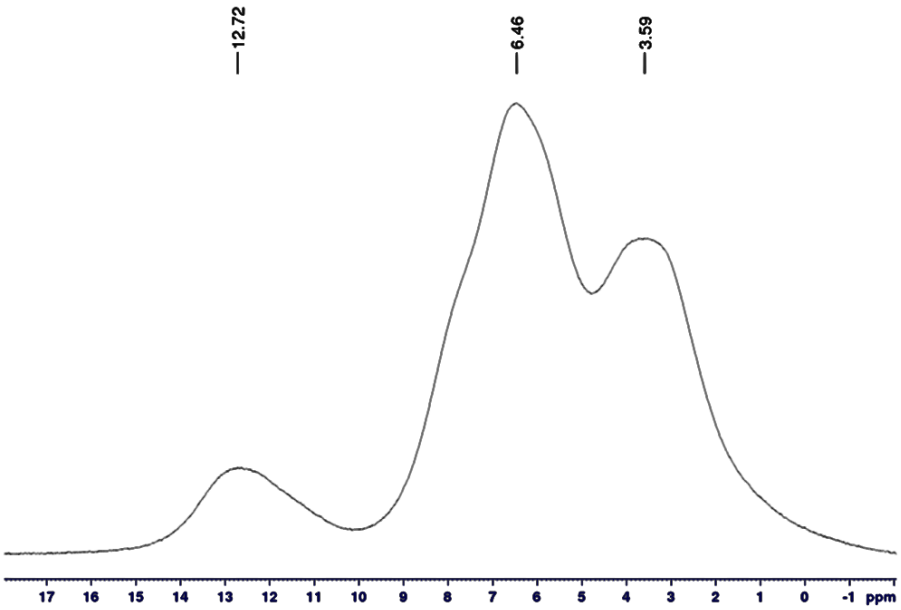


Figure 11. ^{1}H-MAS NMR (solid state 850MHz, 25kHz) of **1b**.

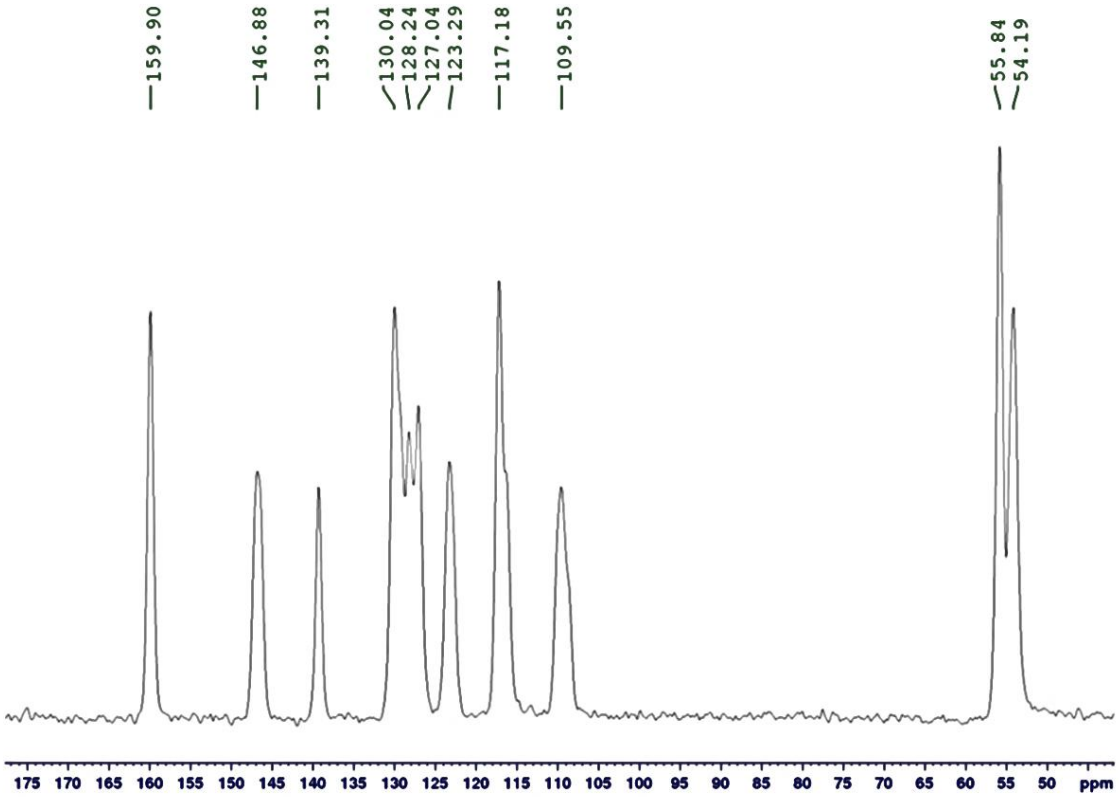


Figure 12. ^{13}C CP-MAS (solid state 125MHz, 15kHz) of **1b**; weak shoulders on the signals at 117.17 and 130.04 ppm and broadening of the signals at 109.55 and 146.88.

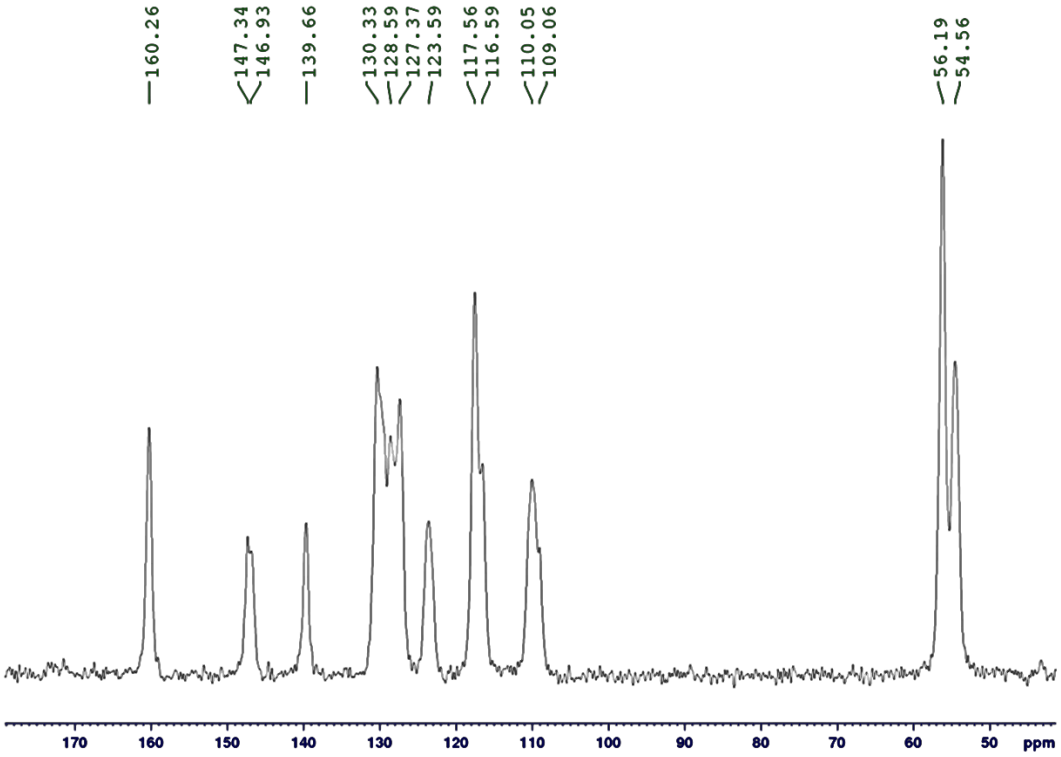


Figure 13. ^{13}C CP-MAS (solid state 212.5 MHz, 25kHz) of **1b.**

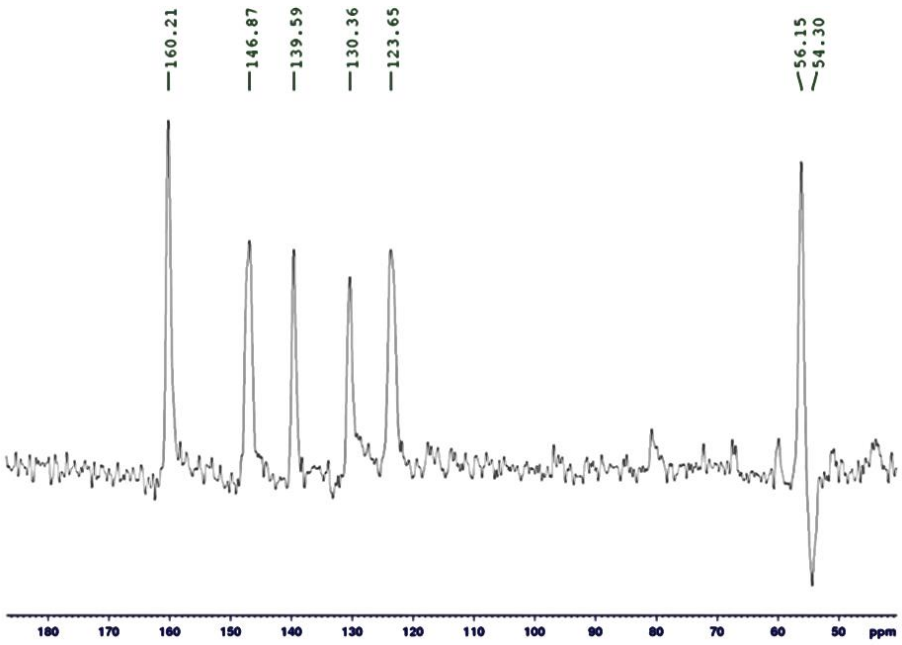
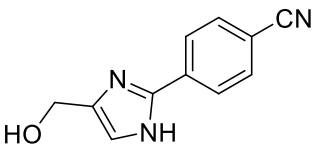


Figure 14. ^{13}C CPPI spectrum (125 MHz, 10 kHz) of **1b**; null signal for CH, negative signal for CH_2, and positive signal for C and CH_3.

Spectra of 4-(4-(hydroxymethyl)-1H-imidazol-2-yl)benzonitrile (1c)



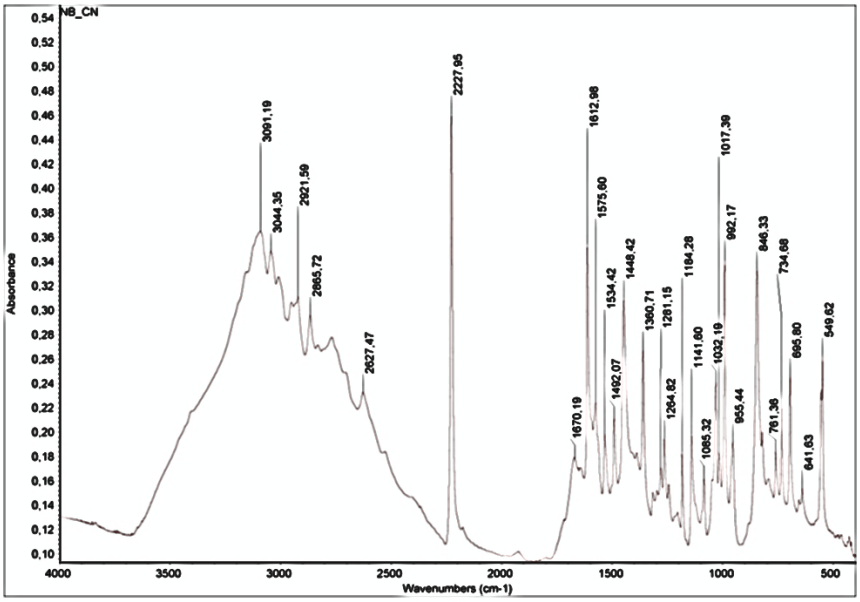


Figure 15. IR spectrum of **1c** in KBr pellets.

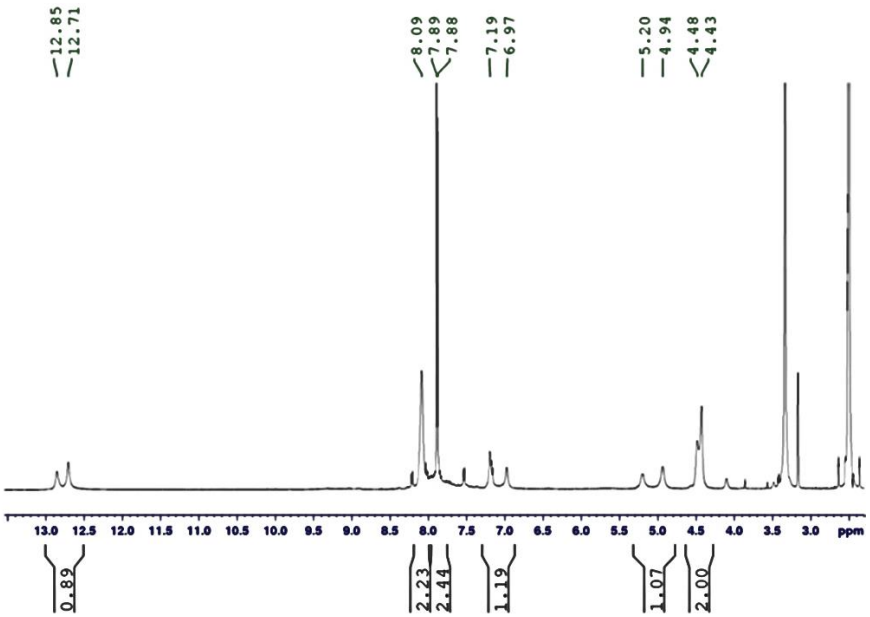


Figure 16. ^{1}H NMR (DMSO-d_6) of **1c** at 298 K.

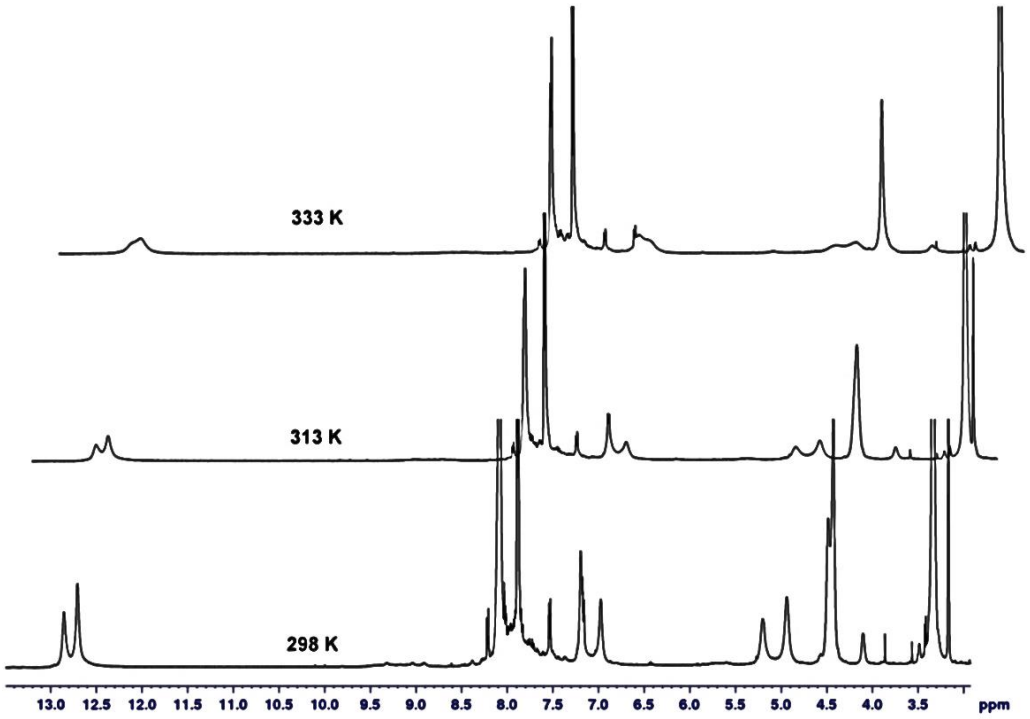


Figure 17. Temperature dependent ^{1}H NMR (DMSO-d_6) of **1c**.

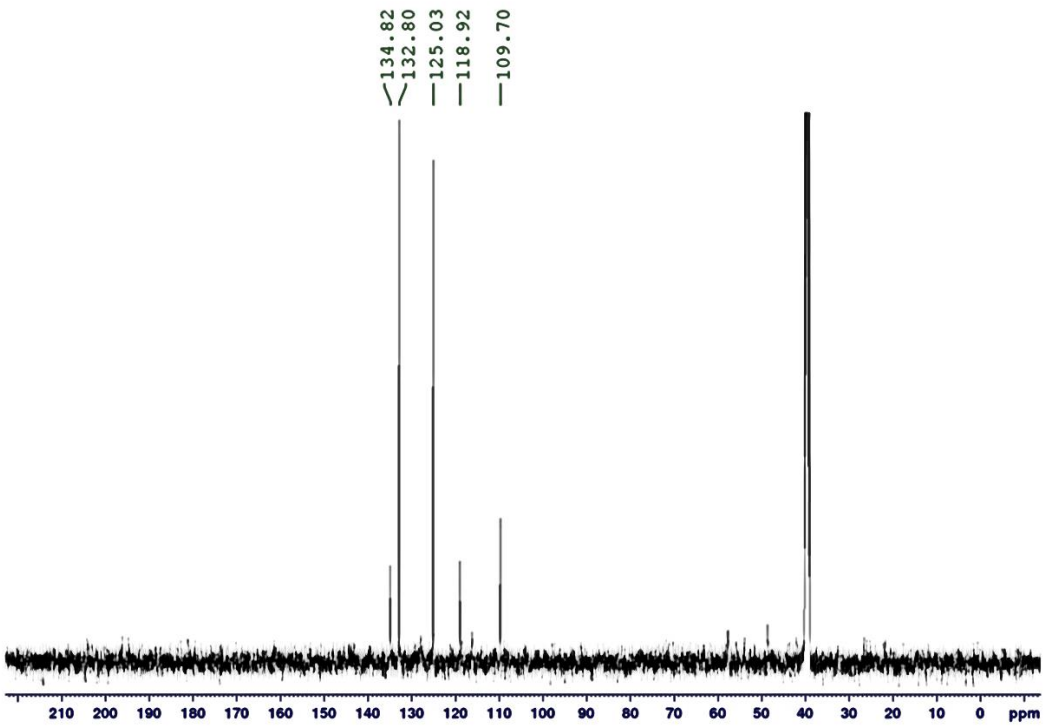


Figure 18. ^{13}C NMR (DMSO-d_6) of **1c** at 298 K.

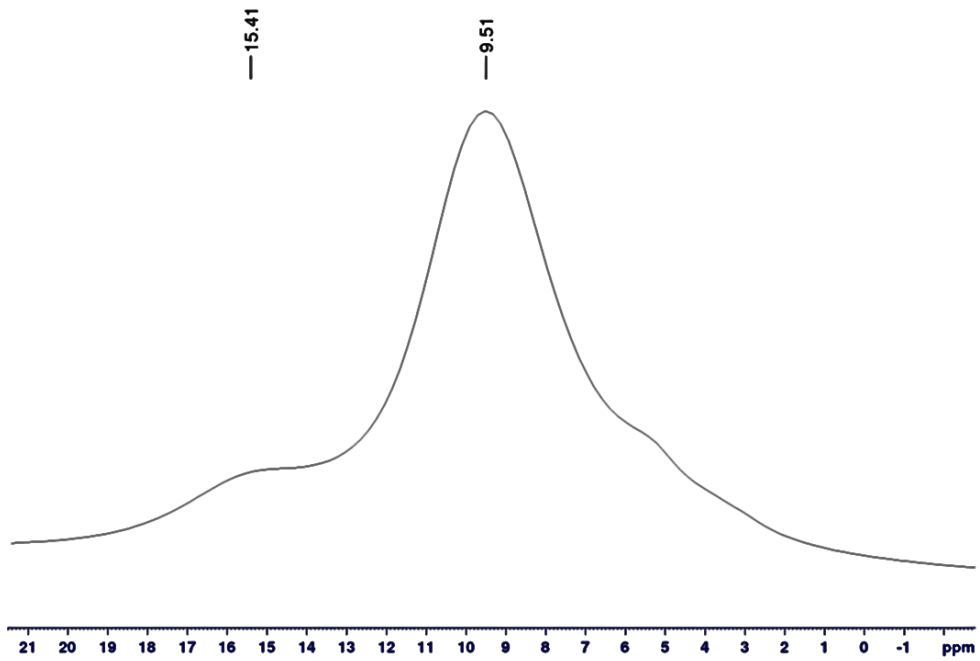


Figure 19. ^{1}H-MAS NMR (solid state 500MHz, 15kHz) of **1c**.

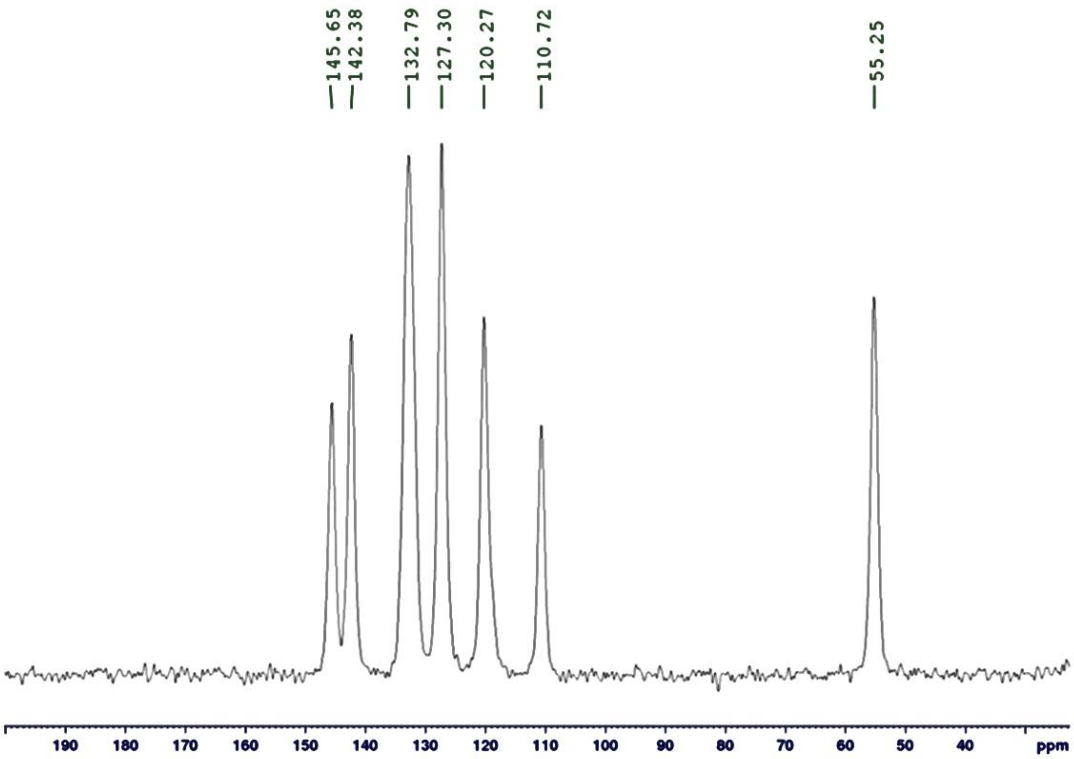
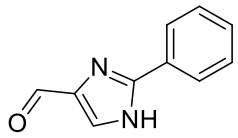


Figure 20. ^{13}C CP-MAS (solid state 125MHz, 15kHz) of **1c**.

Spectra of 2-phenyl-1H-imidazole-4(5)-carbaldehyde (2a)



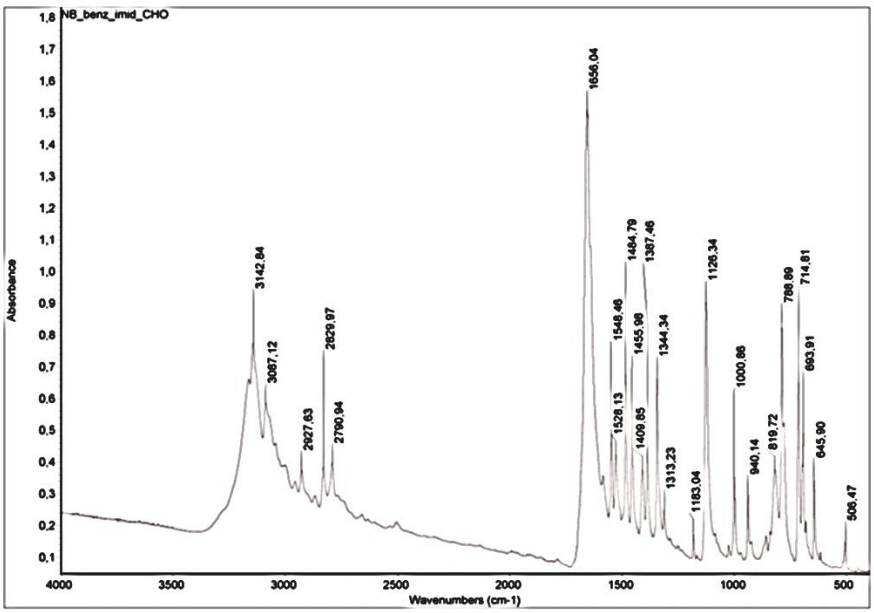


Figure 21. IR spectrum of **2a** in KBr pellets.

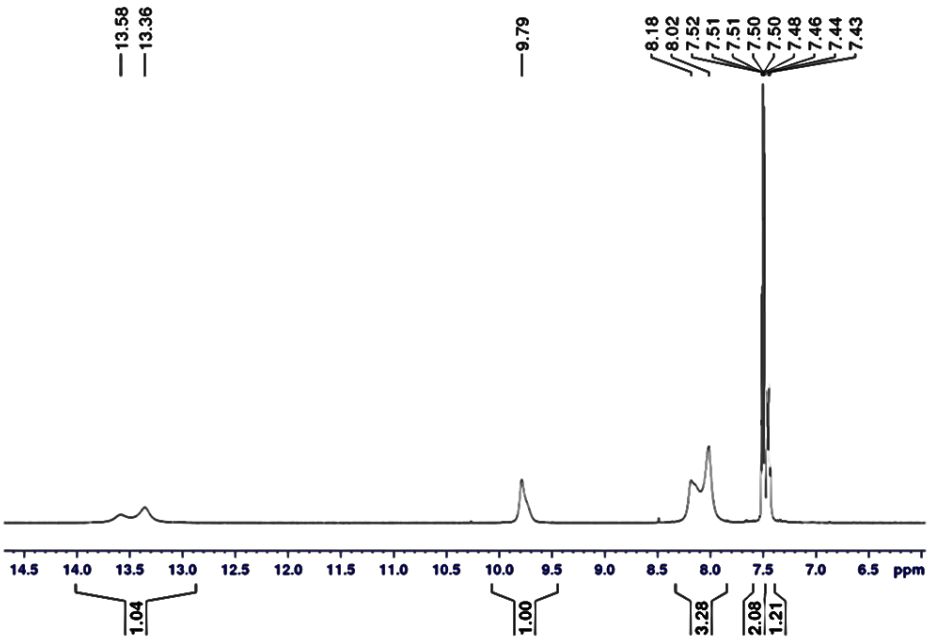


Figure 22. ^{1}H NMR (DMSO-d_6) of **2a** at 298 K.

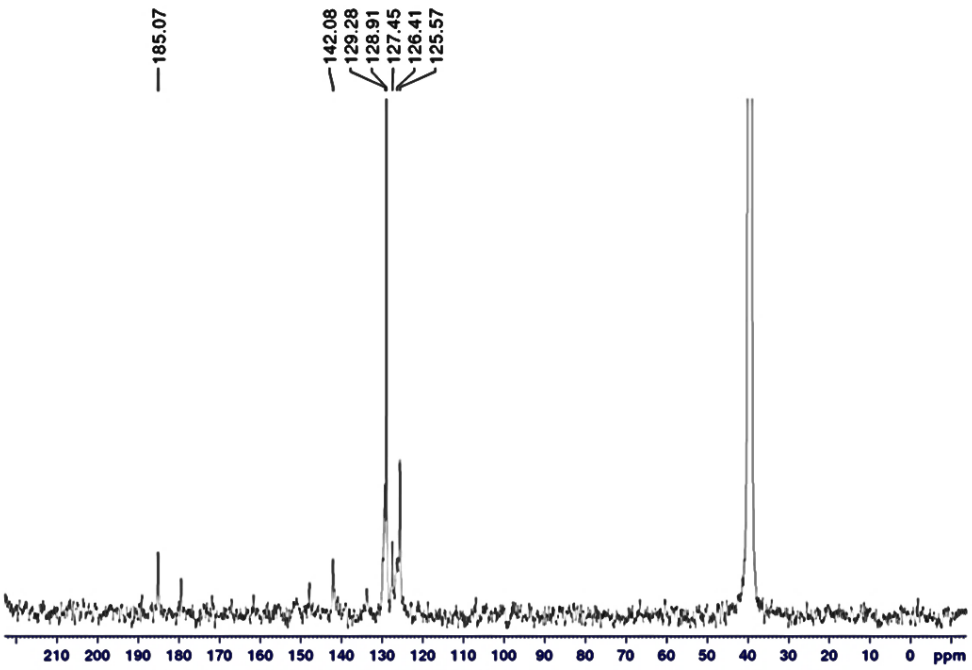


Figure 23. ^{13}C NMR (DMSO-d_6) of **2a** at 298 K (125MHz; NS 512).

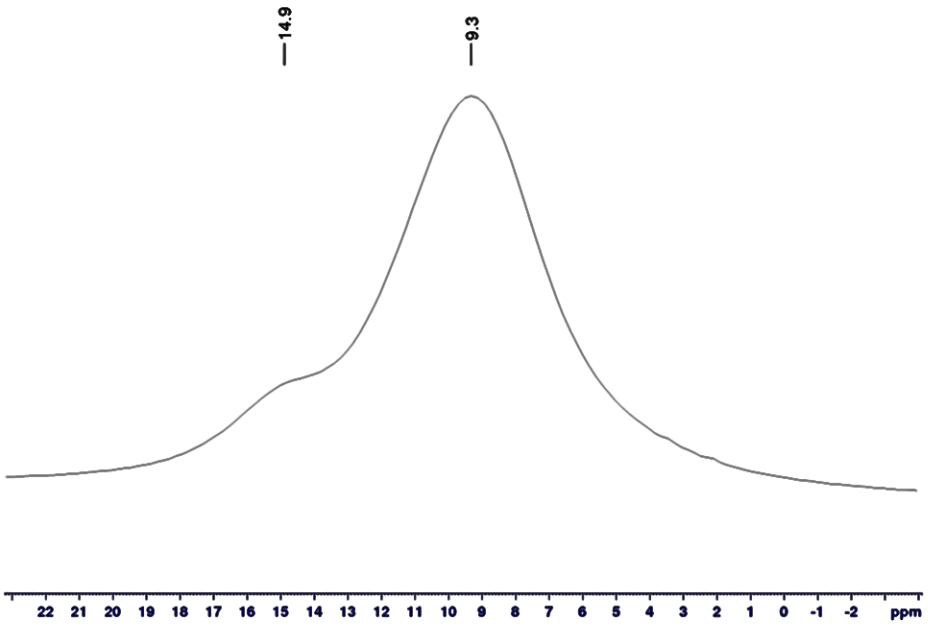


Figure 24. ^{1}H MAS NMR (solid state 500MHz, 15kHz) of **2a.**

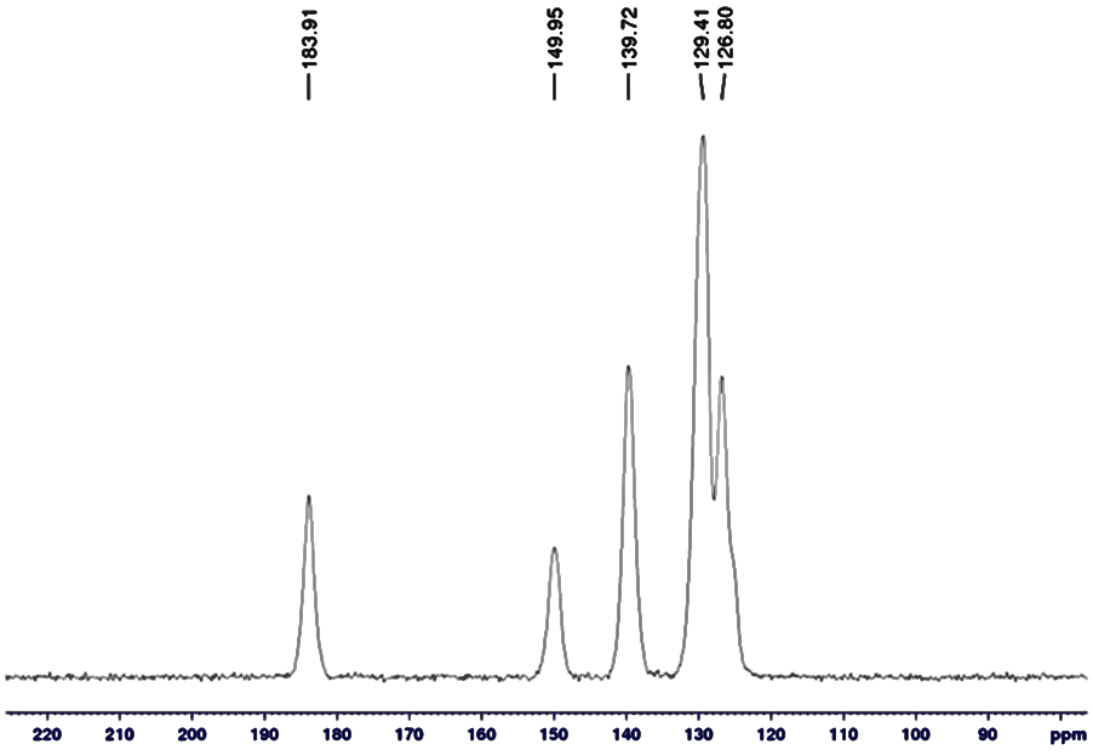


Figure 25. ^{13}C CP-MAS NMR (solid state 500MHz, 15kHz) of **2a.**

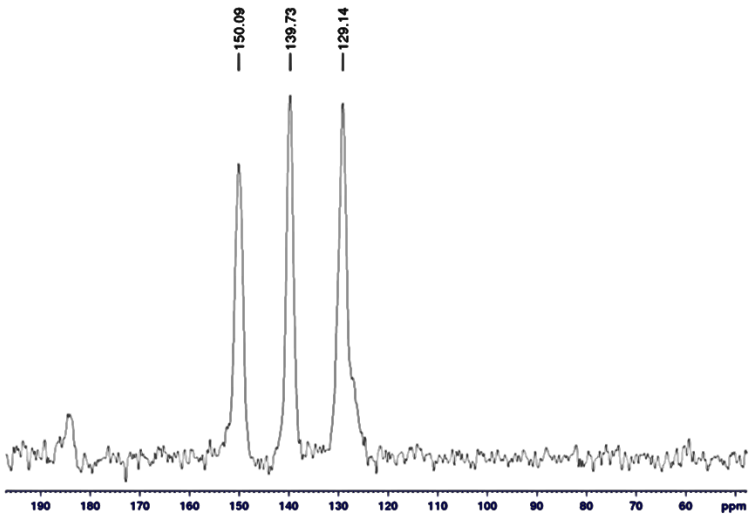
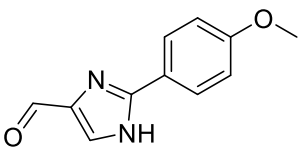


Figure 26. ^{13}C CPPI spectrum (125 MHz, 10 kHz) of **2a**; null signal for CH, negative signal for CH_2, and positive signal for C and CH_3.

Spectra of 2-(4-methoxyphenyl)-1H-imidazole-4-carbaldehyde (2b)



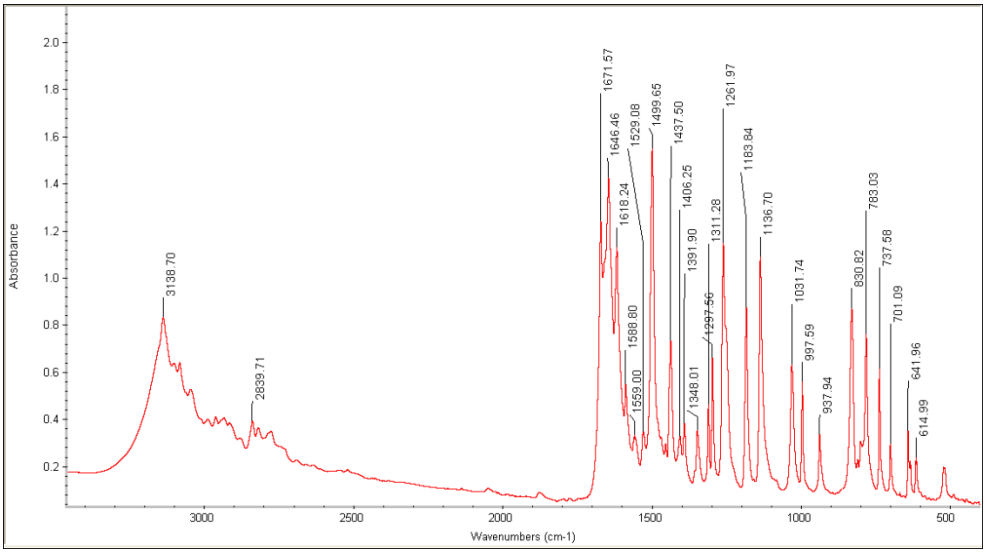


Figure 27. IR spectrum of **2b** in KBr pellets.

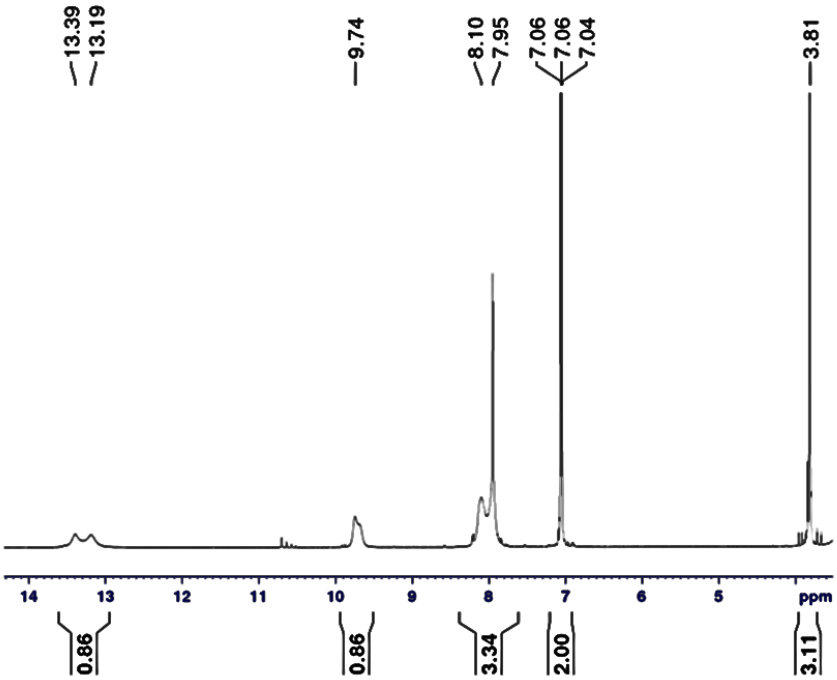


Figure 28. NMR (DMSO-d_6) of **2b** at 298 K.

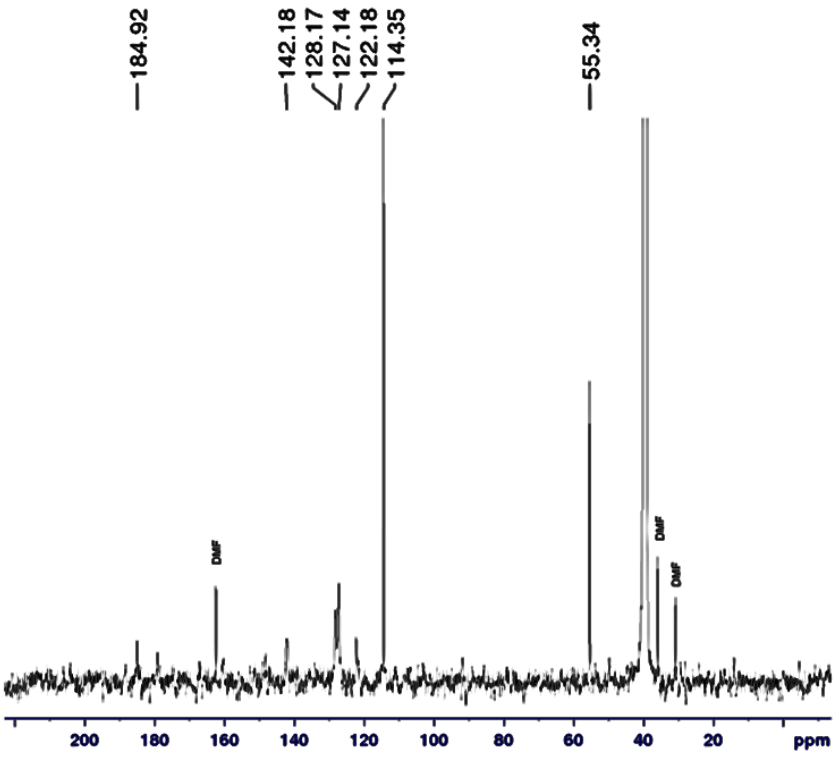


Figure 29. ^{13}C NMR (DMSO-d_6) of **2b** at 298 K (125MHz; NS 1024).

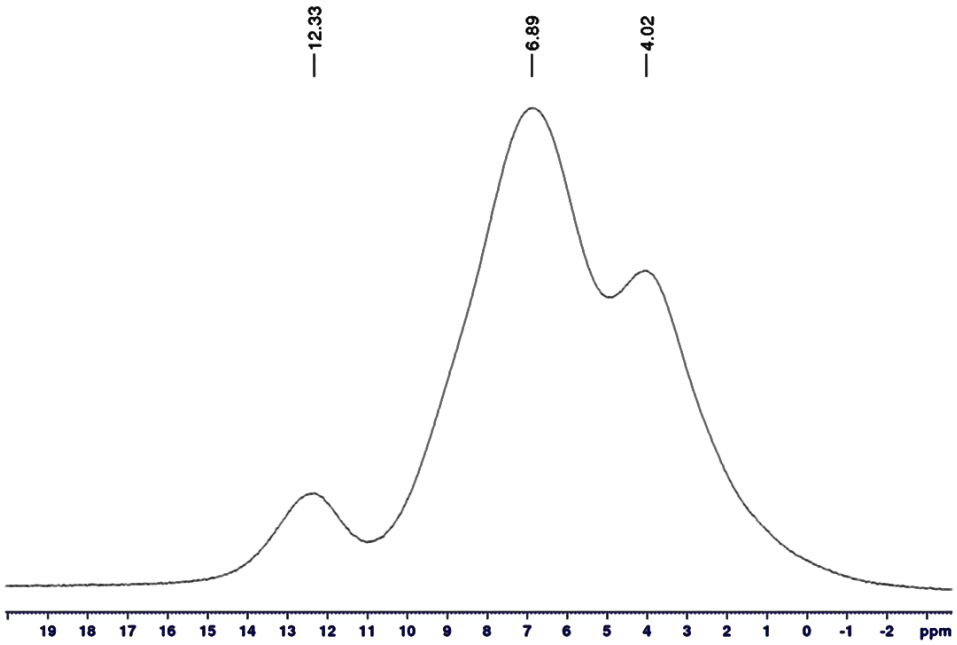


Figure 30. ^{1}H MAS NMR (solid state 850 MHz, 25 kHz) of **2b.**

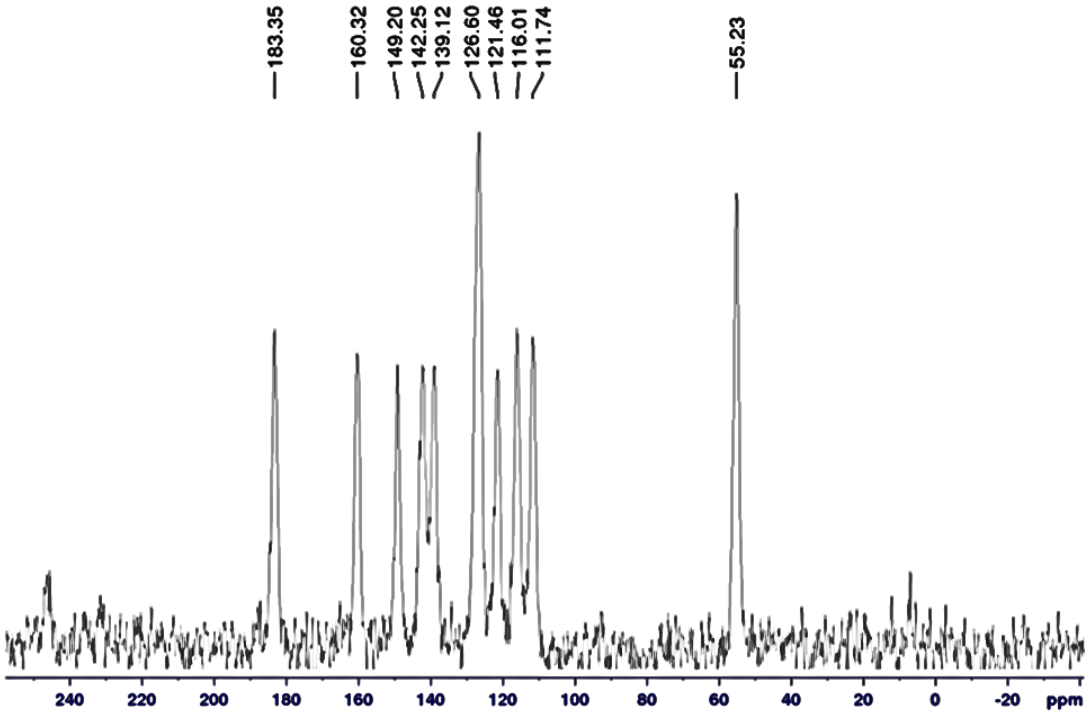


Figure 31. ^{13}C CP-MAS NMR (125 MHz, 15 kHz) of **2b.**

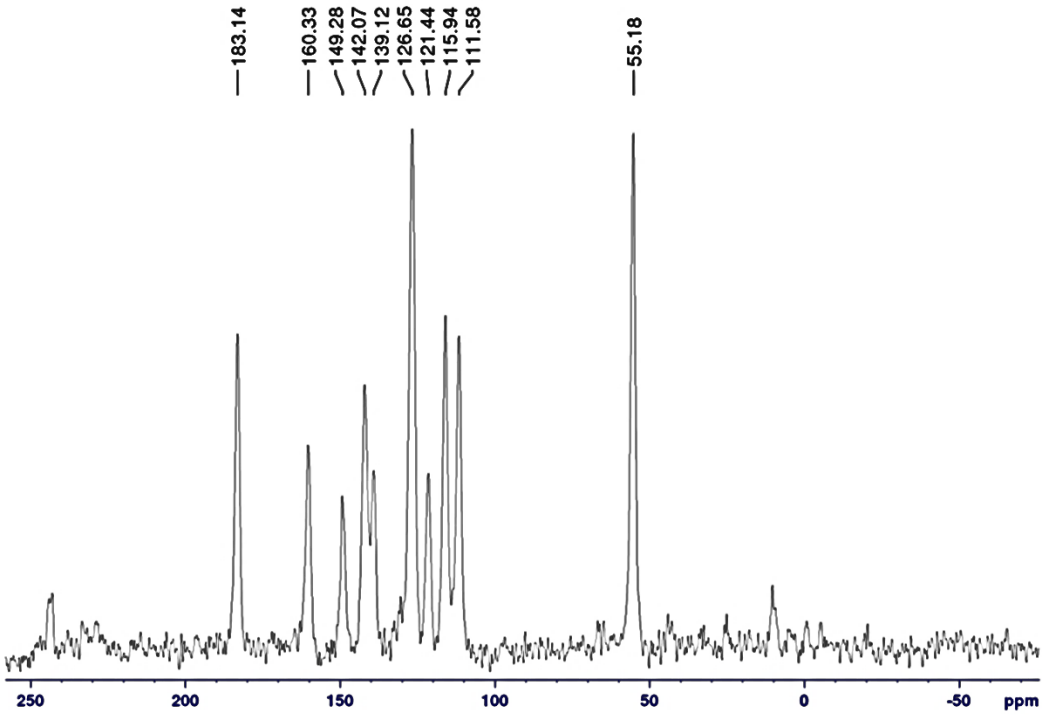


Figure 32. ^{13}C CP-MAS NMR (212.5 MHz, 25 kHz) of **2b.**

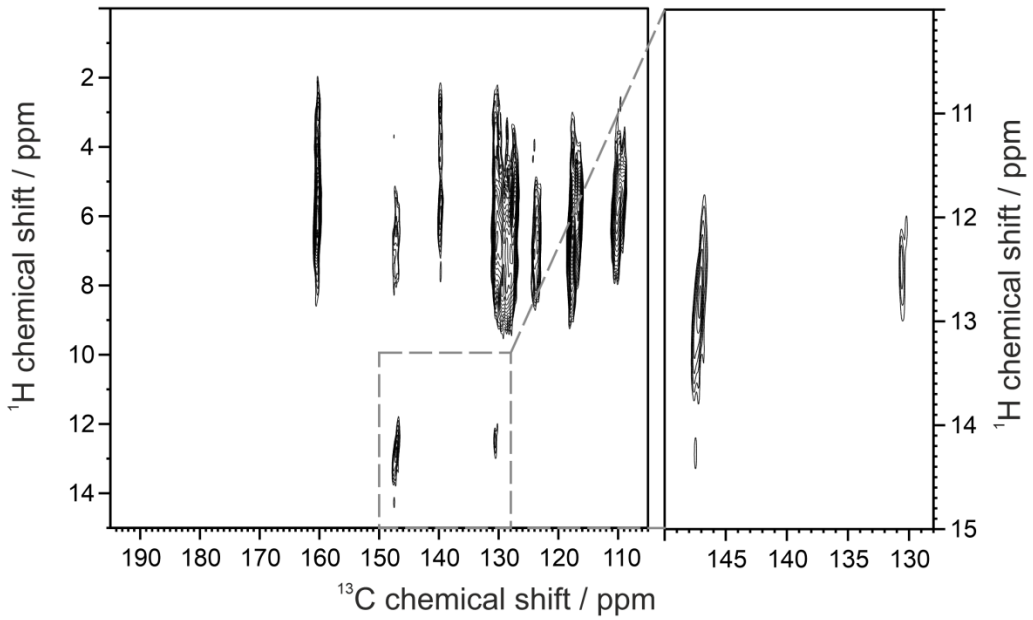


Figure 33. ^{1}H-^{13}C CP-MAS correlation spectrum (212.5 MHz, 25 kHz) of compound **2b**. Right block shows magnified view of the selected area in the correlation spectrum.

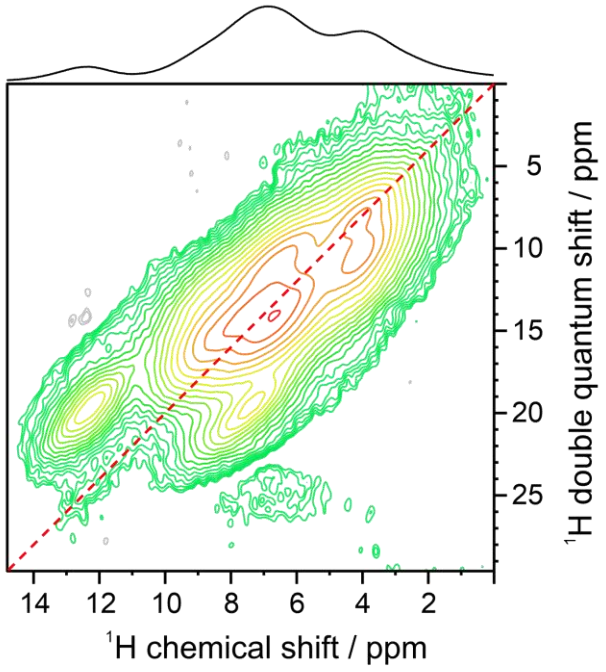


Figure 34. Double quantum-single quantum correlation spectrum of **2b** recorded at 25 kHz MAS, and 1 rotor periods double-quantum recoupling using the BABA-xy16 pulse sequence.

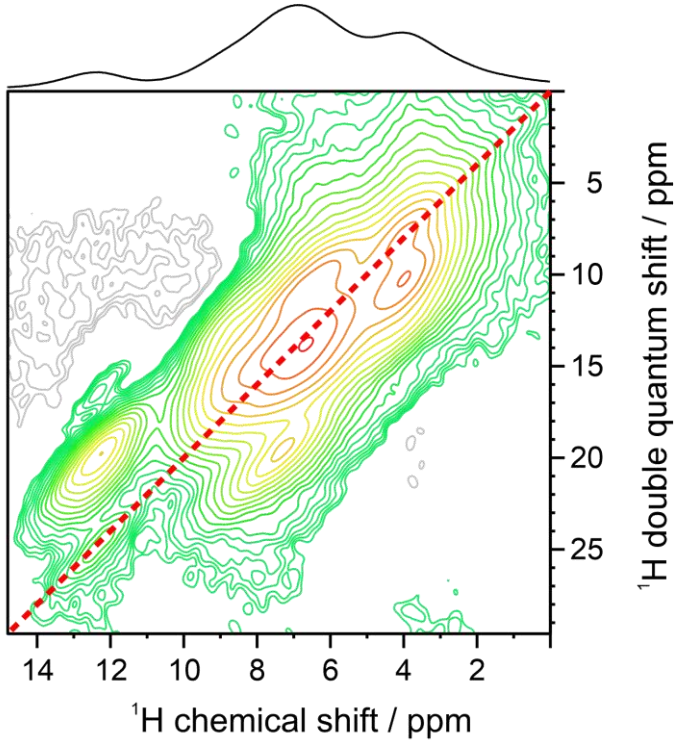
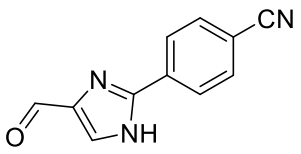


Figure 35. Double quantum-single quantum correlation spectrum of **2b** recorded at 25 kHz MAS, and 4 rotor periods double-quantum recoupling using the BABA-xy16 pulse sequence.

Spectra of 4-(4-formyl-1H-imidazol-2-yl)benzonitrile (2c)



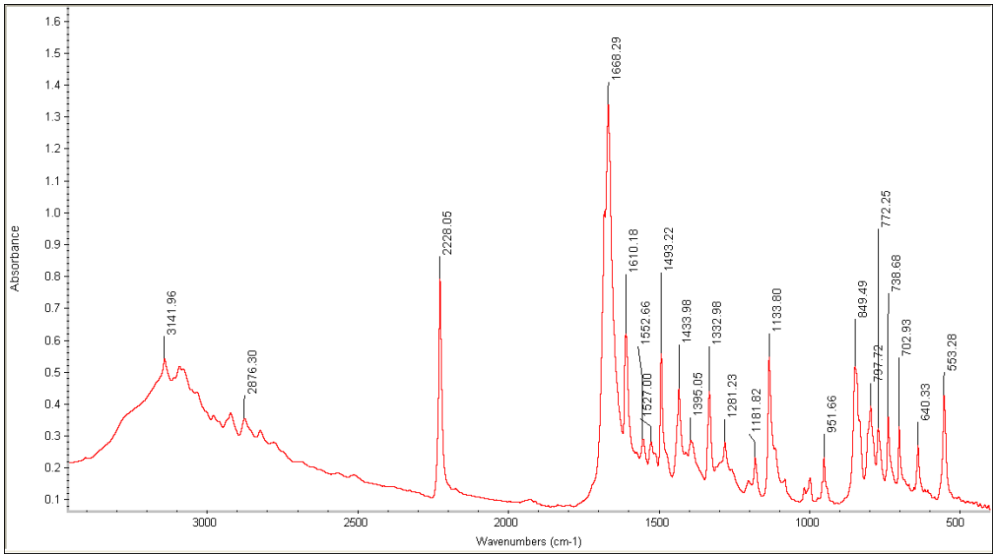


Figure 36. IR spectrum of **2c** in KBr pellets.

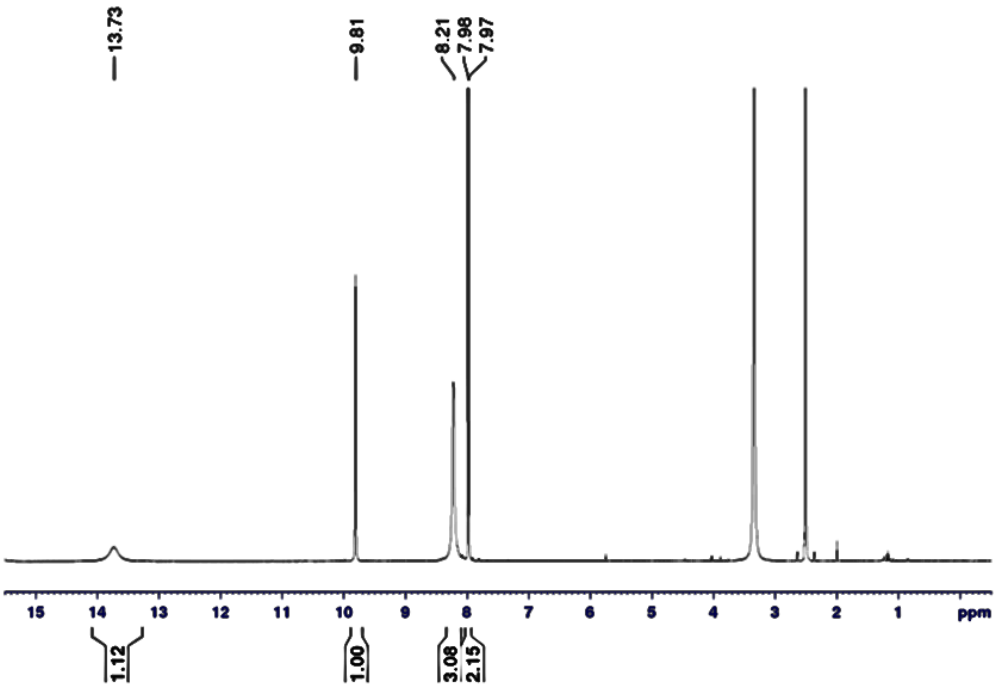


Figure 37. ^{1}H NMR (DMSO-d_6) of **2c** at 298 K.

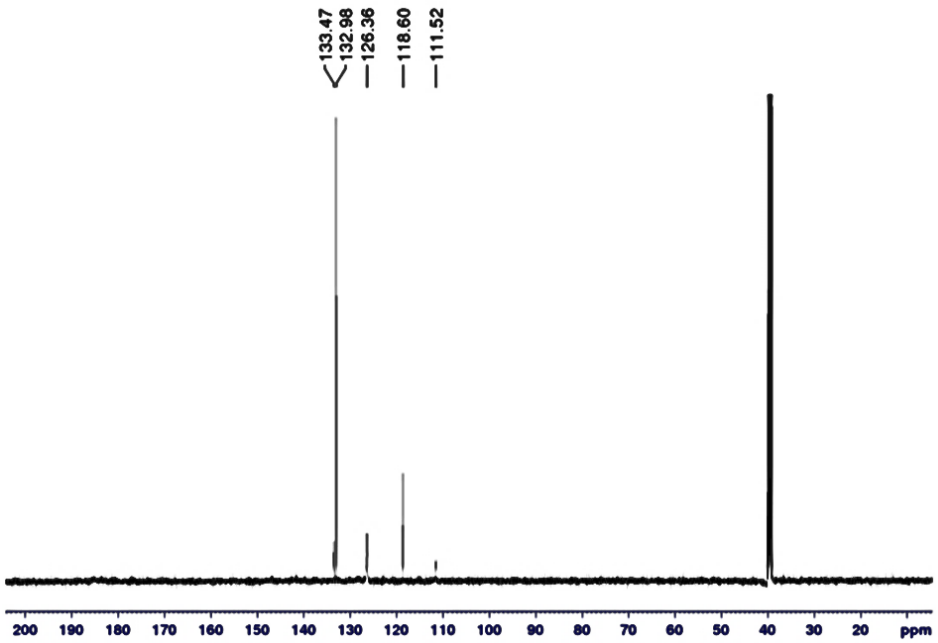


Figure 38. ^{13}C NMR (DMSO-d_6, 125 MHz) of **2c**.

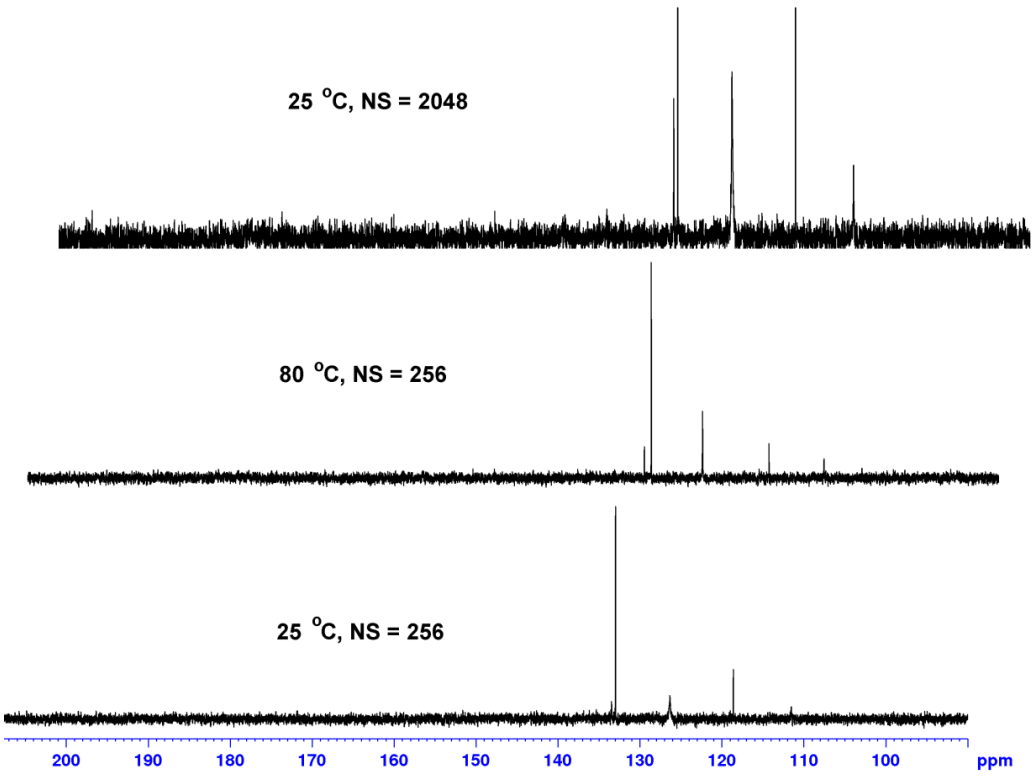


Figure 39. ^{13}C NMR (DMSO-d_6) of **2c** at two different temperatures (25 and 80 ^{0}C) and different scan number (NS) 256 and 2048.

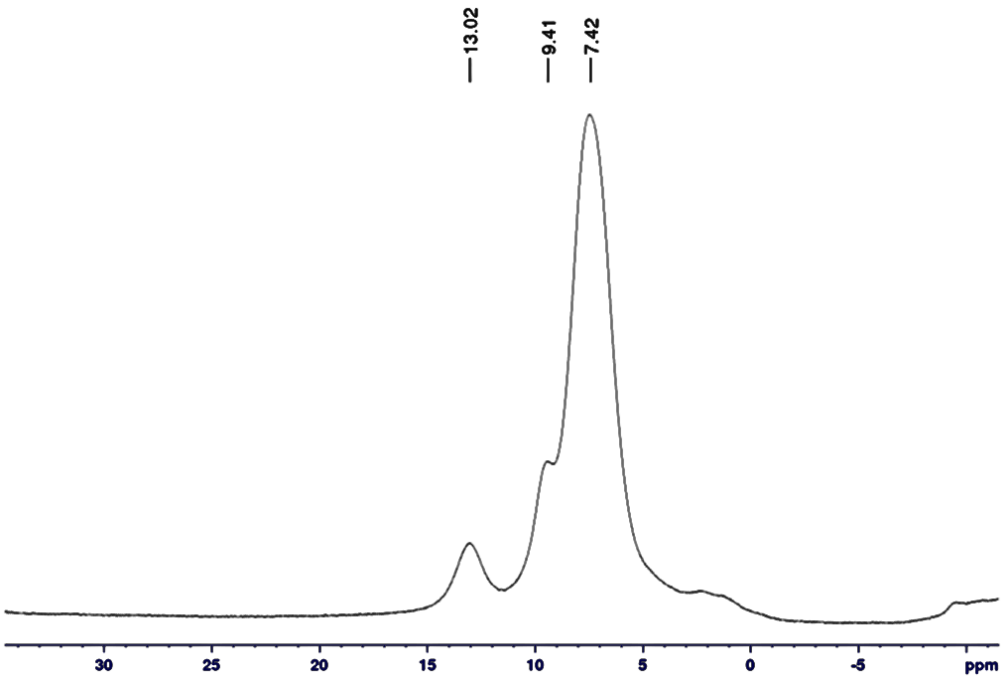


Figure 40. ^{1}H MAS NMR (850 MHz, 29 kHz) of **2c**.

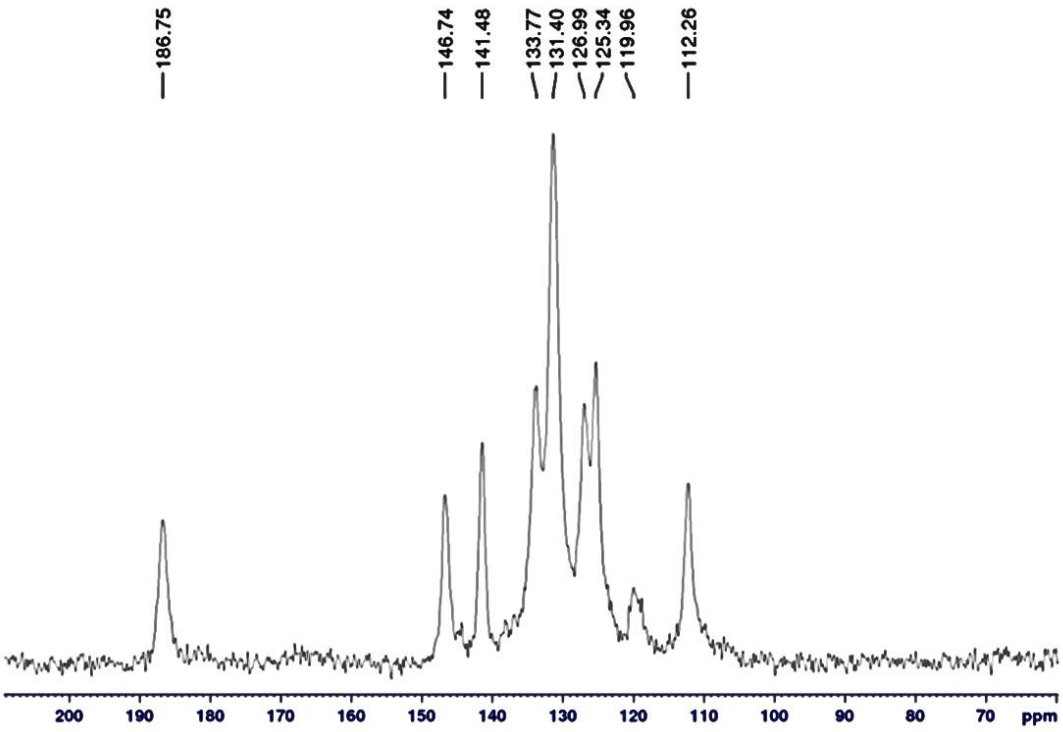


Figure 41. ^{13}C CP-MAS NMR (125 MHz, 10kHz) of **2c**.

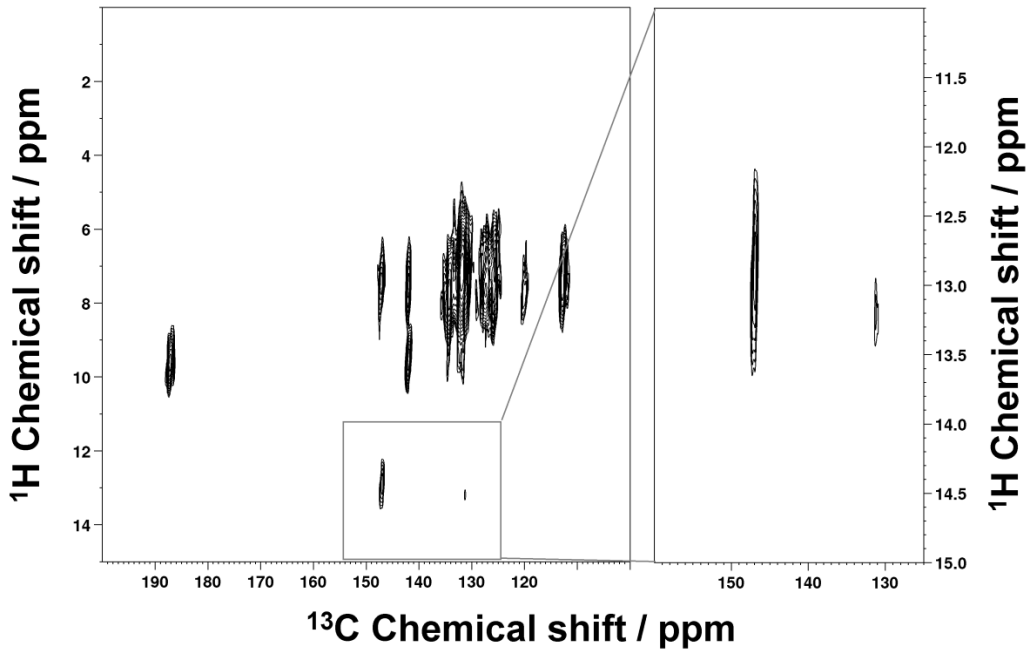


Figure 42. ^{1}H-^{13}C CP-MAS correlation spectrum (212.5 MHz, 25 kHz) of compound **2c**. Right block shows magnified view of the selected area in the correlation spectrum.

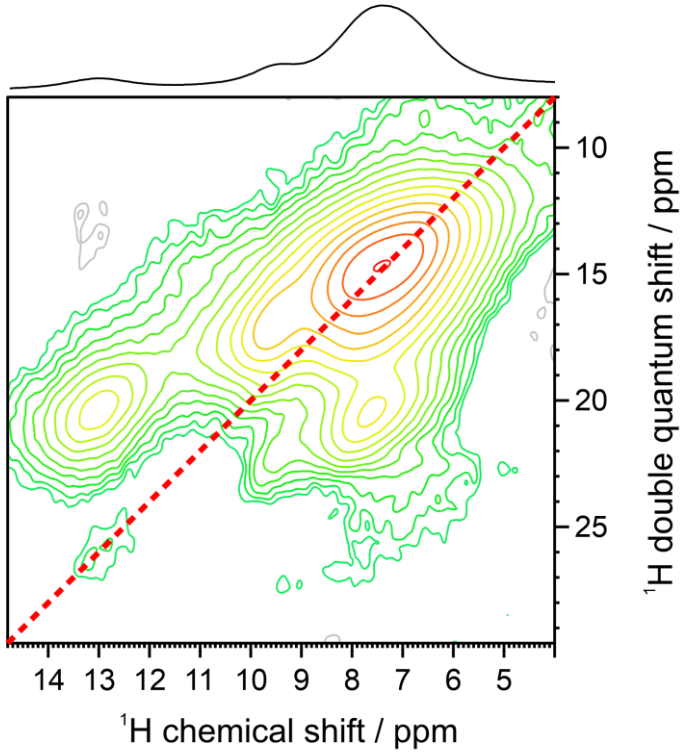


Figure 43. Double quantum-single quantum correlation spectrum of **2c** recorded at 25 kHz MAS, and 1 rotor periods double-quantum recoupling using the BABA-xy16 pulse sequence.

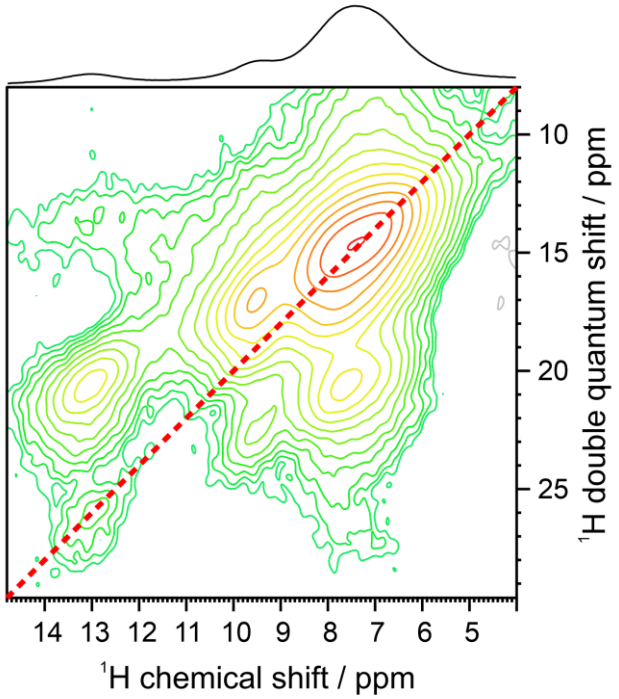
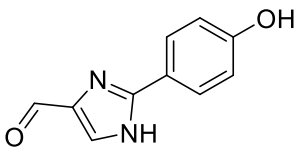


Figure 44. Double quantum-single quantum correlation spectrum of **2c** recorded at 25 kHz MAS, and 2 rotor periods double-quantum recoupling using the BABA-xy16 pulse sequence.

Spectra of 2-(4-hydroxyphenyl)-1H-imidazole-4-carbaldehyde (2d)



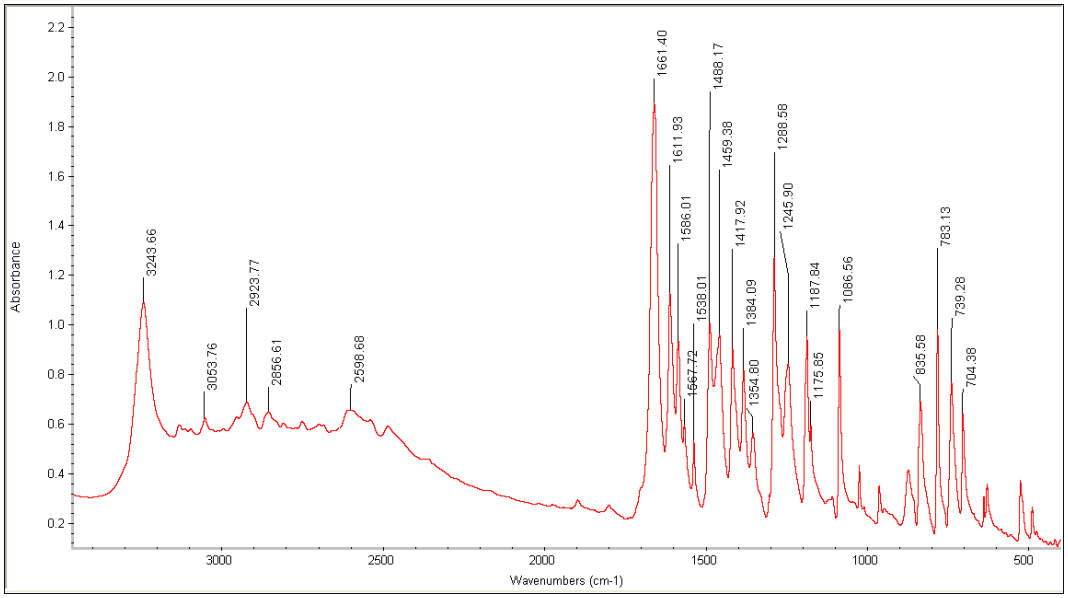


Figure 45. IR spectrum of **2d** in KBr pellets.

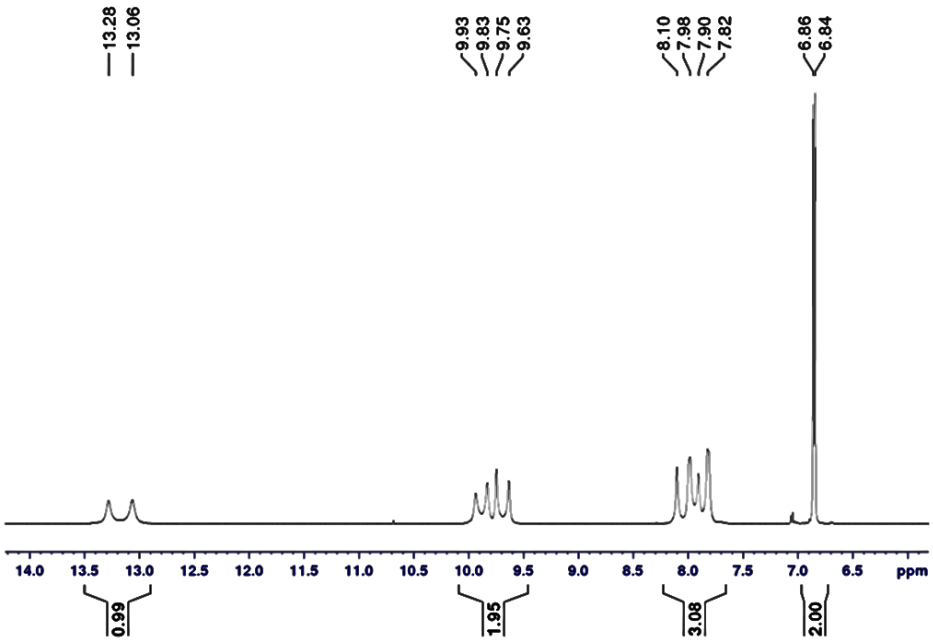


Figure 46. ^{1}H NMR (DMSO-d_6) of **2d** at 298 K (500 MHz, 25mM).

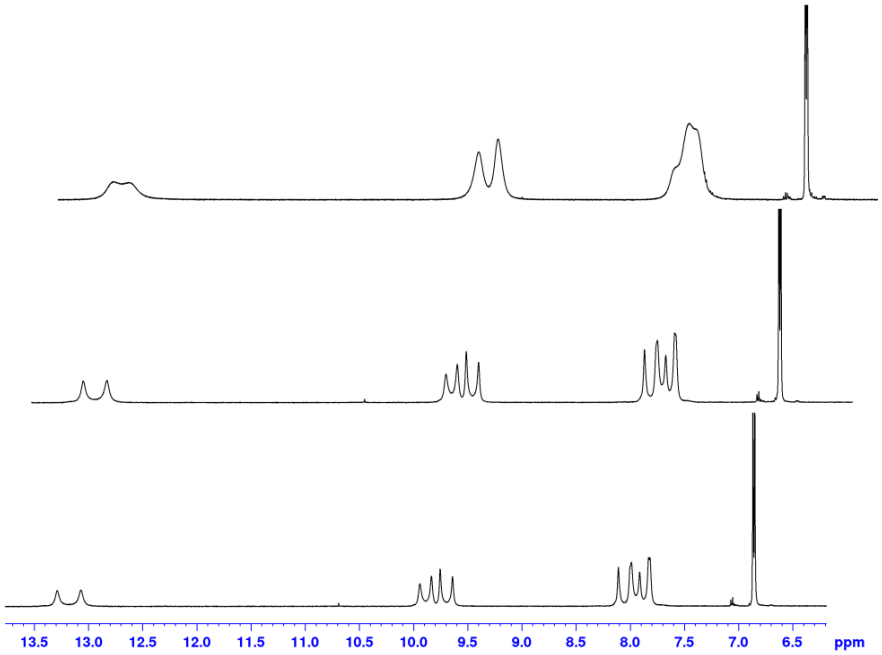


Figure 47. Concentration dependent ^{1}H NMR (DMSO-d_6) spectra of **2d** at 298 K (from bottom to top 13mM, 25mM and > 50 mM).

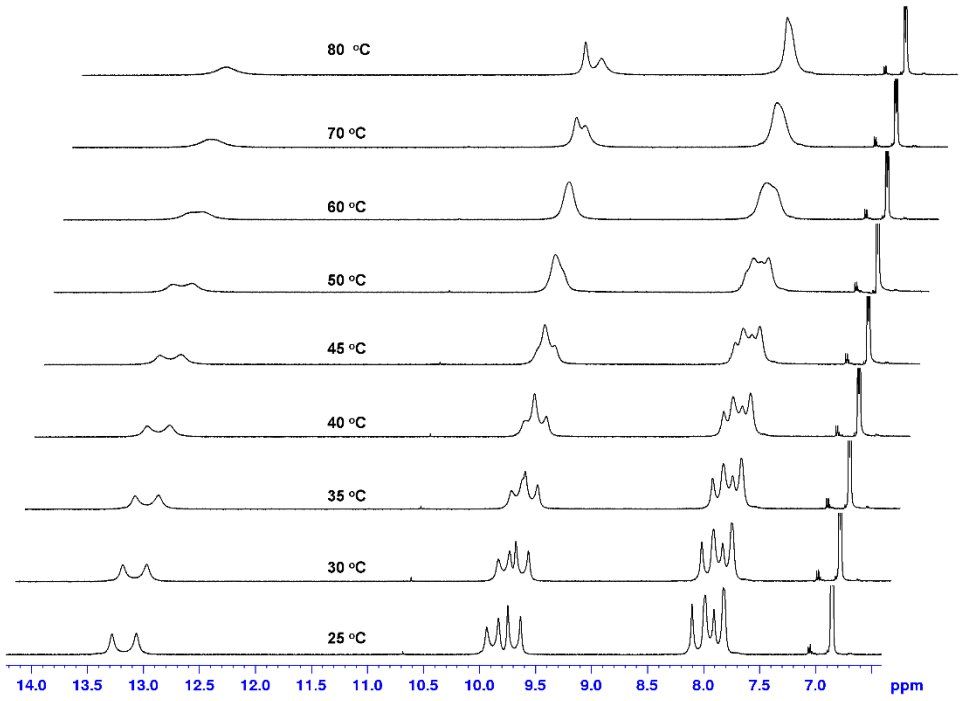


Figure 48. Temperature dependent ^{1}H NMR (DMSO-d_6) spectra of **2d** with concentration of 25mM.

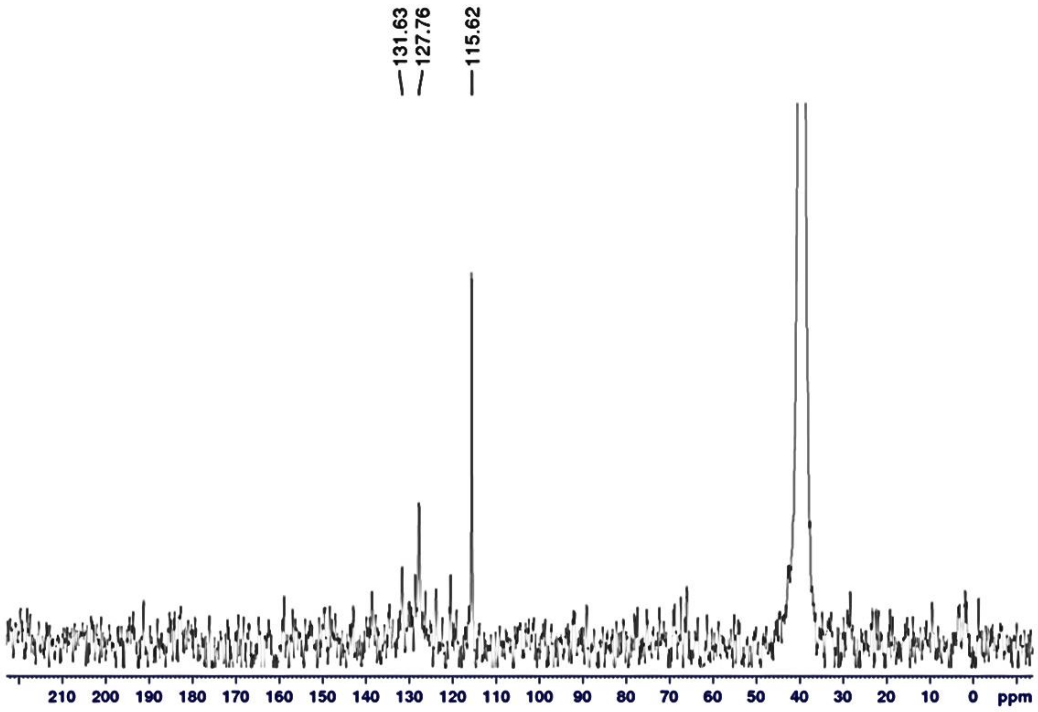


Figure 49. ^{13}C NMR (DMSO-d_6) spectra of **2d**; (125 MHz, NS 1024).

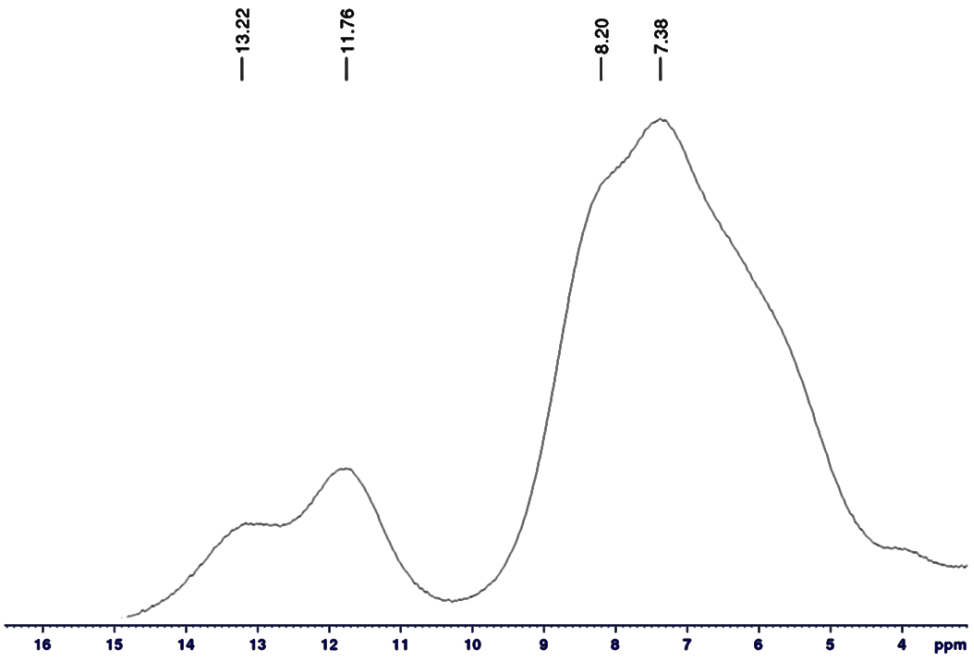


Figure 50. ^{1}H MAS NMR (850 MHz, 29 kHz) of **2d**.

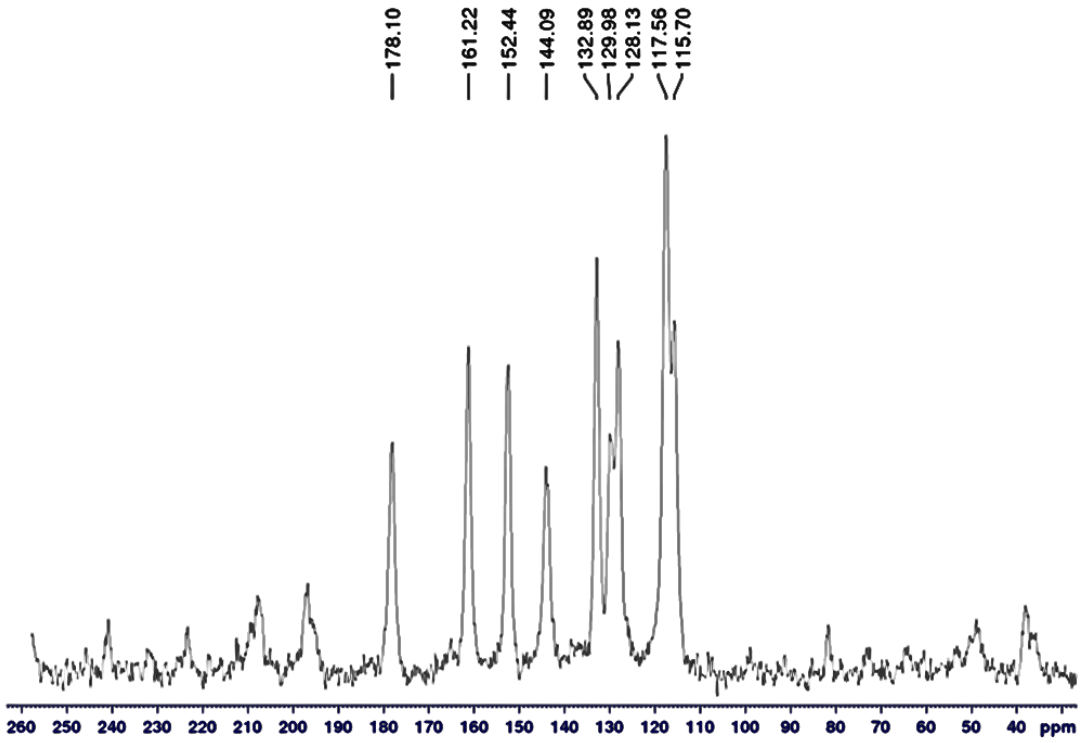
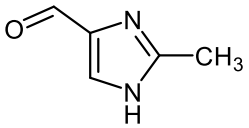


Figure 51. ^{13}C CP-MAS NMR (125 MHz, 10 kHz) of **2d**.

Spectra of 2-methyl-1H-imidazole-4-carbaldehyde



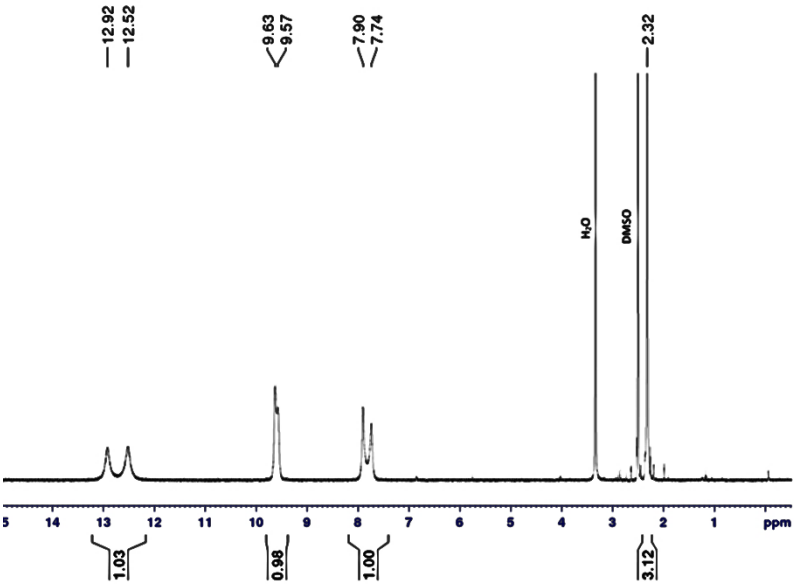


Figure 52. ^{1}H NMR (DMSO-d_6) at 298 K (500 MHz).

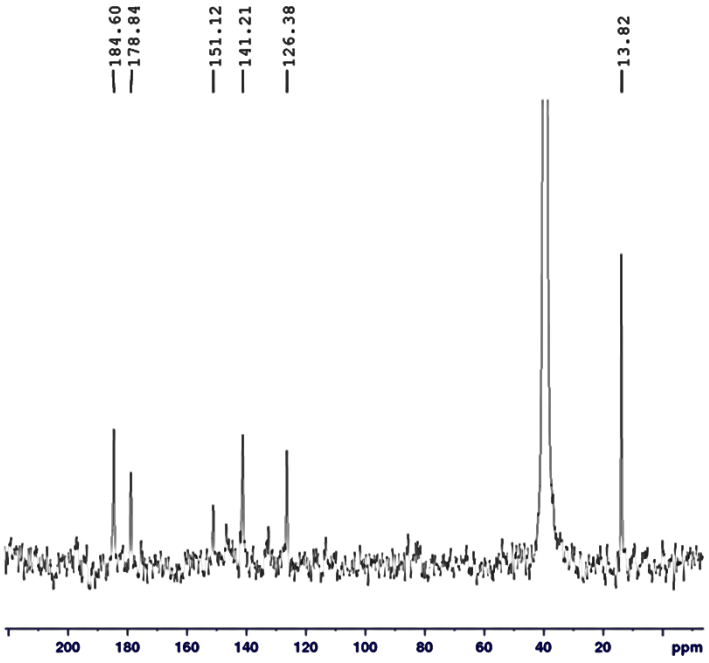


Figure 53. ^{13}C NMR (DMSO-d_6) at 298 K (125 MHz, 512 NS).

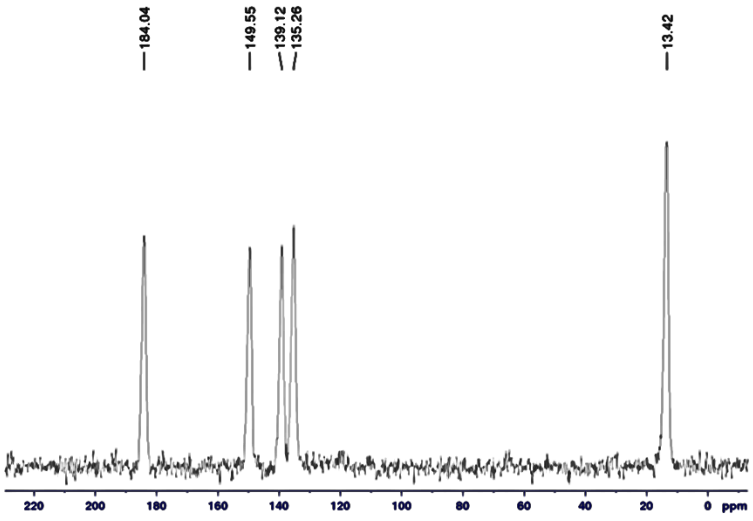


Figure 54. CP-MAS NMR (125 MHz, 15kHz).

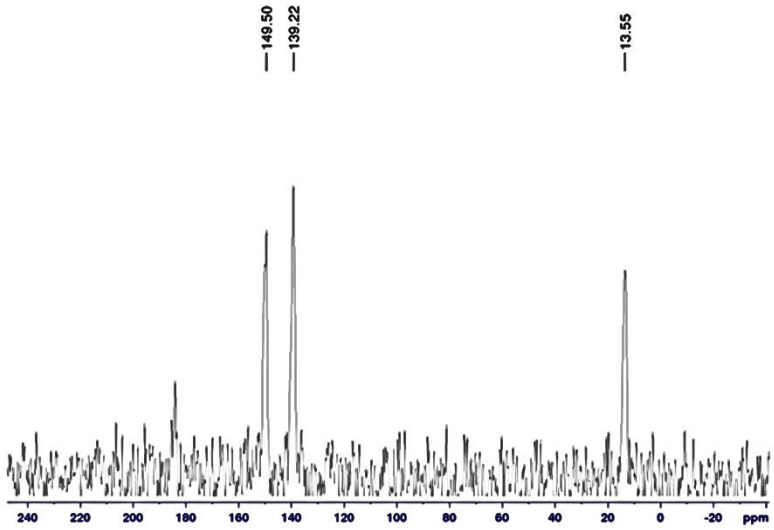


Figure 55. ^{13}C CPPI spectrum (125 MHz, 150 kHz); null signal for CH, negative signal for CH_2, and positive signal for C and CH_3.

Figure 56. Microscope image of the different crystalline phases of **2c** .