

Electronic Supplementary Information for

Dinuclear gold(I) complexes with propylene bridged N-heterocyclic dicarbene ligands: synthesis, structures, trends in reactivities and properties

Cristina Tubaro,^{*a} Marco Baron,^a Michele Costante,^a Marino Basato,^a Andrea Biffis,^a Armando Gennaro,^a Abdirisak Ahmed Isse,^{*a} Claudia Graiff,^b and Gianluca Accorsi^{*c}

^a Dipartimento di Scienze Chimiche, Università di Padova, via Marzolo 1, 35131 Padova, Italy. Tel: +39 049 8275655 (C.T.), +39 049 8275677 (A.A.I.); E-mail: cristina.tubaro@unipd.it, abdirisak.ahmedisse@unipd.it.

^b Dipartimento di Chimica, Università di Parma, Viale delle Scienze 17/A, 43100 Parma, Italy.

^c Istituto per la Sintesi Organica e la Fotoreattività, Consiglio Nazionale delle Ricerche, Via Gobetti 101, 40129 Bologna, Italy. Tel: +39 051 6399816; E-mail: gianluca.accorsi@isof.cnr.it

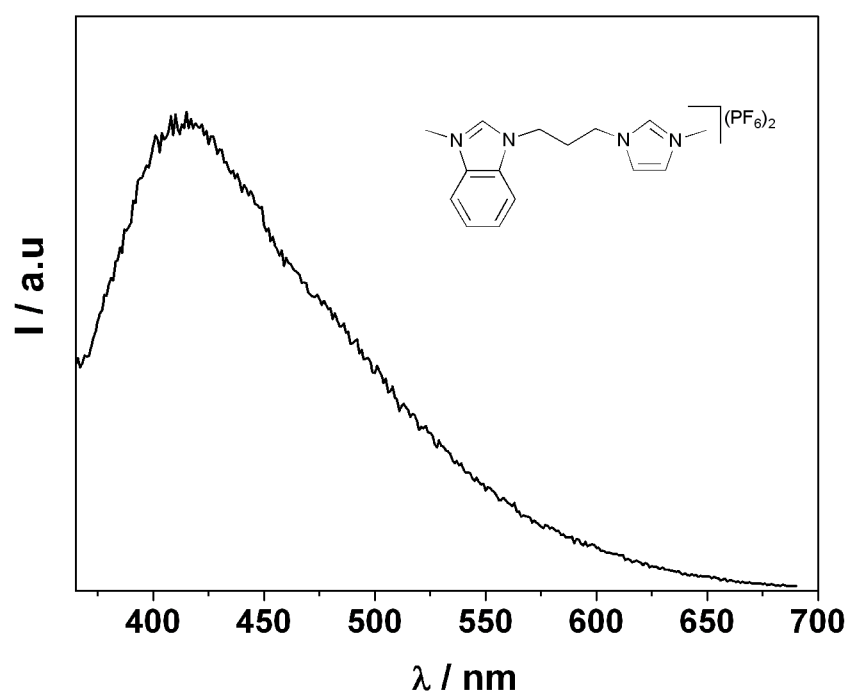


Figure S1. Emission spectrum of the diimidazolium salt precursor of complex **2a** as powder. $\lambda_{\text{exc}} = 350 \text{ nm}$; $\Phi_{\text{em}} < 1\%$; τ = not detected because of the weakness of the signal.

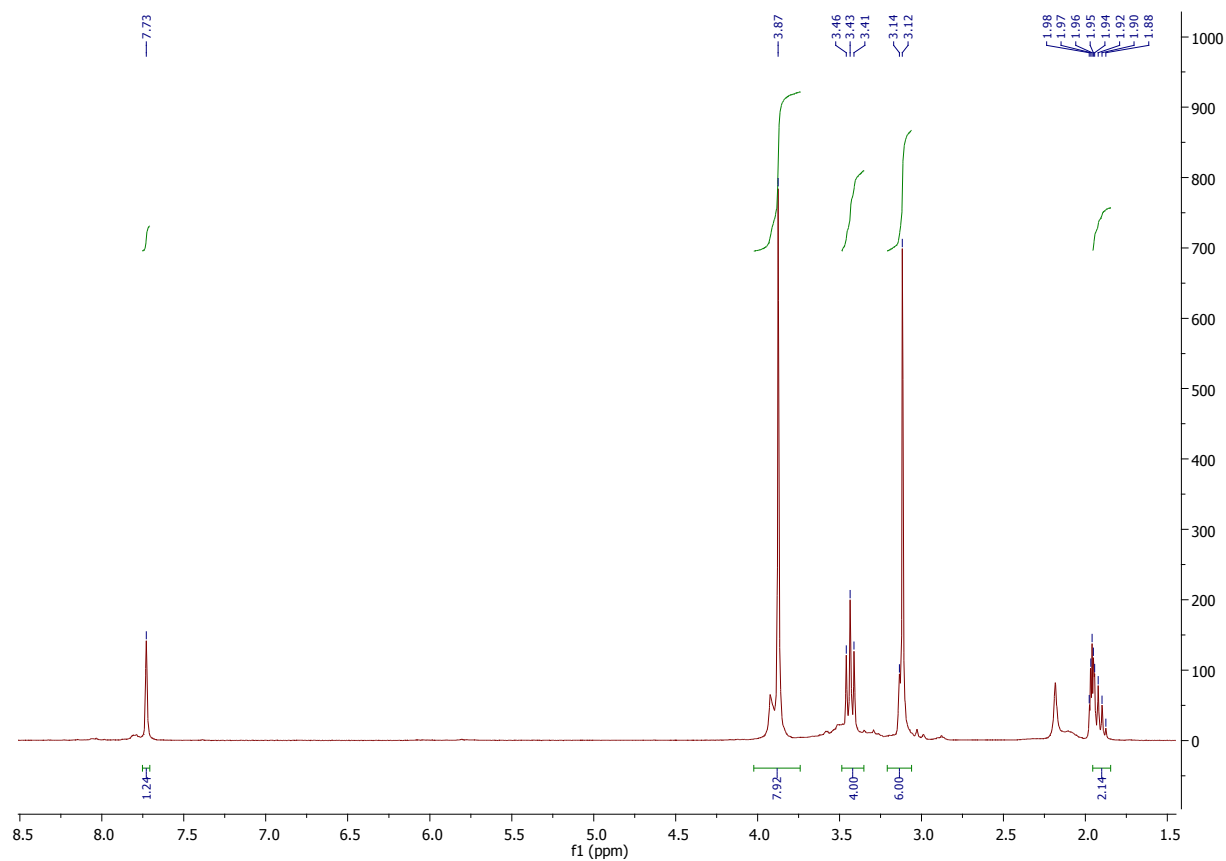


Figure S2. ^1H NMR spectrum in CD_3CN of 1,1'-dimethyl-3,3'-propylene-diimidazolidinium bis(hexafluorophosphate)

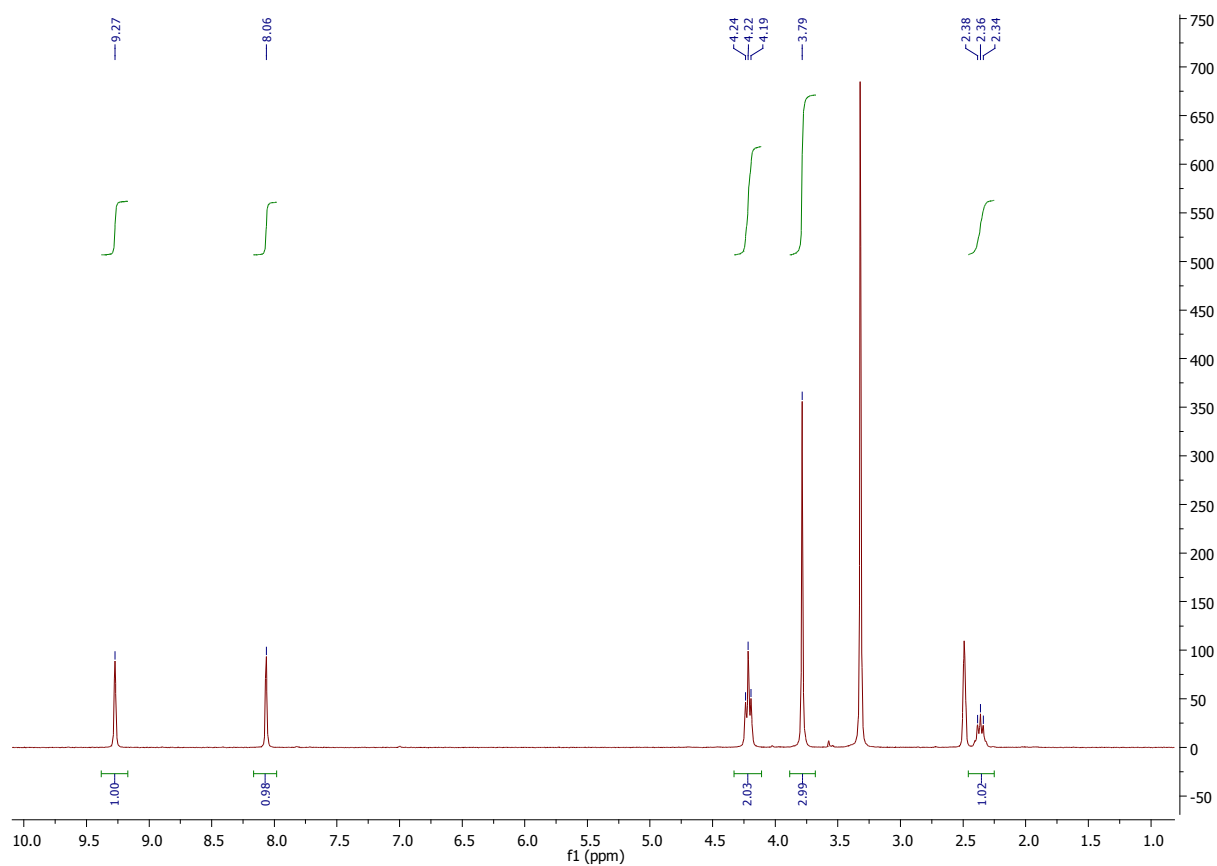


Figure S3. ^1H NMR spectrum in dms0-d_6 of 5,5'-dibromo-1,1'-dimethyl-3,3'-propan-diimidazolium diiodide

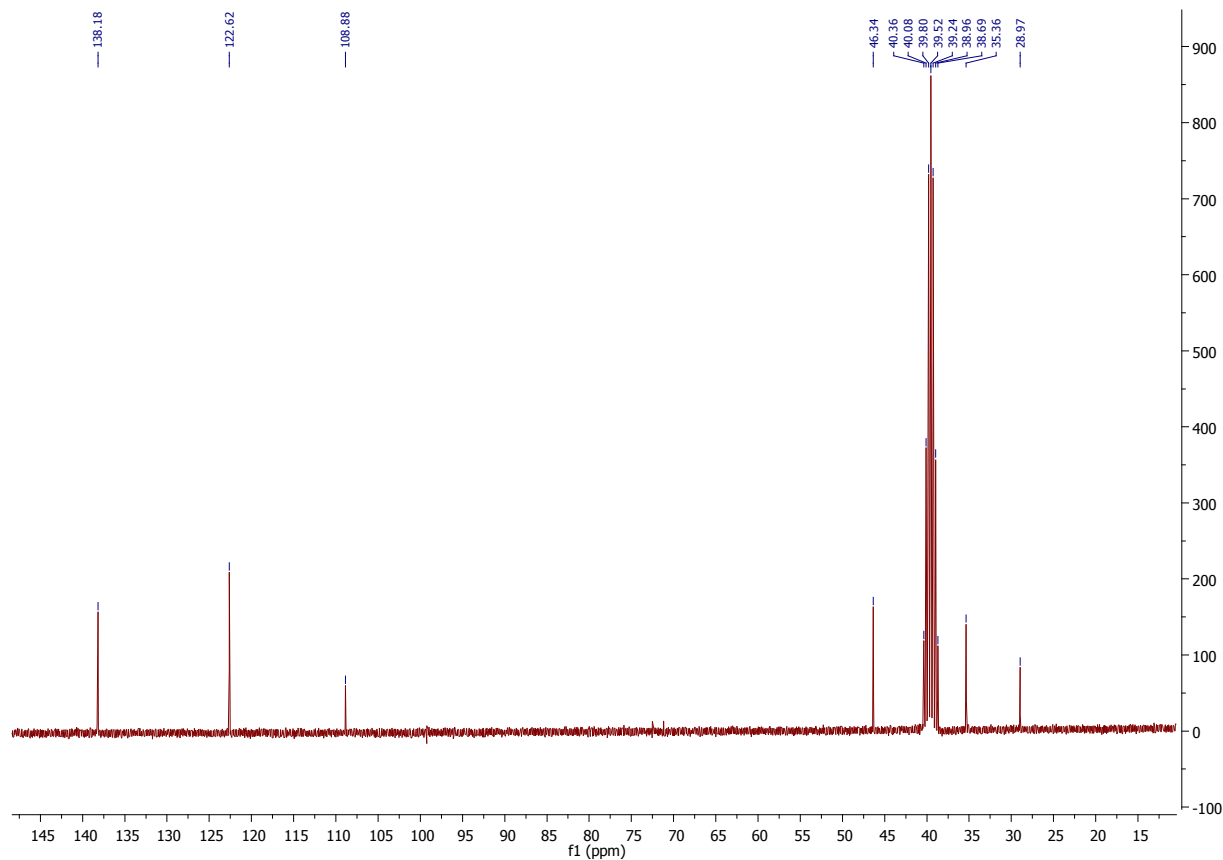


Figure S4. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum in dms0-d_6 of 5,5'-dibromo-1,1'-dimethyl-3,3'-propan-diimidazolium diiodide

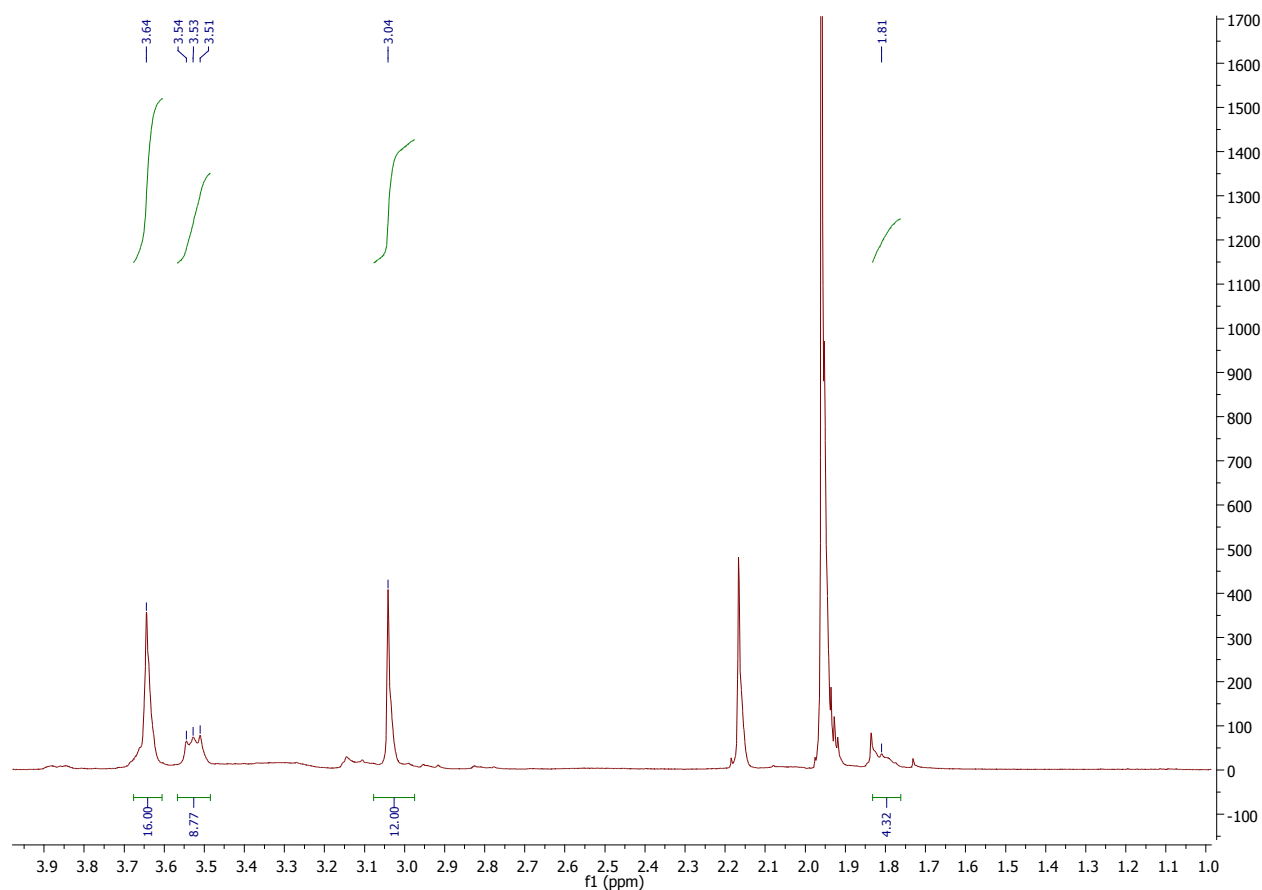


Figure S5. ¹H NMR spectrum in CD₃CN of bis(1,1'-dimethyl-3,3'-propylene-diimidazolidin-2,2'-diylidene)disilver(I) bis(hexafluorophosphate)

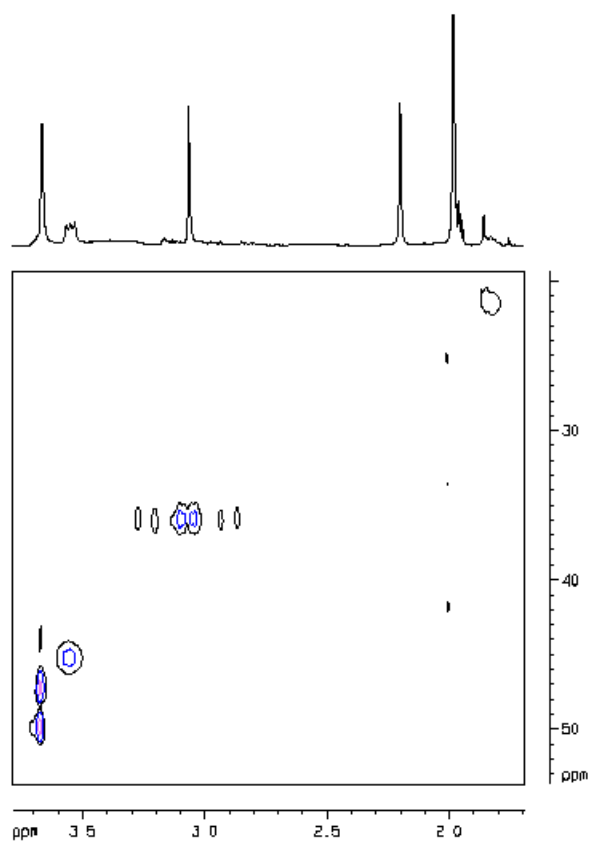


Figure S6. ^1H , ^{13}C HMQC NMR spectrum in CD_3CN of bis(1,1'-dimethyl-3,3'-propylene-diimidazolidin-2,2'-diylidene)disilver(I) bis(hexafluorophosphate)

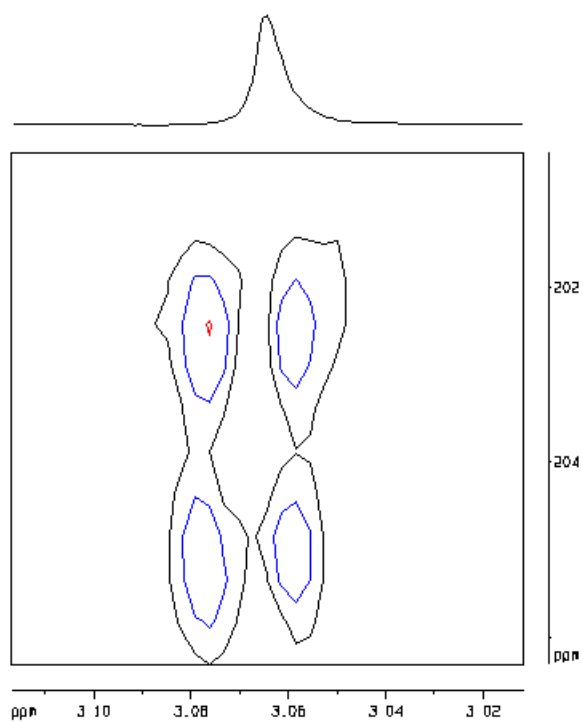


Figure S7. ^1H , ^{13}C HMBC NMR spectrum in CD_3CN of bis(1,1'-dimethyl-3,3'-propylene-diimidazolidin-2,2'-diylidene)disilver(I) bis(hexafluorophosphate)

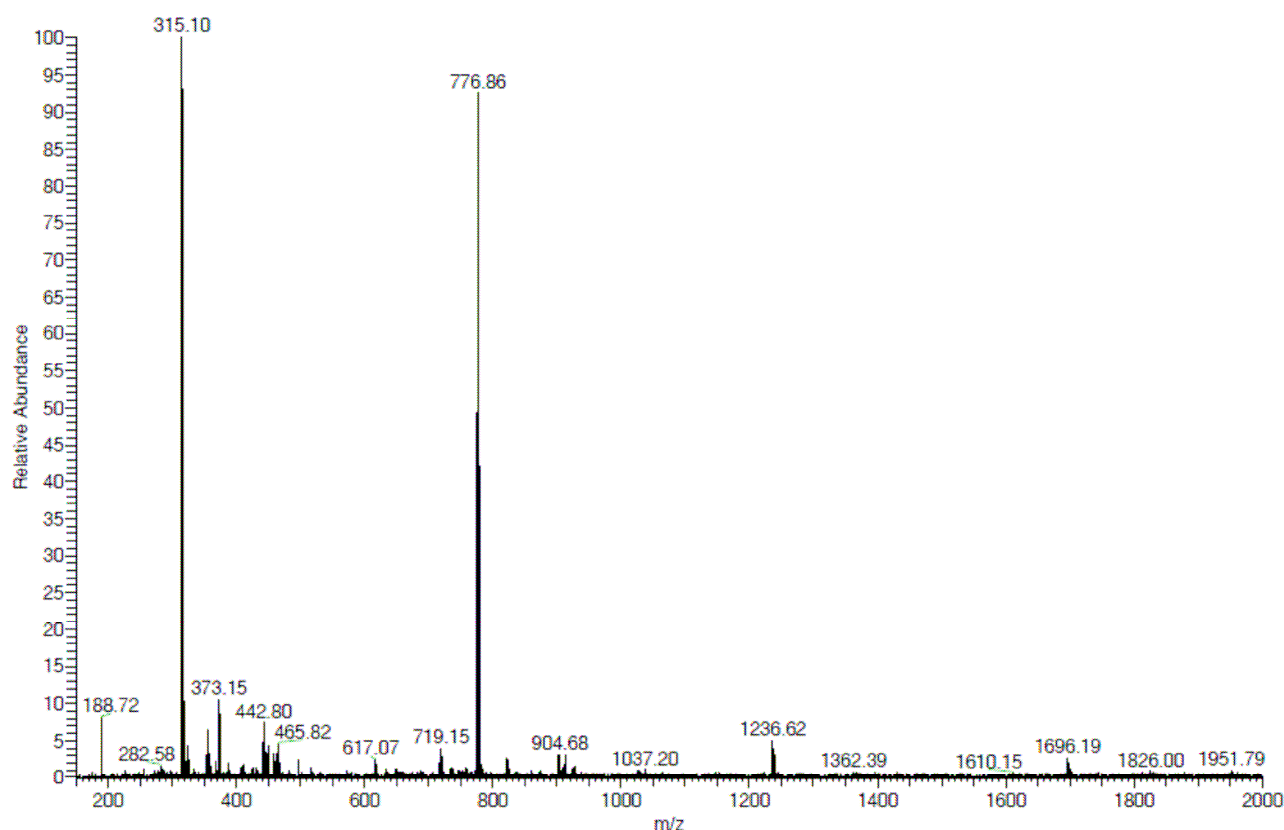


Figure S8. ESI-MS spectrum in CH₃CN of bis(1,1'-dimethyl-3,3'-propylene-diimidazolidin-2,2'-diylidene)disilver(I) bis(hexafluorophosphate)

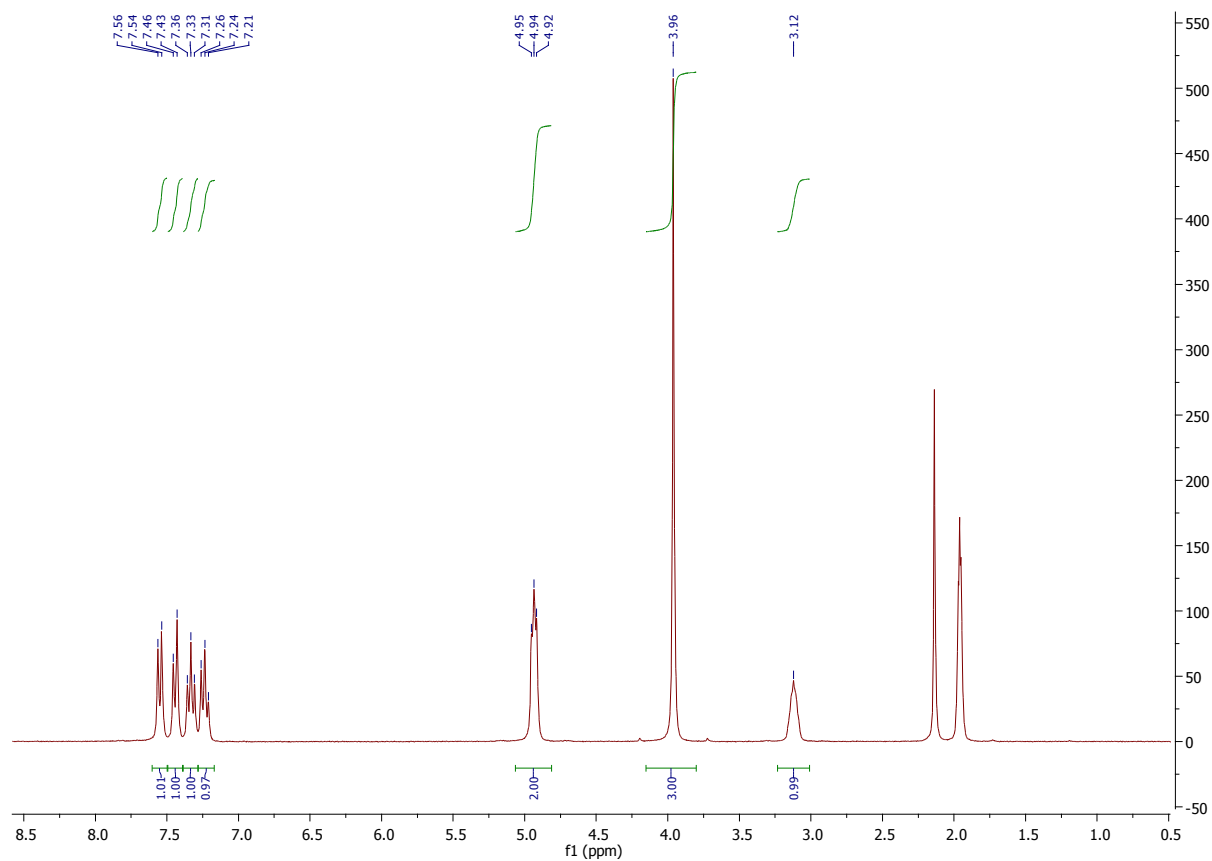


Figure S9. ^1H NMR spectrum in CD_3CN of complex **1a**

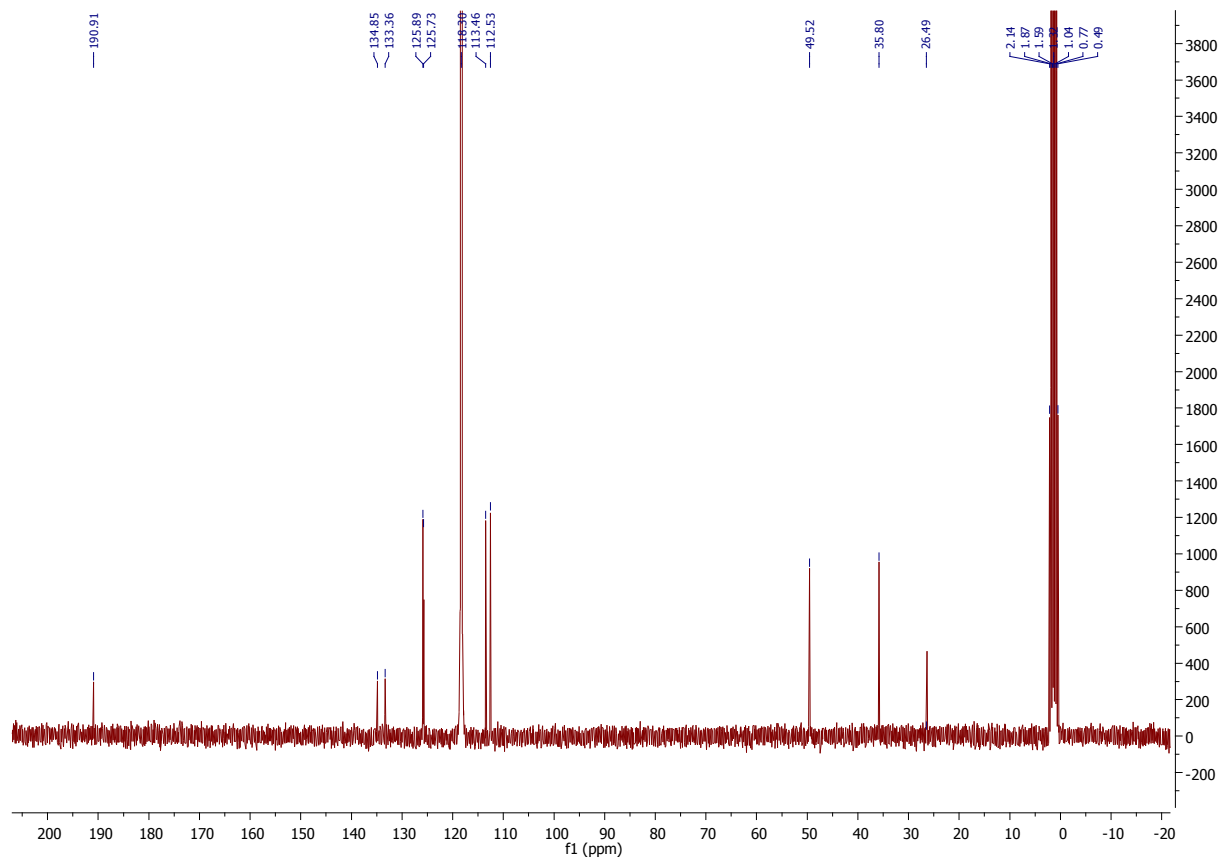


Figure S10. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum in CD_3CN of complex **1a**

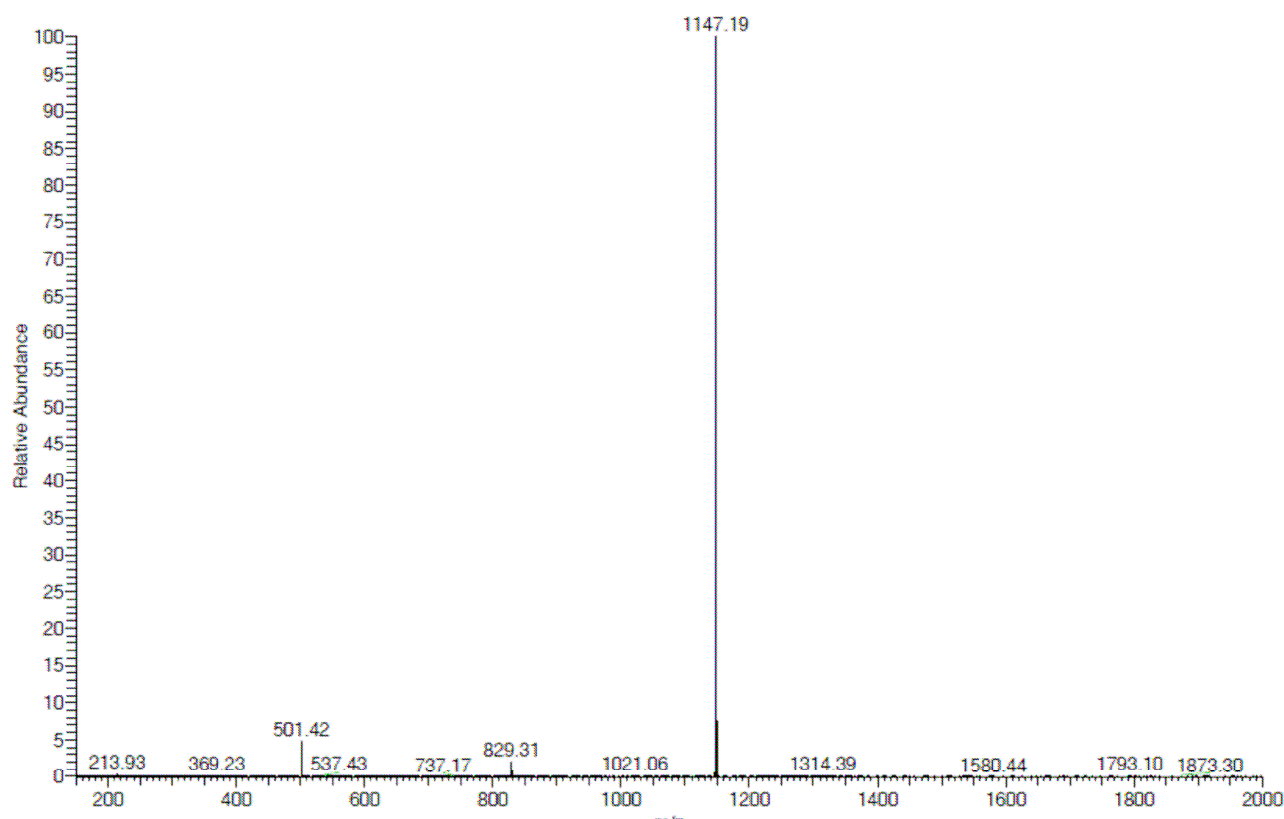


Figure S11. ESI-MS spectrum in CH_3CN of complex **1a**

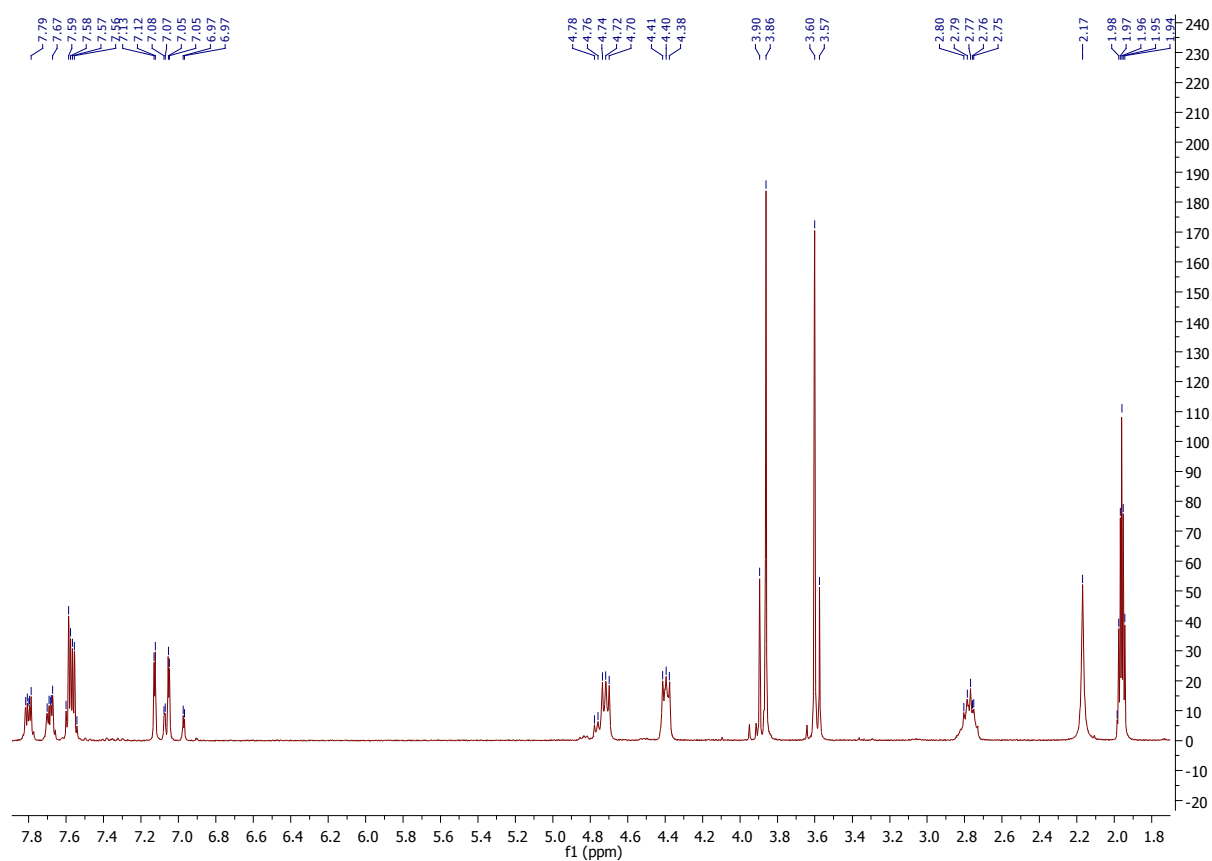


Figure S12. ¹H NMR spectrum in CD₃CN of the mixture **2a/2a'**

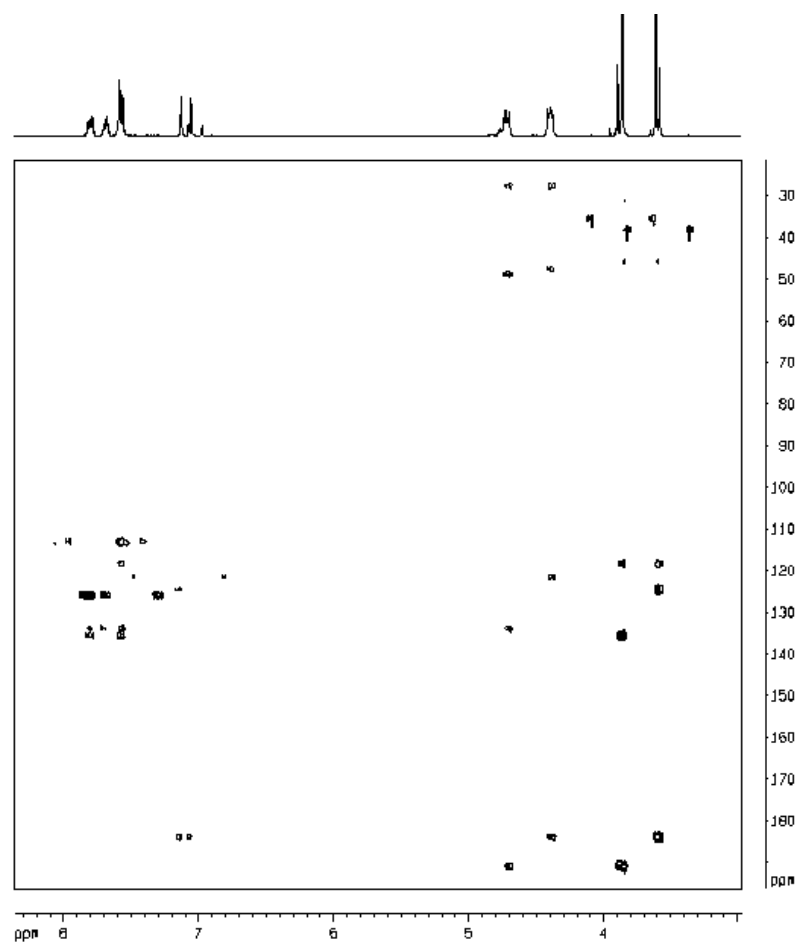


Figure S13. ^1H , ^{13}C HMBC NMR spectrum in CD_3CN of the mixture **2a/2a'**

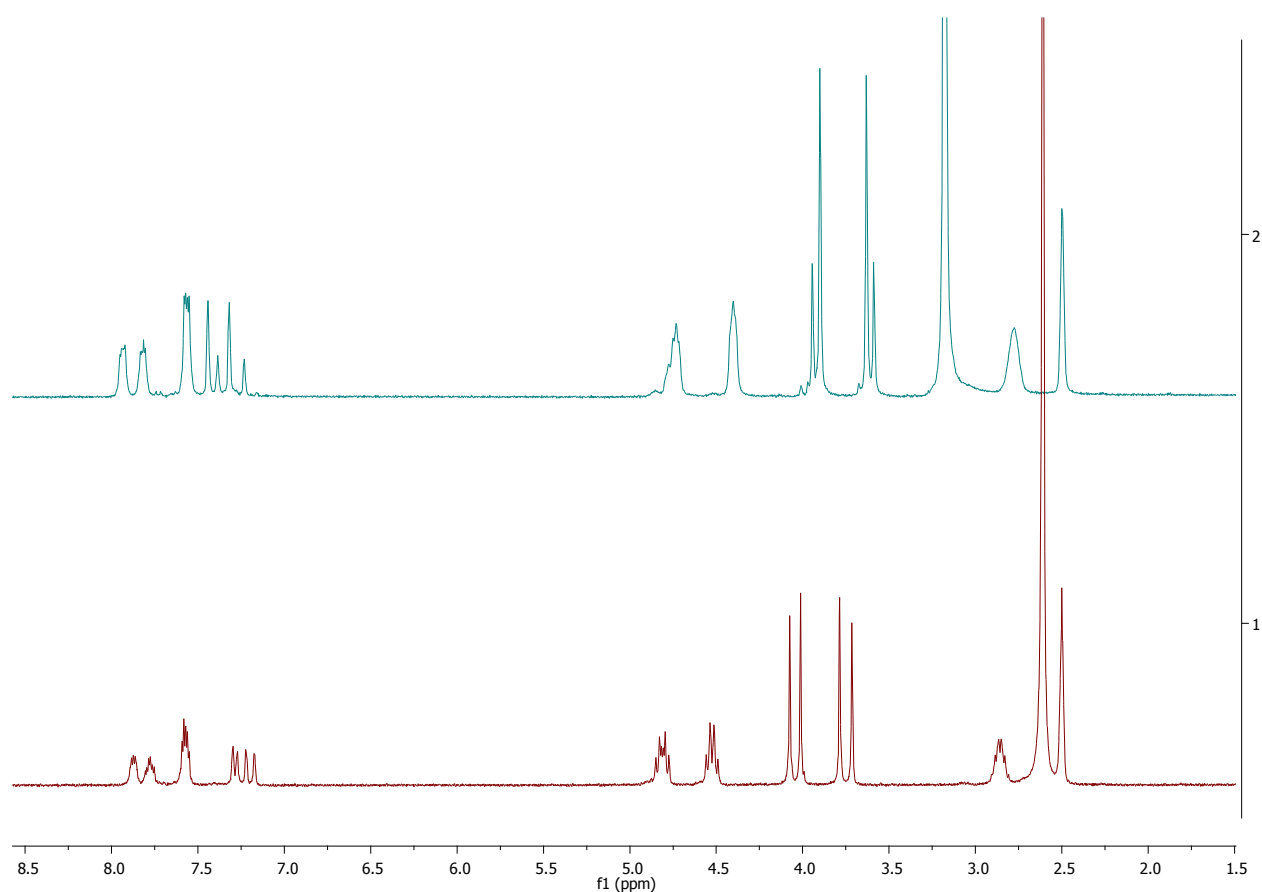


Figure S14. ^1H NMR spectrum in dms0-d_6 of the mixture **2a/2a'** at 25 °C (in green) and after treatment at 150 °C (in red).

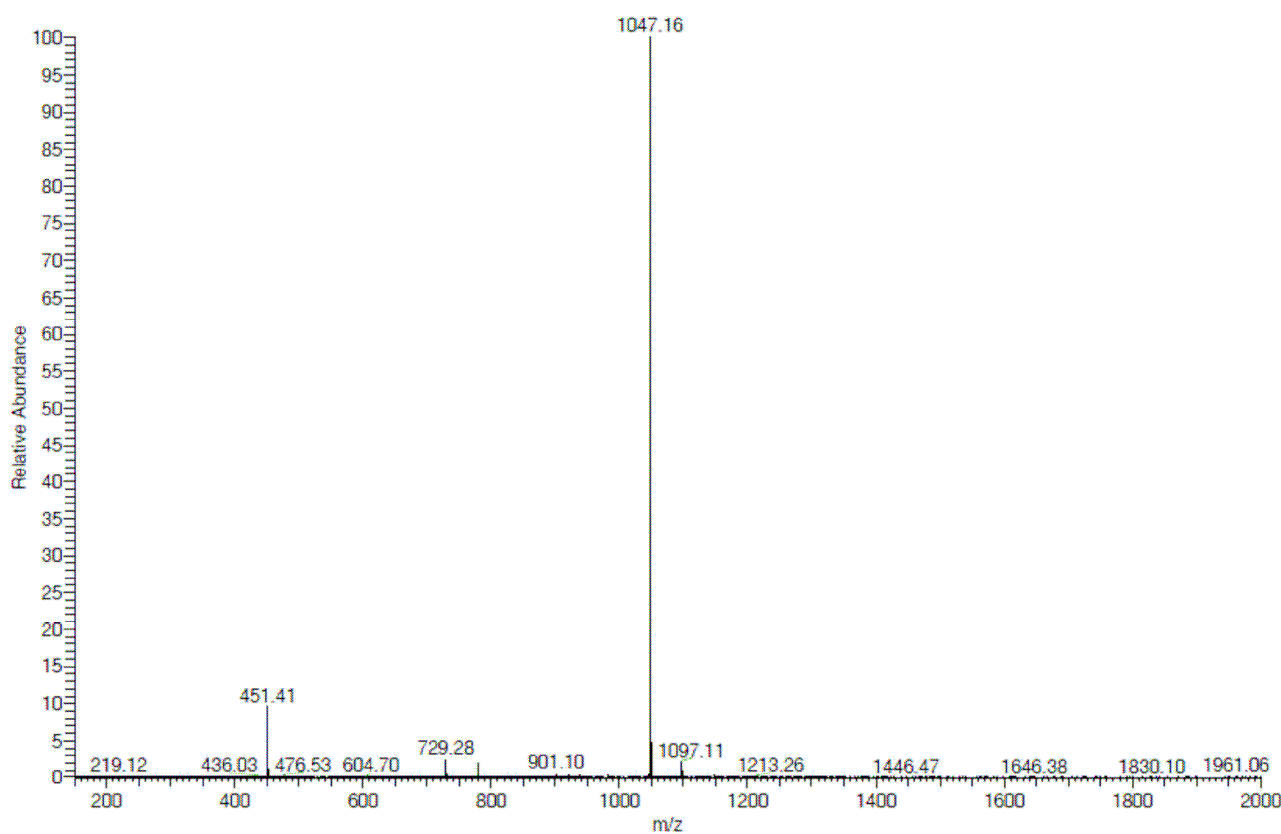


Figure S15. ESI-MS spectrum in CH_3CN of the mixture **2a/2a'**

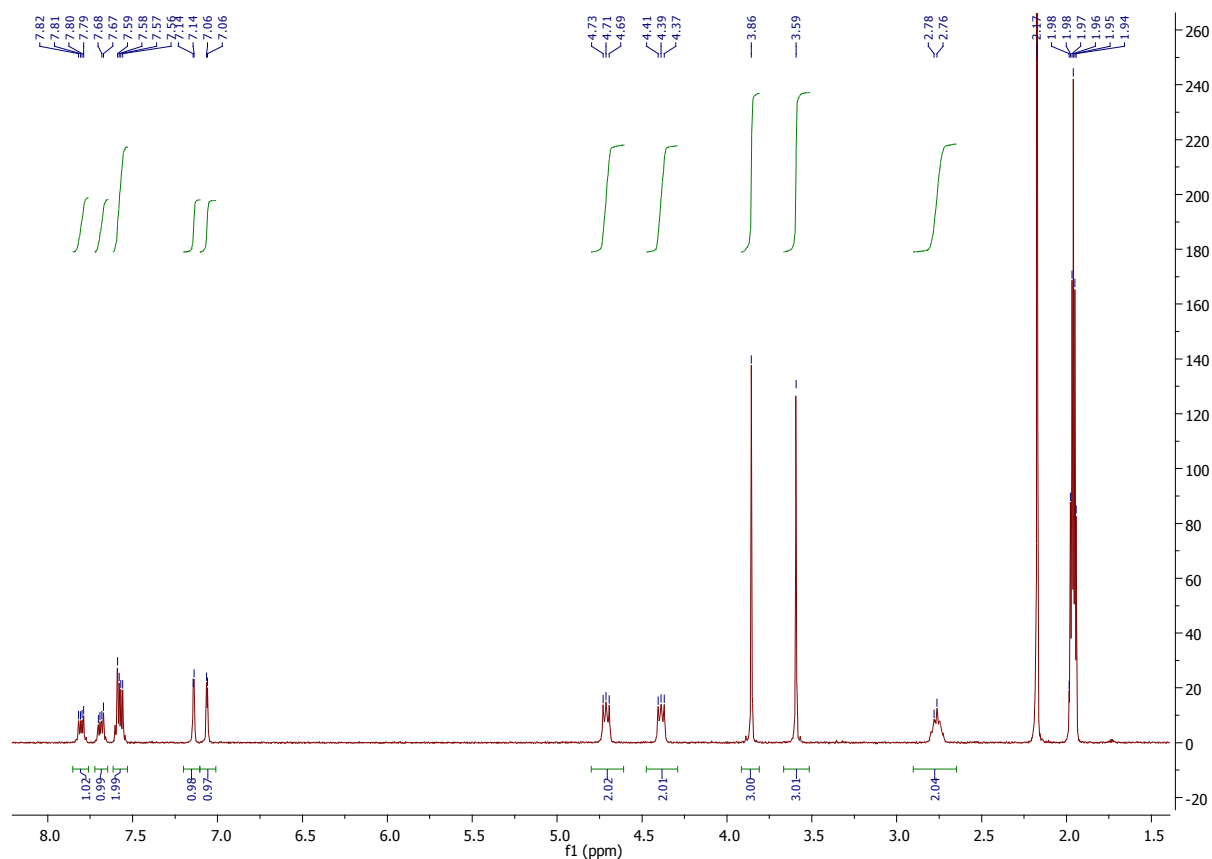


Figure S16. ¹H NMR spectrum in CD₃CN of complex **2a** (from X-ray crystals)

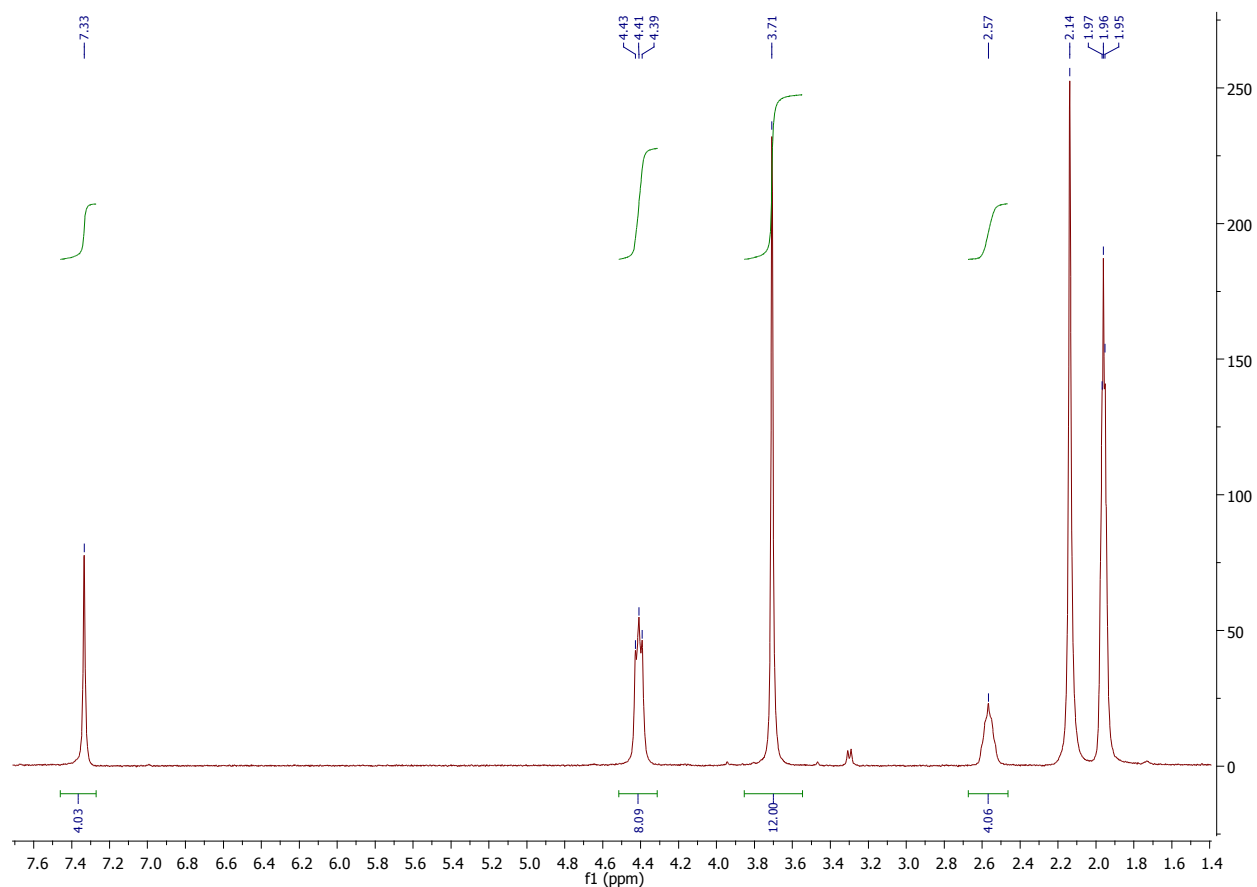


Figure S17. ^1H NMR spectrum in CD_3CN of complex **3a**

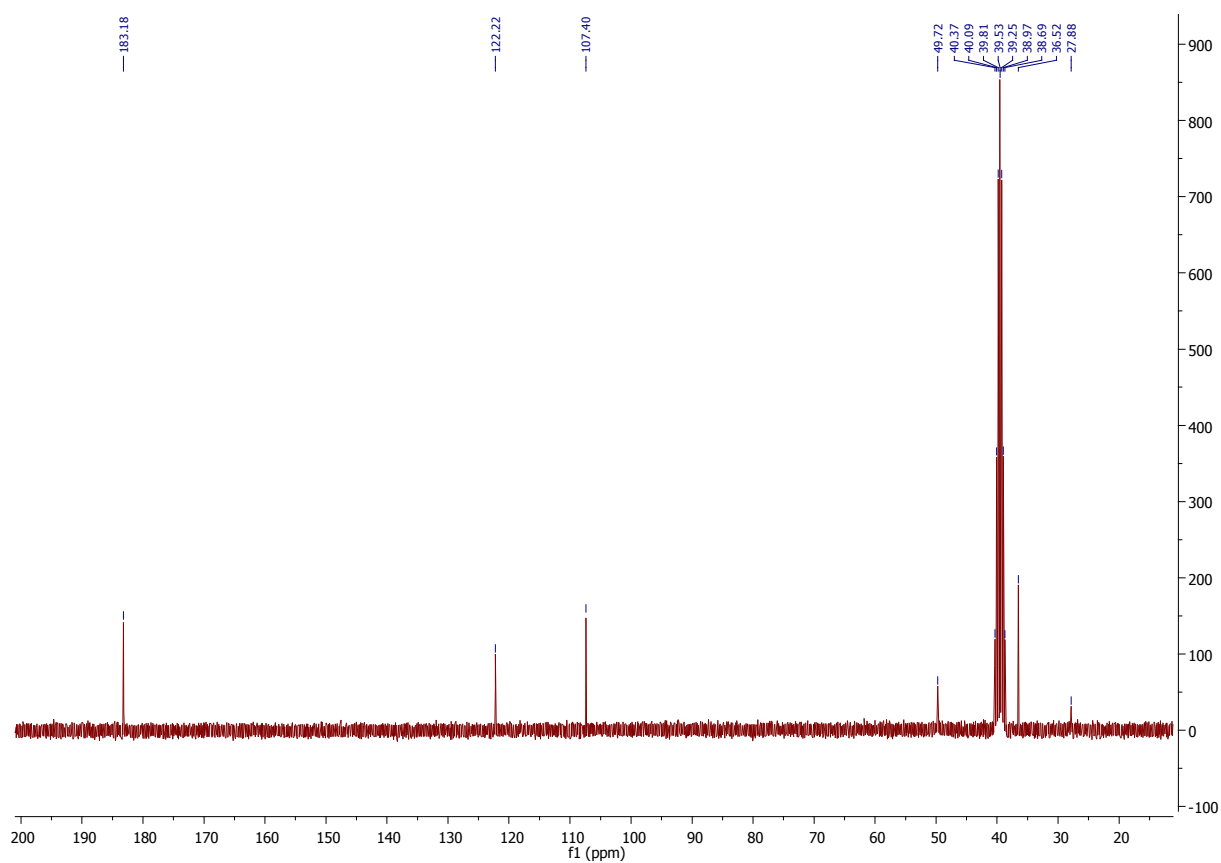


Figure S18. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum in dmsO-d_6 of **3a**

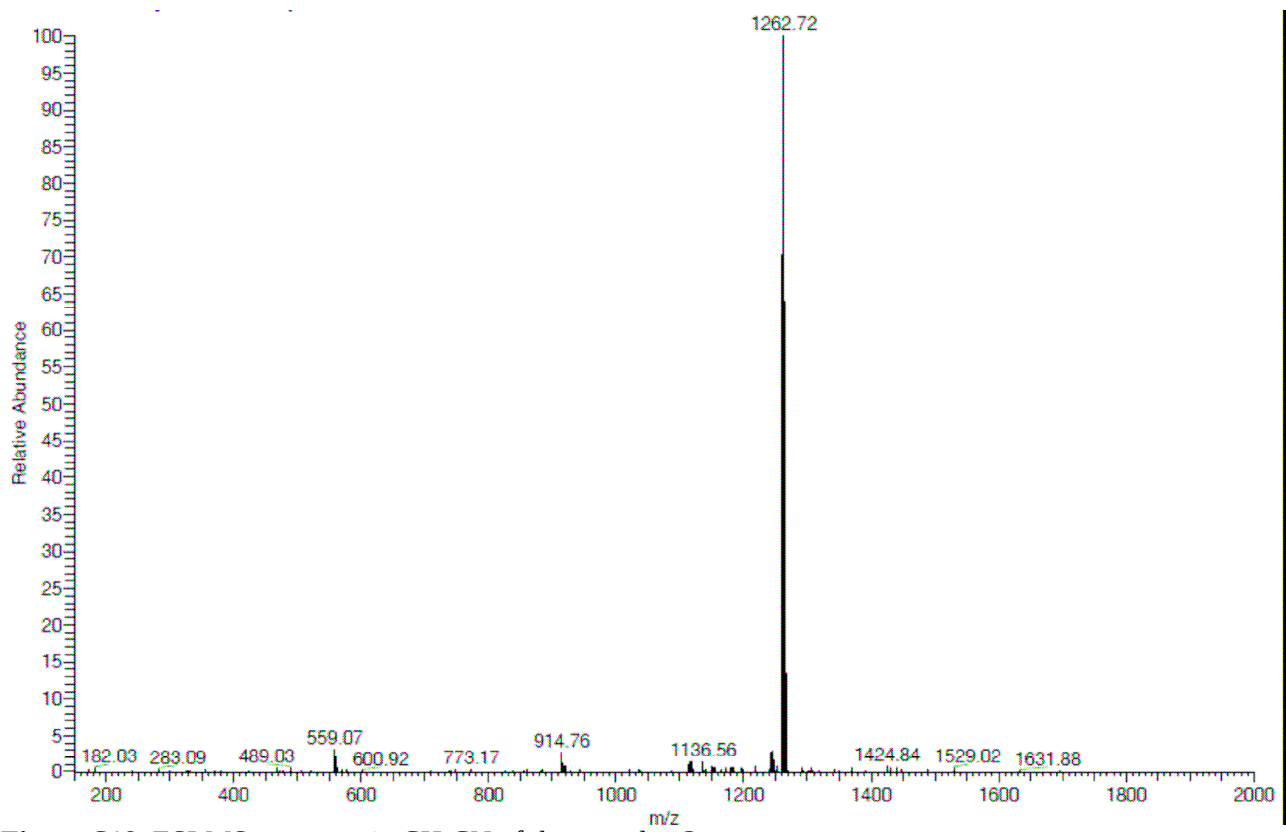


Figure S19. ESI-MS spectrum in CH₃CN of the complex **3a**

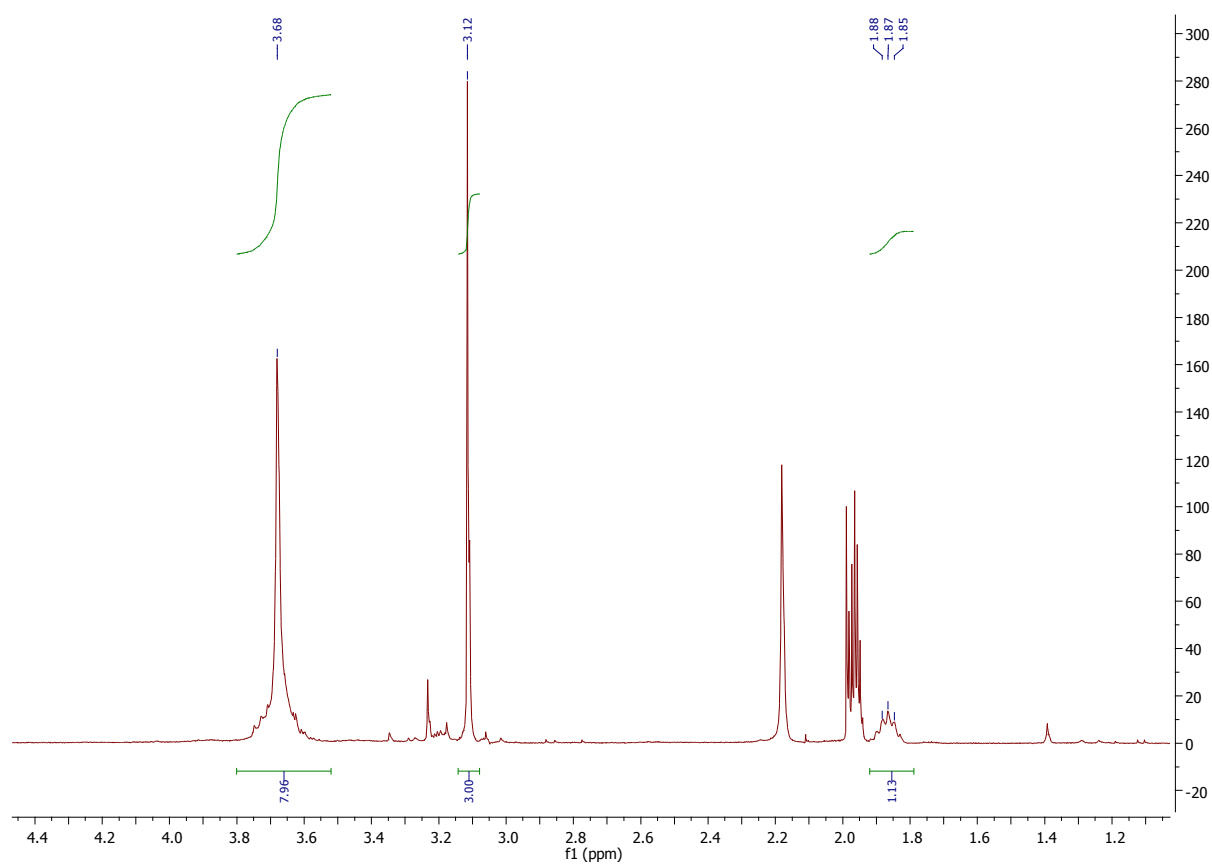


Figure S20. ^1H NMR spectrum in CD_3CN of complex **4a**

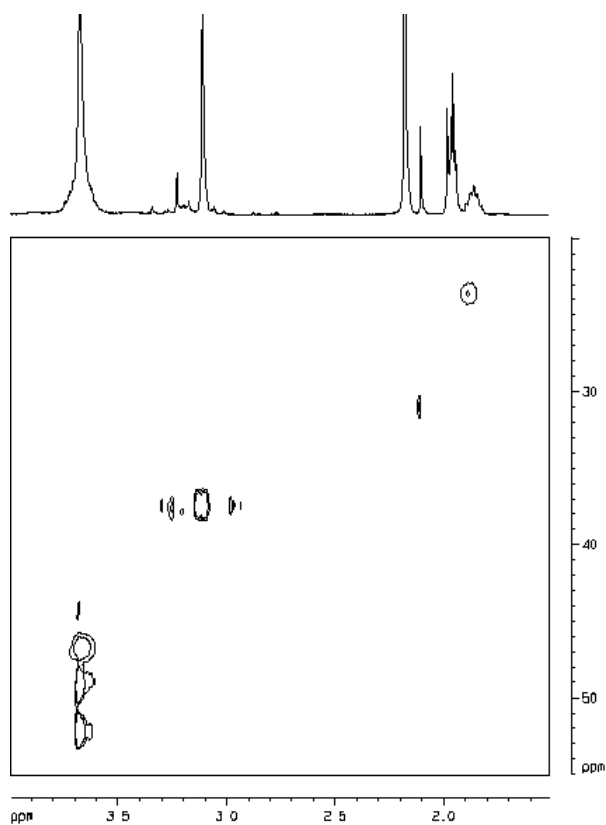


Figure S21. ^1H , ^{13}C HMQC NMR spectrum in CD_3CN of complex **4a**

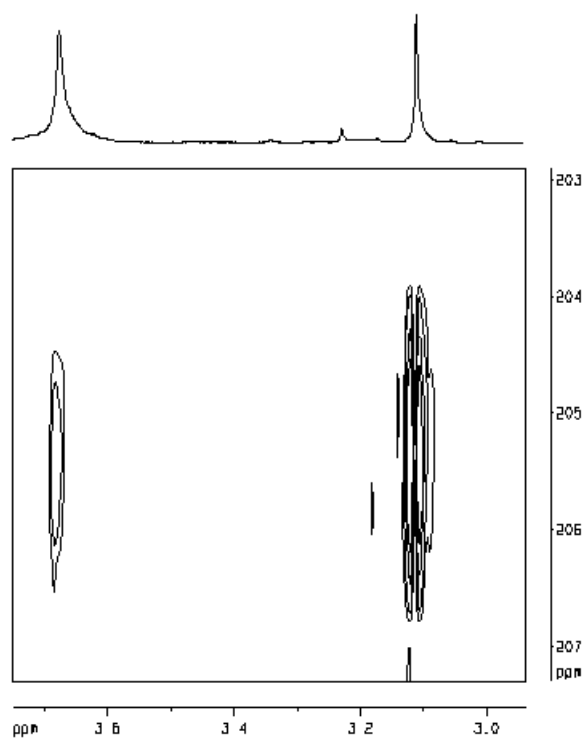


Figure S22. ^1H , ^{13}C HMBC NMR spectrum in CD_3CN of complex **4a**

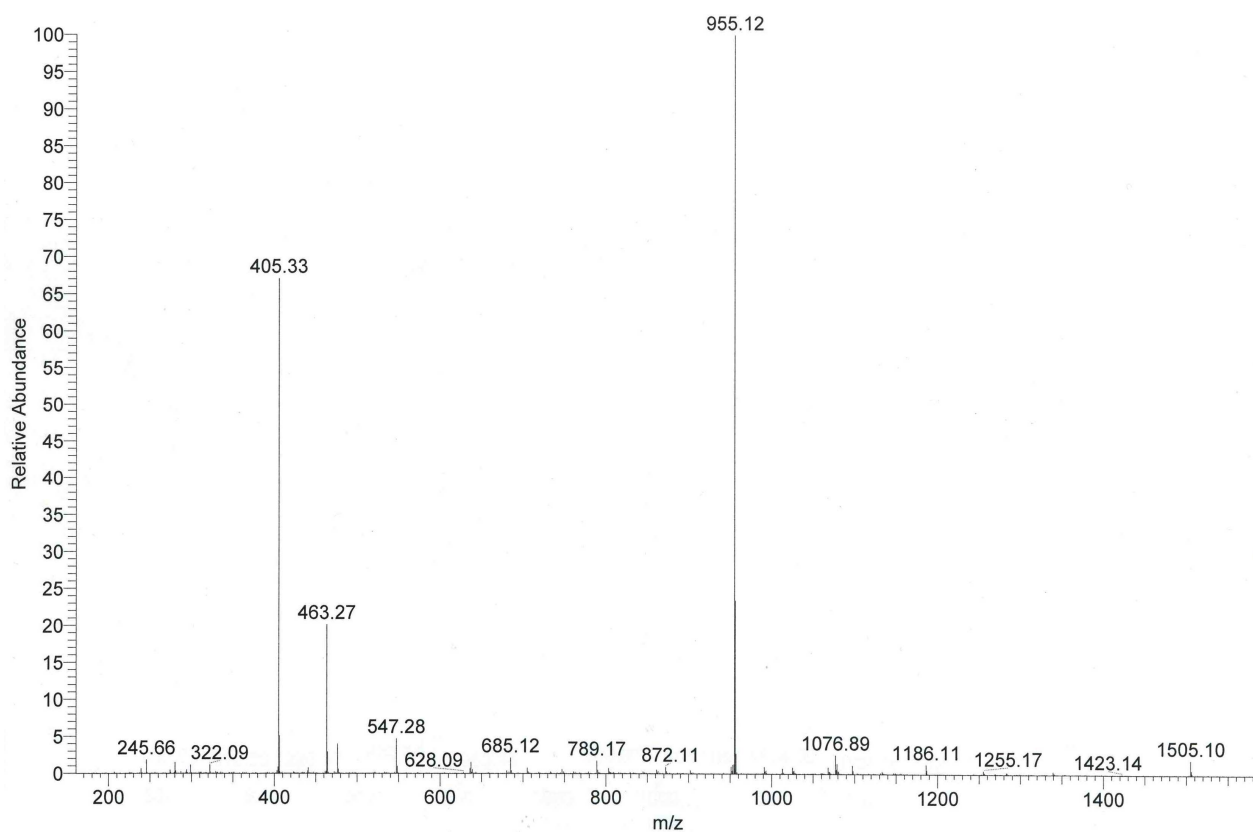


Figure S23. ESI-MS spectrum in CH₃CN of complex **4a**

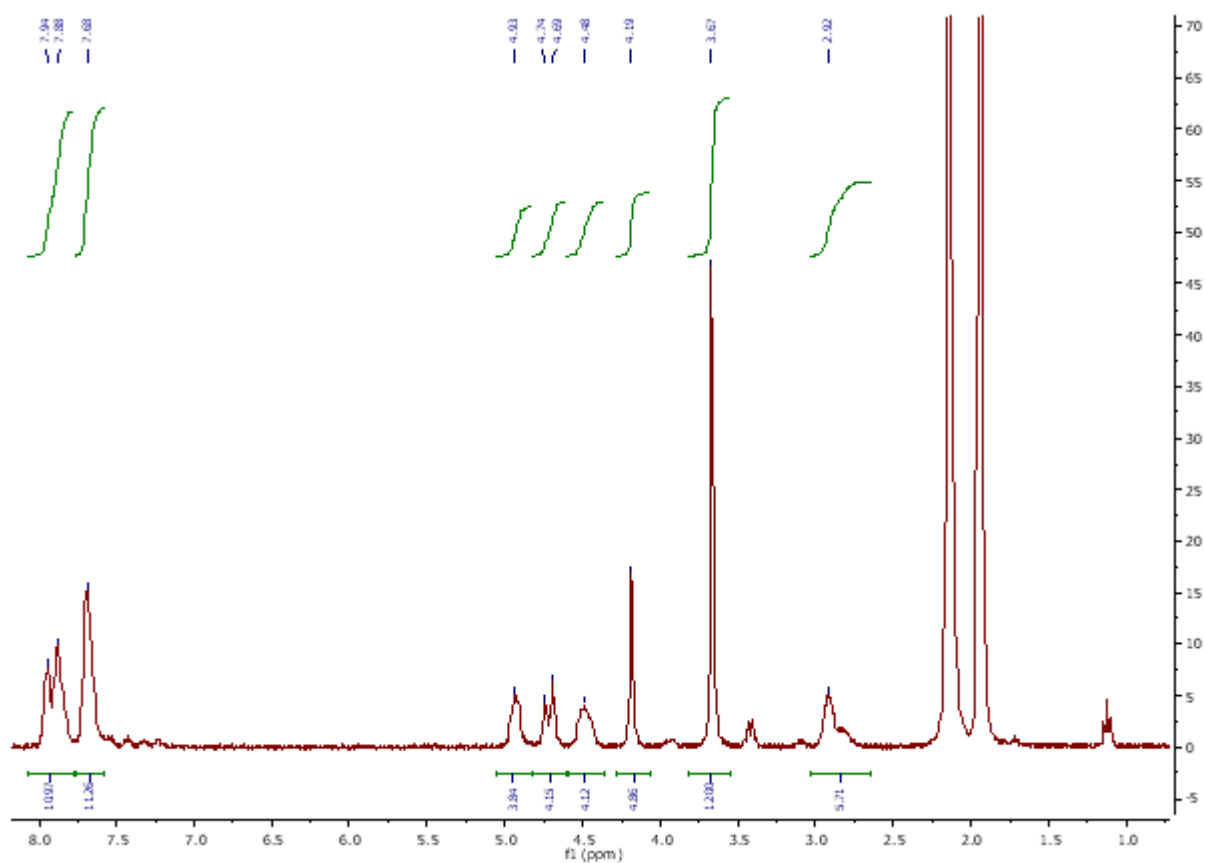


Figure S24. ^1H NMR spectrum in CD_3CN of the mixture **1b/1c**

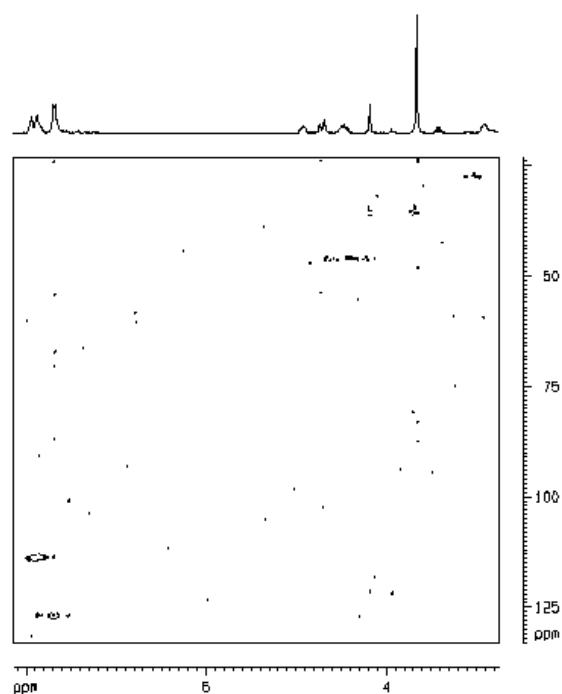


Figure S25. ^1H , ^{13}C HMQC NMR spectrum in CD_3CN of the mixture **1b/1c**

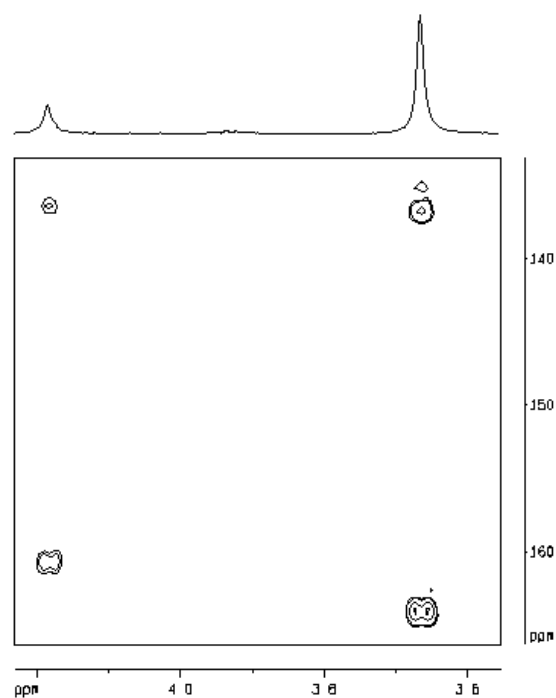


Figure S26. ^1H , ^{13}C HMBC NMR spectrum in CD_3CN of the mixture **1b/1c**

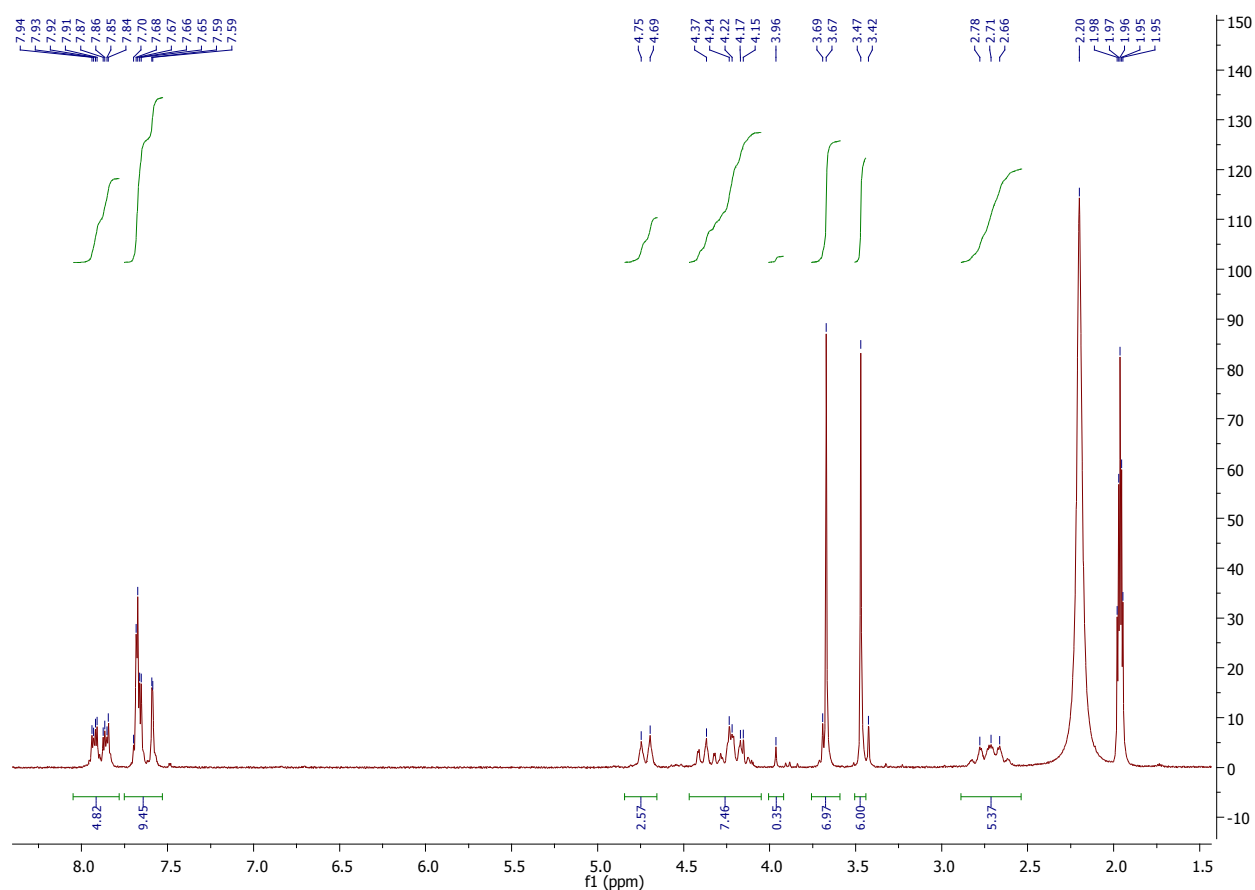


Figure S27. ¹H NMR spectrum in CD₃CN of the mixture **2b/2c**

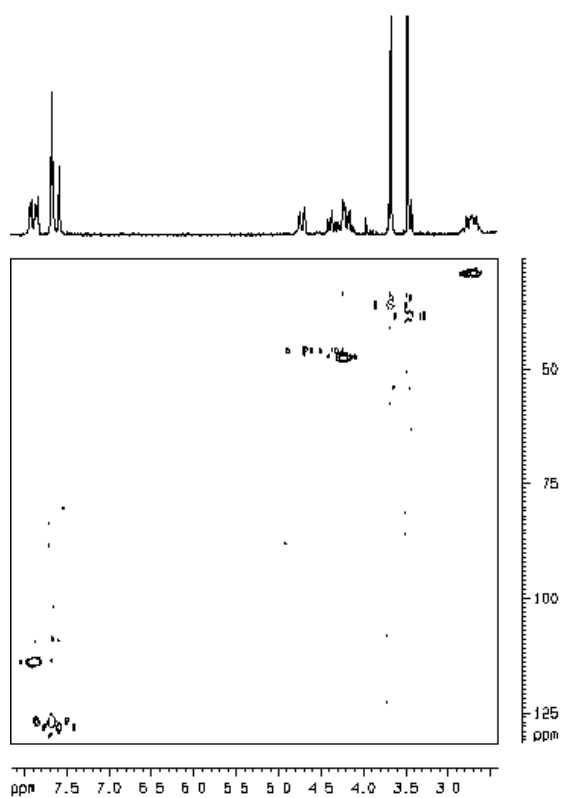


Figure S28. ¹H, ¹³C HMQC NMR spectrum in CD₃CN of the mixture **2b/2c**

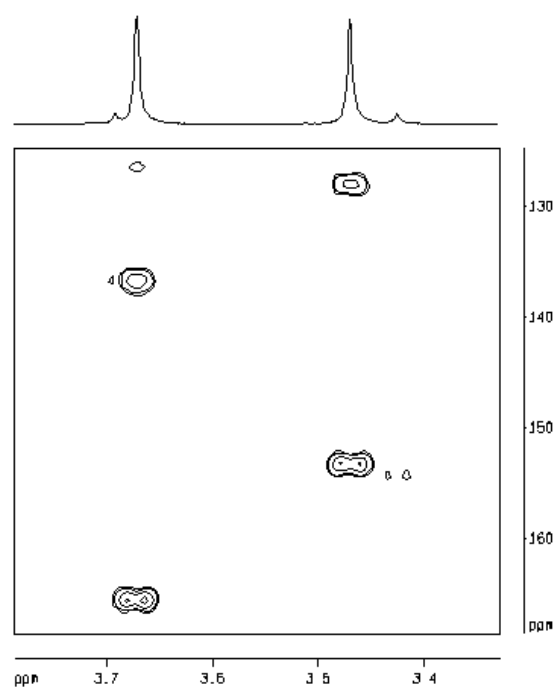


Figure S29. ^1H , ^{13}C HMBC NMR spectrum in CD_3CN of the mixture **2b/2c**

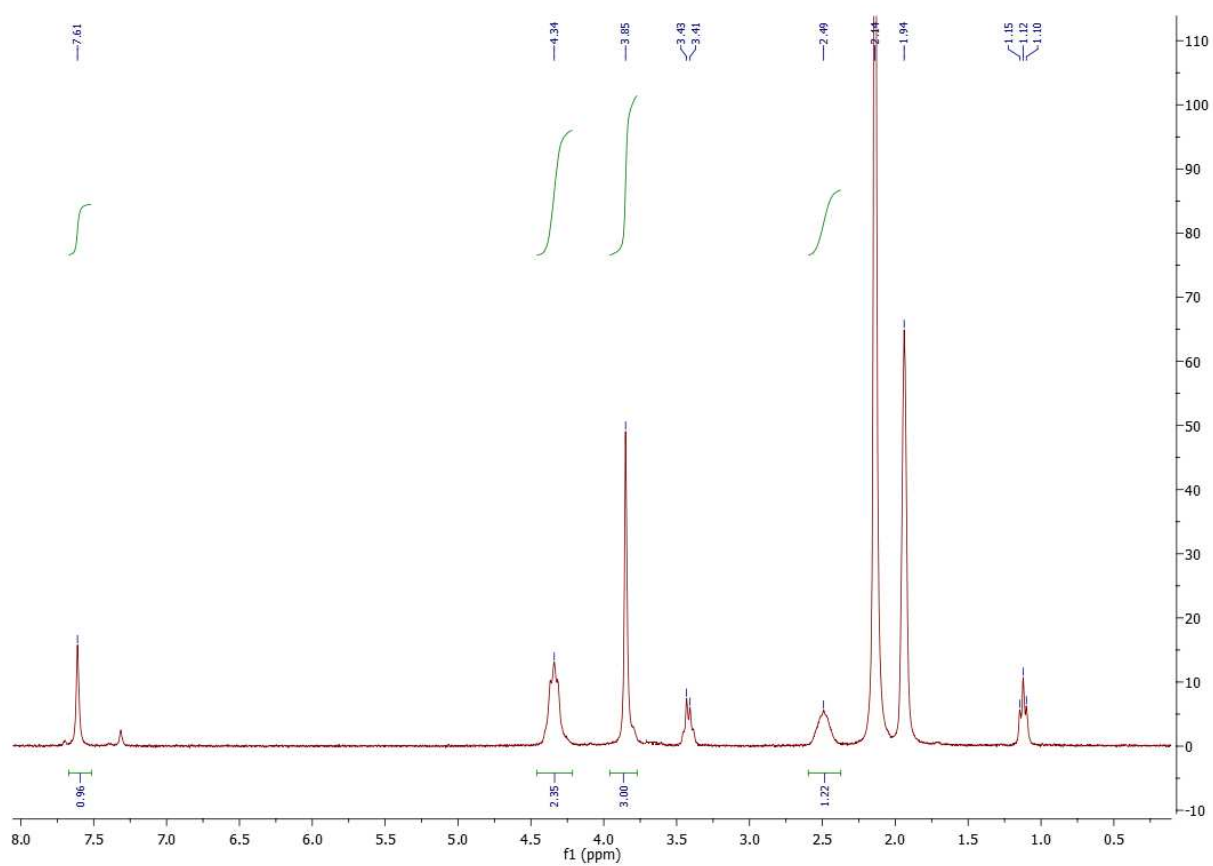


Figure S30. ^1H NMR spectrum in CD_3CN of complex **3c**

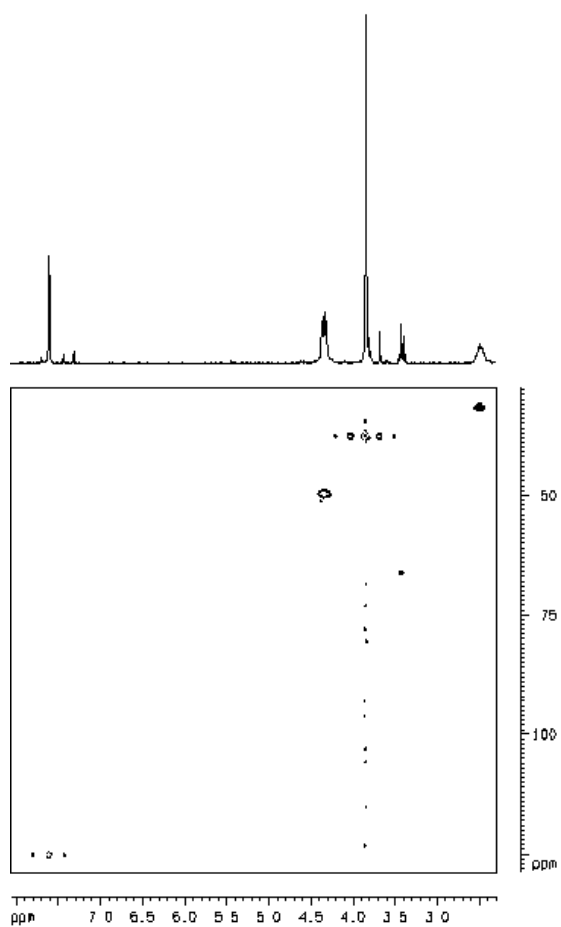


Figure S31. ^1H , ^{13}C HMQC NMR spectrum in CD_3CN of complex **3c**

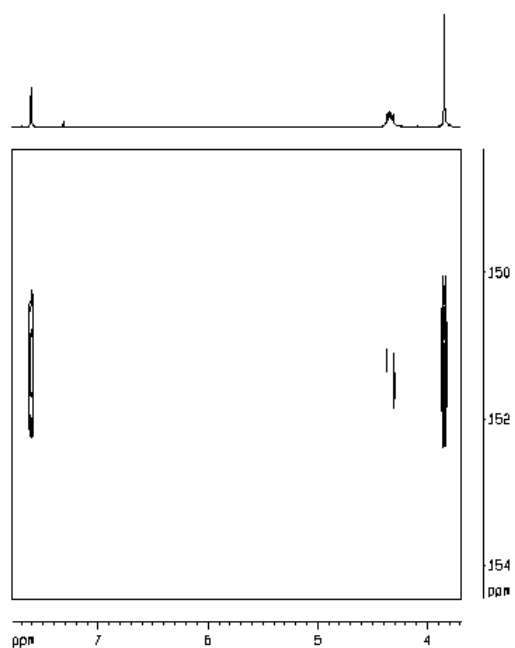


Figure S32. ^1H , ^{13}C HMBC NMR spectrum in CD_3CN of complex **3c**

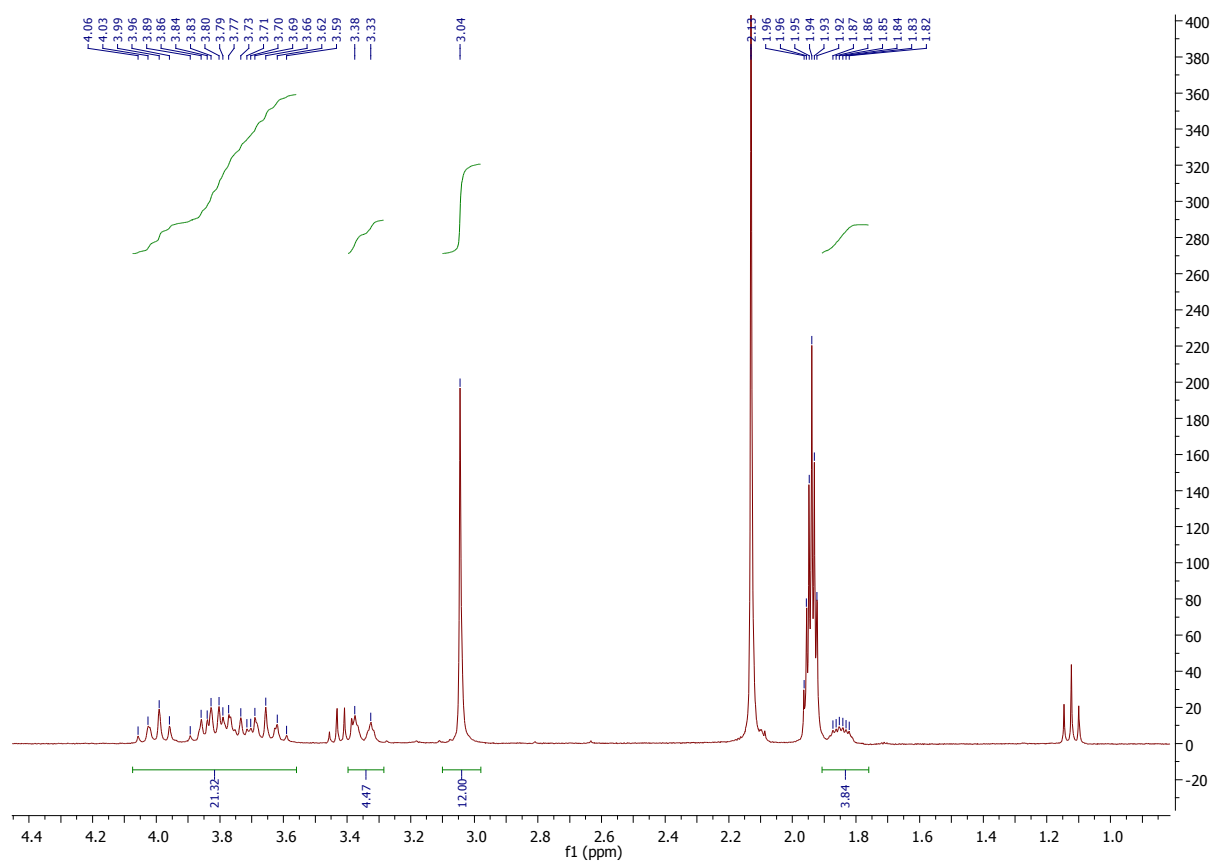


Figure S33. ¹H NMR spectrum in CD₃CN of complex **4b**

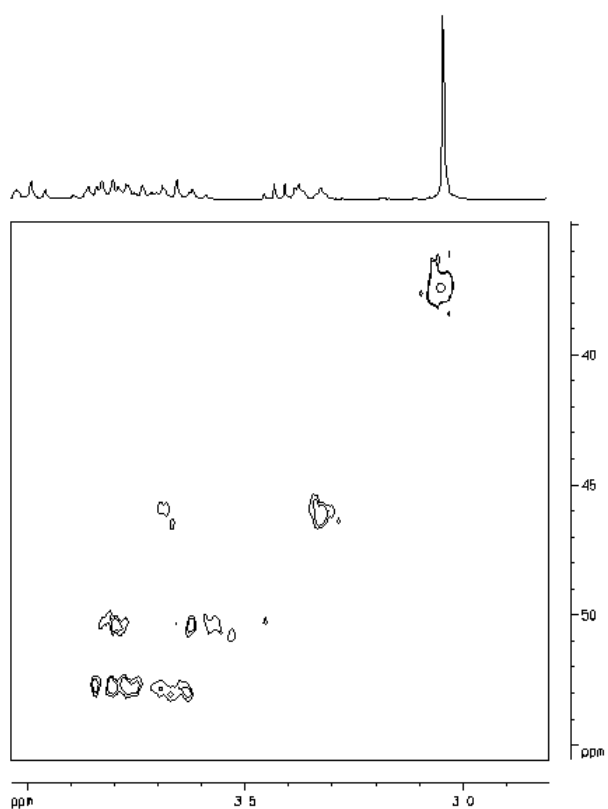


Figure S34. ¹H, ¹³C HMQC NMR spectrum in CD₃CN of complex **4b**

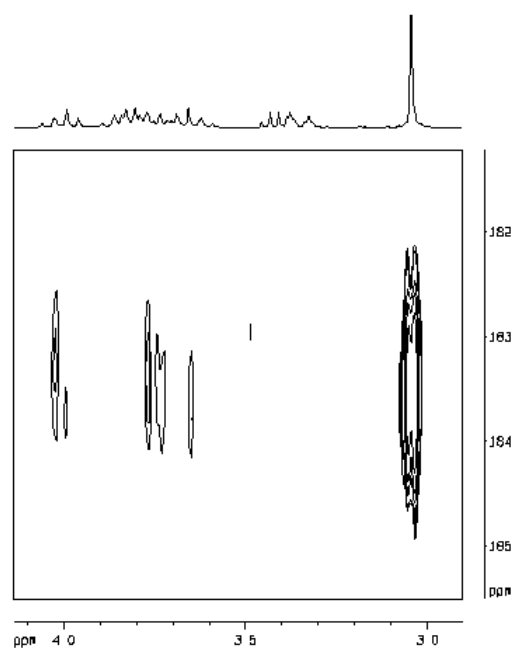


Figure S35. ^1H , ^{13}C HMBC NMR spectrum in CD_3CN of complex **4b**

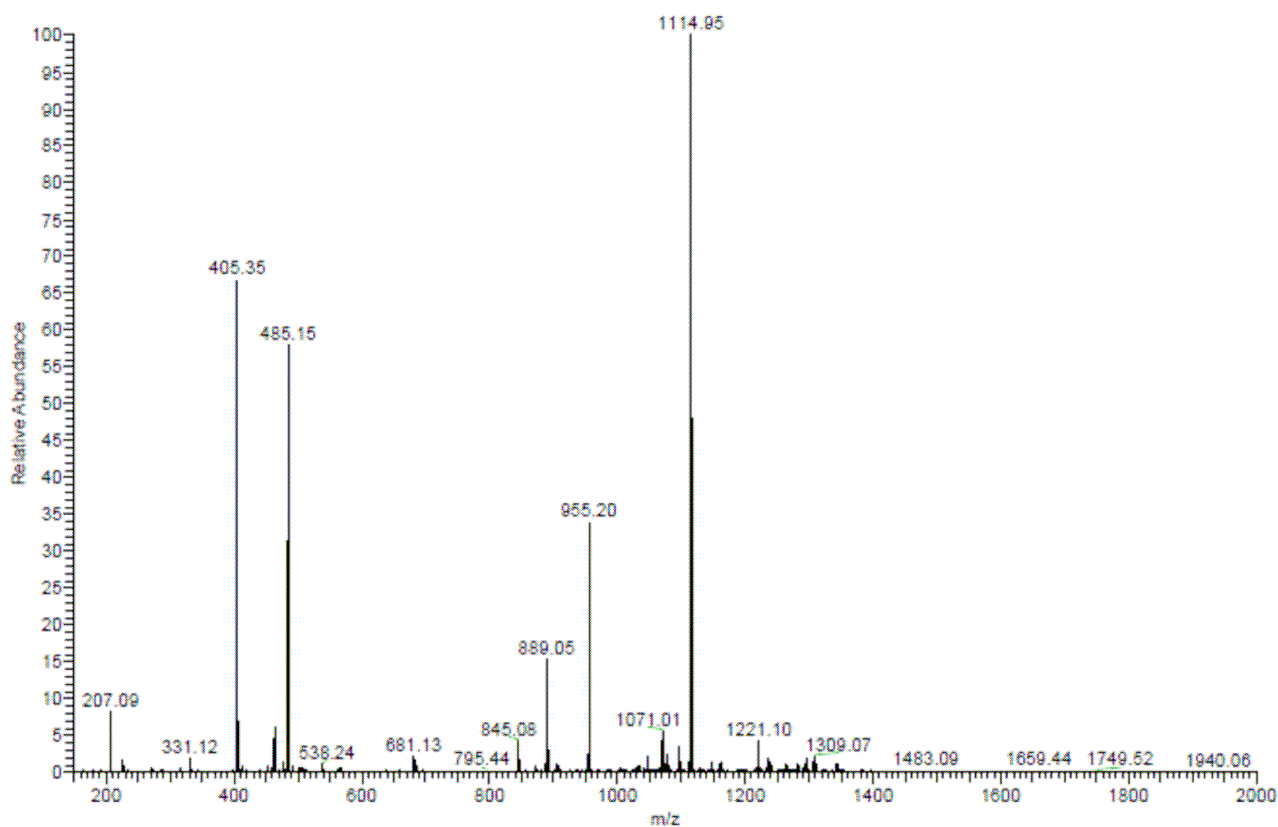


Figure S36. ESI-MS spectrum in CH_3CN of complex **4b**