

Supporting Information
for

A serendipitous self-assembly synthesis of CNN-Pt pincer complexes

Eva Sánchez-Pérez,^{ab} Fernando Santos-Escobar,^b Félix Gutiérrez-Corona,^b Kazimierz Wrobel,^a Katarzyna Wrobel*^a
and Oracio Serrano*^a

^a. Departamento de Química, Sede Pueblito de Rocha, Universidad de Guanajuato, Cerro de la Venada s/n, Guanajuato, Gto., México, C.P. 36040.

^b. Departamento de Biología Experimental, Universidad de Guanajuato, Noria Alta, Guanajuato, Gto., México, C.P. 36020.

Email: katarzyn@ugto.mx

Email: oraciosinh@ugto.mx

Index

Figure S.I.1. A set of ¹³ C{ ¹ H} (blue), APT (red) and DEPT (green) spectra of compound 2	1
Figure S.I.2. NOESY spectra of compound 3	2
All compound's figures.....	3

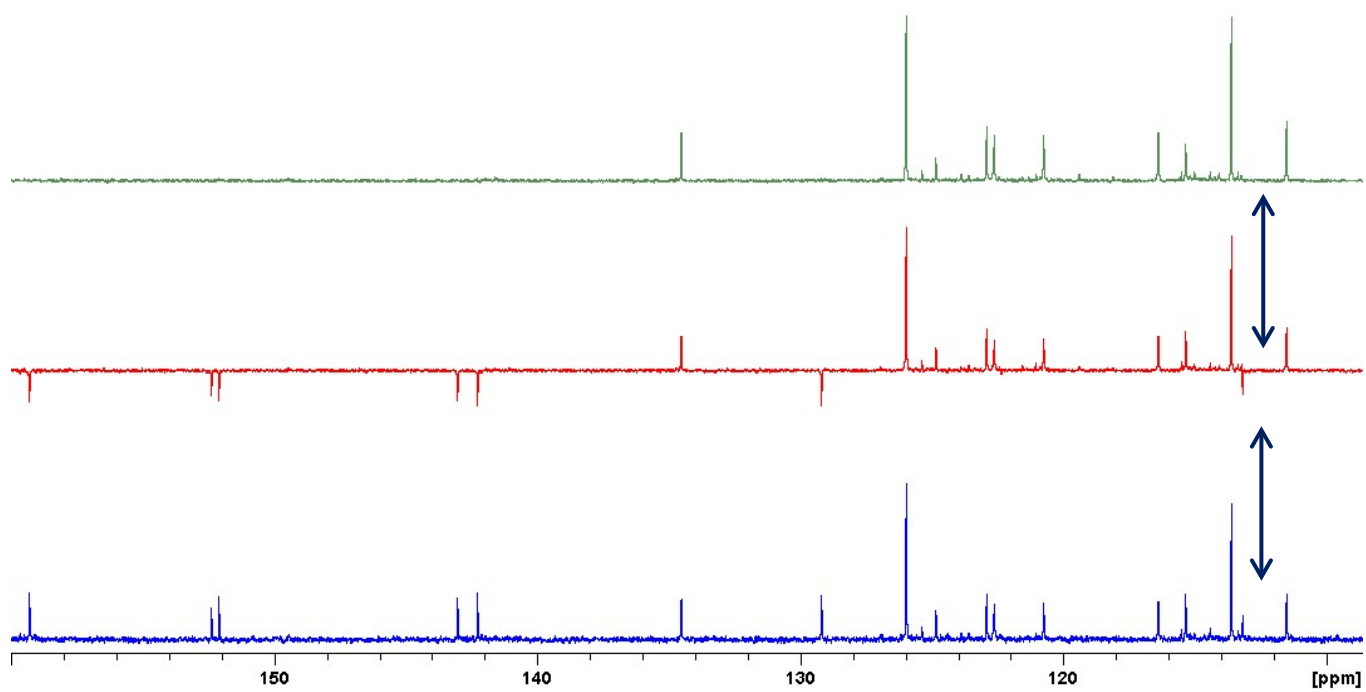


Figure S.I.1. A set of $^{13}\text{C}\{^1\text{H}\}$ (blue), APT (red) and DEPT (green) spectra of compound **2** (Arrows \Leftrightarrow indicate the quaternary carbon of Pt- C_{sp^2} bond).

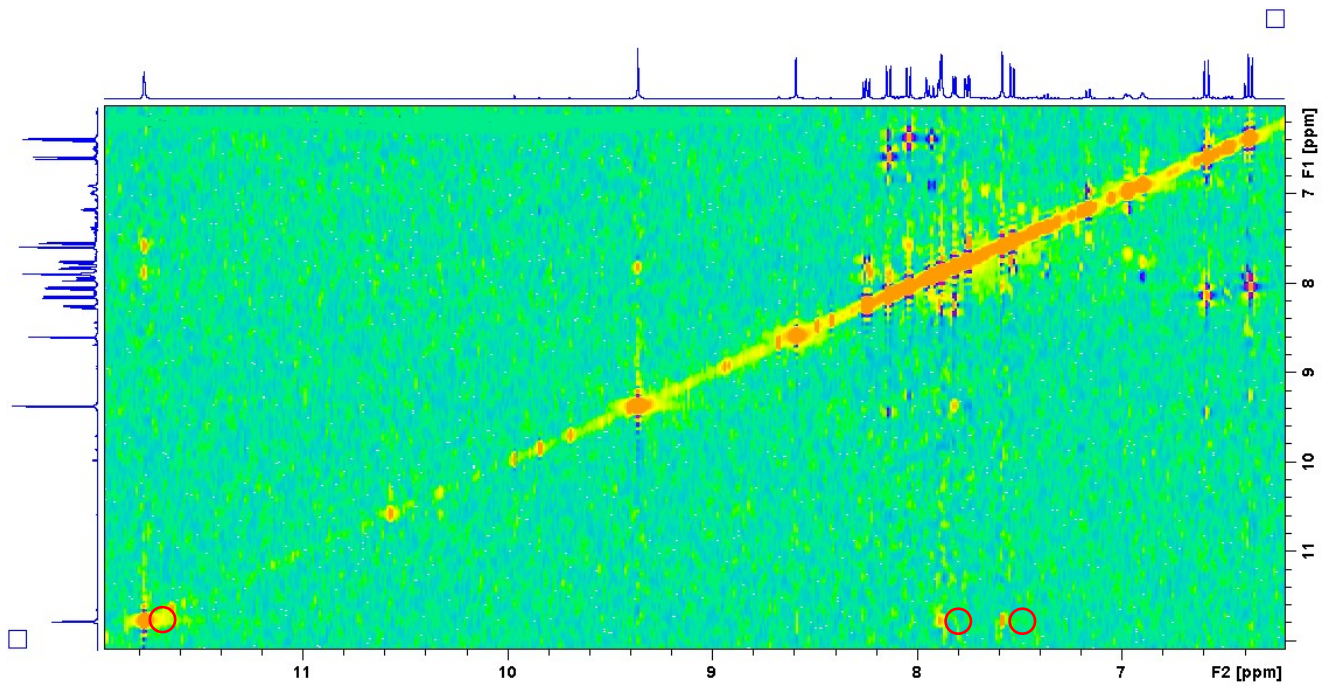


Figure S.I.2. NOESY spectra of compound 3.

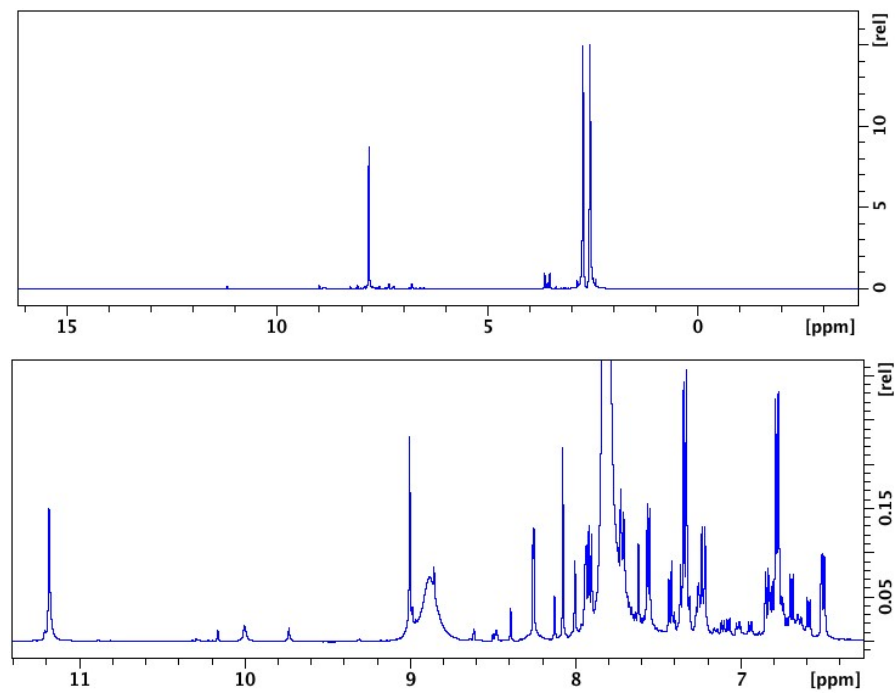


Figure S.I.3. ¹H NMR spectrum of crude solution for the reaction of L_{OMe} and K_2PtCl_4 in DMF (using dms^o-d₆ capillary),
a) full spectra and b) zoom of aromatic region.

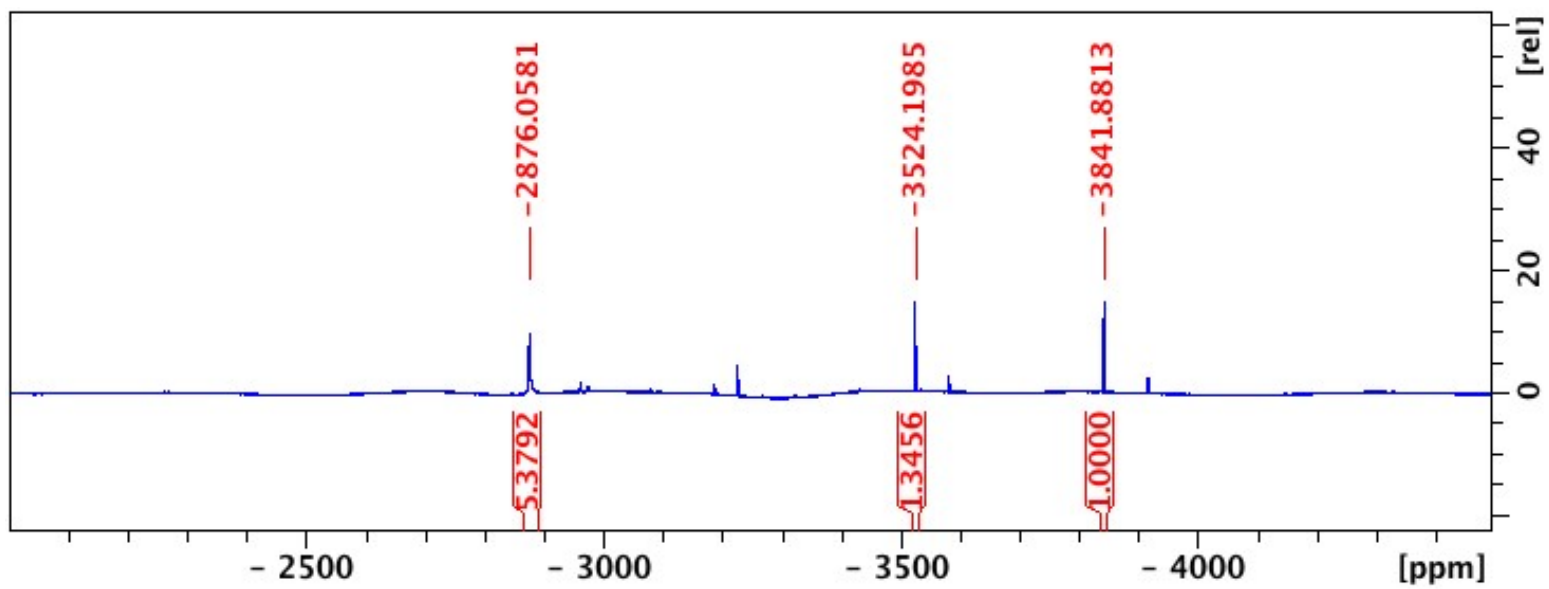


Figure S.I.4. ^{195}Pt NMR of crude solution for the reaction of L_{OMe} and K_2PtCl_4 in DMF.

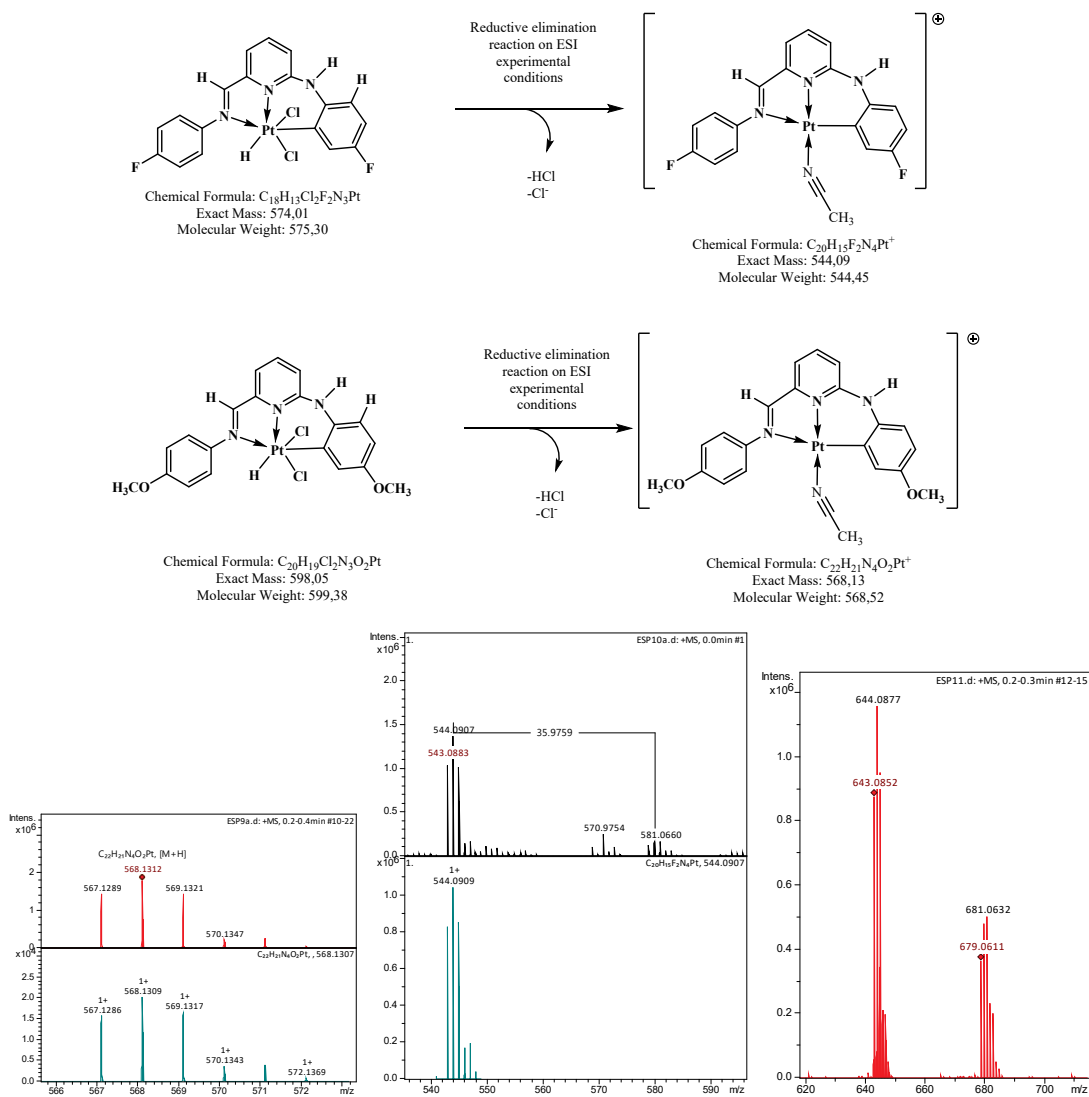


Figure S.I.5. ESI-MS spectra for compounds 1-3.

Spectra for L_{OMe} .

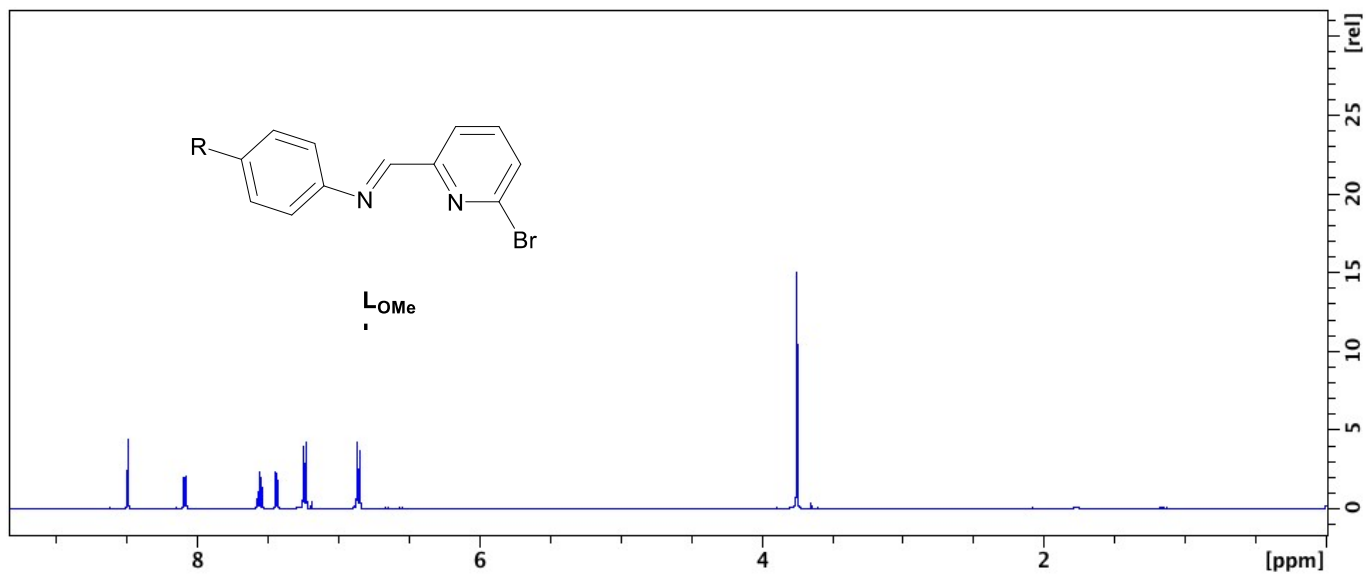


Figure S.I.6. ^1H NMR spectra for compound L_{OMe} (CDCl_3).

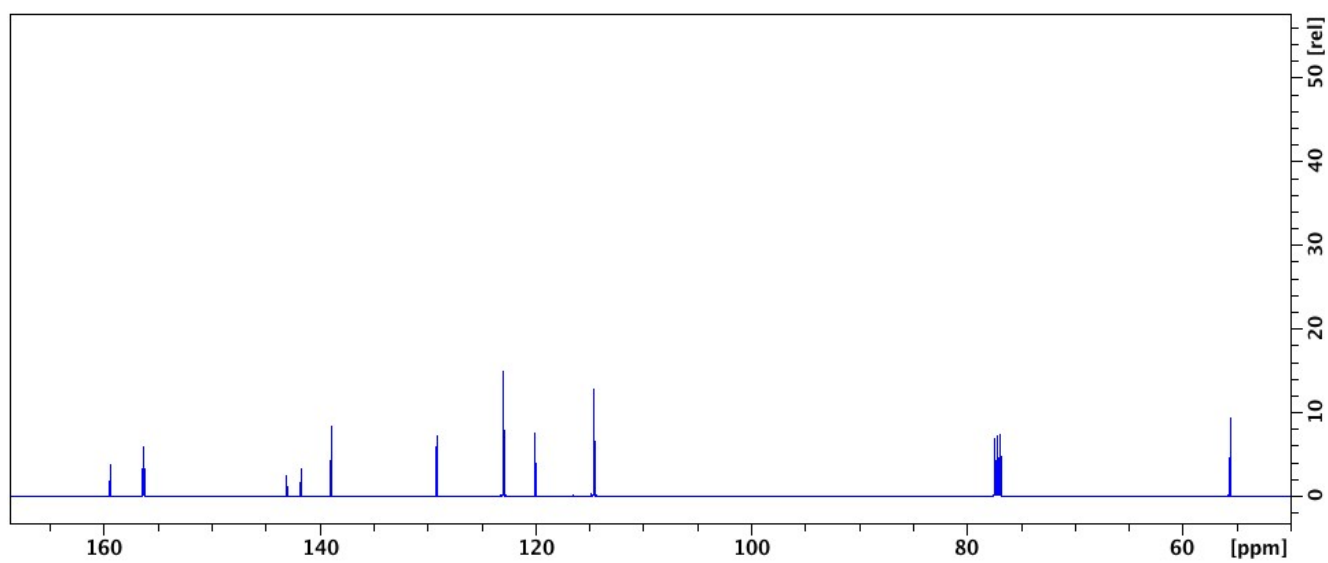


Figure S.I.7. $^{13}\text{C}\{^1\text{H}\}$ NMR spectra for compound L_{OMe} (CDCl_3).

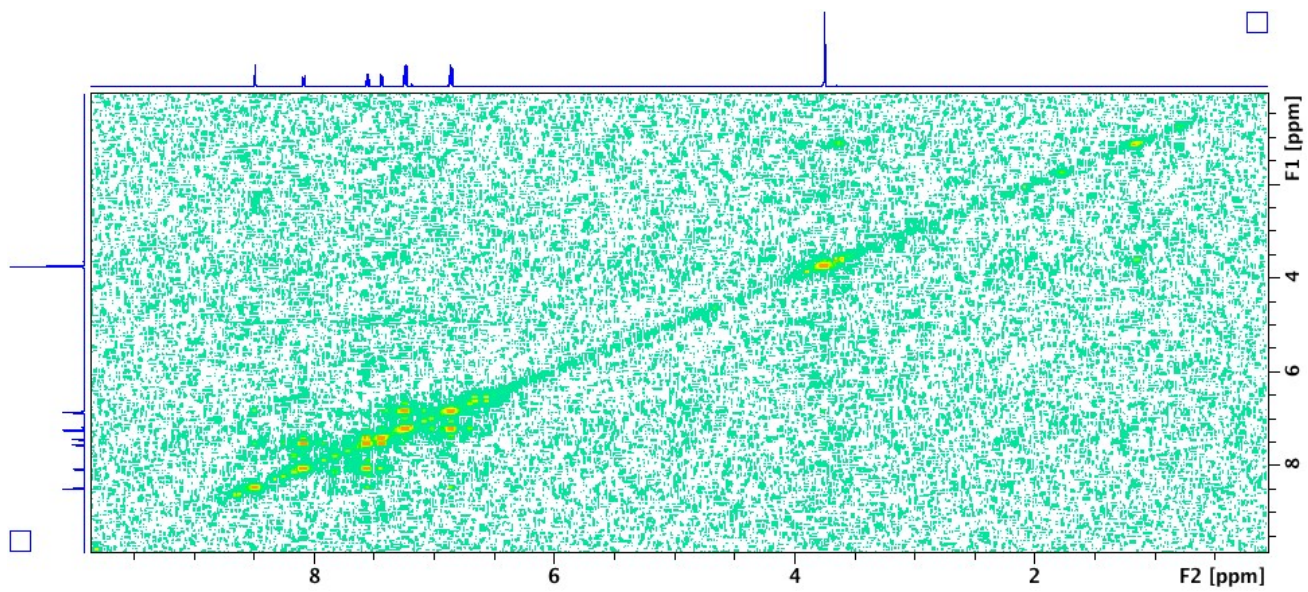


Figure S.I.8. COSY NMR spectra for compound L_{OMe} ($CDCl_3$).

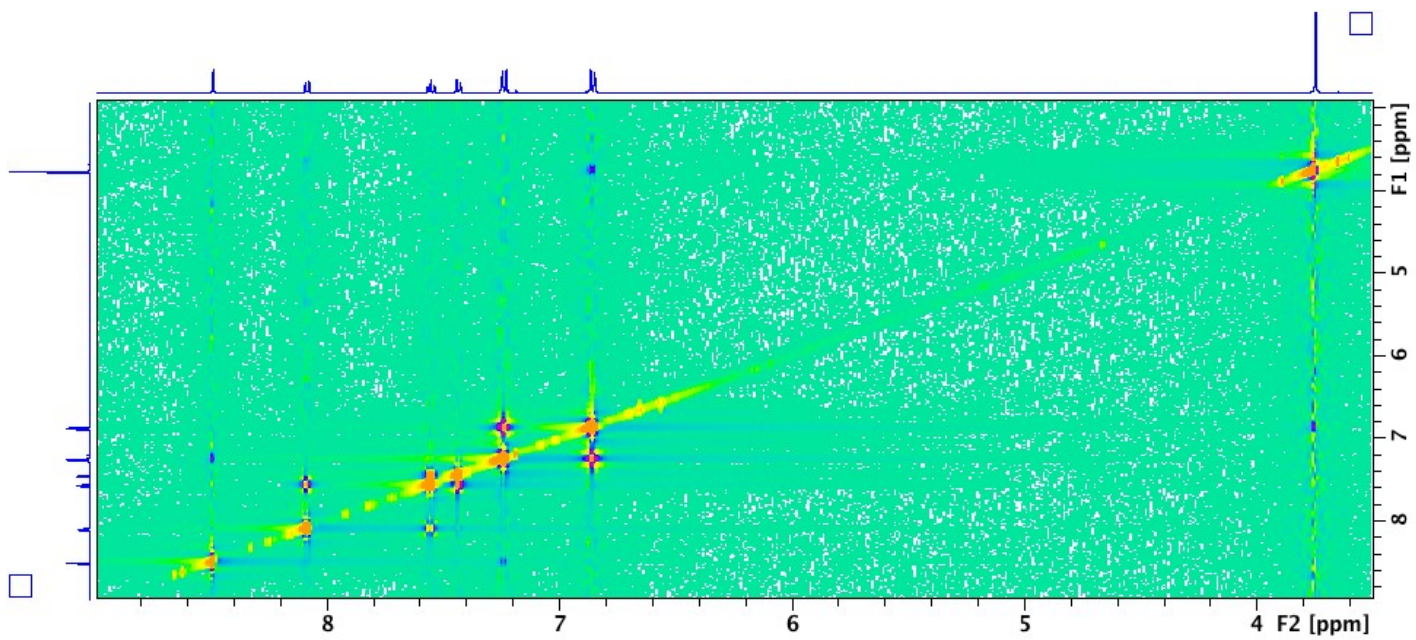


Figure S.I.9. NOESY NMR spectra for compound L_{OMe} ($CDCl_3$).

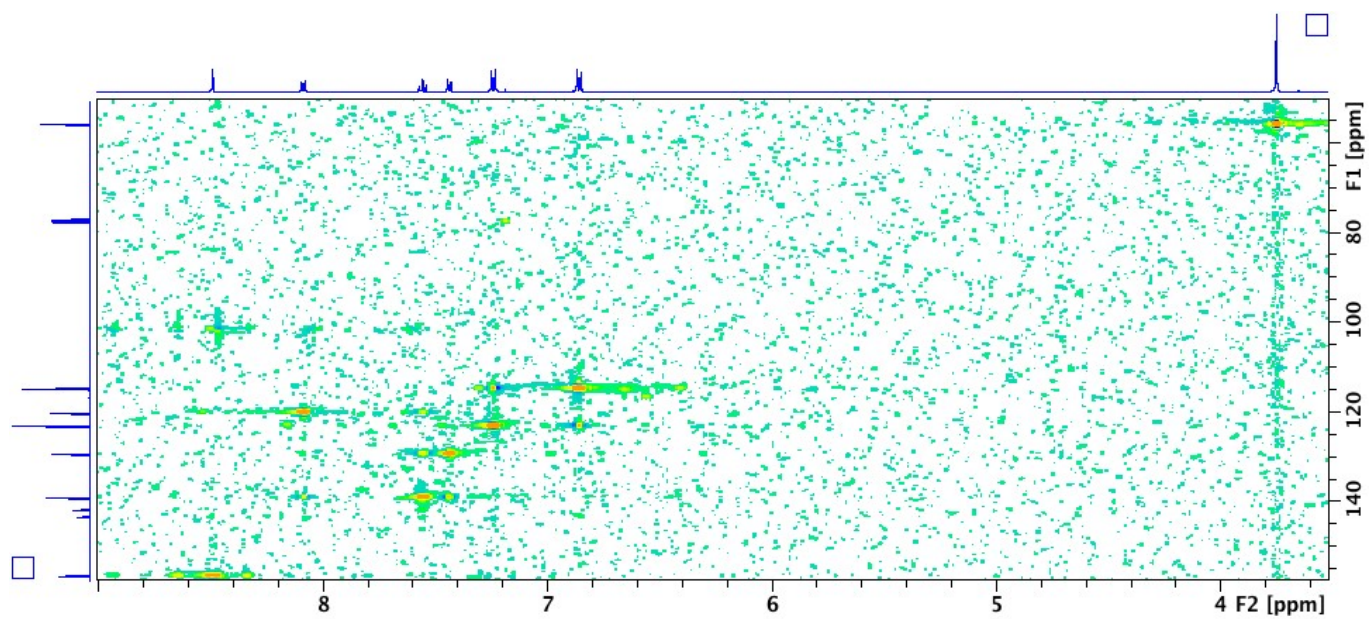


Figure S.I.10. HSQC NMR spectra for compound L_{OMe} ($CDCl_3$).

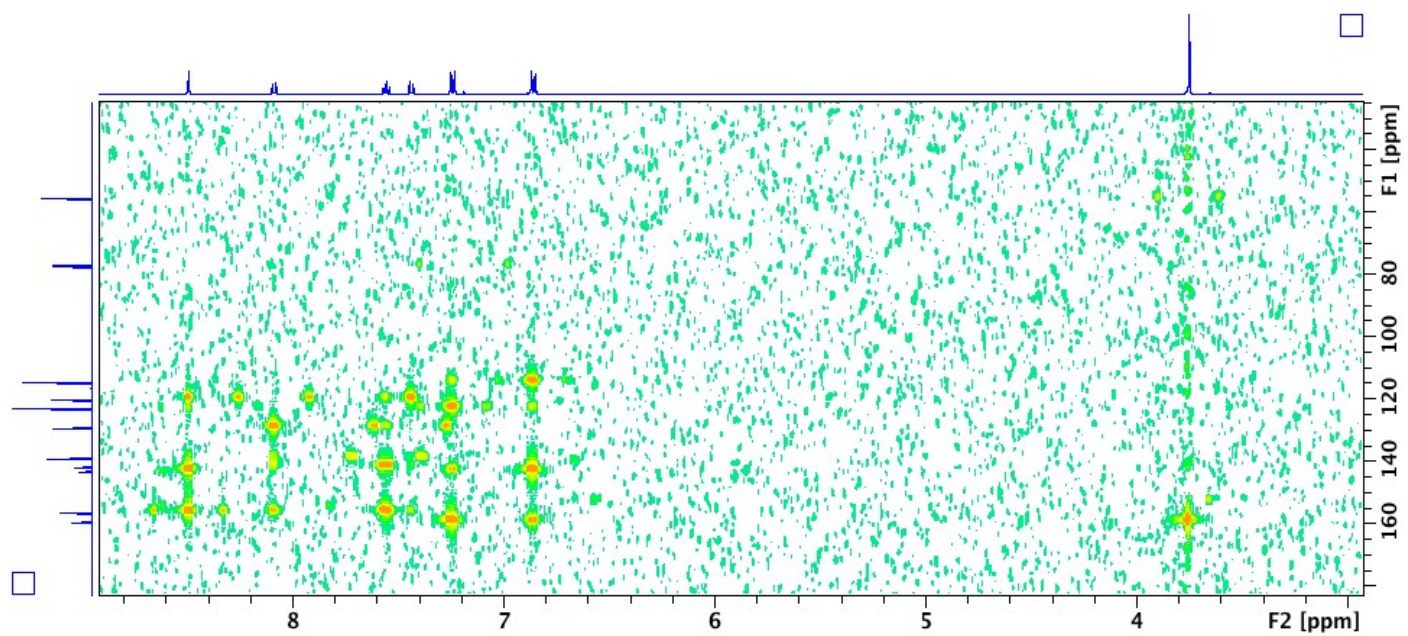


Figure S.I.11. HMBC NMR spectra for compound L_{OMe} ($CDCl_3$).

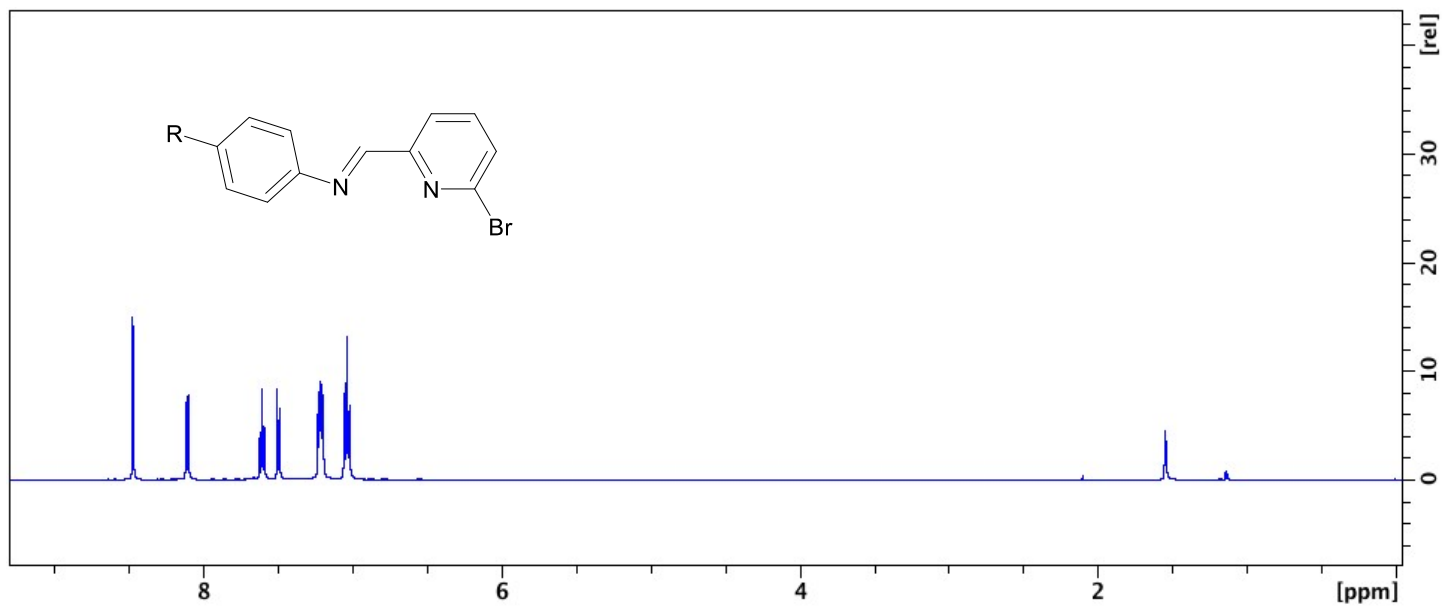


Figure S.I.12. ¹H NMR spectra for compound **L_F** (CDCl₃).

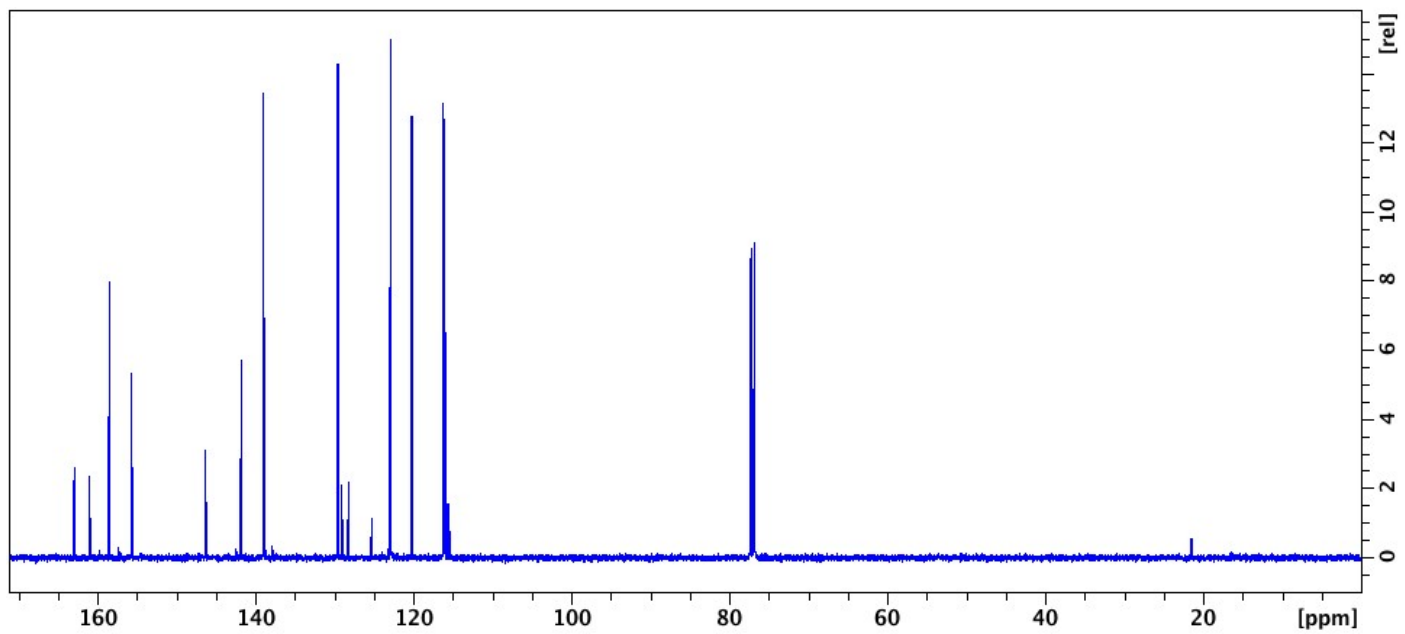


Figure S.I.13. $^{13}\text{C}\{^1\text{H}\}$ NMR spectra for compound L_f (CDCl_3).

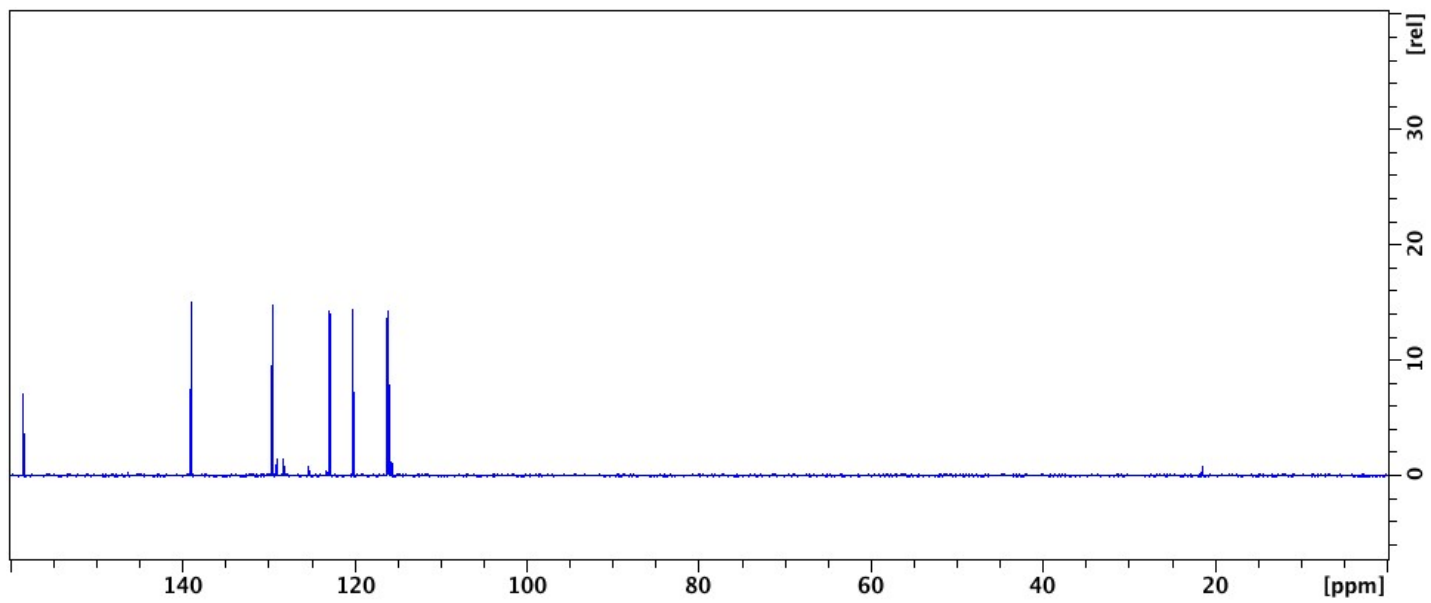


Figure S.I.14. DEPT NMR spectra for compound L_F ($CDCl_3$).

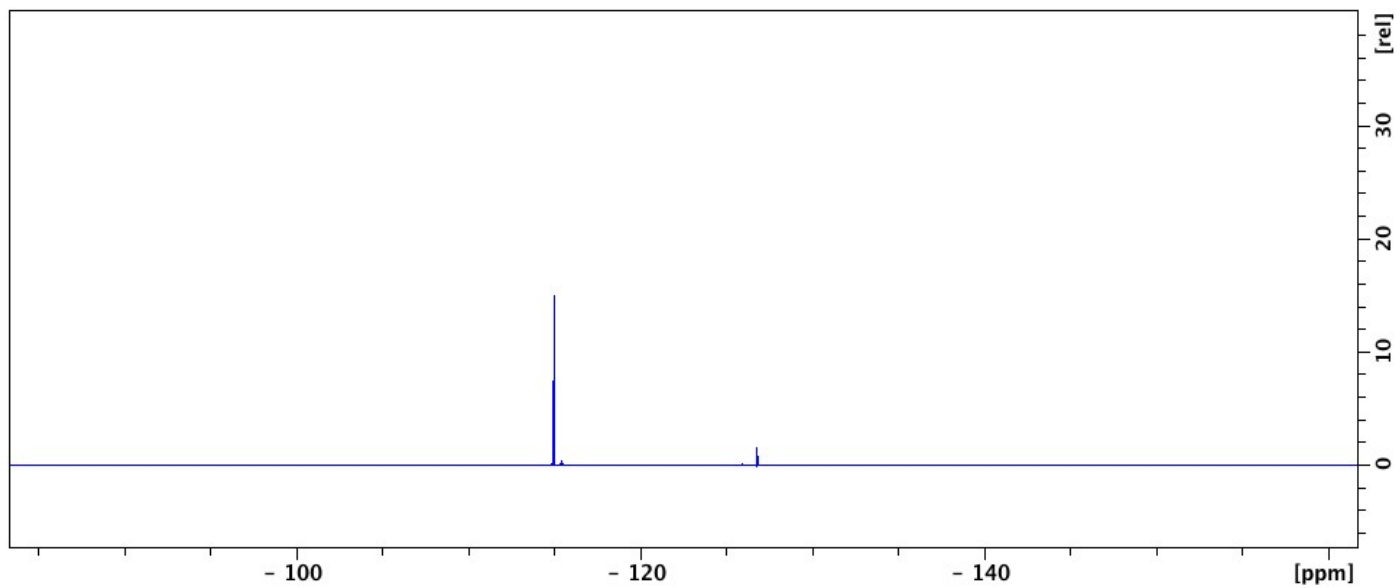


Figure S.I.15. $^{19}\text{F}\{^1\text{H}\}$ NMR spectra for compound L_f (CDCl_3).

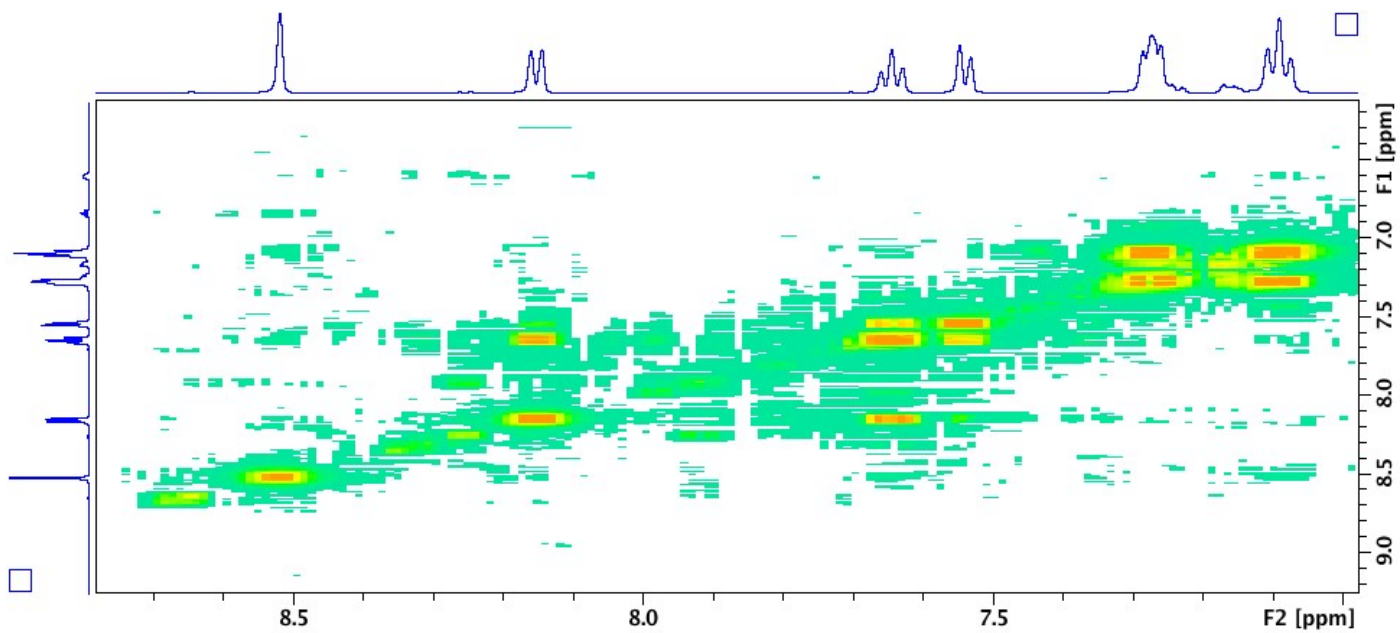


Figure S.I.16. COSY NMR spectra for compound L_f (CDCl_3).

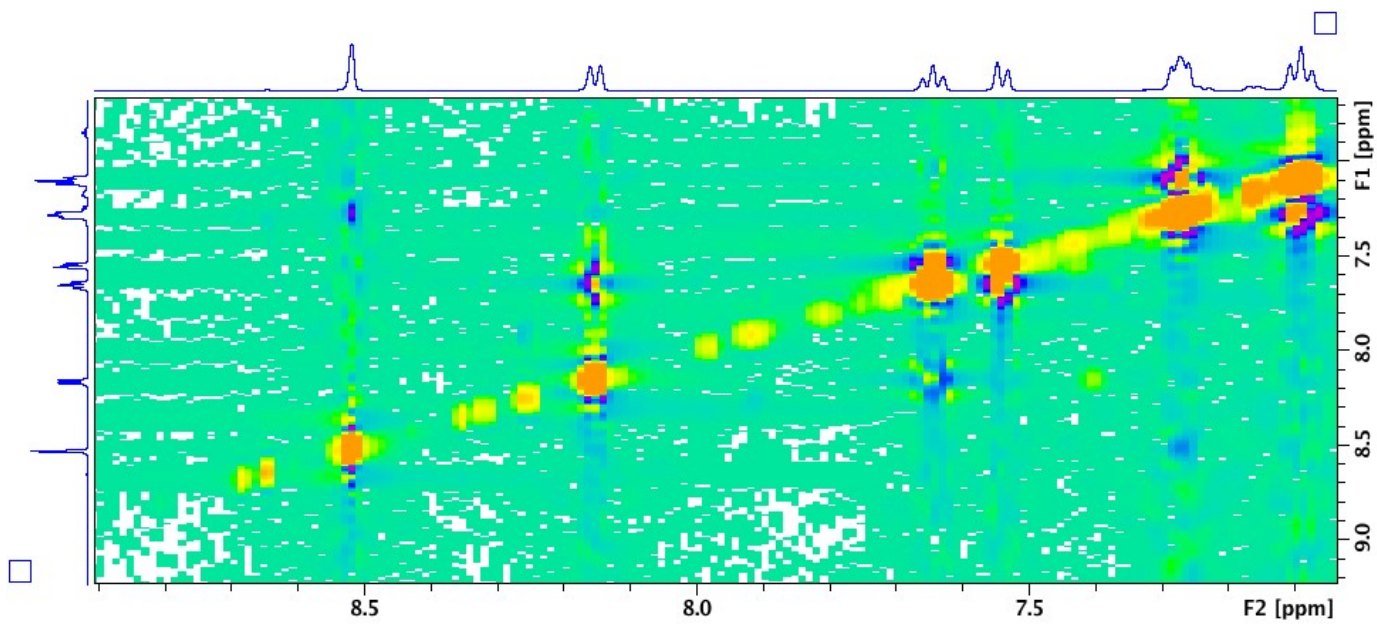


Figure S.I.17. NOESY NMR spectra for compound L_f ($CDCl_3$).

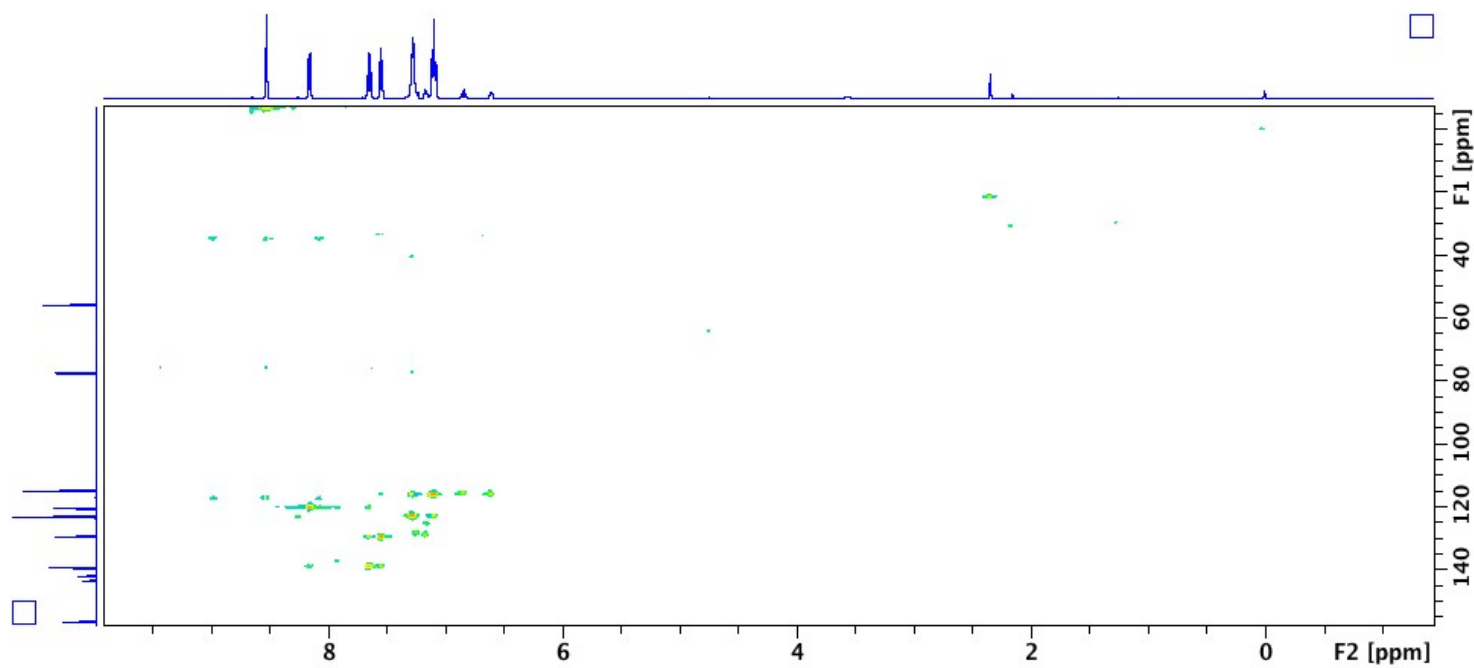


Figure S.I.18. HSQC NMR spectra for compound L_F ($CDCl_3$).

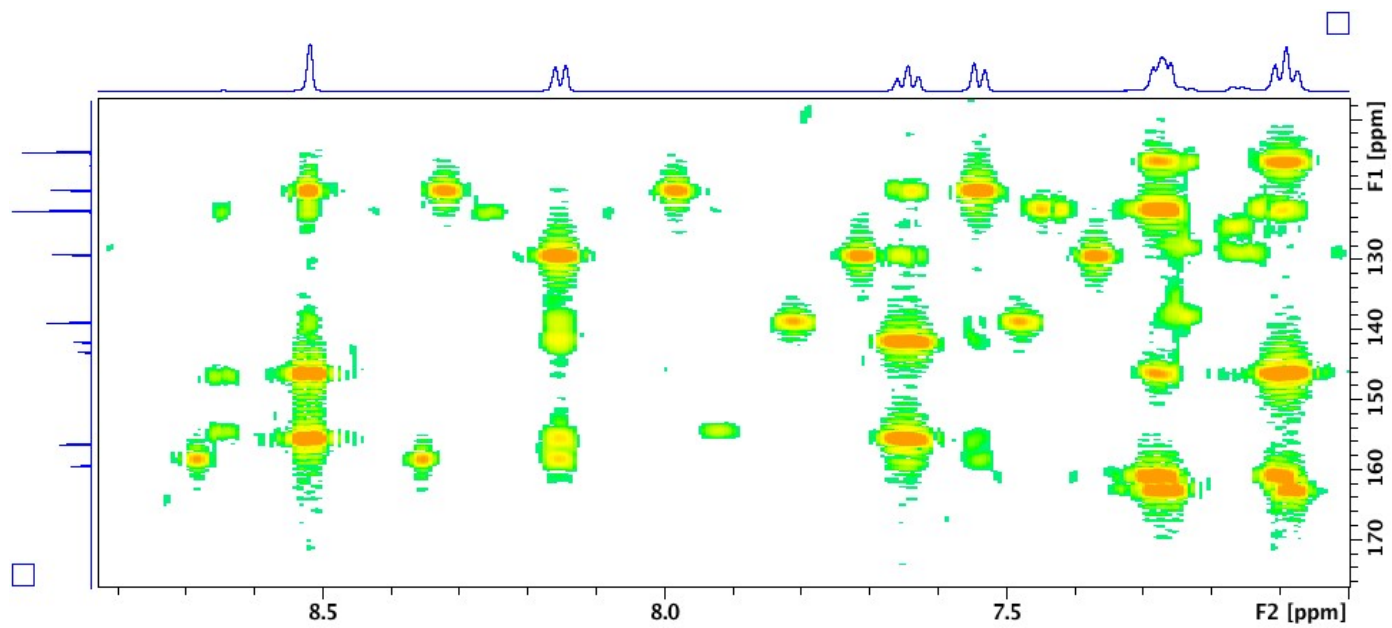


Figure S.I.19. HMBC NMR spectra for compound L_F ($CDCl_3$).

Spectra for L_{cuma} .

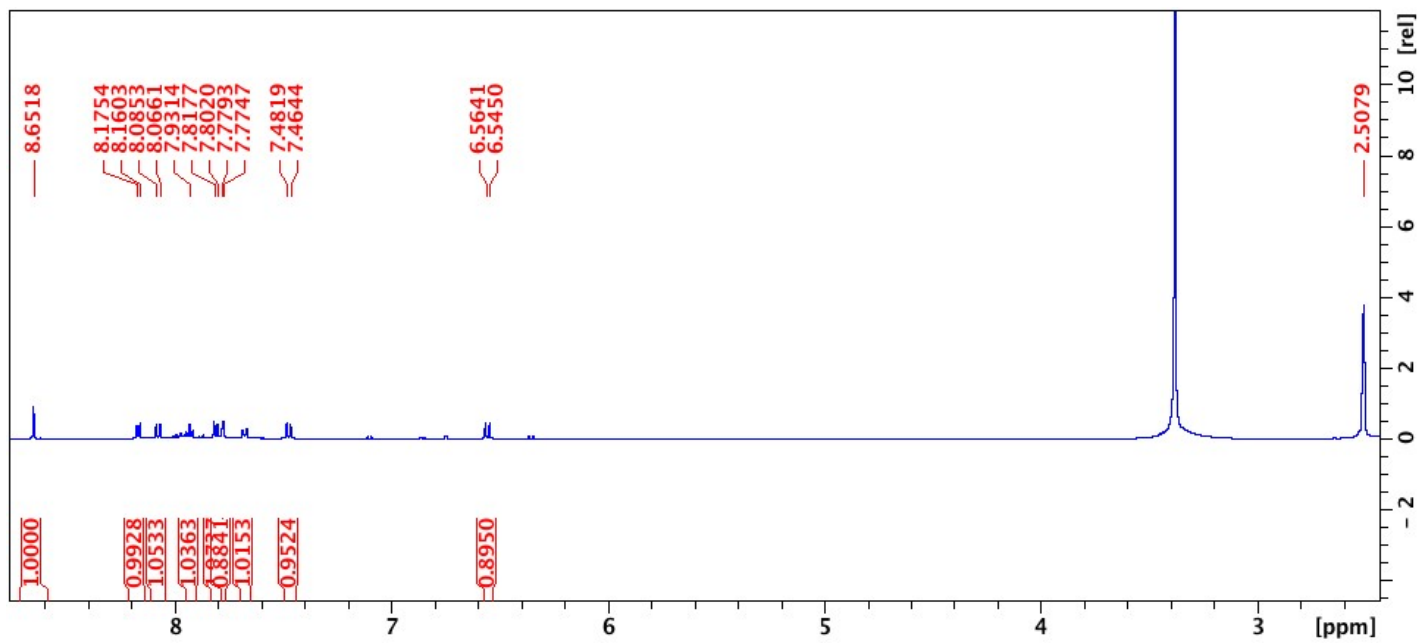


Figure S.I.20. ¹H NMR spectra for compound L_{cuma} (DMSO-d₆).

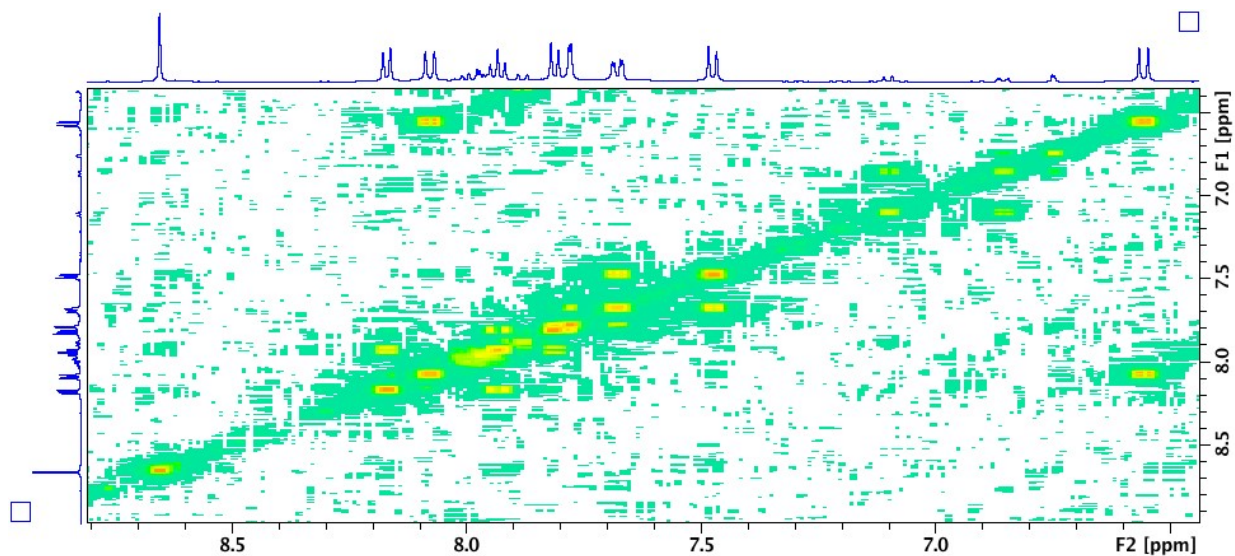


Figure S.I.21. COSY NMR spectra for compound L_{Cuma} (DMSO-d6).

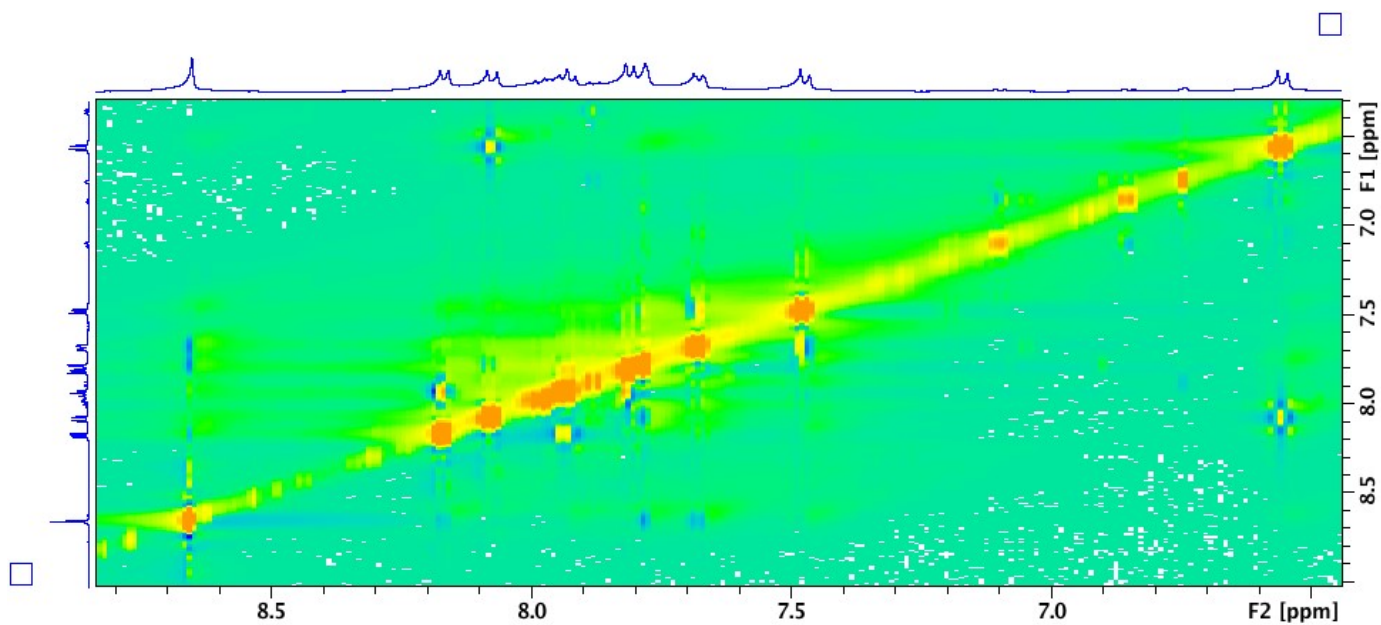


Figure S.I.22. NOESY NMR spectra for compound L_{Cuma} (DMSO-d6).

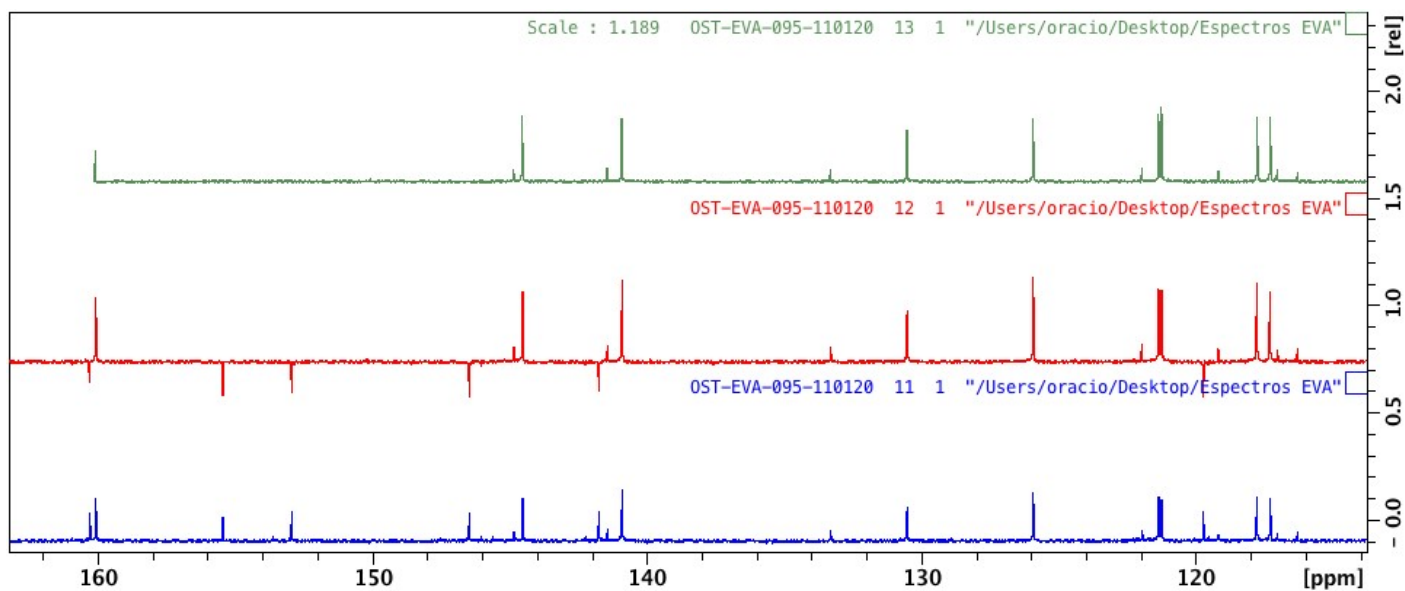


Figure S.I.23. Comparative of $^{13}\text{C}\{^1\text{H}\}$ (blue), APT (red) and DEPT (green) spectrum of compound L_{Cuma} .

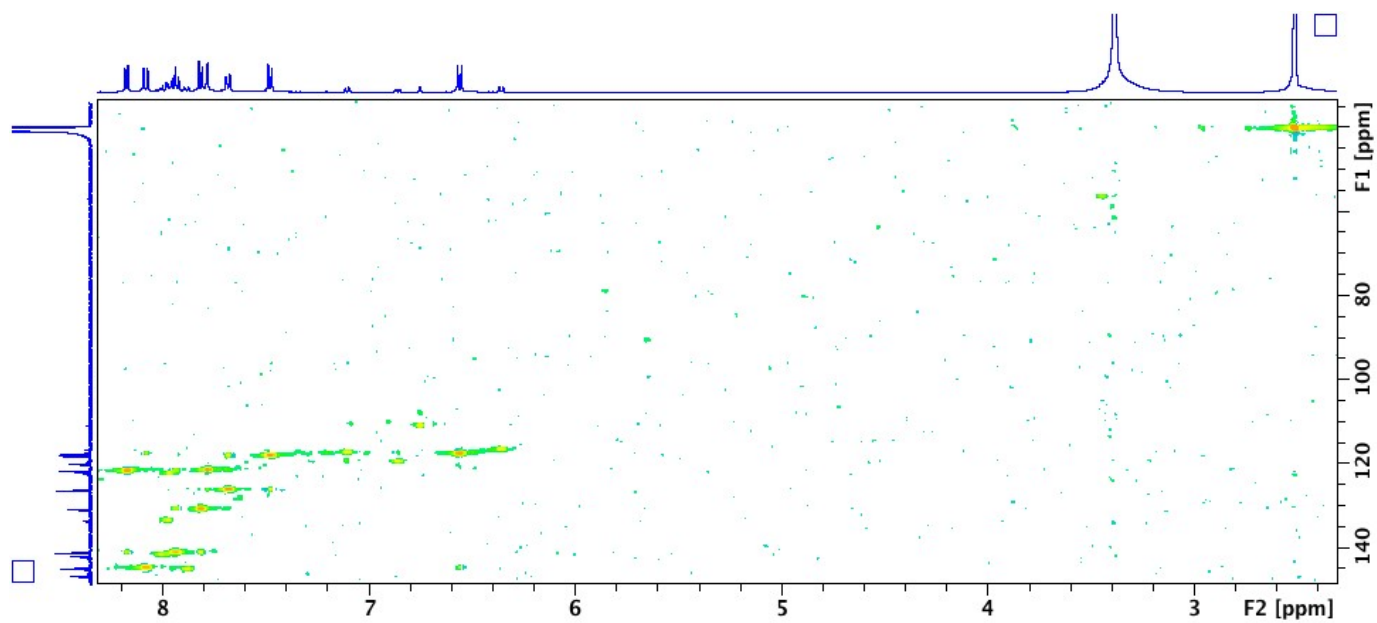


Figure S.I.24. HSQC NMR spectra for compound L_{Cuma} (DMSO-d6).

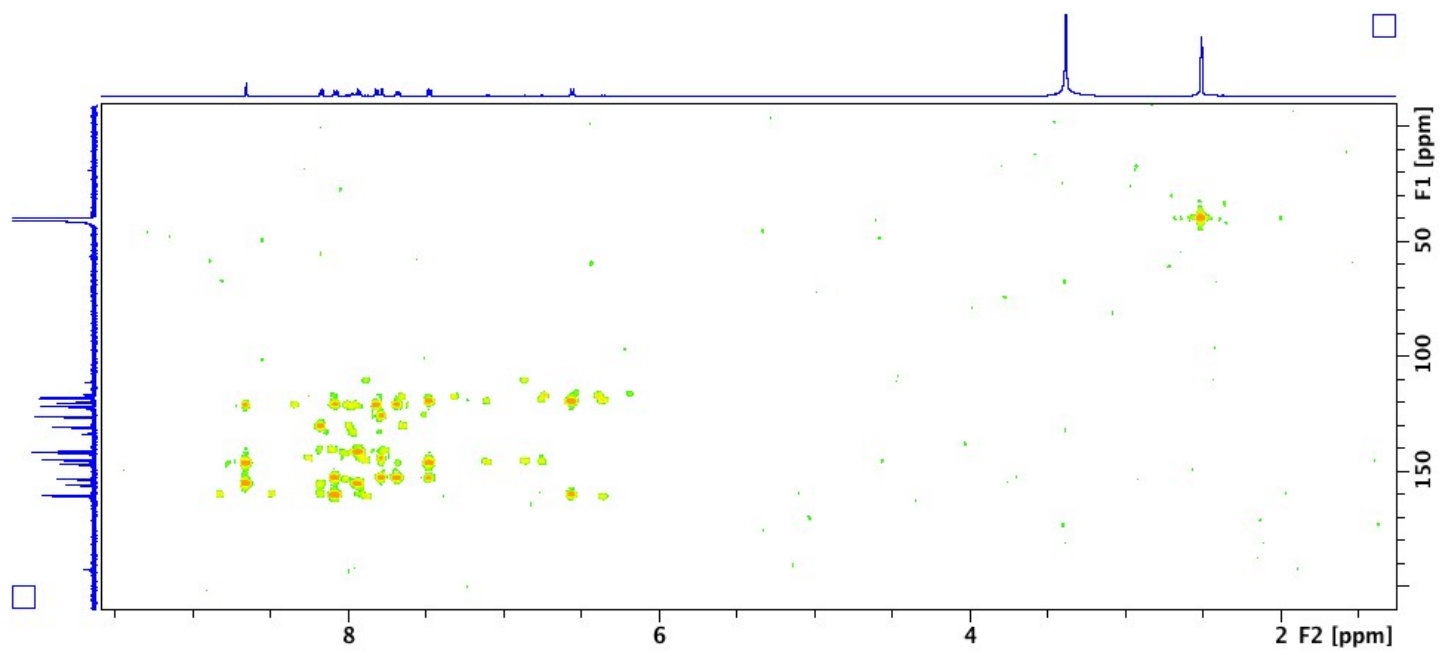
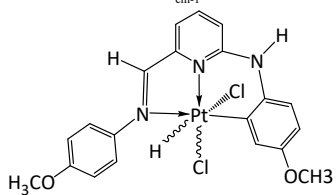
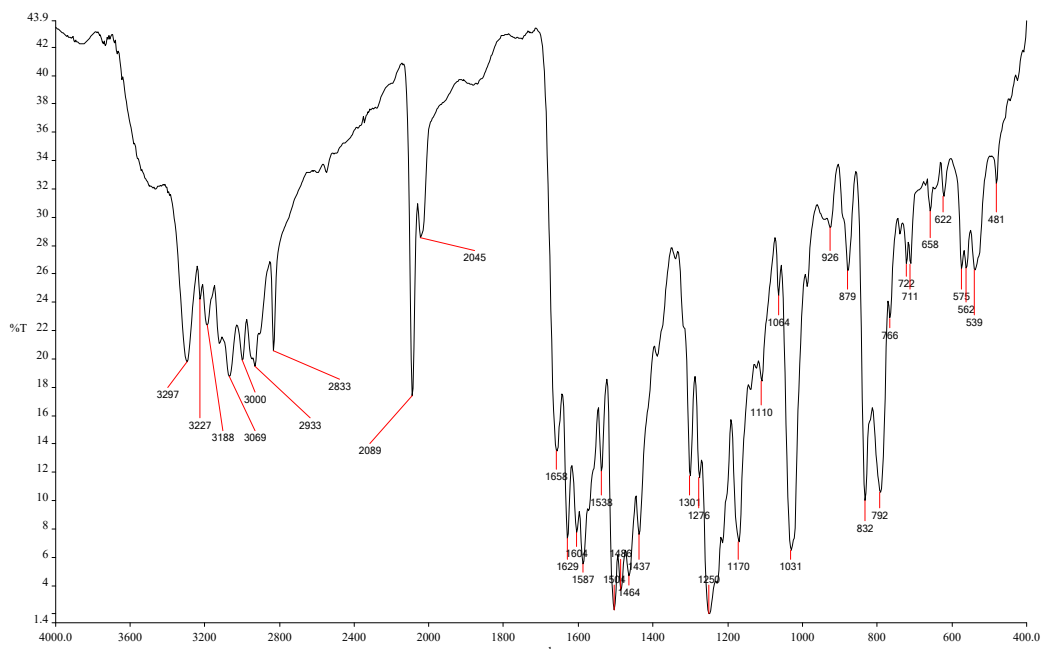
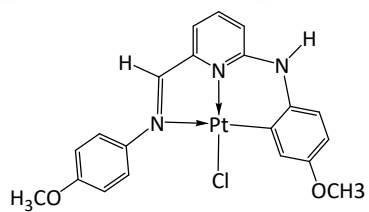
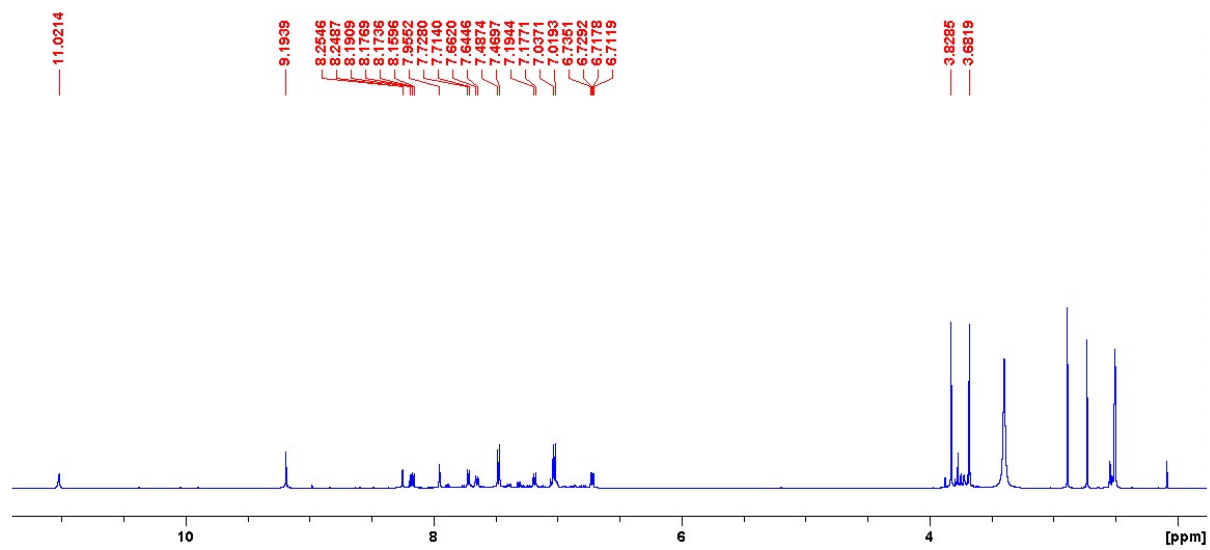


Figure S.I.25. HMBC NMR spectra for compound L_{Cuma} (DMSO-d6).



1b

Figure S.I.26. IR spectra for compound **1b** (KBr disk).



1

Figure S.I.27. ¹H NMR spectra for compound 1.

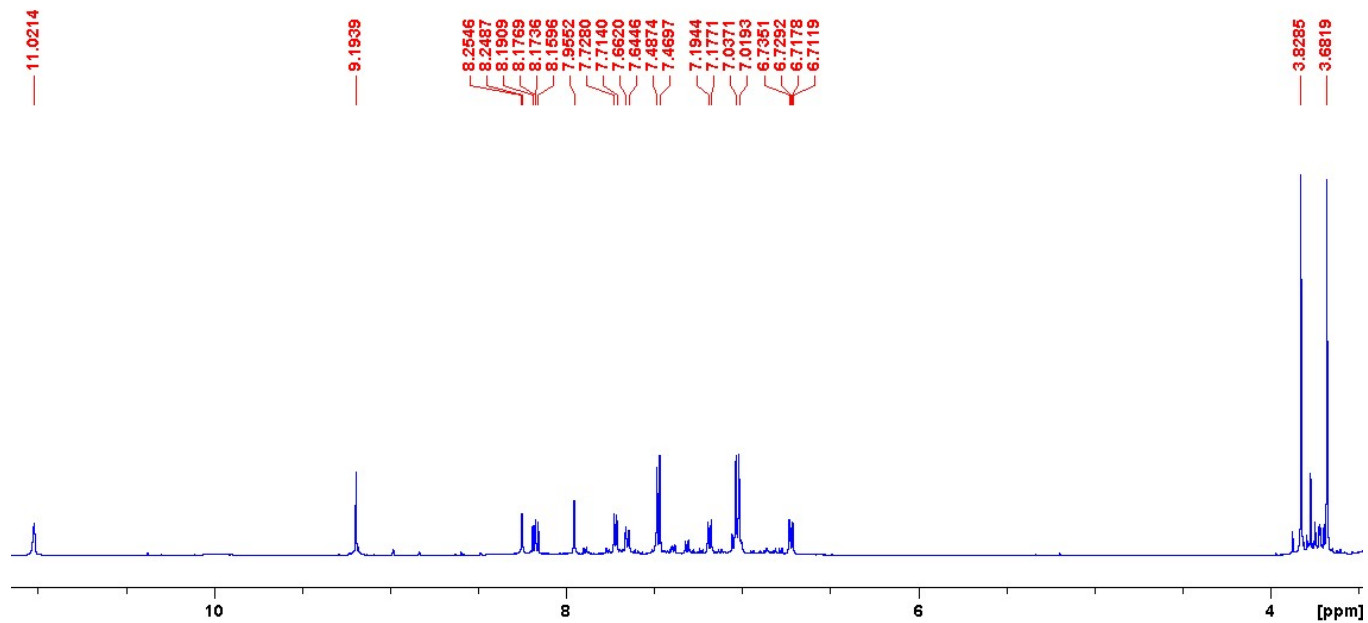


Figure S.I.28. ^1H NMR spectra for compound 1 (Region from 3.5 to 11.2 ppm).

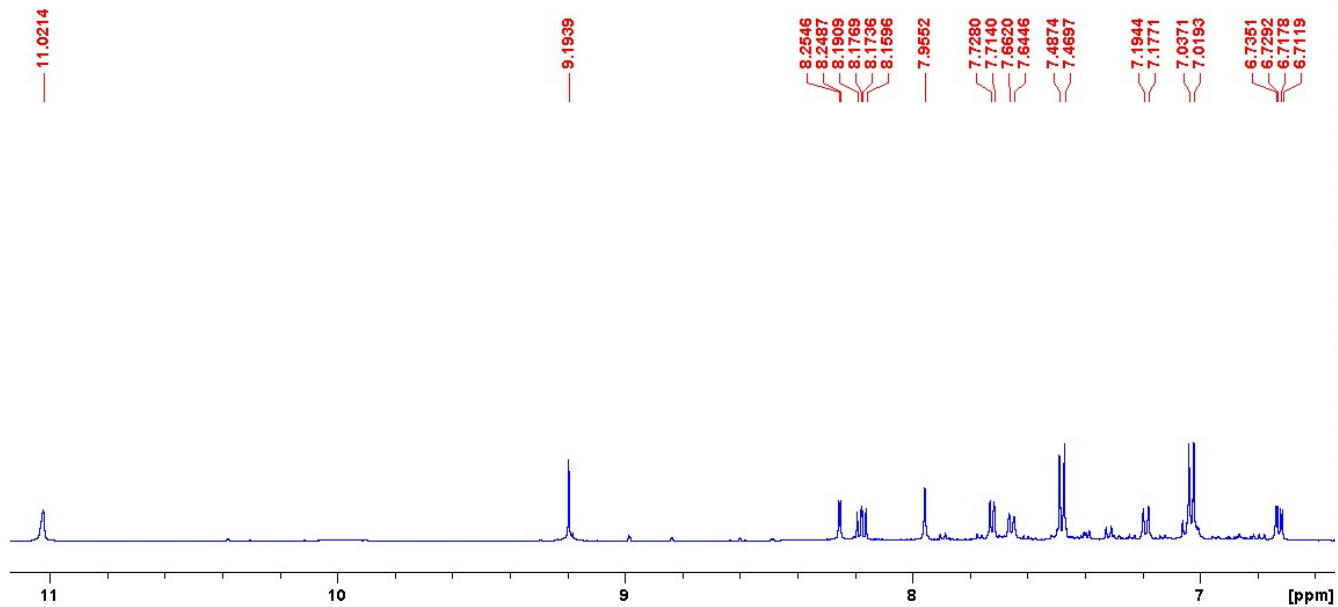


Figure S.I.29. ¹H NMR spectra for compound 1 (Region from 6.5 to 11.2 ppm).

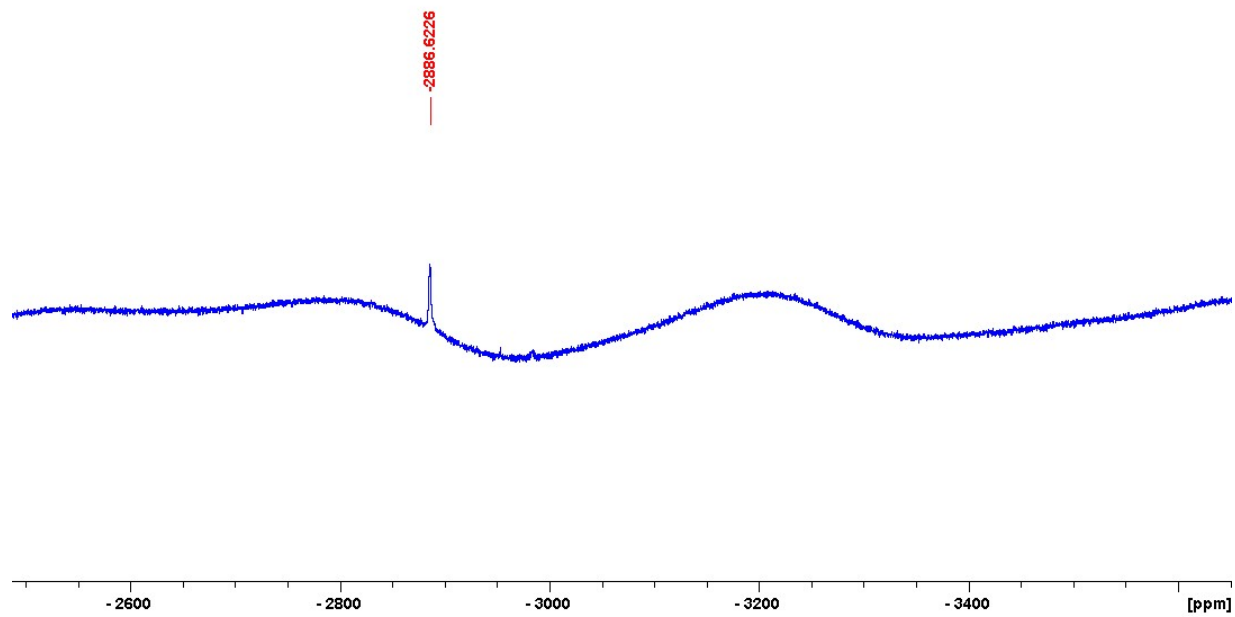


Figure S.I.30. ^{195}Pt NMR spectra for compound 1.

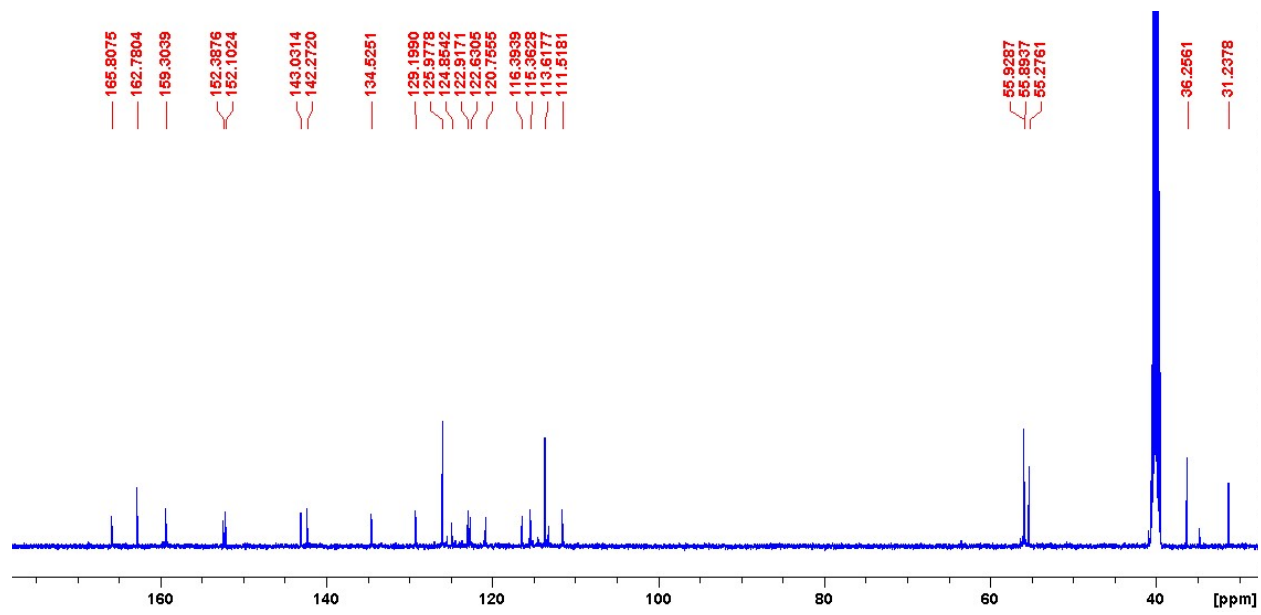


Figure S.I.31. $^{13}\text{C}\{^1\text{H}\}$ NMR spectra for compound **1**.

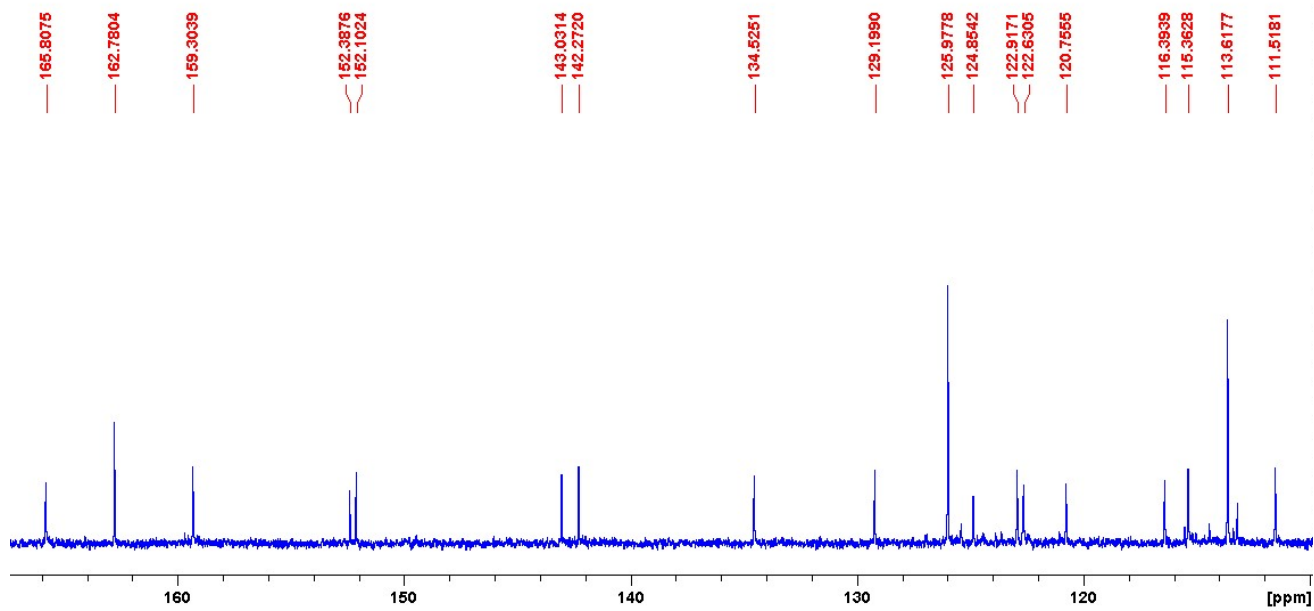


Figure S.I.32. $^{13}\text{C}\{^1\text{H}\}$ NMR spectra for compound 1 (Region from 110 to 168 ppm).

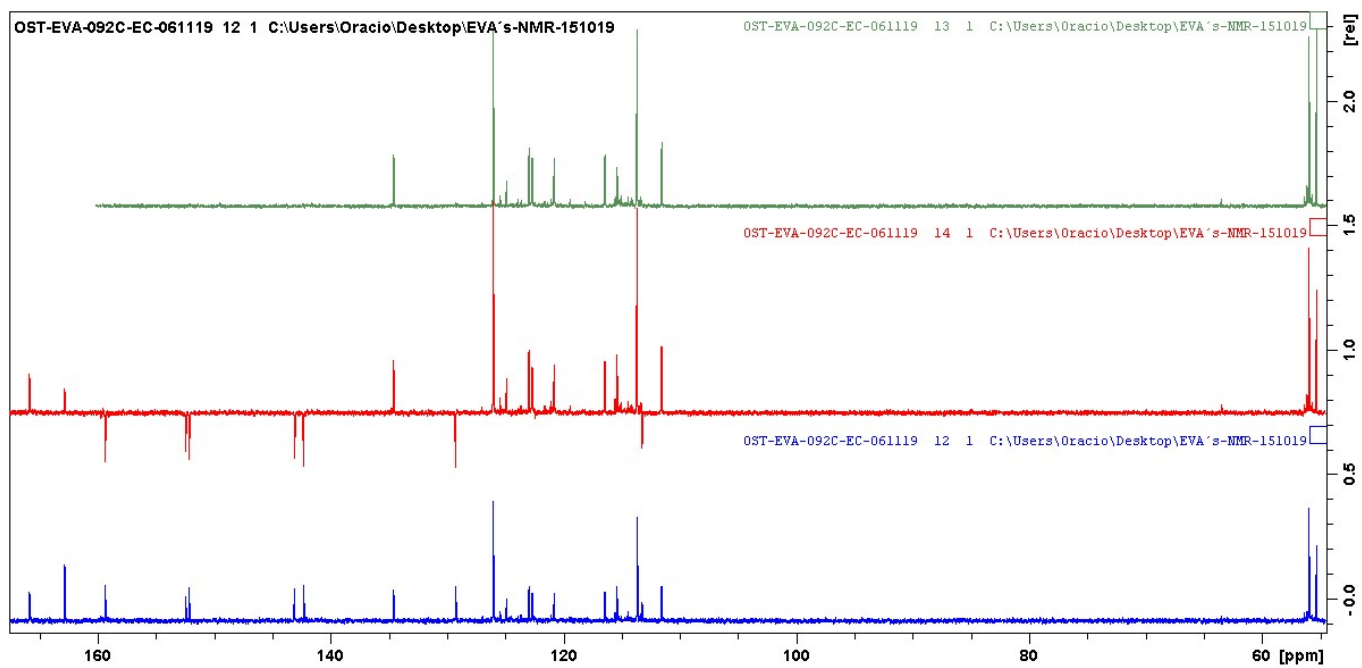


Figure S.I.33. Comparative of $^{13}\text{C}\{^1\text{H}\}$ (blue), APT (red) and DEPT (green) spectrum of compound **1**.

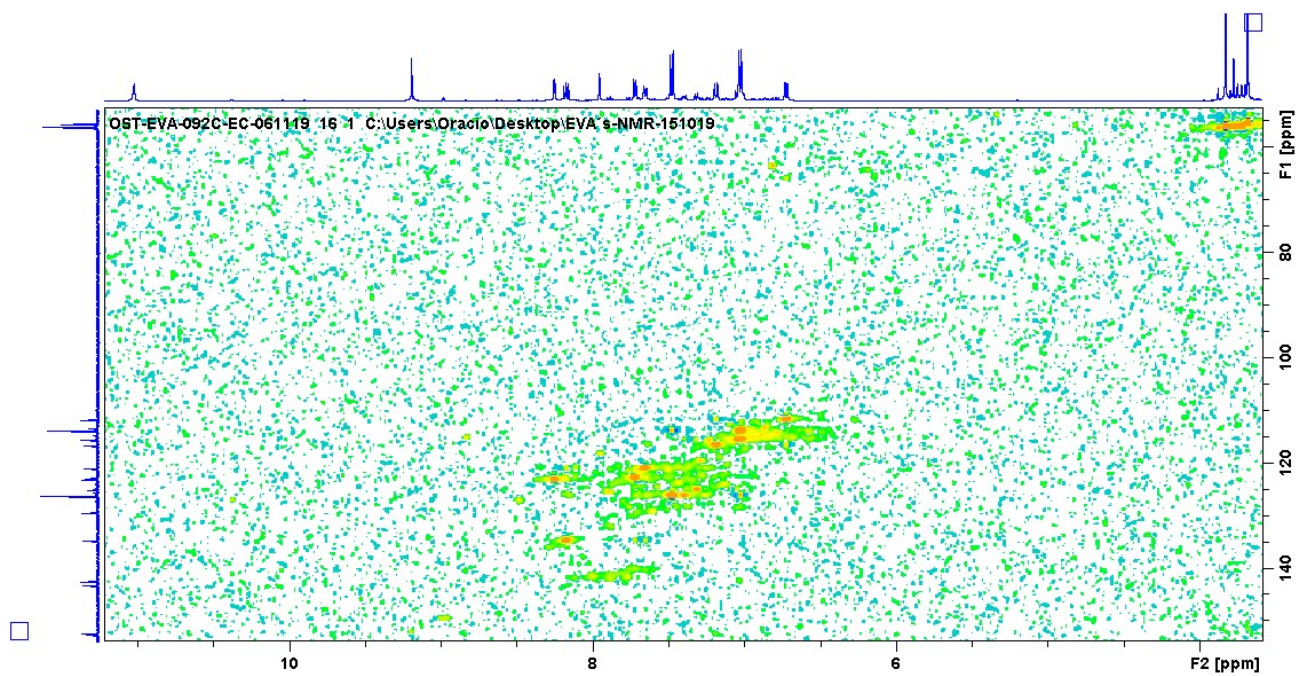


Figure S.I.34. HSQC NMR spectra for compound 1.

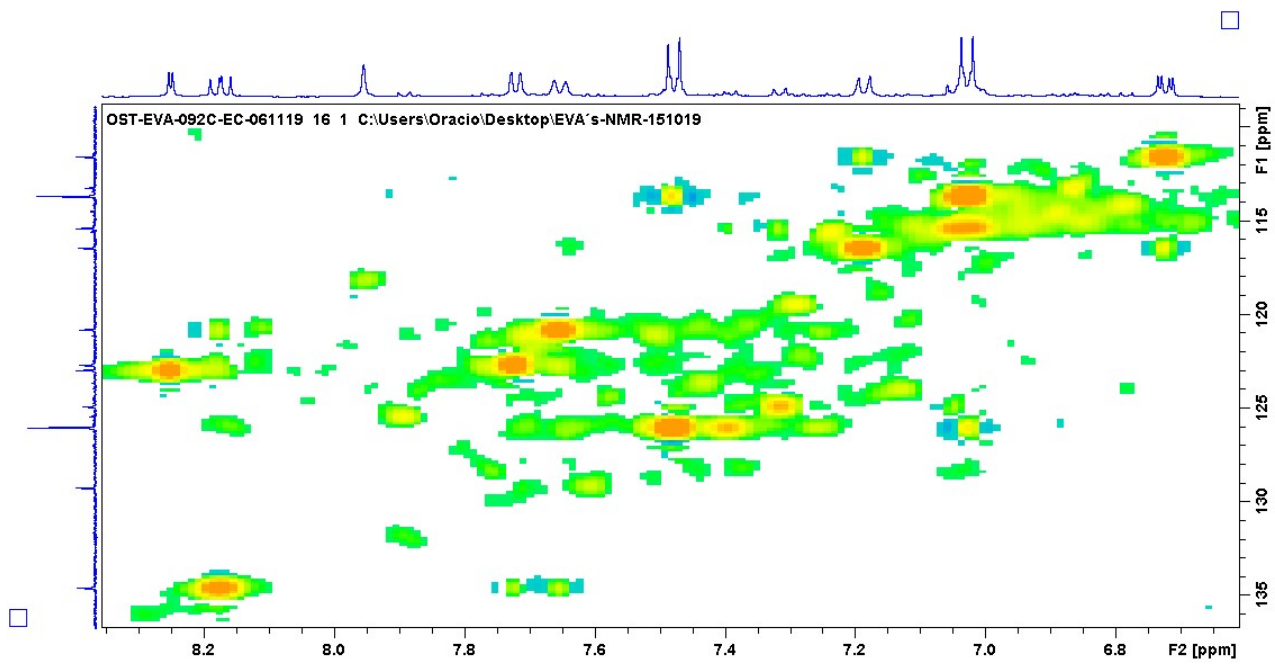


Figure S.I.35. HSQC NMR spectra for compound 1 (Region of aromatics).

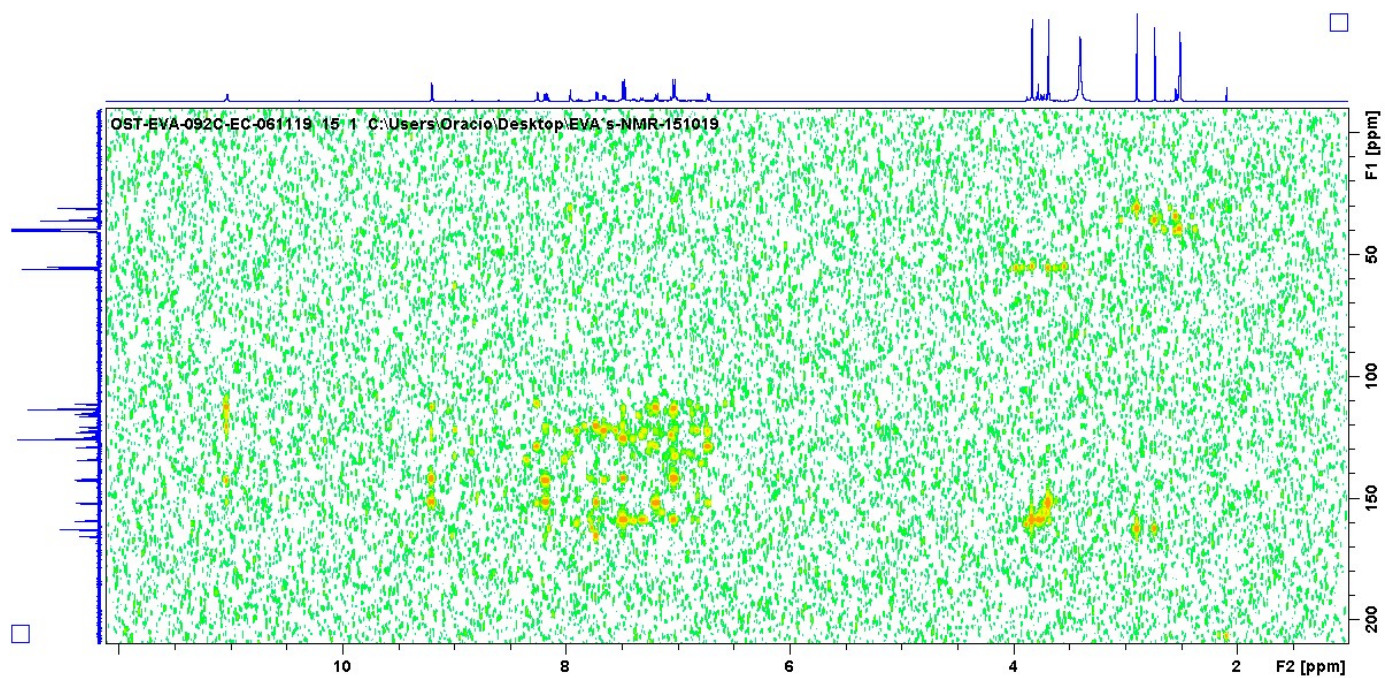
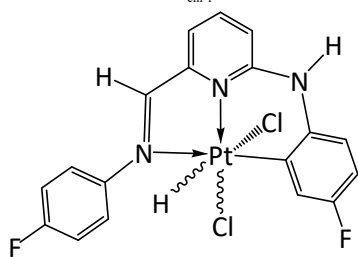
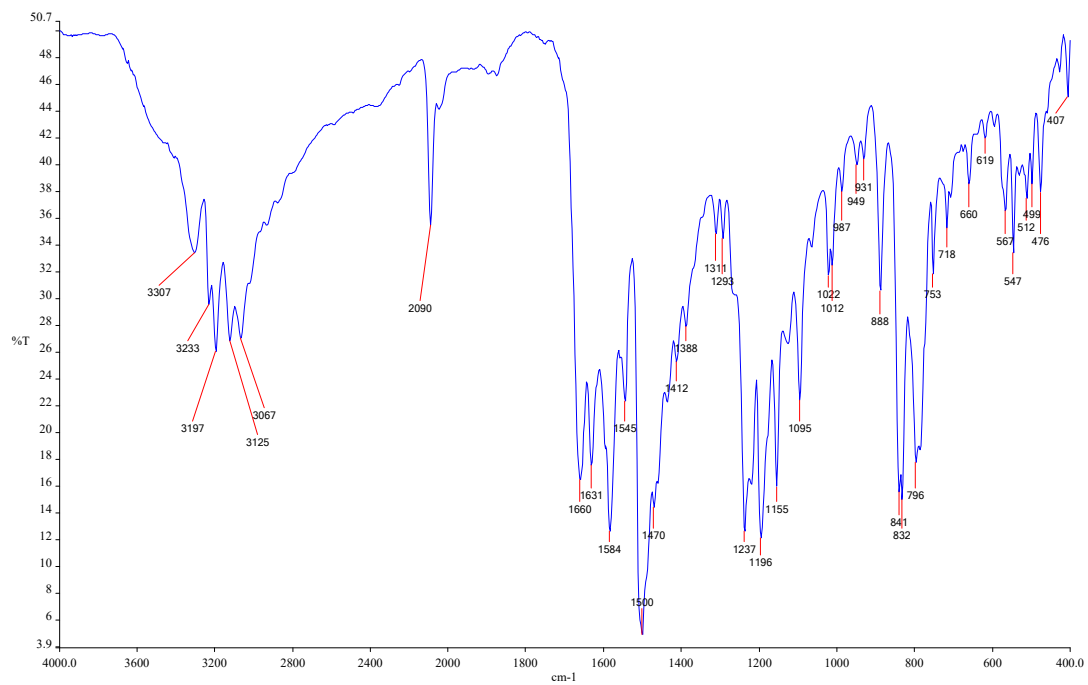


Figure S.I.36. HMBC NMR spectra for compound 1.



2b

Figure S.I.37. IR spectra for compound 2a (KBr disk).

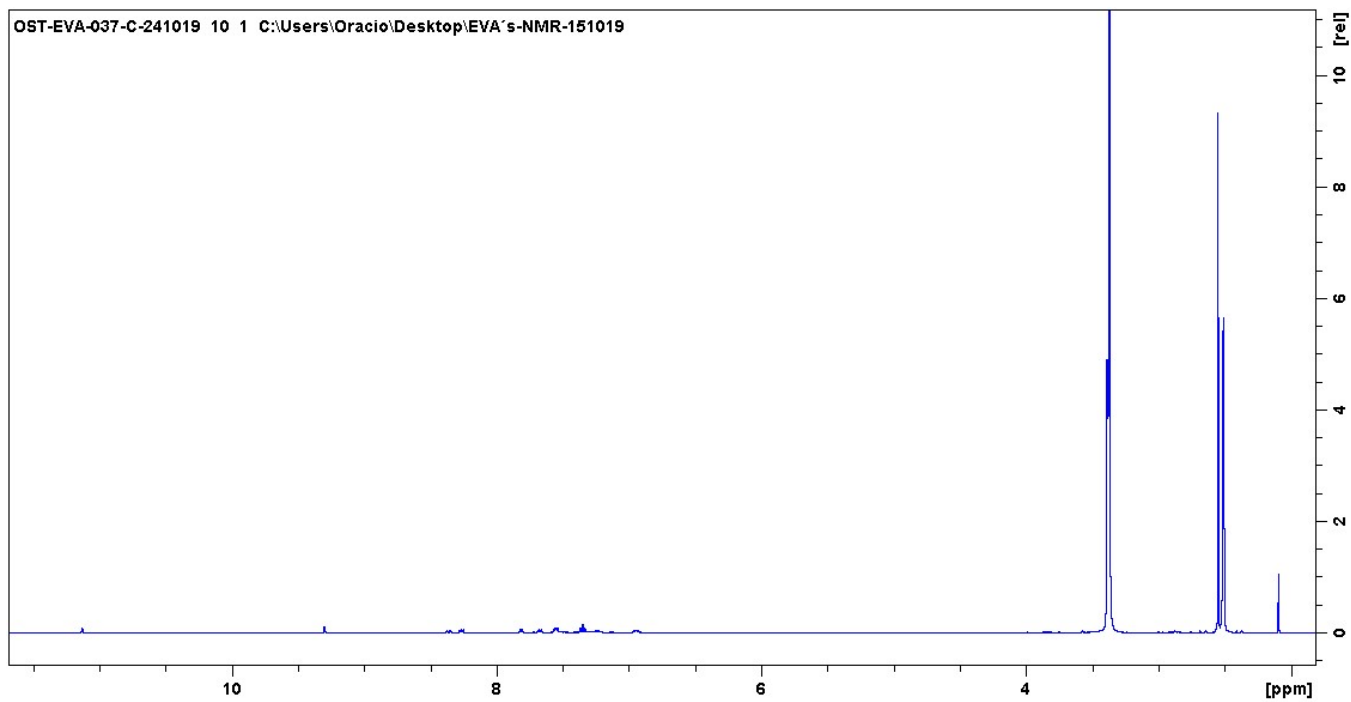


Figure S.I.38. ¹H NMR spectra for compound **2** (DMSO-d₆).

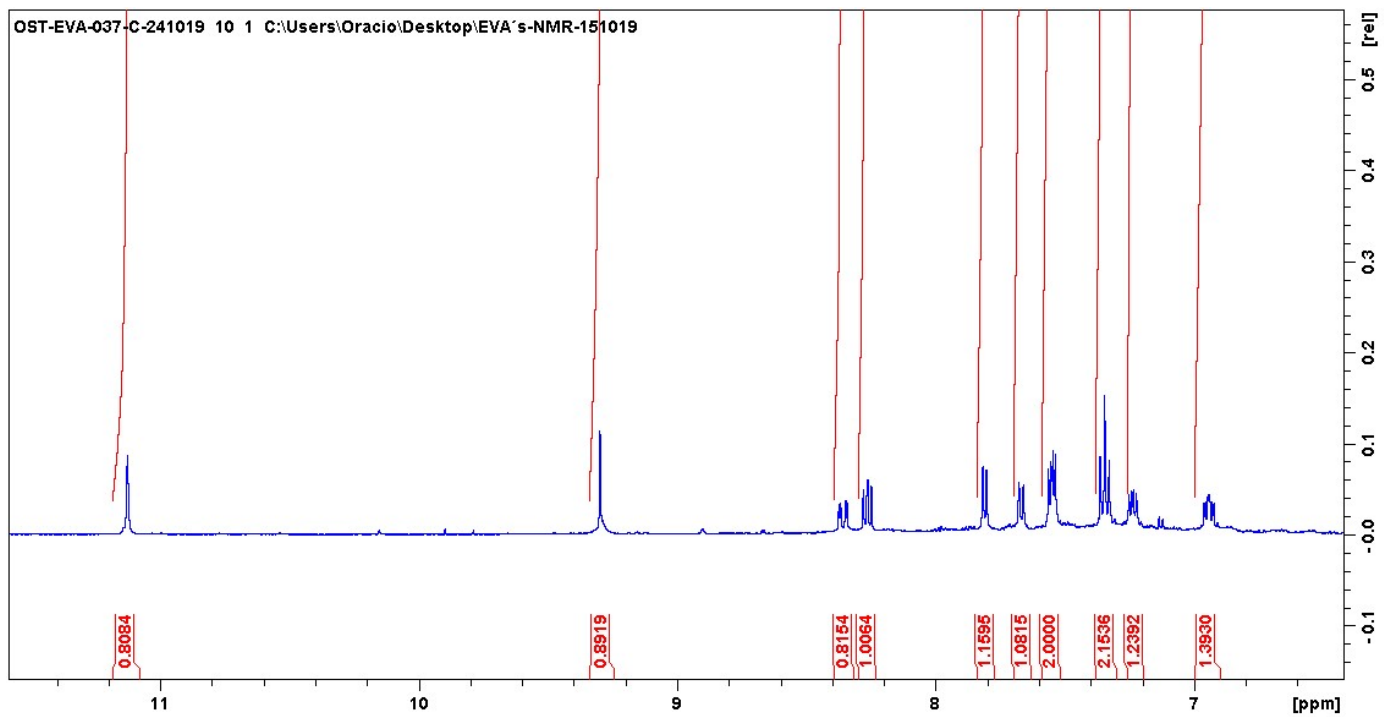


Figure S.I.39. ^1H NMR spectra for compound **2** (DMSO-d_6 , region from 6.6 to 11.6 ppm).

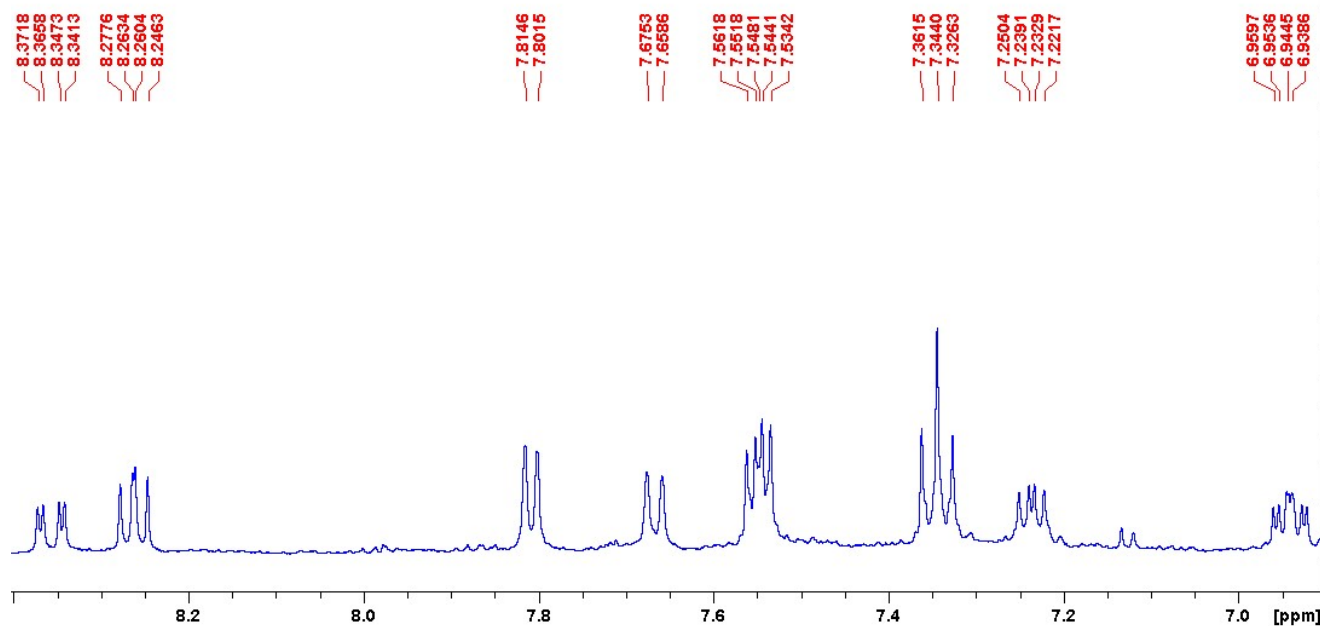


Figure S.I.40. ¹H NMR spectra for compound 2 (DMSO-d₆, region from 6.8 to 8.4 ppm).

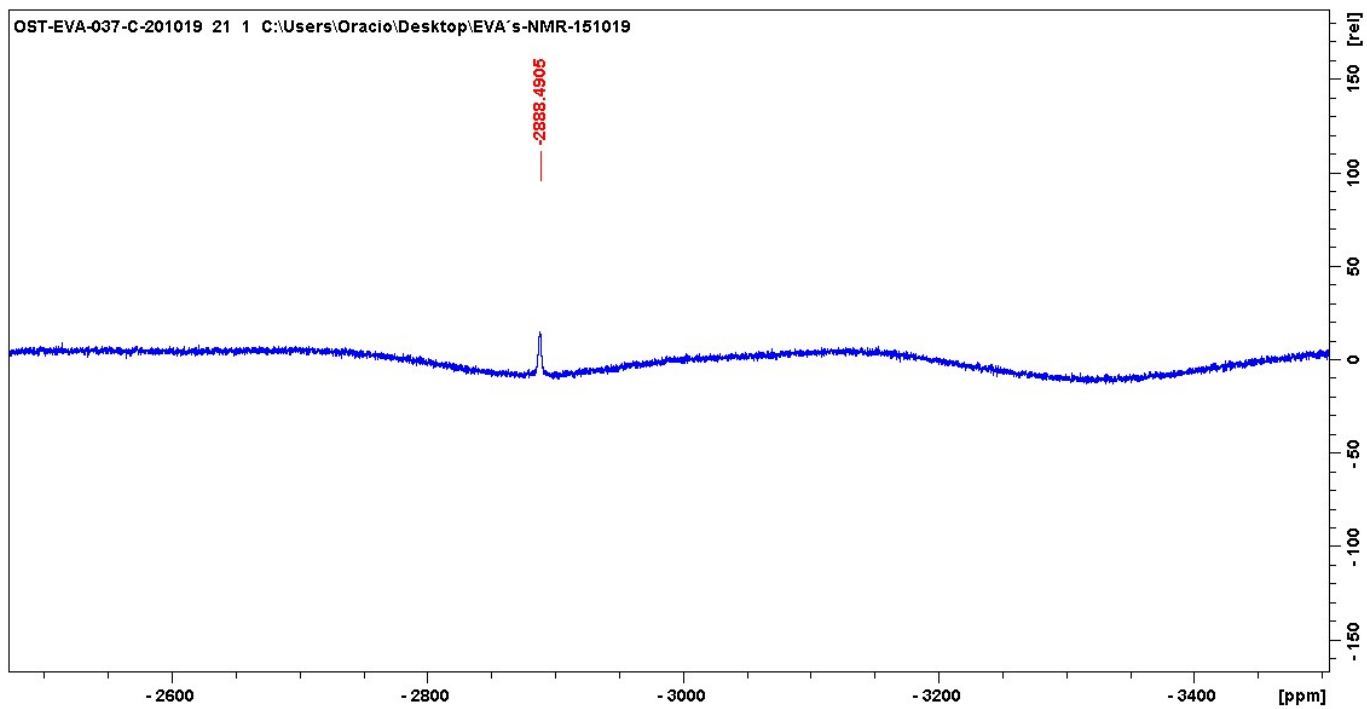


Figure S.I.41. ^{195}Pt NMR spectra for compound **2** (DMSO- d_6).

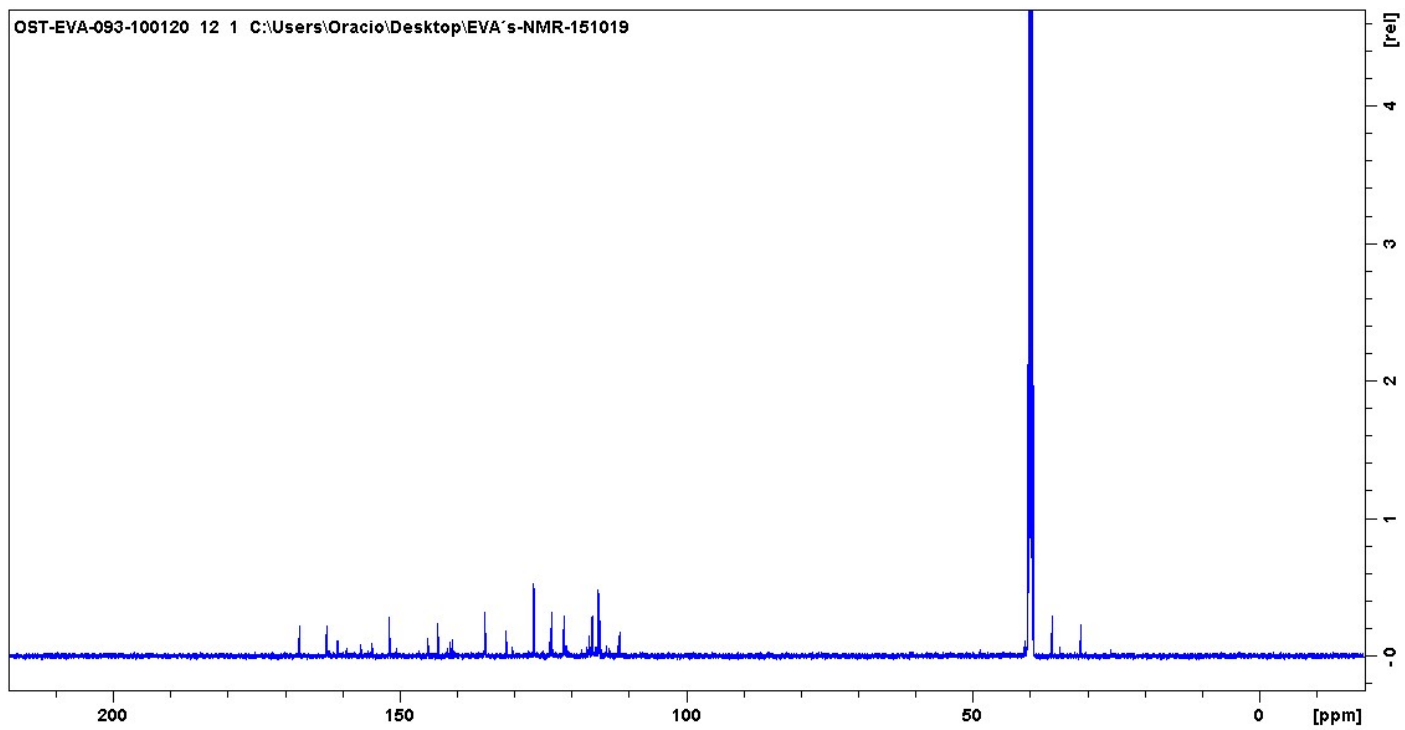


Figure S.I.42. $^{13}\text{C}\{^1\text{H}\}$ NMR spectra for compound **2** (DMSO- d_6).

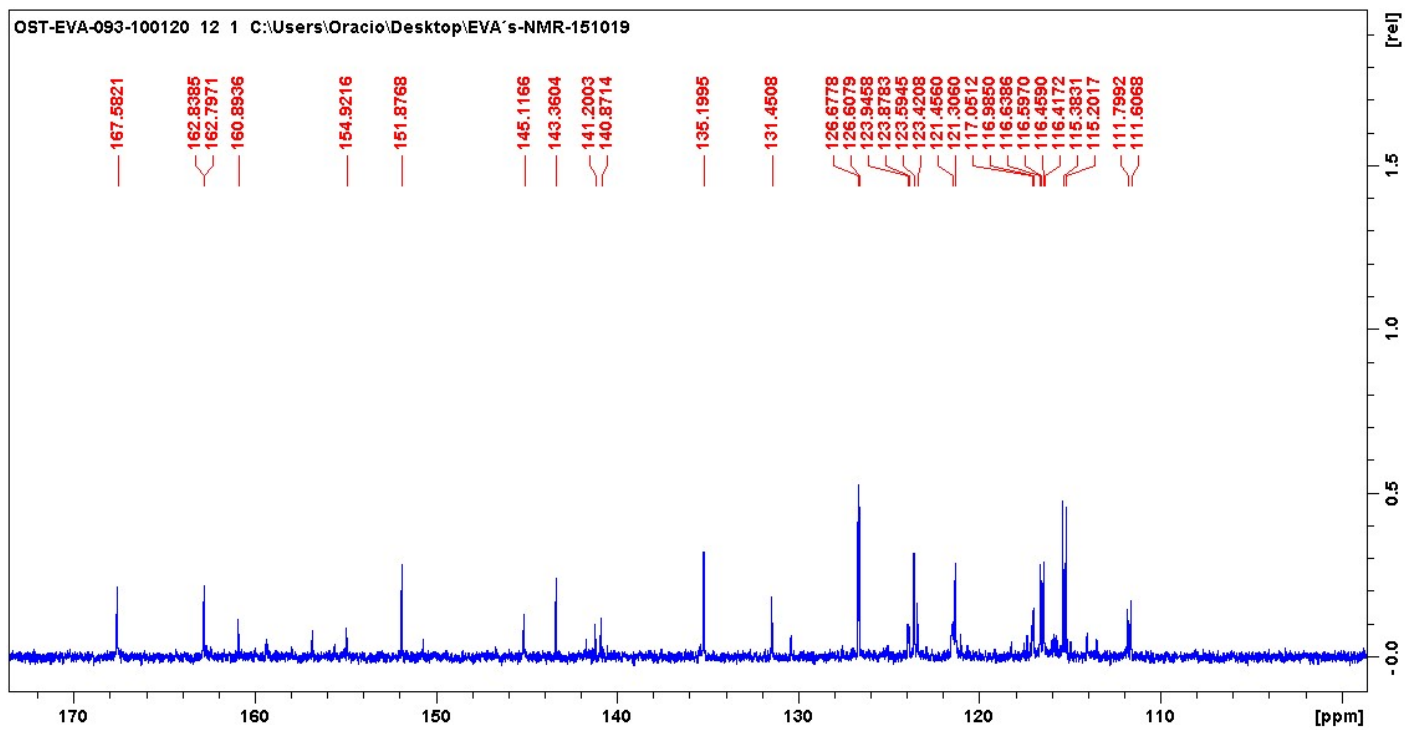


Figure S.I.43. $^{13}\text{C}\{^1\text{H}\}$ NMR spectra for compound **2** (DMSO- d_6 , Region from 100 to 172 ppm).

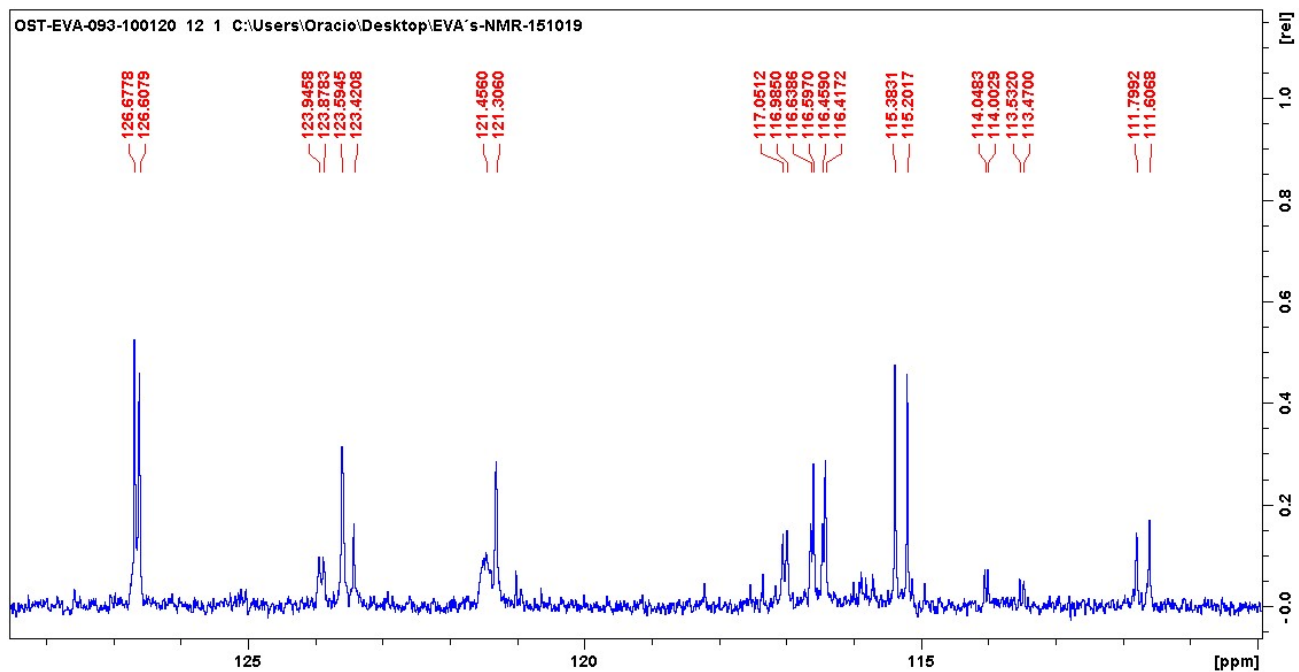


Figure S.I.44. $^{13}\text{C}\{^1\text{H}\}$ NMR spectra for compound **2** (DMSO- d_6 , region from 110 to 129 ppm).

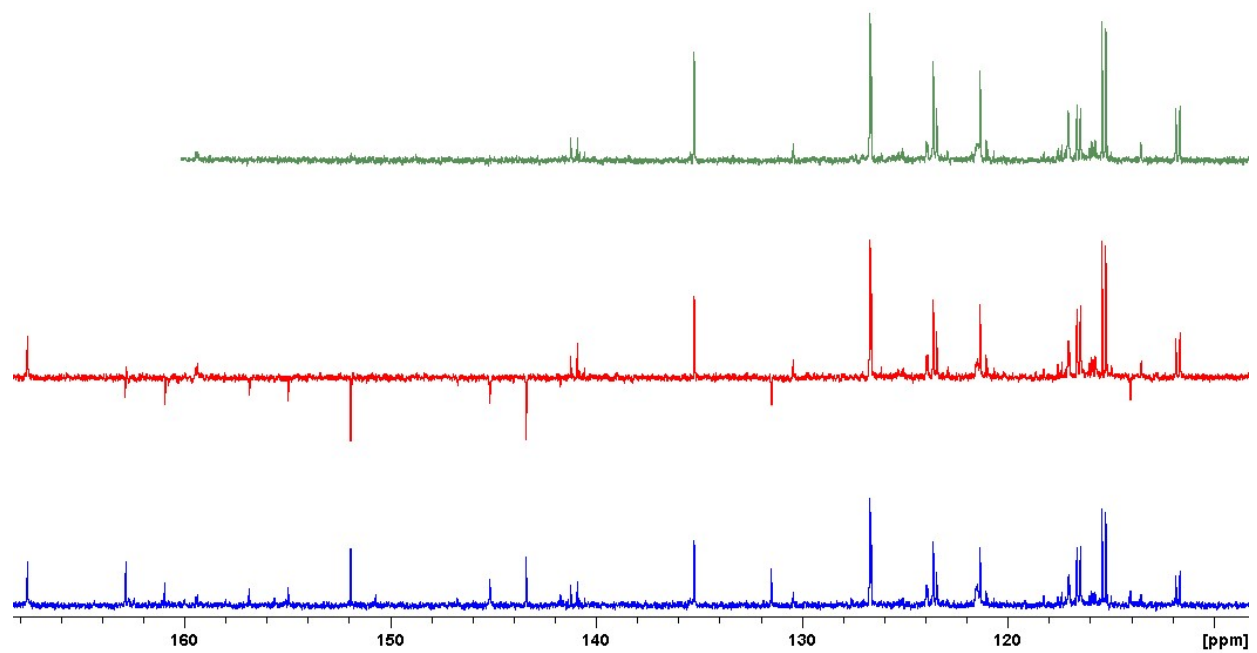


Figure S.I.45. Comparative of ¹³C{¹H} (blue), APT (red) and DEPT (green) spectrum of compound 2 (DMSO-d₆).

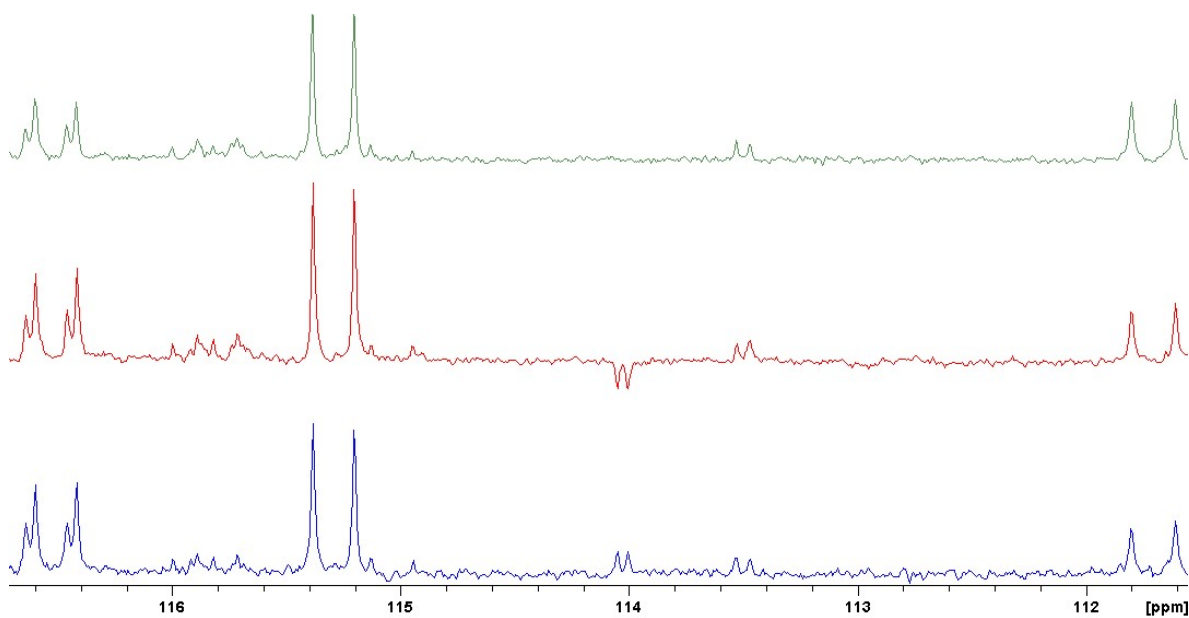


Figure S.I.46. Comparative of $^{13}\text{C}\{^1\text{H}\}$ (blue), APT (red) and DEPT (green) spectrum of compound **2** (DMSO- d_6 , region from 111.6 to 116.8 ppm).

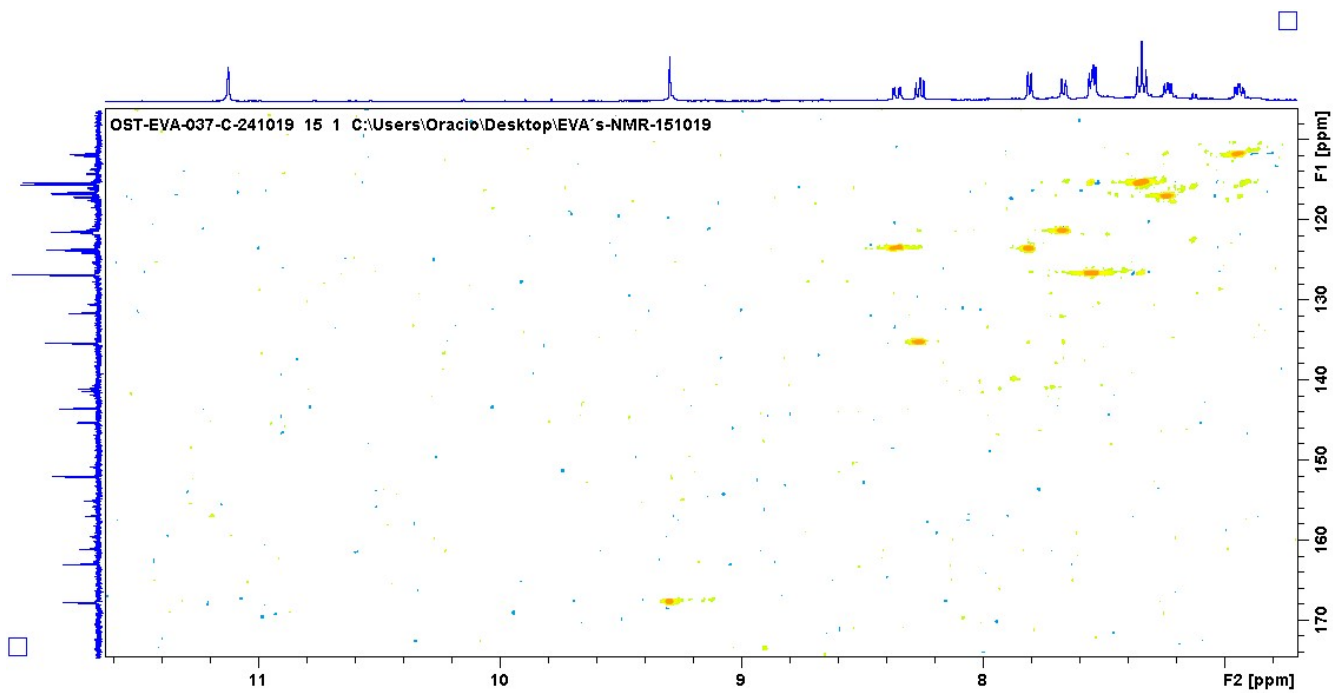


Figure S.I.47. HSQC NMR spectra for compound **2** (DMSO- d_6).

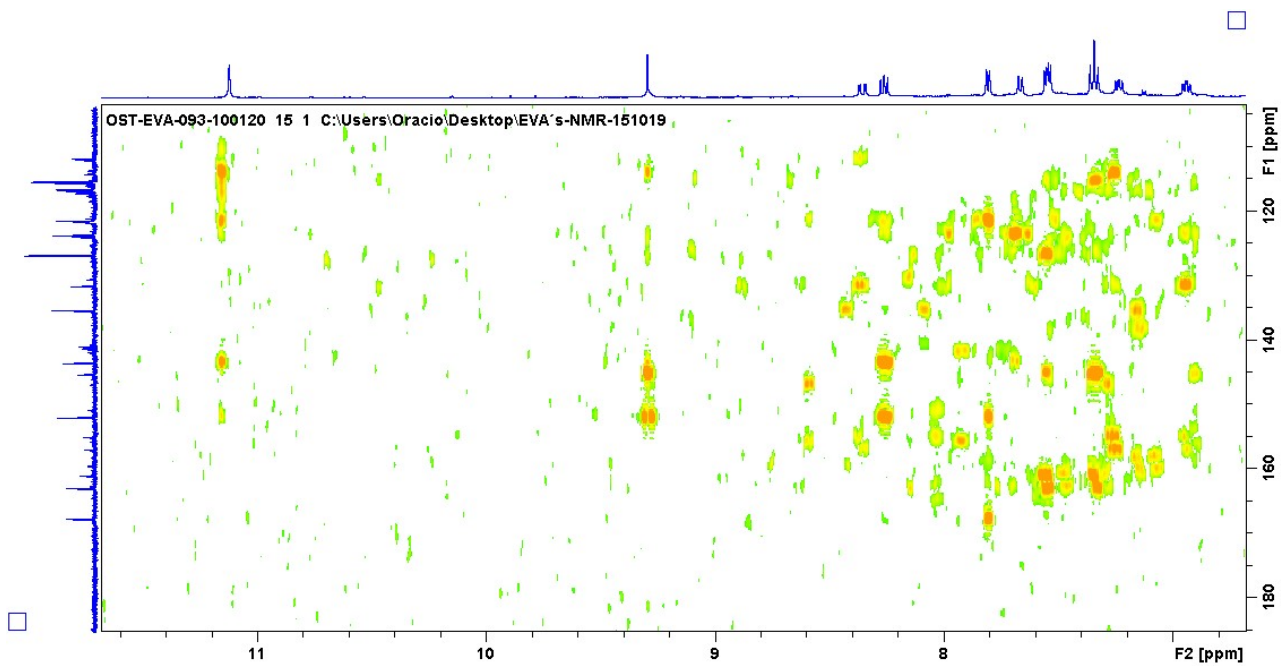


Figure S.I.48. HSQC NMR spectra for compound **2** (DMSO- d_6 , region of aromatics).

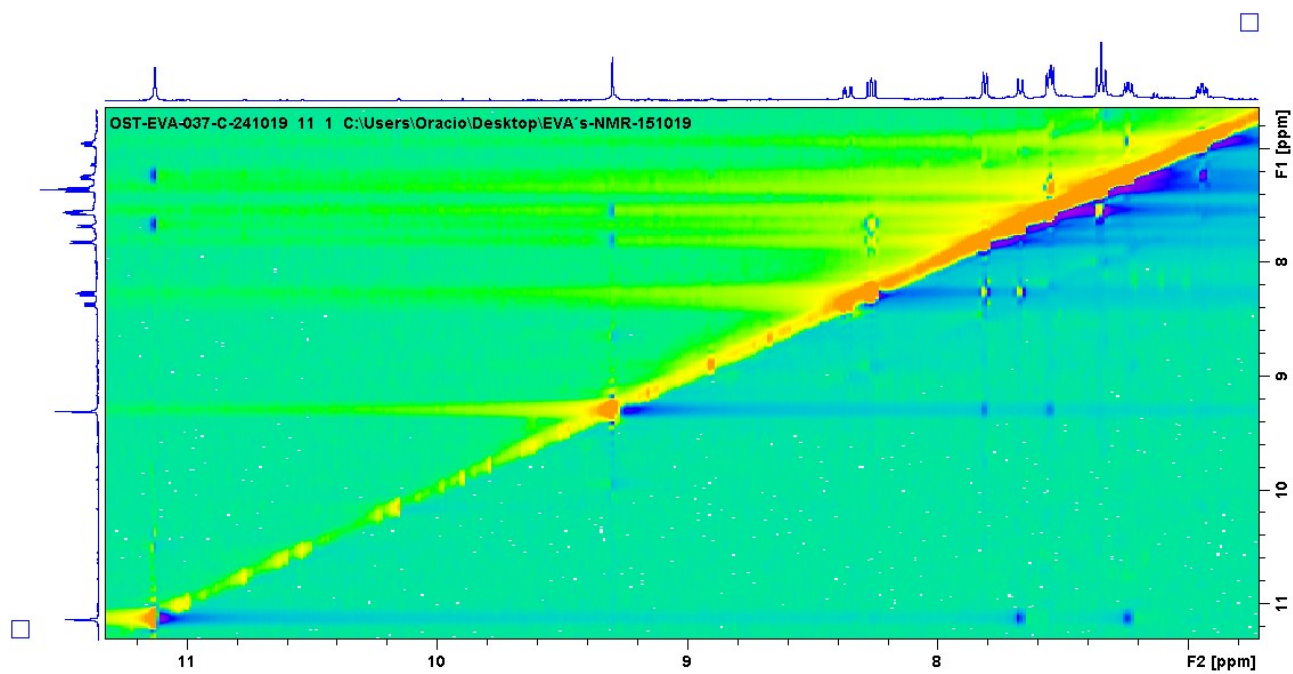


Figure S.I.49. NOESY NMR spectra for compound 2 (DMSO-d₆).

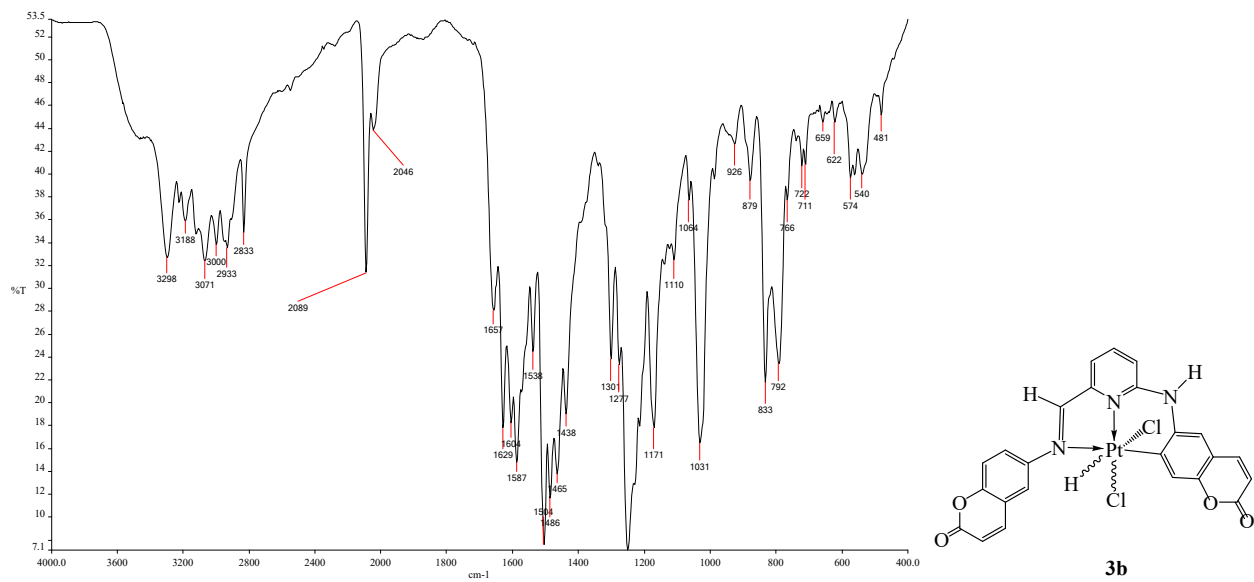


Figure S.I.50. IR spectra for compound **3b** (KBr disk).

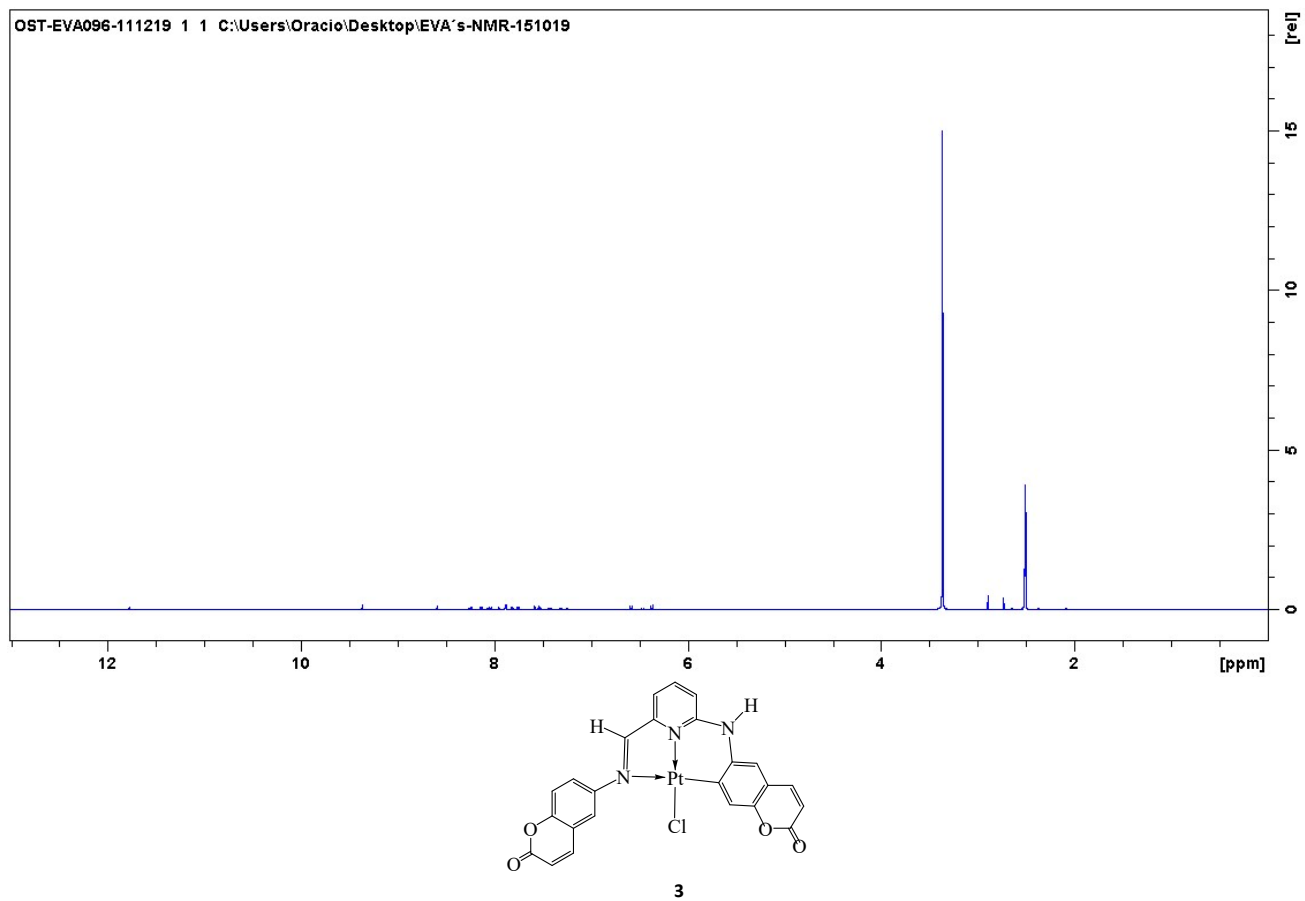


Figure S.I.51. $^{13}\text{C}\{^1\text{H}\}$ NMR spectra for compound **3** (DMSO- d_6).

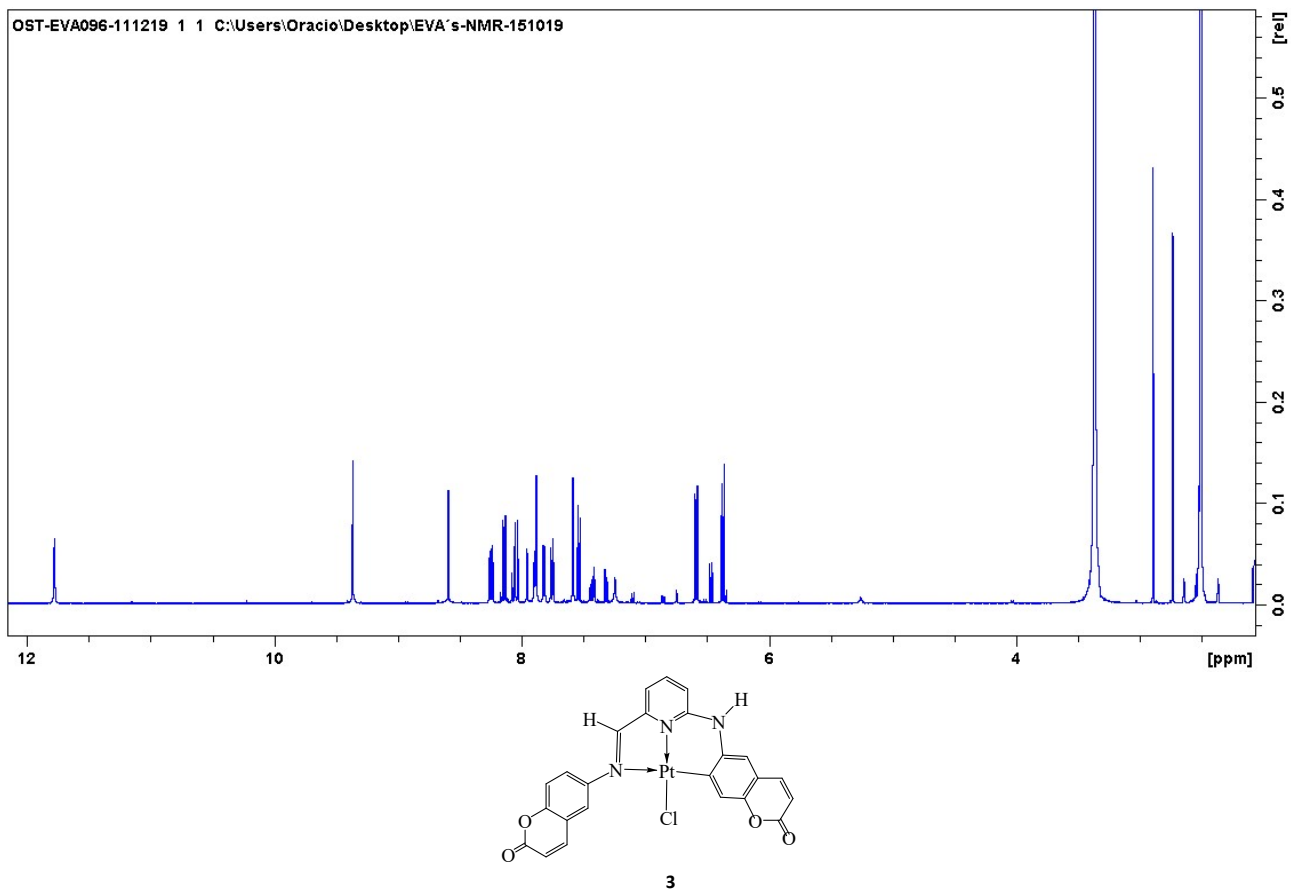


Figure S.I.52. ^1H NMR spectra for compound **3** (DMSO-d_6 , region from 3 to 12 ppm).

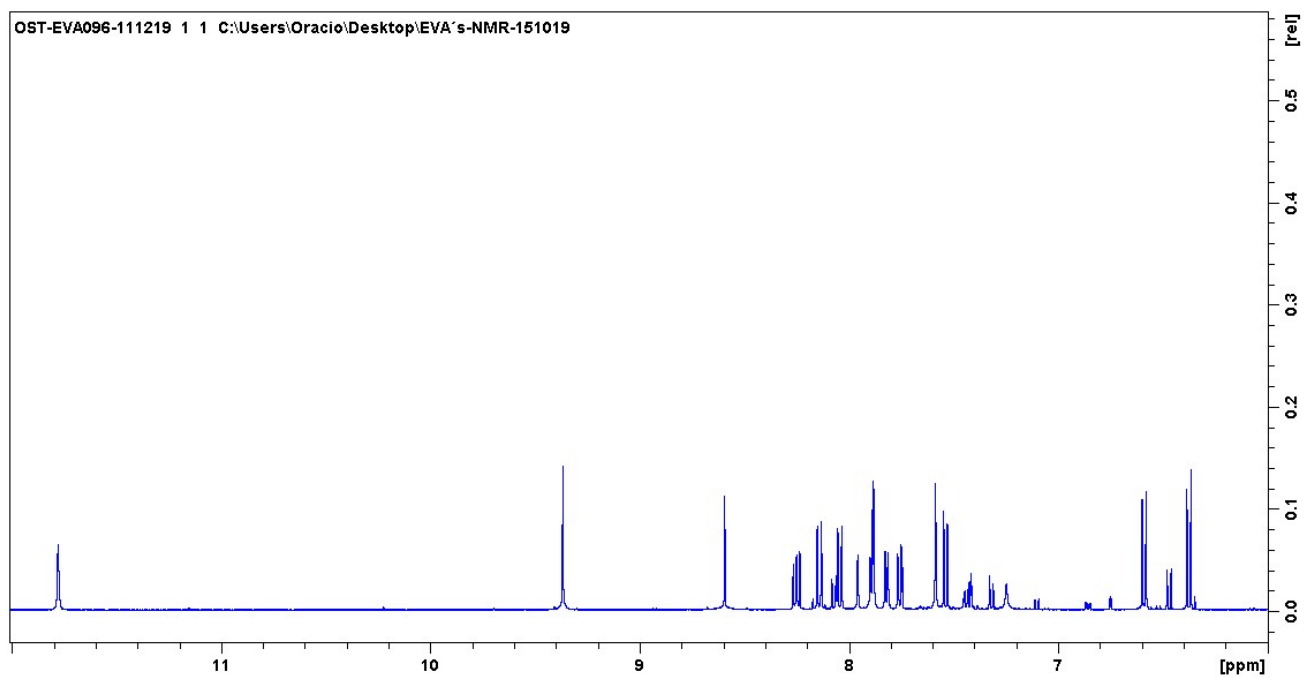


Figure S.I.53. ¹H NMR spectra for compound **3** (DMSO-d₆, region from 6 to 12 ppm).

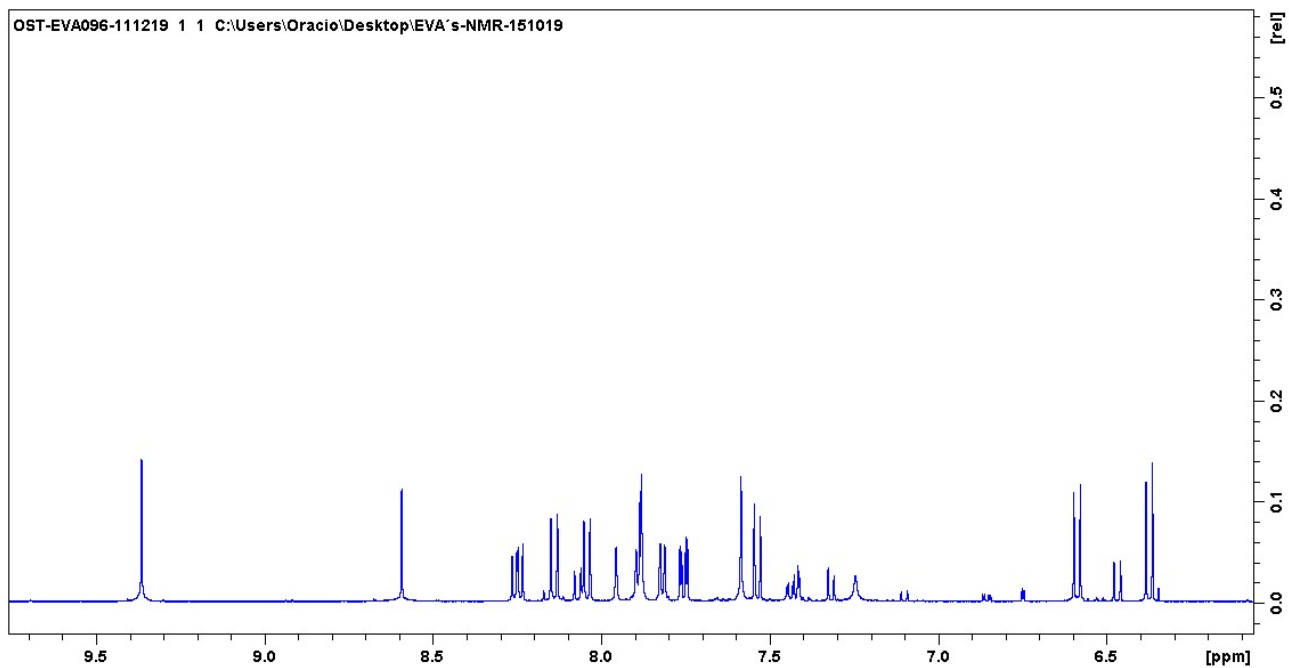


Figure S.I.54. ^1H NMR spectra for compound **3** (DMSO- d_6 , region from 6 to 10 ppm).

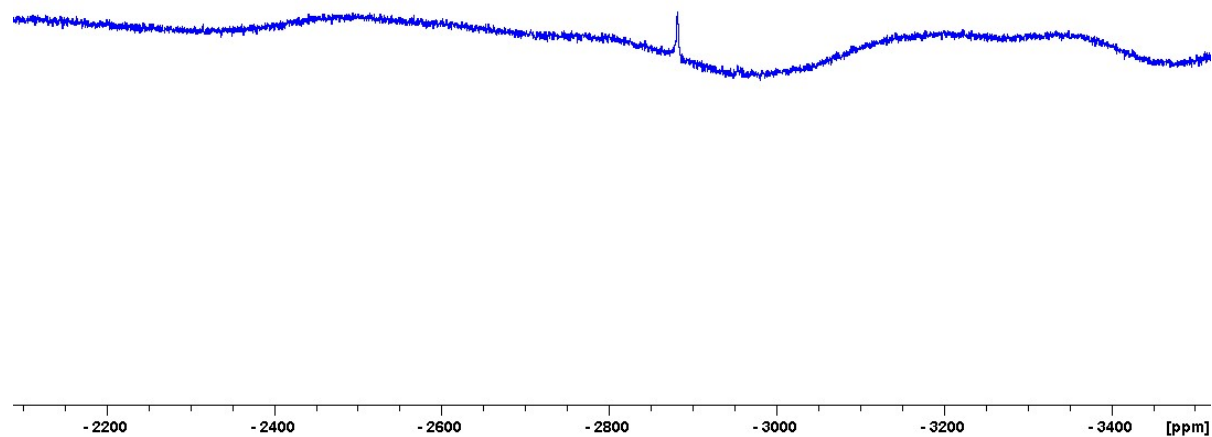


Figure S.I.55. ^{195}Pt NMR spectra for compound **3** (DMSO- d_6).

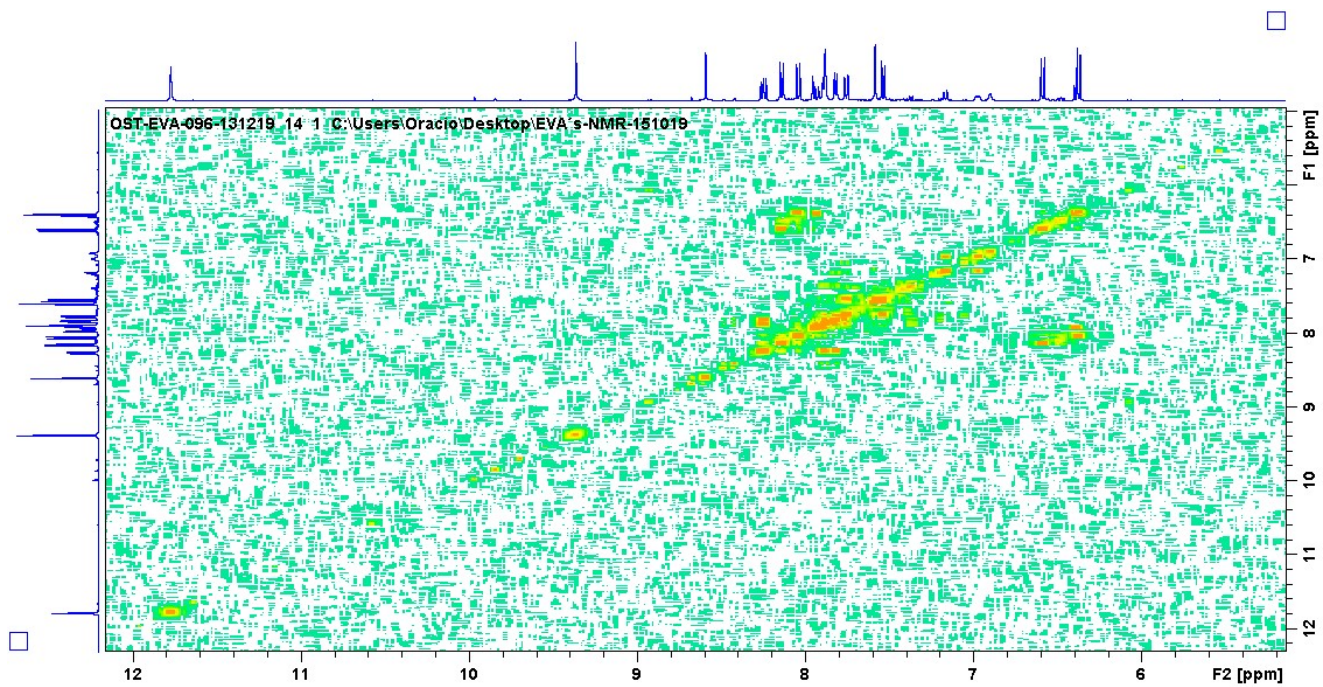


Figure S.I.56. COSY NMR spectra for compound **3** (DMSO- d_6).

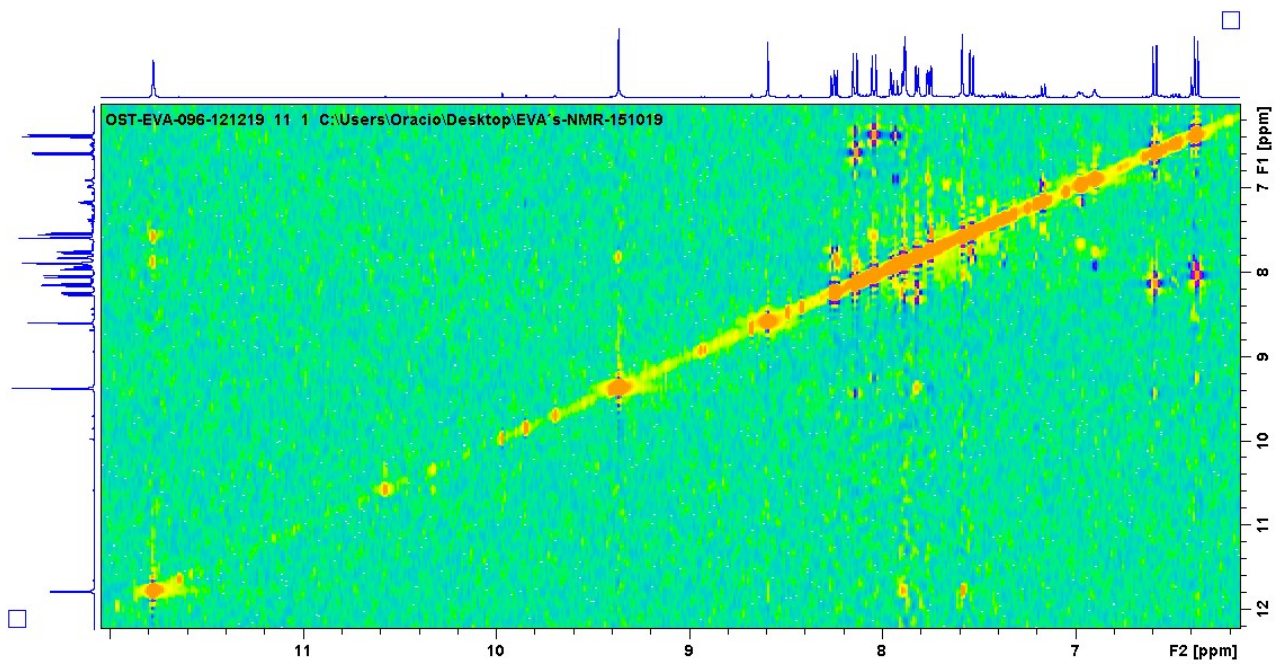


Figure S.I.57. NOESY NMR spectra for compound **3** (DMSO-d₆, region of aromatics).

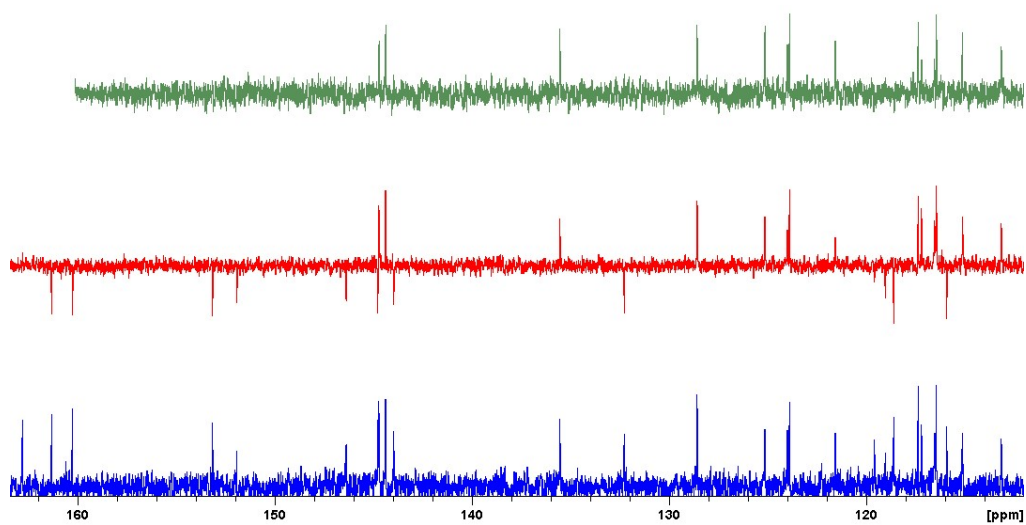


Figure S.I.58. Comparative of $^{13}\text{C}\{^1\text{H}\}$ (blue), APT (red) and DEPT (green) spectrum of compound **3** (DMSO-d_6 , region from 110 to 164 ppm).

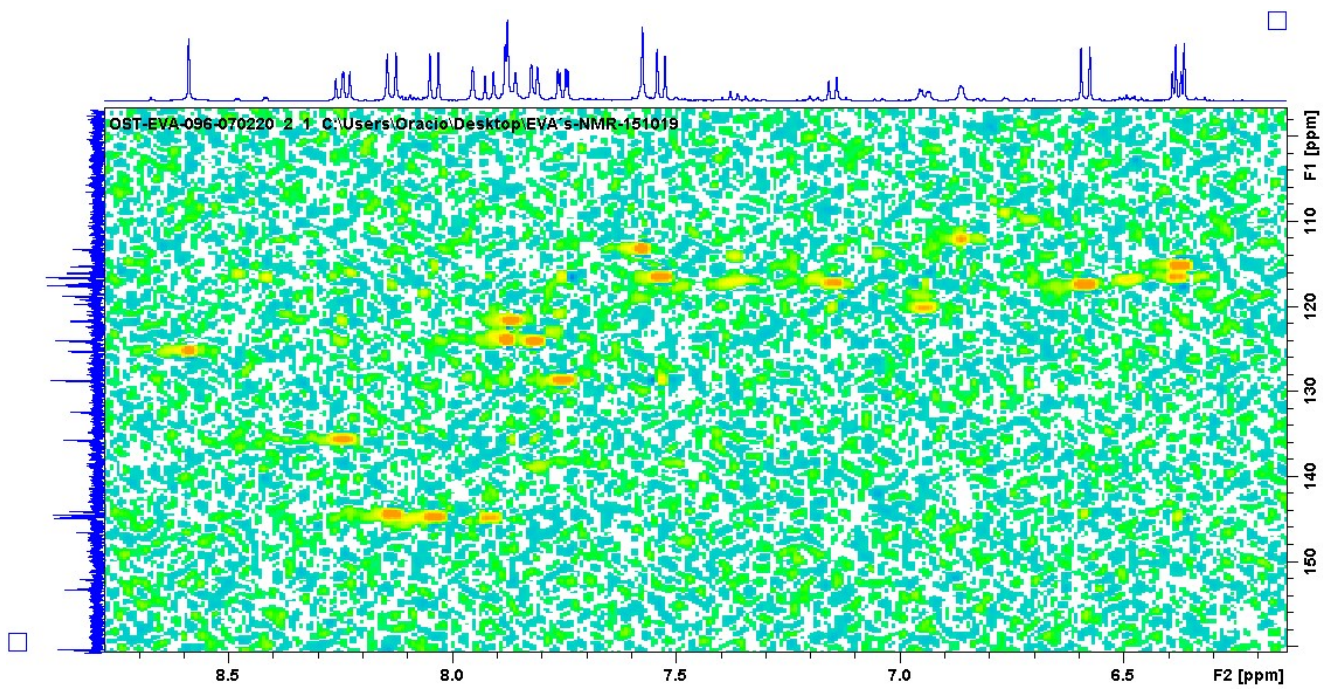


Figure S.I.59. HSQC of compound 3 (DMSO-d₆).