

Supporting Information

Iridium Corroles Exhibit Weak Near-Infrared Phosphorescence but Efficiently Sensitize Singlet Oxygen Formation

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A. UV-vis spectra

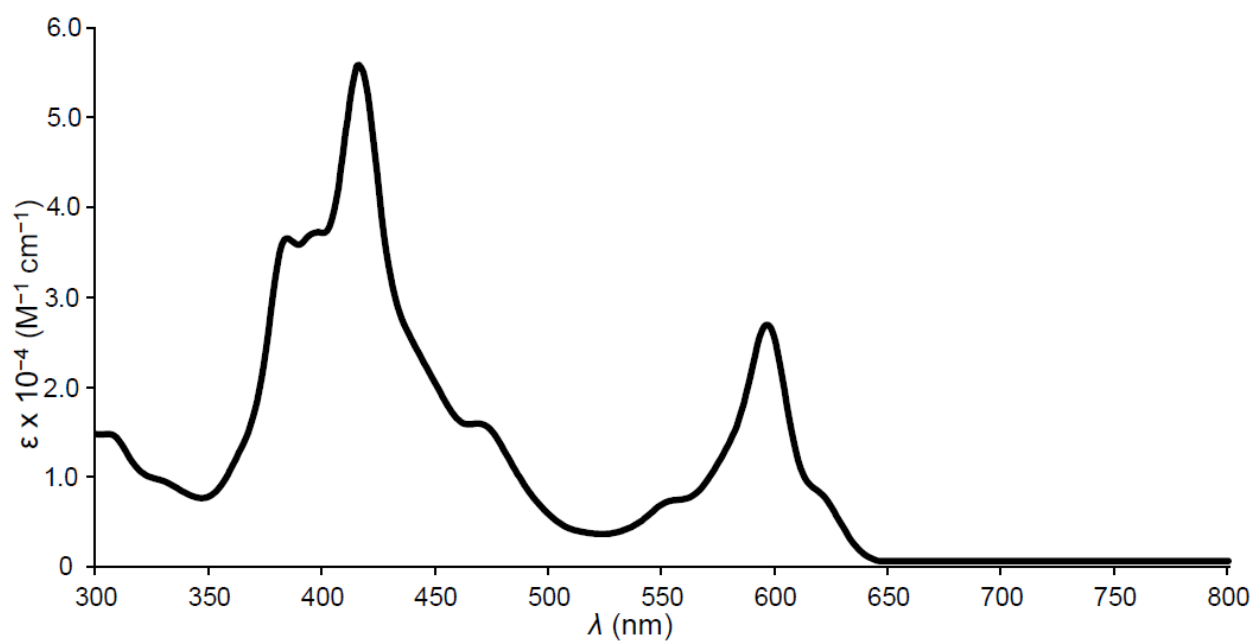


Figure 1. UV-vis spectrum of Ir[TPC]tma₂.

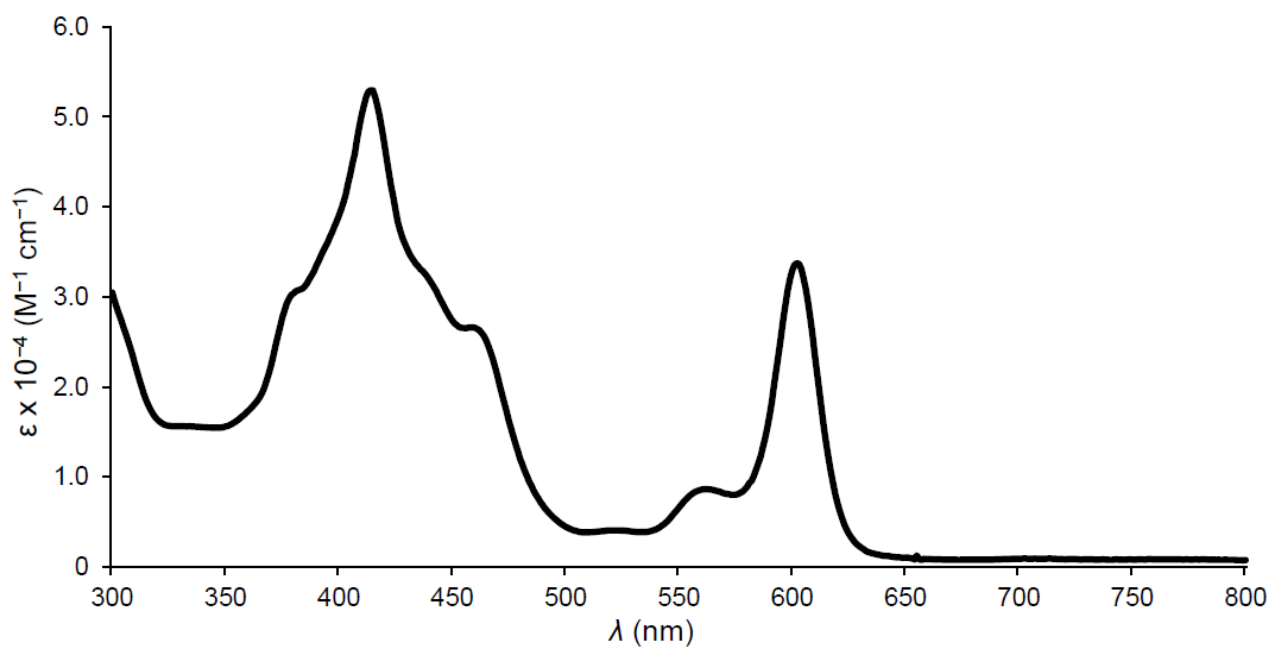


Figure 2. UV-vis spectrum of Ir[TPC]py₂.

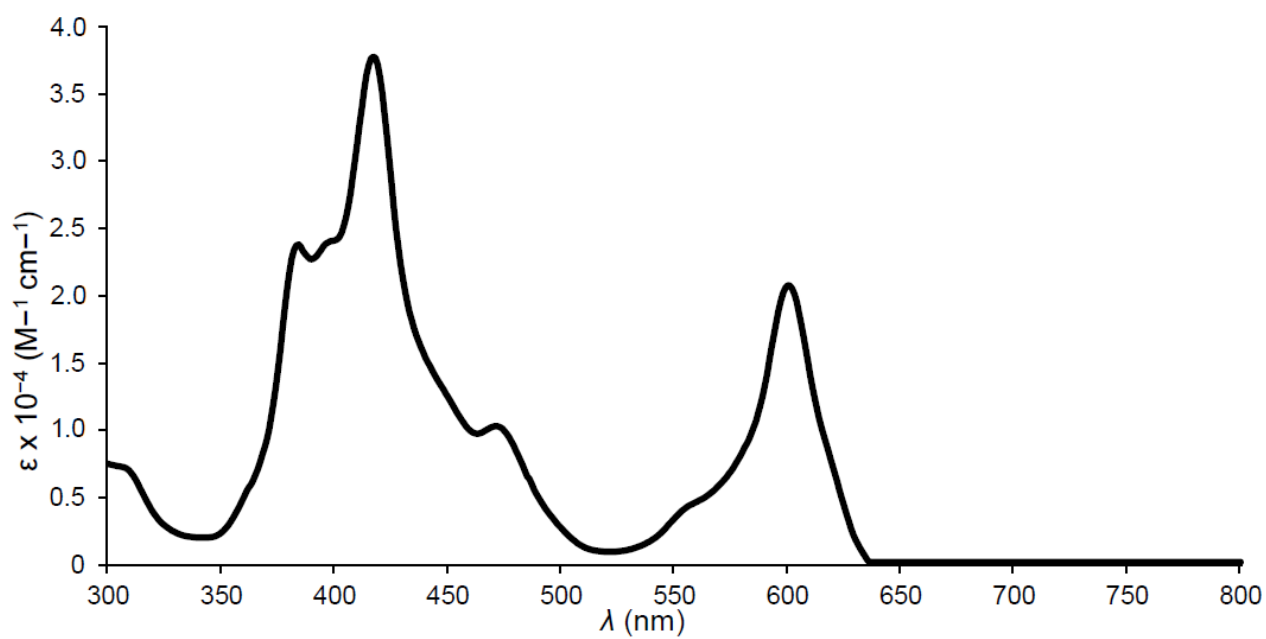


Figure 3. UV-vis spectrum of Ir[TpOMePC]tma₂.

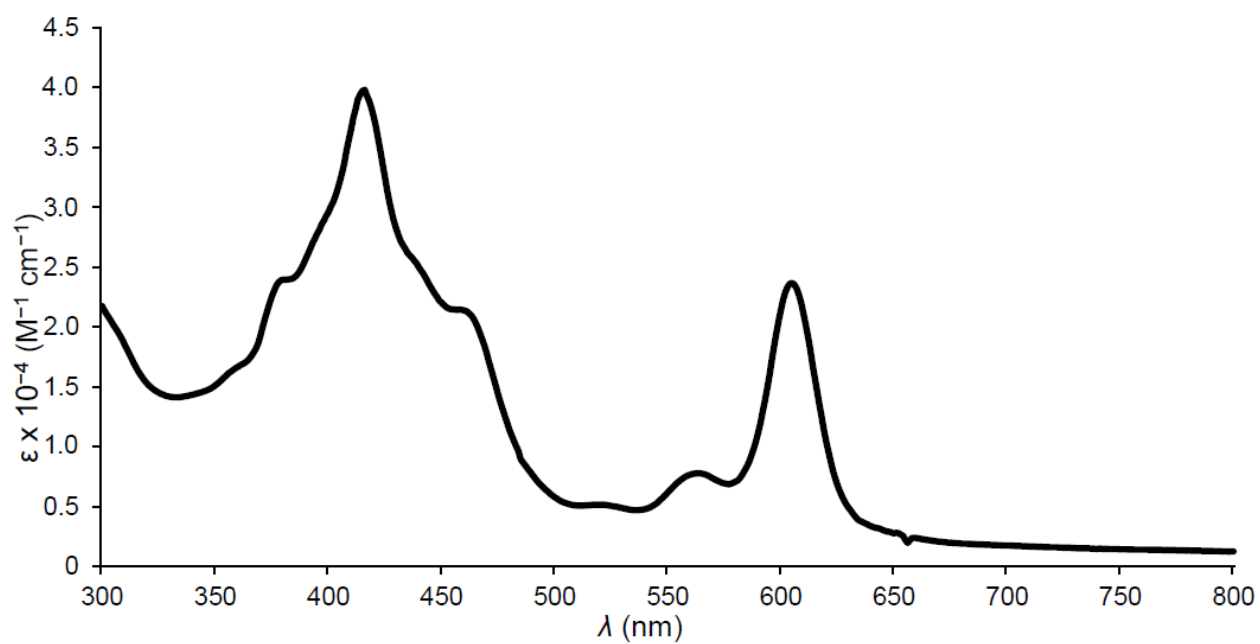


Figure 4. UV-vis spectrum of Ir[TpOMePC]py₂.

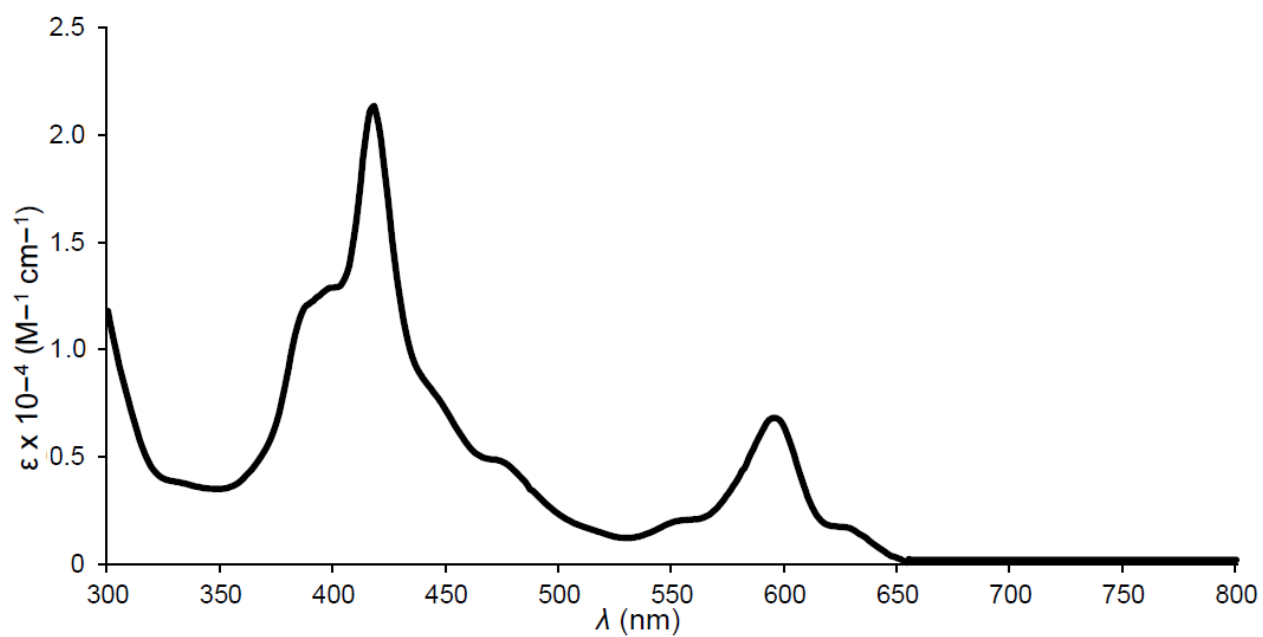


Figure 5. UV-vis spectrum of Ir[TpCF₃PC]tma₂.

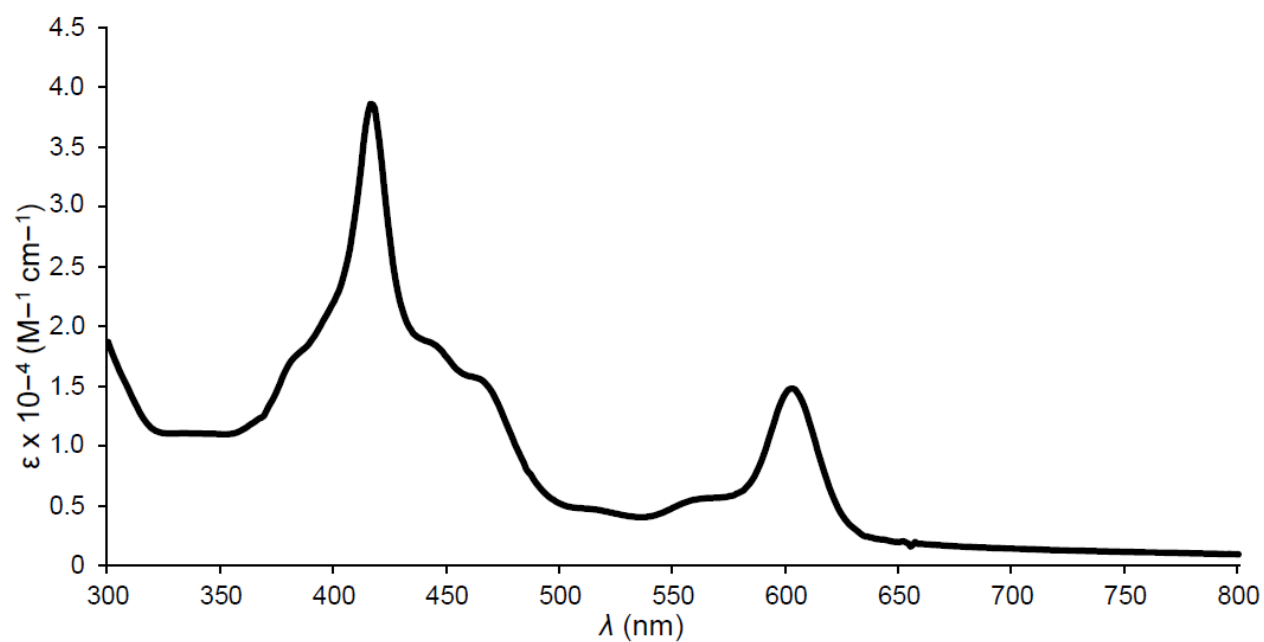


Figure 6. UV-vis spectrum of Ir[TpCF₃PC]py₂.

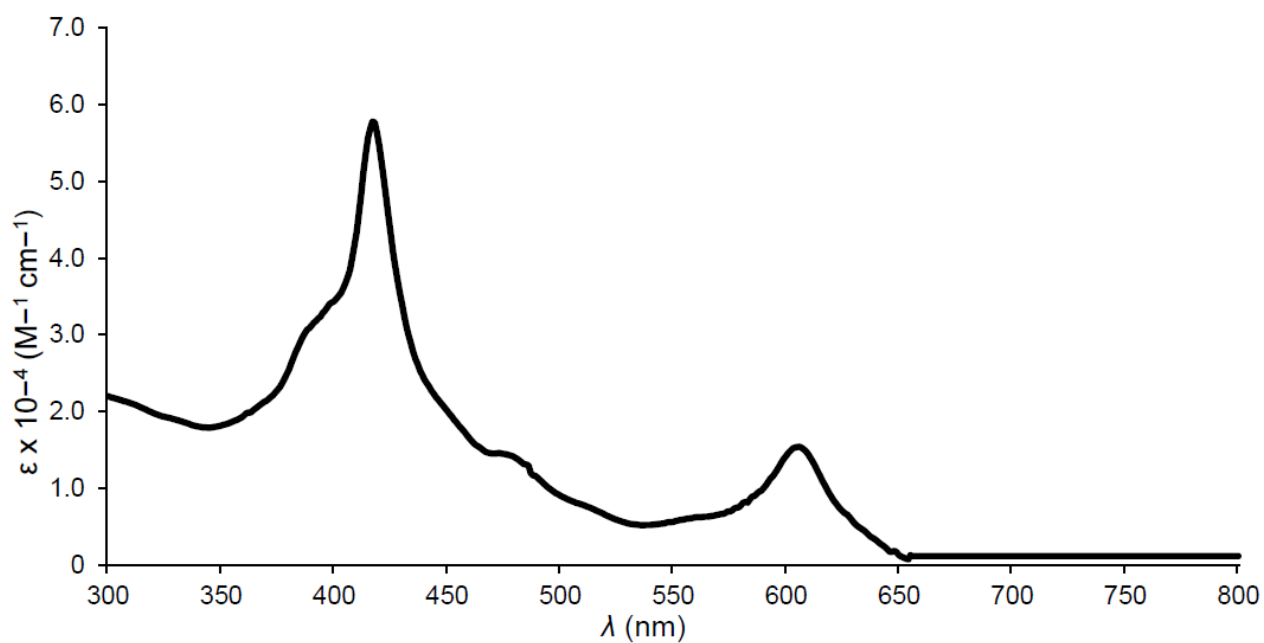


Figure 7. UV-vis spectrum of Ir[TpCF₃PC]dmap₂.

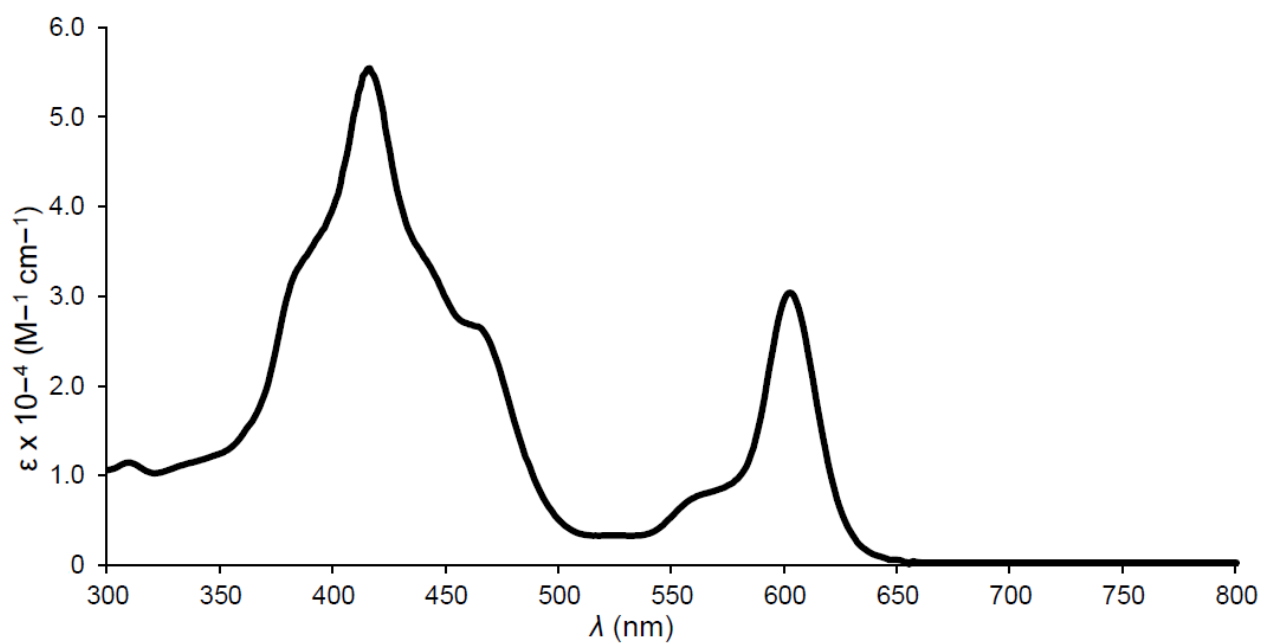


Figure 8. UV-vis spectrum of Ir[TpCF₃PC]4pa₂.

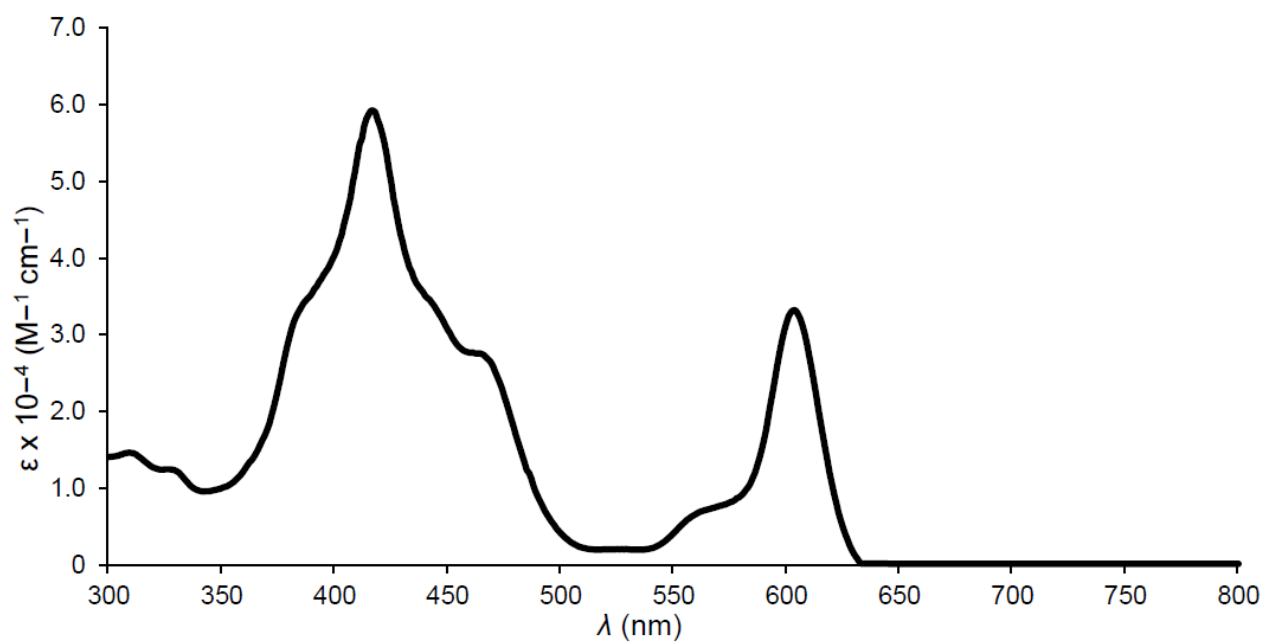


Figure 9. UV-vis spectrum of Ir[TpCF₃PC]isoq₂.

B. Mass spectra

AGI_048_141_posb #1-5 RT: 0.01-0.12 AV: 5 NL: 3.58E7
T: FTMS + p ESI Full ms [600.00-1200.00]

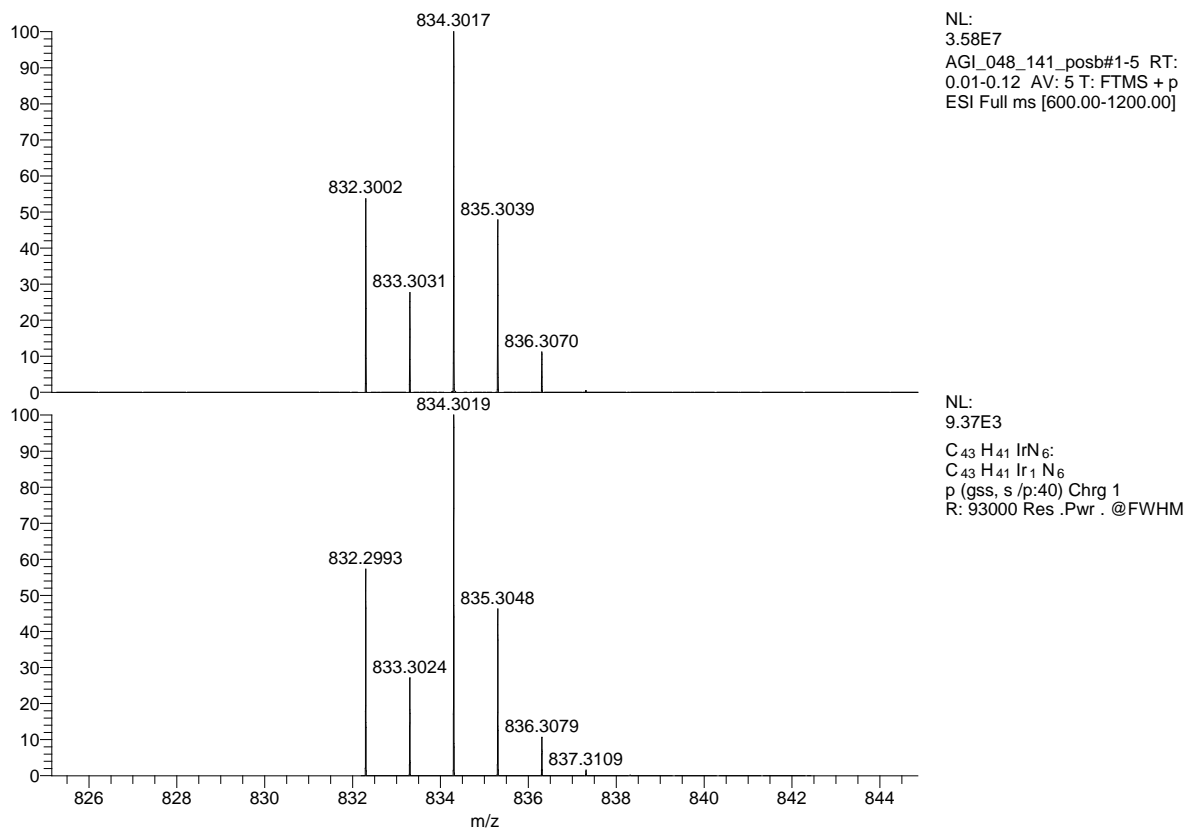
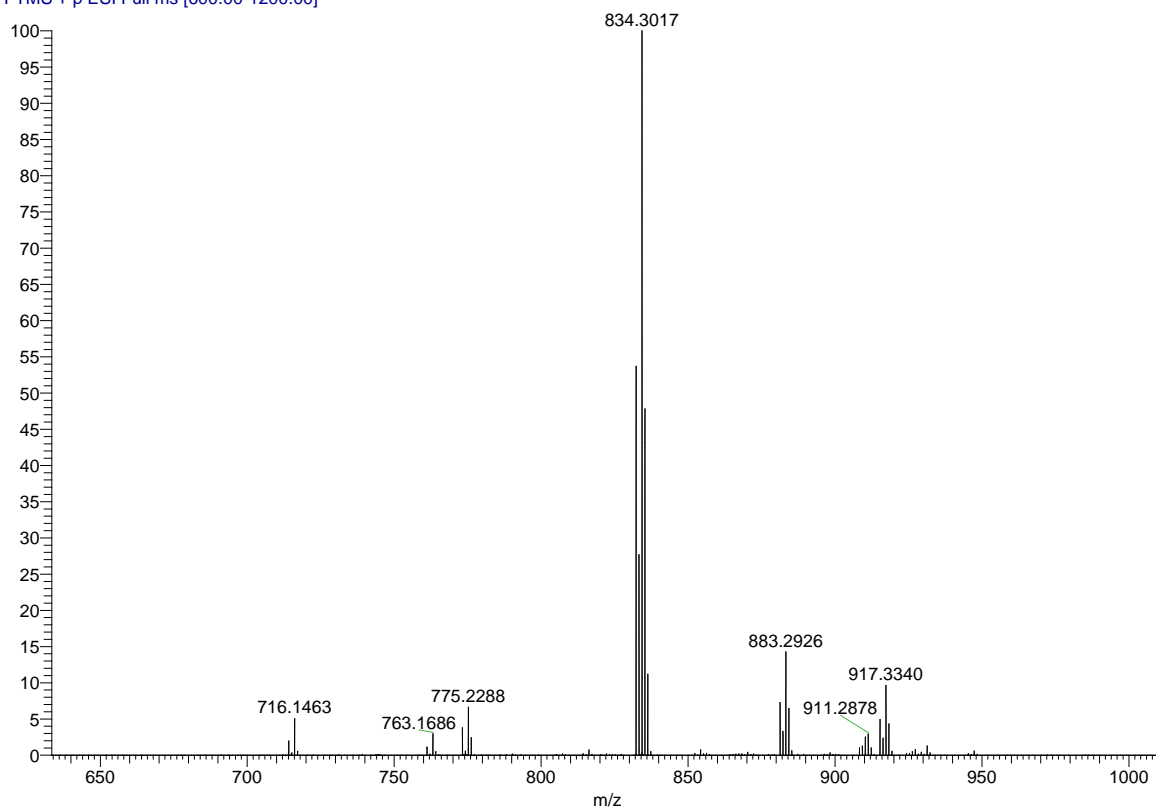


Figure 10. Electrospray ionization mass spectrum of Ir[TPC]tma₂.

AGI_066_168_pos #1-4 RT: 0.02-0.11 AV: 4 NL: 1.01E7
T: FTMS + p ESI Full ms [600.00-1500.00]

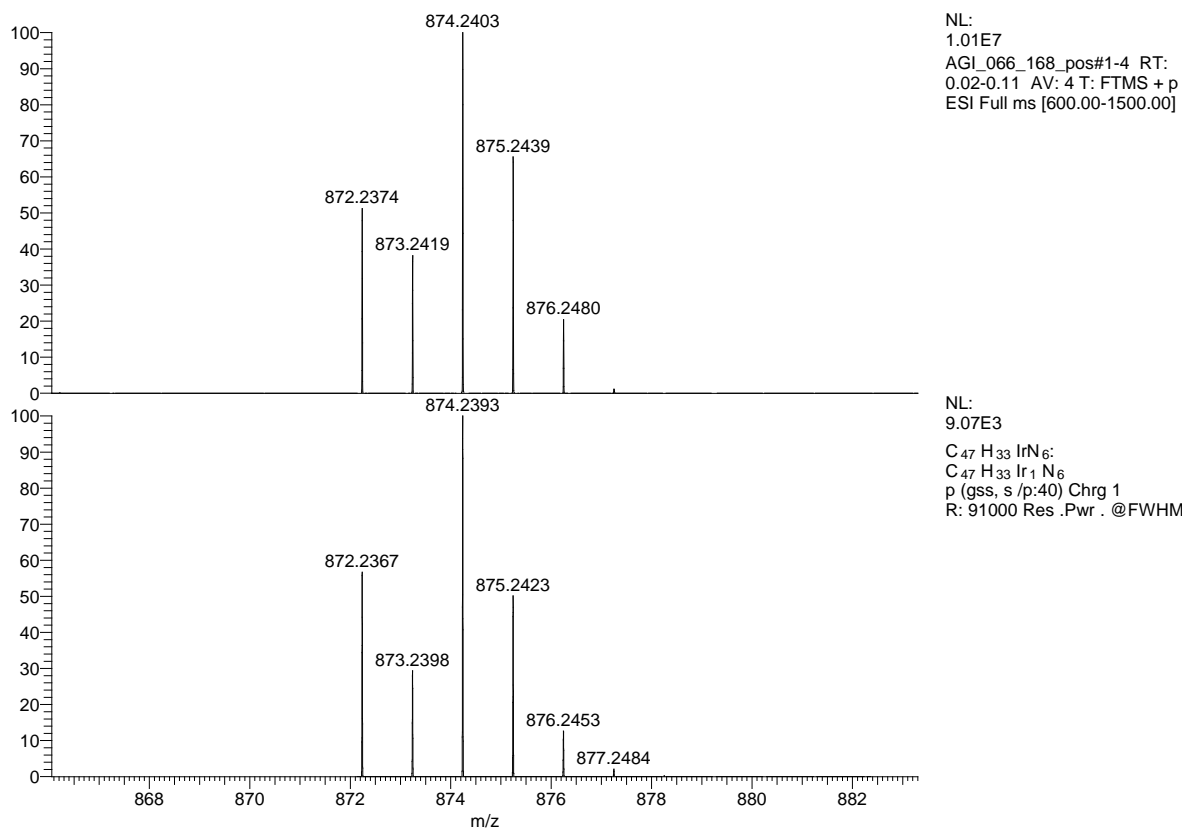
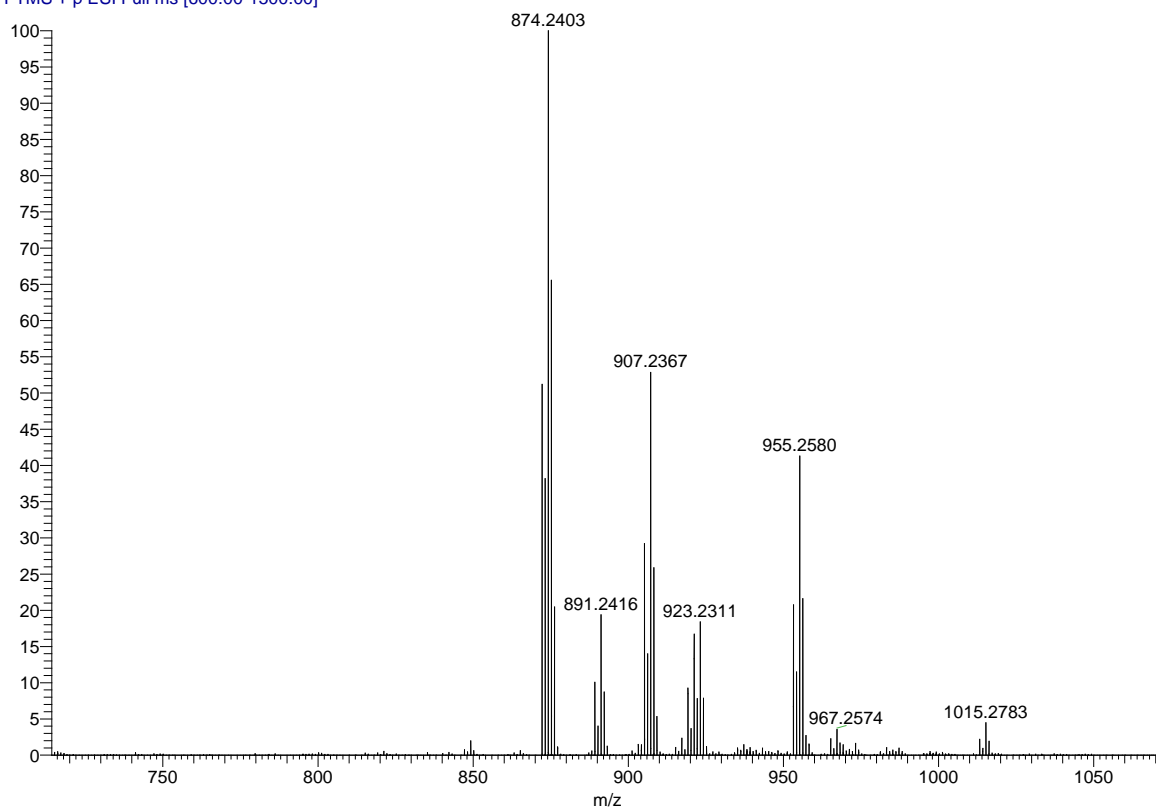


Figure 11. Electrospray ionization mass spectrum of Ir[TPC]py₂.

AGI_056_152_pos #1-4 RT: 0.02-0.11 AV: 4 NL: 1.59E8
T: FTMS + p ESI Full ms [600.00-1200.00]

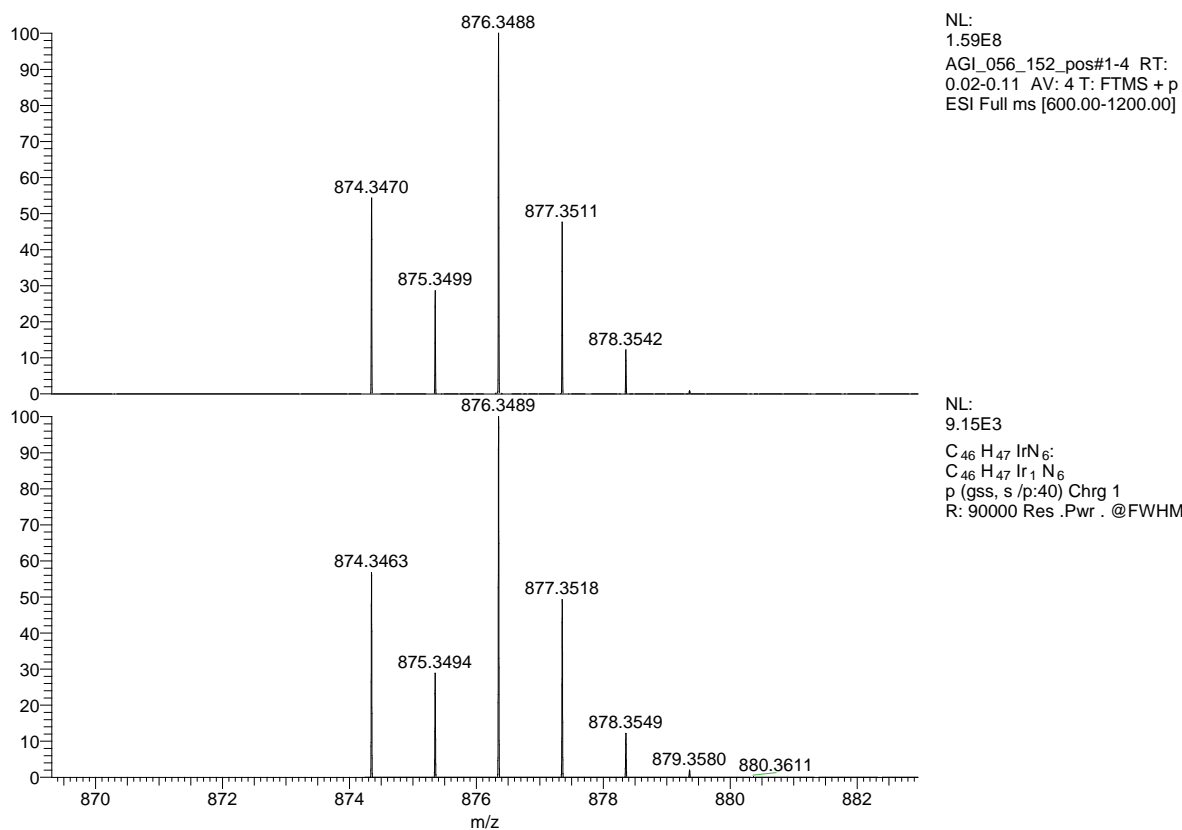
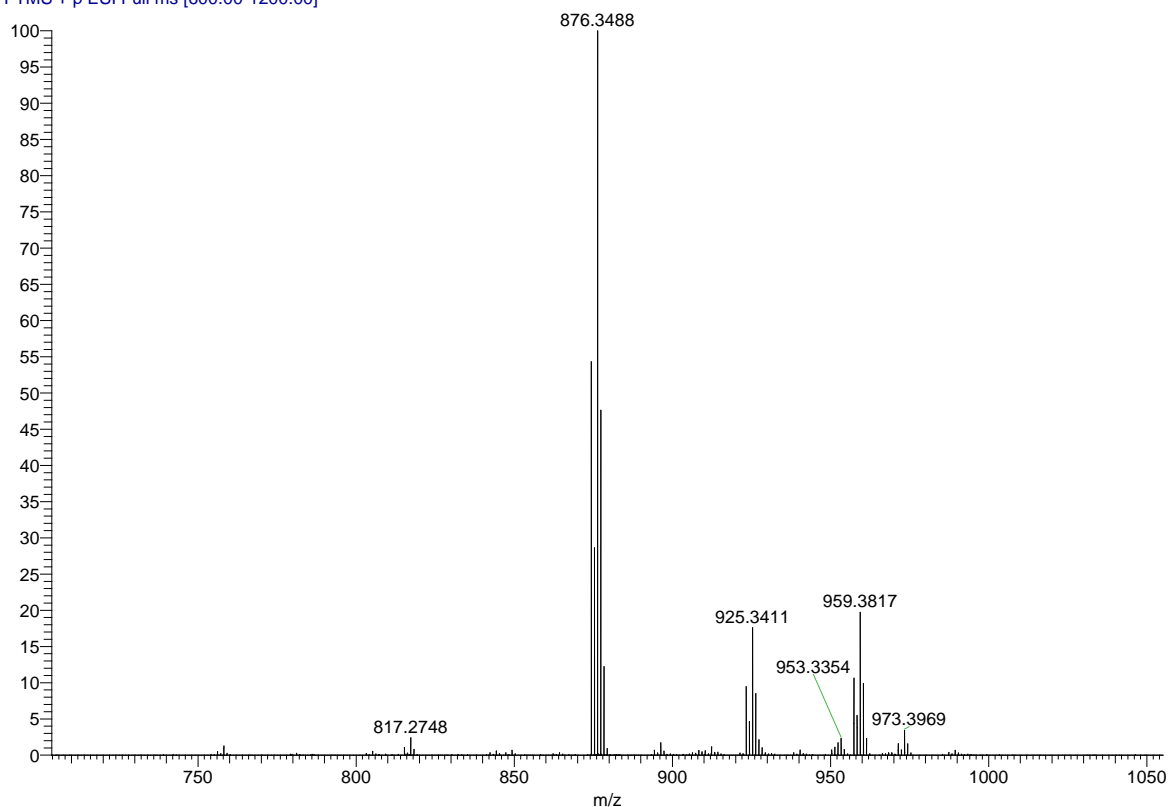


Figure 12. Electrospray ionization mass spectrum of Ir[TpMePC]tma₂.

AGI_058_156 #1-4 RT: 0.02-0.12 AV: 4 NL: 9.42E6
T: FTMS + p ESI Full ms [600.00-1000.00]

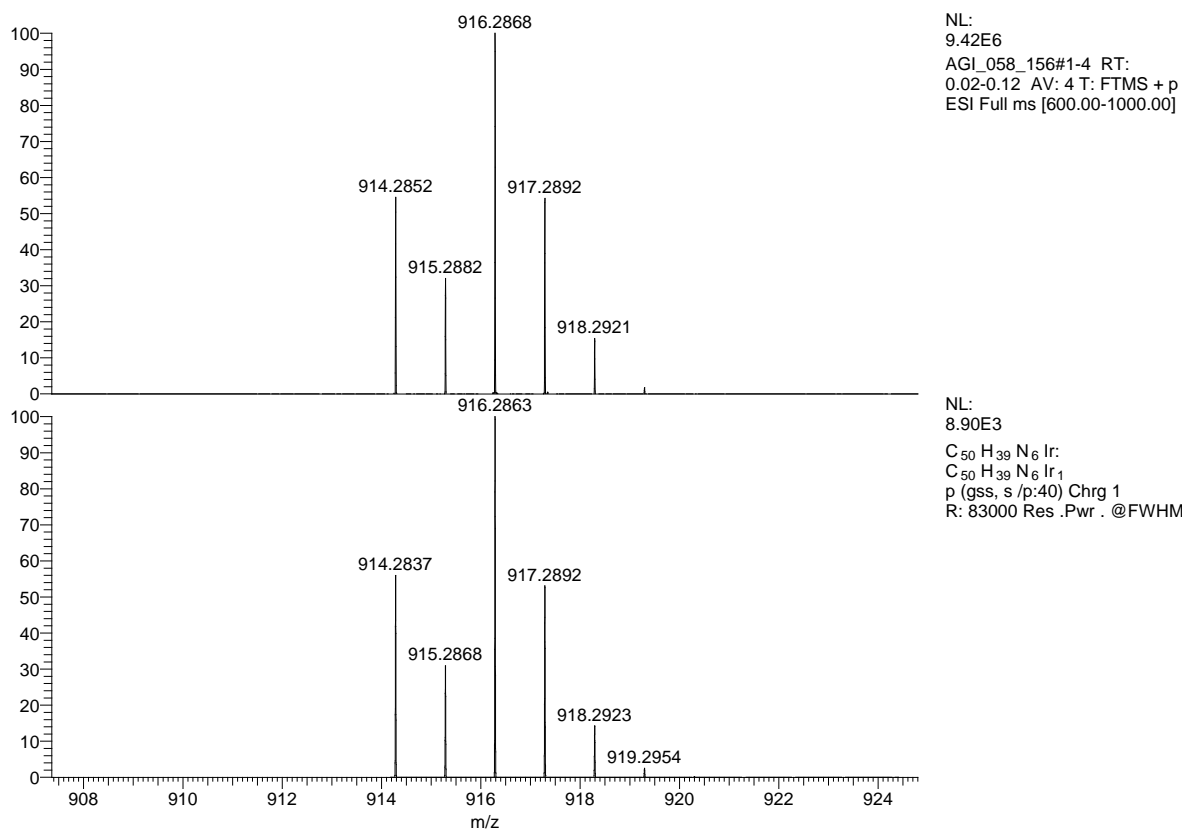
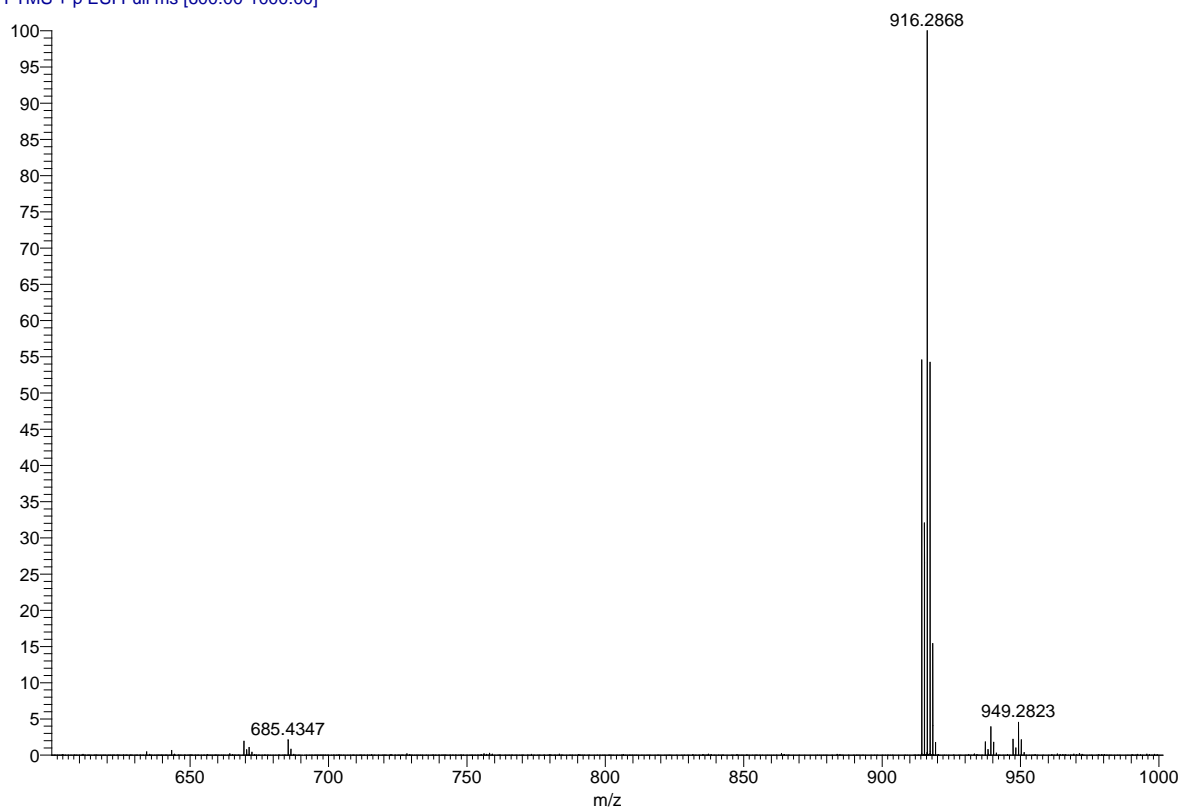


Figure 13. Electrospray ionization mass spectrum of Ir[TpMePC]py₂.

AGI_050_144_pos #1-5 RT: 0.00-0.11 AV: 5 NL: 2.13E7
T: FTMS + p ESI Full ms [600.00-1200.00]

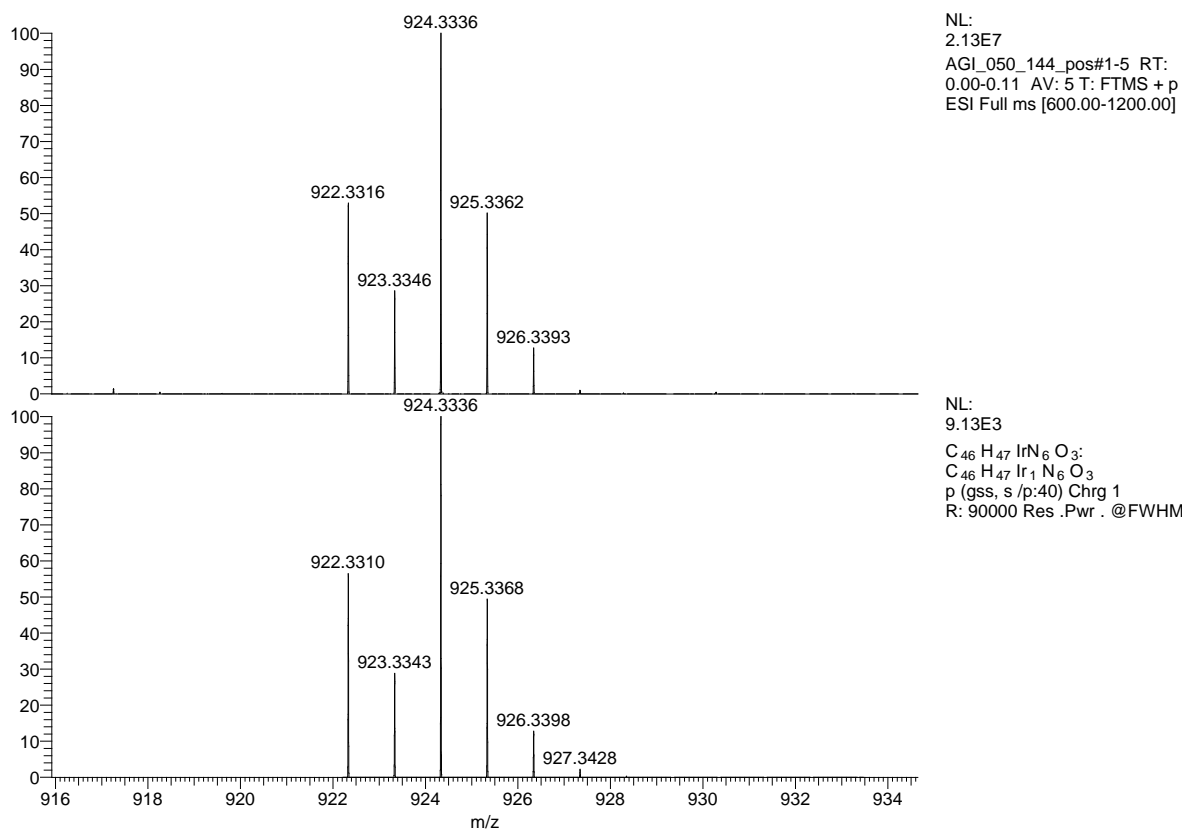
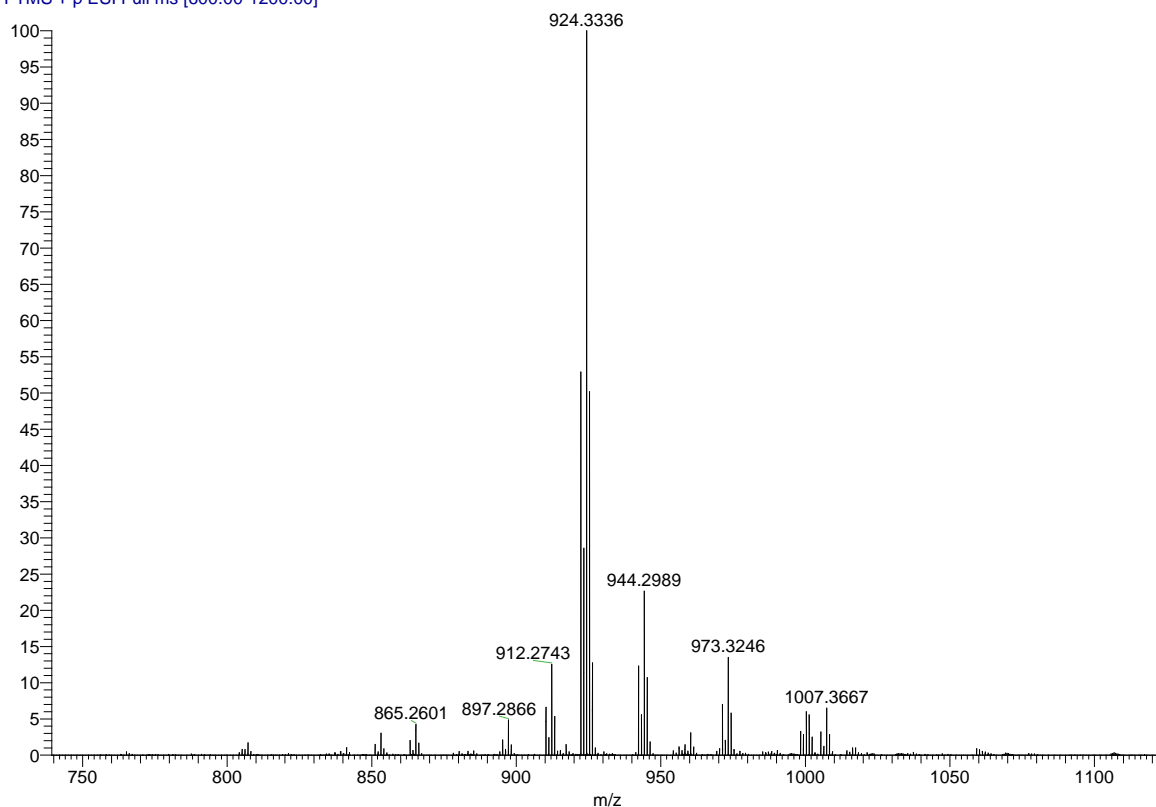


Figure 14. Electrospray ionization mass spectrum of Ir[TpOMePC]tma₂.

p-OMe-py #6 RT: 0.14 AV: 1 NL: 8.58E7
T: FTMS + p ESI Full ms [600.00-1200.00]

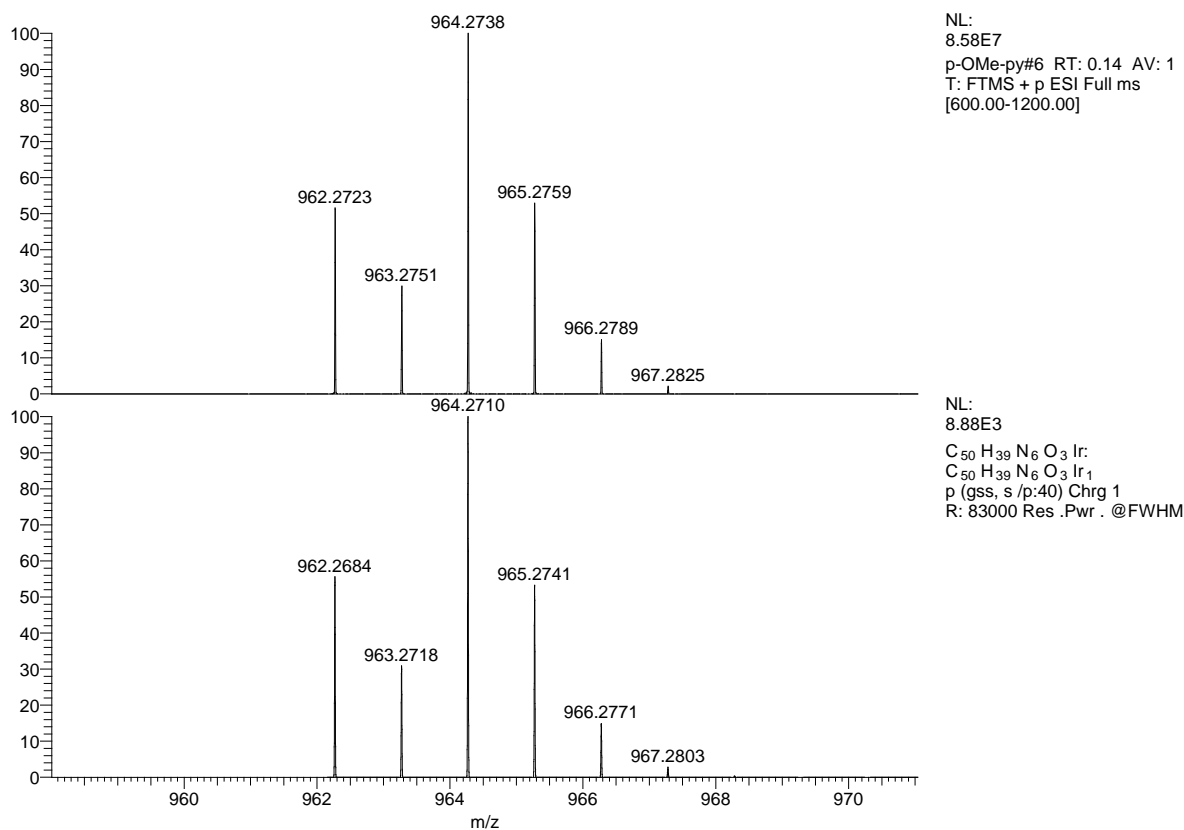
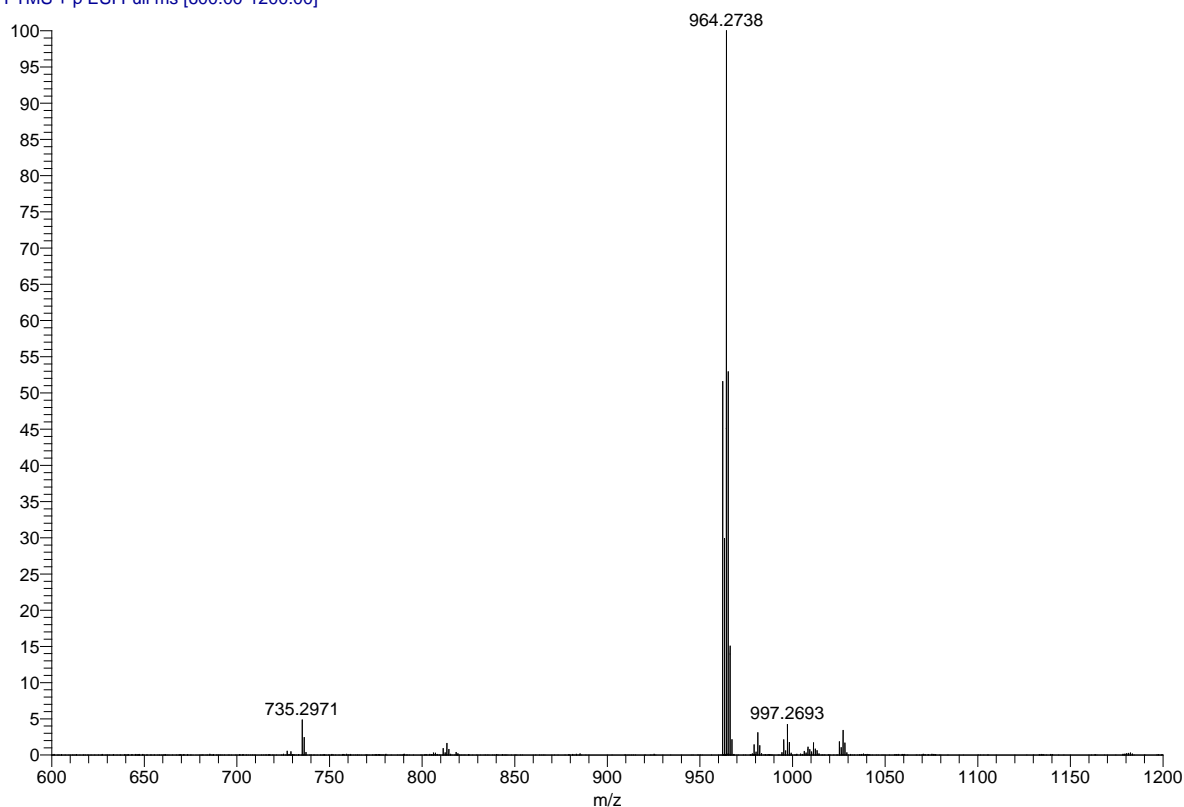
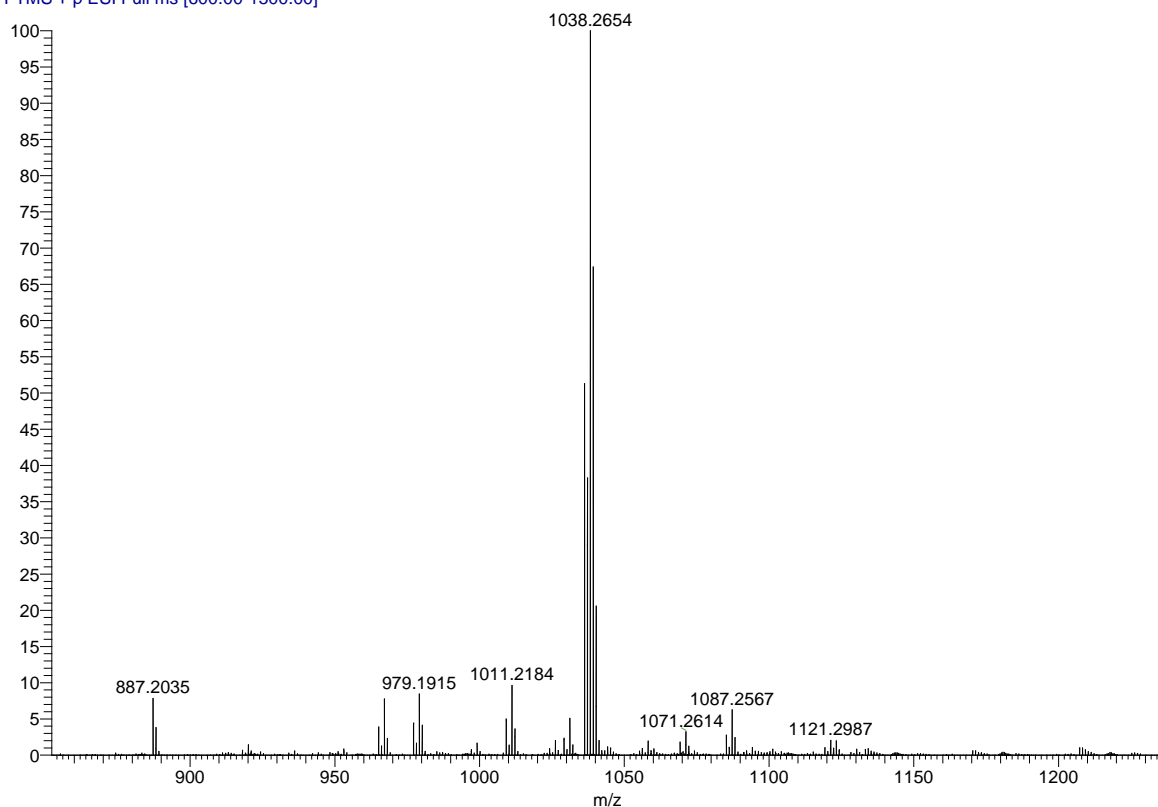
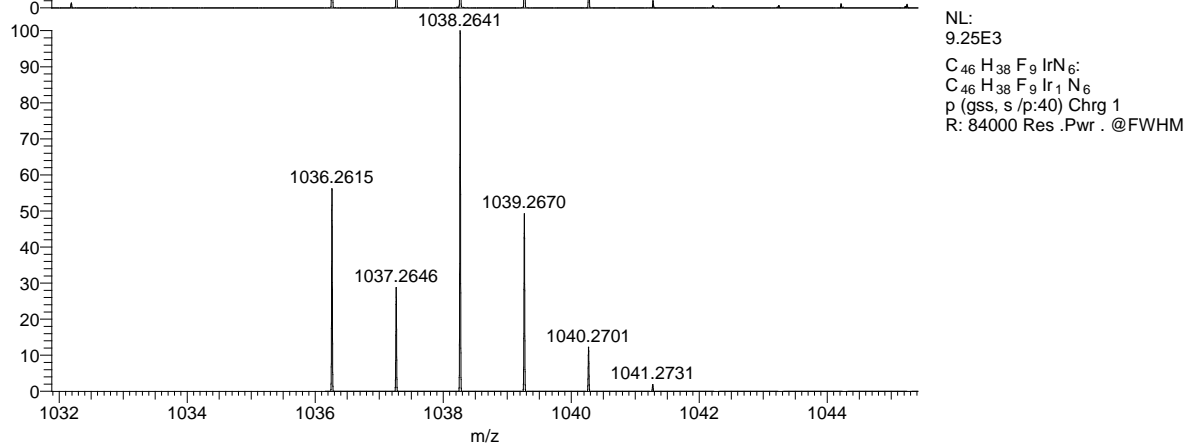


Figure 15. Electrospray ionization mass spectrum of Ir[TpOMePC]py₂.

AGI_055_151_pos #1-5 RT: 0.02-0.13 AV: 5 NL: 1.32E7
T: FTMS + p ESI Full ms [600.00-1500.00]



NL:
1.32E7
AGI_055_151_pos#1-5 RT:
0.02-0.13 AV: 5 T: FTMS + p
ESI Full ms [600.00-1500.00]



NL:
9.25E3
C₄₆ H₃₈ F₉ IrN₆:
C₄₆ H₃₈ F₉ Ir₁ N₆
p (gss, s /p:40) Chrg 1
R: 84000 Res .Pwr . @FWHM

Figure 16. Electrospray ionization mass spectrum of Ir[TpCF₃PC]tma₂.

AGI_068_170_pos #1-5 RT: 0.01-0.12 AV: 5 NL: 1.71E7
T: FTMS + p ESI Full ms [600.00-1500.00]

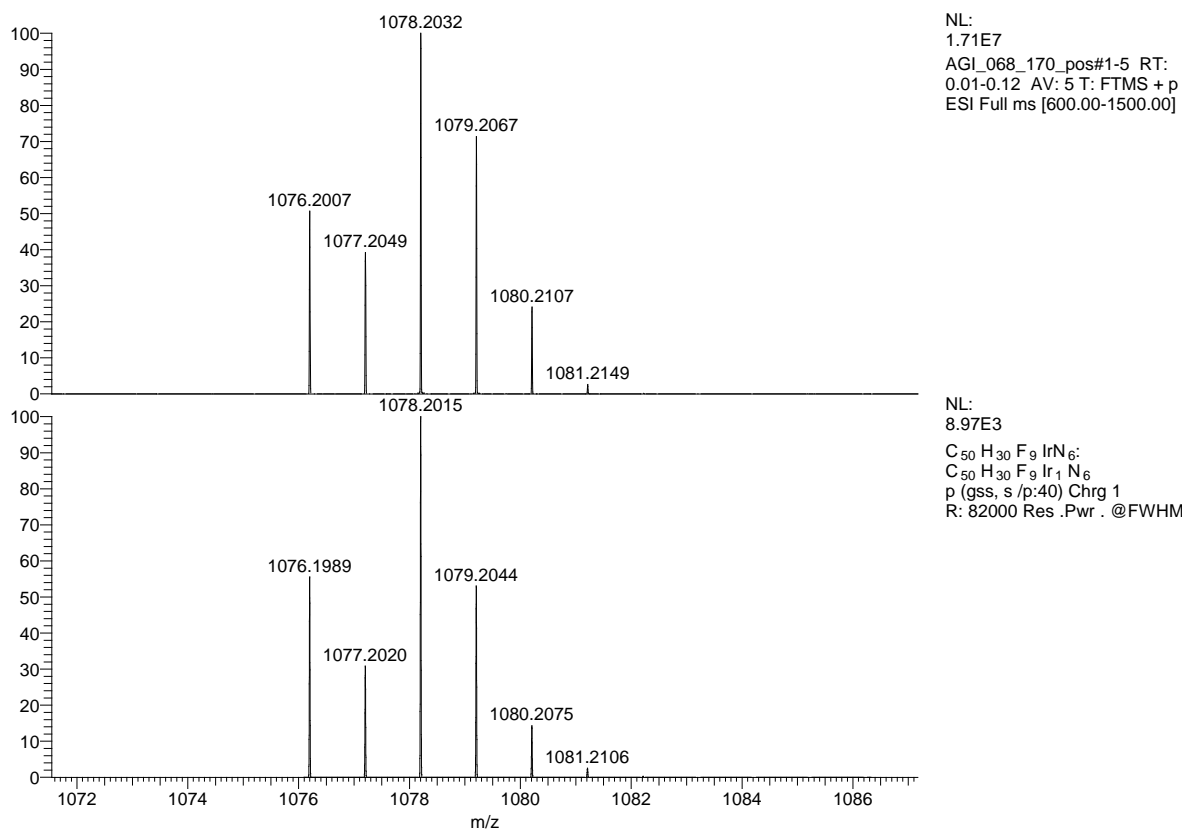
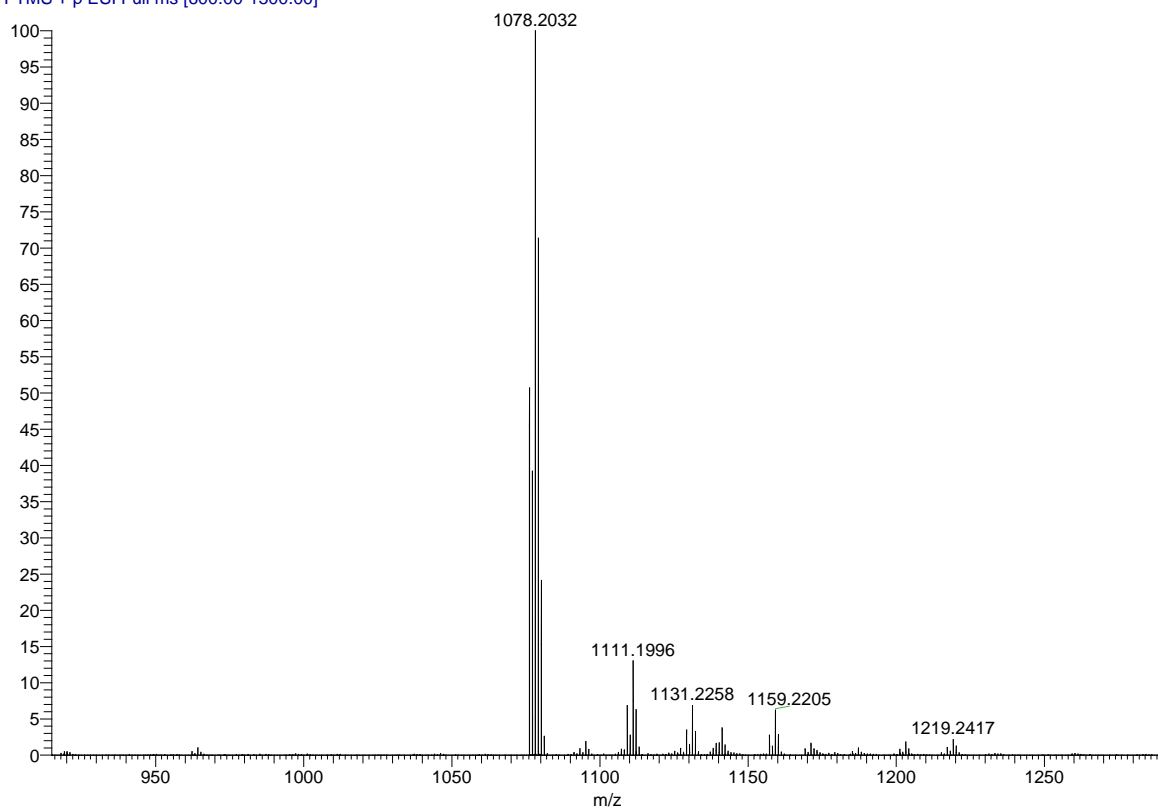


Figure 17. Electrospray ionization mass spectrum of Ir[TpCF₃PC]py₂.

IrpCF3_DMAP #1-5 RT: 0.02-0.12 AV: 5 NL: 8.15E7
T: FTMS + p ESI Full ms [600.00-2000.00]

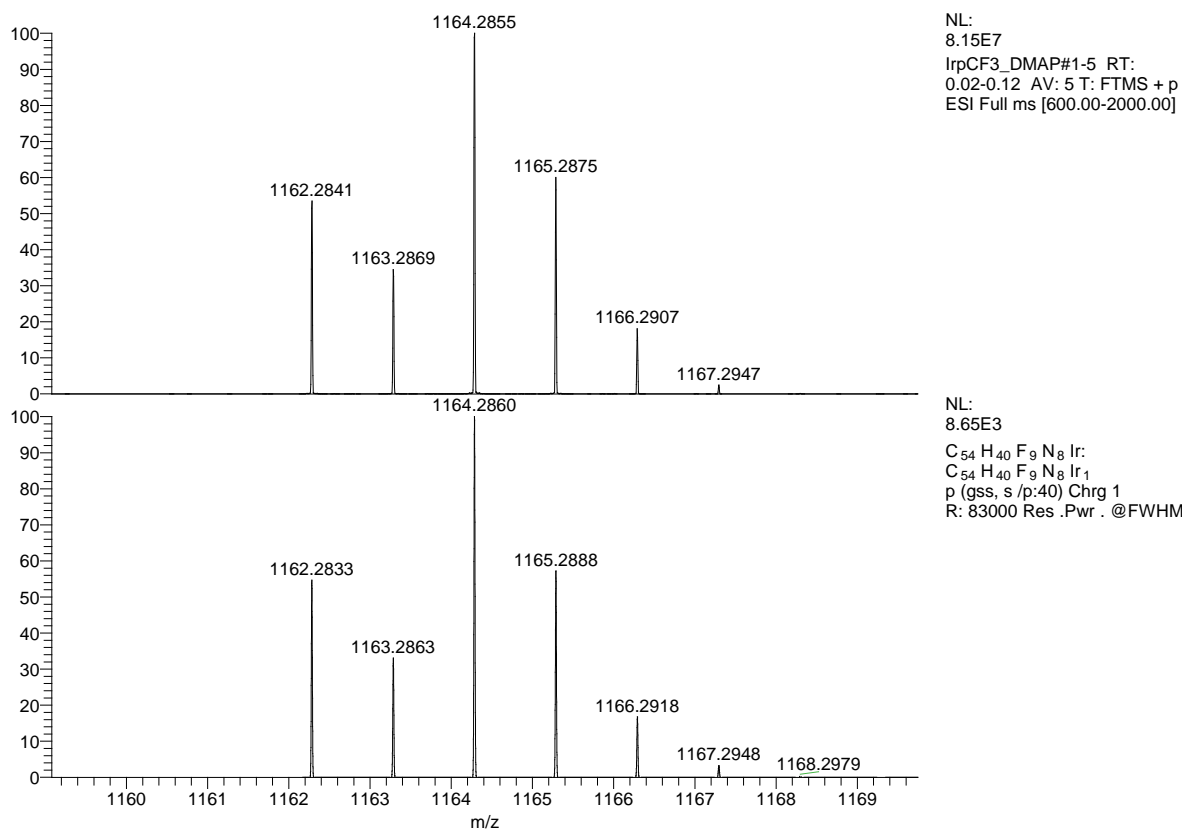
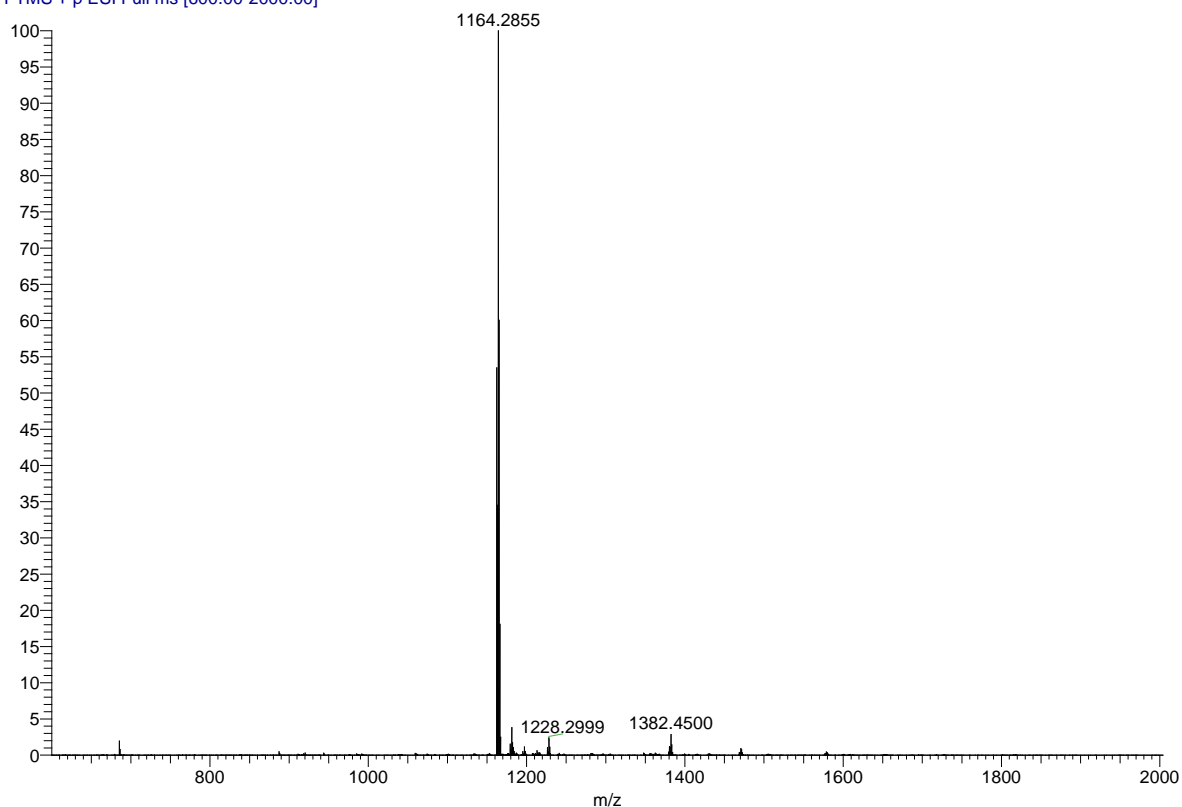
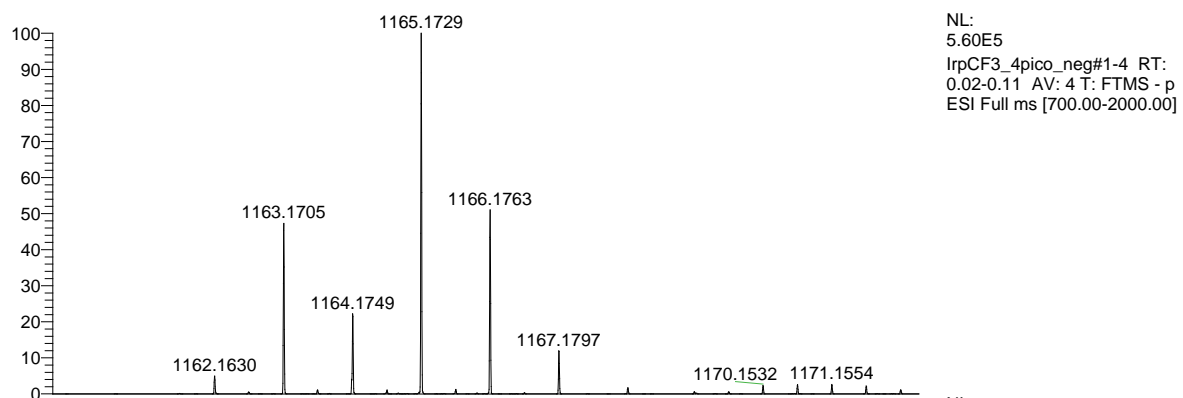
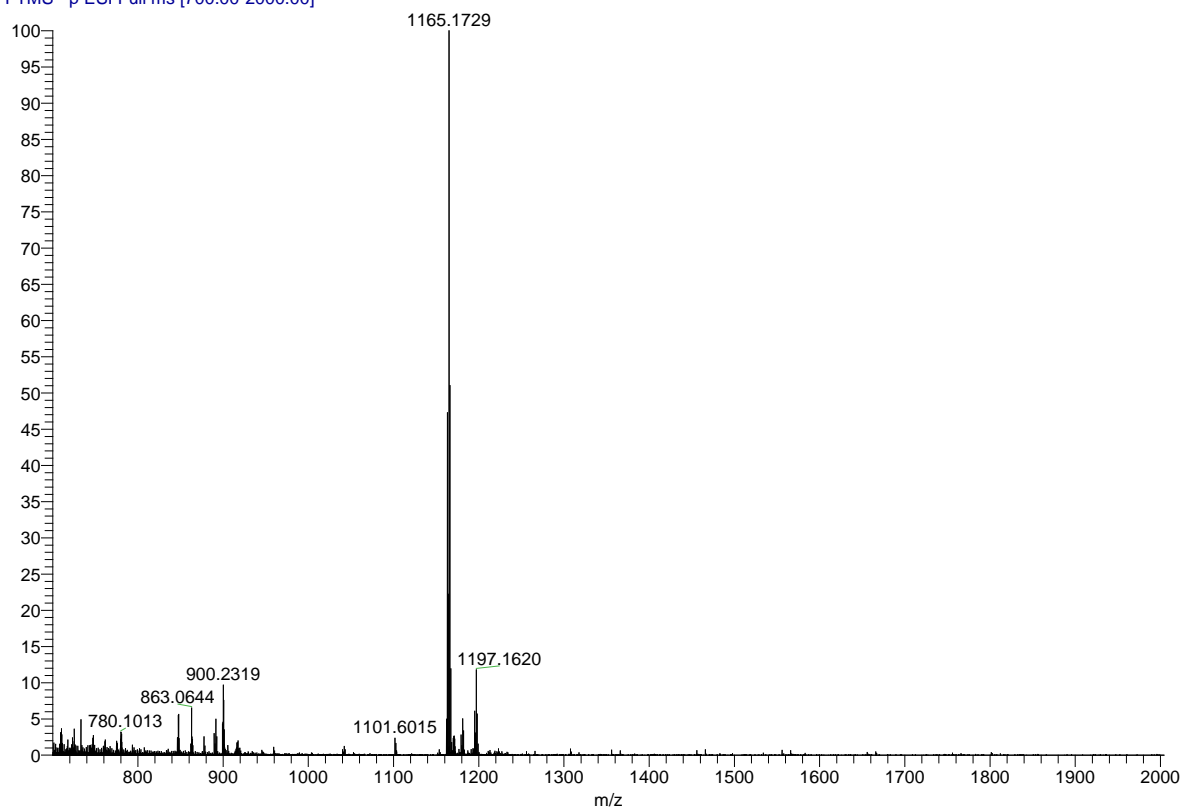
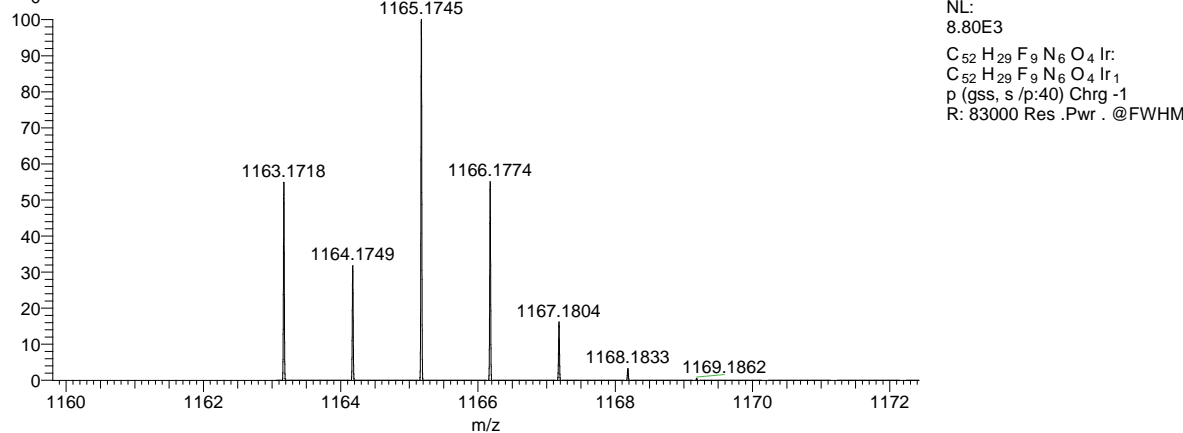


Figure 18. Electrospray ionization mass spectrum of Ir[TpCF₃PC]dmap₂.

IrpCF3_4pico_neg#1-4 RT: 0.02-0.11 AV: 4 NL: 5.60E5
T: FTMS - p ESI Full ms [700.00-2000.00]



NL:
5.60E5
IrpCF3_4pico_neg#1-4 RT:
0.02-0.11 AV: 4 T: FTMS - p
ESI Full ms [700.00-2000.00]



NL:
8.80E3
C₅₂ H₂₉ F₉ N₆ O₄ Ir:
C₅₂ H₂₉ F₉ N₆ O₄ Ir₁
p (gss, s /p:40) Chrg -1
R: 83000 Res .Pwr . @FWHM

Figure 19. Electrospray ionization mass spectrum of Ir[*Tp*CF₃PC]4pa₂.

IrpCF3_isoquinoline_b #2 RT: 0.03 AV: 1 NL: 6.88E7
T: FTMS + p ESI Full ms [700.00-2000.00]

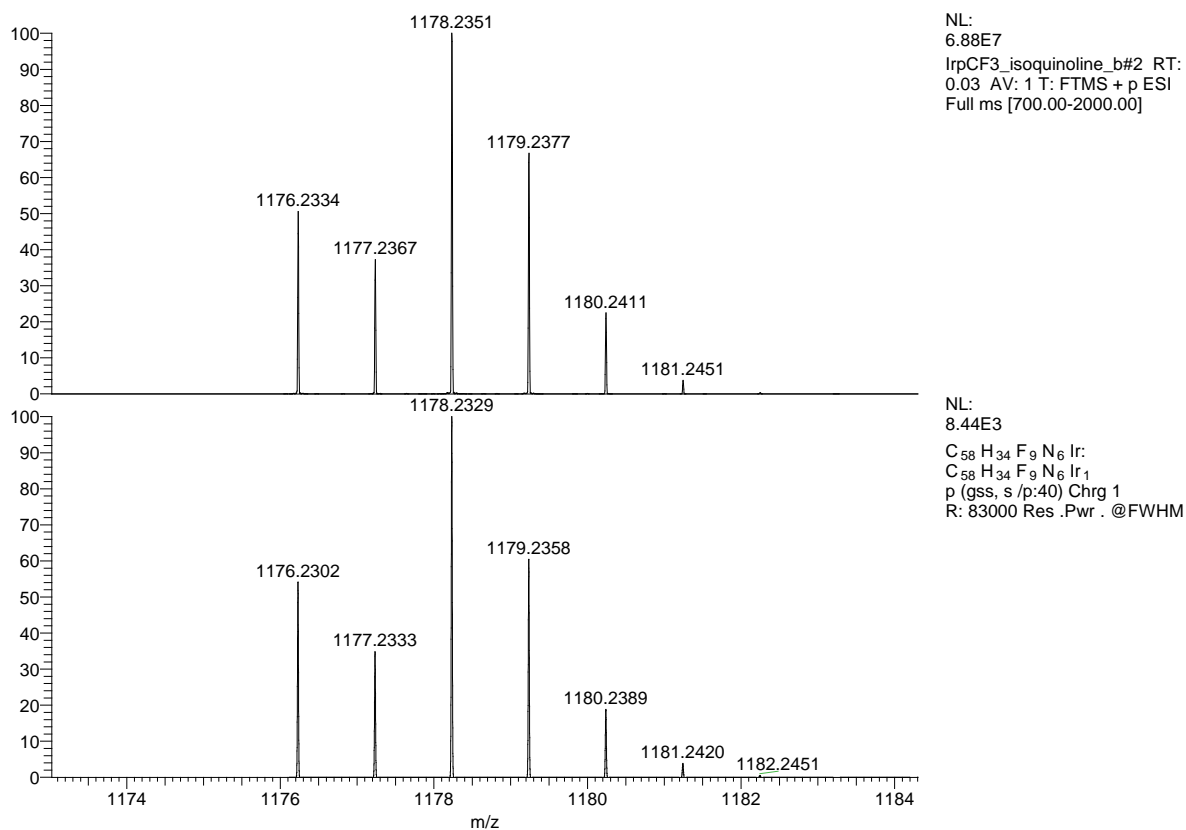
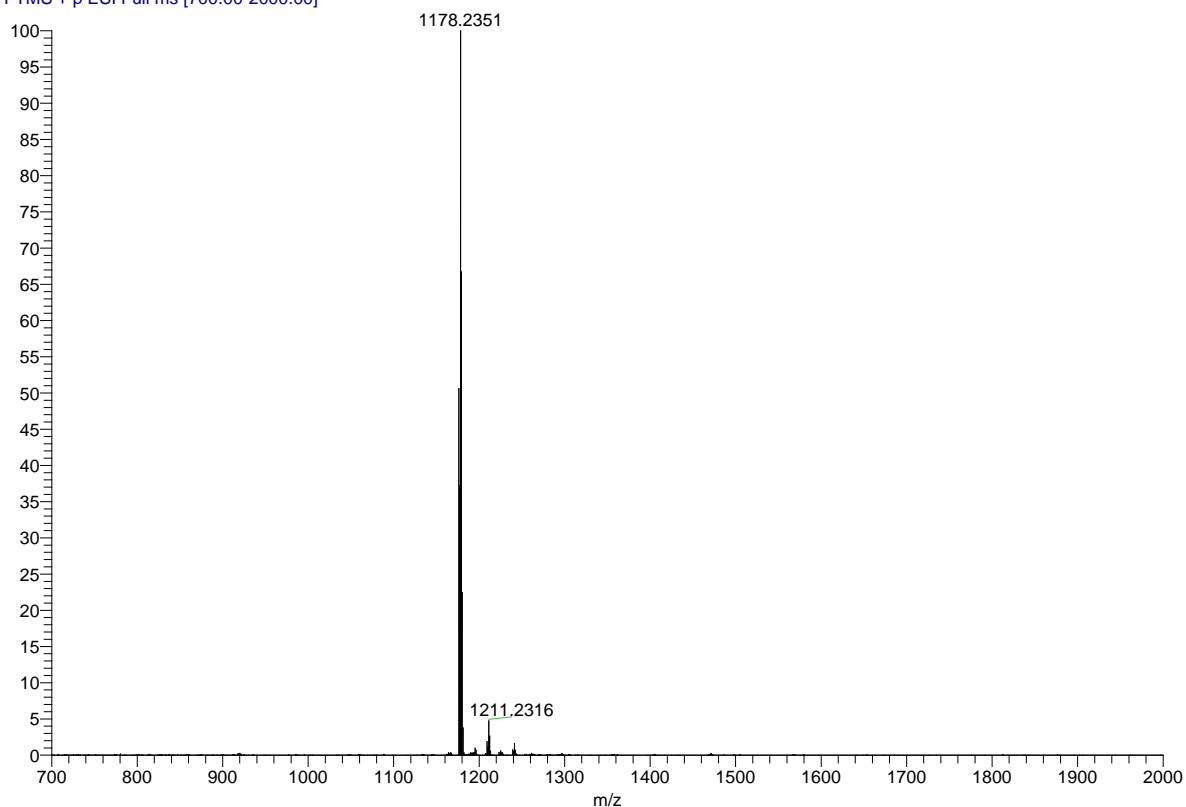


Figure 20. Electrospray ionization mass spectrum of Ir[*Tp*CF₃PC]isoq₂.

C. ^1H NMR spectra

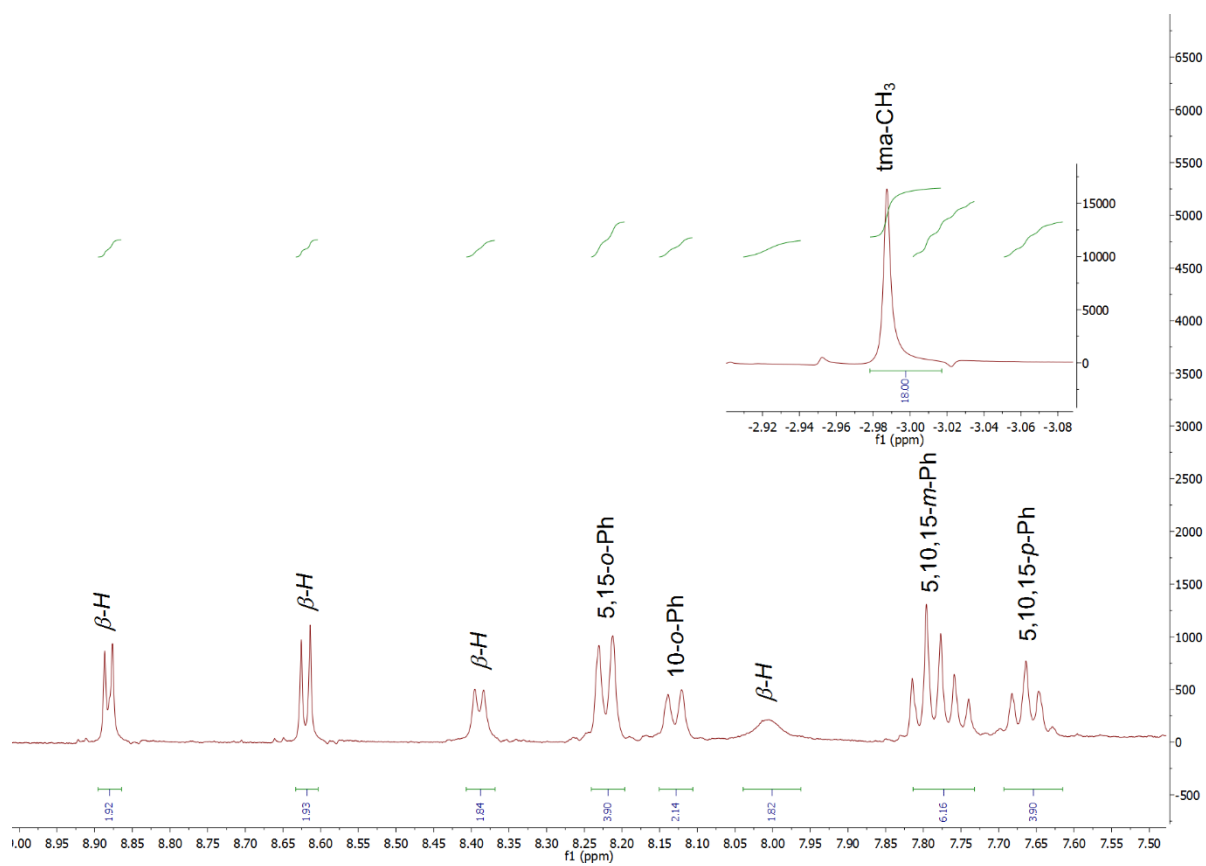


Figure 21. ^1H NMR spectrum of Ir[TPC]tma₂ in acetone-*d*₆.

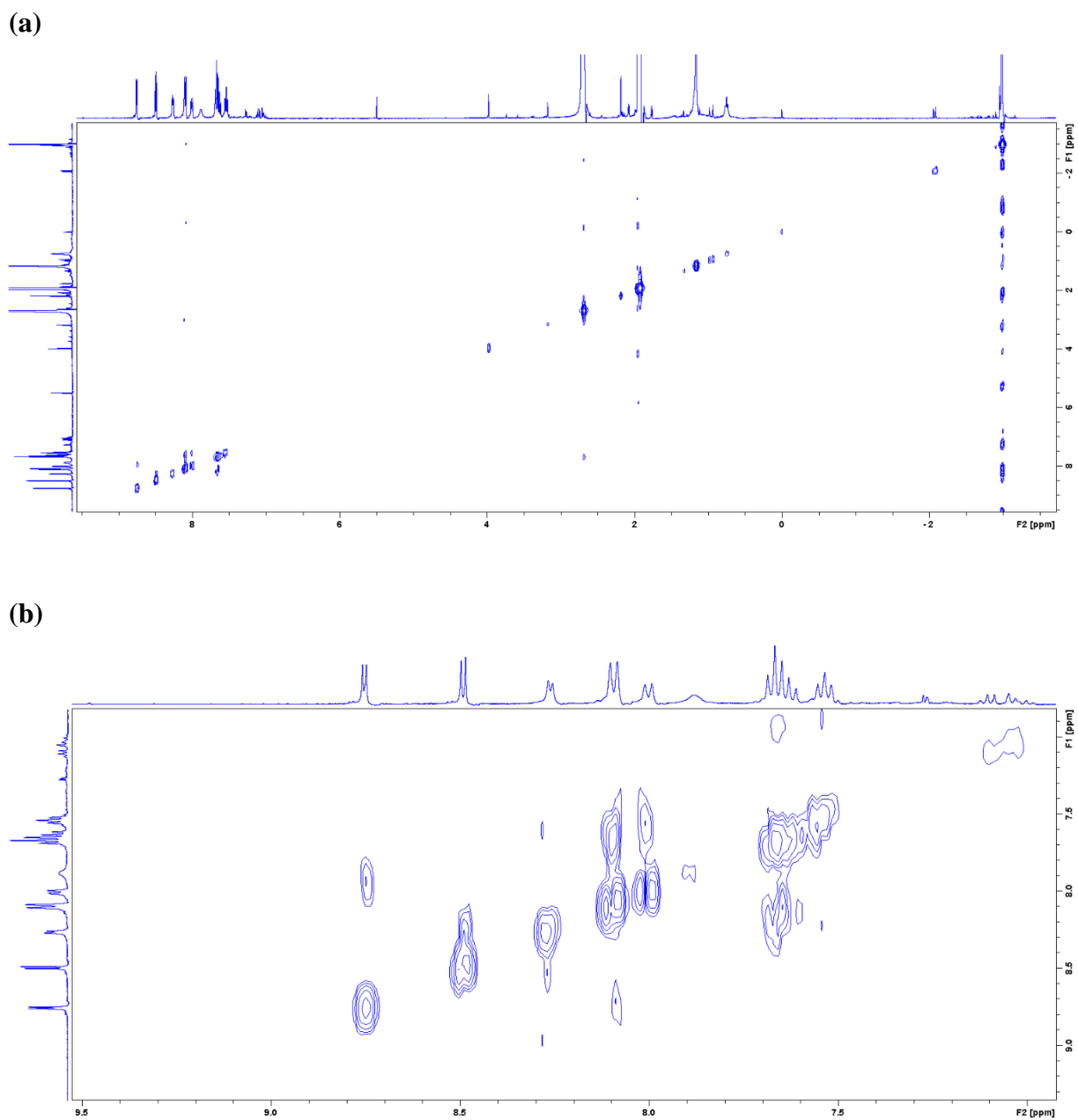


Figure 22. (a) COSY of Ir[TPC]tma₂ in acetone-*d*₆. (b) Close-up of aromatic area.

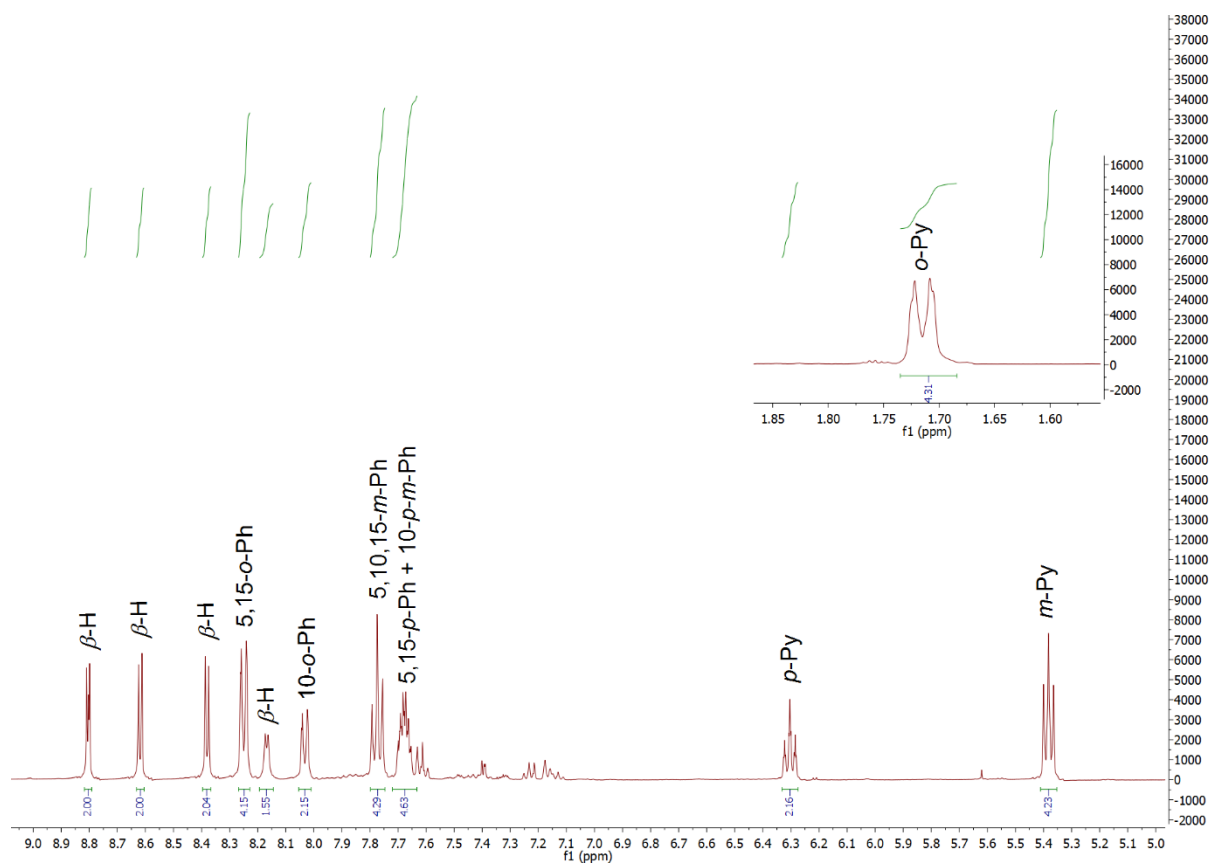


Figure 23. ^1H NMR spectrum of $\text{Ir}[\text{TPC}]\text{py}_2$ in $\text{acetone-}d_6$.

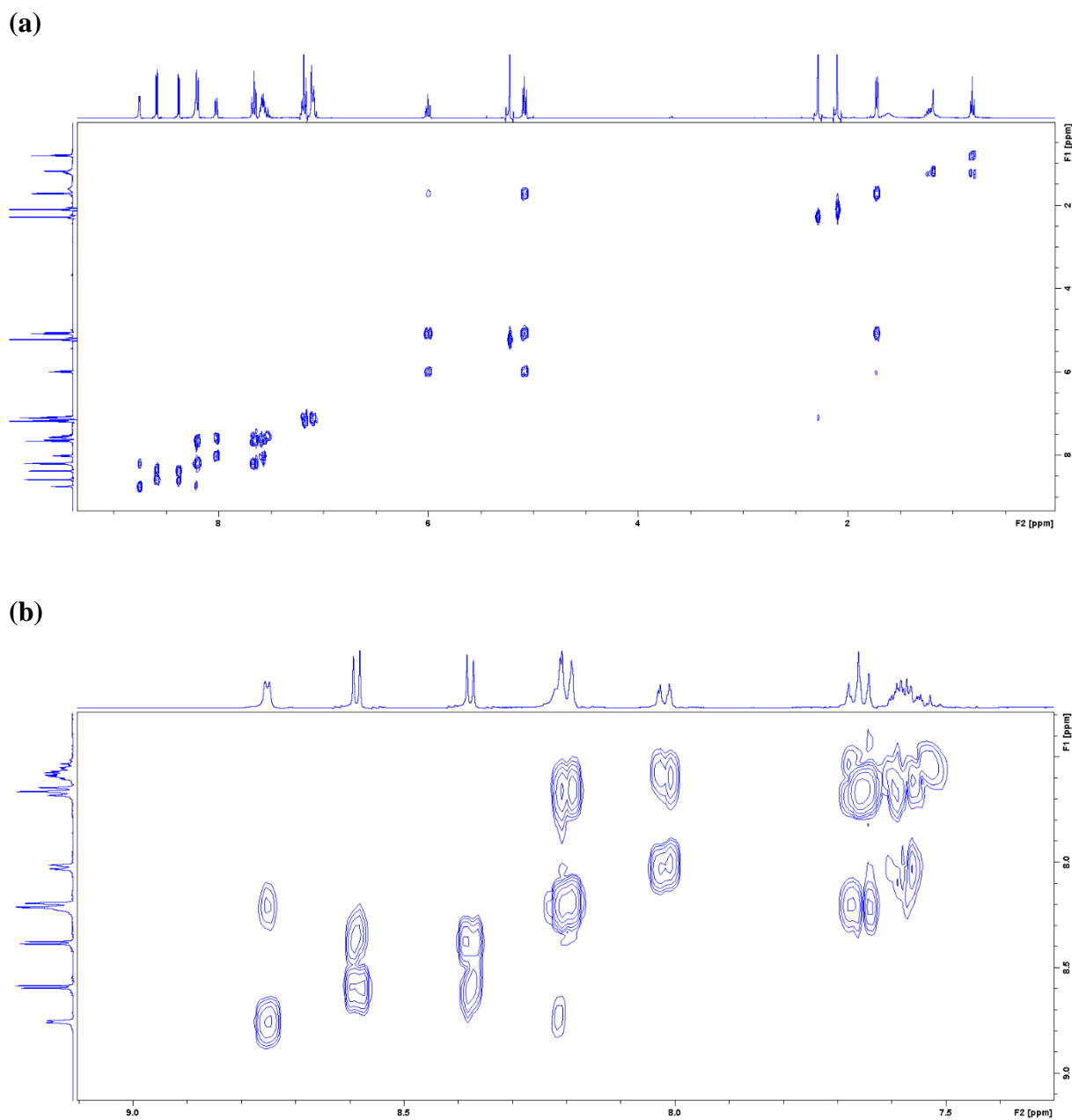


Figure 24. (a) COSY of Ir[TPC]py₂ in acetone-*d*₆. (b) Close-up of aromatic area.

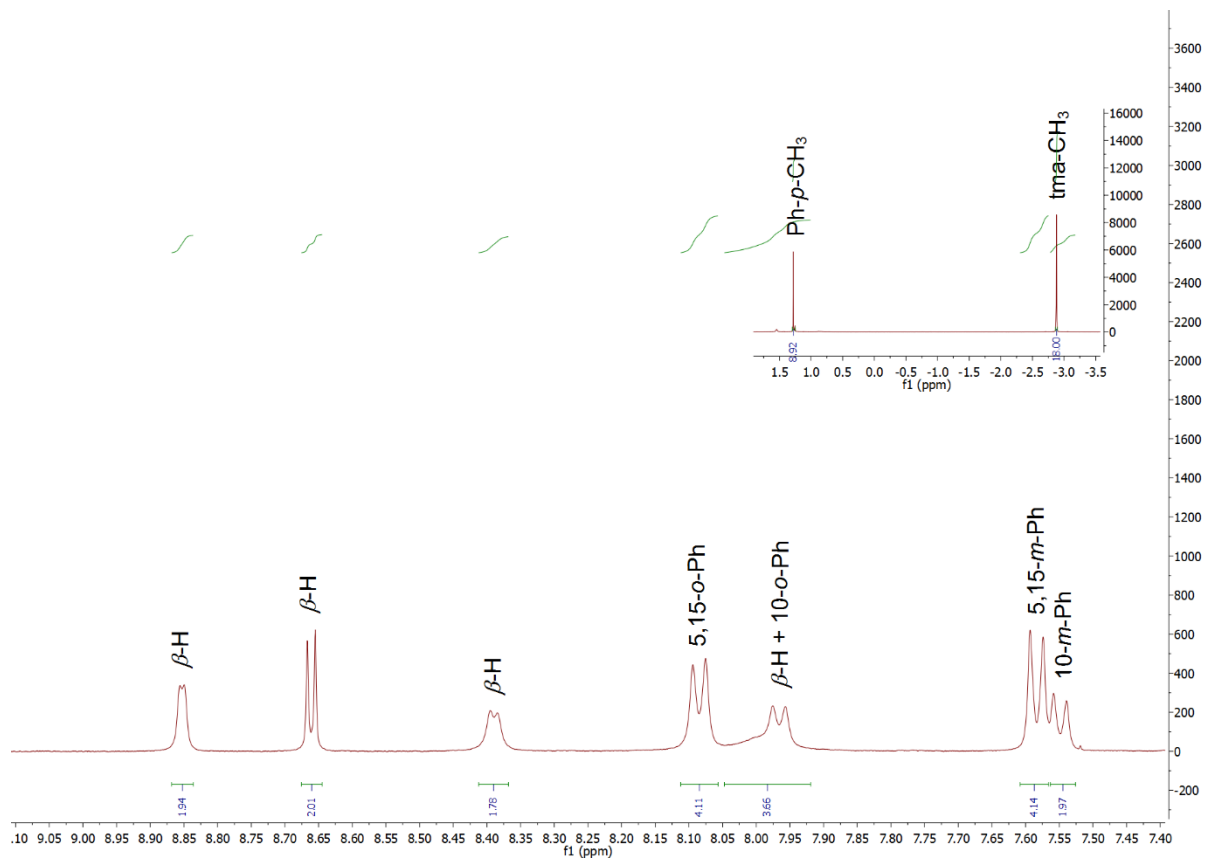


Figure 25. ^1H NMR spectrum of $\text{Ir}[\text{TpMePC}]\text{tma}_2$ in chloroform-*d*.

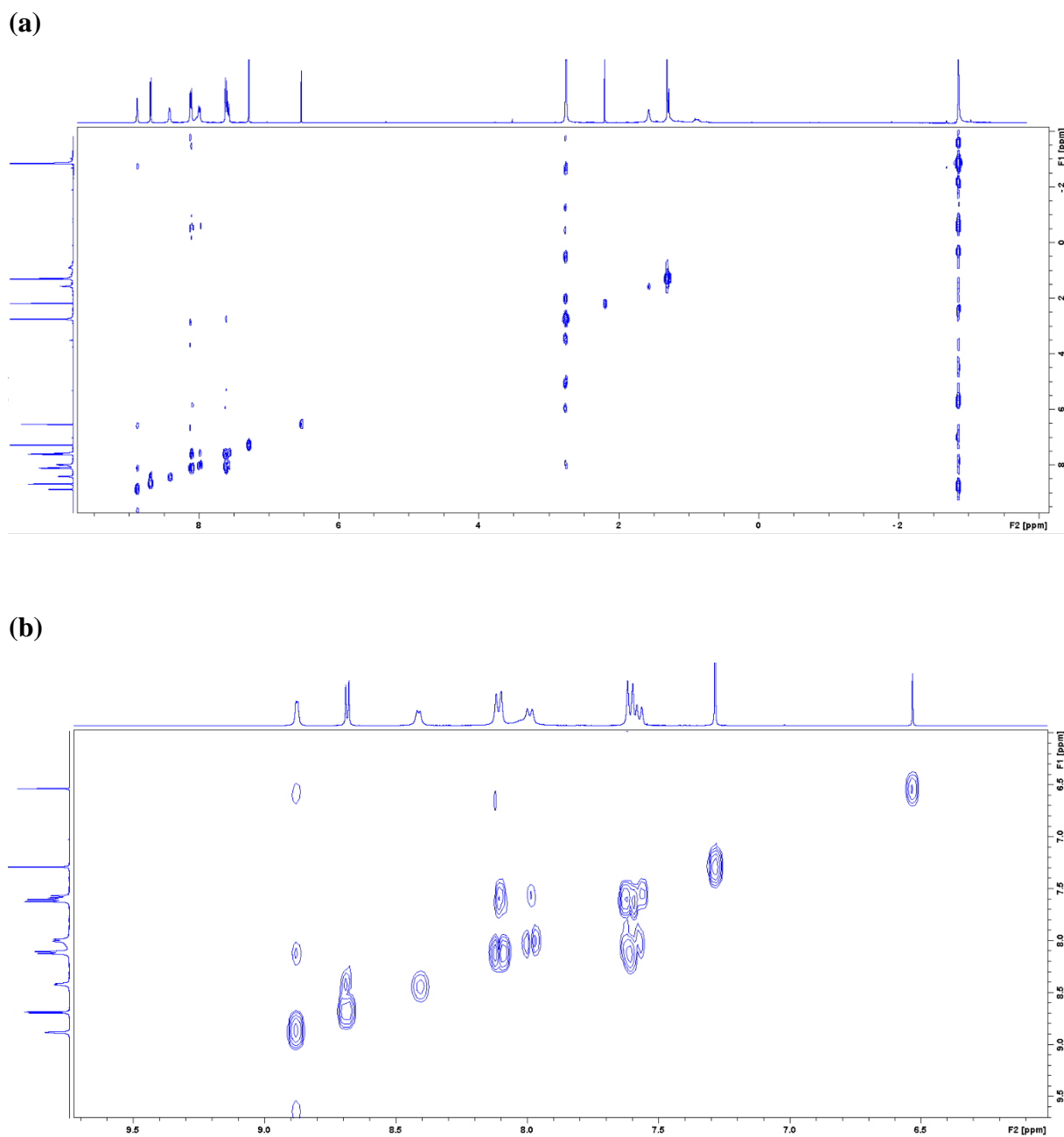


Figure 26. (a) COSY of Ir[*TpMePC*]tma₂ in chloroform-*d*. (b) Close-up of aromatic area.

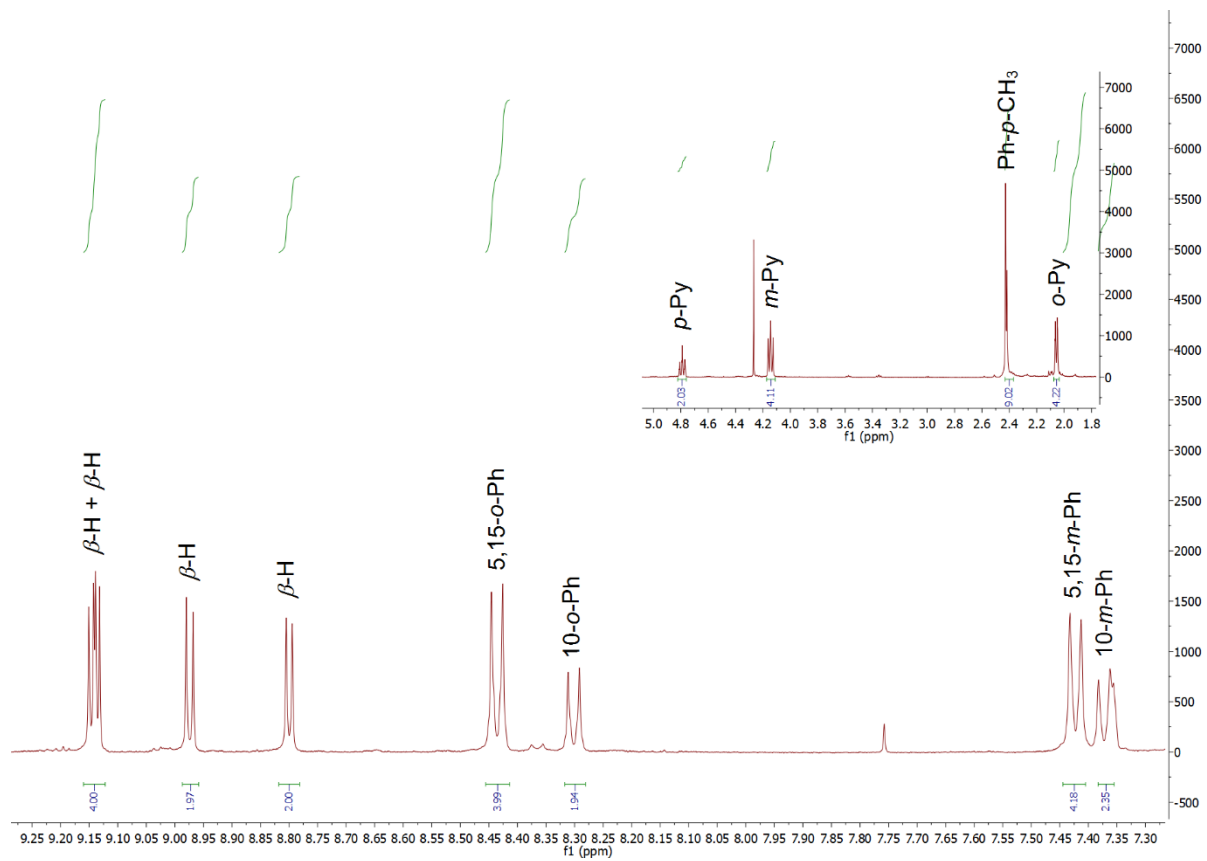


Figure 27. ^1H NMR spectrum of $\text{Ir}[\text{TpMePC}]\text{py}_2$ in $\text{benzene-}d_6$.

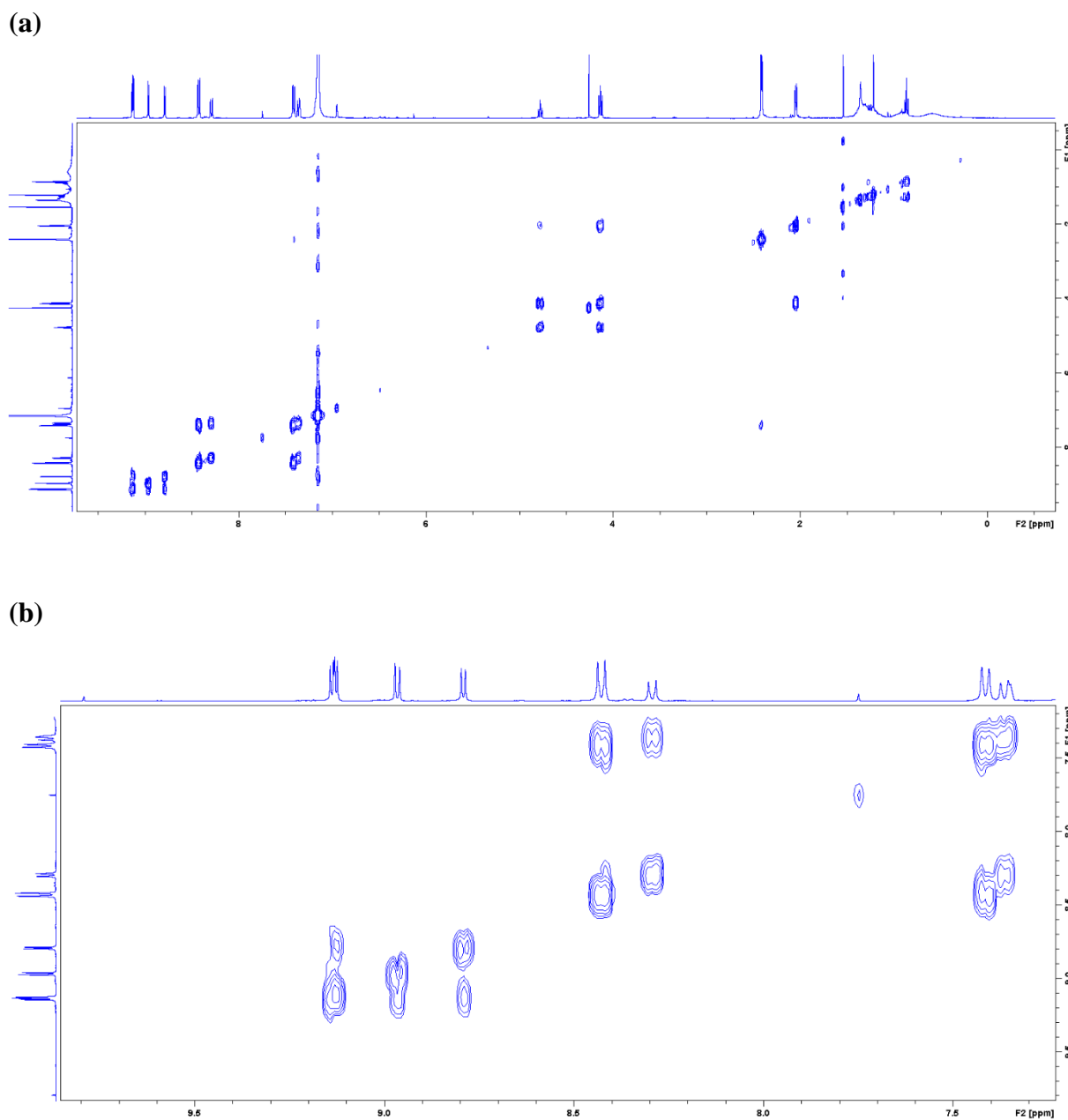


Figure 28. (a) COSY of Ir[TpMePC]py₂ in benzene-*d*₆. (b) Close-up of aromatic area.

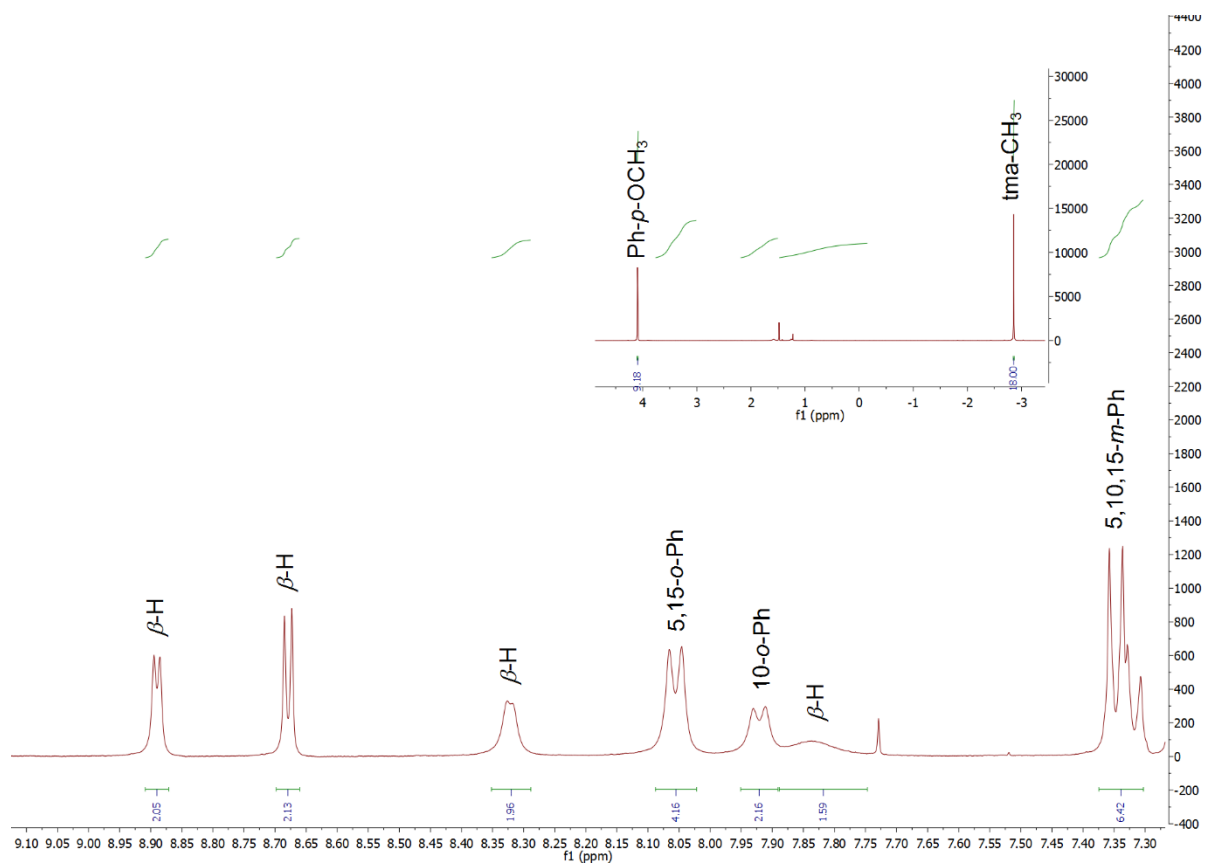


Figure 29. ^1H NMR spectrum of $\text{Ir}[\text{TpOMePC}]\text{tma}_2$ in chloroform-*d*.

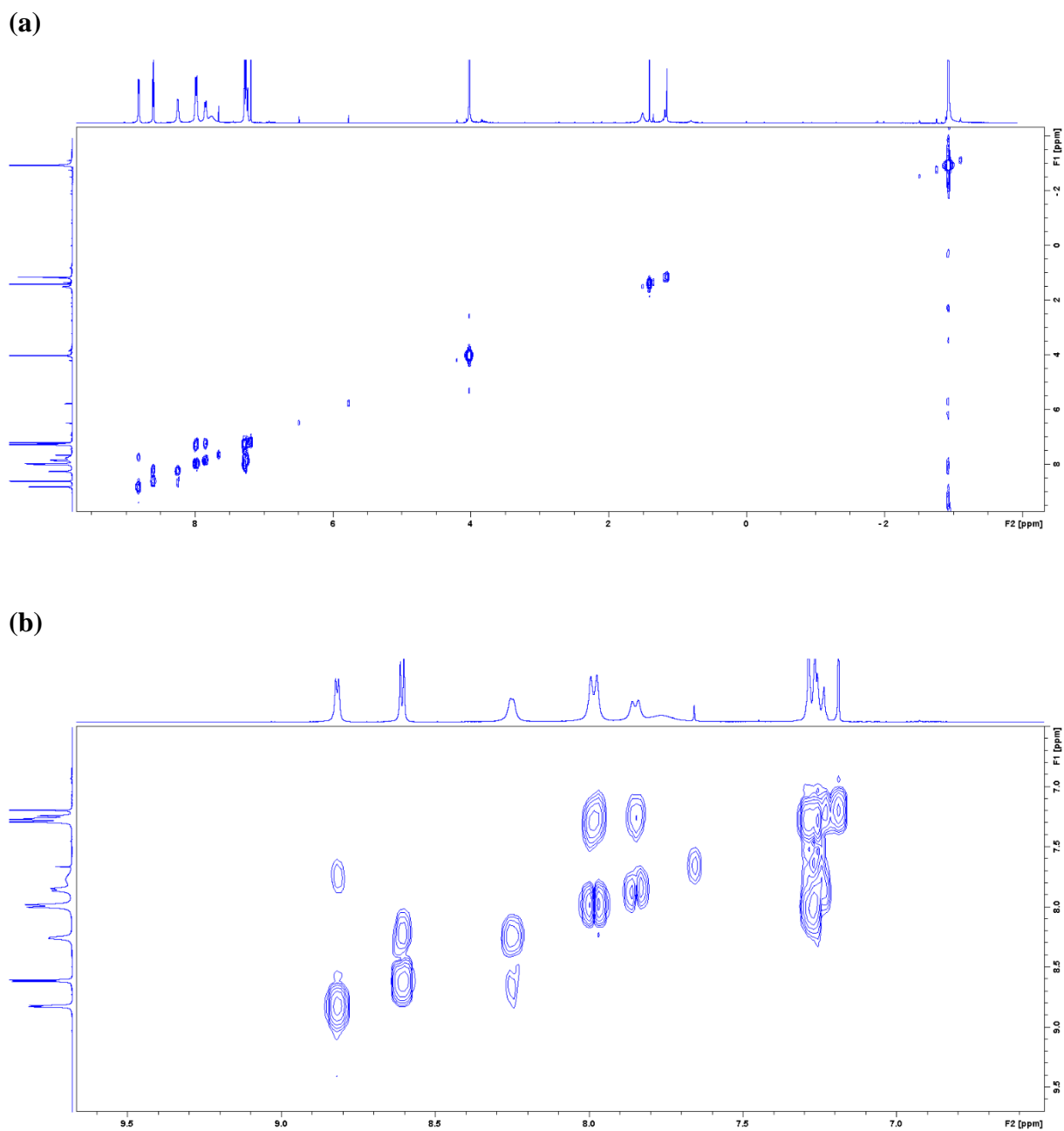


Figure 30. (a) COSY of Ir[TpOMePC]tma₂ in chloroform-*d*. (b) Close-up of aromatic area.

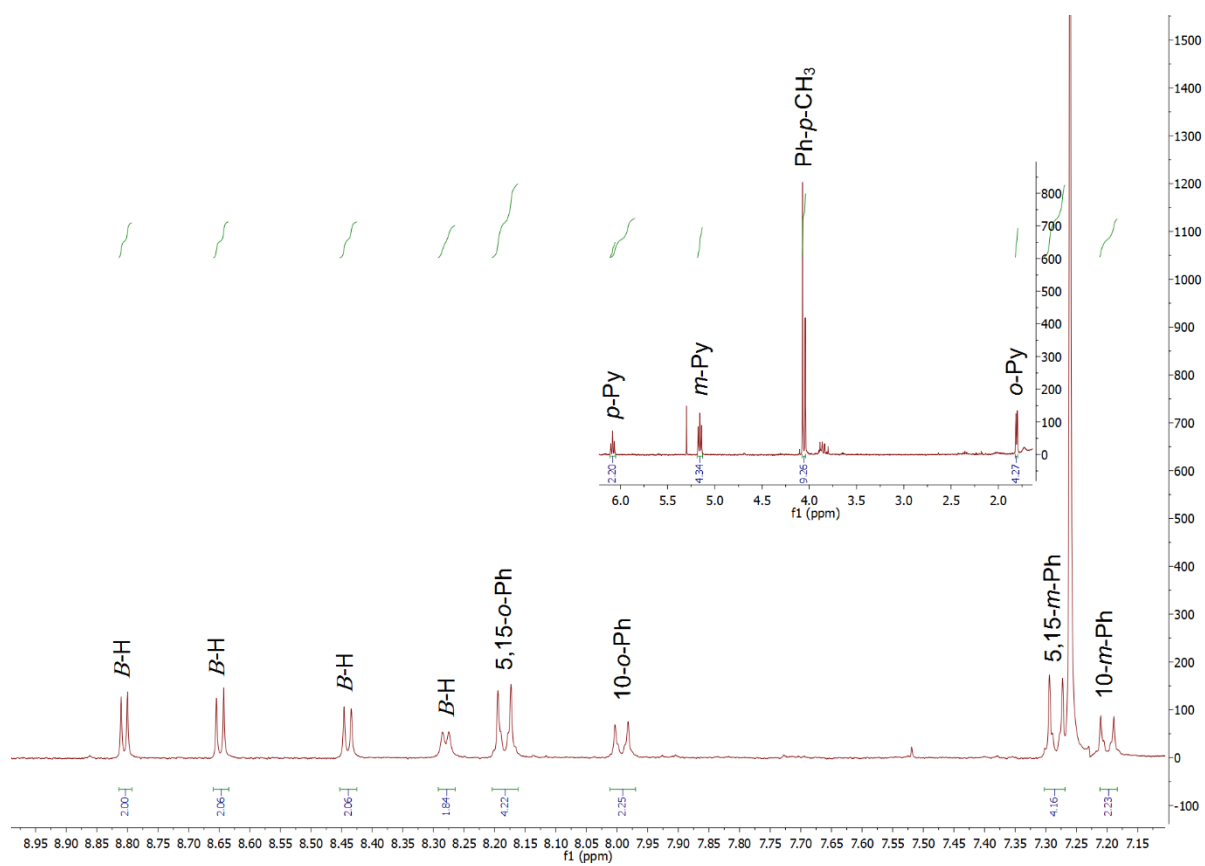


Figure 31. ^1H NMR spectrum of $\text{Ir}[\text{TpOMePC}]\text{py}_2$ in $\text{benzene-}d_6$.

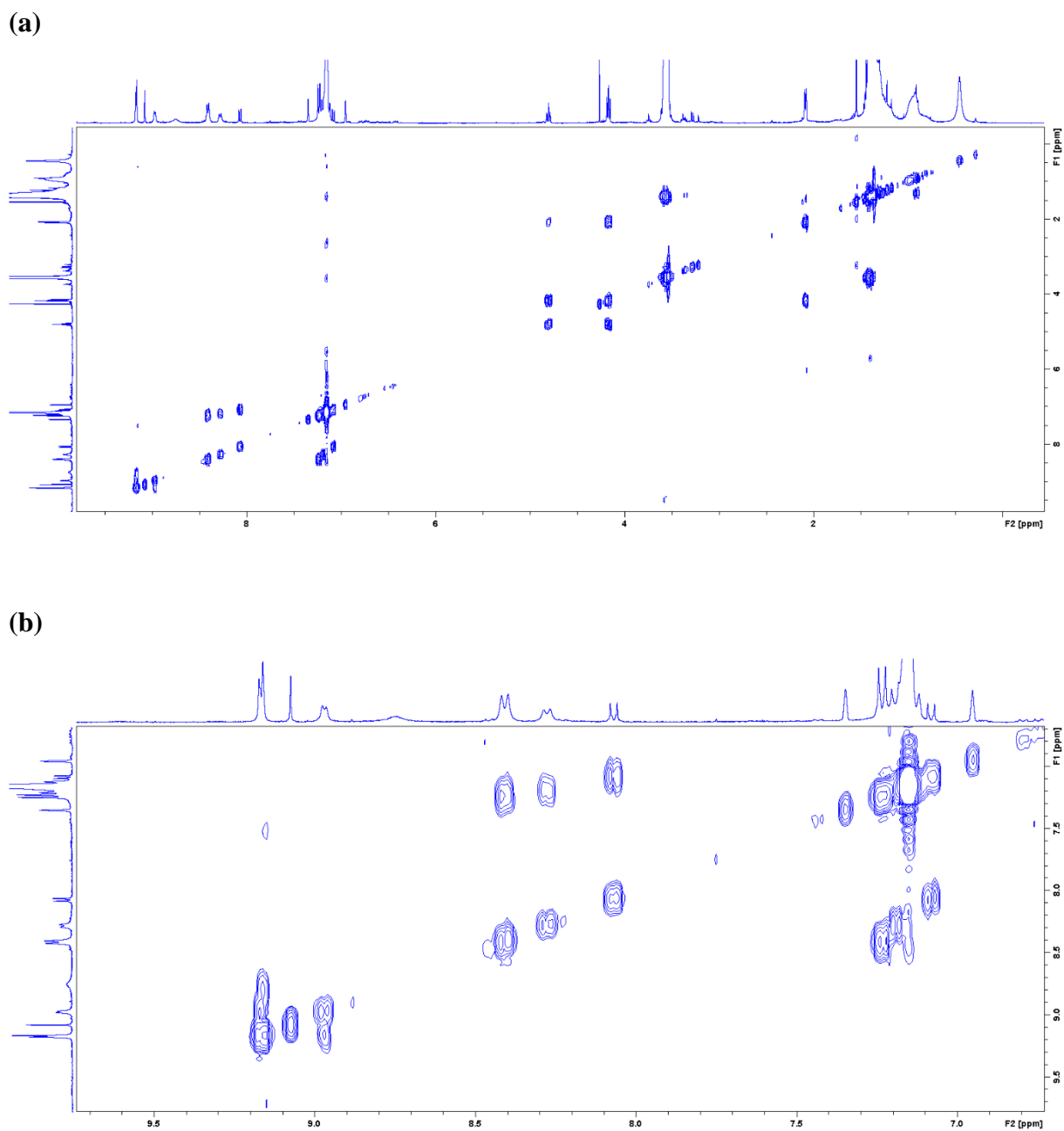


Figure 32. (a) COSY of Ir[TpOMePC]py₂ in benzene-*d*₆. (b) Close-up of aromatic area.

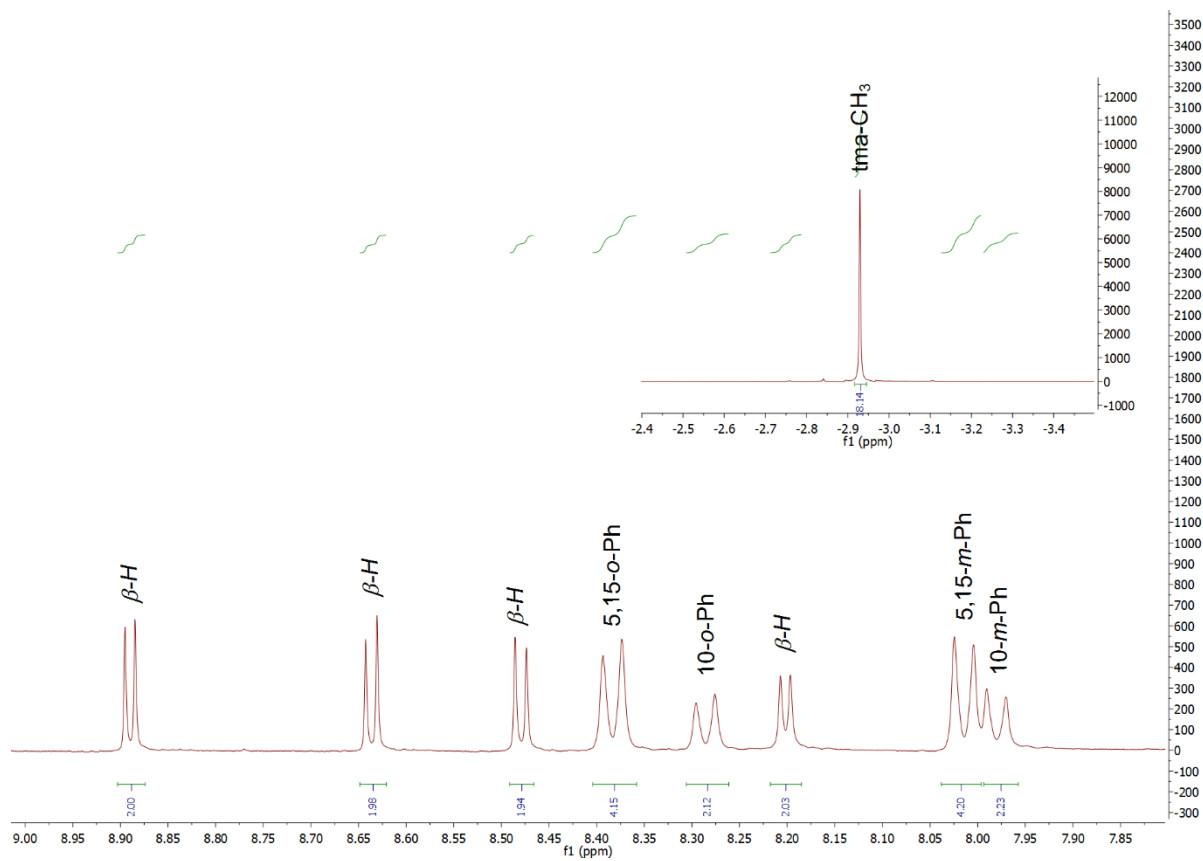


Figure 33. ^1H NMR spectrum of $\text{Ir}[\text{TpCF}_3\text{PC}]\text{tma}_2$ in chloroform-*d*.

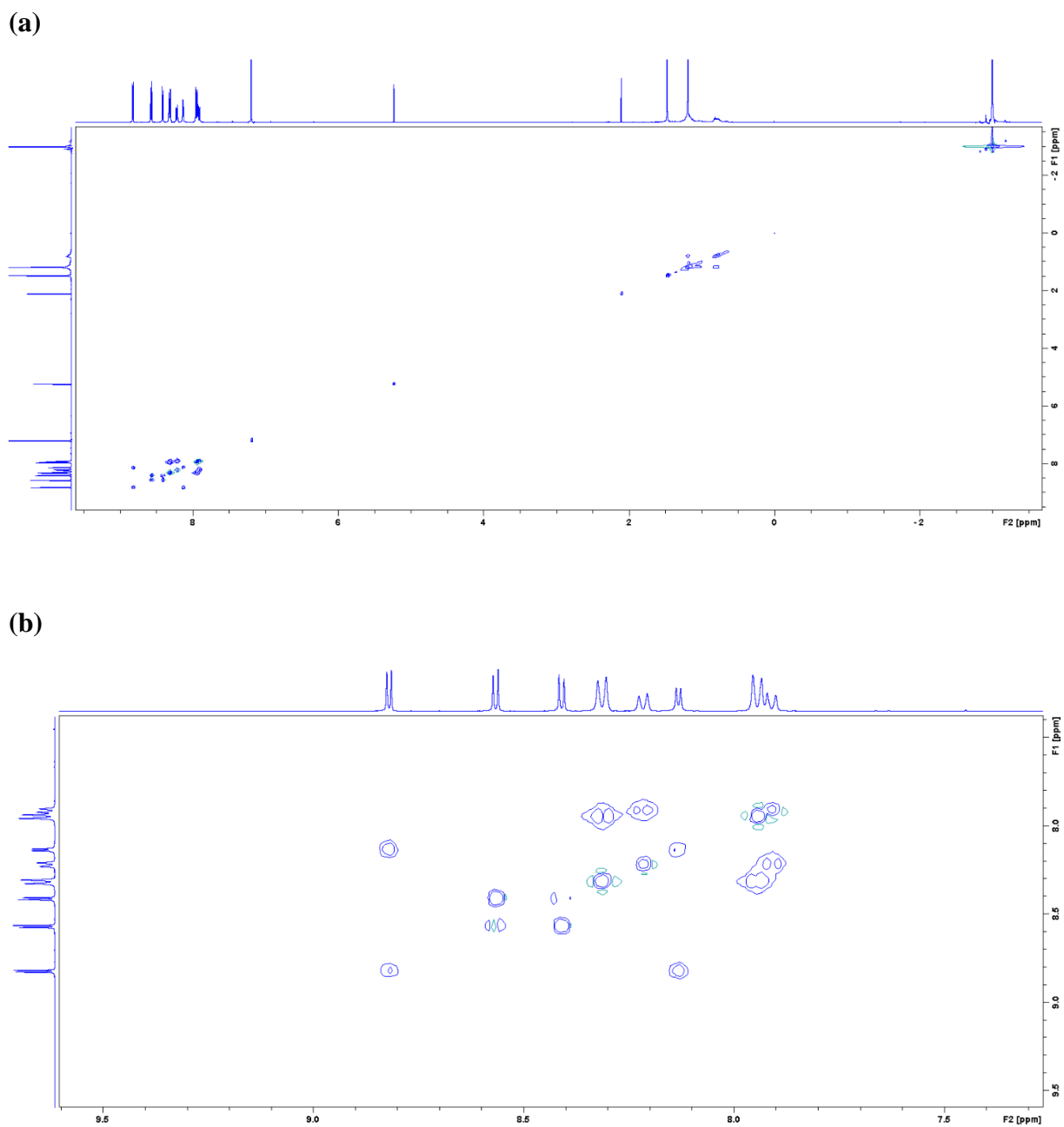


Figure 34. (a) COSY of Ir[TpCF₃PC]tma₂ in chloroform-*d*. (b) Close-up of aromatic area.

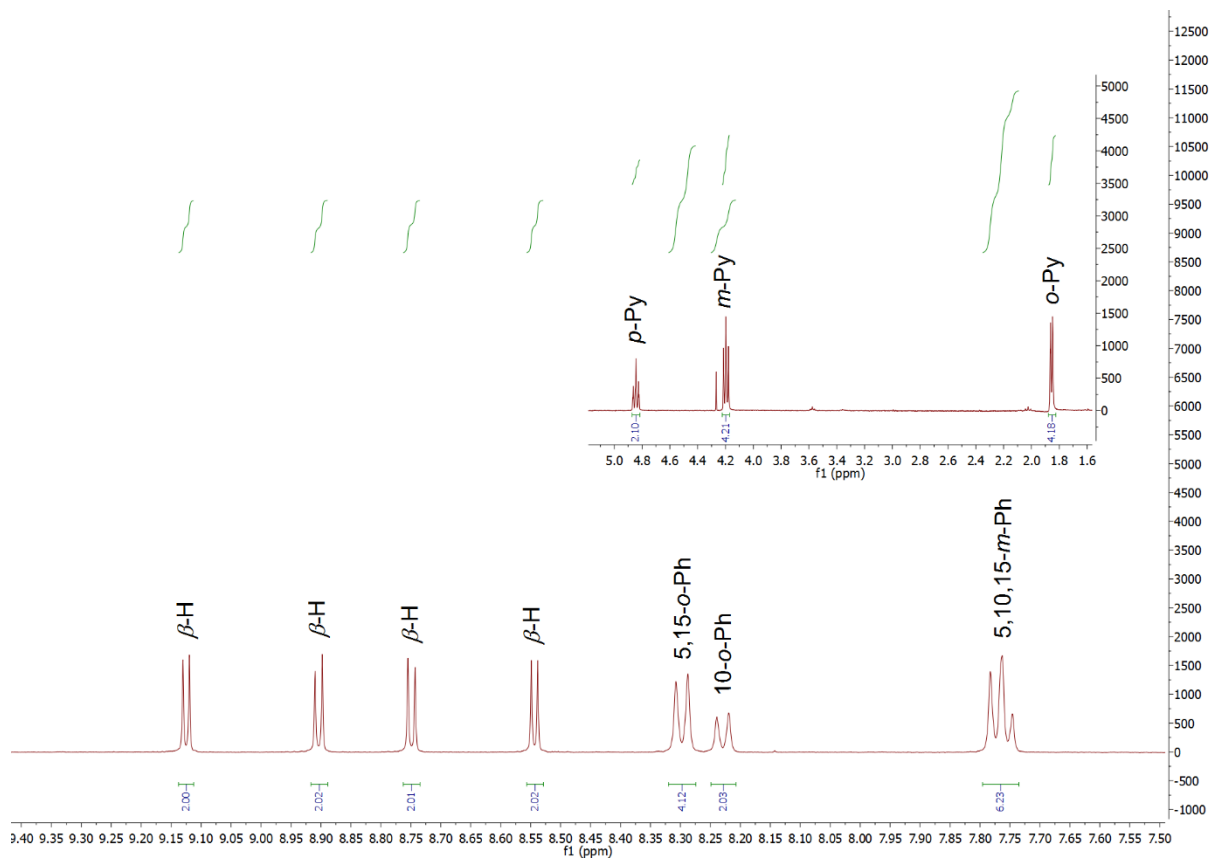


Figure 35. ^1H NMR spectrum of $\text{Ir}[\text{TpCF}_3\text{PC}]\text{py}_2$ in $\text{benzene-}d_6$.

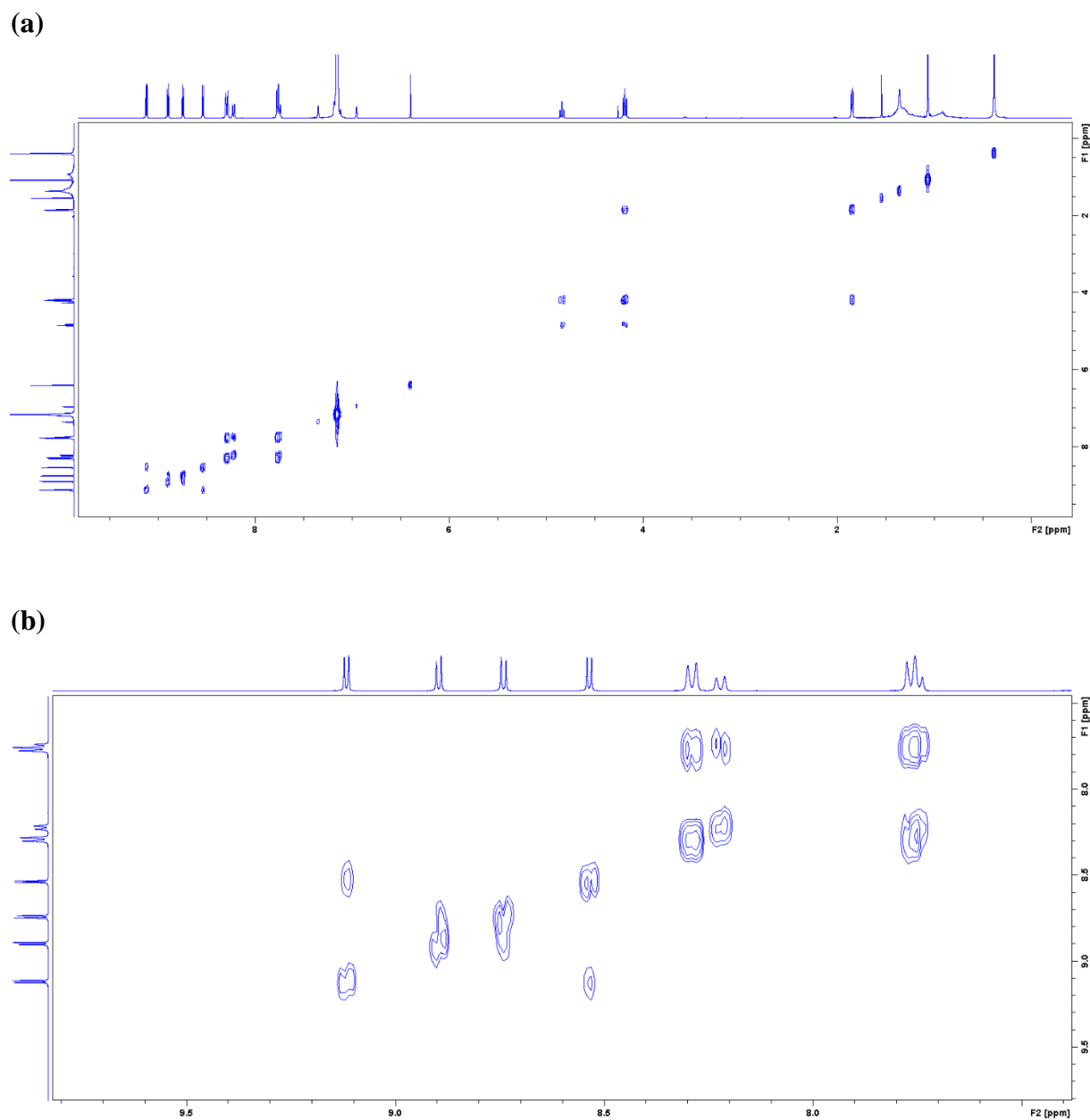


Figure 36. (a) COSY of Ir[TpCF₃PC]py₂ in benzene-*d*₆. (b) Close-up of aromatic area.

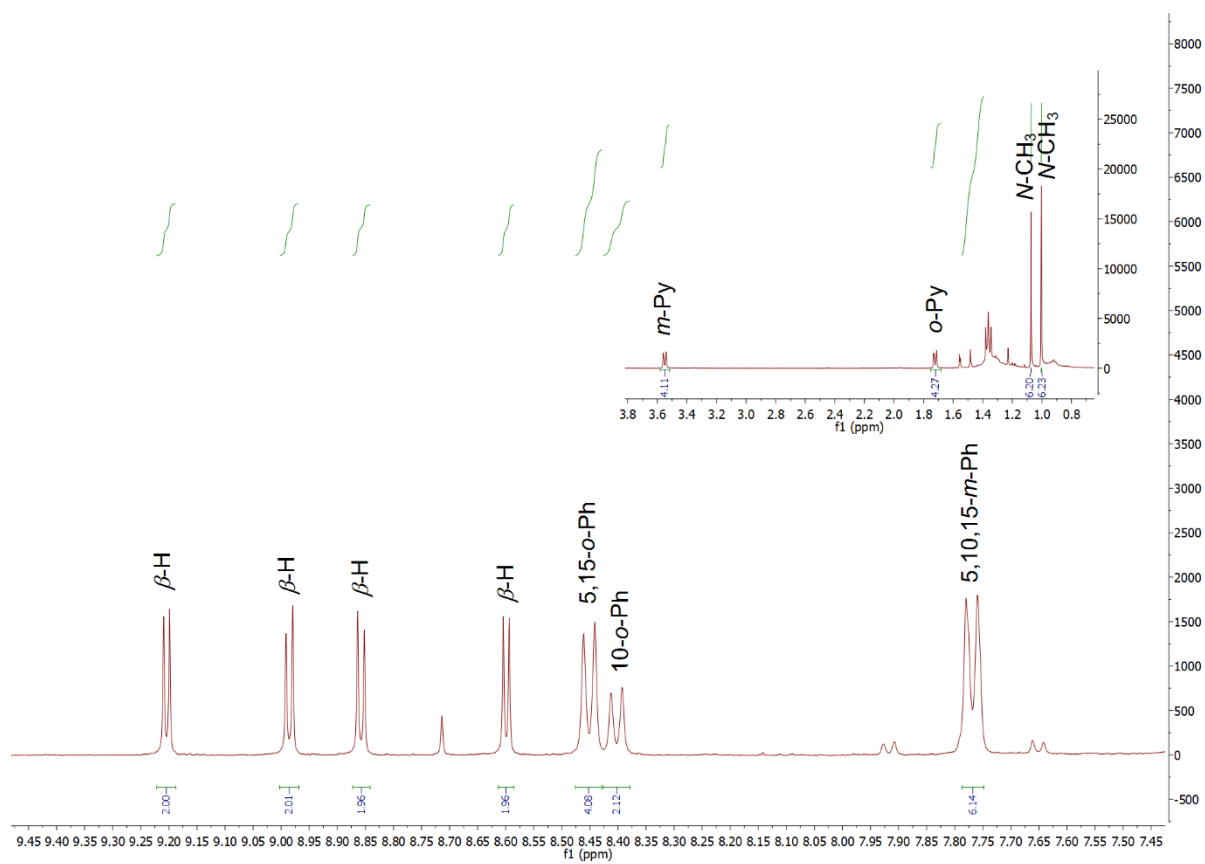


Figure 37. ¹H NMR spectrum of Ir[TpCF₃PC]dmap₂ in benzene-*d*₆.

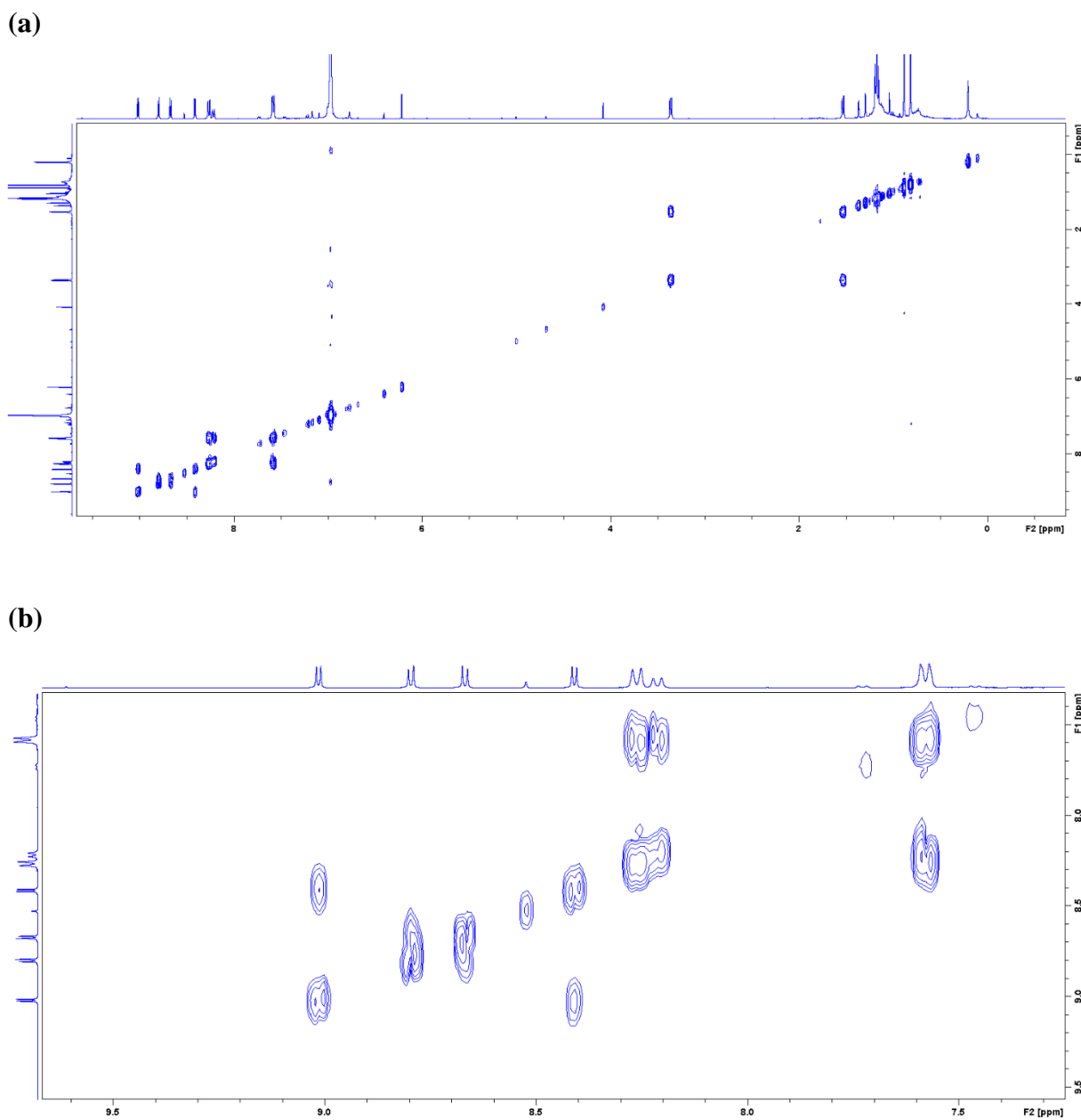


Figure 38. (a) COSY of Ir[TpCF₃PC]dmap₂ in benzene-*d*₆. (b) Close-up of aromatic area.

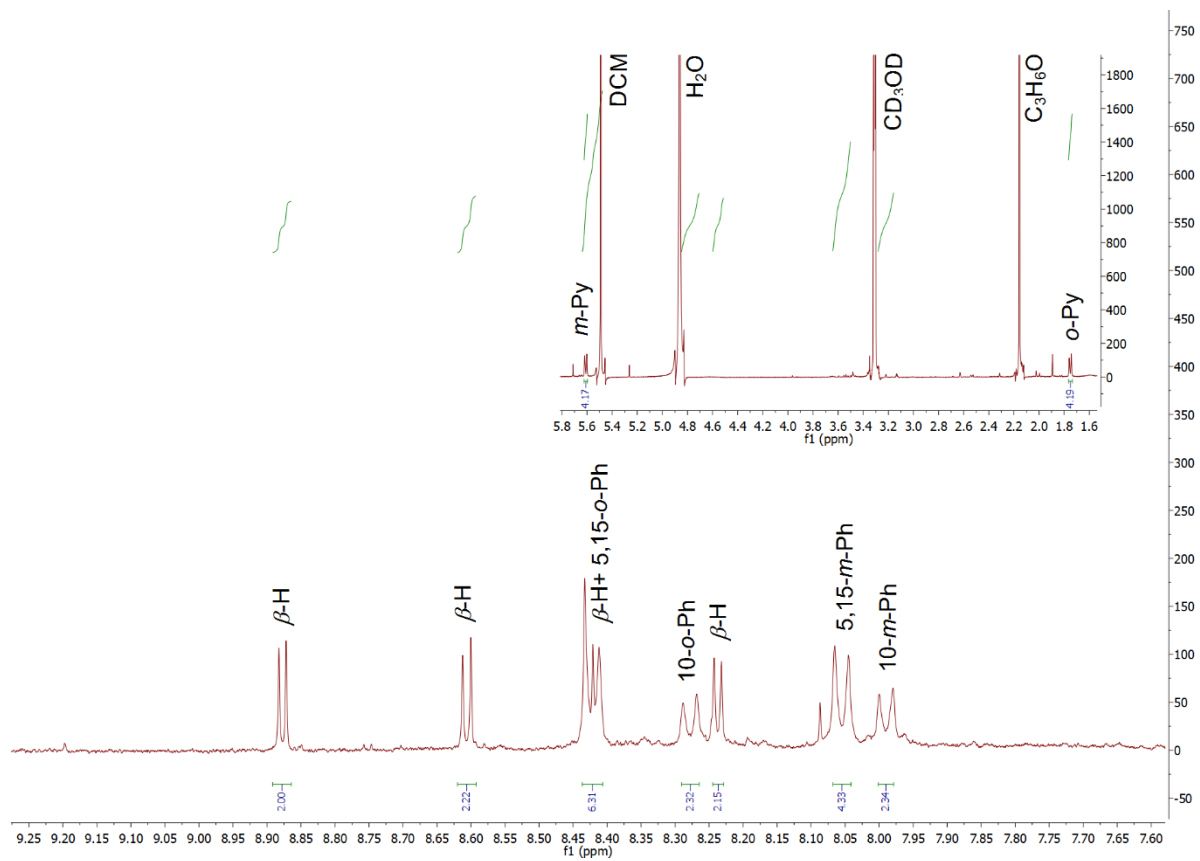


Figure 39. ¹H NMR spectrum of Ir[TpCF₃PC]4pa₂ in methanol-*d*₄.

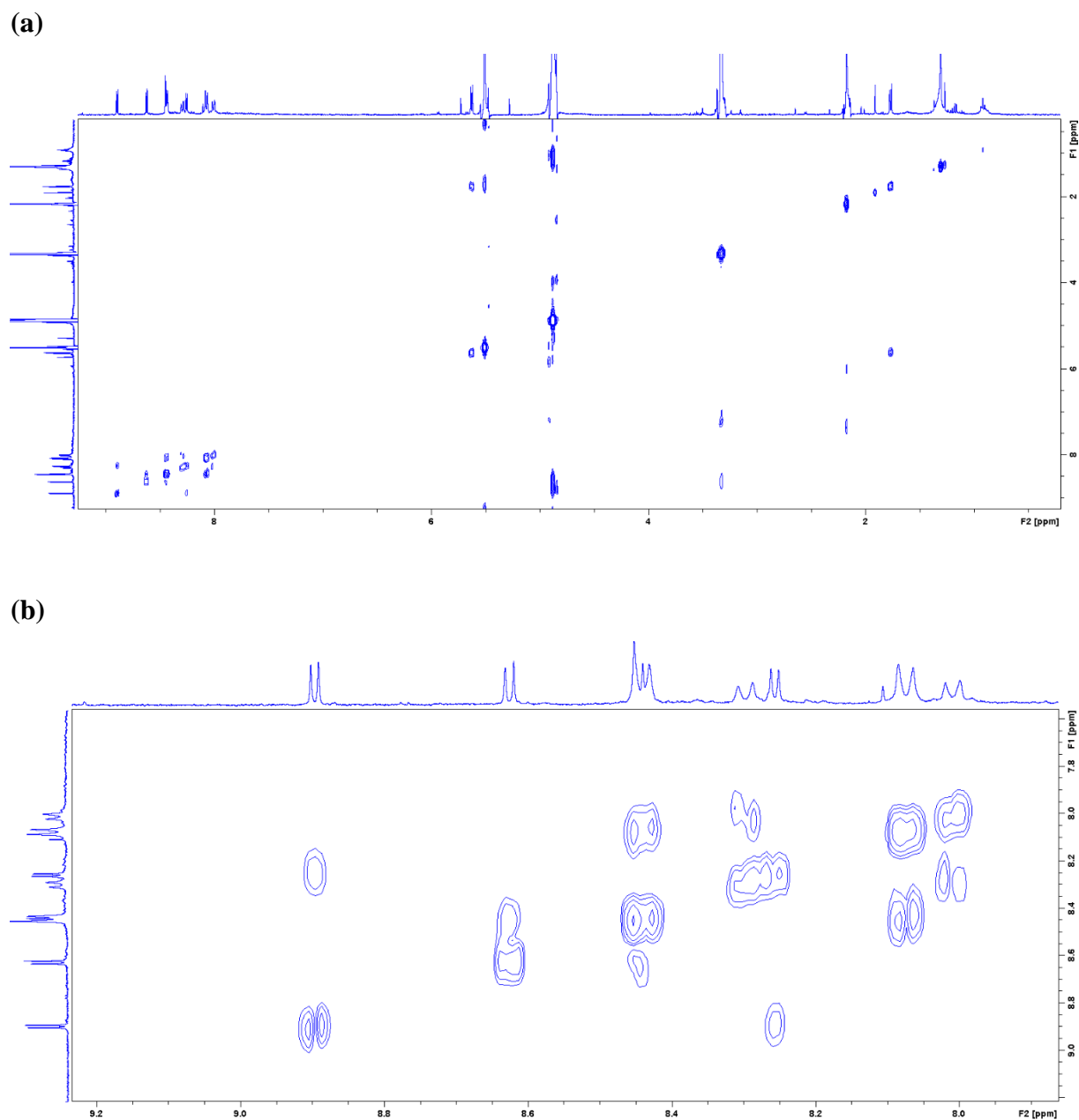


Figure 40. (a) COSY of Ir[TpCF₃PC]4pa₂ in methanol-*d*₄. (b) Close-up of aromatic area.

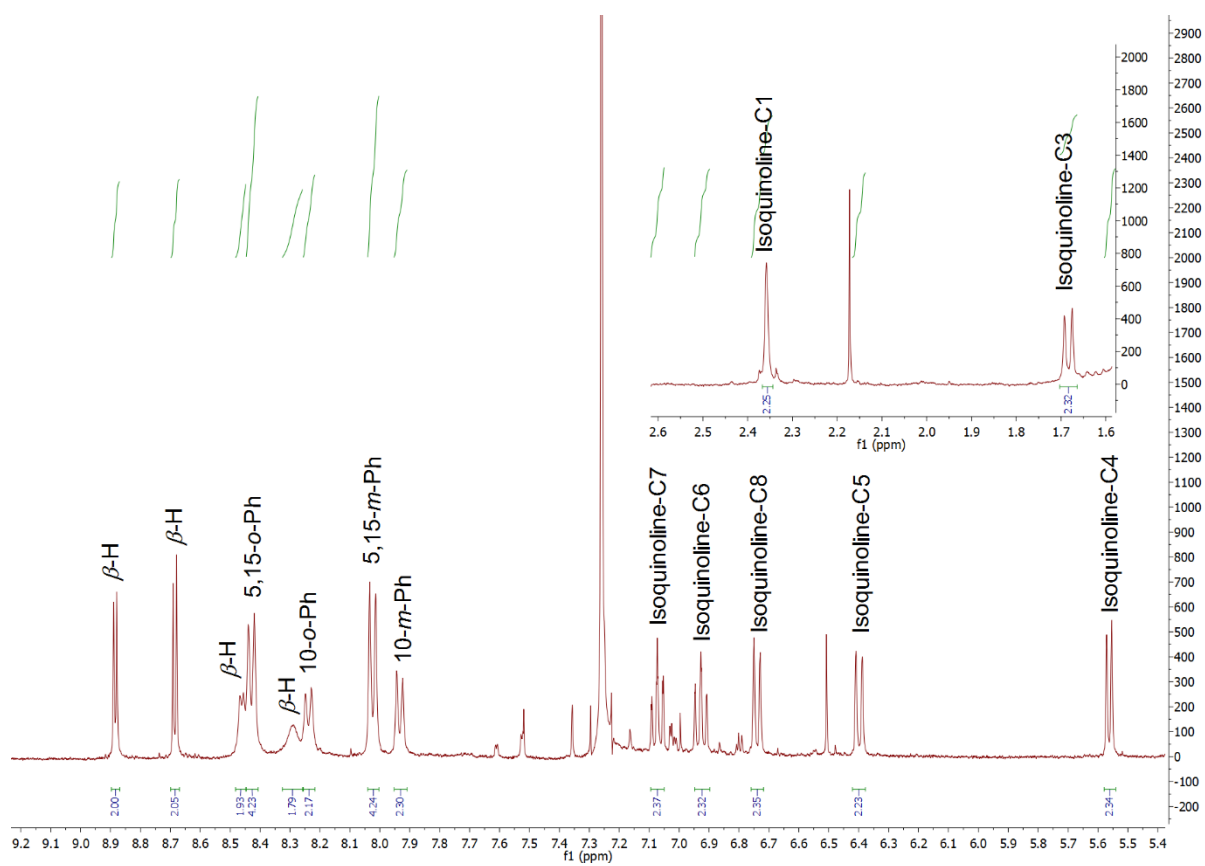


Figure 41. ^1H NMR spectrum of $\text{Ir}[\text{TpCF}_3\text{PC}]\text{isoq}_2$ in chloroform-*d*.

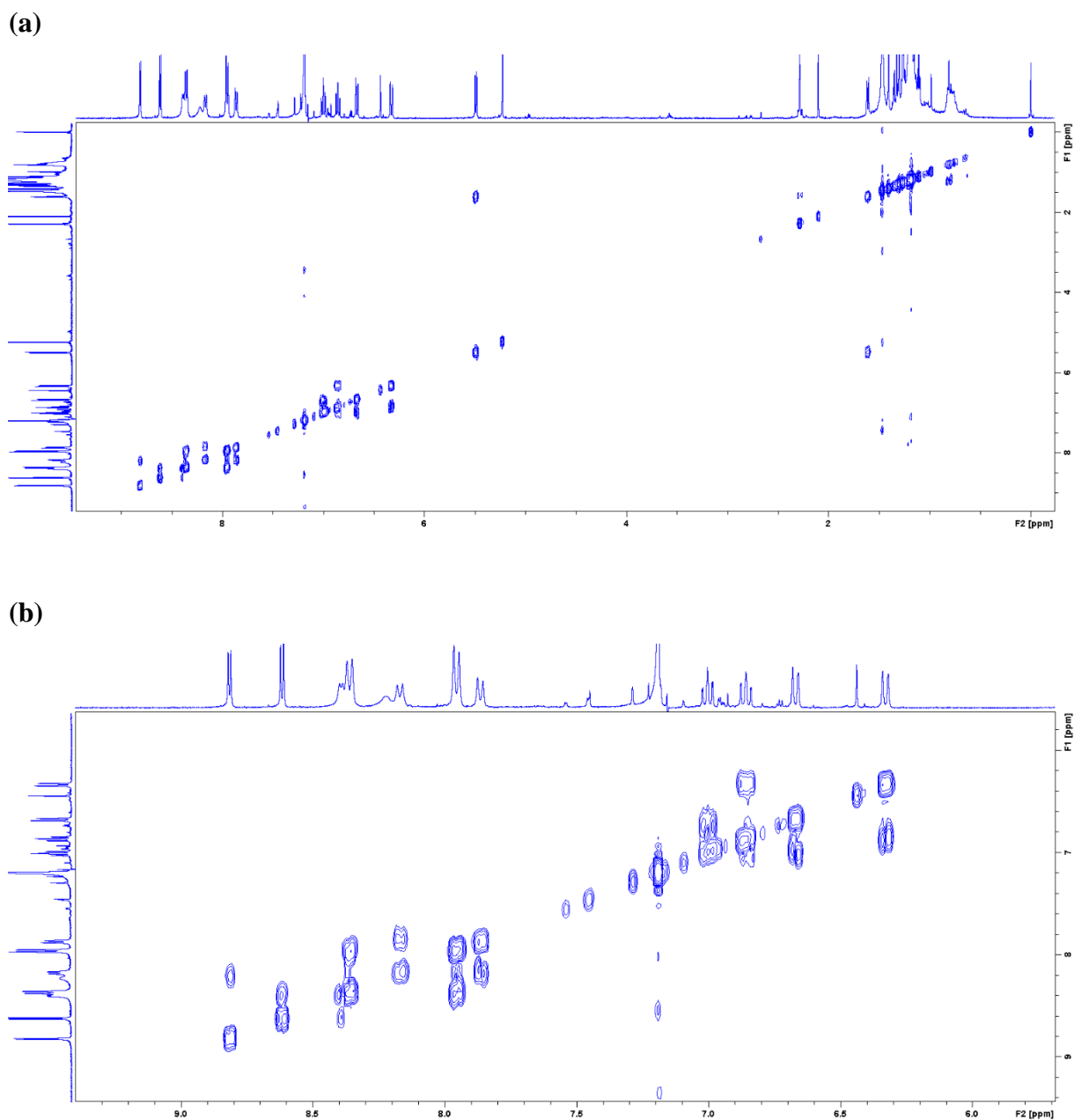


Figure 42. (a) COSY of Ir[TpCF₃PC]isoq₂ in chloroform-*d*. (b) Close-up of aromatic area.