

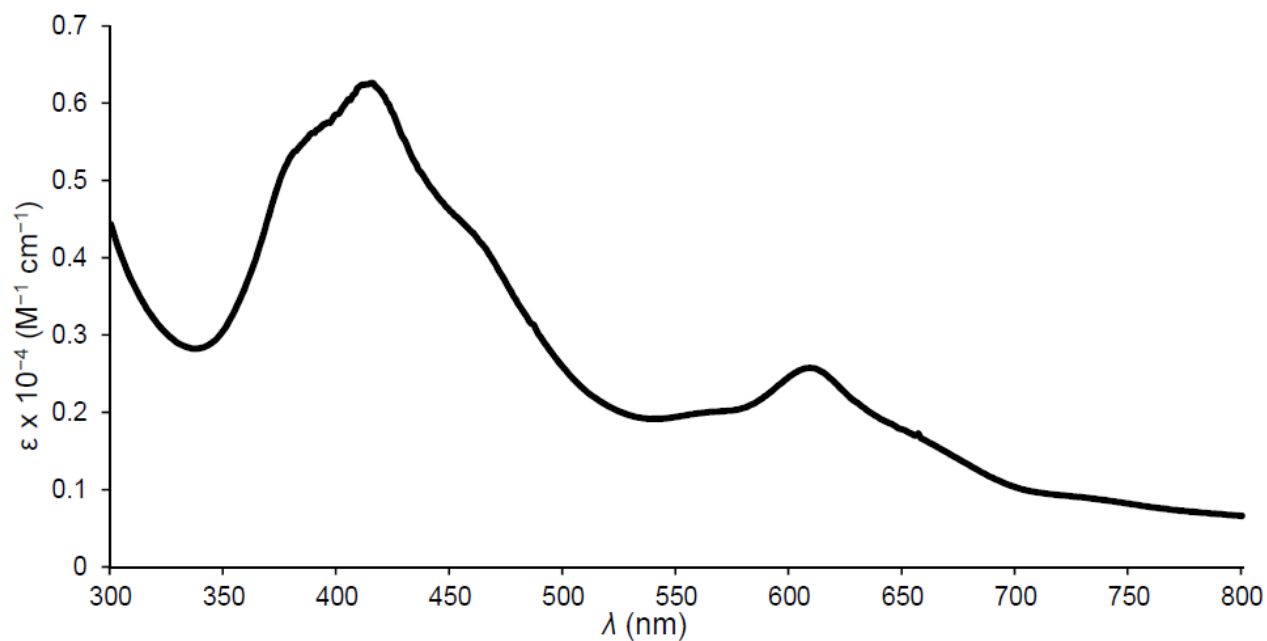
# A Simple, Axial Ligand-Mediated Route to Water-Soluble Iridium Corroles

Ivar K. Thomassen,<sup>a</sup> Daniel Rasmussen,<sup>a</sup> Rune F. Einrem<sup>a</sup> and  
Abhik Ghosh<sup>\*,a</sup>

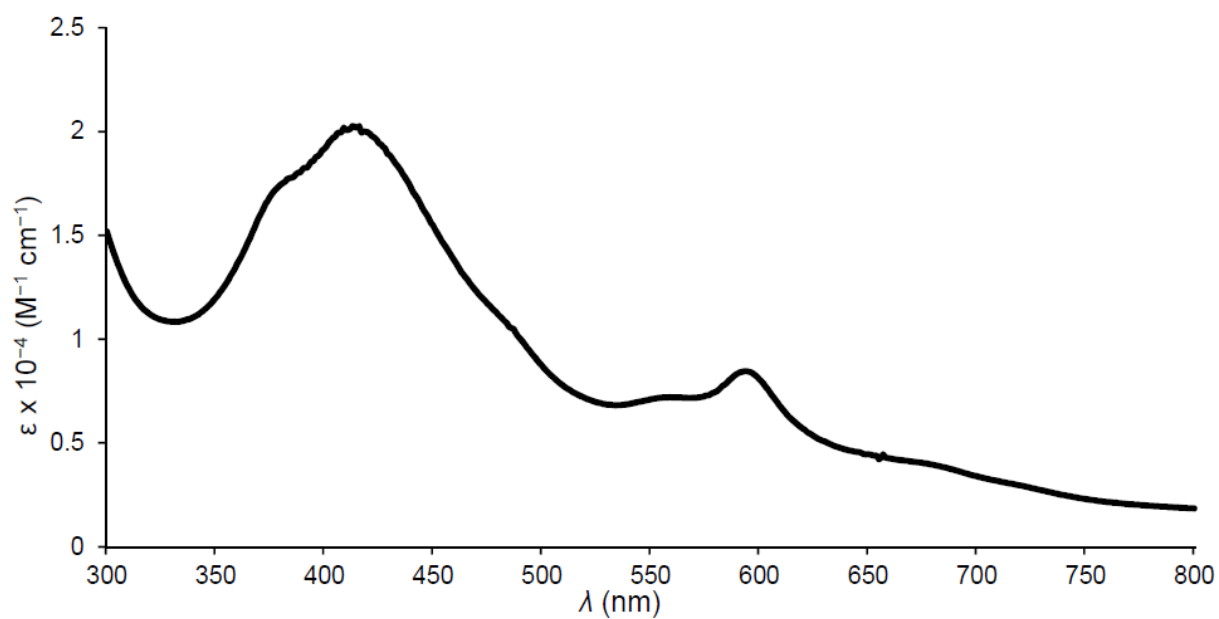
Department of Chemistry, UiT – The Arctic University of Norway, N-9037 Tromsø, Norway;  
Email: [abhik.ghosh@uit.no](mailto:abhik.ghosh@uit.no).

| <b>Contents</b>     | <b>Page</b> |
|---------------------|-------------|
| A. UV-vis spectra   | S2          |
| B. ESI mass spectra | S4          |
| C. NMR spectra      | S10         |

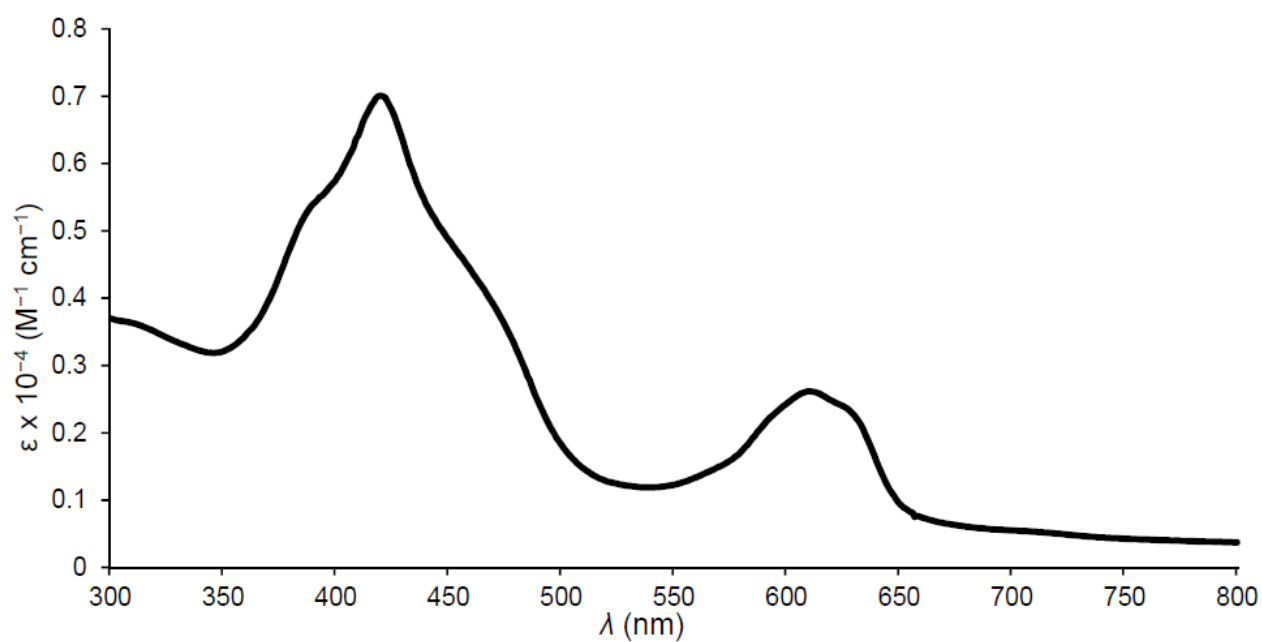
## A. UV-Vis spectra



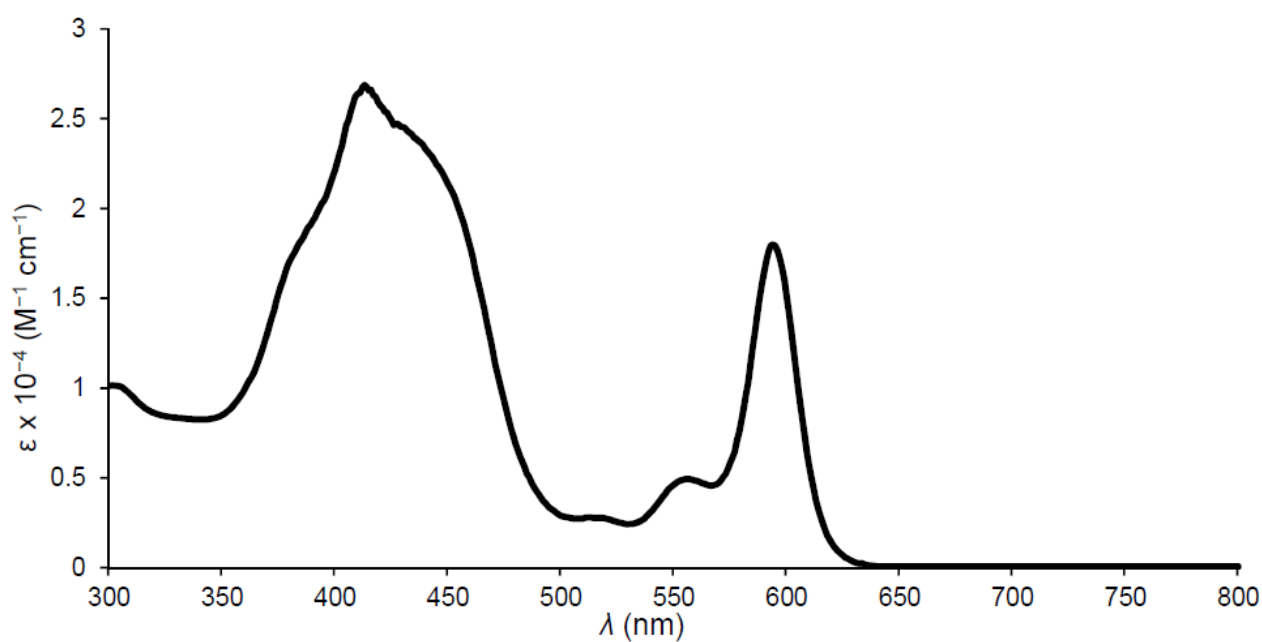
**Figure S1.** UV-vis spectrum of Ir[(TpOMePC)](tcep) in methanol.



**Figure S2.** UV-vis spectrum of Ir[TpOMePC](tppts) in methanol.



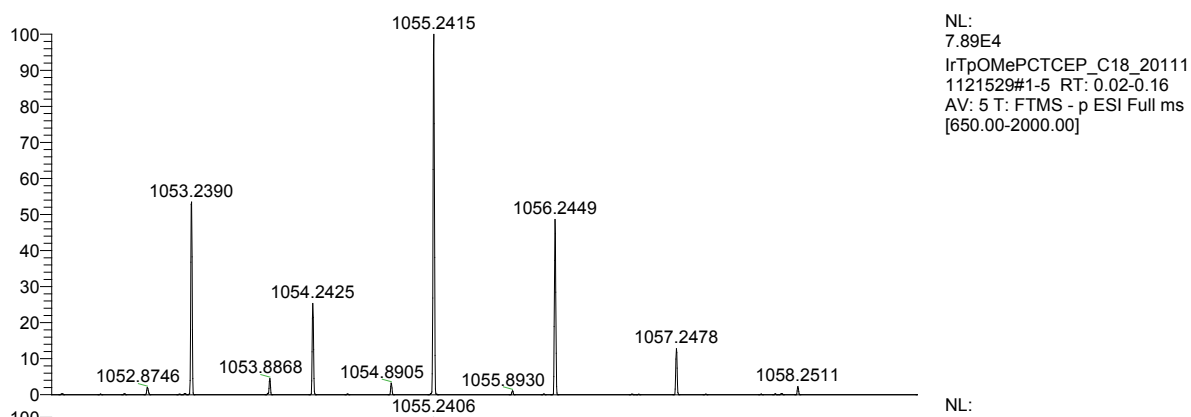
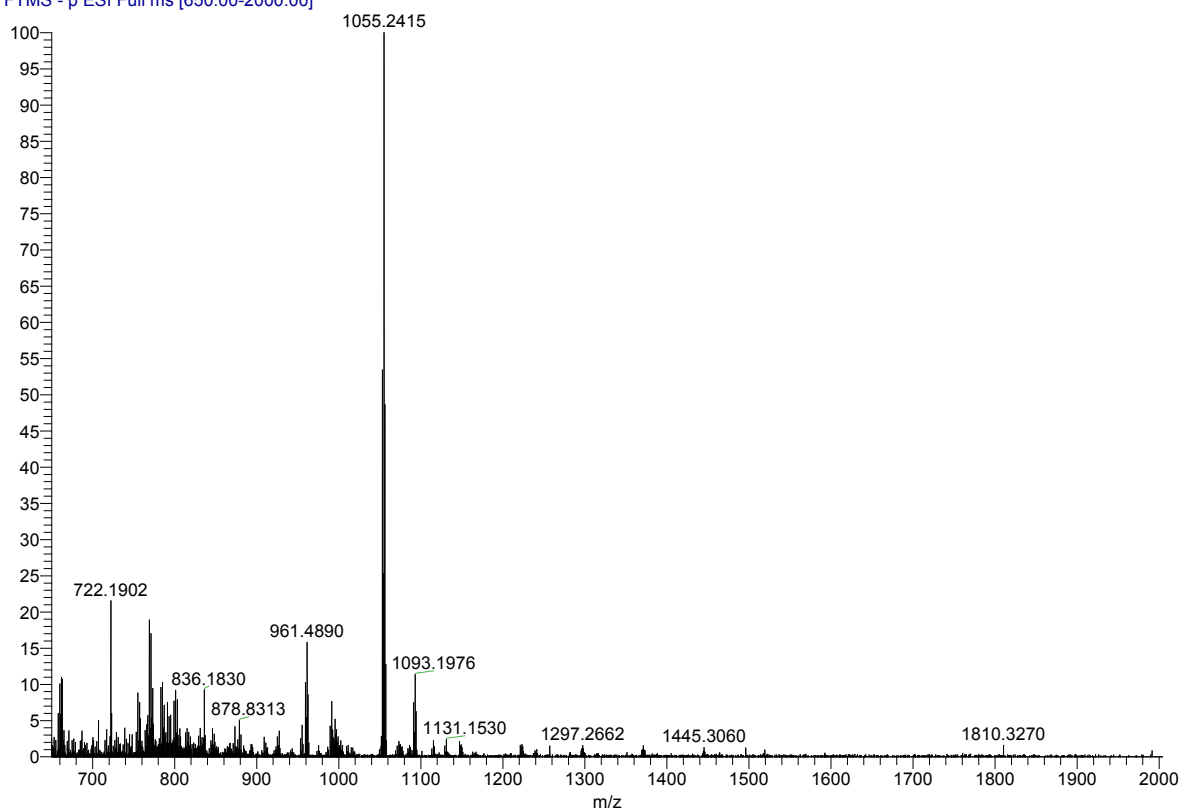
**Figure S3.** UV-vis spectrum of Ir[TpCF<sub>3</sub>PC](tcep) in methanol.



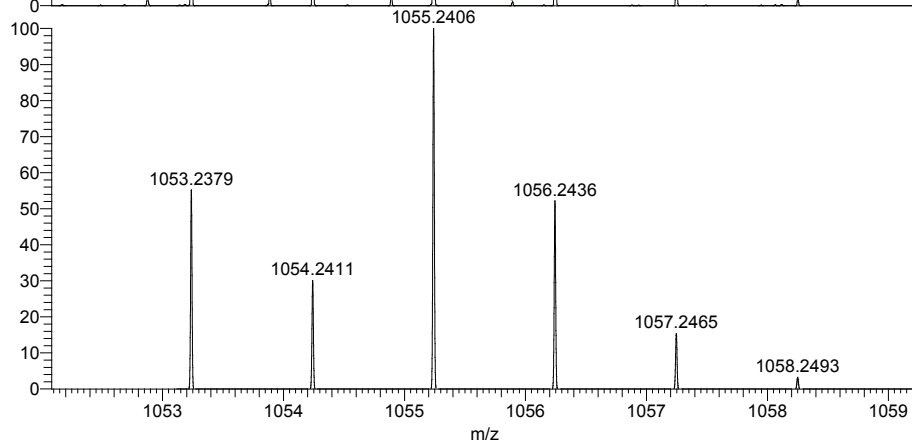
**Figure S4.** UV-vis spectrum of Ir[TpCF<sub>3</sub>PC](tppts) in methanol.

## B. ESI Mass spectra

IrTpOMePCTCEP\_C18\_201111121529 #1-5 RT: 0.02-0.16 AV: 5 NL: 7.89E4  
T: FTMS - p ESI Full ms [650.00-2000.00]



NL:  
7.89E4  
IrTpOMePCTCEP\_C18\_20111  
1121529#1-5 RT: 0.02-0.16  
AV: 5 T: FTMS - p ESI Full ms  
[650.00-2000.00]



NL:  
8.97E3  
IrC<sub>49</sub>H<sub>43</sub>N<sub>4</sub>O<sub>9</sub>P:  
Ir<sub>1</sub>C<sub>49</sub>H<sub>43</sub>N<sub>4</sub>O<sub>9</sub>P<sub>1</sub>  
p (gss, s /p:40) Chrg -1  
R: 81600 Res .Pwr . @FWHM

Figure S5. Negative-mode ESI mass spectra of Ir[TpOMePC](tcep).

IrTpOMePCPhSO3H\_neg #1-5 RT: 0.02-0.13 AV: 5 NL: 1.07E7  
T: FTMS - p ESI Full ms [200.00-2000.00]

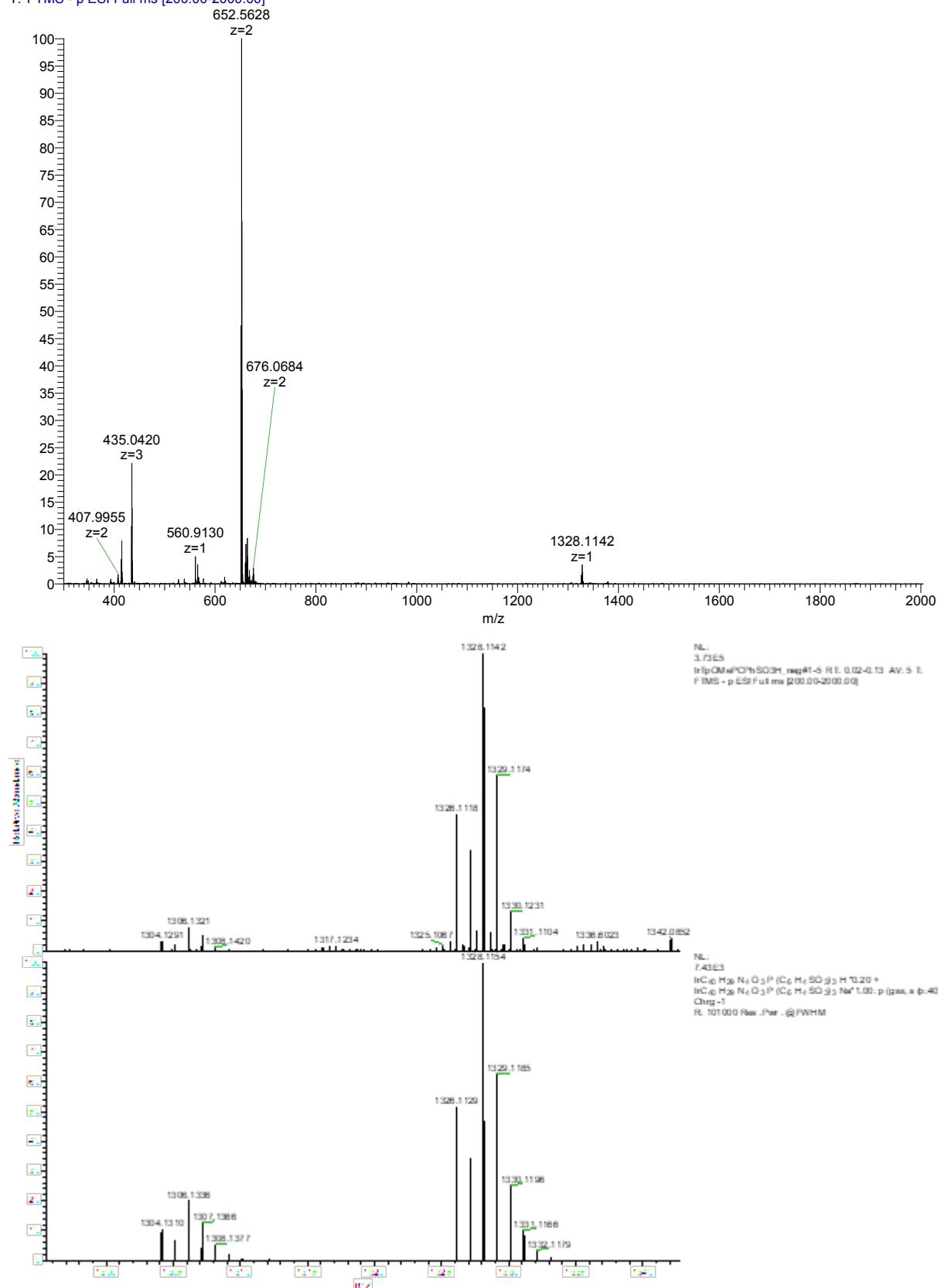


Figure S6. Negative-mode ESI mass spectra of Ir[TpOMePC](tppts) (Z=1). *Contd.*

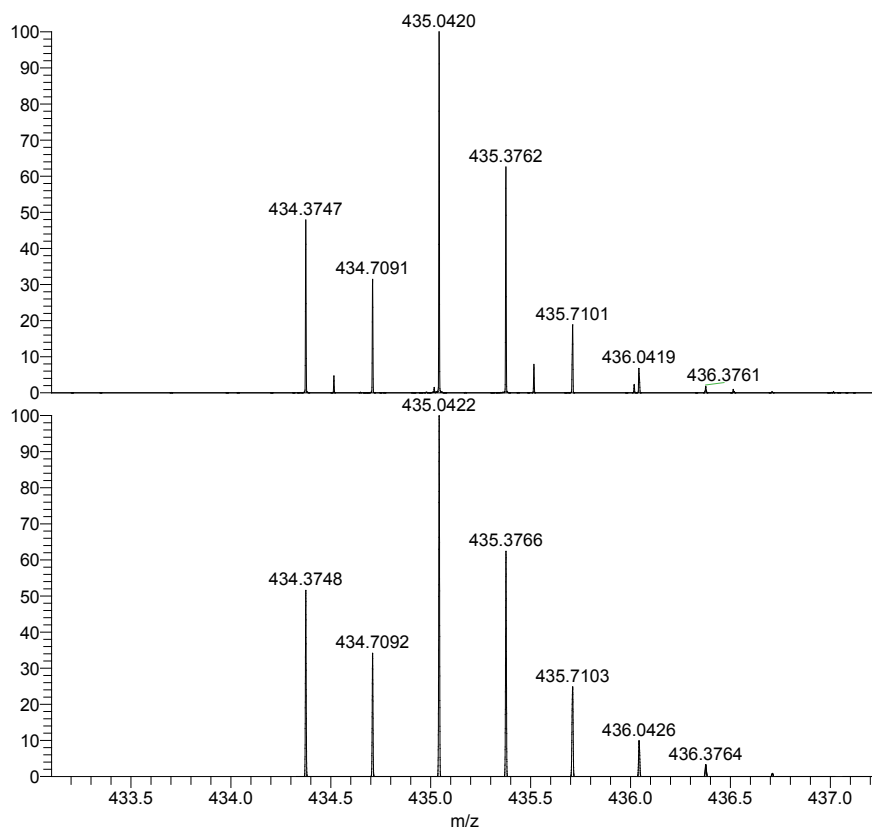
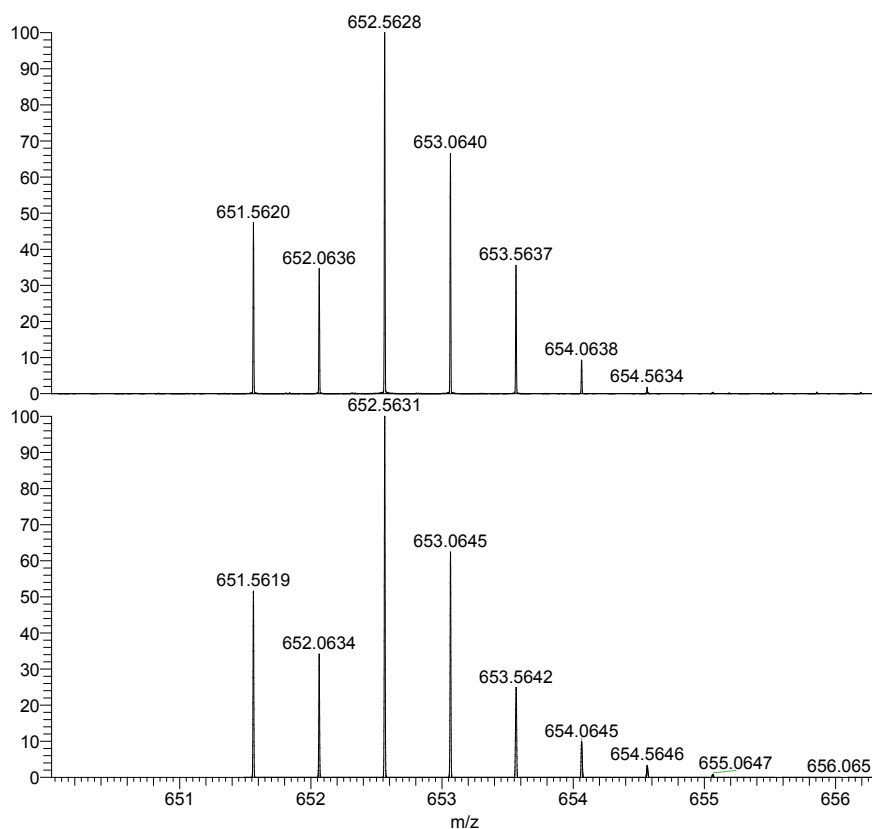
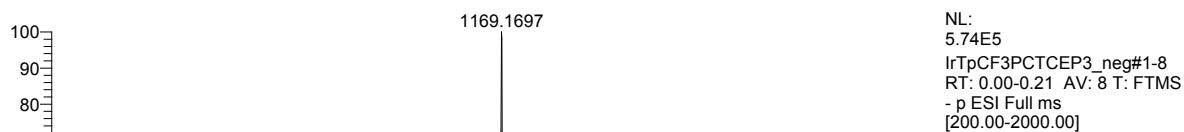
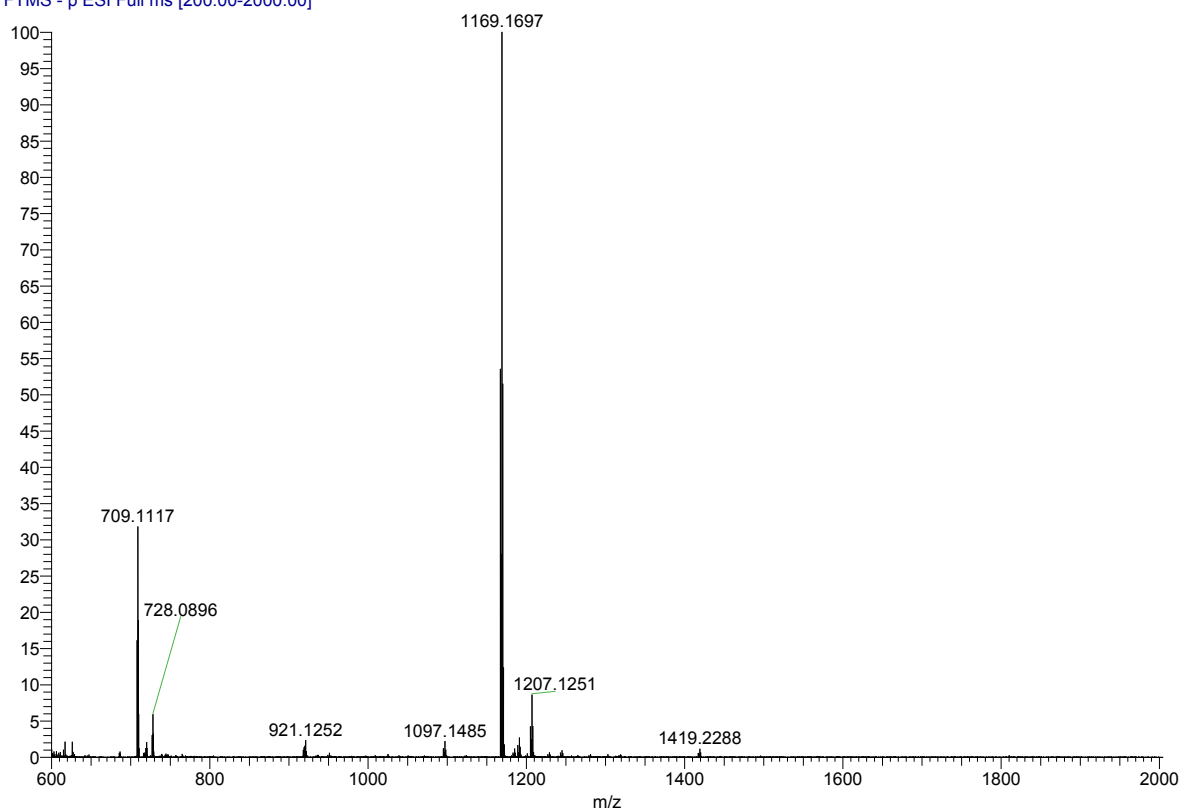
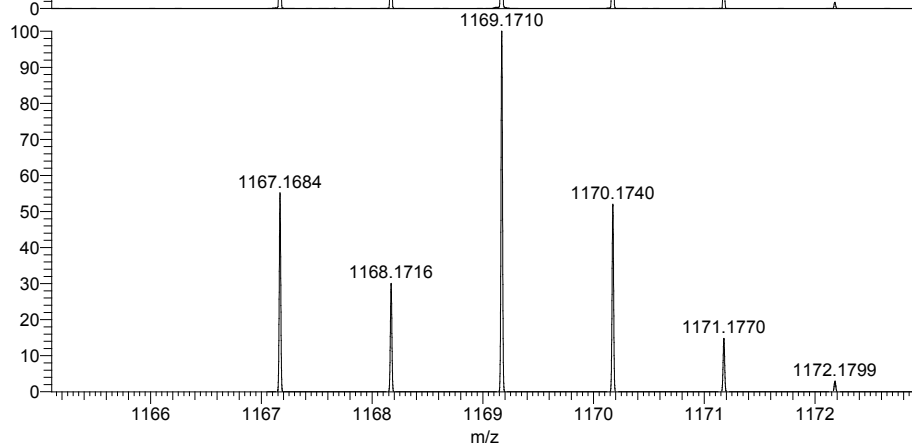


Figure S6 (contd.). Negative-mode ESI mass spectra of Ir[TpOMePC](tppts) (Z=2 and 3).

IrTpCF3PCTCEP3\_neg #1-8 RT: 0.00-0.21 AV: 8 NL: 5.74E5  
T: FTMS - p ESI Full ms [200.00-2000.00]



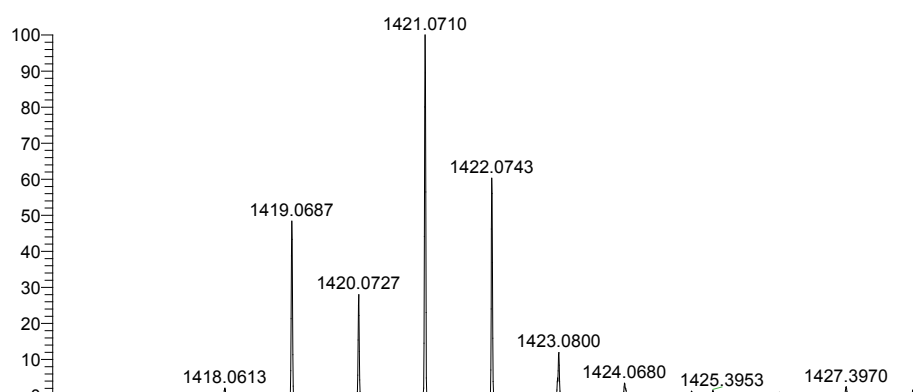
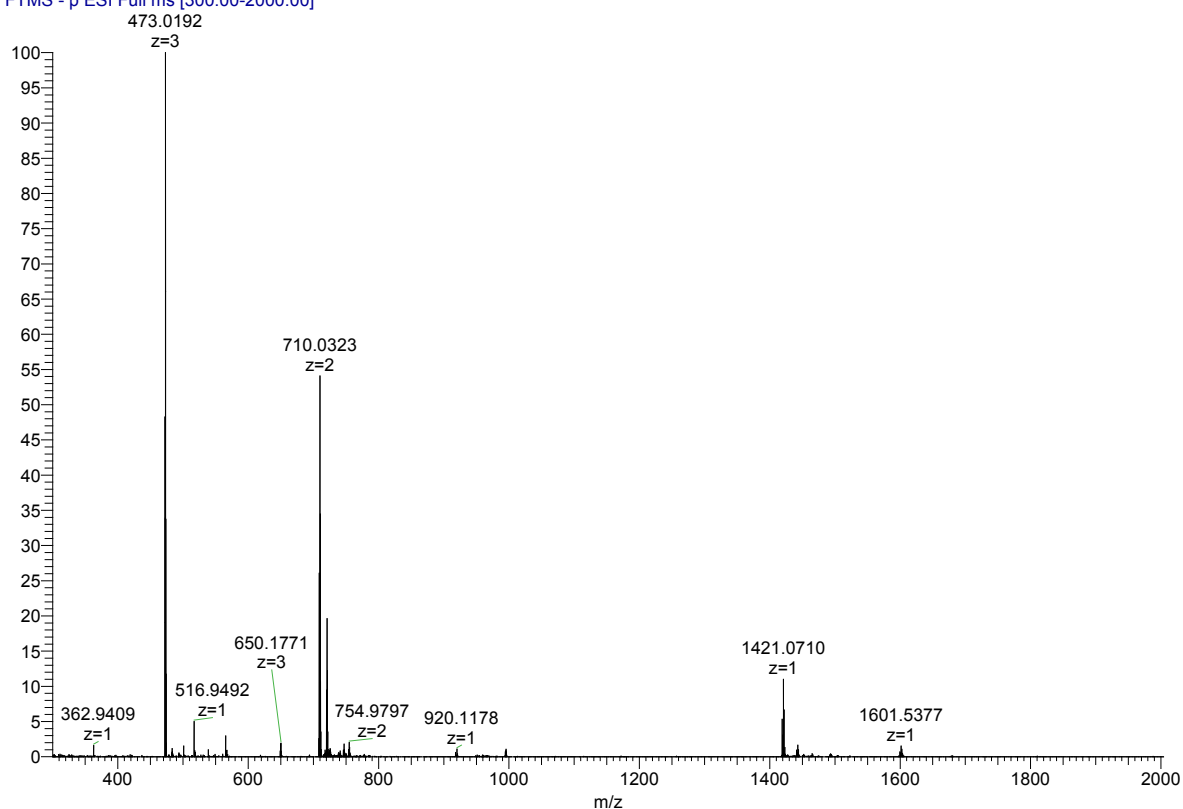
NL:  
5.74E5  
IrTpCF3PCTCEP3\_neg#1-8  
RT: 0.00-0.21 AV: 8 T: FTMS  
- p ESI Full ms  
[200.00-2000.00]



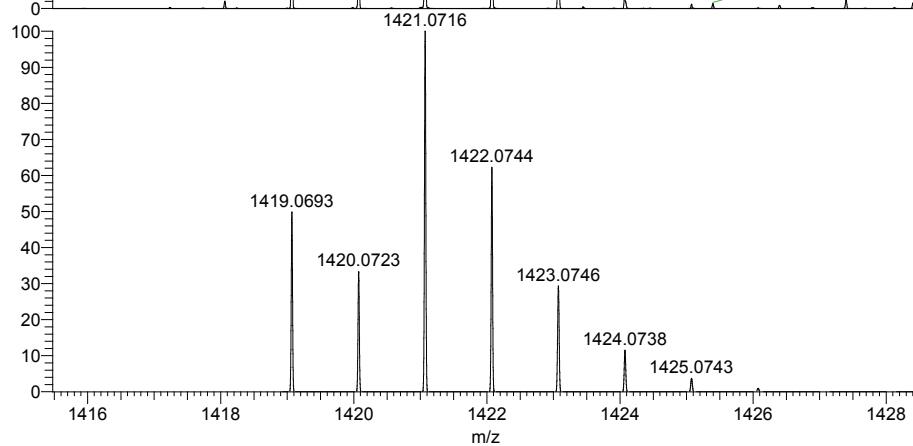
NL:  
9.06E3  
IrC<sub>49</sub>H<sub>34</sub>F<sub>9</sub>N<sub>4</sub>O<sub>6</sub>P:  
Ir<sub>1</sub>C<sub>49</sub>H<sub>34</sub>F<sub>9</sub>N<sub>4</sub>O<sub>6</sub>P<sub>1</sub>  
p (gss, s /p:40) Chrg -1  
R: 78500 Res .Pwr . @FWHM

Figure S7. Negative-mode ESI mass spectra of Ir[(TpCF<sub>3</sub>PC)](tcep).

IrTpCF3PCPh3SO3H\_neg #1-5 RT: 0.01-0.12 AV: 5 NL: 1.10E7  
T: FTMS - p ESI Full ms [300.00-2000.00]



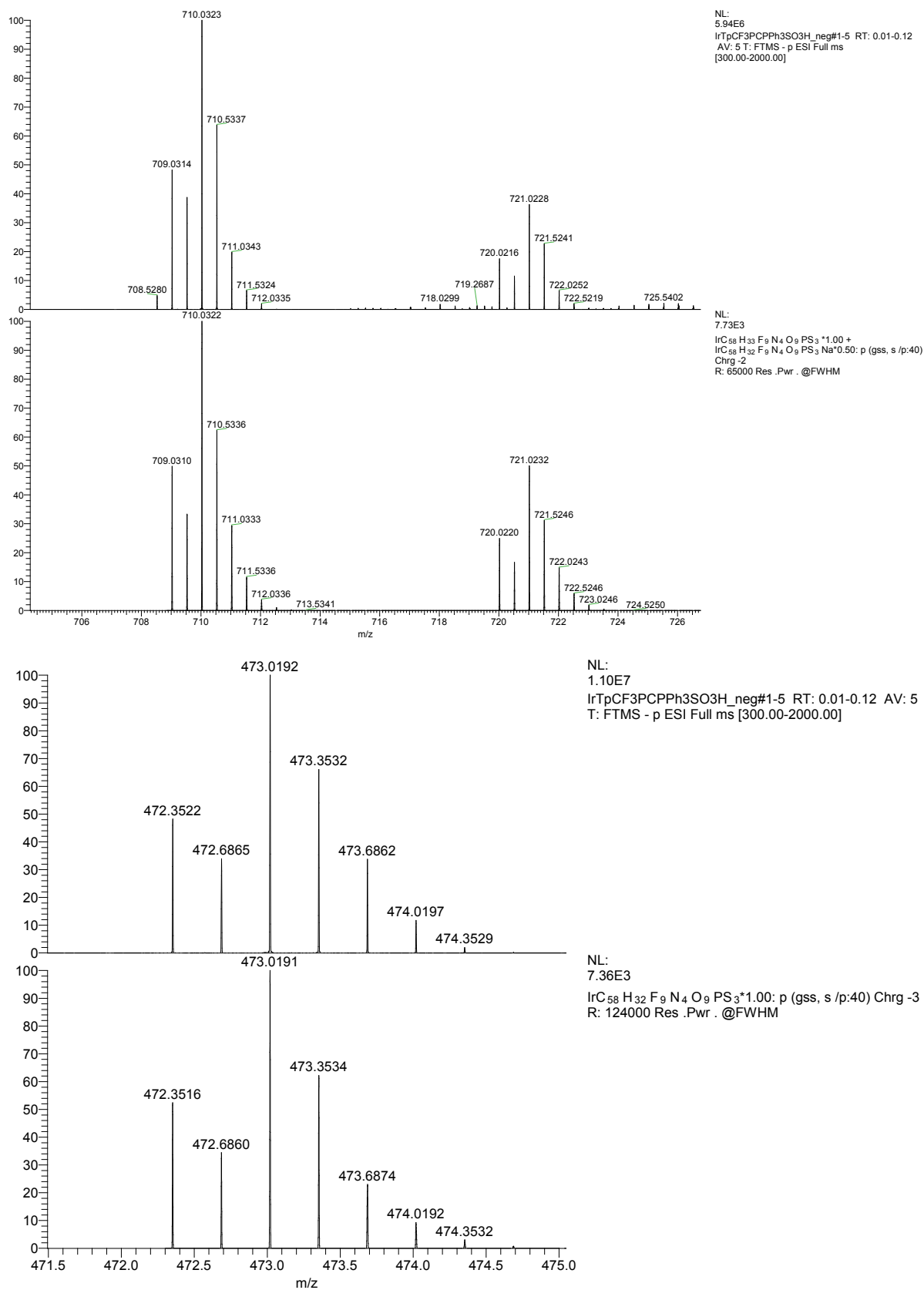
NL:  
1.21E6  
IrTpCF3PCPh3SO3H\_neg#1  
-5 RT: 0.01-0.12 AV: 5 T:  
FTMS - p ESI Full ms  
[300.00-2000.00]



NL:  
7.73E3  
IrC<sub>58</sub>H<sub>34</sub>F<sub>9</sub>N<sub>4</sub>O<sub>9</sub>PS<sub>3</sub>:  
Ir<sub>1</sub>C<sub>58</sub>H<sub>34</sub>F<sub>9</sub>N<sub>4</sub>O<sub>9</sub>P<sub>1</sub>S<sub>3</sub>  
p (gss, s /p:40) Chrg -1  
R: 65000 Res .Pwr . @FWHM

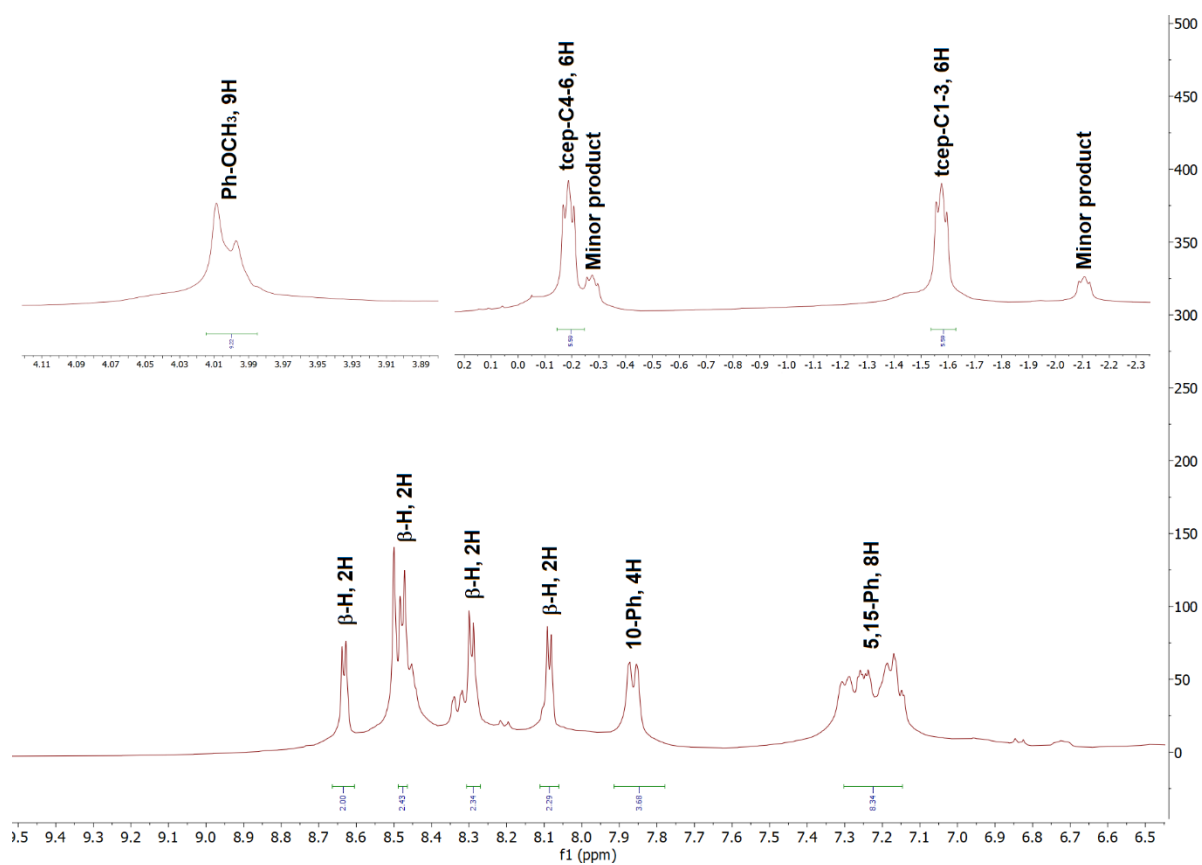
Figure S8. Negative-mode ESI mass spectra of Ir[*TpCF<sub>3</sub>PC*](*tppts*) (*Z*=1). *Contd.*



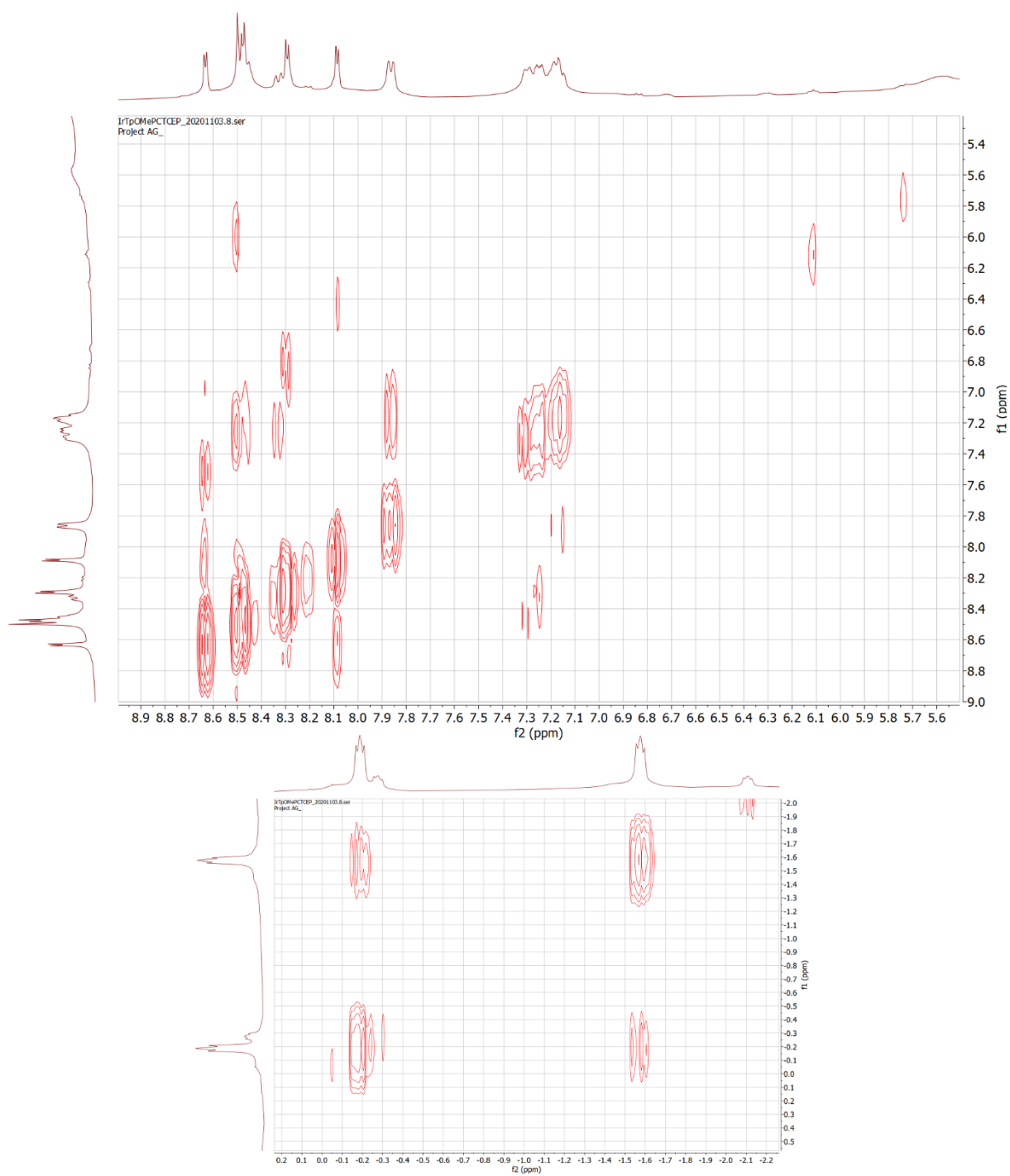


**Figure S8 (contd.).** Negative-mode ESI mass spectra of Ir[*TP*CF<sub>3</sub>PC](*tppts*) (*Z*=2 and 3).

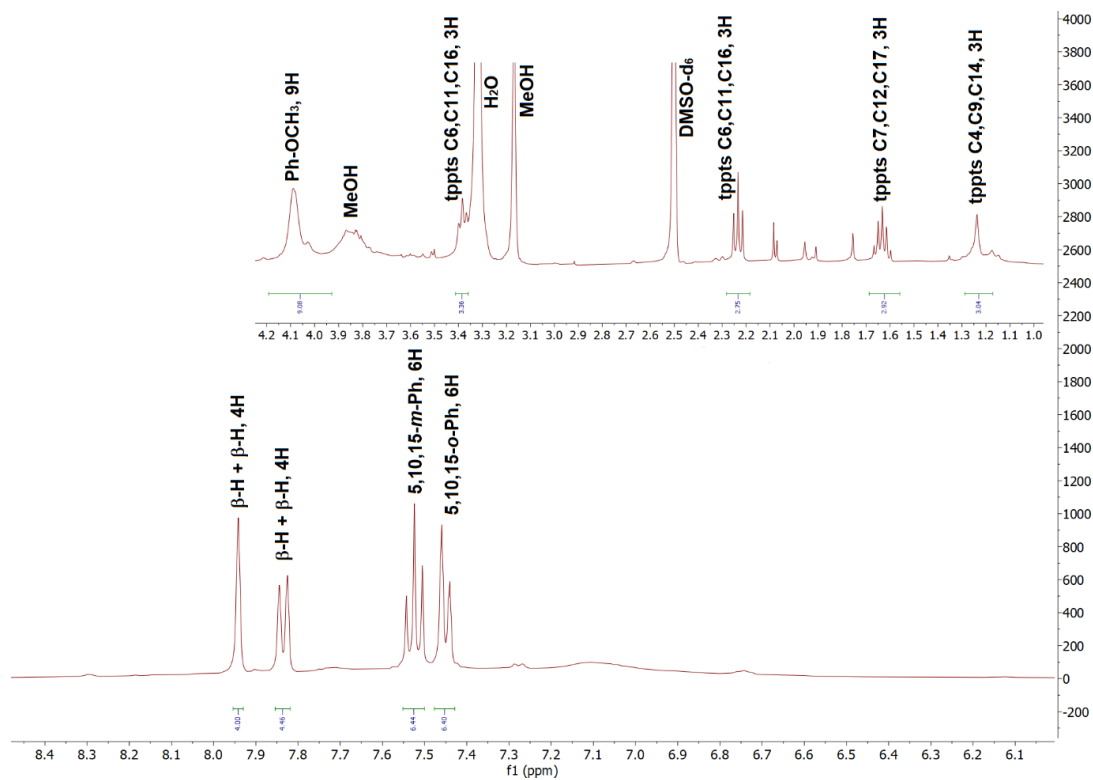
### C. NMR spectra



**Figure S9.** <sup>1</sup>H NMR spectrum of Ir[TpOMePC](tcep) in methanol-*d*<sub>4</sub>.



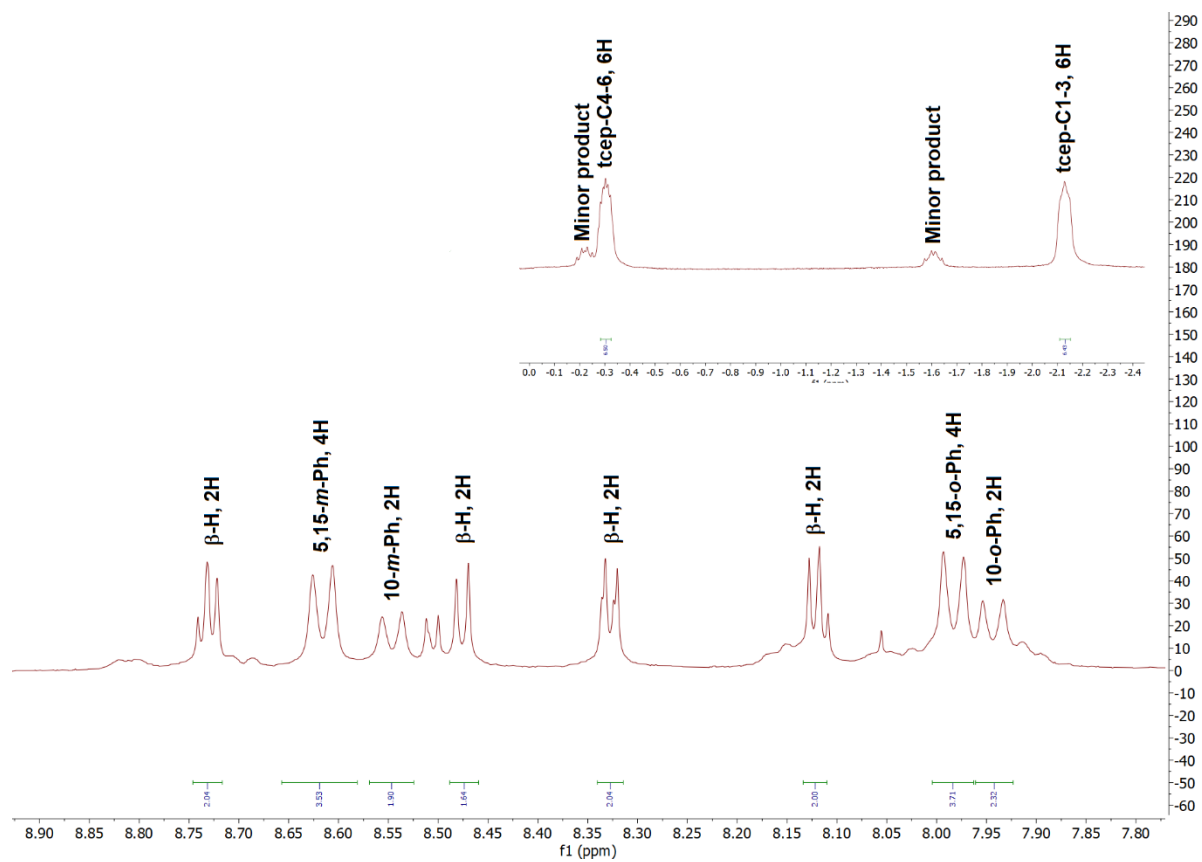
**Figure S10.**  $^1\text{H}$ - $^1\text{H}$  COSY of  $\text{Ir}[\text{TpOMePC}](\text{tcep})$  in  $\text{methanol-}d_4$ . Top: close-up of aromatic area; bottom: close-up of ligand area.



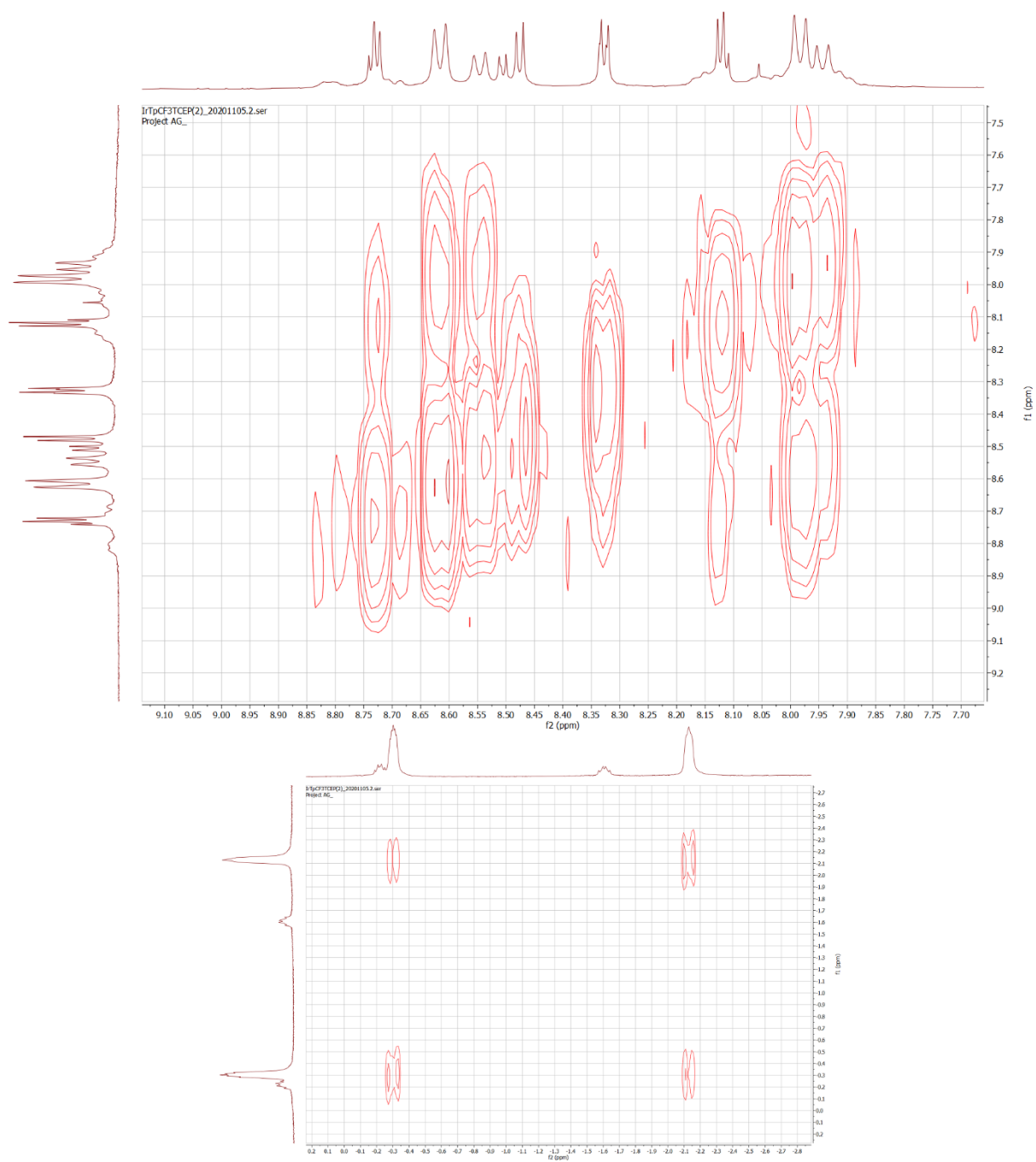
**Figure S11.**  $^1\text{H}$  NMR spectrum of  $\text{Ir}[\text{TpOMePC}](\text{tppts})$  in  $\text{DMSO-}d_6$ .



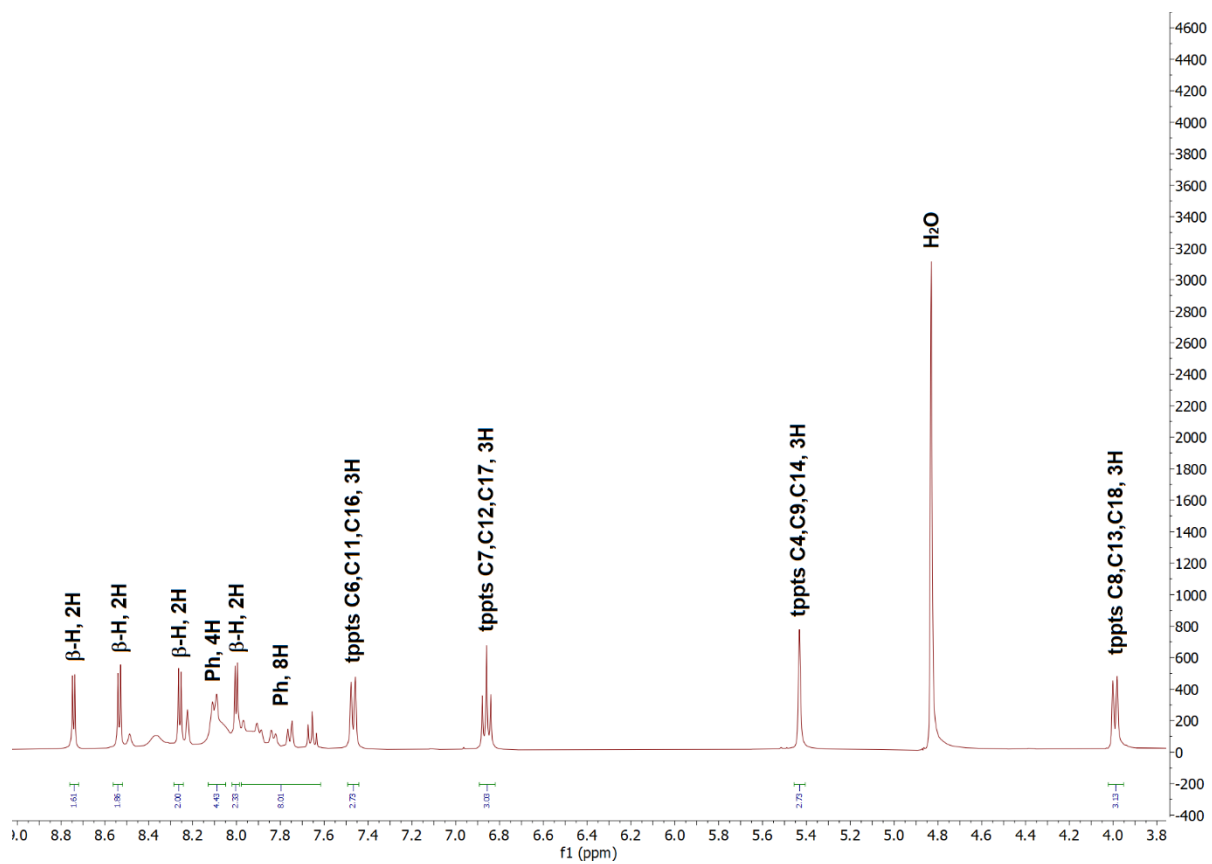
**Figure S12.**  $^1\text{H}$ - $^1\text{H}$  COSY of  $\text{Ir}[\text{TpOMePC}](\text{tppts})$  in  $\text{DMSO-}d_6$ .



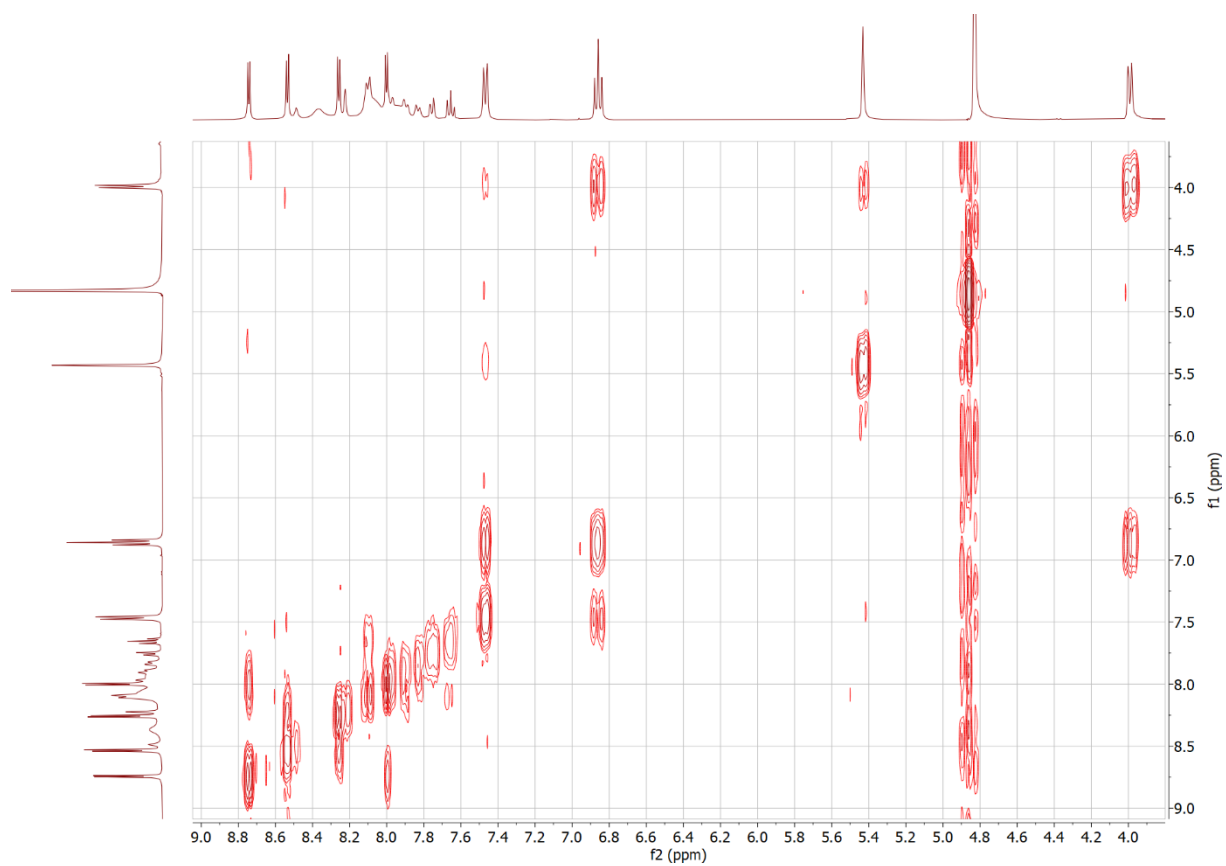
**Figure S13.** <sup>1</sup>H NMR spectrum of Ir[TpCF<sub>3</sub>PC](tcep) in methanol-*d*<sub>4</sub>.



**Figure S14.**  $^1\text{H}$ - $^1\text{H}$  COSY of  $\text{Ir}[\text{TpCF}_3\text{PC}](\text{tcep})$  in  $\text{methanol-}d_4$ . Top: close-up of aromatic area; bottom: close-up of ligand area.



**Figure S15.** <sup>1</sup>H NMR spectrum of Ir[TpCF<sub>3</sub>PC](tppts) in methanol-*d*<sub>4</sub>.



**Figure S16.**  $^1\text{H}$ - $^1\text{H}$  COSY of  $\text{Ir}[\text{TpCF}_3\text{PC}](\text{tppts})$  in  $\text{methanol-}d_4$ .