

## *Supplementary Material*

# Synthesis and Molecular Structure of Perhalogenated Rhenium-Oxo Corroles

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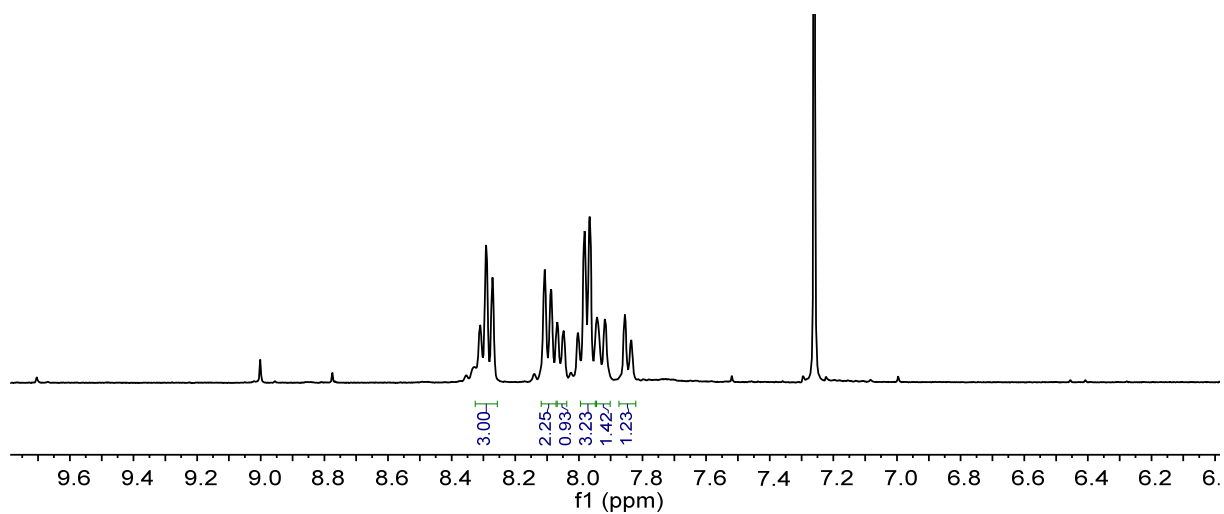
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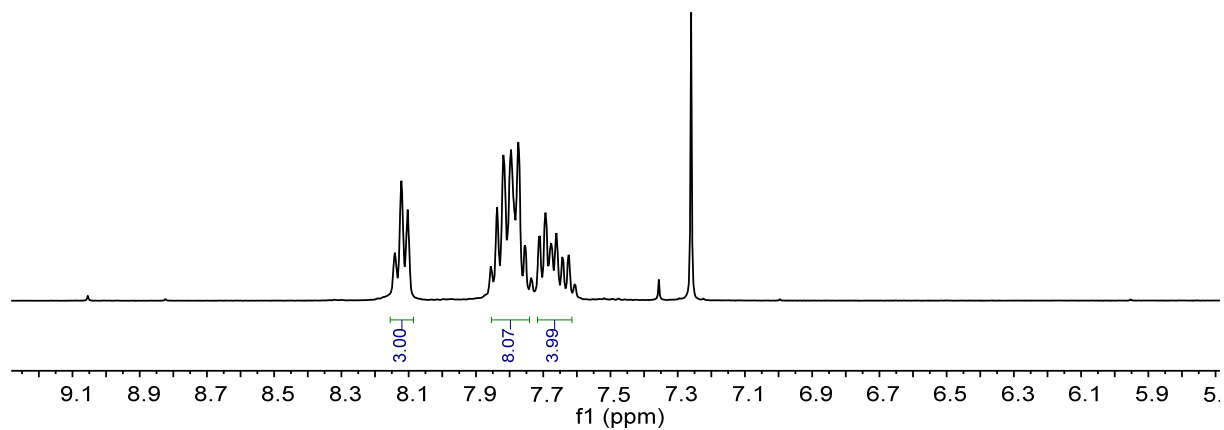
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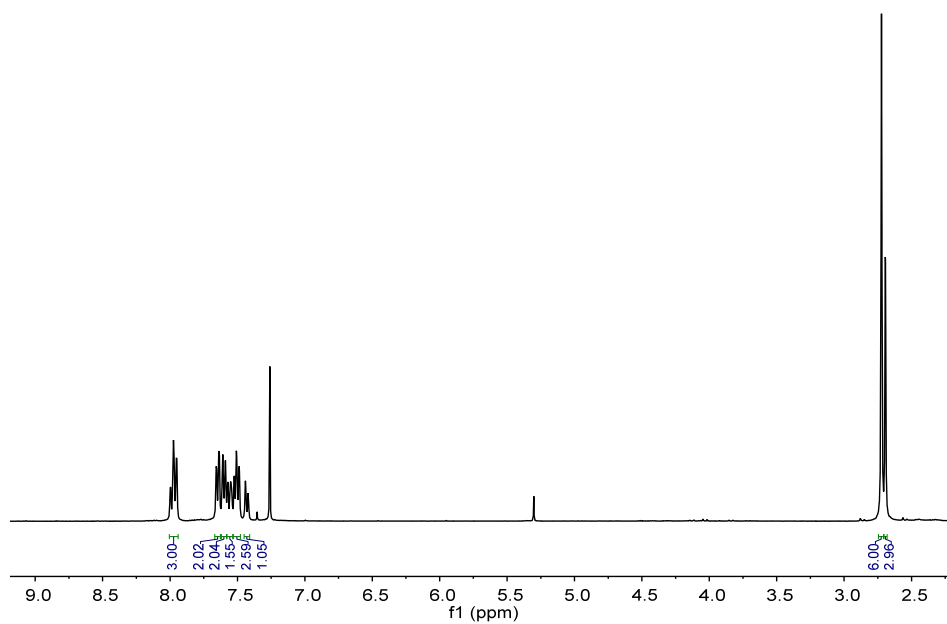
a) NMR Spectra



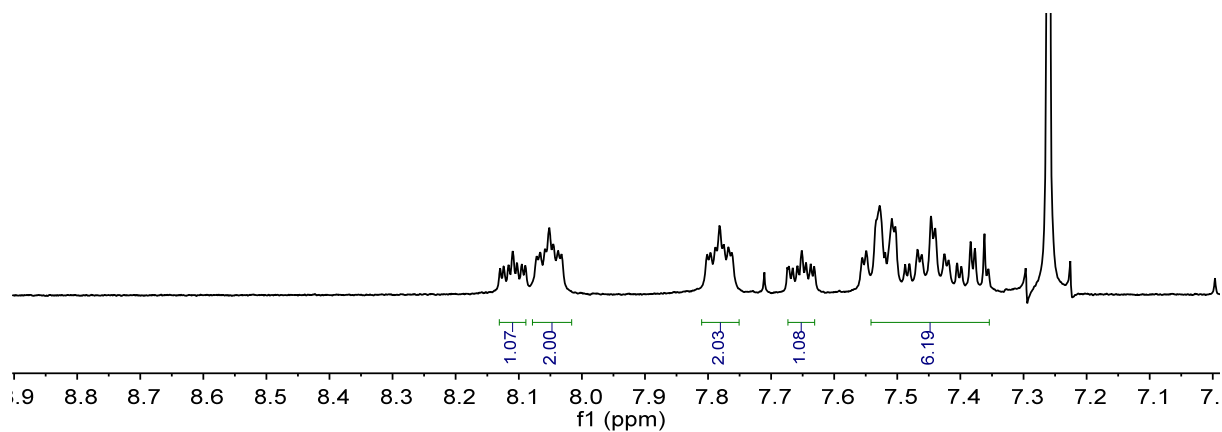
**Figure S1.**  $^1\text{H}$  NMR spectrum of  $\text{Re}[\text{Cl}_8\text{TpCF}_3\text{PC}](\text{O})$  in  $\text{CDCl}_3$  at 298 K.



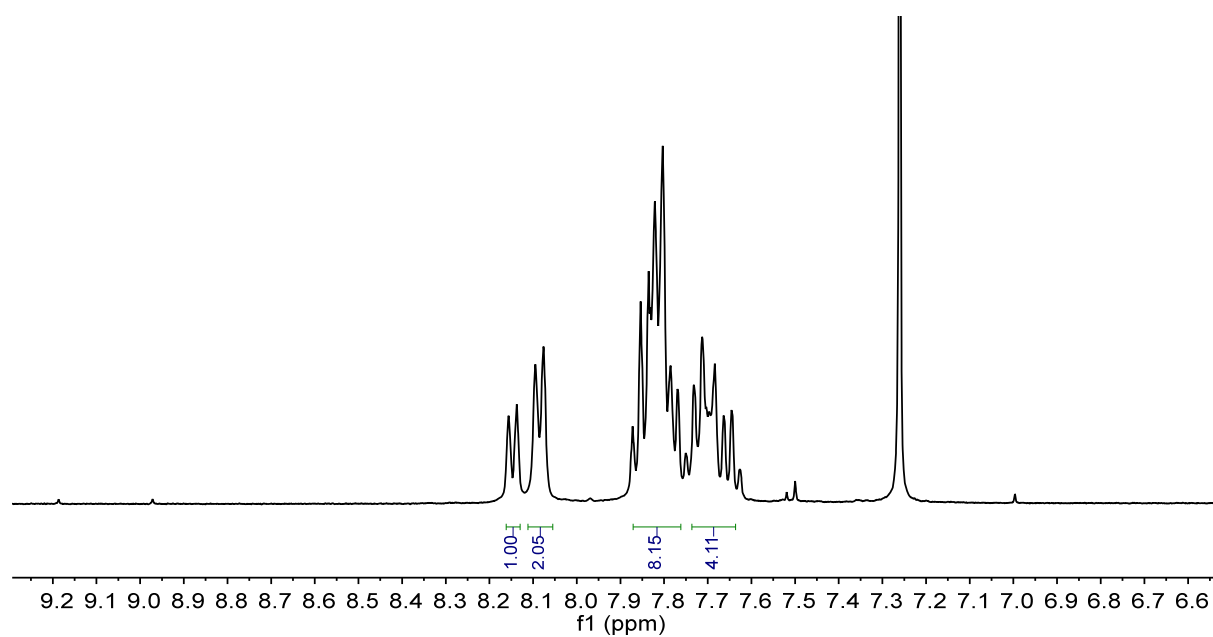
**Figure S2.**  $^1\text{H}$  NMR spectrum of  $\text{Re}[\text{Cl}_8\text{TPC}](\text{O})$  in  $\text{CDCl}_3$  at 298 K.



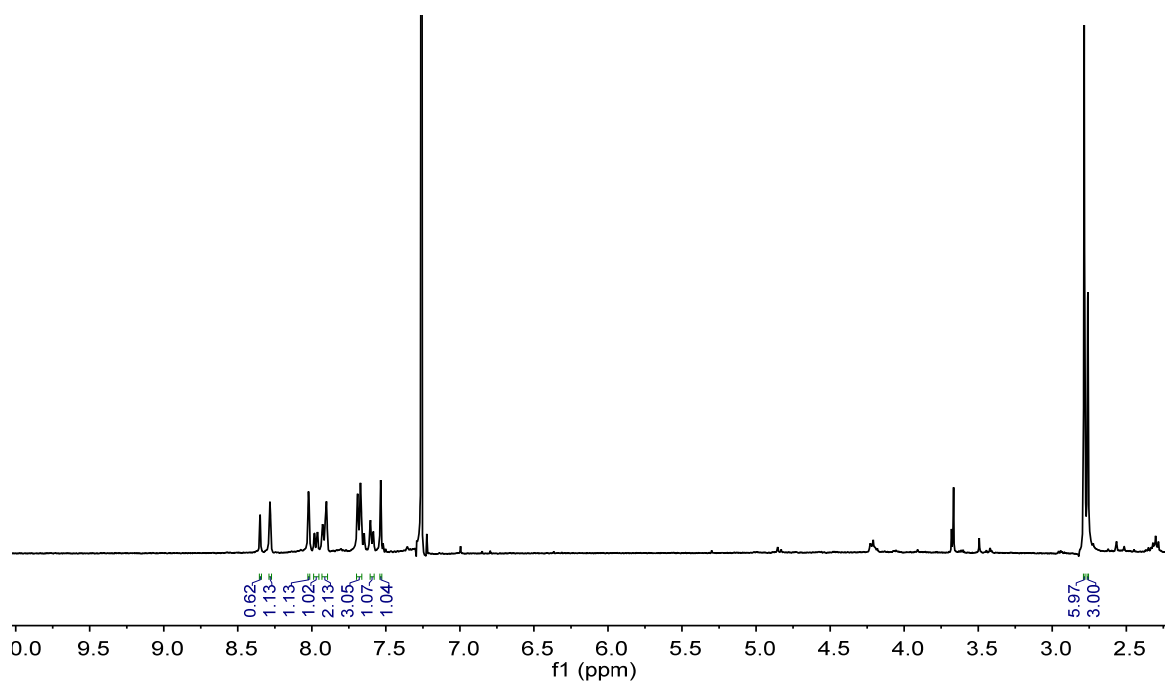
**Figure S3.**  $^1\text{H}$  NMR spectrum of  $\text{Re}[\text{Cl}_8\text{TpCH}_3\text{PC}](\text{O})$  in  $\text{CDCl}_3$  at 298 K.



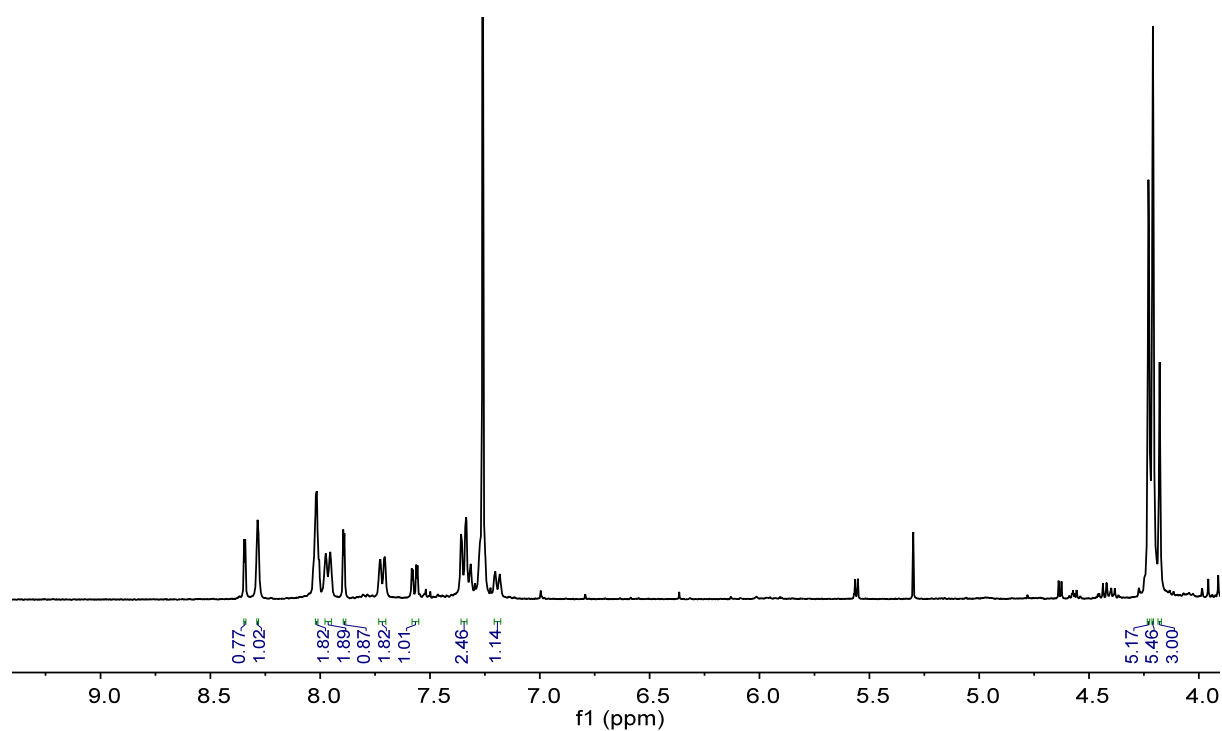
**Figure S4.**  $^1\text{H}$  NMR spectrum of  $\text{Re}[\text{Br}_8\text{TpFPC}](\text{O})$  in  $\text{CDCl}_3$  at 298 K.



**Figure S5.**  $^1\text{H}$  NMR spectrum of  $\text{Re}[\text{Br}_8\text{TPC}](\text{O})$  in  $\text{CDCl}_3$  at 298 K.



**Figure S6.**  $^1\text{H}$  NMR spectrum of  $\text{Re}[\text{Br}_{11}\text{TpCH}_3\text{PC}](\text{O})$  in  $\text{CDCl}_3$  at 298 K.



**Figure S7.**  $^1\text{H}$  NMR spectrum of  $\text{Re}[\text{Br}_{11}\text{TpCH}_3\text{PC}](\text{O})$  in  $\text{CDCl}_3$  at 298 K.

## b) ESI mass Spectra

ReOC8CF3\_171208162313 #1 RT: 0.00 AV: 1 NL: 1.70E5  
T: FTMS + p ESI Full ms [500.00-2000.00]

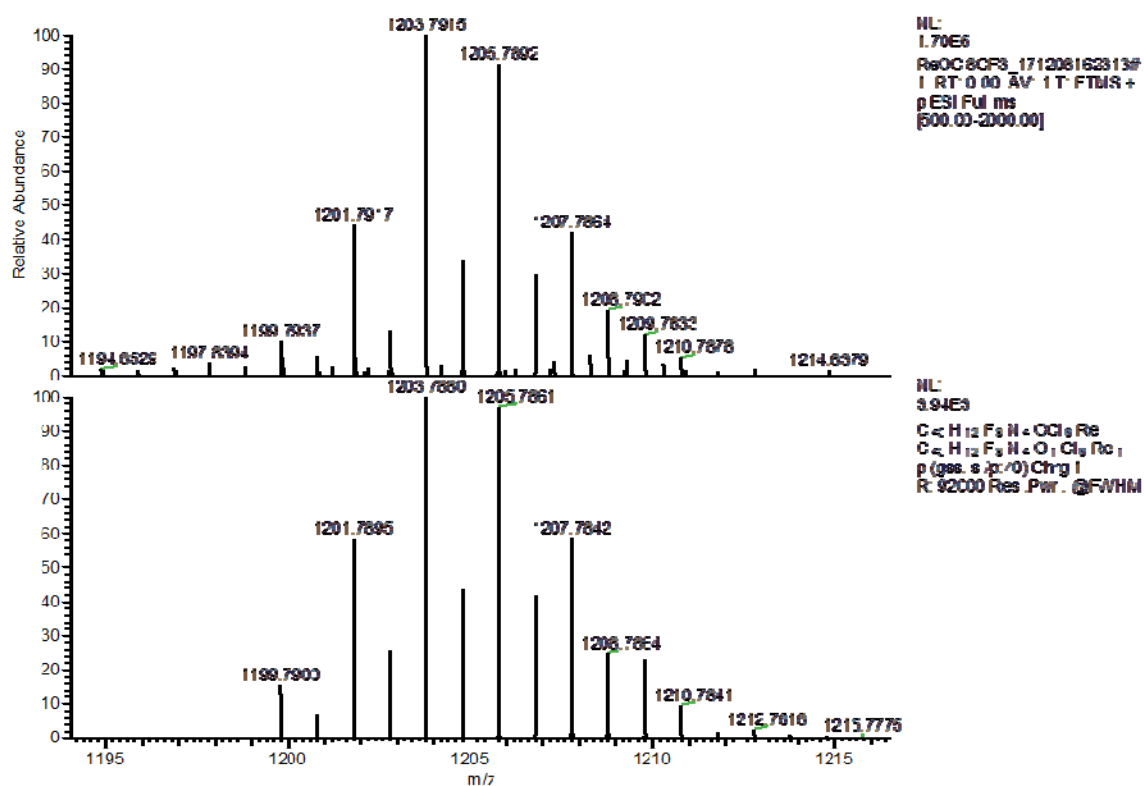
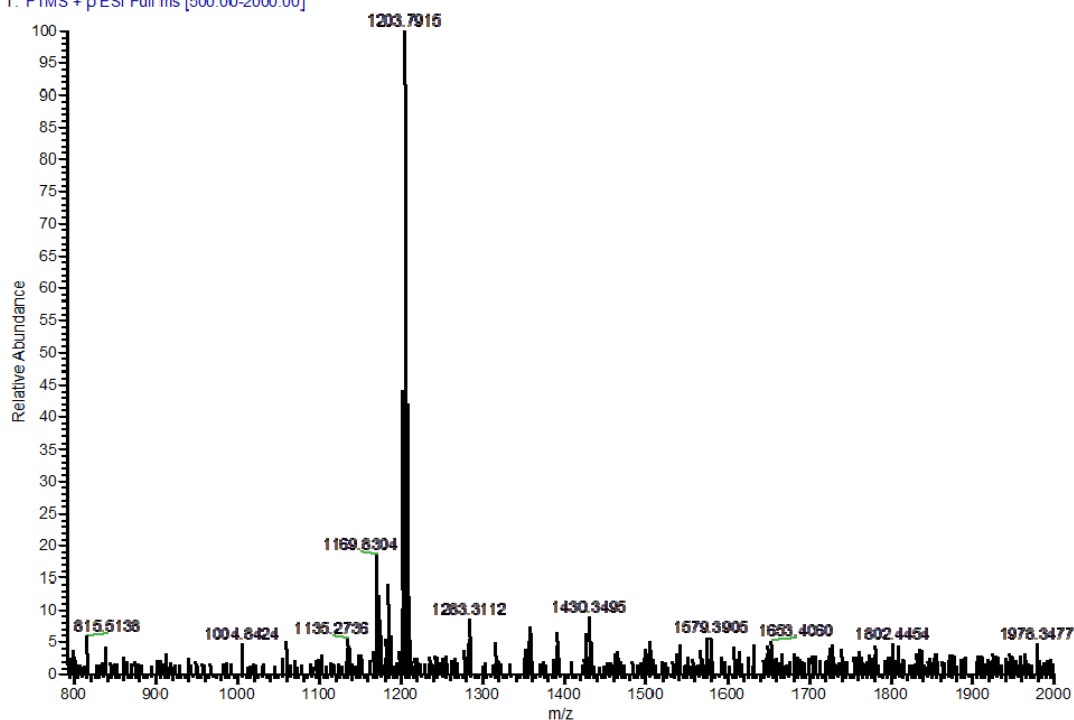


Figure S8. ESI-MS of Re[Cl<sub>8</sub>TpCF<sub>3</sub>PC](O): experimental (top) and simulation (bottom).

ReOC18TPC\_NEG#1-4 RT: 0.00-0.10 AV: 4 NL: 1.13E6  
T: FTMS + p ESI Full ms [700.00-2000.00]

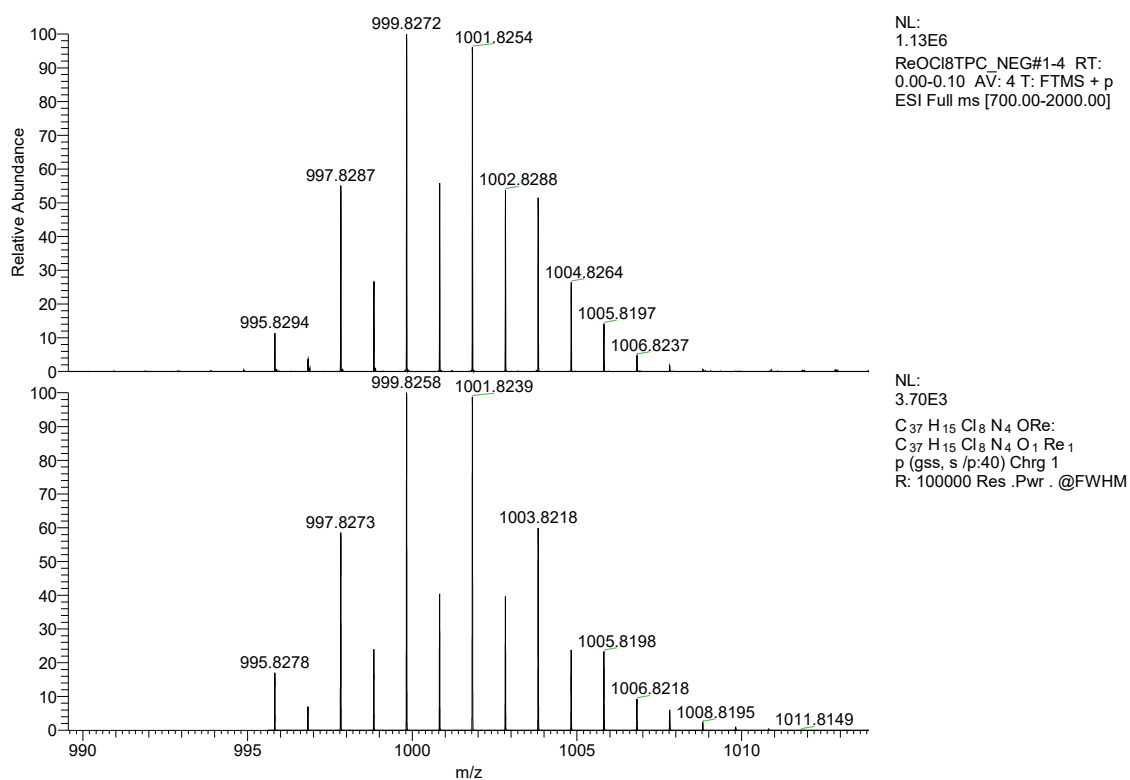
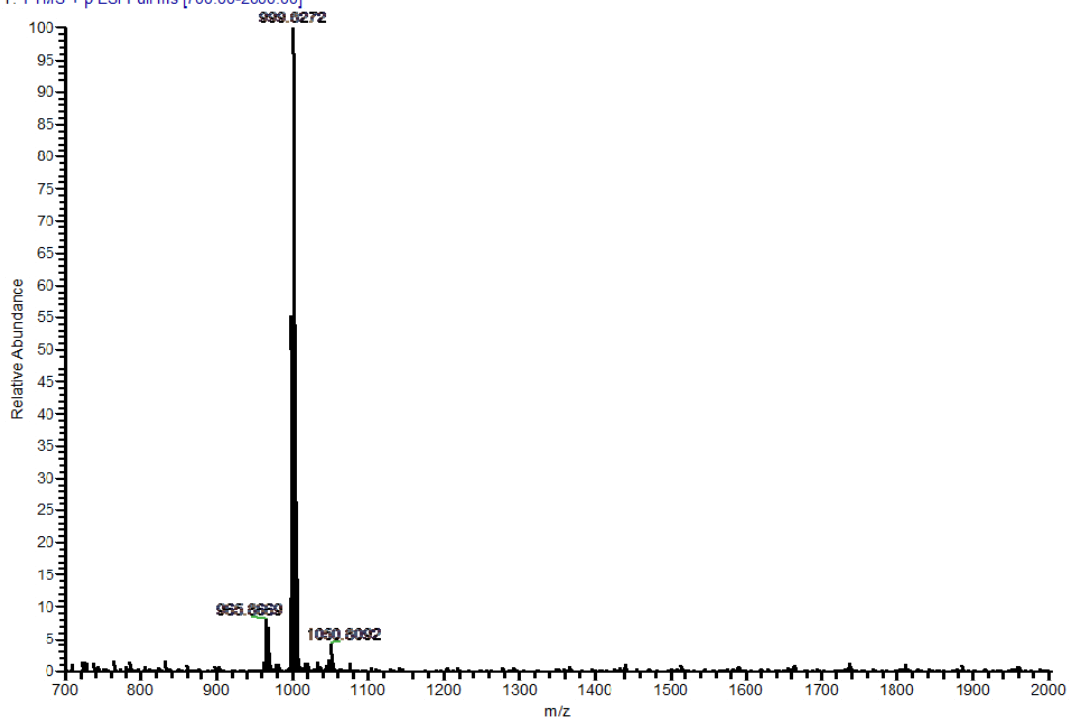
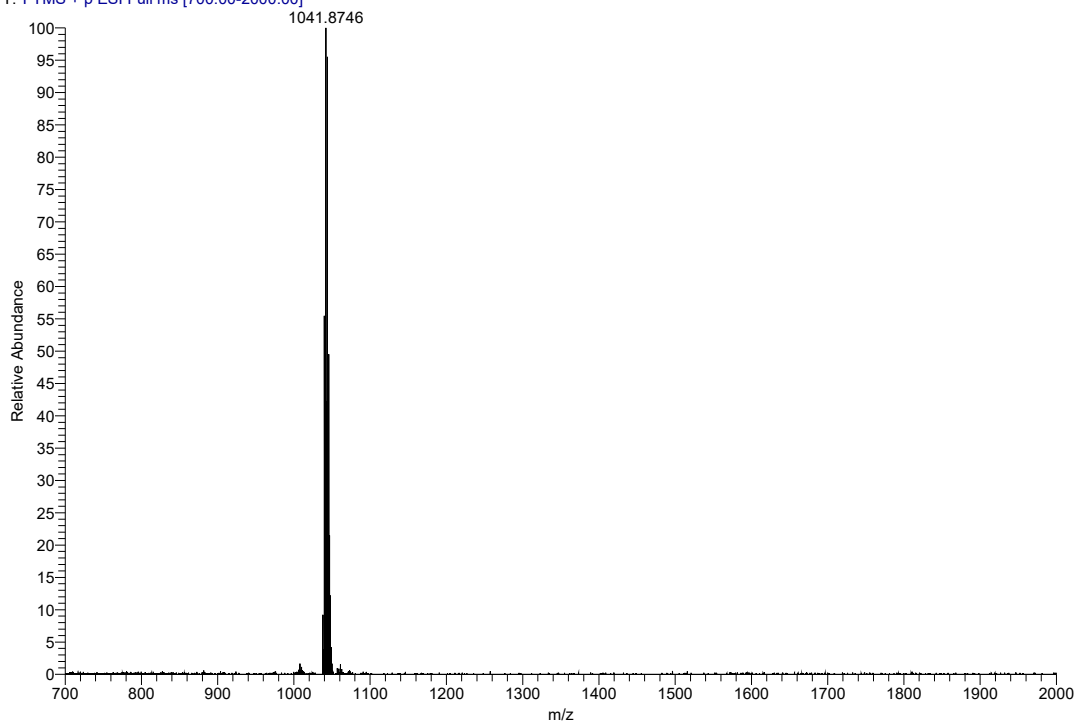
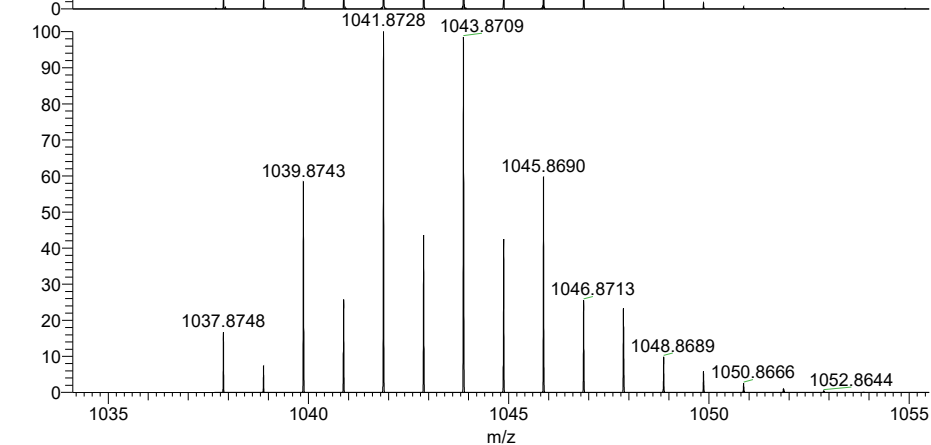


Figure S9. ESI-MS of Re[Cl<sub>8</sub>TPC](O): experimental (top) and simulation (bottom).

ReOC18TpCH3PC\_191212121232 #1 RT: 0.02 AV: 1 NL: 5.27E5  
T: FTMS + p ESI Full ms [700.00-2000.00]



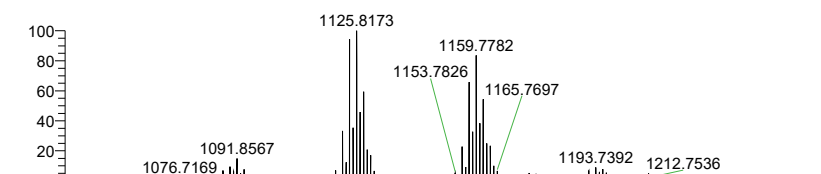
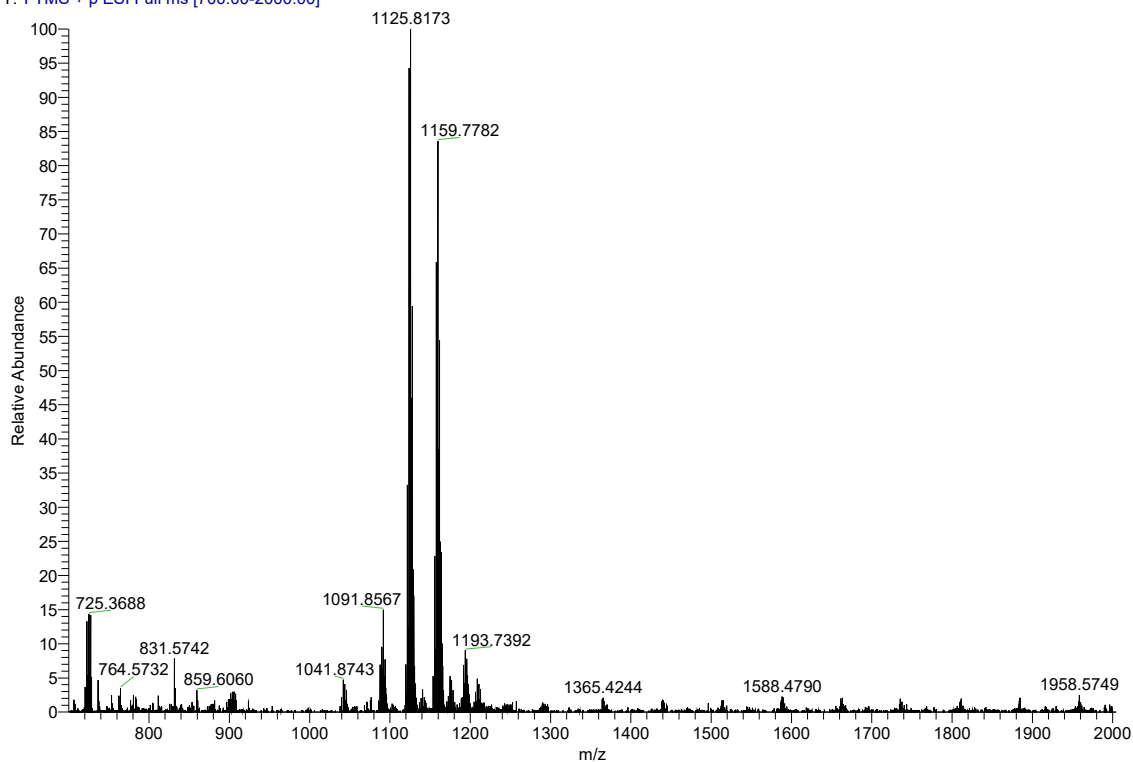
NL:  
5.27E5  
ReOC18TpCH3PC\_1912121212  
32#1 RT: 0.02 AV: 1 T: FTMS  
+ p ESI Full ms  
[700.00-2000.00]



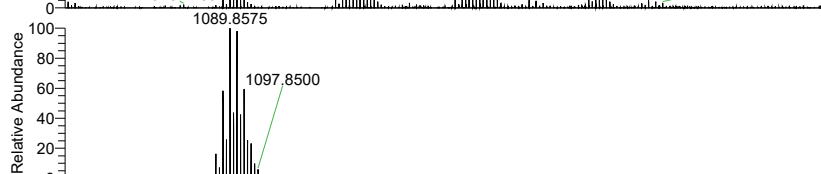
NL:  
3.65E3  
C<sub>40</sub> H<sub>21</sub> Cl<sub>8</sub> N<sub>4</sub> ORe:  
C<sub>40</sub> H<sub>21</sub> Cl<sub>8</sub> N<sub>4</sub> O<sub>1</sub> Re<sub>1</sub>  
p (gss, s /p:40) Chrg 1  
R: 100000 Res .Pwr . @FWHM

Figure S10. ESI-MS of Re[Cl<sub>8</sub>TpCH<sub>3</sub>PC](O): experimental (top) and simulation (bottom).

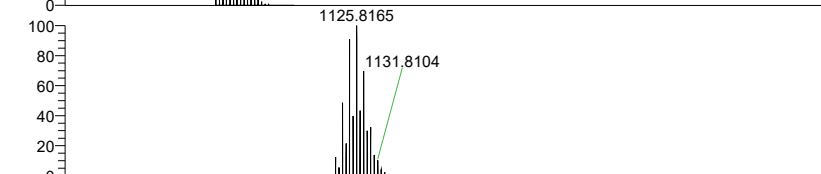
ReOC19TpOCH3PC\_191212121232 #1-3 RT: 0.01-0.06 AV: 3 NL: 2.59E5  
 T: FTMS + p ESI Full ms [700.00-2000.00]



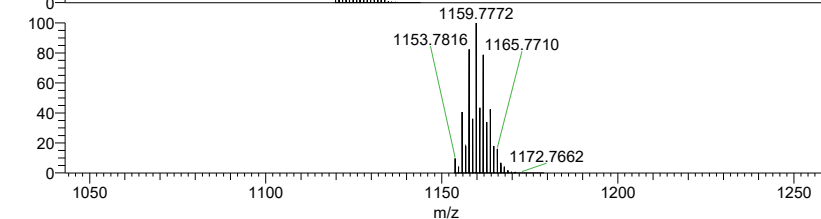
NL:  
 2.59E5  
 ReOC19TpOCH3PC\_19121212  
 1232#1-3 RT: 0.01-0.06 AV: 3  
 T: FTMS + p ESI Full ms  
 [700.00-2000.00]



NL:  
 3.70E3  
 $C_{40}H_{21}Cl_8N_4O_4Re$   
 $C_{40}H_{21}Cl_8N_4O_4Re_1$   
 p (gss, s /p:40) Chrg 1  
 R: 100000 Res .Pwr . @FWHM



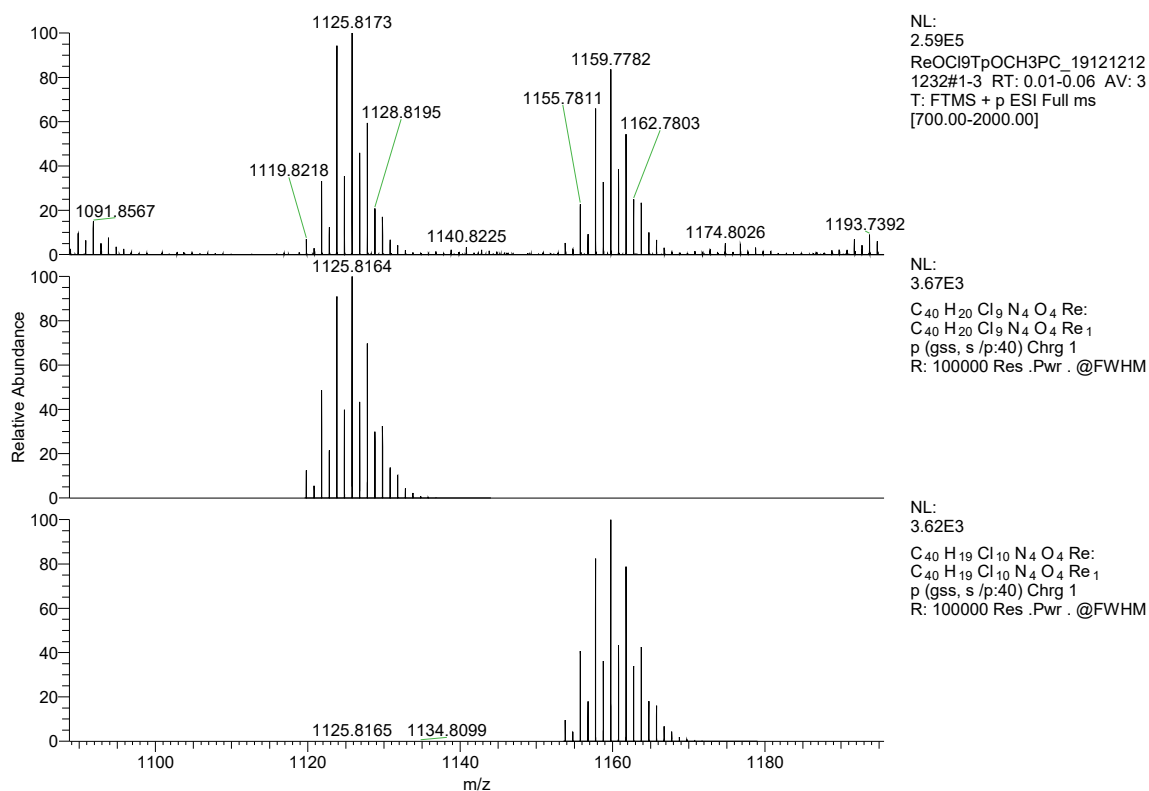
NL:  
 3.67E3  
 $C_{40}H_{20}Cl_9N_4O_4Re$   
 $C_{40}H_{20}Cl_9N_4O_4Re_1$   
 p (gss, s /p:40) Chrg 1  
 R: 100000 Res .Pwr . @FWHM



NL:  
 3.62E3  
 $C_{40}H_{19}Cl_{10}N_4O_4Re$   
 $C_{40}H_{19}Cl_{10}N_4O_4Re_1$   
 p (gss, s /p:40) Chrg 1  
 R: 100000 Res .Pwr . @FWHM

Figure S11. Contd.





**Figure S11.** ESI-MS spectrum of  $\text{Re}[\text{Cl}_9\text{TpOCH}_3\text{PC}](\text{O})$  and  $\text{Re}\{\text{Cl}_{10}\text{TpOCH}_3\text{PC}\}(\text{O})$ : experimental (top) and two simulations (bottom).

ReOBrtTpFPC #1 RT: 0.02 AV: 1 NL: 7.07E5  
T: FTMS + p ESI Full ms [800.00-2000.00]

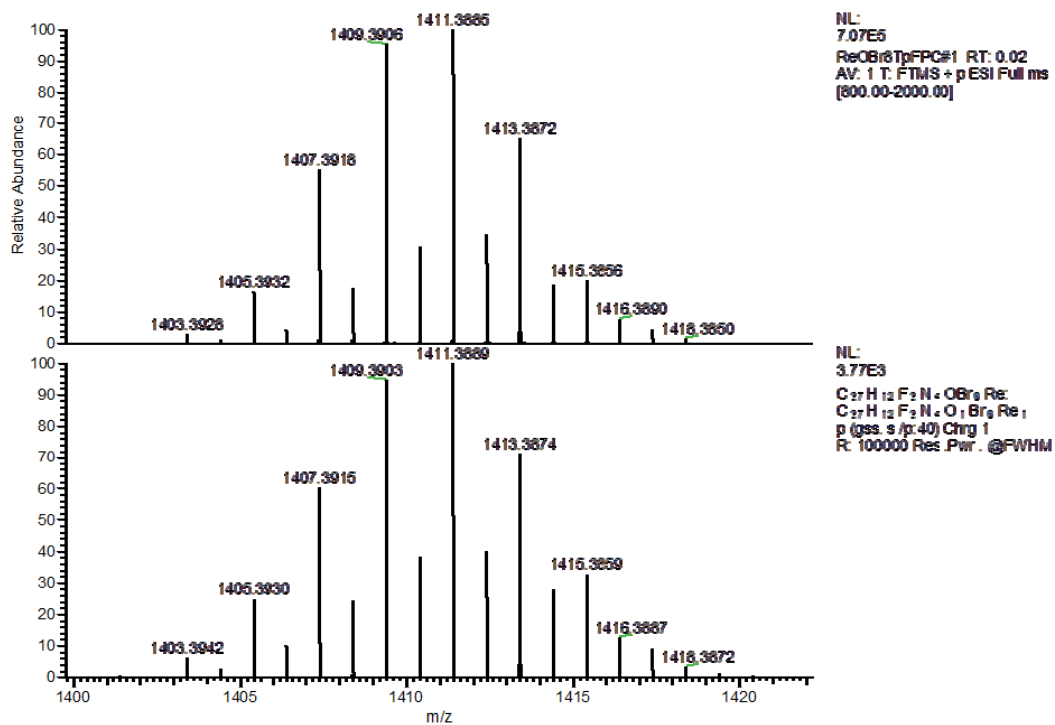
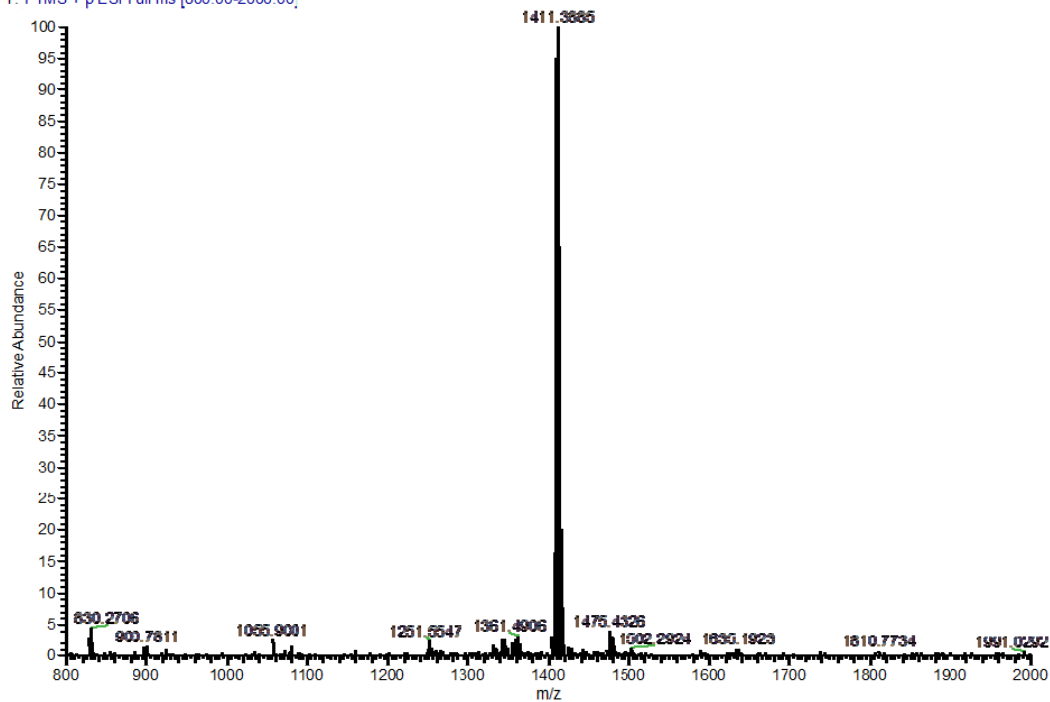
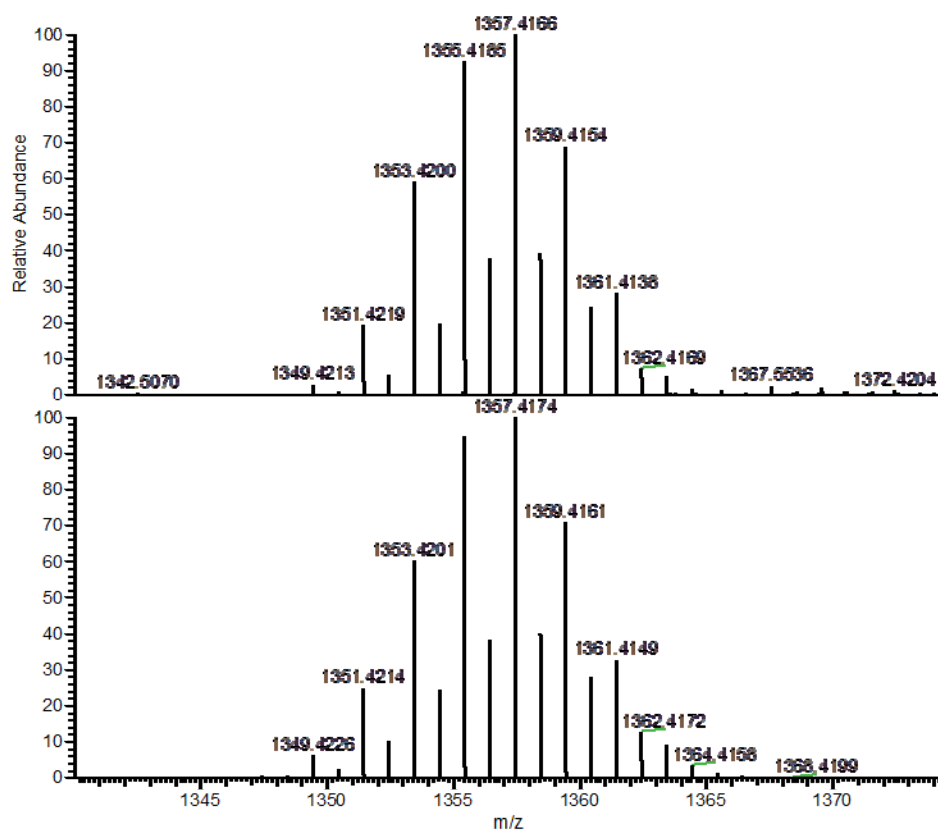
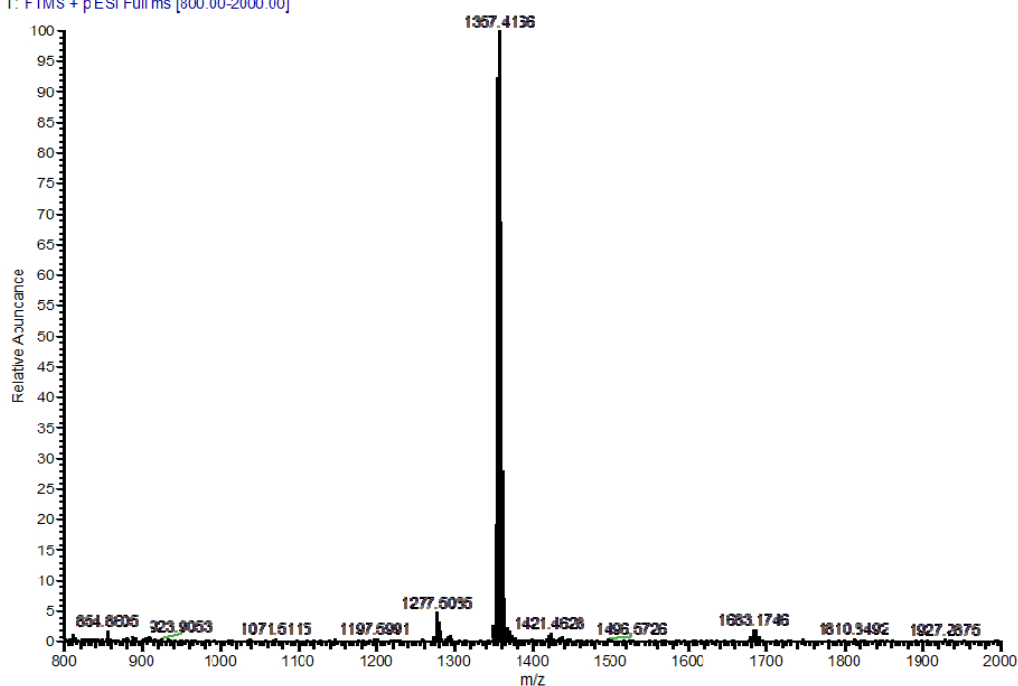


Figure S12. ESI-MS of Re[Br<sub>8</sub>TpFPC](O): experimental (top) and simulation (bottom).

ReOBr8TPC3\_191218152943#1 RT: 0.02 AV: 1 NL: 4.41E5  
T: FTMS + p ESI Full ms [800.00-2000.00]



NL:  
4.41E5  
ReOBr8TPC3\_191218152943  
#1 RT: 0.02 AV: 1 T: FTMS  
+ p ESI Full ms  
[800.00-2000.00]

NL:  
3.60E3  
C<sub>27</sub>H<sub>12</sub>N<sub>2</sub>OBr<sub>8</sub>Re  
C<sub>27</sub>H<sub>12</sub>N<sub>2</sub>O<sub>1</sub>Br<sub>8</sub>Re<sub>1</sub>  
p (gas. s /pr:40) Chrg 1  
R: 92000 Res .Pwr. @FWHM

Figure S13. ESI-MS of Re[Br<sub>8</sub>TPC](O): experimental (top) and simulation (bottom).

ReOBr11TpCH3PC #1 RT: 0.02 AV: 1 NL: 8.57E4  
T: FTMS + p ESI Full ms [800.00-2000.00]

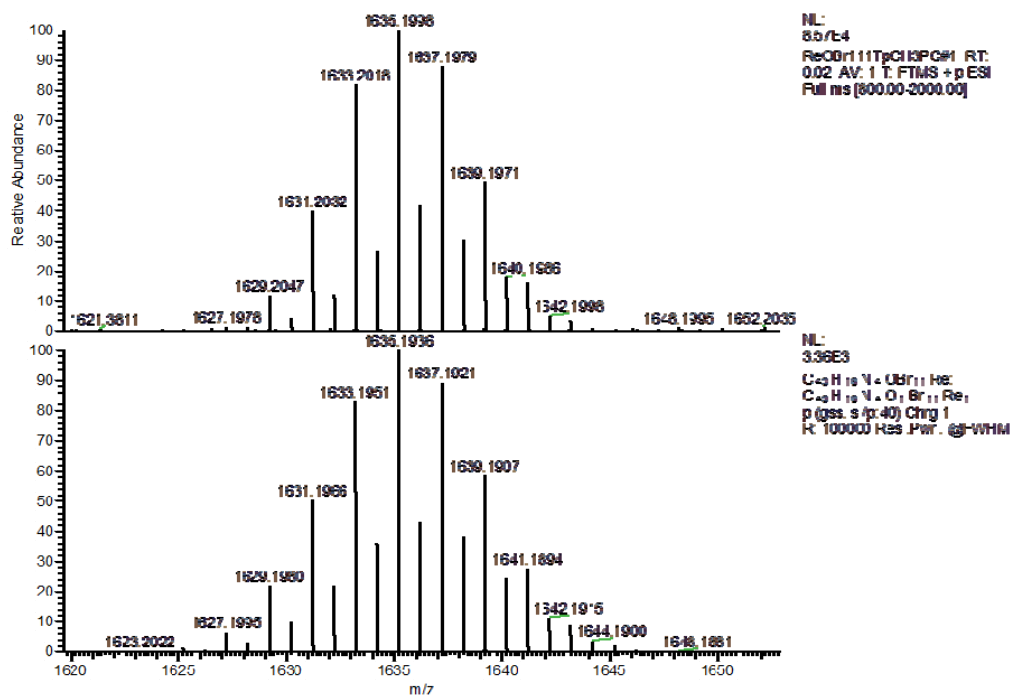
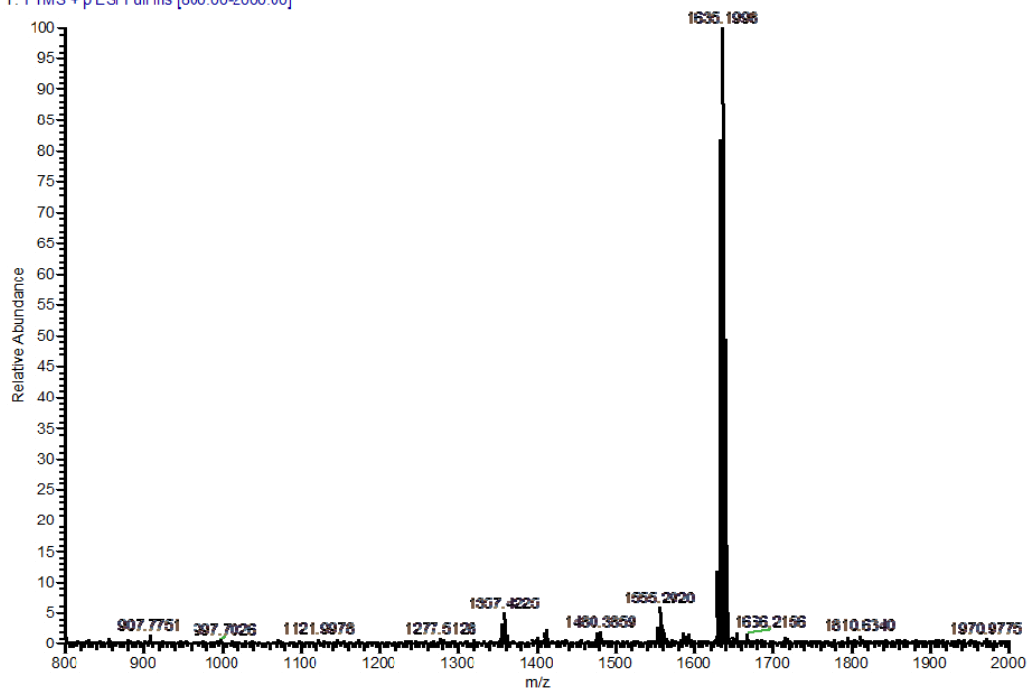


Figure S14. ESI-MS of Re[Br<sub>11</sub>TpCH<sub>3</sub>PC](O): experimental (top) and simulation (bottom).

ReOBr11TpOCH3PC\_pos #1 RT: 0.01 AV: 1 NL: 7.67E5  
T: FTMS + p ESI Full ms [800.00-3000.00]

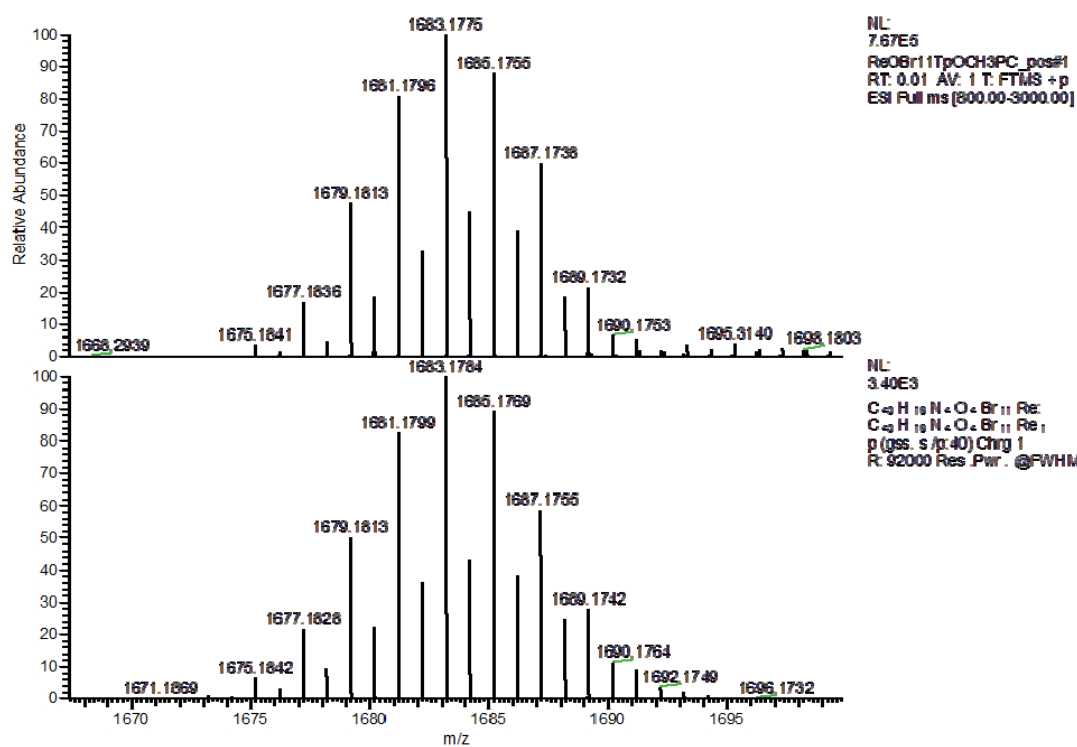
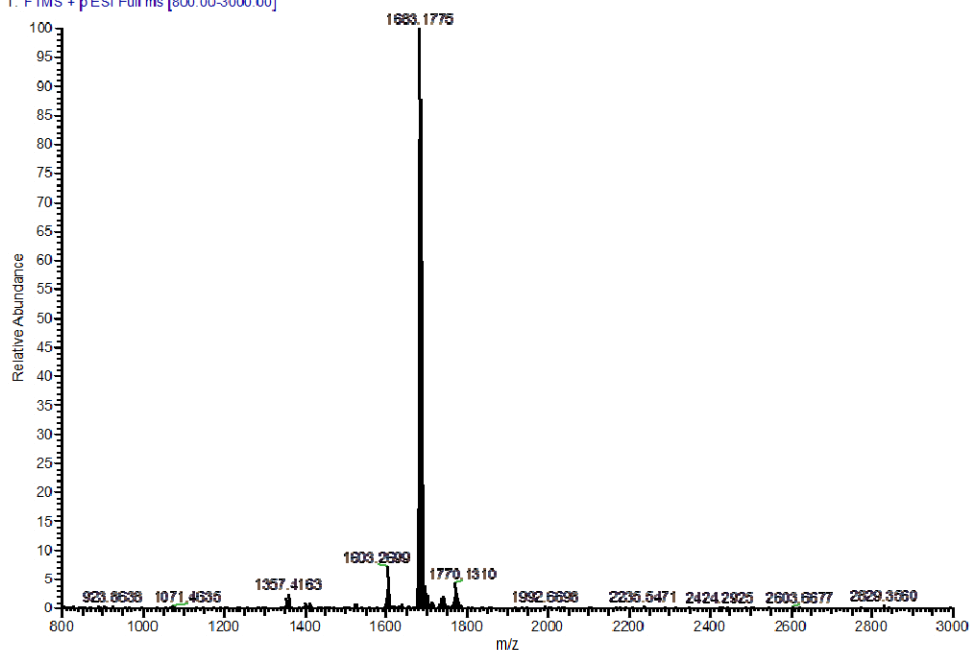


Figure S15. ESI-MS of Re[Br<sub>11</sub>TpOCH<sub>3</sub>PC](O); experimental (top) and simulation (bottom).