

Supporting Information for  
**Synthesis, Mass-Spectrometric Characterization and Polymerization Studies of**  
**Group 4 Dinuclear Bis(metallocene) Complexes**

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**Figure S43.**  $^1\text{H}$  NMR spectrum of **3b'-Hf**.

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**Figure S46.**  $^{13}\text{C}$  NMR spectrum of PE (Table 1, run 1).

**Figure S47.** GPC trace of PE (Table 1, run 1) obtained with **3a-Zr<sub>2</sub>**.

**Figure S48.**  $^{13}\text{C}$  NMR spectrum of PE (Table 1, run 3).

**Figure S49.**  $^{13}\text{C}$  NMR spectrum of PE (Table 1, run 5).

**Figure S50.** GPC trace of PE (Table 1, run 5) obtained with **3b-Zr<sub>2</sub>**.

**Figure S51.** GPC trace of PE (Table 1, run 6) obtained with **3b-Zr<sub>2</sub>**.

**Figure S52.** GPC trace of PE (Table 1, run 7) obtained with **3b'-Zr**.

**Figure S53.** GPC trace of PE (Table 1, run 8) obtained with **3b'-Zr**.

**Figure S54.** GPC trace of PE (Table 1, run 9) obtained with **3c-Zr<sub>2</sub>**.

**Figure S55.** GPC trace of PE (Table 1, run 12) obtained with **3b'-Hf**.

**Figure S57.** GPC trace of PE/PHex (Table 2, run 1) obtained with **3a-Zr<sub>2</sub>**.

**Figure S58.**  $^{13}\text{C}$  NMR spectrum of PE/PHex (Table 2, run 4).

**Figure S59.**  $^{13}\text{C}$  NMR spectrum of PE/PHex (Table 2, run 5).

**Figure S60.** GPC trace of PE/PHex (Table 2, run 5) obtained with **3b-Zr<sub>2</sub>**.

**Figure S61.** GPC trace of PE/PHex (Table 2, run 6) obtained with **3b-Zr<sub>2</sub>**.

**Figure S62.** GPC trace of PE/PHex (Table 2, run 7) obtained with **3b'-Zr**.

**Figure S63.** GPC trace of PE/PHex (Table 2, run 8) obtained with **3b'-Zr**.

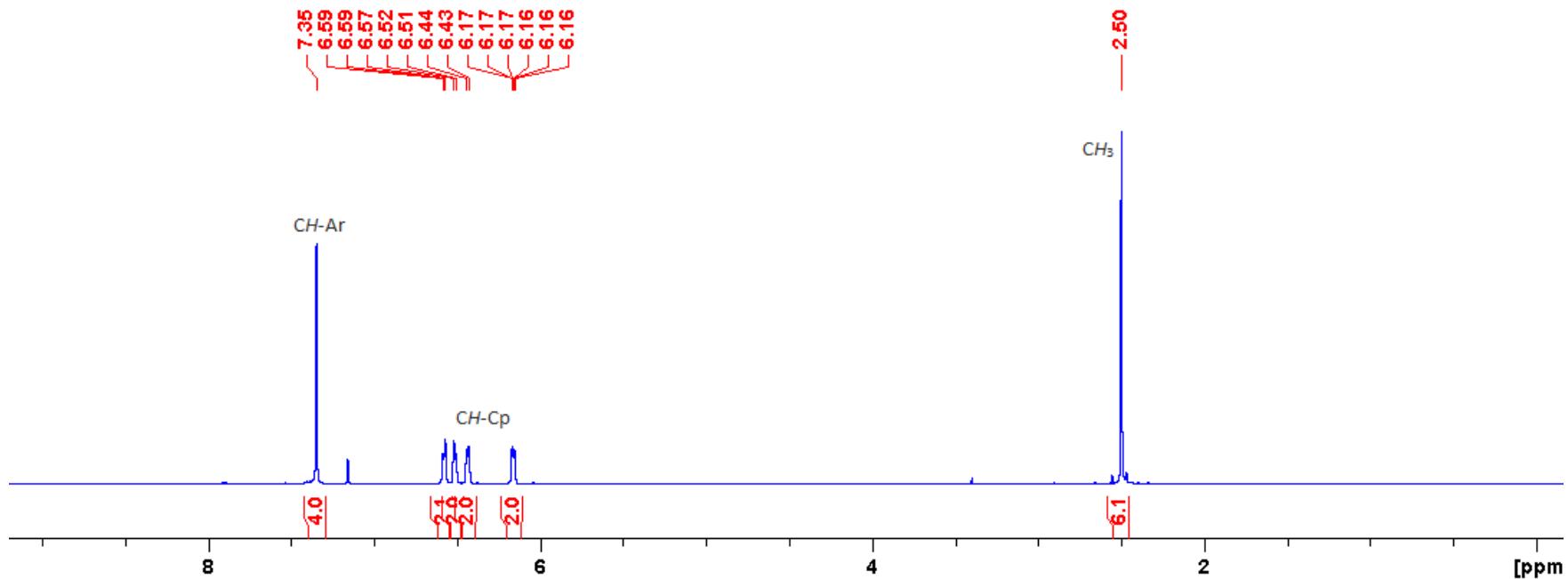
**Figure S64.** GPC trace of PE/PHex (Table 2, run 9) obtained with **3c-Zr<sub>2</sub>**.

**Figure S65.** GPC trace of PE/PHex (Table 2, run 10) obtained with **3a-Hf<sub>2</sub>**.

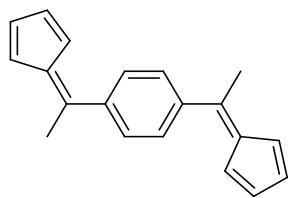
**Figure S66.** GPC trace of PE/PHex (Table 2, run 11) obtained with **3a-Hf<sub>2</sub>**.

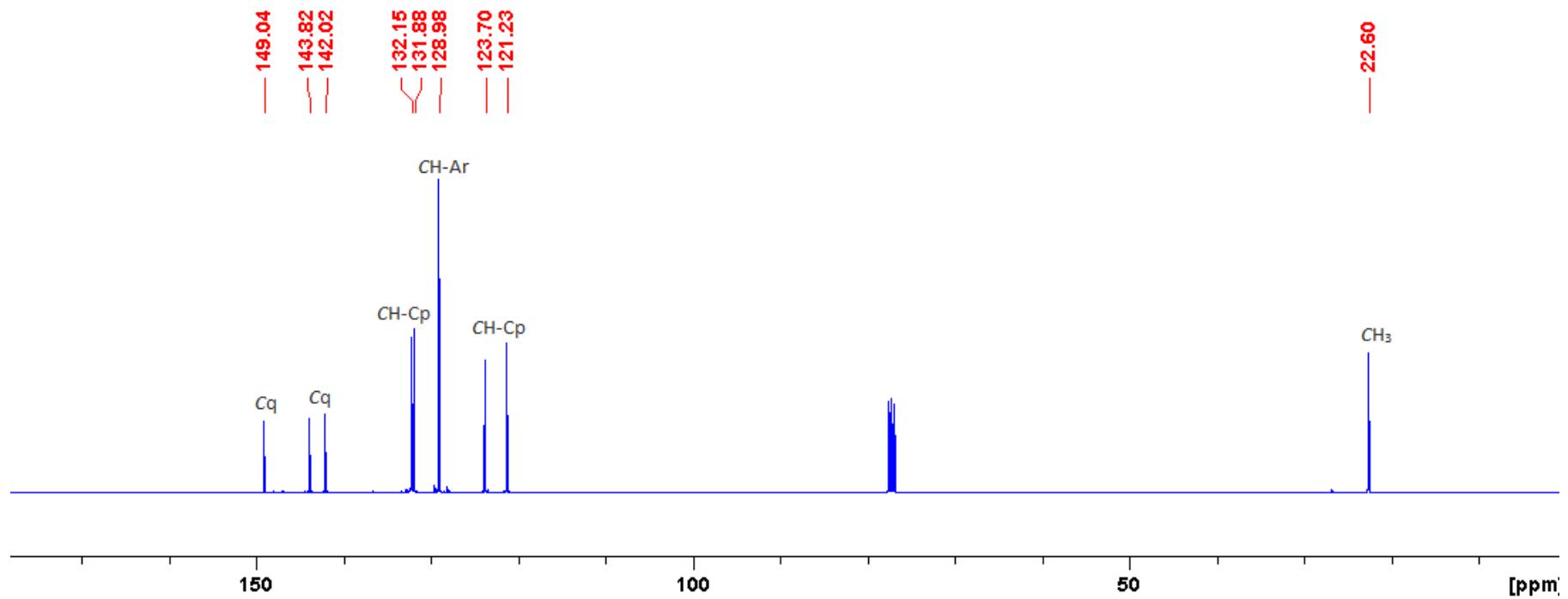
**Figure S67.** Molecular structure of **3a'-Zr**.

**Table S1.** Summary of Crystal and Refinement Data for Compound **3a'-Zr**.

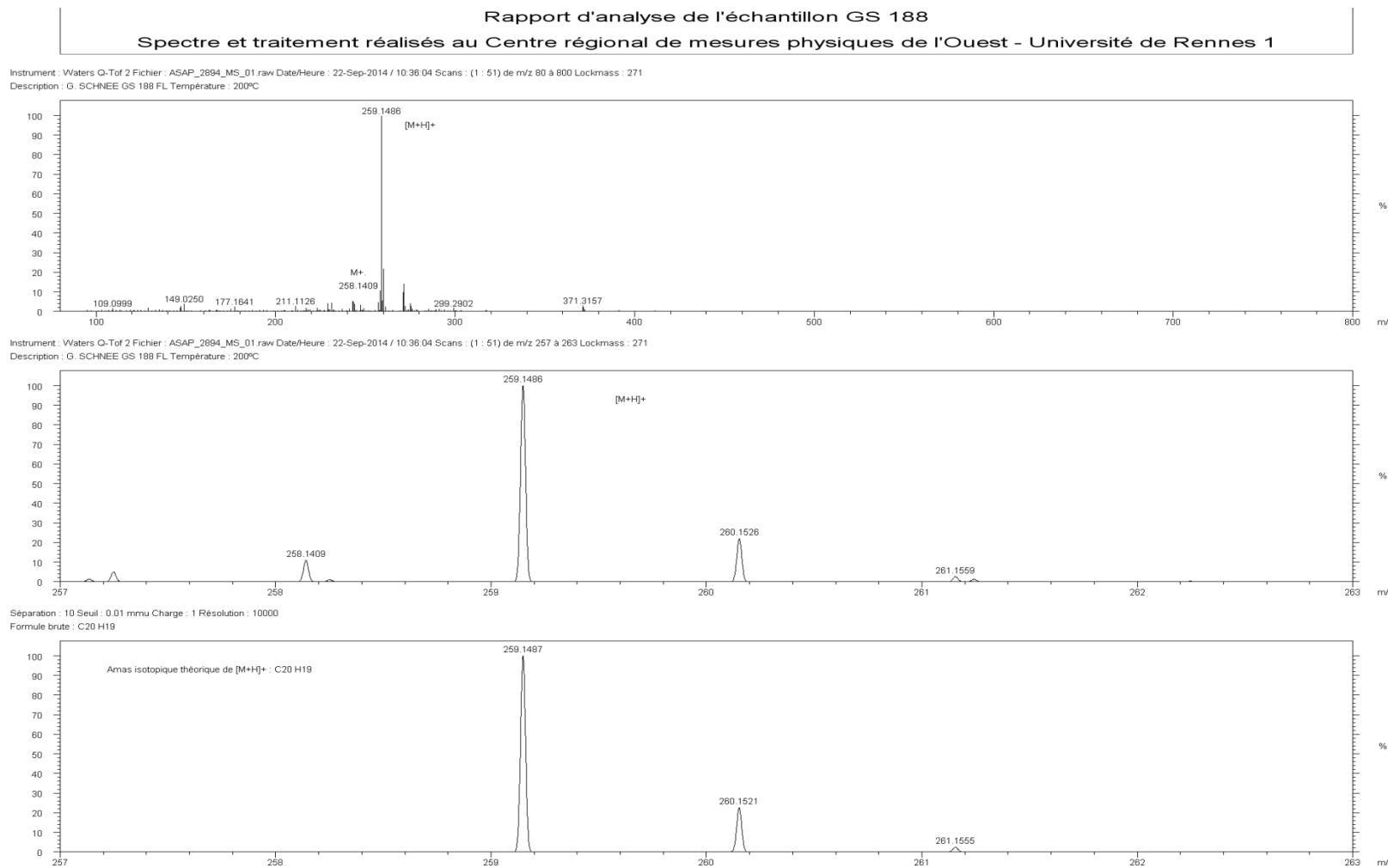


**Figure S1.**  $^1\text{H}$  NMR spectrum ( $\text{CDCl}_3$ , 400 MHz, 25 °C) of **1a**. jfc-gs190-1

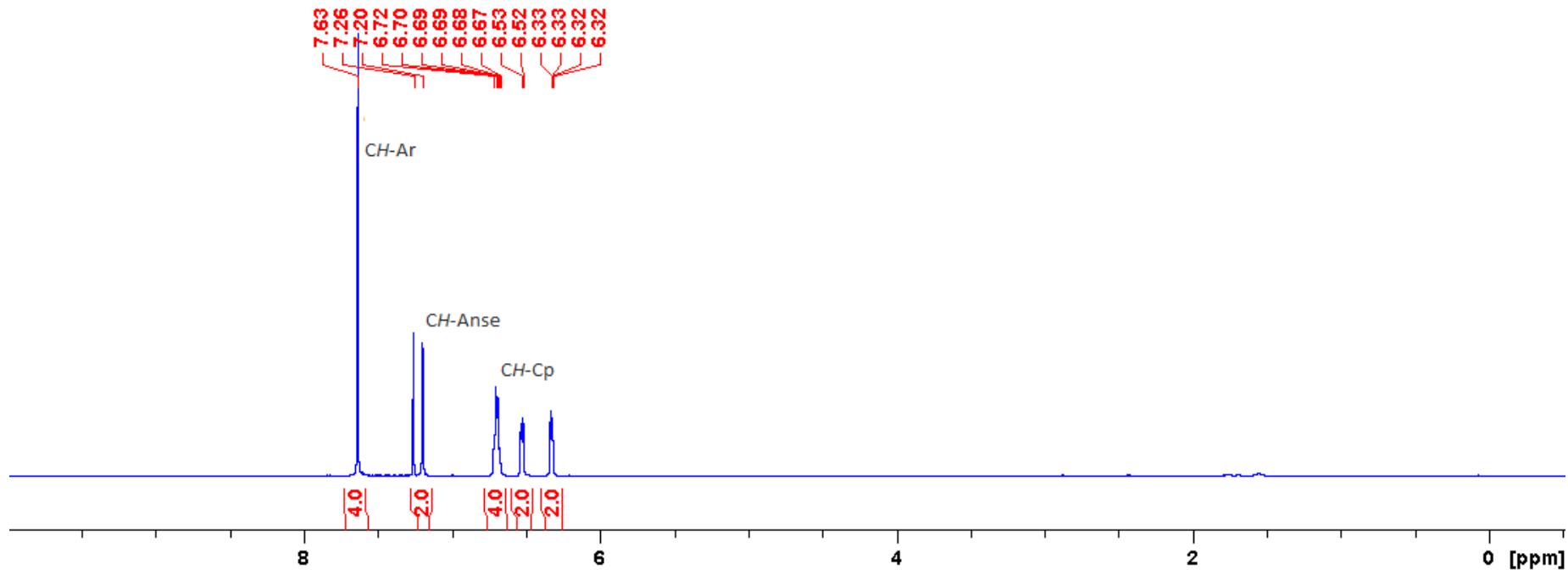




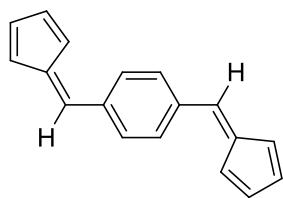
**Figure S2.**  $^{13}\text{C}$  NMR spectrum ( $\text{CDCl}_3$ , 125 MHz, 25 °C) of **1a**.

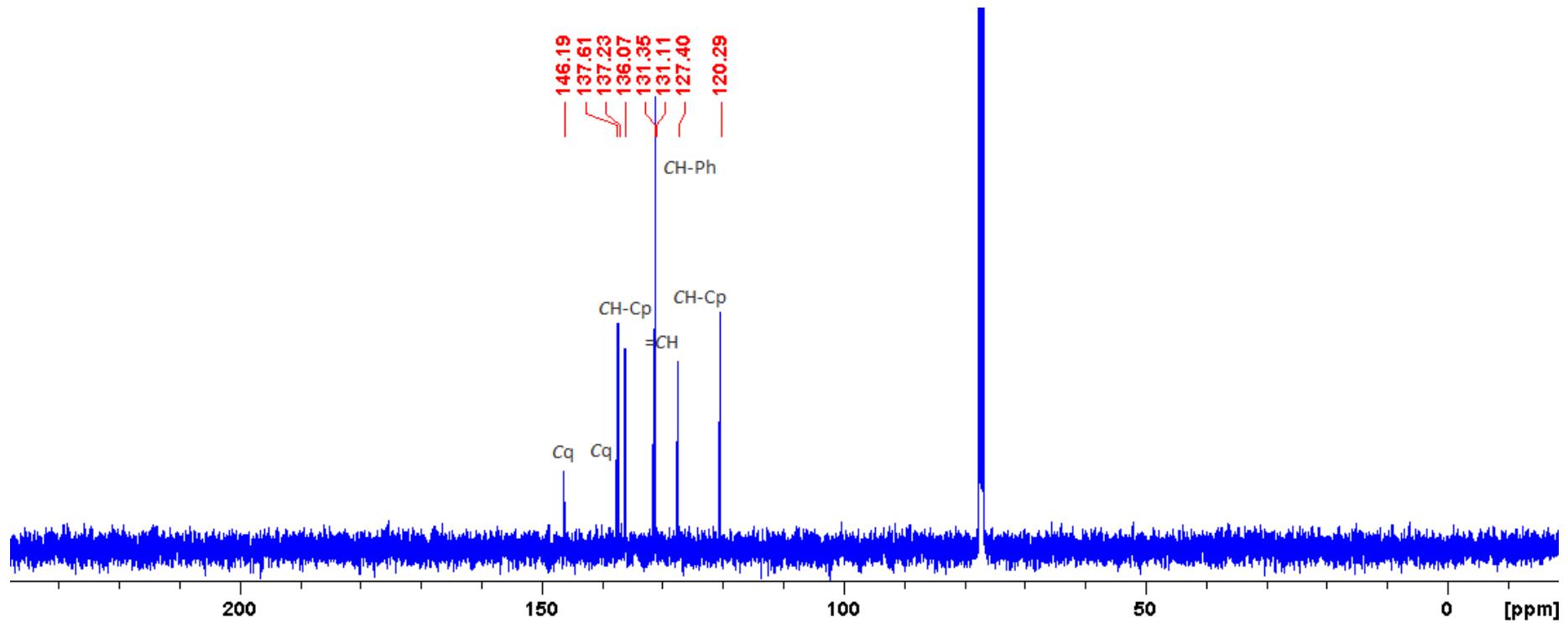


**Figure S3.** ASAP mass spectrum of **1a**.

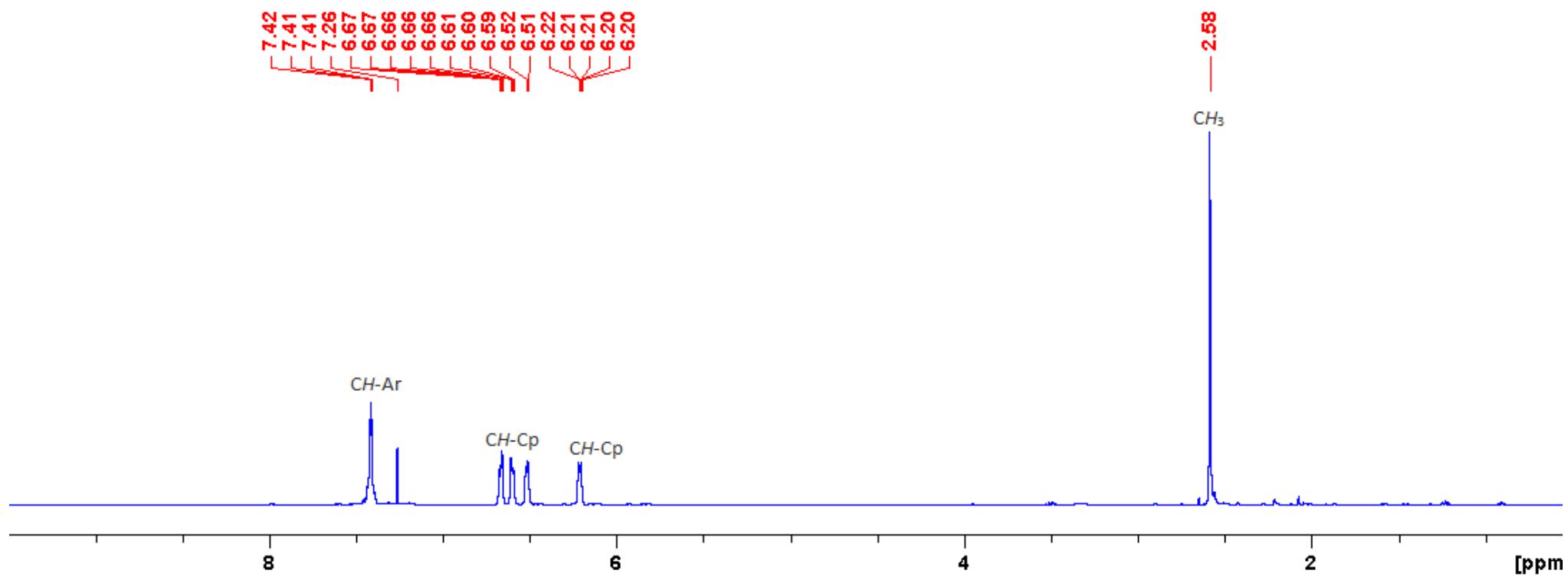


**Figure S4.** <sup>1</sup>H NMR spectrum ( $\text{CDCl}_3$ , 400 MHz, 25 °C) of **1b**.

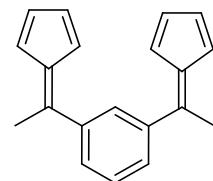


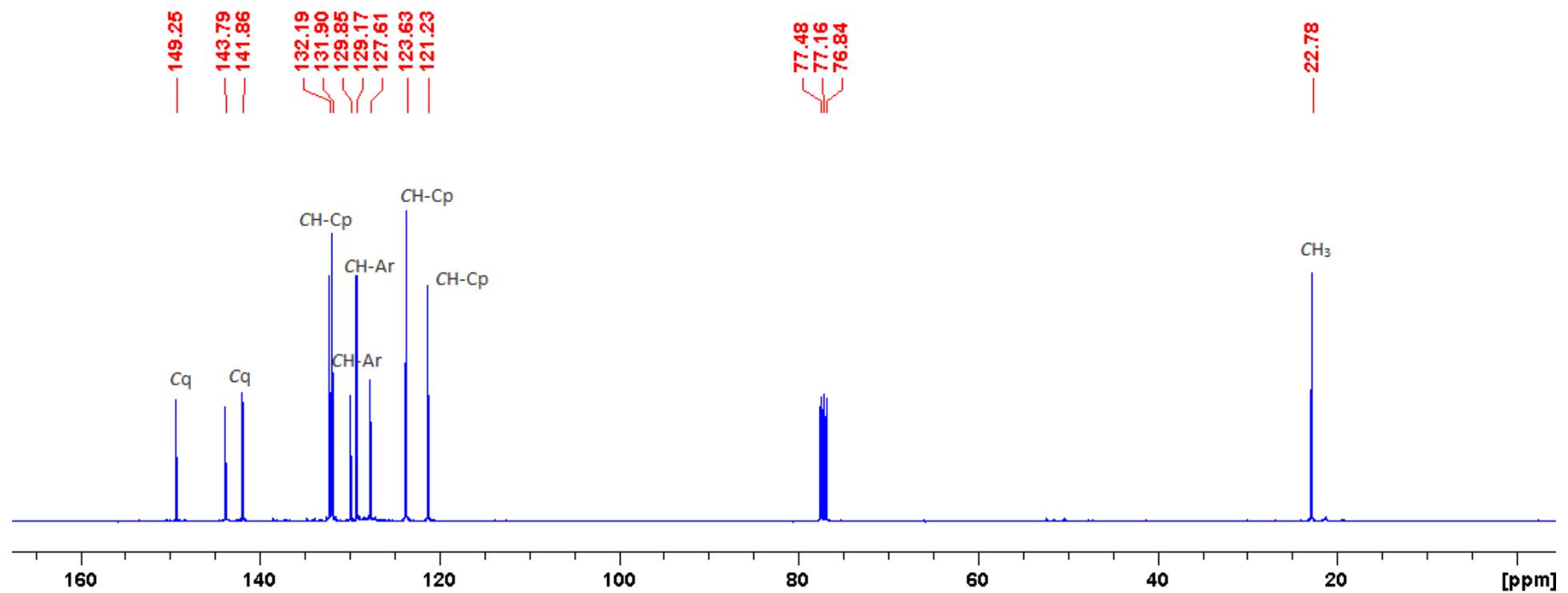


**Figure S5.**  $^{13}\text{C}$  NMR spectrum ( $\text{CDCl}_3$ , 125 MHz, 25 °C) of **1b**.



**Figure S6.**  $^1\text{H}$  NMR spectrum ( $\text{CDCl}_3$ , 400 MHz, 25 °C) of **1c**.

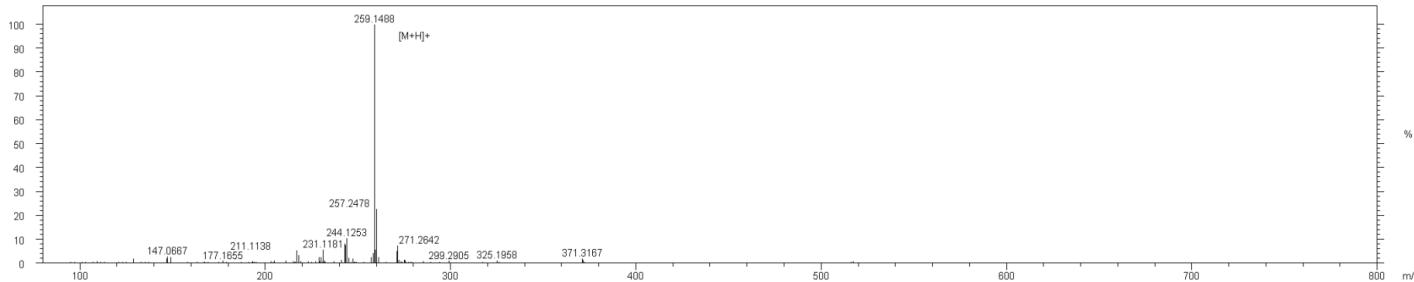




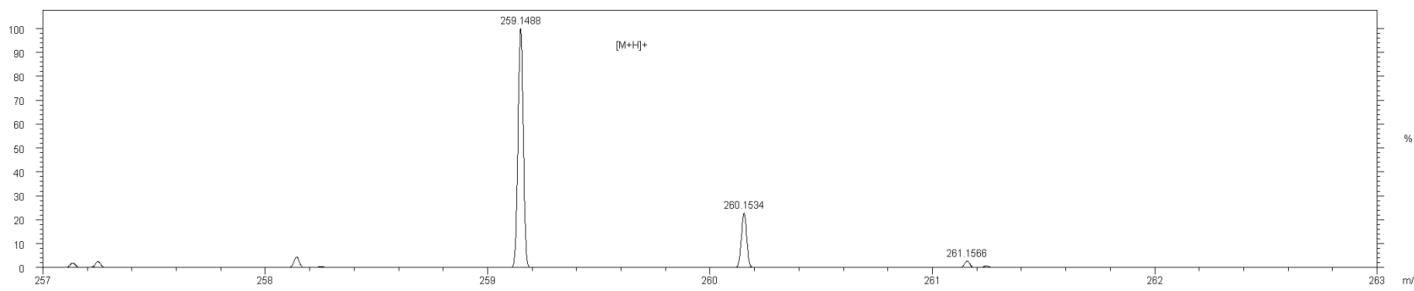
**Figure S7.**  $^{13}\text{C}$  NMR spectrum ( $\text{CDCl}_3$ , 125 MHz, 25 °C) of **1c**.

**Rapport d'analyse de l'échantillon GS 200**  
**Spectre et traitement réalisés au Centre régional de mesures physiques de l'Ouest - Université de Rennes 1**

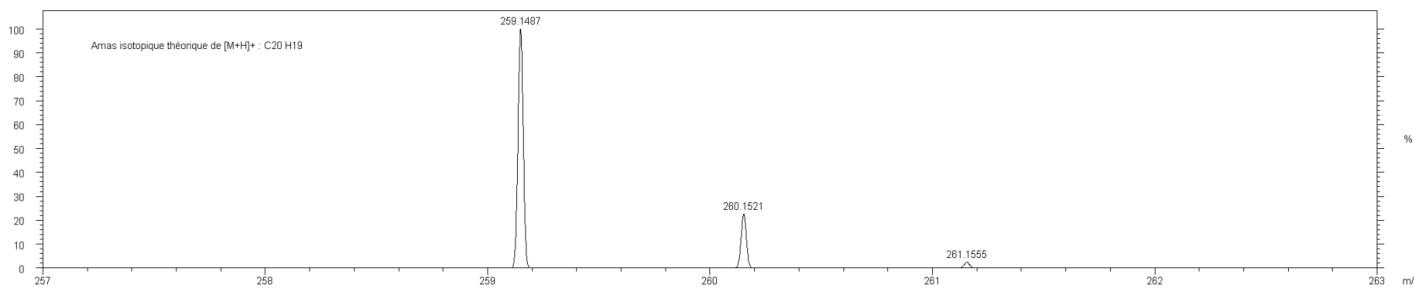
Instrument : Waters Q-ToF 2 Fichier : ASAP\_2895\_MS\_01 raw Date/Horaire : 22-Sep-2014 / 10:16:04 Scans : (1 - 52) de m/z 80 à 800 Lockmass : 411  
 Description : G. SCHNEE GS 200 FL Température : 100°C



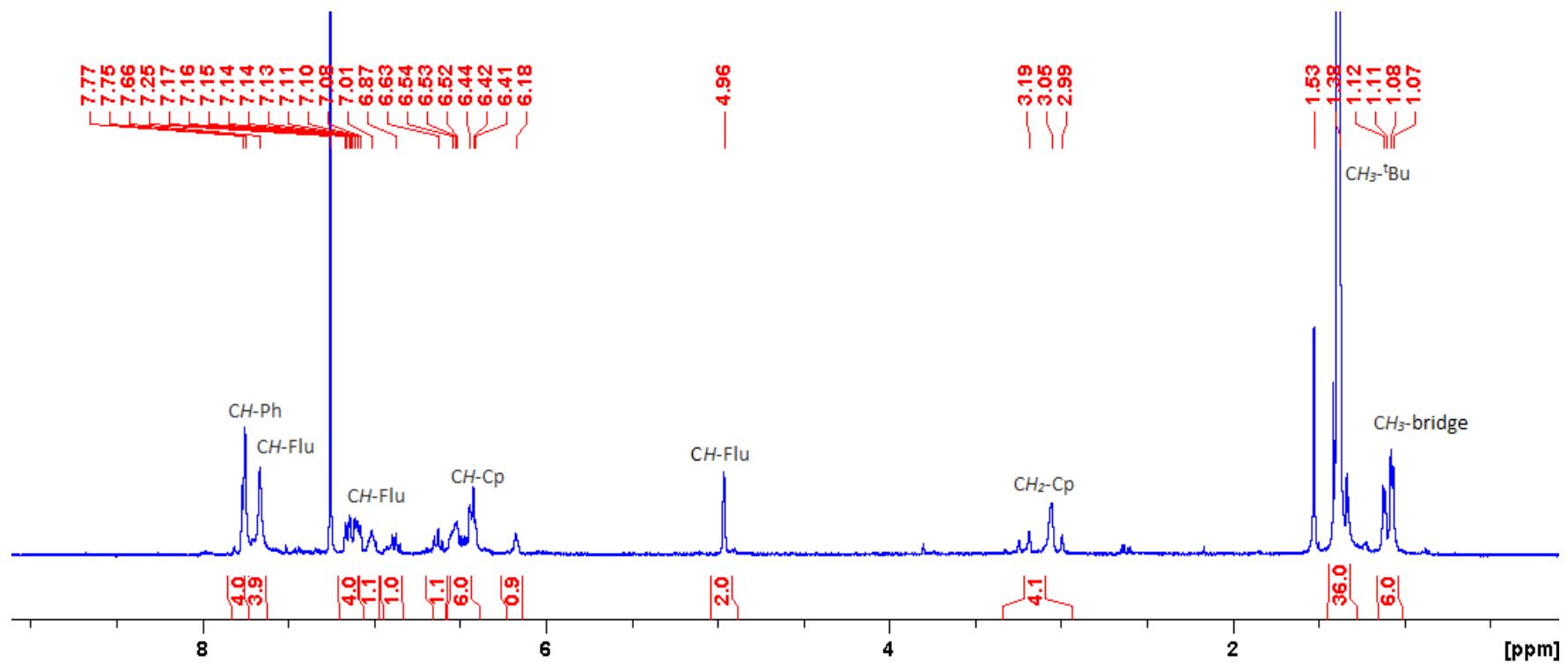
Instrument : Waters Q-ToF 2 Fichier : ASAP\_2895\_MS\_01 raw Date/Horaire : 22-Sep-2014 / 10:16:04 Scans : (1 - 52) de m/z 257 à 263 Lockmass : 411  
 Description : G. SCHNEE GS 200 FL Température : 100°C



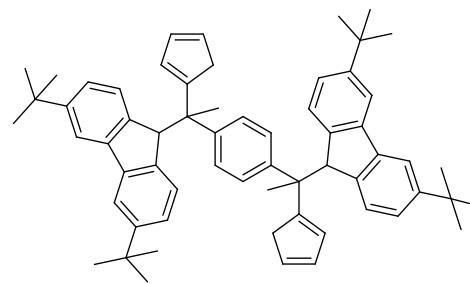
Séparation : 10 Seuil : 0.01 mmu Charge : 1 Résolution : 10000  
 Formule brute : C<sub>20</sub>H<sub>19</sub>

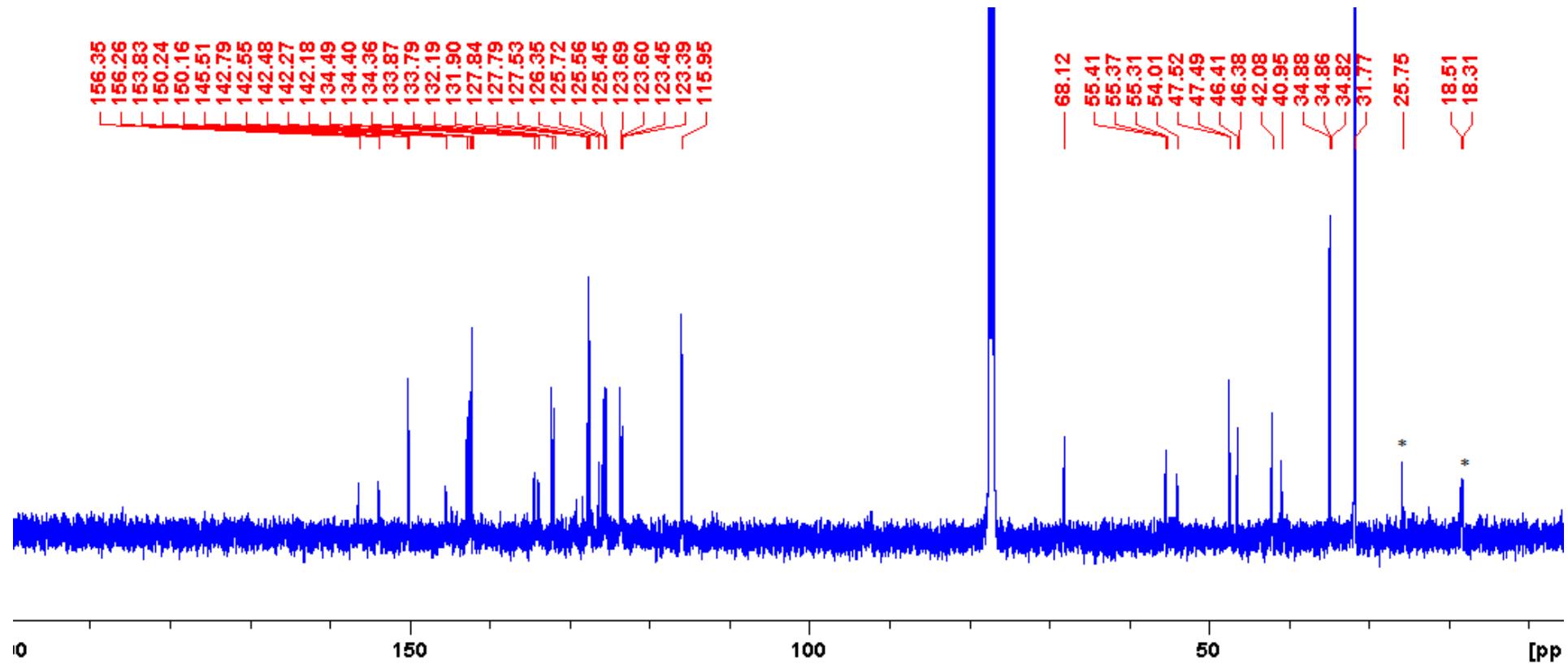


**Figure S8.** ASAP Mass spectrum of **1c**.



**Figure S9.** <sup>1</sup>H NMR spectrum (CDCl<sub>3</sub>, 400 MHz, 25 °C) of **2a**.





**Figure S10.**  $^{13}\text{C}$  NMR spectrum ( $\text{CDCl}_3$ , 125 MHz, 25 °C) of **2a**. (\*) stand for residual solvent peaks)

Centre régional de mesures physiques de l'Ouest (CRMPO) - RAPPORT D'ANALYSE

**Analysis Info**

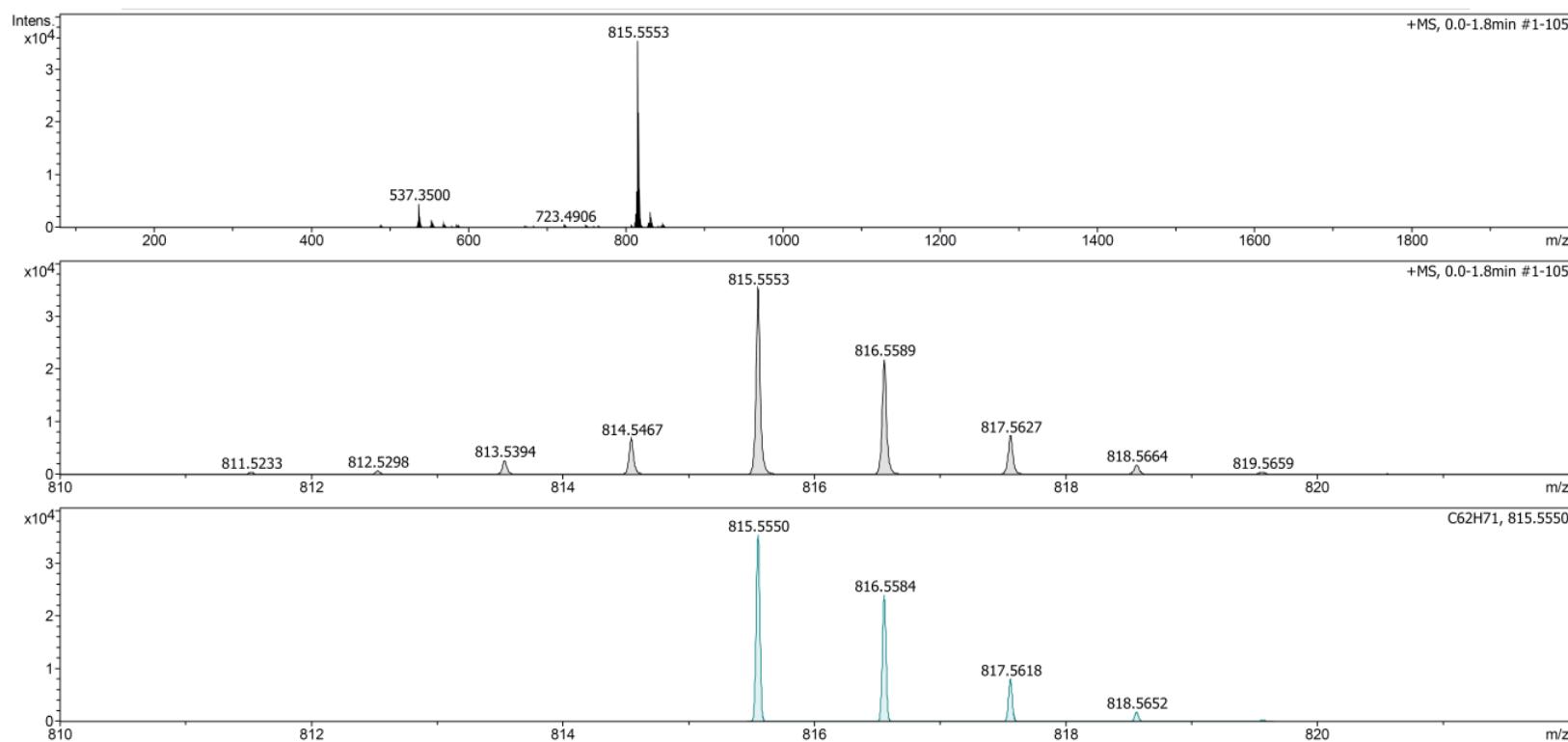
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 Method ASAP\_CRMPO\_tune\_low.m  
 Sample Name LB 20  
 Comment G. SCHNEE LB 20 Température : 255°C

Acquisition Date

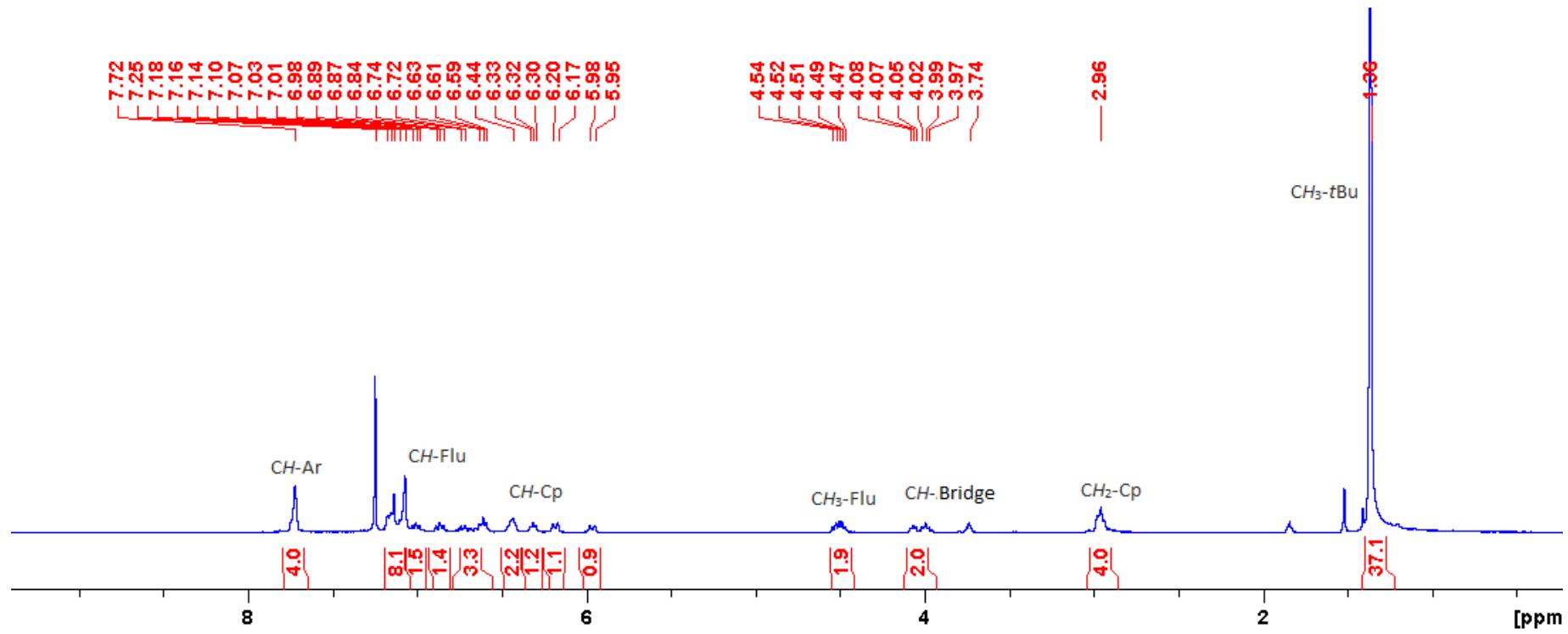
9/25/2014 7:52:24 PM

Operator  
Instrument

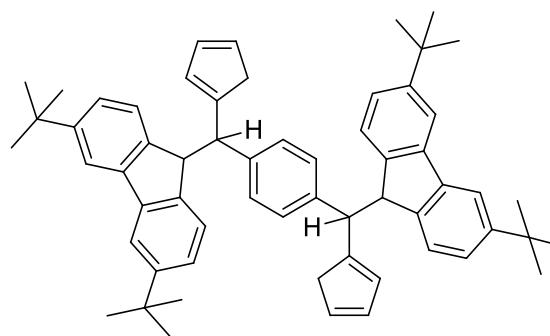
Philippe JÉHAN  
maXis

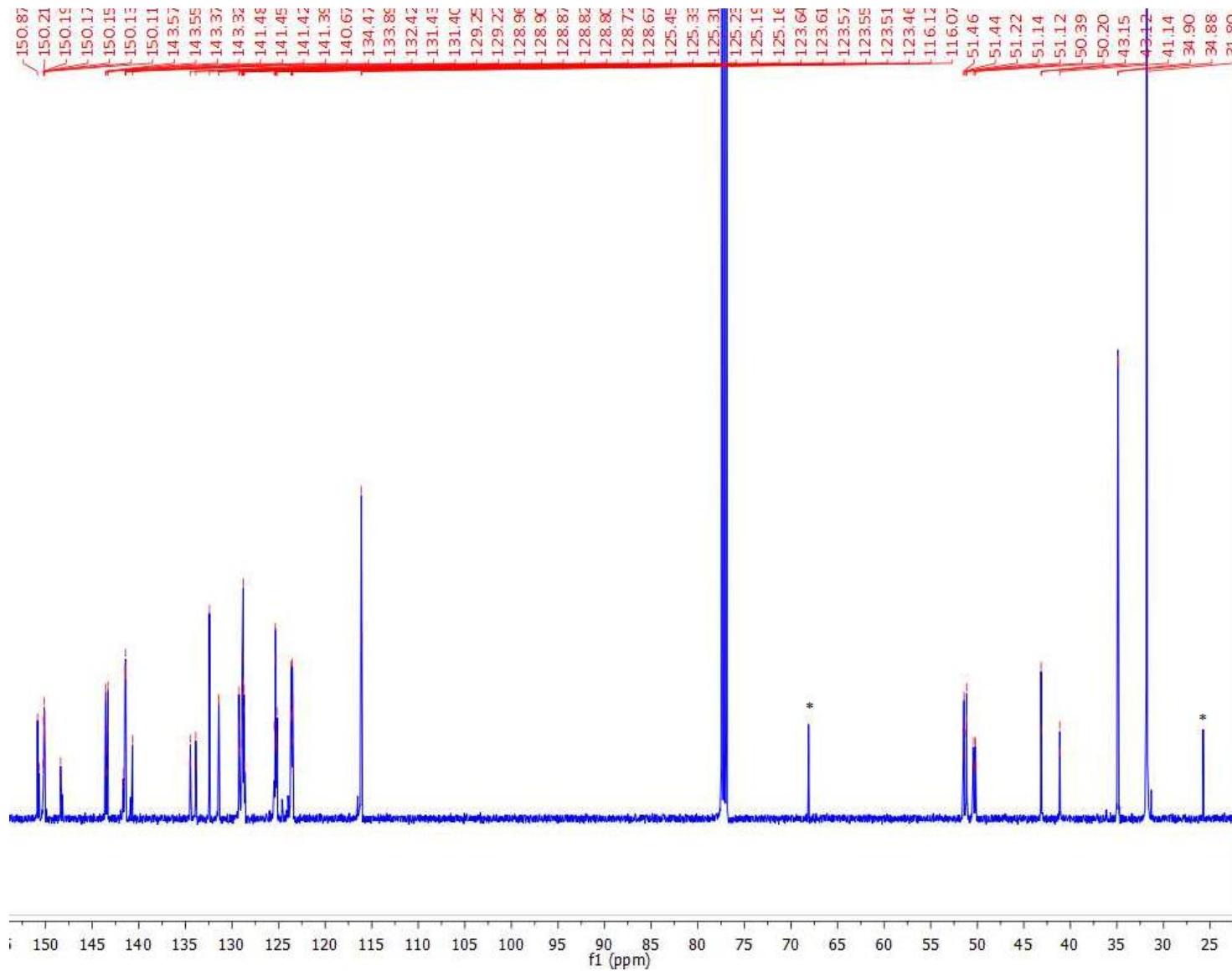


**Figure S11.** ASAP mass spectrum of **2a**.



**Figure S12.** <sup>1</sup>H NMR spectrum ( $\text{CDCl}_3$ , 400 MHz, 25 °C) of **2b**.





**Figure S13.**  $^{13}\text{C}$  NMR spectrum ( $\text{CDCl}_3$ , 125 MHz, 25 °C) of **2b**. (\* stand for residual solvent peaks)

## Centre régional de mesures physiques de l'Ouest (CRMPO) - RAPPORT D'ANALYSE

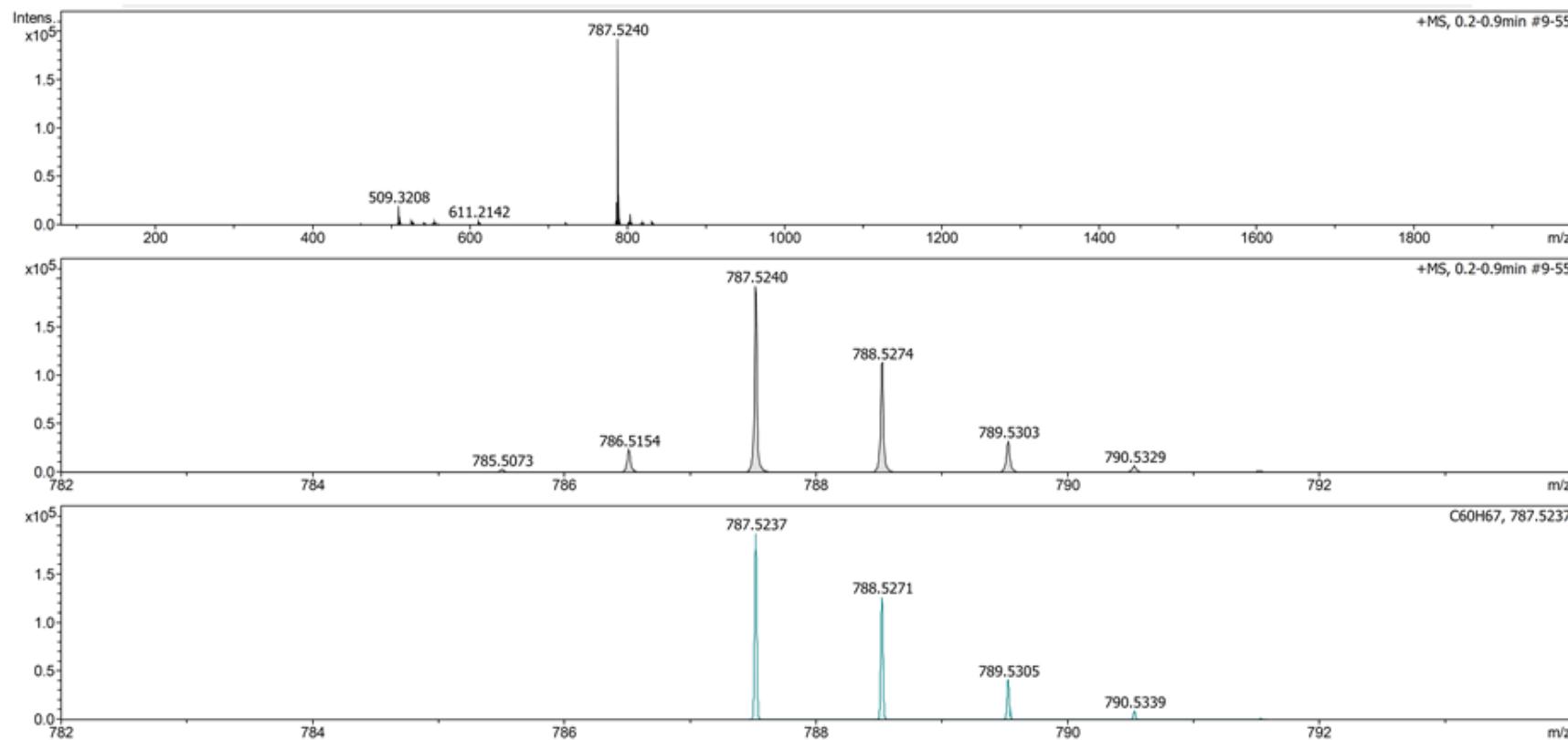
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Sample Name LB 4  
Comment G. SCHNEE LB 4 Température : 230°C

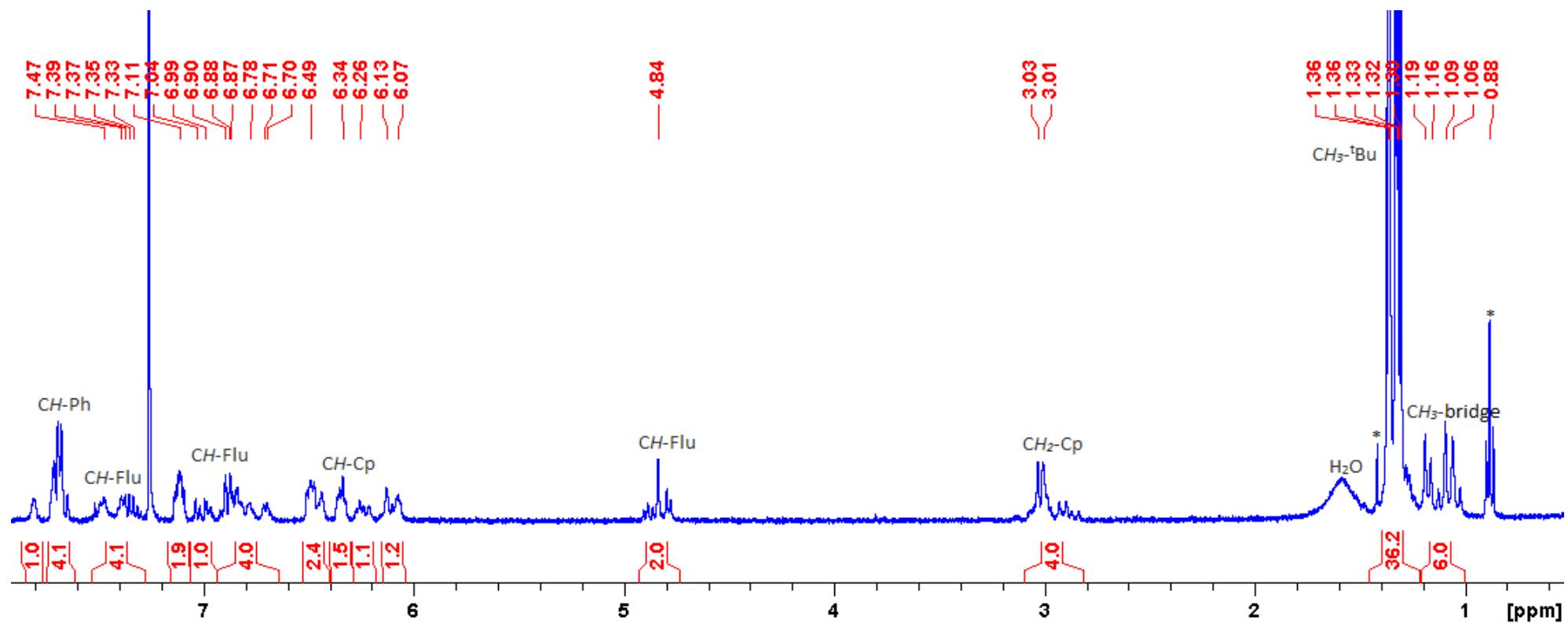
**Acquisition Date**

9/26/2014 3:27:56 PM

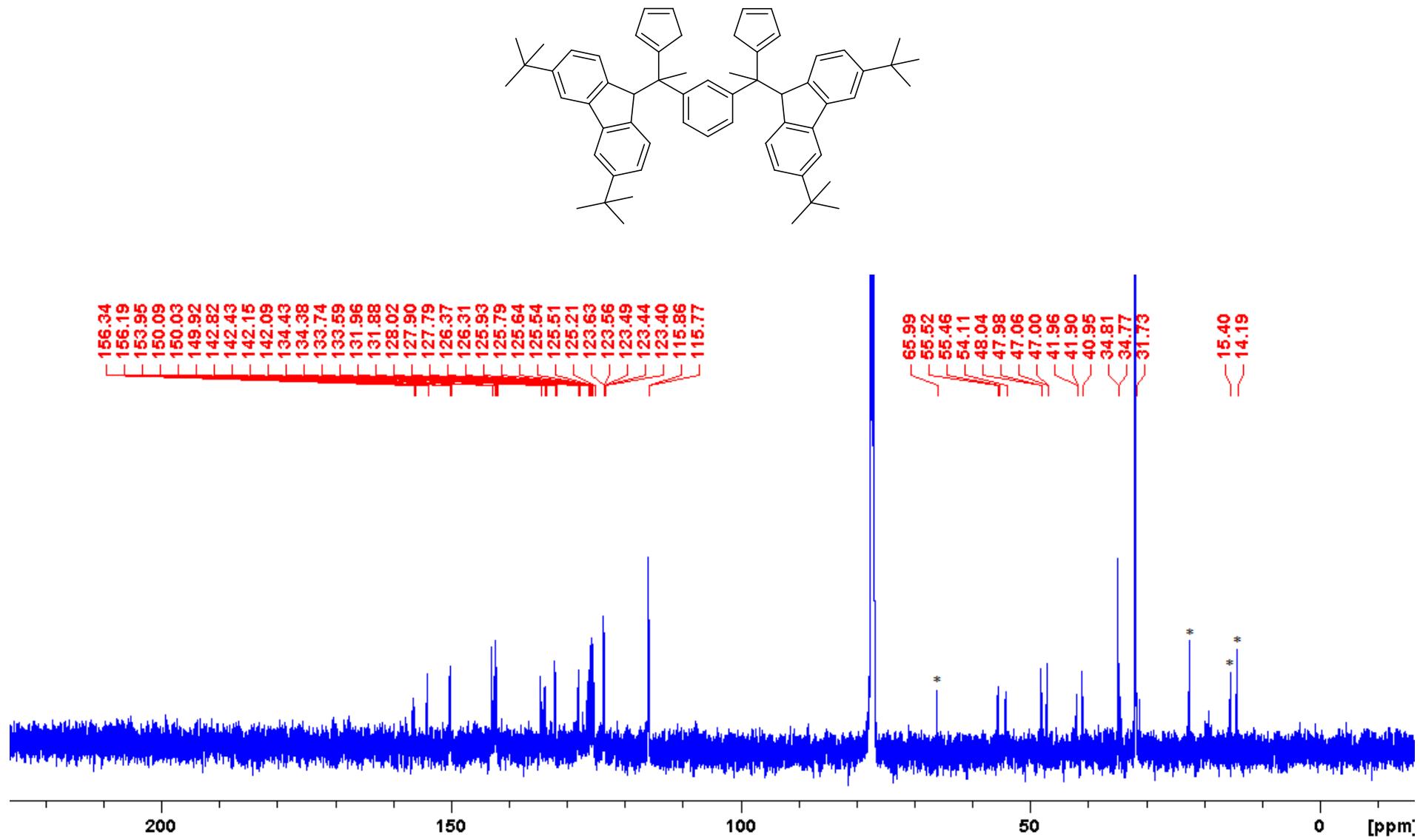
Operator  
Instrument

Philippe JÉHAN  
maXis

**Figure S14.** ASAP mass spectrum of **2b**.



**Figure S15.**  $^1\text{H}$  NMR spectrum ( $\text{CDCl}_3$ , 500 MHz, 25 °C) of **2c**. (\*) stands for residual solvent peak)



**Figure S16.**  $^{13}\text{C}$  NMR spectrum ( $\text{CDCl}_3$ , 125 MHz, 25 °C) of **2c**. (\* stand for residual solvent peaks)

Centre régional de mesures physiques de l'Ouest (CRMPO) - RAPPORT D'ANALYSE

Analysis Info

Analysis Name D:\Data\CRMPO\ASAP\_2997\_MS\_01.d  
Method ASAP\_CRMPO\_tune\_low.m  
Sample Name GS 384  
Comment G. SCHNEE GS 384 Température : 300°C

Acquisition Date

10/29/2014 8:23:01 PM

Operator  
Instrument

Philippe JÉHAN  
maXis

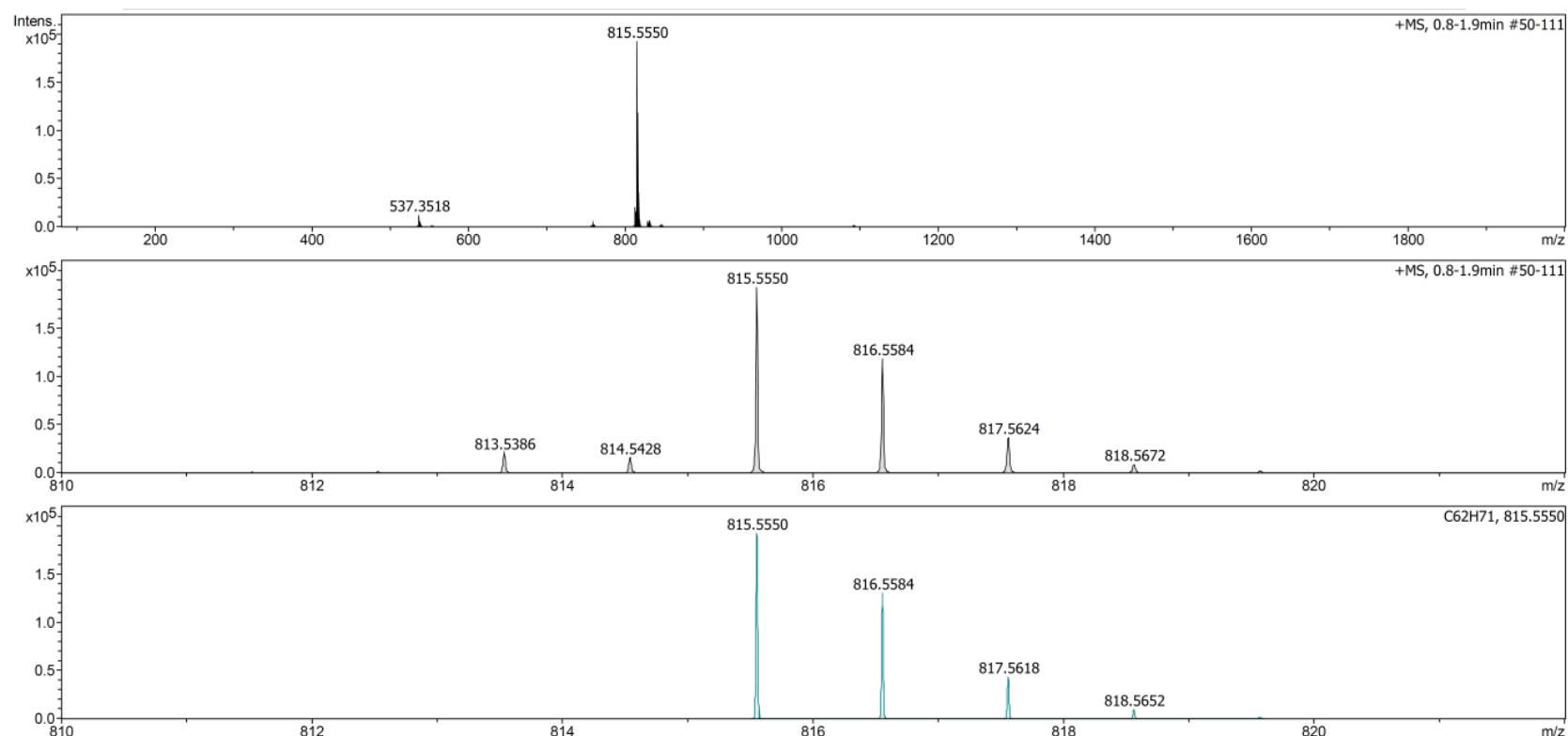
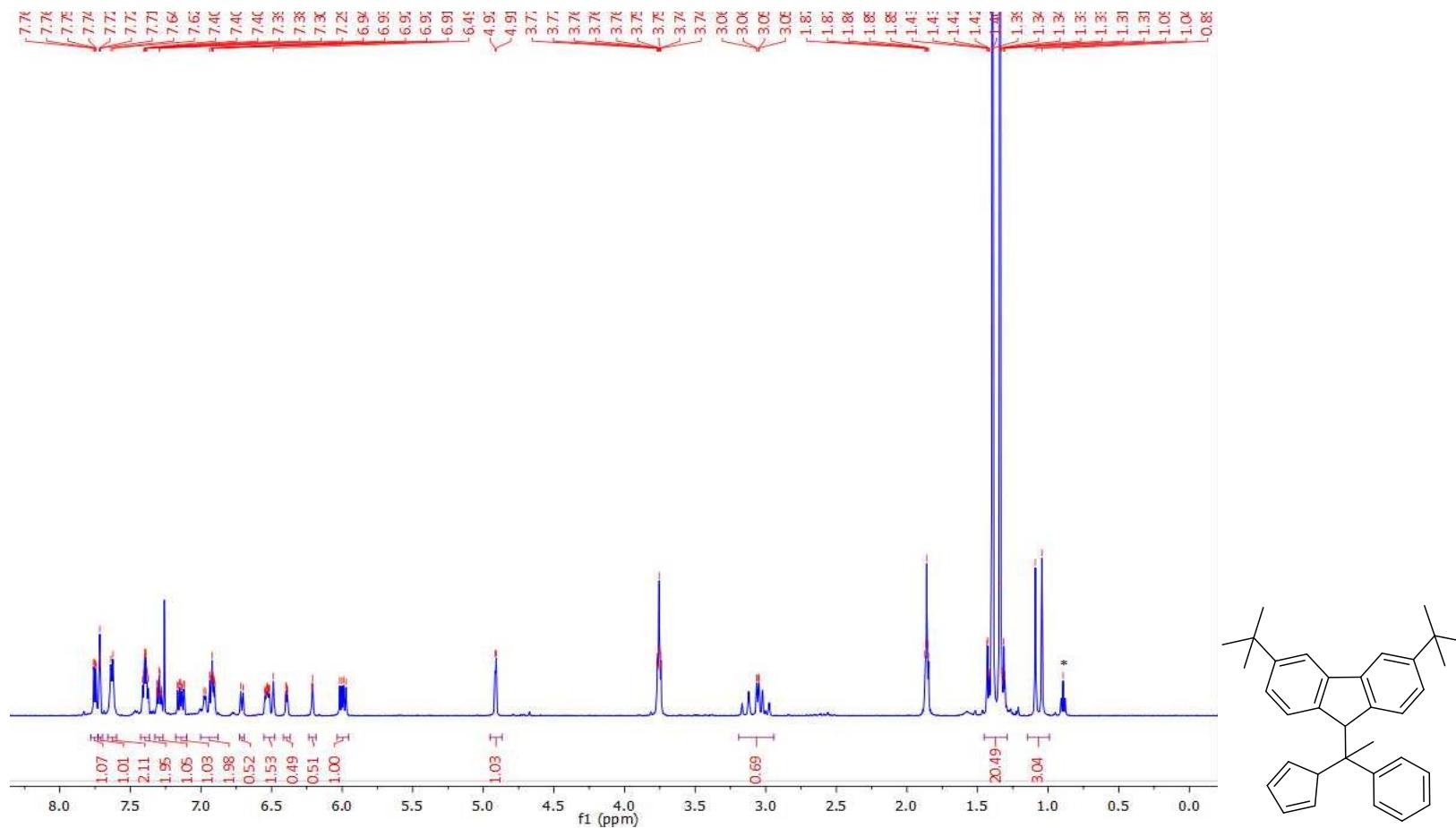
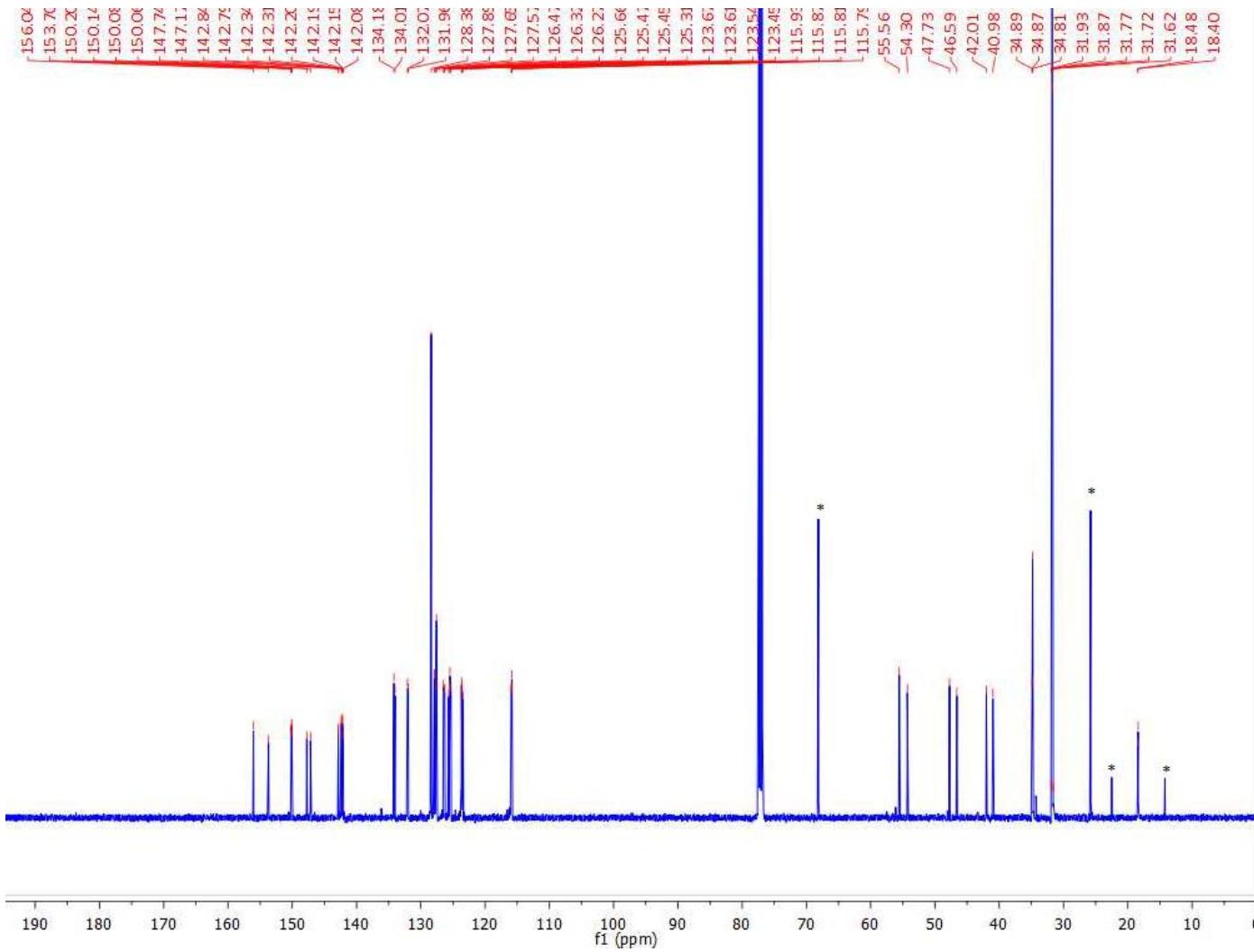


Figure S17. ASAP mass spectrum of **2c**.



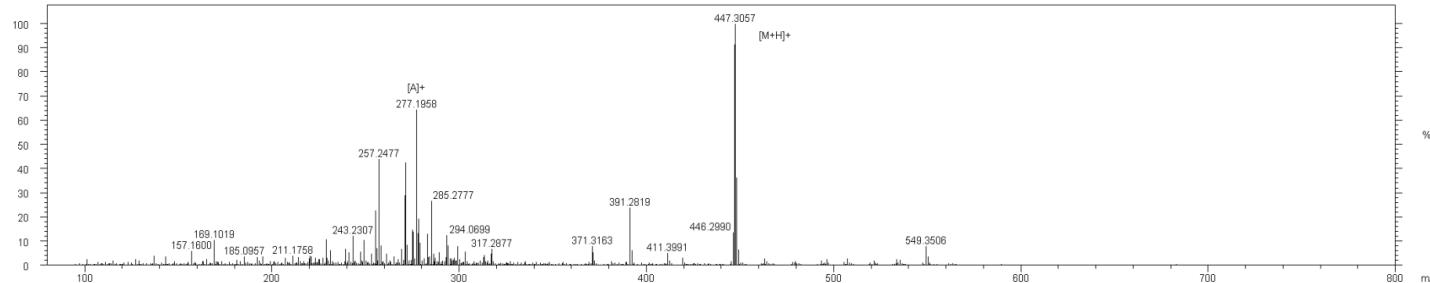
**Figure S18.**  $^1\text{H}$  NMR spectrum ( $\text{CDCl}_3$ , 500 MHz, 25 °C) of **2a'**. (\*residual solvent peak)



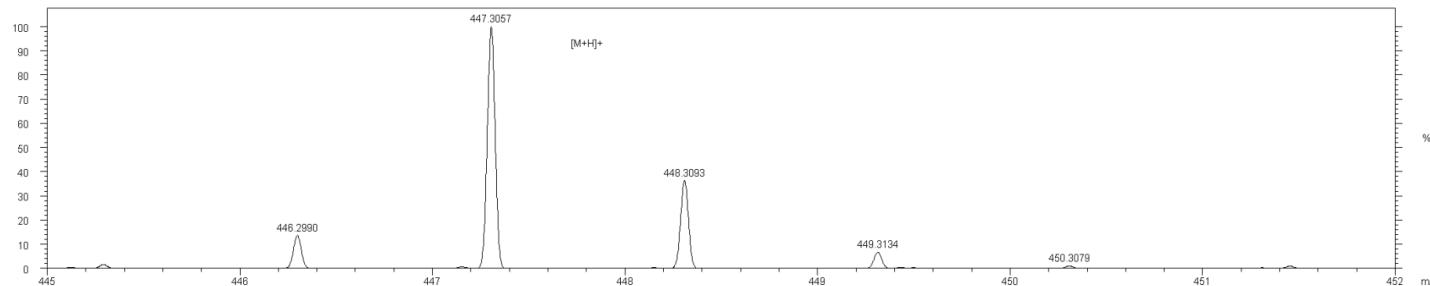
**Figure S19.**  $^{13}\text{C}$  NMR spectrum ( $\text{CDCl}_3$ , 125 MHz, 25 °C) of **2a'**. (\*residual solvent peak)

**Rapport d'analyse de l'échantillon GS 405**  
**Spectre et traitement réalisés au Centre régional de mesures physiques de l'Ouest - Université de Rennes 1**

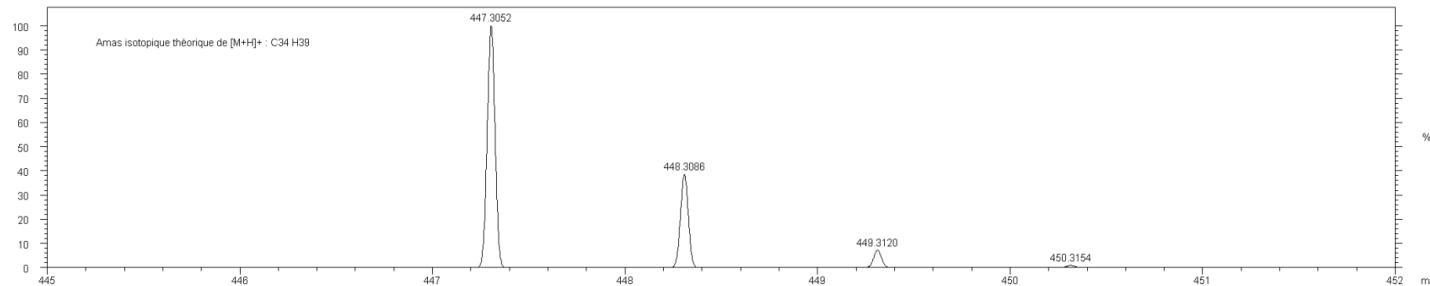
Instrument : Waters Q-ToF 2 Fichier : ASAP\_3136\_MS\_01.raw Date/Heure : 10-Nov-2014 / 15:28:43 Scans : (55 : 103) de m/z 80 à 800 Lockmass : 411  
 Description : G.SCHNEE GS 405 FL Température : 400°C



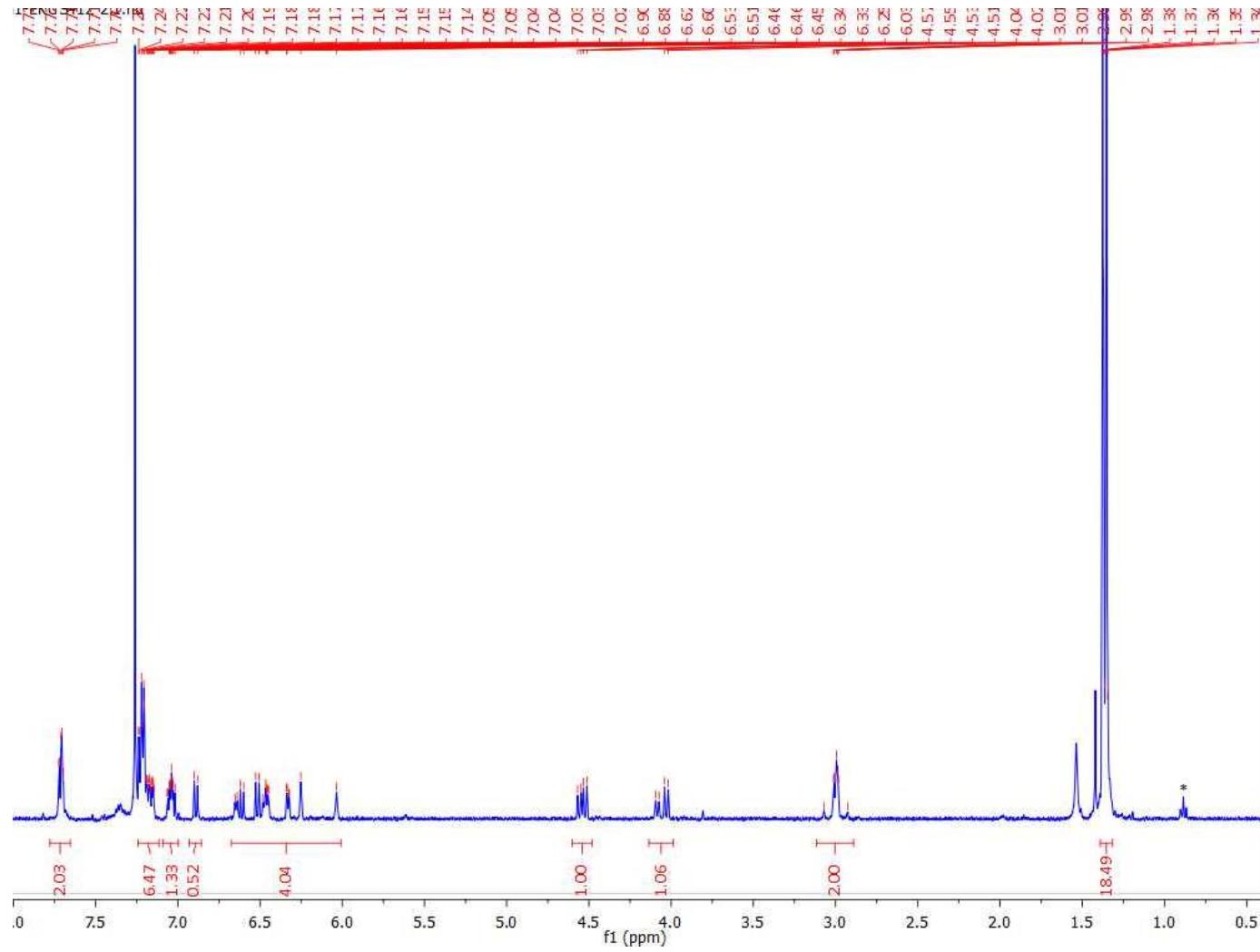
Instrument : Waters Q-ToF 2 Fichier : ASAP\_3136\_MS\_01.raw Date/Heure : 10-Nov-2014 / 15:28:43 Scans : (55 : 103) de m/z 445 à 452 Lockmass : 411  
 Description : G.SCHNEE GS 405 FL Température : 400°C



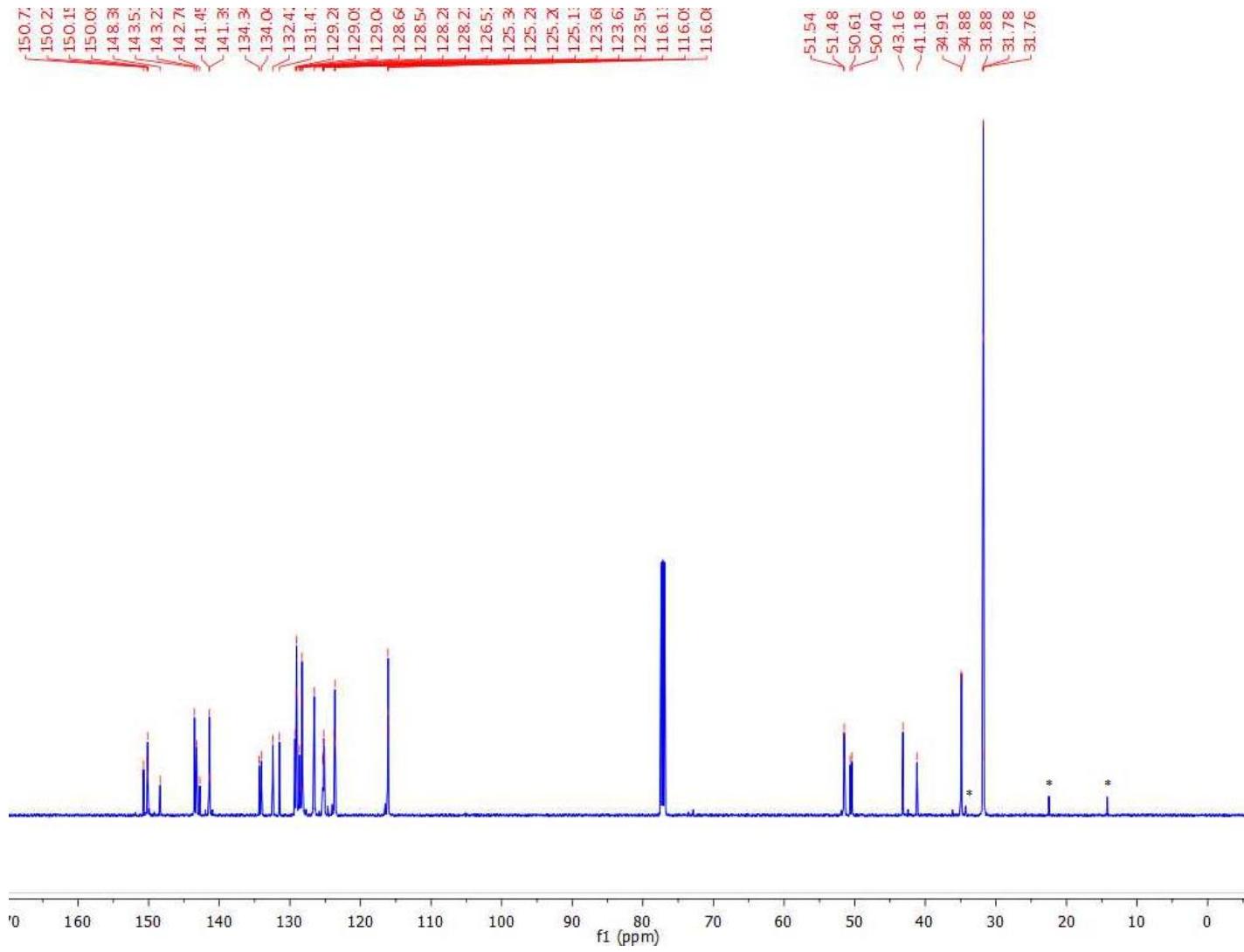
Séparation : 10 Seuil : 0.01 mmu Charge : 1 Résolution : 10000  
 Formule brute : C<sub>34</sub>H<sub>39</sub>



**Figure S20.** ASAP mass spectrum of **2a'**.



**Figure S21.** <sup>1</sup>H NMR spectrum (CDCl<sub>3</sub>, 400 MHz, 25 °C) of **2b'**. (\*stands for residual solvent peak)



**Figure S22.**  $^{13}\text{C}$  NMR spectrum ( $\text{CDCl}_3$ , 125 MHz, 25 °C) of **2b'**. (\*stand for residual solvent peak)

Centre régional de mesures physiques de l'Ouest (CRMPO) - RAPPORT D'ANALYSE

Analysis Info

Analysis Name D:\Data\CRMPO\ASAP\_3091\_MS\_02.d  
Method ASAP\_CRMPO\_tune\_low.m  
Sample Name GS 412  
Comment G. SCHNEE GS 412 Température : 135°C

Acquisition Date

11/10/2014 7:22:31 PM

Operator  
Instrument

Philippe JÉHAN  
maXis

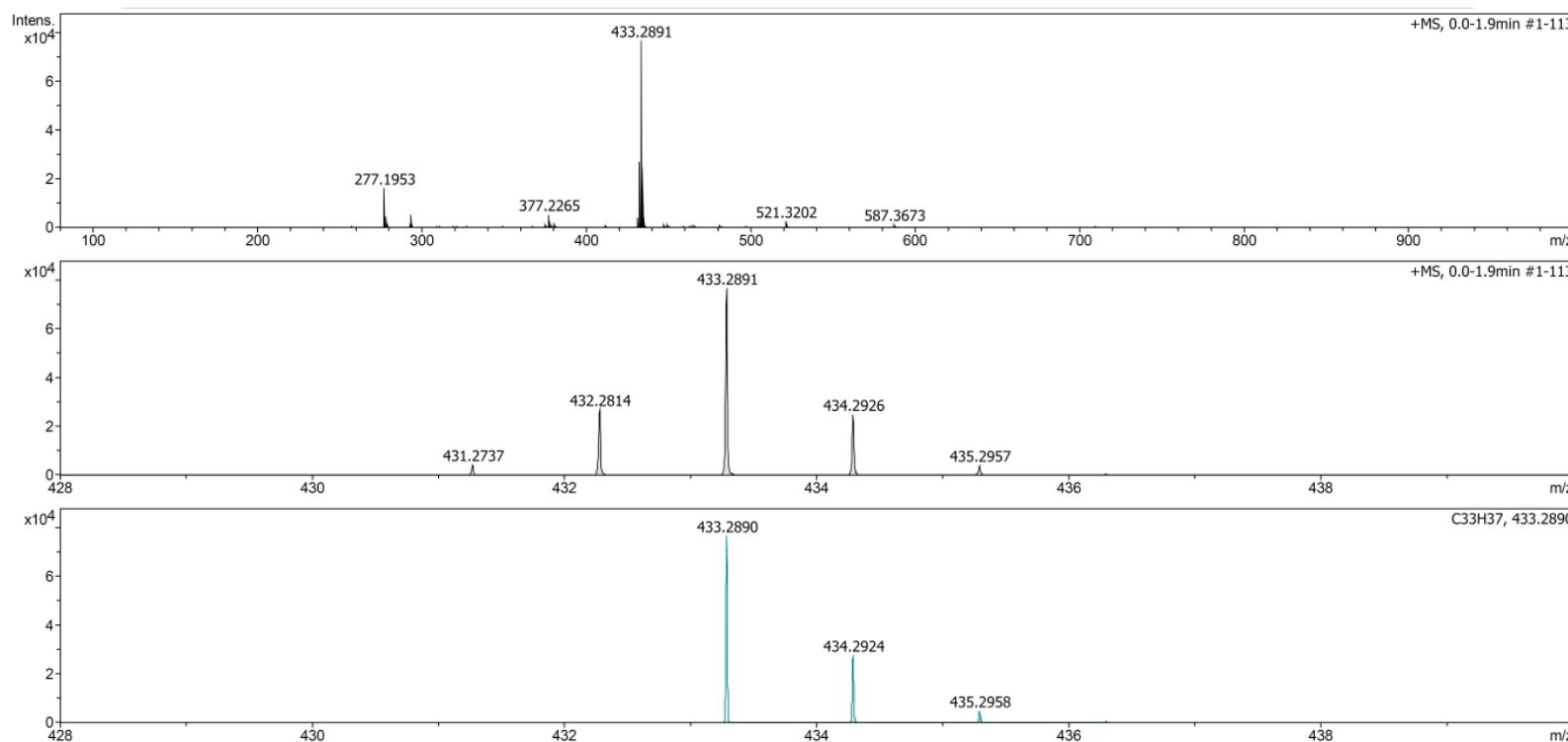
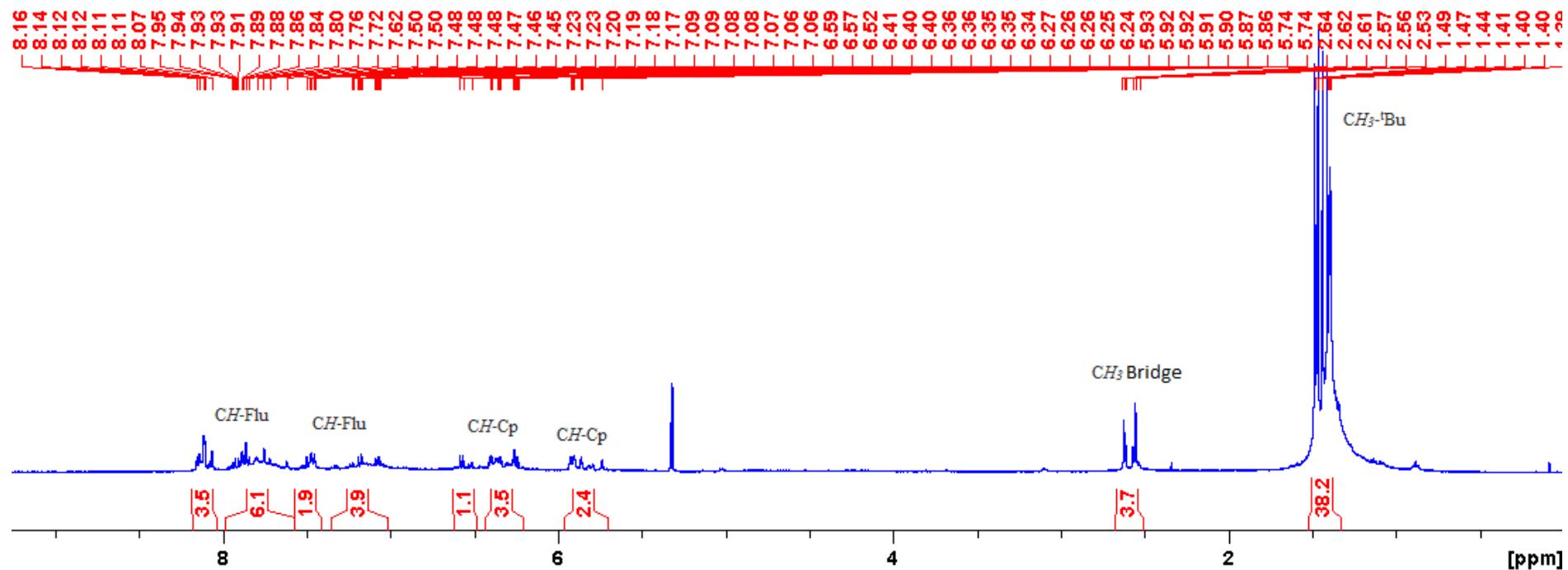
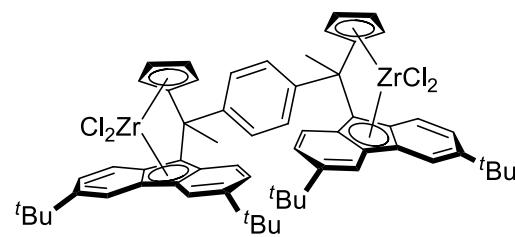
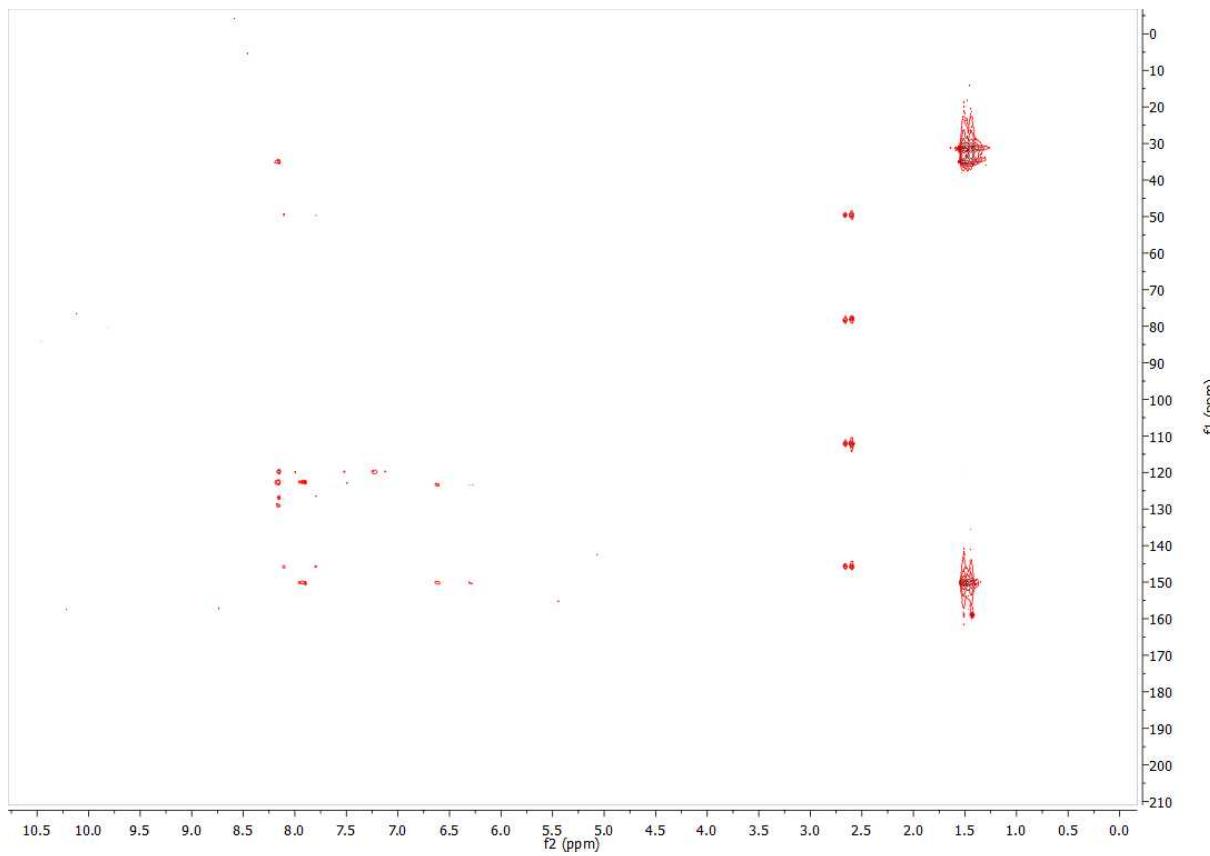


Figure S23. ASAP mass spectrum of 2b'.

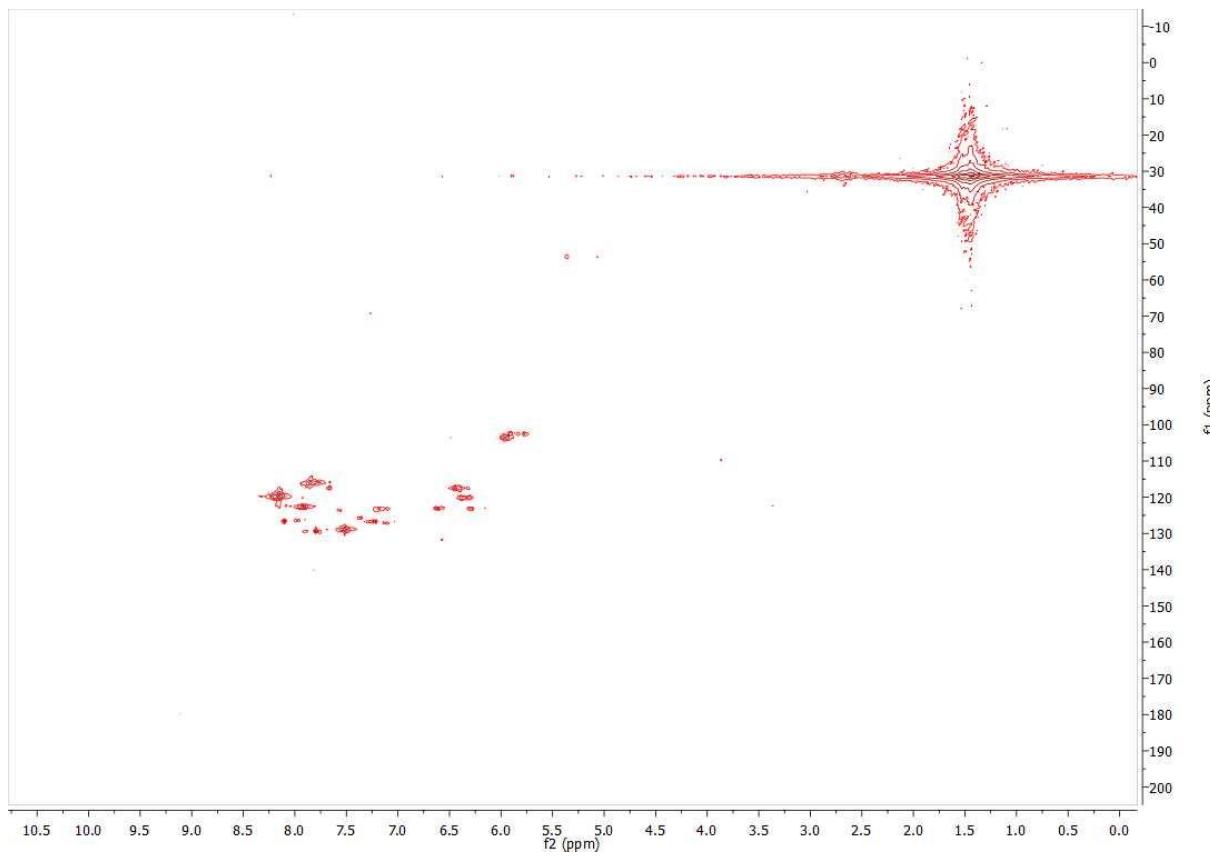


**Figure S24.**  $^1\text{H}$  NMR spectrum ( $\text{CD}_2\text{Cl}_2$ , 500 MHz, 25 °C) of **3a-Zr<sub>2</sub>**.

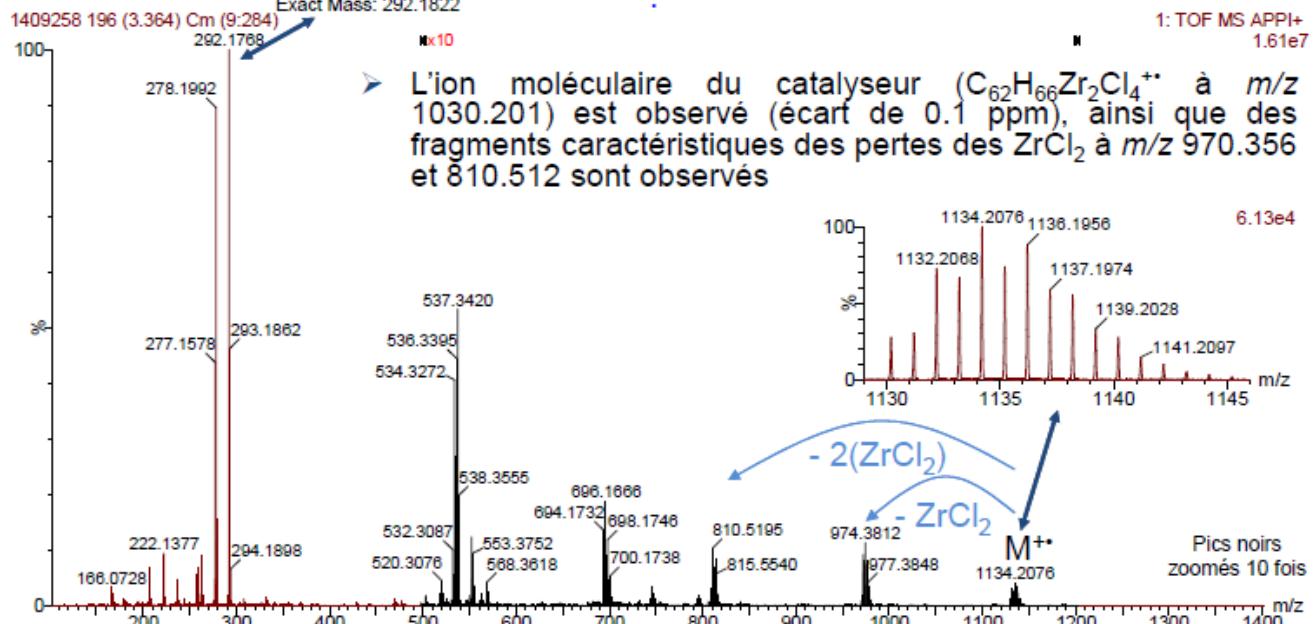
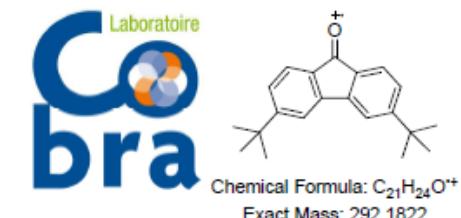




**Figure S25.** HMBC spectrum ( $\text{CD}_2\text{Cl}_2$ , 500 MHz, 25 °C) of **3a-Zr<sub>2</sub>**.

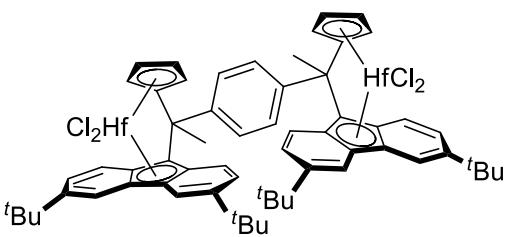
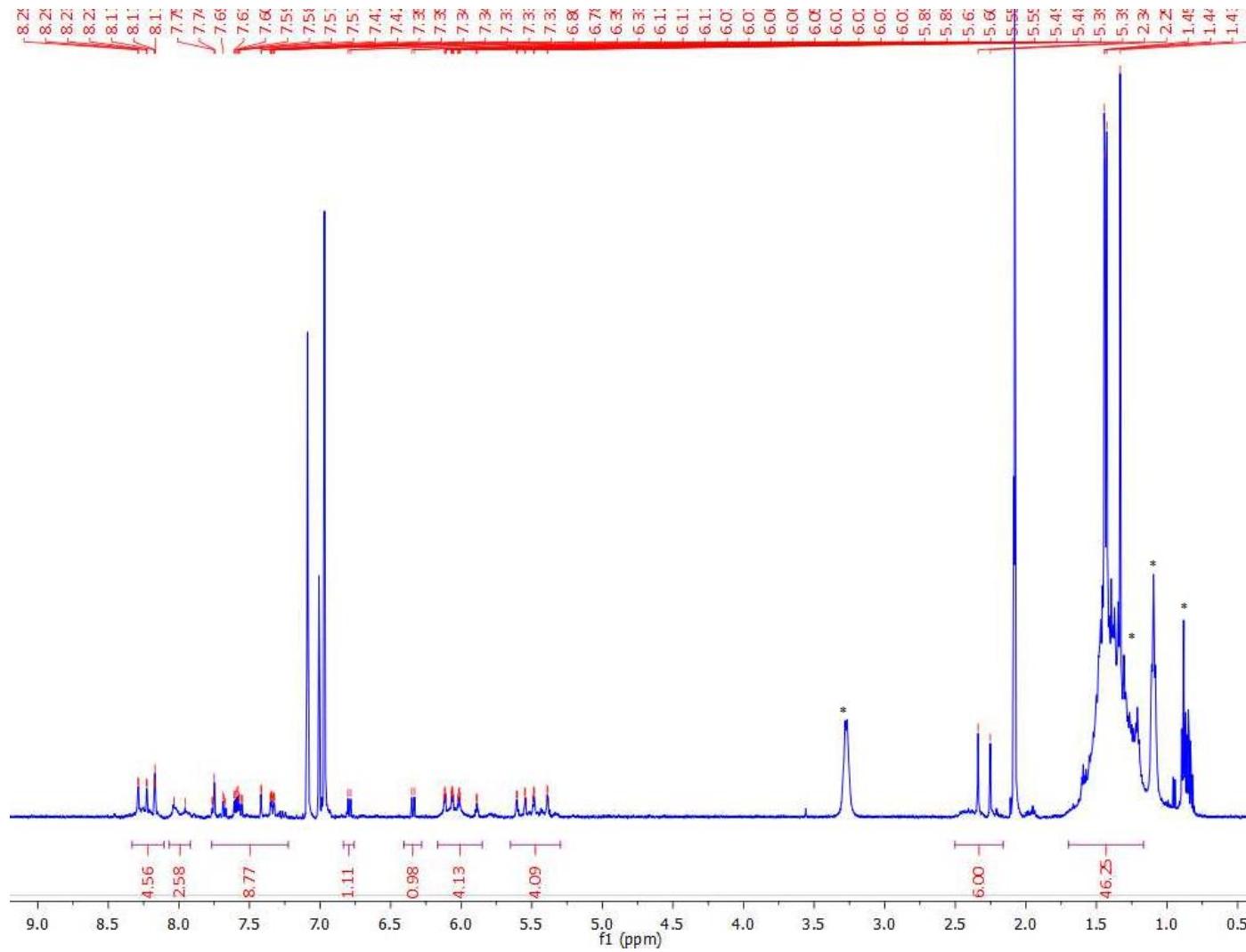


**Figure S26.** HSQC spectrum ( $\text{CD}_2\text{Cl}_2$ , 500 MHz, 25 °C) of **3a-Zr<sub>2</sub>**.

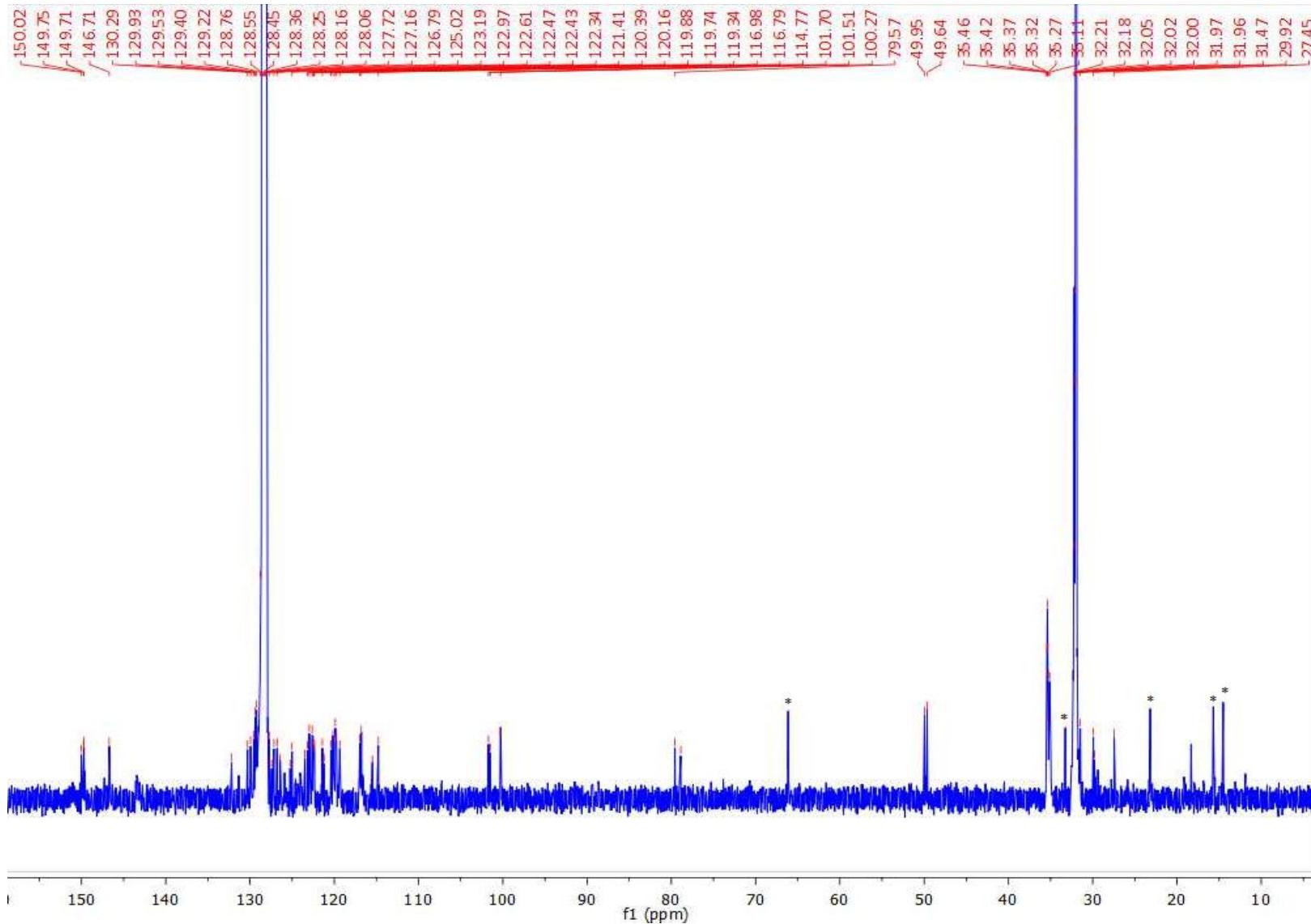


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Figure S27. APPI-IMMS of 3a-Zr<sub>2</sub>.



**Figure S28.**  $^1\text{H}$  NMR spectrum (toluene- $d_8$ , 500 MHz, 25 °C) of **3a-Hf<sub>2</sub>**. (\* stand for residual solvent peaks)



**Figure S29.**  $^{13}\text{C}$  NMR spectrum ( $\text{C}_6\text{D}_6$ , 125 MHz, 25 °C) of **3a-Hf<sub>2</sub>**. (\*residual solvent peak)

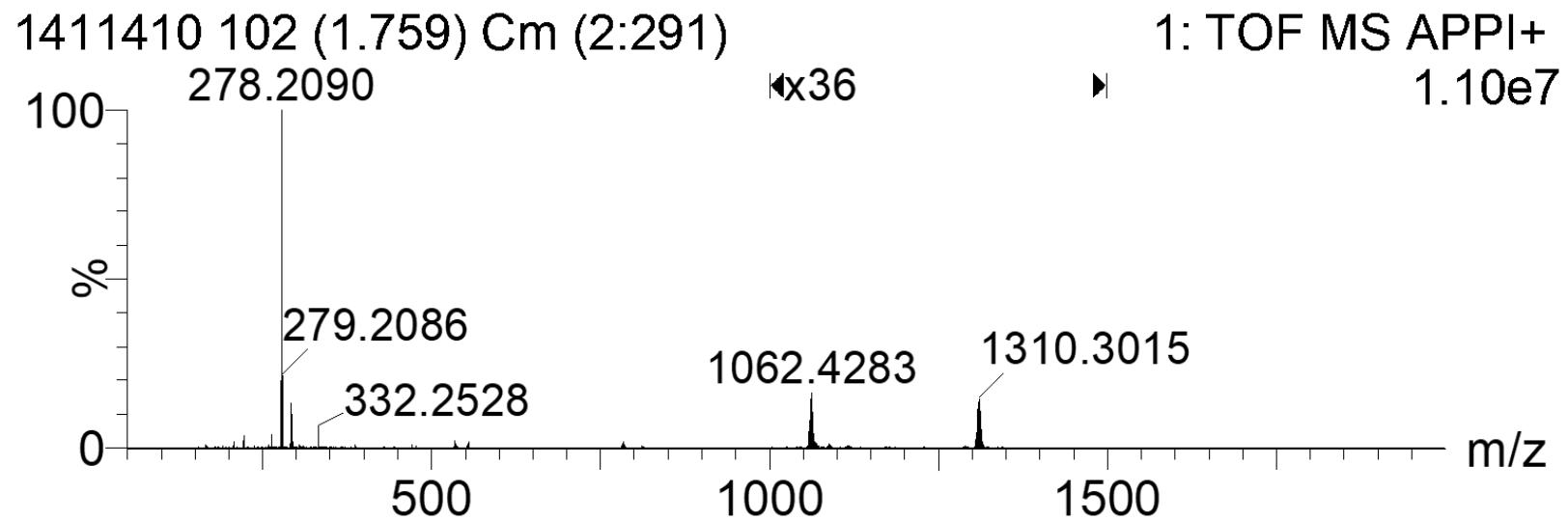
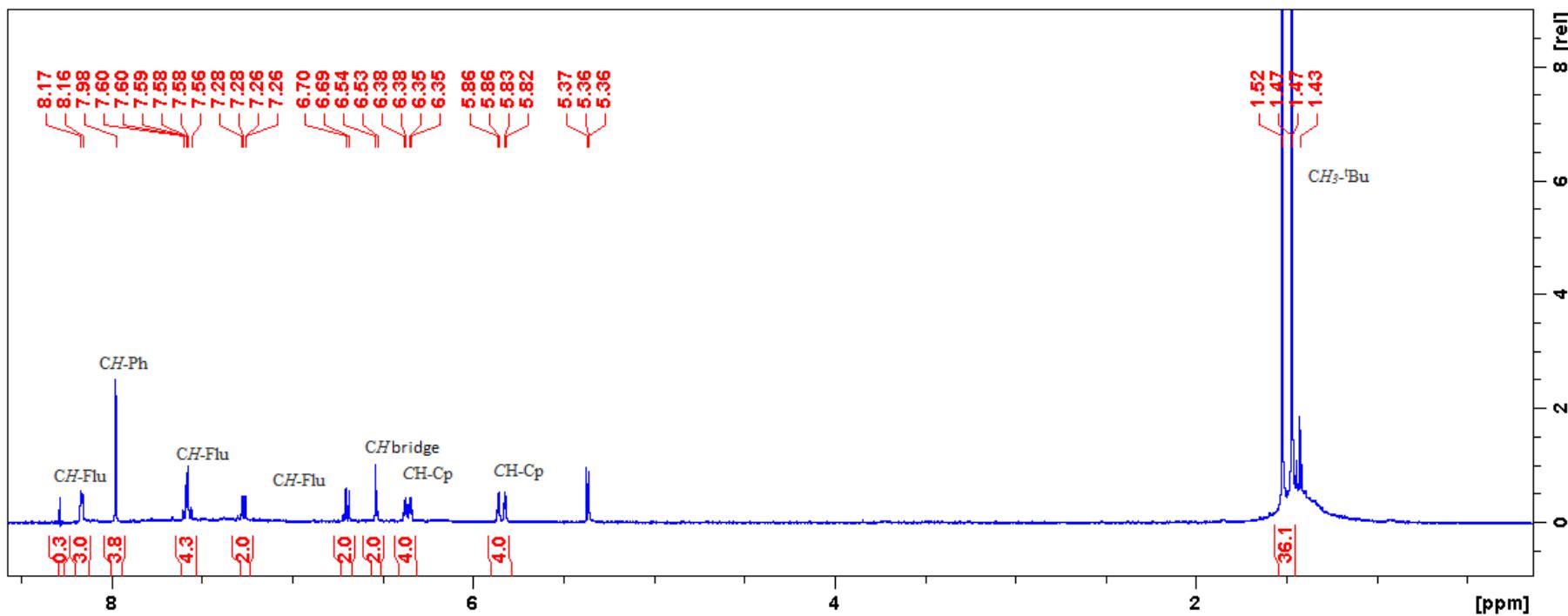
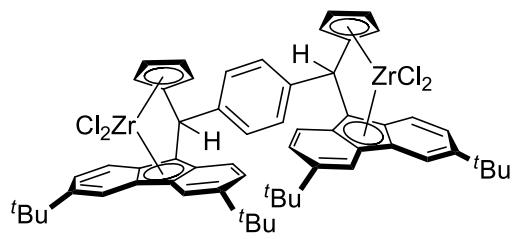
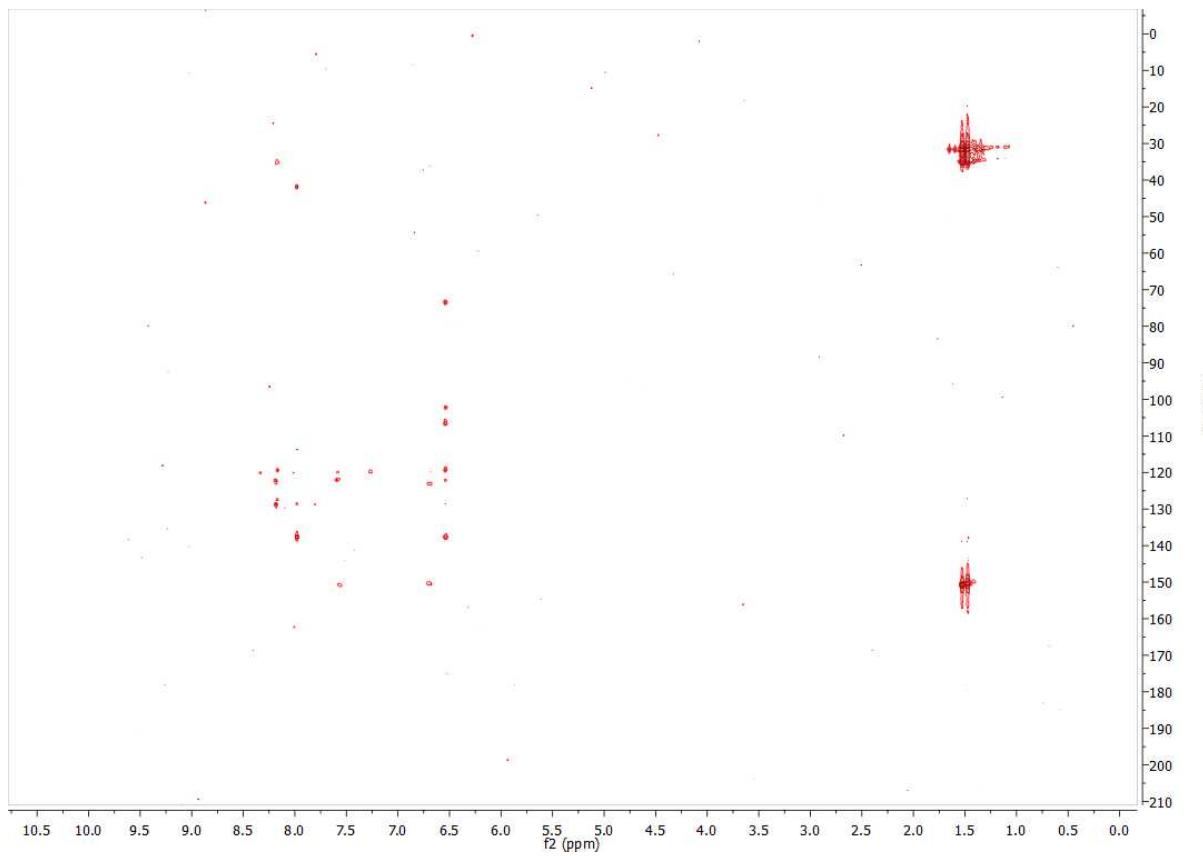


Figure S30. APPI-IMMS of 3a-Hf<sub>2</sub>.

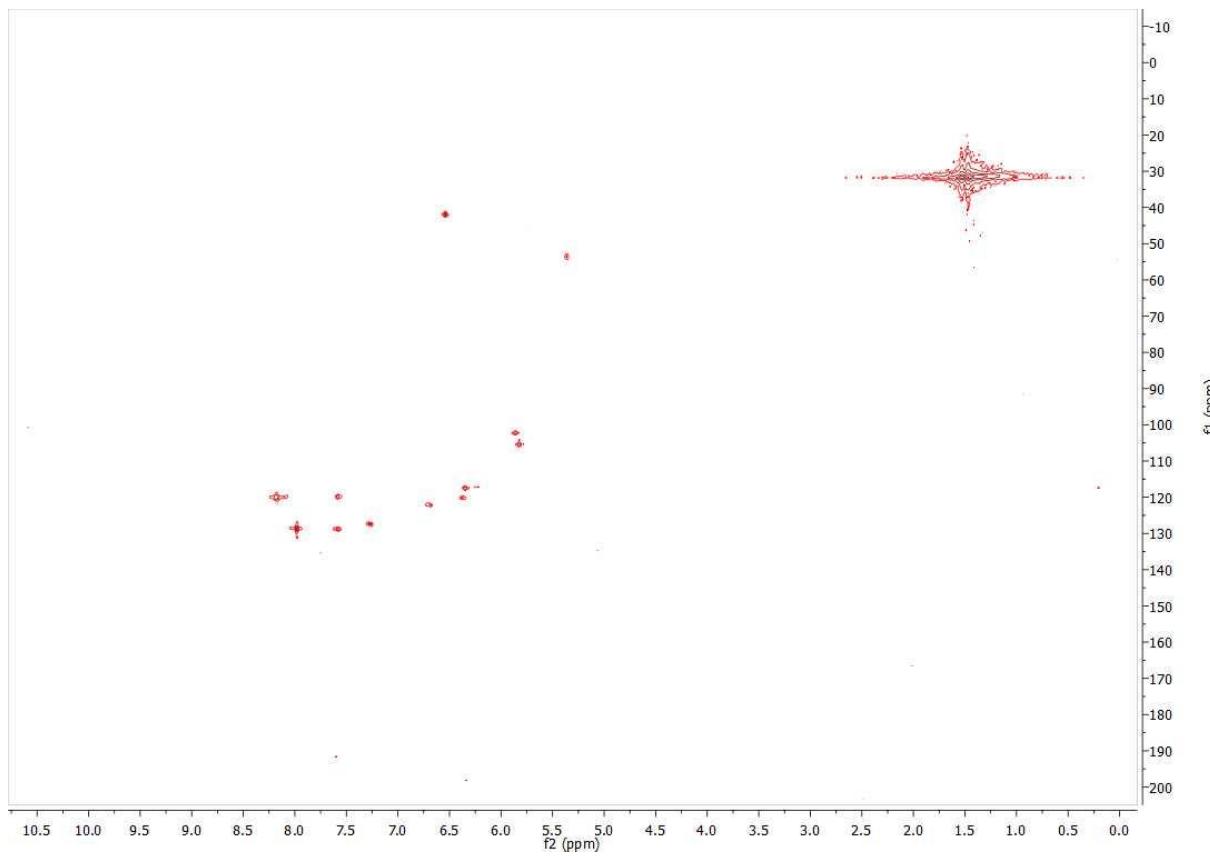


**Figure S31.**  $^1\text{H}$  NMR spectrum ( $\text{CD}_2\text{Cl}_2$ , 500 MHz, 25 °C) of **3b-Zr<sub>2</sub>**.

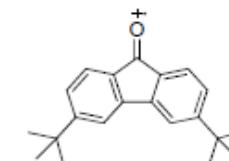




**Figure S32.** HMBC spectrum ( $\text{CD}_2\text{Cl}_2$ , 500 MHz, 25 °C) of **3b-Zr<sub>2</sub>**.



**Figure S33.** HSQC spectrum ( $\text{CD}_2\text{Cl}_2$ , 500 MHz, 25 °C) of **3b-Zr<sub>2</sub>**.



Chemical Formula:  $C_{21}H_{24}O^+$

Exact Mass: 292.1822

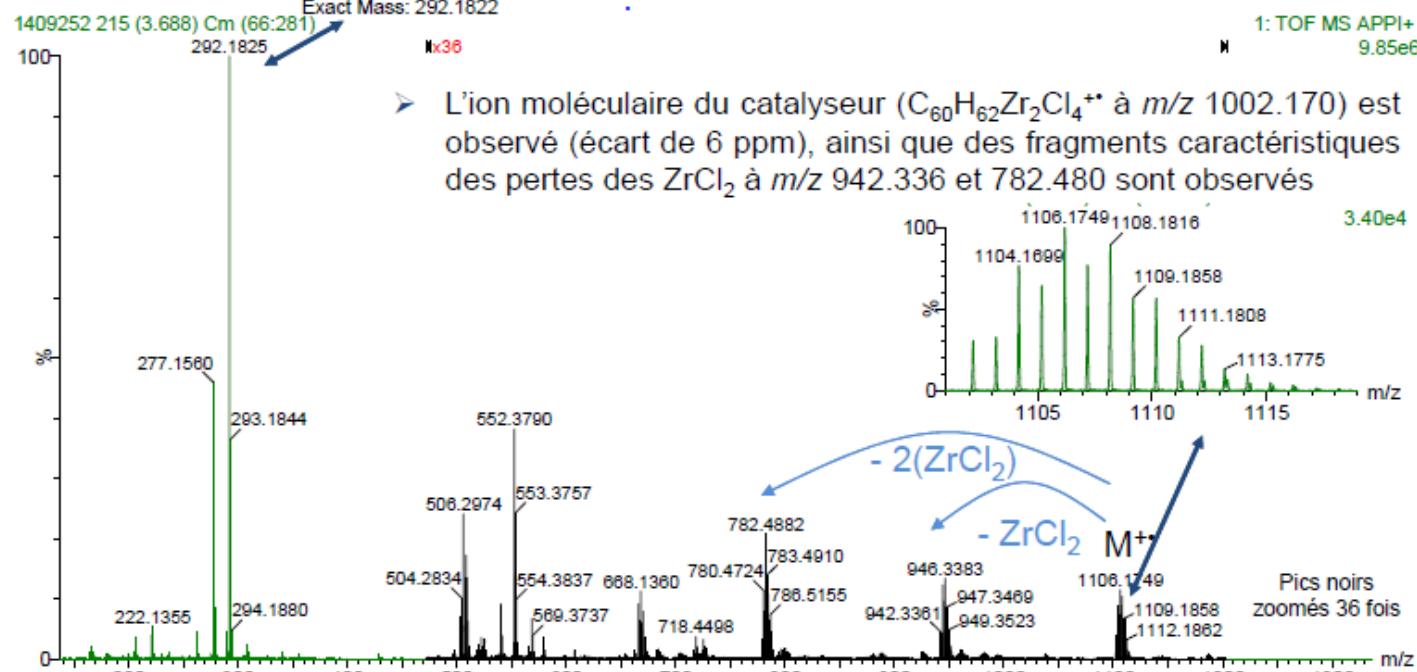
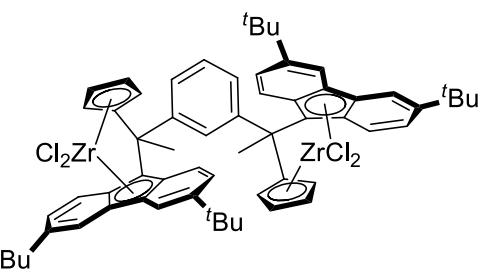
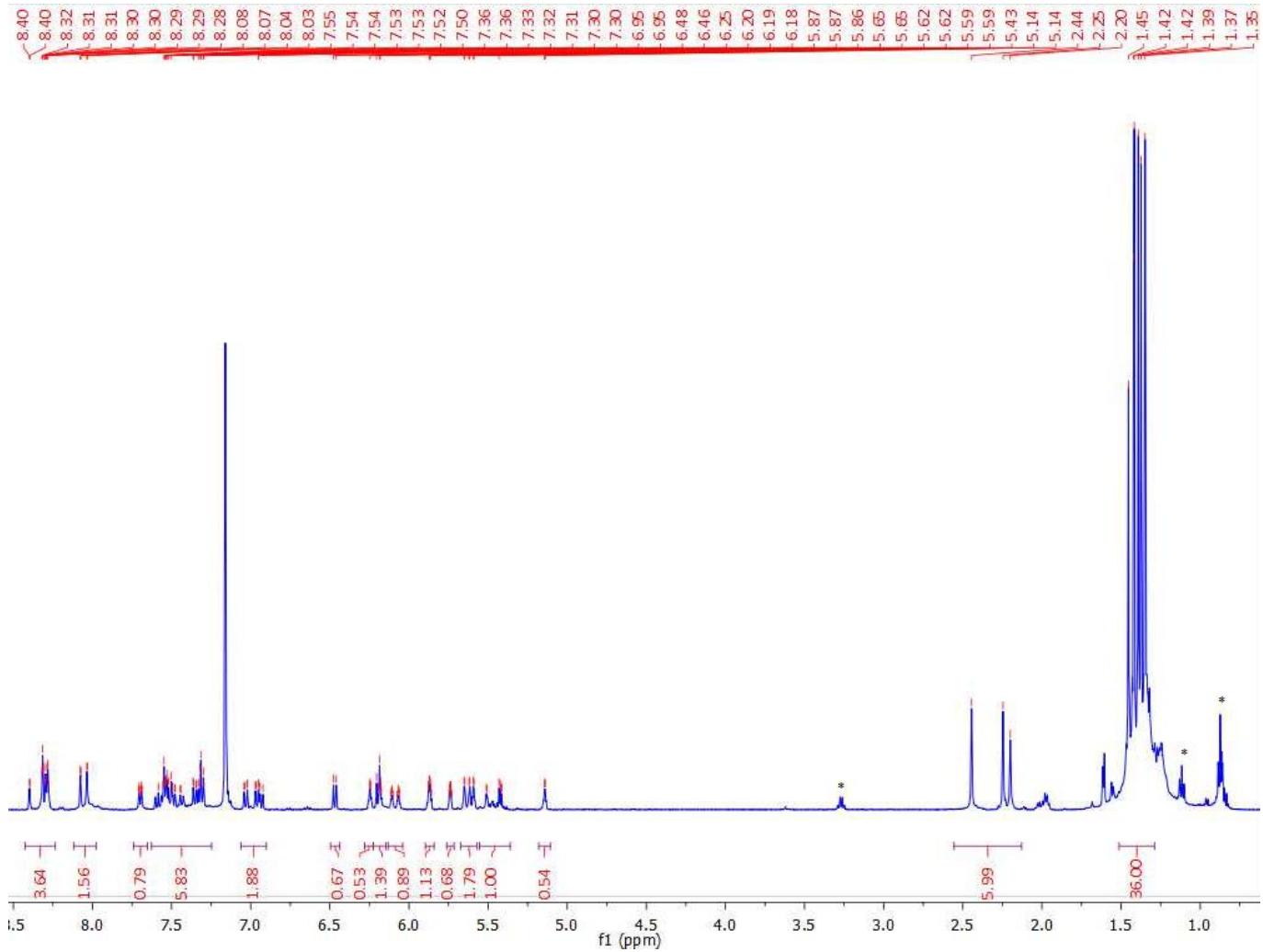
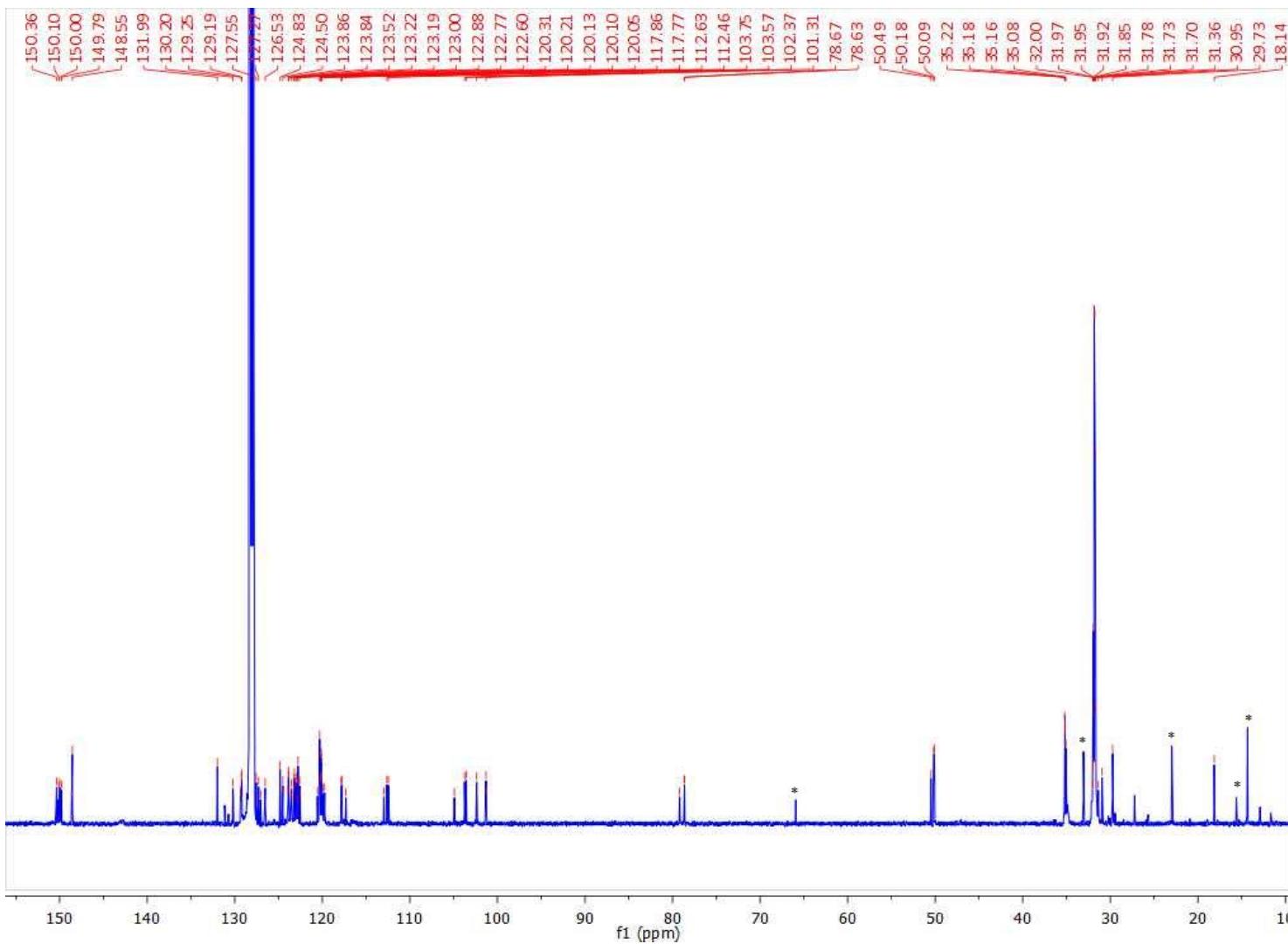


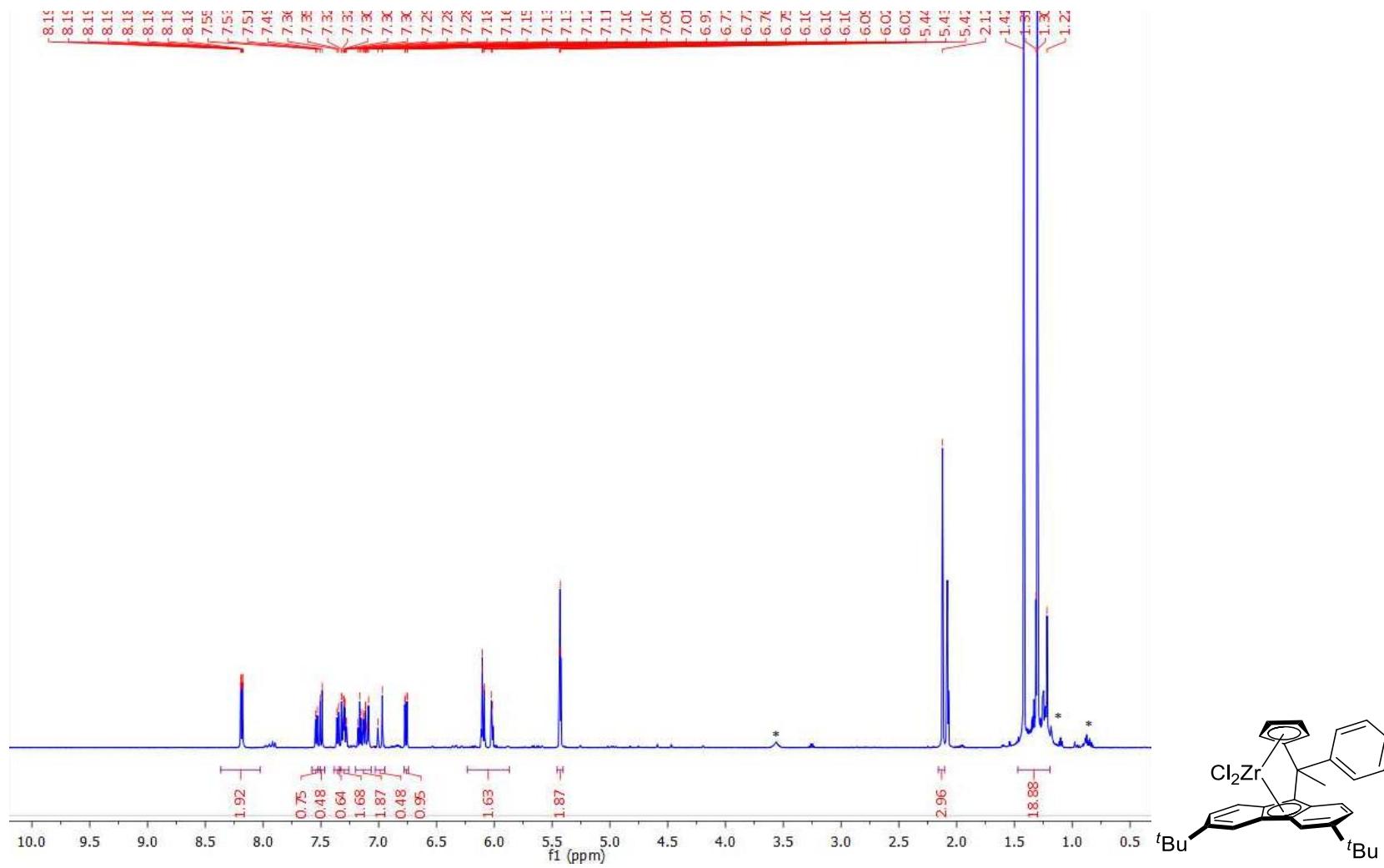
Figure S34. APPI-IMMS of 3b-Zr<sub>2</sub>.



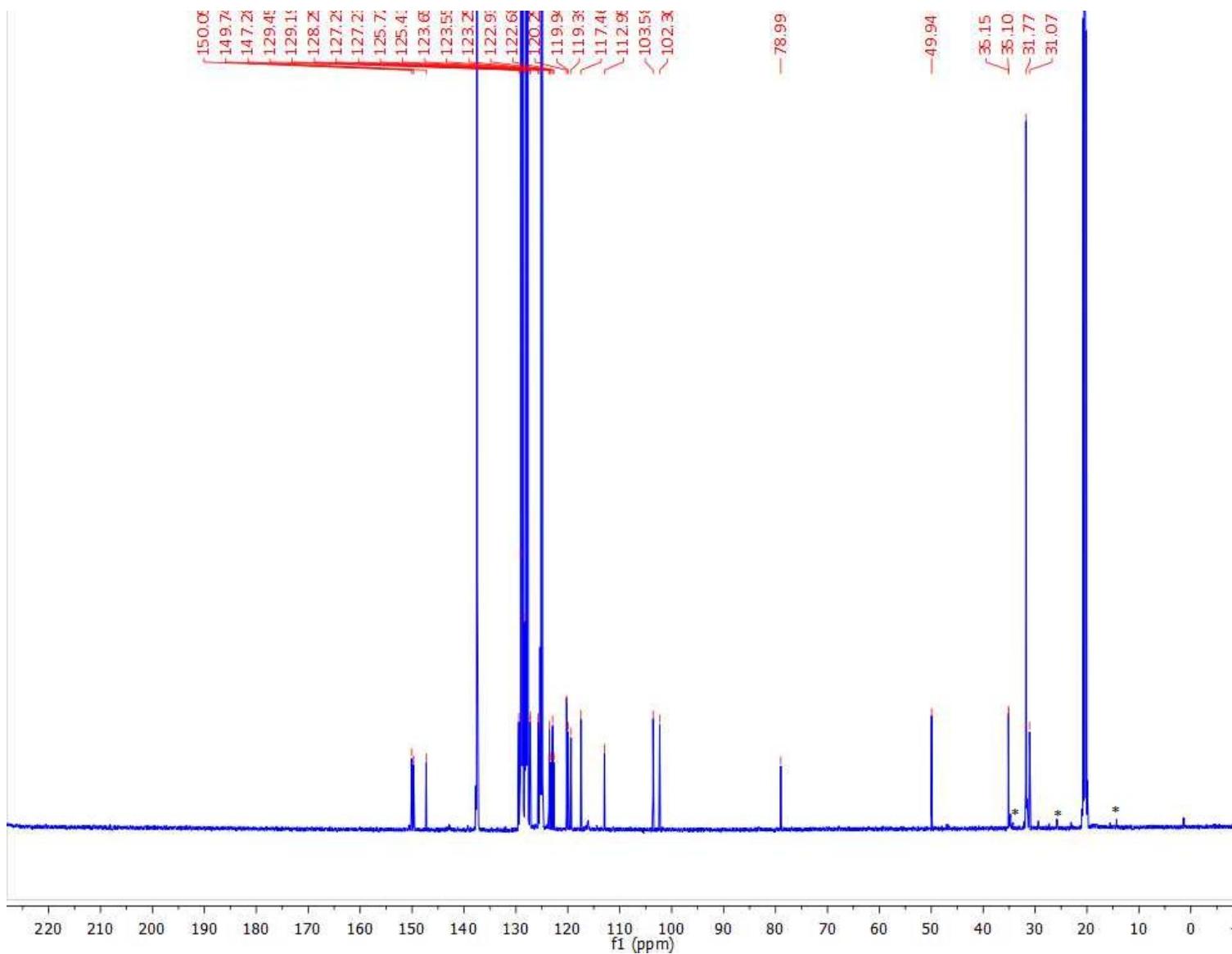
**Figure S35.**  $^1\text{H}$  NMR spectrum ( $\text{C}_6\text{D}_6$ , 500 MHz, 25 °C) of **3c-Zr<sub>2</sub>**. (\* stand for residual solvent peaks)



**Figure S36.**  $^{13}\text{C}$  NMR spectrum ( $\text{C}_6\text{D}_6$ , 125 MHz, 25 °C) of **3c-Zr<sub>2</sub>**. (\*residual solvent peak)



**Figure S37.**  $^1\text{H}$  NMR spectrum (toluene- $d_8$ , 500 MHz, 25 °C) of **3a'-Zr**. (\* stand for residual solvent peaks)



**Figure S38.** <sup>13</sup>C NMR spectrum (toluene-*d*<sub>8</sub>, 125 MHz, 25 °C) of **3a'-Zr**. (\* stand for residual solvent peaks)

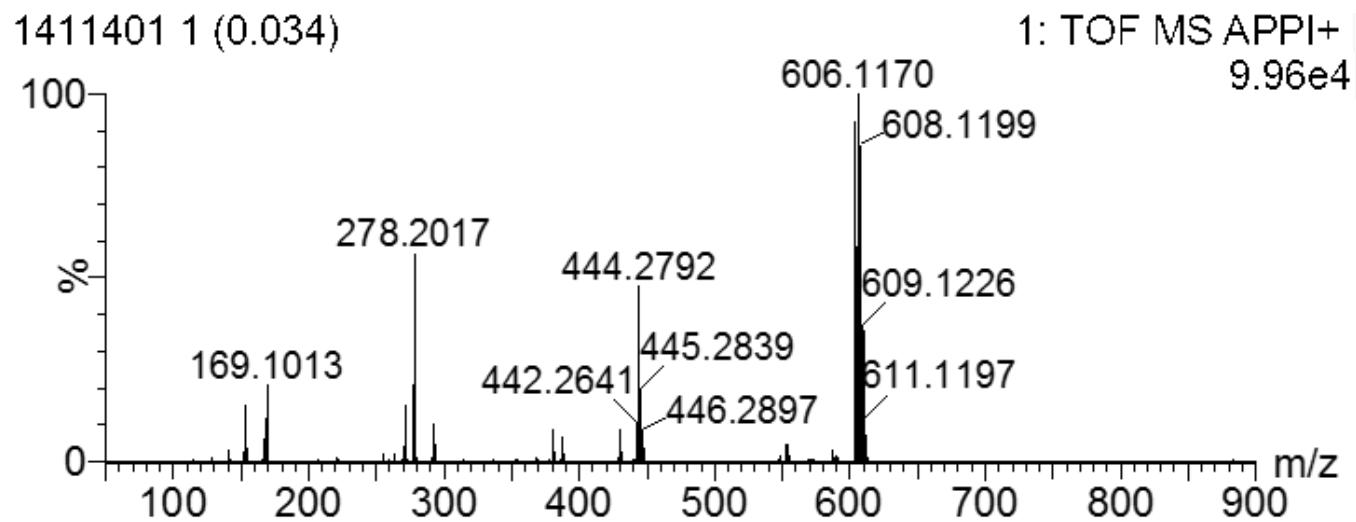
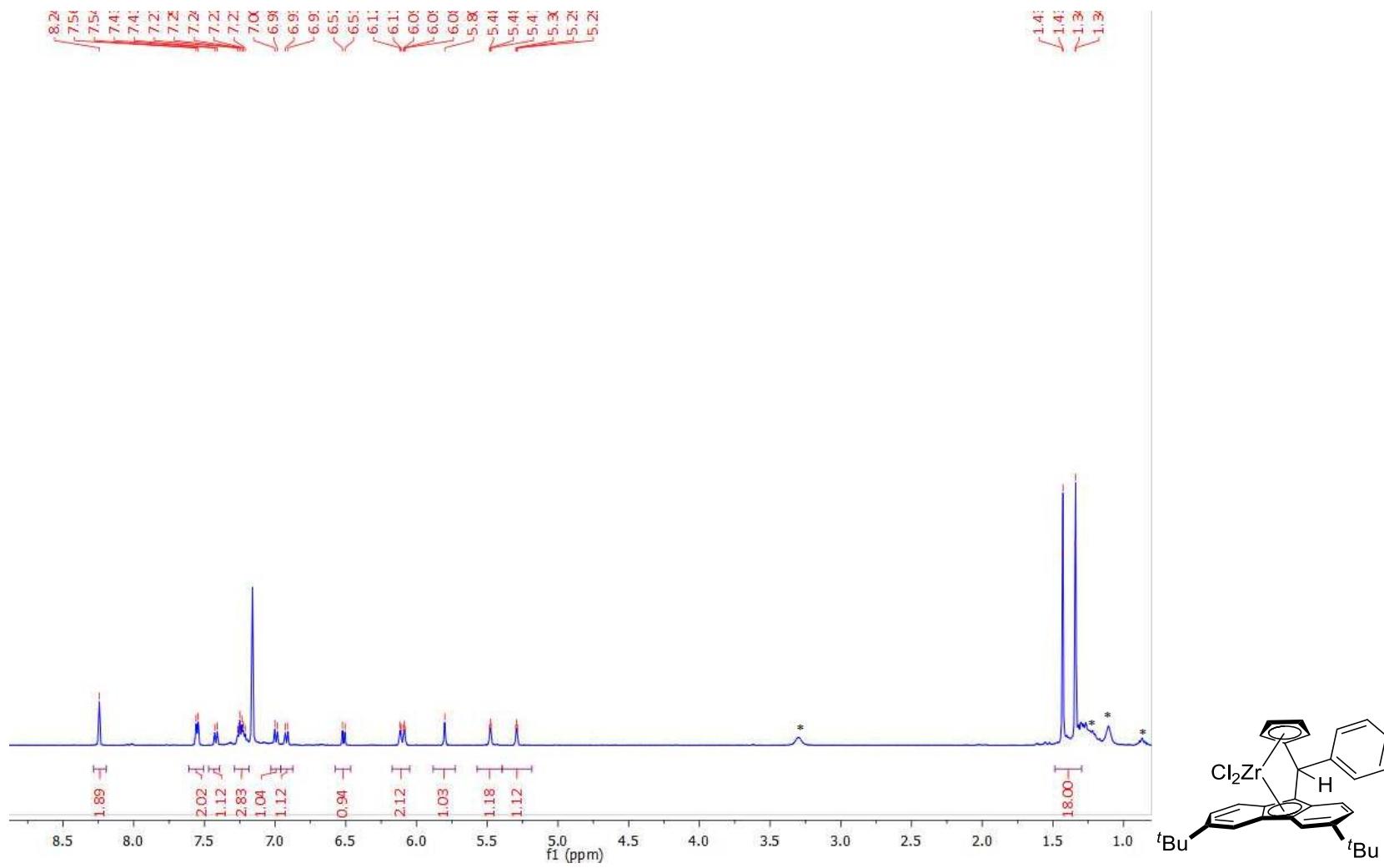
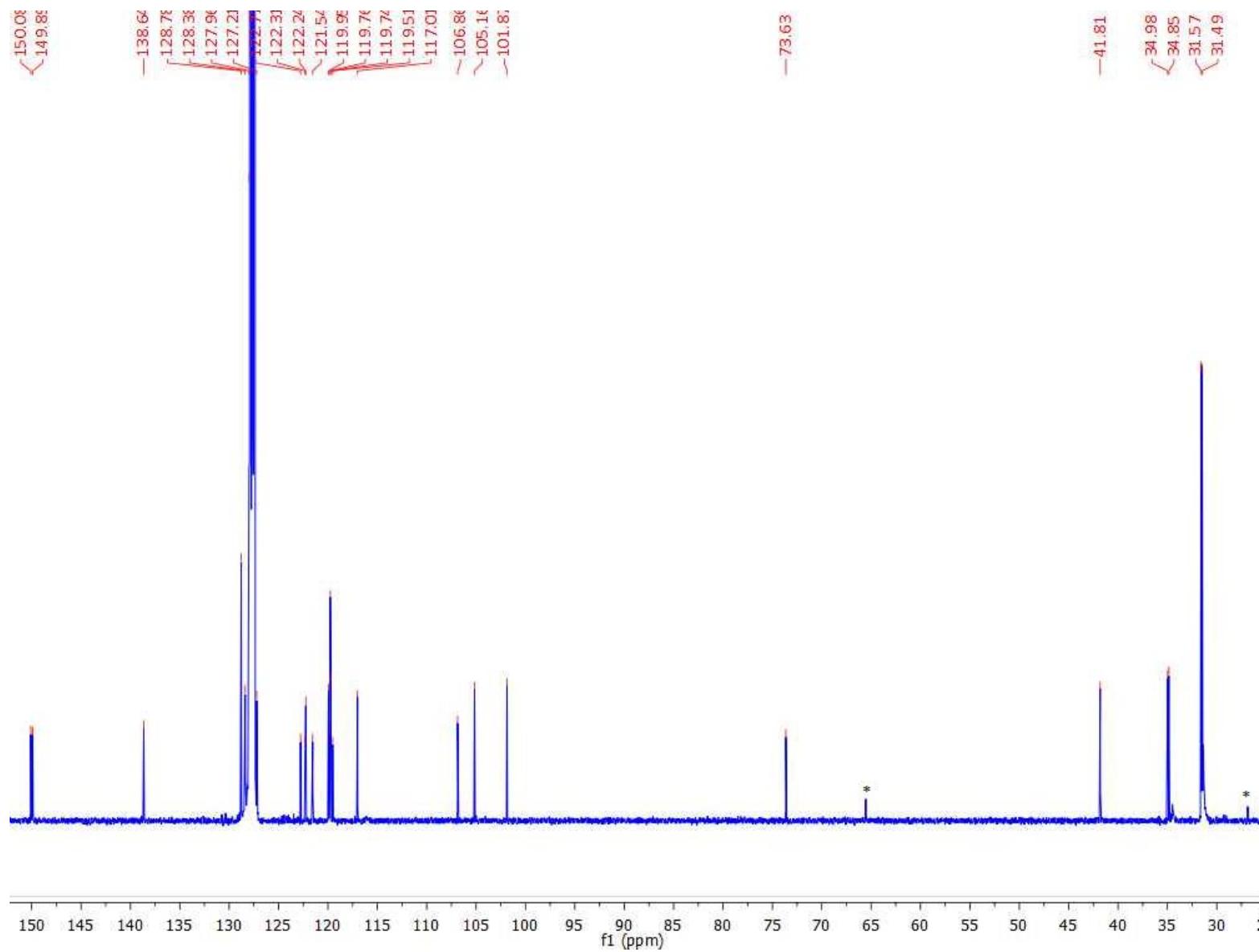


Figure S39. APPI-IMMS of 3a'-Zr.



**Figure S40.**  $^1\text{H}$  NMR spectrum ( $\text{C}_6\text{D}_6$ , 500 MHz, 25 °C) of **3b'**-Zr. (\*residual solvent peak)



**Figure S41.**  $^{13}\text{C}$  NMR spectrum ( $\text{C}_6\text{D}_6$ , 125 MHz, 25 °C) of **3b'-Zr**. (\*residual solvent peak)

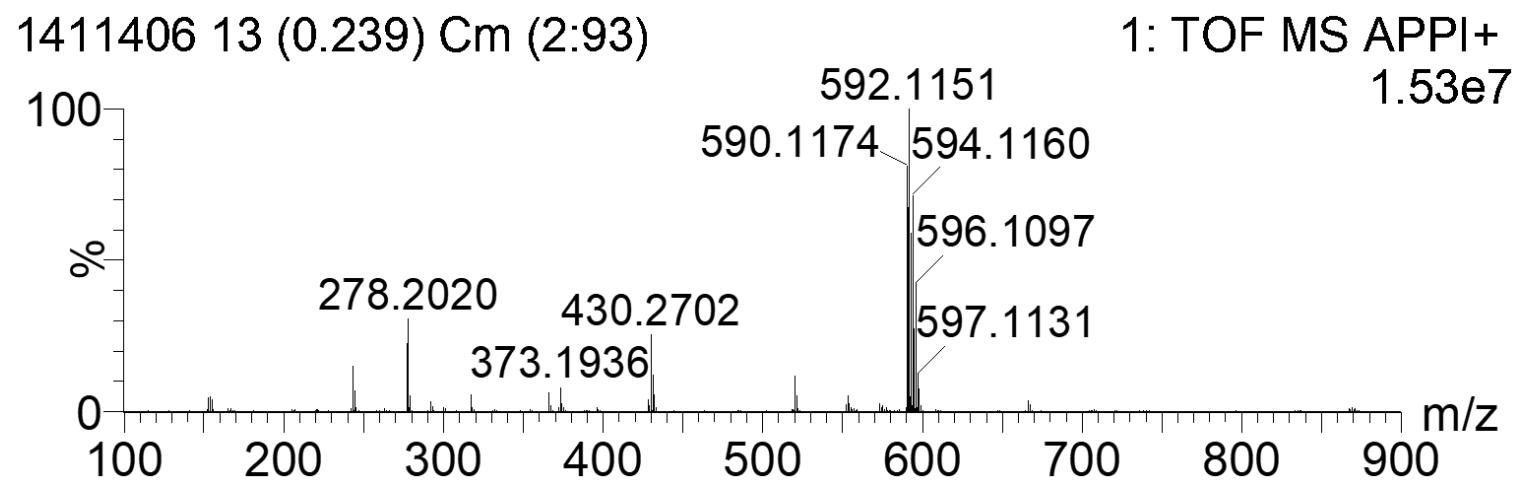
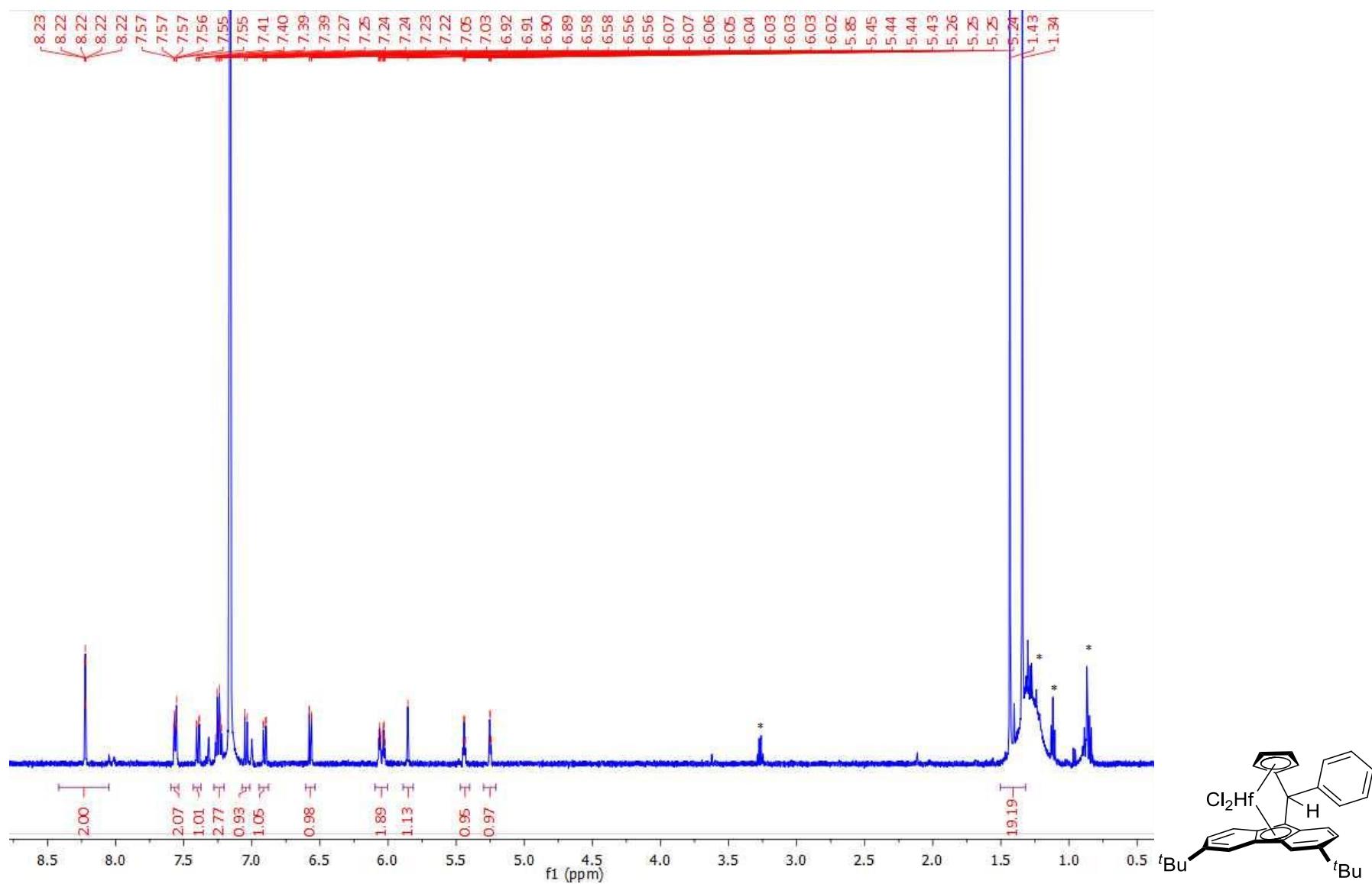
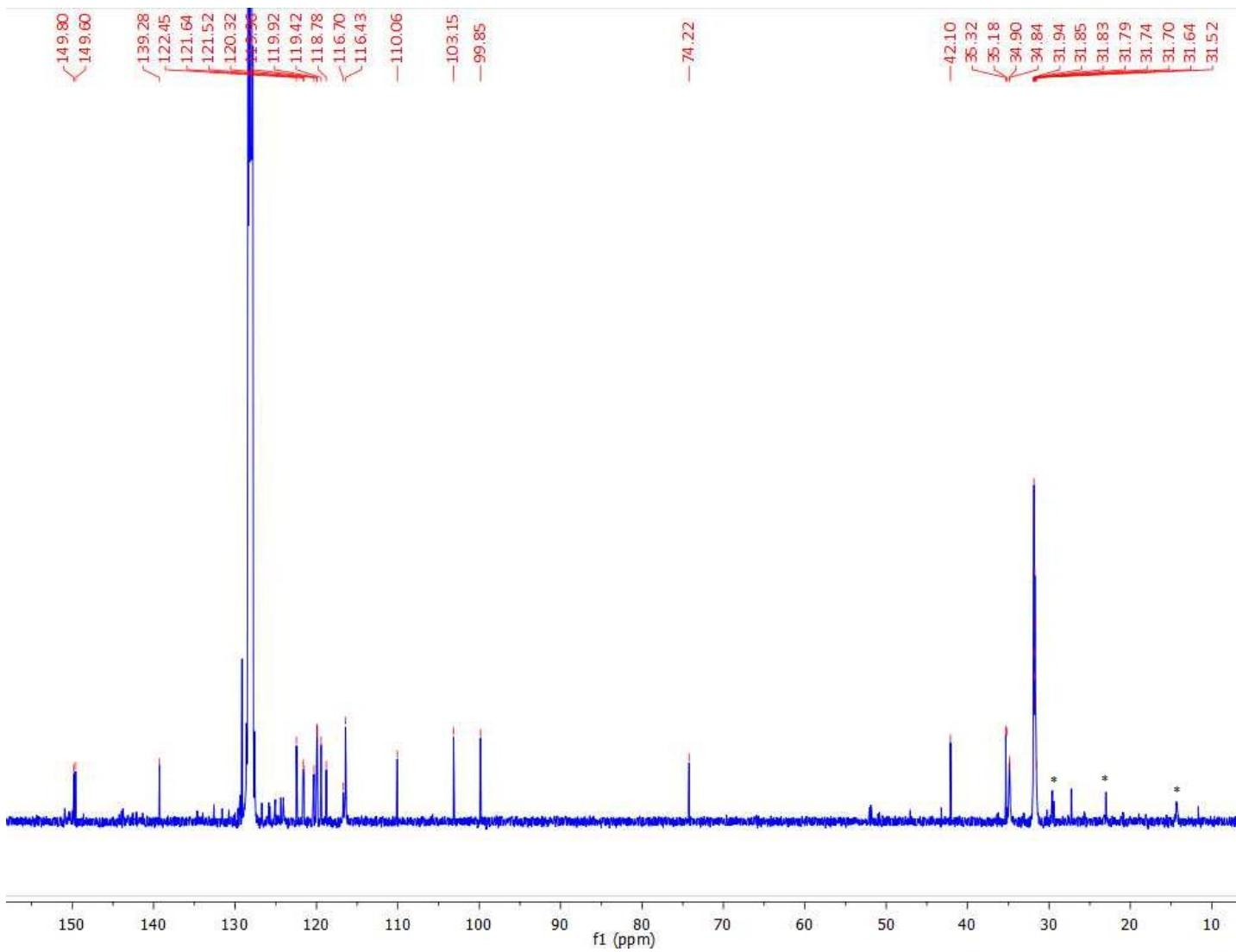


Figure S42. APPI-IMMS of **3b'**-Zr.





**Figure S44.**  $^{13}\text{C}$  NMR spectrum ( $\text{C}_6\text{D}_6$ , 125 MHz,  $25^\circ\text{C}$ ) of **3b'**-Hf. (\*residual solvent peak)

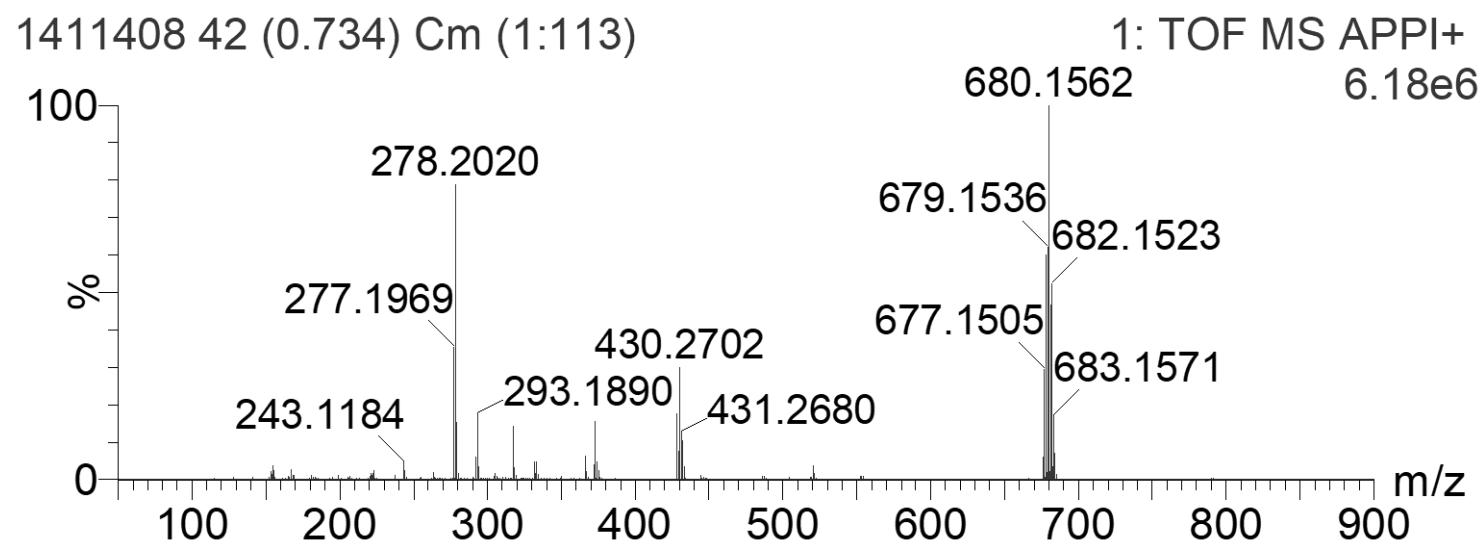
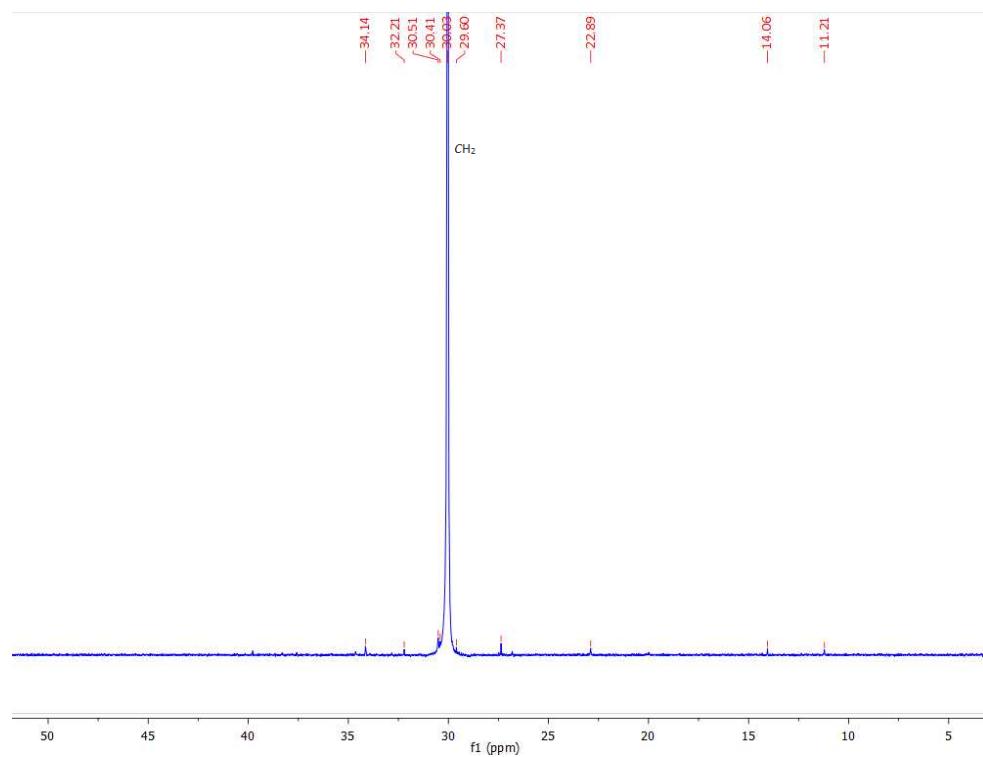
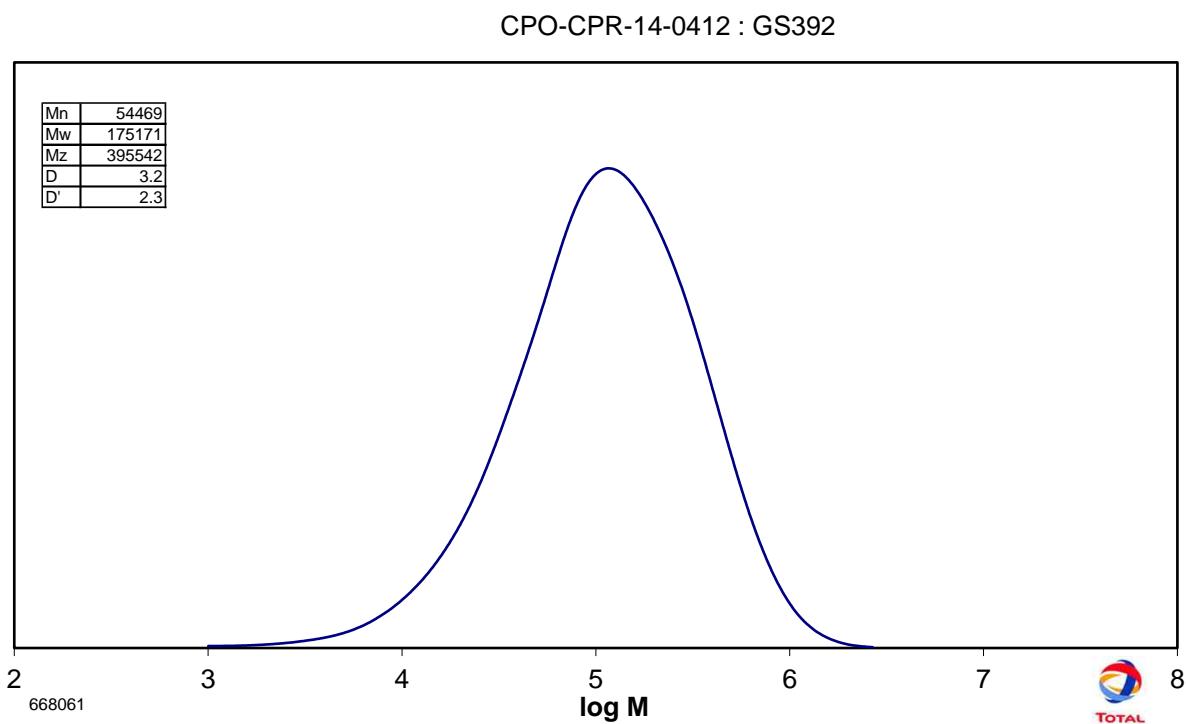


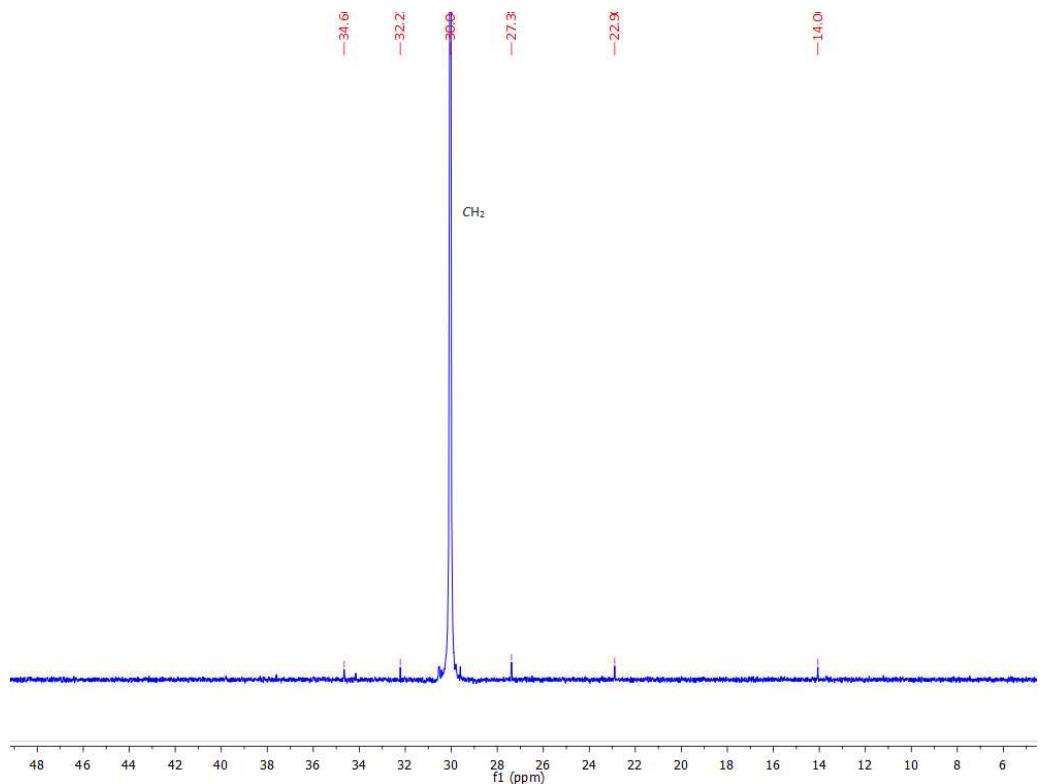
Figure S45. APPI-IMMS of 3b'-Hf.



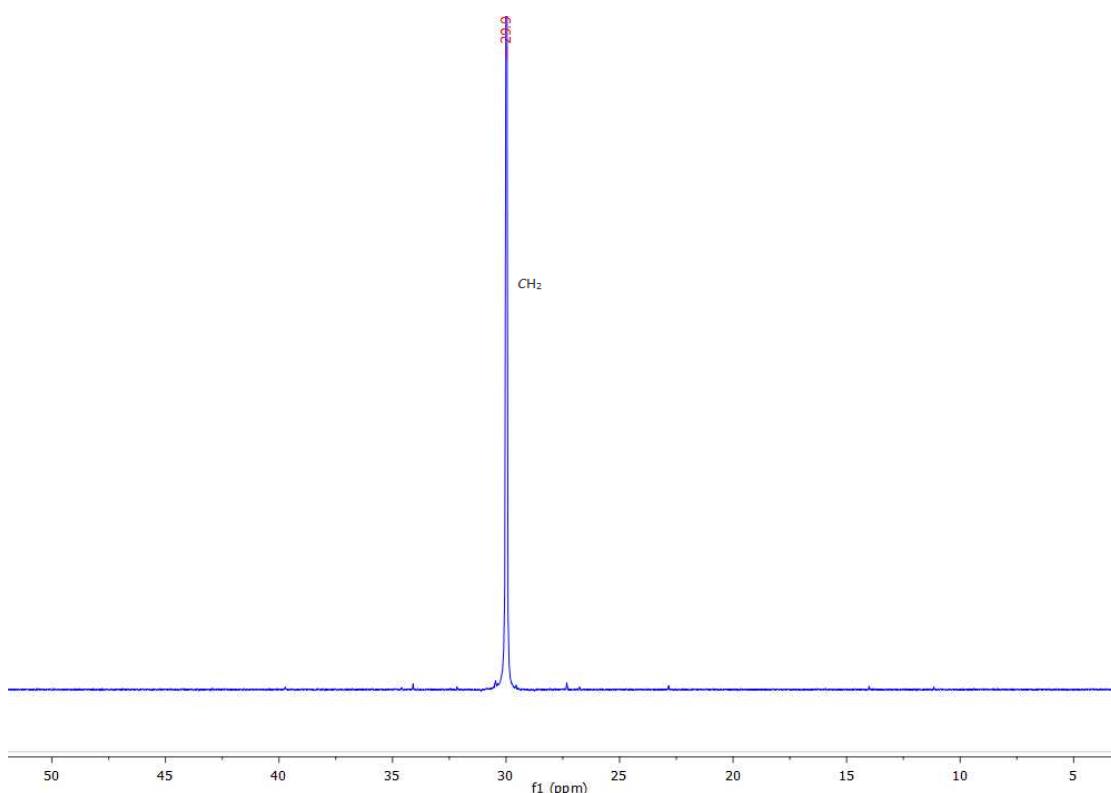
**Figure S46.**  $^{13}\text{C}$  NMR spectrum ( $\text{C}_6\text{D}_3\text{Cl}_3$ , 500 MHz, 100 °C) of PE (Table 1, run 1).



**Figure S47.** GPC trace of PE (Table 1, run 1) obtained with **3a-Zr<sub>2</sub>**.

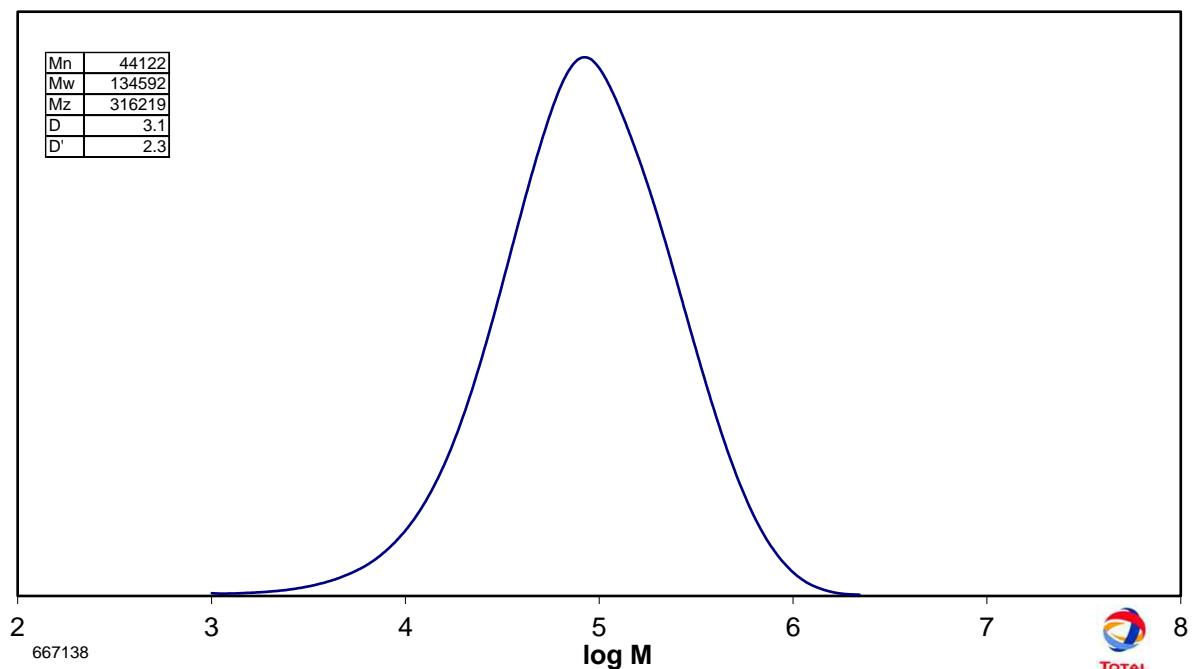


**Figure S48.**  $^{13}\text{C}$  NMR spectrum ( $\text{C}_6\text{D}_3\text{Cl}_3$ , 500 MHz, 100 °C) of PE (Table 1, run 3).



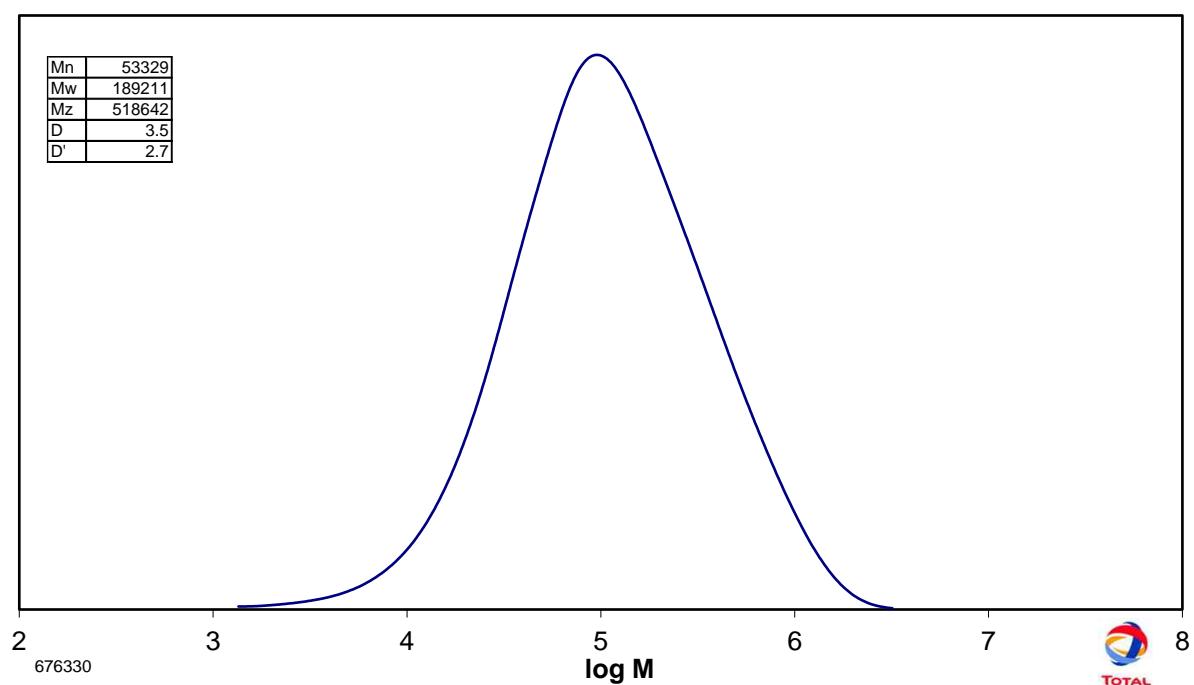
**Figure S49.**  $^{13}\text{C}$  NMR spectrum ( $\text{C}_6\text{D}_3\text{Cl}_3$ , 500 MHz, 100 °C) of PE (Table 1, run 5).

CPO-CPR-14-0380 : GS381



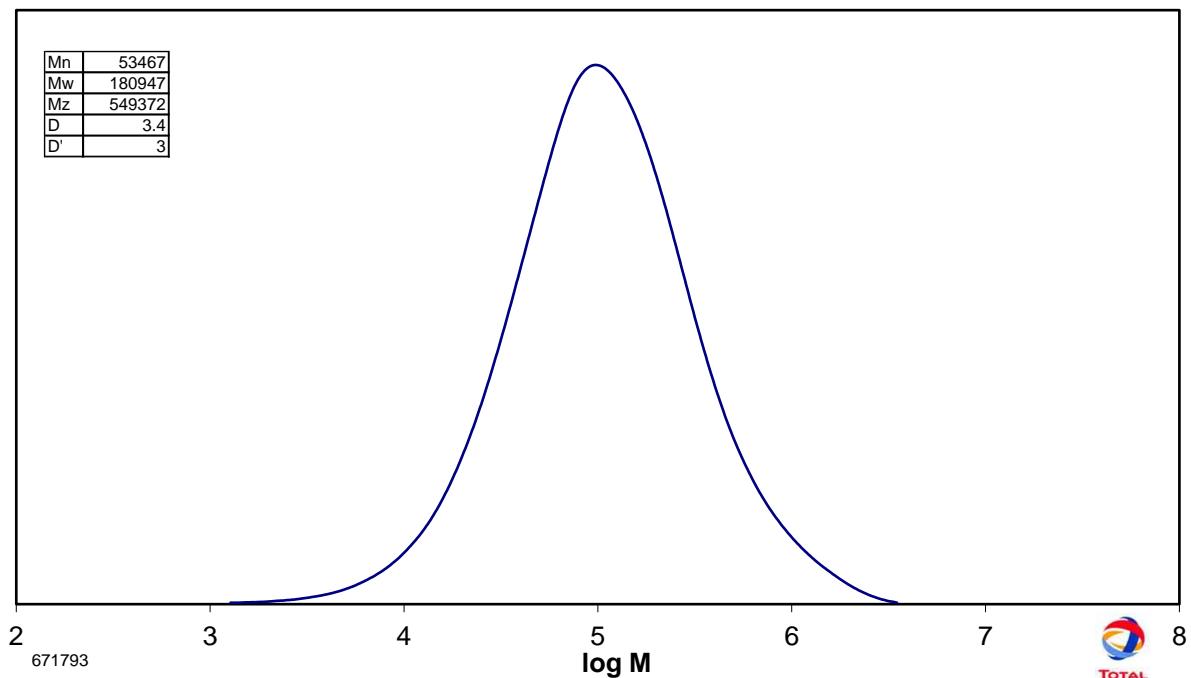
**Figure S50.** GPC trace of PE (Table 1, run 5) obtained with **3b-Zr<sub>2</sub>**.

CPO-CPR-15-0029 : GS381 2



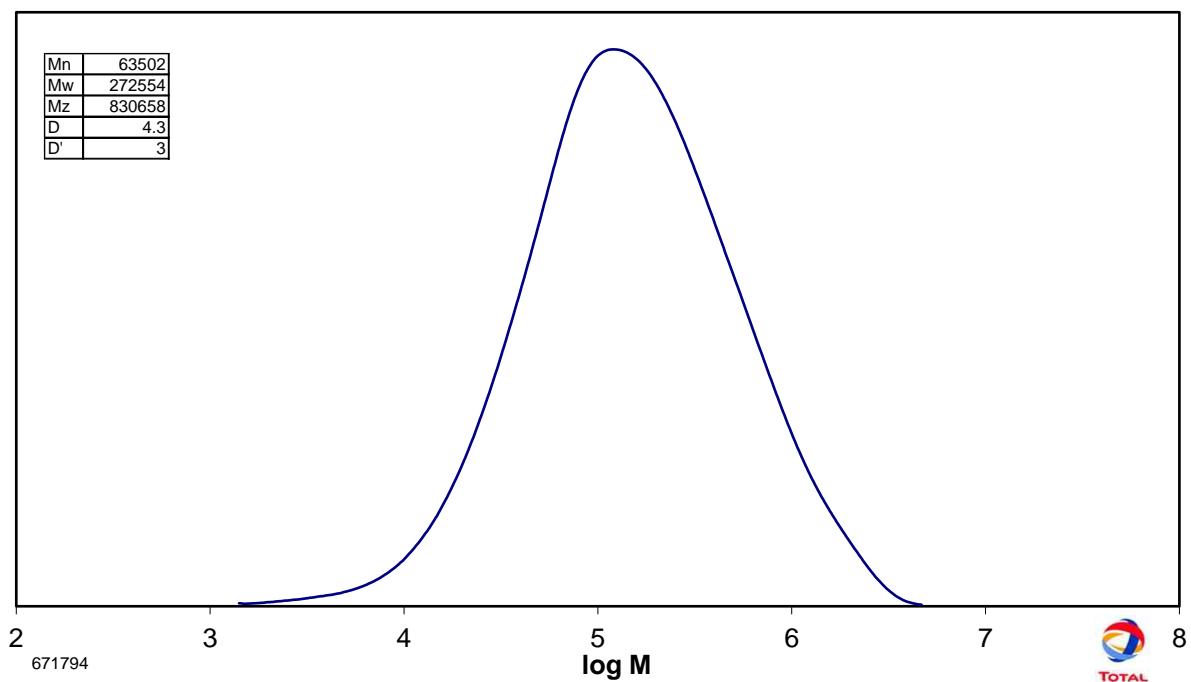
**Figure S51.** GPC trace of PE (Table 1, run 6) obtained with **3b-Zr<sub>2</sub>**.

CPO-CPR-14-0481 : GS418 PE exp Rennes



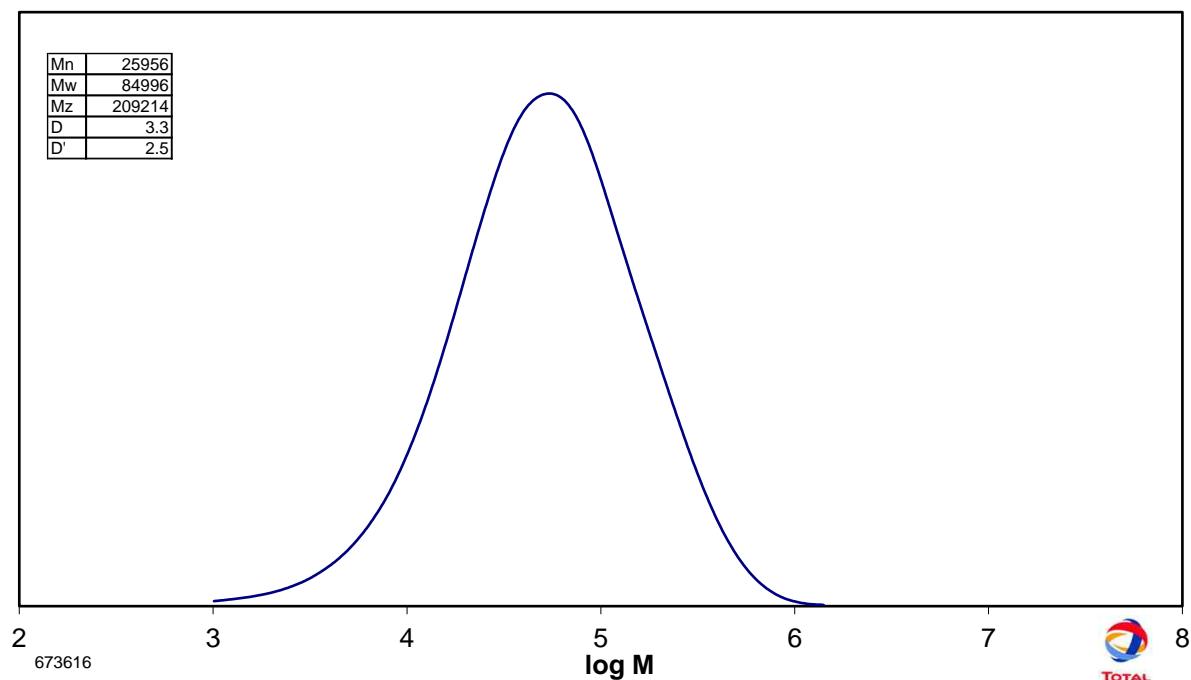
**Figure S52.** GPC trace of PE (Table 1, run 7) obtained with **3b'-Zr**.

CPO-CPR-14-0481 : GS418 2 PE exp Rennes



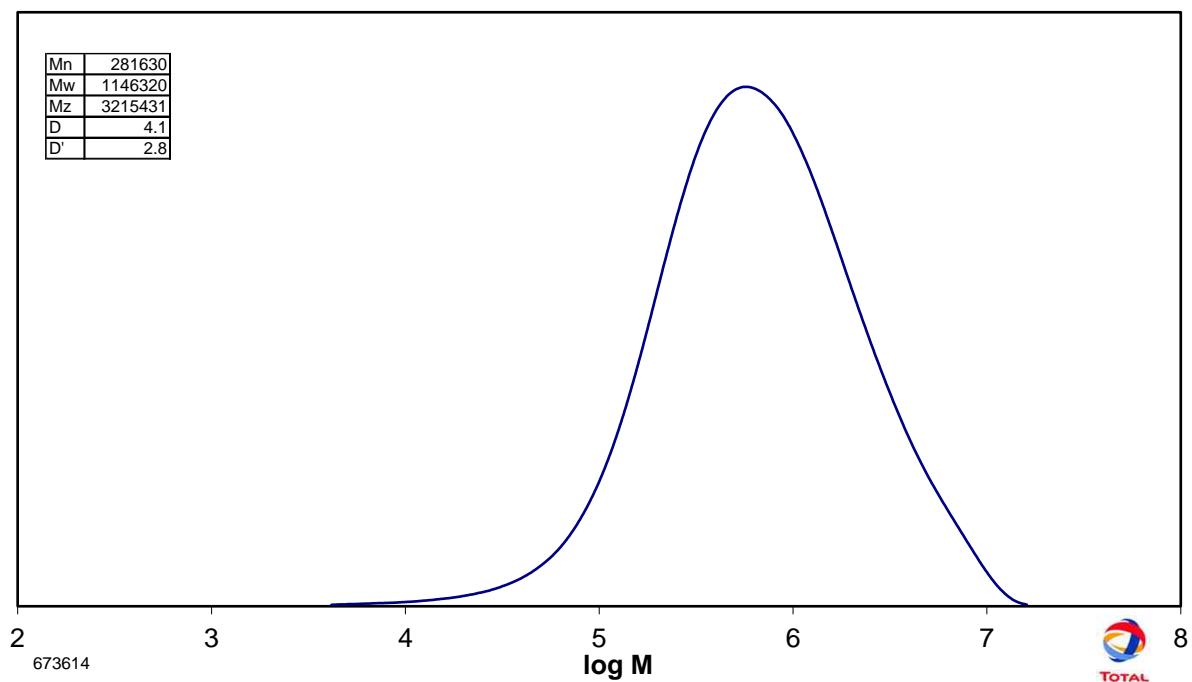
**Figure S53.** GPC trace of PE (Table 1, run 8) obtained with **3b'-Zr**.

CPO-CPR-14-0513 : CRUMBS PE (GS432)

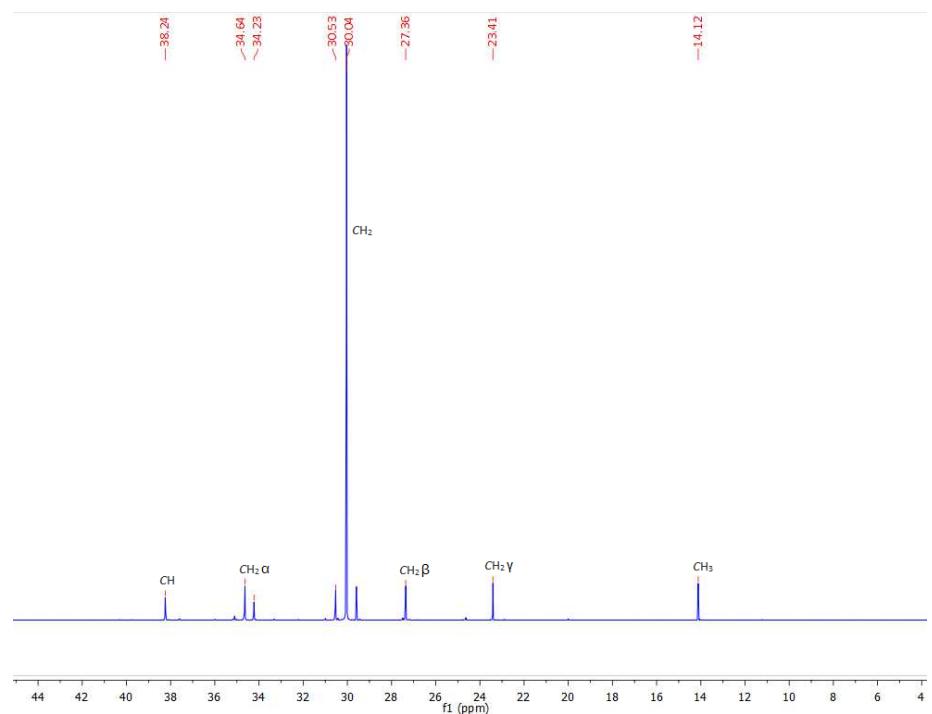


**Figure S54.** GPC trace of PE (Table 1, run 9) obtained with **3c-Zr<sub>2</sub>**.

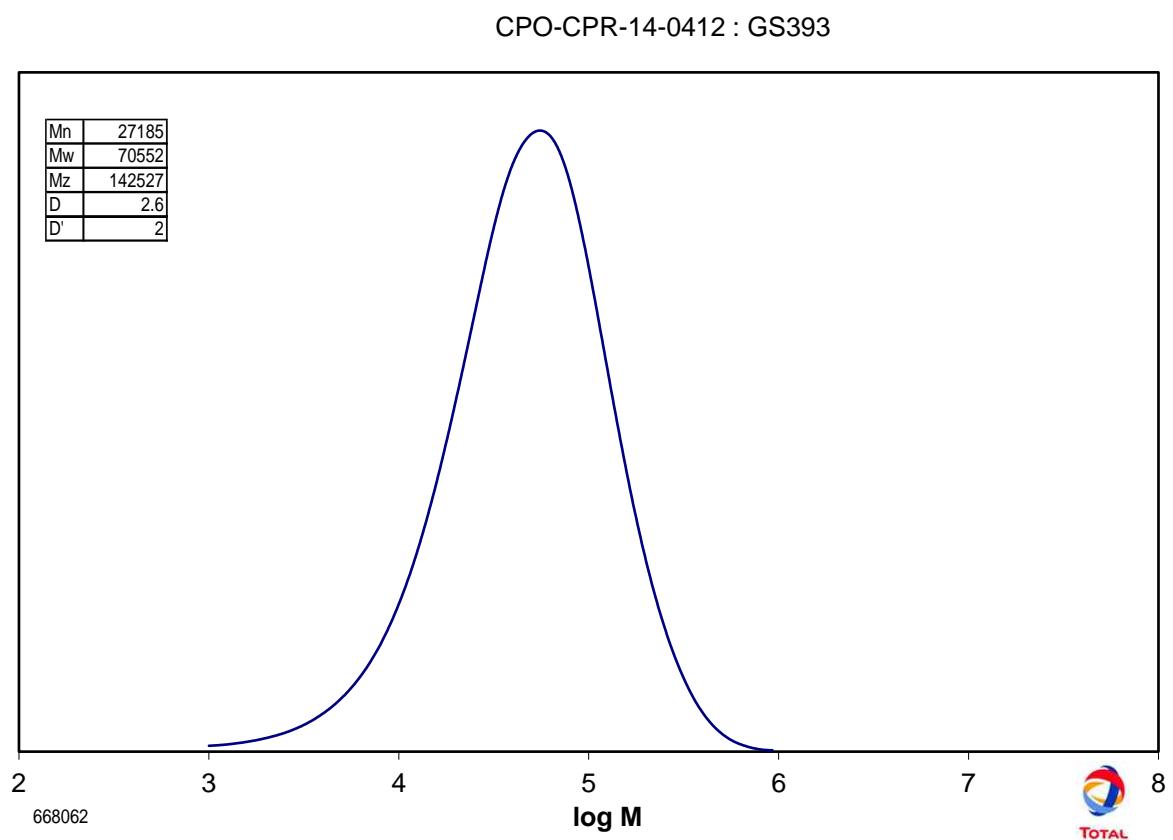
CPO-CPR-14-0513 : CRUMBS PE (GS430)



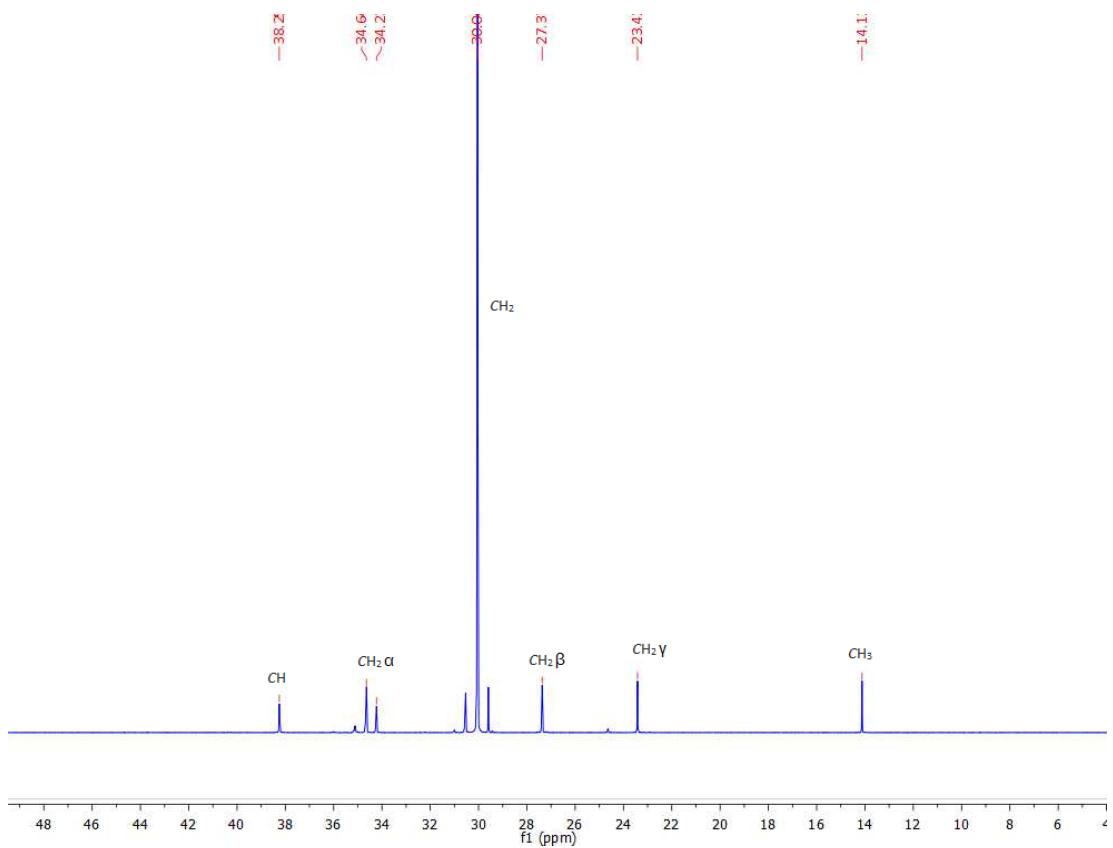
**Figure S55.** GPC trace of PE (Table 1, run 12) obtained with **3b'-Hf**.



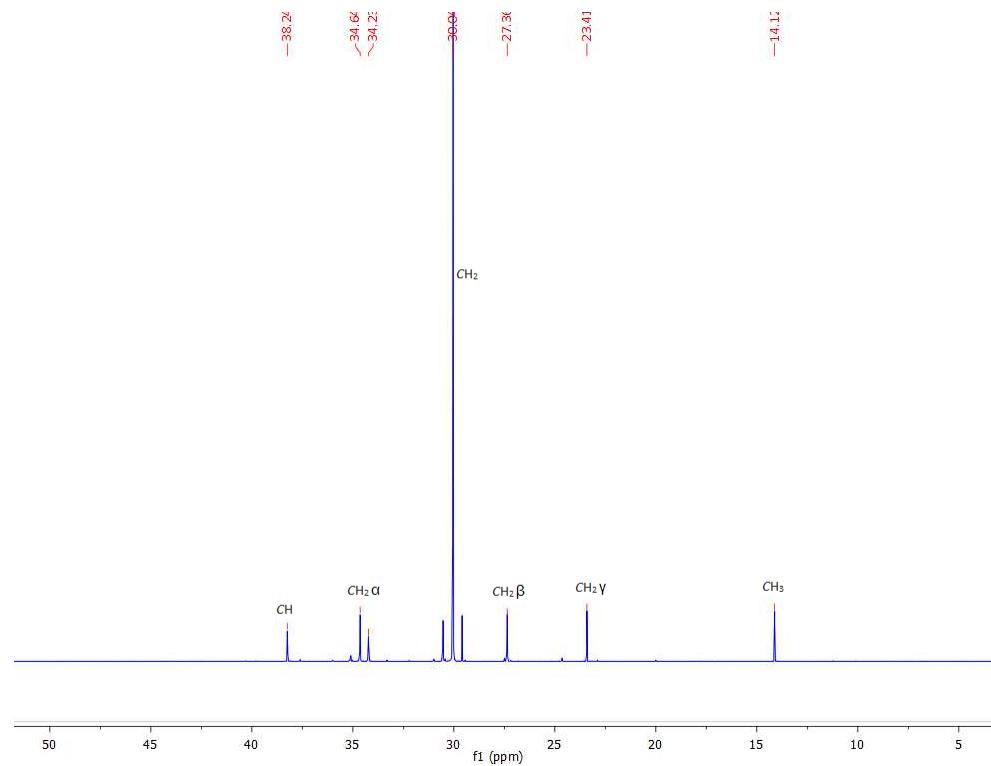
**Figure S56.**  $^{13}\text{C}$  NMR spectrum ( $\text{C}_6\text{D}_3\text{Cl}_3$ , 500 MHz, 100 °C) of PE/PHex (Table 2, run 1).



**Figure S57.** GPC trace of PE/PHex (Table 2, run 1) obtained with **3a-Zr<sub>2</sub>**.

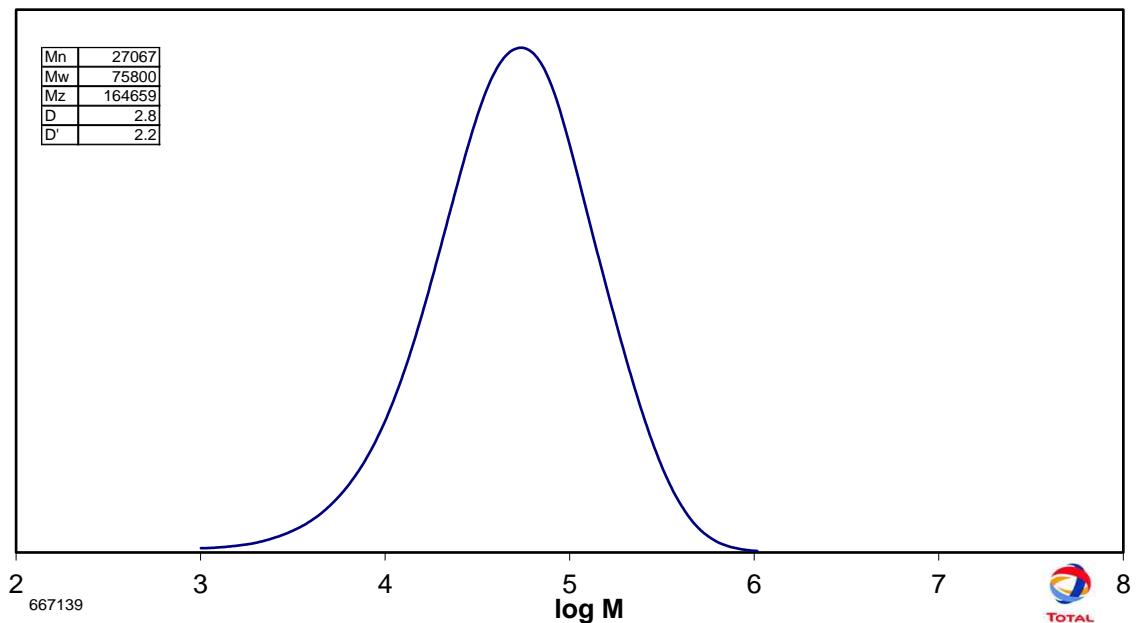


**Figure S58.**  $^{13}\text{C}$  NMR spectrum ( $\text{C}_6\text{D}_3\text{Cl}_3$ , 500 MHz, 100 °C) of PE/PHex (Table 2, run 4).



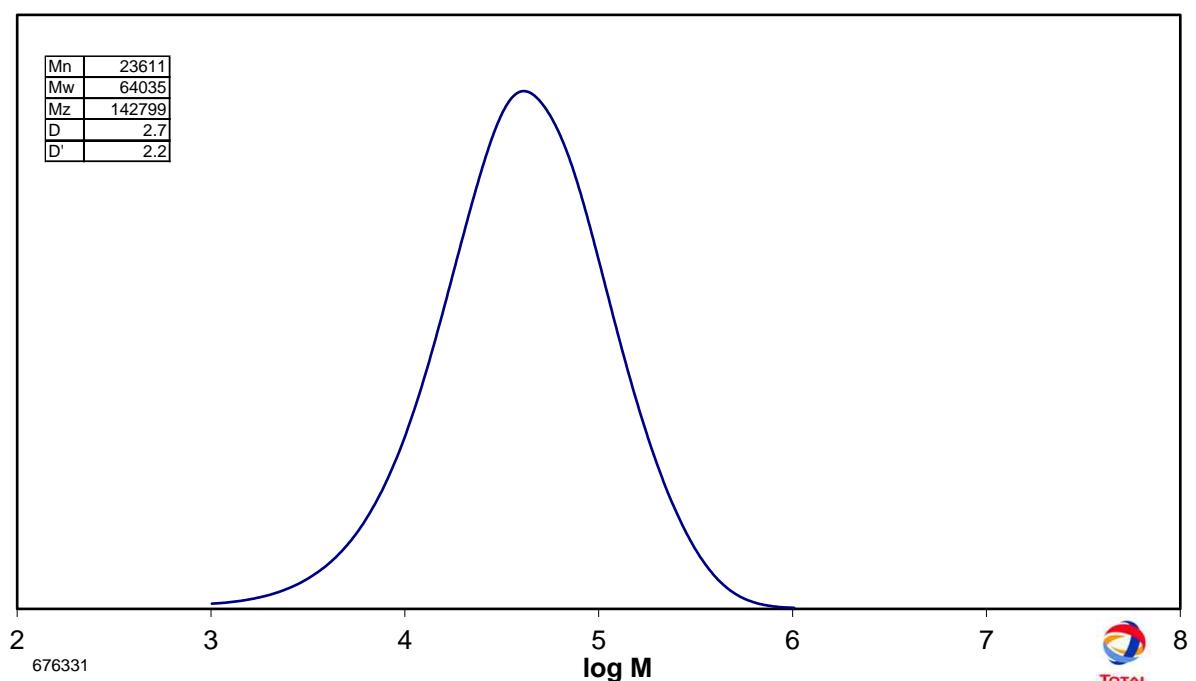
**Figure S59.**  $^{13}\text{C}$  NMR spectrum ( $\text{C}_6\text{D}_3\text{Cl}_3$ , 500 MHz, 100 °C) of PE/PHex (Table 2, run 5).

CPO-CPR-14-0380 : GS382



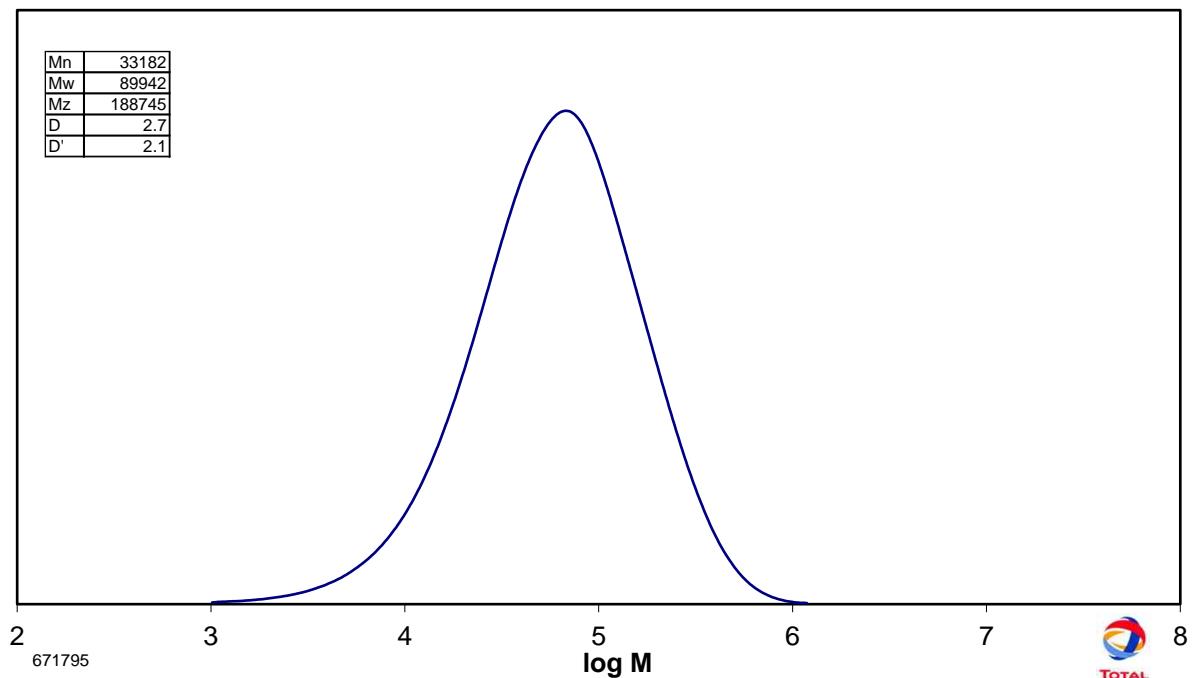
**Figure S60.** GPC trace of PE/PHex (Table 2, run 5) obtained with **3b-Zr<sub>2</sub>**.

CPO-CPR-15-0029 : GS382 2

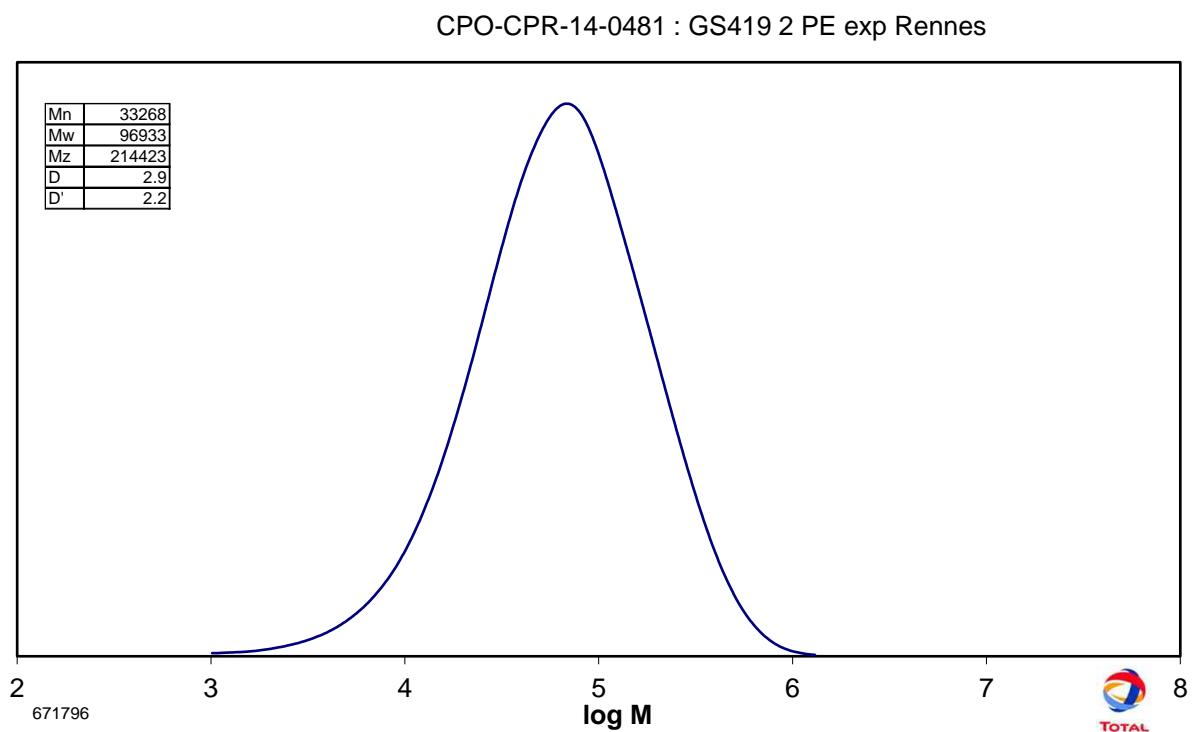


**Figure S61.** GPC trace of PE/PHex (Table 2, run 6) obtained with **3b-Zr<sub>2</sub>**.

CPO-CPR-14-0481 : GS419 PE exp Rennes

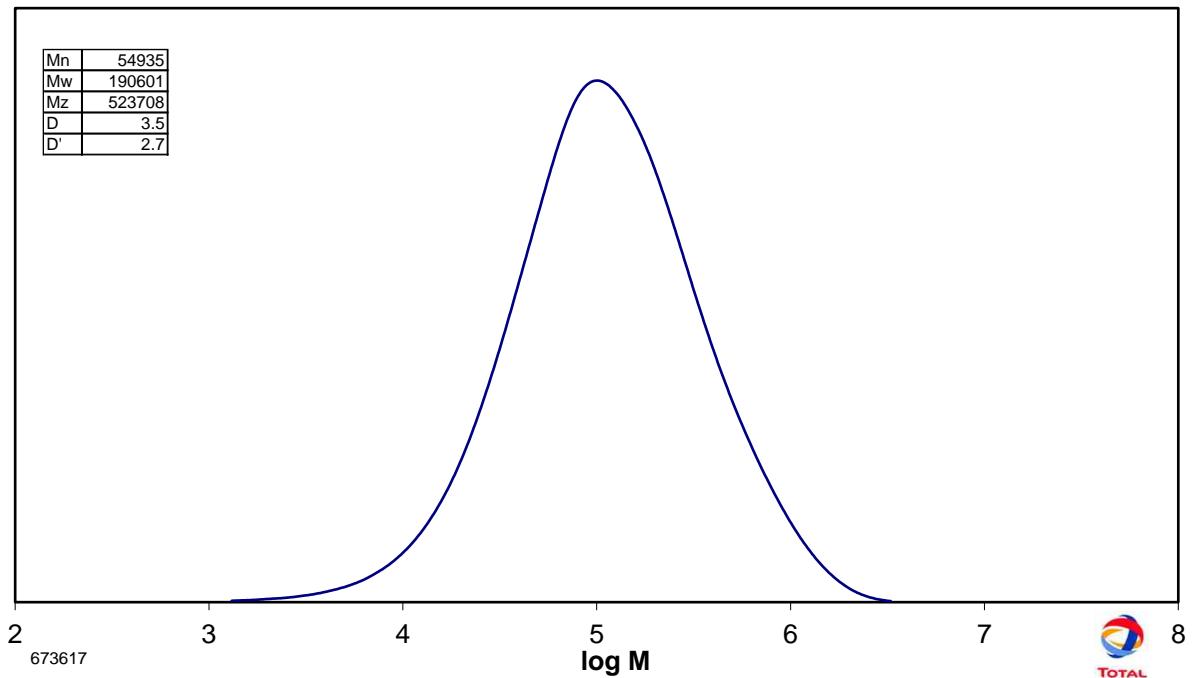


**Figure S62.** GPC trace of PE/PHex (Table 2, run 7) obtained with **3b'-Zr**.



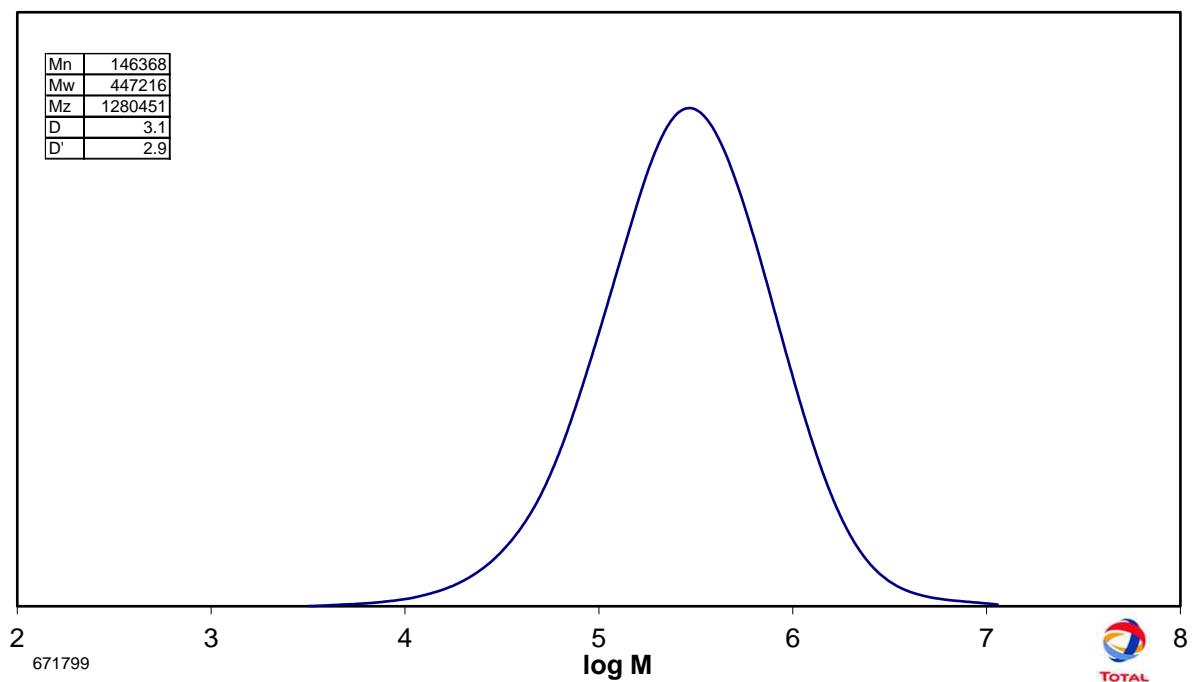
**Figure S63.** GPC trace of PE/PHex (Table 2, run 8) obtained with **3b'-Zr**.

CPO-CPR-14-0513 : CRUMBS PE (GS433)

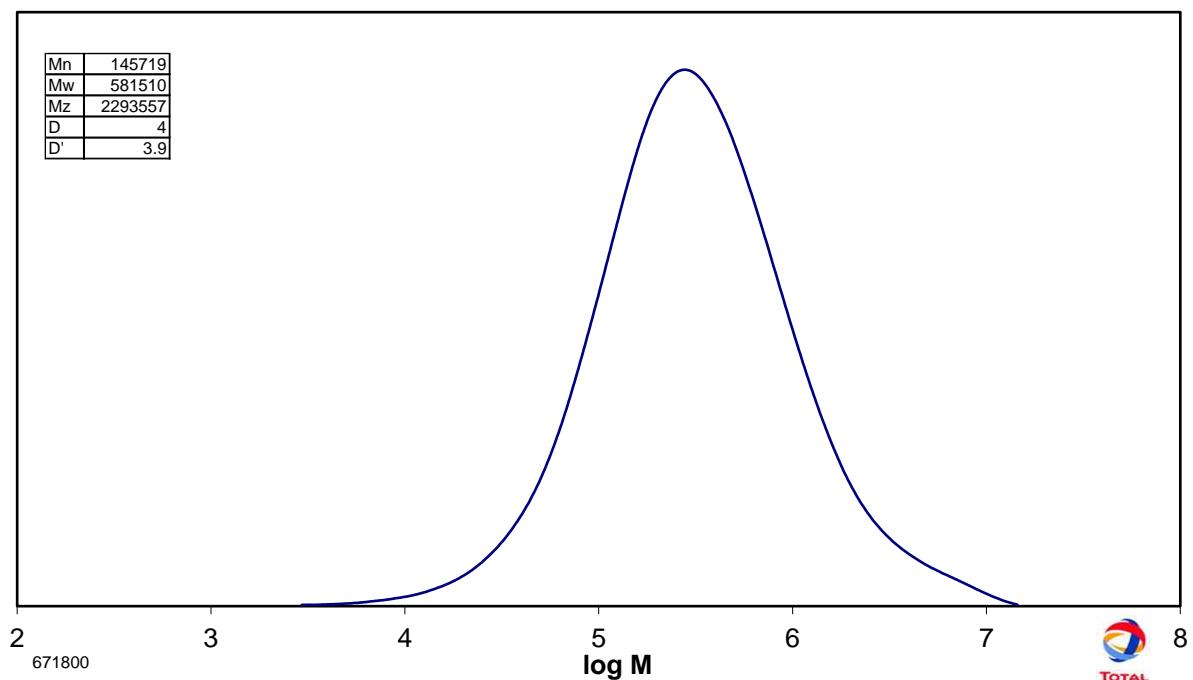


**Figure S64.** GPC trace of PE/PHex (Table 2, run 9) obtained with **3c-Zr<sub>2</sub>**.

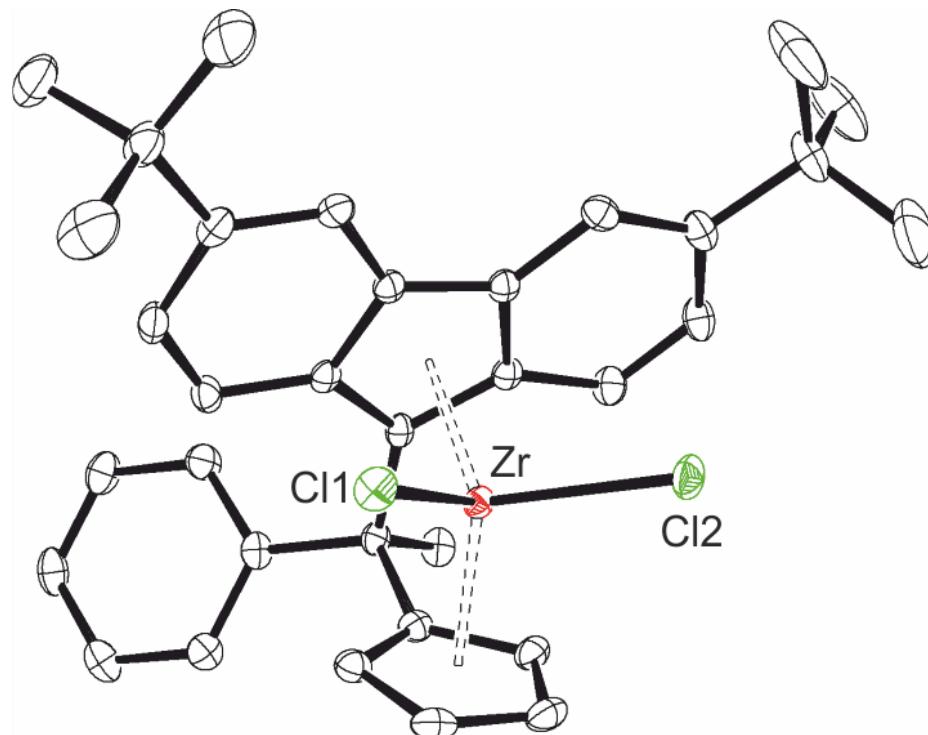
CPO-CPR-14-0481 : GS416 PE exp Rennes



**Figure S65.** GPC trace of PE/PHex (Table 2, run 10) obtained with **3a-Hf<sub>2</sub>**.



**Figure S66.** GPC trace of PE/PHex (Table 2, run 11) obtained with **3a-Hf<sub>2</sub>**.



**Figure S67.** Molecular structure of **3a'-Zr** (ellipsoids drawn at the 50% probability level; all hydrogen atoms are omitted for clarity).

**Table S1.** Summary of Crystal and Refinement Data for Compound **3a'-Zr**.

3a-Zr	
Empirical formula	C <sub>34</sub> H <sub>36</sub> Cl <sub>2</sub> Zr
Formula weight	606.75
Temperature, <i>K</i>	150(2)
Wavelength, Å	0.71073
Crystal system	orthorhombic
space group	<i>P c c n</i>
a, Å	15.8912(19)
b, Å	31.664(4)
c, Å	11.9600(13)
β, deg	90
Volume, Å <sup>3</sup>	6018.0(12)
Z	8
Calculated density, g.cm <sup>-3</sup>	1.339
Absorption coefficient, mm <sup>-1</sup>	0.564
Crystal size, mm	0.46 x 0.21 x 0.11
no. of rflns collected	91512
no. of indep rflns	6899 [R(int) = 0.0457]
Max. and min. transmission	0.940 and 0.886
Data / restraints / parameters	6899 / 0 / 341
Final <i>R</i> indices [ <i>I</i> >2σ]	<i>R</i> 1 <sup>a</sup> = 0.025, <i>wR</i> 2 <sup>b</sup> = 0.0573
<i>R</i> indices (all data)	<i>R</i> 1 <sup>a</sup> = 0.0321, <i>wR</i> 2 <sup>b</sup> = 0.0613
Goodness-of-fit on F <sup>2</sup>	1.064
Largest diff. peak and hole, e.Å <sup>-3</sup>	0.343 and -0.316