

Supporting Information Available.

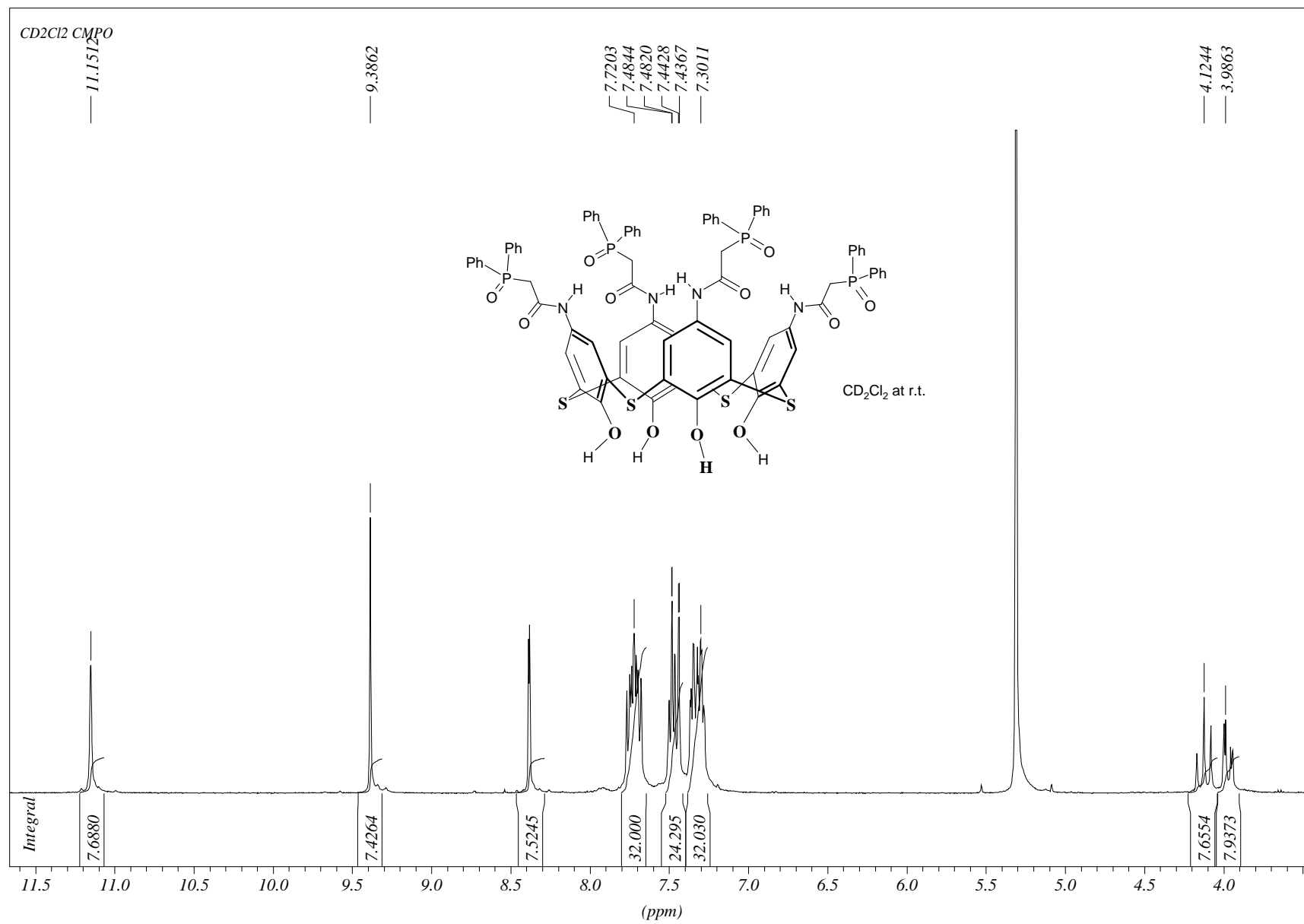
**Hydrogen Bonded Dimers of a Thiocalixarene Substituted by Carbamoylmethylphosphineoxide  
Groups at the Wide Rim**

**Oleg Kasyan,<sup>a</sup> Vitaly Kalchenko,<sup>a</sup> Michael Bolte<sup>b</sup> and Volker Böhmer**

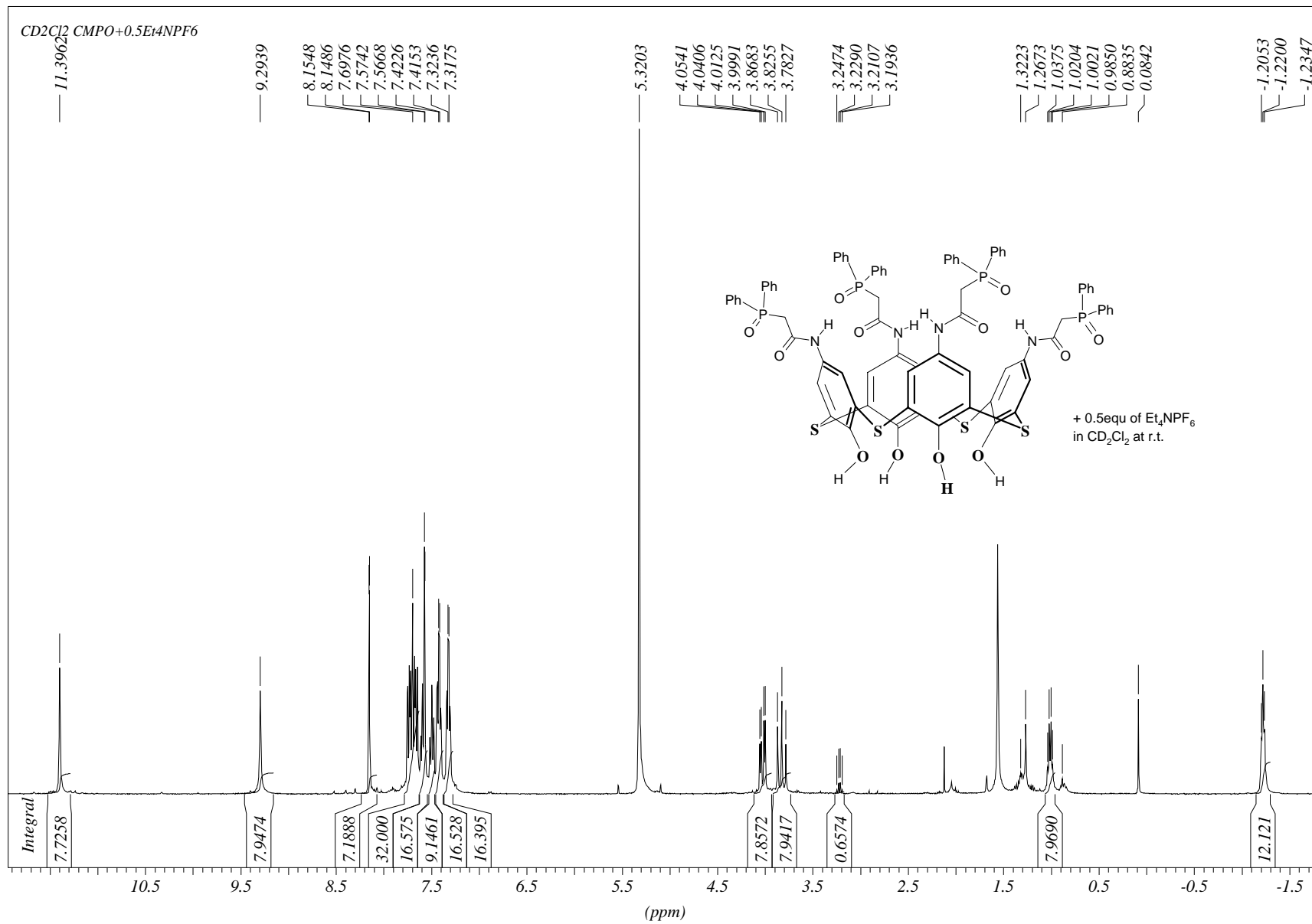
**TABLE OF CONTENTS**

<b>General Experimental Procedures</b> .....	S1
<b>Figure S1.</b> <sup>1</sup> H NMR spectrum of <b>2</b> in CD <sub>2</sub> Cl <sub>2</sub> .....	S2
<b>Figure S2.</b> <sup>1</sup> H NMR spectrum of <b>2</b> in CD <sub>2</sub> Cl <sub>2</sub> in the presence of Et <sub>4</sub> NPF <sub>6</sub> .....	S3
<b>Figure S3.</b> <sup>1</sup> H NMR spectrum of <b>2</b> in CD <sub>2</sub> Cl <sub>2</sub> in the presence of C <sub>10</sub> H <sub>10</sub> CoPF <sub>6</sub> .....	S4
<b>Figure S4.</b> <sup>1</sup> H NMR spectrum of <b>2</b> in CDCl <sub>3</sub> in the presence of Et <sub>3</sub> NHCl .....	S5
<b>Figure S5.</b> <sup>1</sup> H NMR spectrum of <b>2</b> in CD <sub>2</sub> Cl <sub>2</sub> the presence of Et <sub>3</sub> NHCl .....	S6
<b>Figure S6.</b> <sup>1</sup> H NMR spectrum of <b>2</b> in toluene-d <sub>8</sub> in the presence of Et <sub>3</sub> NHCl .....	S7
<b>Figure S7.</b> <sup>1</sup> H NMR spectrum of <b>2</b> in CDCl <sub>3</sub> .....	S8
<b>Figure S8.</b> <sup>1</sup> H NMR spectrum of <b>2</b> in C <sub>2</sub> D <sub>2</sub> Cl <sub>4</sub> at 120°C in the presence of Et <sub>4</sub> NPF <sub>6</sub> .....	S9
<b>Figure S9.</b> <sup>1</sup> H NMR spectrum of <b>2</b> in C <sub>2</sub> D <sub>2</sub> Cl <sub>4</sub> in the presence of Et <sub>4</sub> NPF <sub>6</sub> .....	S10
<b>Figure S10.</b> ESI-MS spectrum of <b>2</b> .....	S11
<b>Figure S11.</b> ESI-MS spectrum of <b>2</b> in the presence of C <sub>10</sub> H <sub>10</sub> CoPF <sub>6</sub> .....	S12
<b>Figure S12.</b> ESI-MS spectrum of <b>2</b> in the presence of Et <sub>4</sub> NPF <sub>6</sub> .....	S13
<b>Figure S13.</b> The part of ESI-MS spectrum of <b>2</b> in the presence of Et <sub>3</sub> NHCl .....	S14

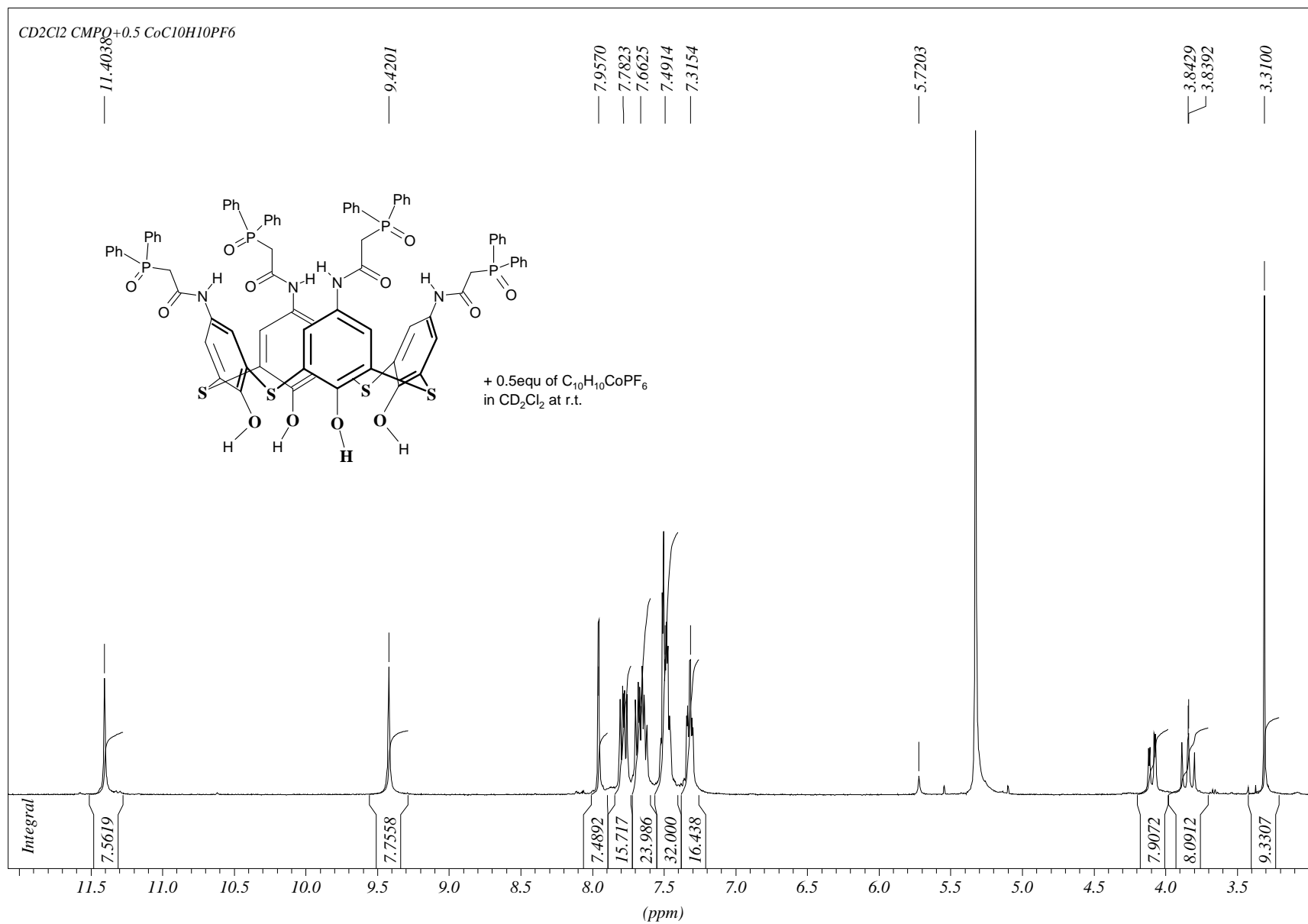
**General Experimental Procedures.** <sup>1</sup>H NMR spectra were recorded on a Bruker Avance DRX 400 instrument at 400 MHz using the solvent signals as internal reference.



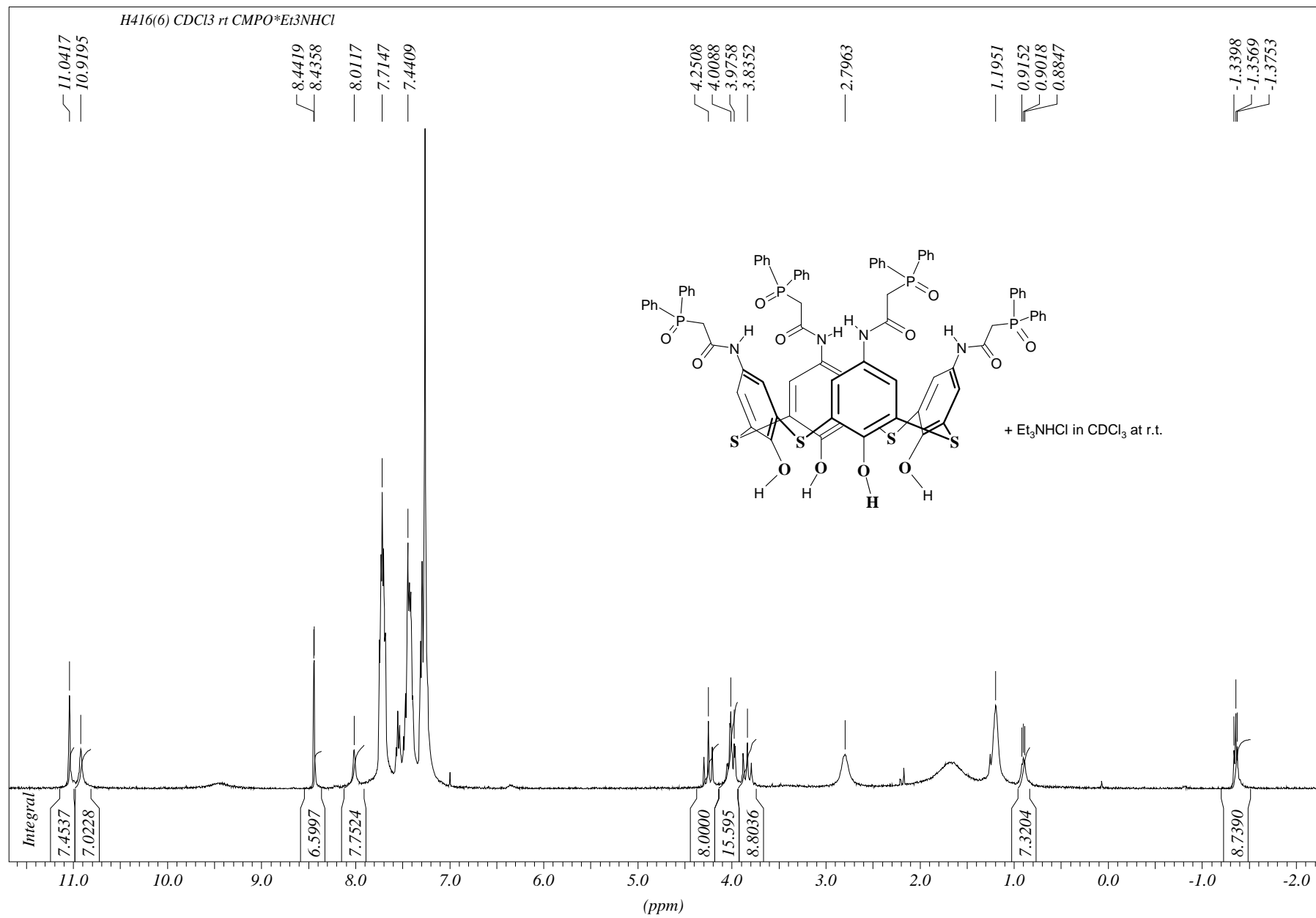
**Figure S1.** <sup>1</sup>H NMR spectrum of **2** in CD<sub>2</sub>Cl<sub>2</sub>



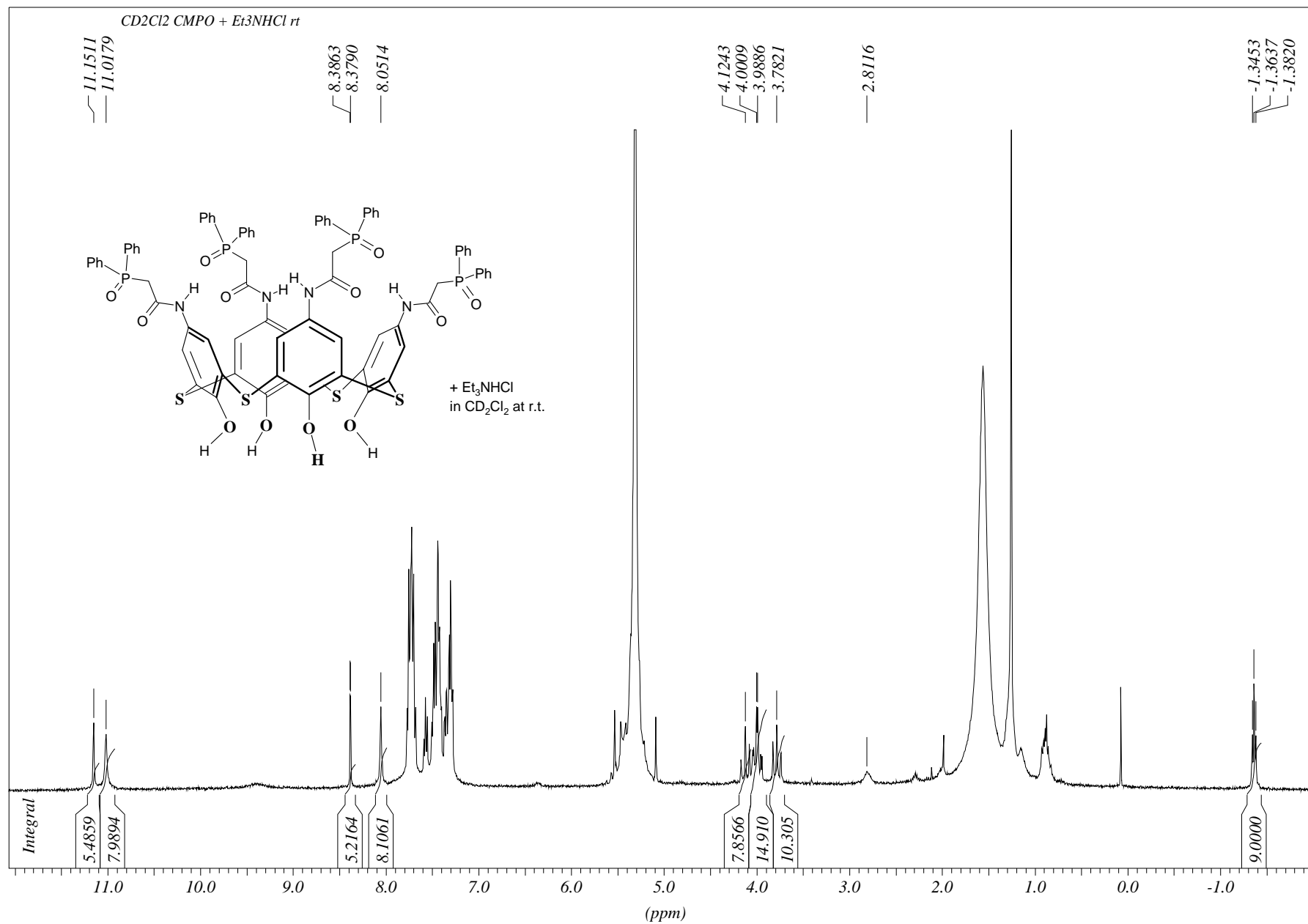
**Figure S2.** <sup>1</sup>H NMR spectrum of **2** in CD<sub>2</sub>Cl<sub>2</sub> in the presence of Et<sub>4</sub>NPF<sub>6</sub>



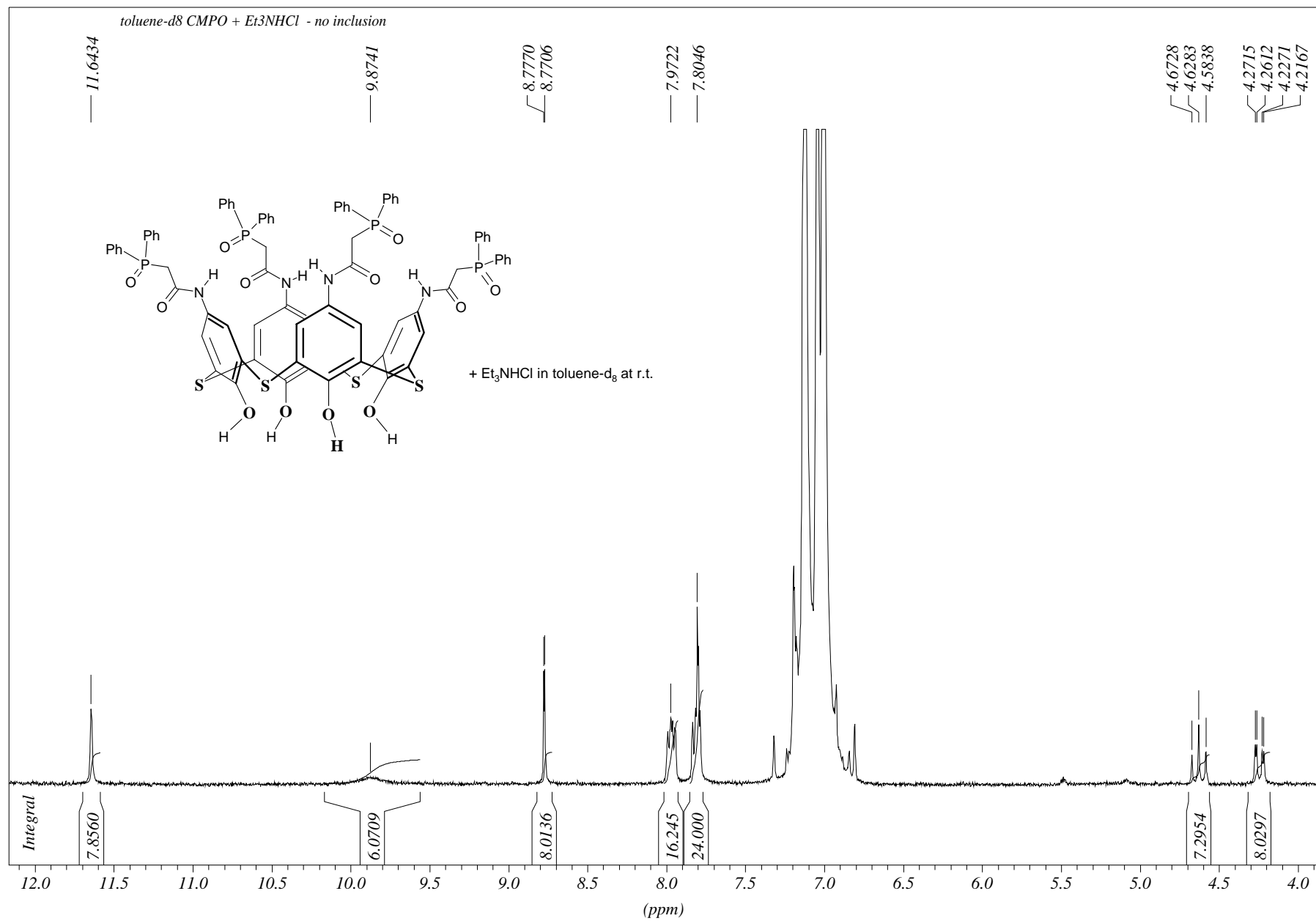
**Figure S3.** <sup>1</sup>H NMR spectrum of **2** in CD<sub>2</sub>Cl<sub>2</sub> in the presence of C<sub>10</sub>H<sub>10</sub>CoPF<sub>6</sub>



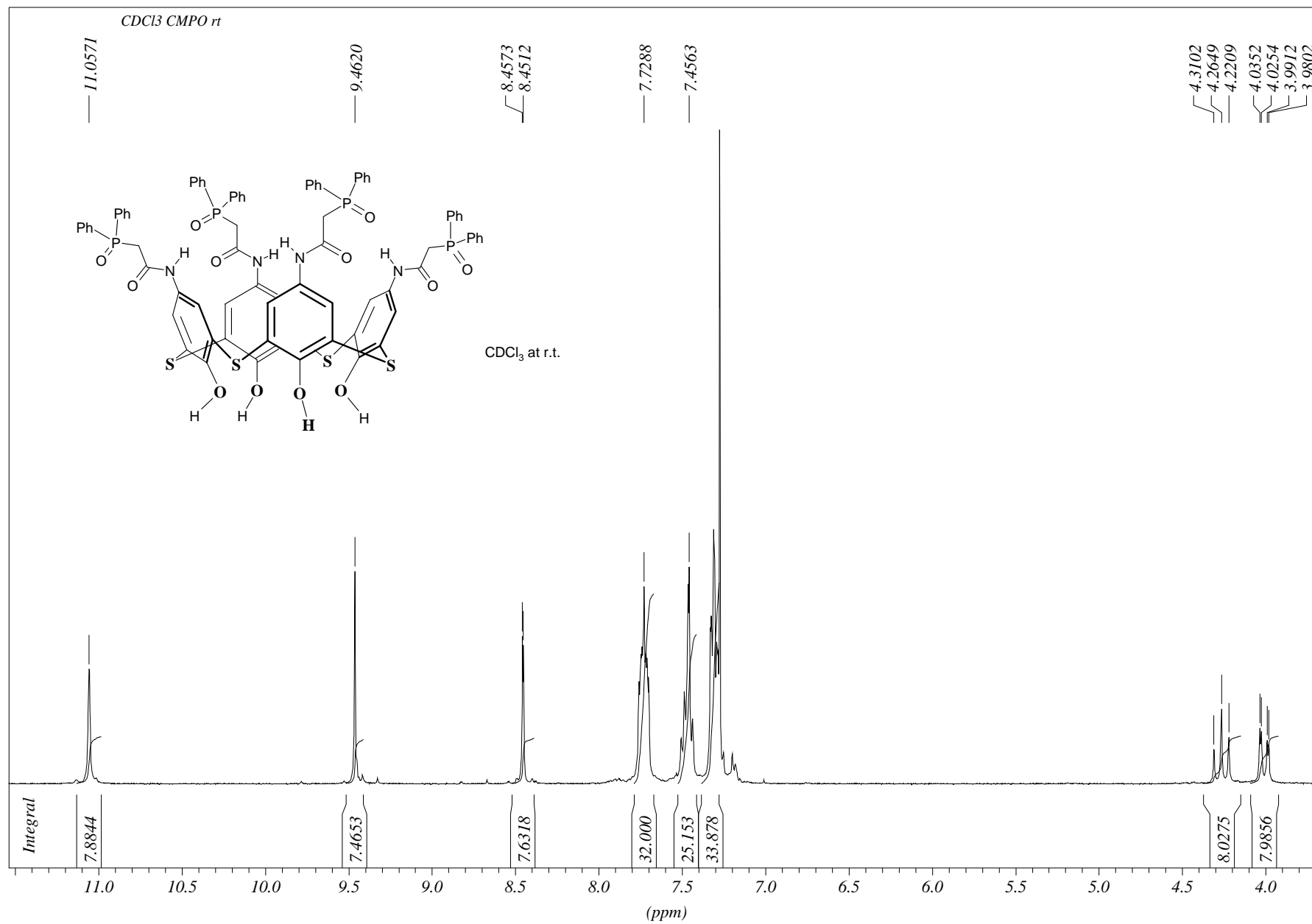
**Figure S4.** <sup>1</sup>H NMR spectrum of **2** in CDCl<sub>3</sub> in the presence of Et<sub>3</sub>NHCl



**Figure S5.** <sup>1</sup>H NMR spectrum of **2** in CD<sub>2</sub>Cl<sub>2</sub> the presence of Et<sub>3</sub>NHCl

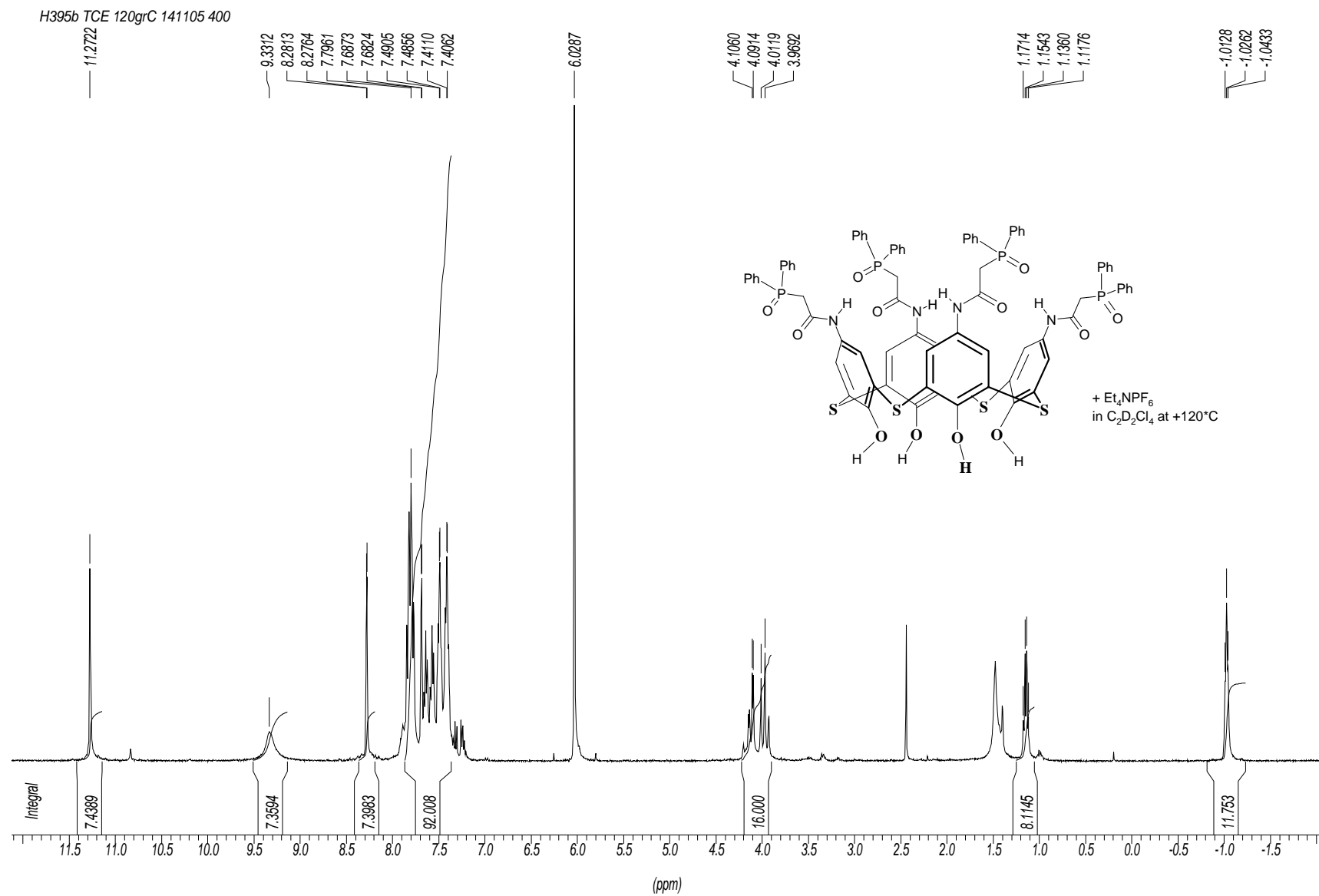


**Figure S6.** <sup>1</sup>H NMR spectrum of **2** in toluene-d<sub>8</sub> in the presence of Et<sub>3</sub>NHCl

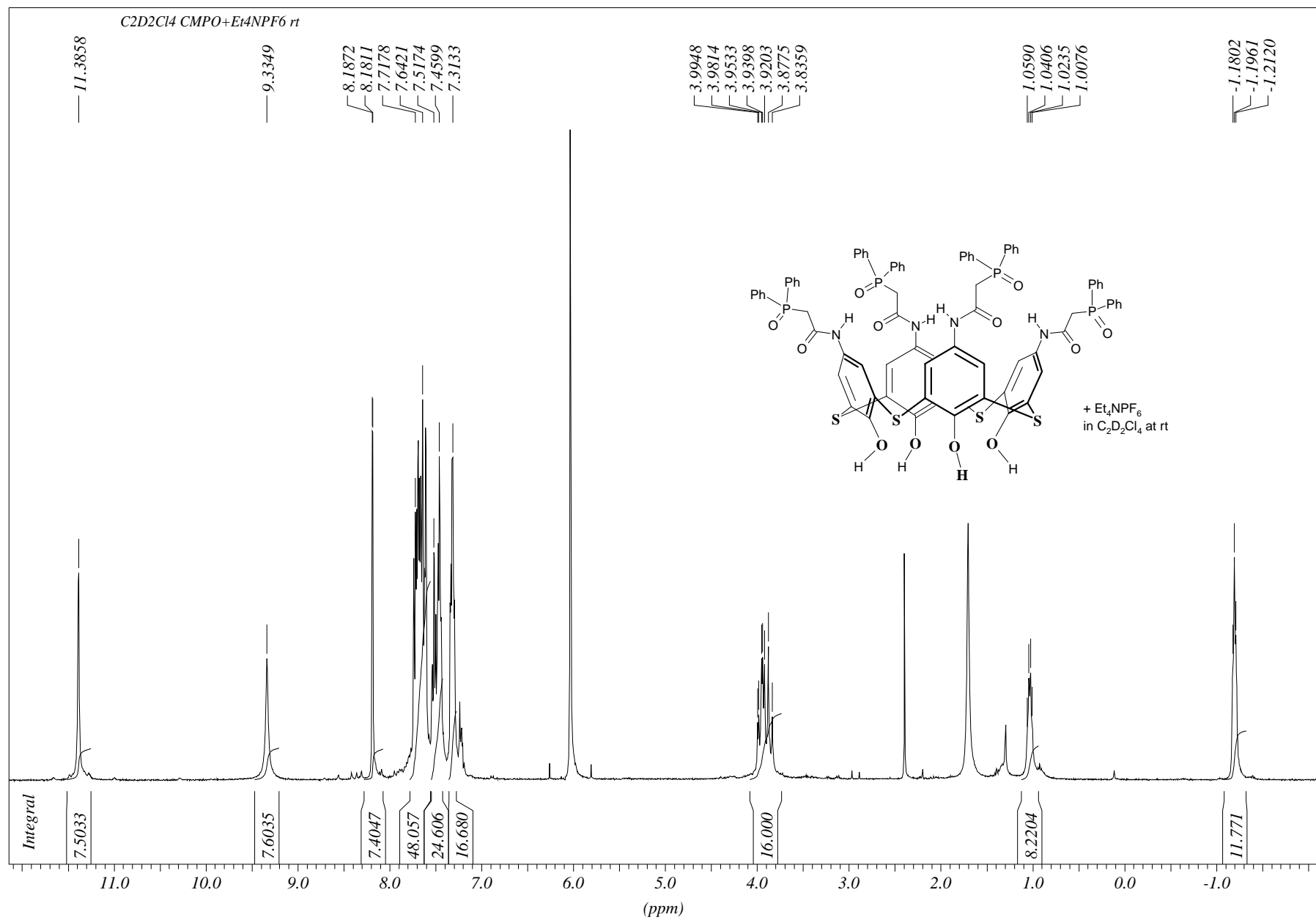


**Figure S7.** <sup>1</sup>H NMR spectrum of **2** in CDCl<sub>3</sub>





**Figure S8.**  $^1\text{H}$  NMR spectrum of **2** in  $\text{C}_2\text{D}_2\text{Cl}_4$  at  $120^\circ\text{C}$  in the presence of  $\text{Et}_4\text{NPF}_6$



**Figure S9.**  $^1\text{H}$  NMR spectrum of **2** in  $\text{C}_2\text{D}_2\text{Cl}_4$  in the presence of  $\text{Et}_4\text{NPF}_6$

**Kasyan, H348**

ESI3057 3 (0.135) Cm (3:23)

1: TOF MS ES+  
5.39e4

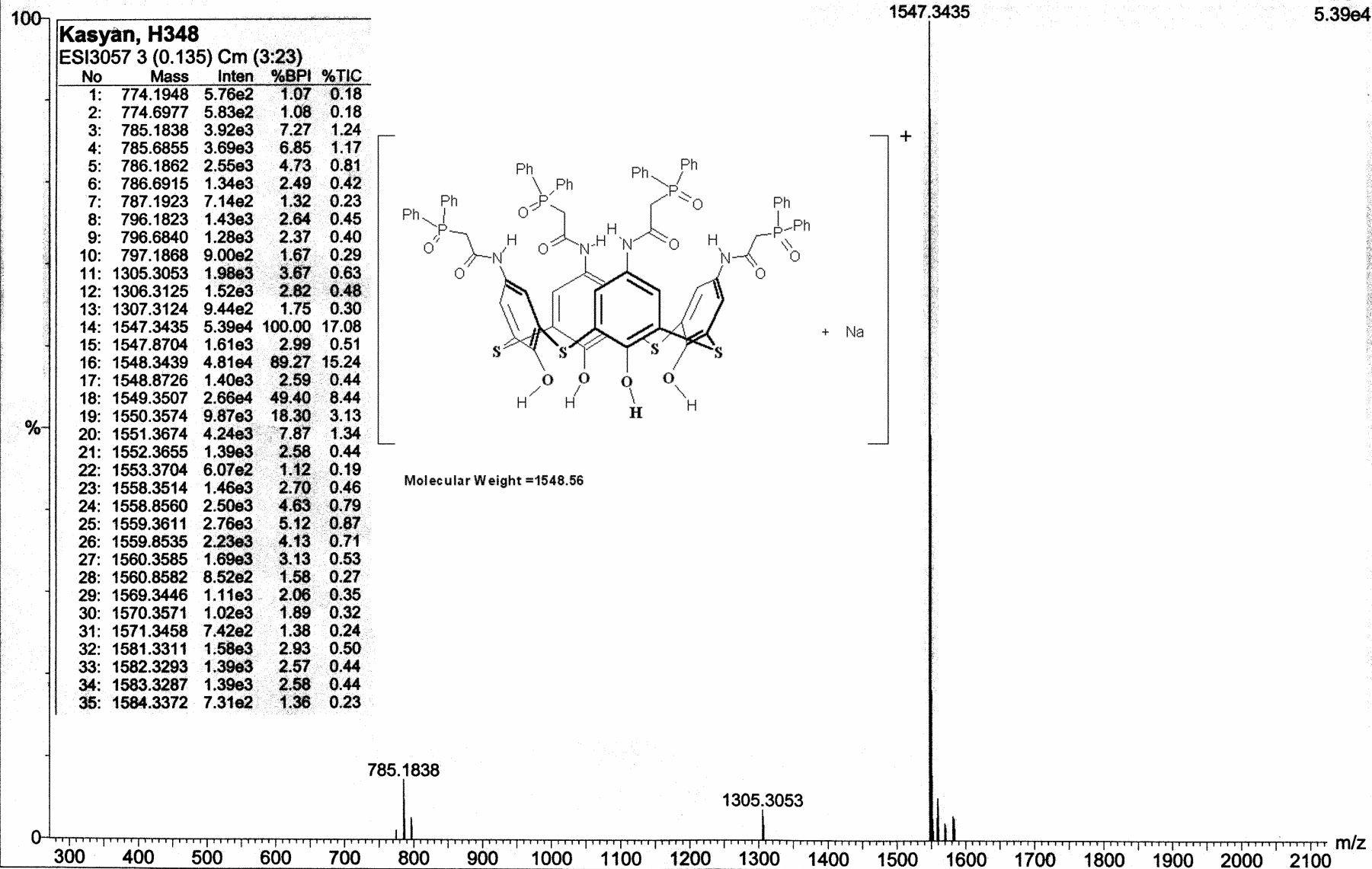
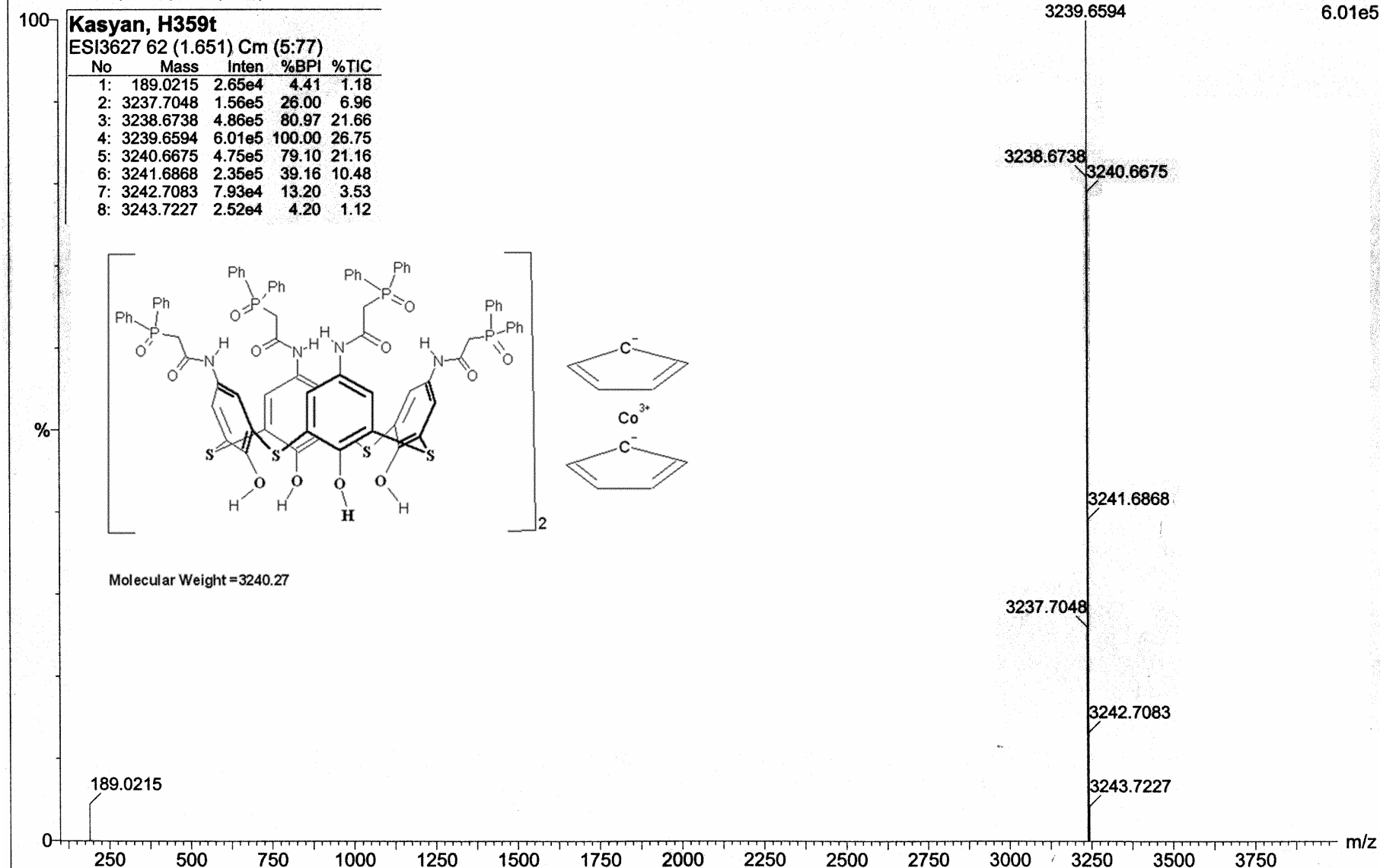


Figure S10. ESI-MS spectrum of 2

**Kasyan, H359t**

ESI3627 62 (1.651) Cm (5:77)

1: TOF MS ES+  
6.01e5**Figure S11.** ESI-MS spectrum of **2** in the presence of  $C_{10}H_{10}CoPF_6$

Kasyan, H359x10

ESI3626 61 (1.628) Cm (5:85)

1: TOF MS ES+  
7.21e5

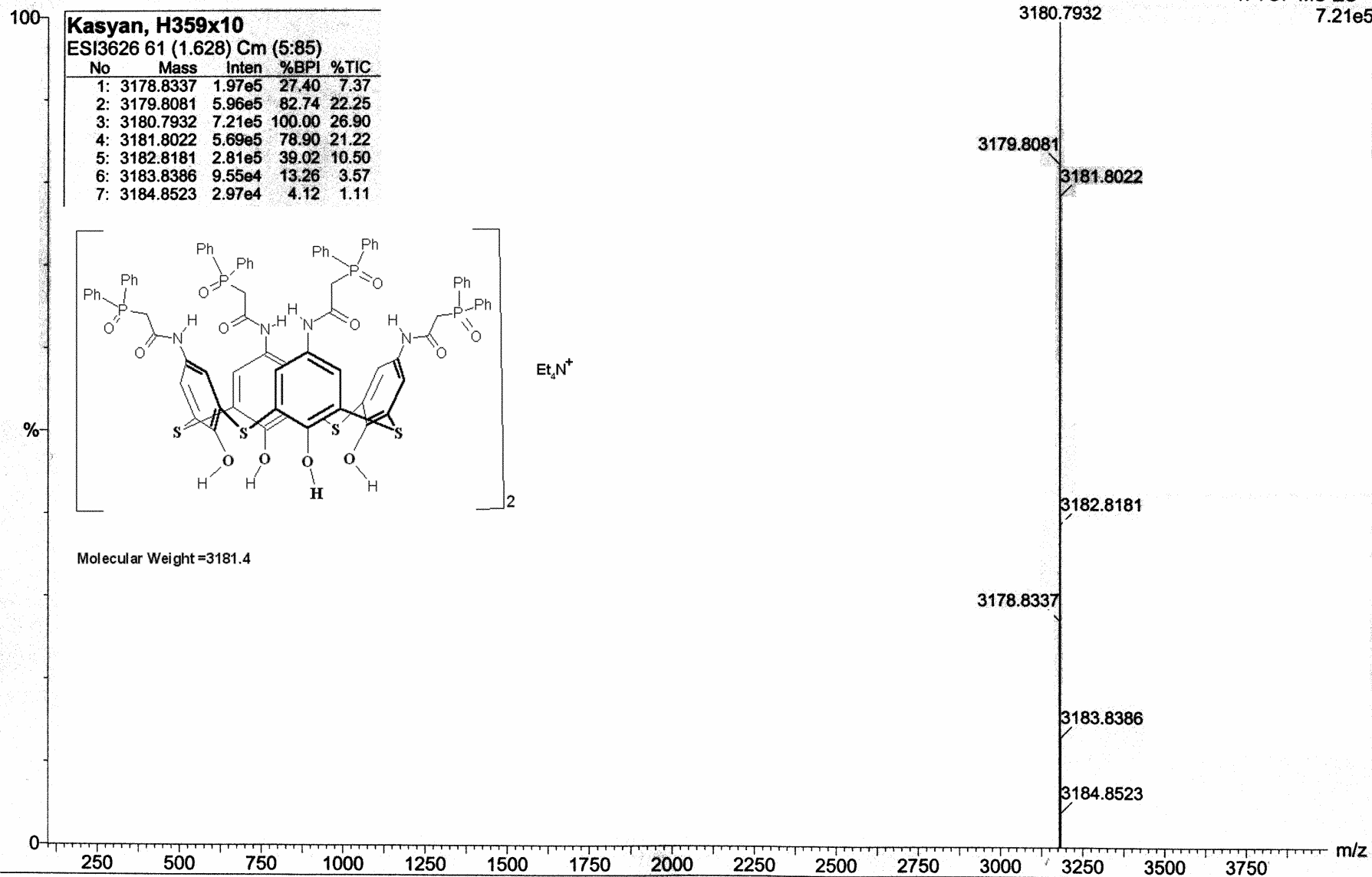
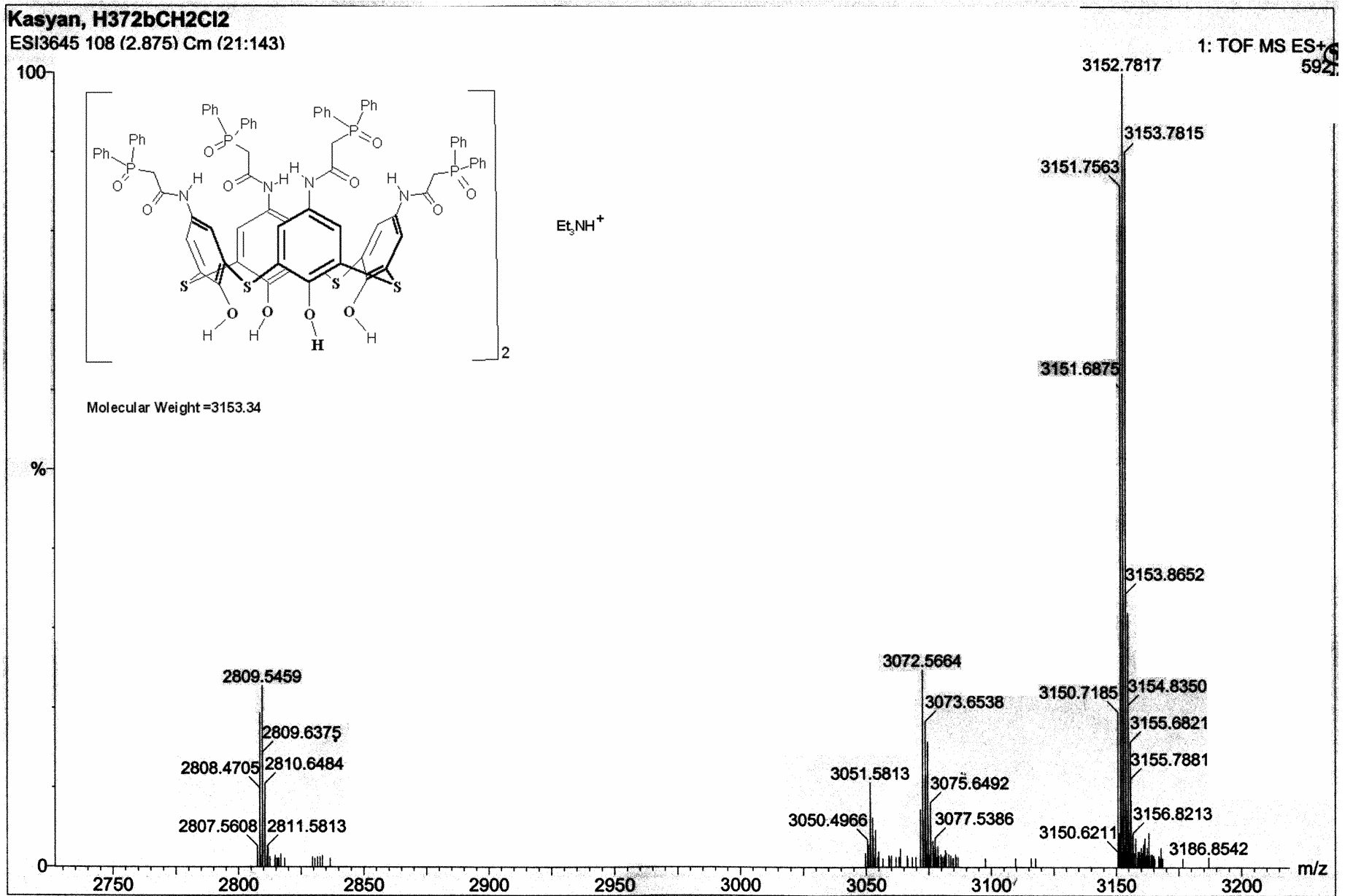


Figure S12. ESI-MS spectrum of **2** in the presence of  $\text{Et}_4\text{NPF}_6$



**Figure S13.** The part of ESI-MS spectrum of **2** in the presence of  $\text{Et}_3\text{NHCl}$