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SUPPORTING INFORMATION

Title: Selective Catalytic Hydration of Alkynes in the Presence of Au-Cavitands: A Study in Structure–Activity Relationships

Author(s): Mami Inoue, Katto Ugawa, Tomoyuki Maruyama, Tetsuo Iwasawa*

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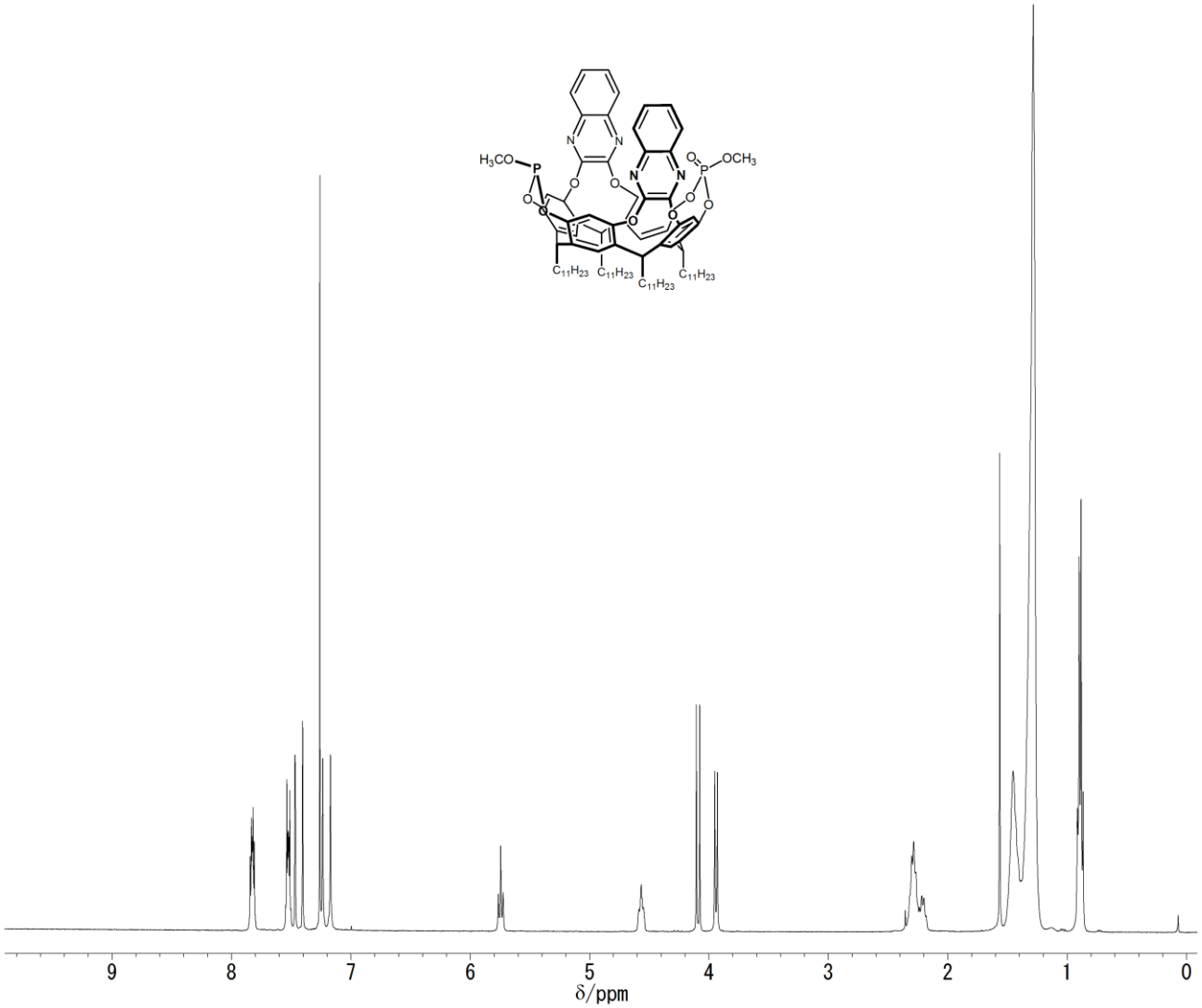
1) Compound **2** (^{1}H NMR spectrum in $CDCl_3$)



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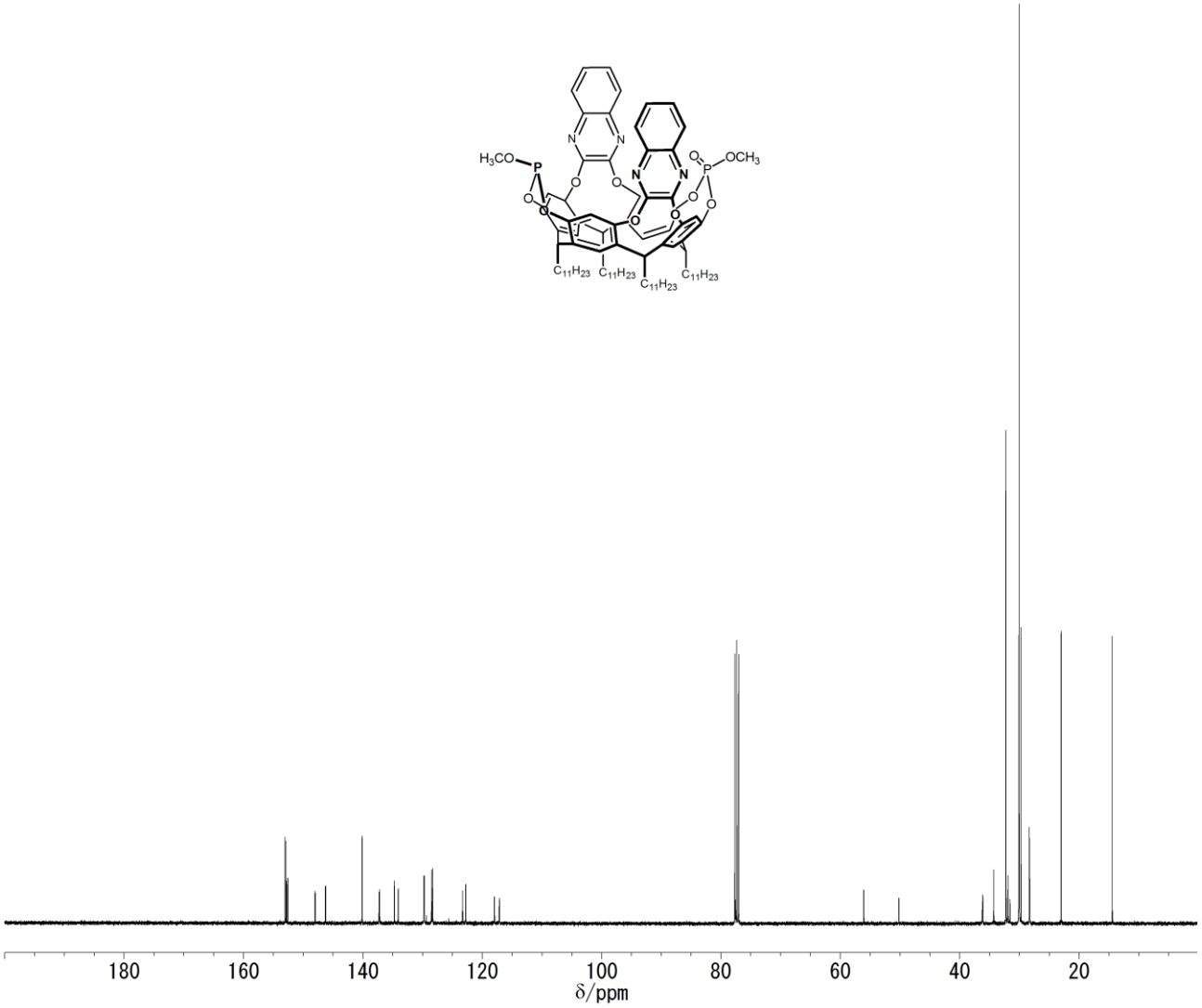

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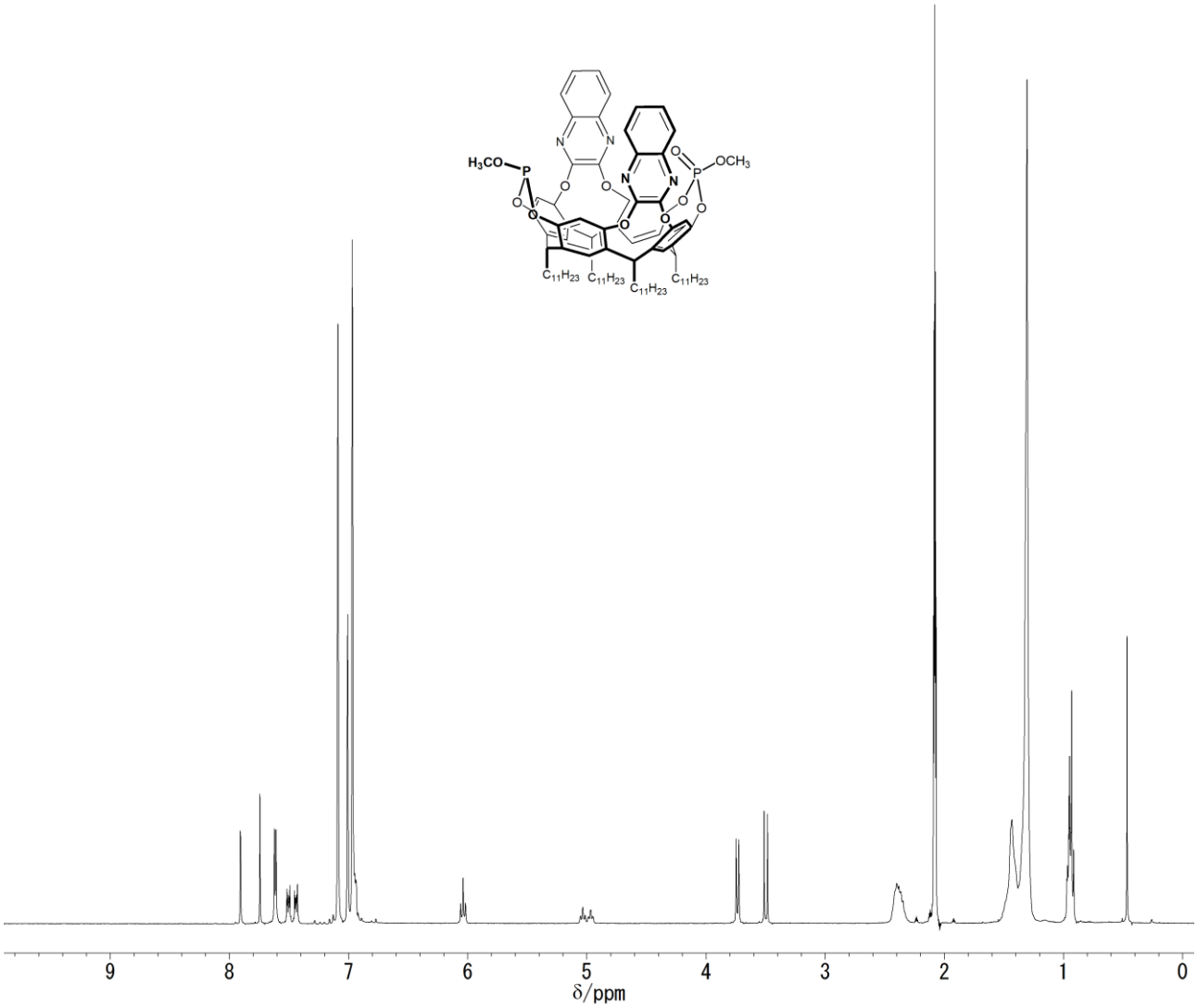

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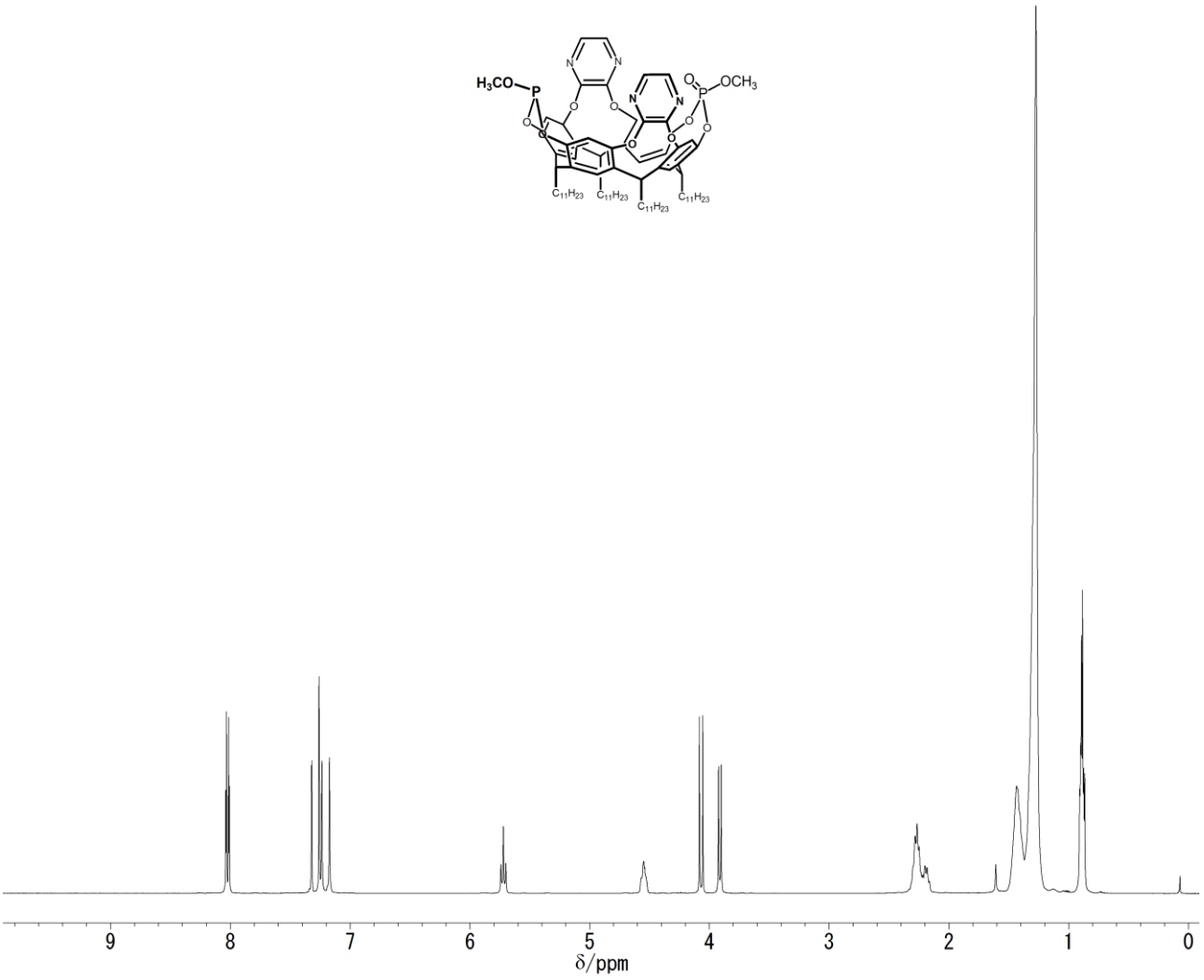

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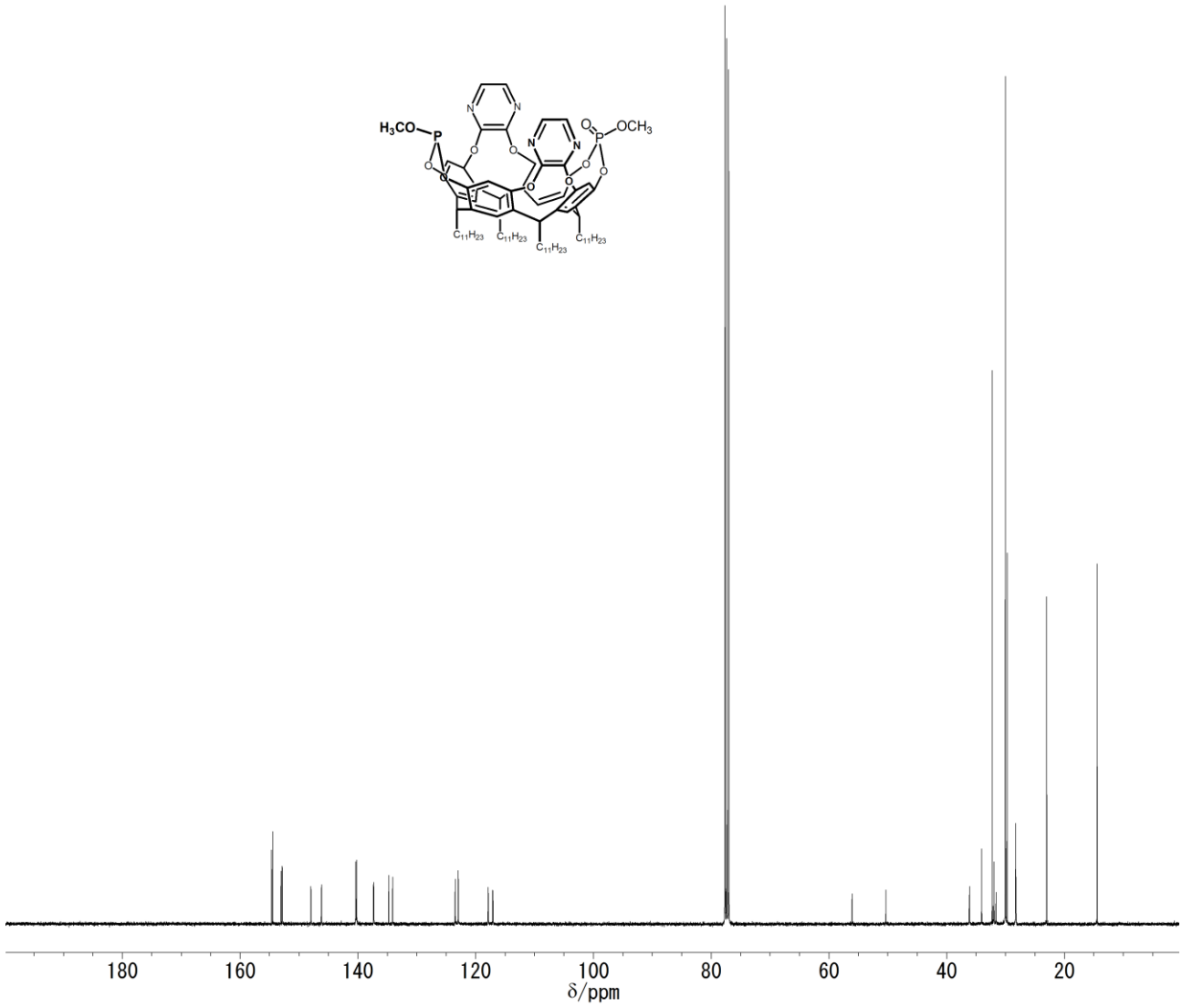

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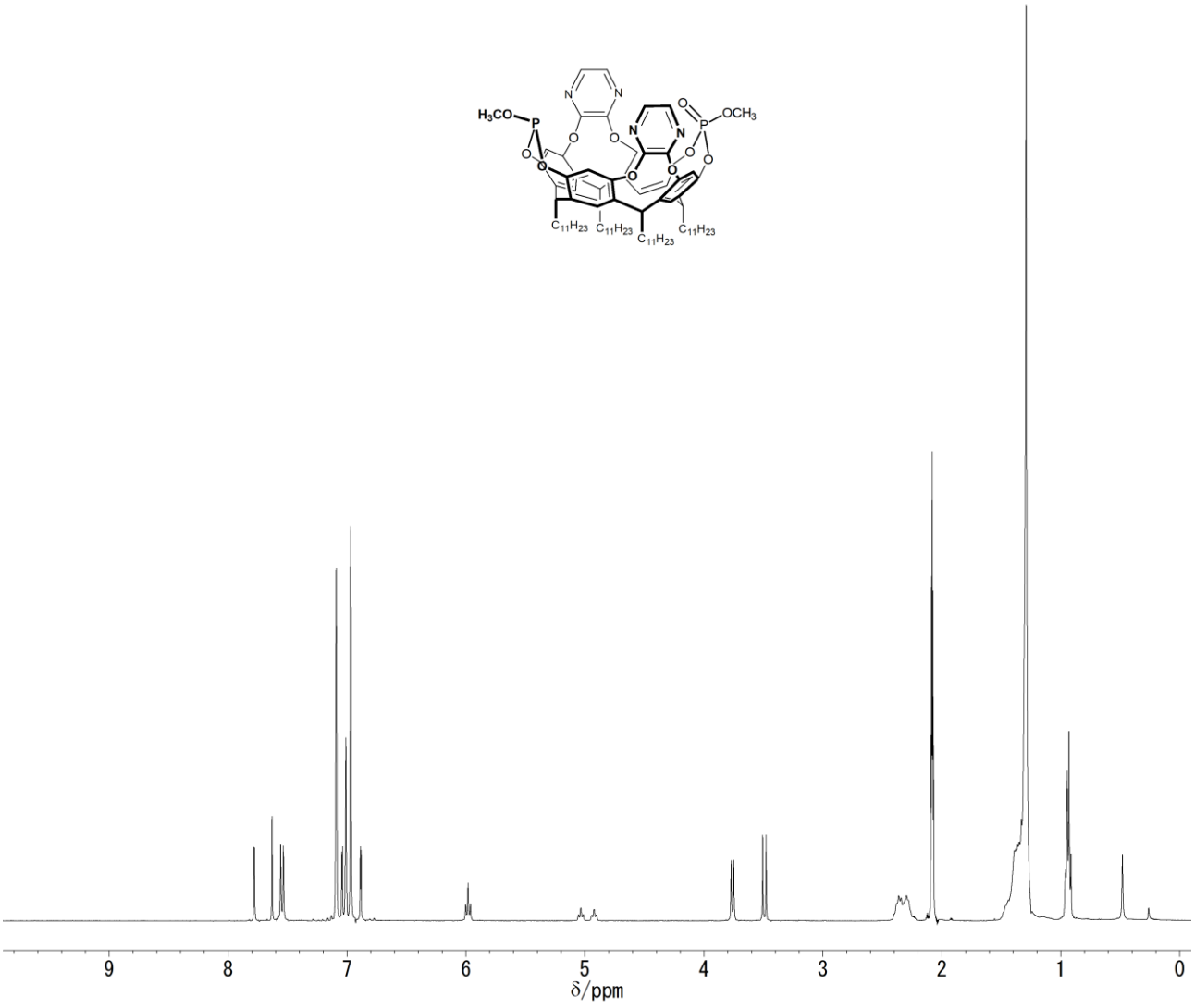

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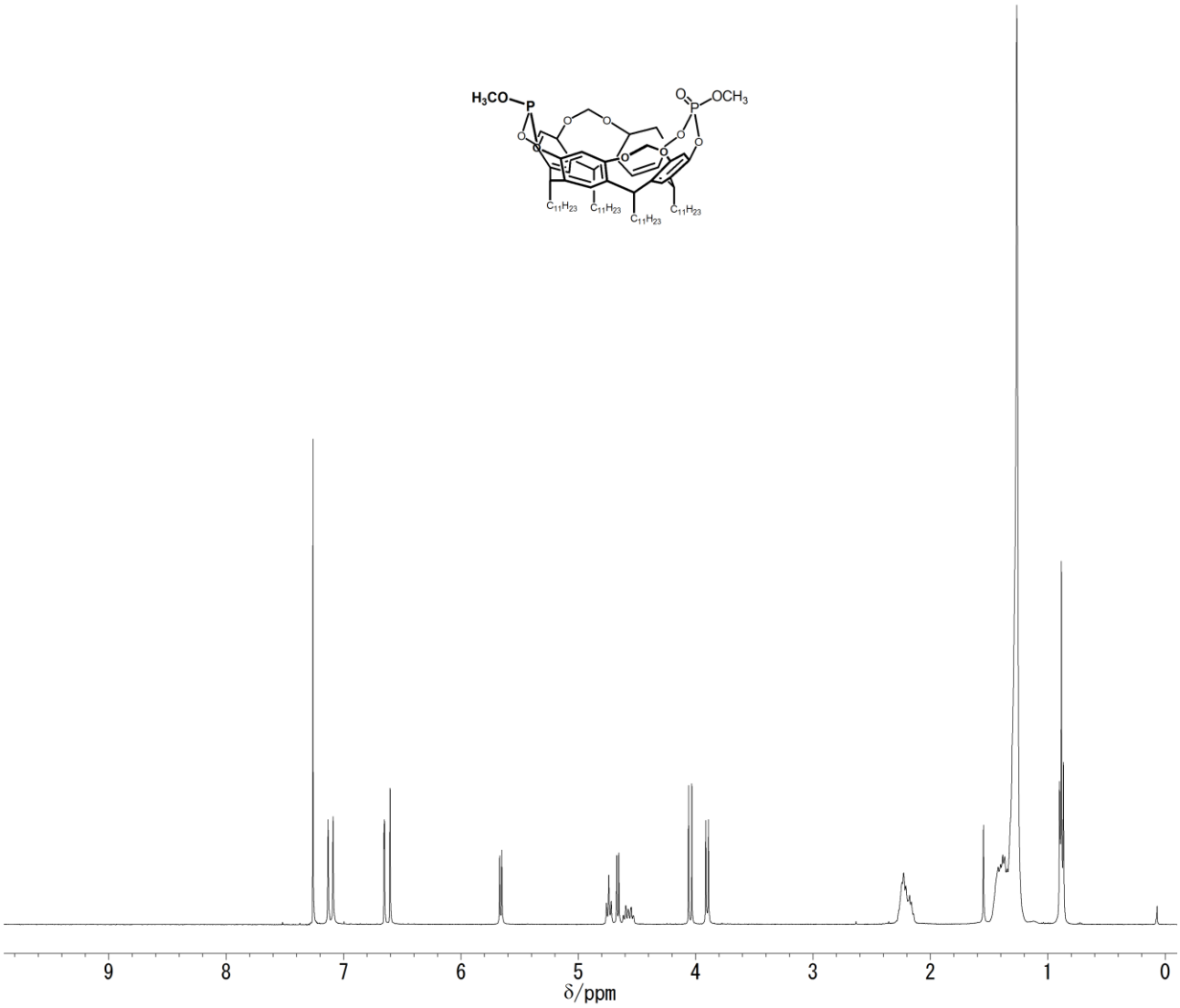

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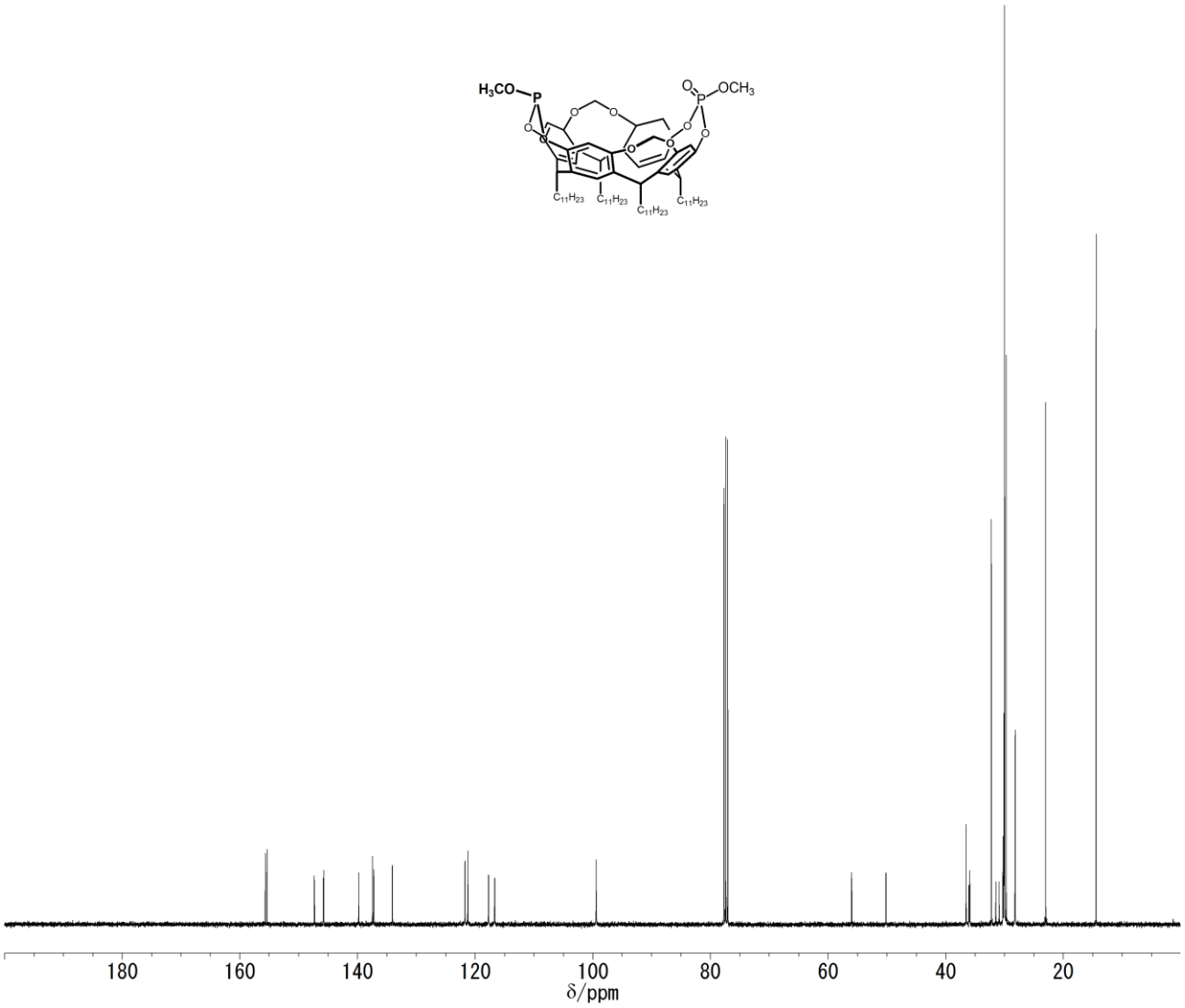

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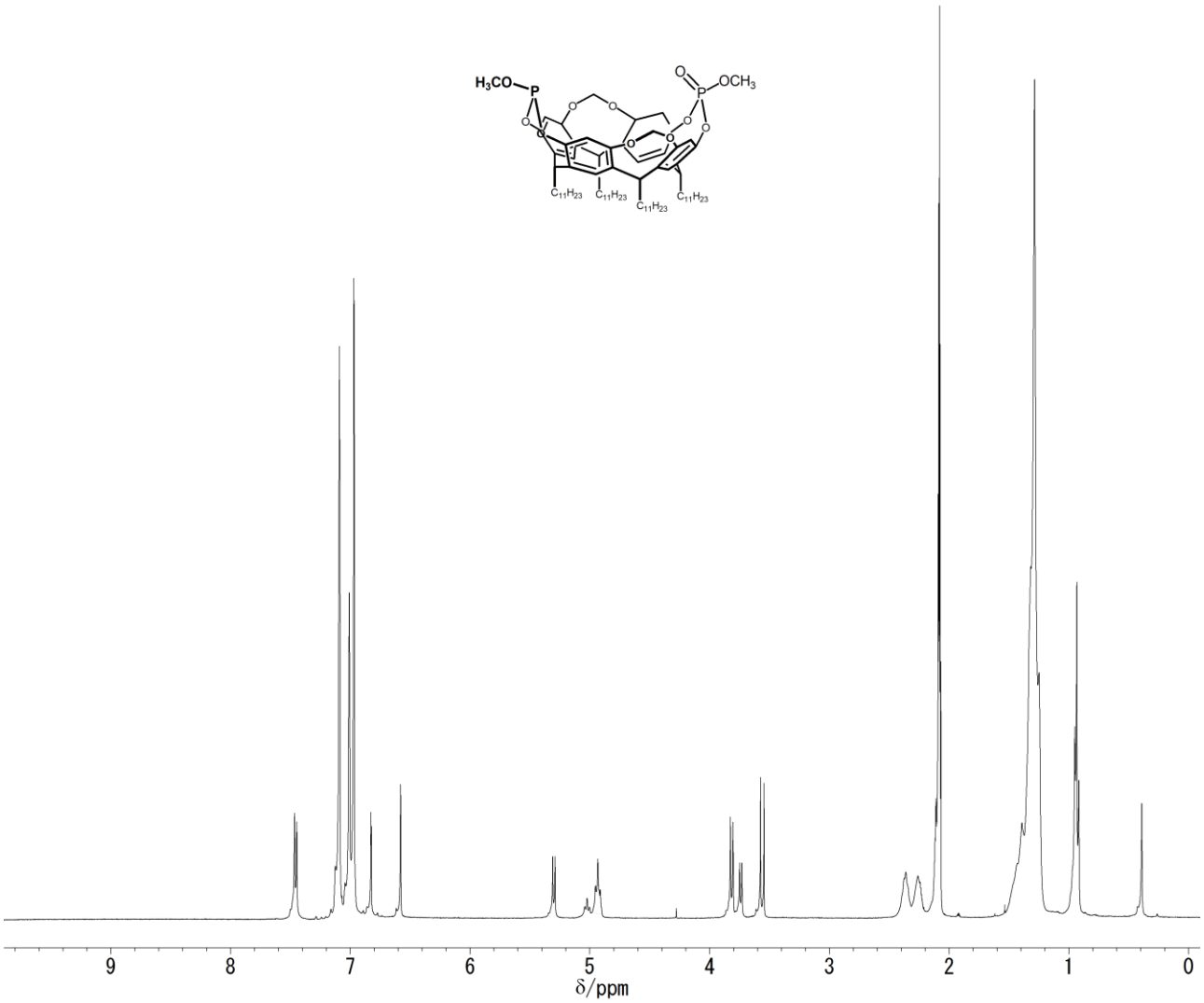

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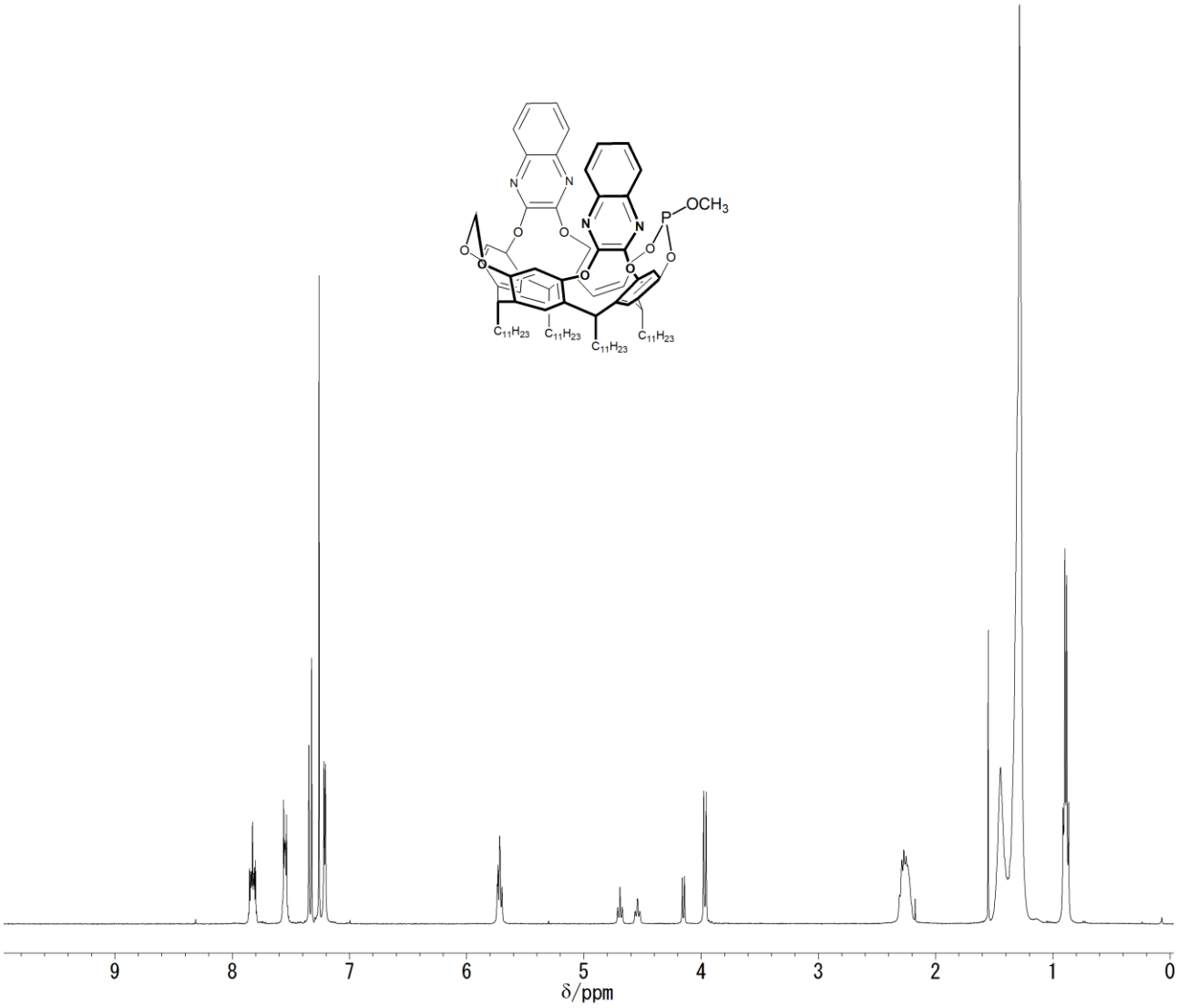

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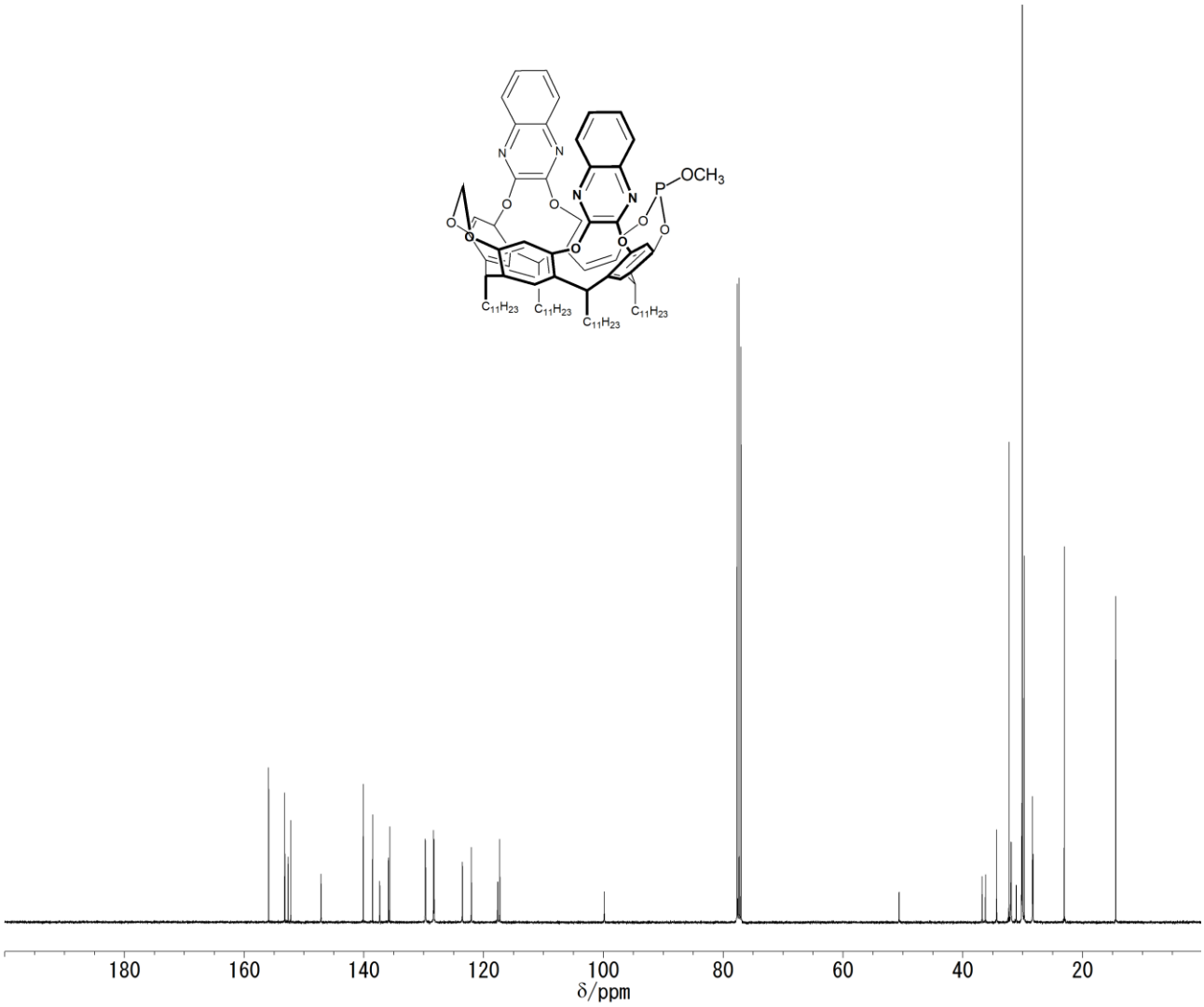

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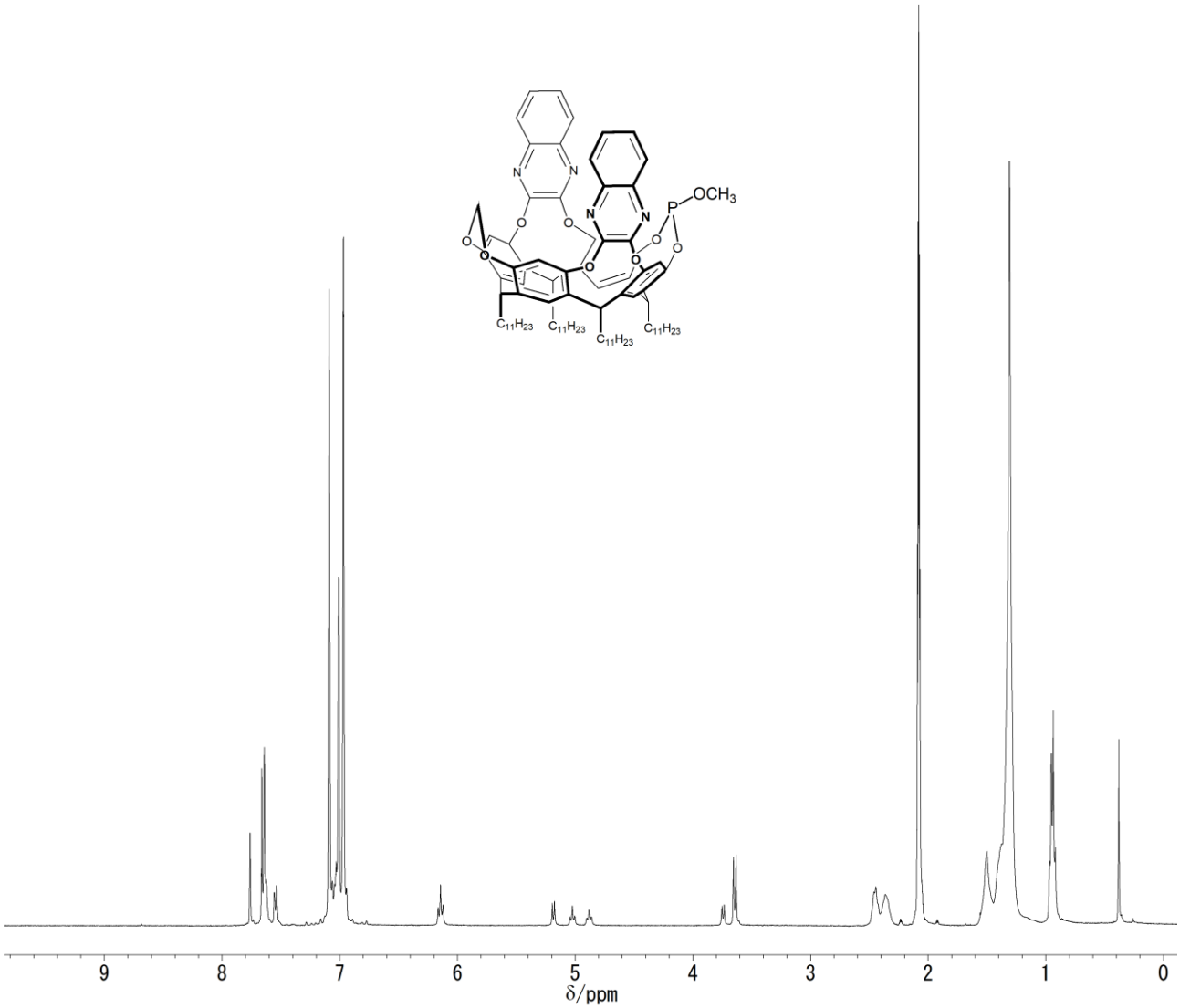

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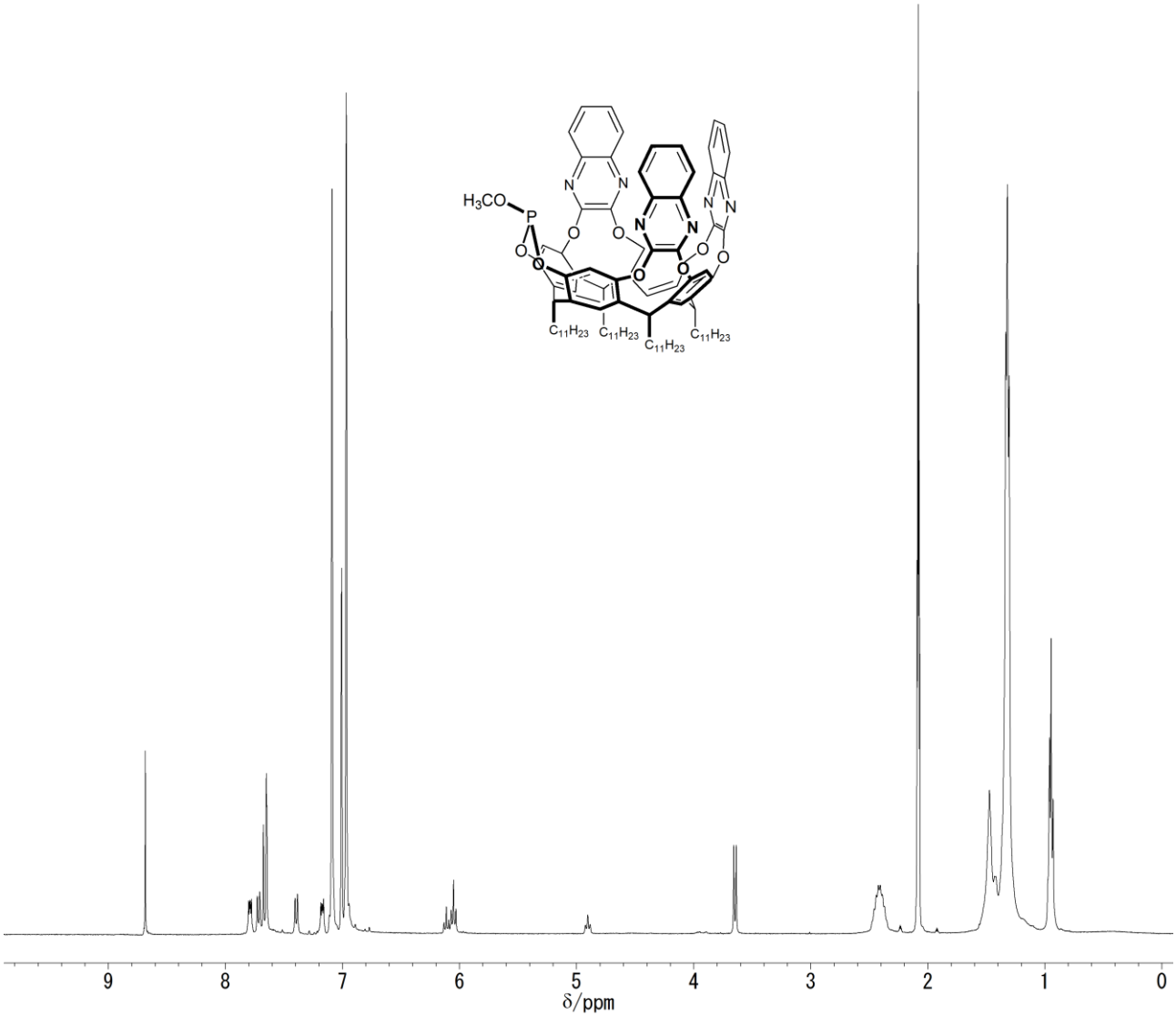

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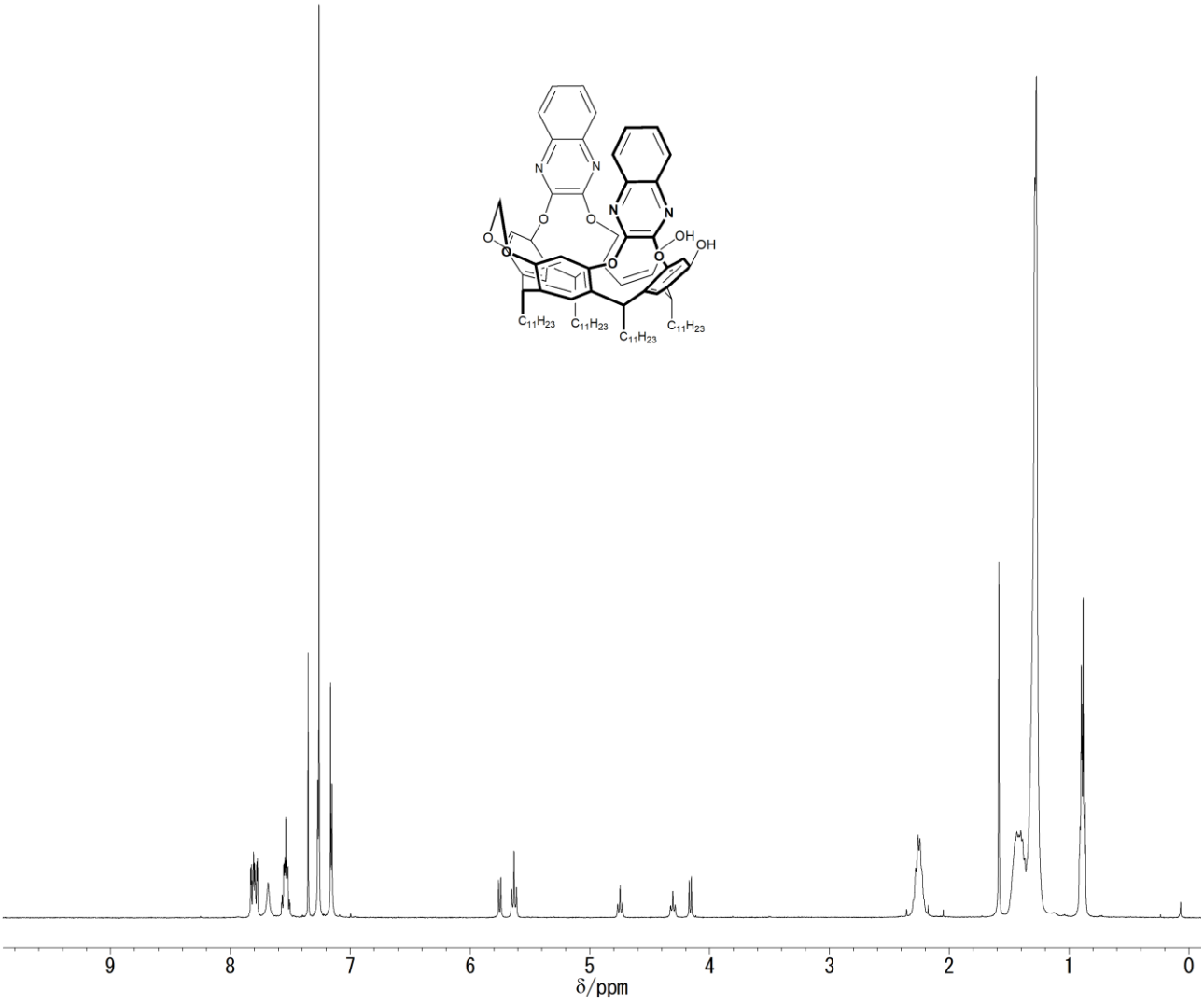
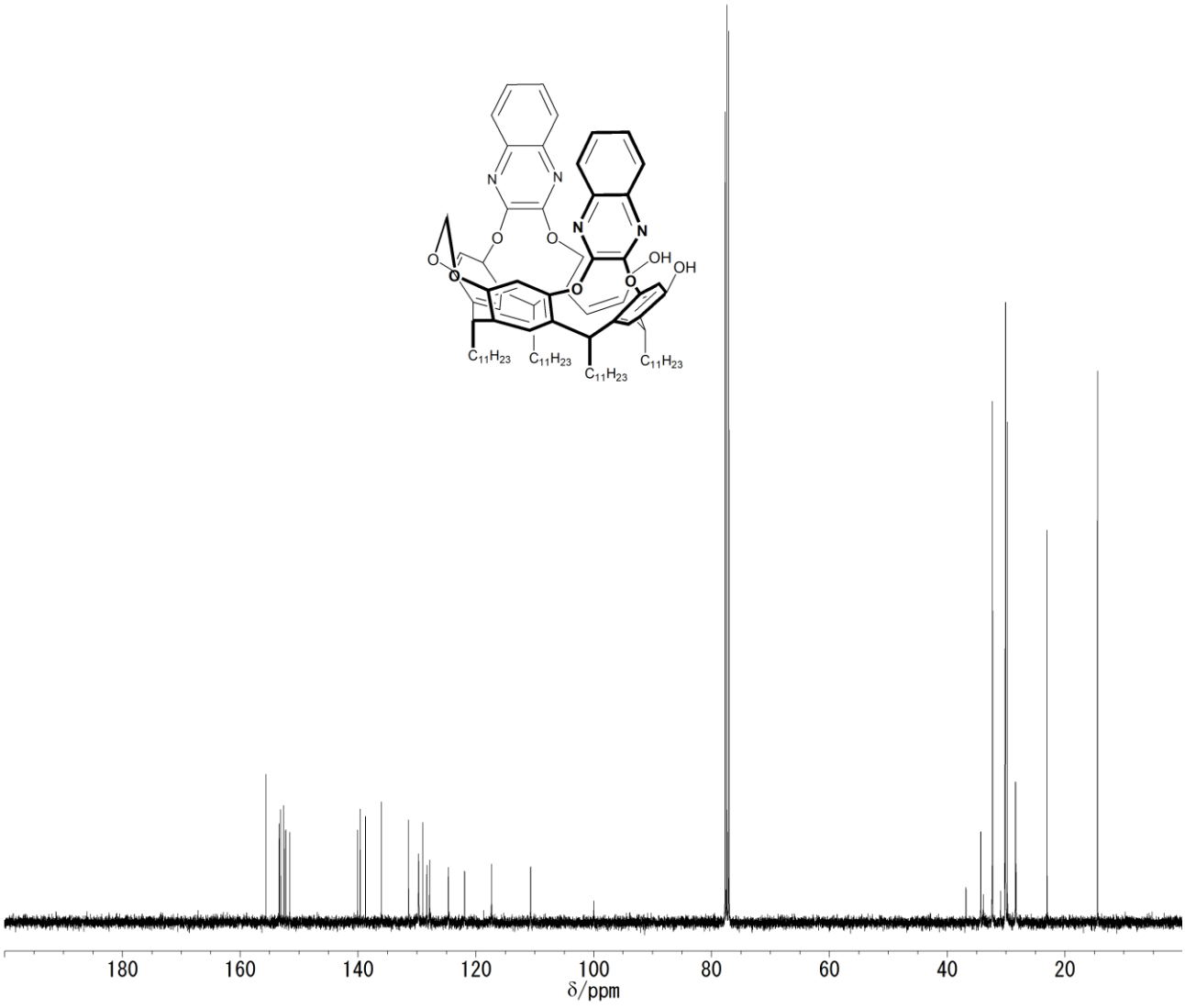


Compound **10** (^{13}C NMR spectrum in $CDCl_3$)



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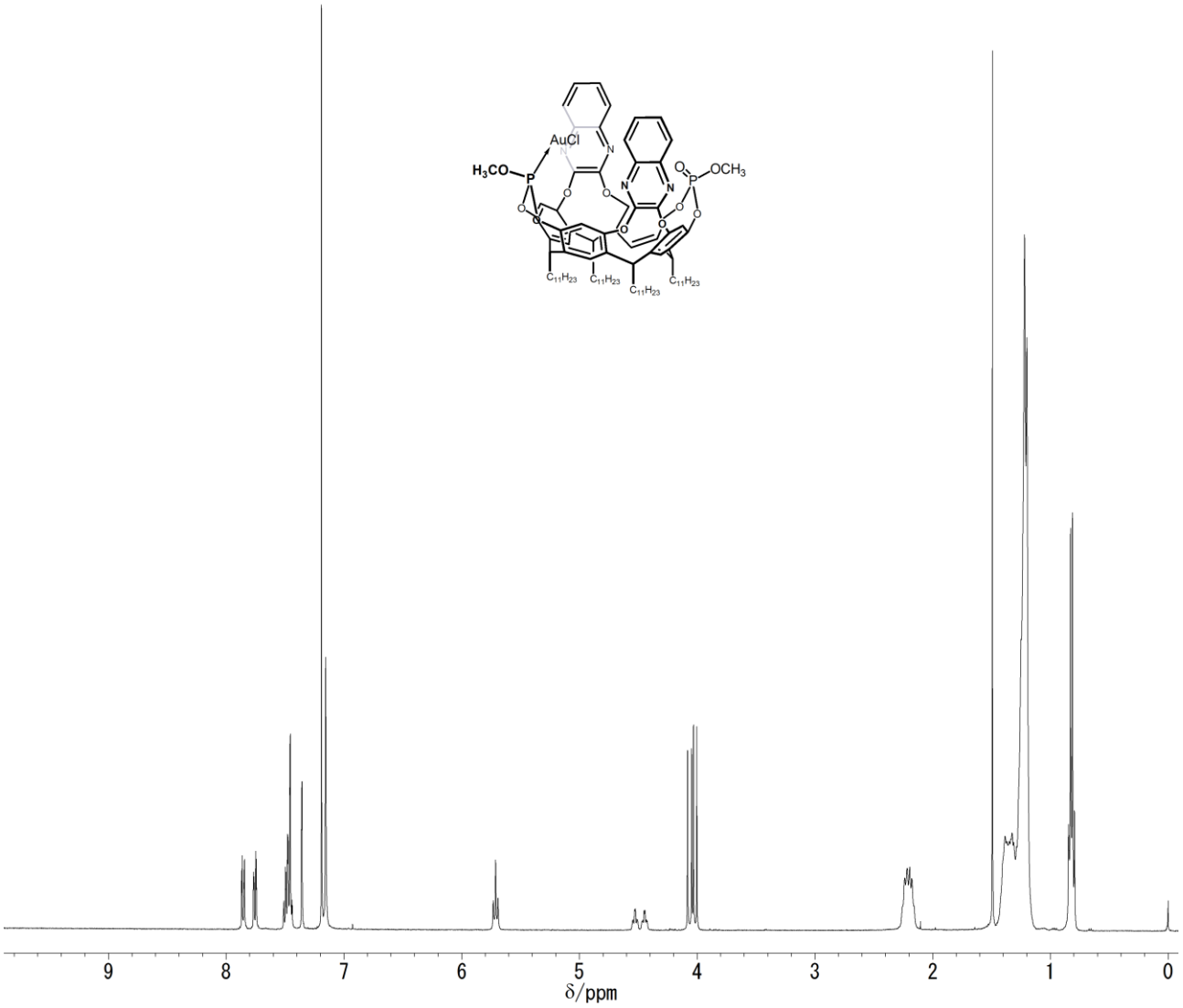

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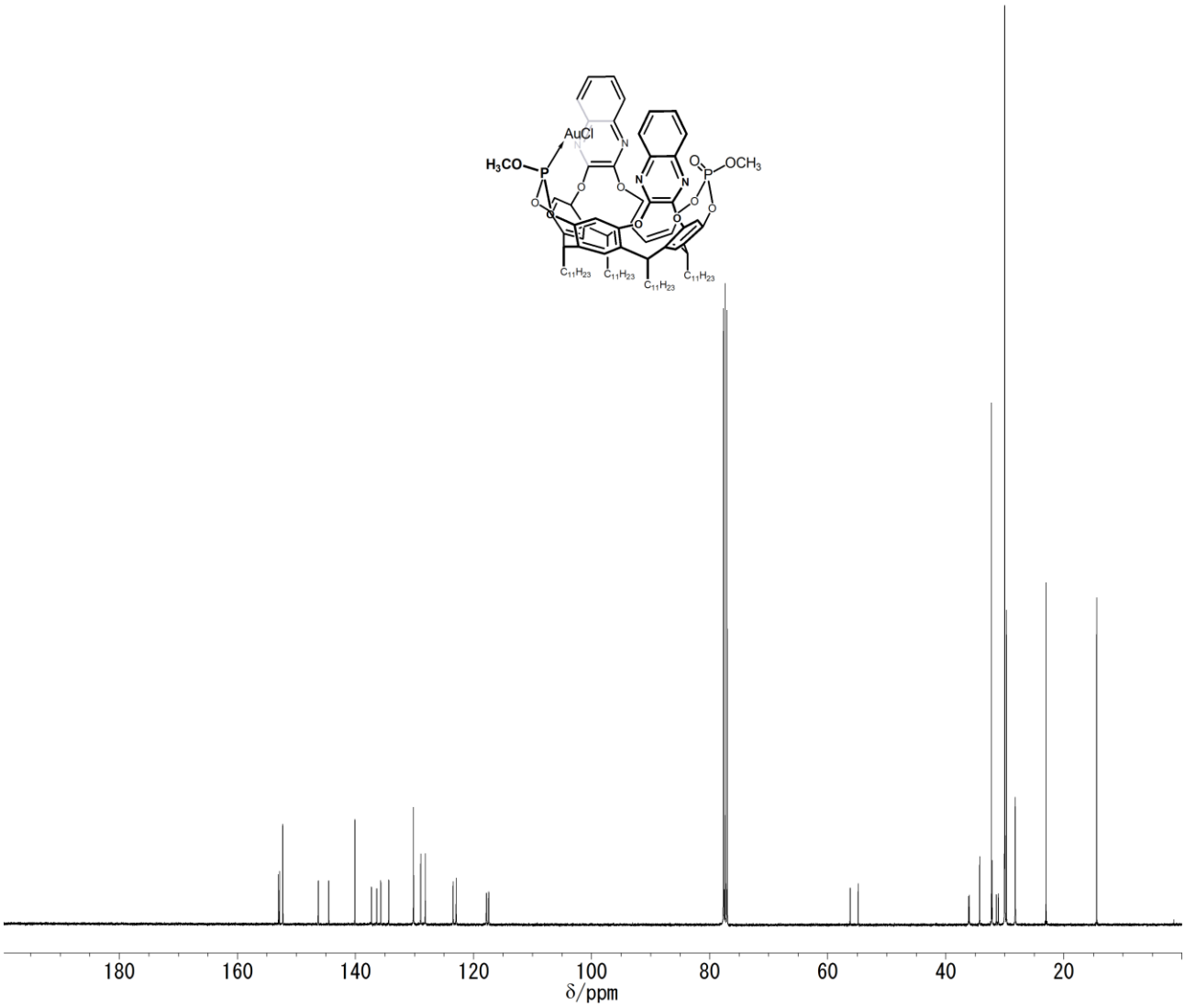

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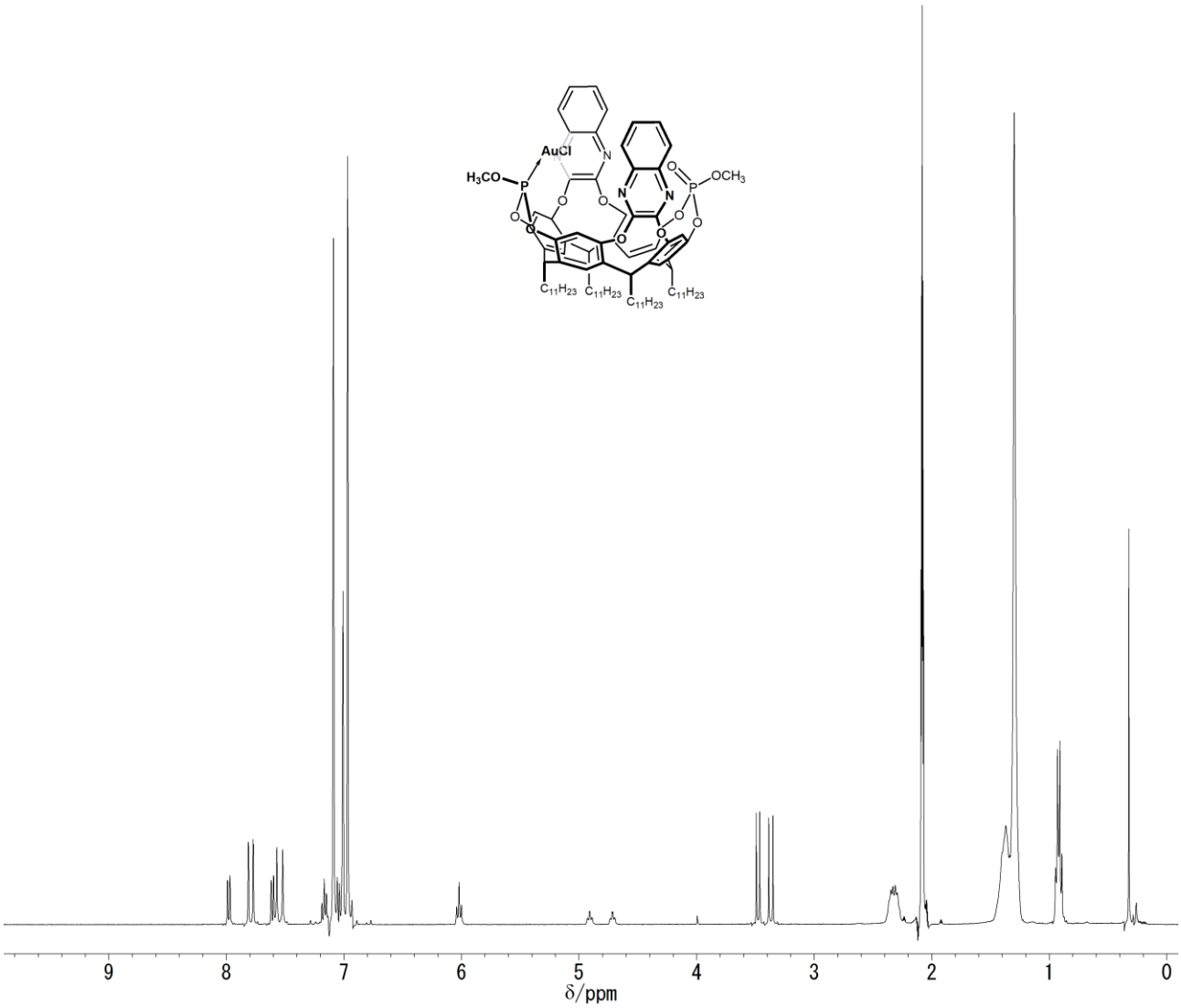

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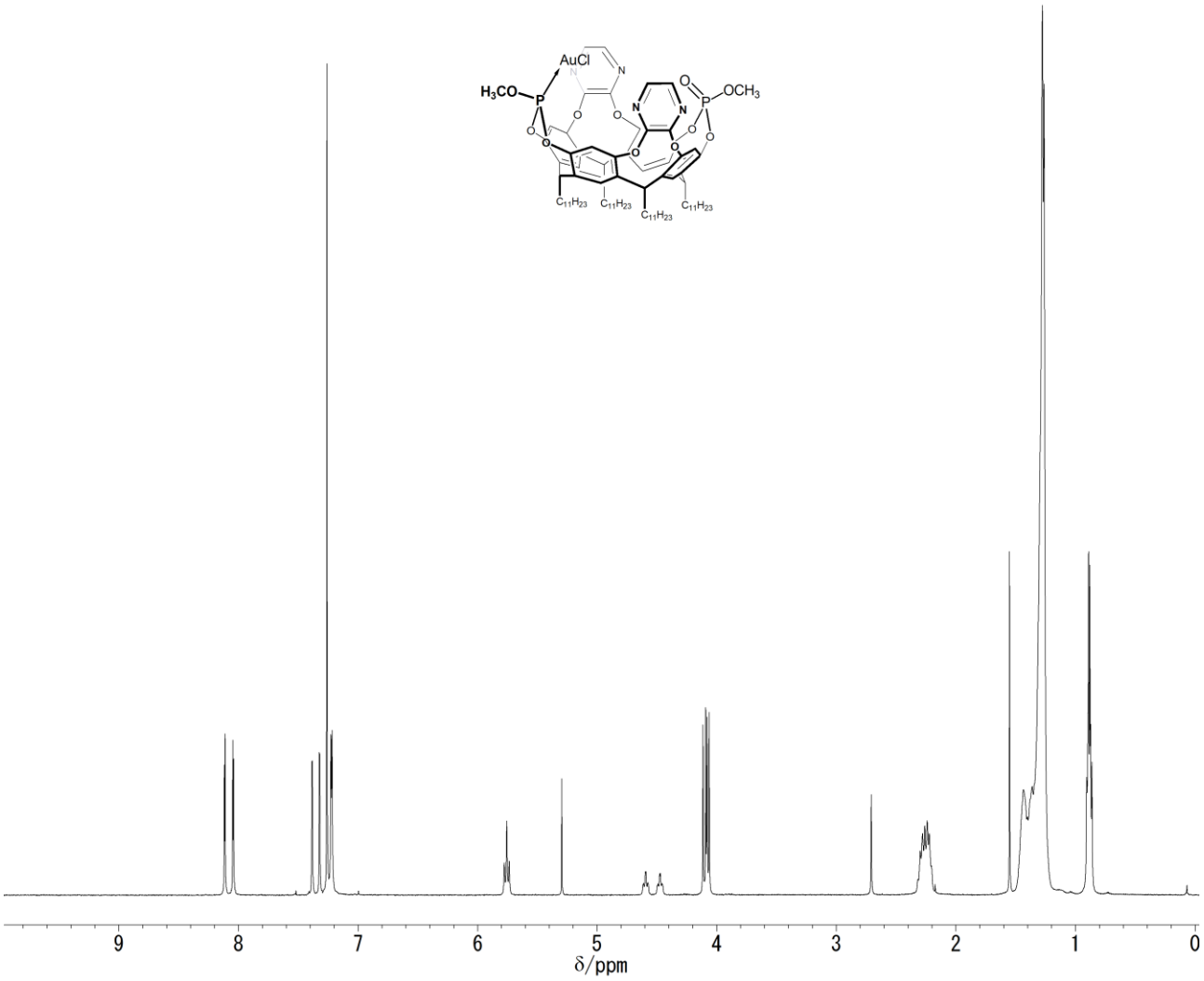

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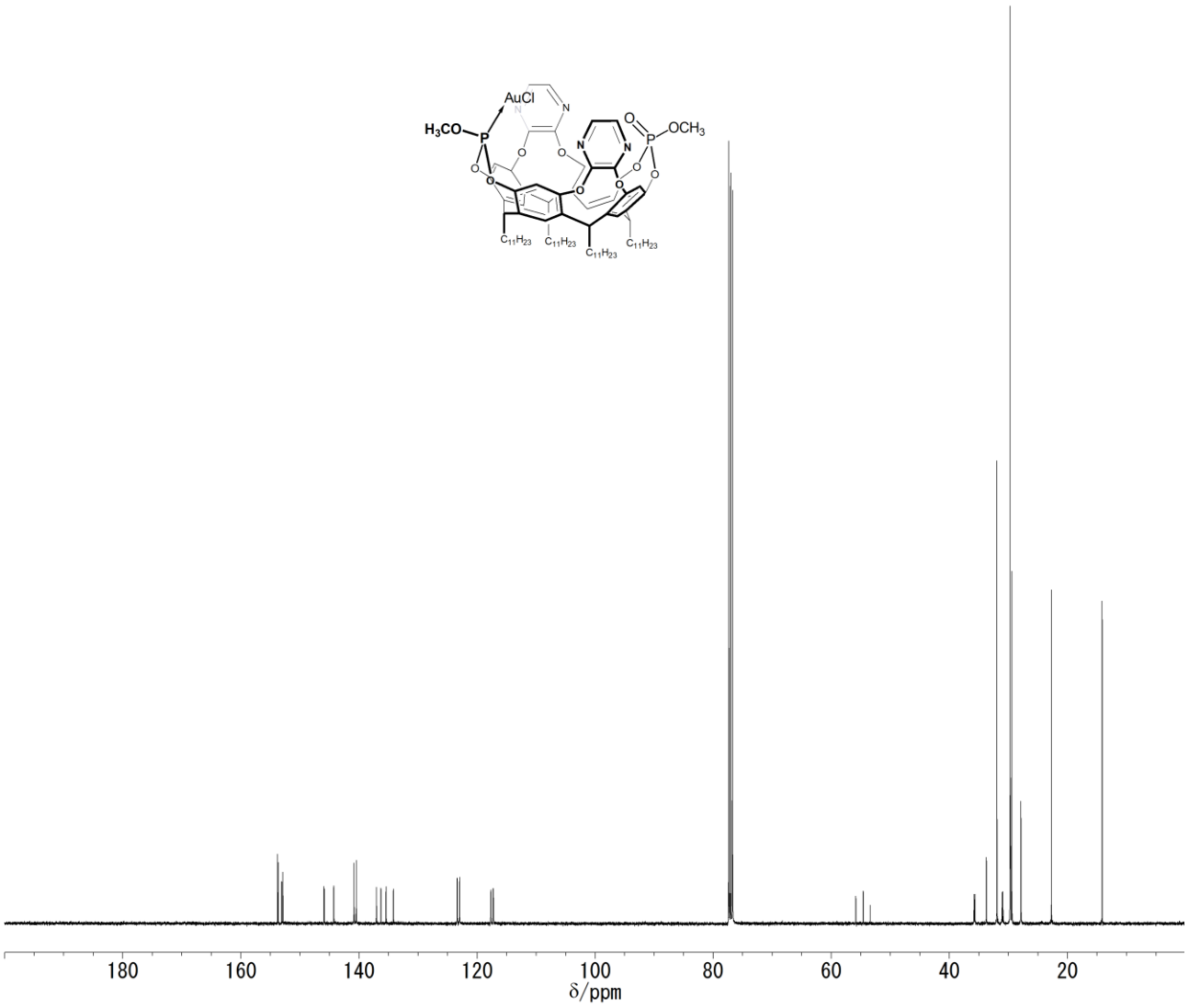

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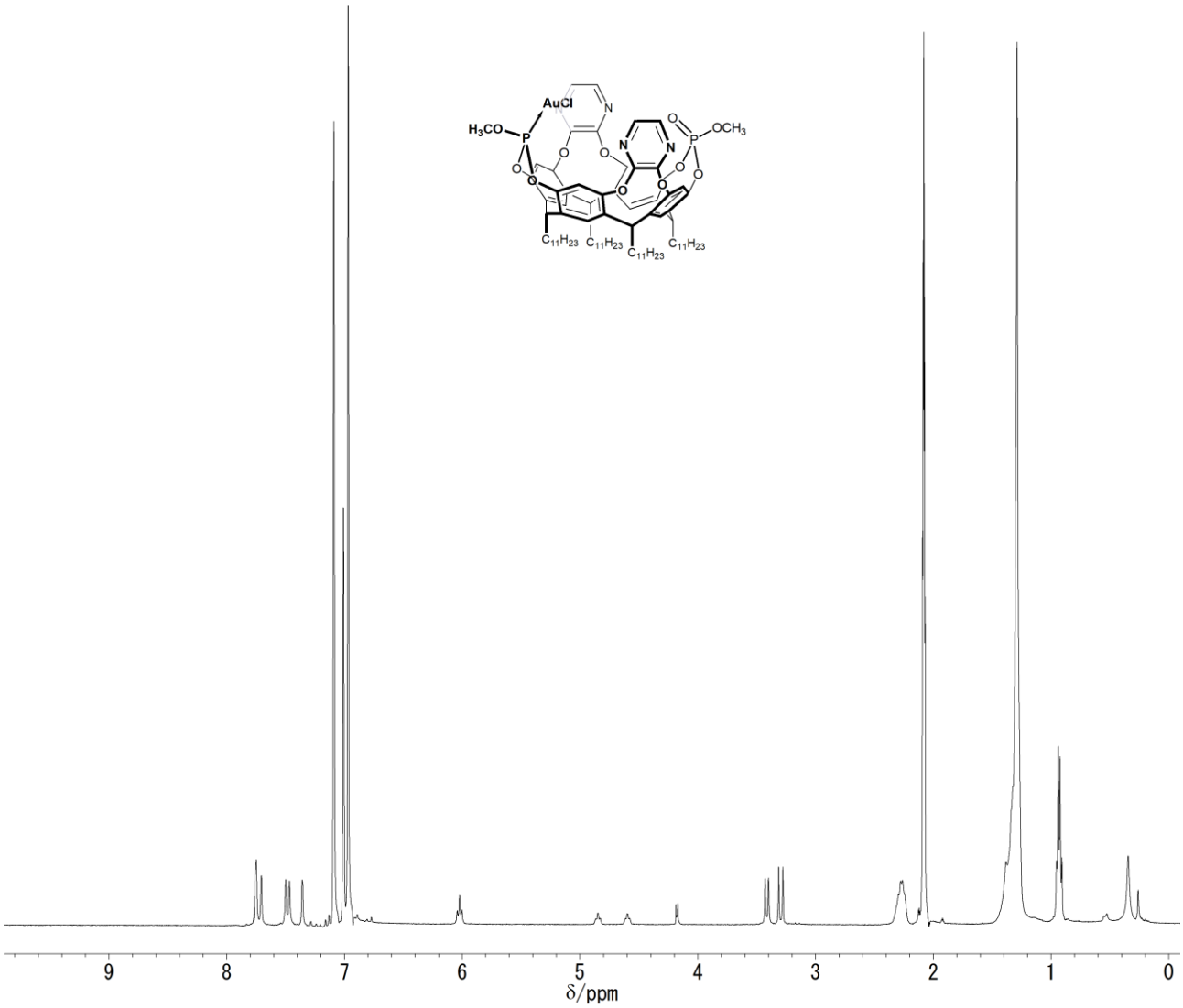
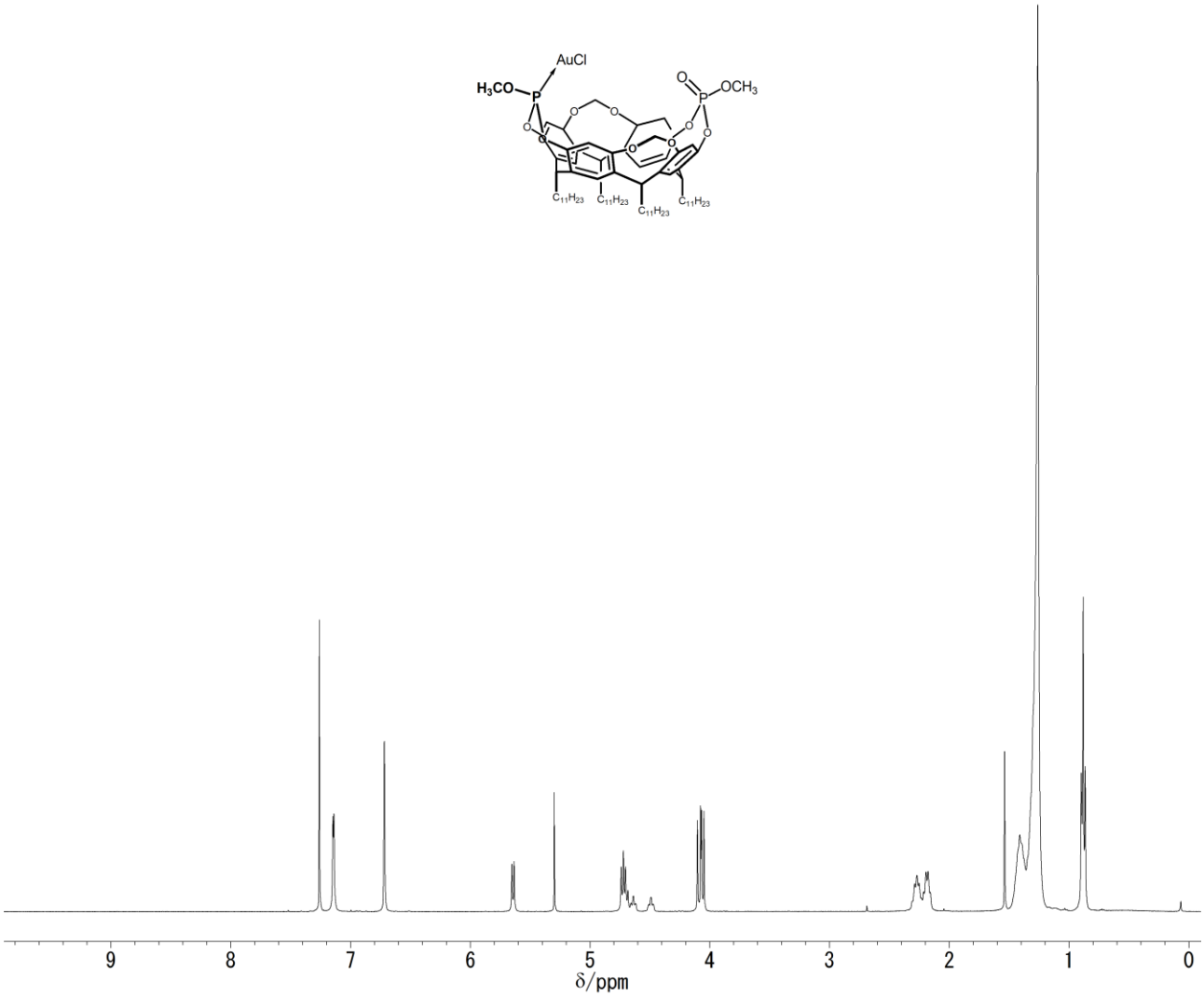
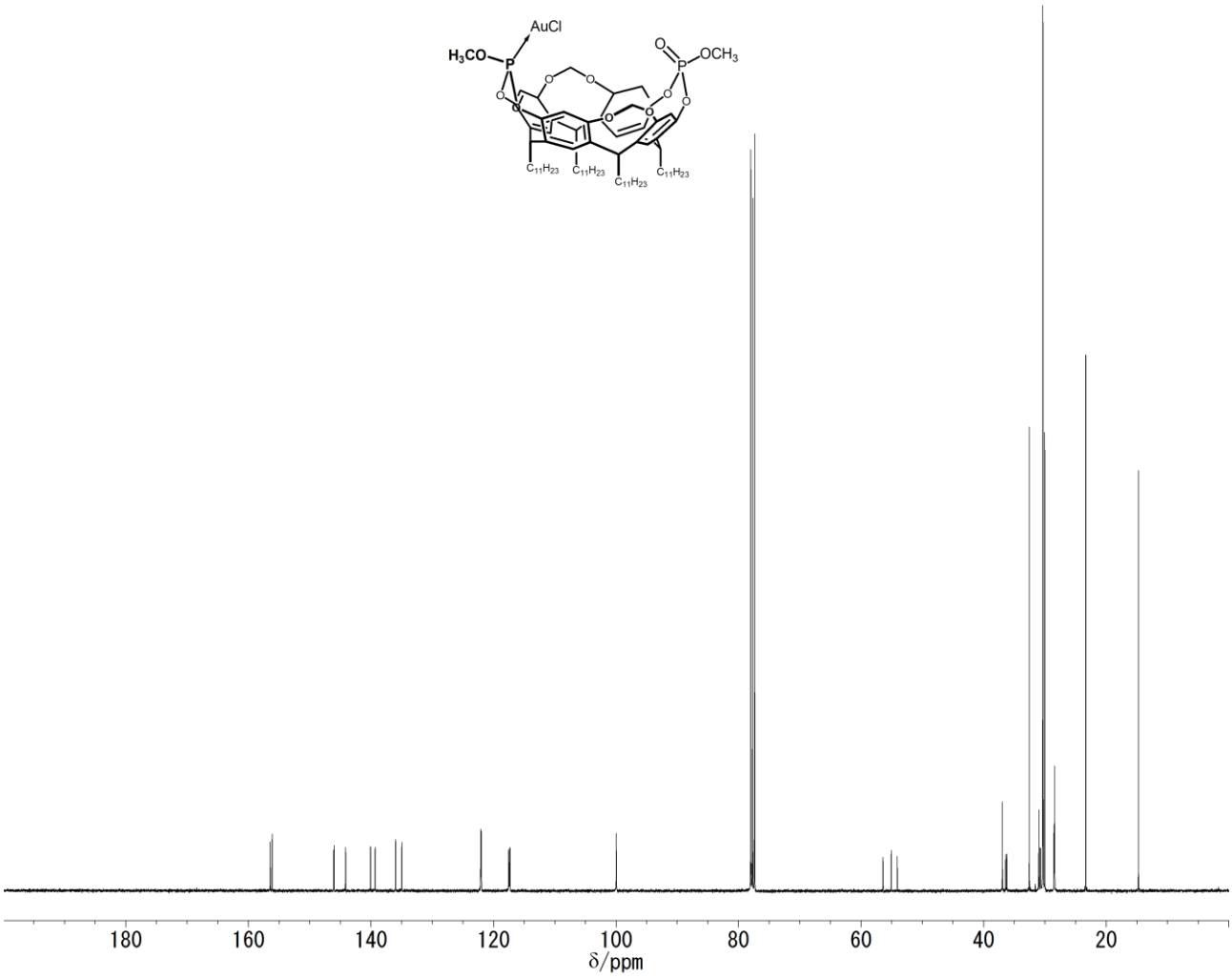


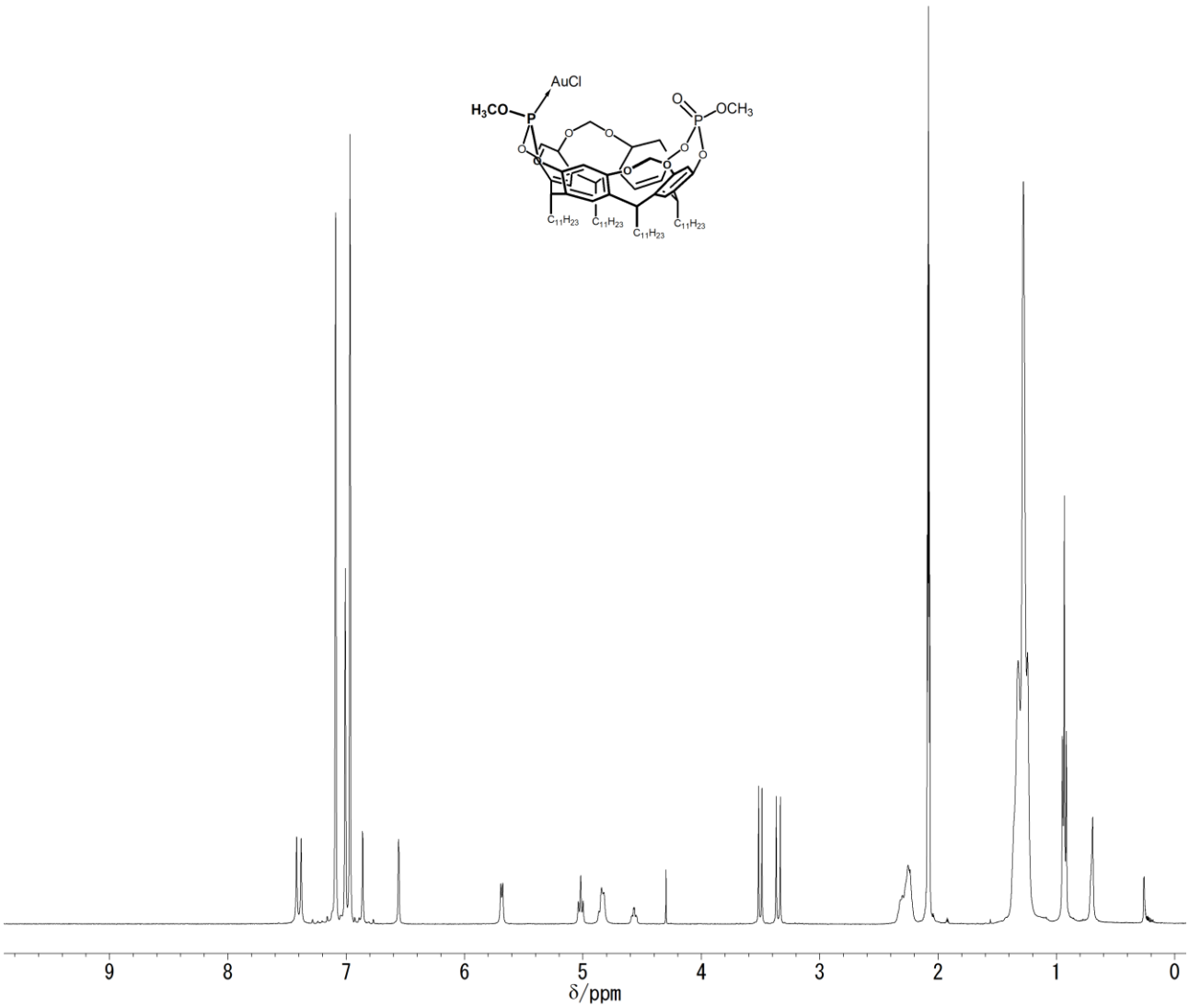
Compound **6**•AuCl (^{1}H NMR spectrum in $CDCl_3$)



Compound **6**•AuCl (^{13}C NMR spectrum in $CDCl_3$)



Compound **6**•AuCl (^{1}H NMR spectrum in [D8]toluene)



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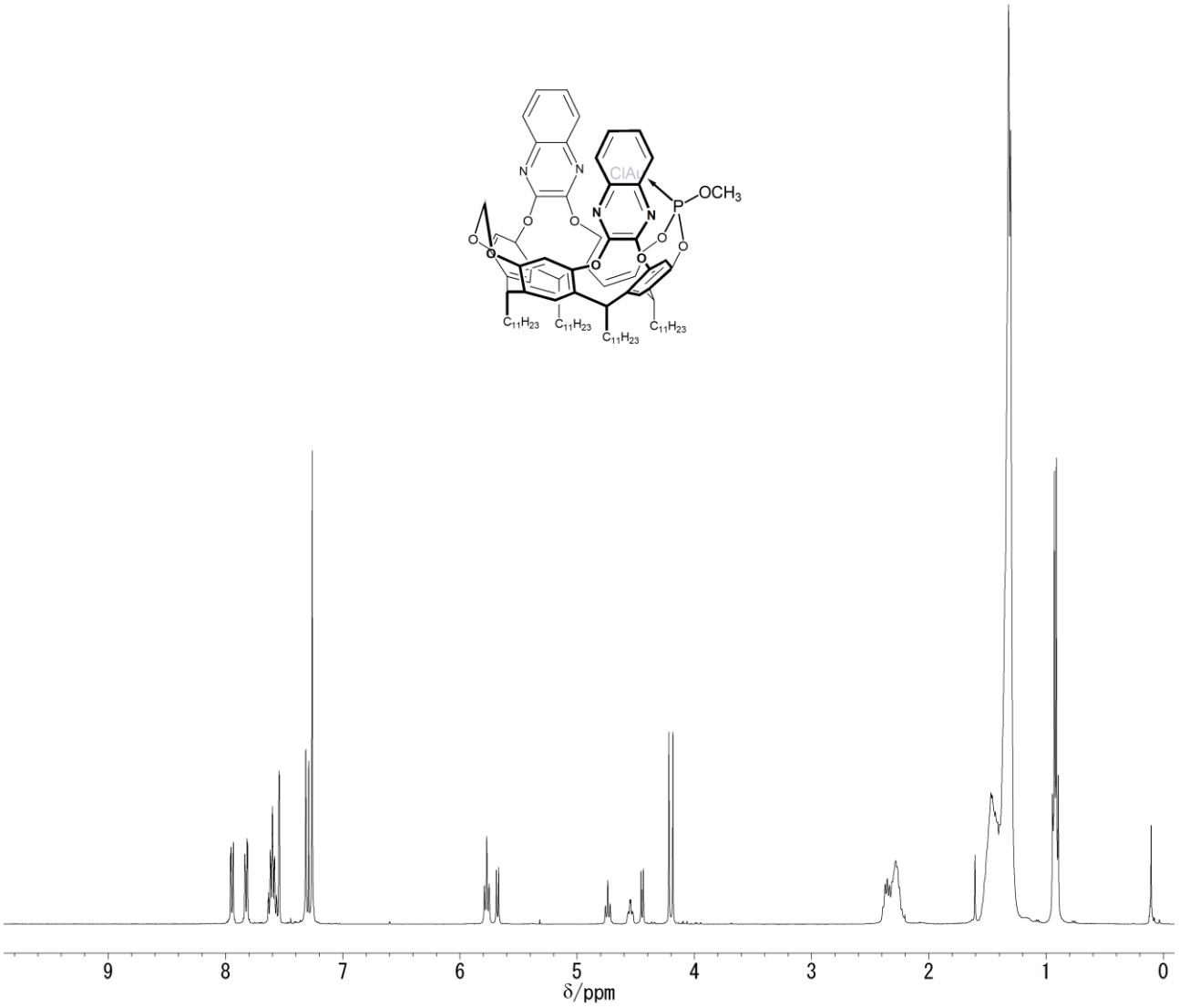

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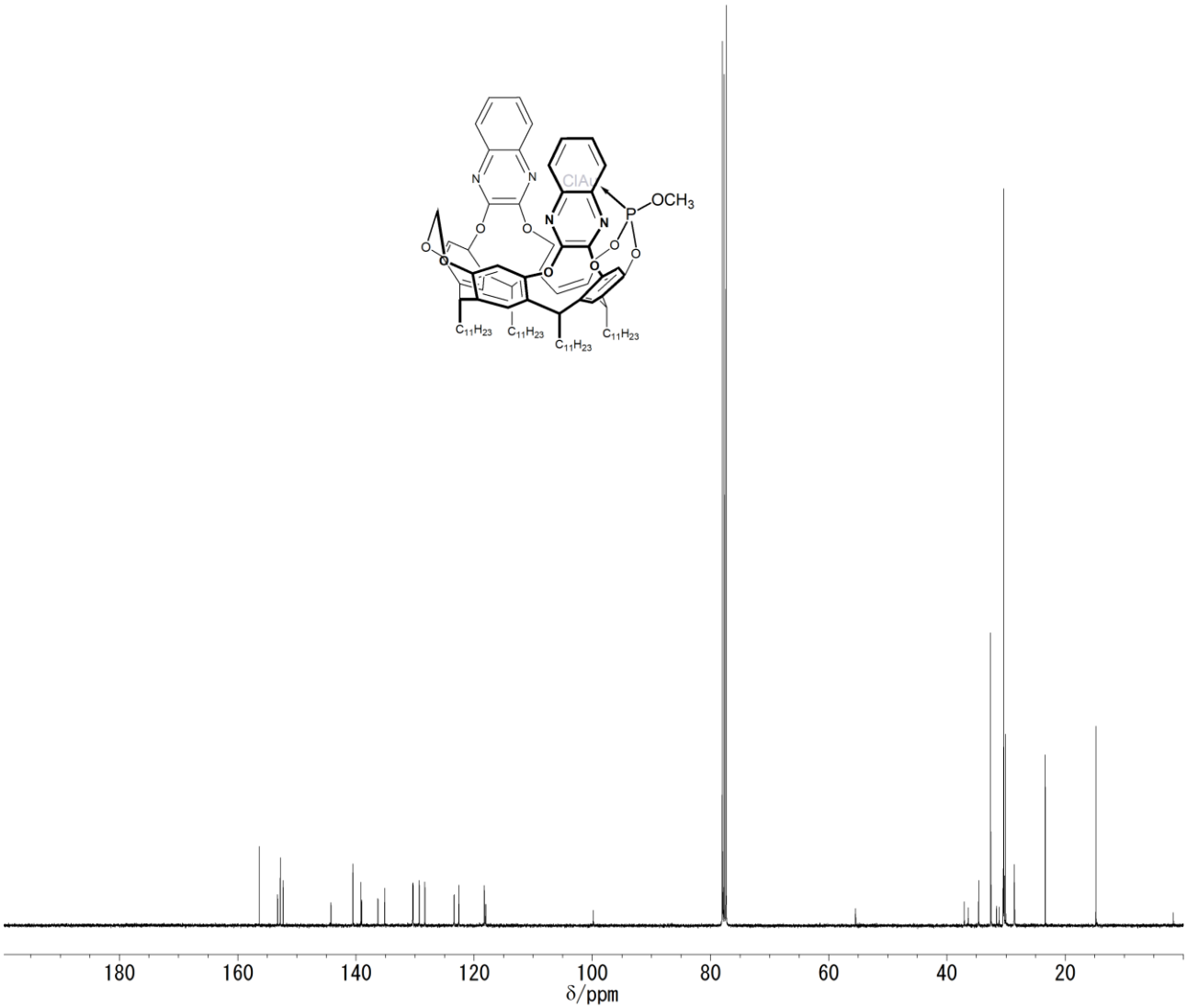

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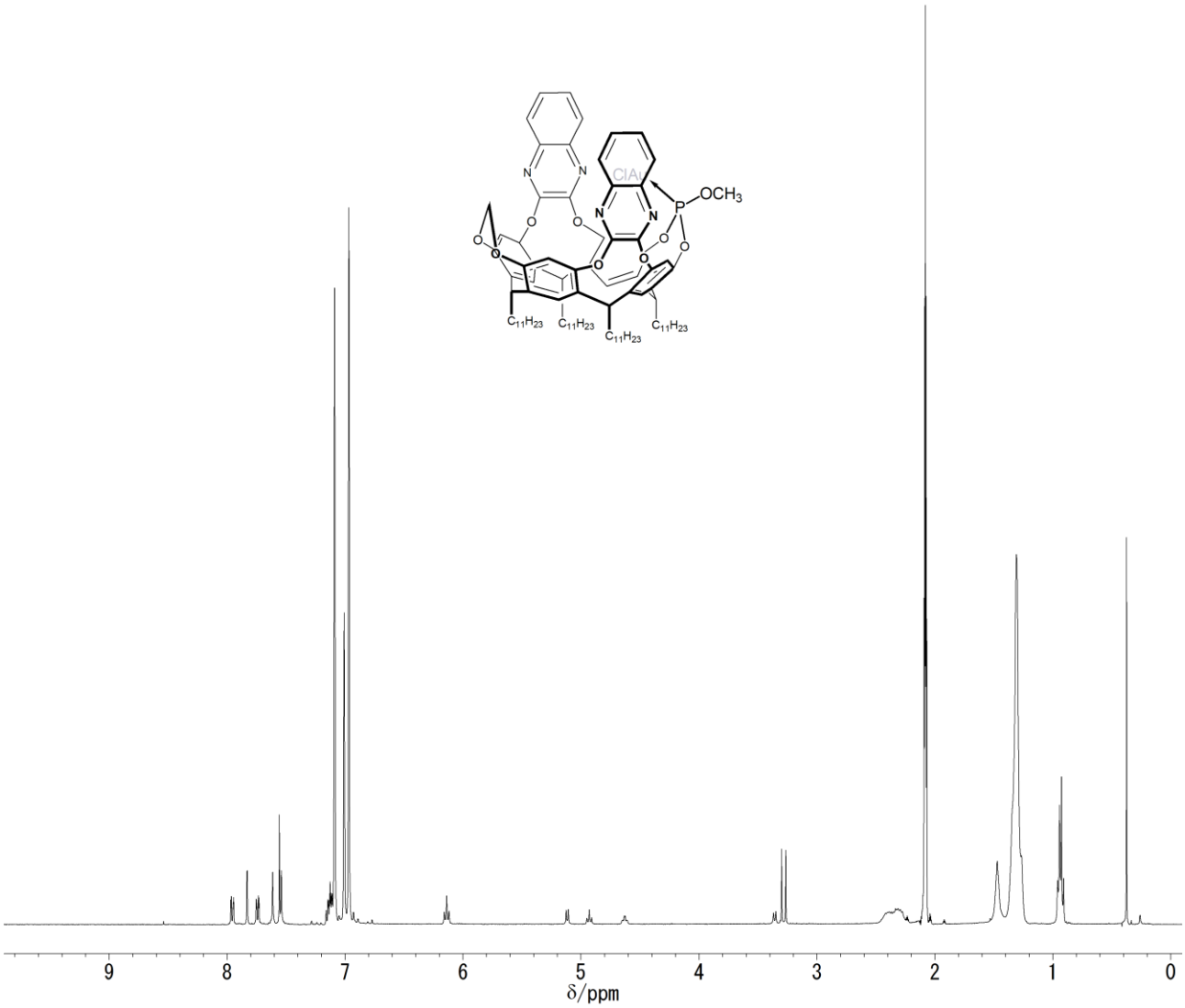

2) The stack of ^{1}H NMR spectra (Figure 1S) for representative procedure of hydration reactions of 2-octyne **7d** (Table 2, entry 14), in which [D_8]toluene was used.

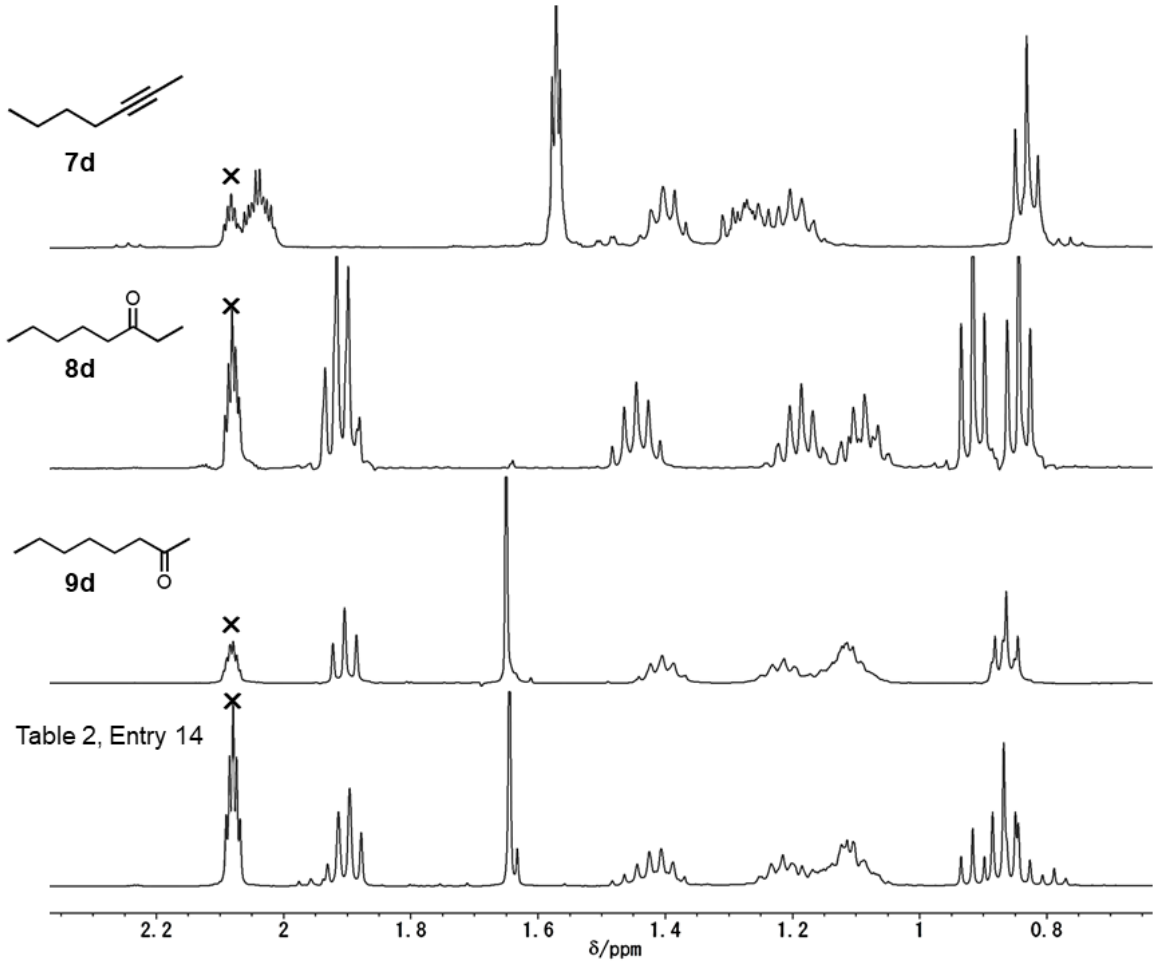

Figure S1. Portions of ^{1}H NMR spectra (400 MHz, toluene-d_8) for determination of NMR yields in Table 2, entry 14; the top, 2-octyne **7d**; and the second and third from the top, the commercially available authentic samples of 3-octanone **8d** and 2-octanone **9d**; the bottom, the resultant product of **8d** (12%) and **9d** (88%).

3) The data of HRMS (ESI) for **2**•AuCl.

==== Shimadzu LCMSsolution 分析レポート ====

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分析日時 : 2018/05/23 18:39:41

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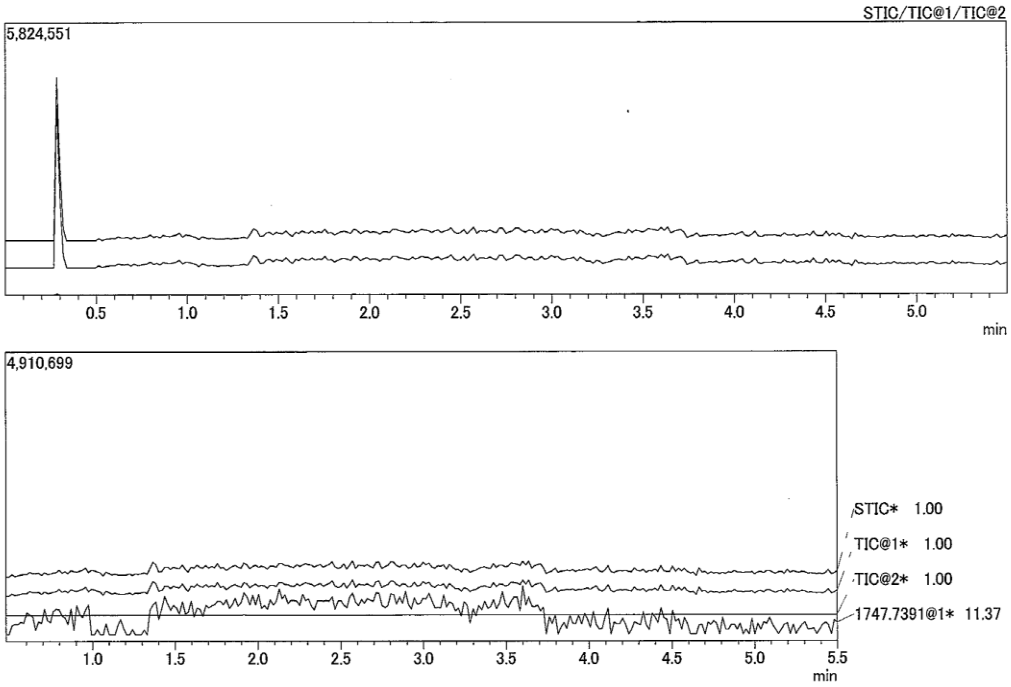

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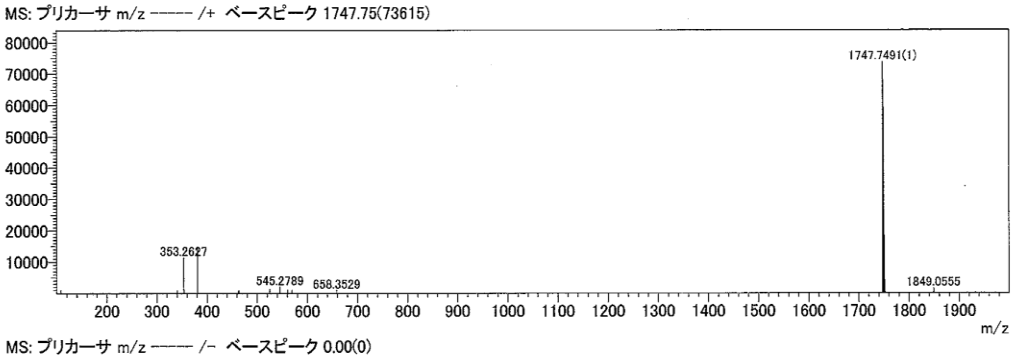

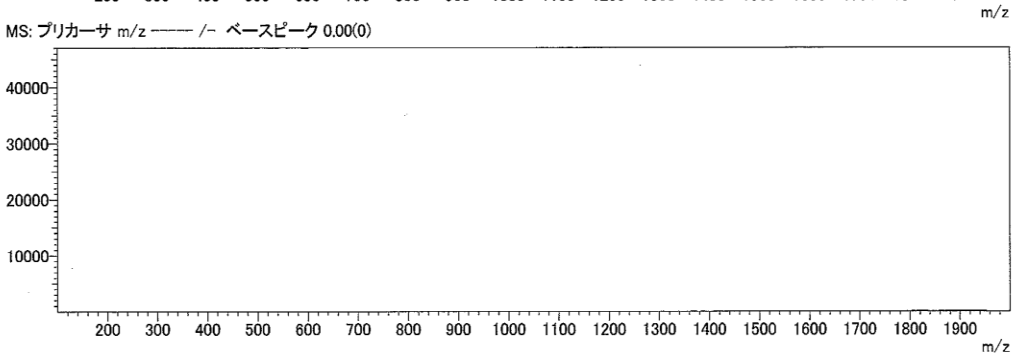

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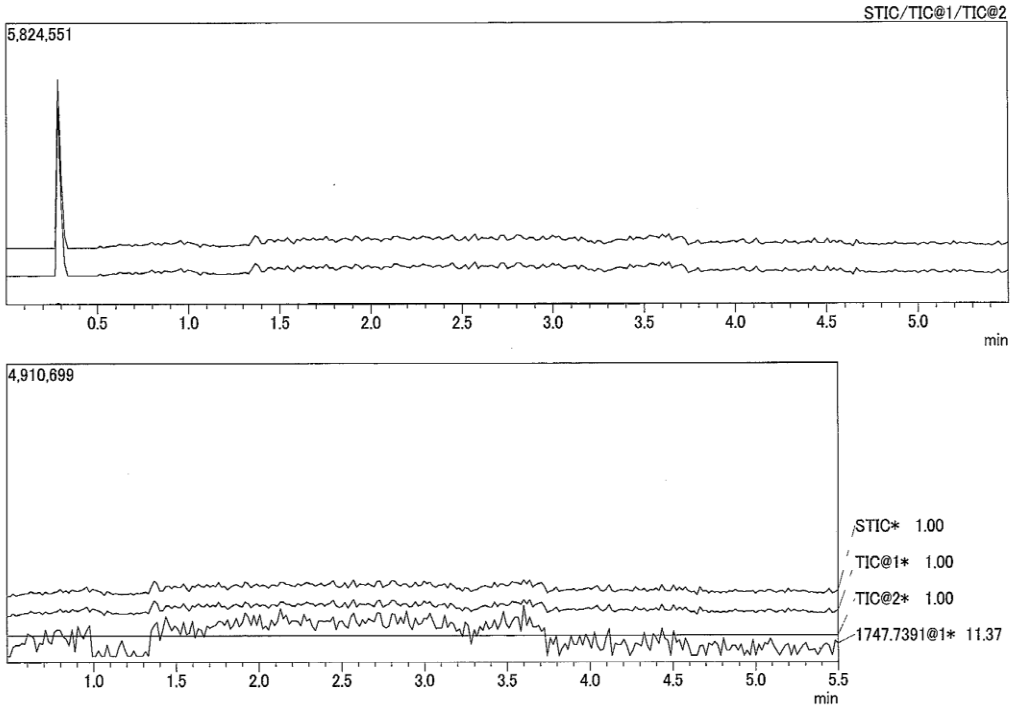

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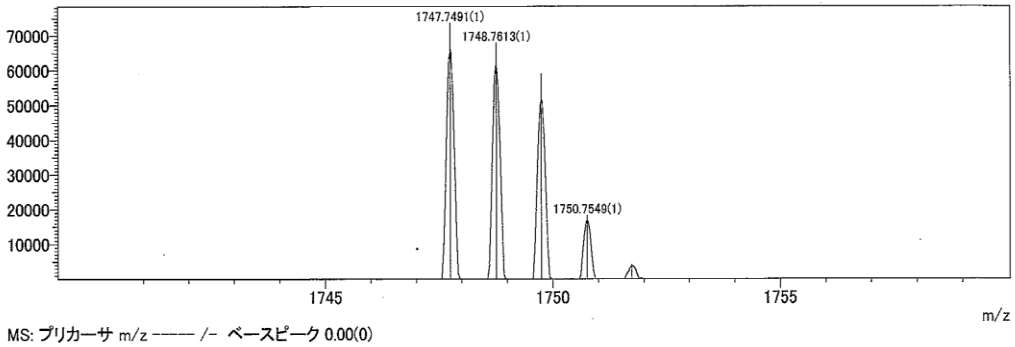

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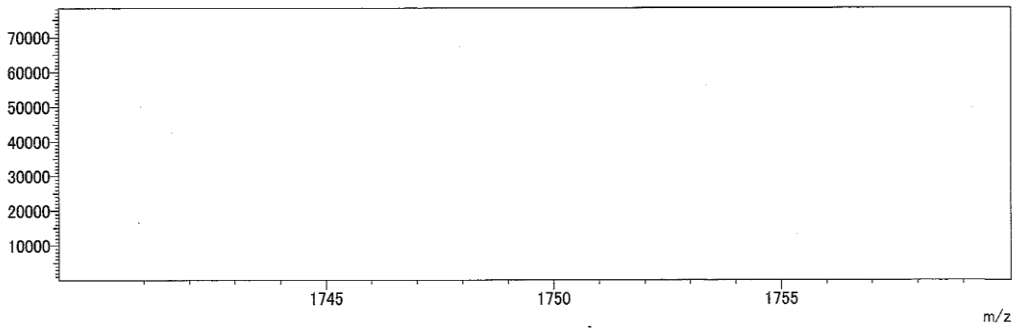

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