

# **Supporting Information**

**for**

## **Structural conditions required for the bridge**

## **lithiation and substitution of a basic calix[4]arene**

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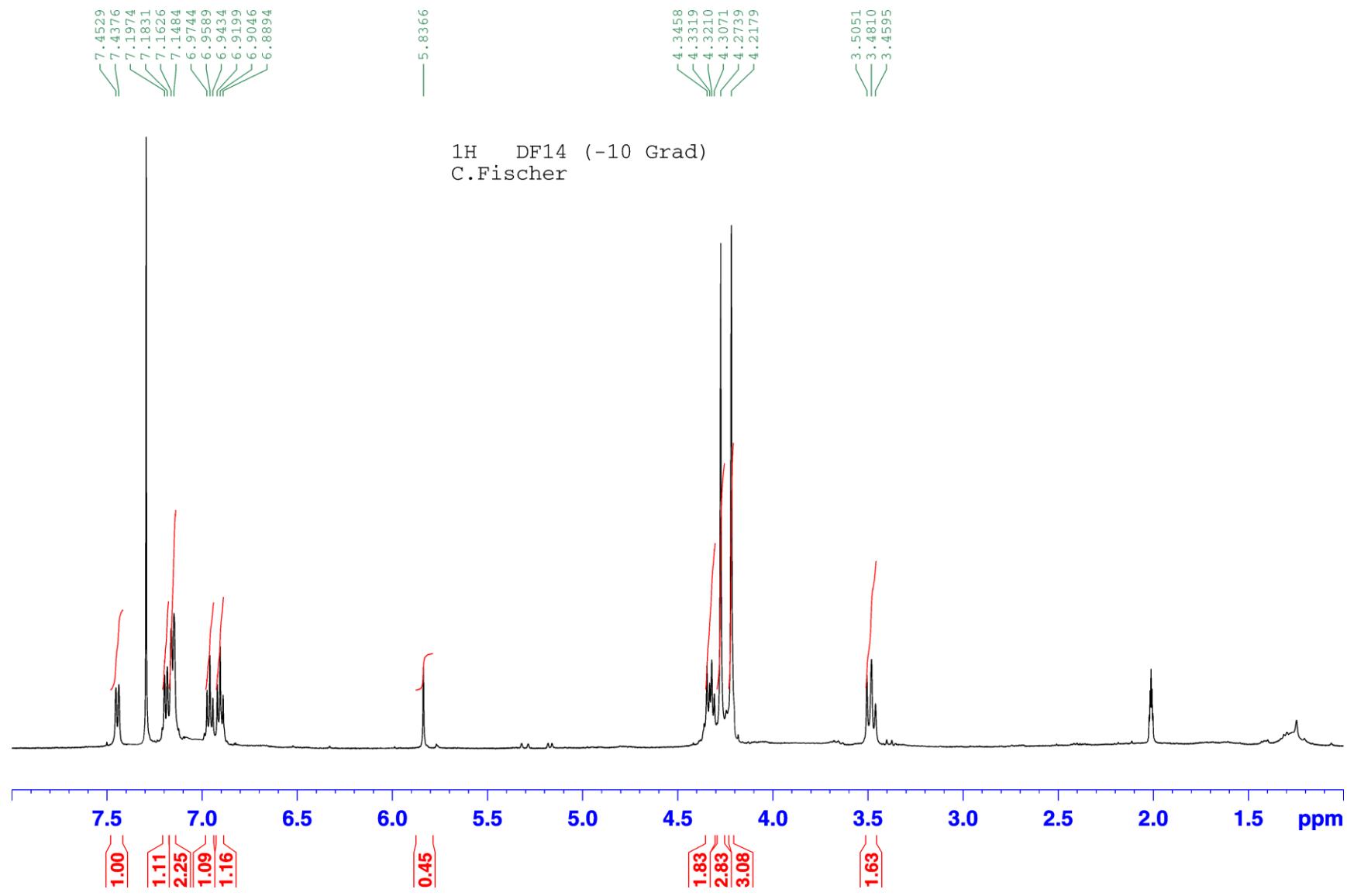
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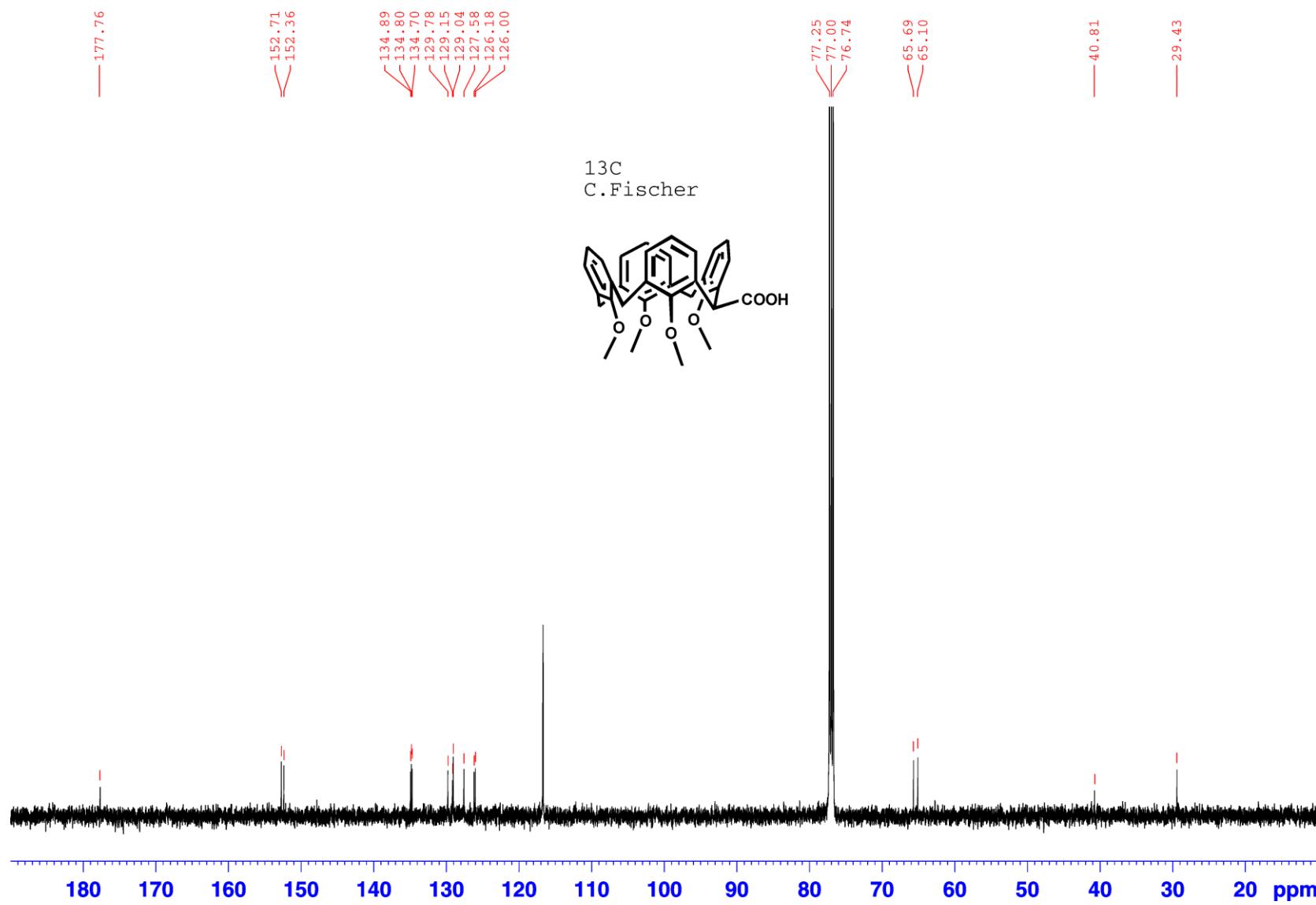
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### **<sup>1</sup>H NMR and <sup>13</sup>C NMR spectra of compounds 5, 11–14 and crystal packing illustration of mixed ether 12.**

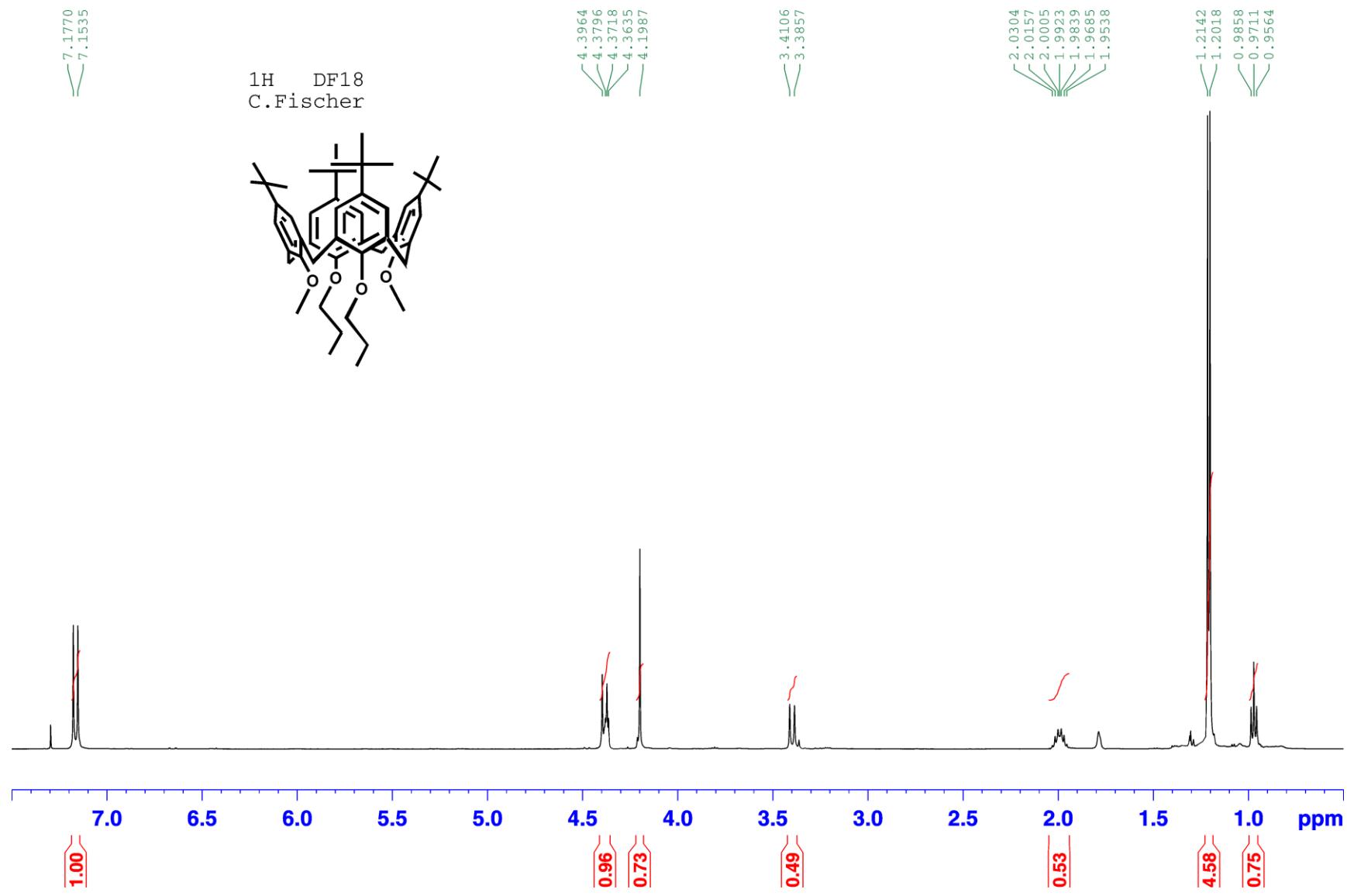
<sup>1</sup> H NMR and <sup>13</sup> C NMR spectra of compounds 5, 11, 12, 13 and 14 .....	S2–S11
Crystal packing illustration of mixed ether 12 .....	S12



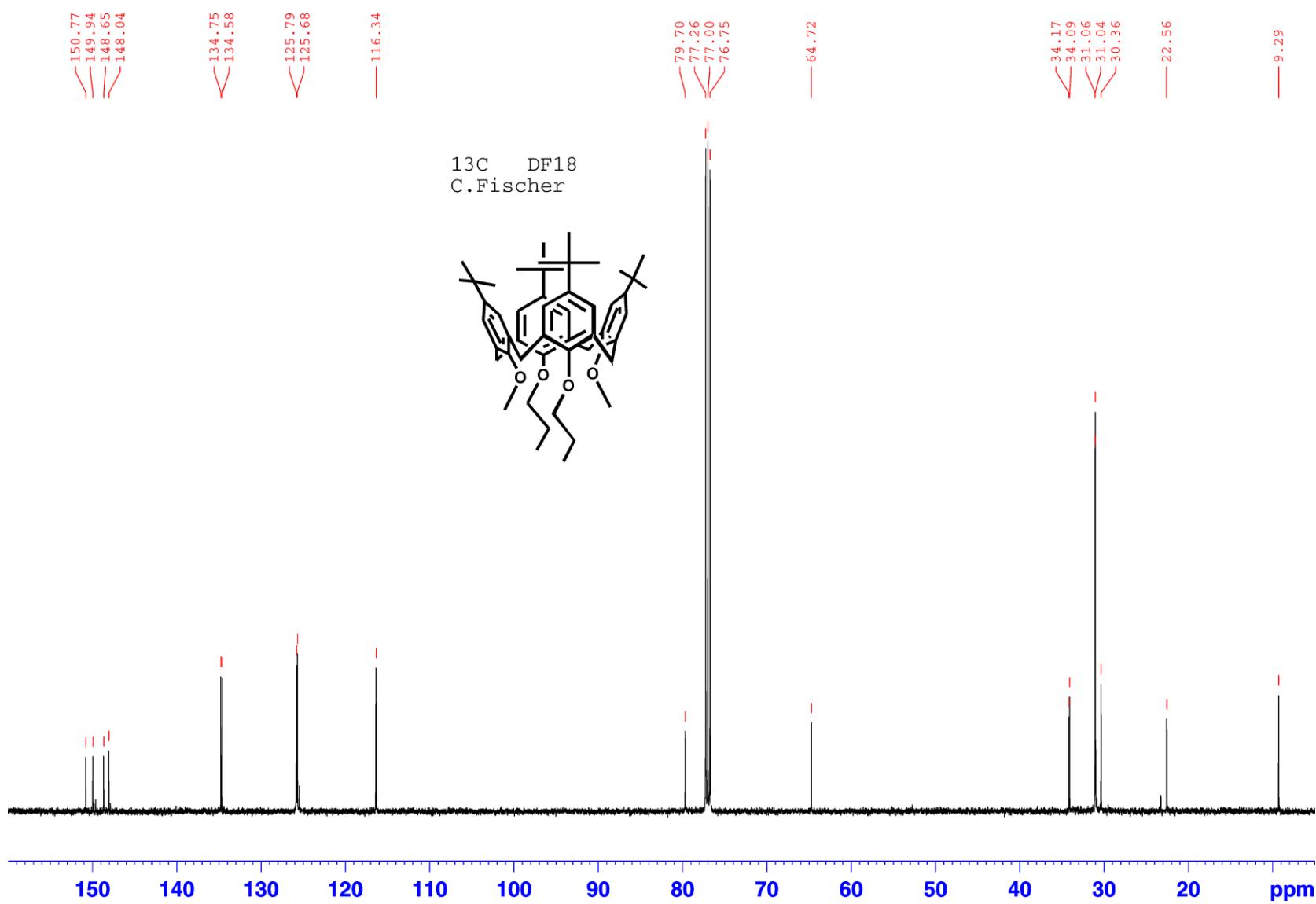
**Figure S1:**  $^1\text{H}$  NMR spectrum of **5** in  $\text{CDCl}_3$  (incl. NaI/acetonitrile- $d_3$ ) at 263 K.



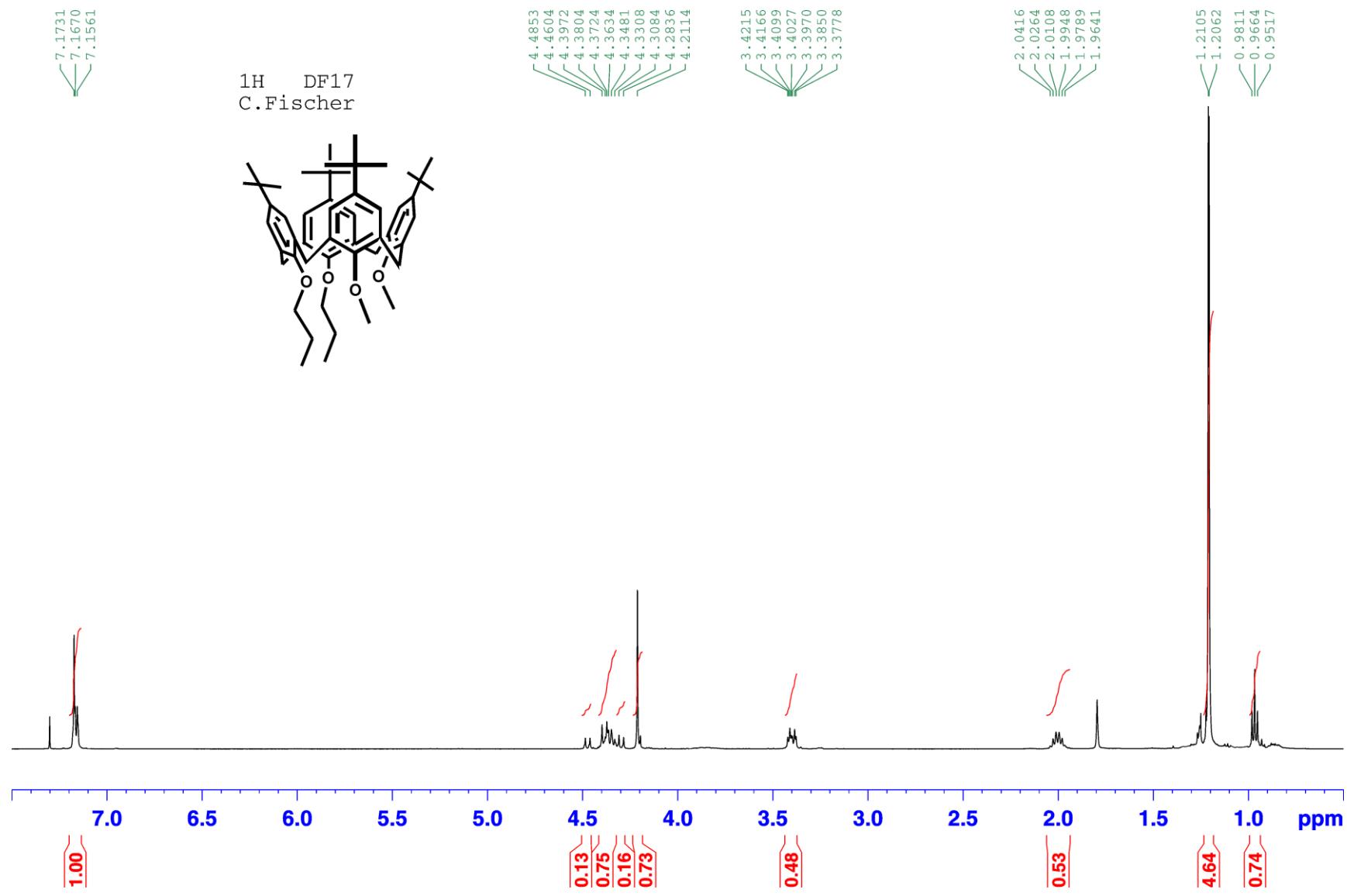
**Figure S2:**  $^{13}\text{C}$  NMR spectrum of **5** in  $\text{CDCl}_3$  (incl. NaI/acetonitrile- $d_3$ ) at 263 K.



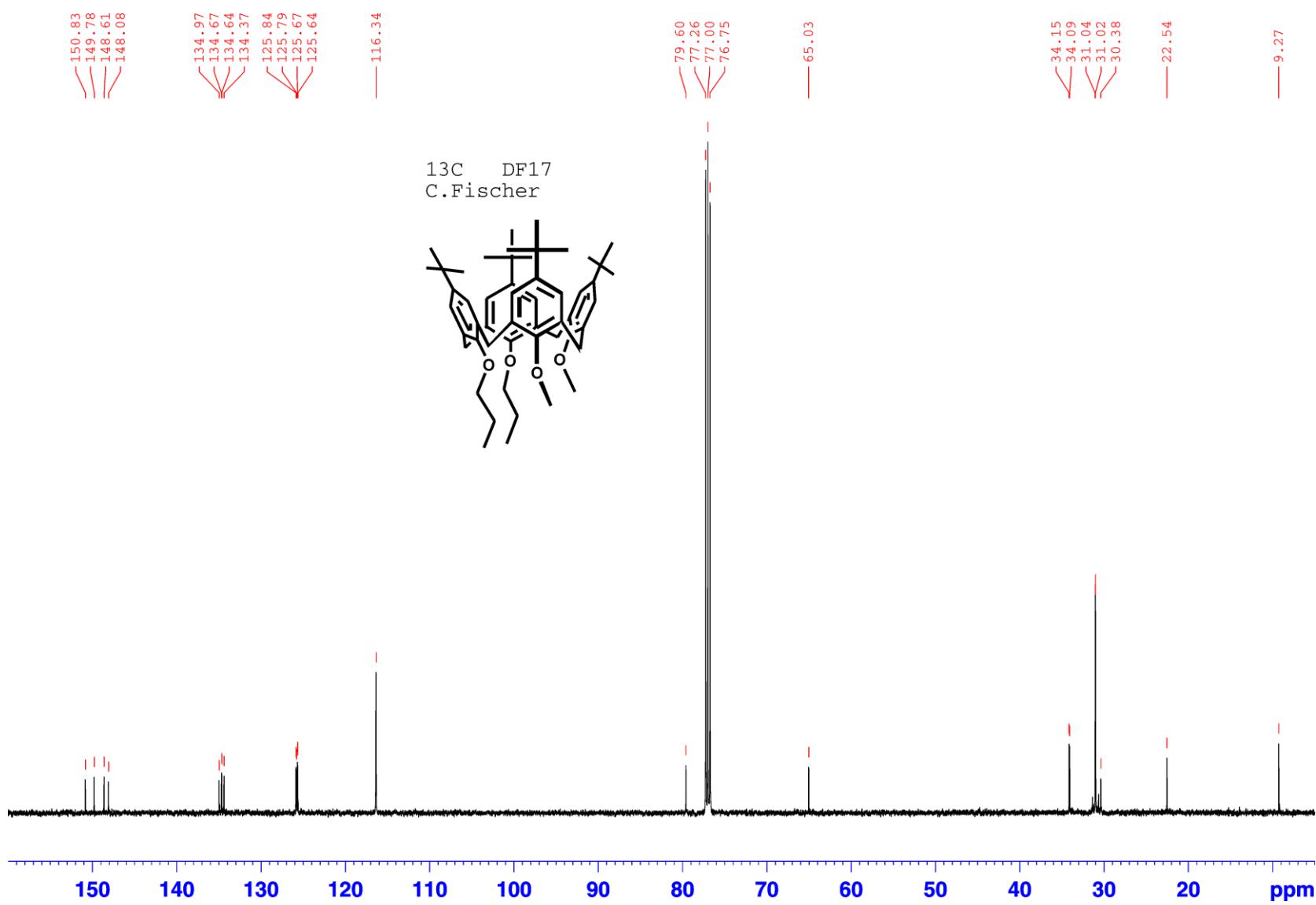
**Figure S3:**  $^1\text{H}$  NMR spectrum of **11** in  $\text{CDCl}_3$  (incl.  $\text{NaI}/\text{acetonitrile}-d_3$ ) at 293 K.



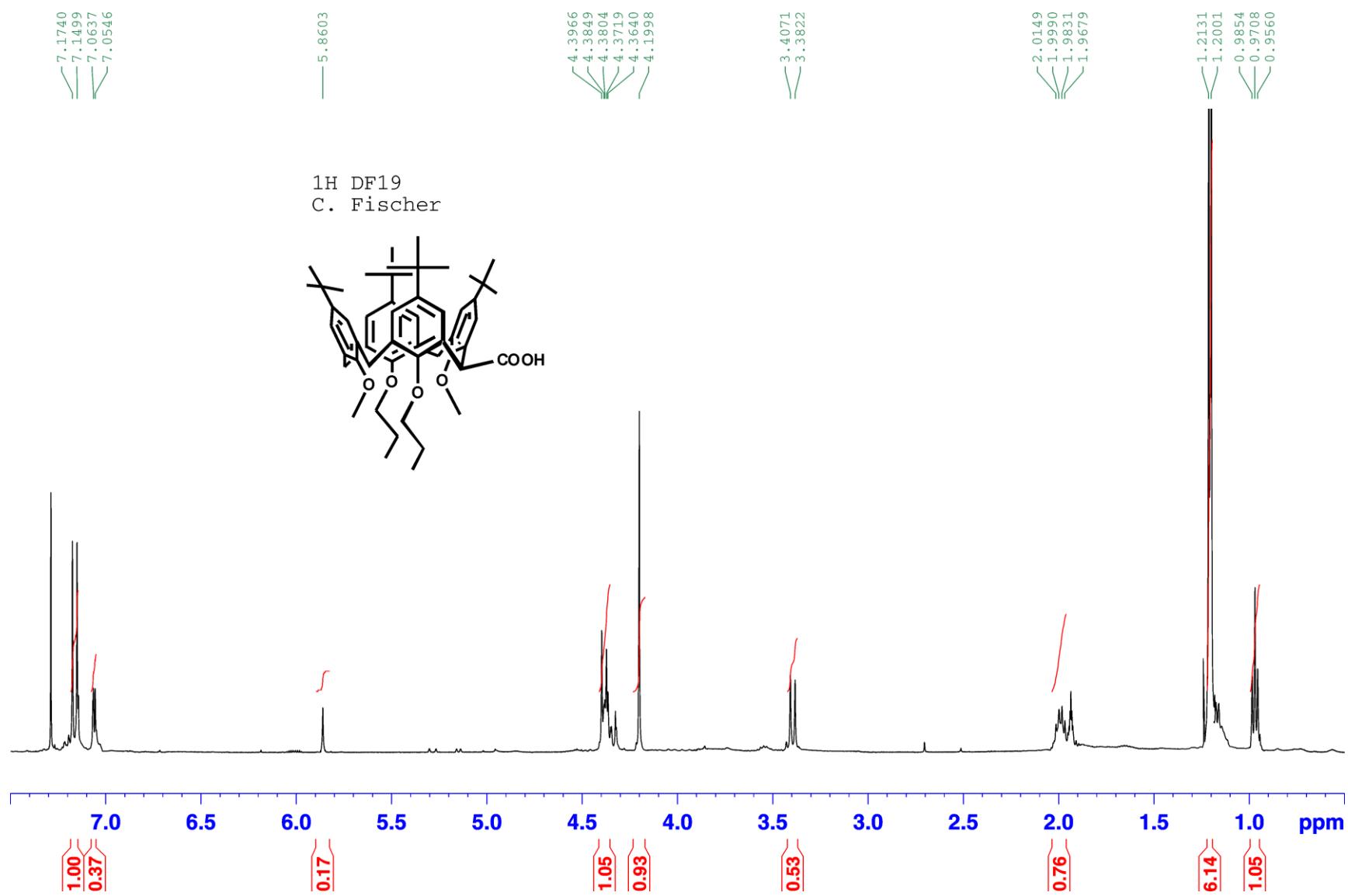
**Figure S4:** <sup>13</sup>C NMR spectrum of **11** in CDCl<sub>3</sub> (incl. NaI/acetonitrile-d<sub>3</sub>) at 293 K.



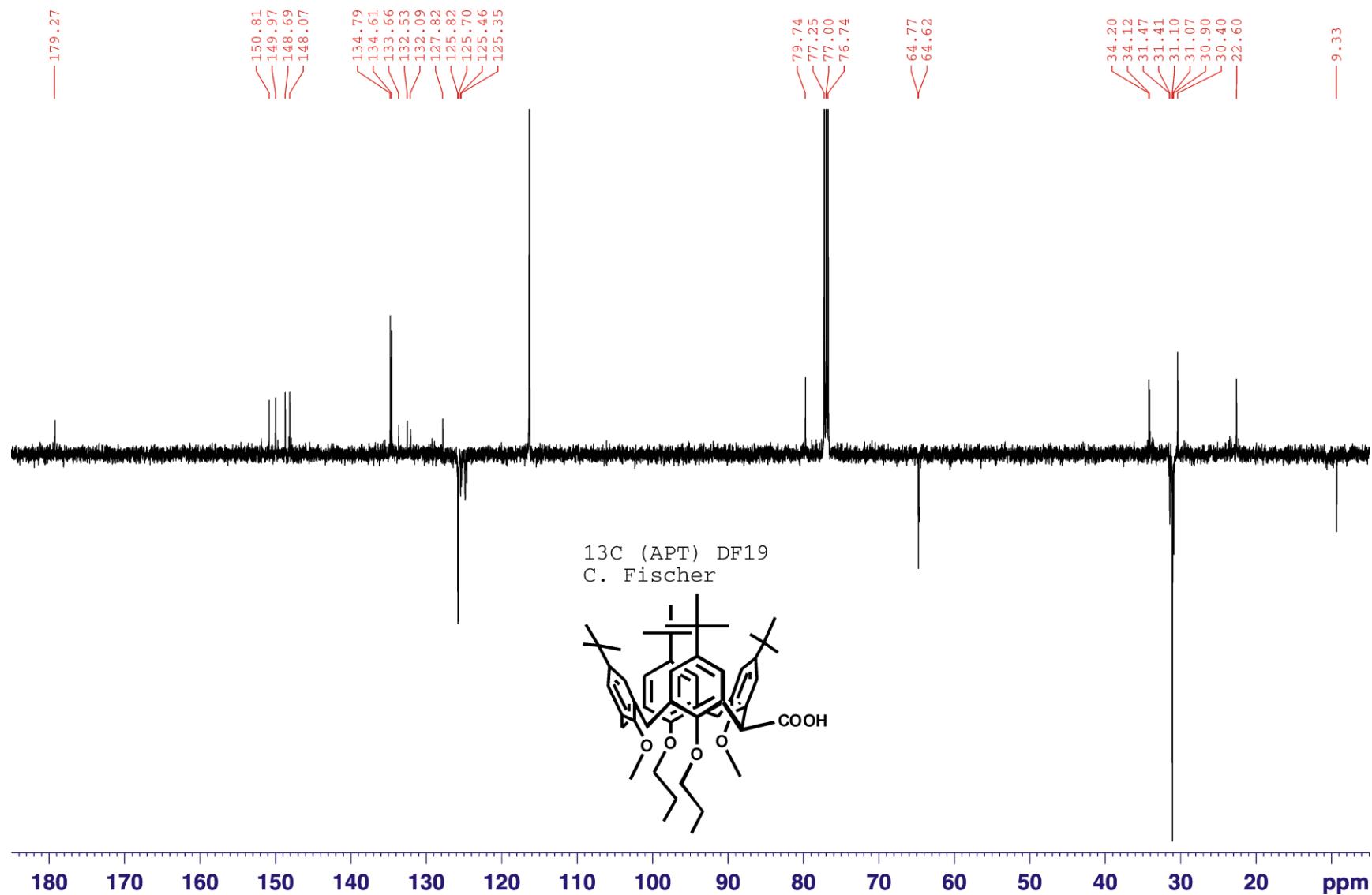
**Figure S5:** <sup>1</sup>H NMR spectrum of **12** in CDCl<sub>3</sub> (incl. NaI/acetonitrile-d<sub>3</sub>) at 293 K.



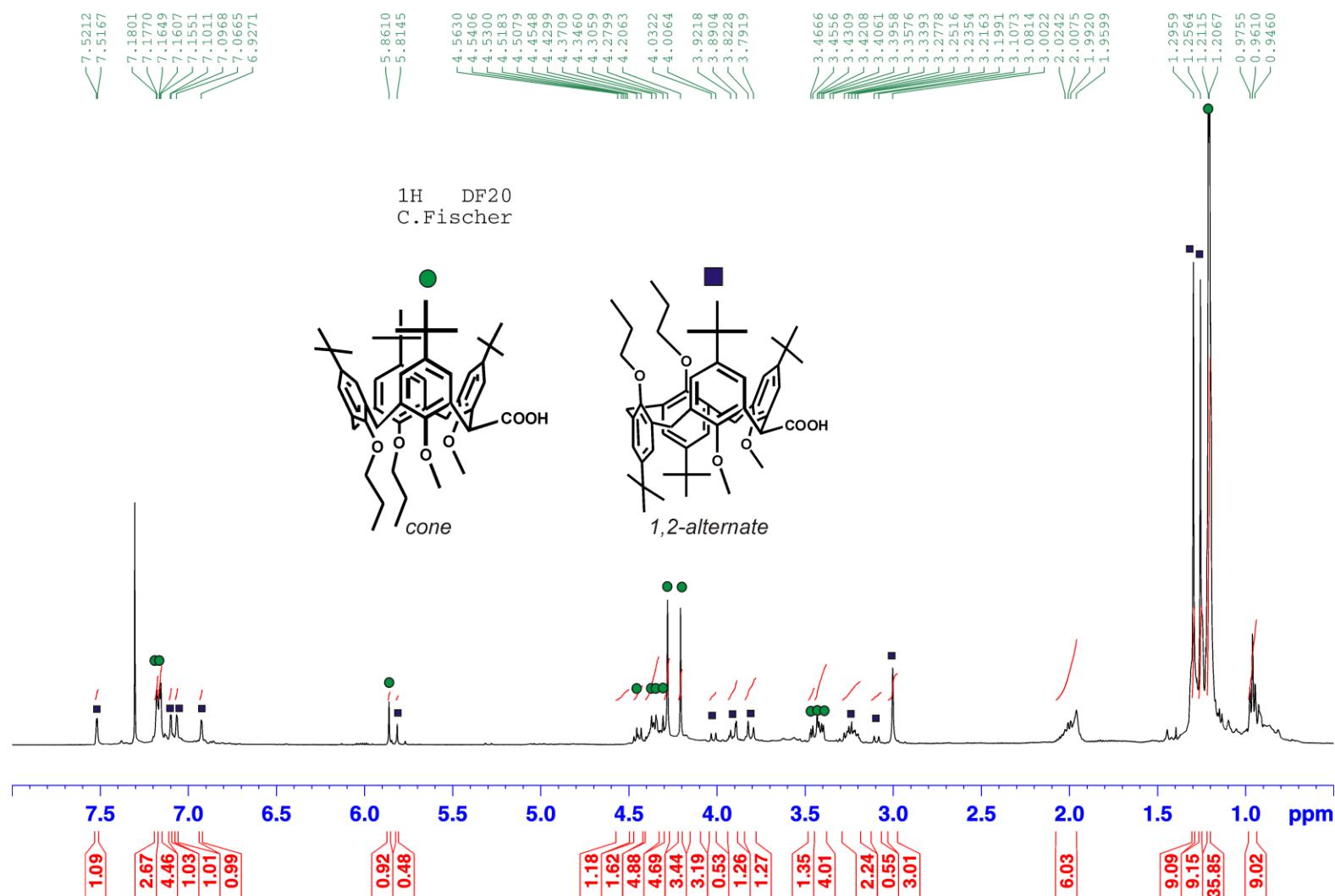
**Figure S6:** <sup>13</sup>C NMR spectrum of **12** in CDCl<sub>3</sub> (incl. NaI/acetonitrile-d<sub>3</sub>) at 293 K.



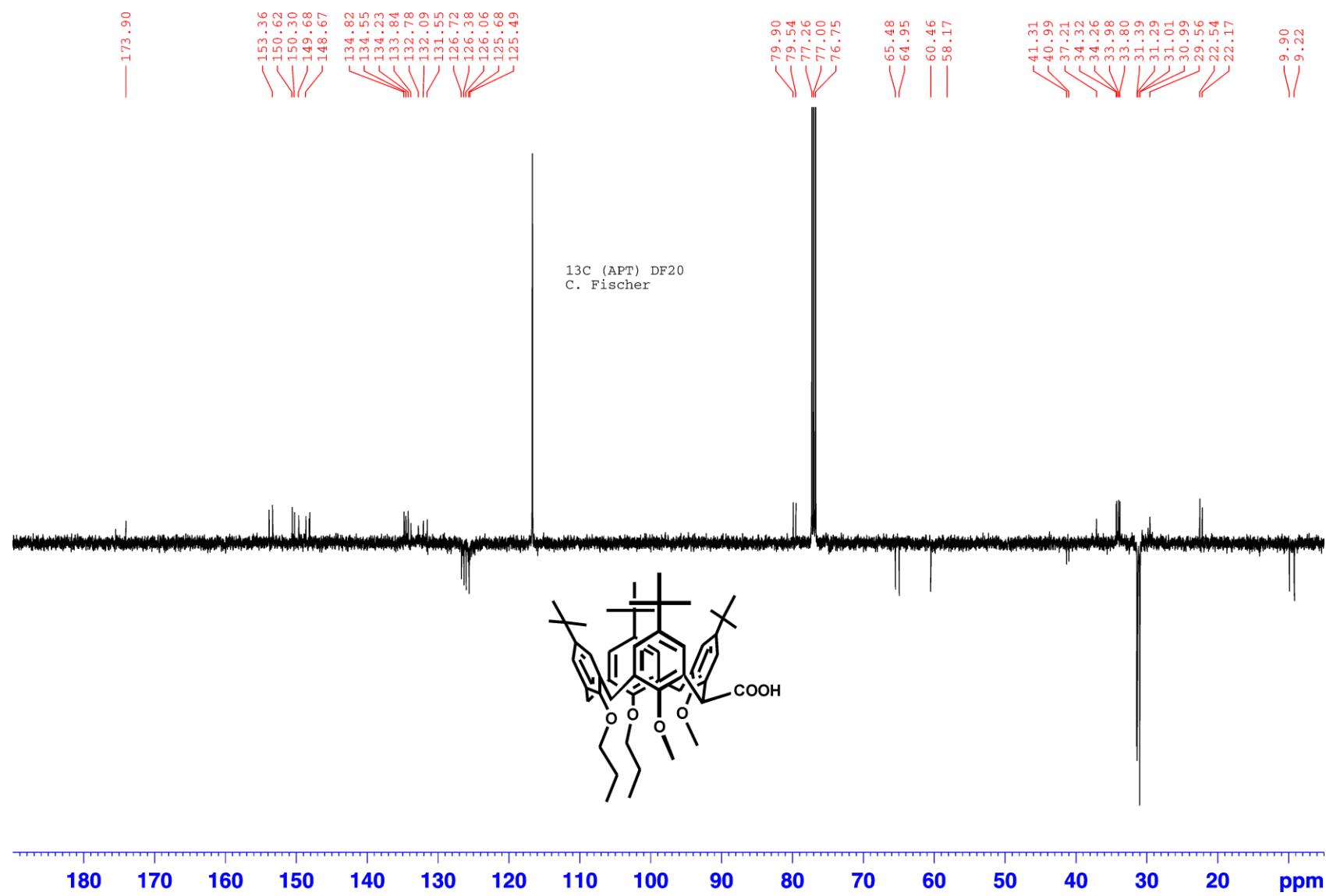
**Figure S7:** <sup>1</sup>H NMR spectrum of **13** in CDCl<sub>3</sub> (incl. NaI/acetonitrile-d<sub>3</sub>) at 293 K.



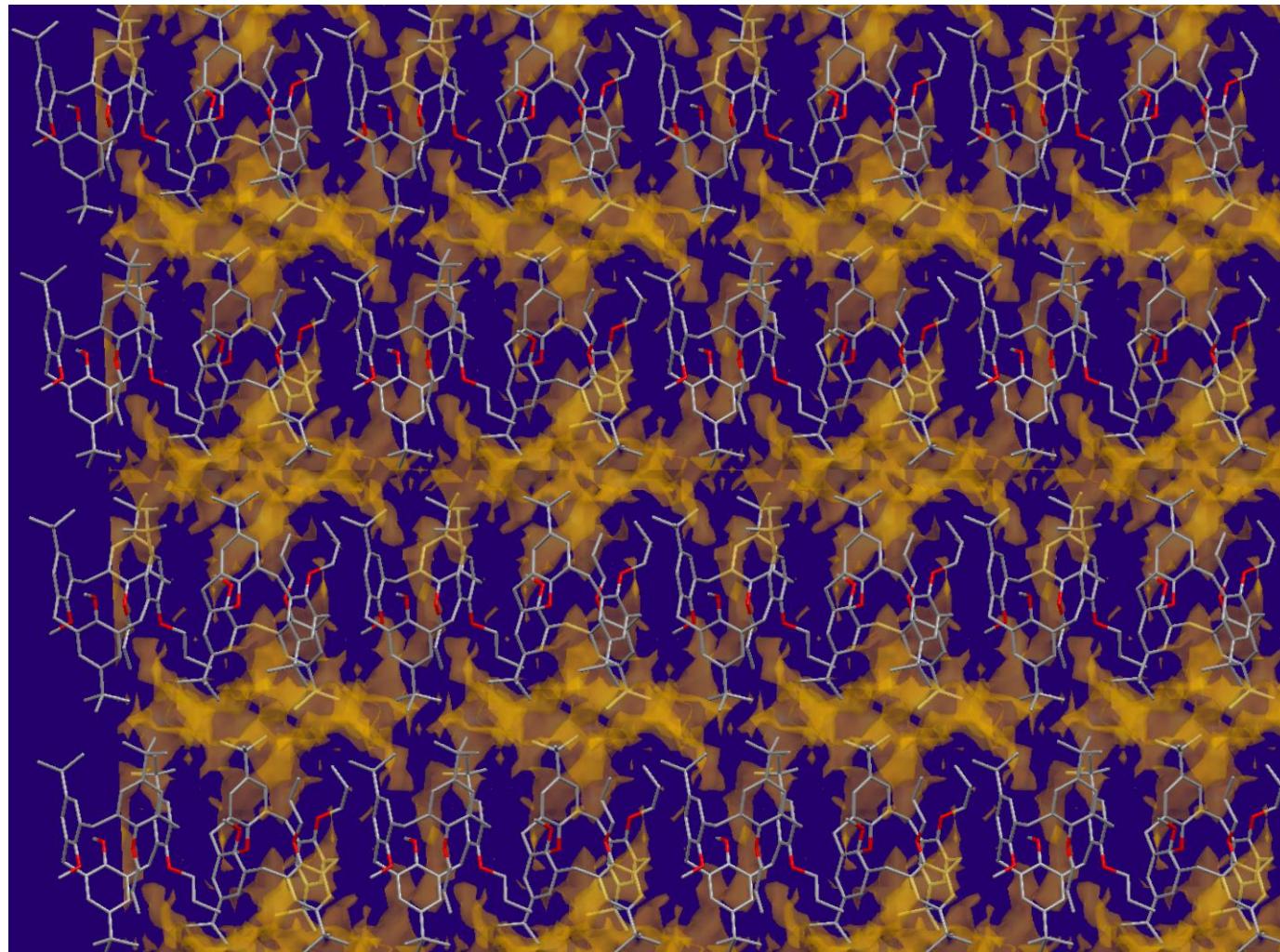
**Figure S8:**  $^{13}\text{C}$  APT NMR spectrum of **13** in  $\text{CDCl}_3$  (incl. NaI/acetonitrile- $d_3$ ) at 293 K.



**Figure S9:** <sup>1</sup>H NMR spectrum of **14** in CDCl<sub>3</sub> (incl. NaI/acetonitrile-d<sub>3</sub>) at 293 K with assignment of the resonances of the two different conformers.



**Figure S10:**  $^{13}\text{C}$  APT NMR spectrum of **14** in  $\text{CDCl}_3$  (incl. NaI/acetonitrile- $d_3$ ) at 293 K.



**Figure S11:** Packing motif of structure **12** along the crystallographic *c*-direction. The yellow areas denote solvent accessible empty voids.