Supplementary data for

Arylation of thiacalix[4]arenes using organomercurial intermediates

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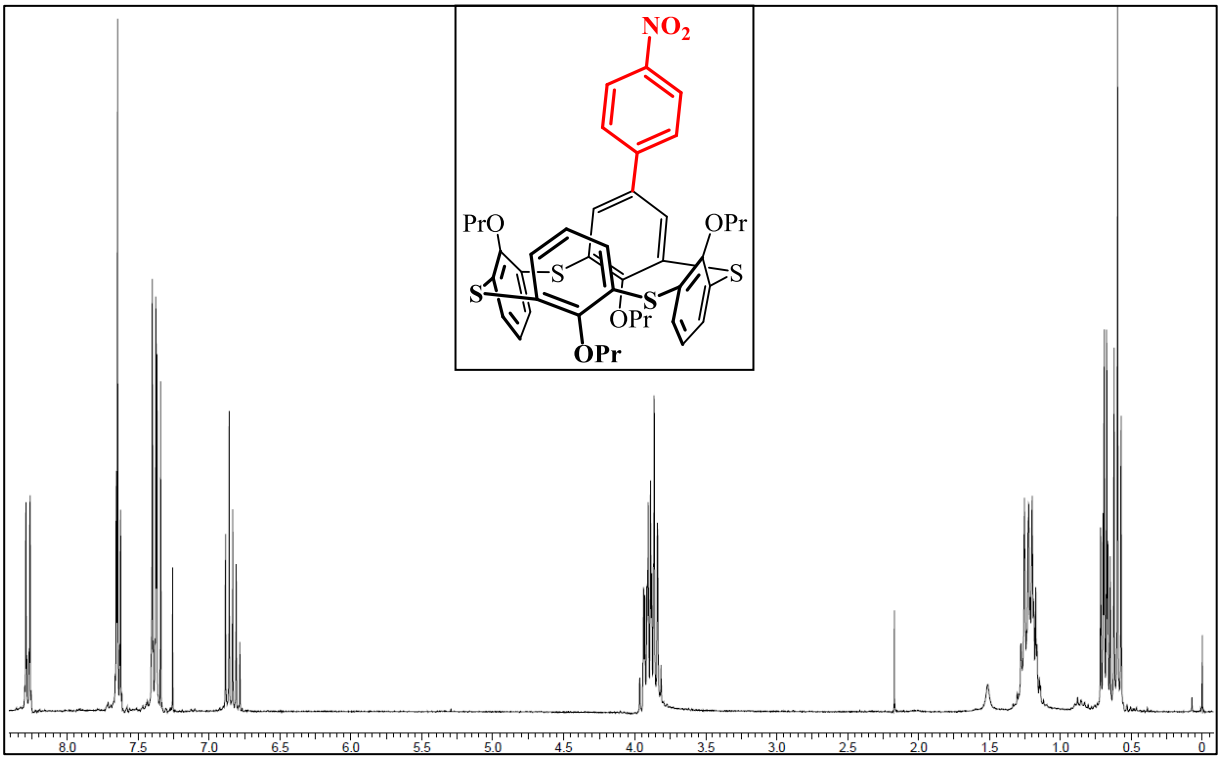


Figure 1: ^{1}H NMR spectrum ($CDCl_3$, 300 MHz, 298 K) of compound **4**

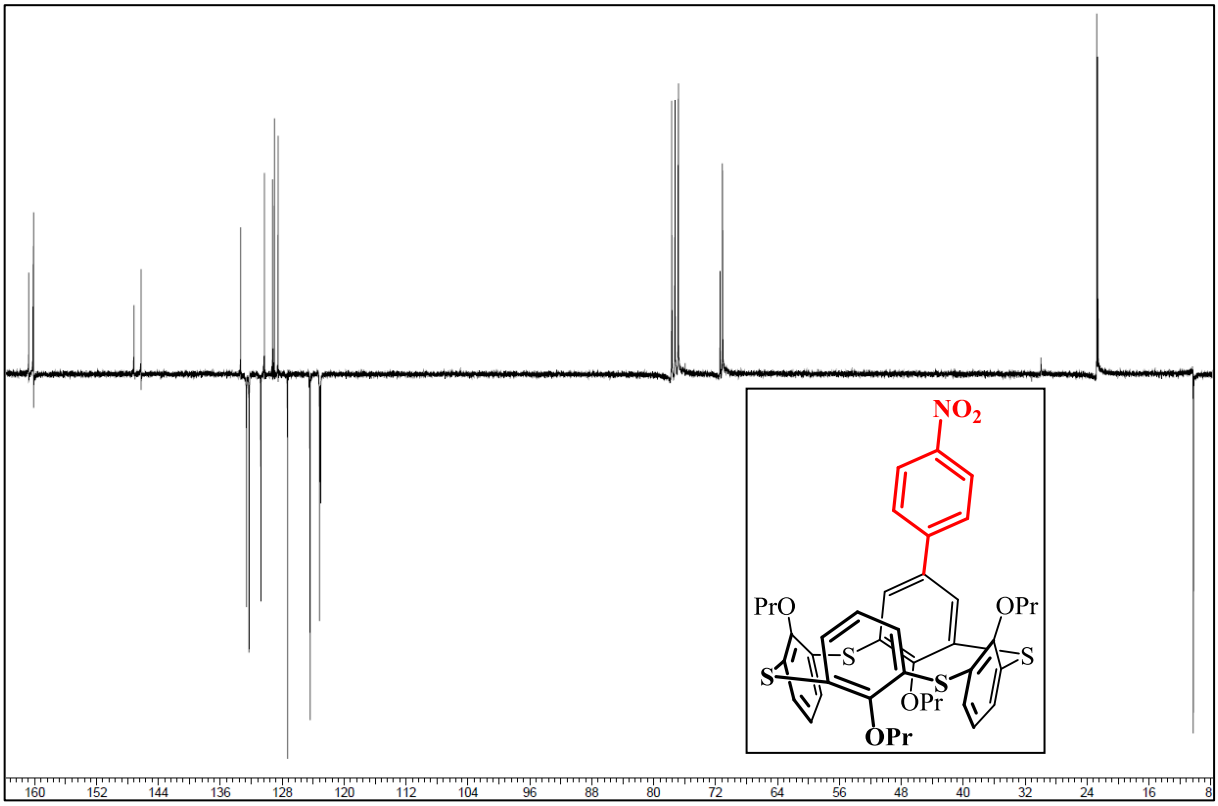


Figure 2: ^{13}C NMR spectrum ($CDCl_3$, 75 MHz, 298 K) of compound **4**

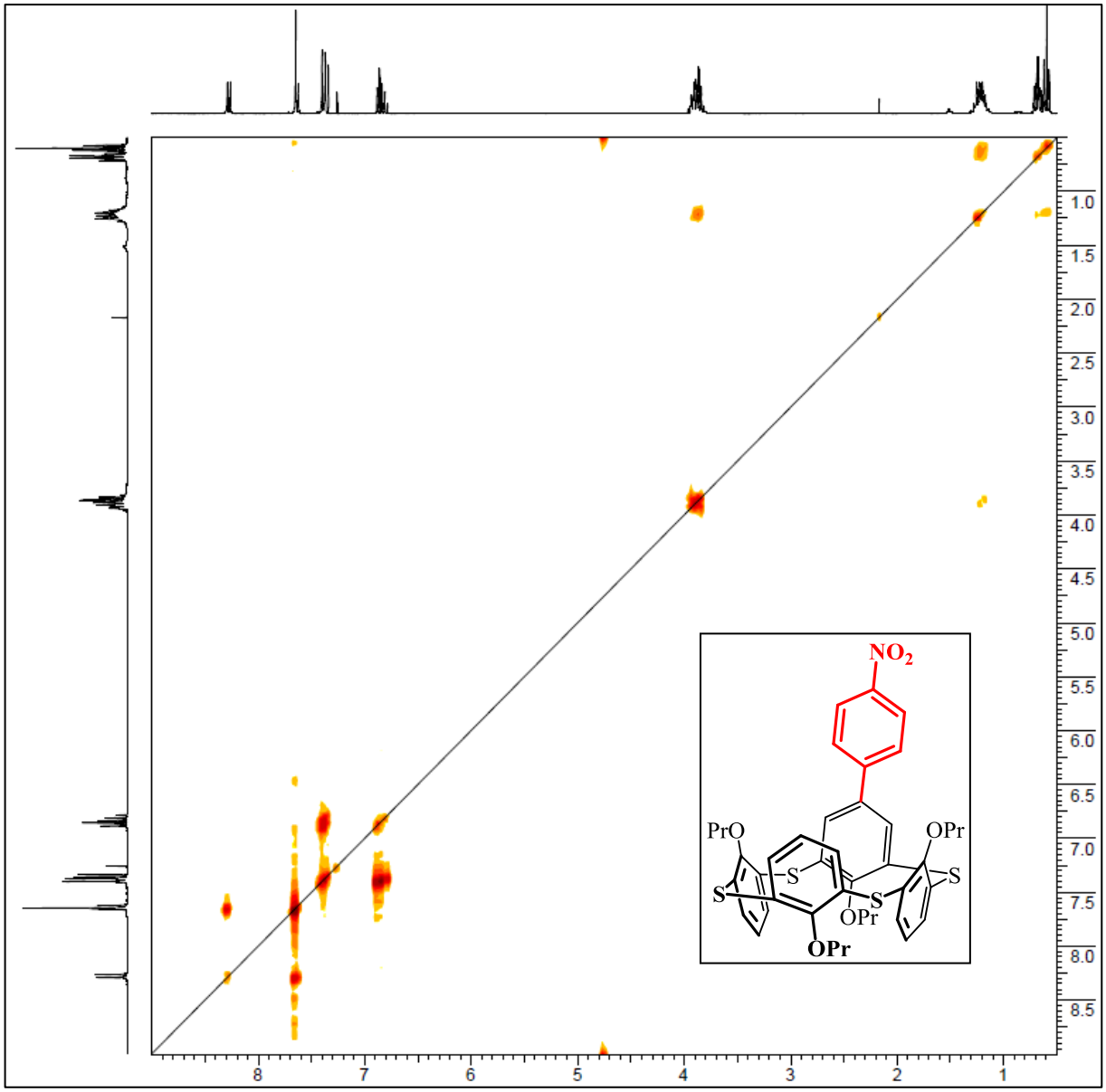
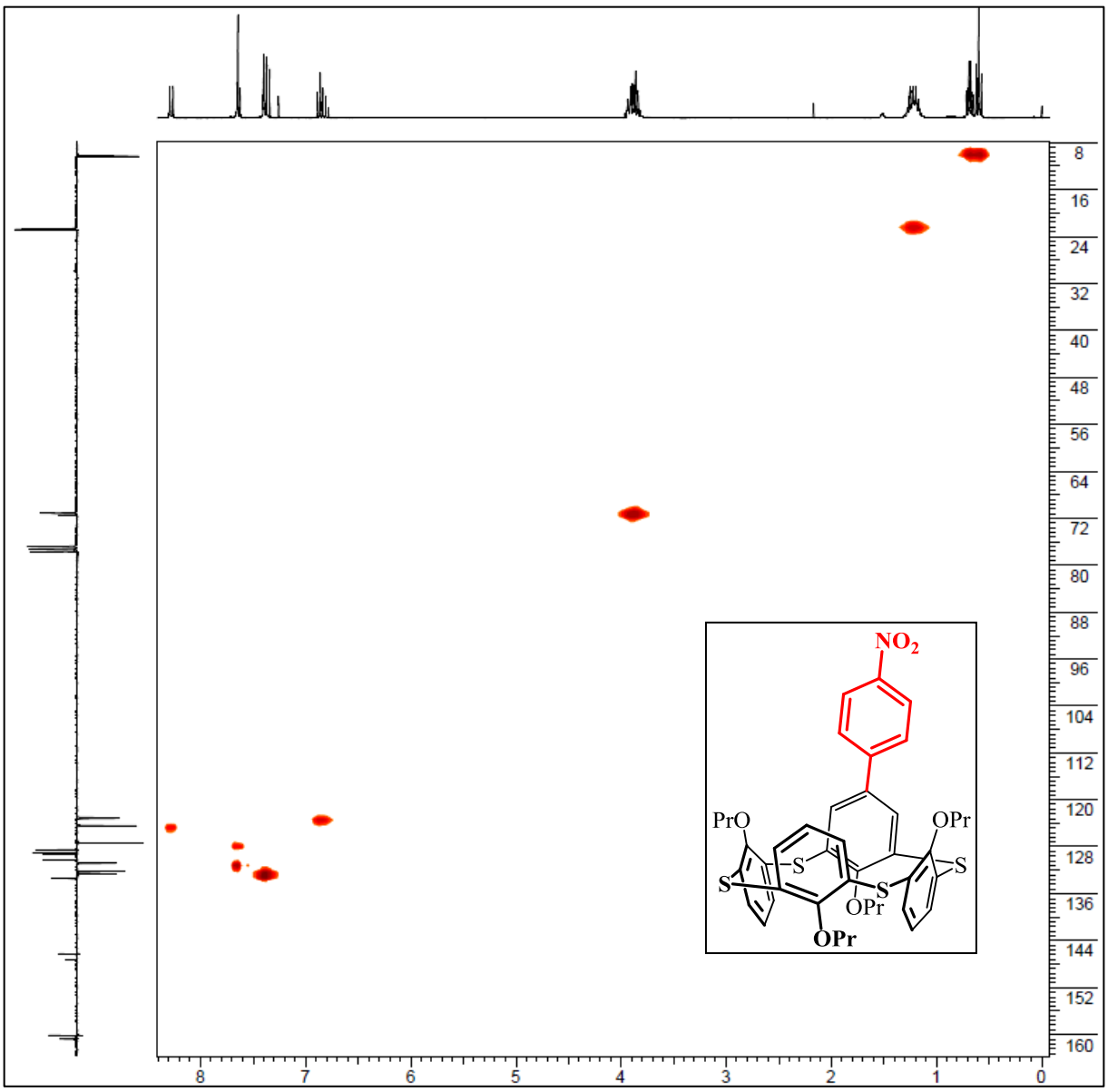


Figure 3: ^{1}H-^{1}H gCOSY 2D NMR spectrum ($CDCl_3$, 300 MHz, 298 K) of compound **4**



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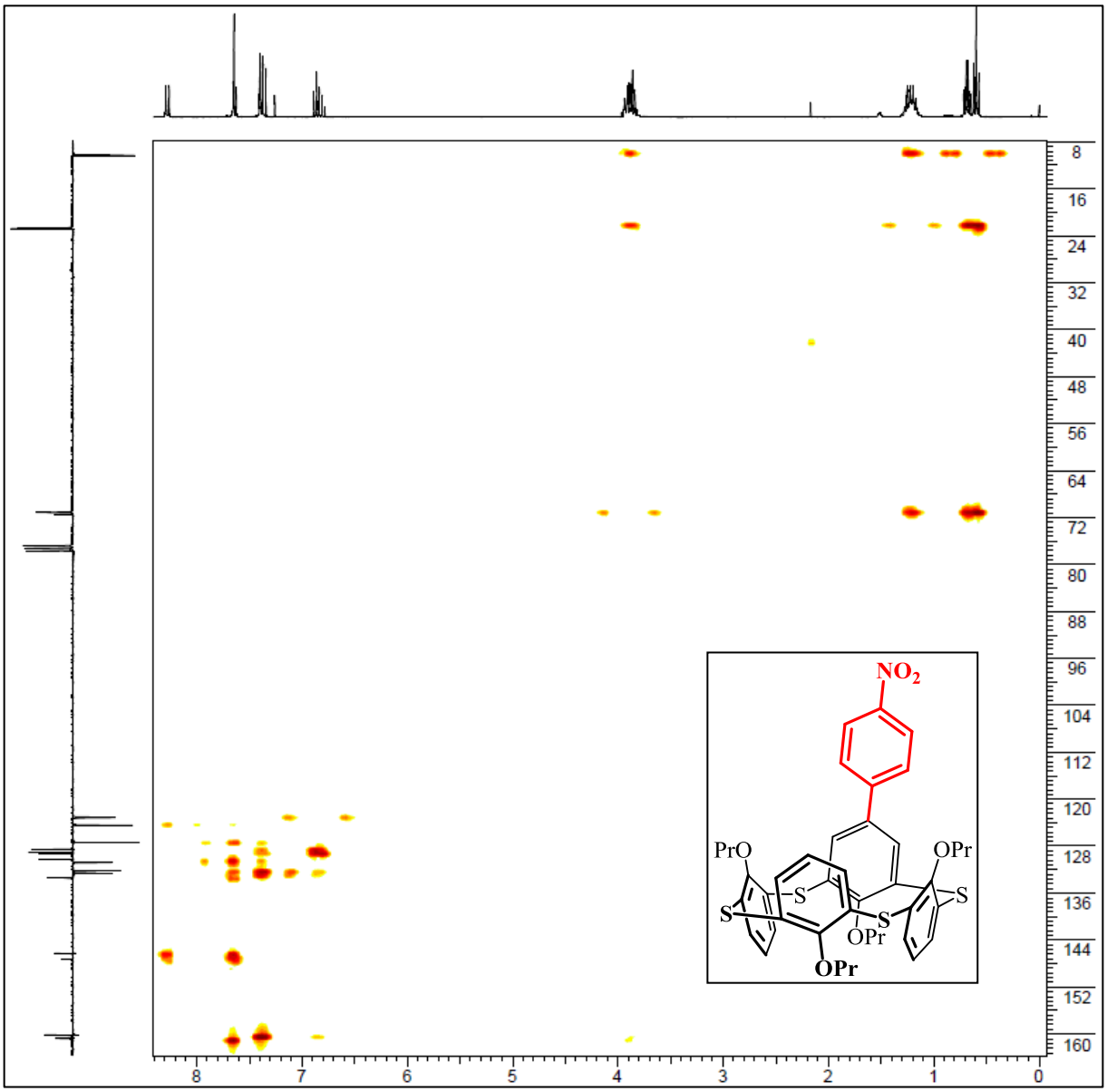

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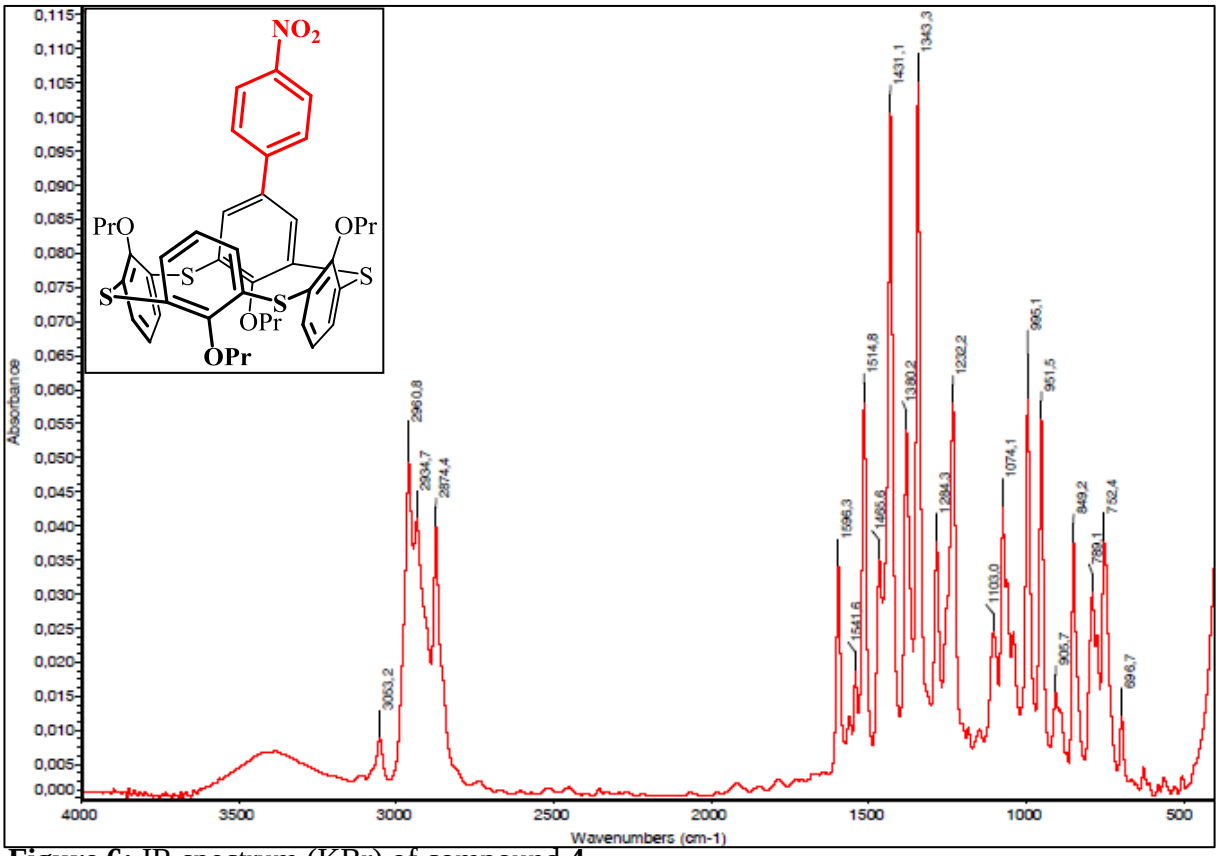


Figure 6: IR spectrum (KBr) of compound **4**

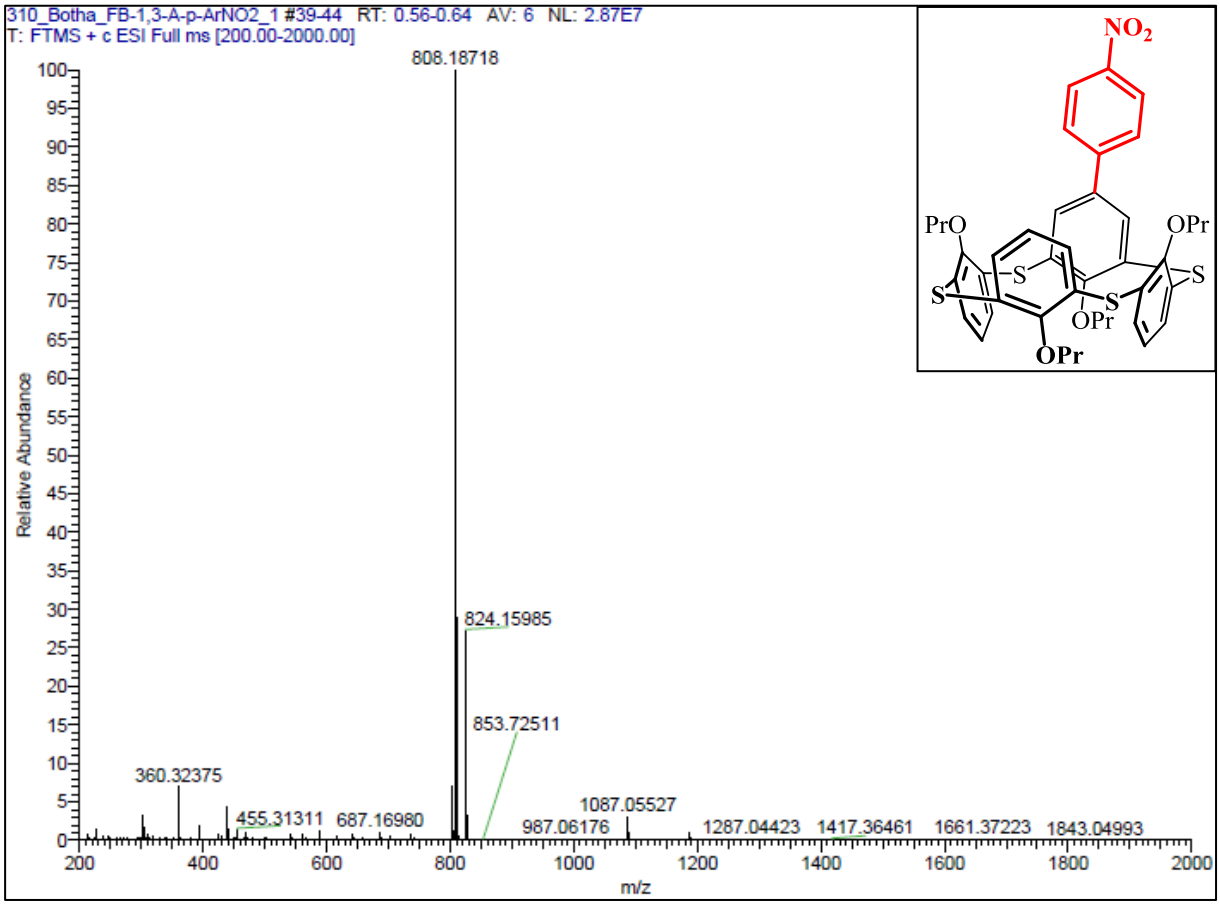
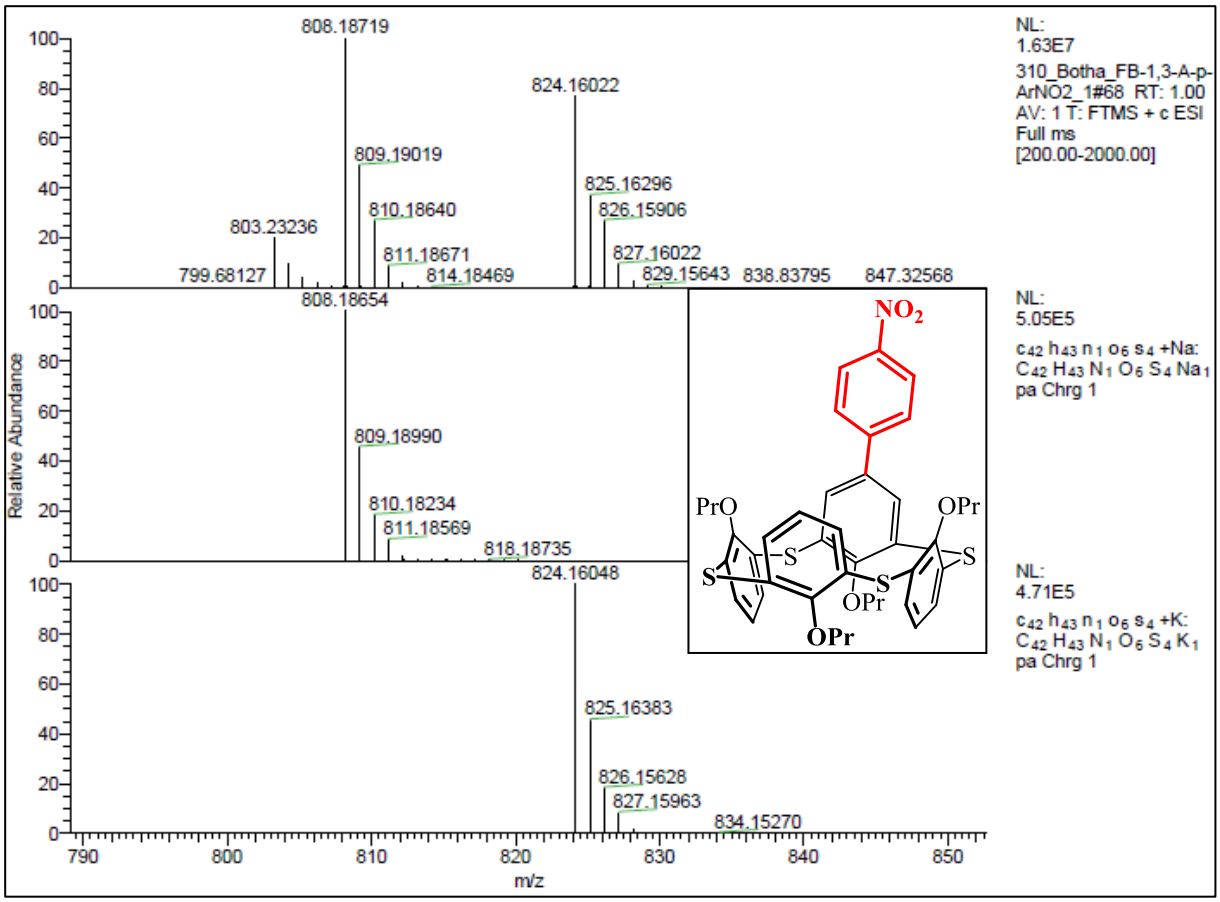


Figure 7: HRMS spectrum of compound **4**



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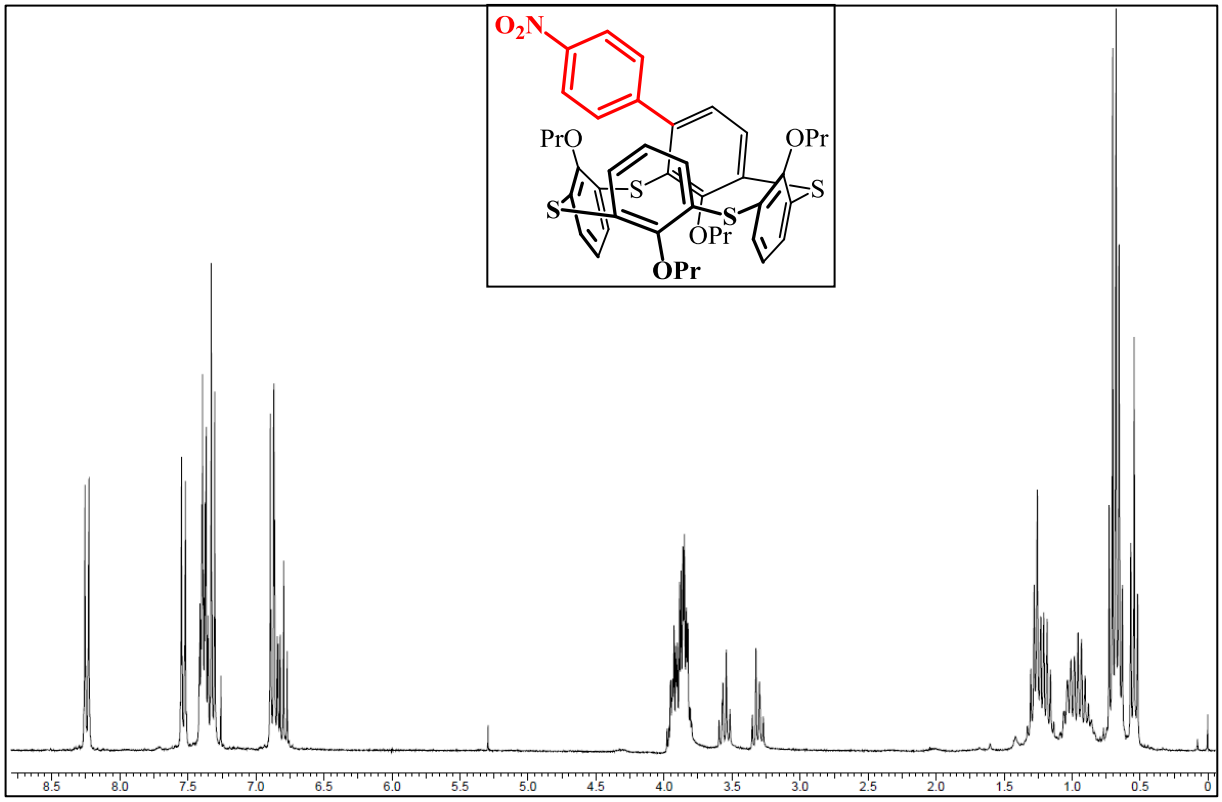
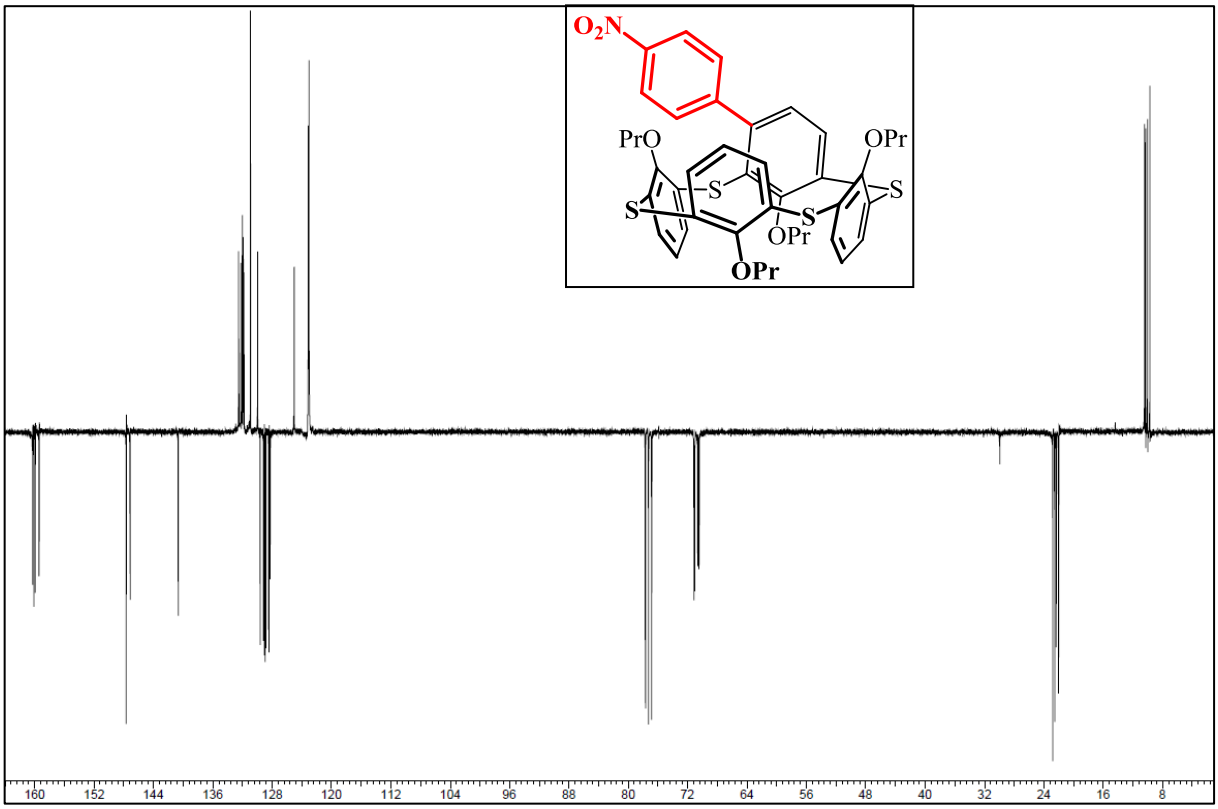


Figure 9: ^{1}H NMR spectrum ($CDCl_3$, 300 MHz, 298 K) of compound **5**



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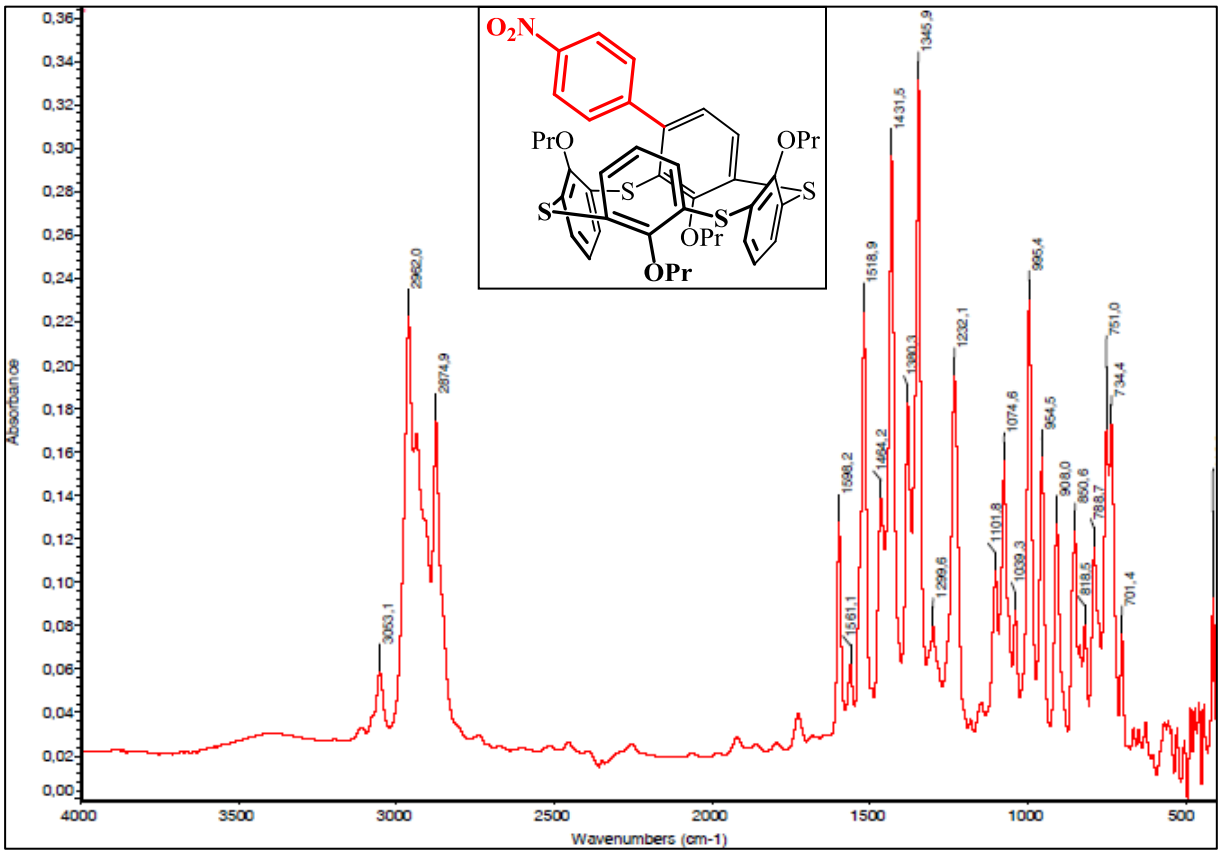

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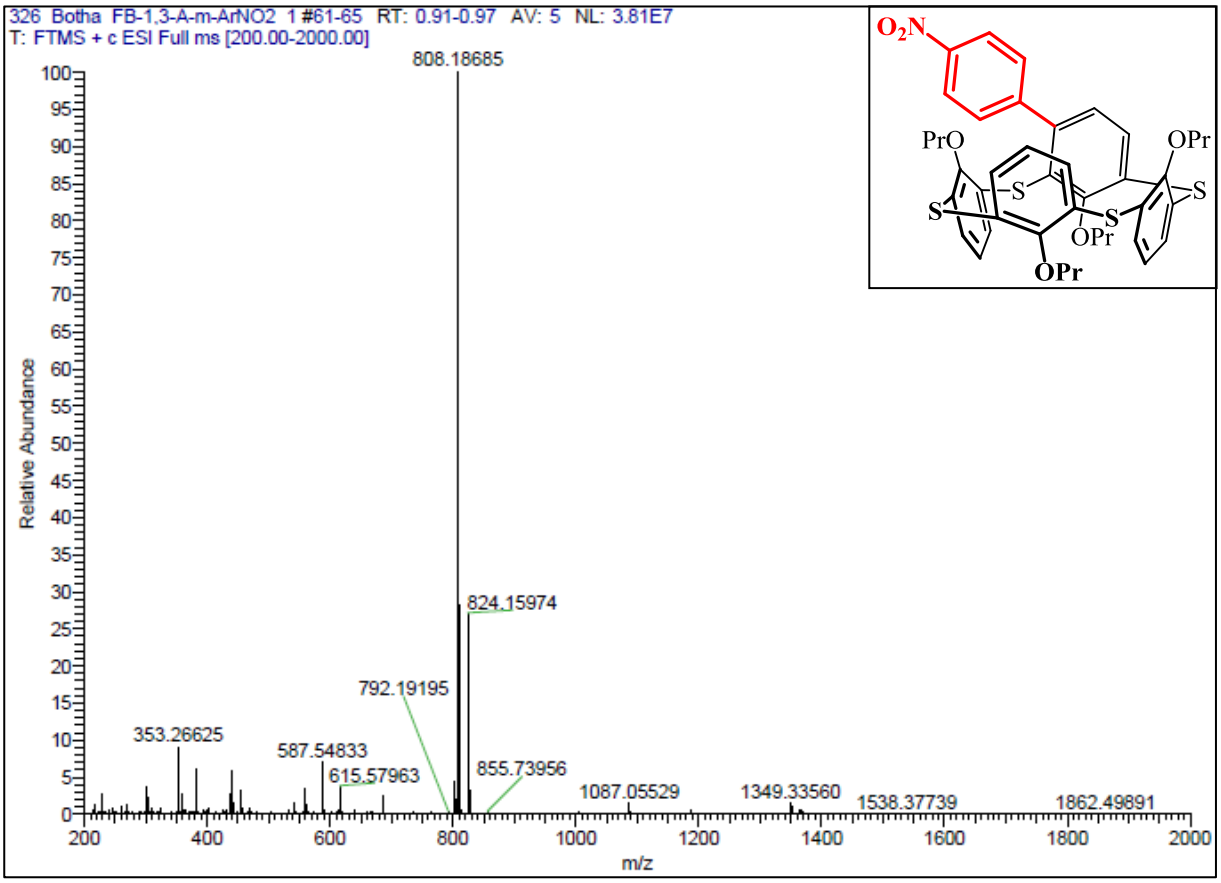

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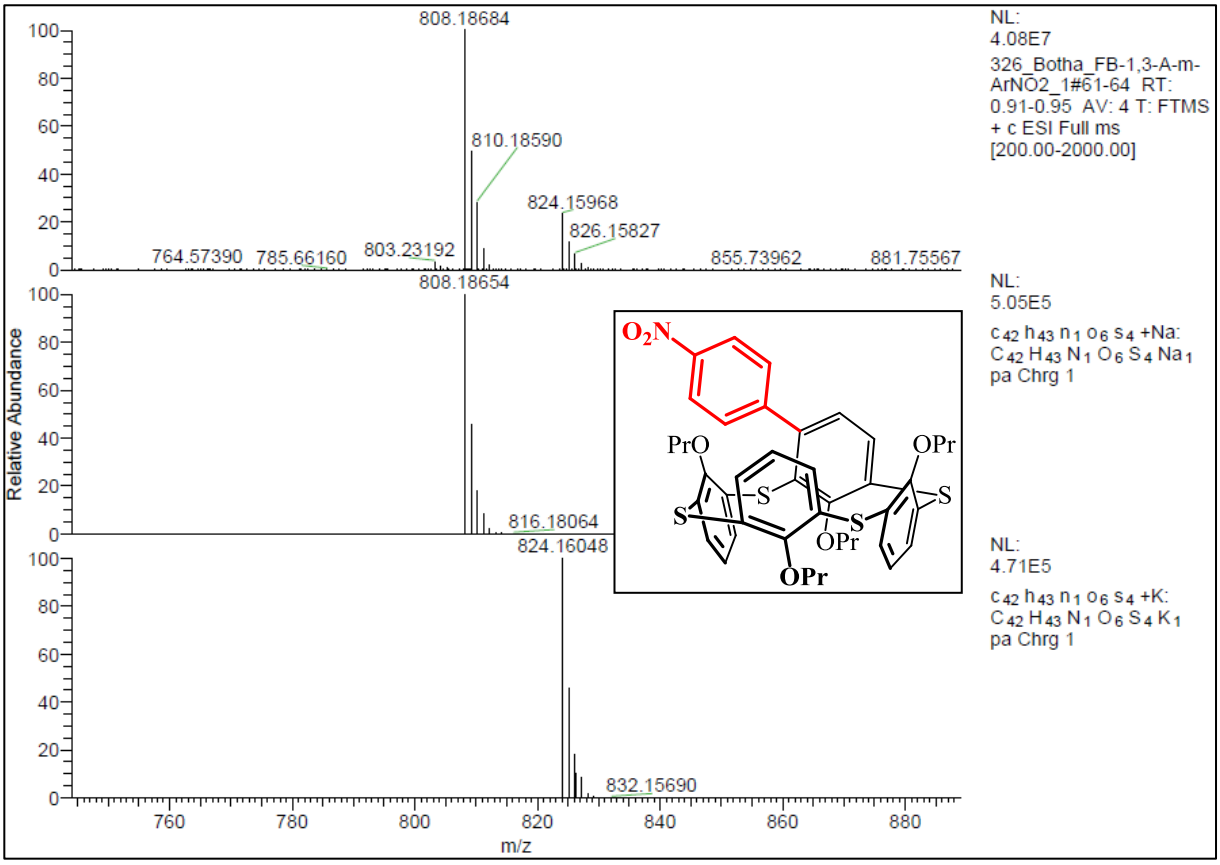

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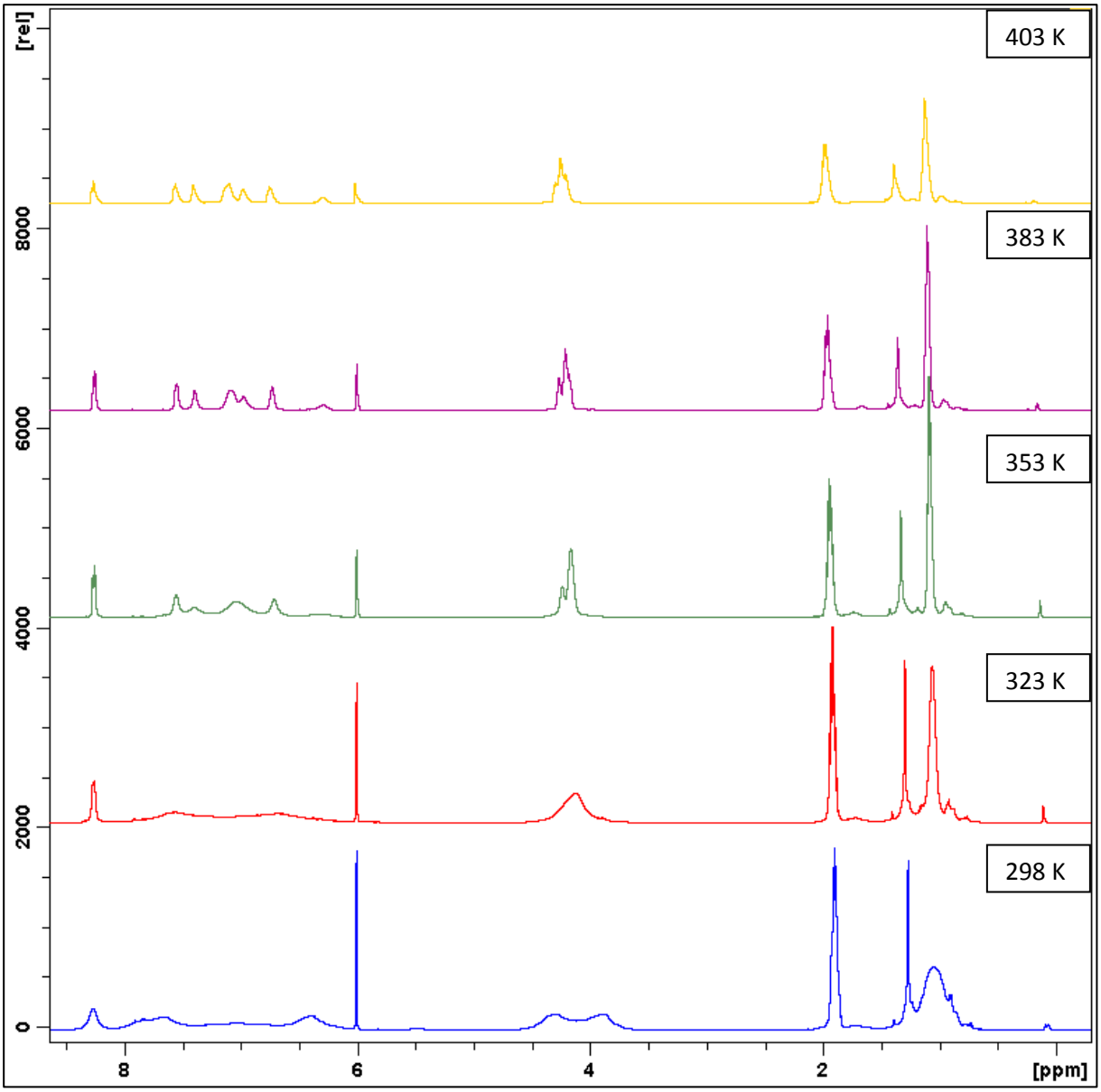
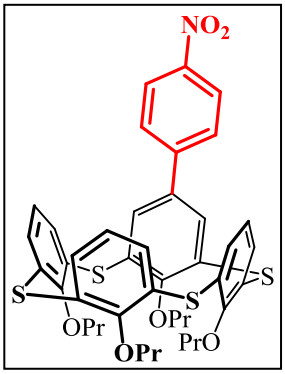
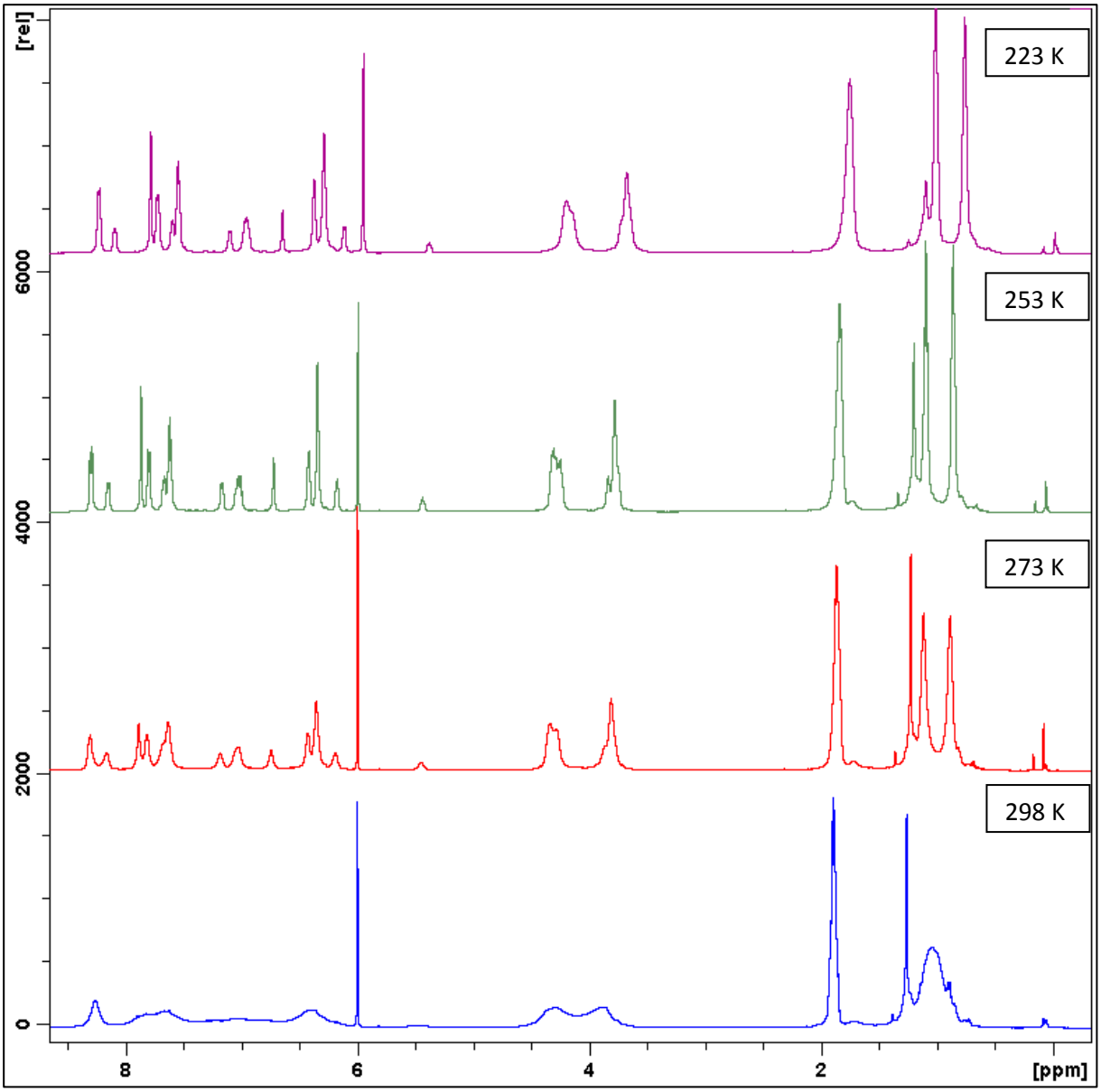


Figure 14: Temperature dependent ^{1}H NMR spectra ($C_2D_2Cl_4$, 500.1 MHz) of compound **9**





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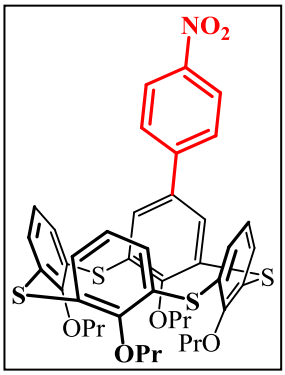

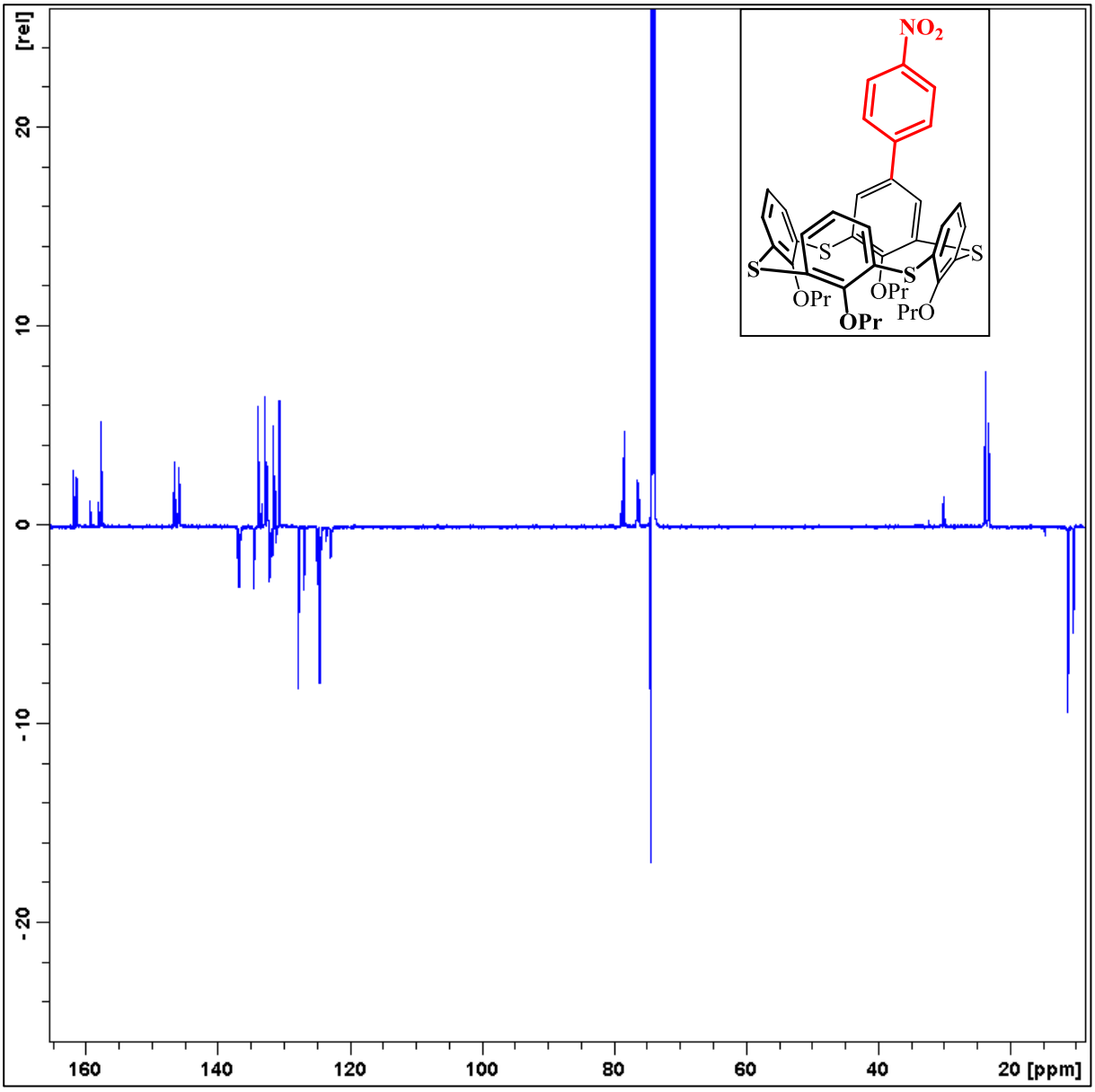

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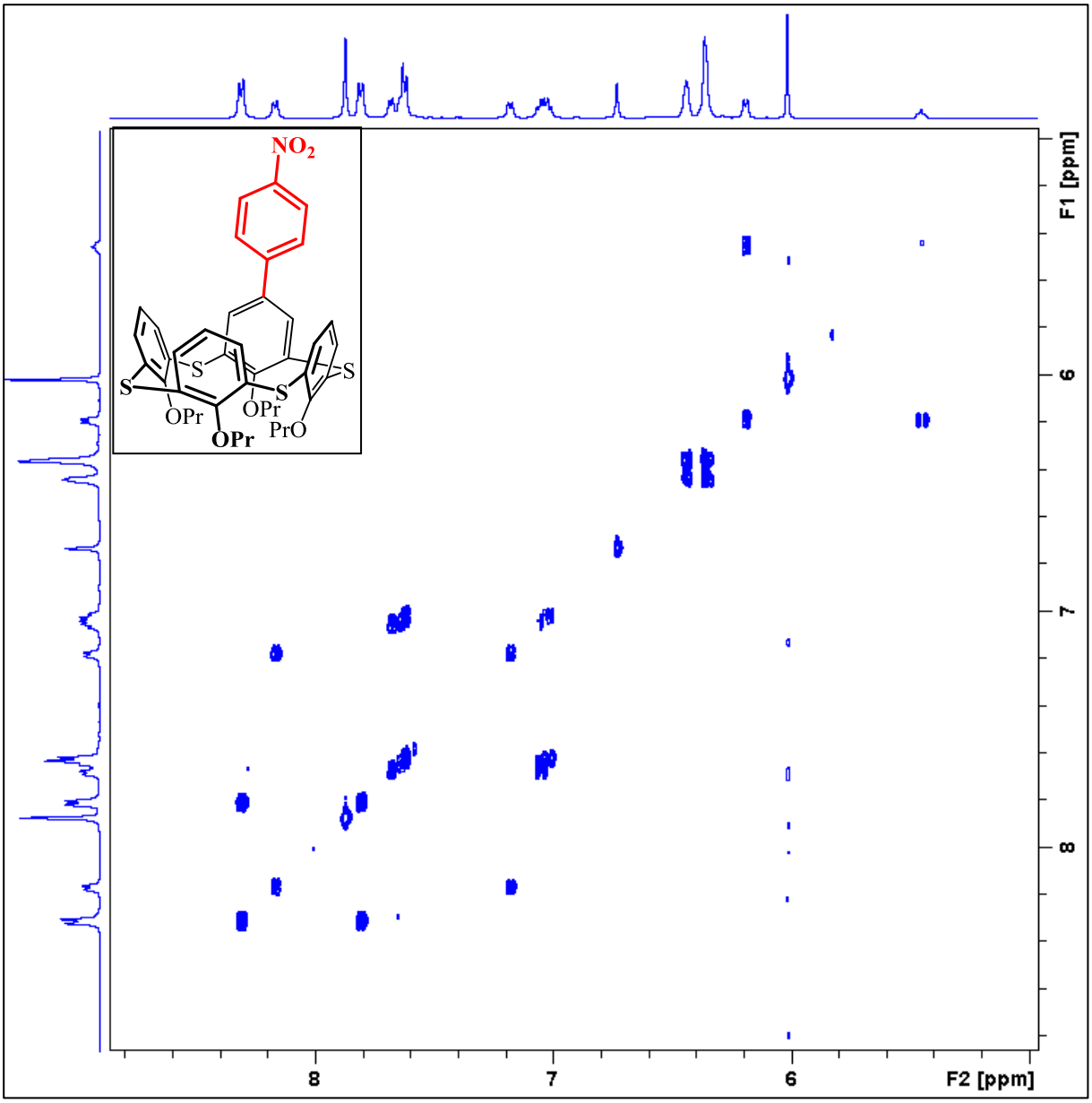

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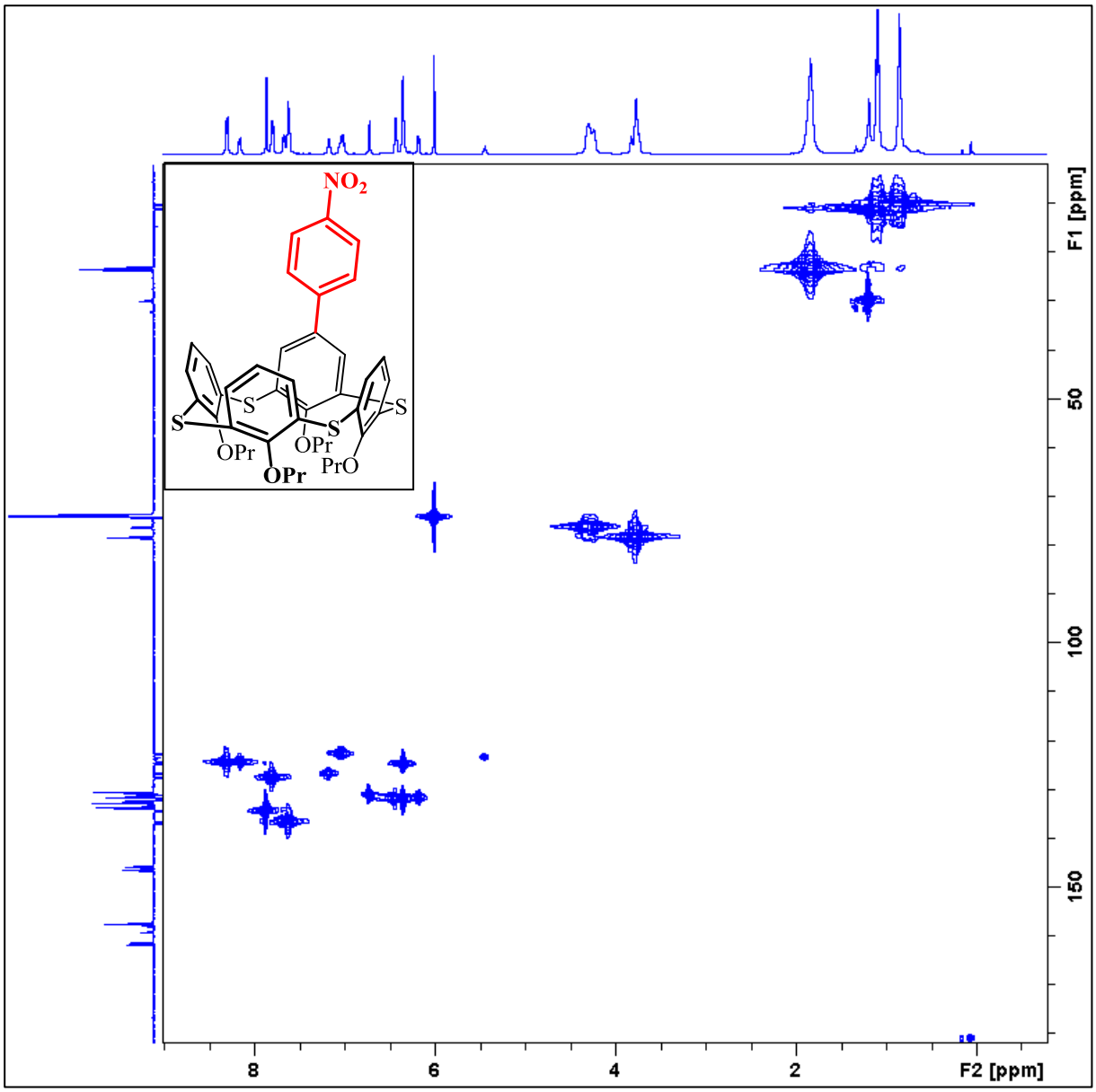

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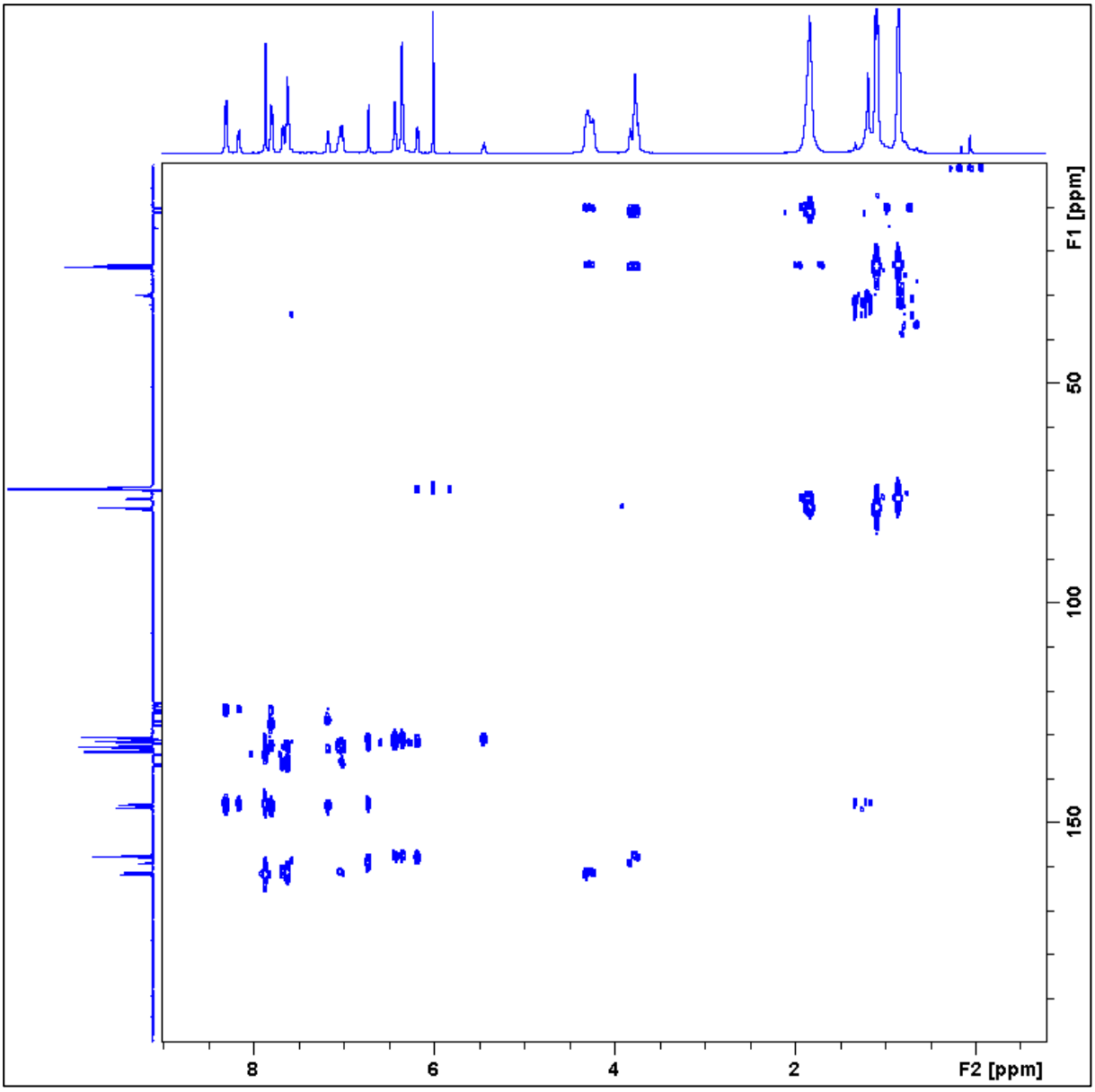

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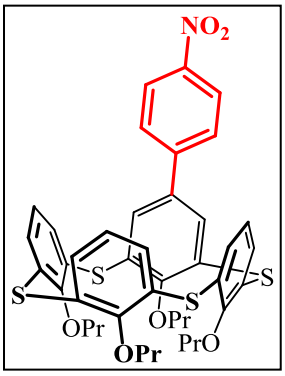


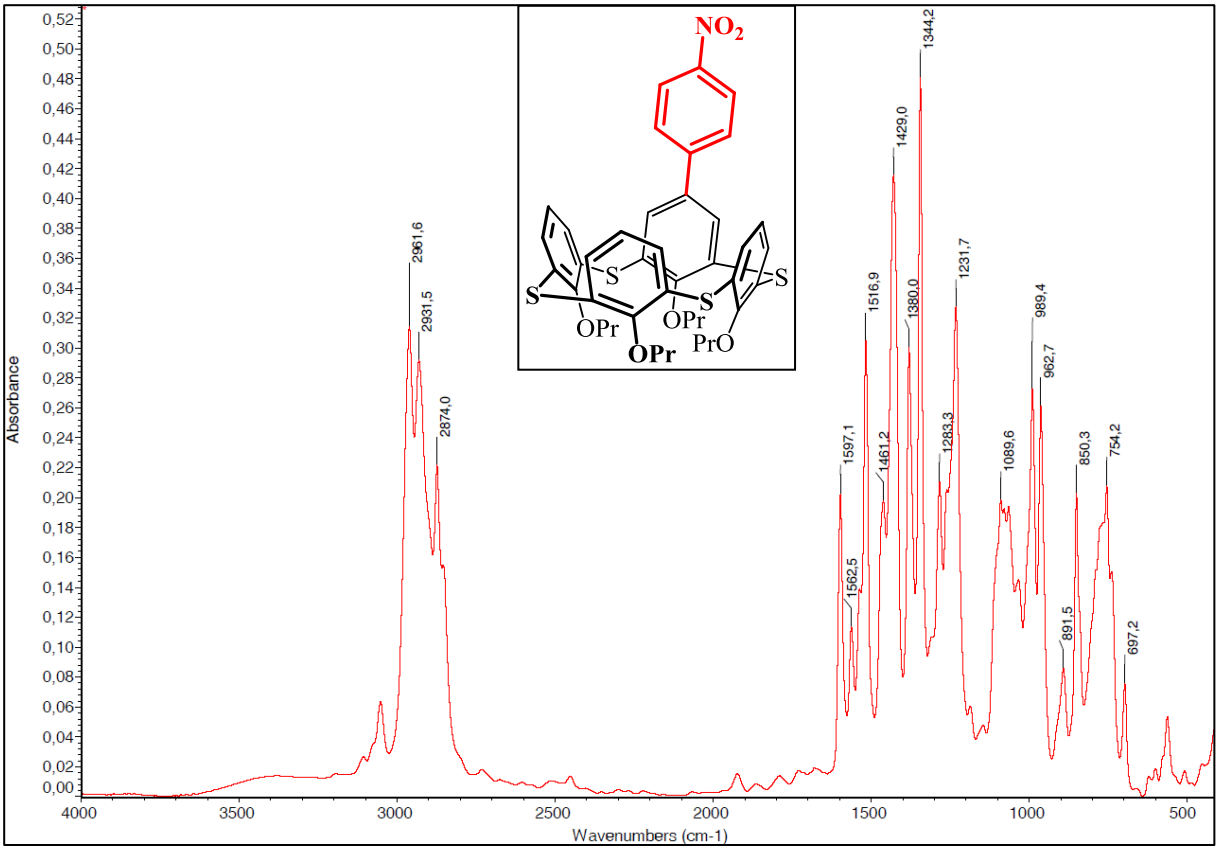
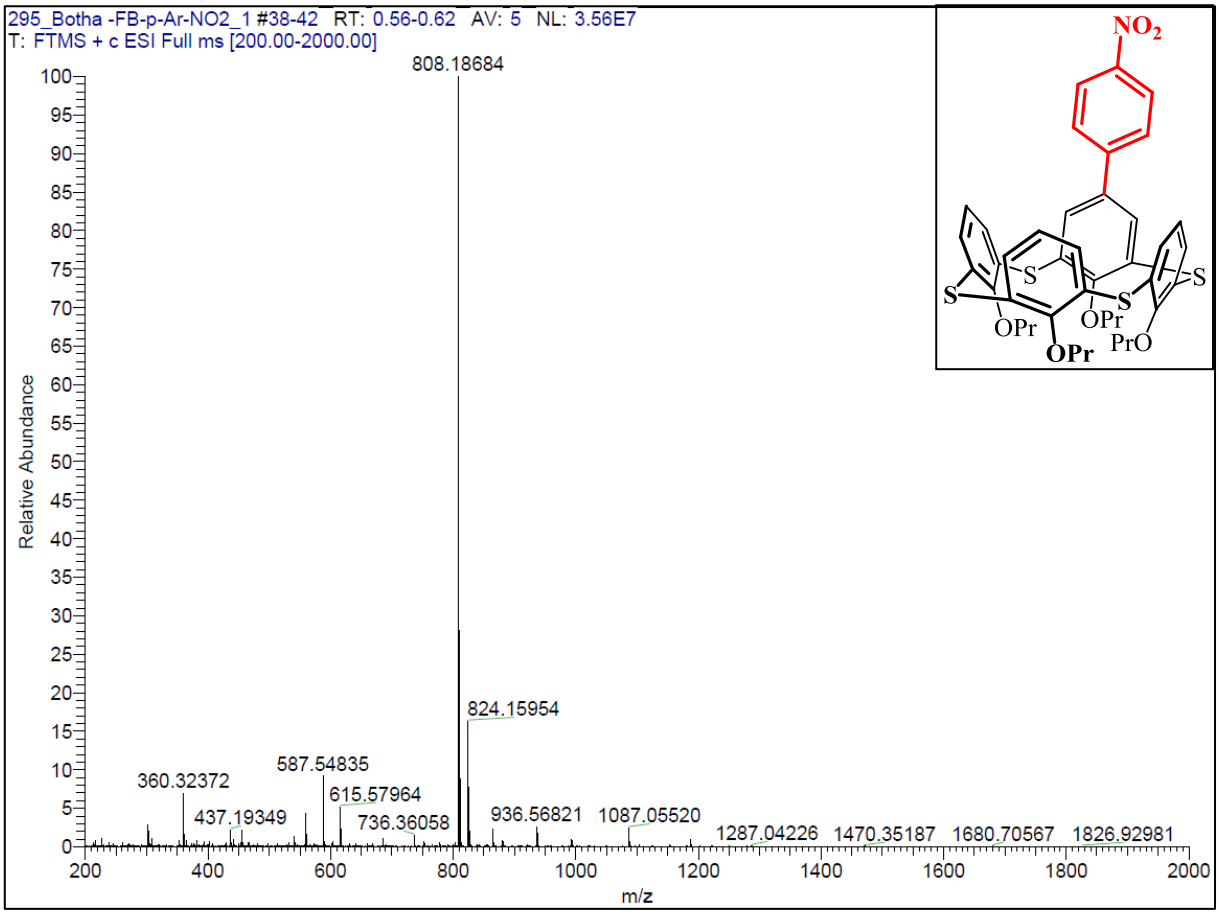


Figure 20: IR spectrum (KBr) of compound **9**



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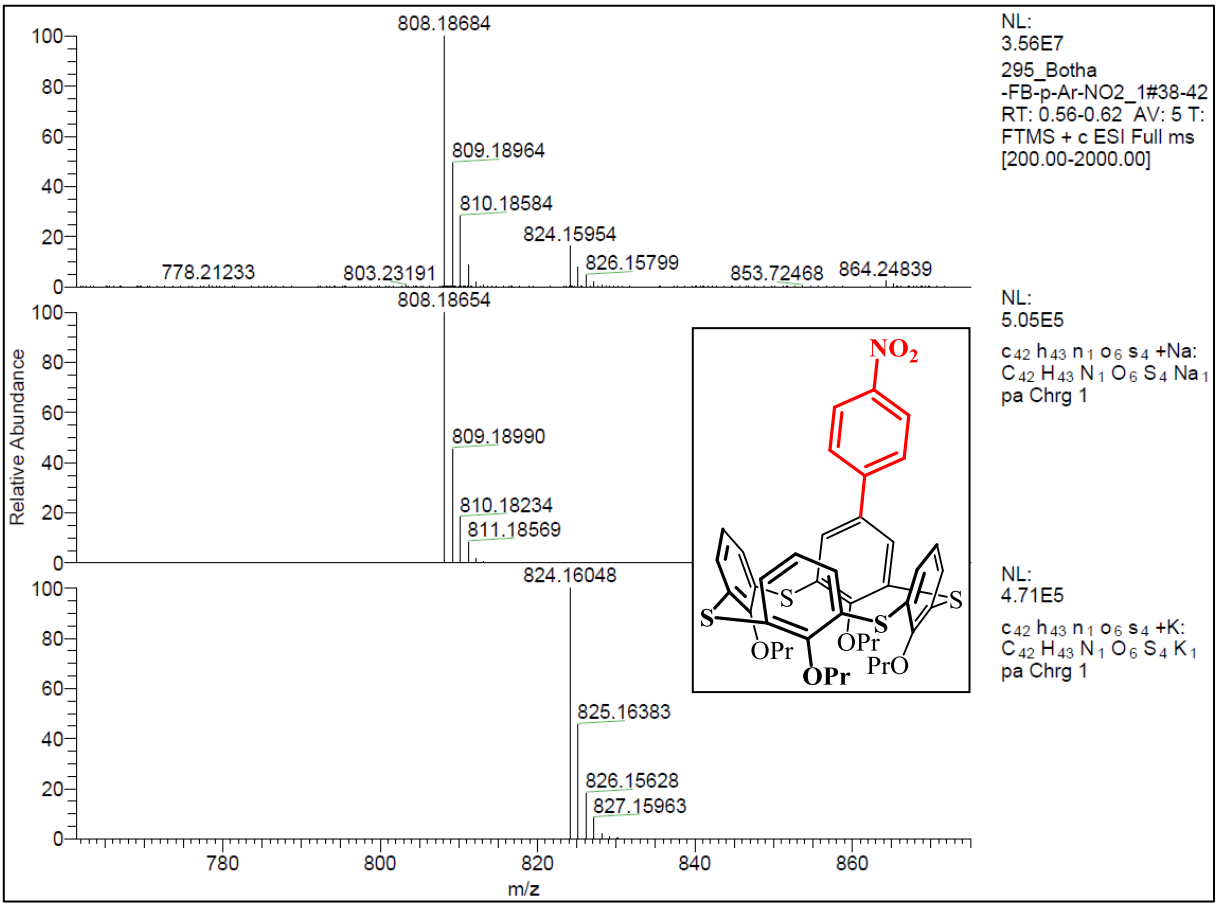

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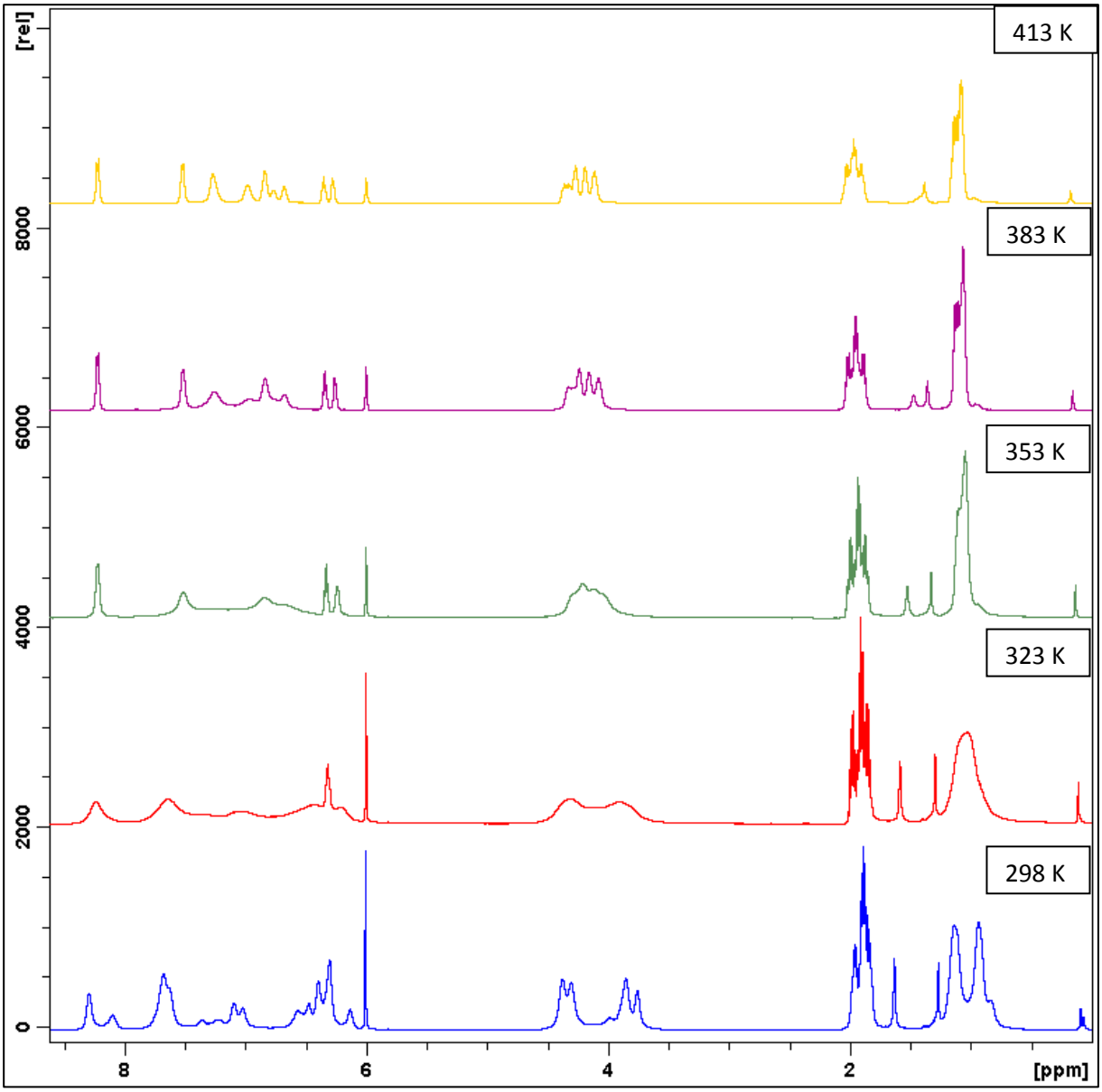

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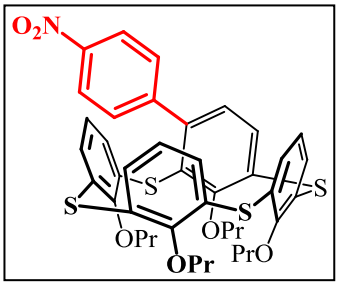

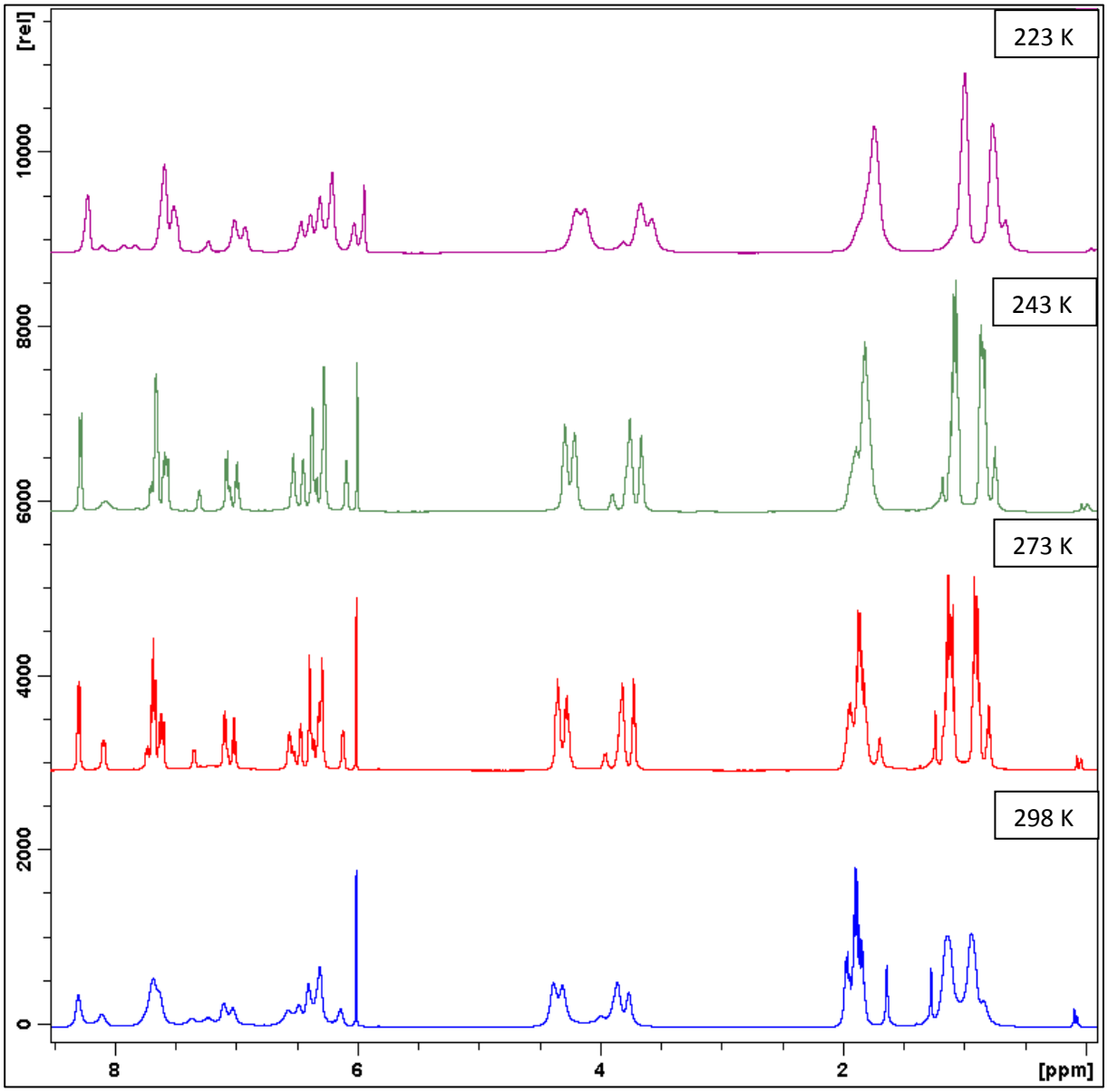

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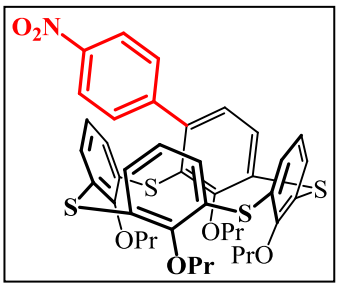


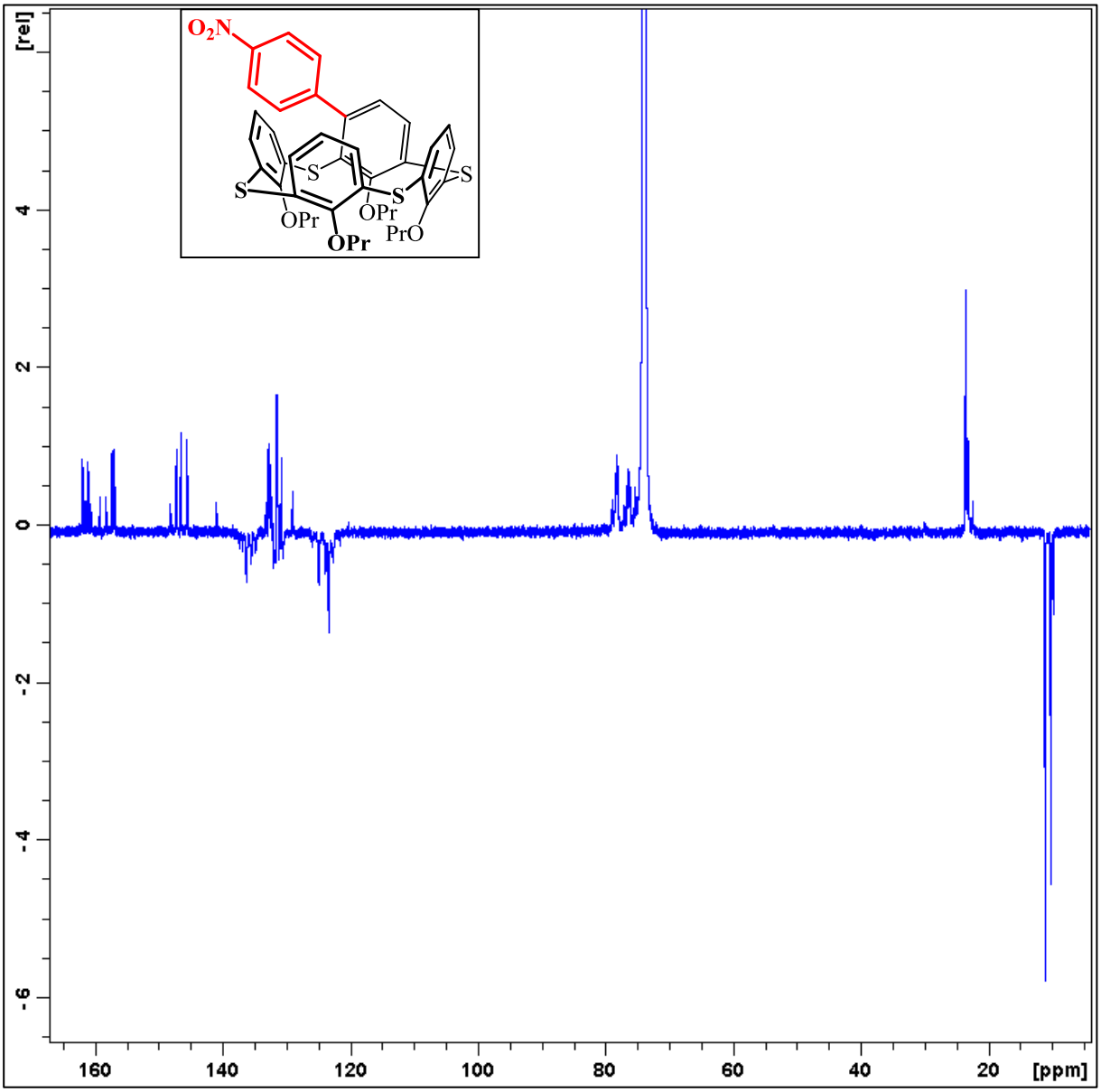
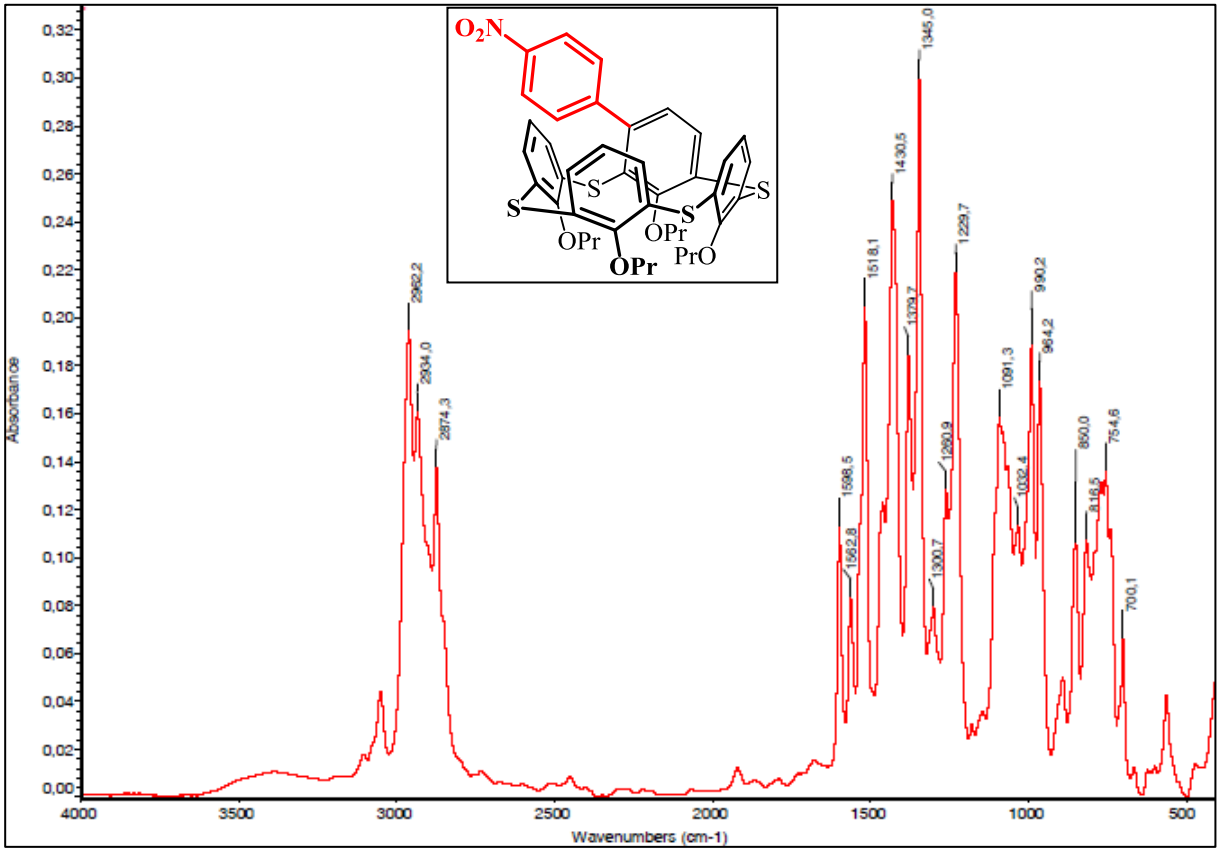


Figure 25: ^{13}C NMR spectrum ($C_2D_2Cl_4$, 125 MHz, 223 K) of compound **10**



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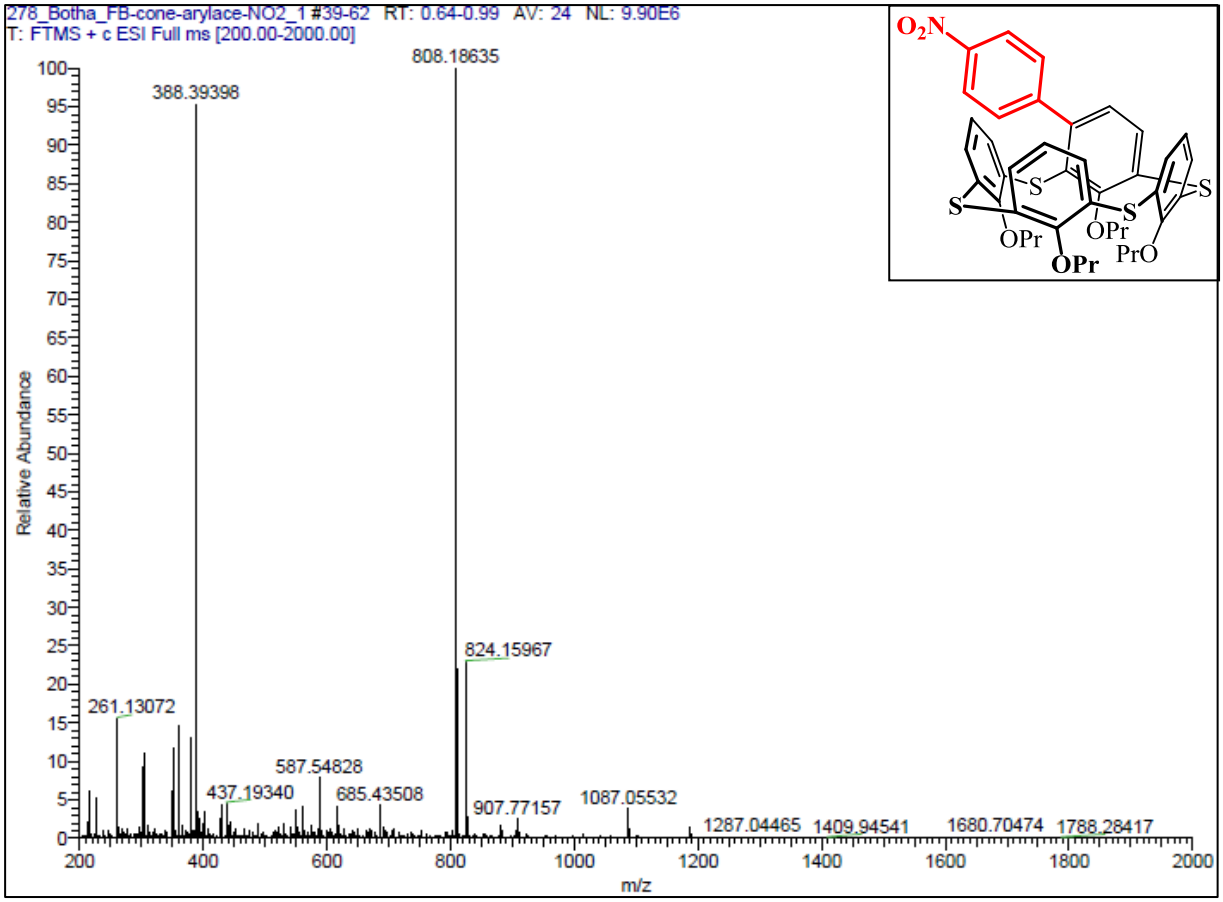
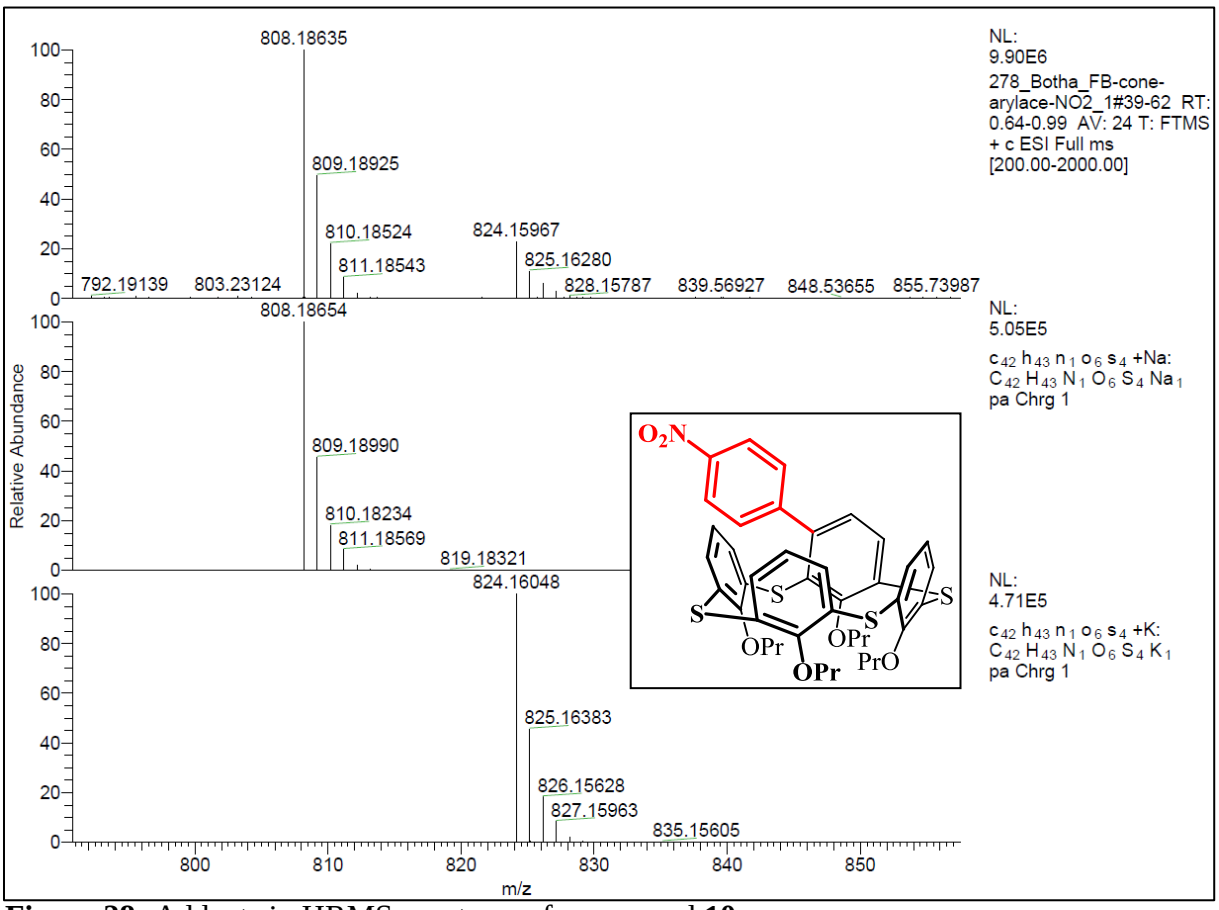


Figure 27: HRMS spectrum of compound **10**



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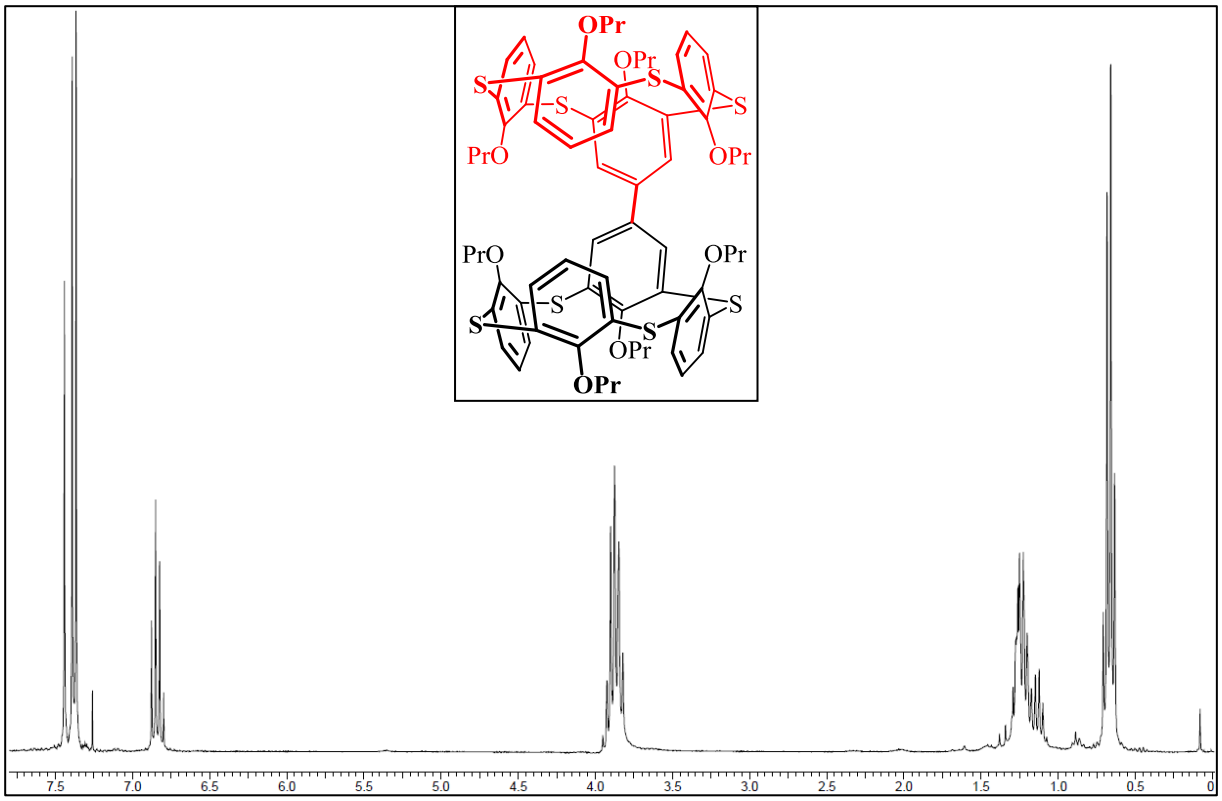
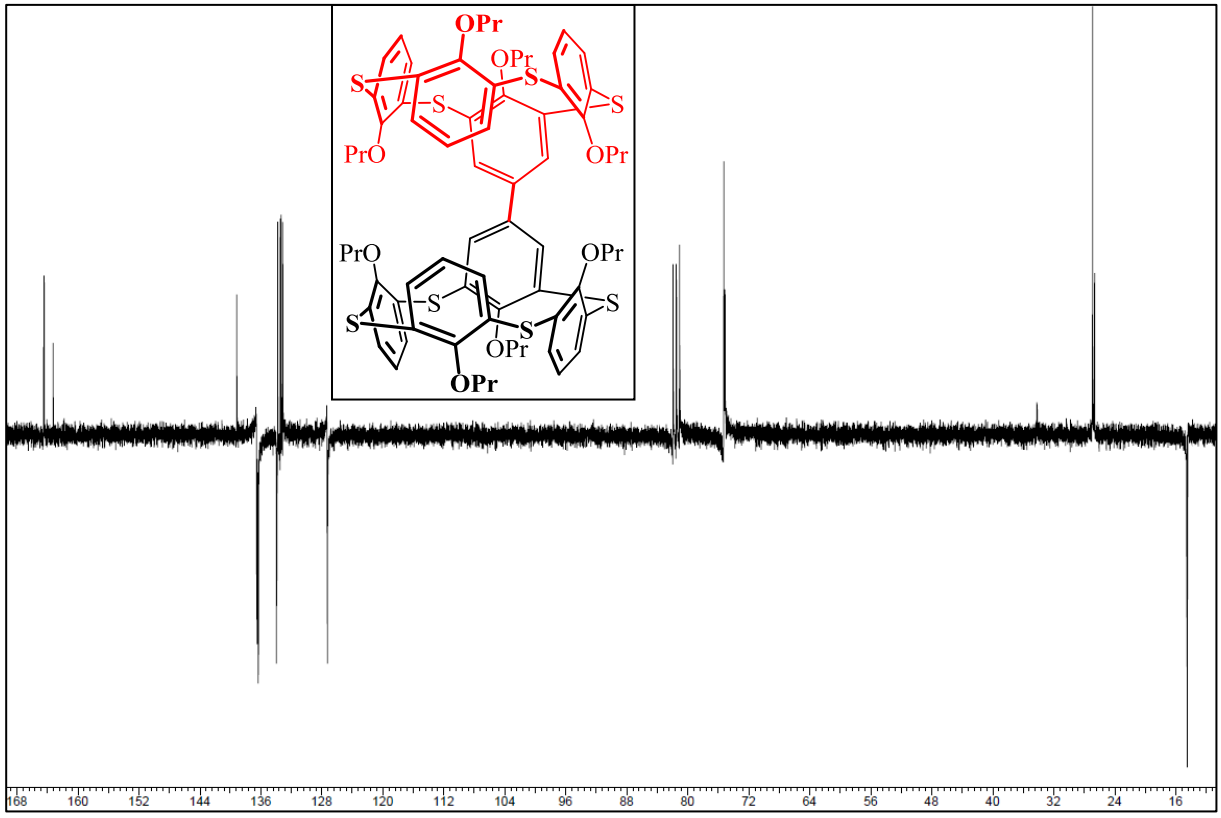


Figure 29: ^{1}H NMR spectrum ($CDCl_3$, 300 MHz, 298 K) of compound **11**



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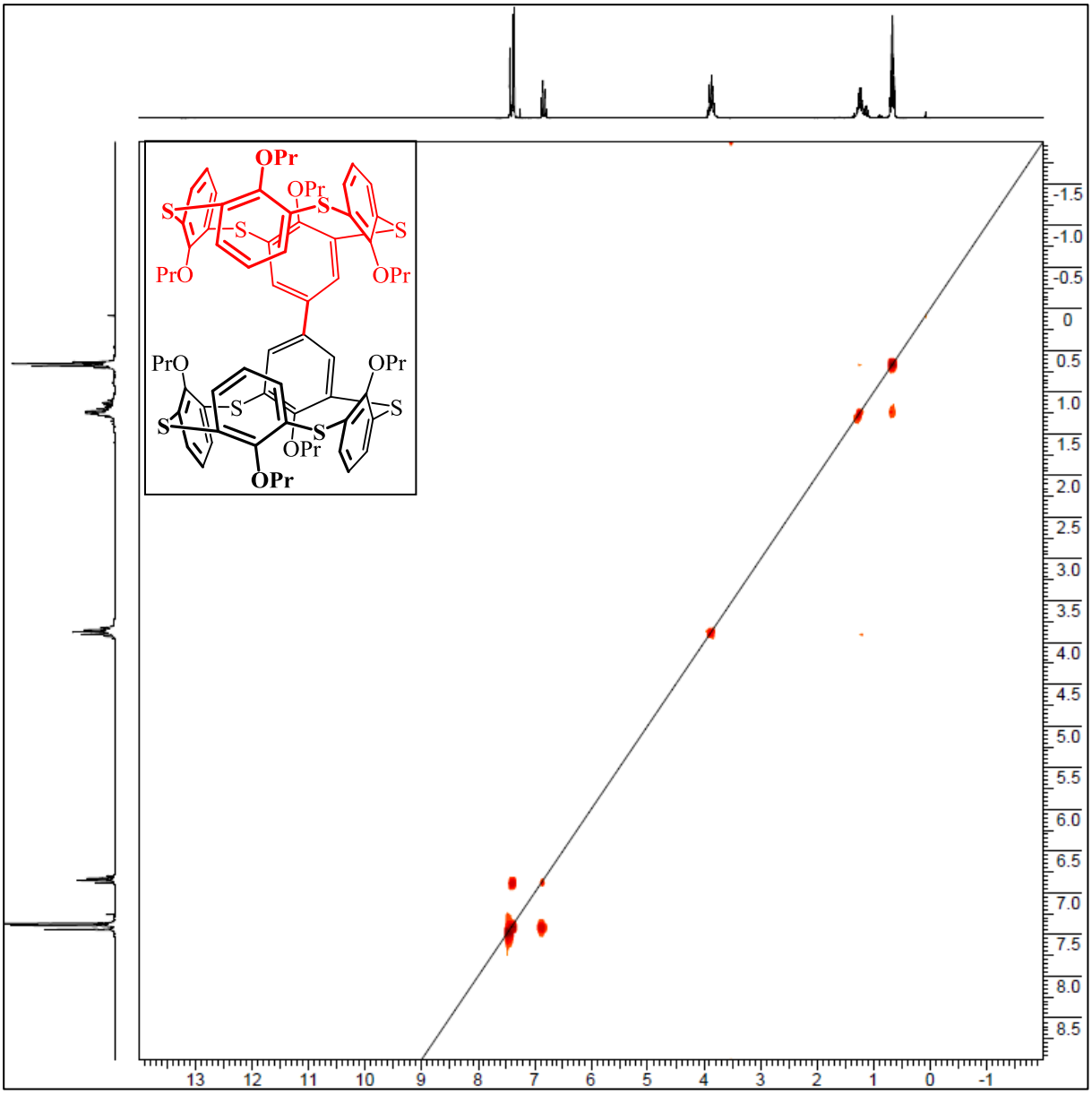

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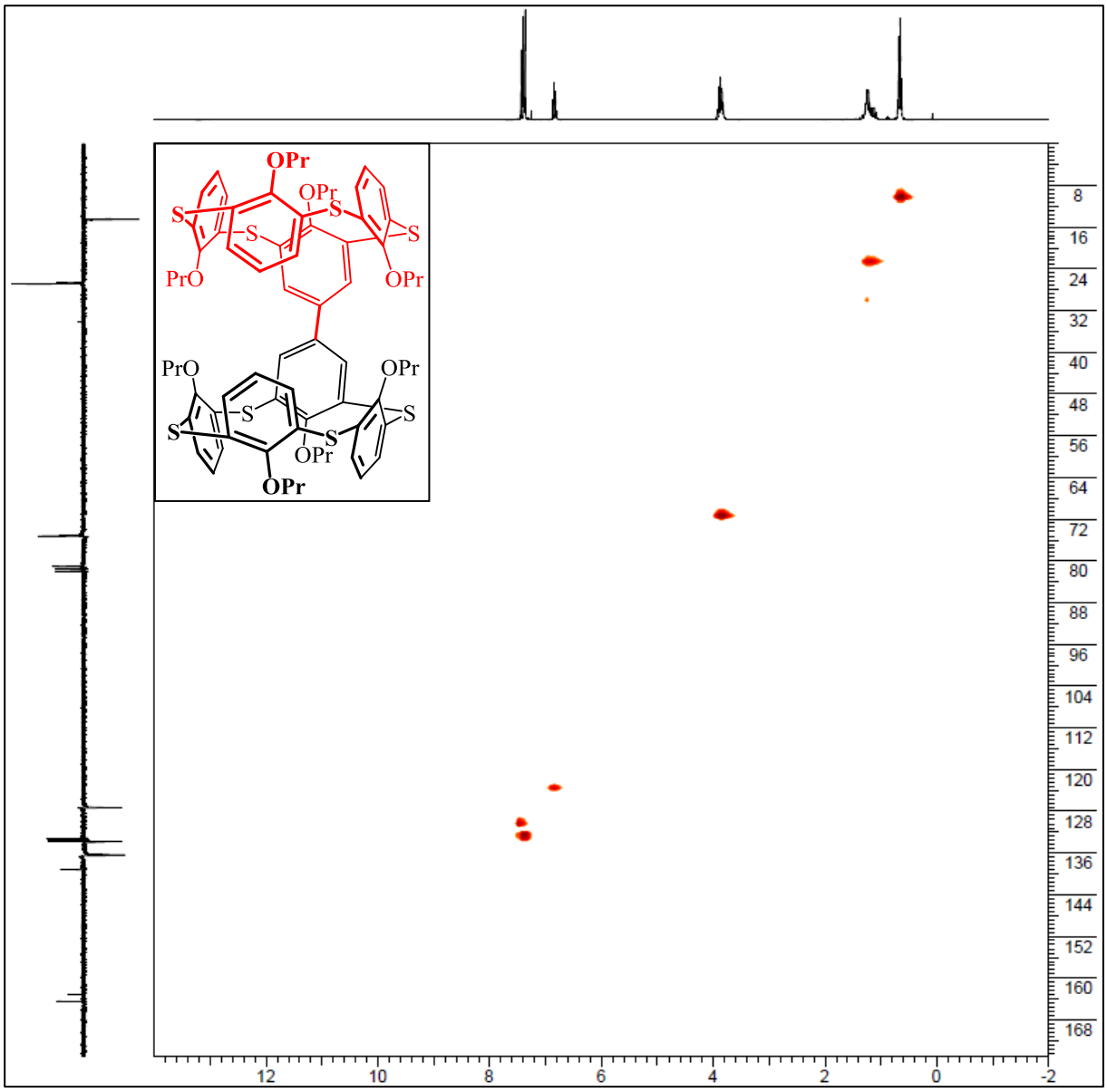

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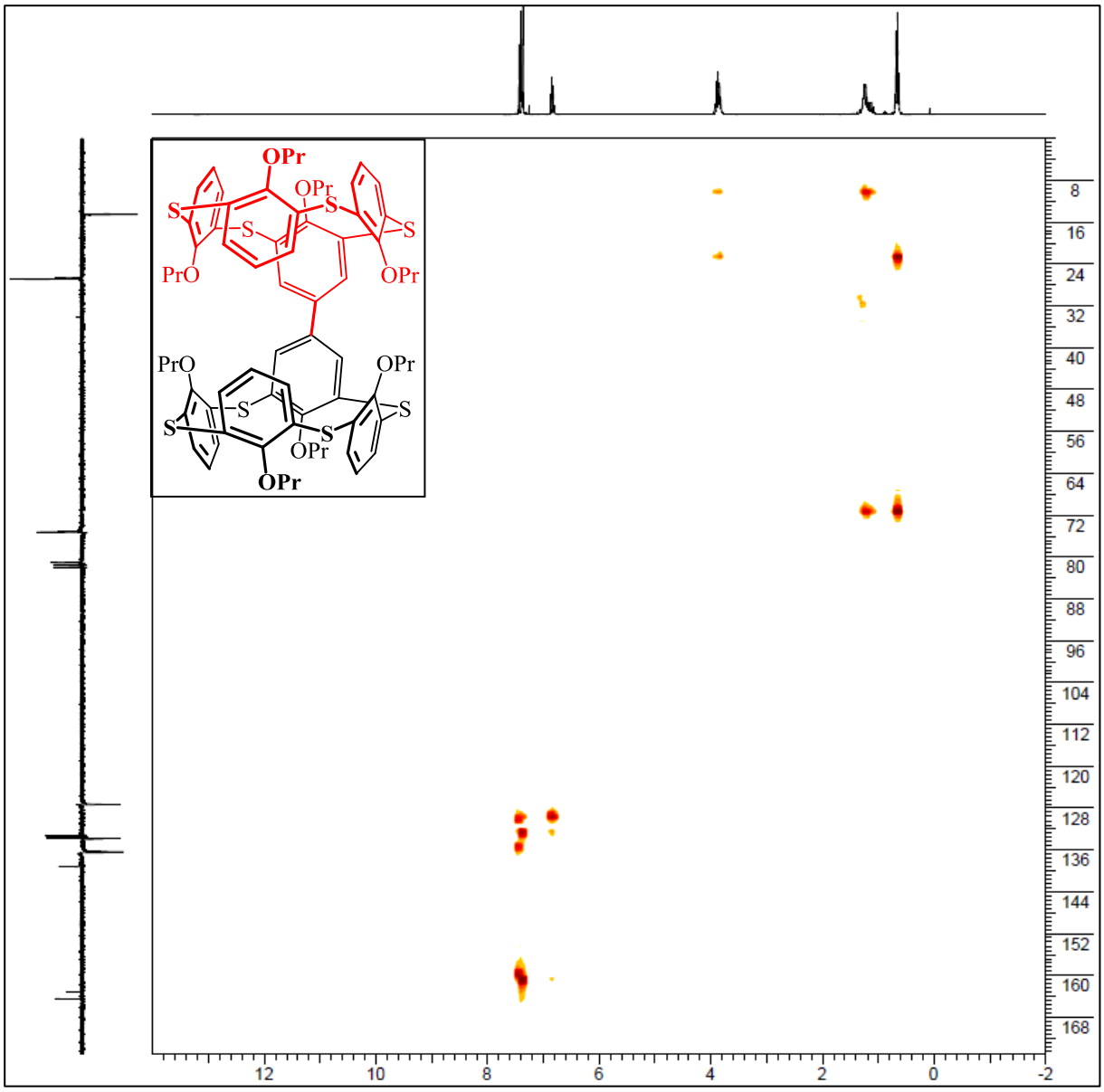
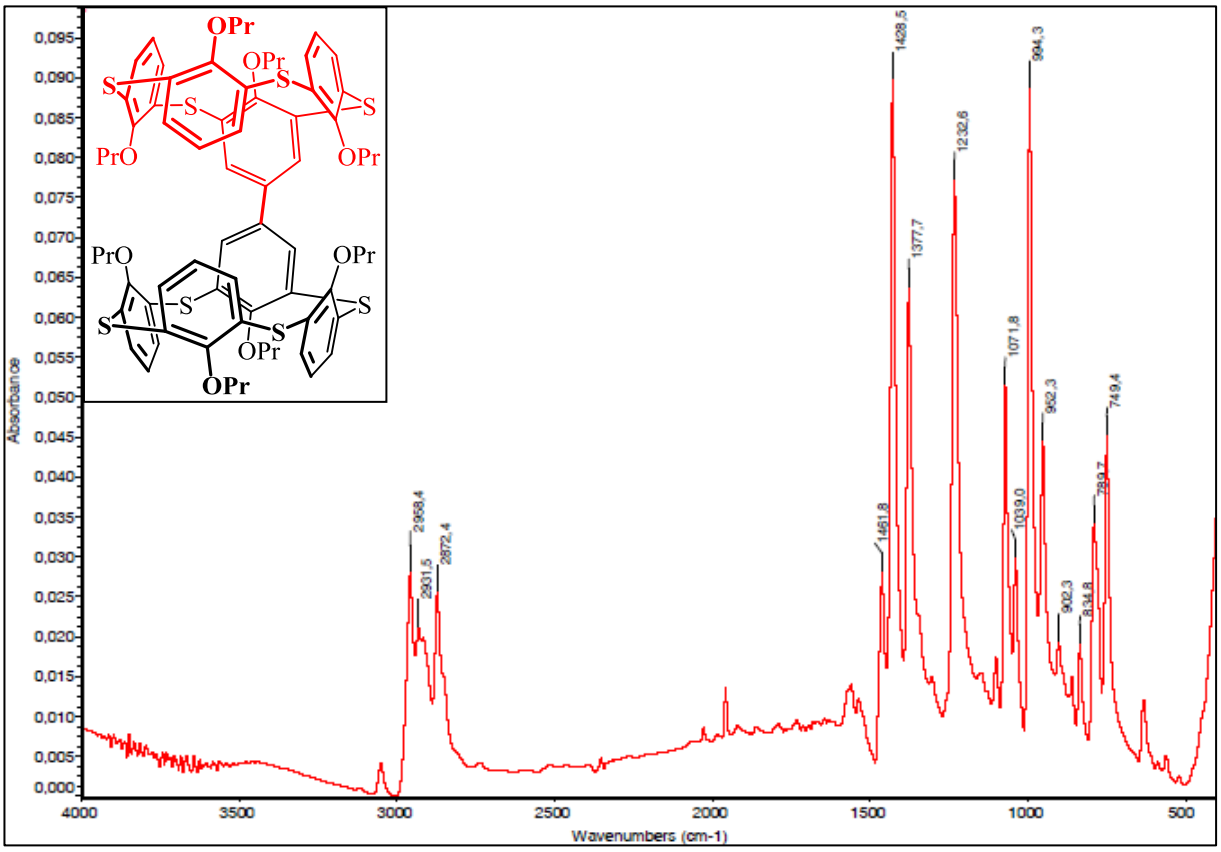


Figure 33: ^{1}H-^{13}C gHMBC 2D NMR spectrum ($CDCl_3$, 300 MHz, 298 K) of compound **11**



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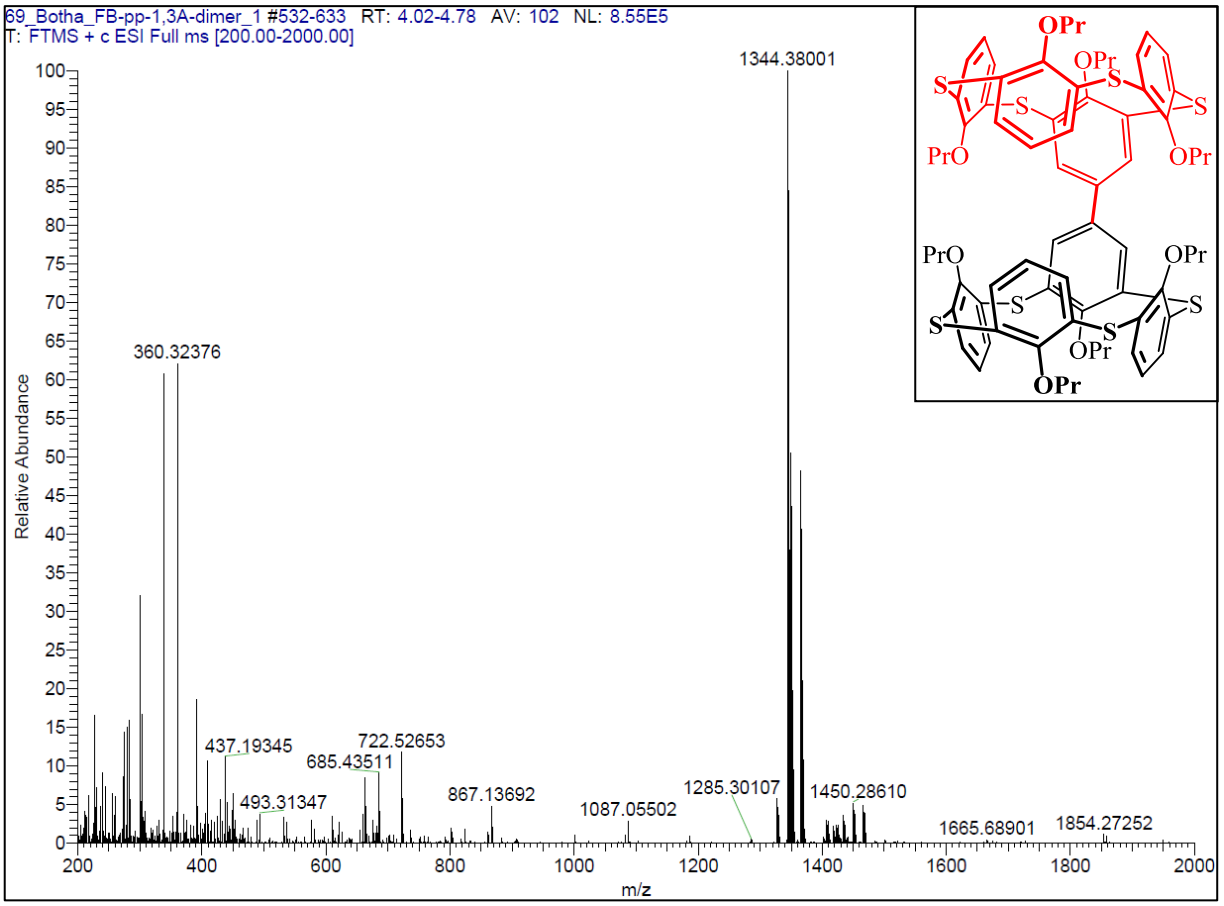

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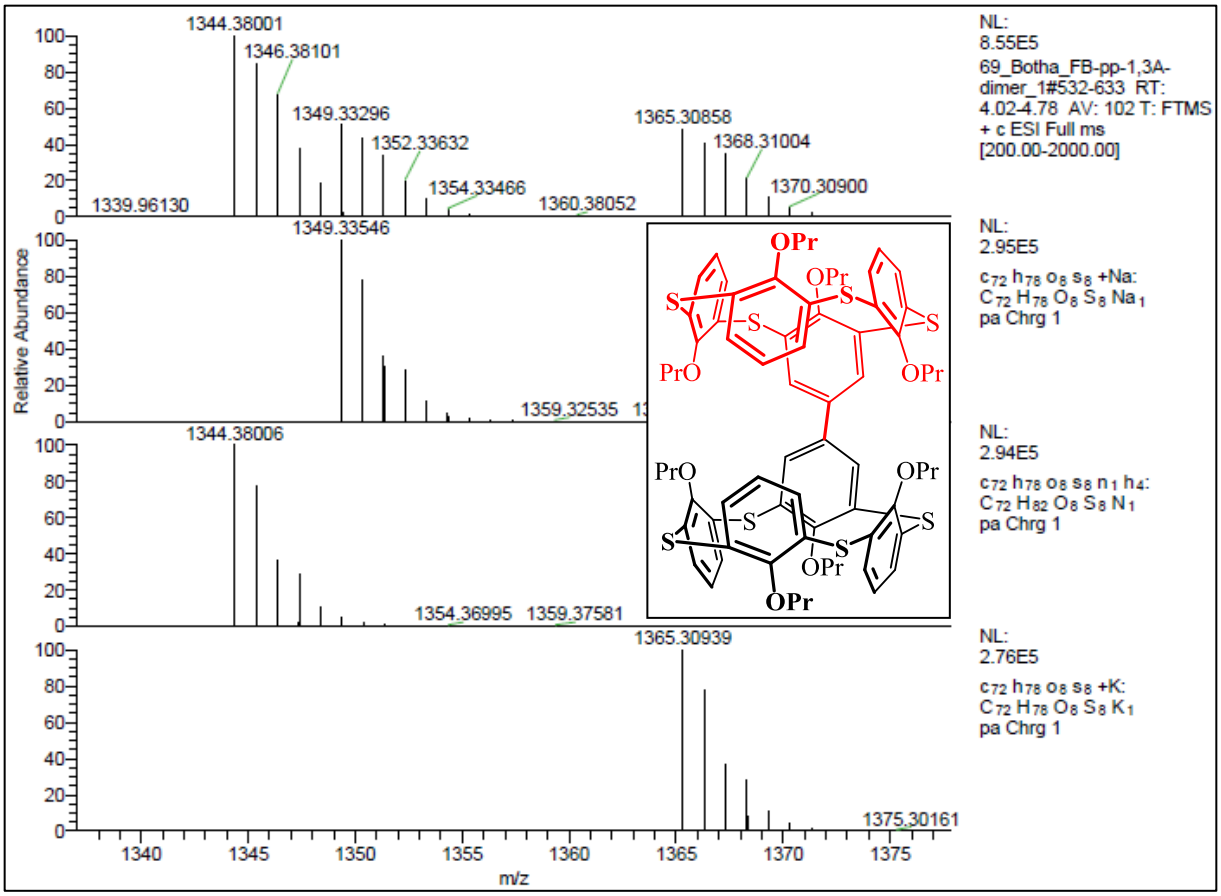

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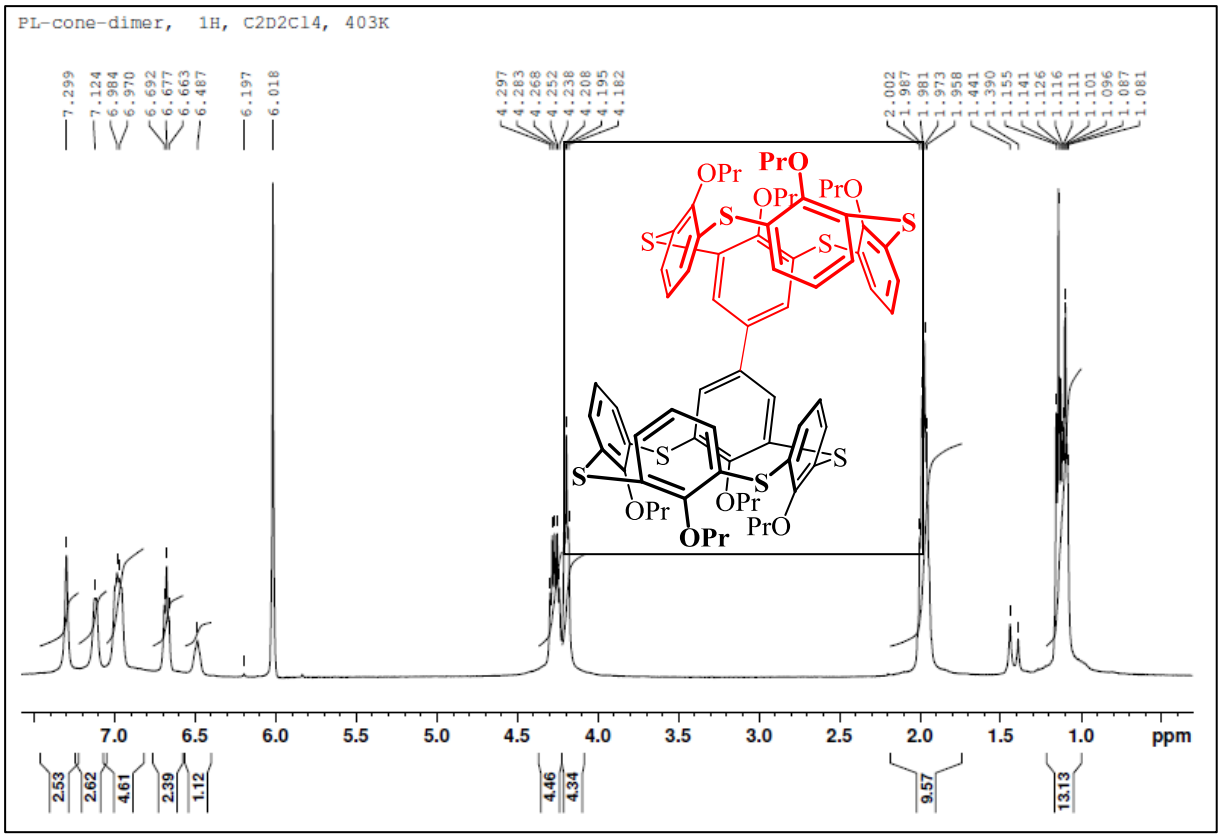


Figure 37: ^{1}H NMR spectrum ($C_2D_2Cl_4$, 500 MHz, 403 K) of compound **13**

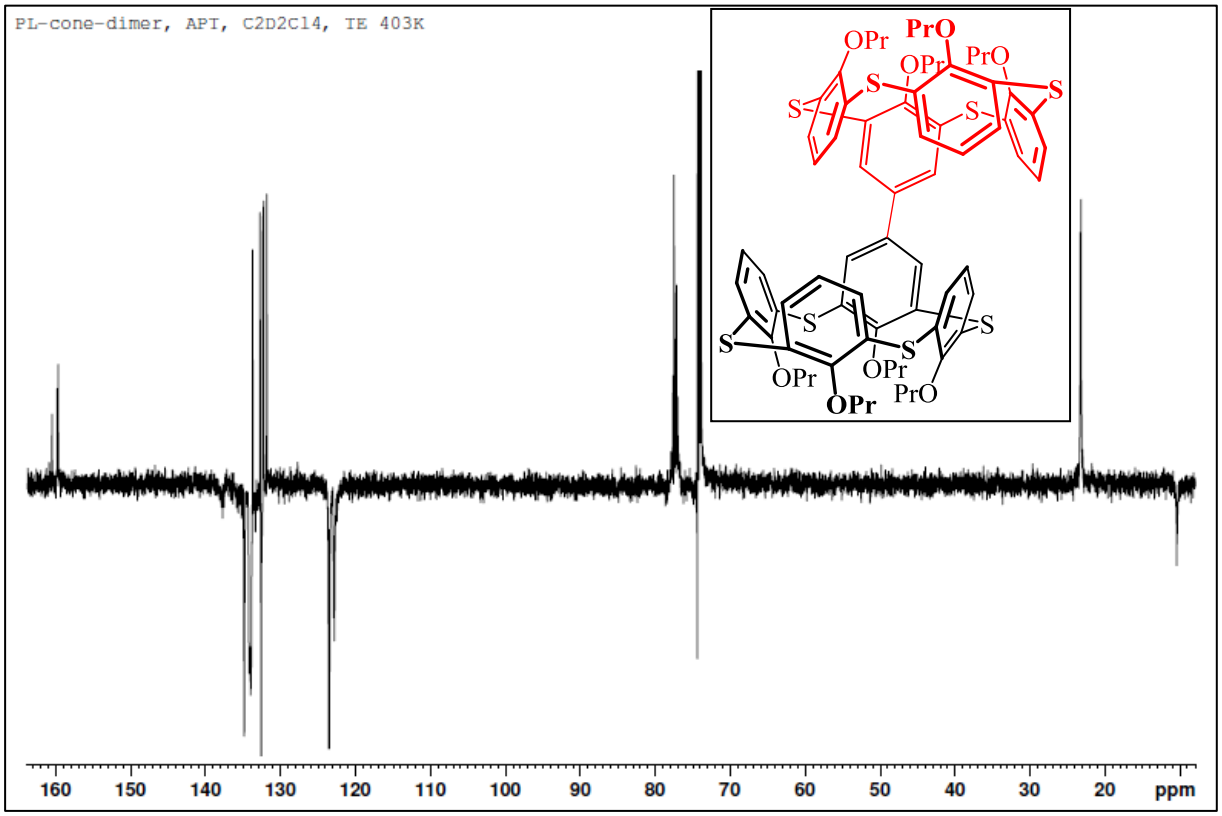


Figure 38: ^{13}C NMR spectrum ($C_2D_2Cl_4$, 125 MHz, 403 K) of compound **13**

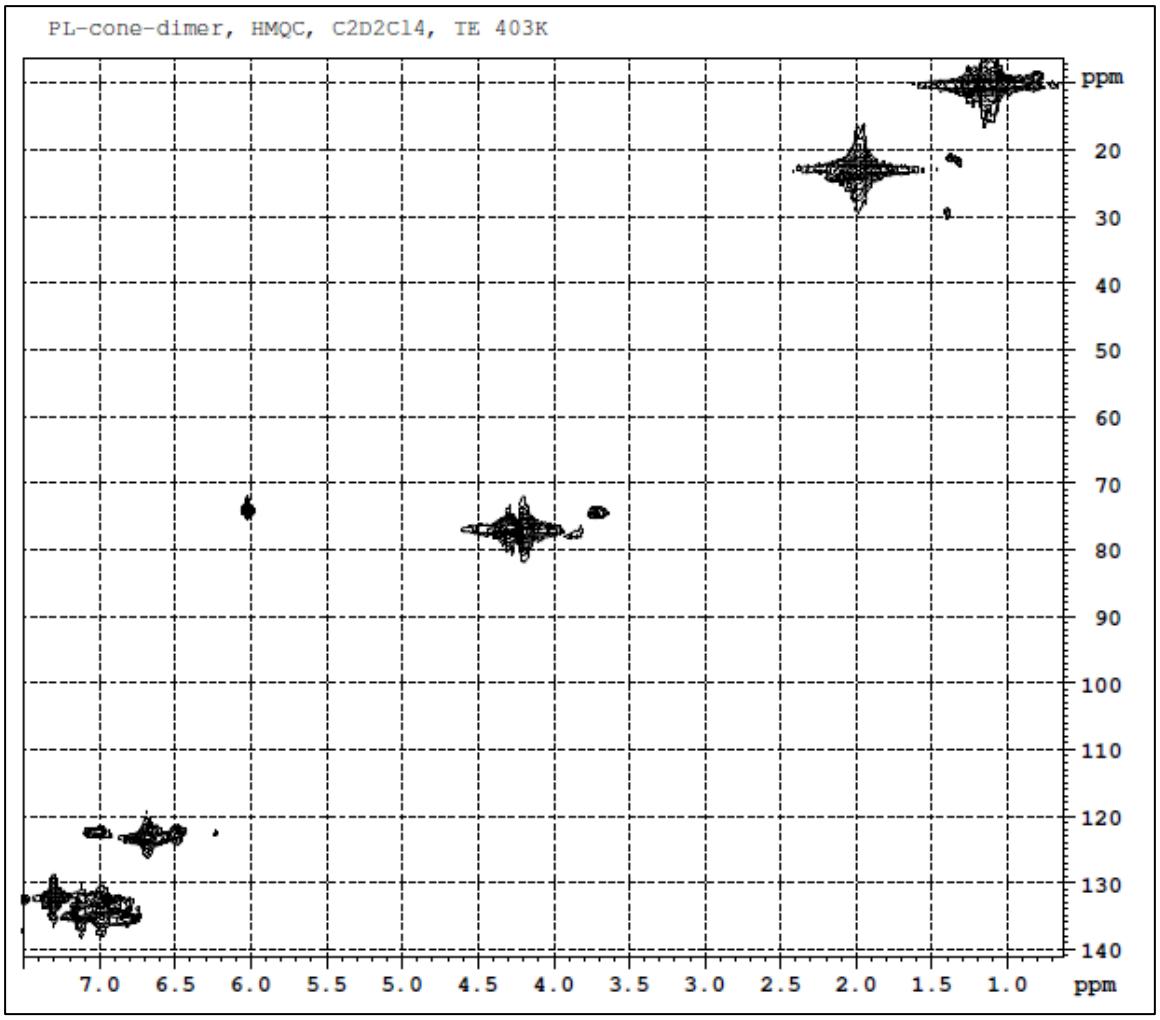
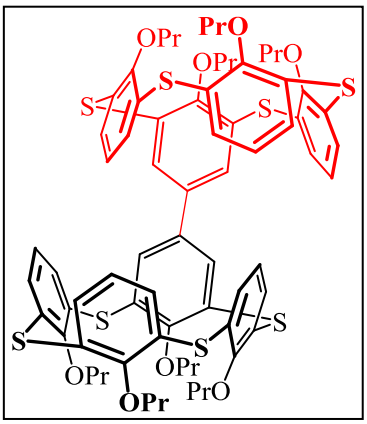


Figure 39: ^{1}H-^{13}C gHMQC 2D NMR spectrum ($C_2D_2Cl_4$, 500 MHz, 403 K) of compound **13**



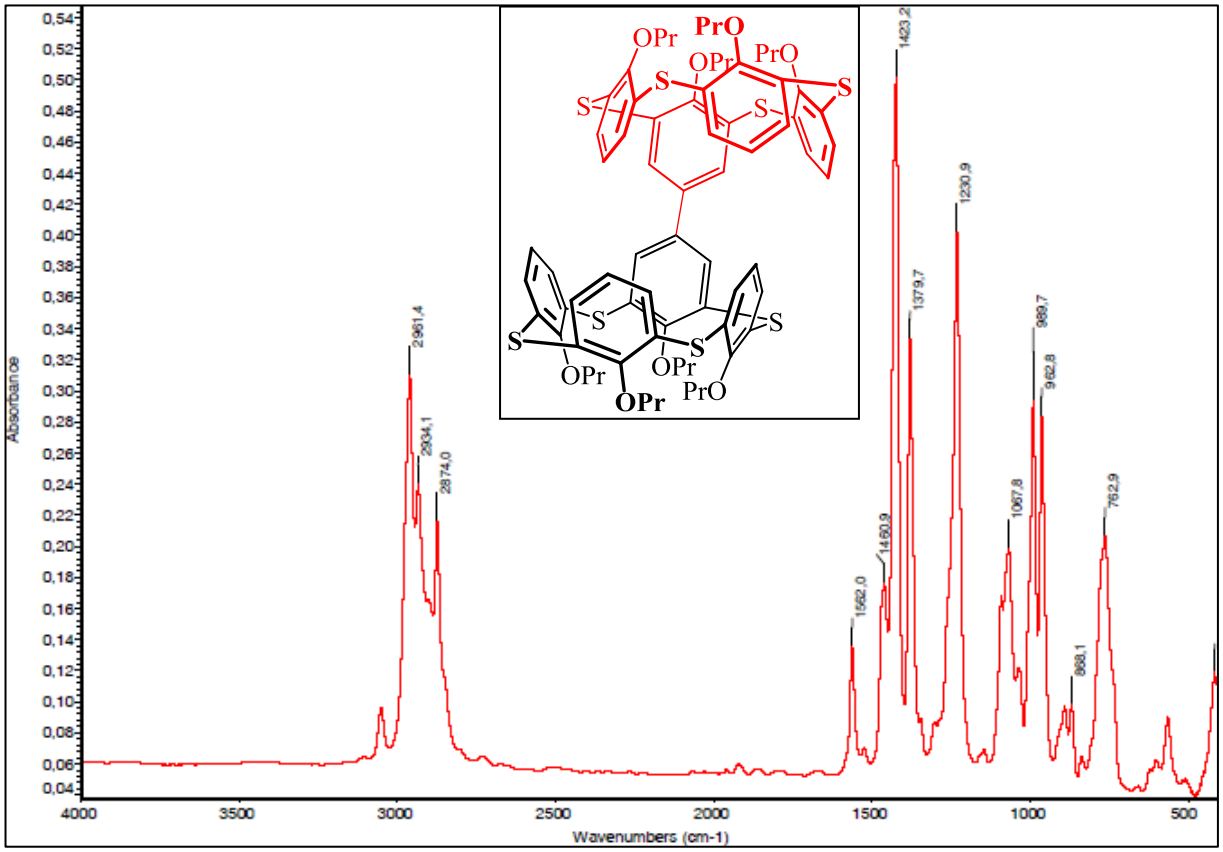


Figure 40: IR spectrum (KBr) of compound **13**

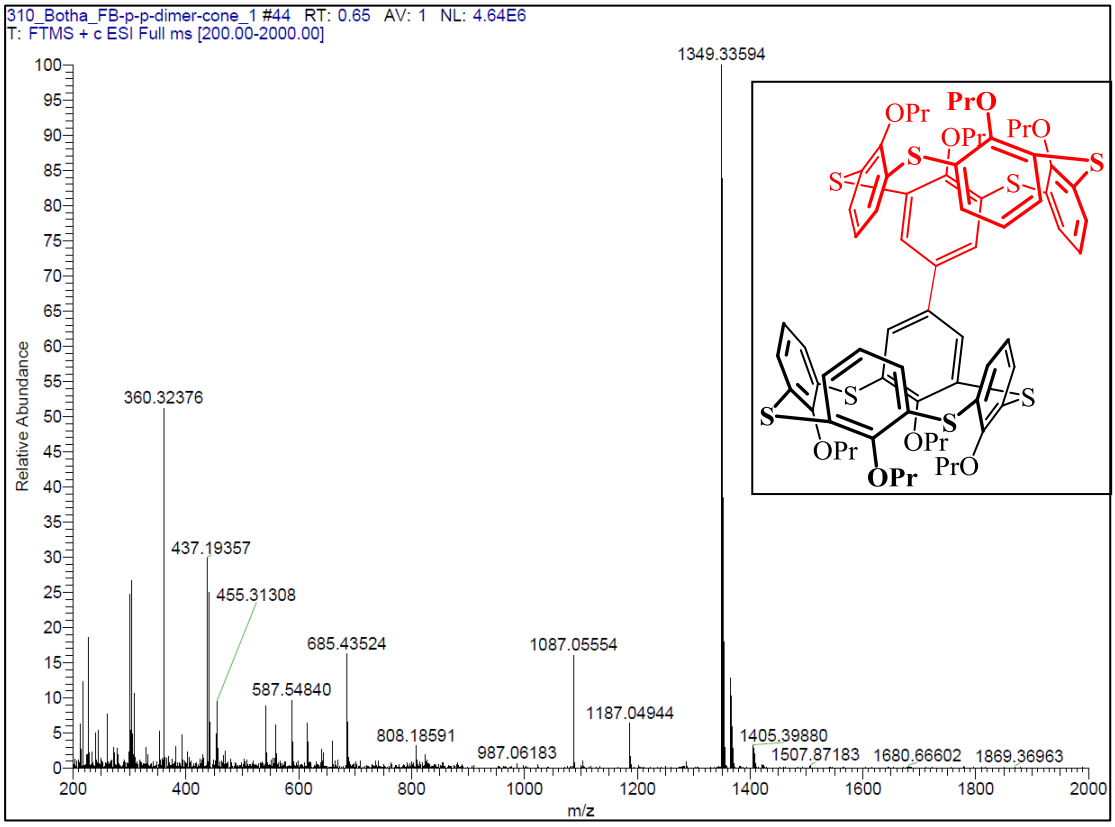


Figure 41: HRMS spectrum of compound **13**

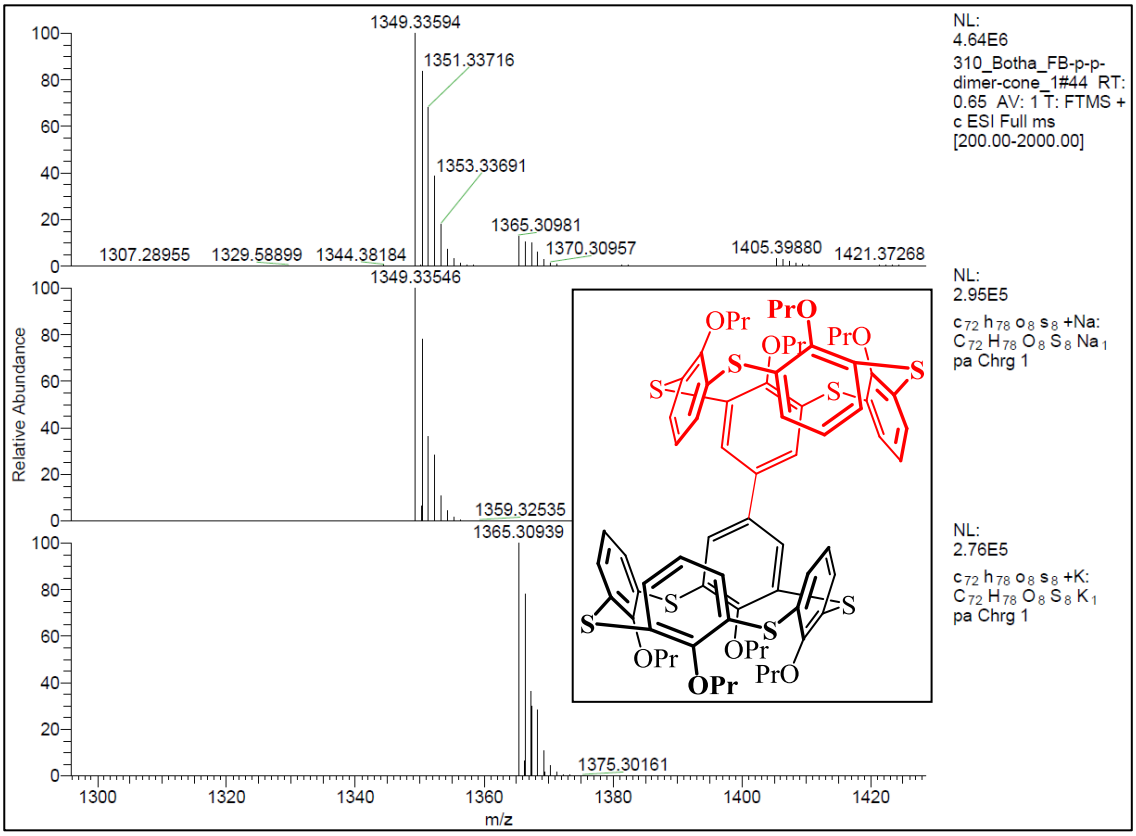


Figure 42: Adducts in HRMS spectrum of compound **13**

2. Crystallographic data

The following figures show the numbering used in the crystallographic study.

Structures are depicted with displacement ellipsoids drawn at the 50% probability level. The hydrogen atoms were omitted for sake of figures legibility (in case of **4**, **5** and **9** the weakly occupied atoms were omitted as well). In case of **13** symmetry code: (i) -x,-y+2,-z+1.

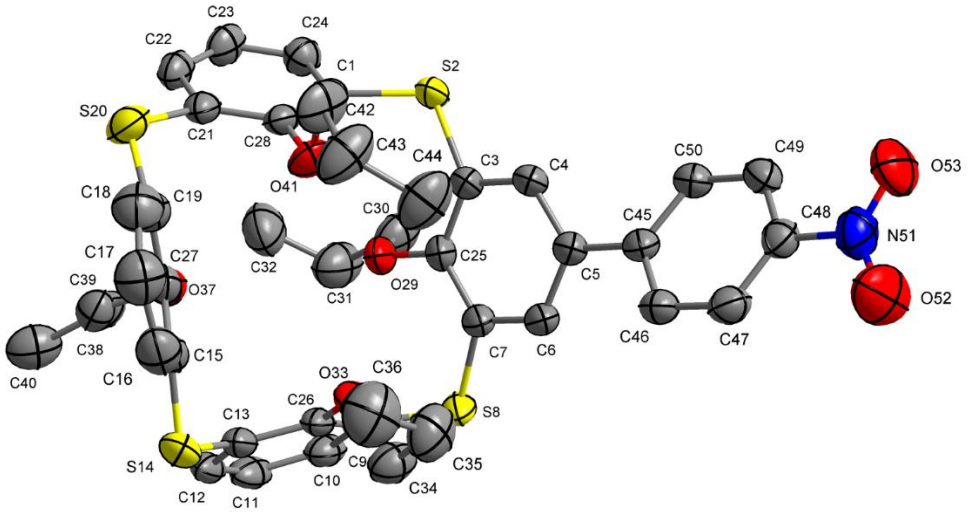


Figure 43: ORTEP drawing of compound **4**

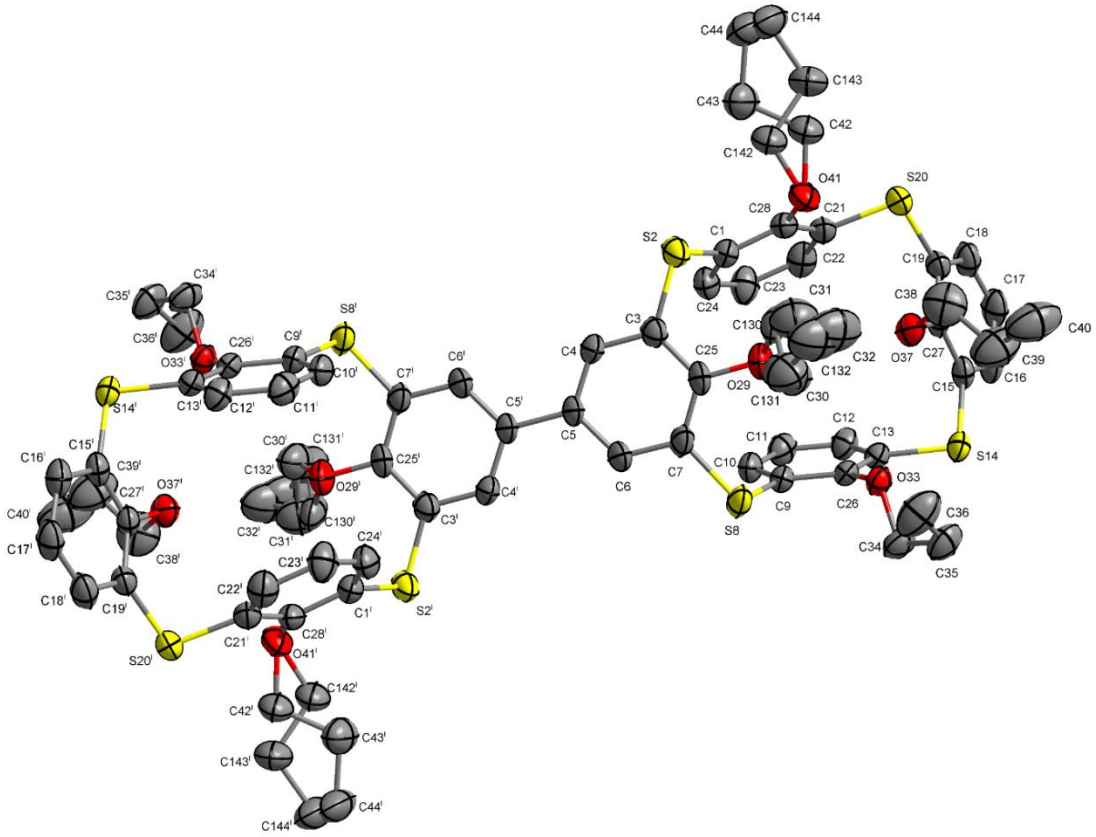


Figure 44: ORTEP drawing of compound **13**

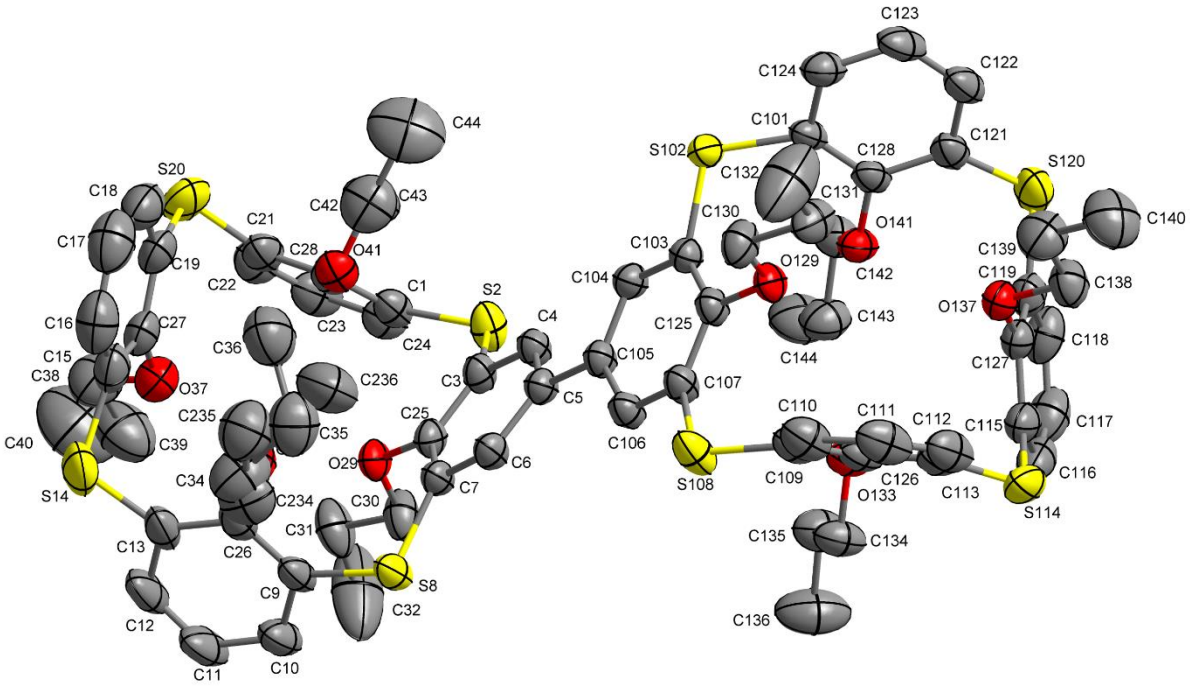


Figure 45: ORTEP drawing of compound **11**

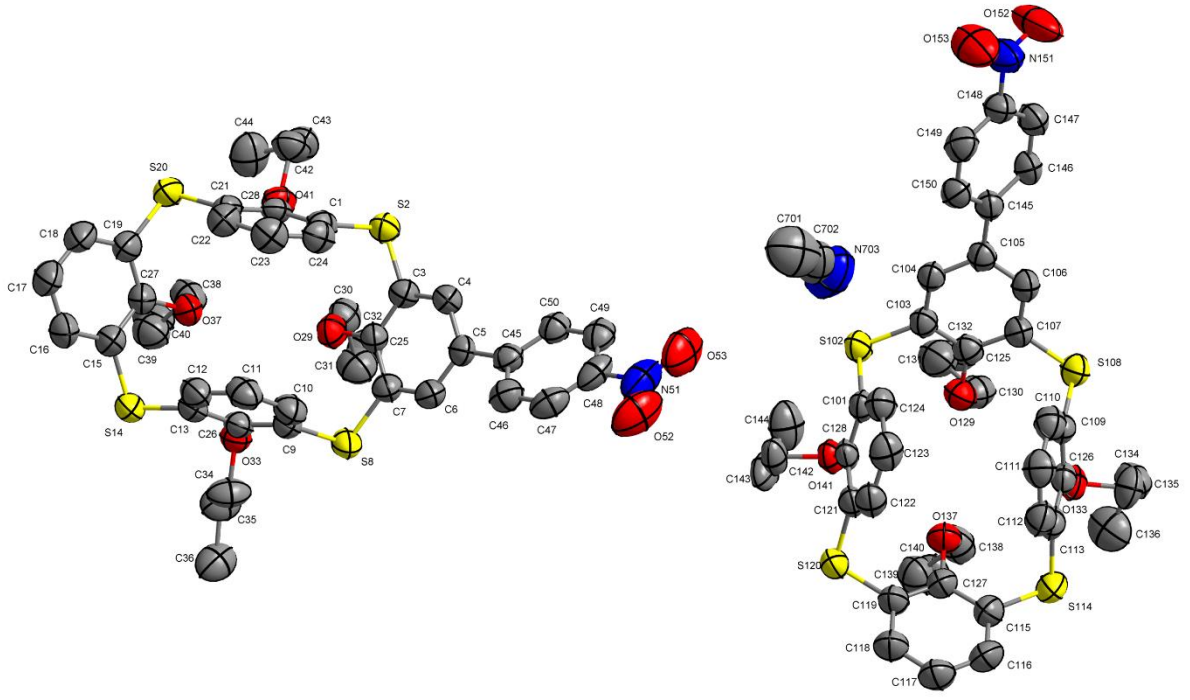


Figure 46: ORTEP drawing of compound **9** (CH_3CN solvate)

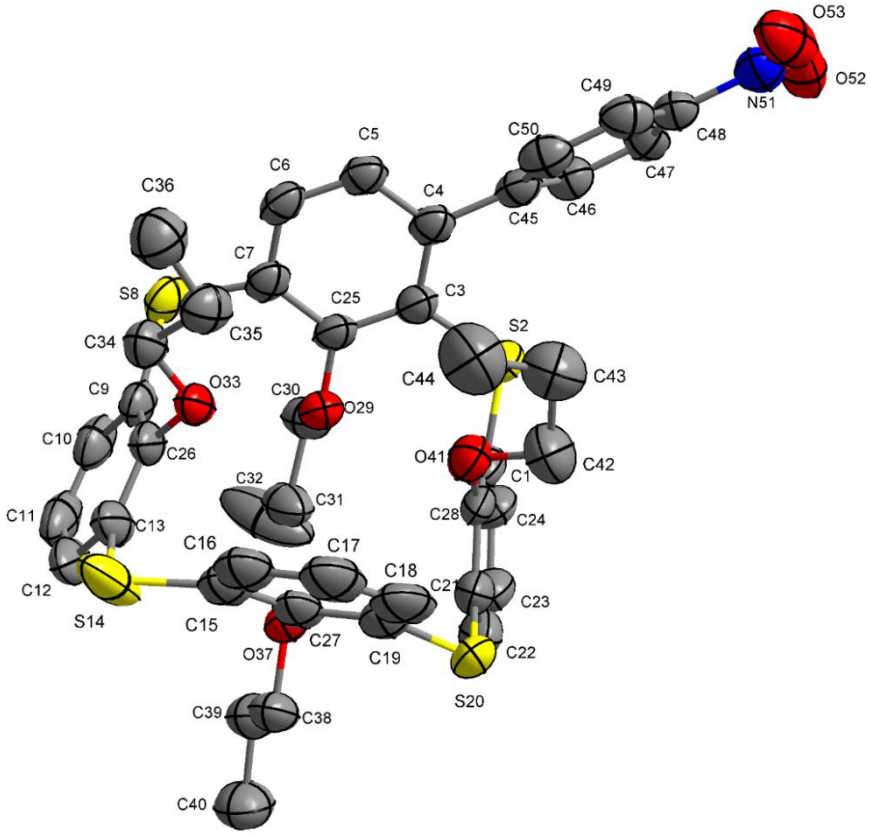


Figure 47: ORTEP drawing of compound **5**

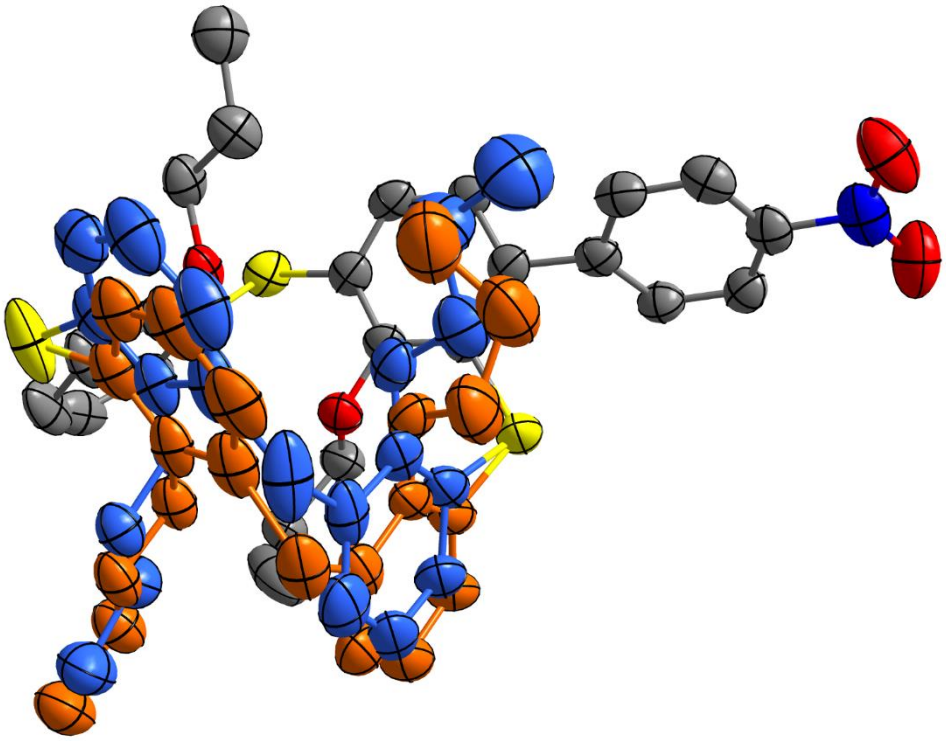


Figure 48: Disorder in **5**. The weakly occupied fragment is depicted in blue, the strongly occupied in orange.

3. Spectral data of impure compounds

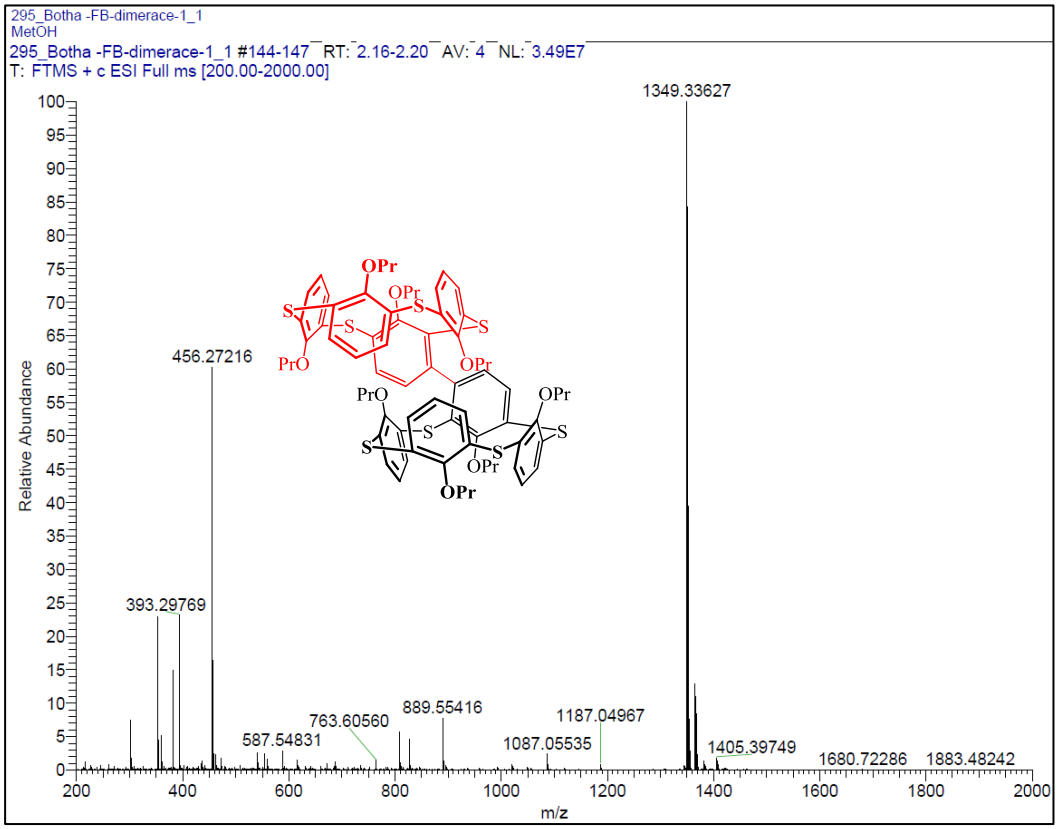


Figure 49: HRMS spectrum of compound **12**

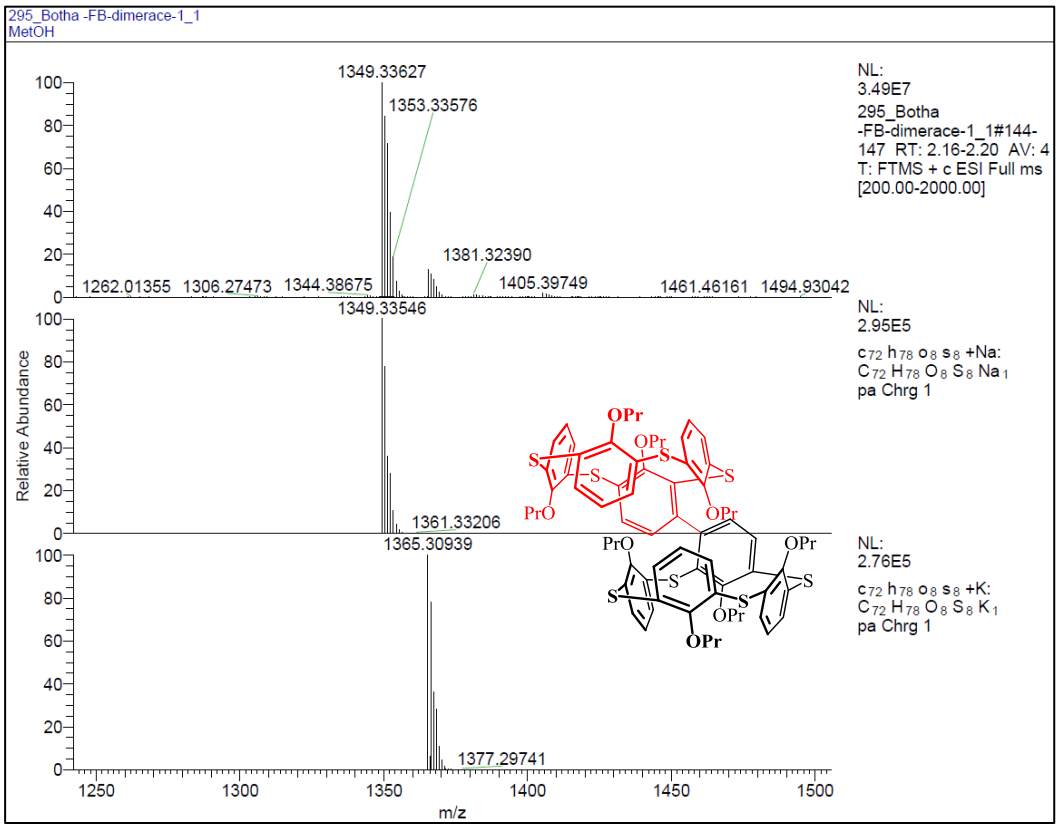


Figure 50: Adducts in HRMS spectrum of compound **12**

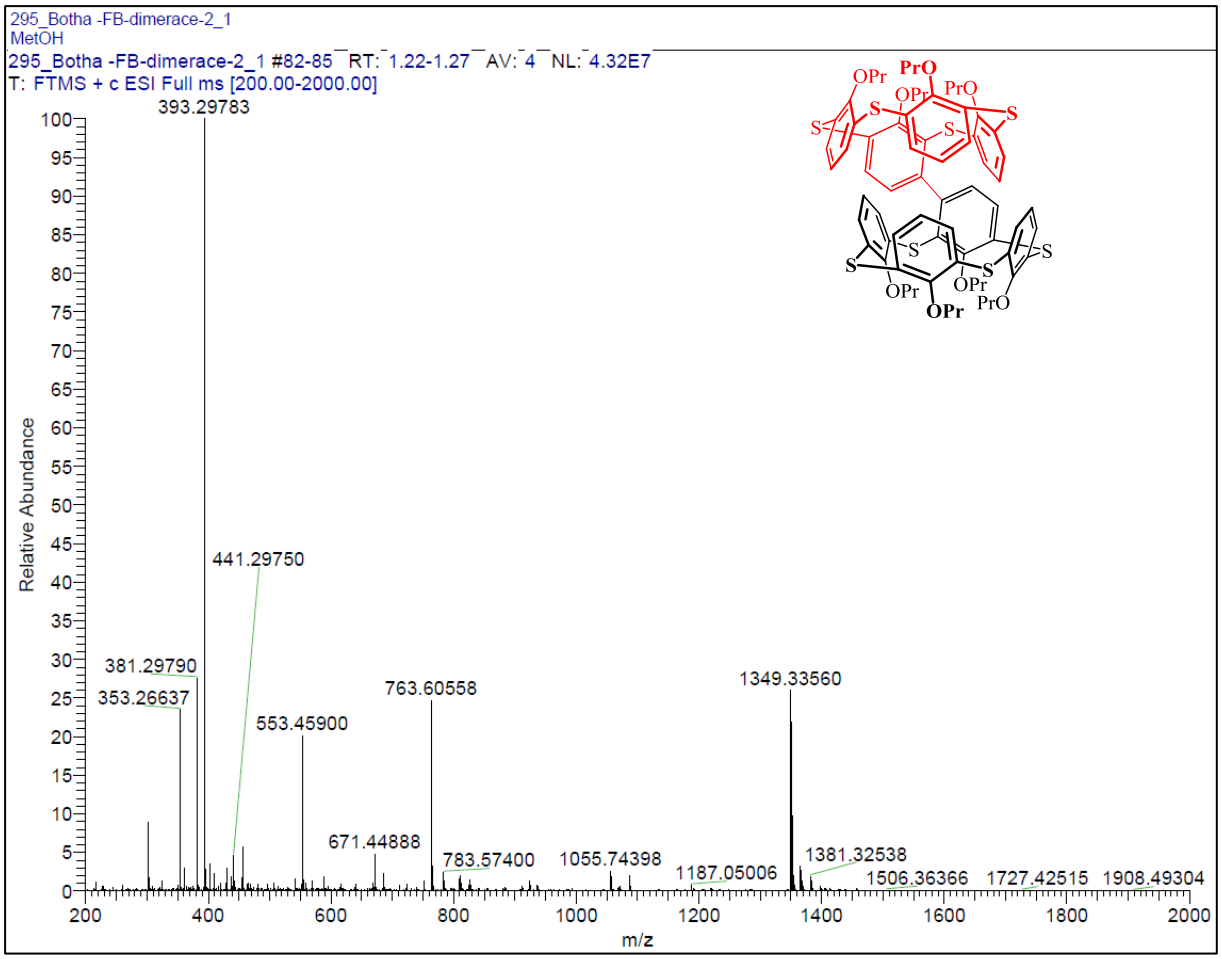


Figure 51: HRMS spectrum of compound **14**

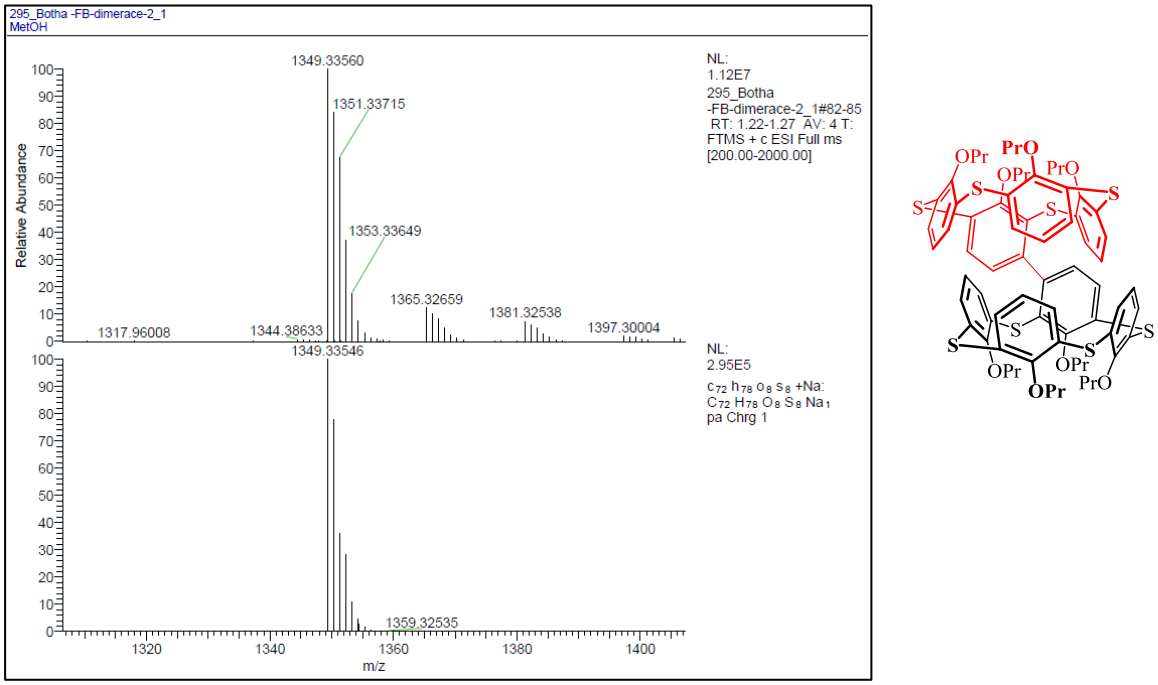


Figure 52: Adducts in HRMS spectrum of compound **14**