

## Supporting Information

for

### Click synthesis and complexation properties of a new unsymmetrical macrocycle bearing 1,4-dioxabenzene and triazole units

by

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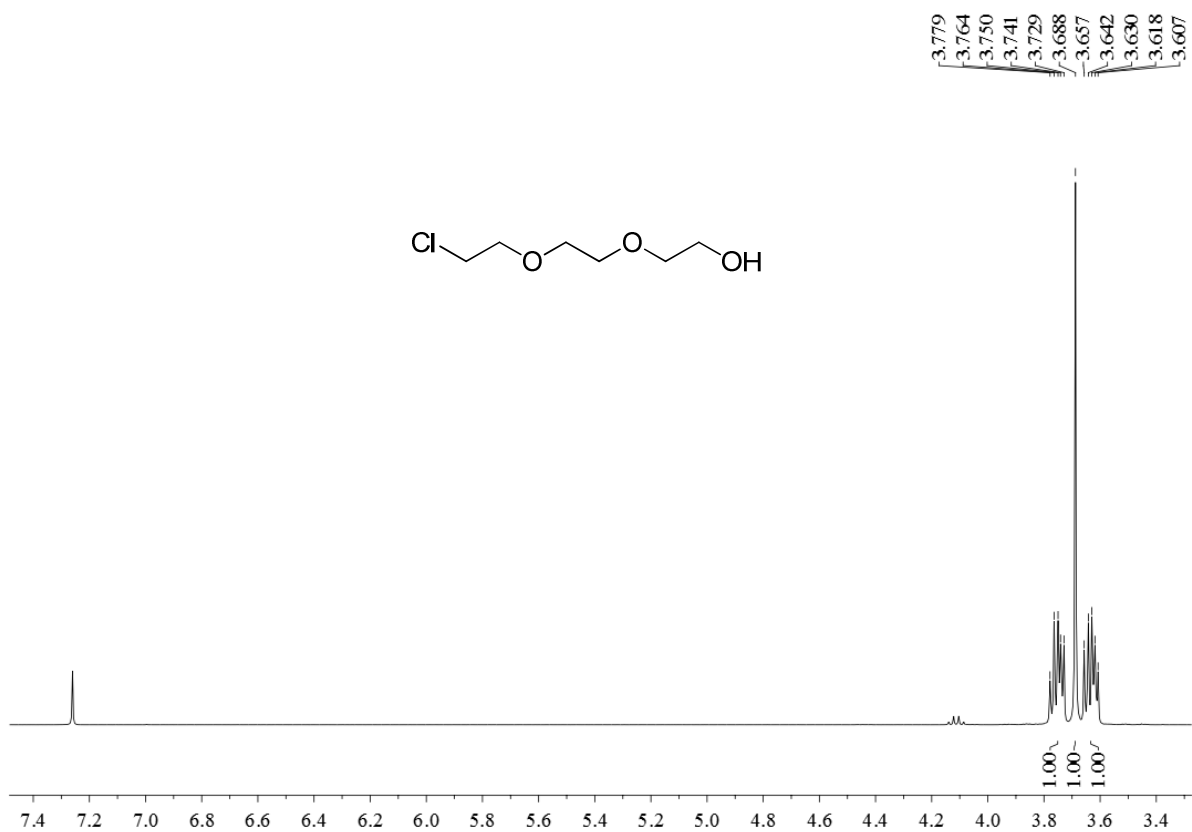
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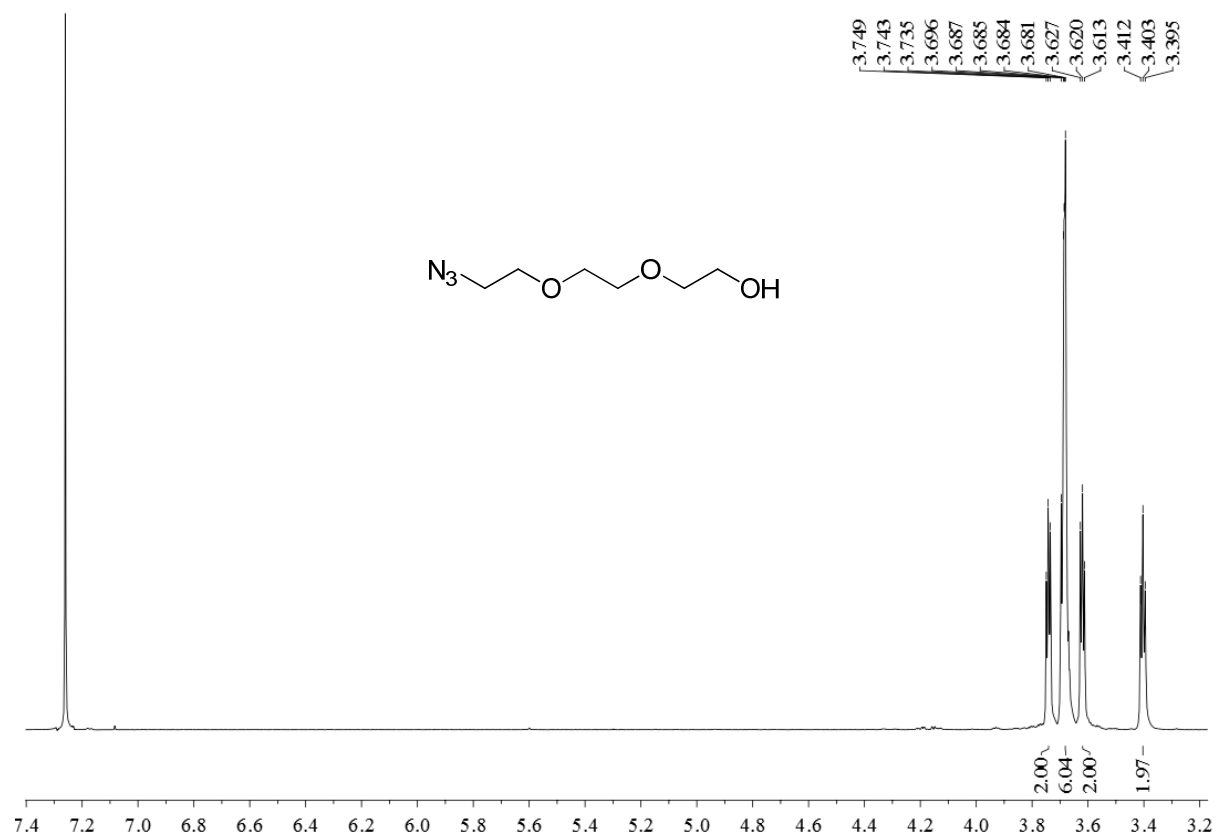
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**Figure S1.** <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz) spectrum of compound 1.



**Figure S2.** <sup>1</sup>H NMR (CDCl<sub>3</sub>, 600 MHz) spectrum of compound 2.

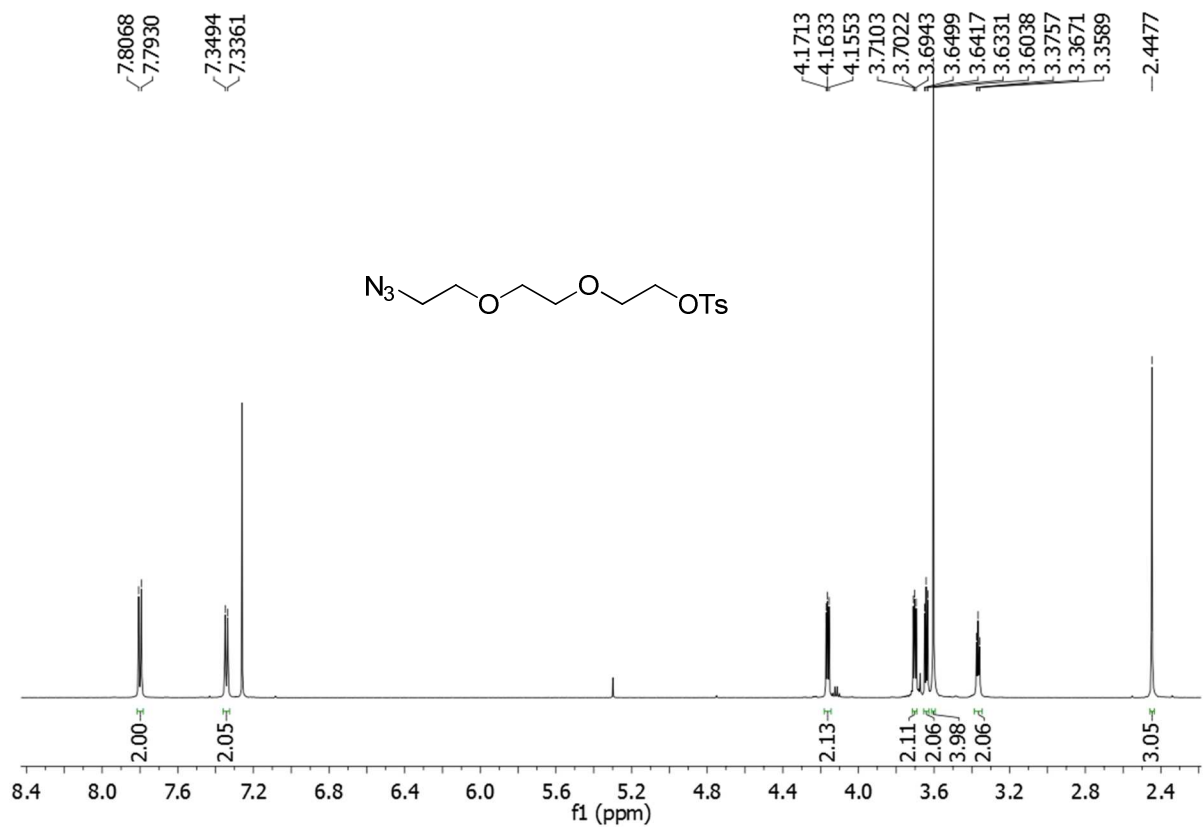


Figure S3. <sup>1</sup>H NMR (CDCl<sub>3</sub>, 600 MHz) spectrum of compound 3.

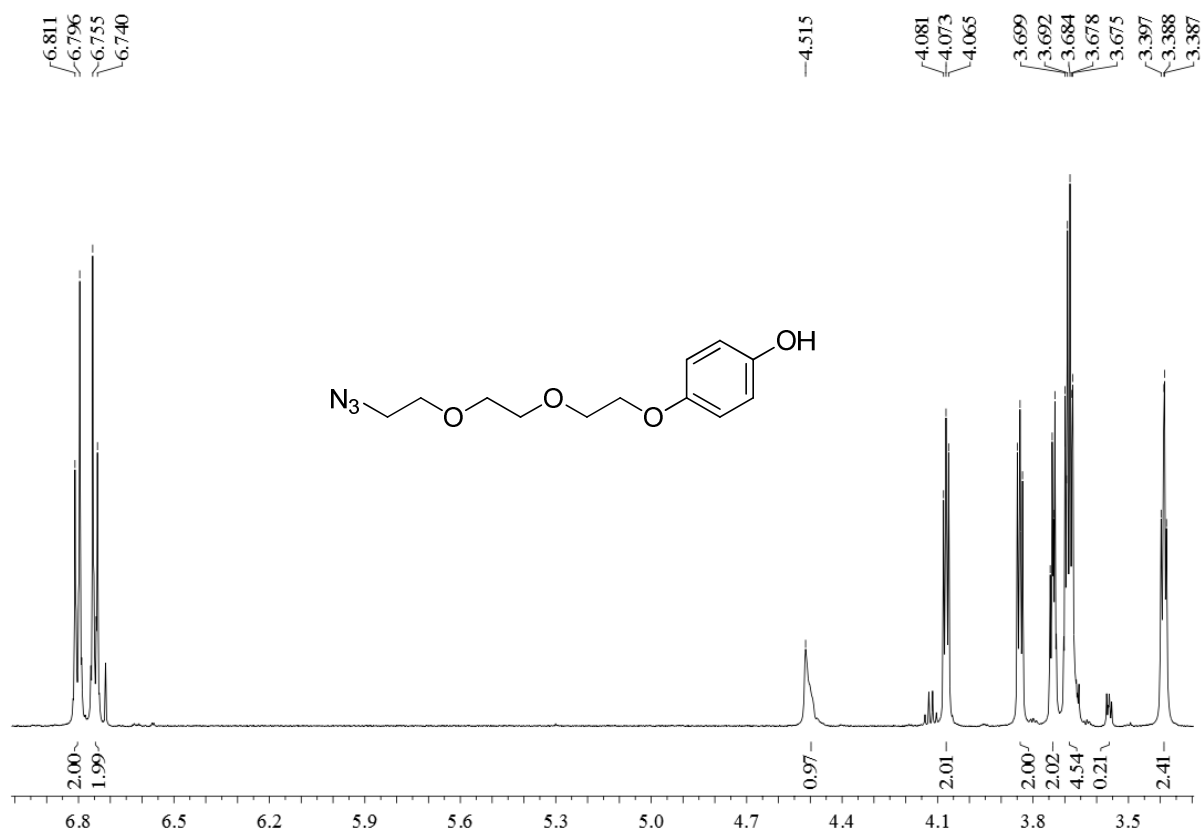
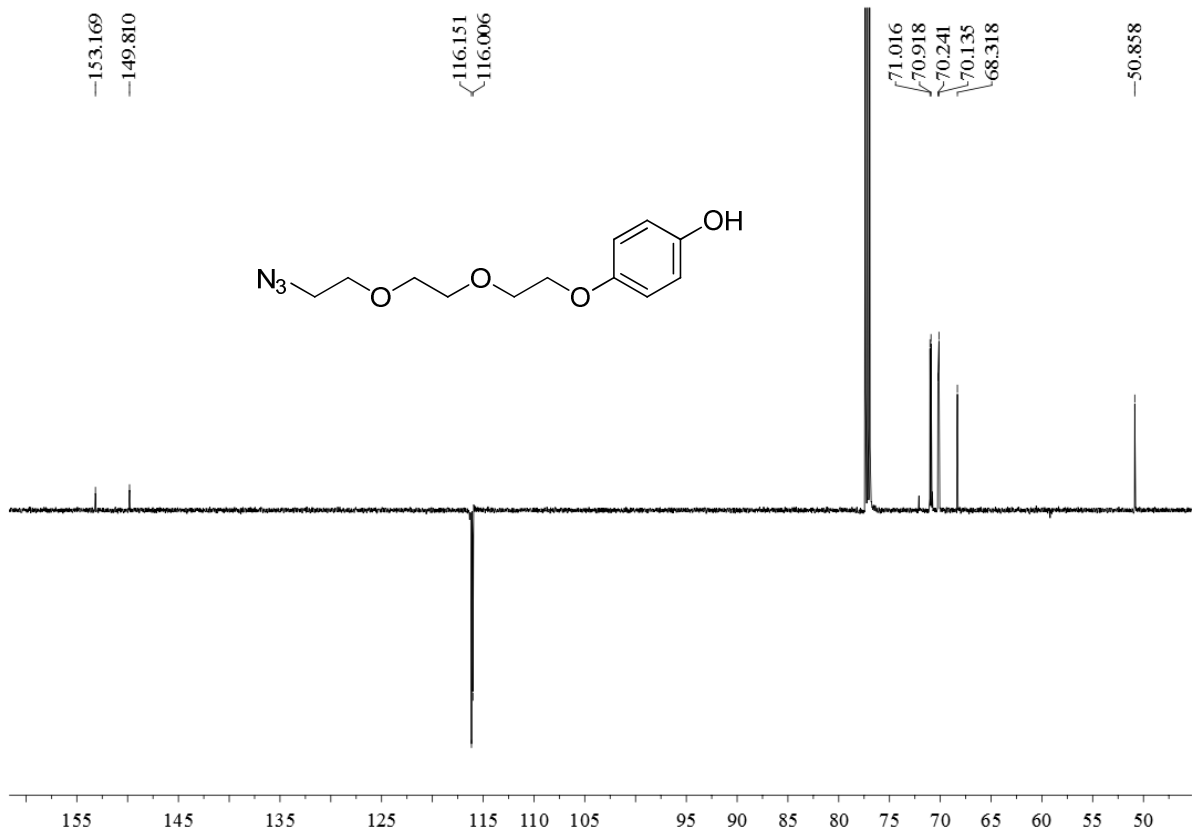
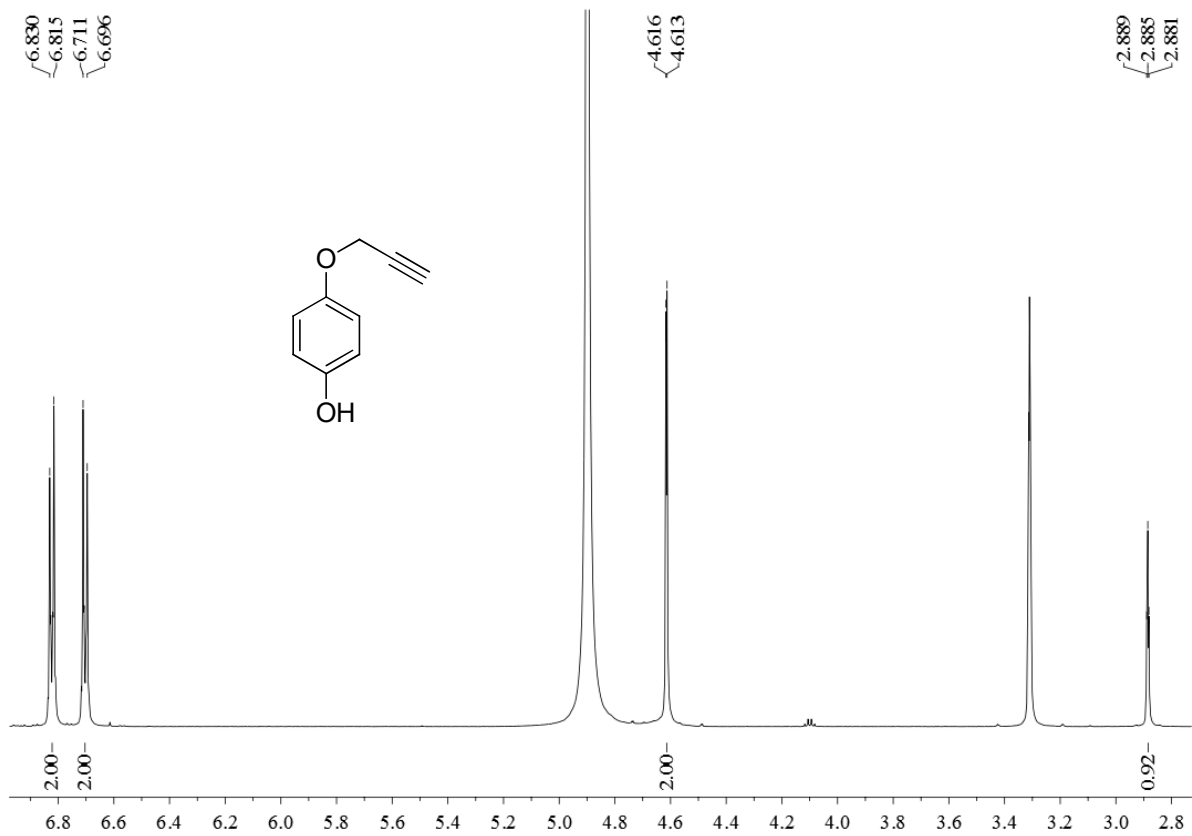


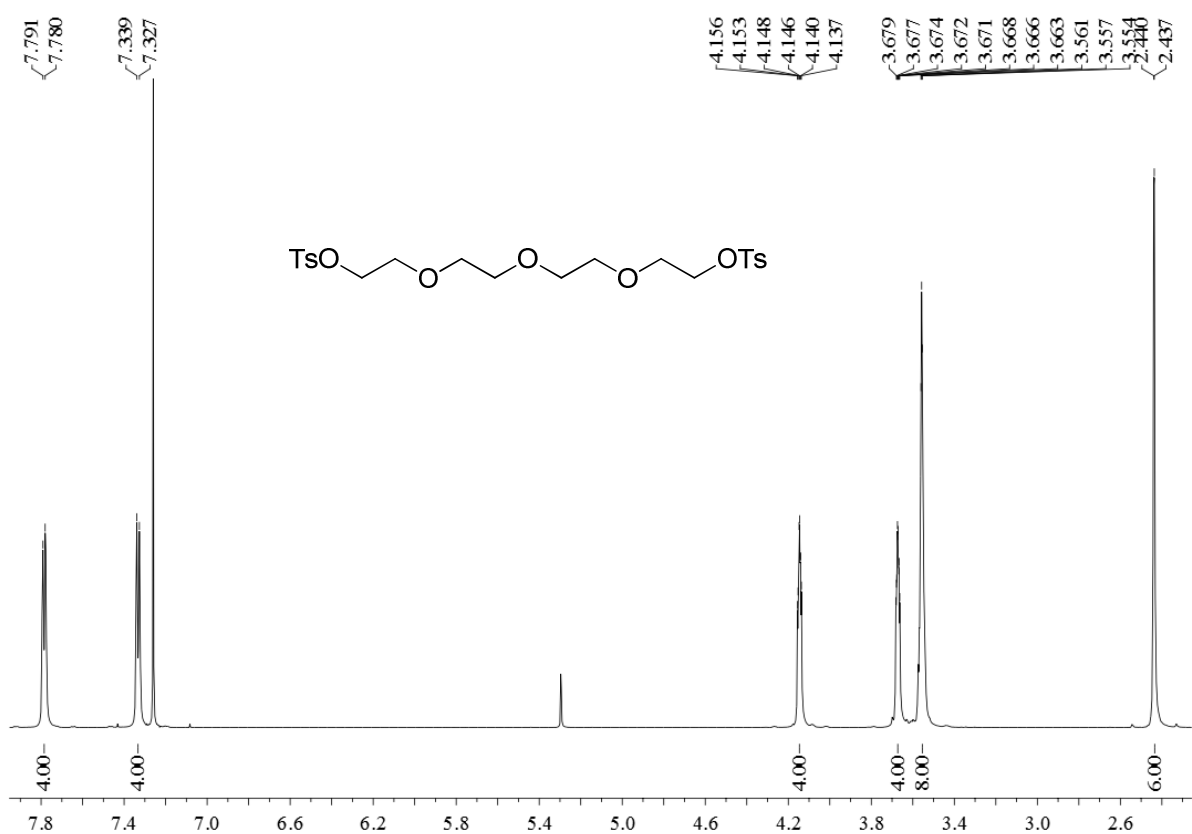
Figure S4. <sup>1</sup>H NMR (CDCl<sub>3</sub>, 600 MHz) spectrum of compound 4.



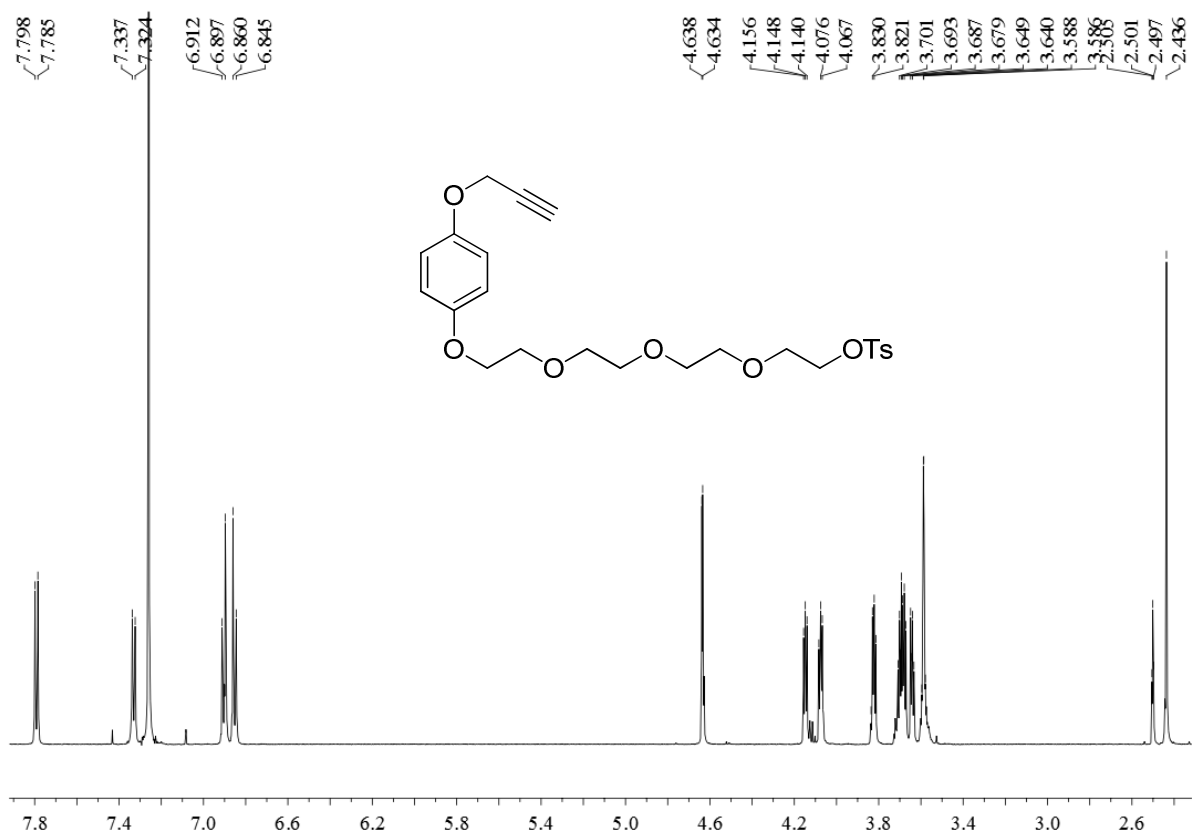
**Figure S5.** <sup>13</sup>C-APT-NMR (CDCl<sub>3</sub>, 150 MHz) spectrum of compound 4.



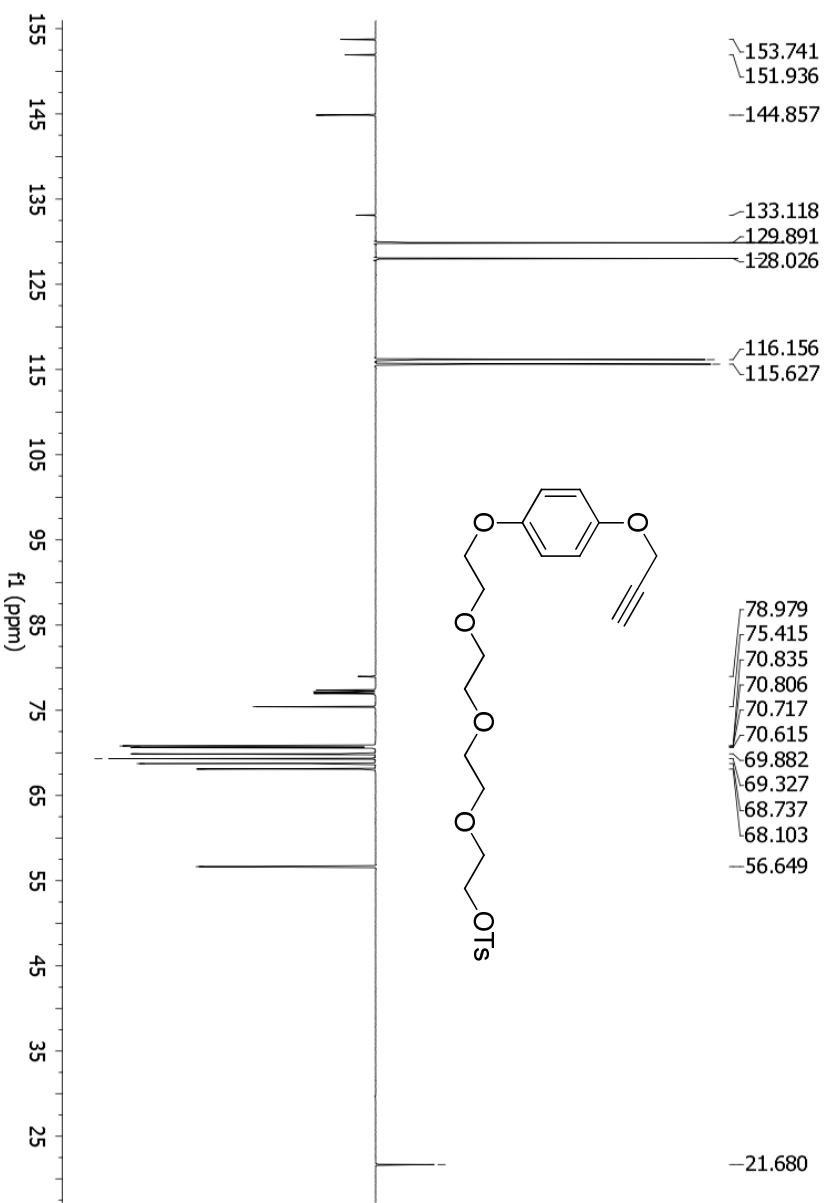
**Figure S6.** <sup>1</sup>H NMR (MeOD, 600 MHz) spectrum of compound 5.



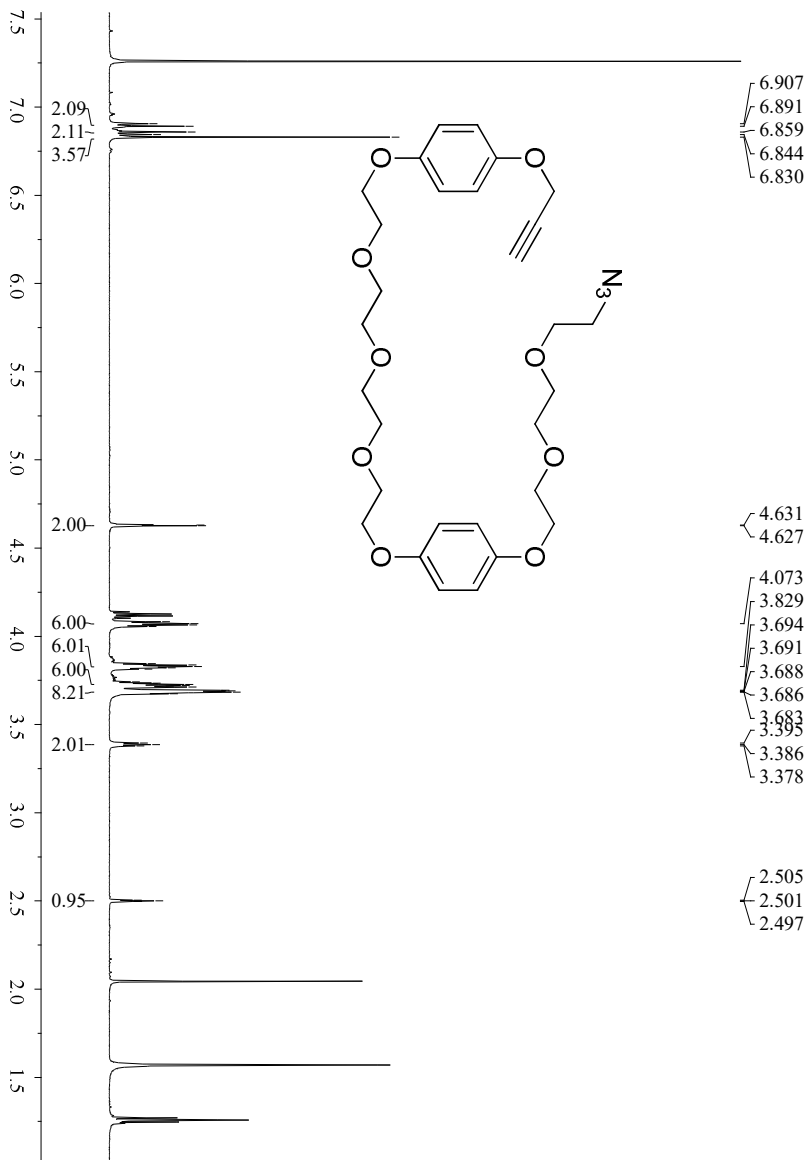
**Figure S7.**  $^1\text{H NMR}$  (CDCl<sub>3</sub>, 600 MHz) spectrum of compound 6.



**Figure S8.**  $^1\text{H NMR}$  (CDCl<sub>3</sub>, 600 MHz) spectrum of compound 7.



**Figure S9.** <sup>13</sup>C NMR (CDCl<sub>3</sub>, 150 MHz) spectrum of compound **7**.



**Figure S10.**  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 600 MHz) spectrum of compound **8**.

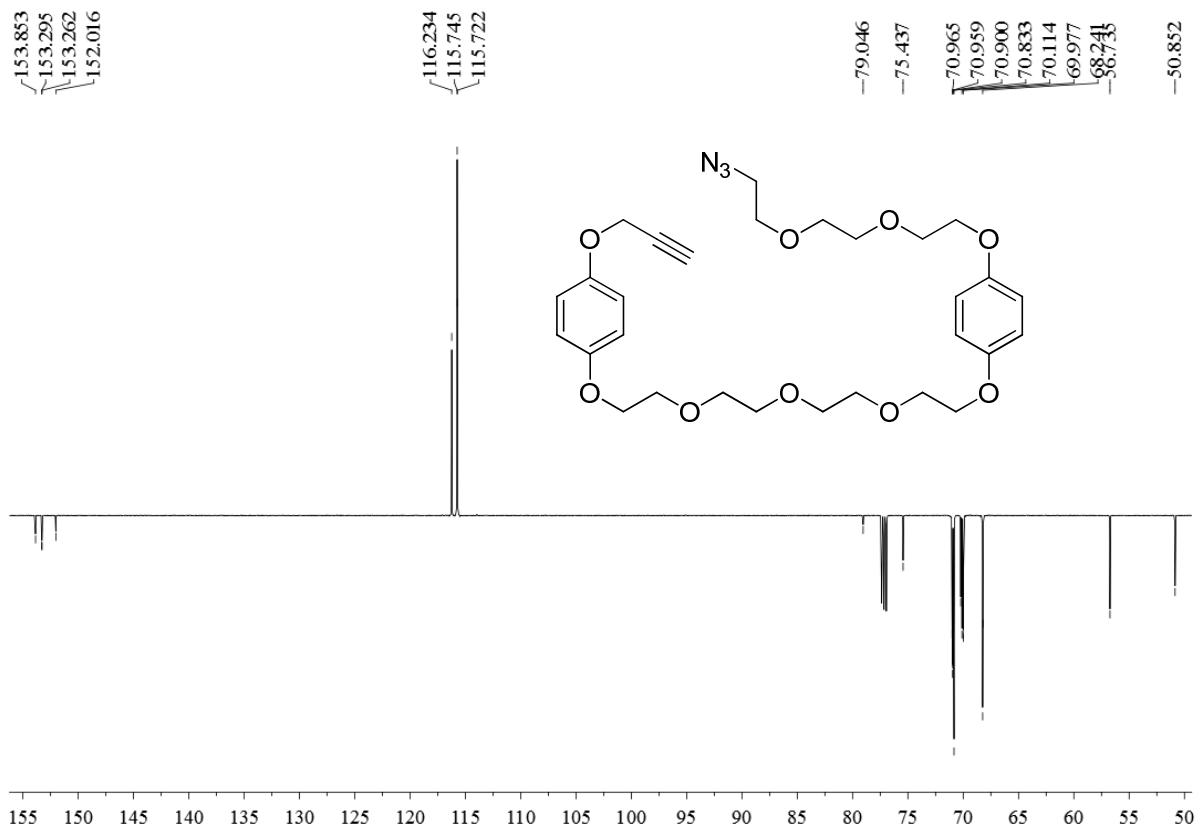
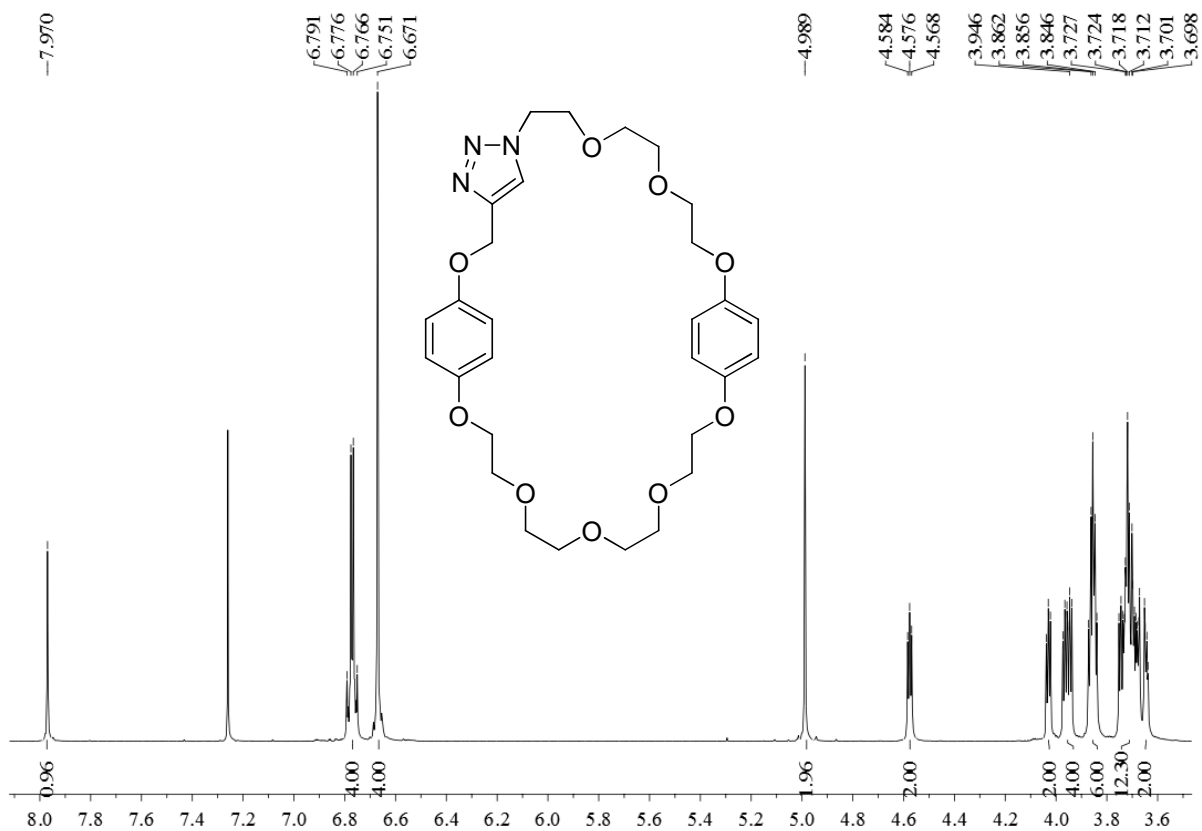
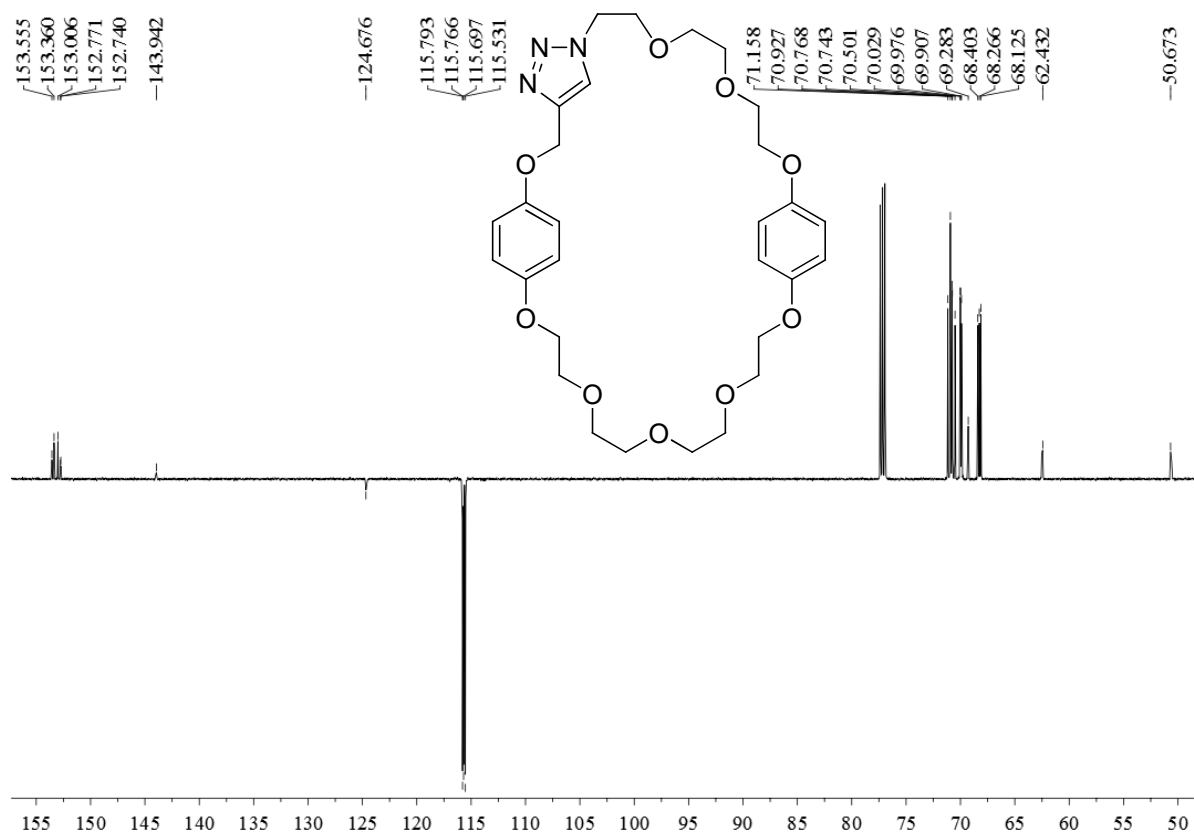


Figure S11.  $^{13}\text{C}$ -APT NMR (CDCl<sub>3</sub>, 150 MHz) spectrum of compound 8.

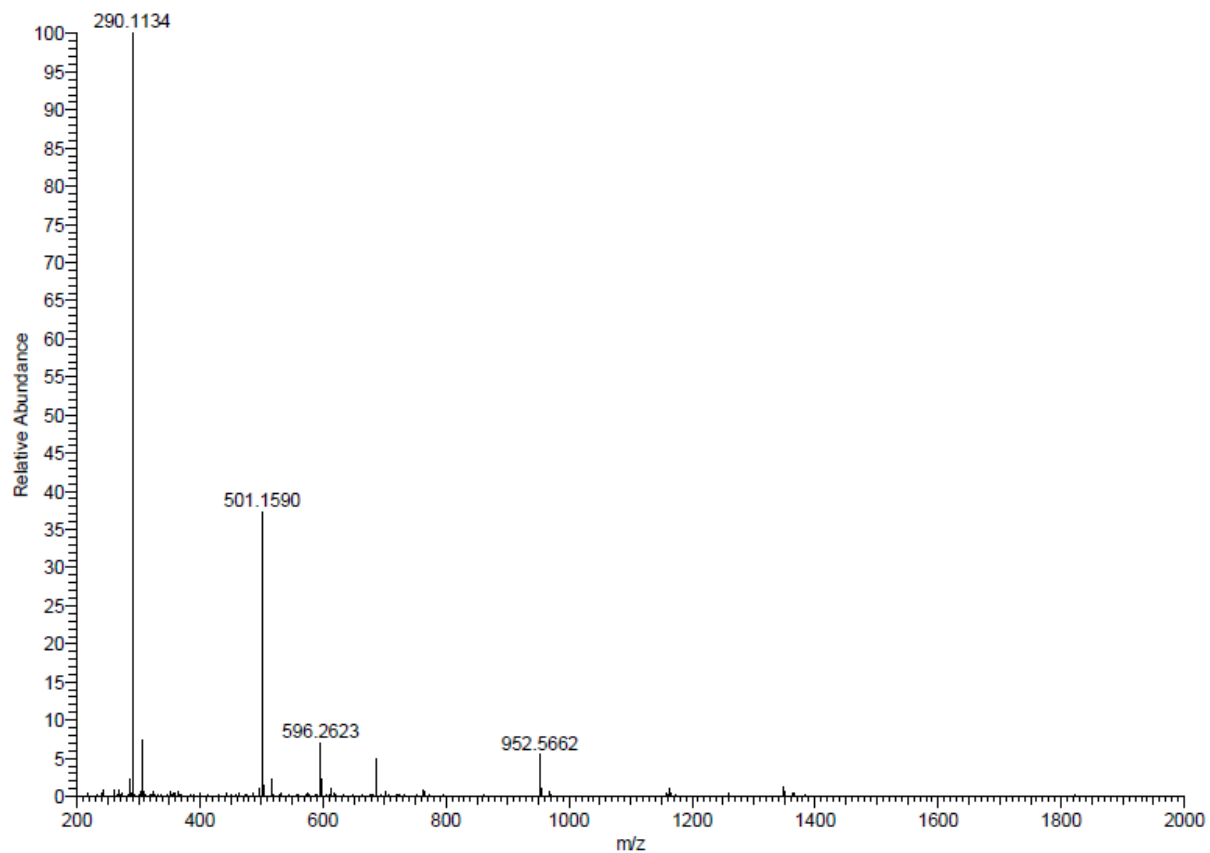




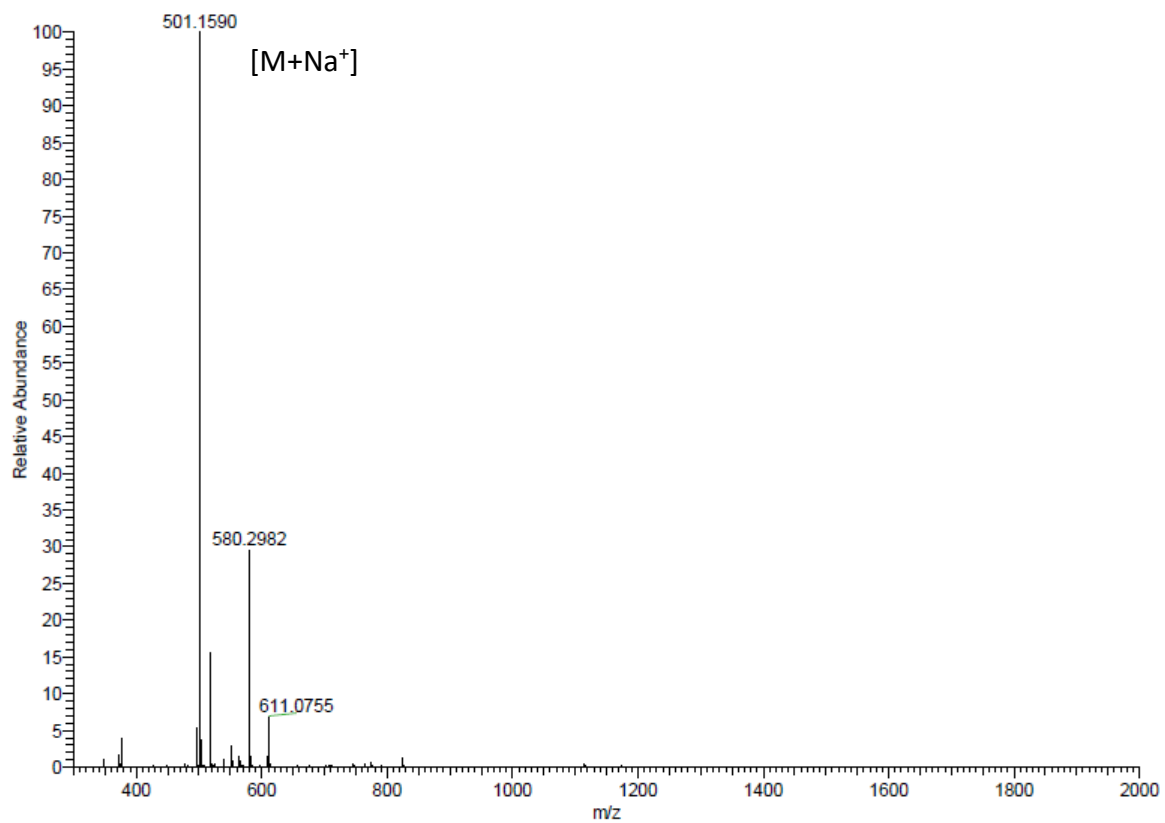
**Figure S12.**  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 600 MHz) spectrum of compound **9**.



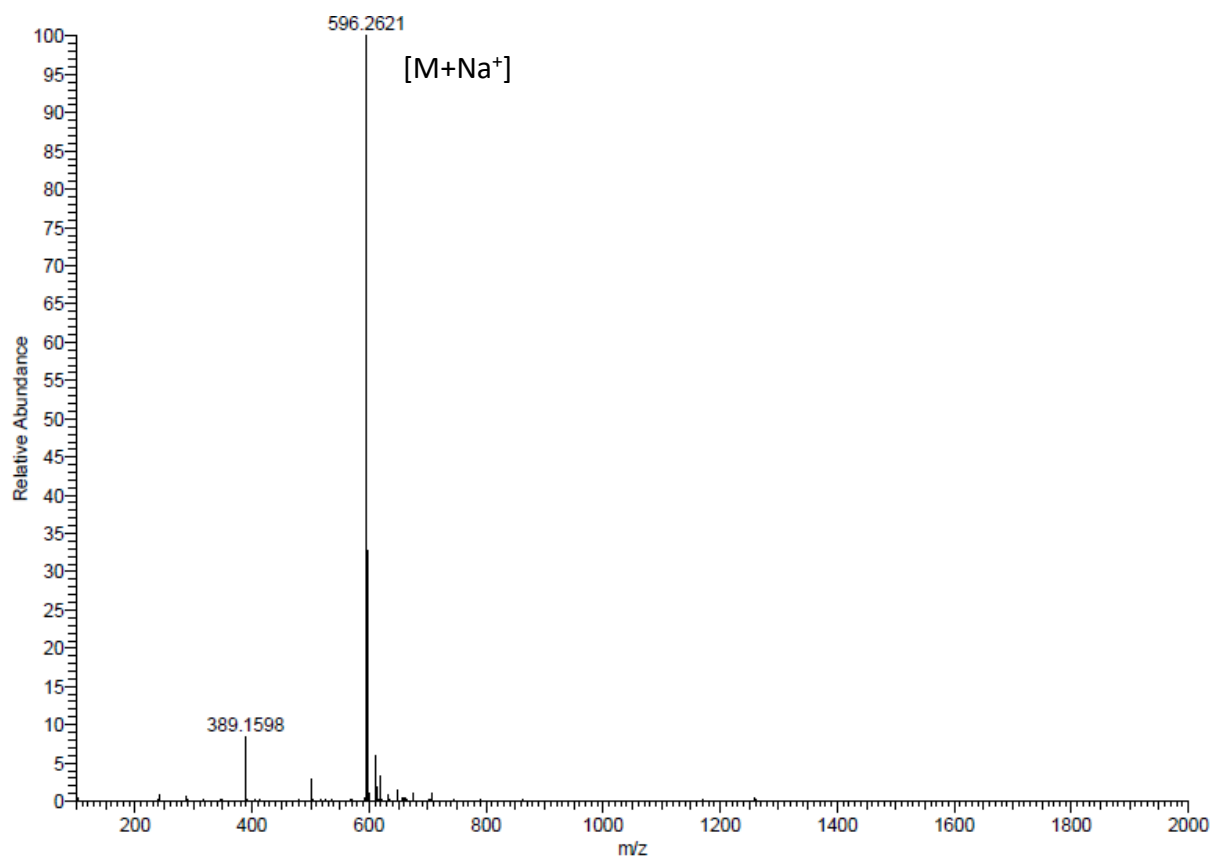
**Figure S13.**  $^{13}\text{C}$ -APT NMR ( $\text{CDCl}_3$ , 150 MHz) spectrum of compound **9**.



**Figure S14.** ESI(+)-HRMS spectrum of **4**.



**Figure S15.** ESI(+)-HRMS spectrum of **7**.



**Figure S16.** ESI(+)-HRMS spectrum of **8**.

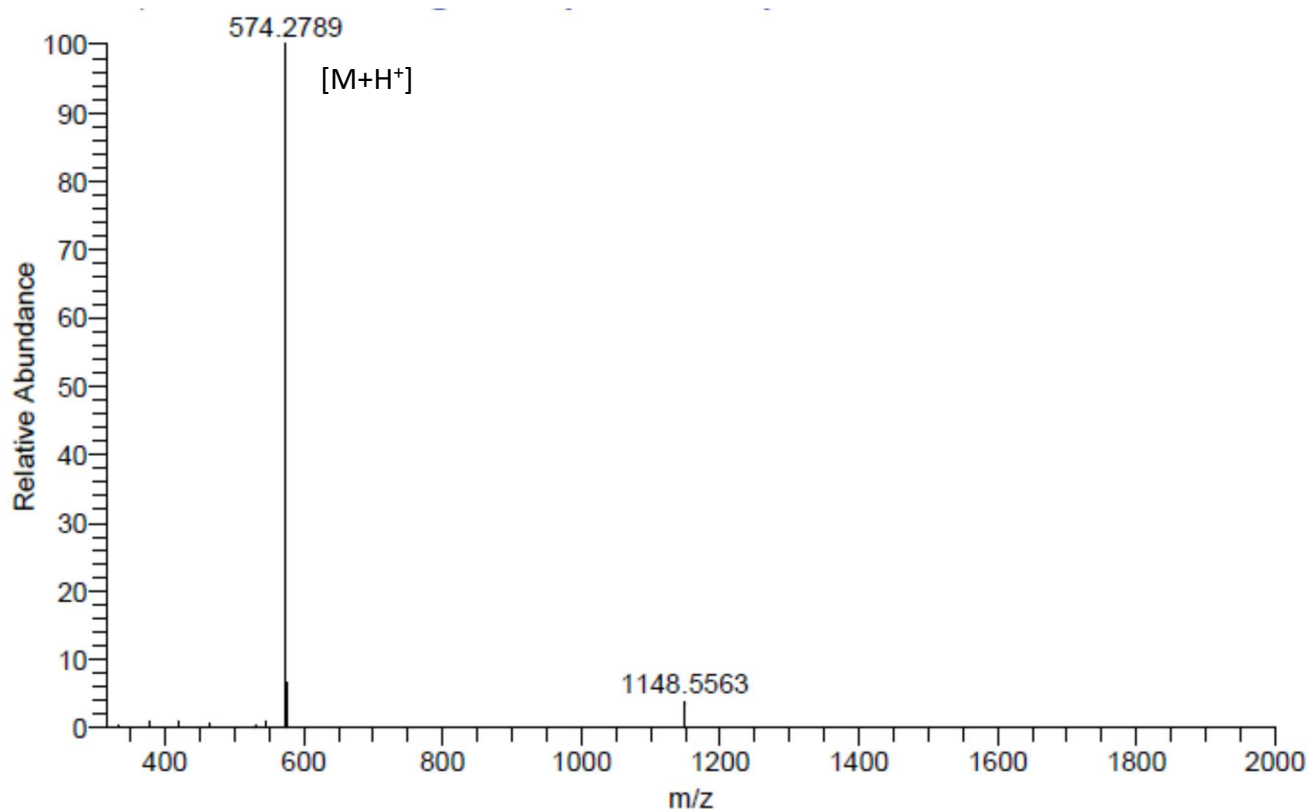


Figure S17. ESI(+)-HRMS spectrum of 9.

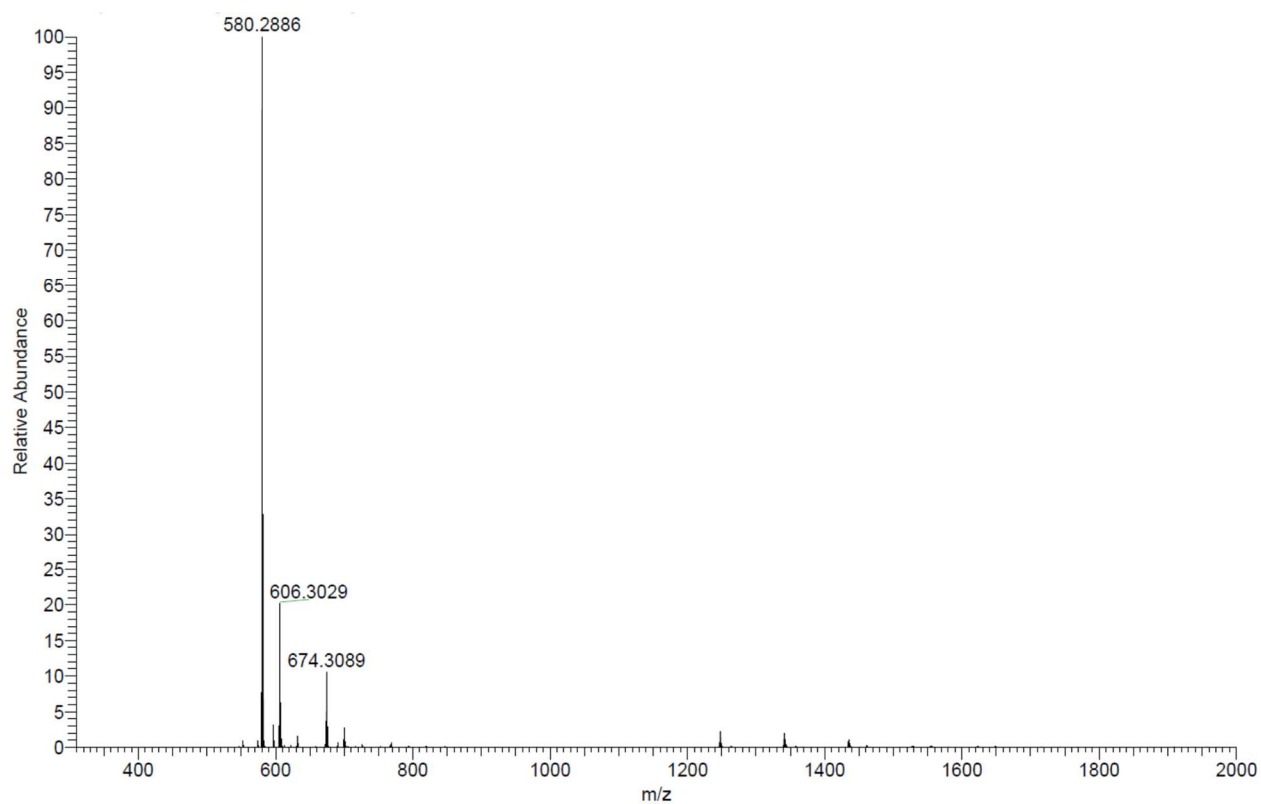
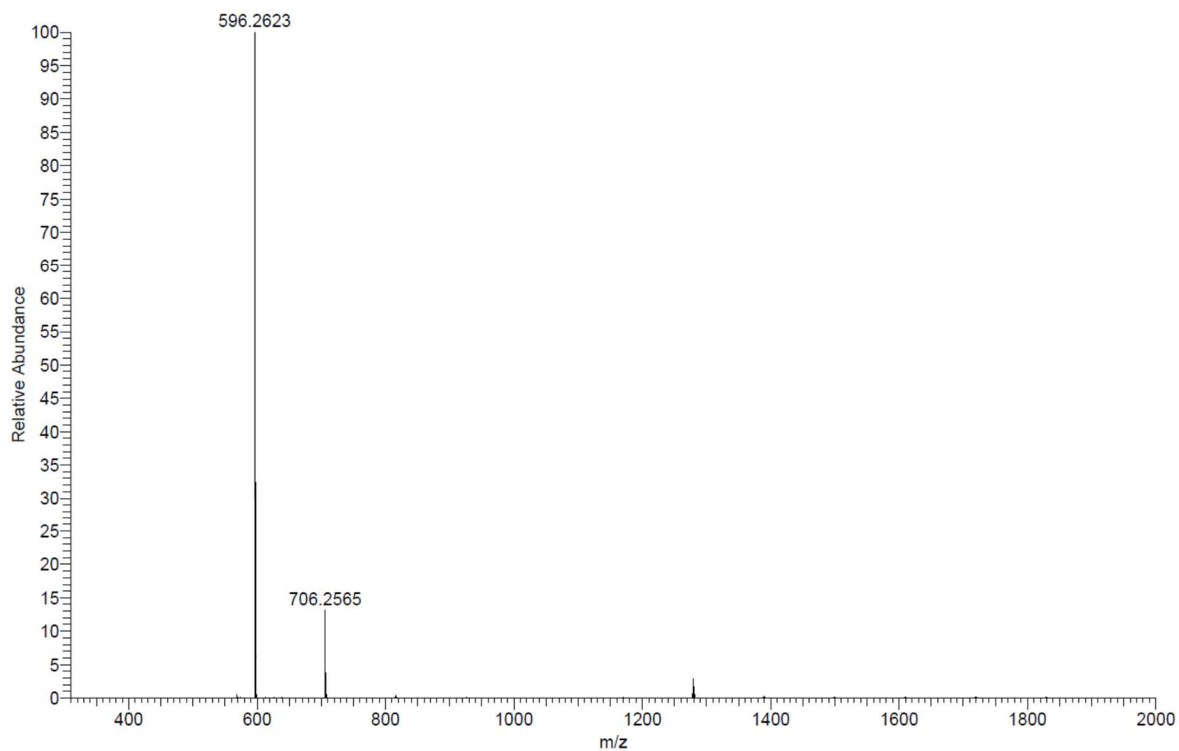
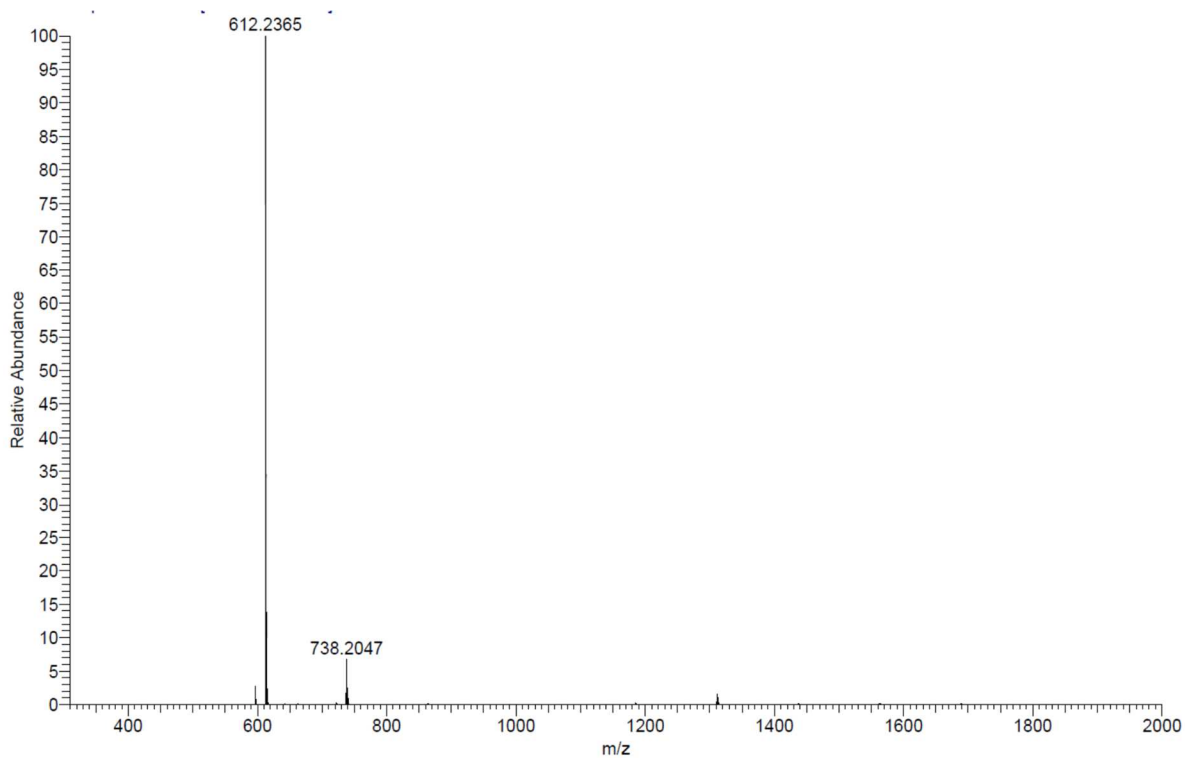


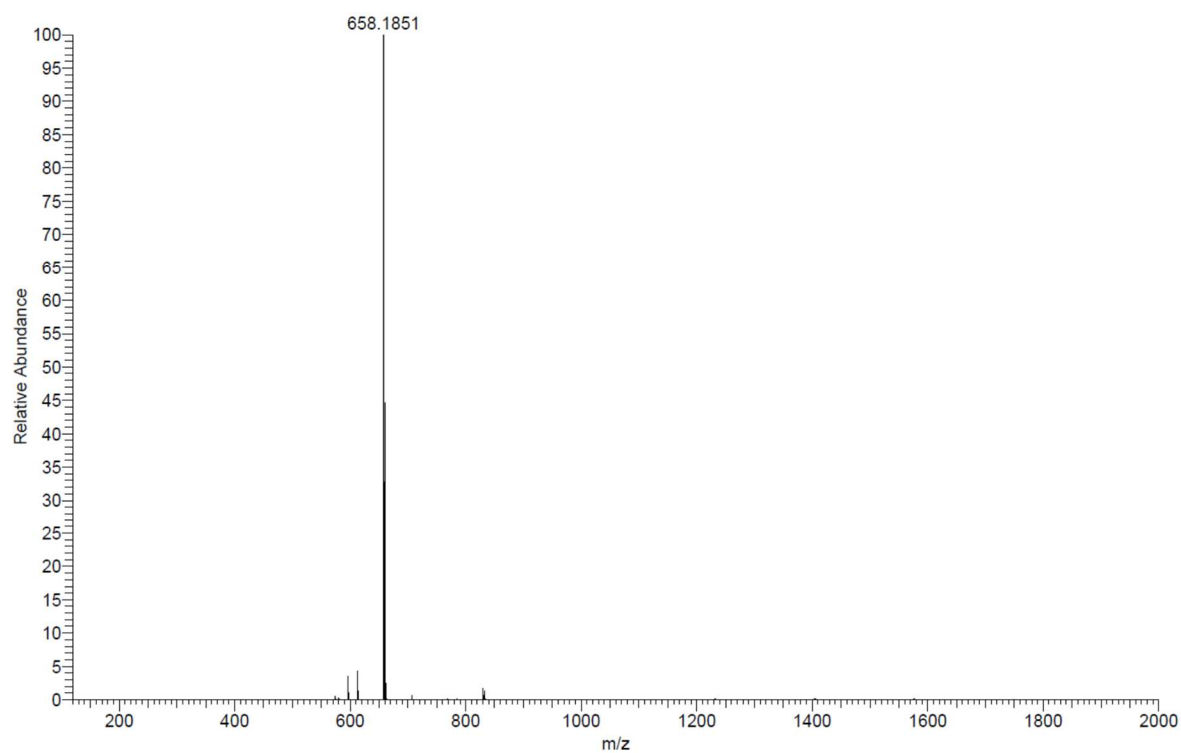
Figure S18. ESI(+)-HRMS spectrum of 9•Li<sup>+</sup> complex



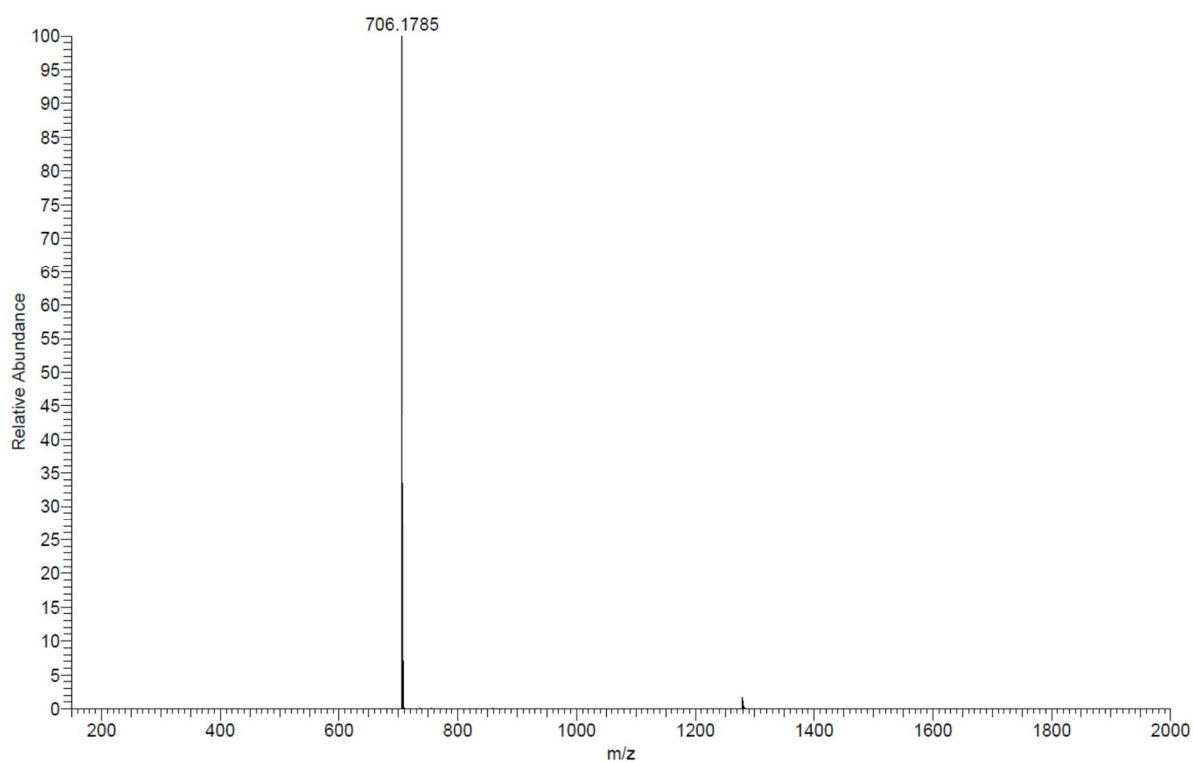
**Figure S19.** ESI(+)-HRMS spectrum of **9•Na<sup>+</sup>** complex



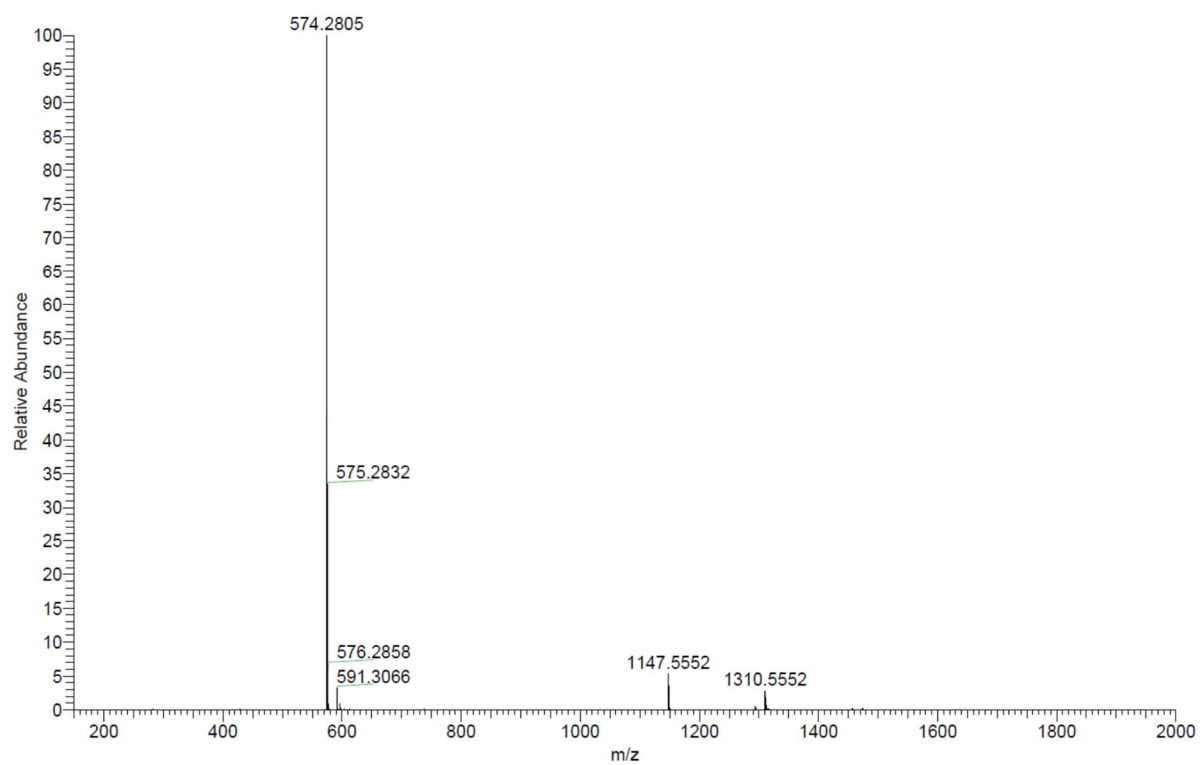
**Figure S20.** ESI(+)-HRMS spectrum of **9•K<sup>+</sup>** complex



**Figure S21.** ESI(+)-HRMS spectrum of **9•Rb<sup>+</sup>** complex



**Figure S22.** ESI(+)-HRMS spectrum of **9•Cs<sup>+</sup>** complex



**Figure S23.** ESI(+)-HRMS spectrum of **9•NH<sub>4</sub><sup>+</sup>** complex