

*Supplementary information*

# Arylamine Analogs of Methylene Blue: Substituent Effect on Aggregation Behavior and DNA Binding

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## Content

- 2 ..... FIGURE S1.  $^1\text{H}$  NMR SPECTRUM OF THE COMPOUND PTZA, DMSO- $D_6$ , 300 K, 400 MHZ.
- 2 ..... FIGURE S2.  $^1\text{H}$  NMR SPECTRUM OF THE COMPOUND PTZ1, DMSO- $D_6$ , 300 K, 400 MHZ.
- 3 ..... FIGURE S3.  $^1\text{H}$  NMR SPECTRUM OF THE COMPOUND PTZ2, DMSO- $D_6$ , 300 K, 400 MHZ.
- 3 ..... FIGURE S4.  $^{13}\text{C}$  NMR SPECTRUM OF THE COMPOUND PTZA, DMSO- $D_6$ , 300 K, 100 MHZ.
- 4 ..... FIGURE S5.  $^{13}\text{C}$  NMR SPECTRUM OF THE COMPOUND PTZ1, DMSO- $D_6$ , 300 K, 100 MHZ.
- 4 ..... FIGURE S6.  $^{13}\text{C}$  NMR SPECTRUM OF THE COMPOUND PTZ2, DMSO- $D_6$ , 300 K, 100 MHZ.
- 5 ..... FIGURE S7. FT-IR SPECTRUM OF THE COMPOUND PTZA.
- 5 ..... FIGURE S8. FT-IR SPECTRUM OF THE COMPOUND PTZ1.
- 5 ..... FIGURE S9. FT-IR SPECTRUM OF THE COMPOUND PTZ2.
- 6 ..... FIGURE S10. HRMS SPECTRUM OF THE COMPOUND PTZA.
- 6 ..... FIGURE S11. HRMS SPECTRUM OF THE COMPOUND PTZ1.
- 7 ..... FIGURE S12. HRMS SPECTRUM OF THE COMPOUND PTZ2.
- 7 ..... FIGURE S13.  $1/[\text{DNA}]$  VERSUS  $\text{A}_0/(\text{A} - \text{A}_0)$  PLOT FOR MB-DNA UV-VIS TITRATION.
- 8 ..... FIGURE S14.  $1/[\text{DNA}]$  VERSUS  $\text{A}_0/(\text{A} - \text{A}_0)$  PLOT FOR PTZ1-DNA UV-VIS TITRATION.

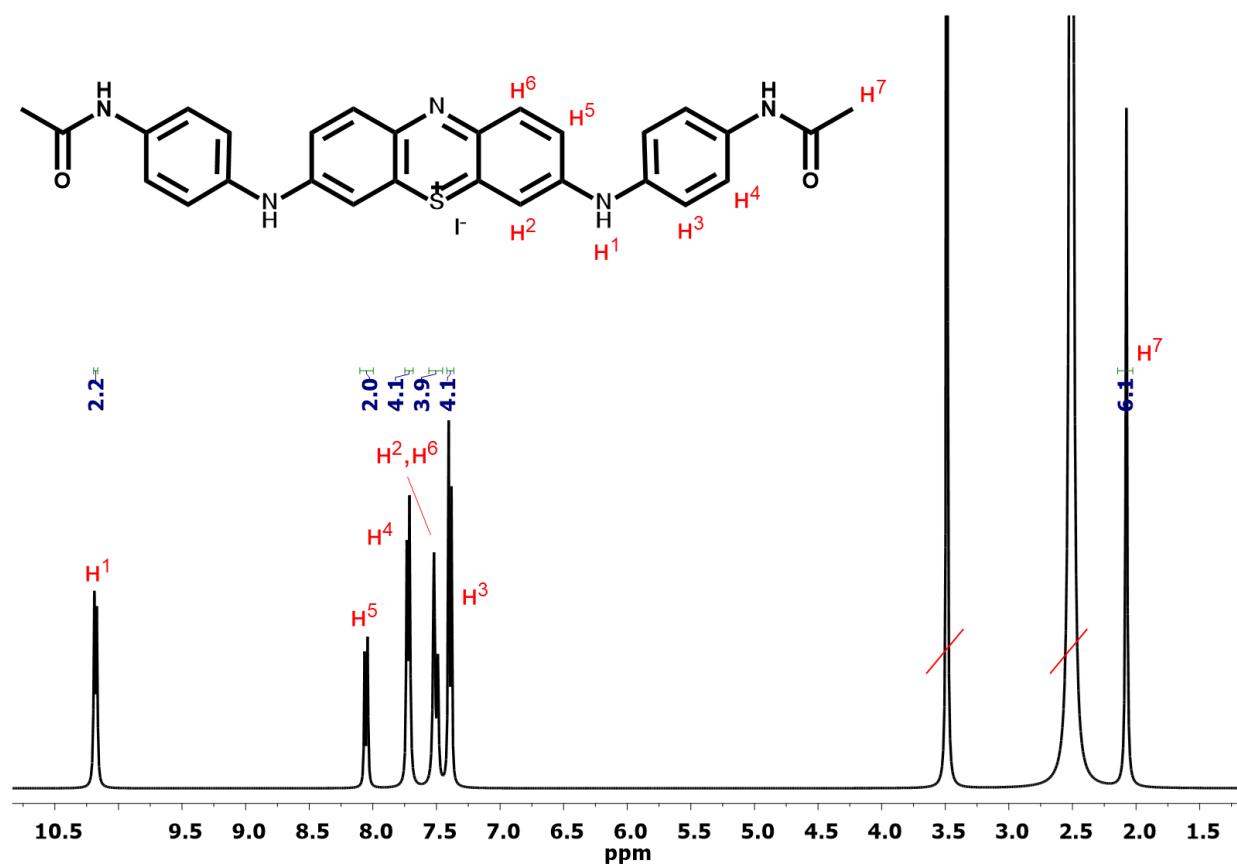


Figure S1. <sup>1</sup>H NMR spectrum of the compound **PTZa**, DMSO-d<sub>6</sub>, 300 K, 400 MHz.

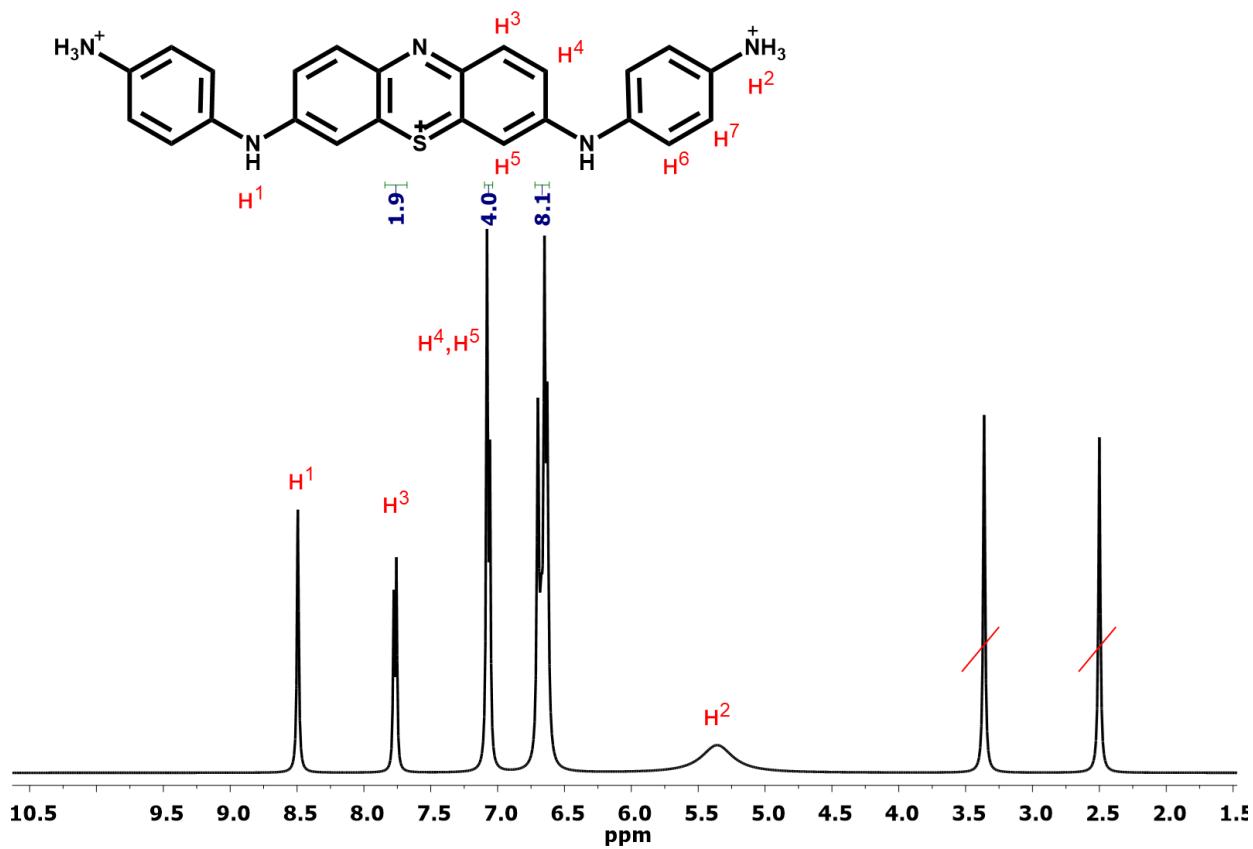


Figure S2. <sup>1</sup>H NMR spectrum of the compound **PTZ1**, DMSO-d<sub>6</sub>, 300 K, 400 MHz.

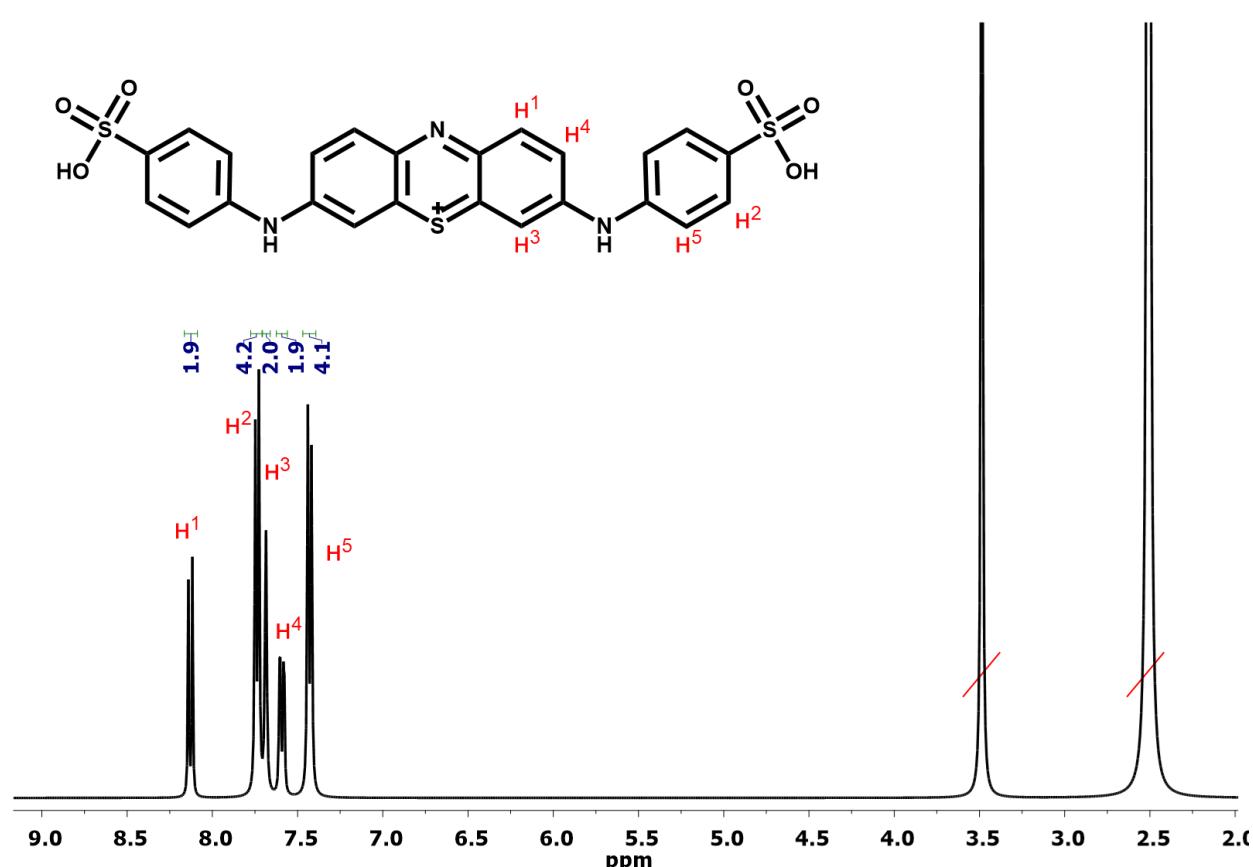


Figure S3. <sup>1</sup>H NMR spectrum of the compound **PTZ2**, DMSO-*d*<sub>6</sub>, 300 K, 400 MHz.

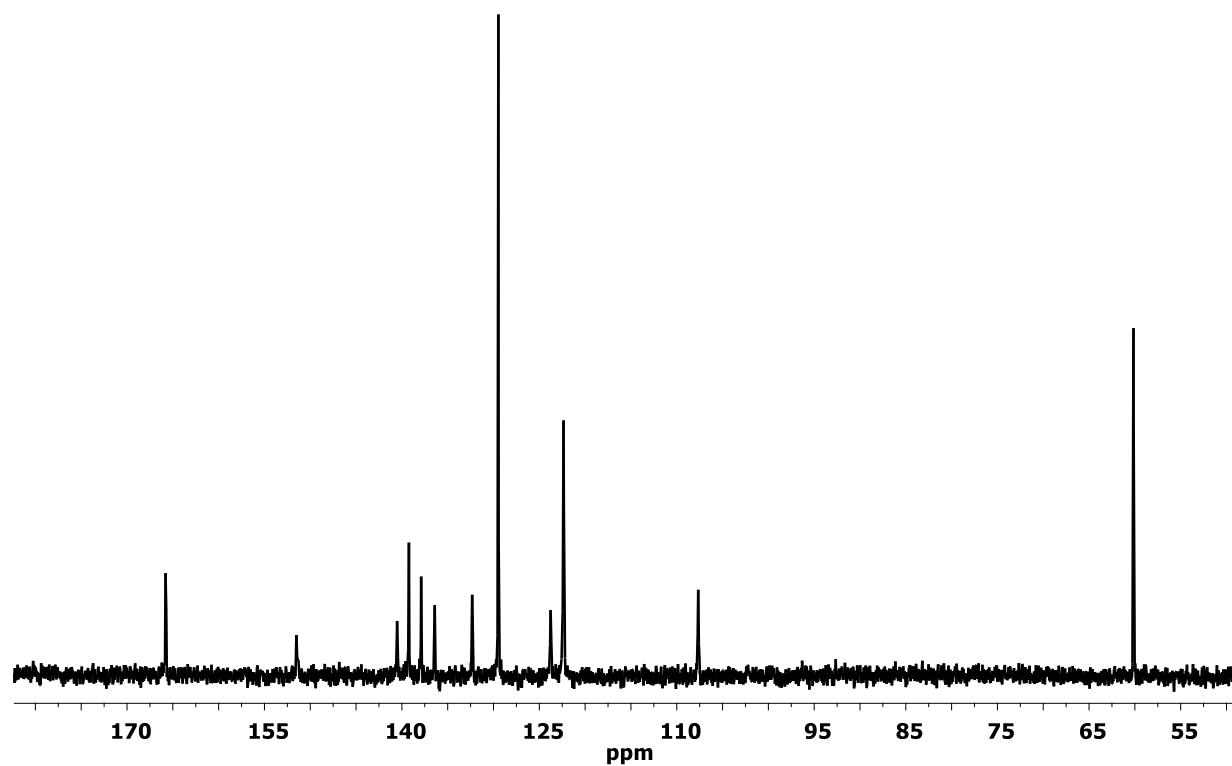


Figure S4. <sup>13</sup>C NMR spectrum of the compound **PTZa**, DMSO-*d*<sub>6</sub>, 300 K, 100 MHz.

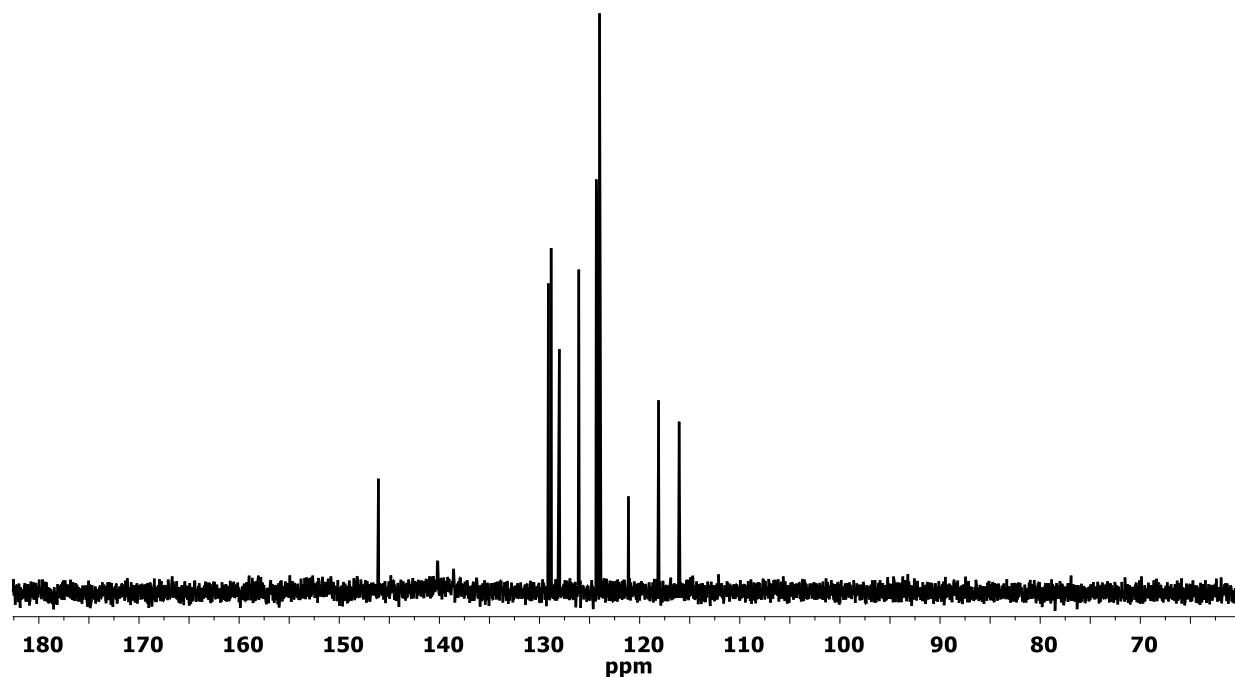


Figure S5. <sup>13</sup>C NMR spectrum of the compound **PTZ1**, DMSO-*d*<sub>6</sub>, 300 K, 100 MHz.

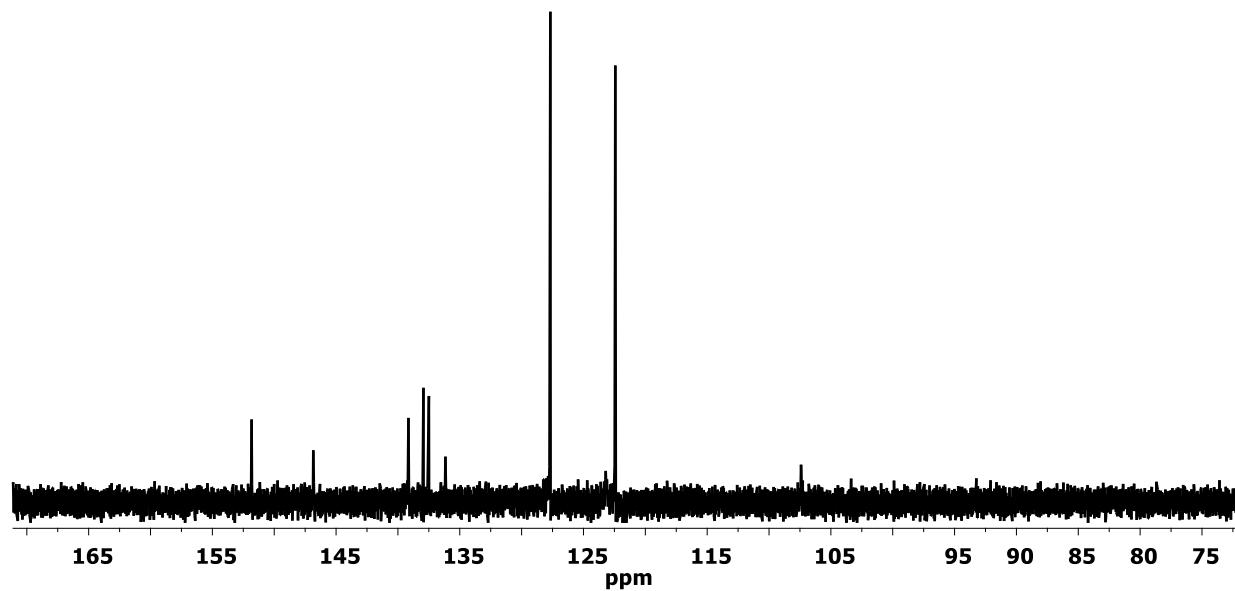


Figure S6. <sup>13</sup>C NMR spectrum of the compound **PTZ2**, DMSO-*d*<sub>6</sub>, 300 K, 100 MHz.

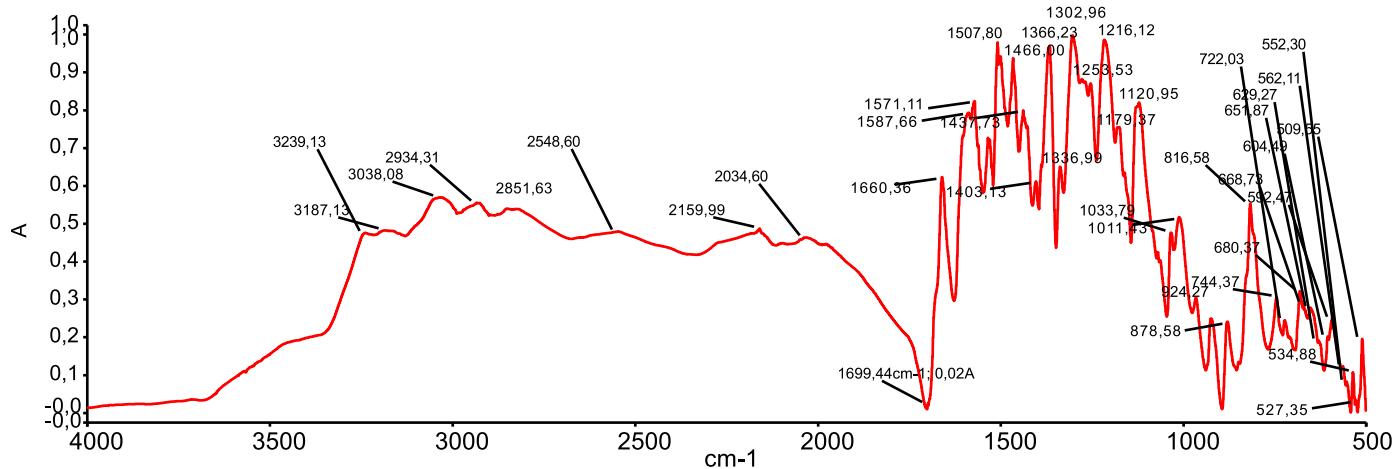


Figure S7. FT-IR spectrum of the compound **PTZa**.

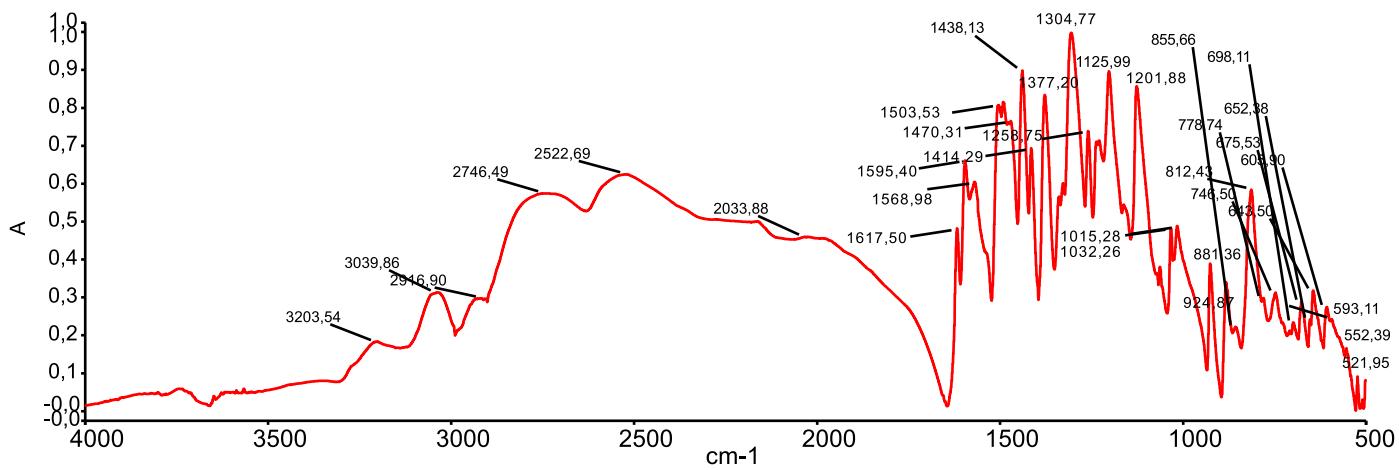


Figure S8. FT-IR spectrum of the compound **PTZ1**.

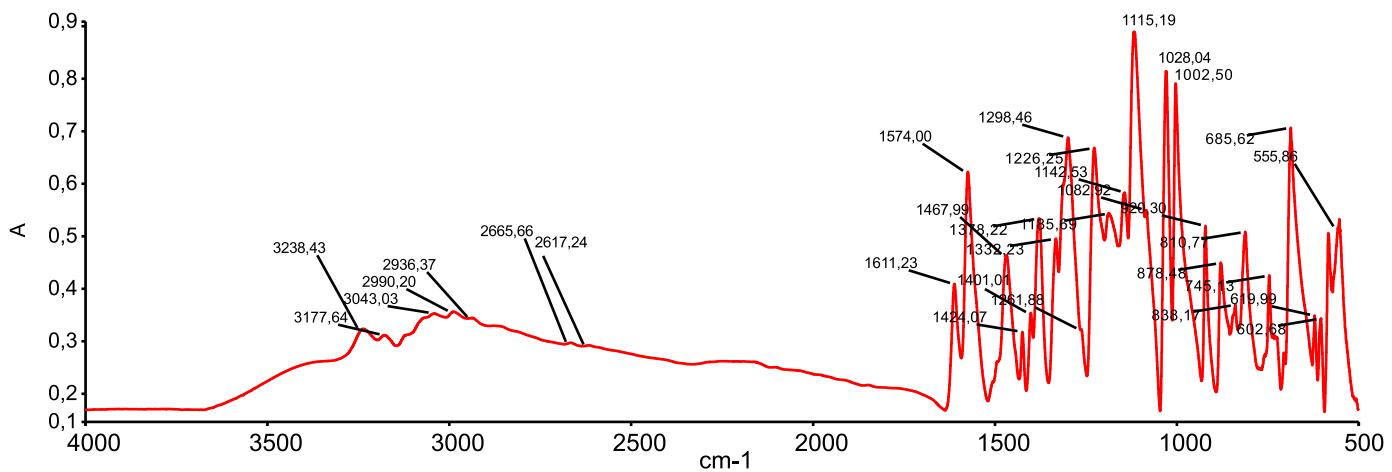


Figure S9. FT-IR spectrum of the compound **PTZ2**.

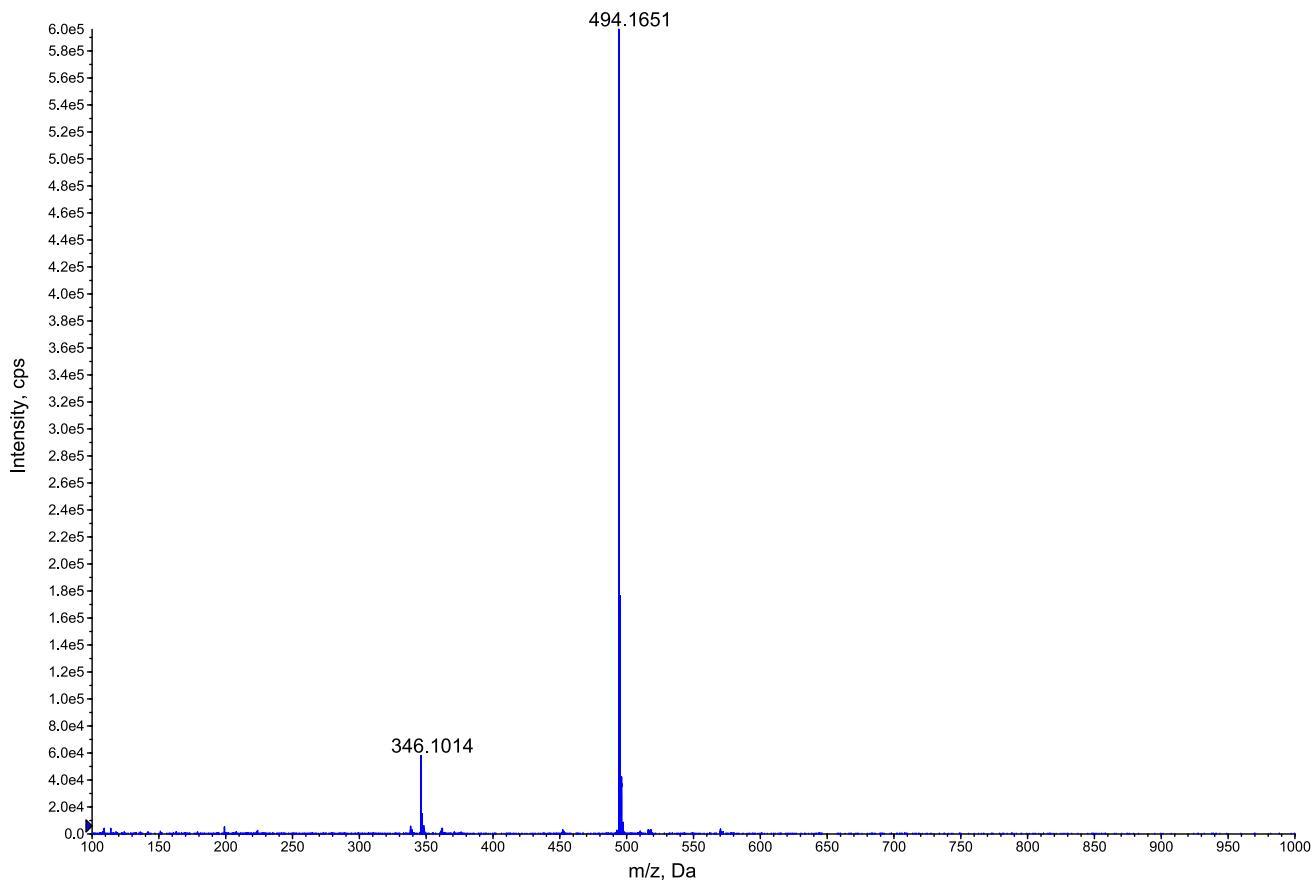


Figure S10. HRMS spectrum of the compound PTZa.

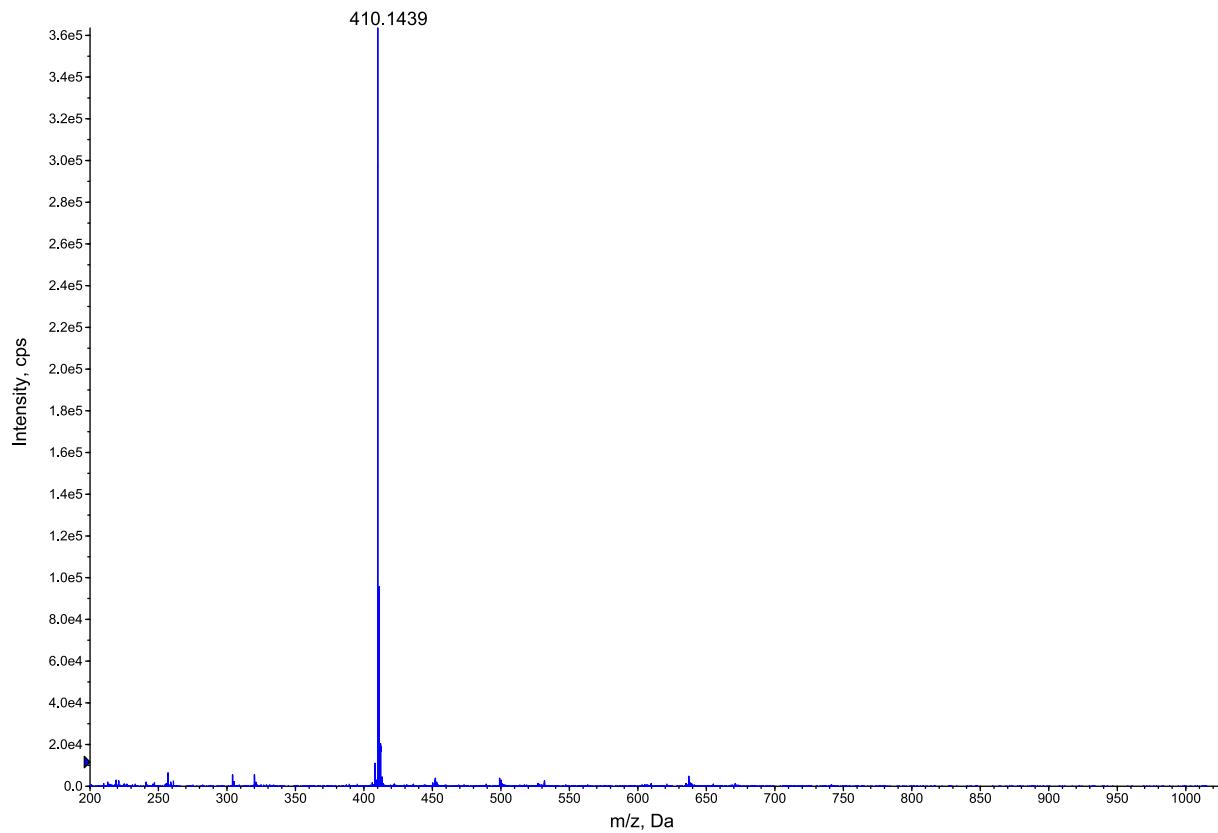


Figure S11. HRMS spectrum of the compound PTZ1.

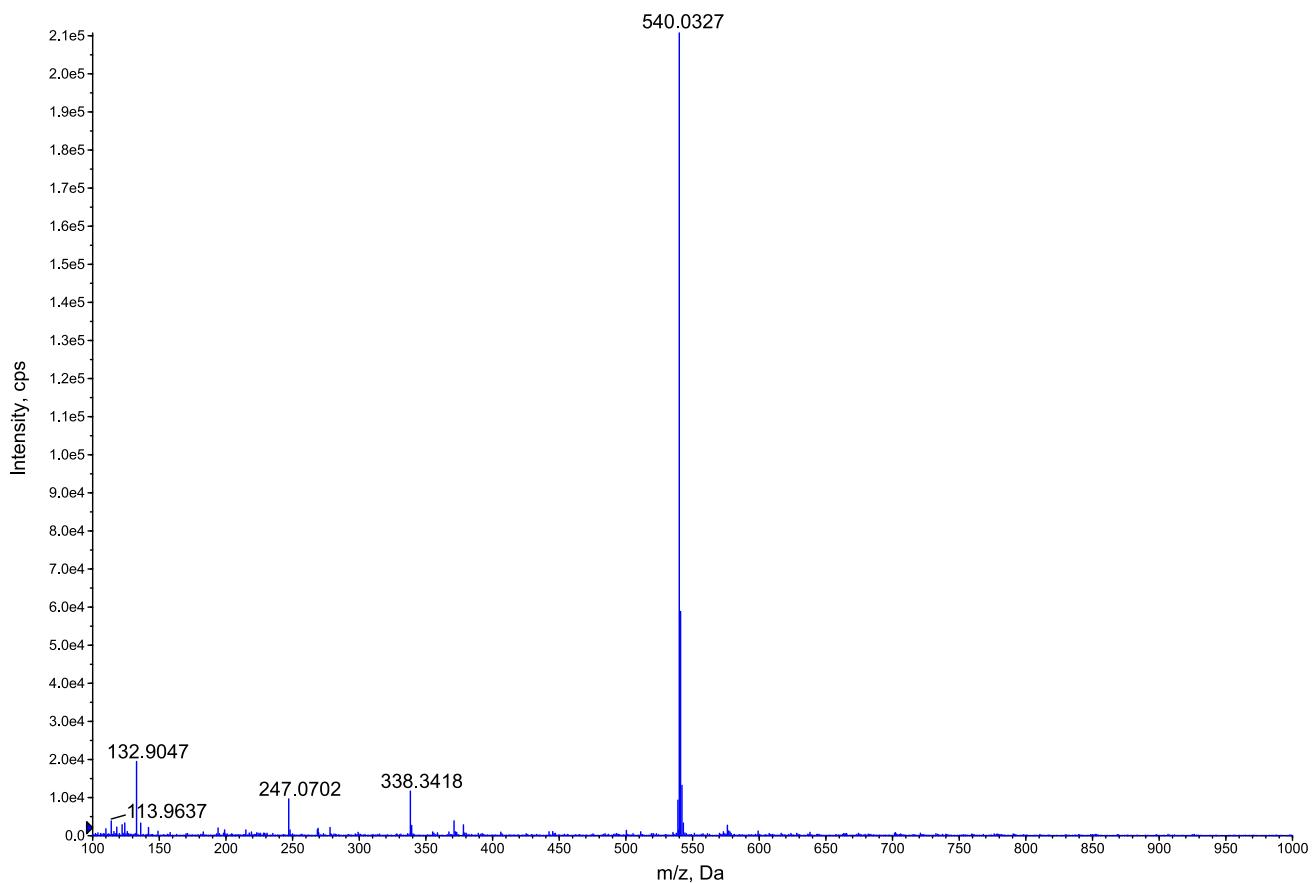


Figure S12. HRMS spectrum of the compound **PTZ2**.

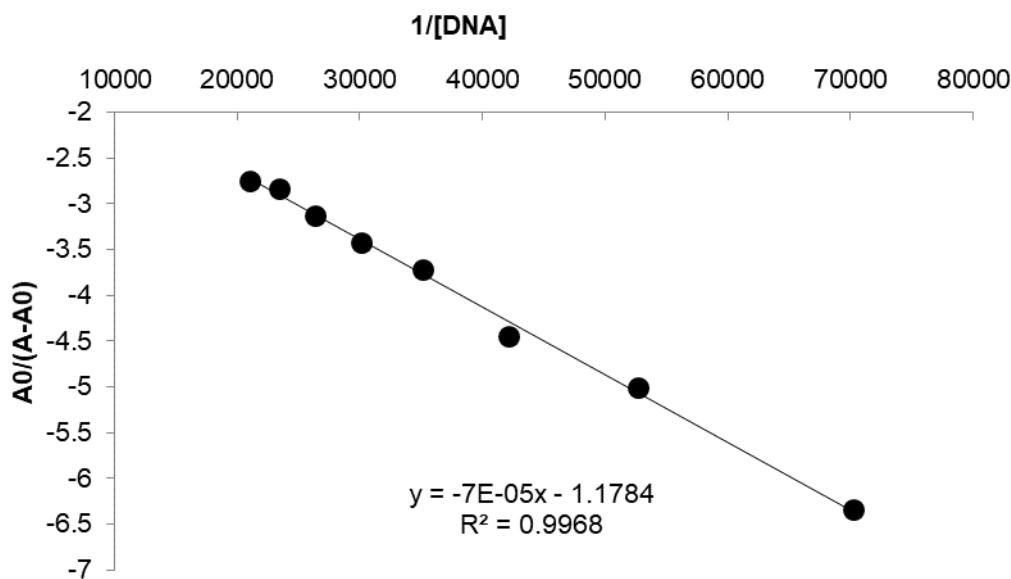


Figure S13.  $1/[\text{DNA}]$  versus  $A_0/(A - A_0)$  plot for **MB**-DNA UV-Vis titration.

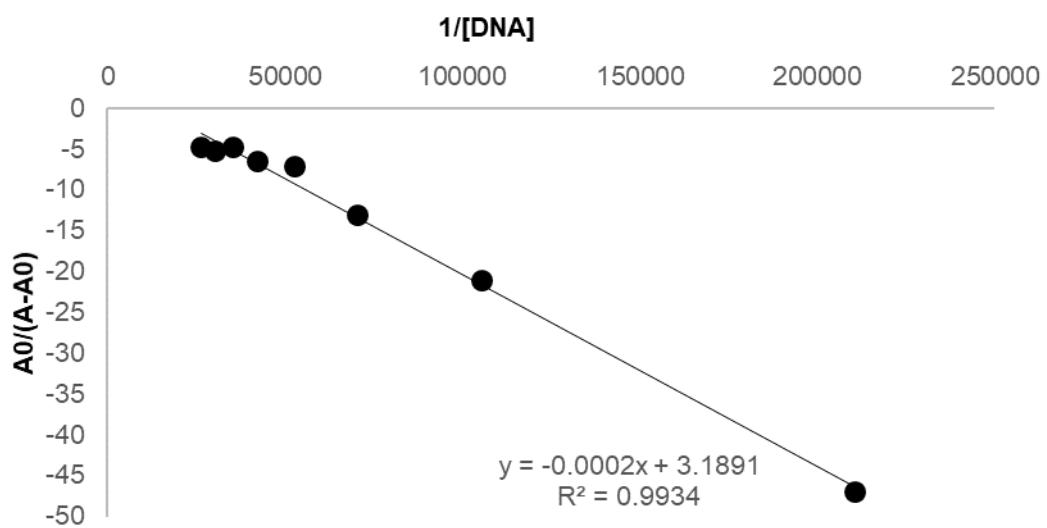


Figure S14.  $1/[\text{DNA}]$  versus  $A_0/(A - A_0)$  plot for **PTZ1**-DNA UV-Vis titration.