

## Supplementary Material

### Novel peptidomimetics: synthesis, characterization, and molecular modeling studies

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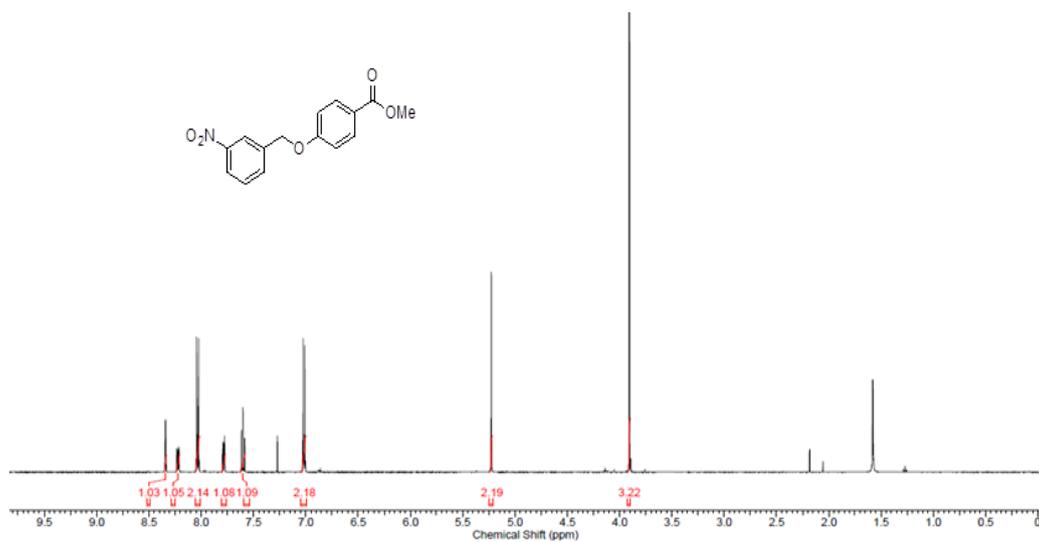
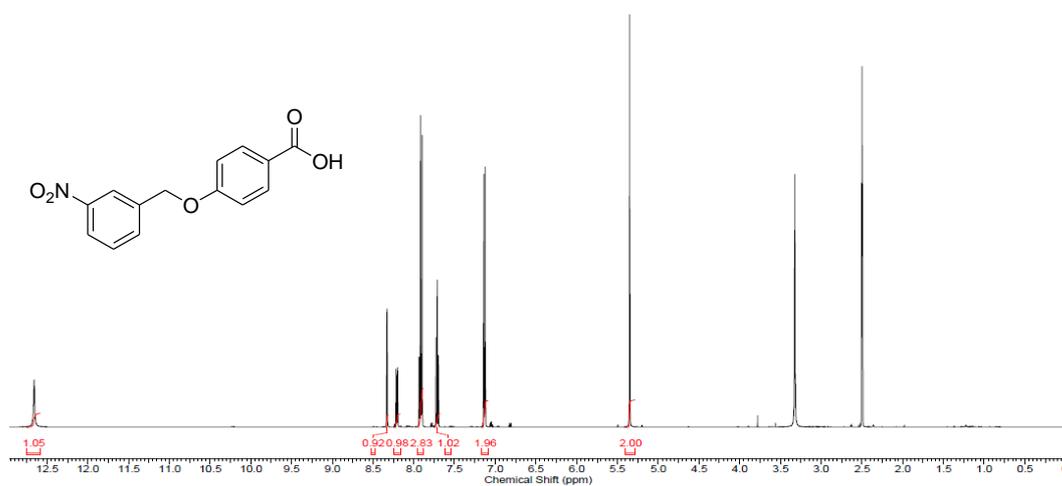
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## 1. IR and NMR Spectra of all the synthesized compounds

Figure S1. <sup>1</sup>H NMR spectrum (500 MHz, CDCl<sub>3</sub>) of 5a.Figure S2. <sup>1</sup>H NMR spectrum (500 MHz, CDCl<sub>3</sub>) of 6a.

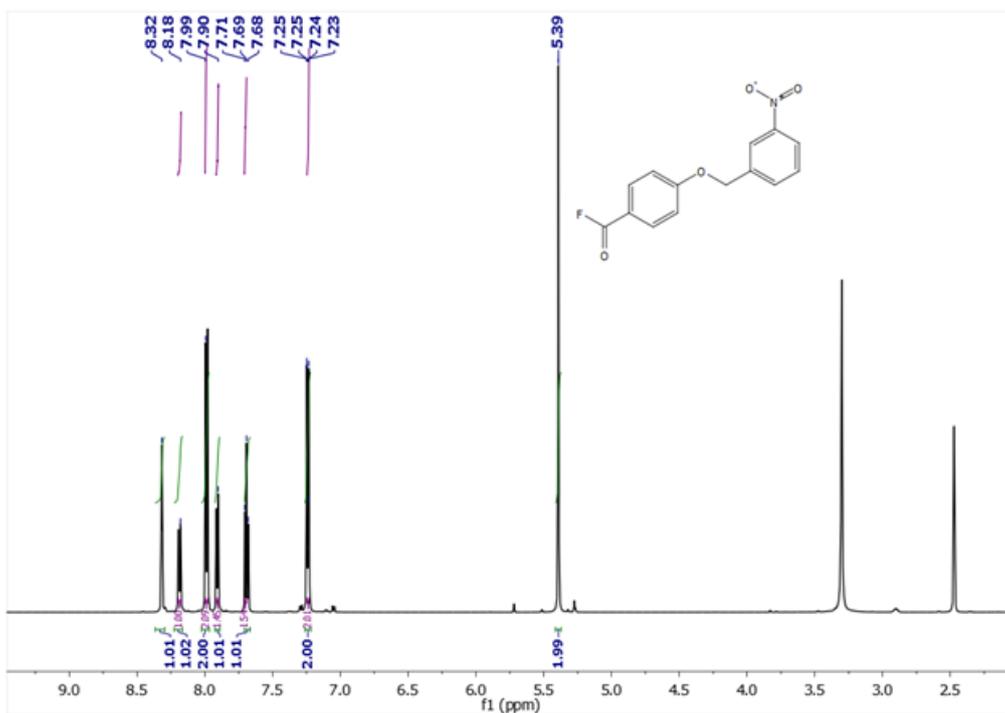


Figure S3.  $^1\text{H}$  NMR spectrum (500 MHz,  $\text{DMSO-}d_6$ ) of 7a.

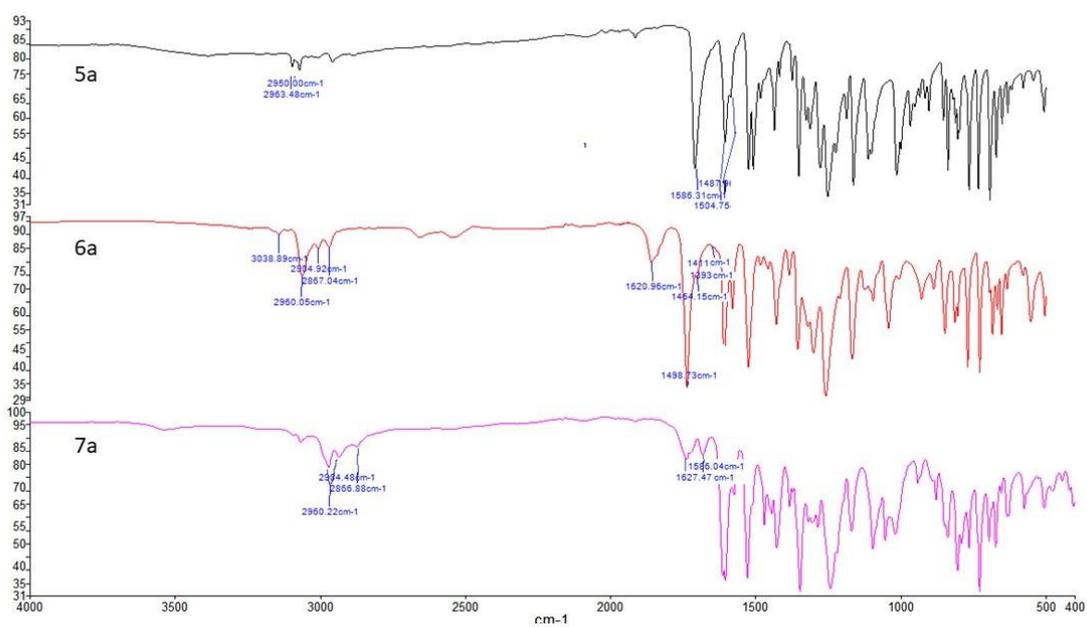


Figure S4. IR spectrum (ATR) of 5a, 6a and 7a.

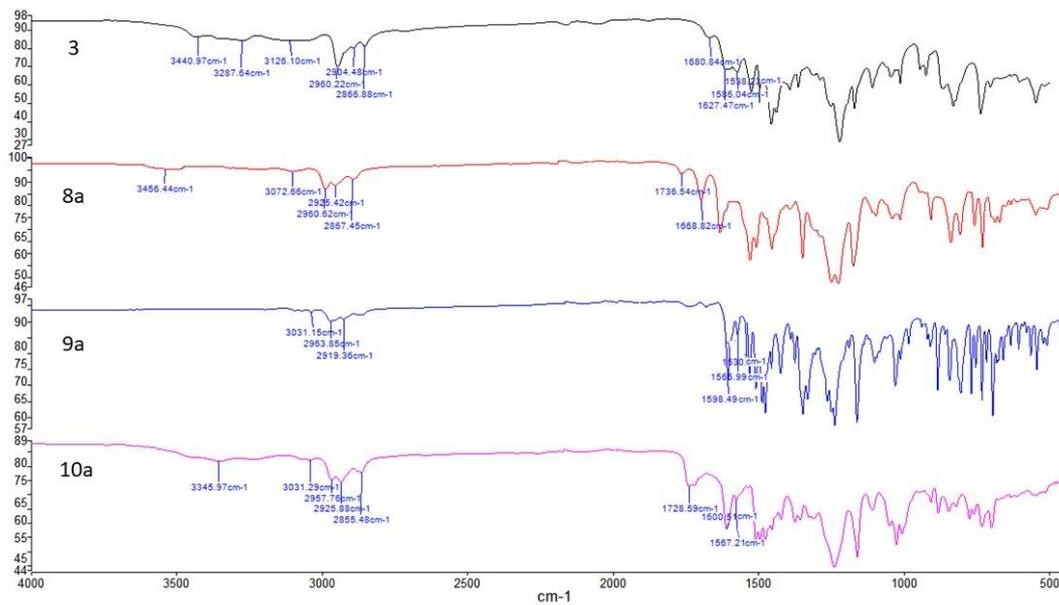


Figure S5. IR spectrum (ATR) of 3, 8a, 9a and 10a.

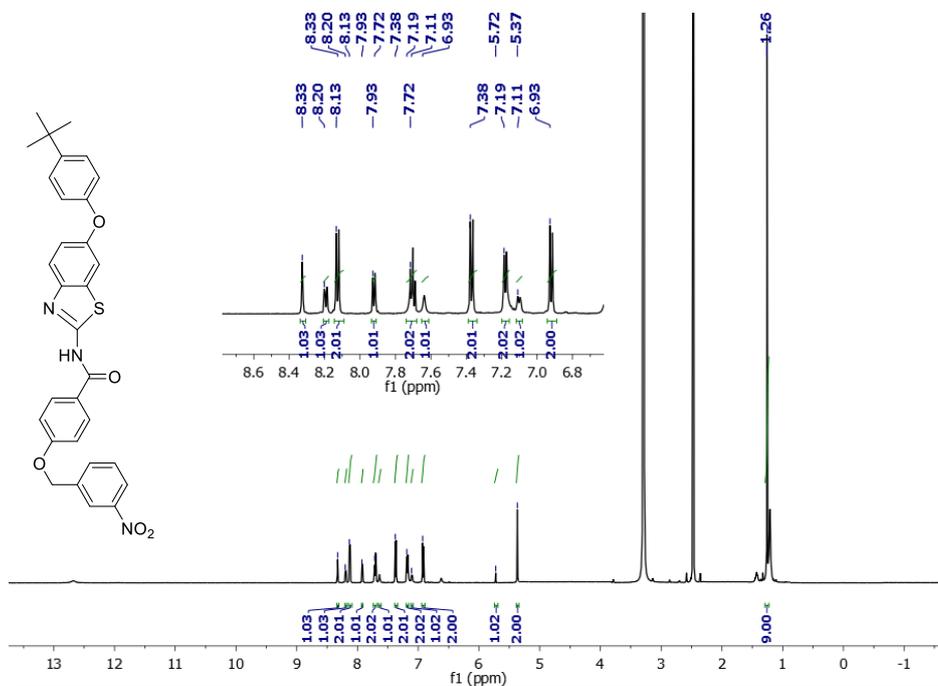
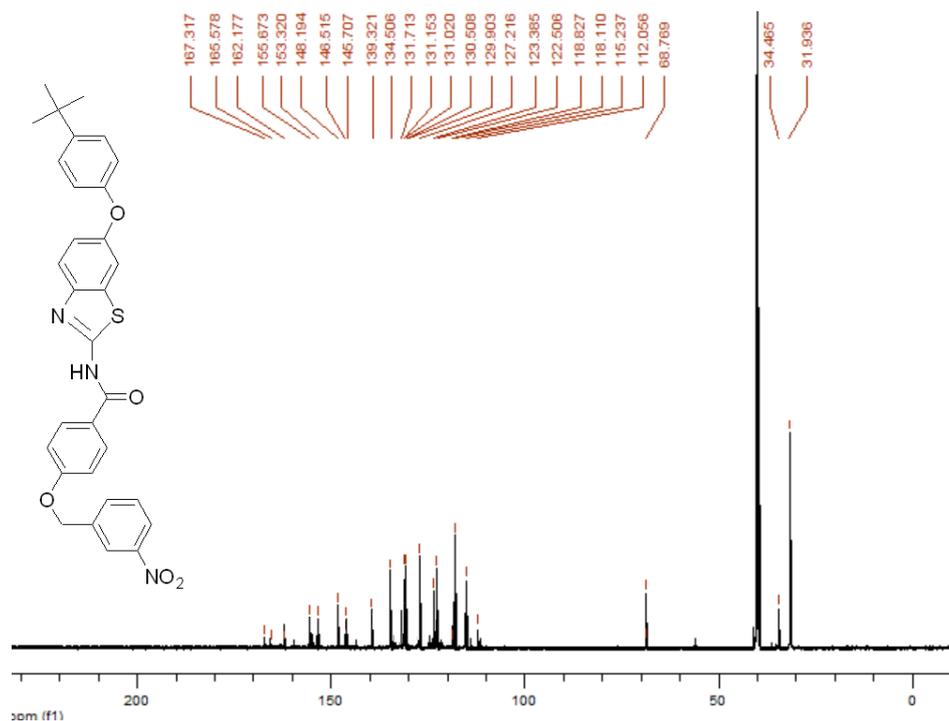
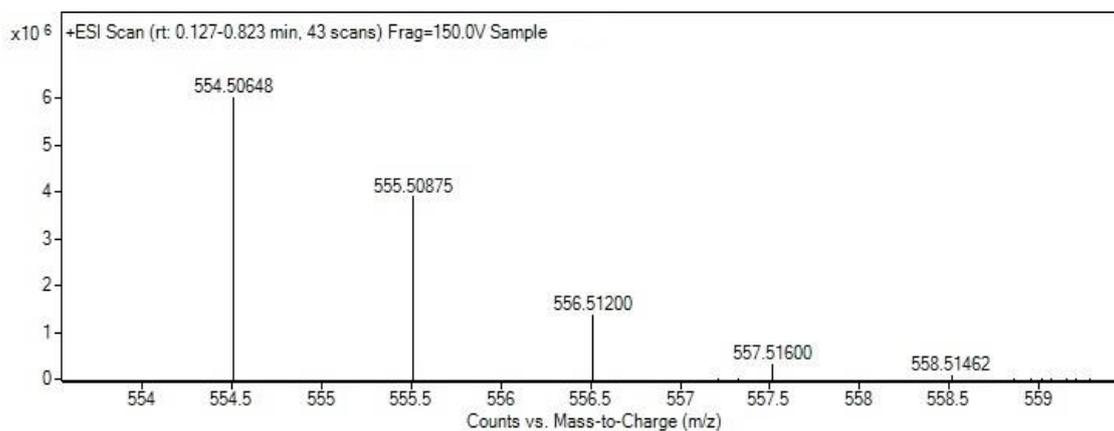


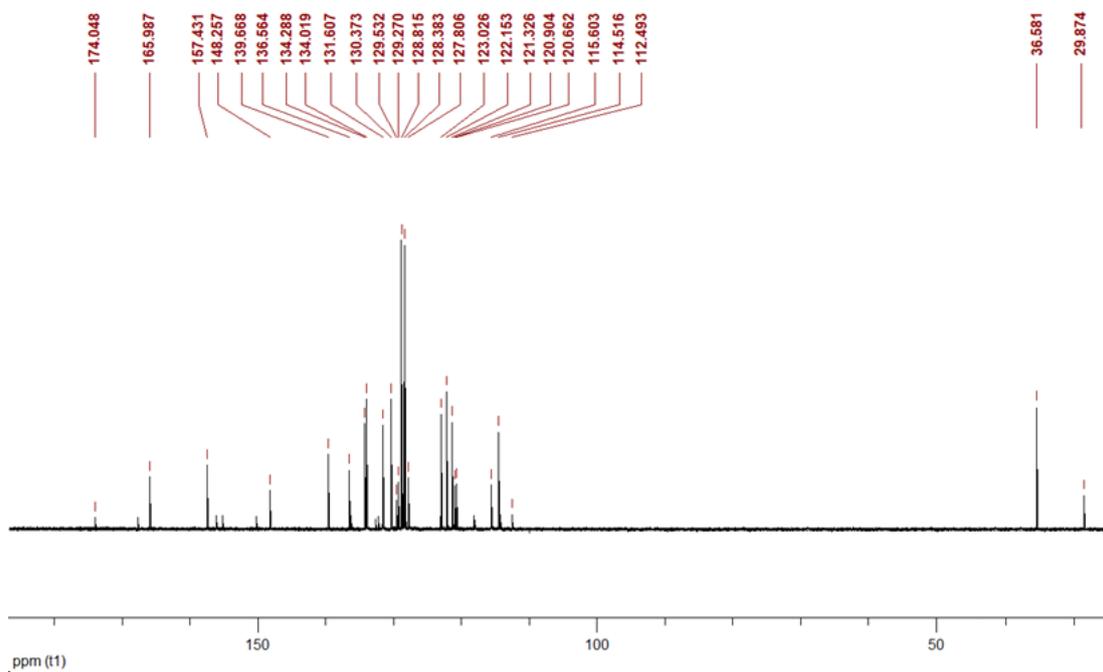
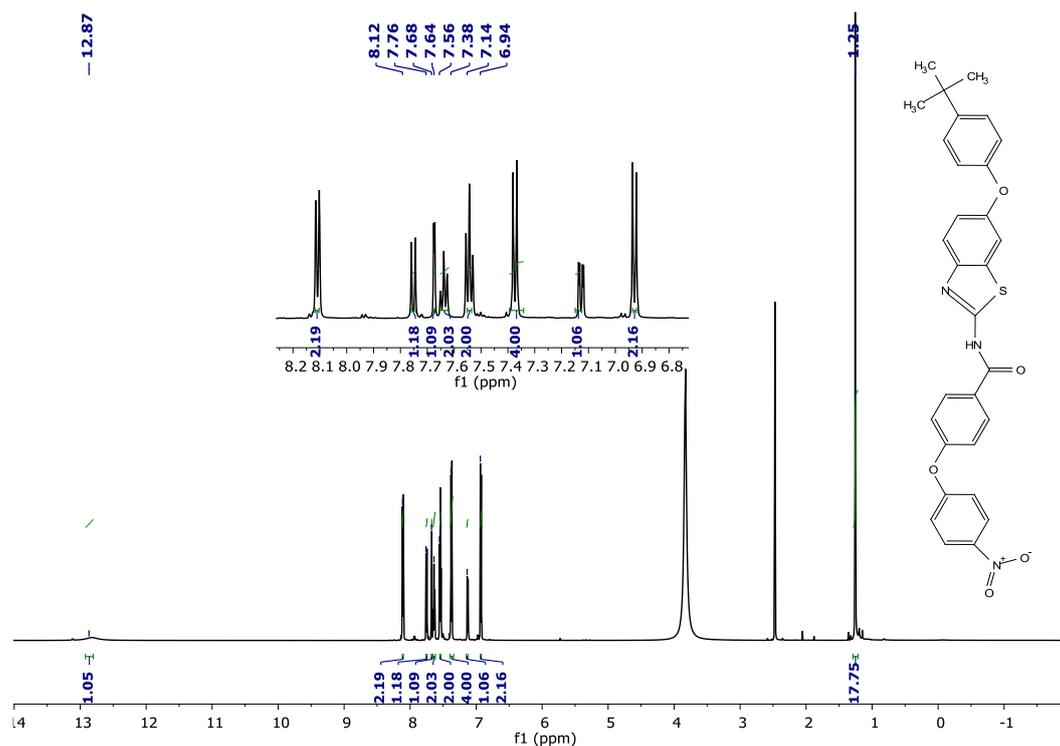
Figure S6. <sup>1</sup>H NMR spectrum (500 MHz, DMSO-*d*<sub>6</sub>) of 8a.



**Figure S7.**  $^{13}\text{C}$  NMR spectrum (126 MHz,  $\text{DMSO-}d_6$ ) of **8a**.



**Figure S8.** LC-HRMS spectrum of **8a**.



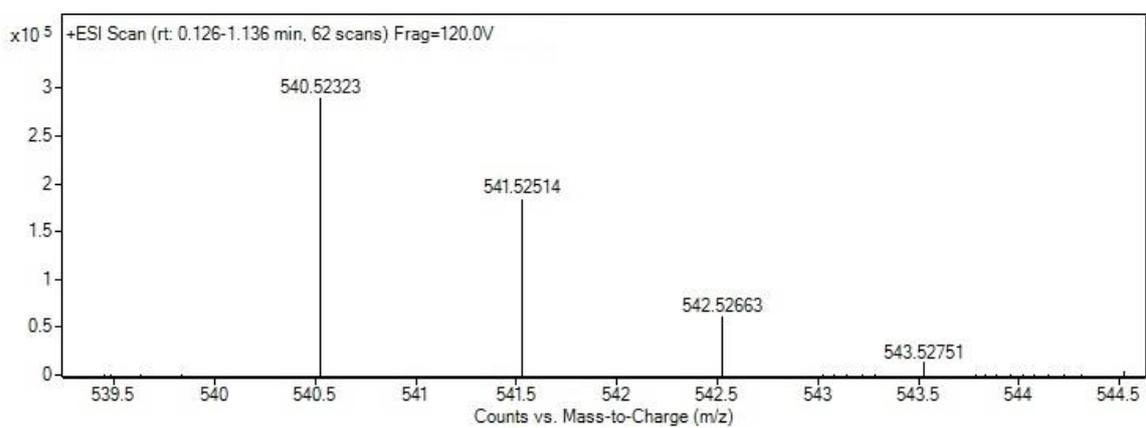


Figure S11. LC-HRMS spectrum of **8b**.

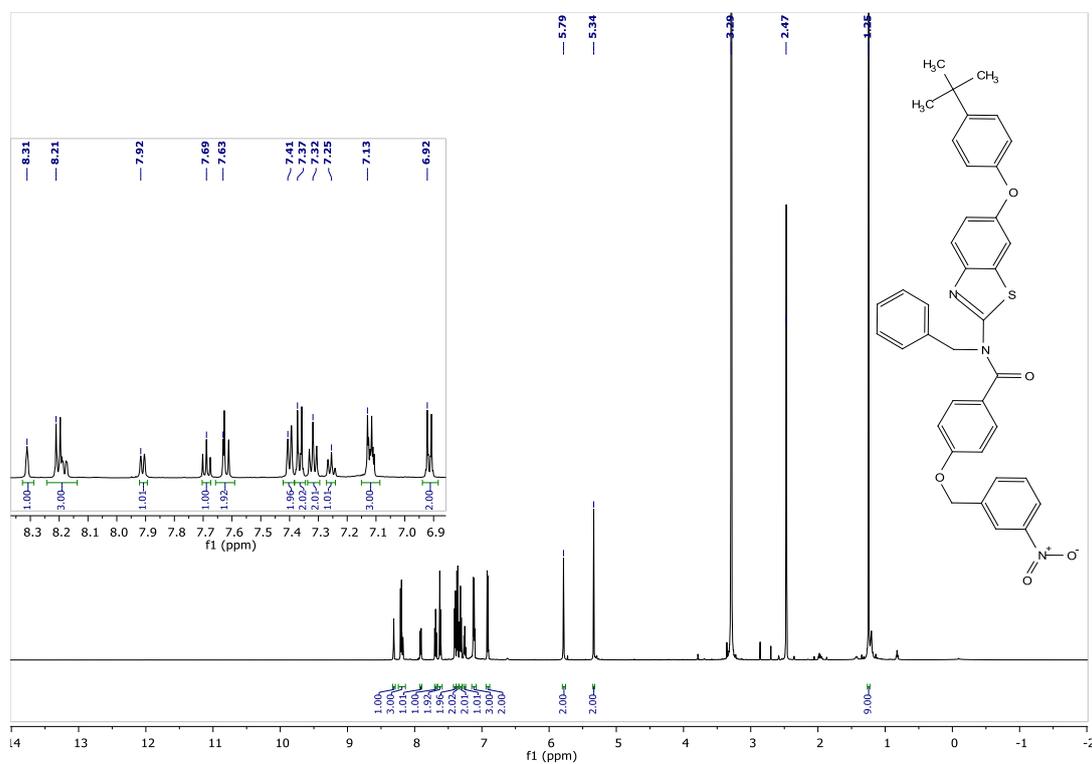


Figure S12. <sup>1</sup>H NMR spectrum (500 MHz, DMSO-d<sub>6</sub>) of **9a**.

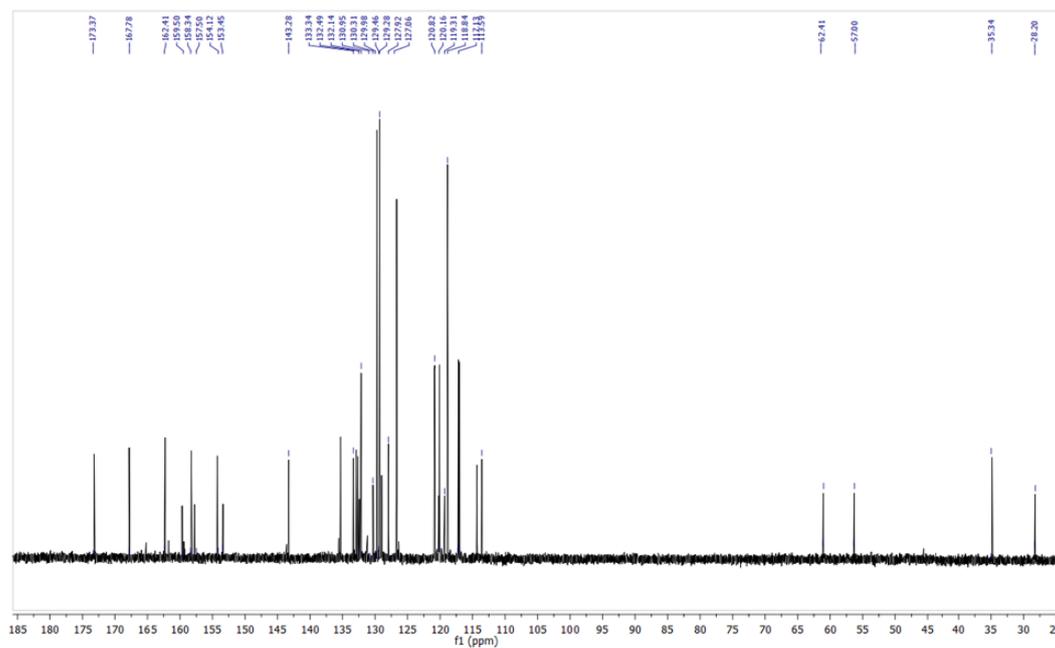


Figure S13.  $^{13}\text{C}$  NMR spectrum (126 MHz,  $\text{DMSO-}d_6$ ) of **9a**.

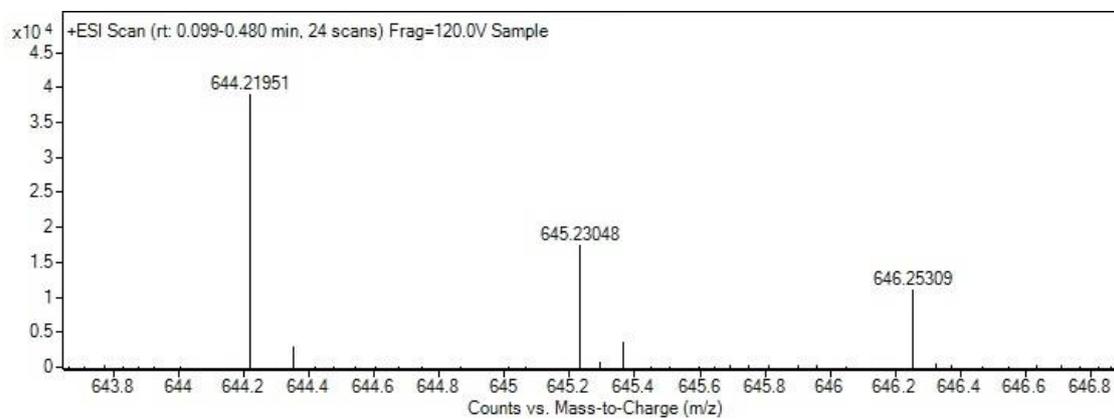
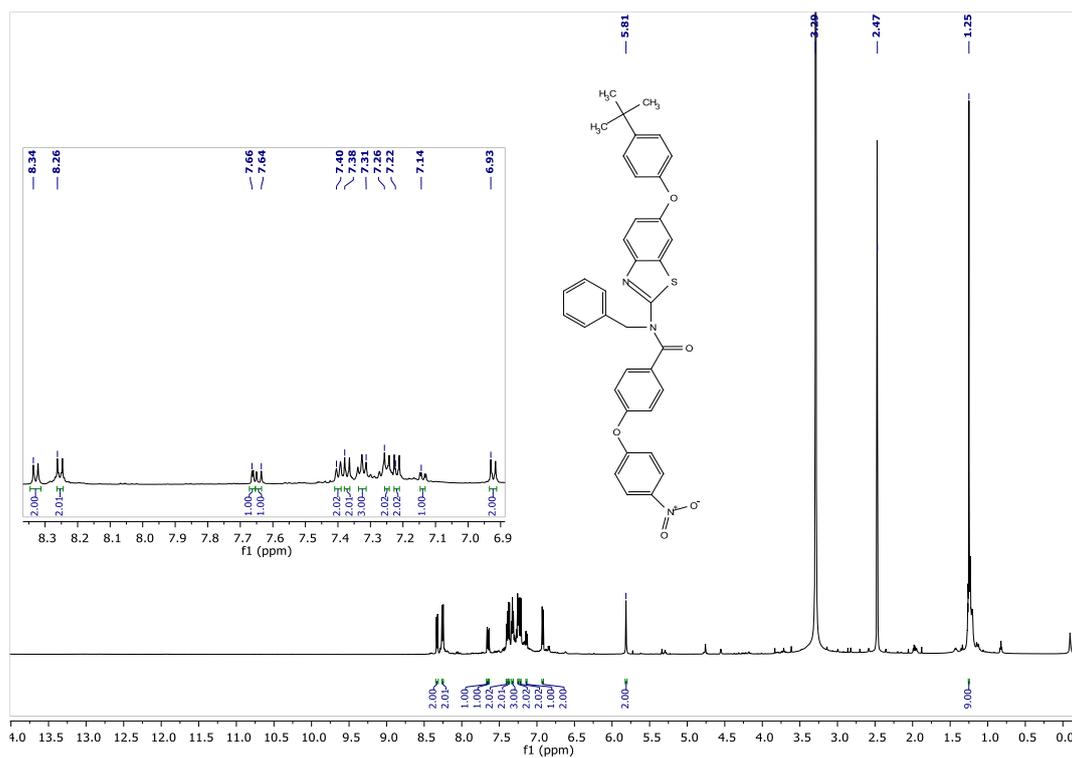
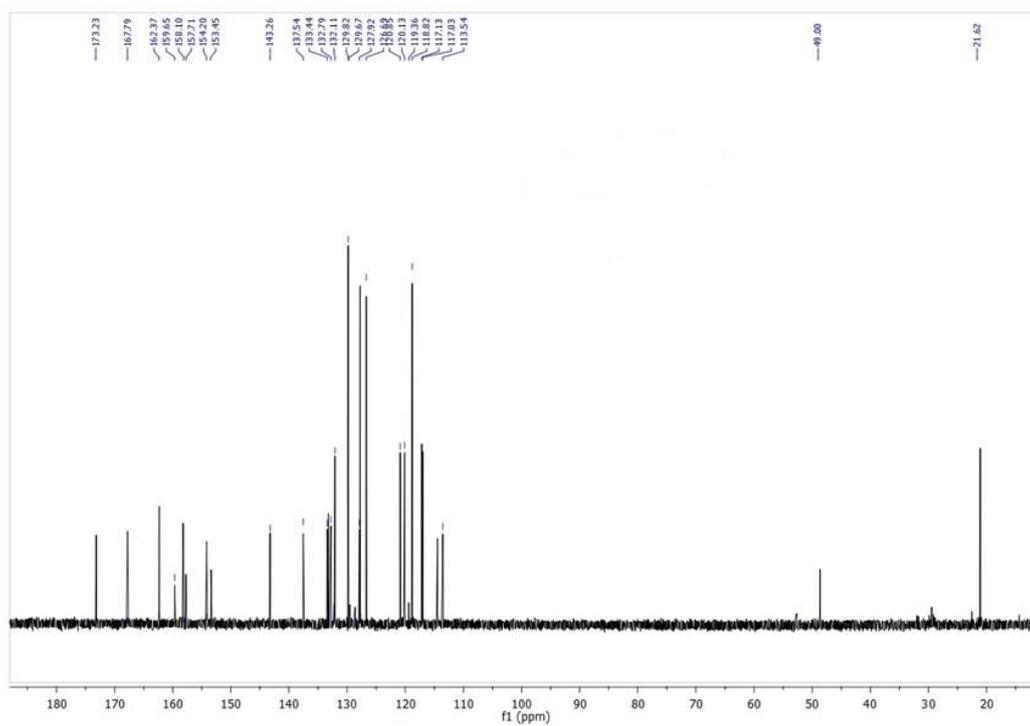


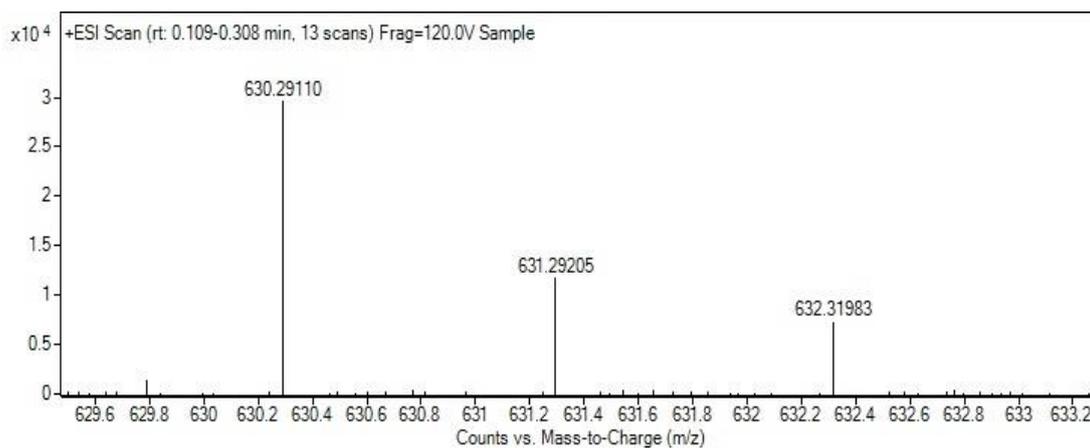
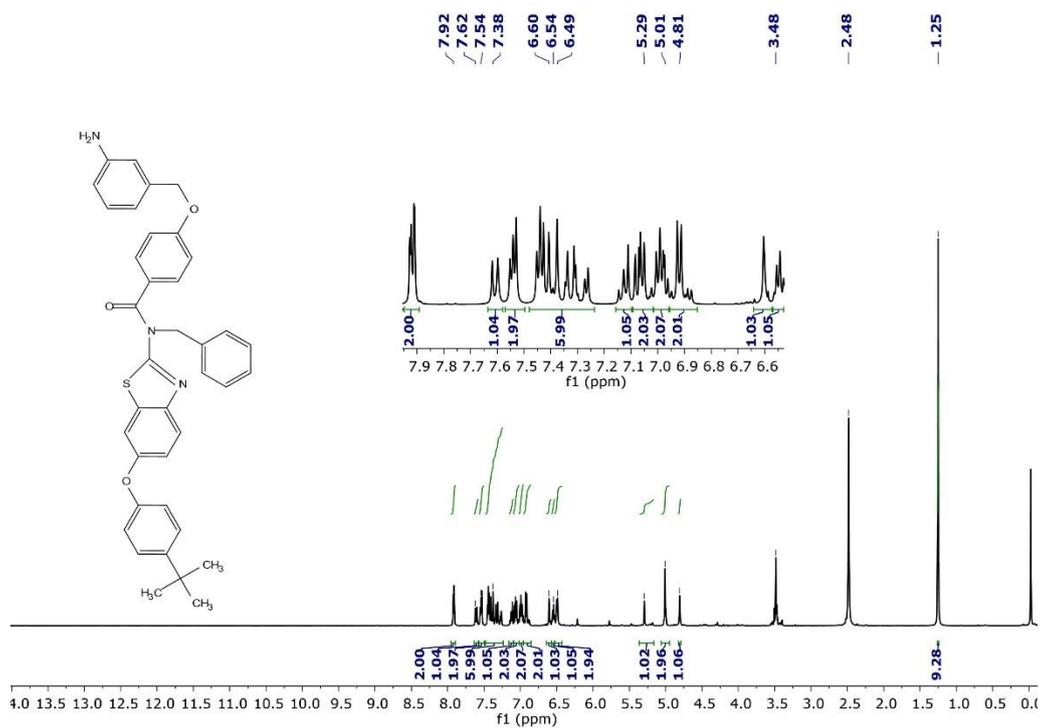
Figure S14. LC-HRMS spectrum of **9a**.



**Figure S15.**  $^1\text{H}$  NMR spectrum (500 MHz,  $\text{DMSO}-d_6$ ) of **9b**.



**Figure S16.**  $^{13}\text{C}$  NMR spectrum (126 MHz,  $\text{DMSO}-d_6$ ) of **9b**.

**Figure S17.** LC-HRMS spectrum of **9b**.**Figure S18.** <sup>1</sup>H NMR spectrum (500 MHz, DMSO-*d*<sub>6</sub>) of **10a**.

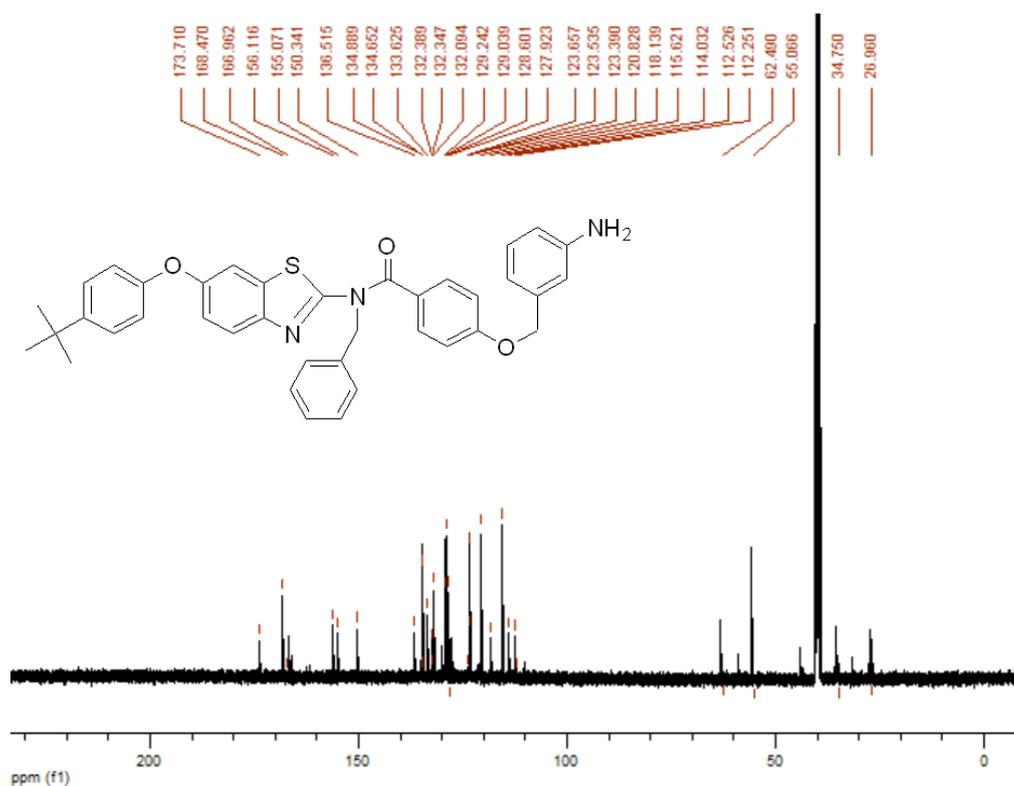


Figure S19. <sup>13</sup>C NMR spectrum (126 MHz, DMSO-*d*<sub>6</sub>) of 10a.

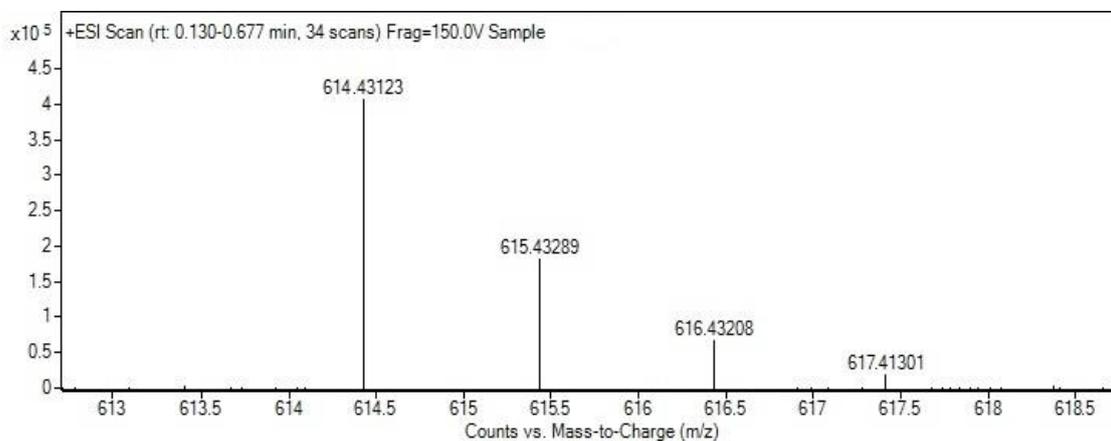


Figure S20. LC-HRMS spectrum of 10a.

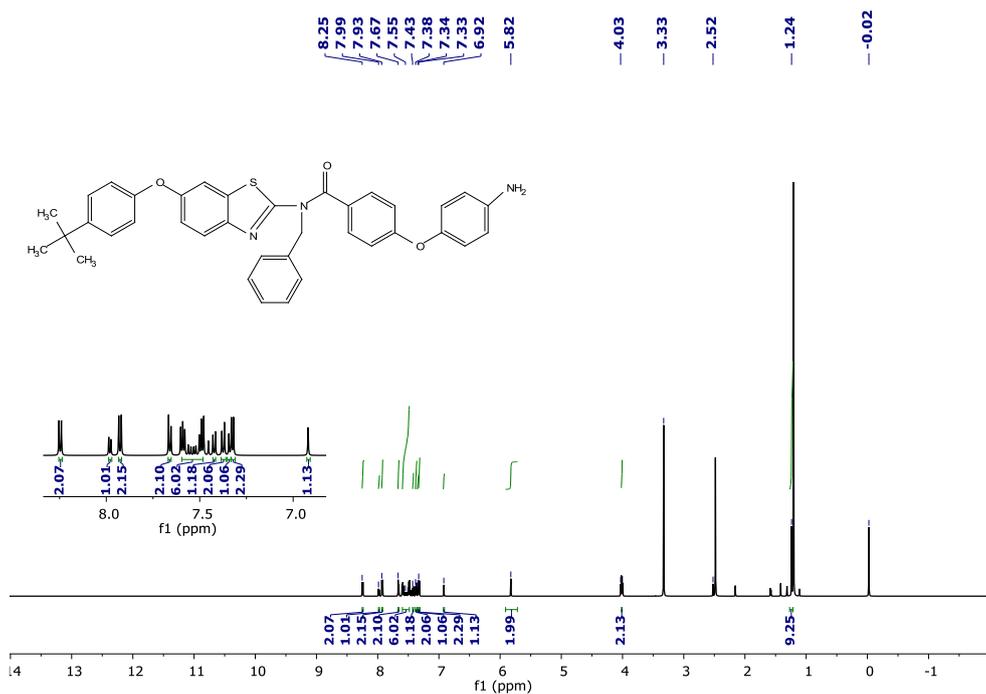


Figure S21. <sup>1</sup>H NMR spectrum (500 MHz, DMSO-*d*<sub>6</sub>) of **10b**.

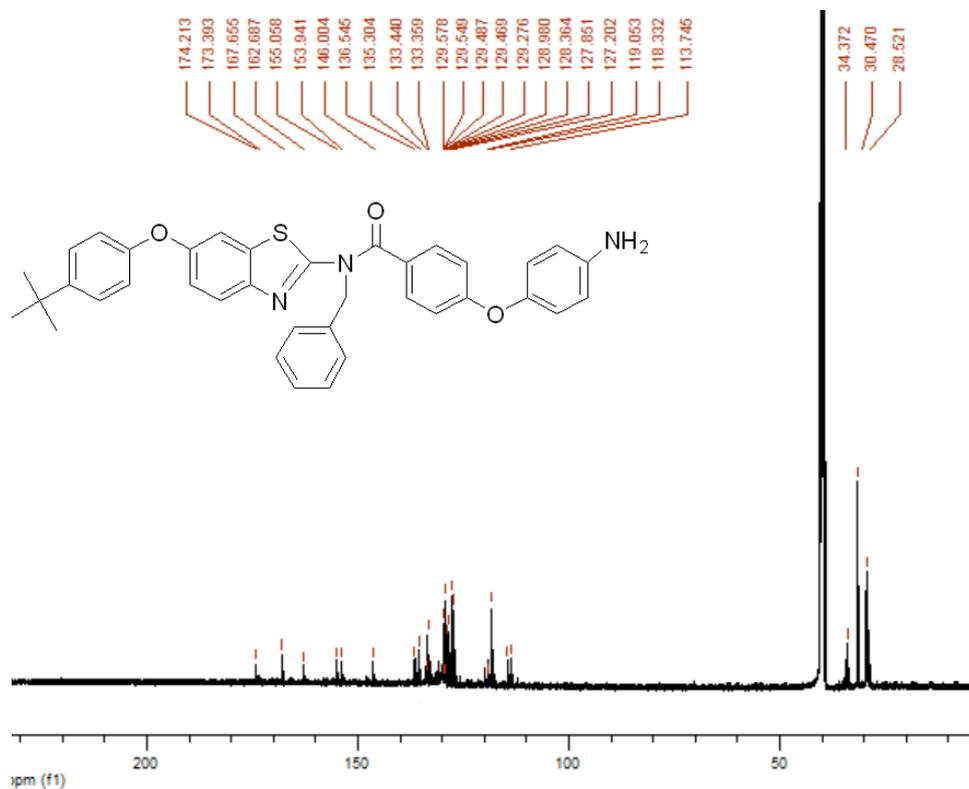


Figure S22. <sup>13</sup>C NMR spectrum (126 MHz, DMSO-*d*<sub>6</sub>) of **10b**.

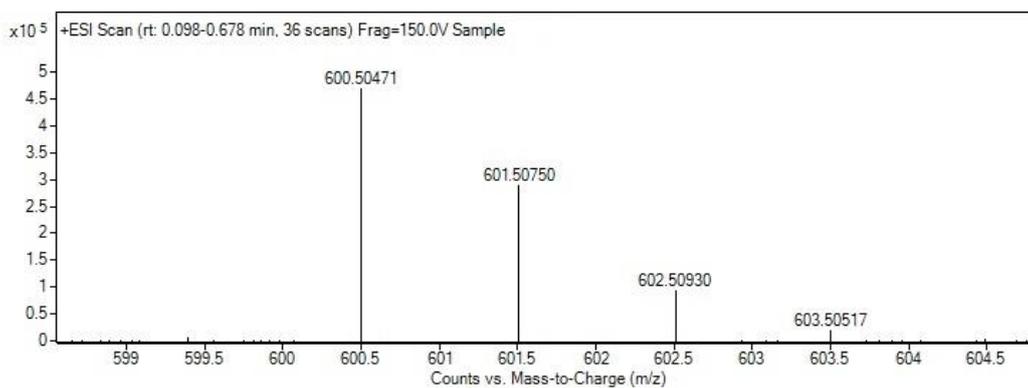


Figure S23. LC-HRMS spectrum of **10b**.

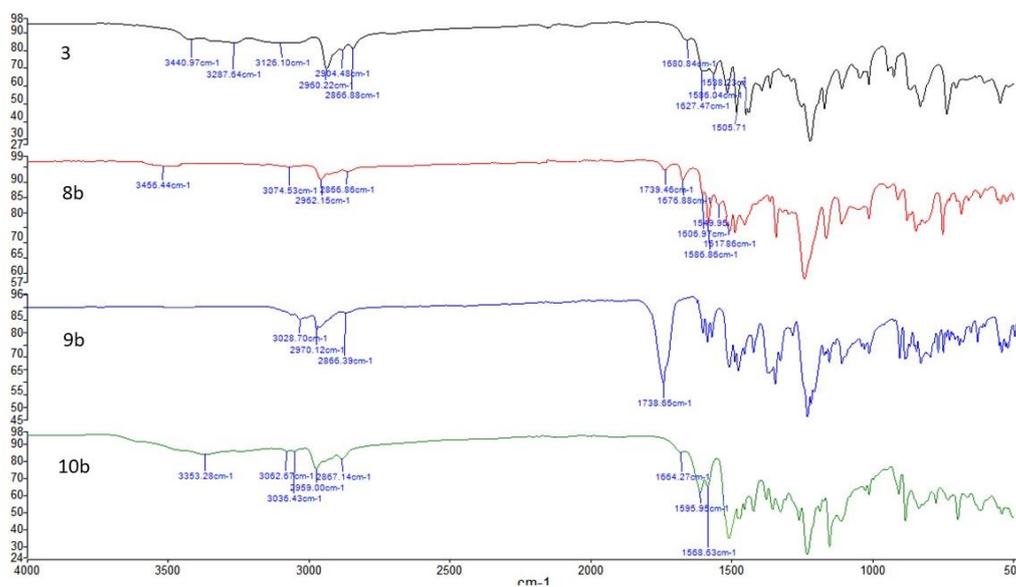


Figure S24. IR spectrum (ATR) of **3**, **8b**, **9b** and **10b**.

## 2. 2D Diagrams of interactions involved in molecular docking

Table S1. 2D diagrams of interactions involved between PD-L1 and novel peptidomimetics

