

## Supporting Information

# Interactions of Arene Ruthenium Metallaprisms with Human Proteins

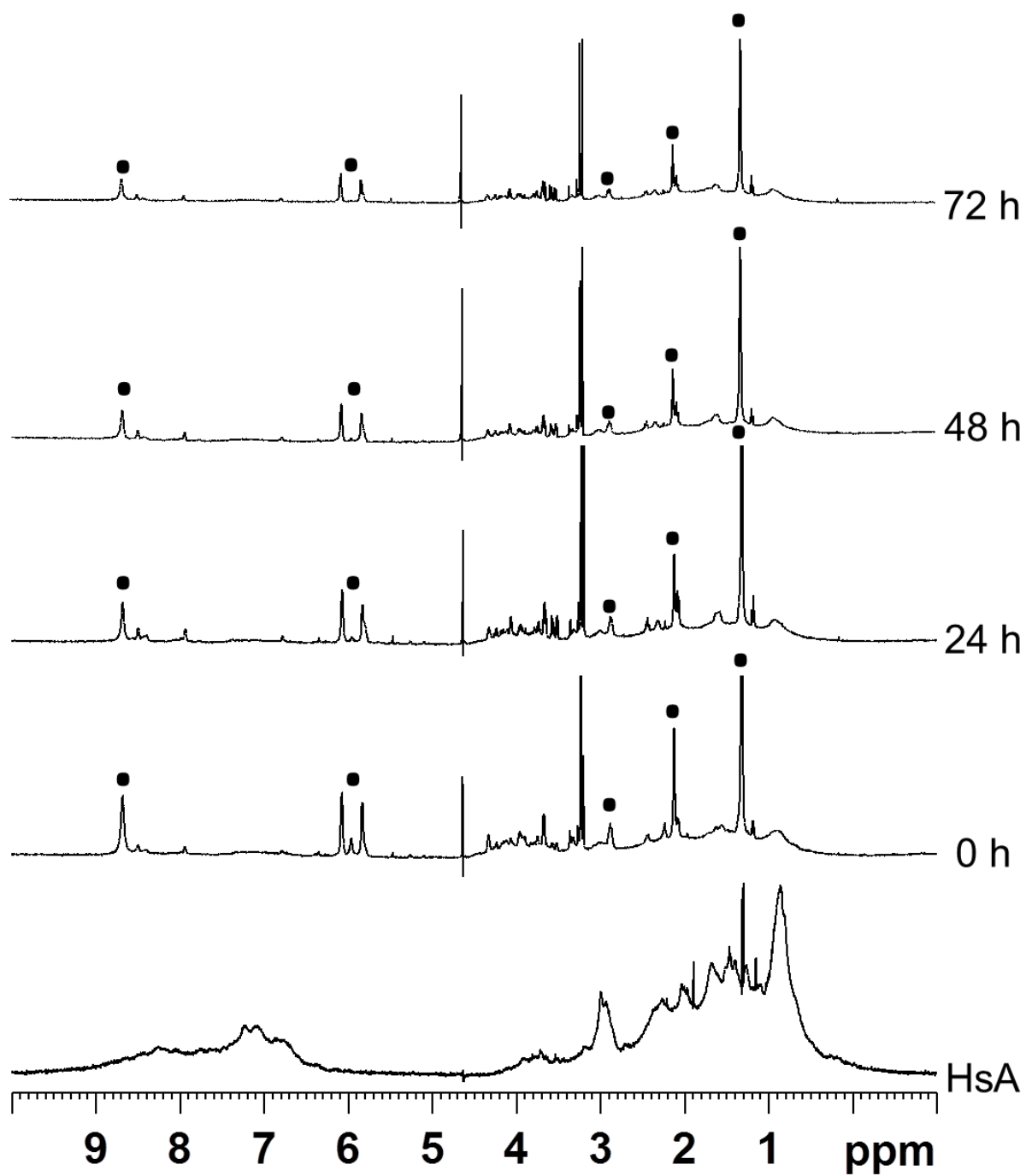
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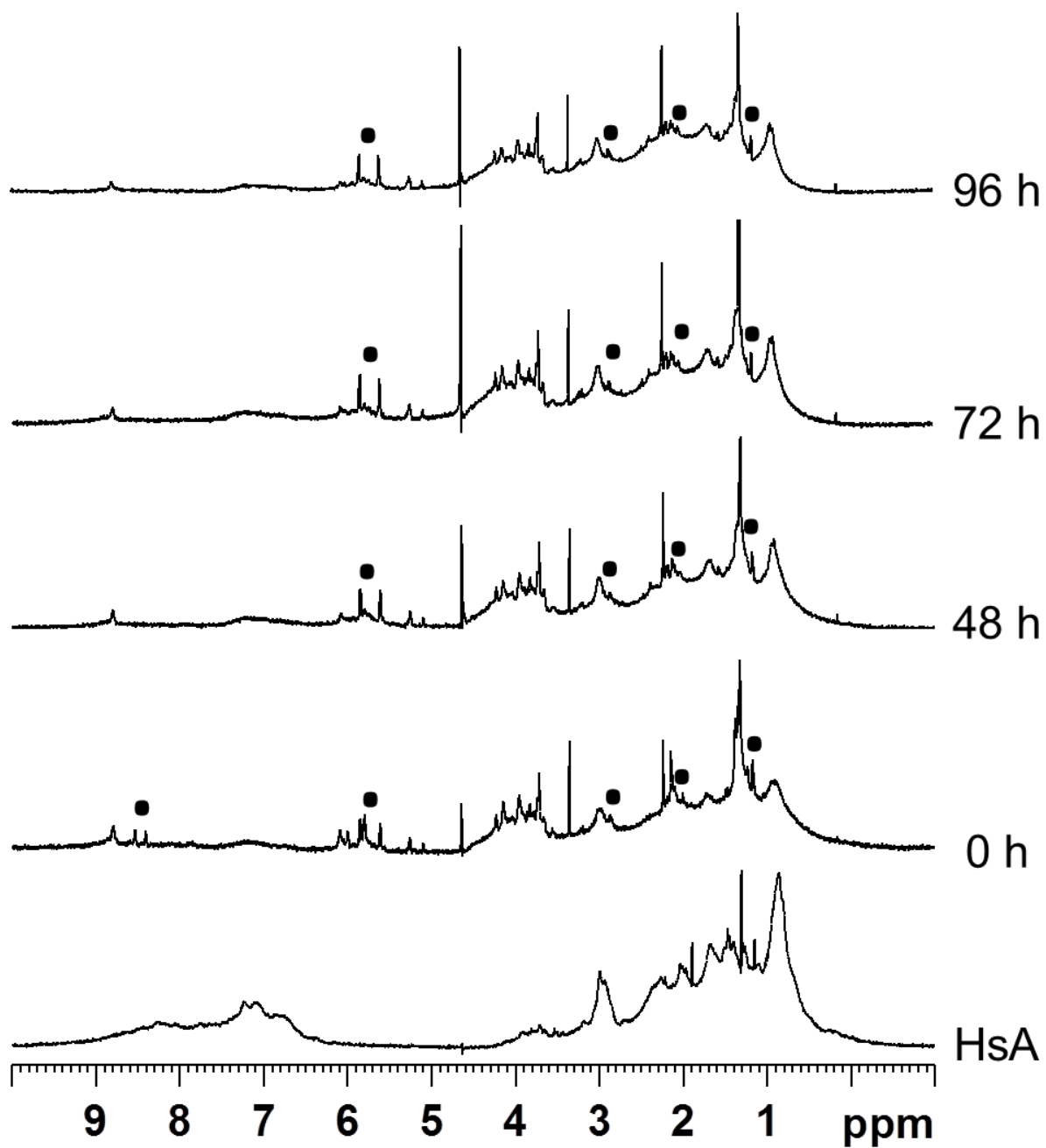
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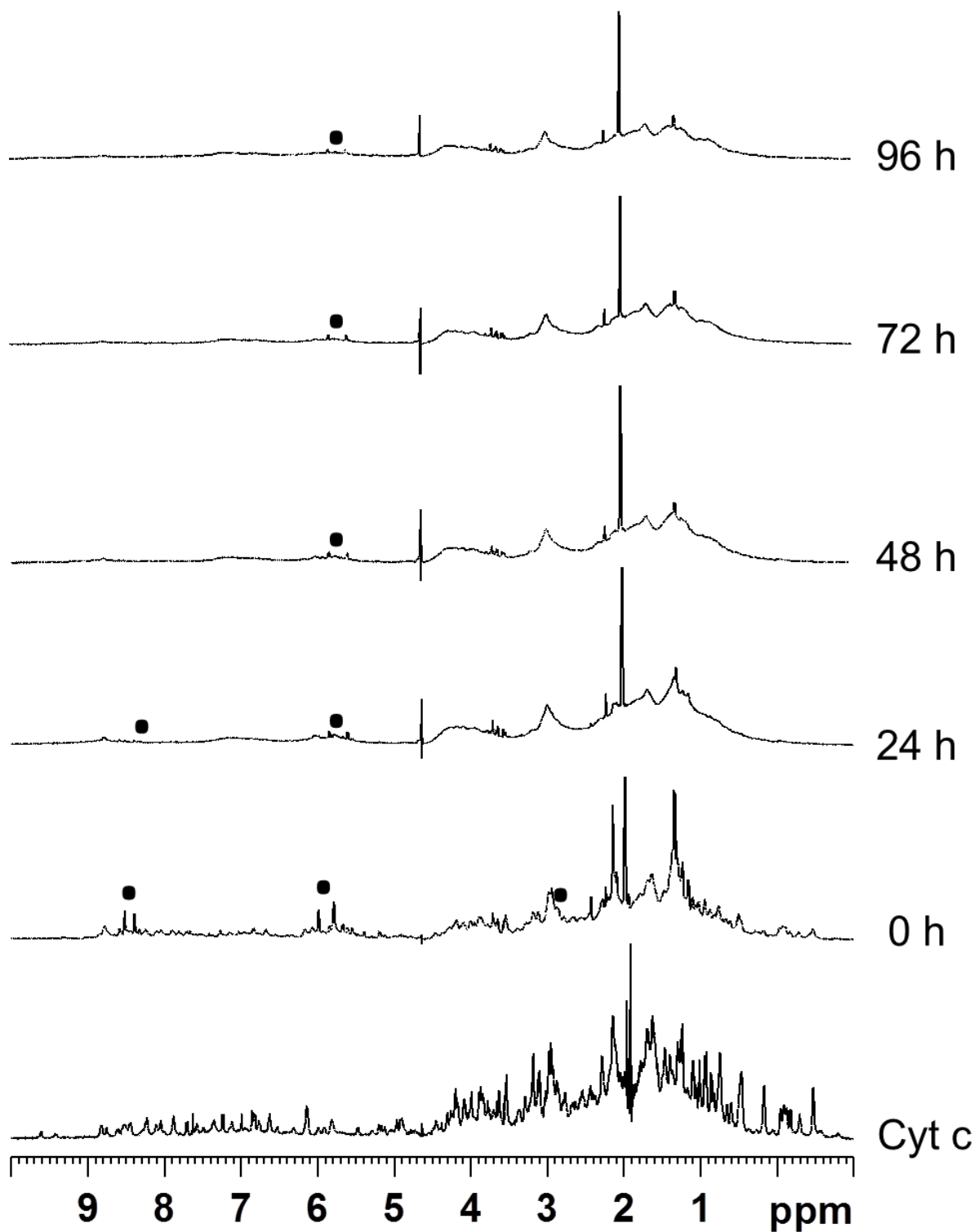
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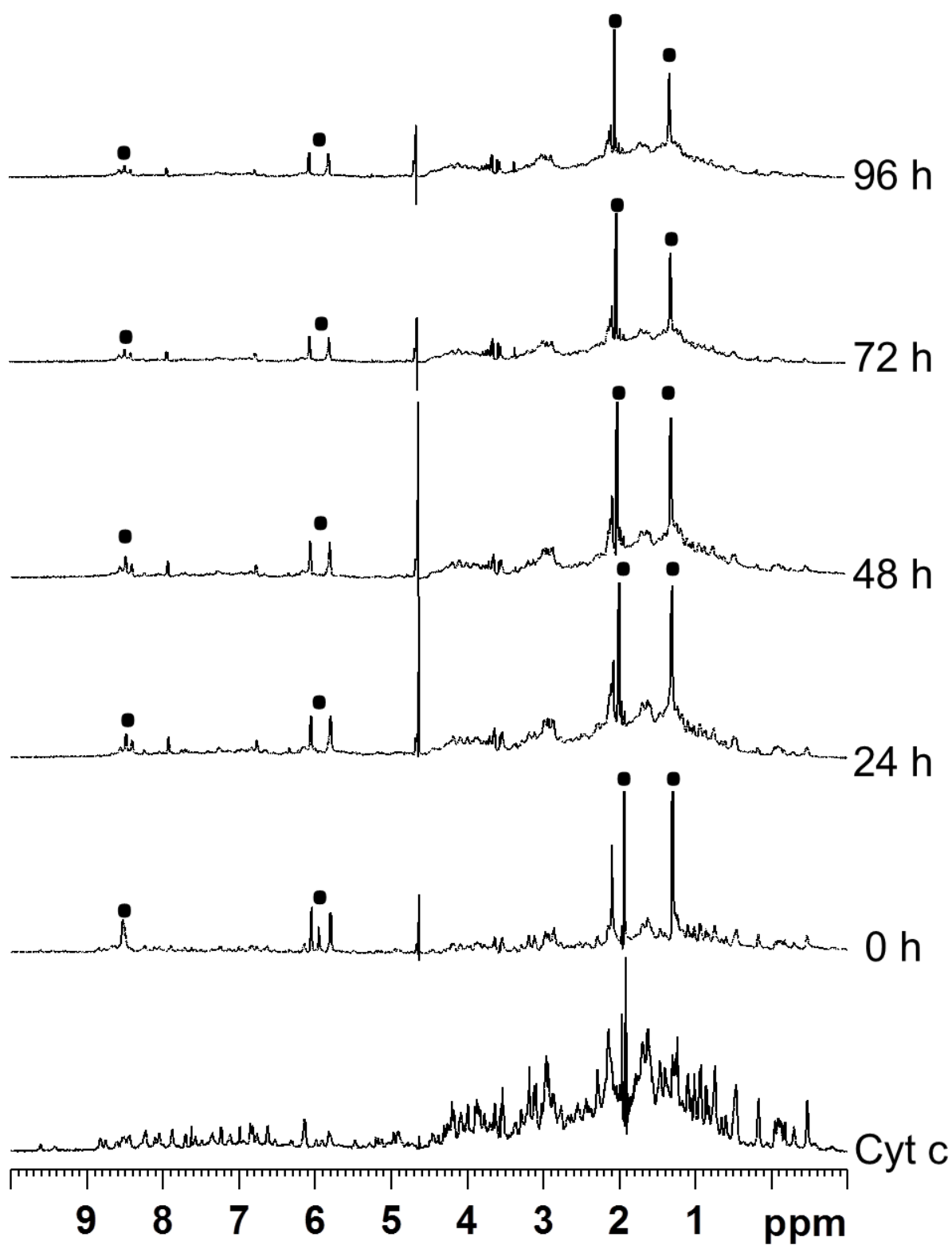
**Figure S1.** <sup>1</sup>H NMR spectra of the mixture HsA / [2]<sup>6+</sup> dissolved in D<sub>2</sub>O and recorded at 37 °C. The spectrum of free HsA was added at the bottom for comparison. The resonances for the metallaprism are highlighted by (■).



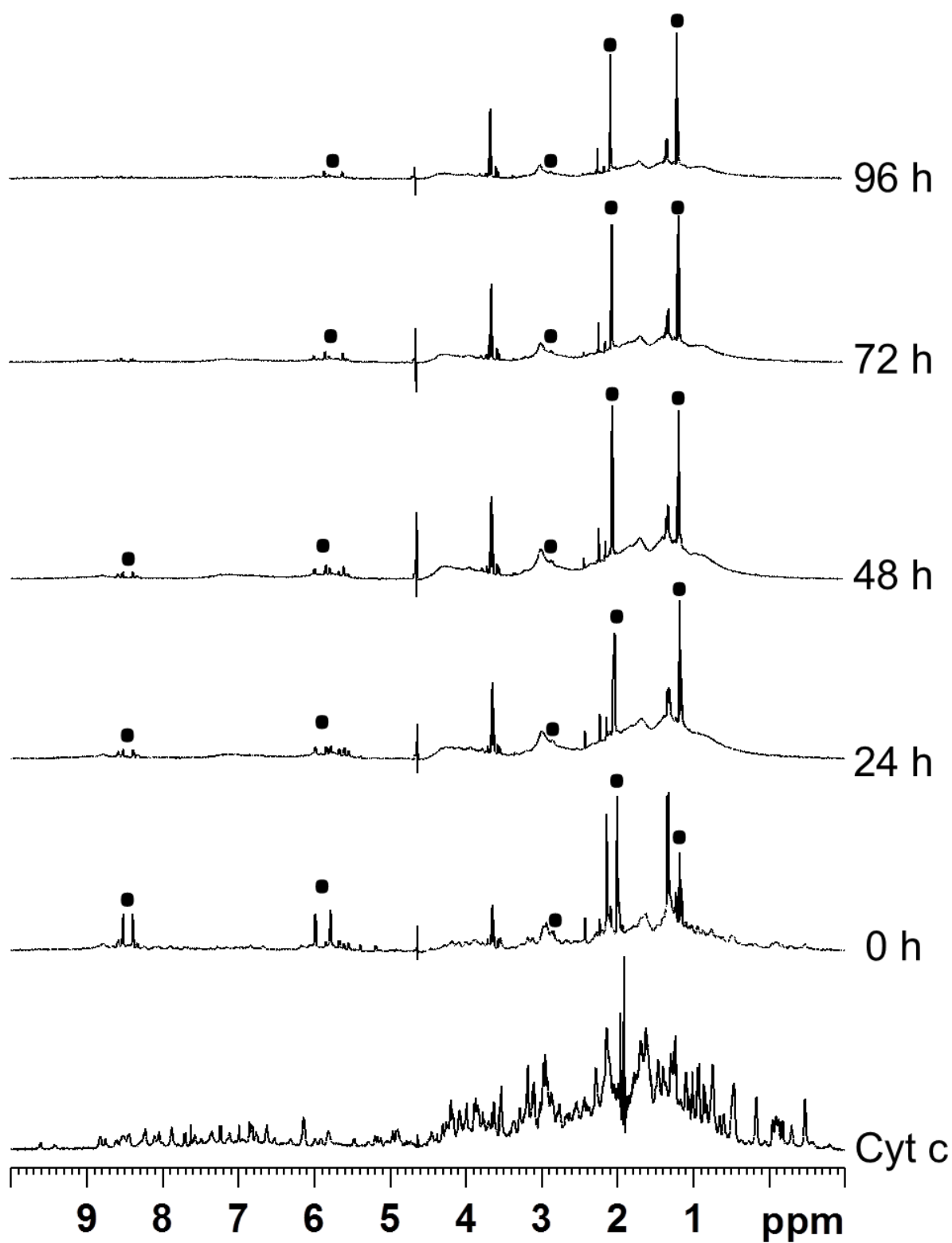
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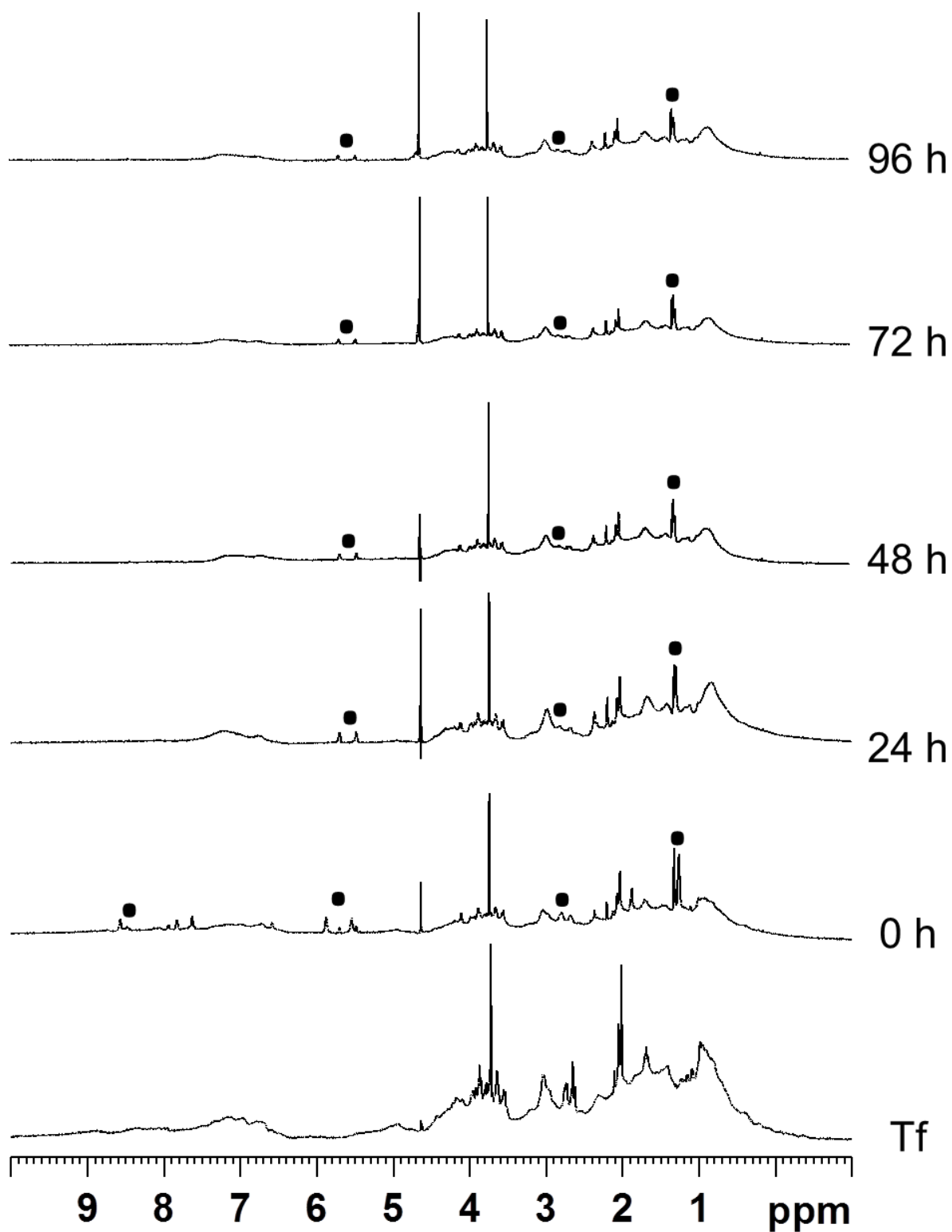
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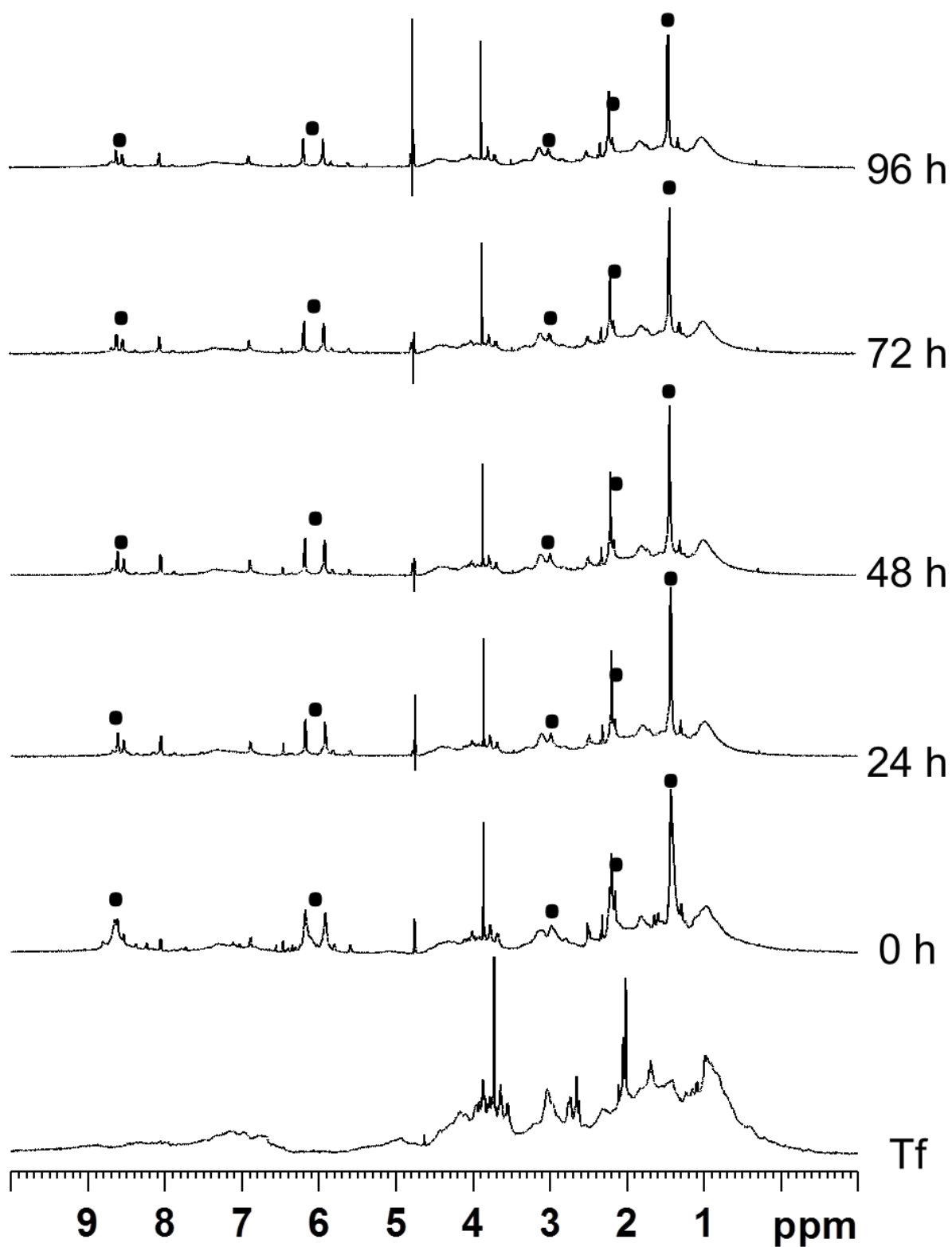
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**Figure S5.** <sup>1</sup>H NMR spectra of the mixture Cyt c / [3]<sup>6+</sup> dissolved in D<sub>2</sub>O and recorded at 37°C. The spectrum of free Cyt c was added at the bottom for comparison. The resonances for the metallaprism are highlighted by (■).

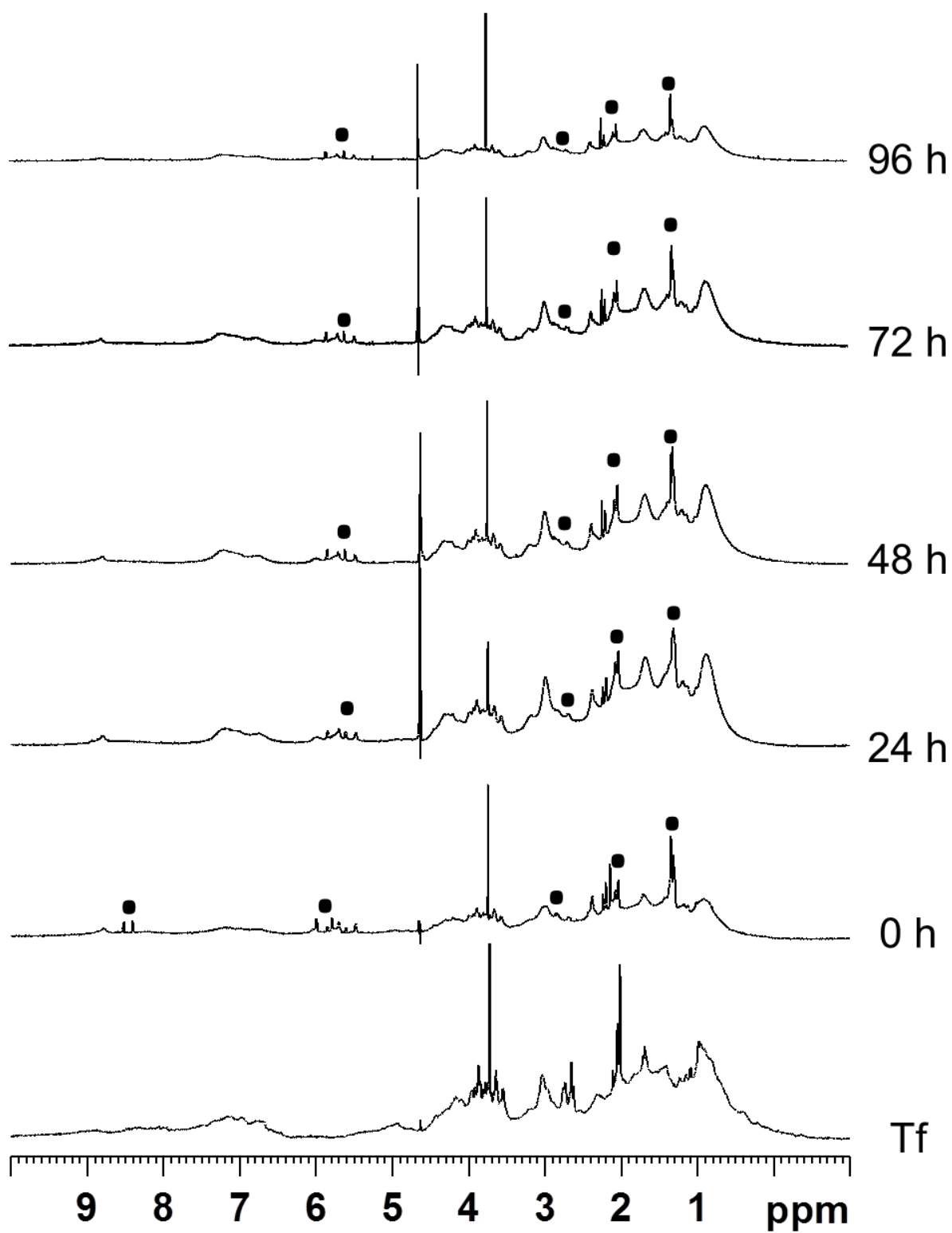


**Figure S6.** <sup>1</sup>H NMR spectra of the mixture Tf / [1]<sup>6+</sup> dissolved in D<sub>2</sub>O and recorded at 37°C. The spectrum of free Tf was added at the bottom for comparison. The resonances for the metallaprism are highlighted by (■).

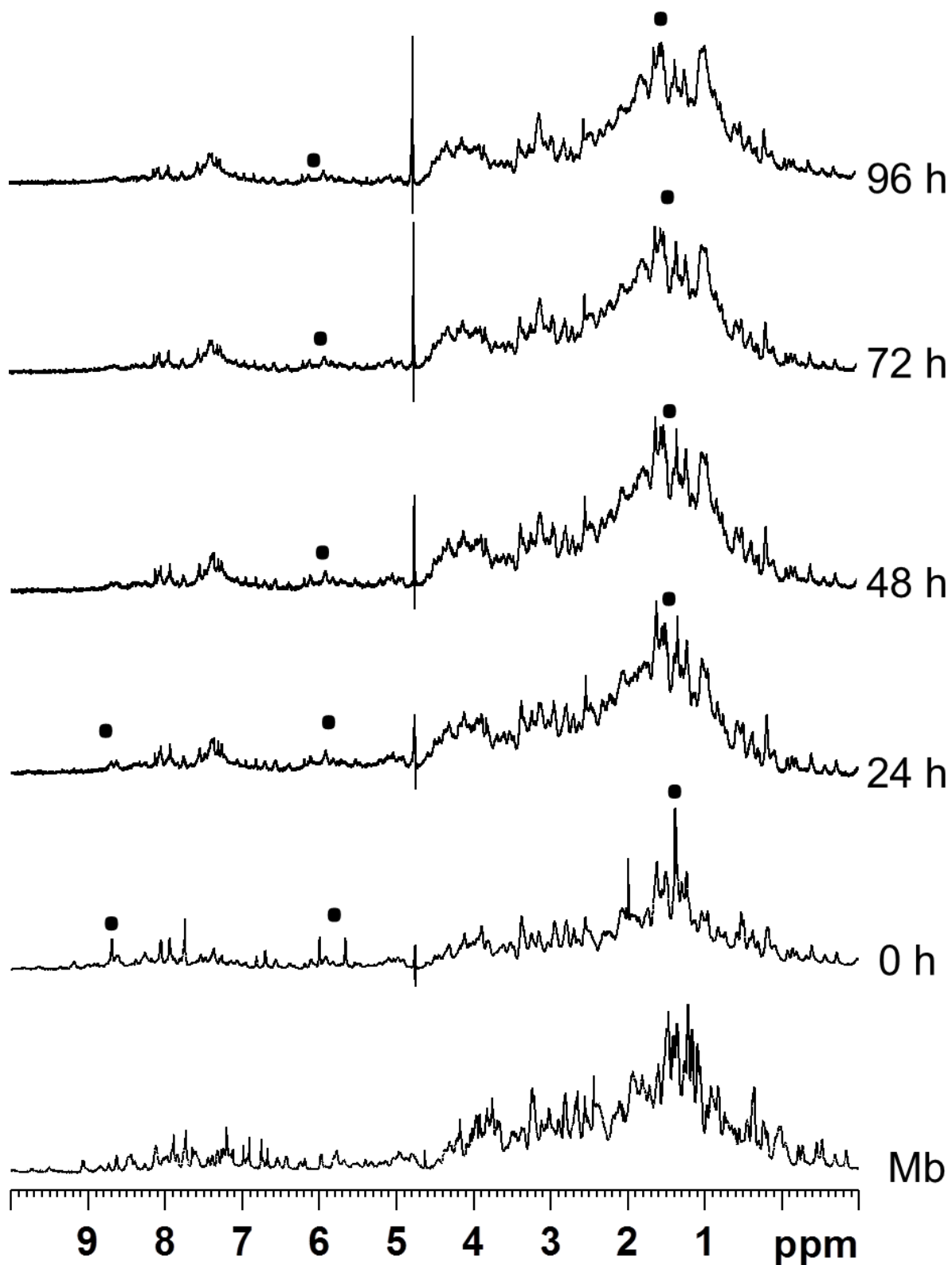


**Figure S7.** <sup>1</sup>H NMR spectra of the mixture Tf / [2]<sup>6+</sup> dissolved in D<sub>2</sub>O and recorded at 37°C. The spectrum of free Tf was added at the bottom for comparison. The resonances for the metallaprism are highlighted by (■).

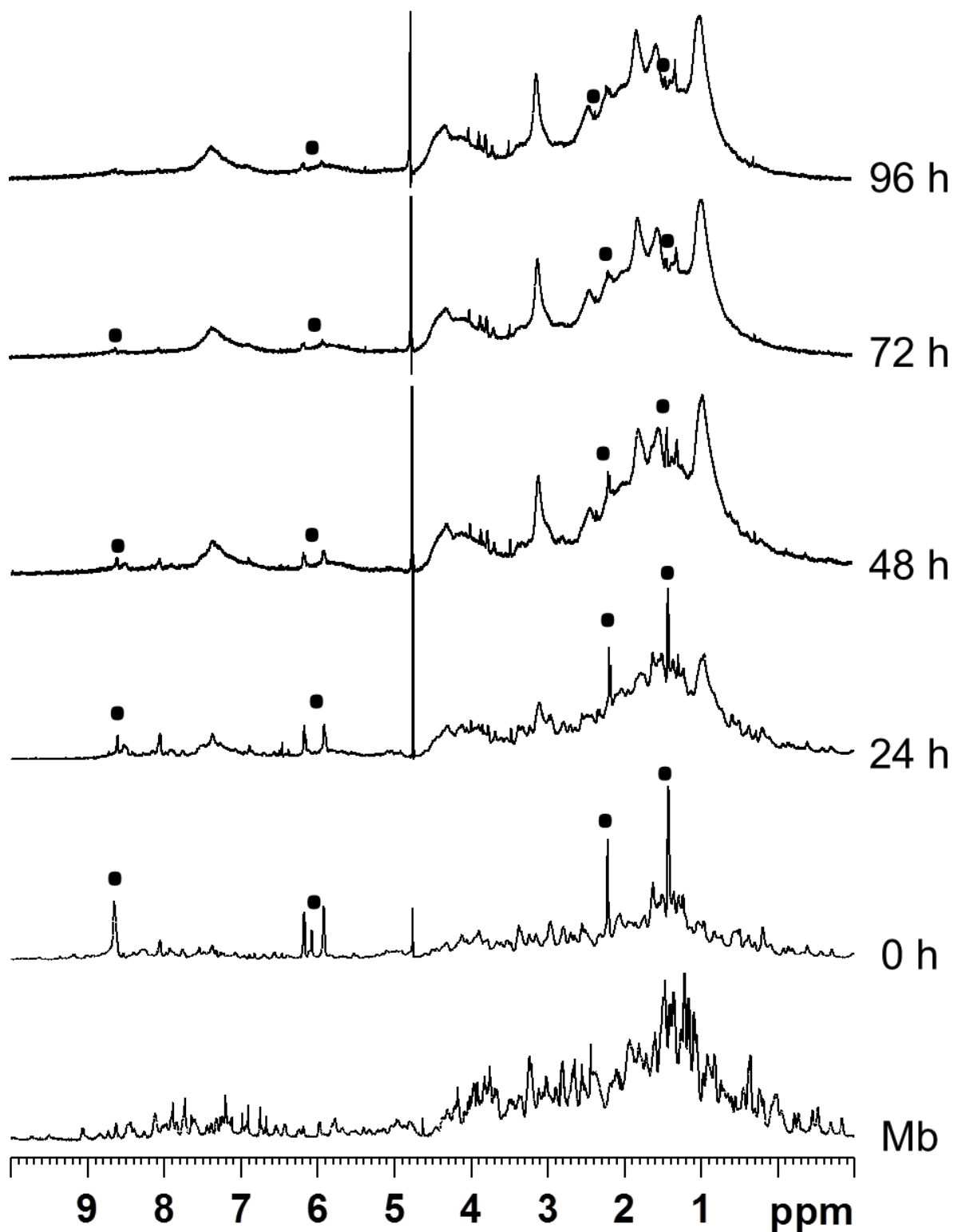




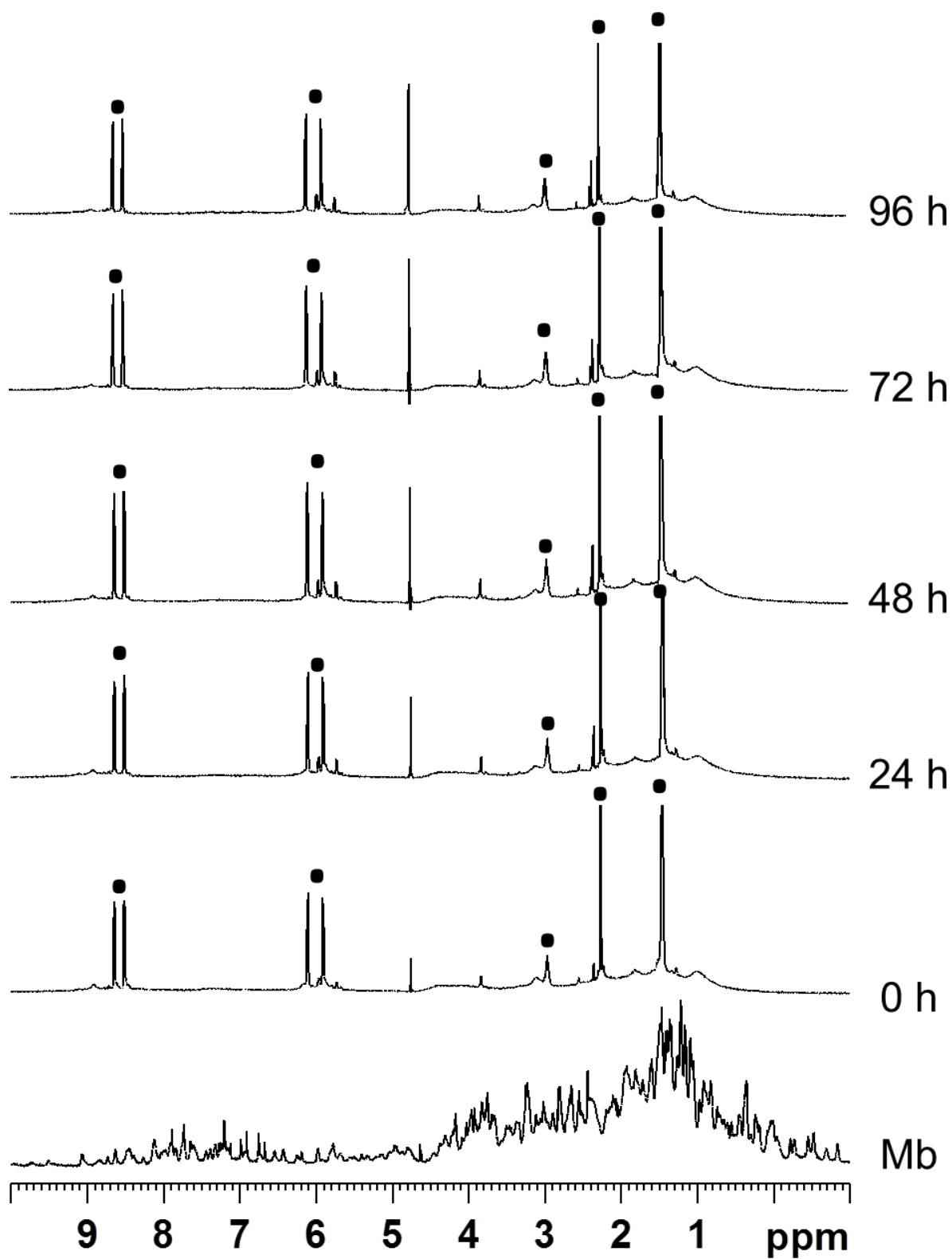
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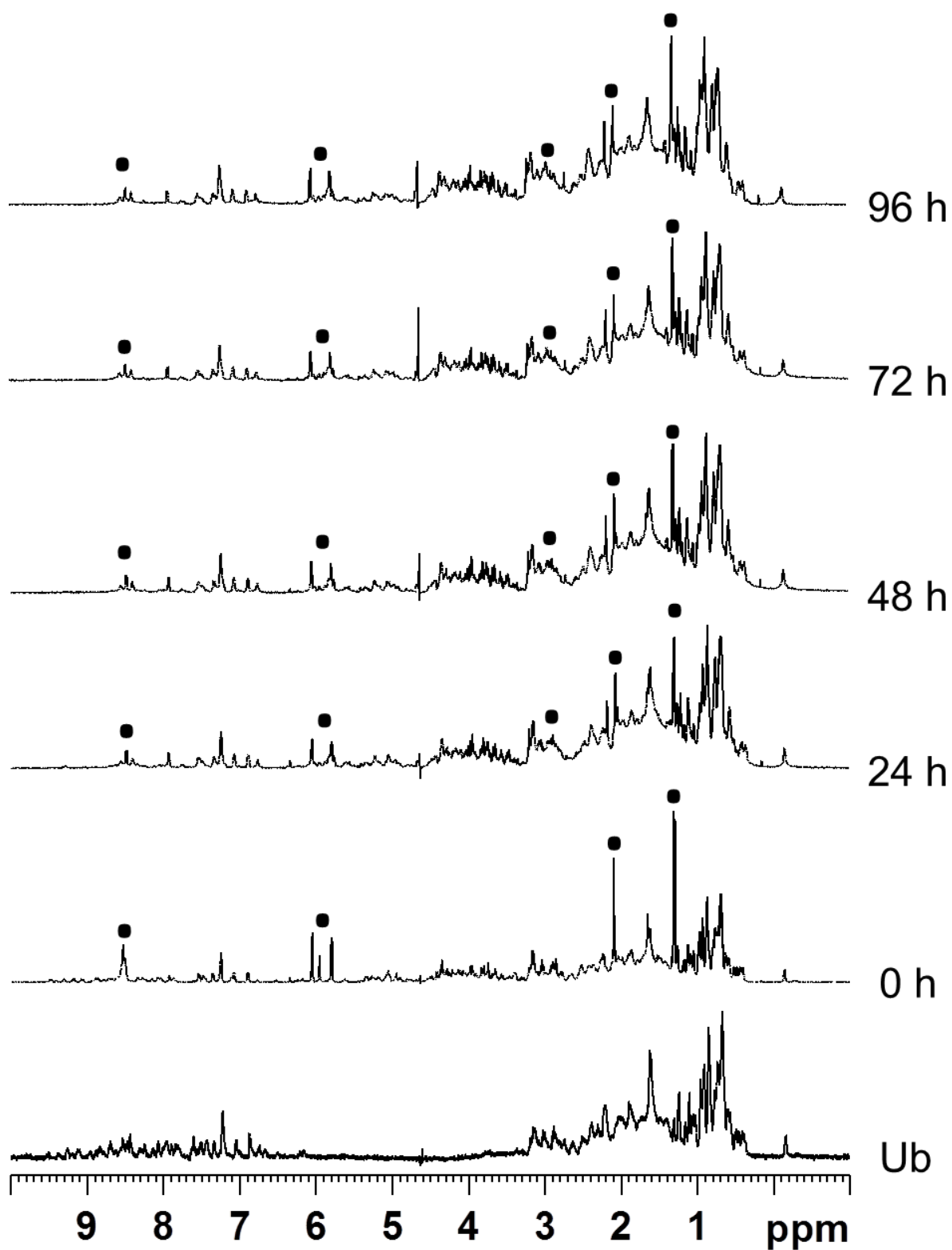
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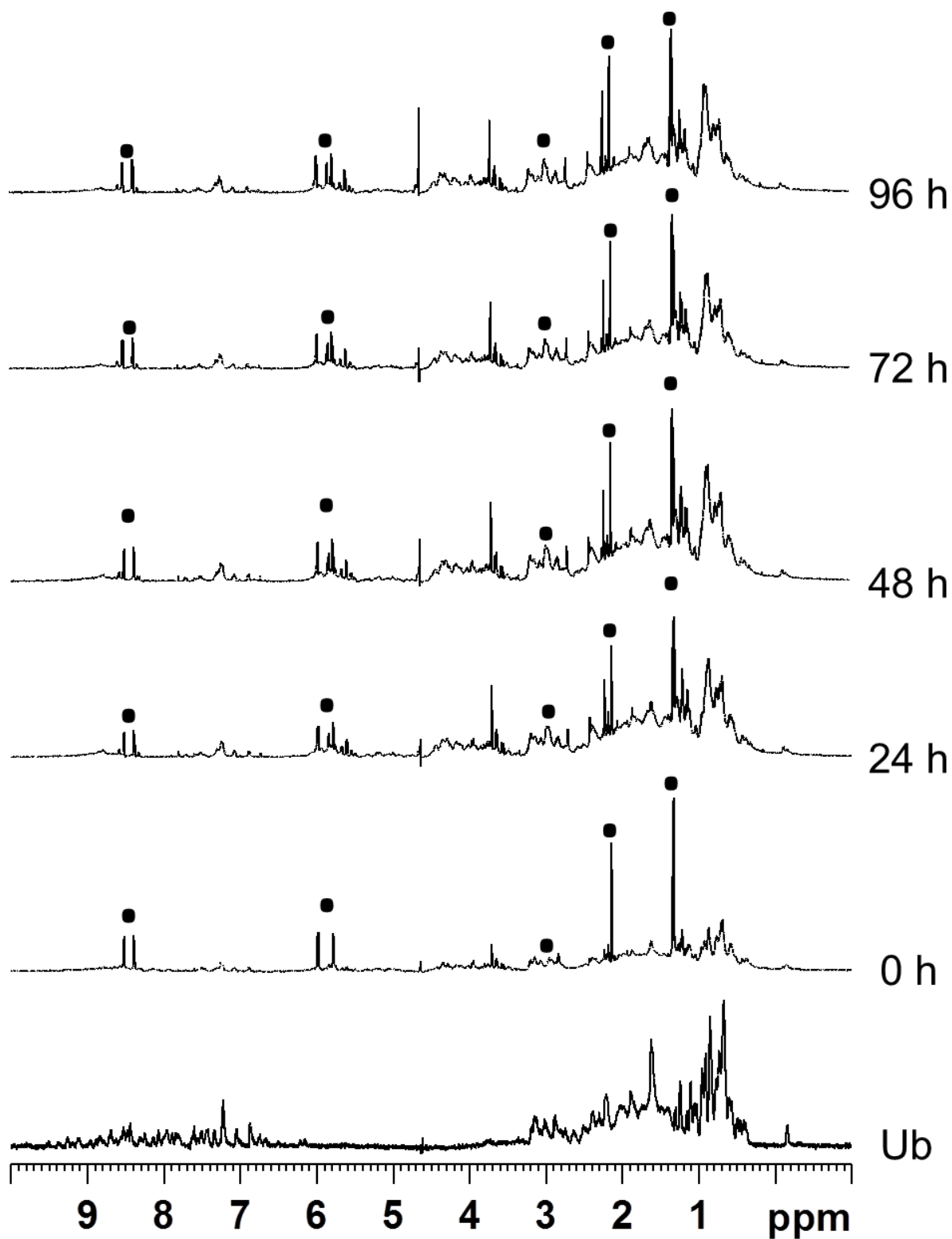
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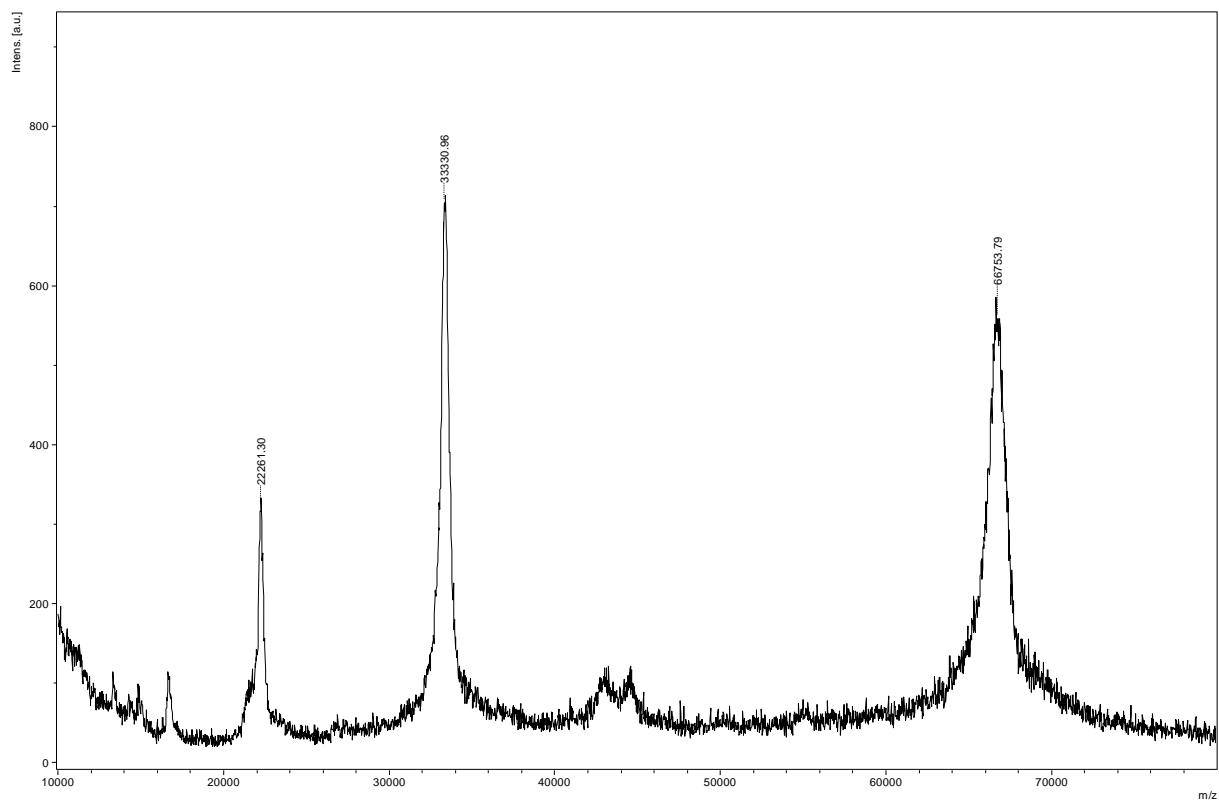
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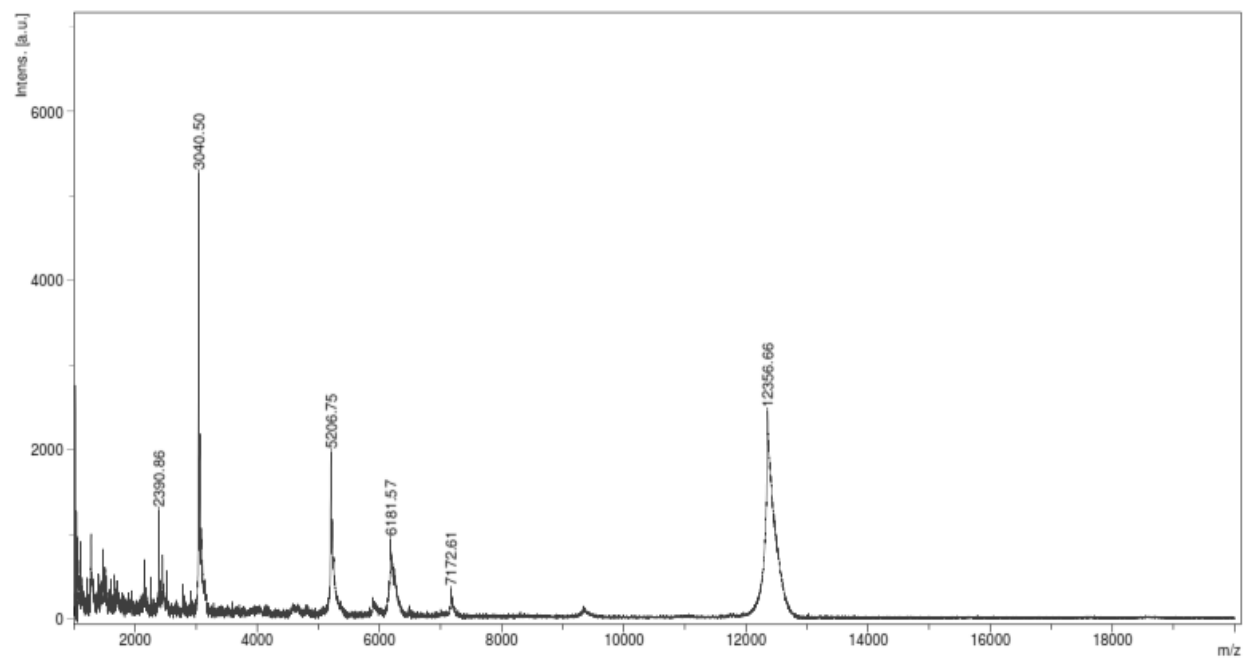
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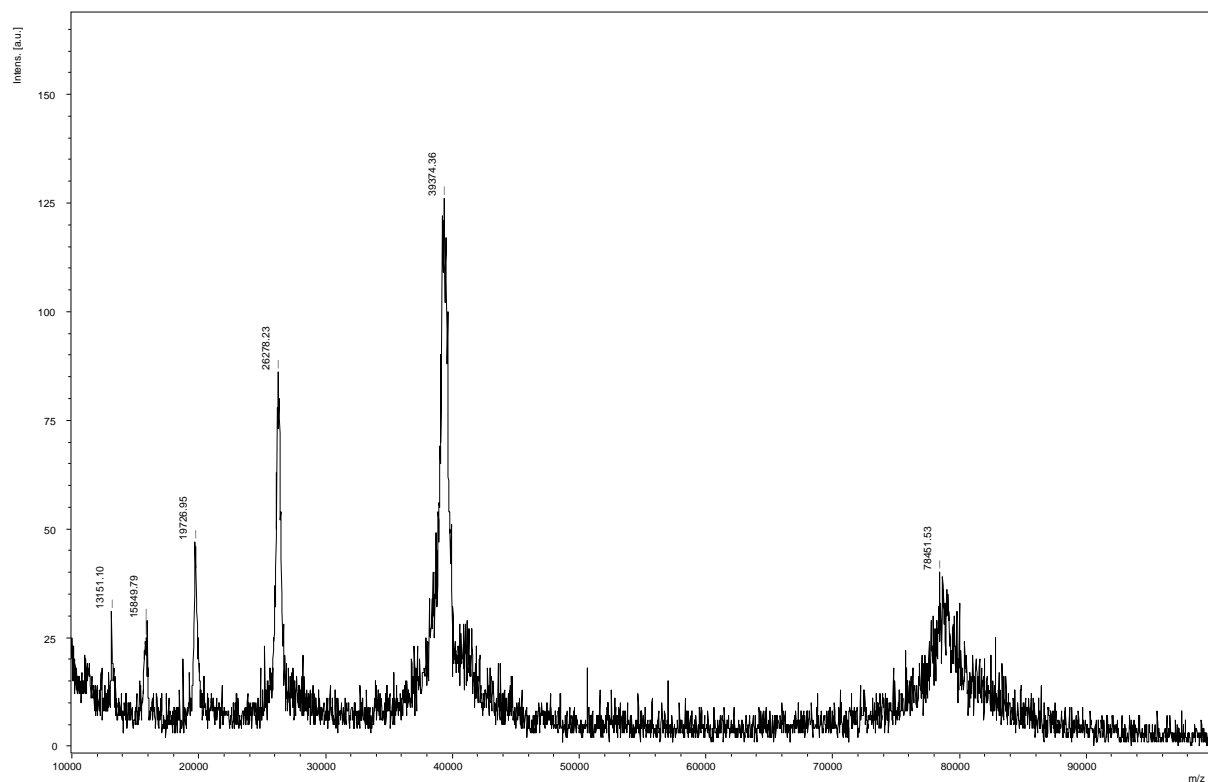
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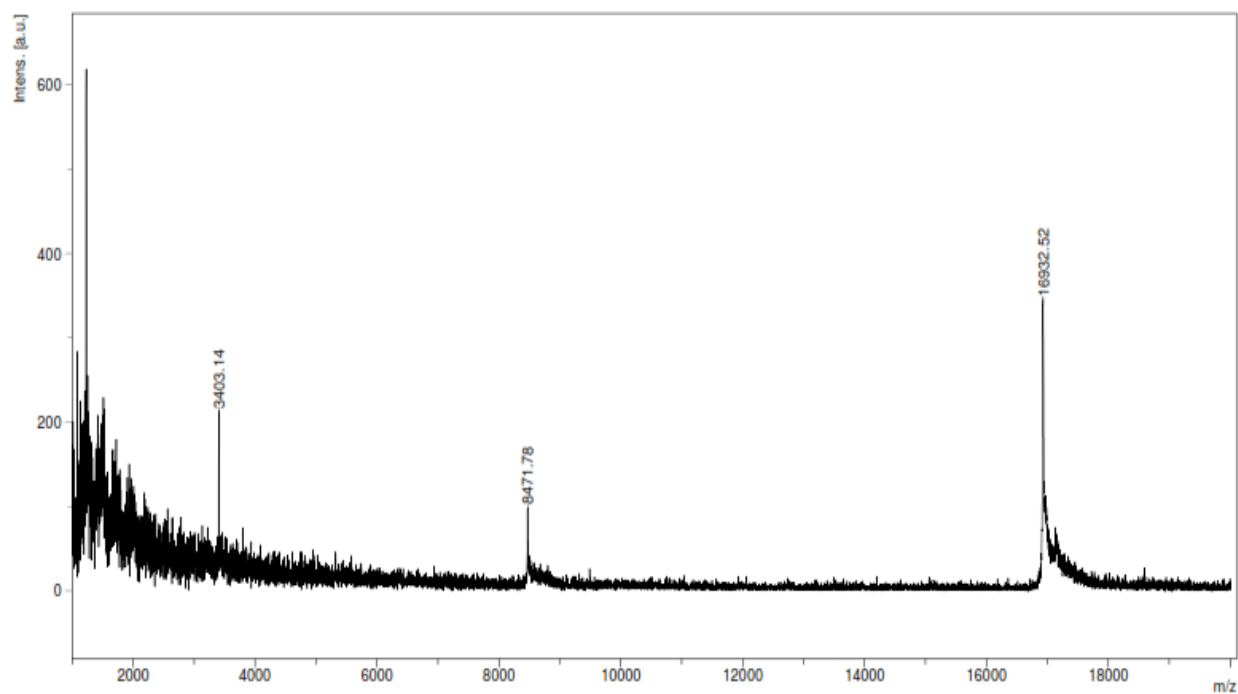
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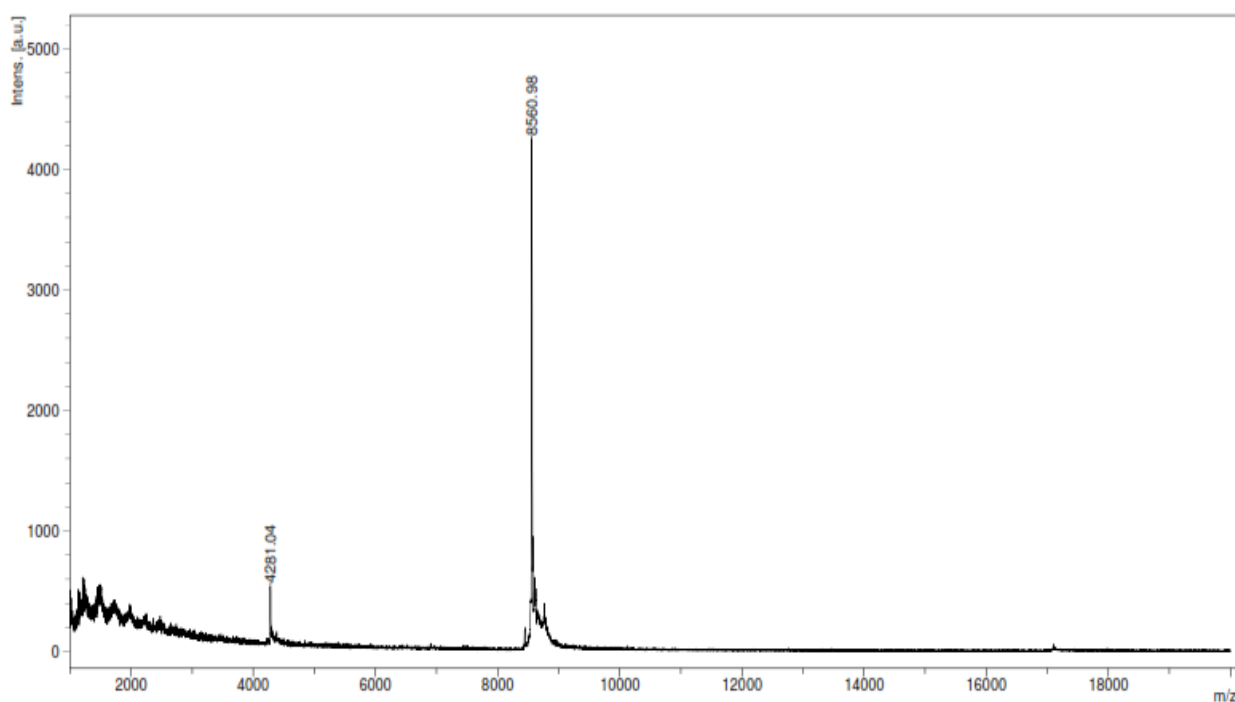


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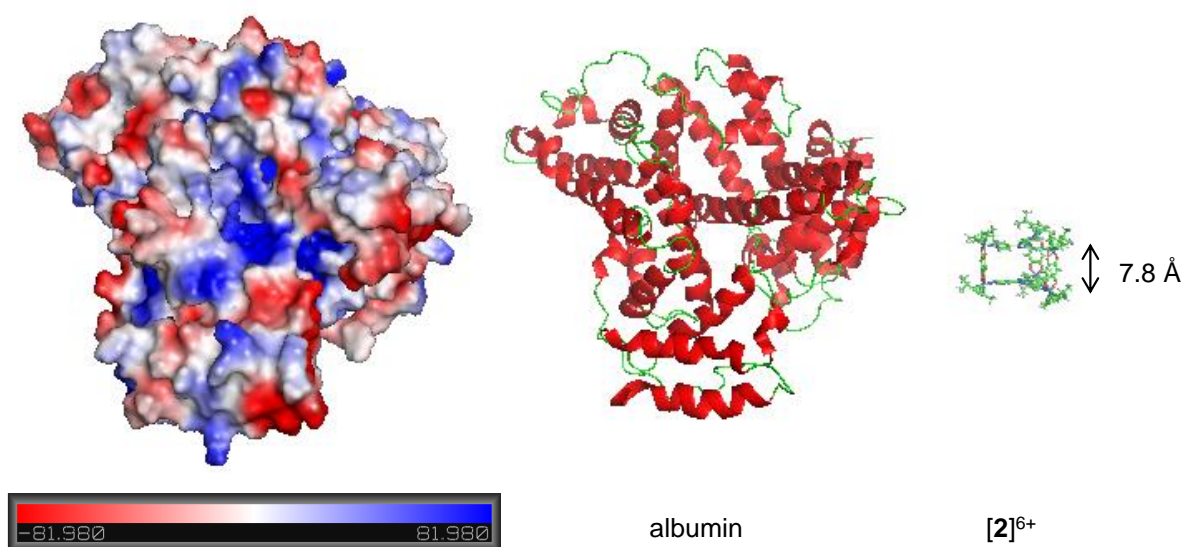


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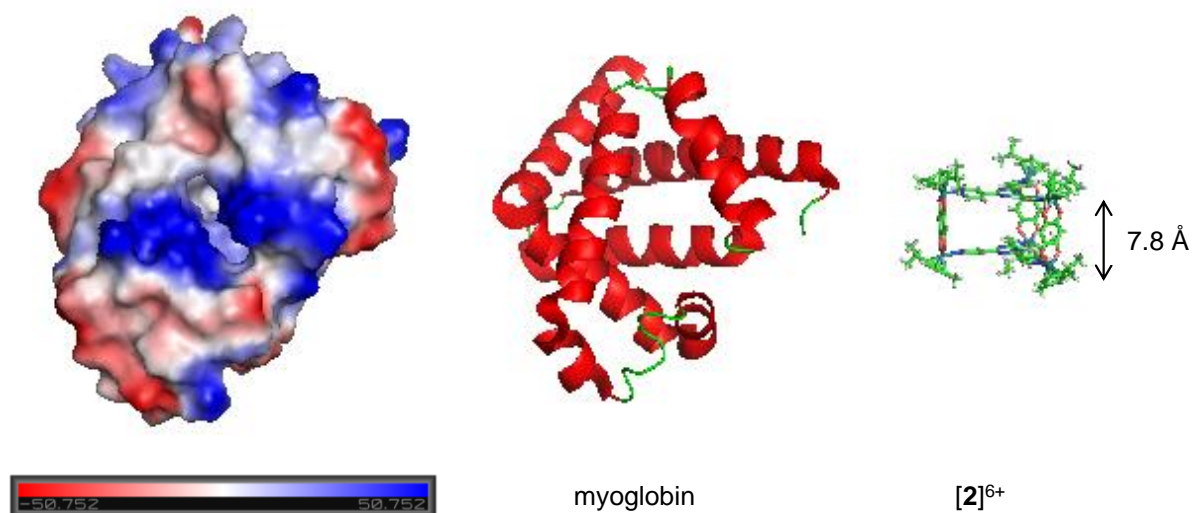




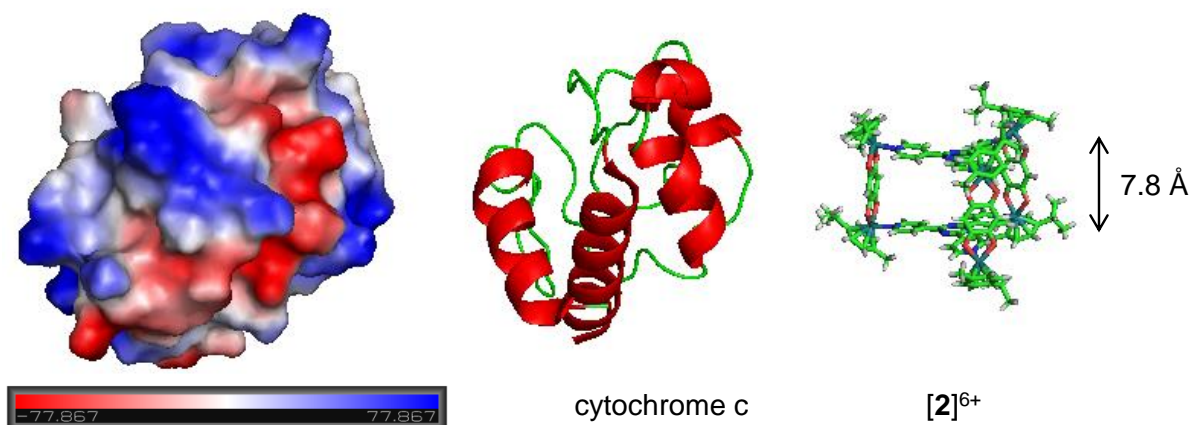
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**Figure S19.** Electrostatic potentials on the protein surface modelled with PyMOL (v 1.7.2.1) (left). The sequence was modelled from the RSCB pdb file 1UOR.<sup>1</sup> Areas of negative potentials are shown in red, of positive potentials in blue and of neutral potentials in white. The structure of the protein created from the same pdb file is shown in the middle. The structure of metallaprism [2]<sup>6+</sup> (right) was added to highlight the difference in sizes.



**Figure S20.** Electrostatic potentials on the protein surface modelled with PyMOL (v 1.7.2.1) (left). The sequence was modelled from the RSCB pdb file 4DC8.<sup>2</sup> Areas of negative potentials are shown in red, of positive potentials in blue and of neutral potentials in white. The structure of the protein created from the same pdb file is shown in the middle. The structure of metallaprism  $[2]^{6+}$  (right) was added to highlight the difference in sizes.



**Figure S21.** Electrostatic potentials on the protein surface modelled with PyMOL (v 1.7.2.1) (left). The sequence was modelled from the RSCB pdb file 1HRC.<sup>3</sup> Areas of negative potentials are shown in red, of positive potentials in blue and of neutral potentials in white. The structure of the protein created from the same pdb file is shown in the middle. The structure of metallaprism  $[2]^{6+}$  (right) was added to highlight the difference in sizes.

## References

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- 2 D. J. Kissick, C. M. Dettmar, M. Becker, A. M. Mulichak, V. Cherezov, S. L. Ginell, K. P. Battaile, L. J. Keefe, R. F. Fischetti and G. J. Simpson, *Acta Crystallogr., Sect. D: Biol. Crystallogr.*, 2013, **69**, 843-851.
- 3 G. W. Bushnell, G. V. Louie and G. D. Brayer, *J. Mol. Biol.*, 1990, **214**, 585-595.