

Supporting Information for

Phthalocyanine-functionalized magnetic silica nanoparticles as anion chemosensors

João M. M. Rodrigues,^{1,*} Andreia S. F. Farinha,^{2,*} Zhi Lin,³ José A. S. Cavaleiro,¹ Augusto C. Tomé¹ and João P. C. Tomé^{4,*}

¹LAQV-REQUIMTE, Department of Chemistry, University of Aveiro, 3810-193 Aveiro, Portugal

²Water Desalination and Reuse Center (WDRC), Division of Biological and Environmental Sciences (BESE), King Abdullah University of Science and Technology (KAUST) Thuwal, 23955-6900, Saudi Arabia

³CICECO and Department of Chemistry, University of Aveiro, 3810-193 Aveiro, Portugal

⁴CQE, Departamento de Engenharia Química, Instituto Superior Técnico, Universidade de Lisboa, 1049-001 Lisboa, Portugal

* Correspondence: jrodrigues@ua.pt; andreia.farinha@kaust.edu.sa; jtome@tecnico.ulisboa.pt

Index

1	NMR, MS and TEM image of the new compounds.....	2
2	UV-Vis titration of Pc1 and MSNP-Pc1 with different anions	5
2.1	Titration of Pc1 with anions (tetrabutylammonium salts) in DMSO	5
2.2	Titration of MSNP-Pc1 with anions (tetrabutylammonium salts) in DMSO	8
2.3	Titration of MSNP-Pc1 with anions (tetrabutylammonium salts) in water	12
3	Fluorescence titrations of Pc1 and MSNP-Pc1 with different anions	16
3.1	Titration of Pc1 with anions (tetrabutylammonium salts) in DMSO	16
3.2	Titration of MSNP-Pc1 with anions (tetrabutylammonium salts) in DMSO	19
3.3	Titration of MSNP-Pc1 with anions (tetrabutylammonium salts) in water	23

1. NMR, MS and TEM image of the new compounds

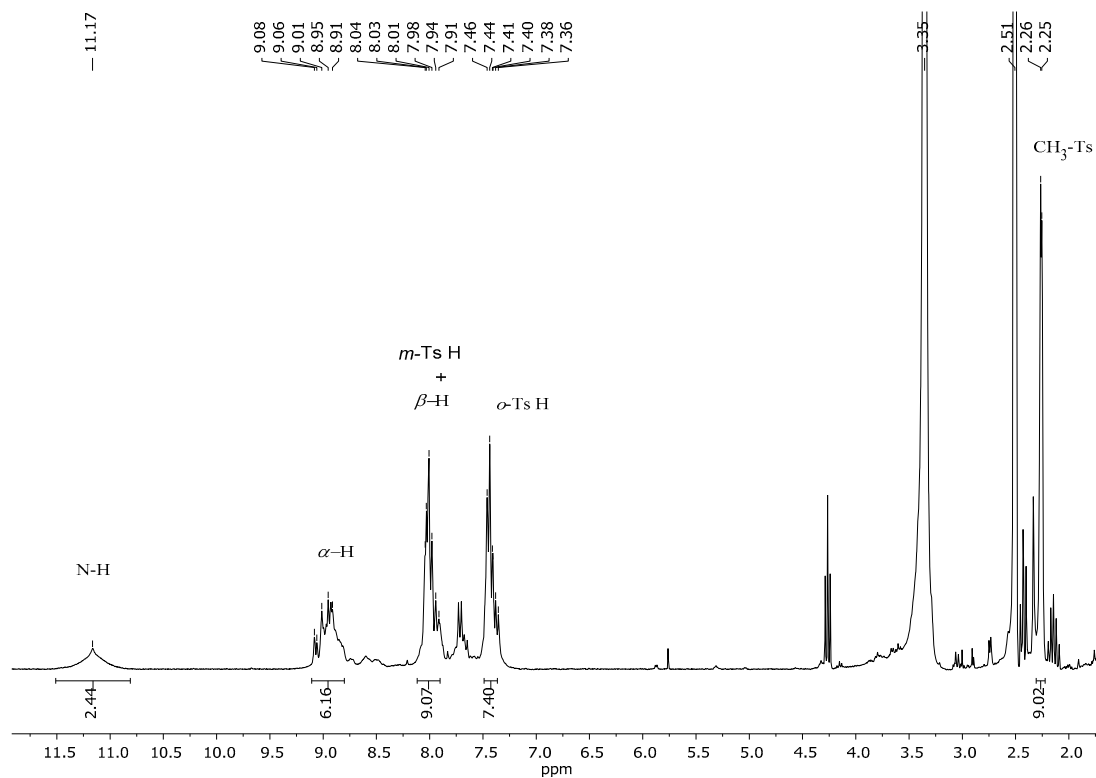


Figure S1. ^1H NMR spectrum of Pc1 in $\text{DMSO-}d_6$.

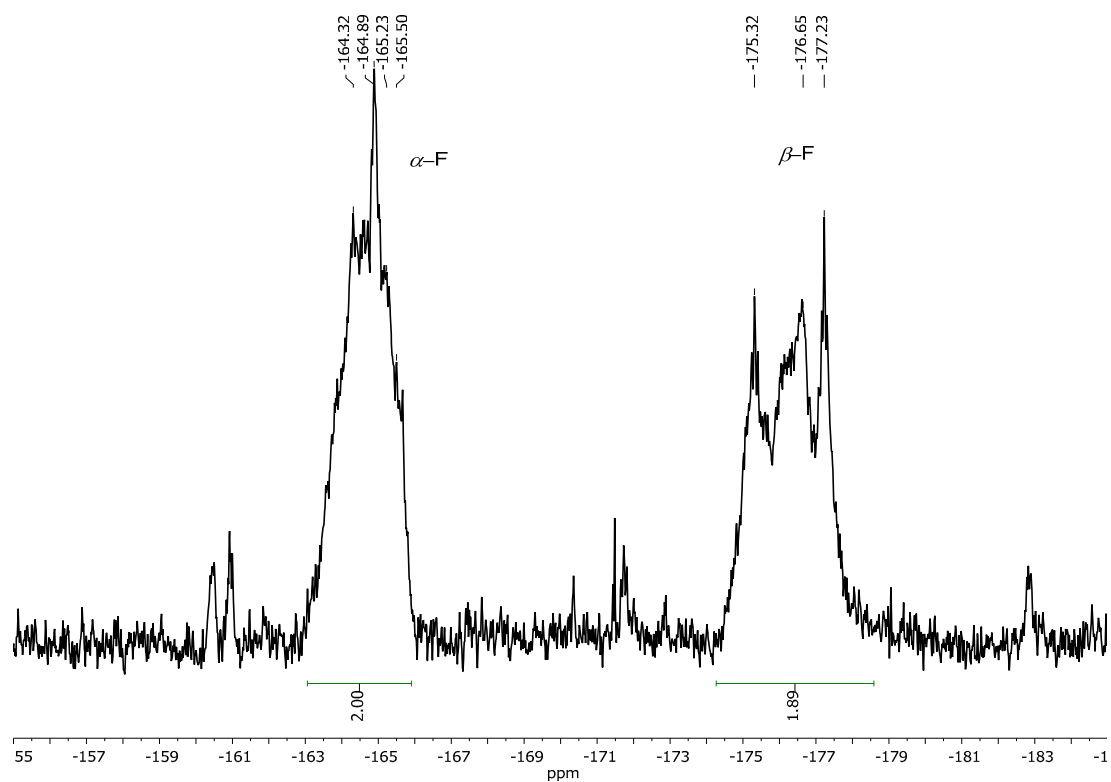


Figure S2. ^{19}F NMR spectrum of Pc1 in $\text{DMSO-}d_6$.

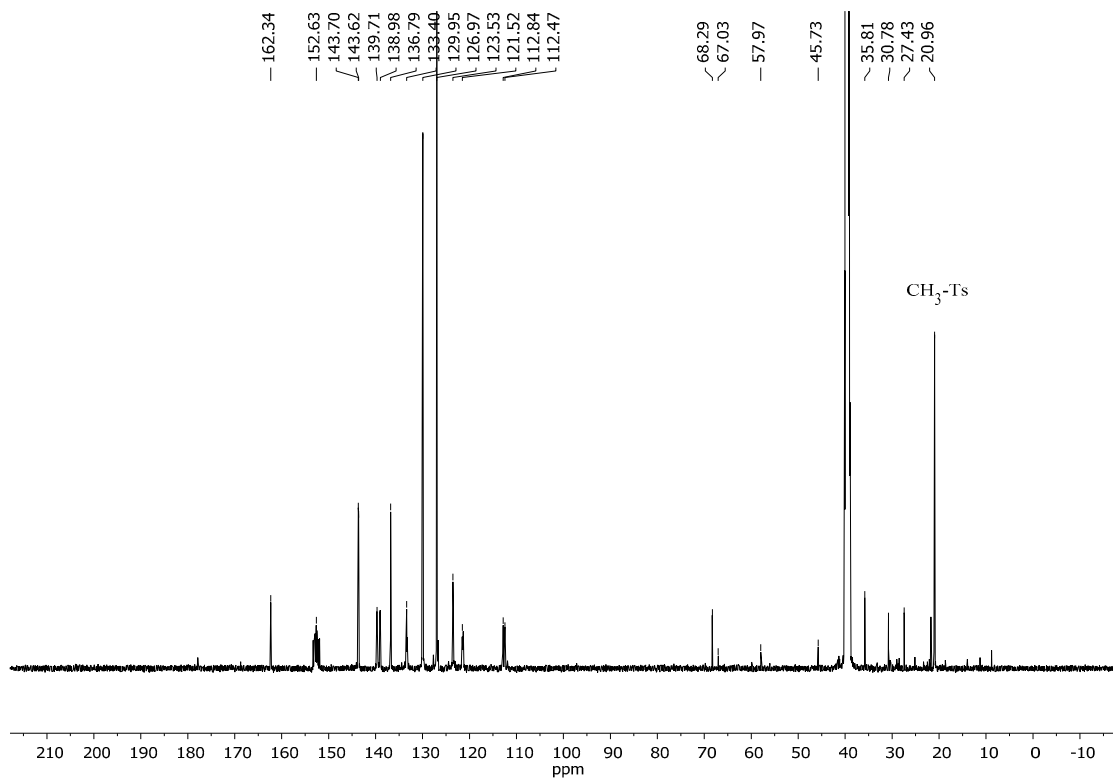


Figure S3. ^{13}C NMR spectrum of Pc1 in $\text{DMSO-}d_6$.

JR11-Pc3NHTs4F #30-32 RT: 0.83-0.89 AV: 3 NL: 5.54E4
 T: FTMS + p ESI SIM ms [1148.00-1168.00]

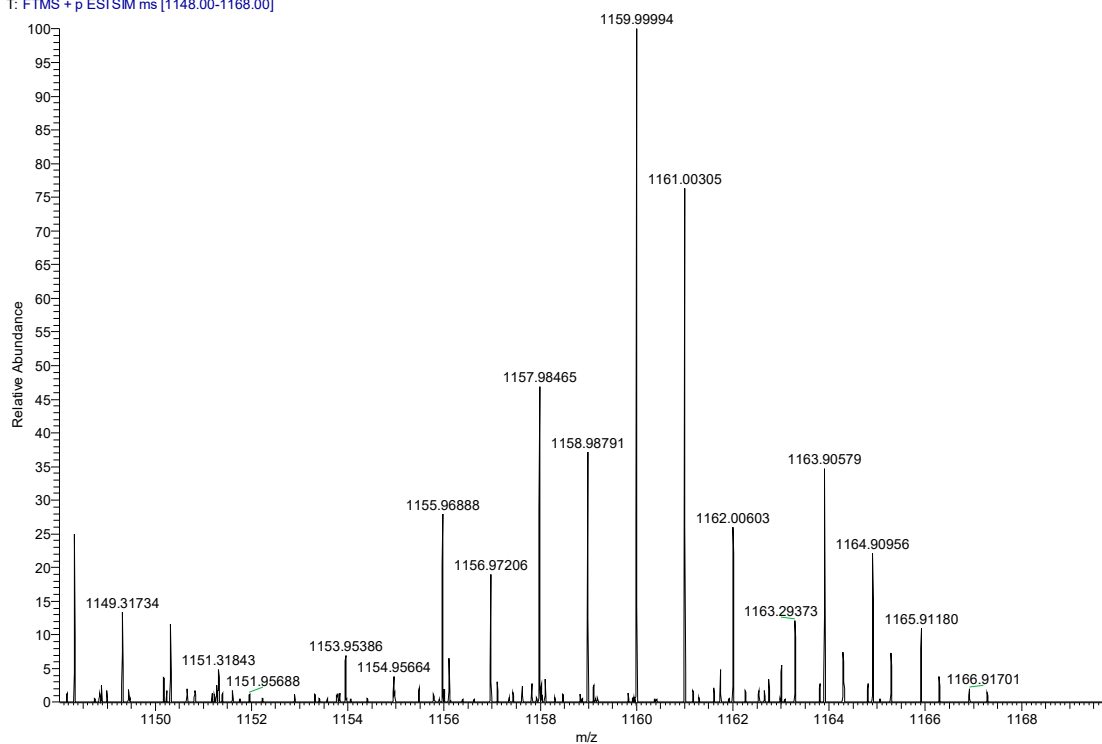


Figure S4. High resolution electrospray ionization mass spectrum (ESI MS) of Pc1.

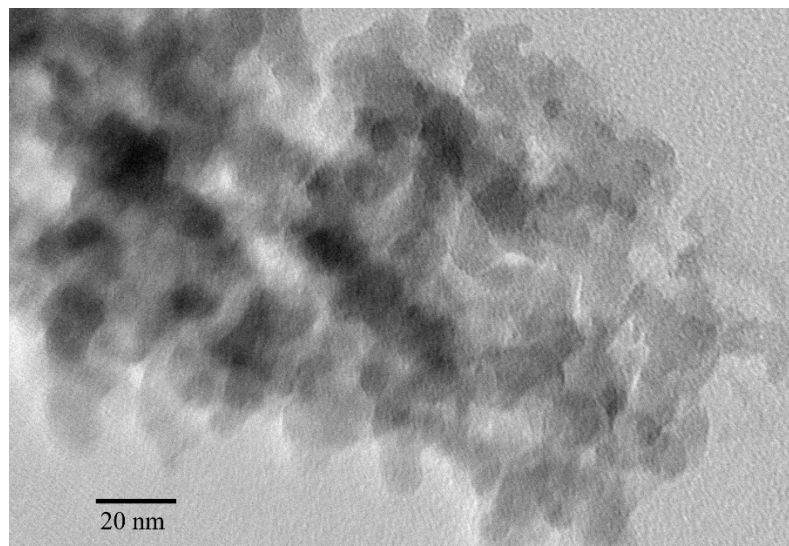


Figure S5. Transmission electron microscopy (TEM) of MSNP.

2. UV-Vis titration of Pc1 and MSNP-Pc1 with different anions

2.1. Titration of Pc1 with anions (tetrabutylammonium salts) in DMSO

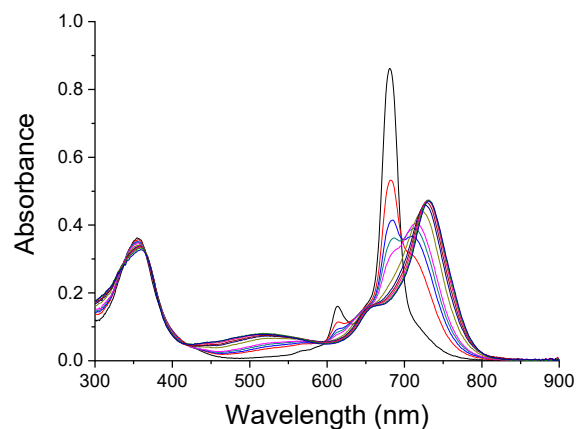


Figure S6. Titration of Pc1 with acetate anion.

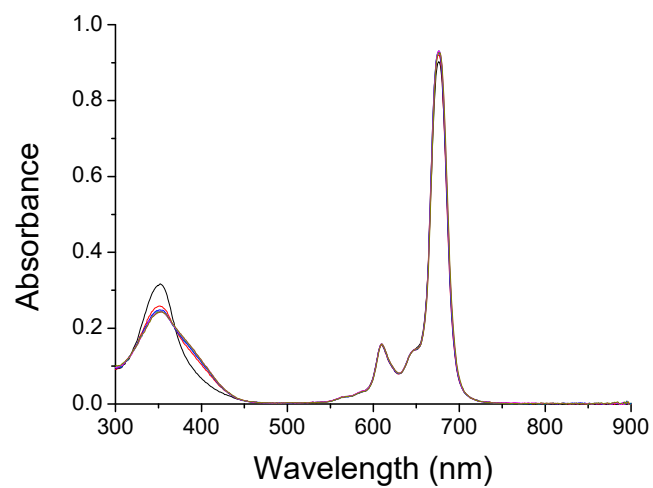


Figure S7. Titration of Pc1 with bromide anion.

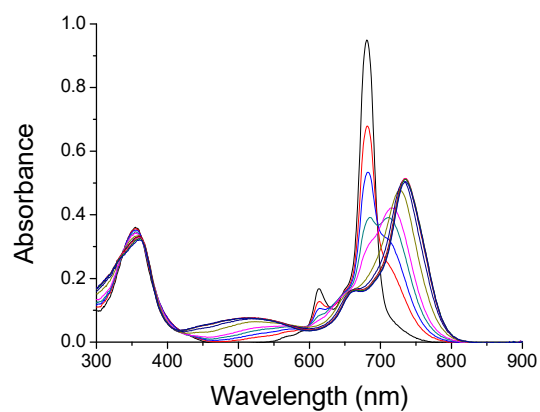


Figure S8. Titration of Pc1 with fluoride anion.

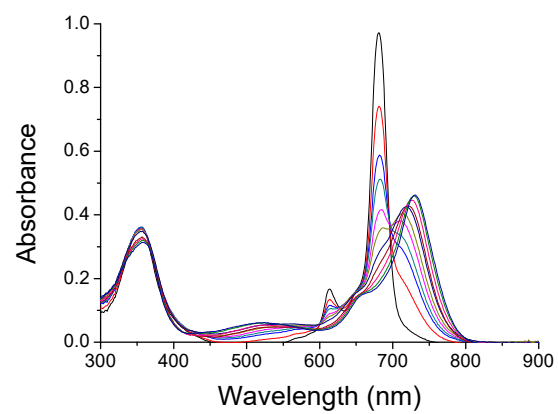


Figure S9. Titration of Pc1 with dihydrogen phosphate anion.

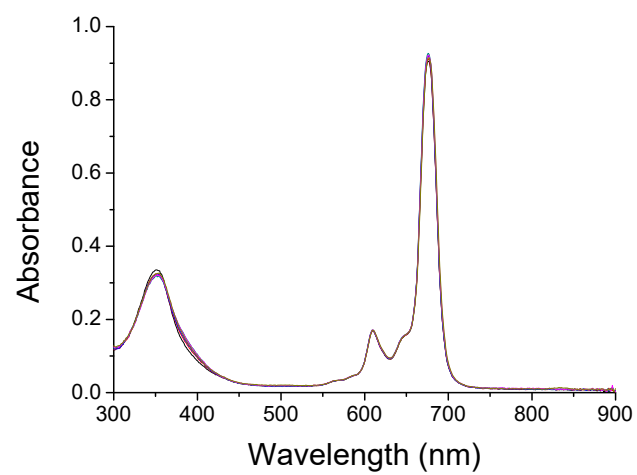


Figure S10. Titration of Pc1 with hydrogen sulfate anion.

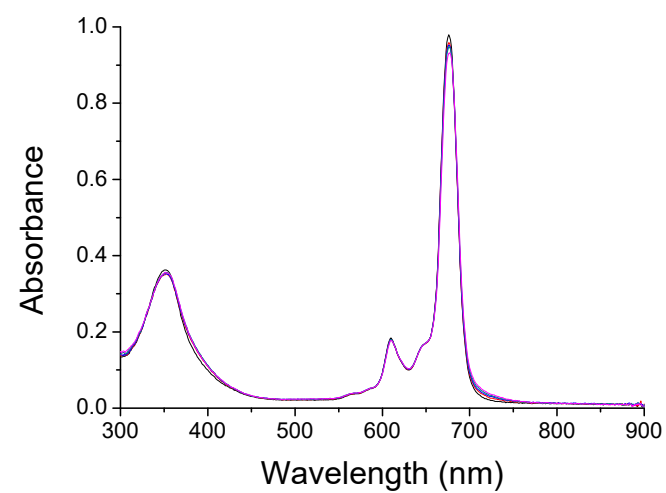


Figure S11. Titration of Pc1 with nitrate anion.

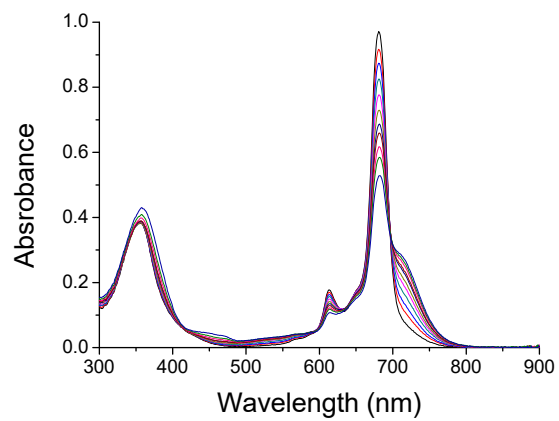


Figure S12. Titration of Pc1 with nitrite anion.

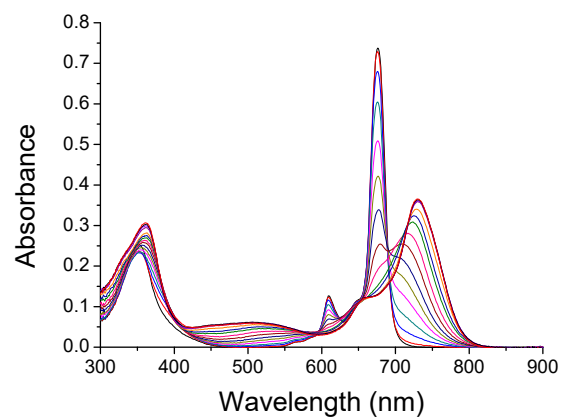


Figure S13. Titration of Pc1 with hydroxide anion.

2.2. Titration of MSNP-Pc1 with anions (tetrabutylammonium salts) in DMSO

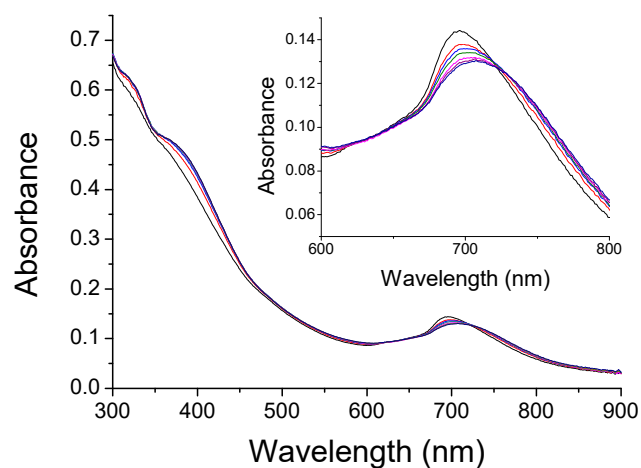


Figure S14. Titration of MSNP-Pc1 with acetate anion.

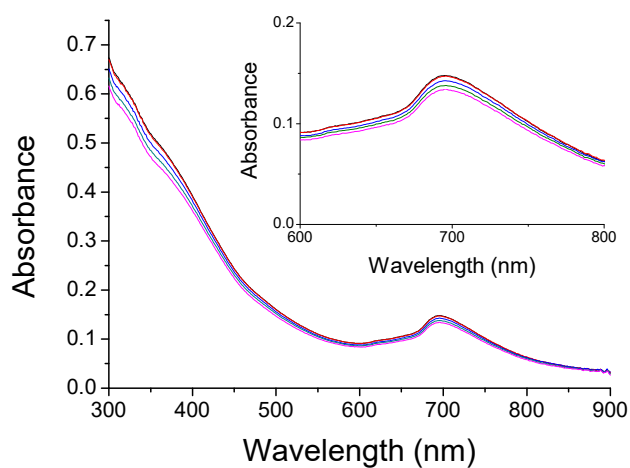


Figure S15. Titration of MSNP-Pc1 with bromide anion.

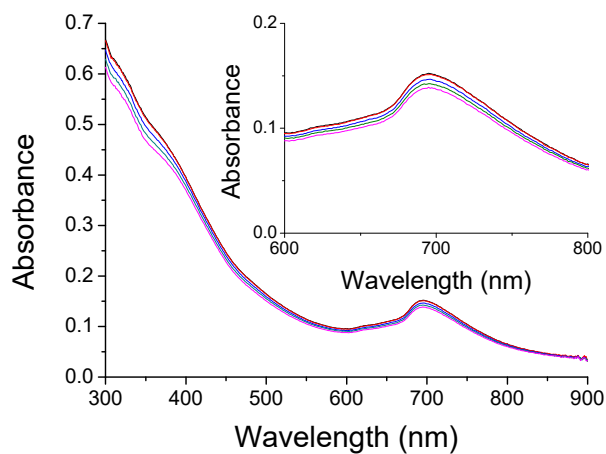


Figure S16. Titration of MSNP-Pc1 with chloride anion.

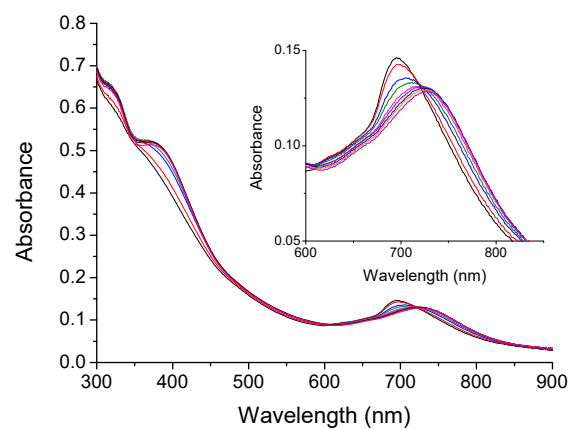


Figure S17. Titration of MSNP-Pc1 with cyanide anion.

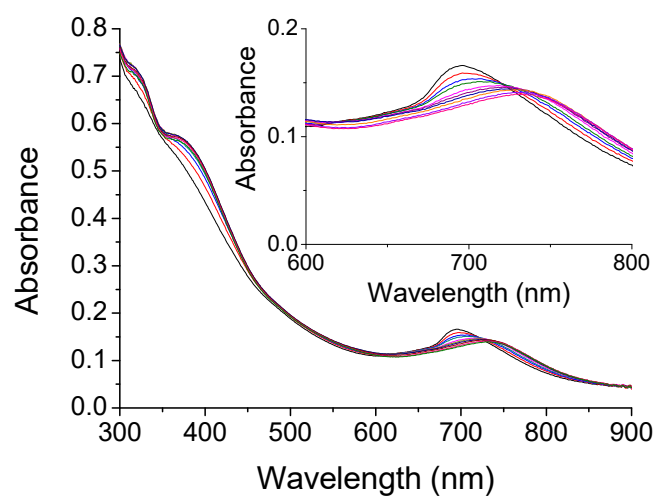


Figure S18. Titration of MSNP-Pc1 with fluoride anion.

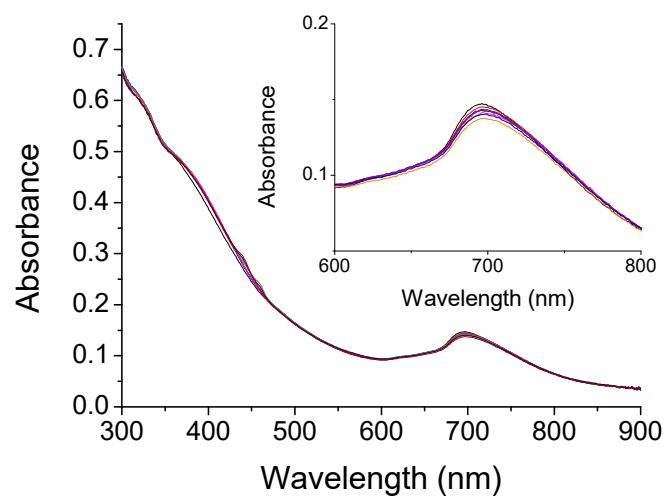


Figure S19. Titration of MSNP-Pc1 with dihydrogen phosphate anion.

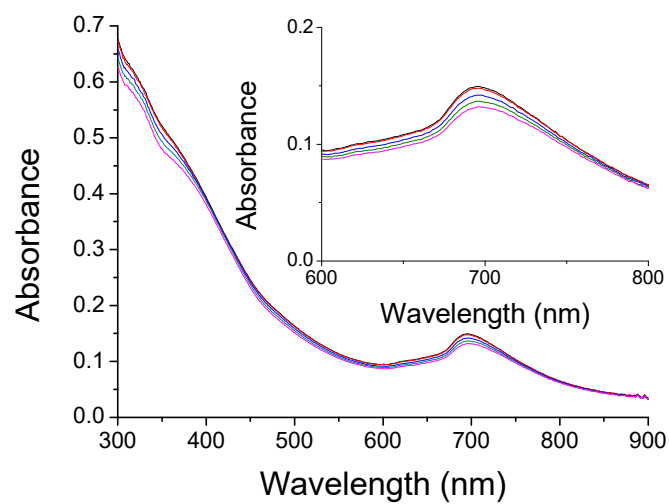


Figure S20. Titration of MSNP-Pc1 with hydrogen sulfate anion.

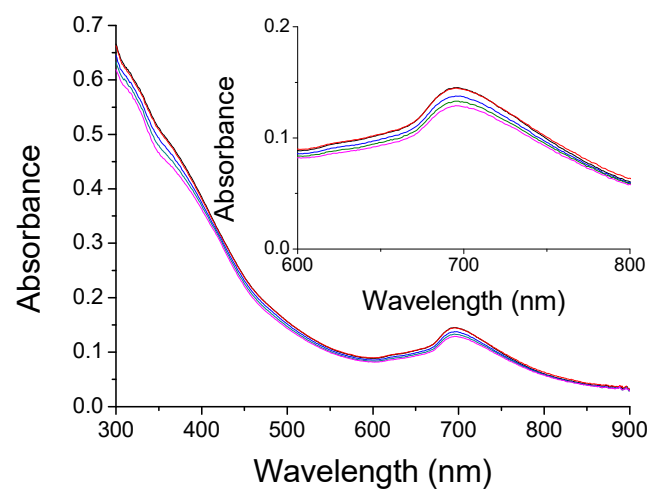


Figure S21. Titration of MSNP-Pc1 with nitrate anion.

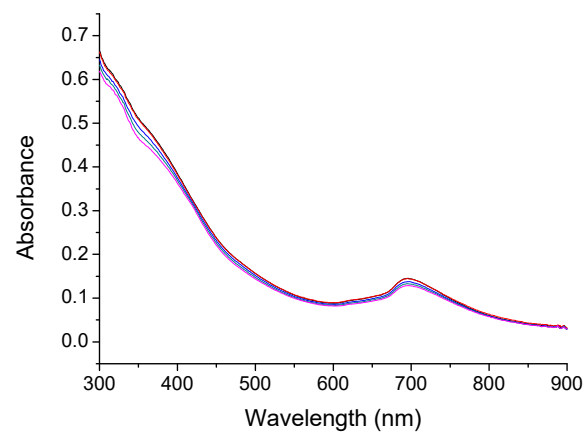


Figure S22. Titration of MSNP-Pc1 with nitrite anion.

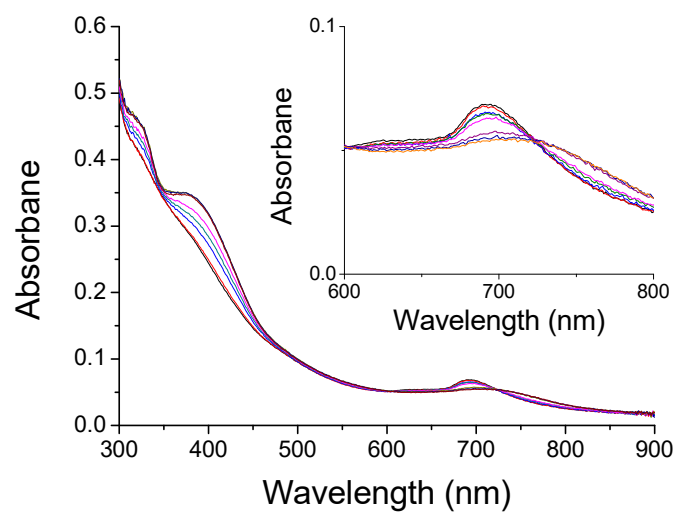


Figure S23. Titration of MSNP-Pc1 with hydroxide anion.

2.3. Titration of MSNP-Pc1 with anions (tetrabutylammonium salts) in water

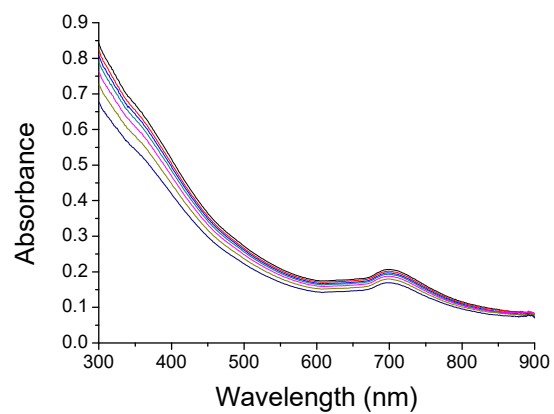


Figure S24. Titration of MSNP-Pc1 with acetate anion.

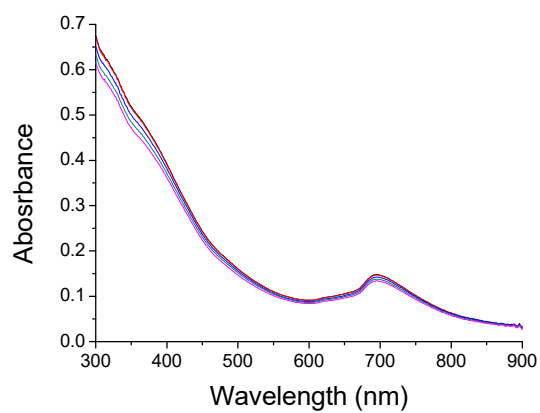


Figure S25. Titration of MSNP-Pc1 with bromide anion.

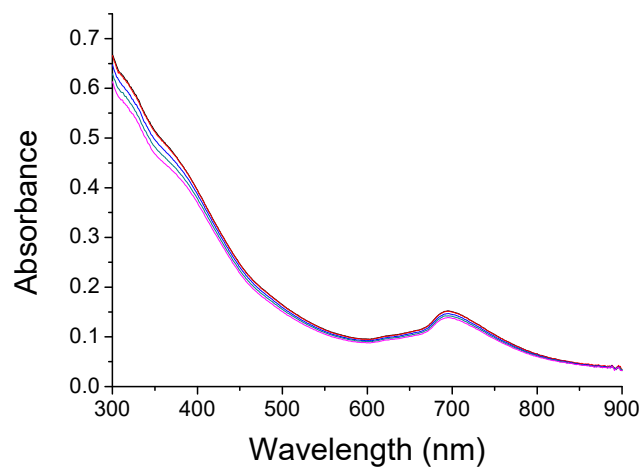


Figure S26. Titration of MSNP-Pc1 with chloride anion.

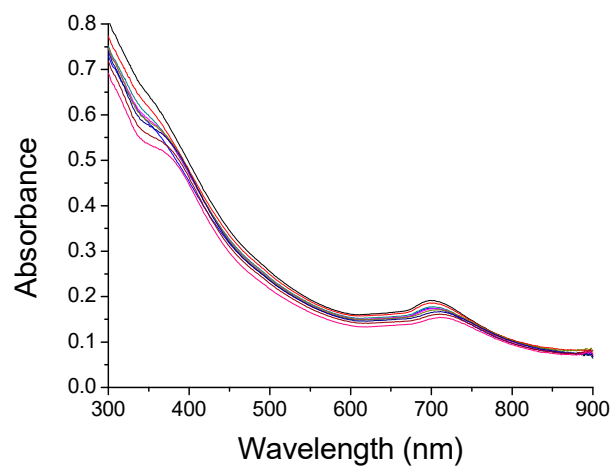


Figure S27. Titration of MSNP-Pc1 with cyanide anion.

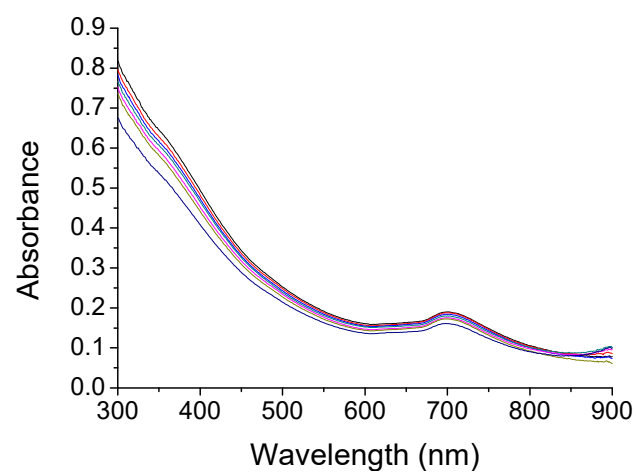


Figure S28. Titration of MSNP-Pc1 with fluoride anion.

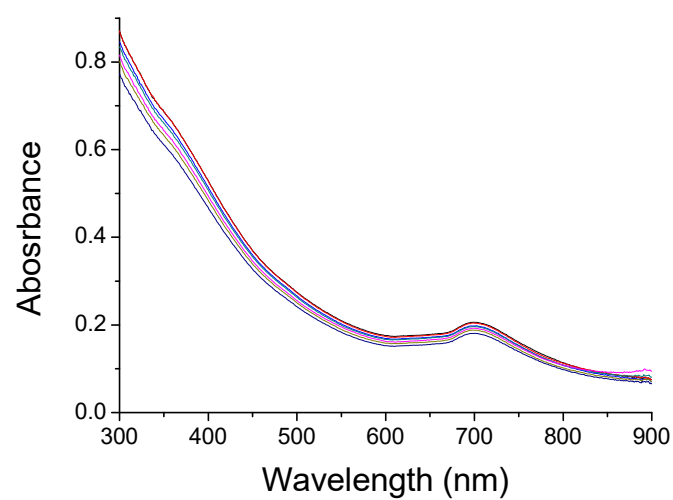


Figure S29. – Titration of MSNP-Pc1 with dihydrogen phosphate anion.

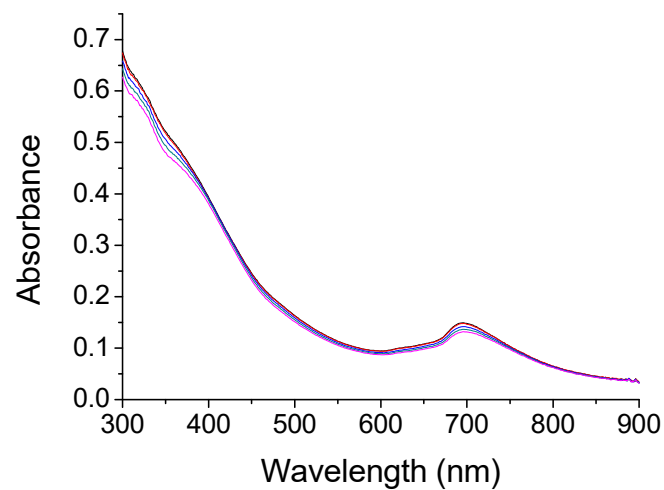


Figure S30. Titration of MSNP-Pc1 with hydrogen sulfate anion.

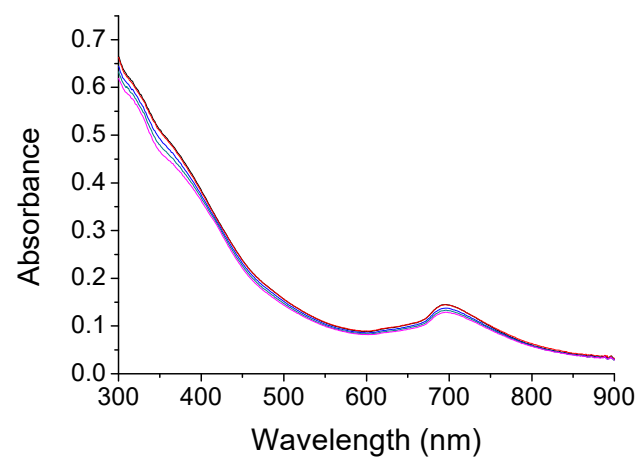


Figure S31. Titration of MSNP-Pc1 with nitrate anion.

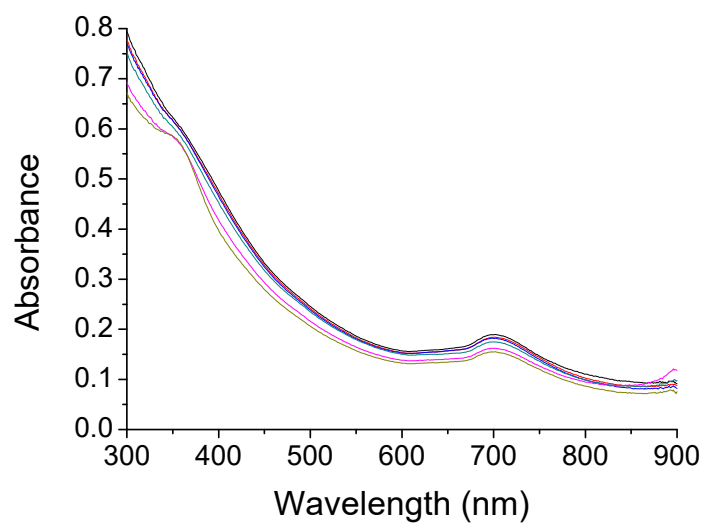


Figure S32. Titration of MSNP-Pc1 with nitrite anion.

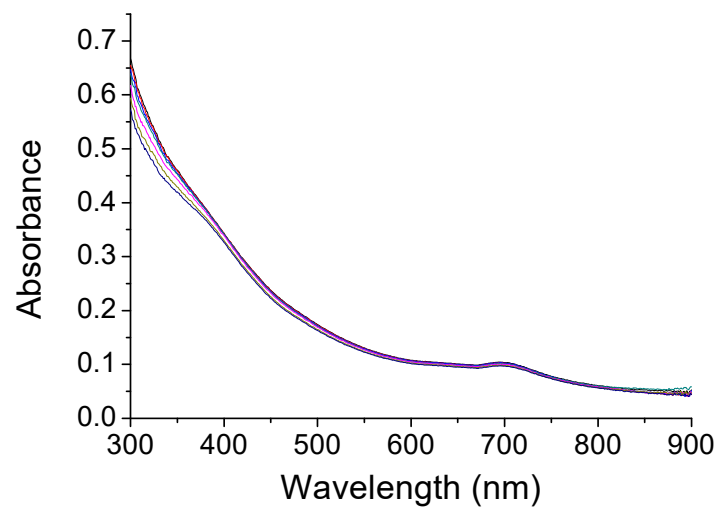


Figure S33. Titration of MSNP-Pc1 with hydroxide anion.

3. Fluorescence titrations of Pc1 and MSNP-Pc1 with different anions

3.1. Titration of Pc1 with anions (tetrabutylammonium salts) in DMSO

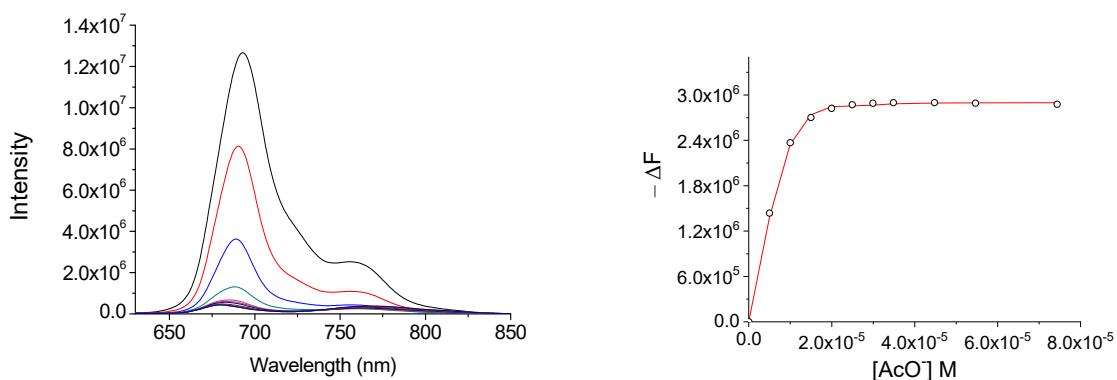


Figure S34. Titration of Pc1 with acetate anion (left), and the plot of the experimental data and corresponding fit to a 1:2 binding model (right).

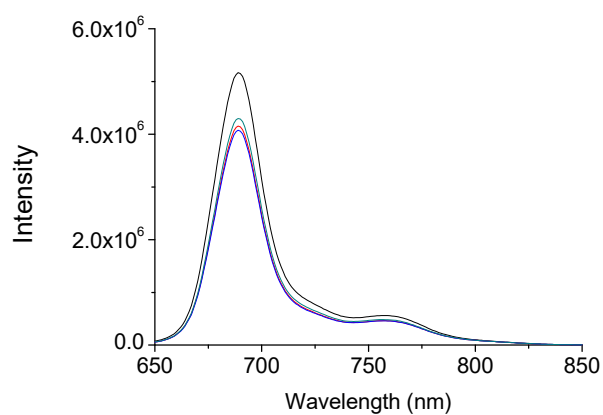


Figure S35. Titration of Pc1 with bromide anion.

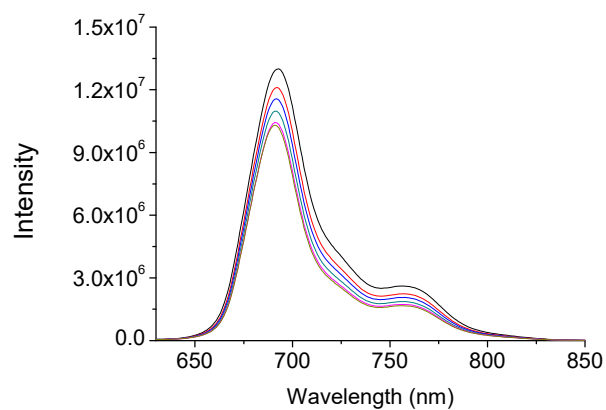


Figure S36. Titration of Pc1 with chloride anion.

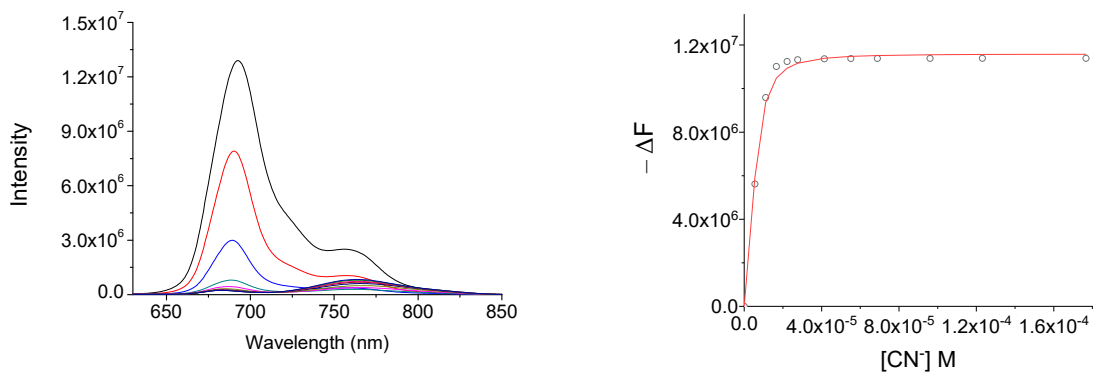


Figure S37. Titration of **Pc1** with cyanide anion (left), and the plot of the experimental data and corresponding fit to a 1:2 binding model (right).

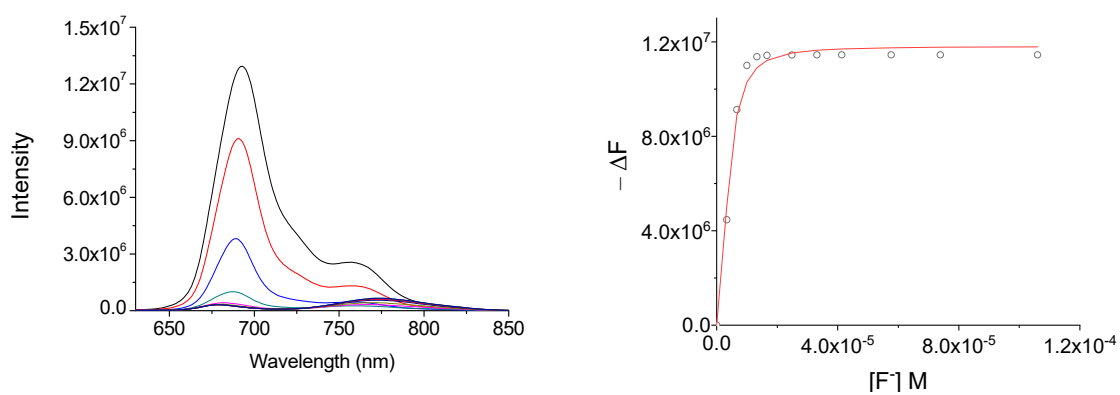


Figure S38. Titration of **Pc1** with fluoride anion (left), and the plot of the experimental data and corresponding fit to a 1:2 binding model (right).

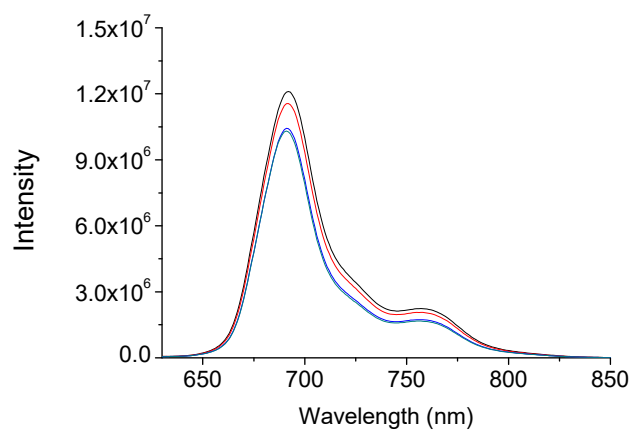


Figure S39. Titration of **Pc1** with hydrogen sulfate anion.

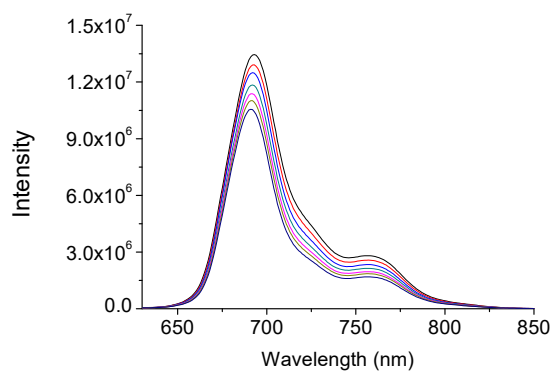


Figure S40. Titration of **Pc1** with nitrate anion.

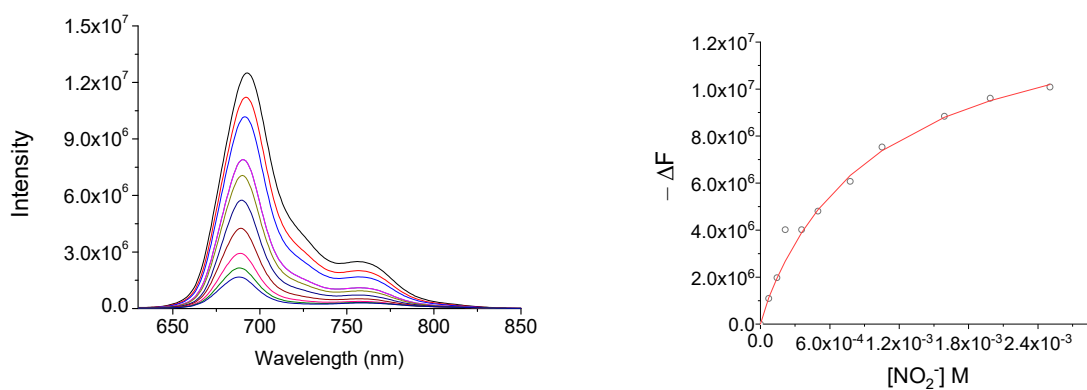


Figure S41. – Titration of **Pc1** with nitrite anion (left), and the plot of the experimental data and corresponding fit to a 1:2 binding model (right).

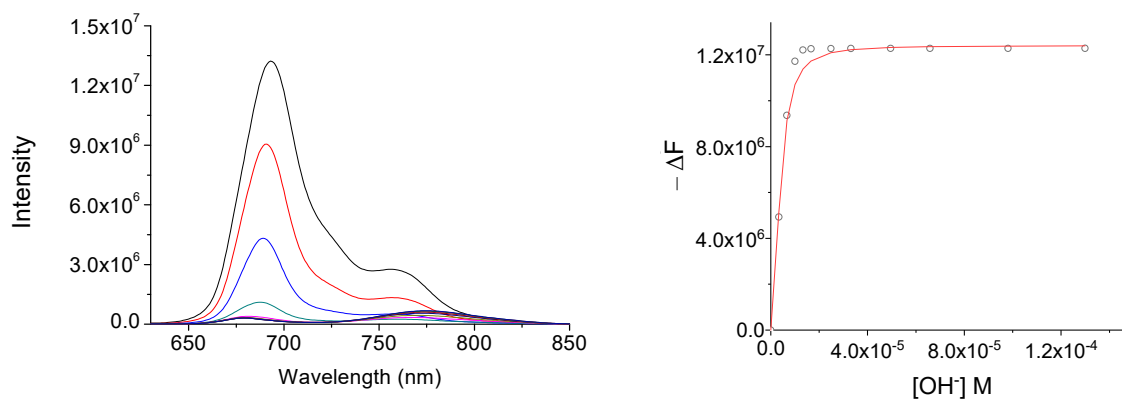


Figure S42. Titration of **Pc1** with hydroxide anion (left), and the plot of the experimental data and corresponding fit to a 1:2 binding model (right).

3.2. Titration of MSNP-Pc1 with anions (tetrabutylammonium salts) in DMSO

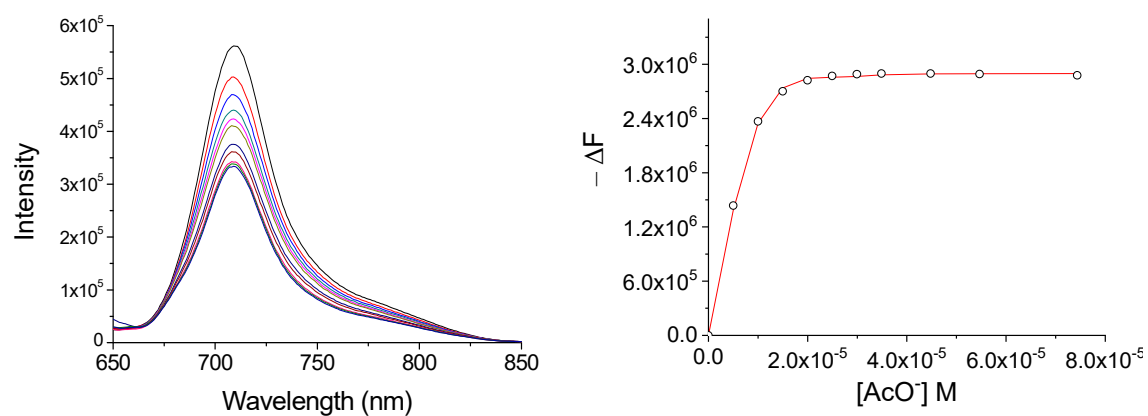


Figure S43. Titration of MSNP-Pc1 with acetate anion (left), and the plot of the experimental data and corresponding fit to a 1:2 binding model (right).

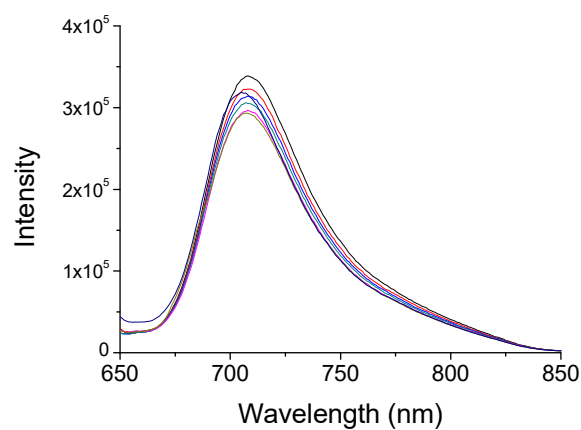


Figure S44. Titration of MSNP-Pc1 with bromide anion.

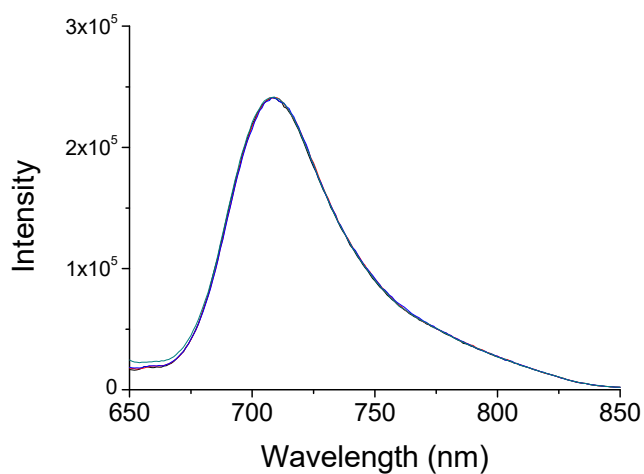


Figure S45. Titration of MSNP-Pc1 with chloride anion.

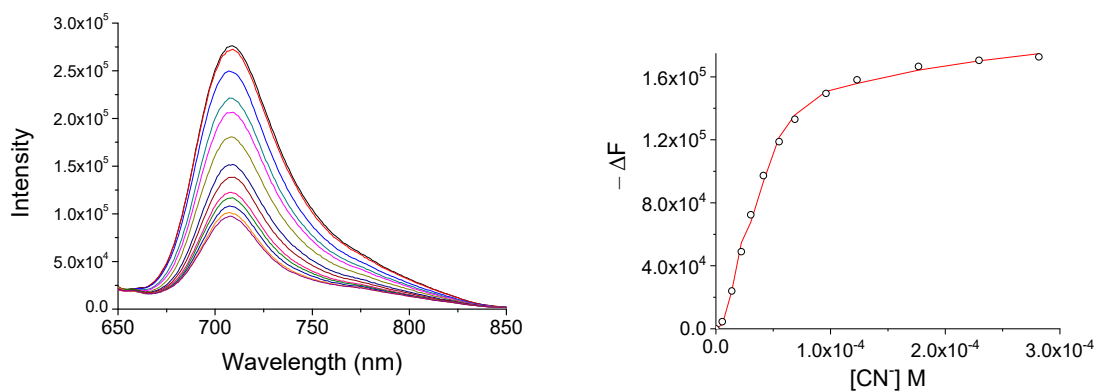


Figure S46. Titration of MSNP-Pc1 with cyanide anion (left), and the plot of the experimental data and corresponding fit to a 1:2 binding model (right).

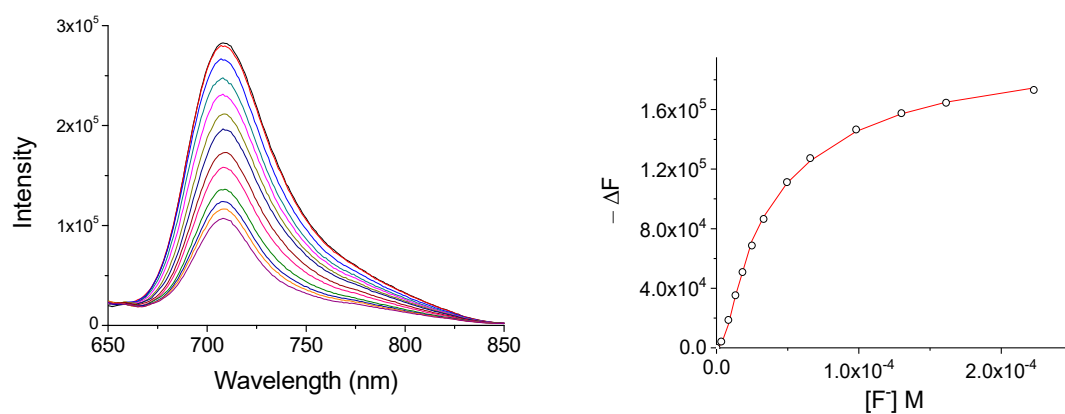


Figure S47. Titration of MSNP-Pc1 with fluoride anion (left), and the plot of the experimental data and corresponding fit to a 1:2 binding model (right).

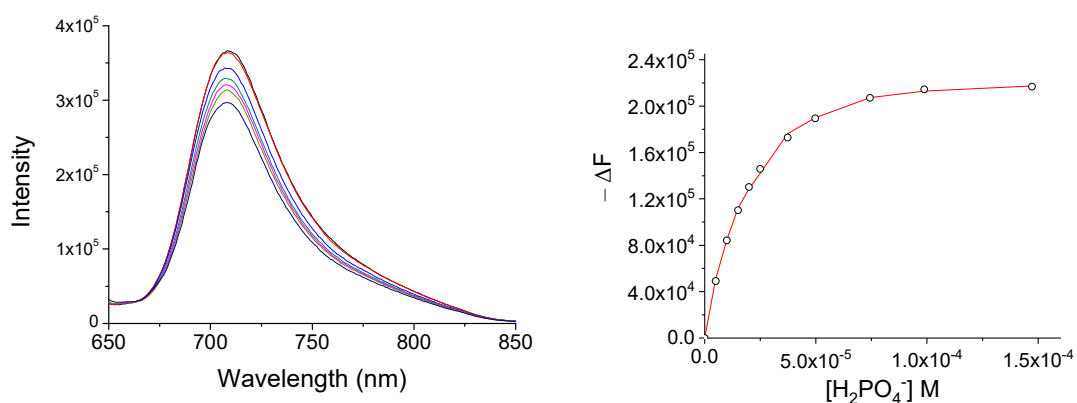


Figure S48. Titration of MSNP-Pc1 with dihydrogen phosphate anion (left), and the plot of the experimental data and corresponding fit to a 1:2 binding model (right).

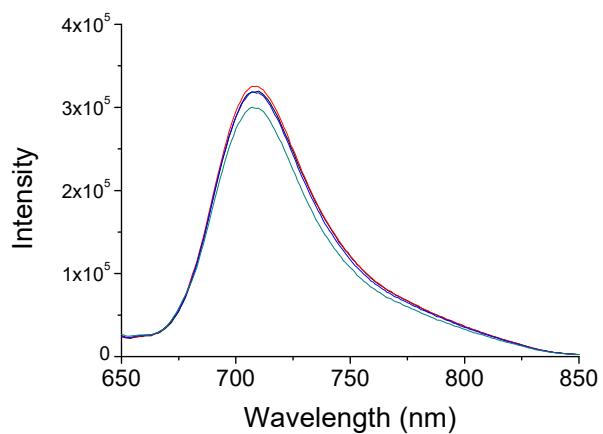


Figure S49. Titration of MSNP-Pc1 with hydrogen sulfate anion.

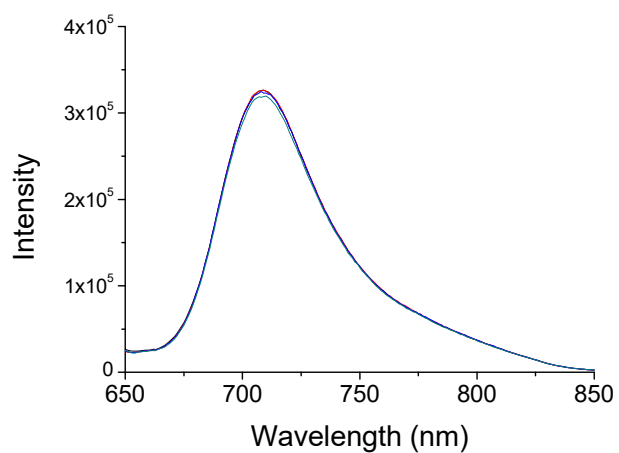


Figure S50. Titration of MSNP-Pc1 with nitrate anion.

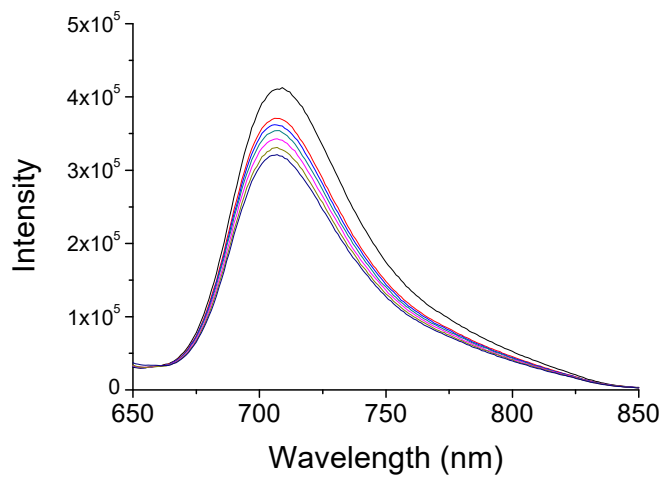


Figure S51. Titration of MSNP-Pc1 with nitrite anion.

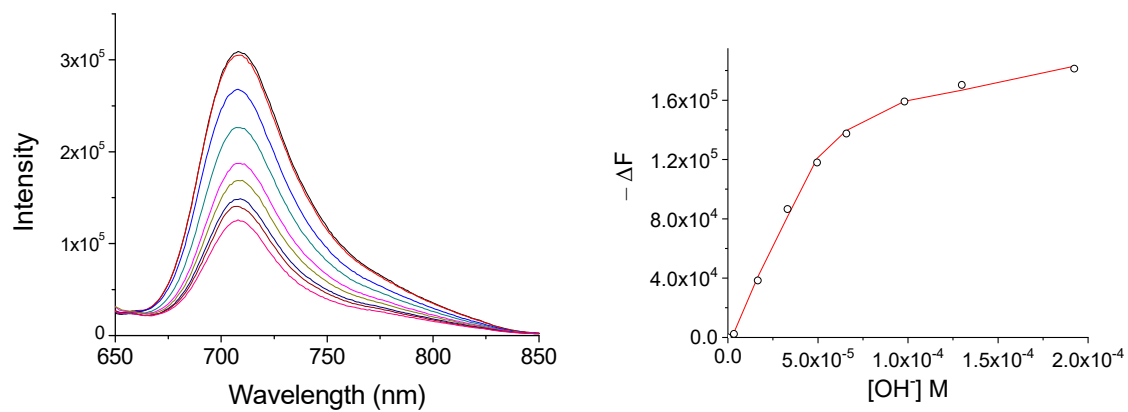


Figure S52. Titration of MSNP-Pc1 with hydroxide anion (left), and the plot of the experimental data and corresponding fit to a 1:2 binding model (right).

3.3. Titration of MSNP-Pc1 with anions (tetrabutylammonium salts) in water

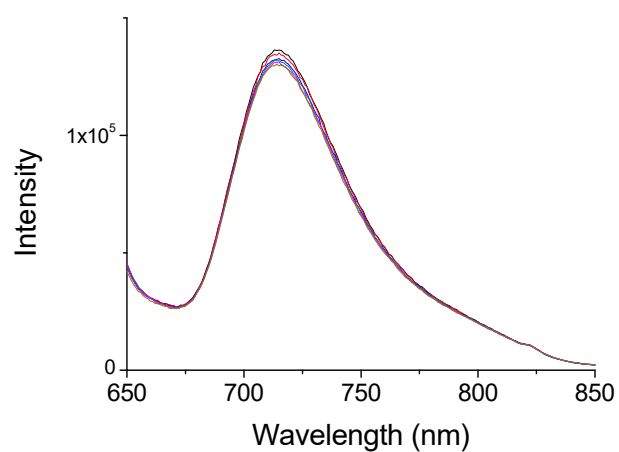


Figure S53. Titration of MSNP-Pc1 with acetate anion.

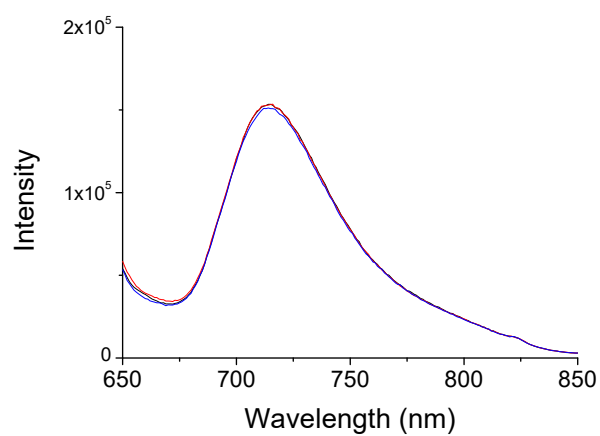


Figure S54. Titration of MSNP-Pc1 with bromide anion.

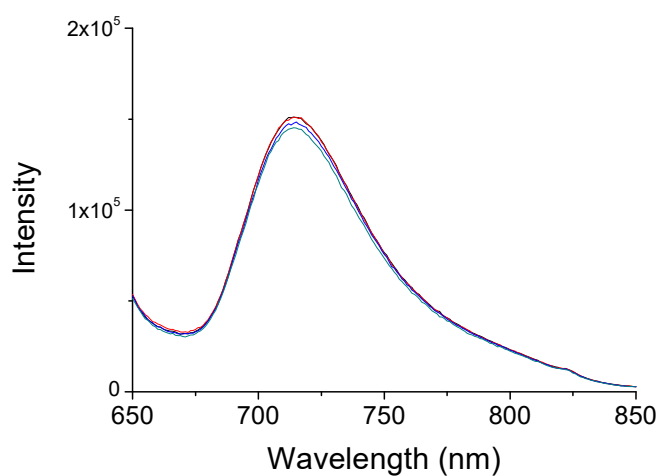


Figure S55. Titration of MSNP-Pc1 with chloride anion.

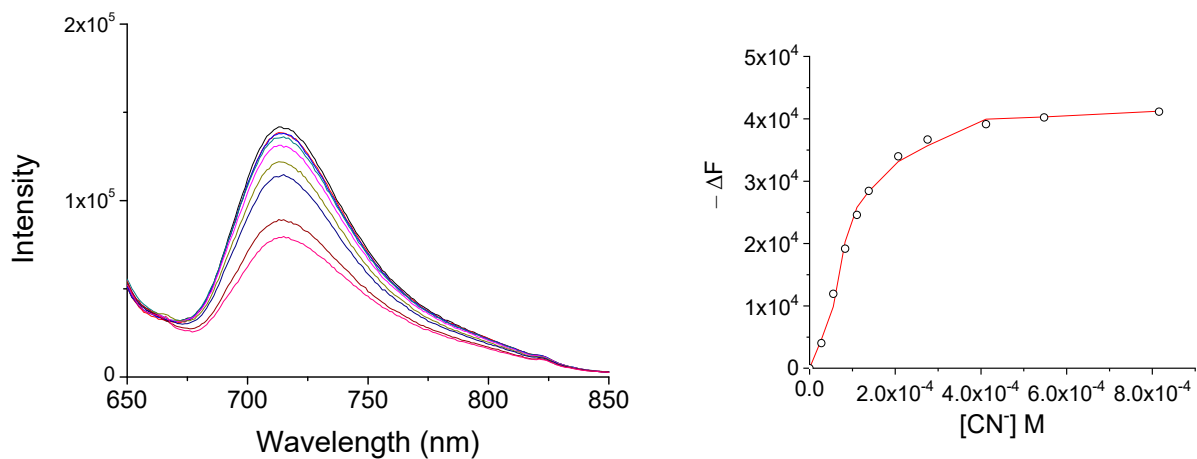


Figure S56. Titration of MSNP-Pc1 with cyanide anion (left), and the plot of the experimental data and corresponding fit to a 1:2 binding model (right).

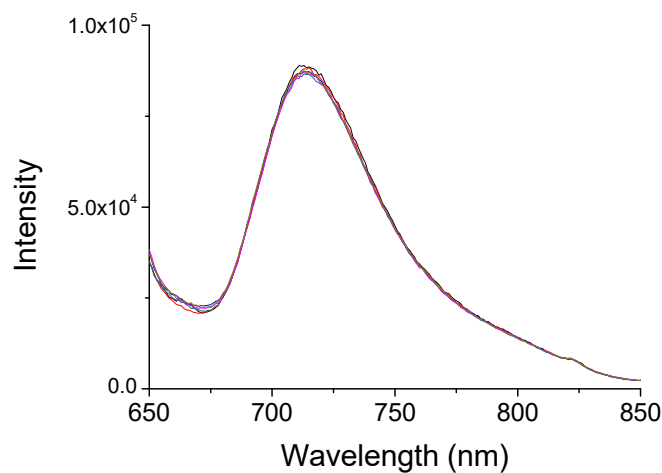


Figure S57. Titration of MSNP-Pc1 with fluoride anion.

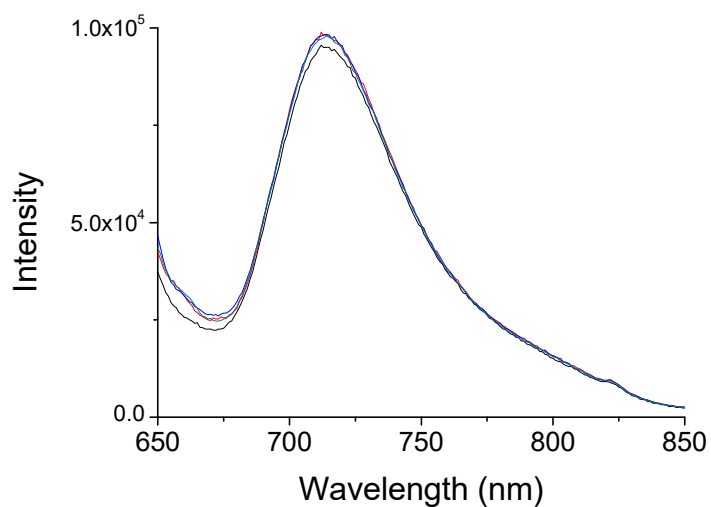


Figure S58. Titration of MSNP-Pc1 with dihydrogen phosphate anion.

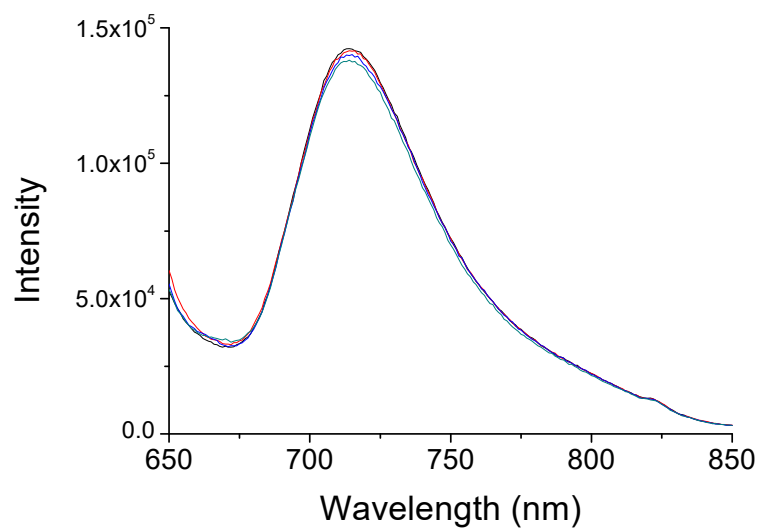


Figure S59. Titration of MSNP-Pc1 with hydrogen sulfate anion.

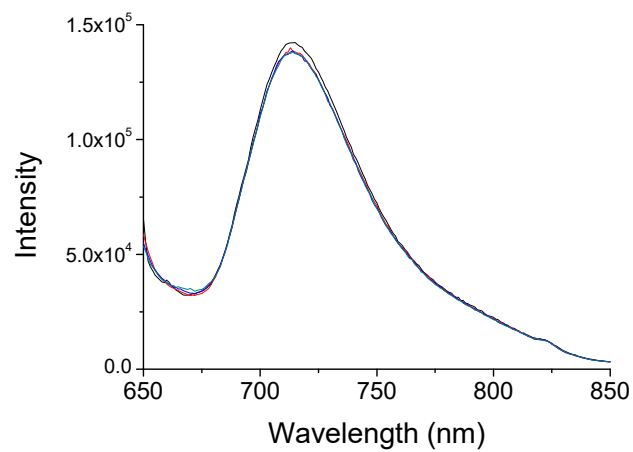


Figure S60. Titration of MSNP-Pc1 with nitrate anion.

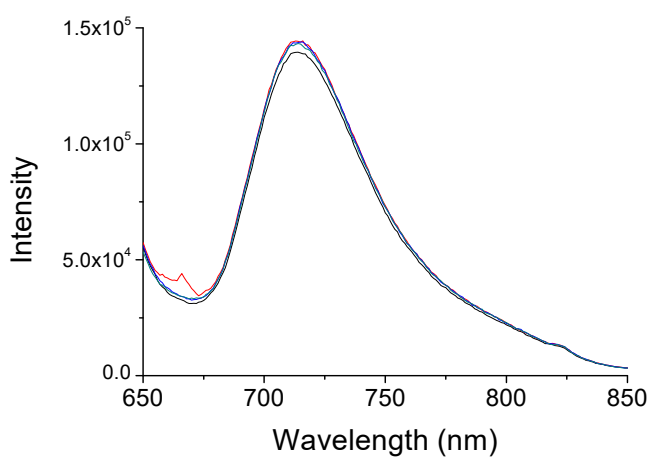


Figure S61. Titration of MSNP-Pc1 with nitrite anion.