Time and Concentration-Dependent Reactivity of Cys, Hcy and GSH on the Diels-Alder-Grafted 1,3,5-Tris Conjugate of Calix[6]arene To Bring Selectivity for Cys: Spectroscopy and Microscopy, and Its Reactivity in Cells

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SI01. Characterization of P_1:

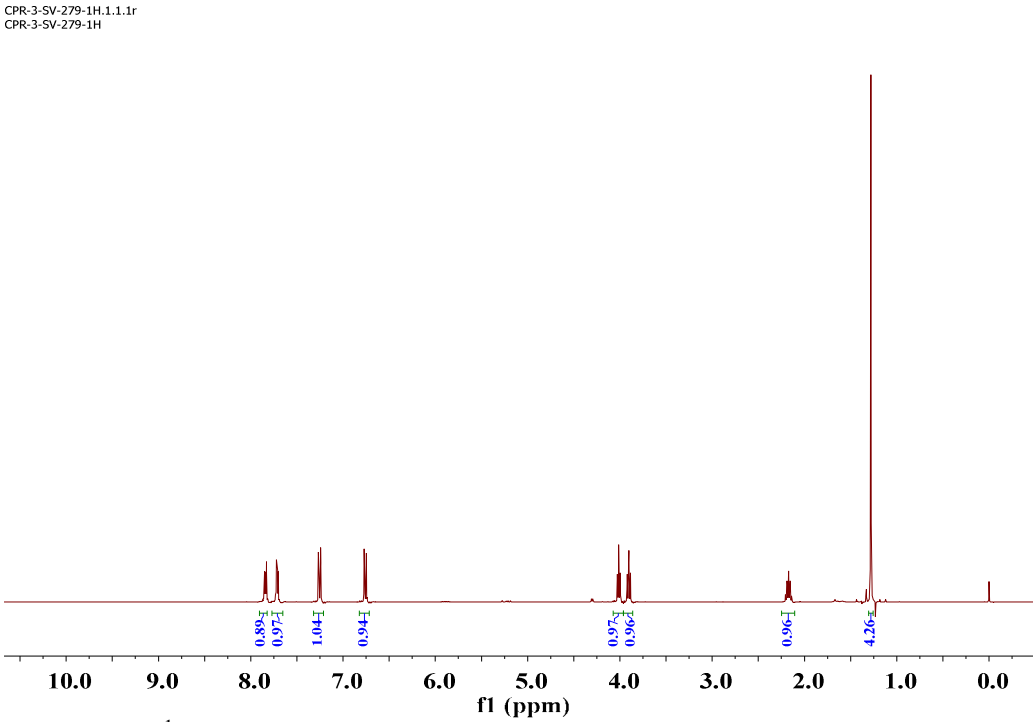


Figure S01. ^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of P_1.

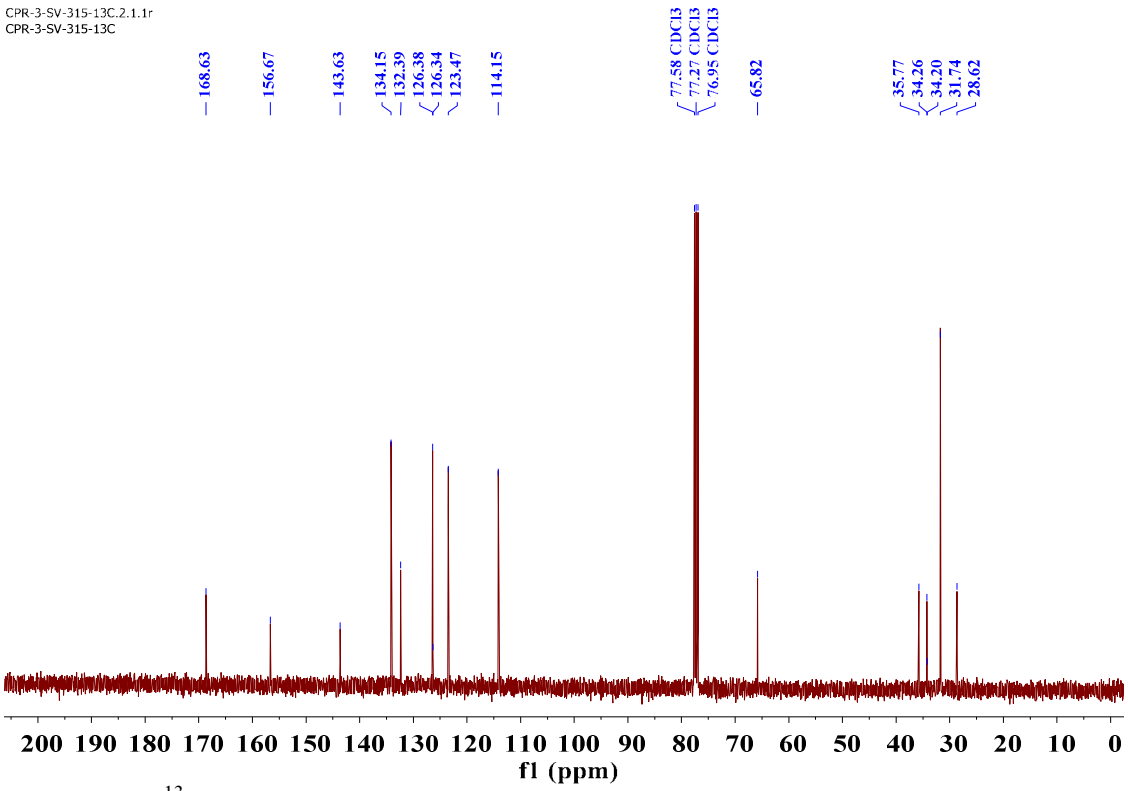


Figure S02. ^{13}C NMR spectrum ($CDCl_3$, 100 MHz) of P_1

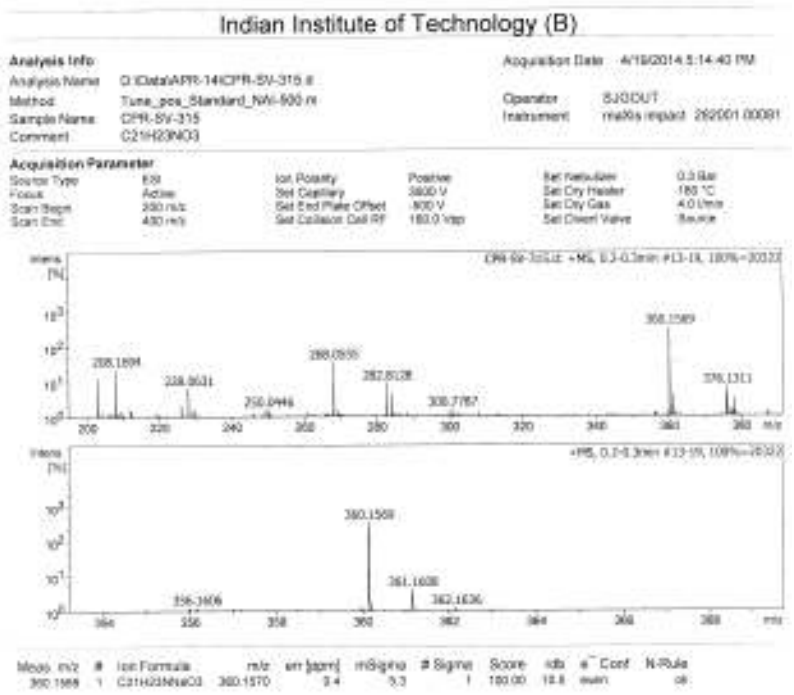


Figure S03. HRMS spectrum of $\mathbf{P_1}$.

SI02. Characterization of $\mathbf{P_2}$:

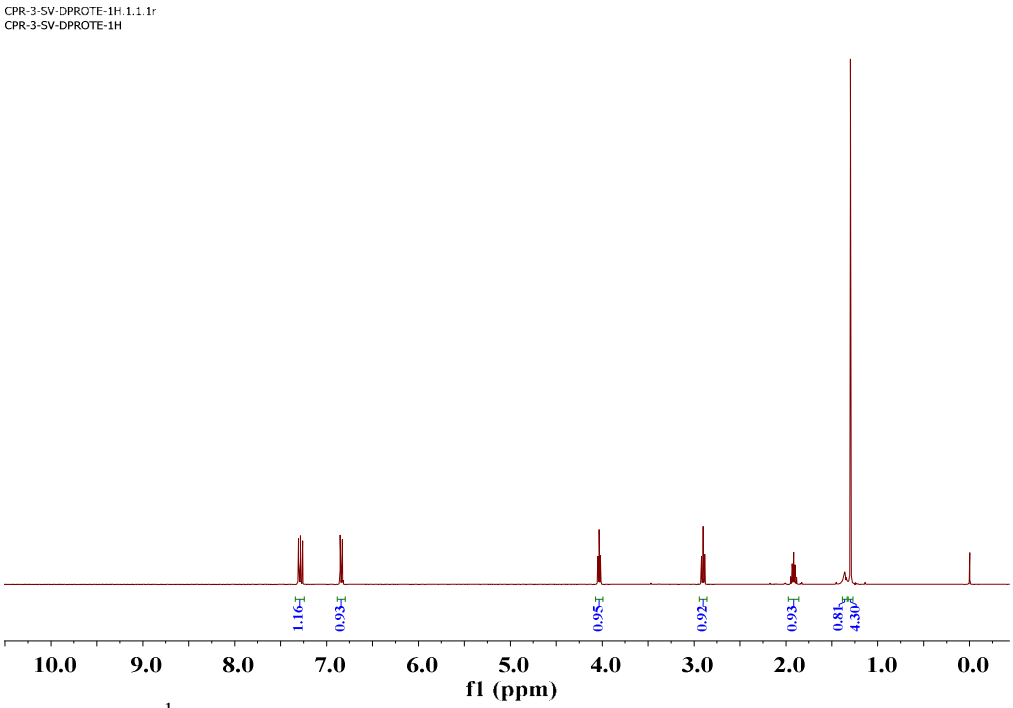


Figure S04. ^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of $\mathbf{P_2}$.

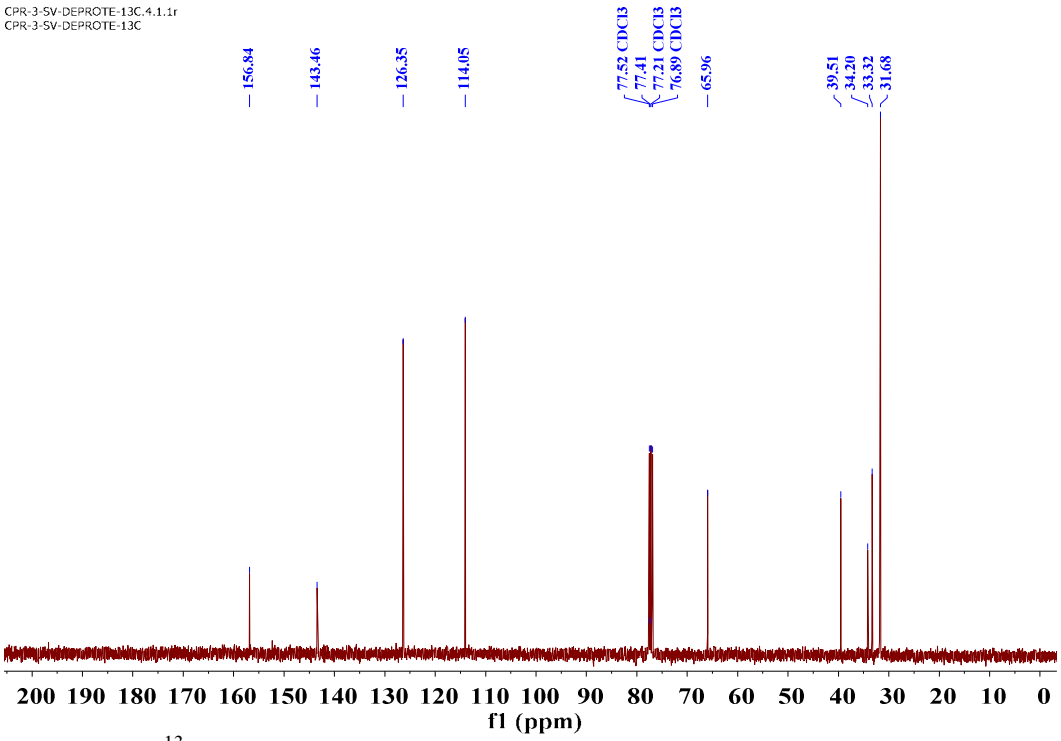


Figure S05. ^{13}C NMR spectrum ($CDCl_3$, 100 MHz) of $\mathbf{P_2}$.

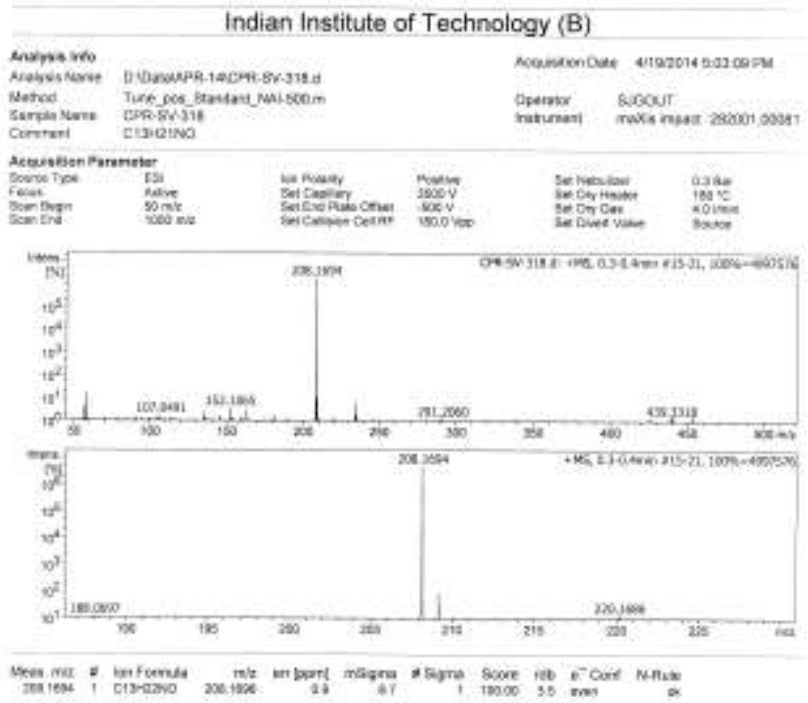


Figure S06. HRMS spectrum of $\mathbf{P_2}$.

SI03. Characterization of P_3

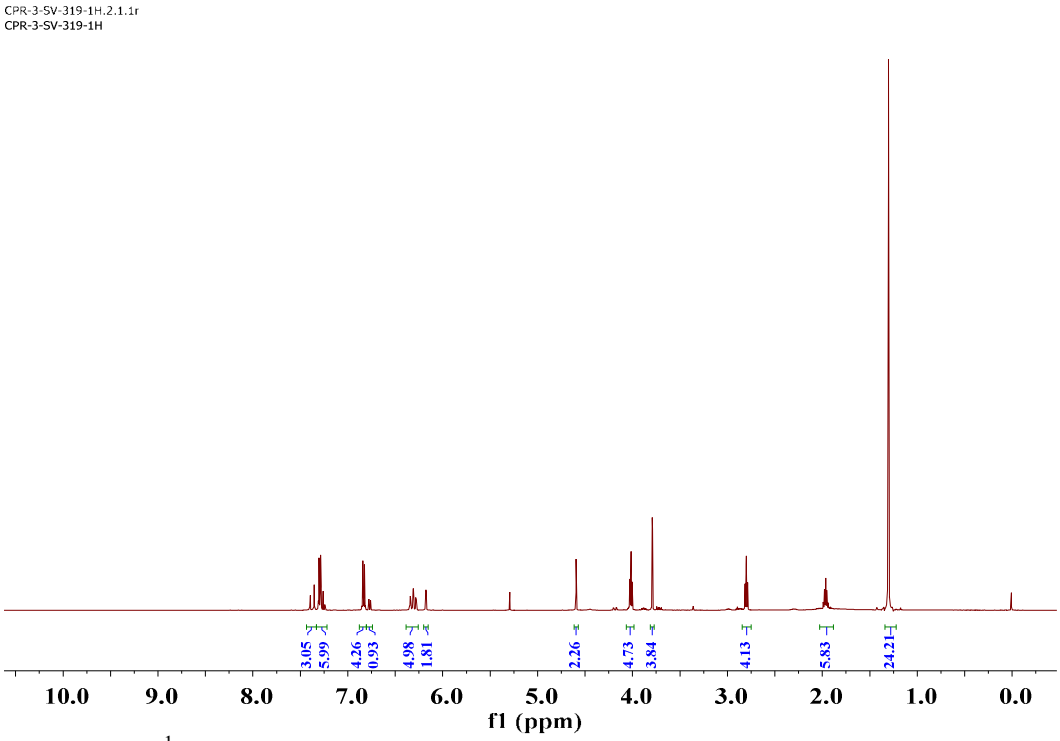


Figure S07. ^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of $\mathbf{P_3}$.

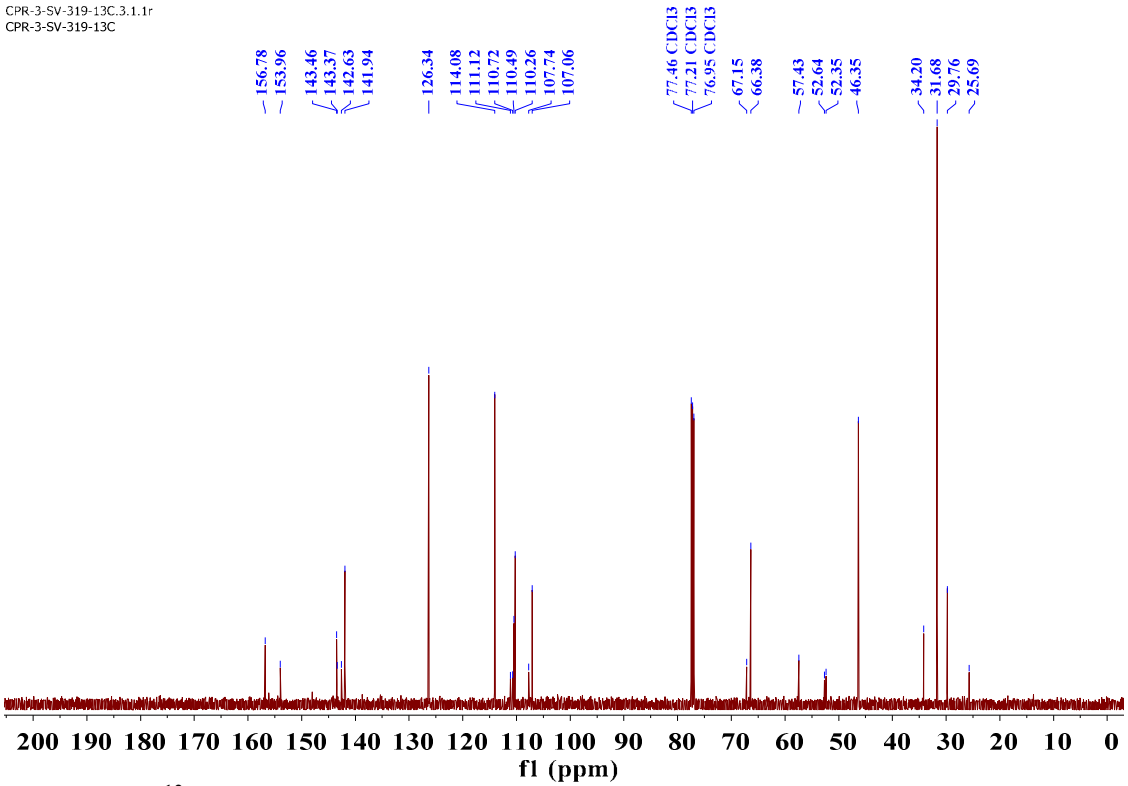


Figure S08. ^{13}C NMR spectrum ($CDCl_3$, 100 MHz) of $\mathbf{P_3}$.

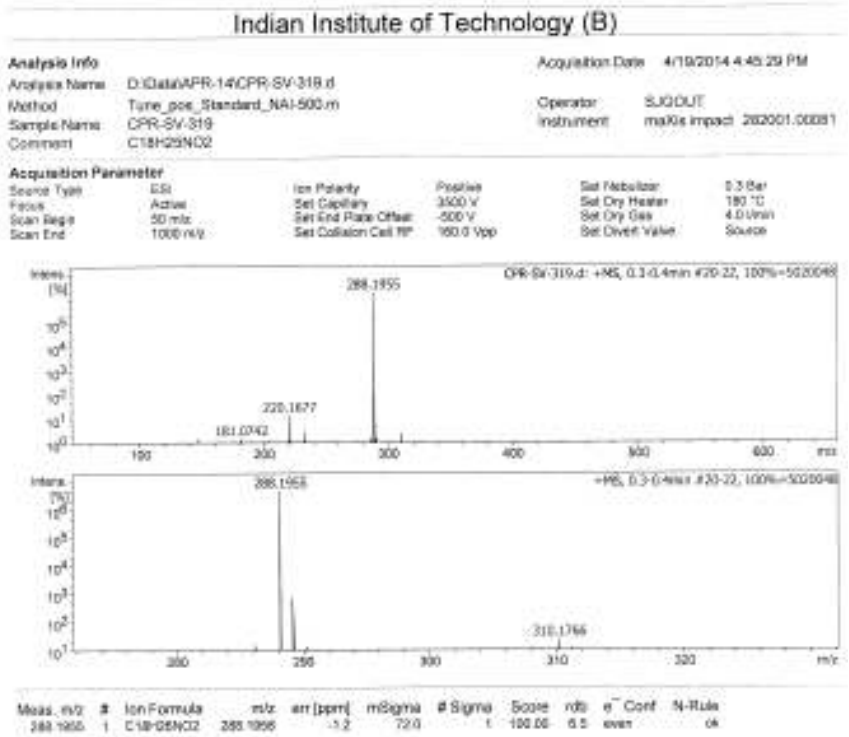


Figure S09. HRMS spectrum of $\mathbf{P_3}$.

SI04. Characterization of $\mathbf{P_4}$

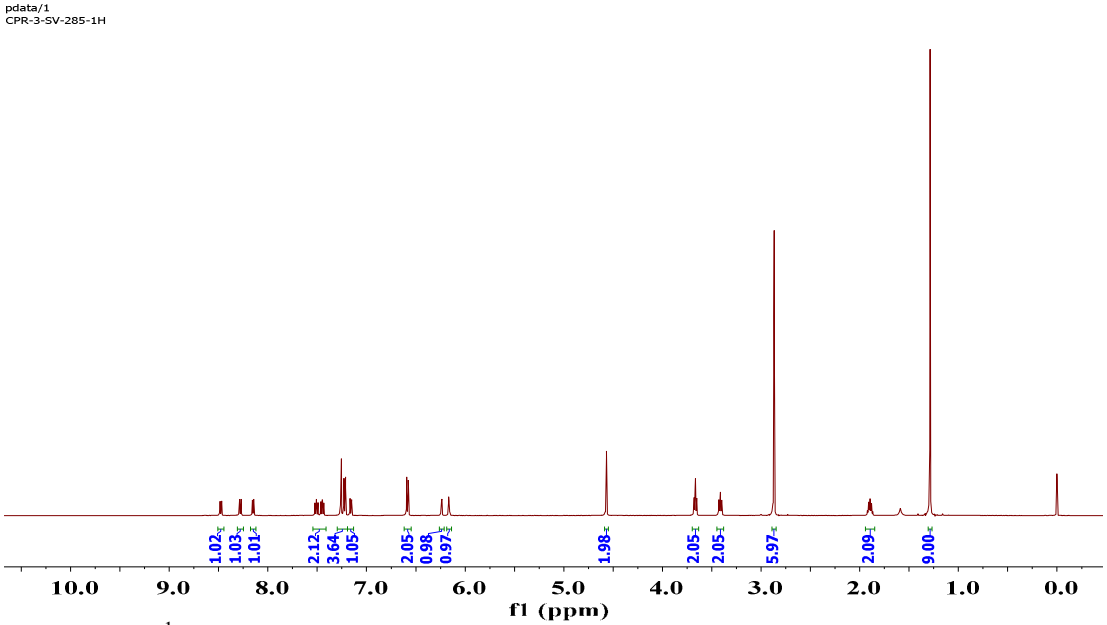


Figure S10. ^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of $\mathbf{P_4}$.

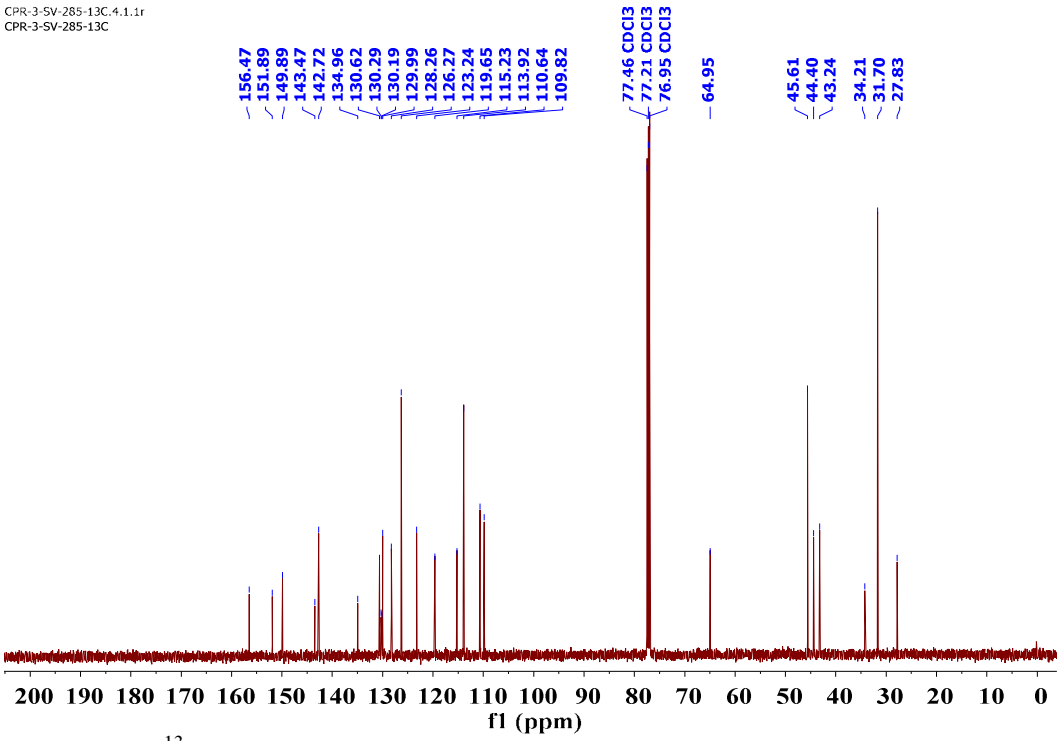


Figure S11. ^{13}C NMR spectrum ($CDCl_3$, 100 MHz) of $\mathbf{P_4}$.

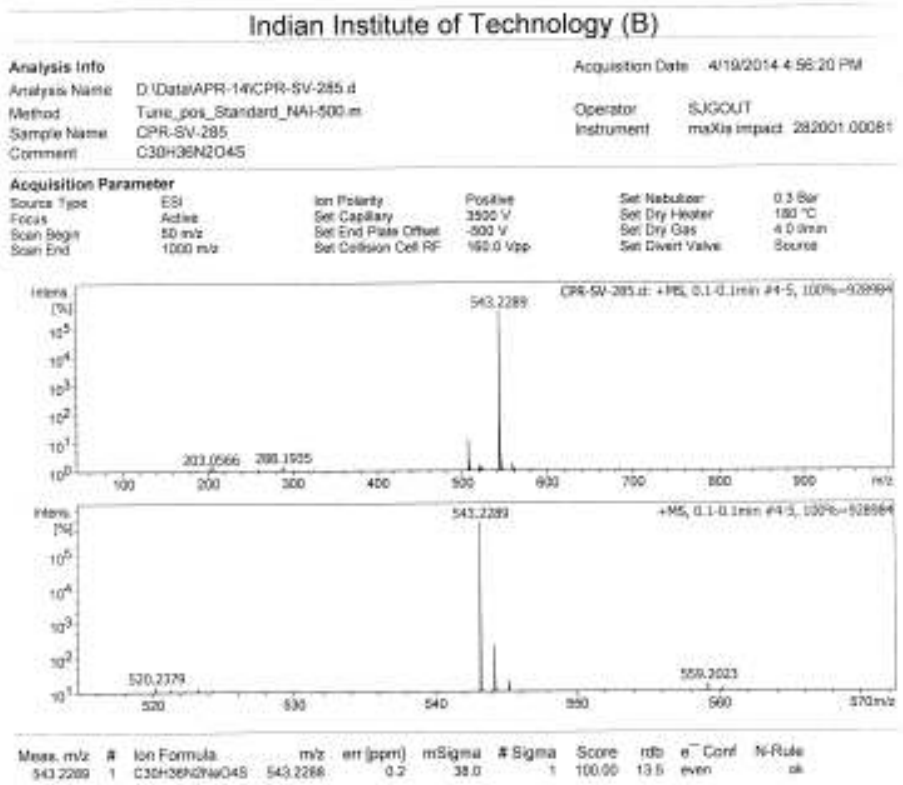


Figure S12. HRMS spectrum of $\mathbf{P_4}$.

SI05. Characterization of L_1

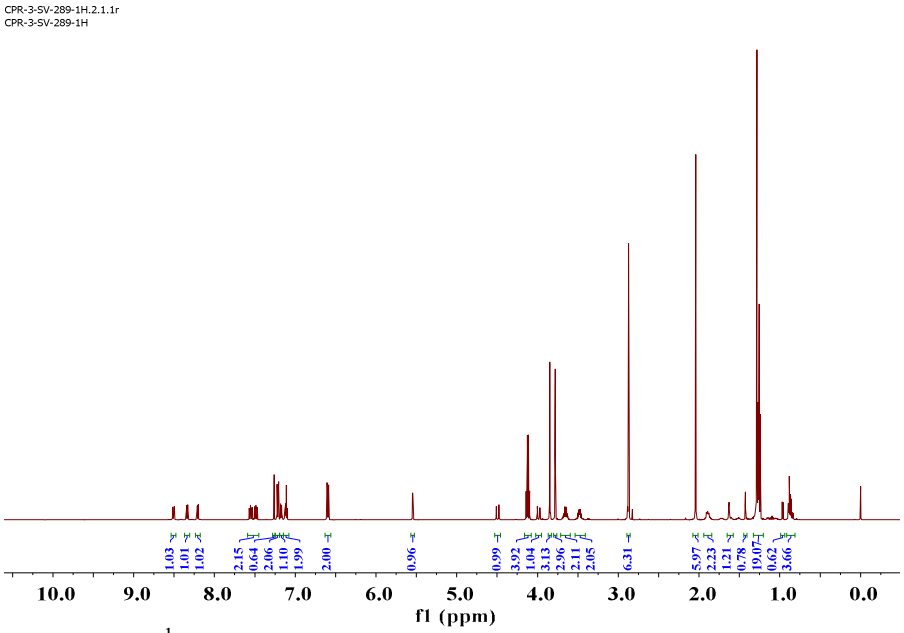


Figure S13. ^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of L_1.

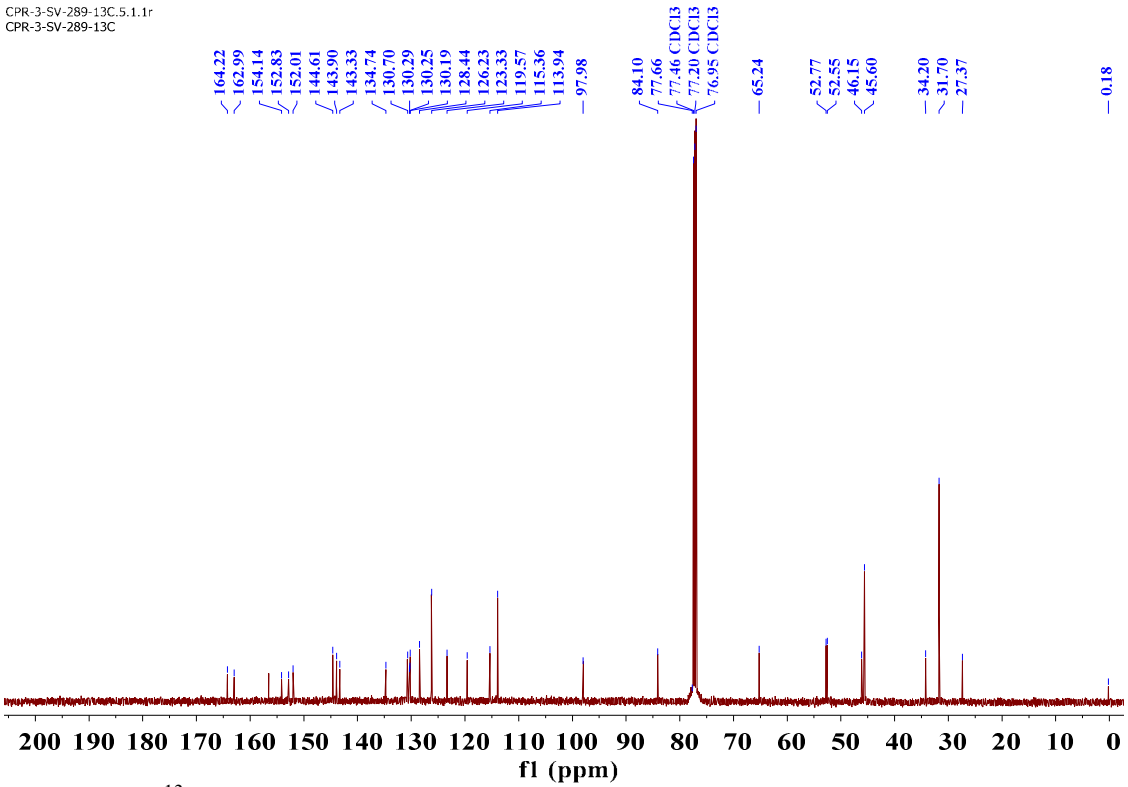


Figure S14. ^{13}C NMR spectrum ($CDCl_3$, 125 MHz) of L_1

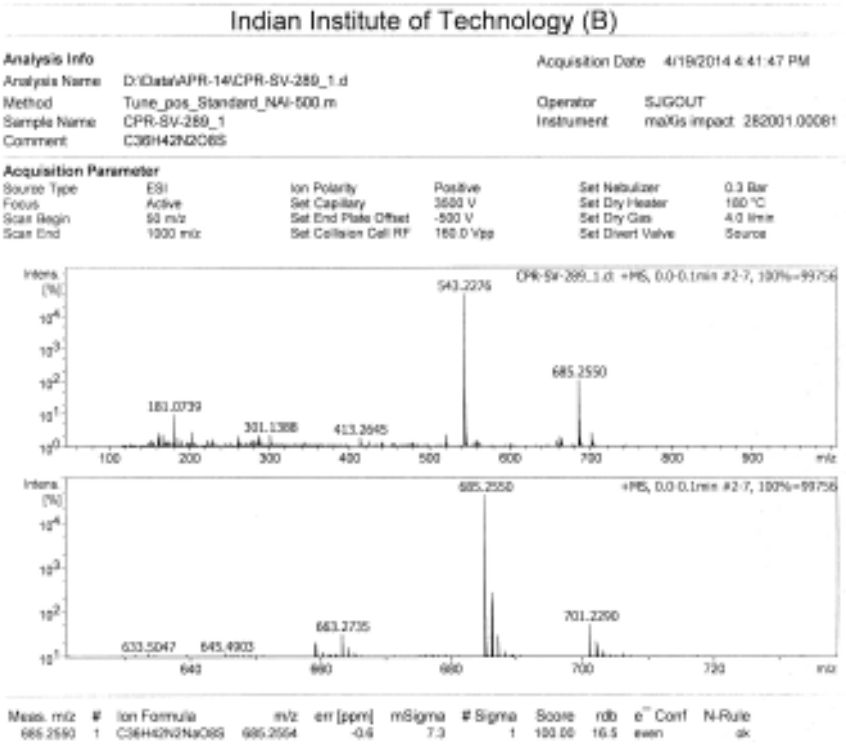
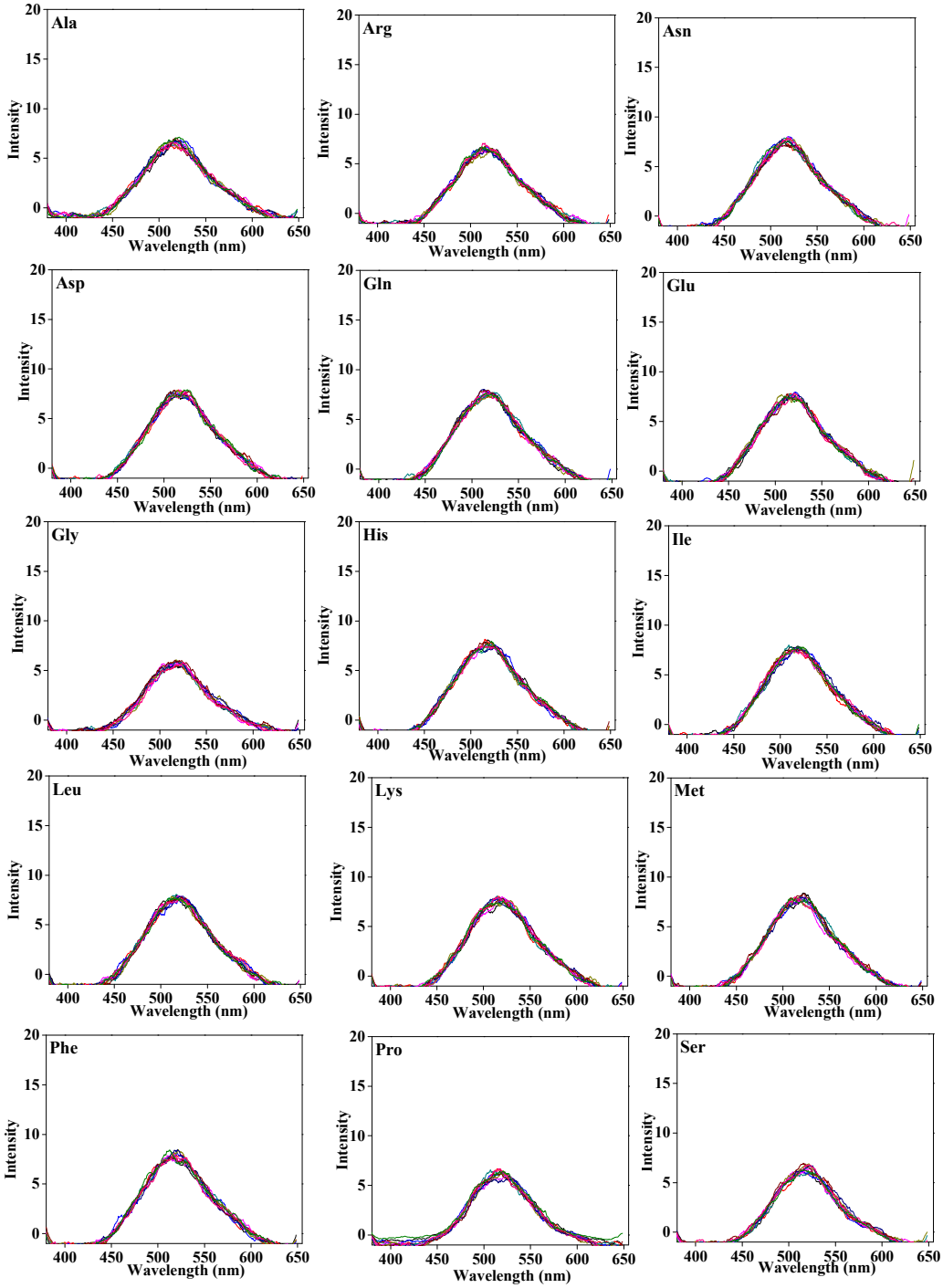


Figure S15. HRMS spectrum of $\mathbf{L_1}$.

SI06. Fluorescence studies of L_1 with amino acids



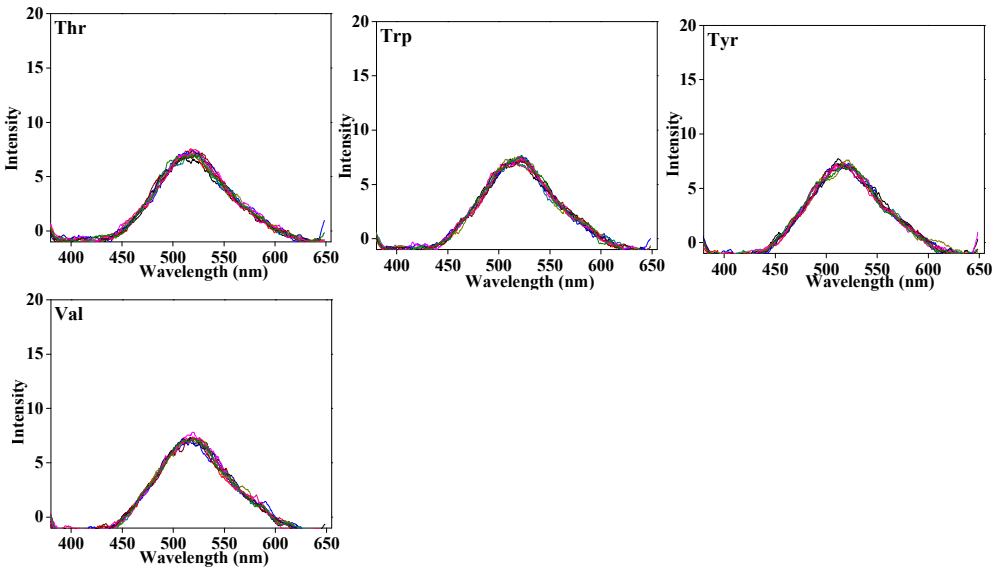


Figure S16. Fluorescence titration studies of **L** with amino acids.

SI07. Characterization of P_6

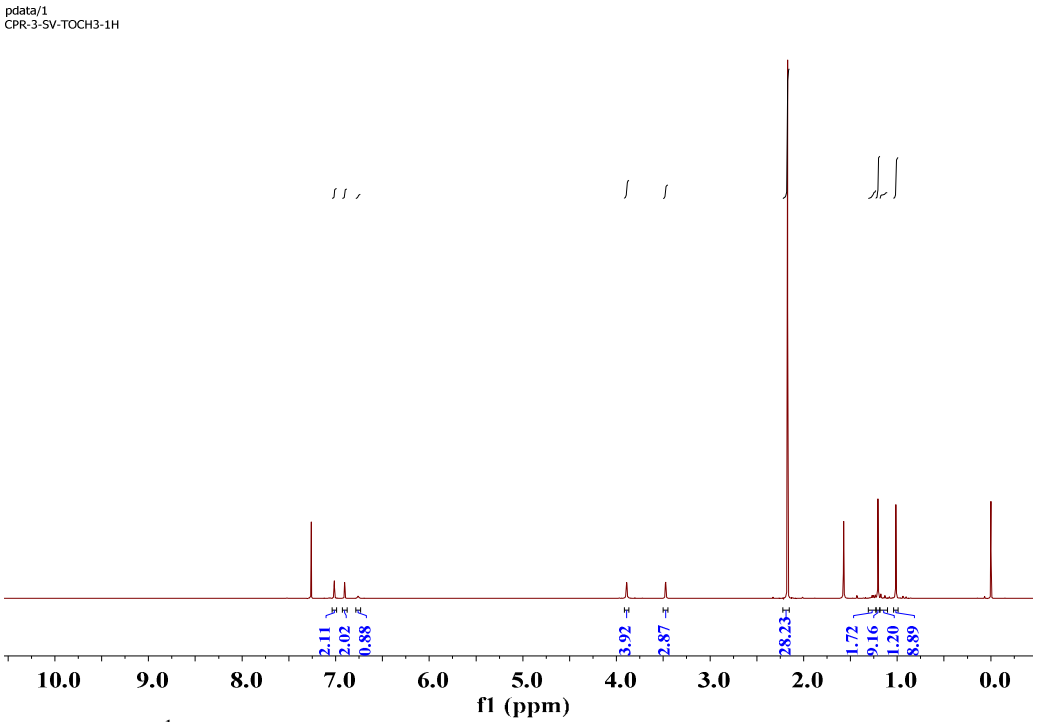


Figure S17. ^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of $\mathbf{P_6}$.

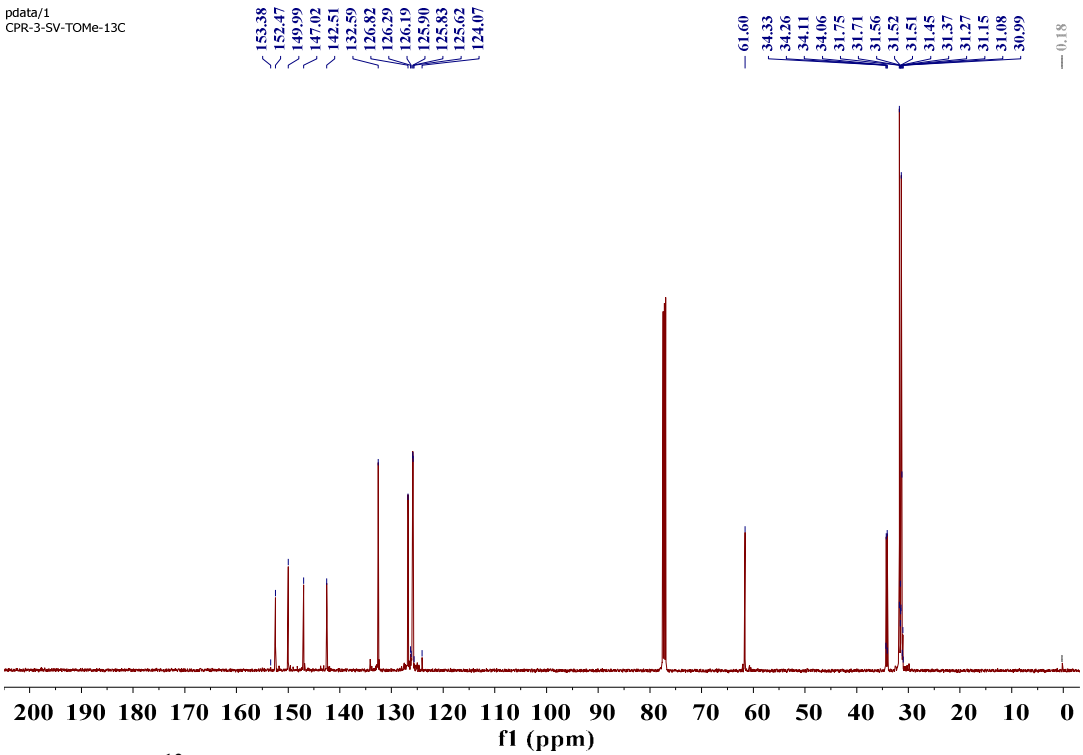


Figure S18. ^{13}C NMR spectrum ($CDCl_3$, 125 MHz) of $\mathbf{P_6}$.

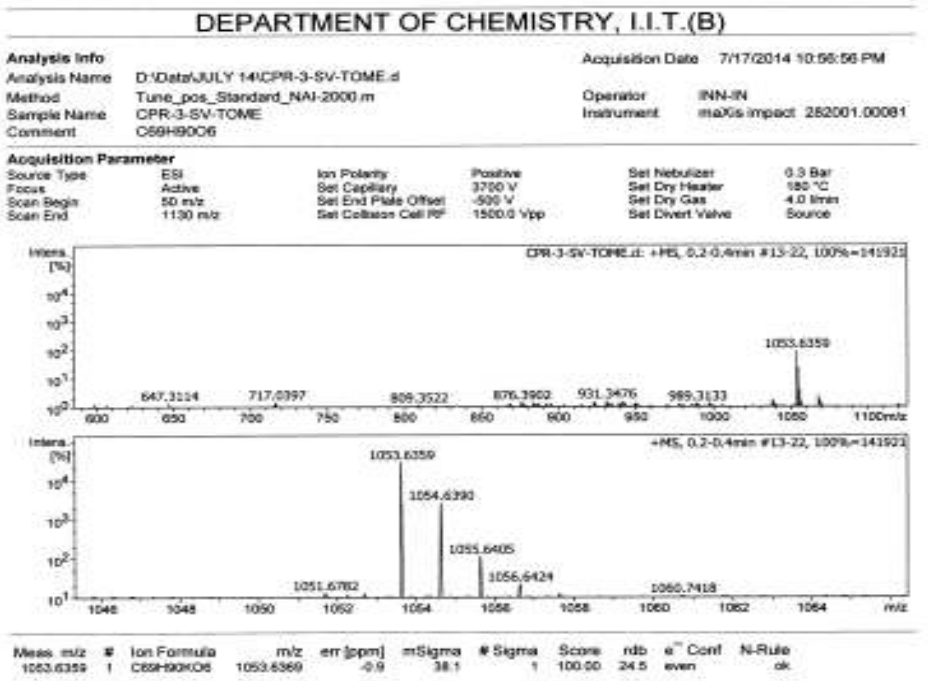


Figure S19. HRMS spectrum of $\mathbf{P_6}$.

SI08. Characterization of $\mathbf{P_7}$

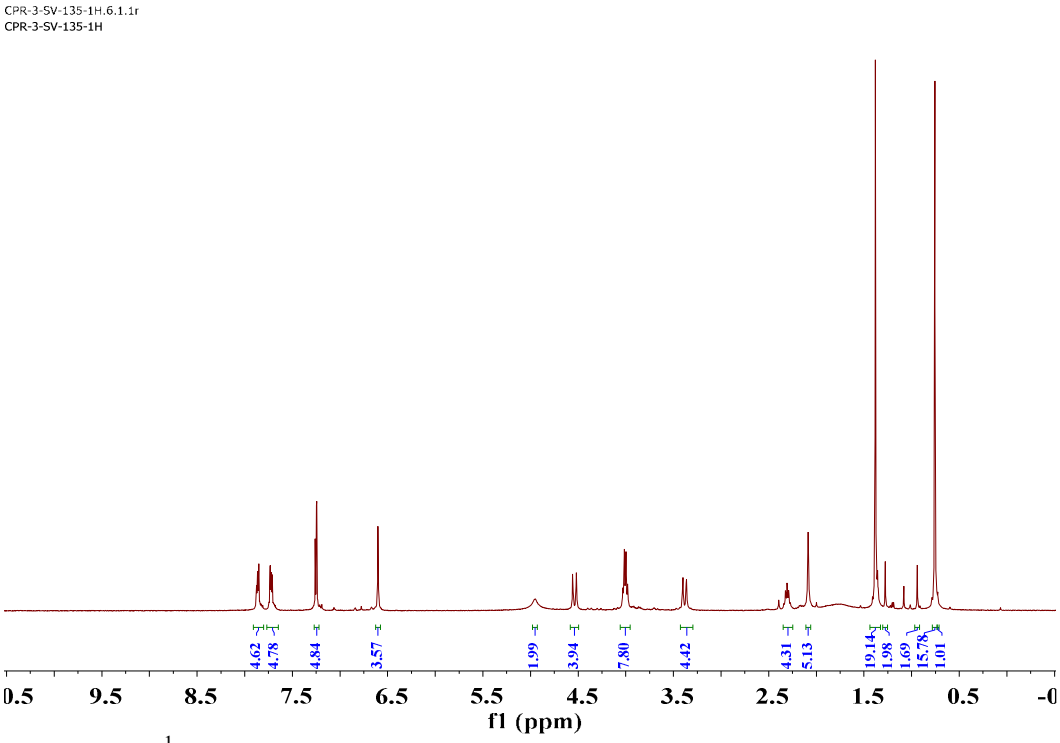


Figure S20. ^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of $\mathbf{P_7}$.

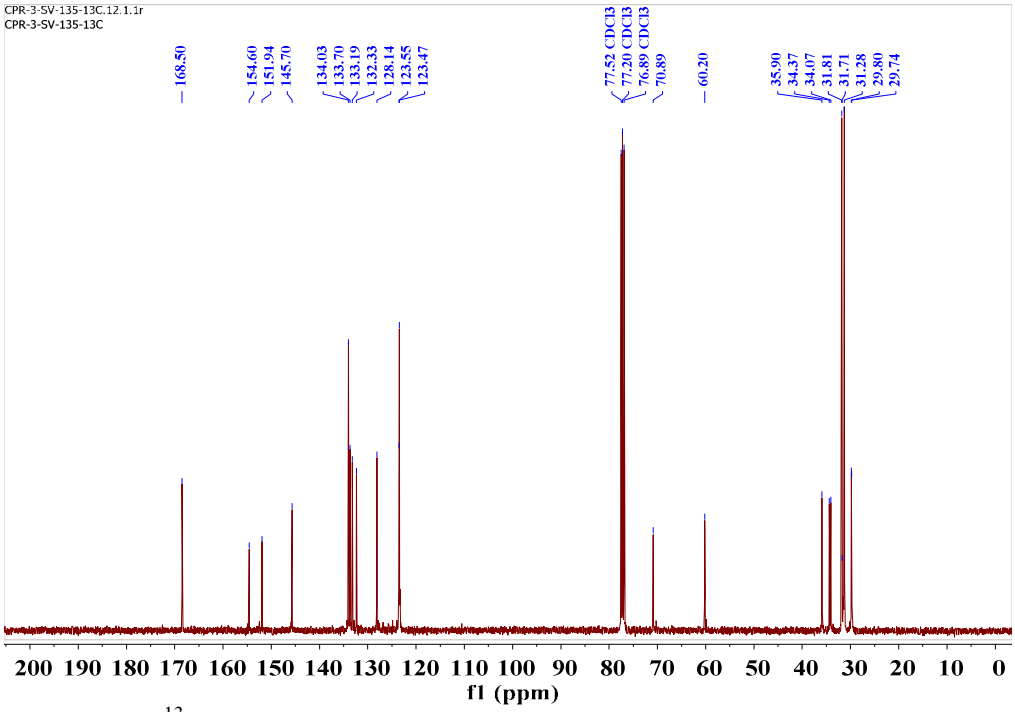


Figure S21. ^{13}C NMR spectrum ($CDCl_3$, 100 MHz) of $\mathbf{P_7}$

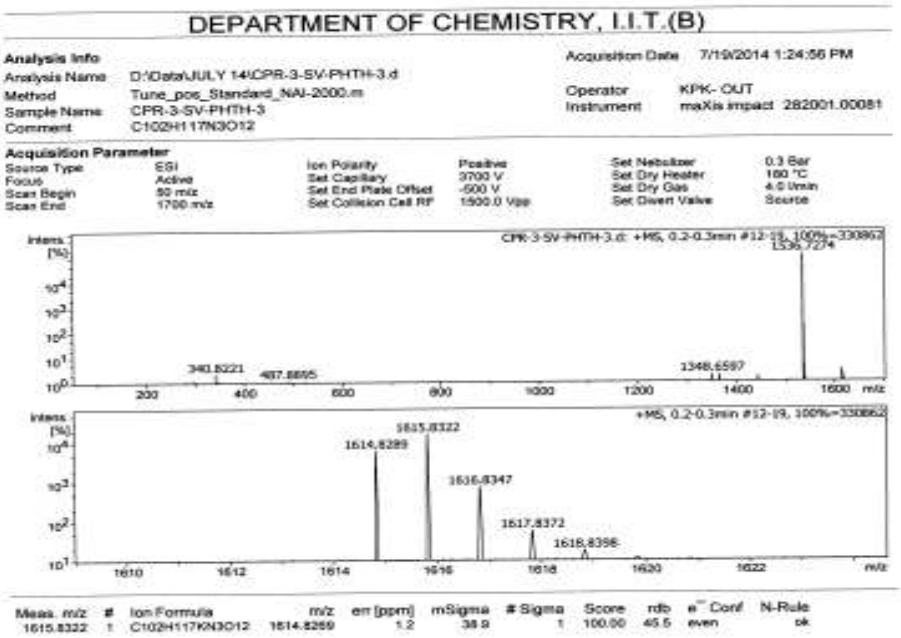


Figure S22. HRMS spectrum of $\mathbf{P_7}$.

SI9. Characterization of P_8

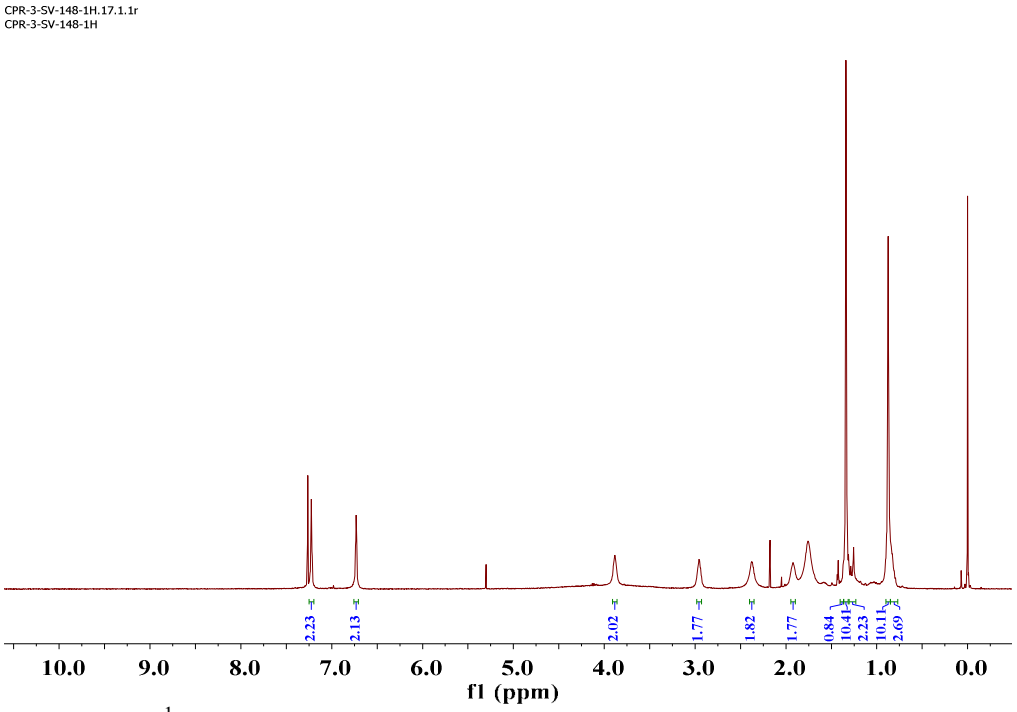


Figure S23. ^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of $\mathbf{P_8}$.

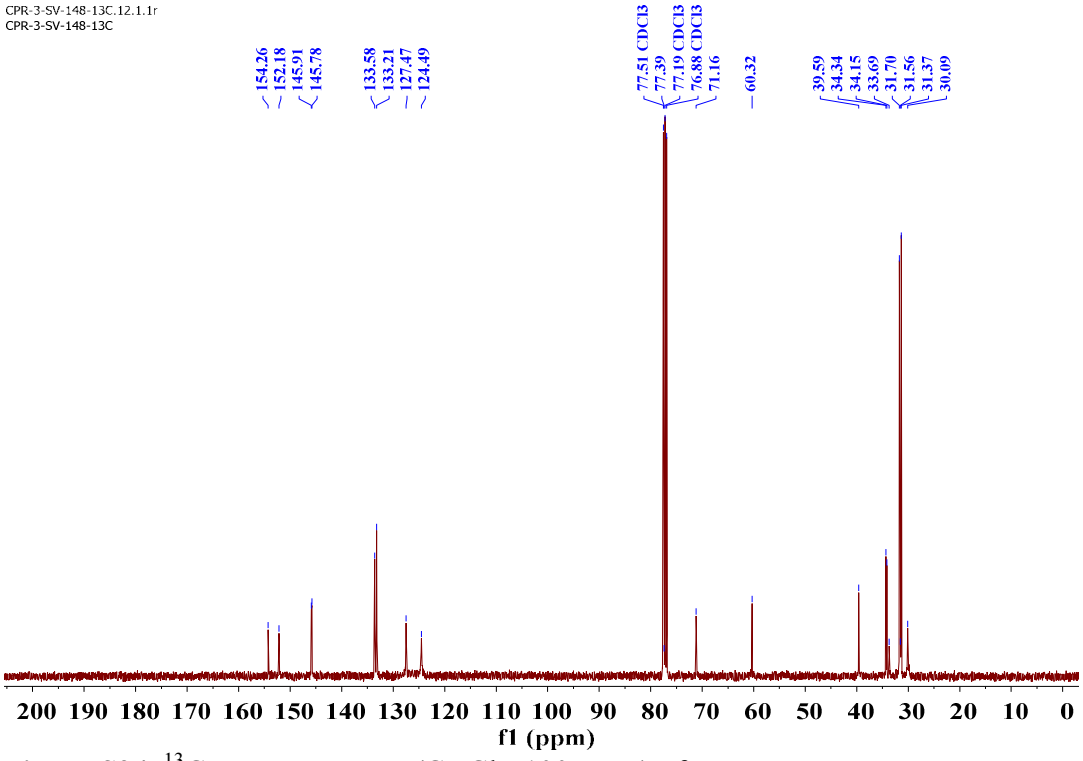


Figure S24. ^{13}C NMR spectrum ($CDCl_3$, 100 MHz) of $\mathbf{P_8}$.

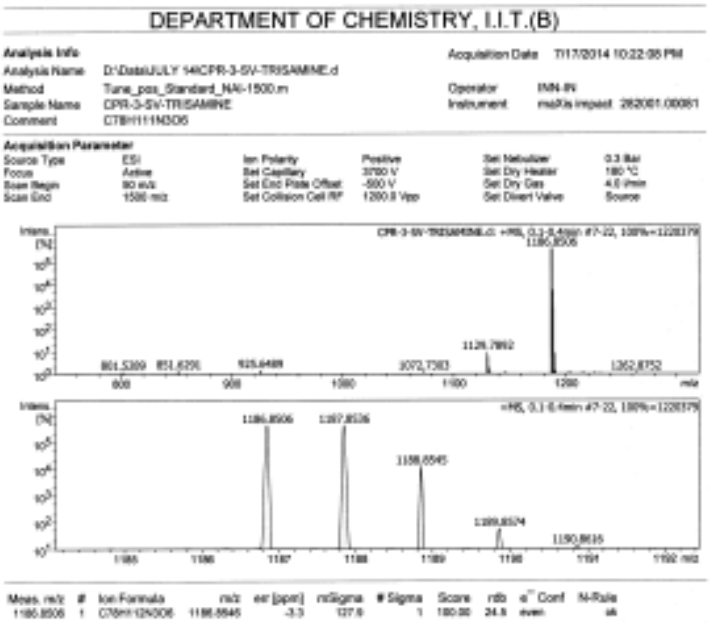


Figure S25. HRMS spectrum of **P_8**.

SI10. Characterization of P_9

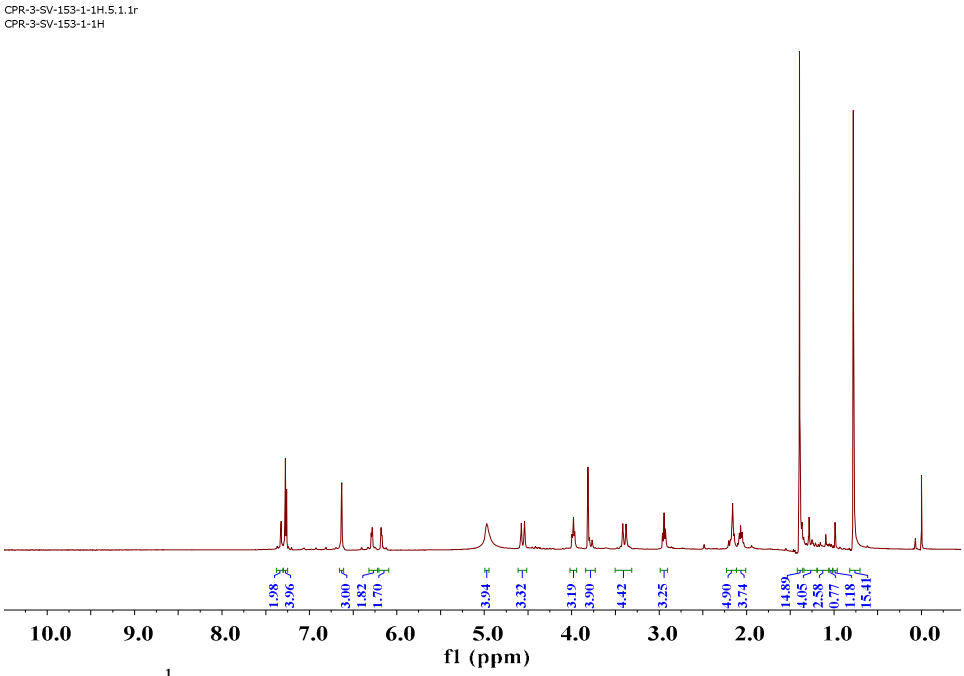


Figure S26. ^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of **P_9**.

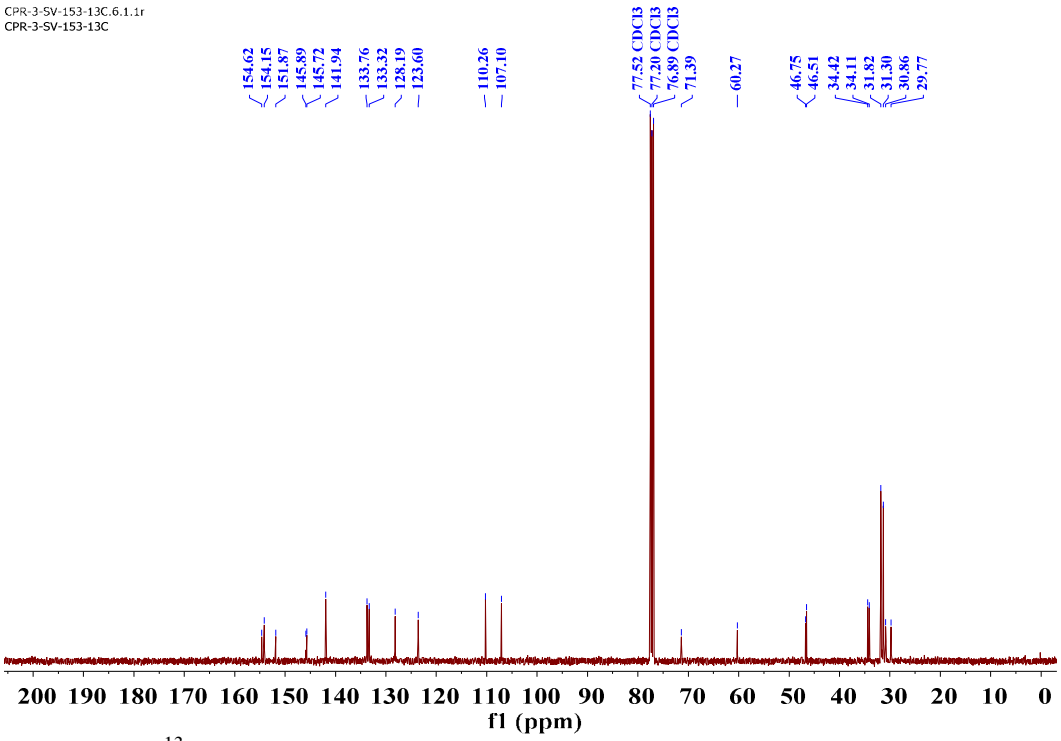


Figure S27. ^{13}C NMR spectrum ($CDCl_3$, 100 MHz) of **P_9**.

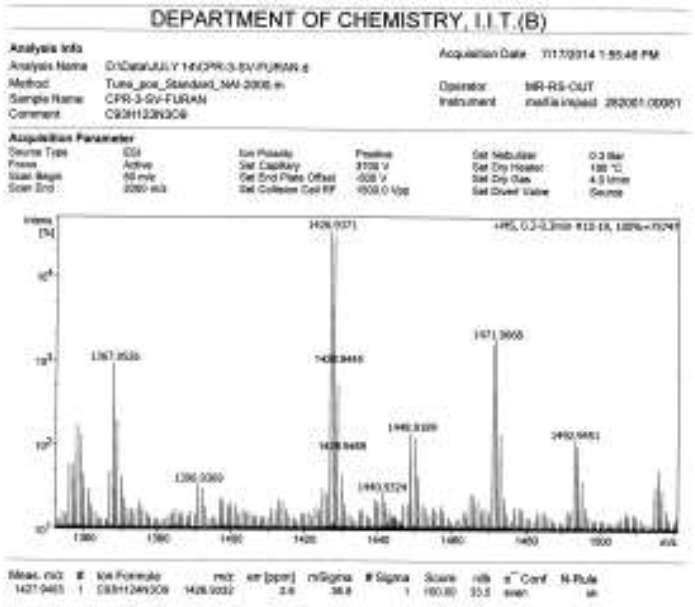


Figure S28. HRMS spectrum of **P_9**.

SI11. Characterization of P_{10}

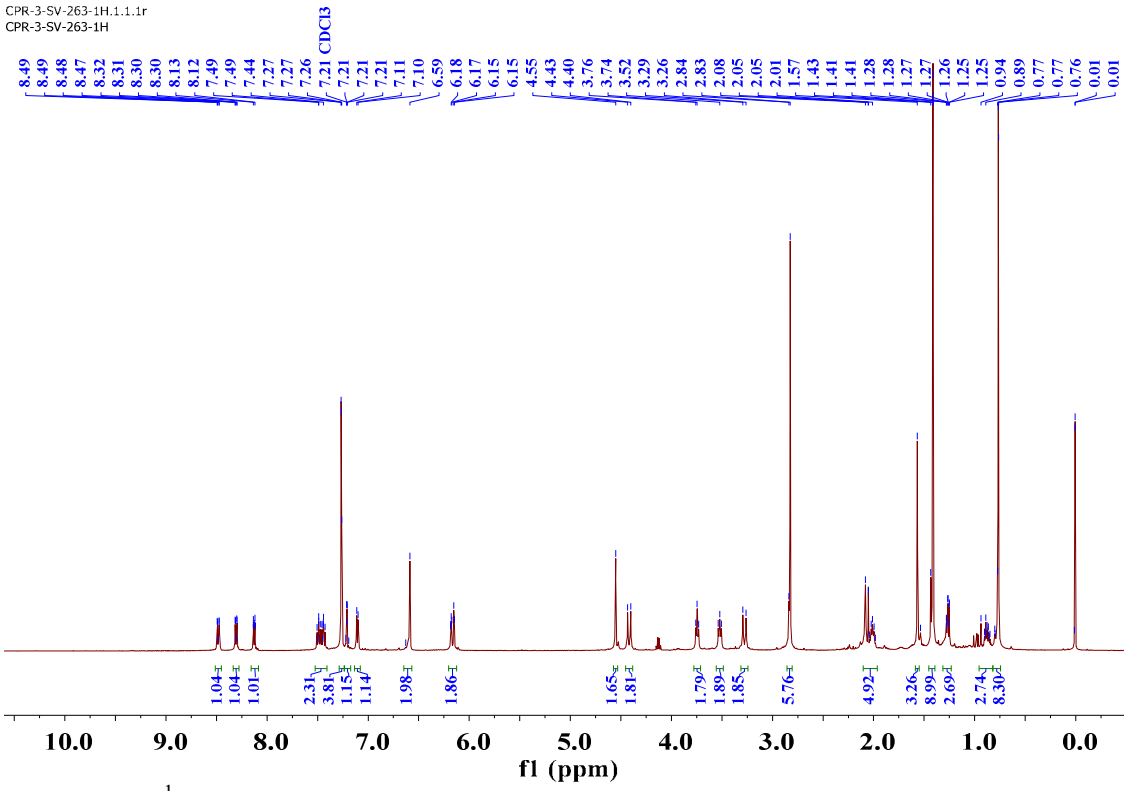


Figure S29. ^{1}H NMR spectrum ($CDCl_3$, 500 MHz) of $\mathbf{P_{10}}$.

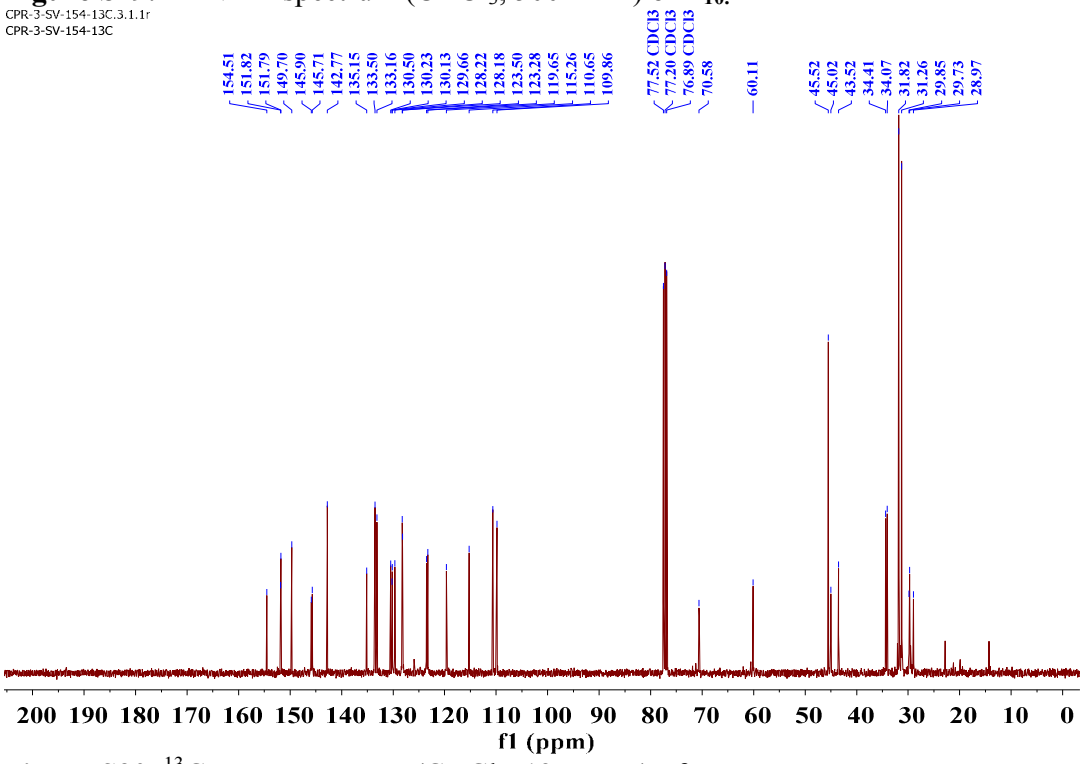


Figure S30. ^{13}C NMR spectrum ($CDCl_3$, 125 MHz) of $\mathbf{P_{10}}$.

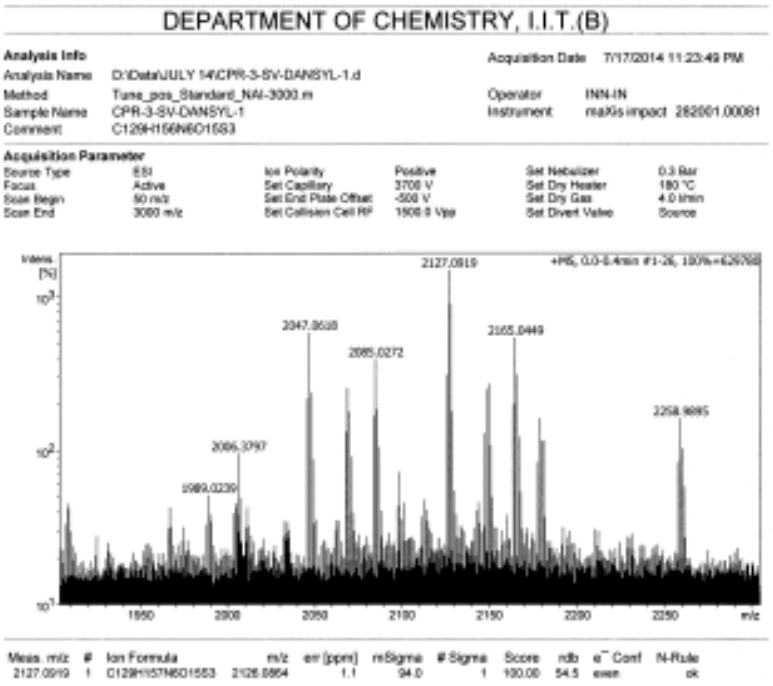


Figure S31. HRMS spectrum of $\mathbf{P_{10}}$.

SI12. Characterization of $\mathbf{L_2}$

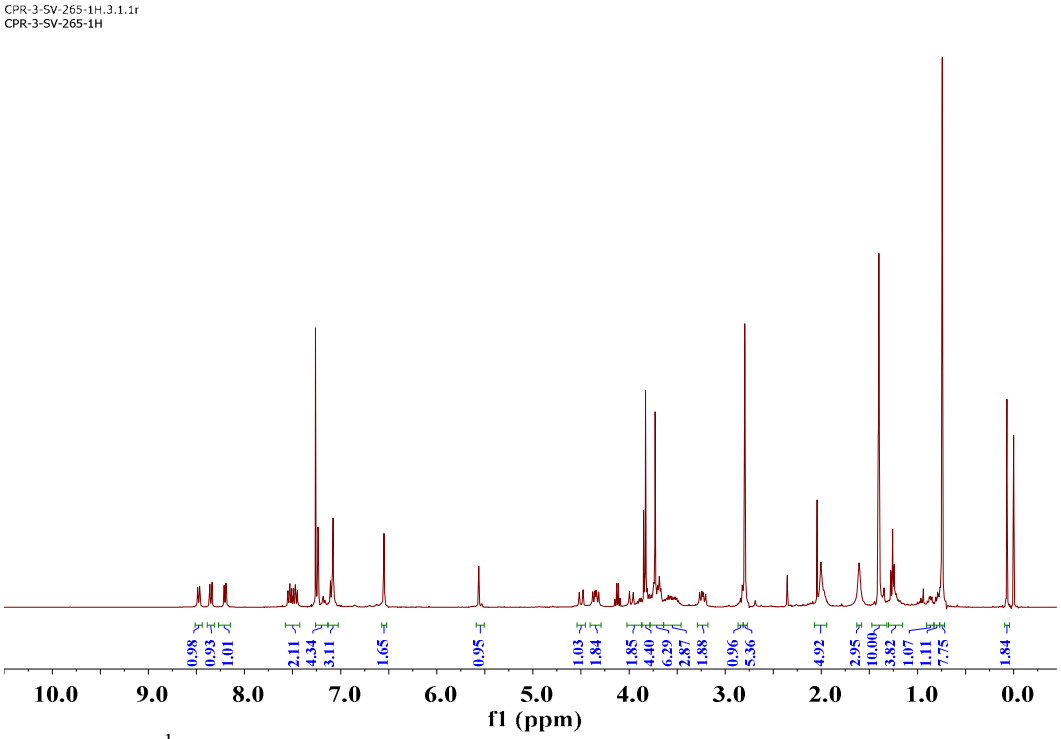


Figure S32. ^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of $\mathbf{L_2}$.

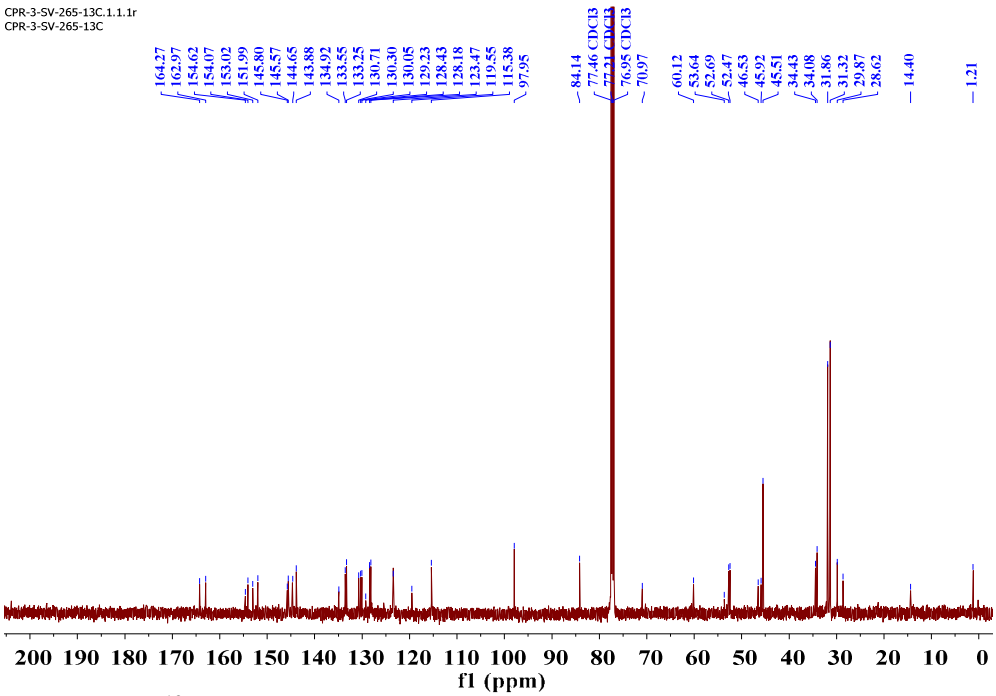


Figure S33. ^{13}C NMR spectrum ($CDCl_3$, 100 MHz) of $\mathbf{L_2}$.

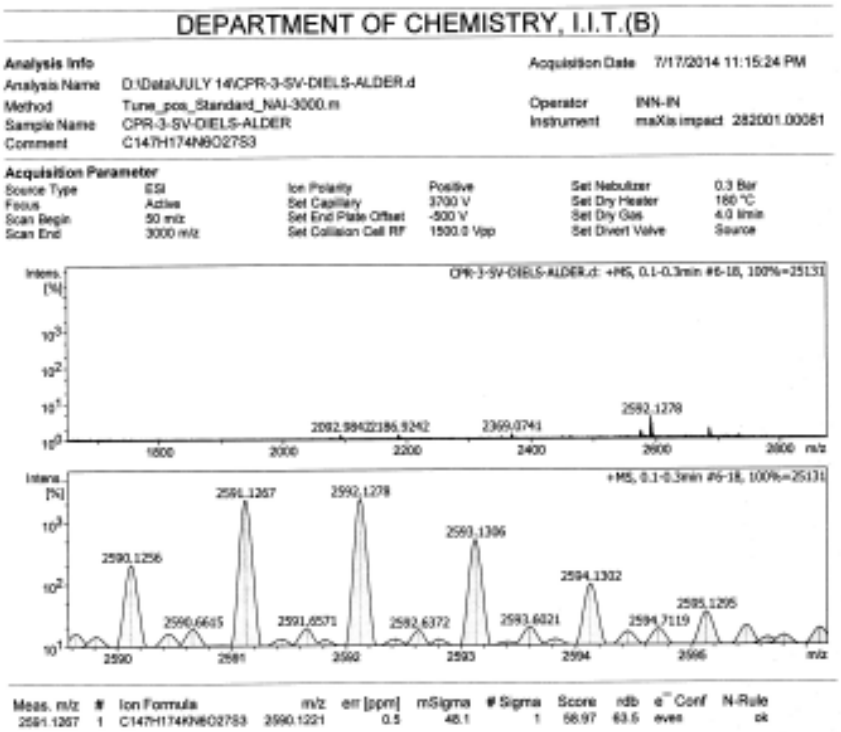


Figure S34. HRMS spectrum of $\mathbf{L_2}$.

SI13. Parametric details of the 2D NMR experiments carried out with P_{10} and L_2

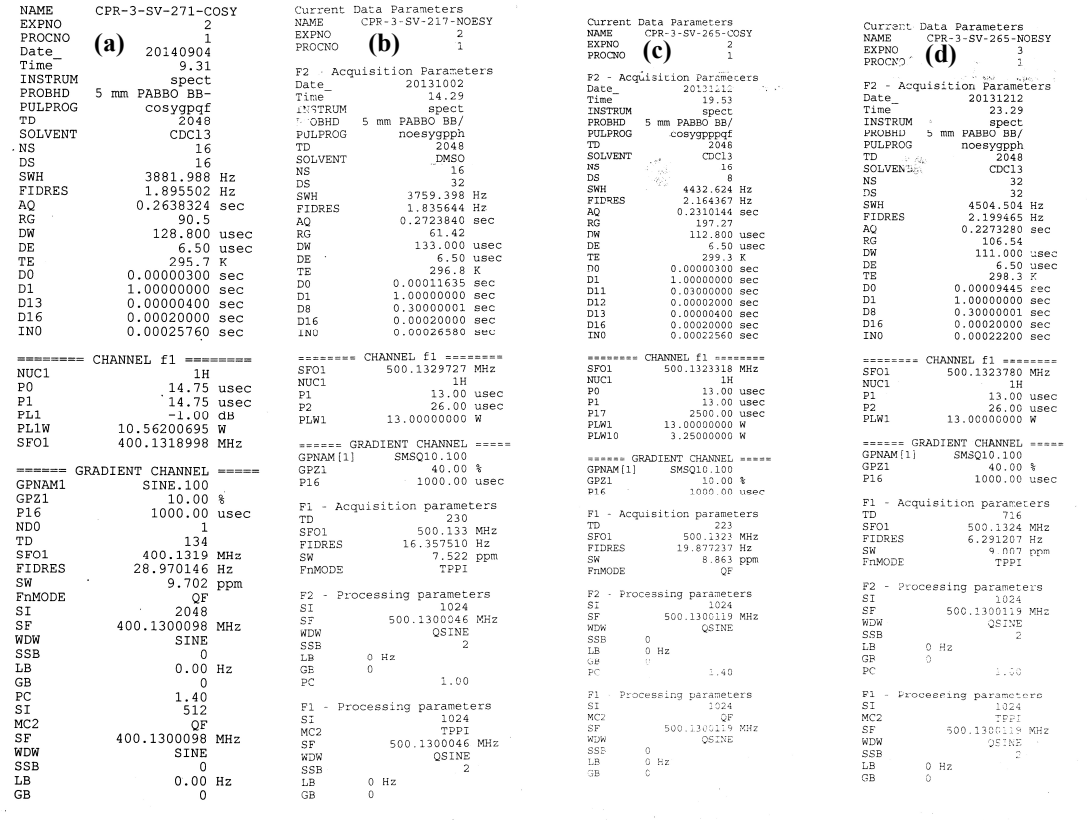
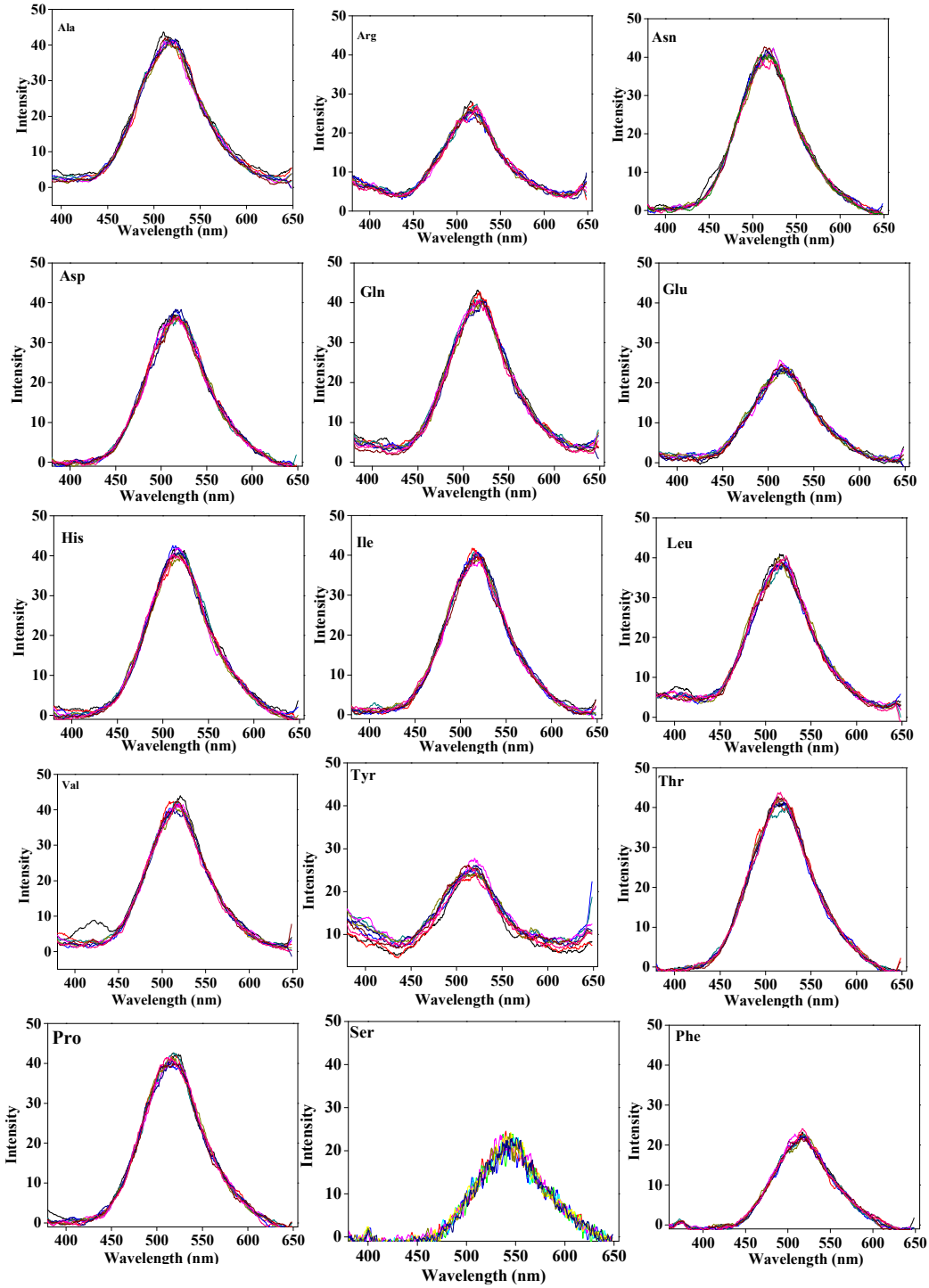


Figure S35. 2D NMR details for P_{10} and L_2 (a) & (b) COSY and NOESY for P_{10}; (c) & (d) COSY and NOESY for L_2.

SI14. Fluorescence studies of L_2 with amino acids



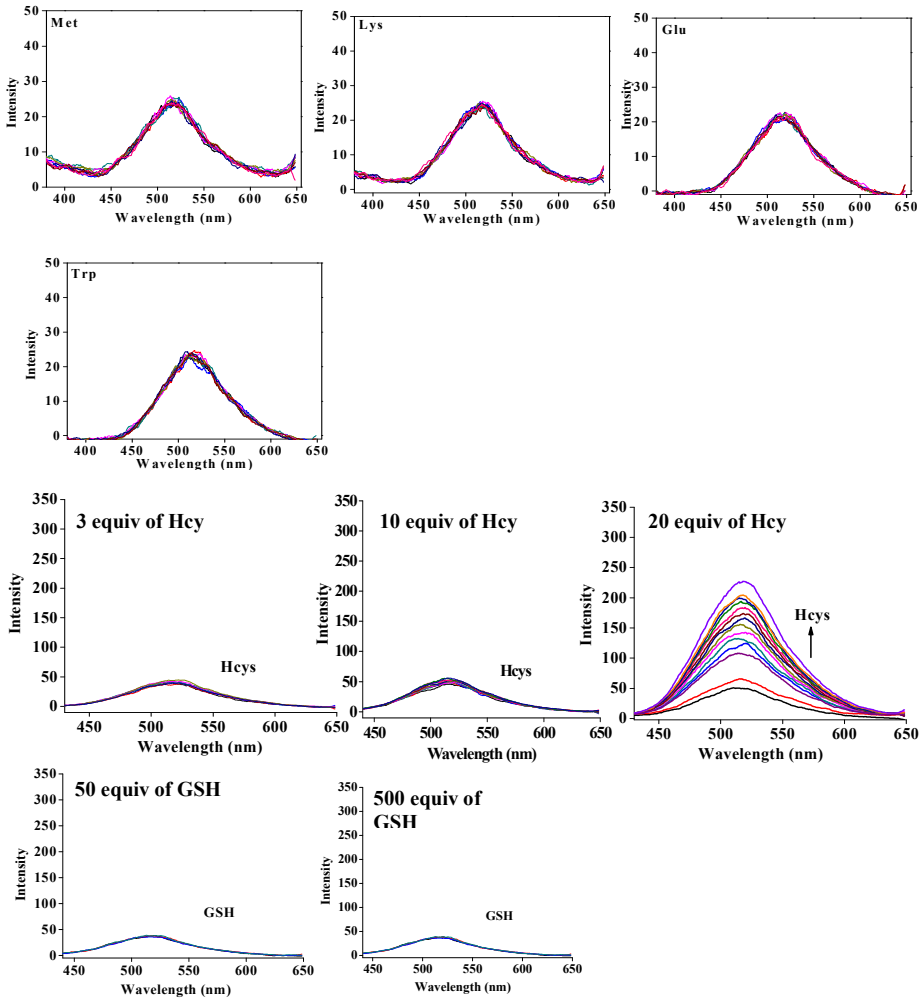


Figure S36. Fluorescence titration studies of $\mathbf{L_2}$ with amino acids.

SI 15. SEM images of L_2 with GSH

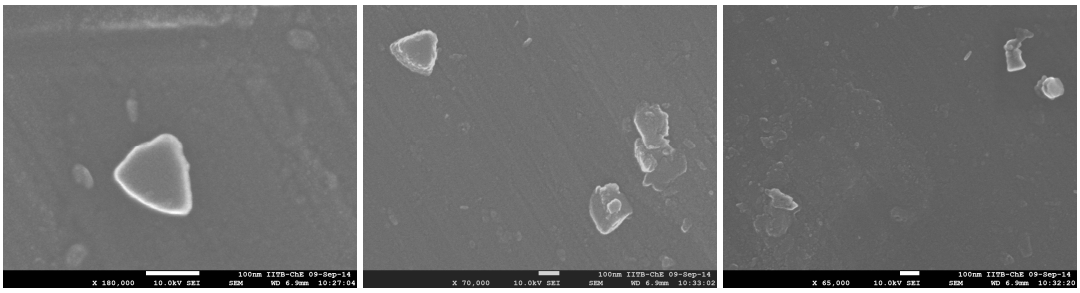


Figure S37. SEM images of $\mathbf{L_2}$ with the reaction of GSH (1:5).