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Synthesis, Characterization and Protein Sensing of Cysteine Doped Polyanaline

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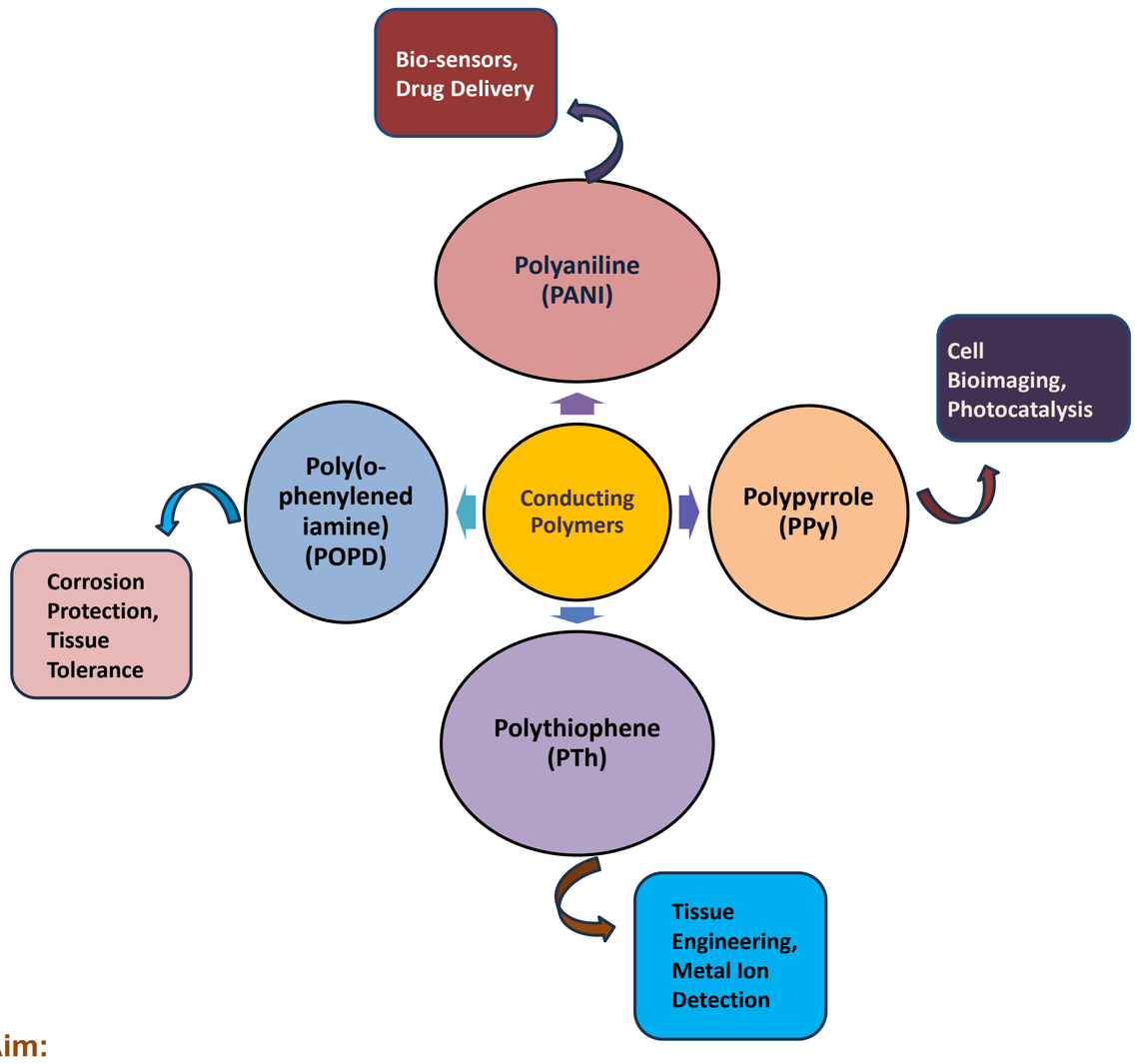
INTRODUCTION & AIM

Introduction:

Conducting polymers (CPs) such as polyaniline (PANI), polypyrrole (PPy), polythiophene (PTh), poly(o-phenylenediamine) (POPD), and polyethylene dioxy thiophene (PEDOT) are wellknown for their outstanding electroactive and optoelectronic properties [1–2]. Water-soluble conjugated polymers are reported to exhibit remarkable fluorescent properties and are reported to be utilized in designing fluorescent probes, bio-macromolecule determination, cell bioimaging, and so on [3].



Aim:

In this paper, oligomers of polyaniline (PANI) modified with cysteine (Cys) were synthesized via using different mole ratios of aniline: Cysteine (80:20, 50:50, and 20:80) followed by ultrasound-assisted polymerization of PANI.

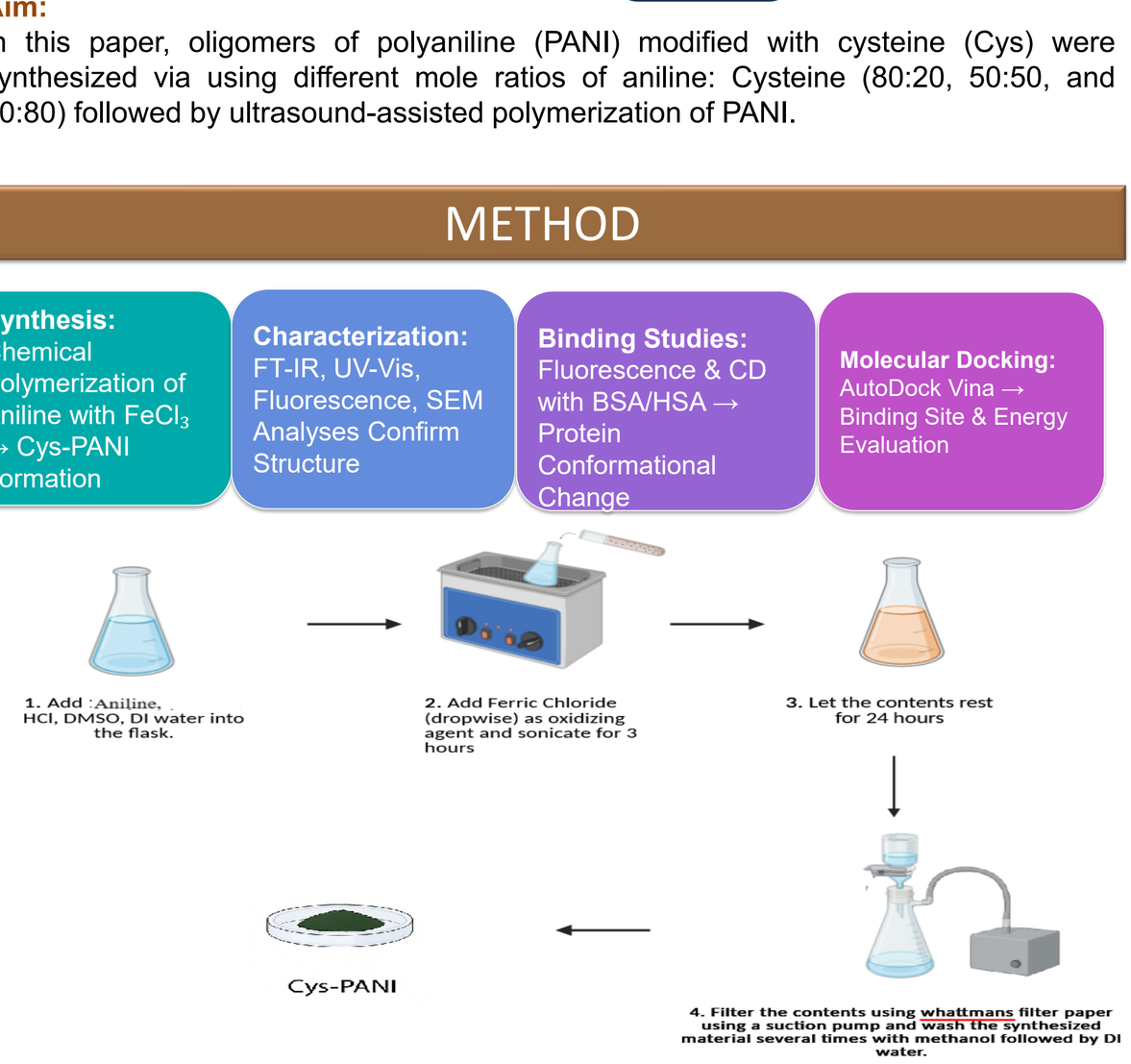
METHOD

Synthesis: Chemical Polymerization of Aniline with $FeCl_3$ → Cys-PANI Formation

Characterization: FT-IR, UV-Vis, Fluorescence, SEM Analyses Confirm Structure

Binding Studies: Fluorescence & CD with BSA/HSA → Protein Conformational Change

Molecular Docking: AutoDock Vina → Binding Site & Energy Evaluation



Schematic Diagram for the Synthesis of Cys-PANI Oligomers

RESULTS & DISCUSSION

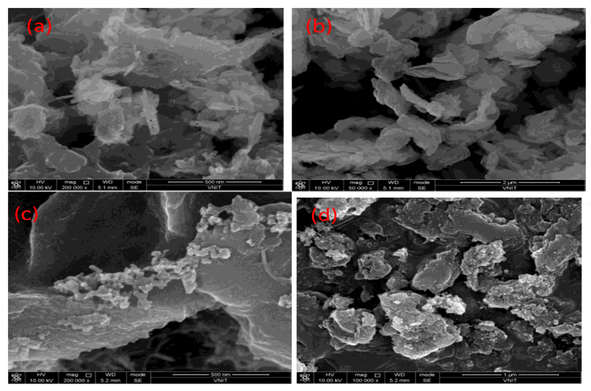


FIGURE 1 | SEM images of the Cys-PANI oligomers formed via Chemical Polymerization (a) PANI, (b), Cys-PANI/20-80, (c) Cys-PANI/50-50, and (d) Cys-PANI/80-20.

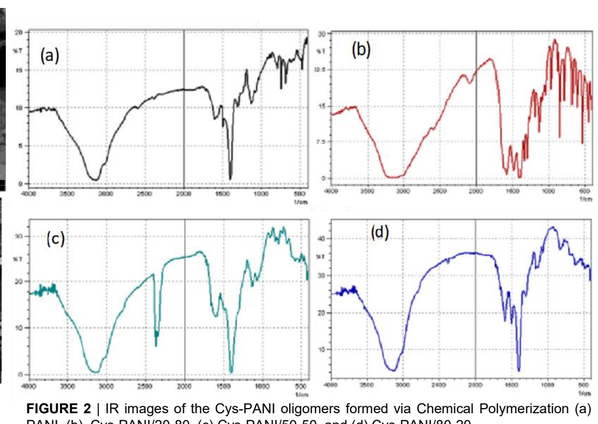


FIGURE 2 | IR images of the Cys-PANI oligomers formed via Chemical Polymerization (a) PANI, (b), Cys-PANI/20-80, (c) Cys-PANI/50-50, and (d) Cys-PANI/80-20.

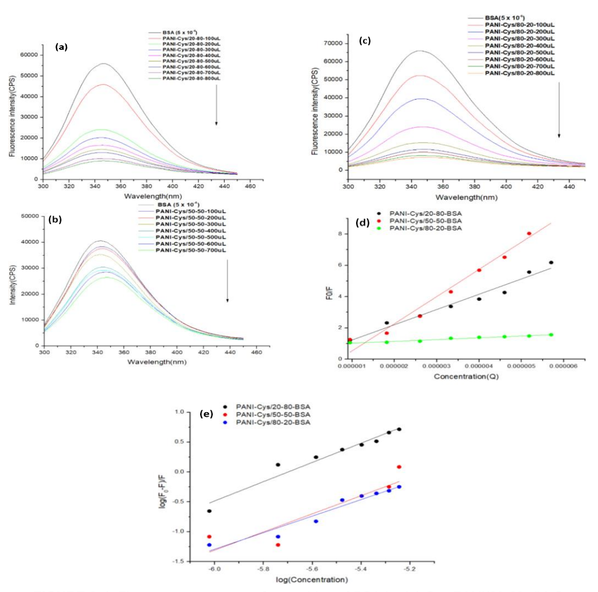


FIGURE 3 | Fluorescence spectra of quenching of BSA by (a) Cys-PANI/80-20, (b) Cys-PANI/50-50, (c) Cys-PANI/20-80, (d) stern volmer plot for of fluorescence quenching of BSA, and (e) plot of log F_0-F/F versus log concentration.

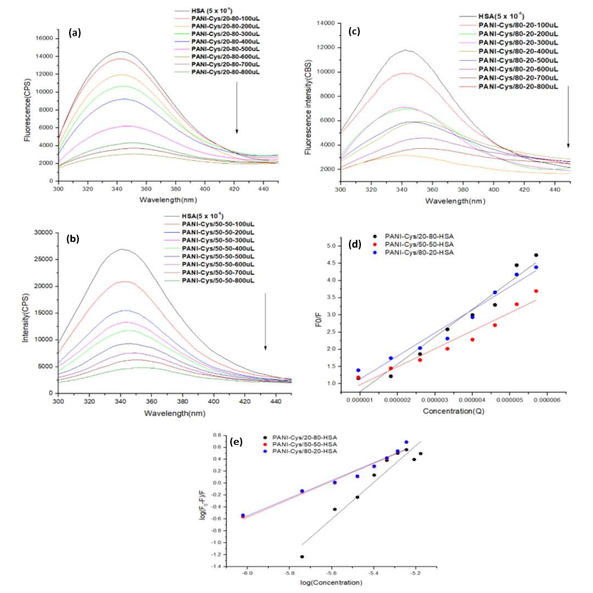


FIGURE 4 | Fluorescence spectra of quenching of HSA by the Cys-PANI oligomers: (a) Cys-PANI/80-20, (b) Cys-PANI/50-50, (c) Cys-PANI/20-80, (d) Stern Volmer plot for fluorescence quenching of HSA, and (e) plot of log F_0-F/F versus log concentration.

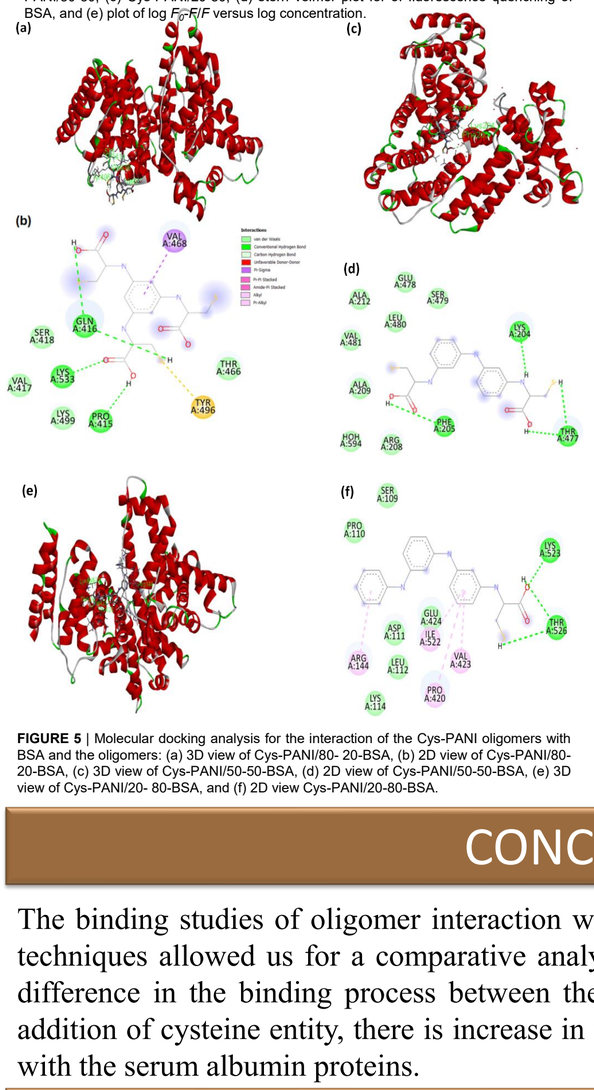


FIGURE 5 | Molecular docking analysis for the interaction of the Cys-PANI oligomers with BSA and the oligomers: (a) 3D view of Cys-PANI/80- 20-BSA, (b) 2D view of Cys-PANI/80-20-BSA, (c) 3D view of Cys-PANI/50-50-BSA, (d) 2D view of Cys-PANI/50-50-BSA, (e) 3D view of Cys-PANI/20- 80-BSA, and (f) 2D view Cys-PANI/20-80-BSA.

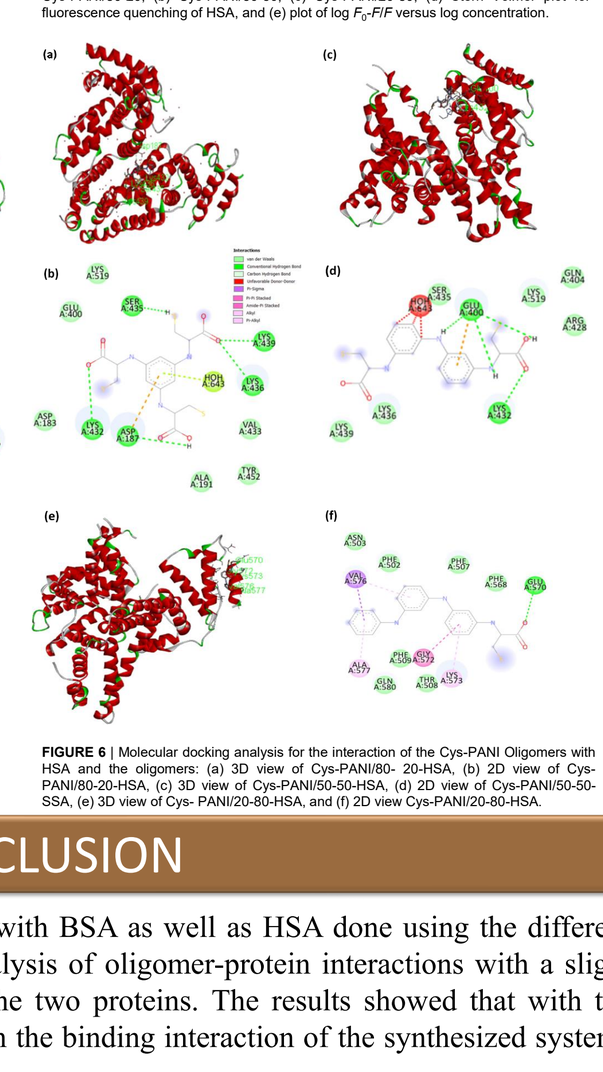


FIGURE 6 | Molecular docking analysis for the interaction of the Cys-PANI Oligomers with HSA and the oligomers: (a) 3D view of Cys-PANI/80- 20-HSA, (b) 2D view of Cys-PANI/80-20-HSA, (c) 3D view of Cys-PANI/50-50-HSA, (d) 2D view of Cys-PANI/50-50-SSA, (e) 3D view of Cys- PANI/20-80-HSA, and (f) 2D view Cys-PANI/20-80-HSA.

CONCLUSION

The binding studies of oligomer interaction with BSA as well as HSA done using the different techniques allowed us for a comparative analysis of oligomer-protein interactions with a slight difference in the binding process between the two proteins. The results showed that with the addition of cysteine entity, there is increase in the binding interaction of the synthesized systems with the serum albumin proteins.

FUTURE WORK/REFERENCES

The binding energy values calculated showed that these polymers could potentially be used in fabricating protein sensors.

1- J. Huang and R. Kaner, *Conjugated Polymers: Theory, Synthesis, Prop- erties, and Characterization*, 3rd ed., eds. T. A. Skotheim and J. Reyn- olds (CRC Press, 2006).

2-S. Myrick, F. Nwanze, A. F. Adcock, X. Dong, L. Yang, and U. Riaz, “Graphene Oxide-Modified Polythiophene Nanohybrids: Antibacterial Properties and Sonophotocatalytic Degradation of Dyes Under Visible- Light Irradiation,” *International Journal of Polymeric Materials and Polymeric Biomaterials* 73 (2024): 1451–1460.