

DEVELOPMENT OF AN APTAMER-BASED SURFACE-ENHANCED RAMAN SPECTROSCOPY (SERS) SENSOR FOR THE QUANTITATIVE ANALYSIS OF FLUORIDE IONS

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Theme: Good Health and Well-Being (SDG 3)

Research Problem

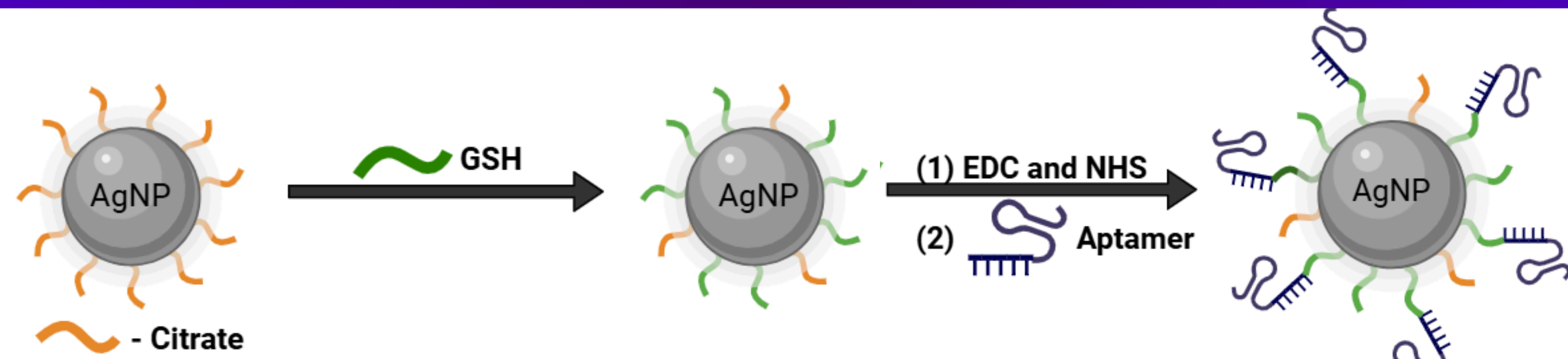


- Prevent fluoride-related diseases.
- Ensure good health and well-being for all.

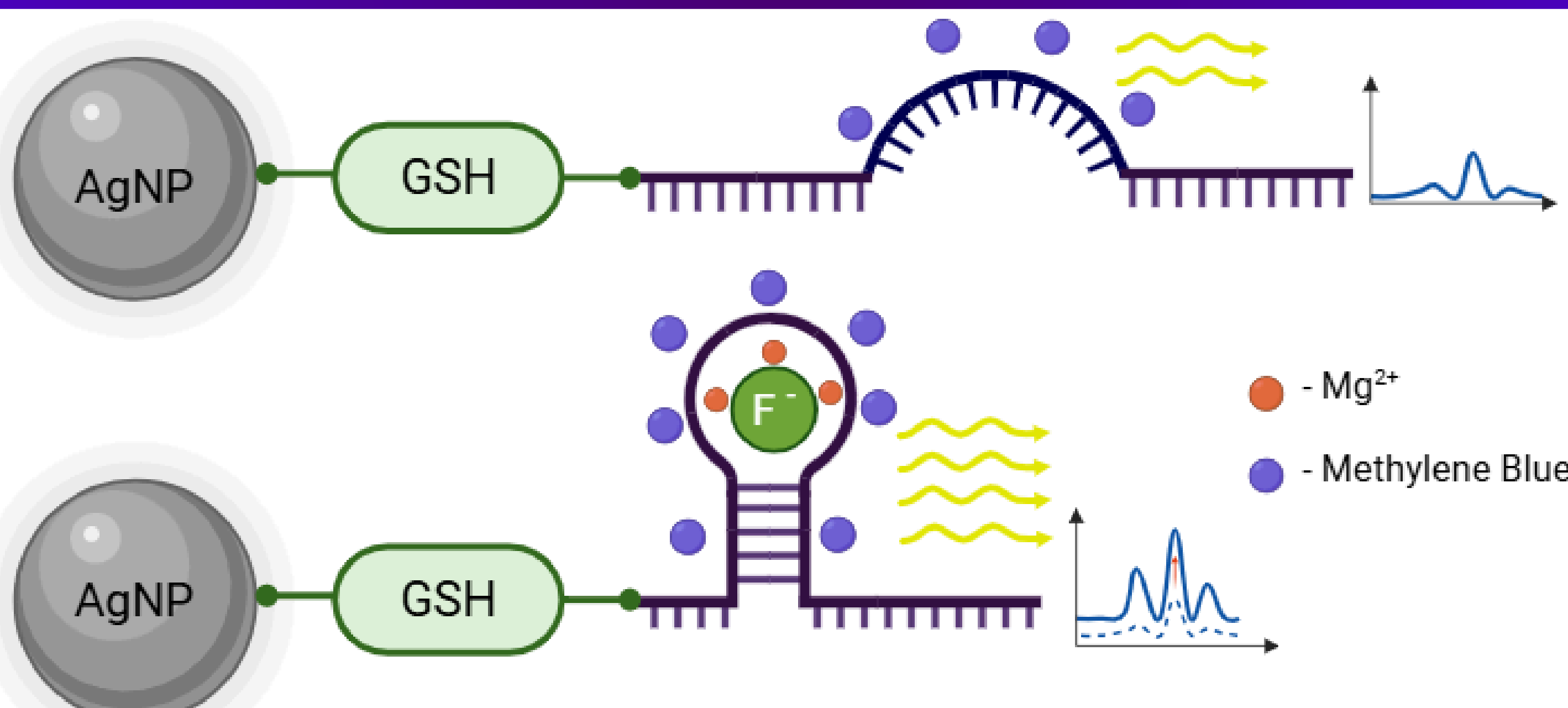
Main Objective

Development of a simple and sensitive method for trace-level fluoride detection for healthcare, industrial, and environmental applications.

Methodology for Sensor Development



Operating Mechanism of the SERS-Based Sensor



Optimizing the EDC, NHS Concentrations

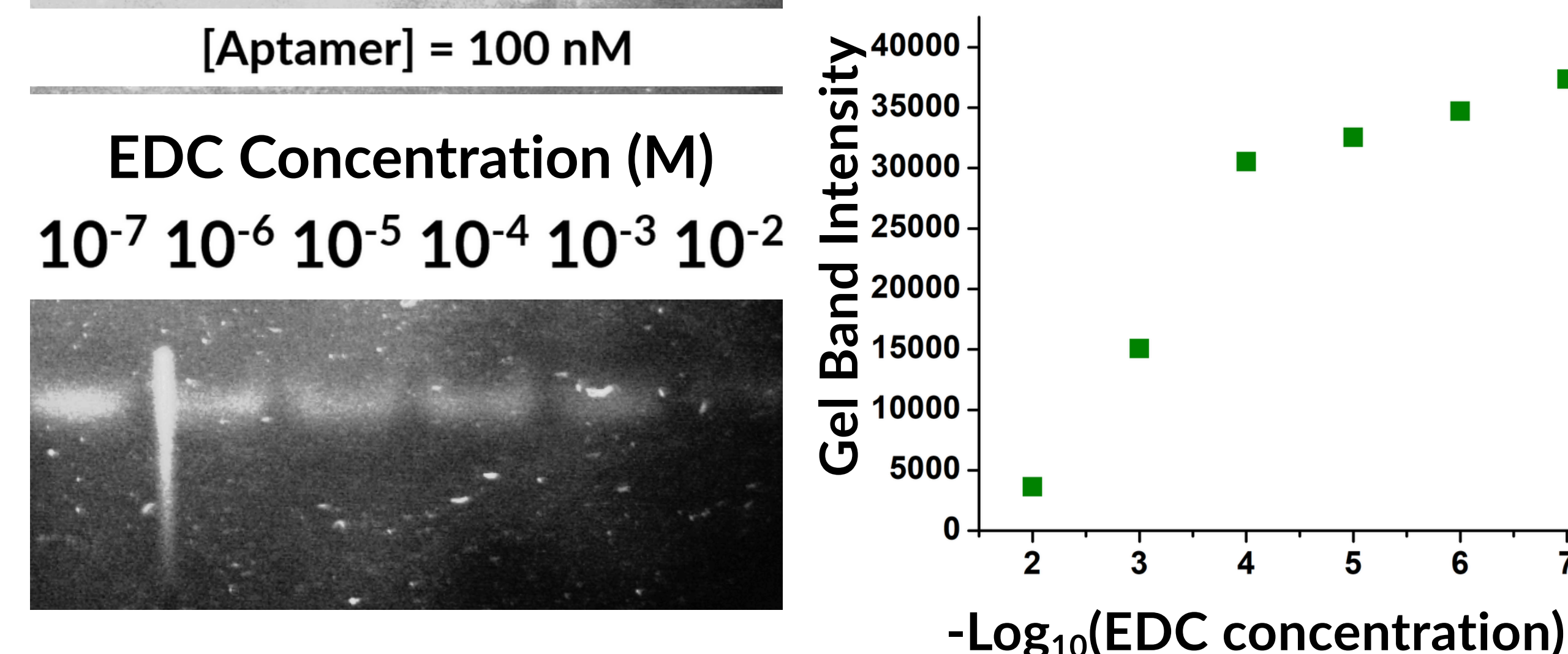


Figure 3: Increasing the EDC/NHS concentrations decreases unbound aptamer levels. (with [NHS] = 2 × [EDC]).

Optimizing the Aptamer Concentration

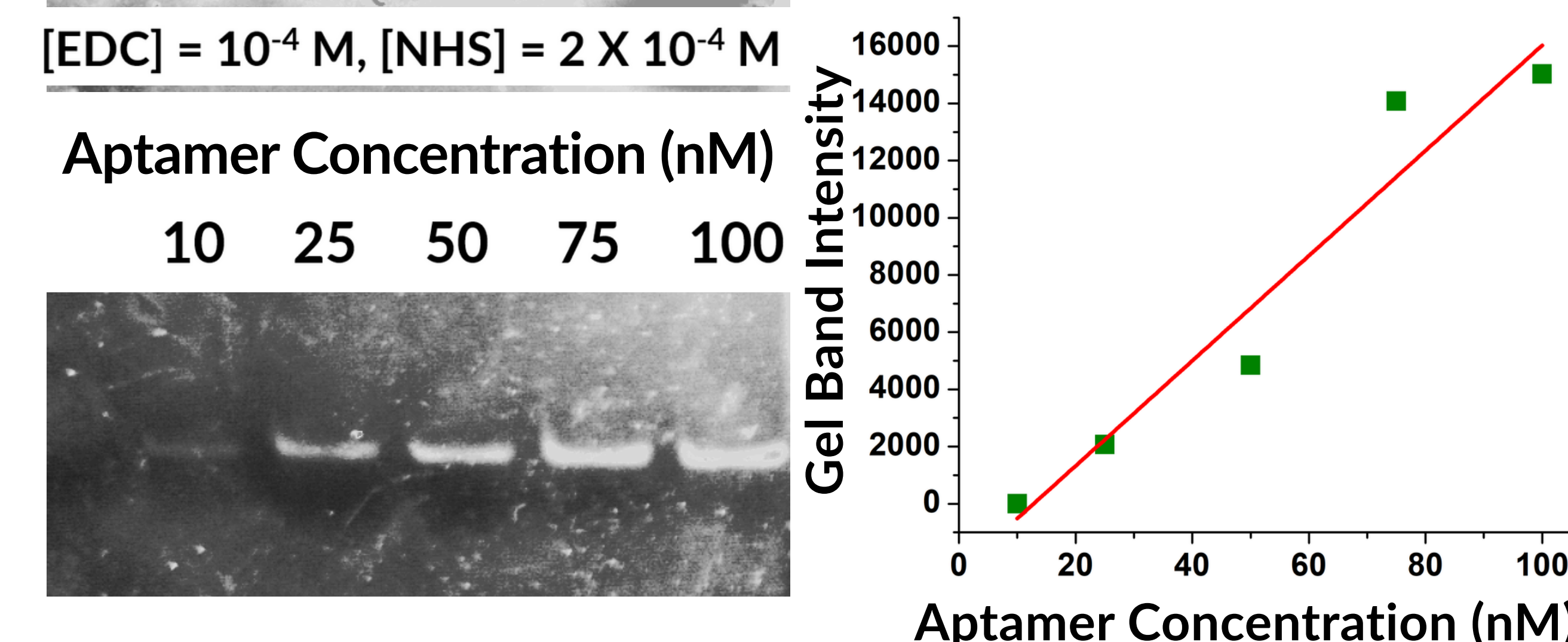


Figure 4: Increasing the aptamer concentration increases the unbound aptamer levels.

SERS Assay

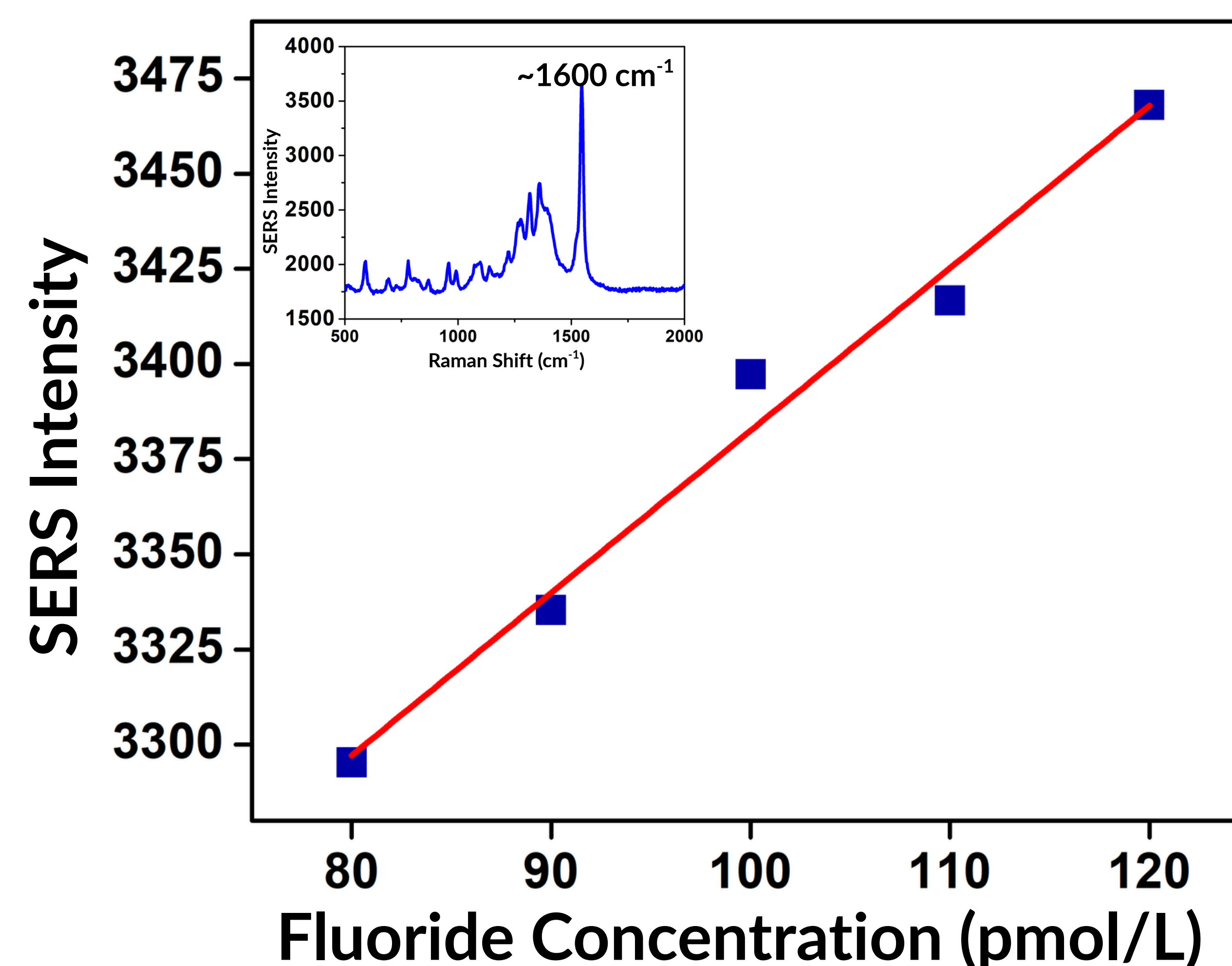


Figure 5: Linear relationship between average SERS intensity of the ~1600 cm⁻¹ MB peak and fluoride concentration, enabling quantitative detection.

Computational Study

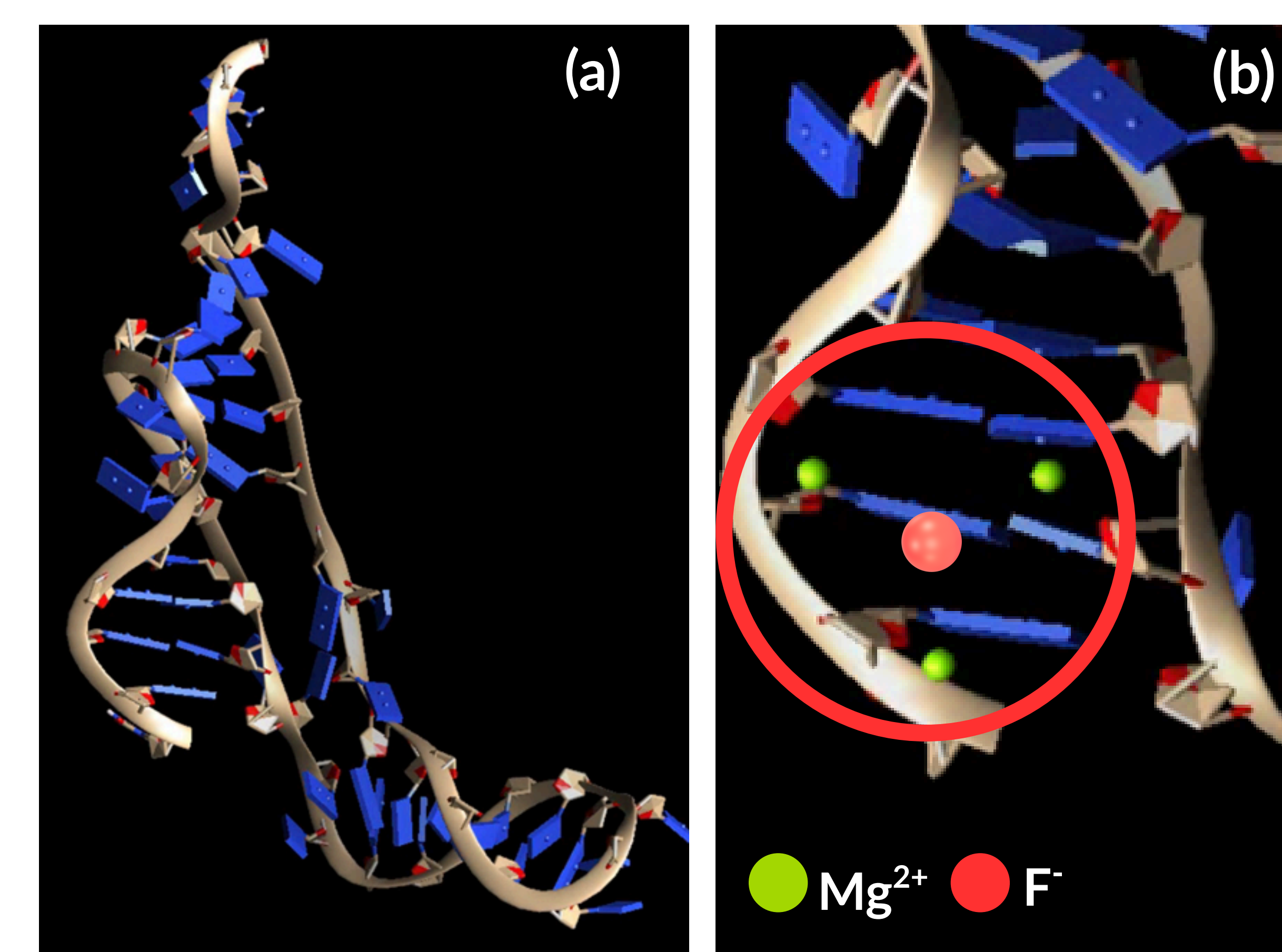
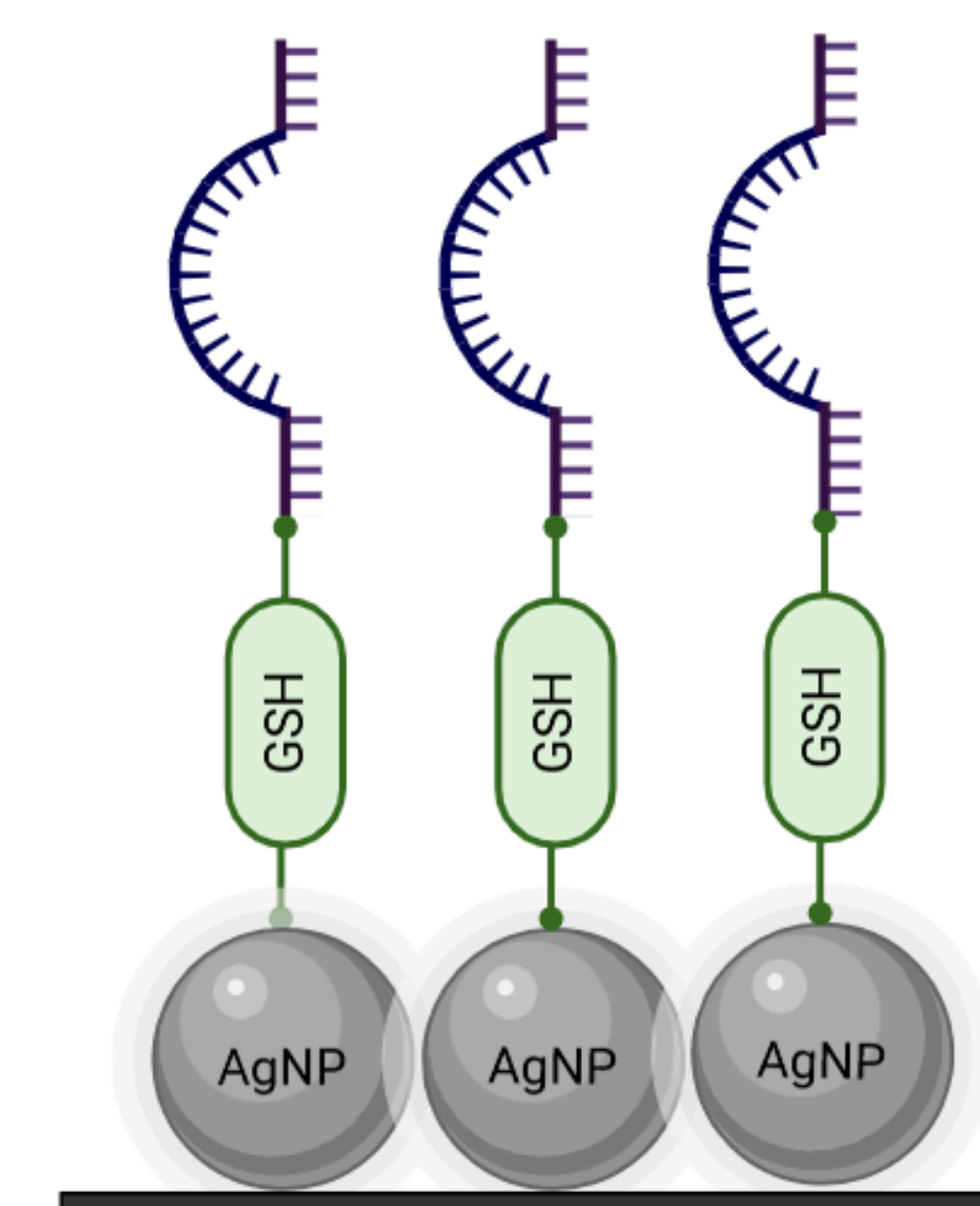


Figure 6: (a) Stabilized aptamer structure after AlphaFold3 prediction followed by MD simulation. (b) Predicted fluoride binding pocket by GNINA. (Affinity = -4.67 kcal/mol)

Conclusion

- The biosensor exhibited a linear correlation between the SERS intensity of the ~1600 cm⁻¹ methylene blue peak and fluoride concentrations ranging from 80 to 120 pM, demonstrating its potential as a facile and reliable platform for detecting trace levels of fluoride.
- Computational analyses further revealed a plausible binding pocket within the DNA aptamer, indicating comparable behavior to its RNA- fluoride riboswitch analogue.

Future Work



References

- Ren, A.; Rajashankar, K. R.; Patel, D. J. Fluoride ion encapsulation by Mg²⁺ ions and phosphates in a fluoride riboswitch. *Nature*, 2012, 486, 85–89. DOI: 10.1038/nature11152.
- Husser, C.; Vuilleumier, S.; Ryckelynck, M. FluorMango, an RNA-Based Fluorogenic Biosensor for the Direct and Specific Detection of Fluoride. *Small* 2022, 18, 2205232. DOI: 10.1002/smll.202205232.
- Bartczak, D. and Kanaras, A. G., Preparation of Peptide-Functionalized Gold Nanoparticles Using One Pot EDC/Sulfo-NHS Coupling, *Langmuir*, 2011, 27, 491–500, DOI: 10.1021/la2022177.