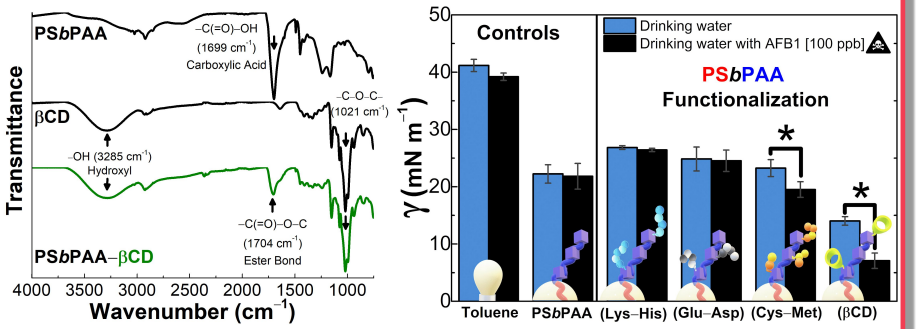
Design and Characterization of Smart Polymers for Rapid Sensing of Aflatoxin B1

Research Question

- **Which natural molecules**—from amino acids to a short−chain carbohydrate—can efficiently **form receptors capable of entrapping Aflatoxin B1** in aqueous environments?

Characterization and Functionalization



Methodology

- We leveraged infrared spectroscopy to observe overlapping peaks in transmittance and identify **successful synthesis of our new sensing system**:
  A polymer functionalized with natural host molecules.

- After characterization, Interfacial Tension Analysis (γ) revealed **PS*b*PAA-(Cys-Met)** and **PS*b*PAA-βCD** best entrapped Aflatoxin B1.

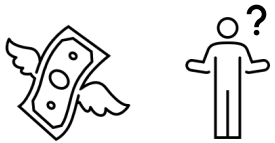
Conclusion

- We found that host molecules **with specialized sulfur groups or hydrophobic cavities best sensed Aflatoxin B1** in both groundwater and drinking water, demonstrating the potential advantage of hydrophobic sites for entrapping carcinogenic contaminants.

Introduction

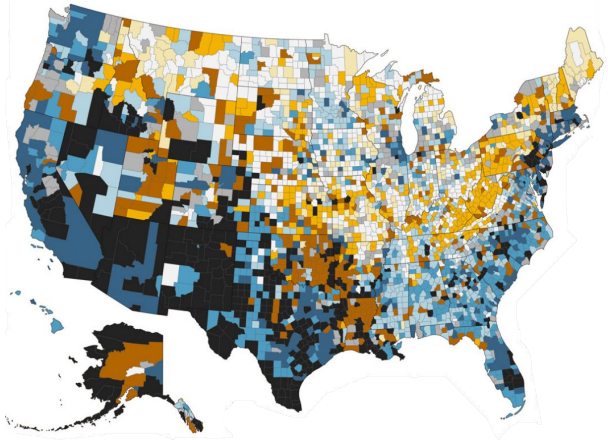
- Water contamination and pollution are major concerns on the global spectrum, **affecting both agricultural and drinking water**

- The demand for **water contaminant receptors is high**, yet modern approaches are extremely expensive and complex



- In past studies, polymeric structures have been presented as possible means for constructing detectors, **by modifying a base copolymer with various functional groups to retrieve distinctive analyte interactions**

All drinking water violations and health-based drinking water violations



Unequal access to safe drinking water!

Research Question

- Our study works to use cost effective methods to combine affordable molecules with the base molecule:

  Poly(styrene)-*block*-poly(acrylic acid)

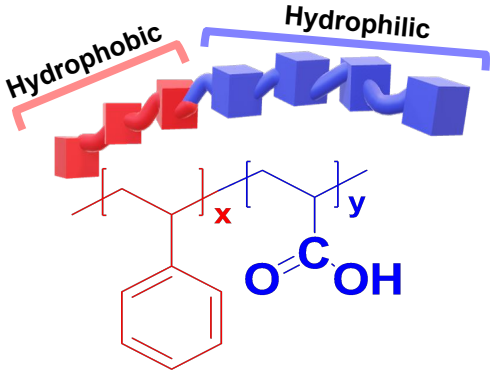
- **PS*b*PAA** is an amphiphilic polymer that contains a hydrophobic and hydrophilic end, allowing for many various reactions with **host molecules!**

Our main question is:

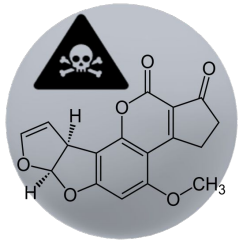
- **Which natural host molecules** can efficiently **form PS*b*PAA receptors capable of entrapping Aflatoxin B1** in aqueous environments?

Control Polymer

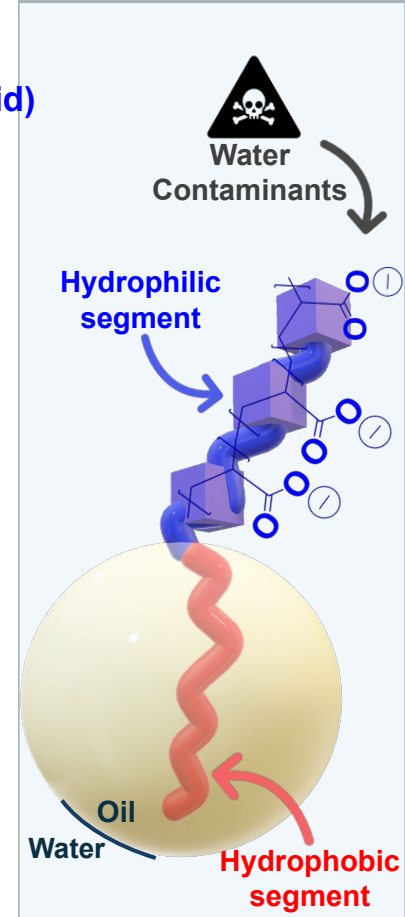
Poly(styrene)−*block*−poly(acrylic acid)



Aflatoxin B1



Unregulated water biohazard, a toxin made by fungi *(Aspergillus)*



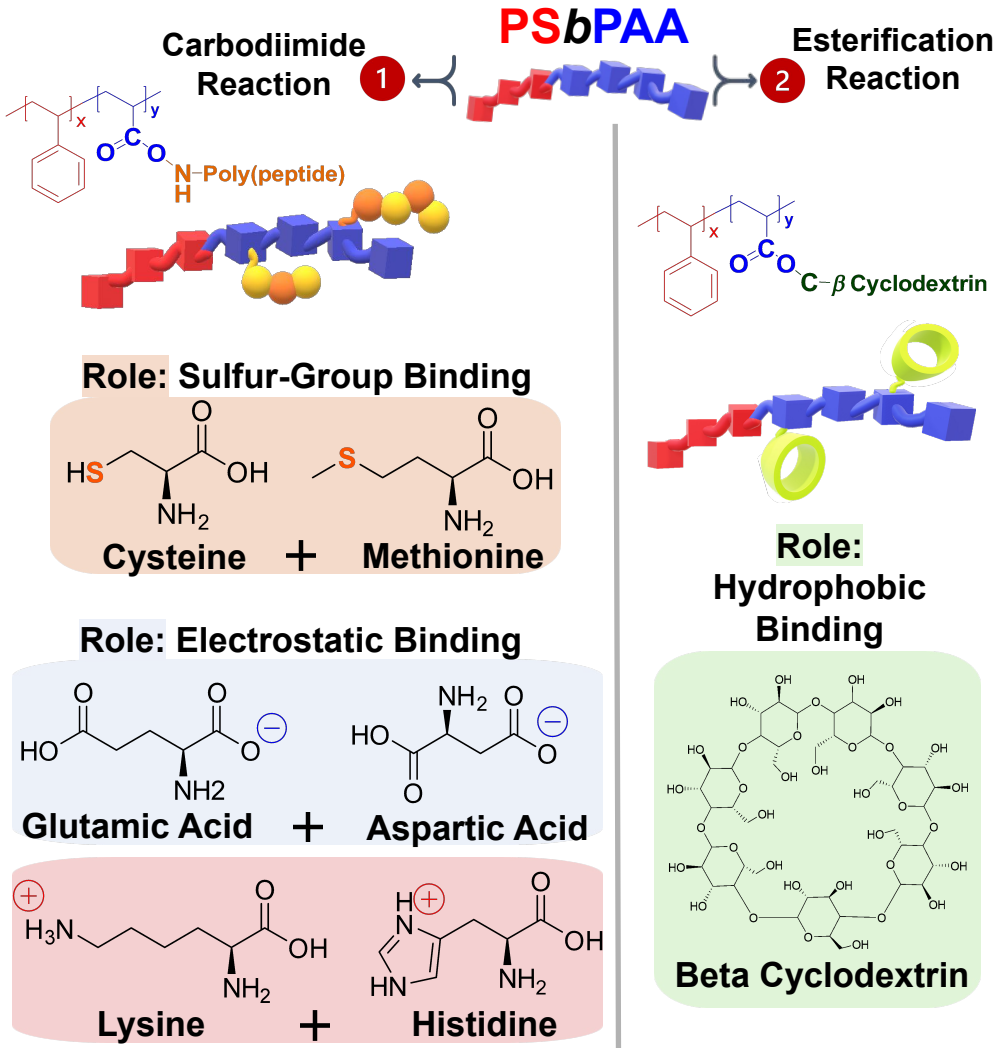
Methodology: Part 1

1. Synthesis of Functionalized Polymers

- Carbodiimide (1) and Esterification (2) reactions were used to synthesize **new sensing systems** potentially capable of **forming Host-Guest complexes with Aflatoxin B1** through electrostatic, hydrophobic, and possible sulfur-group interaction

- The Carbodiimide reactions attached 3 dipeptides to the base molecule (**PS*b*PAA**) via interactions between **amines (–NH_2)** and **carboxylates (–COO^-)**

- The Esterification reaction attached 1 carbohydrate (βCD) via interactions between **hydroxyl (–OH)** and **carboxylate (–COO^-)** groups



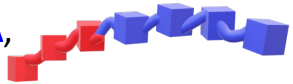
Methodology: Part 2

2. Primary Characterization Technique

- Next, the products of the reactions were characterized using **Fourier–Transform Infrared (FTIR) spectroscopy** to test for successful synthesis of receptors

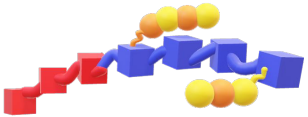
- We completed several evaluations to test:

PS*b*PAA,



each host molecule,

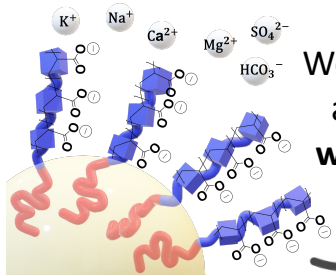
and **each receptor** (**PS*b*PAA +** host molecule) separately, each acting as a control for one another



Part 3

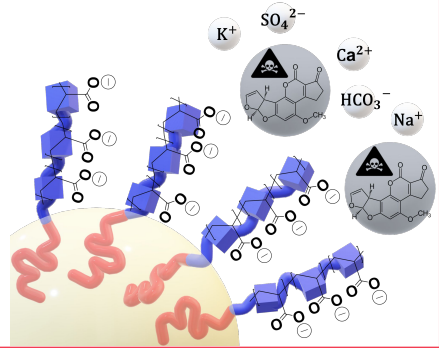
3. Sensing Technique for Detection of Aflatoxin B1

- **Interfacial Tension Analysis** was applied to observe how much the interfacial performance of the smart receptor was affected by the addition of Aflatoxin B1



We first tested the receptors in drinking water and synthetic groundwater **to ensure they weren't affected by salts** or any other water components before adding AFB1

- Next, a tiny dose of 100 parts per billion of the biohazard AFB1 was added



Results: Part 1

1. Characterization

- We can observe from the results of the **Infrared Spectroscopy** that the aligning in the peaks or frequencies display the successful synthesis of the receptors

- **New bands were observed**, while the consistency of certain frequencies shows how some functional groups of the controls have not been altered after receptor synthesis, further illustrating that **expected chemical bonds are present within the final product**

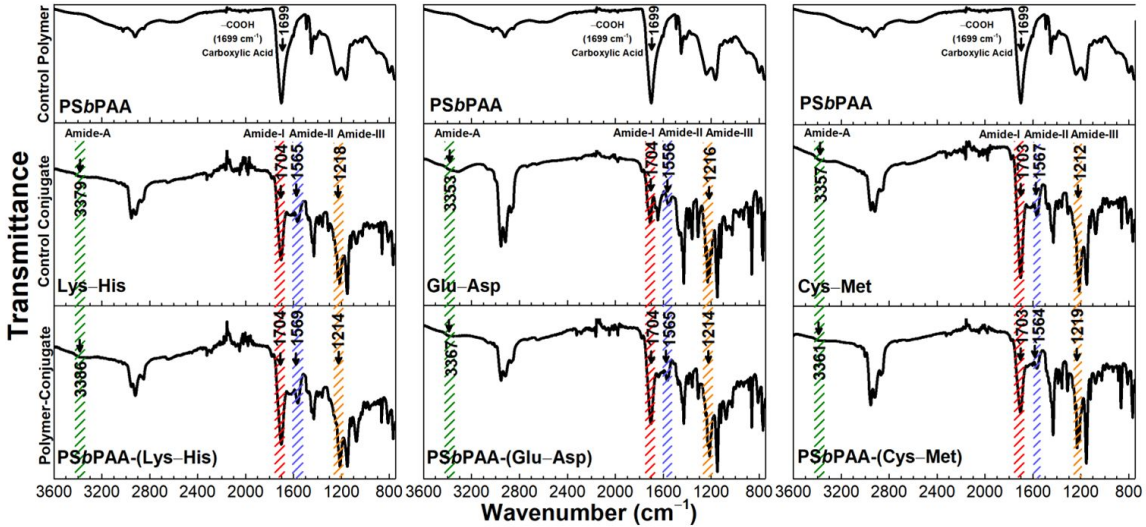


Figure 1: Infrared spectra used to identify amide bands in PS*b*PAA with amino acids

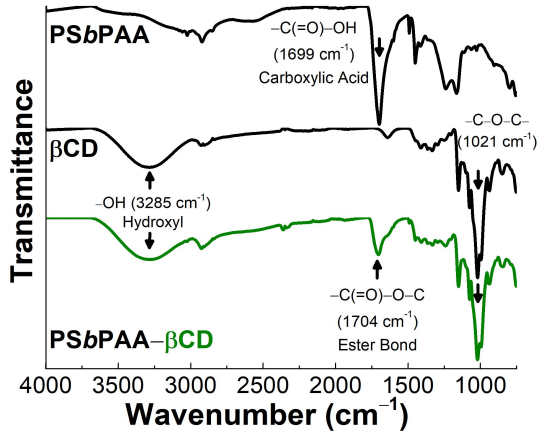


Figure 2: Infrared spectra used to identify ester bands in PS*b*PAA with carbohydrate βCD

Results: Part 2

2. Smart Functionalization

- All natural host molecules **(Lys-His), (Glu-Asp), (Cys-Met) and (BCD)** were incorporated in **PS*b*PAA** to provide **stability under harsh conditions**.

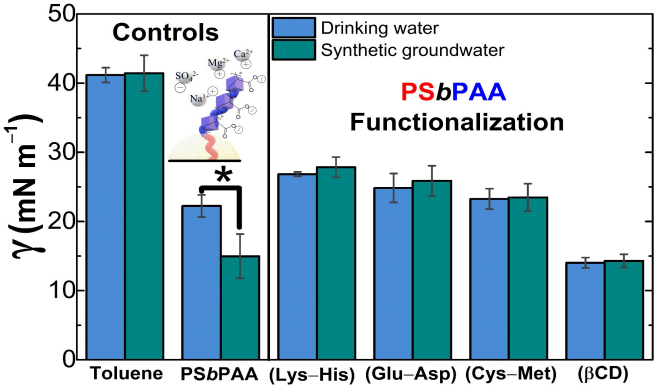


Figure 3 shows their **similar interfacial performance** in both drinking water and high-salinity groundwater, which confirmed their smart trend.

Part 3

3. Selective Sensing

- Next, we expected to see a change in interfacial tension **(γ)** with the addition of Aflatoxin B1, where greater interfacial change is caused by more sensitivity in the receptor

From **Figure 4**, we can observe a statistically significant change in the interfacial tension in **PS*b*PAA–(Cys–Met)** and **PS*b*PAA–βCD**

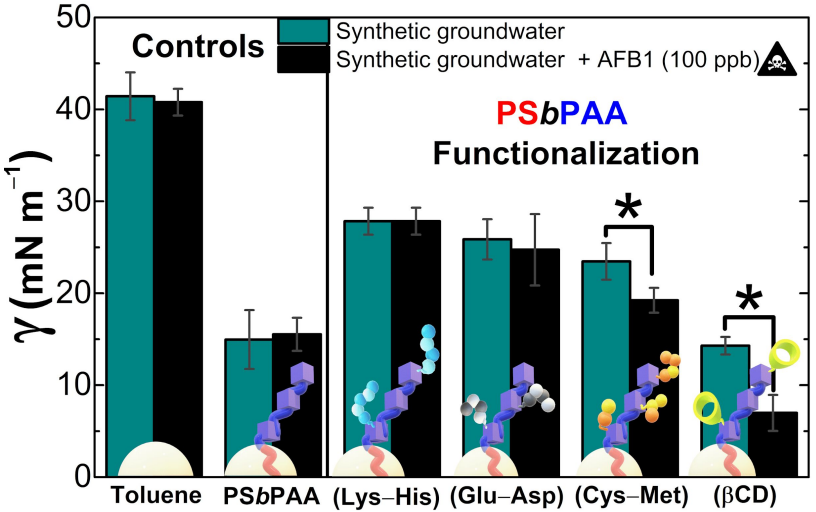


Figure 4: Two receptors selectivity detect AFB1.

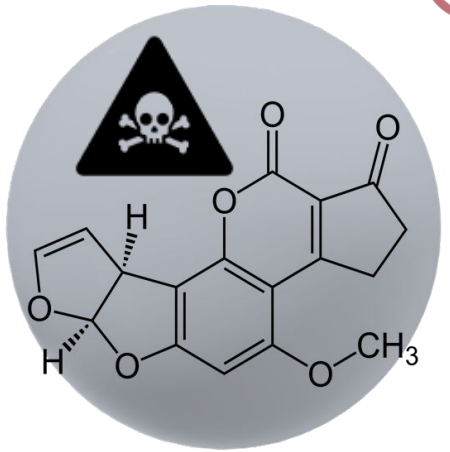
The same trend was found in drinking water!

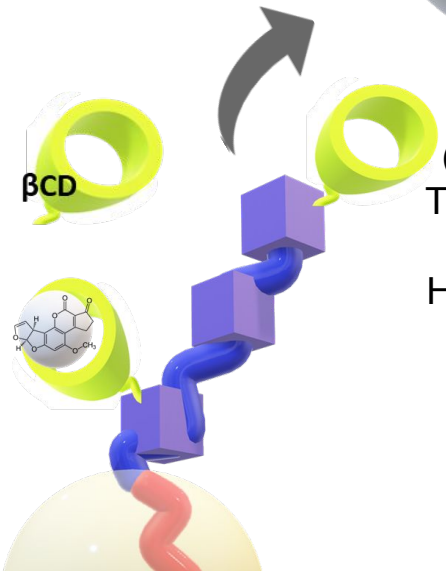
Discussion

- Our results revealed that the receptors performed very well in synthetic groundwater and drinking water, not interfering with any salts, proving their capability of acting as adequate complexes in practical applications

- We found that **(βCD)** and **(Cys-Met)** were the only molecules within the receptors that detected Aflatoxin B1, displaying the advantages of both hydrophobic interactions and interactions with specialized sulfur groups

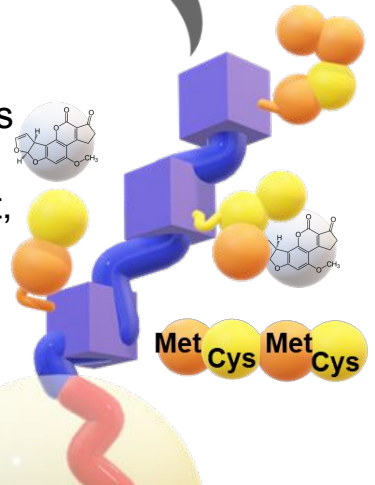
Aflatoxin B1





Conclusion

(95% confidence)
The interaction was dominated by:
Hydrophobic effect, followed by a possible thiol-π interaction

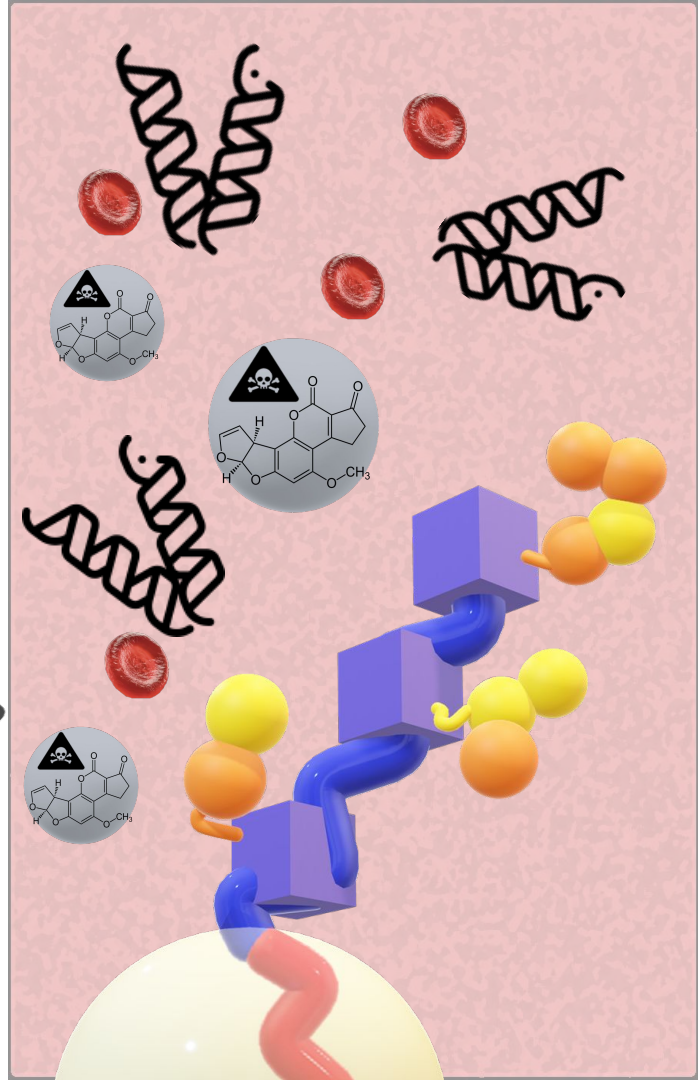


Next Steps

- Ultimately, our study presents the ability to construct economical water-contaminant detectors, addressing challenges regarding water pollution and access

- We can improve our study in future by evaluating **Interfacial Tension Analysis** in **Albumin,** a protein commonly found in human blood to mimic the detection of Aflatoxin B1 in human bloodstreams

- We can also **test more host molecules that present sulfur group interactions** to more accurately draw conclusions between the capability of detecting Aflatoxin B1 and the presence of specialized sulfur groups in available analytes



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