Biocompatible Strategies for polyvinyl chloride(PVC) Microplastic Adsorption in Human Brain: Exploring Polyphenol and Nitrile-Based Interactions with PVC

Aldiyar Balgabay

Under the direction of

Dr. Haiyan Fan
Research Superviser
Nazarbayev University, Department of Chemistry

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Abstract

Widespread use of plastic has led to the problem where tiny plastic particles (¡5mm), called microplastics (MPs), are now found even in the human body. It was discovered that the highest concentration of MPs is in the human brain. Among the most common types of plastic are polyethylene (75%), polypropylene (13%), and polyvinyl chloride (7%). However, polyethylene and polypropylene are both chemically inert and therefore less toxic. In contrast, PVC contains chloride groups, which makes it more dangerous for the human organism. There are several known methods to interact with PVC, such as using reactive oxides like SiO_2 or TiO_2 through degradation mechanisms, magnetic forces, adsorption via activated carbon or biochar, or plasmonic catalysis with metal nanoparticles. However, none of these methods are inherently safe for the biological environment of the brain without special modifications. After analyzing literature, it was found that organic compounds containing aromatic rings, hydroxyl, carbonyl, and amino groups can effectively react with PVC nanoparticles. Therefore, it was assumed that polyphenol nanoparticles synthesized from black tea using ethylenediamine (EDA) could be a potential solution for brain microplastic pollution. To find the optimal tea-to-EDA ratio for nanoparticle synthesis, tea was mixed with EDA in three different proportions: 1g tea: 4 ml of EDA, 1: 6, and 1: 8. Fluorescence spectroscopy showed that the 1:6 ratio gave the best results. FTIR analysis was used to confirm the presence of functional groups. All key groups were detected, except the carbonyl group. Another finding was that polyphenols most likely interact with EDA via hydrogen bonding. This same mechanism may potentially be used in PVC–polyphenol interaction. This research is still in progress, and further investigation is required to prove the existence of interaction between PVC and tea-based polyphenol nanoparticles.

1 Introduction

Plastic pollution became a noticeable issue back in the mid-20th century, when the mass production of polymers sharply increased[14]. However, it is only in recent years that more attention has been paid to microplastics—tiny fragments(from 1 nm to 5 mm) that form when larger plastic items break down.[9, 13] The amount of microplastics (MPs) in the environment is rapidly increasing, both in the air and in water. Recent studies have shown that microplastics are now being detected inside the human body, especially in the kidneys, lungs, and even the brain.[9, 13]

There are three main ways MPs can enter the body: through food, through the olfactory bulb (via inhalation), and through the skin's pores[1, 6]. To quantify the amount of micro- and nanoplastics (MNPs) in human brain tissue, a team of researchers from the University of New Mexico examined the brains of deceased individuals. Their findings revealed that, on average, the brain contains 75% more MPs than the other listed organs. Since the majority of this brain plastic consisted of polyethylene (PE, around 75%) and polypropylene (PP, 13%), and polyvinyl chloride (PVC, around 7%).[13]

However, it was found that polyeathylene is the least toxic MP in this list[12]. On the other hand, PVC is chemically active, due to its chloride groups, and probably can cause huge neurotoxic effects on the human body.[15] Studies on *Clarias gariepinus* have demonstrated that PVC microparticles reduce the activity of key antioxidant enzymes in the brain, such as SOD, CAT, and GPx, increase lipid peroxidation, and disrupt acetylcholinesterase function, which is a critical enzyme in neurotransmission.[8] These findings indicate a high neurotoxic potential of PVC, making it a priority target for further investigation regarding the potential impact of microplastics on the human brain.

Although this area of research is still in its early stages and reliable data remains limited, the initial findings already point to serious potential risks. For instance, the same New Mexico study reported that individuals suffering from dementia had 4–5 times more micro- and nanoplastic (MNP) particles in their brains compared to those with no signs of neurodegenerative disease.[13] Moreover, it was found that MP accumulation significantly increased neuroinflammation, microtubule disruption, and neuronal cell death after global cerebral ischemia.[10]

One of the hardest parts of this project is that interacting with nanoplastics (NPs) in biological systems is very challenging, especially since most existing methods for reducing microplastics (MPs) involve reactive oxides like SiO_2 or TiO_2 through degradation mechanisms, magnetic forces (such as magnetite Fe_3O_4), adsorption using activated carbon or biochar, or plasmonic catalysis with metal nanoparticles.[5, 16] However, none of these methods can be directly used in the brain without serious modifications due to toxicity

and harsh conditions.

Adsorption, for instance, doesn't always require activated carbon or biochar.[16] For example, Azo Dye Reactive Yellow 2 (RY2) has been used to interact with PVC.[17] It's not ideal for the brain because of its toxicity and the conditions required for the interaction to occur. But it still serves as a good example to understand which functional groups are effective for adsorbing PVC. RY2 contains multiple azo groups, aromatic rings, and sulfonate groups.

Similarly, Jia Li's research showed that PVC microplastics can adsorb antibiotics such as sulfadiazine (SDZ), amoxicillin (AMX), tetracycline (TC), ciprofloxacin (CIP), and trimethoprim (TMP). They tested five types of MPs (PE, PVC, PP, polyamide (PA), and polystyrene (PS)) to investigate how different MPs interact with these pollutants.[11] According to their data, PVC showed relatively strong interaction with CIP, which contains aromatic rings, nitrogen atoms, carbonyl, and hydroxyl groups.

Another study by Fang Wang and her team[16] focused on identifying how different organic compounds and mechanisms can attract MPs. For PVC specifically, the mechanisms involved include electrostatic interaction, hydrophobic interaction, surface complexation, pore filling, and various noncovalent bonds. Many of the effective molecules, such as pyrines, phenanthrenes, tylosin, and bisphenol A, contain aromatic rings and multiple oxygen atoms.

From another perspective, perfluorooctanesulfonamide might be a good match for brain-like environments in terms of interaction ability, but the high fluorine content could be too toxic for use in neural tissues.

In addition to these approaches, some studies suggest that acetonitrile may interact with halogen-containing molecules through a σ-hole mechanism,[4] where the electron pair from the nitrile group donates into the electrophilic region of the halogen atom. This opens up the possibility of identifying an organic-based solution capable of creating electrostatic or noncovalent interactions strong enough to bind with PVC—while remaining safe for the brain and not causing neurotoxicity.[16]

Based on this information, it is thought that polyphenols nanoparticles[7] extracted from black tea (usind ethyldiamine as a formemr of nanoparticles[3, 18]), due to their rich content of aromatic rings and hydroxyl groups, are capable of interacting effectively with PVC microparticles through π–π stacking, hydrogen bonding, and potential donor–acceptor interactions with chlorine σ-holes. Therefore, polyphenol-based nanoparticles synthesized from black tea components may serve as biocompatible sorbents for the capture or deactivation of PVC microplastics in biological systems or environmental media.

2 Methodology

2.1 Synthesis of tea-based nanoparticles

To synthesize polyphenol-based nanoparticles, we used black tea as a natural polyphenol source. We took 0.5 grams of black tea and mixed it with ethylenediamine (EDA), which acts as a nitrogen-rich cross-linking agent that helps nanoparticle formation and improves fluorescence.

To find the best ratio to create nanoparticles, three mixtures with different tea-to-EDA ratios were created:

- 1:4 (0.5g tea : 2 mL EDA),
- 1:6 (0.5g tea : 3 mL EDA),
- 1:8 (0.5g tea : 4 mL EDA).

Each mixture was filled with distilled water up to 40 mL total volume. The mixtures were sealed in heat-resistant capsules to prevent evaporation and were heated at 200°C for 6 hours in a laboratory muffle furnace. This thermal process supports carbonization and formation of fluorescent nanoparticles.

2.2 Fluariscent spectroscopy

After cooling, the solutions became concentrated. 0.5 mL of each sample was transferred to small transparent 1.5 mL capsules, discilated water was added until full and subjected to a visual dilution test under UV illumination from below. After each try the concentration of solution was halfed by removing 0.75mL of solution and fillingit with water. Rhis ws done multipule times until the emission wasn't xilible throughout the entire solution. This method relies on the principle that fluorescent nanoparticles tend to aggregate in concentrated solutions, leading to quenching effects and uneven light distribution. When UV light was applied from the bottom, samples that were overly concentrated displayed fluorescence limited to the bottom layer, indicating insufficient dispersion of nanoparticles. In contrast, evenly dispersed fluorescence throughout the sample indicated an optimal dilution level, where nanoparticles were adequately dispersed and aggregation was minimized, ensuring more reliable optical analysis in subsequent tests.

To investigate the distribution of tea-derived polyphenol nanoparticles in each mixture, fluorescence spectroscopy was performed at two excitation wavelengths, 350 nm and 400 nm. This dual-wavelength approach was used to capture the distinct photophysical responses of nanoparticles of varying size and aggregation states, as well as their potential interactions with ethylenediamine. The comparative fluorescence intensity enabled us to

identify the dominant nanoparticle population and its optimal excitation conditions.

2.3 Solid-state FTIR analysis

To enable solid-state infrared analysis, the concentrated mixtures were poured into three separate glass dishes and left to evaporate at room temperature for 72 hours. This slow evaporation process facilitated the formation of dry films containing polyphenol-based nanoparticles. Once fully dried, these residues were collected and prepared for Fourier-transform infrared (FTIR) spectroscopy.

FTIR spectroscopy was chosen to identify the key functional groups within the synthesized nanoparticles, particularly those responsible for their chemical reactivity and potential binding interactions with polymeric materials such as polyvinyl chloride (PVC). The analysis focused on detecting characteristic vibrational bands associated with hydroxyl (O–H), carbonyl (C=O), amine (N–H), and aromatic (C=C) groups.

Spectra were collected in the range of 4000–500 $cm^{-}1$, with a resolution of 2 $cm^{-}1$ and averaging 32 scans per sample. Comparative interpretation of the spectra across the three tea-to-EDA ratios allowed us to assess the influence of synthesis conditions on the chemical composition of the nanoparticles. Stronger or sharper peaks in regions corresponding to O–H, C=O, and aromatic vibrations were interpreted as indicators of more abundant surface functionality, which may enhance the nanoparticles' ability to form intermolecular interactions with plastic surfaces, such as hydrogen bonding or π–π interactions with polymer chains.

2.4 Future analysis

The diluted samples in capsules will be analyzed using UV-based methods, potentially to measure emission properties or quantum yield. The exact method will be clarified later.

3 Results and Discussion

3.1 Visual Observations After Synthesis

After making three mixtures, each of 40 mL of their solution, they were heated in the laboratory muffle furnace. After 6 hours of heating in the muffel furnace, the solutions turned dark brown and emitted a sharp, unpleasant odor reminiscent of ammonia. This suggests the occurrence of a chemical reaction, likely involving the interaction between ethylenediamine (EDA) and the polyphenolic compounds in tea. The changes in color and smell indicate that the synthesis of nanoparticles likely occurred.

3.2 Preliminary Fluorescence Testing

To assess the fluorescent properties of the synthesized nanoparticles and determine their suitability for further analysis, 0.5 mL of the concentrated solution was transferred into 1.5 mL capsuls and diluted with distilled water. Due to their size-dependent optical properties, nanoparticles can exhibit quantum confinement effects, allowing them to emit fluorescence upon interaction with UV light. This makes UV testing a useful preliminary method for evaluating both the presence and behavior of the particles under excitation.

In more concentrated solutions, the fluorescence was barely visible and mostly located at the bottom of the capsul. This is likely due to *self-quenching*, a phenomenon where high concentrations of nanoparticles and surrounding molecules absorb each other's photon[2]. After sequential dilution and thorough mixing, each time replacing 750 µL with water, the fluorescence gradually became more pronounced. By the fourth dilution, the emission was visible throughout the entire solution, indicating a more favorable concentration for fluorescence studies.

3.3 Fluorescence Spectroscopy Results

Fluorescence spectroscopy was then conducted using two excitation wavelengths — 350 nm and 400 nm — for three samples: undiluted, moderately diluted, and highly diluted solutions.

Under 350 nm excitation, the diluted solution from capsul 2 displayed the highest emission peak around 500 nm, corresponding to a yellow-brown fluorescence. This observation aligns with visual inspection and suggests a high population of well-dispersed, small-sized nanoparticles.

In contrast, under 400 nm excitation, the undiluted sample from capsul 2 and 3 exhibited the highest peak. This may indicate the presence of larger or more aggregated particles that respond more efficiently to longer-wavelength excitation.

This dual behavior highlights the heterogeneous nature of the nanoparticle population. Dilution likely reduces aggregation, allowing smaller, more efficient emitters to dominate the fluorescence profile at shorter excitation wavelengths. Overall, capsul 2 appears to contain the optimal balance of concentration and dispersion for efficient nanoparticle fluorescence, making it the most suitable candidate for further applications.

3.4 FTIR Spectroscopy Analysis

The FTIR spectra of different samples showed little variation, suggesting that the primary chemical structure remains similar across all conditions. However, characteristic

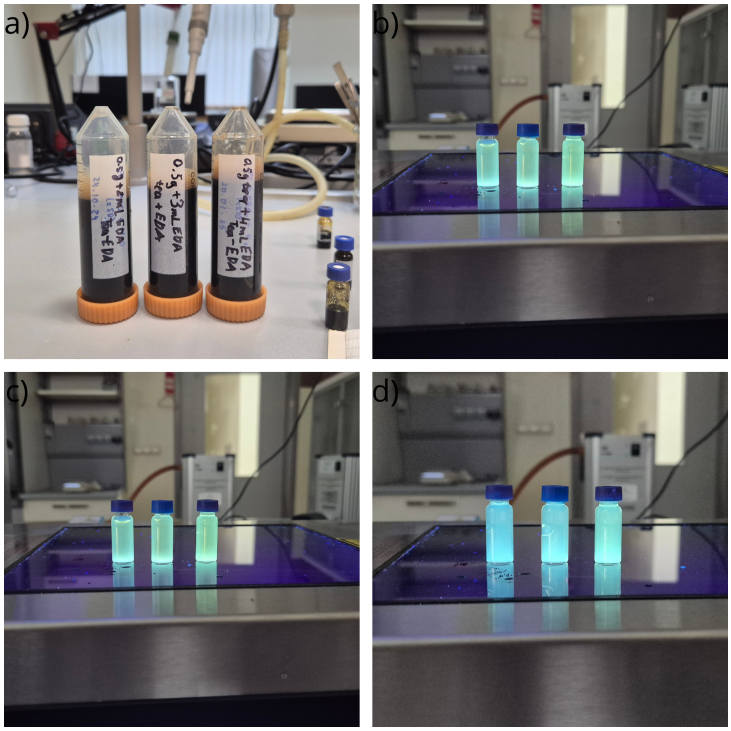


Figure 1: a) Solutions after muffel furnace, b) First try under UV light, c) second try under UV light, d) fourth try under UV light

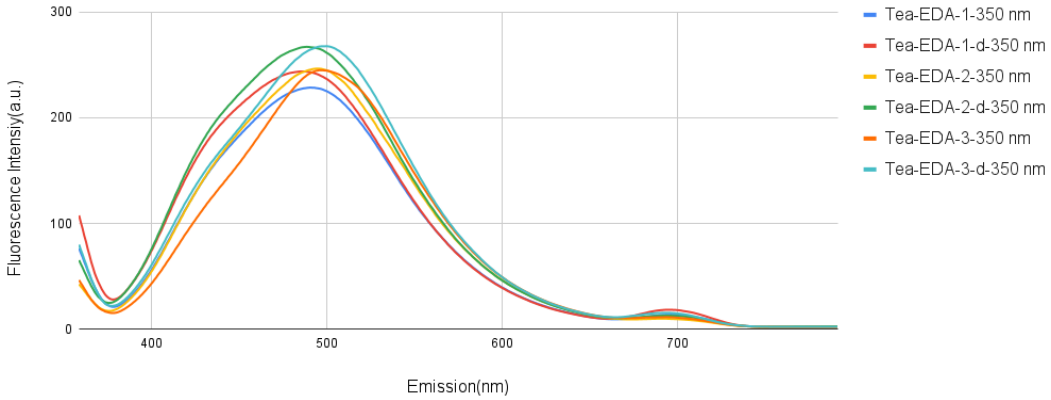


Figure 2: Fluorescent Spectroscopy at 350 nm

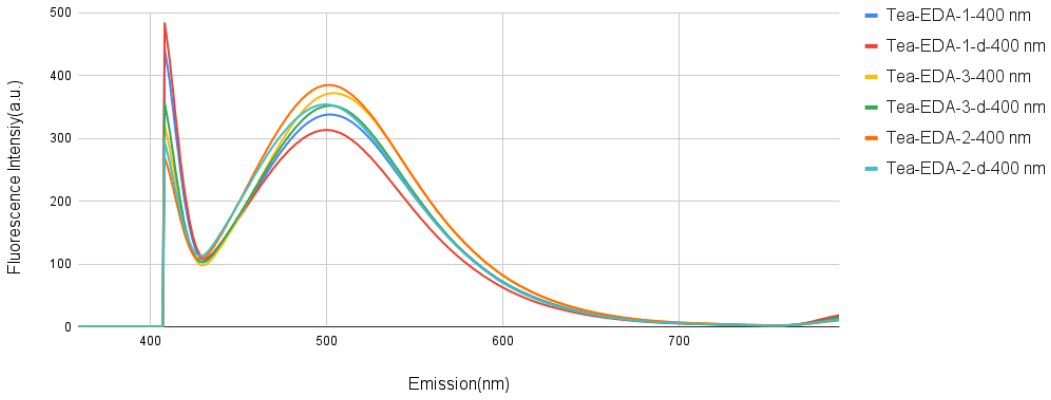


Figure 3: Fluorescent Spectroscopy at 400 nm

peaks corresponding to N–H and O–H likely originating from the polyphenol structures and ethylenediamine, respectively stretching vibrations were observed in the 3000–3400 cm^{-1} region creatind wide peak. A strong absorption band at approximately 3340 cm^{-1} demonstrates stroong intermolecular hydrogen bonding between N-H and O-H due to the shift from 3300-3500 cm^{-1} for amines and 3200-3600 cm^{-1} for hydroxy groups to 3000-3400 cm^{-1} region.

In addition, a distinct peak at 2930 cm^{-1} is attributed to the asymmetric stretching of C–H bonds in methylene and methyl groups. This confirms the presence of aliphatic hydrocarbon chains, which are typical components of both polyphenolic structures and ethylenediamine-modified systems. The combination of these signals confirms the successful synthesis of functionalized polyphenol nanoparticles with hydrophilic and hydrophobic characteristics, supporting their potential interaction with hydrophobic pollutants such as PVC micro- and nanoparticles.

Finally, paek at 1310 cm^{-1} must be C-N straching or O-H bending, along with a prominent C=C stretching from aromatic rings band near 1480 cm^{-1}, and N-H bending at 1560 cm^{-1}. These features support the presence of polyphenolic structures and the potential incorporation of EDA.[2] However, there wasn't fonund any peak at around 1700 cm^{-1} that could be related to C=O group. This can lower owr chances to effectively interract with MNPs.

But, still, the retention of these peaks suggests that EDA did not break down the polyphenolic framework but likely formed hydrogen bonds or other non-covalent interactions. This may have contributed to stabilization of the nanoparticle surfaces, enhancing their water solubility and potential biocompatibility.

4 Conclusion

The aim of this project was to synthesize polyphenol-based nanoparticles from tea extract that could potentially interact with micro- and nanoplastics, specifically polyvinyl chloride (PVC) fragments. Based on the experimental results, it can be concluded that the synthesis of polyphenol nanoparticles using ethylenediamine (EDA) as a stabilizing and reacting agent is indeed feasible. The visual changes, fluorescence emission, and FTIR analysis all support the successful formation of polyphenol-based nanoparticles.

Among all tested conditions, the most optimal synthesis ratio was found to be 1 gram of tea to 6 mL of EDA. This ratio produced the most stable and highly fluorescent nanoparticles, as confirmed by UV testing and fluorescence spectroscopy. The consistent emission profiles and FTIR signatures across dilutions further validate the reproducibility and chemical integrity of the synthesized nanoparticles.

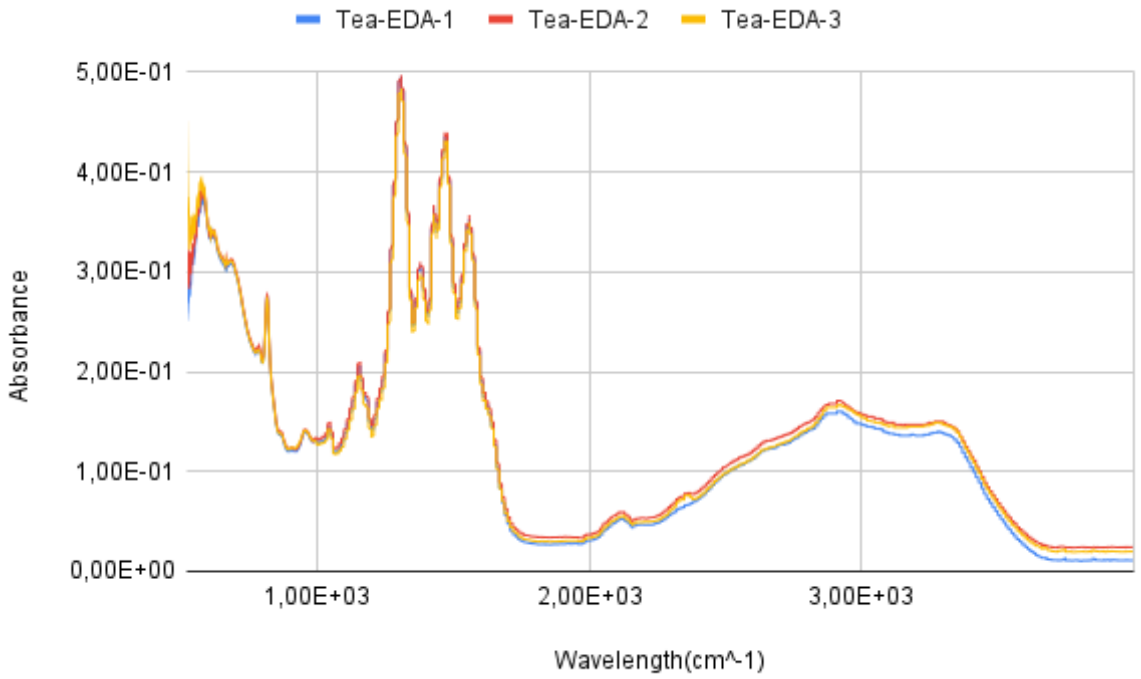


Figure 4: FTIR Spectroscopy

However, the interaction between the synthesized nanoparticles and PVC-based micro- and nanoplastics could not be confirmed within the scope of this study. Future work should focus on optimizing the interaction conditions, possibly through surface modification of nanoparticles, or by using more sensitive detection methods such as DLS (Dynamic Light Scattering), TEM (Transmission Electron Microscopy), or zeta potential analysis.

Overall, the project successfully demonstrates a green and accessible method for synthesizing functional nanoparticles from natural sources like tea, offering a promising direction for future applications in environmental cleanup and nanomaterial development.

5 Limitations and Future Plans

One of the key limitations of this project was the inability to experimentally test the interaction between polyphenol nanoparticles and polyvinyl chloride (PVC) micro-/nanoplastics. The primary reason for this was the lack of specialized equipment and facilities required for the synthesis or characterization of PVC micro-/nanoparticles. Additionally, the project did not receive sufficient funding to purchase commercially available PVC particles.

Despite this, based on data from existing literature, there is strong evidence to suggest that some form of interaction between polyphenol nanoparticles and PVC micro-/nanoplastics is likely. However, experimental confirmation remains necessary.

In future studies, once PVC micro-/nanoplastics are either synthesized or obtained, it will be possible to explore these interactions more rigorously. A promising direction involves in vivo testing: by pre-labeling PVC particles with a fluorescent or other biological marker and injecting them into the mice's organism, it would be possible to track their behavior in the blood vessels. Subsequently, the polyphenol nanoparticles could be delivered to the brain via the blood-brain barrier (BBB), allowing researchers to investigate not only the potential interaction between nanoparticles and PVC, but also the biosafety of polyphenols and the systemic toxicity of PVC-based plastics.

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