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Covalent functionalization of fullerene C_{60} with polyethyleneimine

Malena L. Boffadossi, Sofía C. Santamarina, Milena B. Boarini, Edgardo N. Durantini and María E. Milanesio

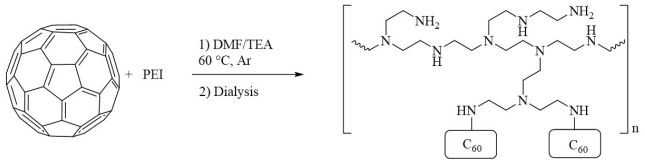
IDAS-CONICET, Departamento de Química, FCEFQyN, Universidad Nacional de Río Cuarto, Río Cuarto, Córdoba, Argentina.

INTRODUCTION & AIM

Several families of photosensitizers (PSs) have been evaluated for microbial inactivation [1,2]. These compounds are photostable, absorb visible light, and generate reactive oxygen species (ROS), but their poor solubility causes aggregation that limits photoactivity. Covalent functionalization, including polycationic fragments, enhances solubility, biological activity, and bacterial membrane interaction. The development of covalent functionalization strategies for C_{60} fullerene has enabled the incorporation of chemical groups capable of improving its biological activity [2]. The inclusion of polycationic fragments in the PS structure increases its ability to interact with bacterial membranes, enhancing microbial inactivation. Polyethylenimine (PEI) is a polycationic polymer with protonable amino groups that confer positive charges, enabling interaction with microbial membranes [3]. Based on this property, a new C_{60}-PEI conjugate was synthesized as a potential photodynamic agent.

RESULTS & DISCUSSION

Fullerene derivative functionalized with polyethyleneimine (C_{60}-PEI) was synthesized from the reaction between C_{60} fullerene and PEI using *N,N*-dimethylformamide (DMF) as solvent and in the presence of triethylamine (TEA) *(Scheme 1)*. The reaction mixture was kept under stirring at 60 °C and subsequently purified by dialysis in aqueous solution, yielding the C_{60}-PEI conjugate as the final product [3].



Scheme 1. *Synthesis of C_{60}-PEI*

Spectroscopic studies of C_{60}-PEI were carried out and compared with reference C_{60} fullerene using DMF and water as solvents *(Figure 1)*. The conjugate showed weaker absorption bands in the 300-800 nm range, which are characteristic of substituted C_{60} fullerenes *(Figure 1)* [1,3]. The absorption spectrum of C_{60}-PEI in water confirms the presence of PEI in the fullerene structure.

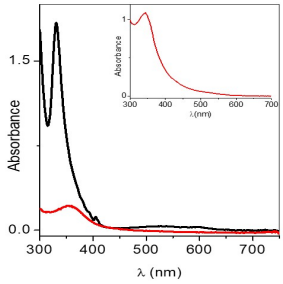


Figure 1. *Absorption spectra of C_{60}-PEI (red solid line) and C_{60} (black solid line) in DMF. Inset: absorption spectra of C_{60}-PEI in water.*

The photodynamic properties of the fullerene derivative were evaluated in DMF and water using anthracene derivatives: 9,10-dimethylanthracene (DMA) and 2´-(anthracene-9,10-diyl)bis (methylmalonate) tetrasodium salt (ABMM) [3]. From the observed rate constants (k_{obs}), singlet oxygen quantum yields (Φ_Δ) for C_{60}-PEI were determined, yielding values of 0.15 in DMF and 0.70 in water *(Figure 2)*. The high Φ_Δ of the PS in water compared to the organic medium could indicate, in addition to considerable photodynamic activity, an association between the cationic PS and the anionic substrate ABMM. Nevertheless, these results demonstrate that the conjugate exhibits photodynamic activity in both organic and aqueous media, suggesting that the incorporation of the polymer improves the solubility of C_{60} fullerene in polar systems.

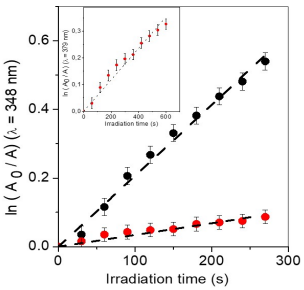


Figure 2. *First-order plots for the photooxidation of DMA photosensitized by C_{60} (●) and C_{60}-PEI (●) in DMF. Inset: First-order plots for the photooxidation of ABMM photosensitized by C_{60}-PEI (●) in water. λ_{irr} = 450-700 nm.*

CONCLUSION

A C_{60} fullerene derivative modified with a polymer precursor of positive charges was synthesized to be used as a potential photosensitizer for the photodynamic inactivation of microorganisms. Absorption spectroscopic studies indicated that the conjugate exhibits a characteristic spectrum of substituted fullerenes and that the presence of PEI allows the solubilization of fullerene in water. Likewise, photodynamic studies confirmed that C_{60}-PEI generates oxygen singlet ($O_2(^1\Delta_g)$) in both organic and aqueous media. Taken together, the results suggest that C_{60}-PEI possesses suitable properties for application as a photodynamic agent in microbial inactivation.

FUTURE WORK / REFERENCES

1. Heredia, D. A.,; Durantini, A. M.; Durantini, J. E.; Durantini, E. N. Fullerene C_{60} derivatives as antimicrobial photodynamic agents. *J. Photochem. Photobiol. C: Photochem. Rev.* **2022**, *51*, 100471.
2. Yin, R.; Wang, M.; Huang, Y.-Y; Landi, G.; Vecchio, D.; Chiang, L. Y; Hamblin, M. R. Antimicrobial photodynamic inactivation with decacationic functionalized fullerenes: oxygen-independent photokilling in presence of azide and new mechanistic insights. *Free Radic. Biol. Med.* 2015, *79*, 14.
3. Gsponer, N. S.; Baigorria, E.; Durantini, E. N.; Milanesio, M. E. Fullerene C_{60}-chitosan conjugate applied in the photoinactivation of Staphylococcus aureus. *Eur. Polym. J.* **2024**, *204*, 11678.