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RESEARCH

Photophysical characterization of tetrahydroxyphenyl porphyrin Zn(II) and V(IV) complexes: experimental and DFT study

Carlos Diaz-Uribe · Daily Rangel · William Vallejo · Roger Valle · Yoan Hidago-Rosa · Ximena Zarate · Eduardo Schott

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Abstract Photodynamic therapy (PDT) is a promising technique for the treatment of various diseases. In this sense, the singlet oxygen quantum yield (Φ_Δ) is a physical–chemical property that allows to stablish the applicability of a potential photosensitizers (PS) as a drug for PDT. In the herein report, the Φ_Δ of three photosensitizers was determined: metal-free tetrahydroxyphenyl porphyrin (THPP), THPP-Zn and the THPP-V metal complexes. Their biological application was also evaluated. Therefore, the in vitro study was carried out to assess their biological activity against *Escherichia coli*. The metal-porphyrin complexes exhibited highest activities against the bacterial strain *Escherichia coli*. at the highest concentration (175 µg/mL) and show better activity than the free base ligand (salts and blank solution). Results indicated a relation between Φ_Δ and the inhibitory activity against *Escherichia coli*, thus, whereas higher is the Φ_Δ, higher is the inhibitory activity. The values of the Φ_Δ and the inhibitory activity follows the tendency THPP-Zn > THPP > THPP-V. Furthermore, quantum chemical calculations allowed to gain deep insight into the electronic and optical properties of THPP-Zn macrocycle, which let to verify the most

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C. Diaz-Uribe (✉) · D. Rangel · W. Vallejo
Grupo de Investigación en Fotoquímica y Fotobiología. Programa de Química. Facultad de Ciencias Básicas, Universidad del Atlántico, 081007 Puerto Colombia, Colombia
e-mail: carlosdiaz@mail.uniatlantico.edu.co

R. Valle
Programa de Biología, Facultad de Ciencias Básicas, Universidad del Atlántico, 081007 Puerto Colombia, Colombia

Y. Hidago-Rosa · E. Schott (✉)
Departamento de Química Inorgánica, Facultad de Química y Farmacia, Centro de Energía UC, Centro de Investigación en Nanotecnología y Materiales Avanzados CIEN-UC, Pontificia, Universidad Católica de Chile, Avenida Vicuña Mackenna, 4860 Santiago, Chile
e-mail: maschotte@gmail.com

Y. Hidago-Rosa
Facultad de Ingeniería, Universidad Finis Terrae, Av. Pedro de Valdivia, 1509 Santiago, Providencia, Chile

X. Zarate (✉)
Facultad de Ingeniería, Instituto de Ciencias Químicas Aplicadas, Universidad Autónoma de Chile, Av. Pedro de Valdivia 425, Santiago, Chile
e-mail: ximena.zarate@uautonoma.cl

E. Schott
Millennium Nucleus in Catalytic Processes Towards Sustainable Chemistry (CSC), Santiago, Chile

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