

# Photodynamic effect of 5,10,15,20-tetrakis(4-carboxyphenyl)porphyrin and (Zn<sup>2+</sup> and Sn<sup>4+</sup>) derivatives against *Leishmania* spp in the promastigote stage: experimental and DFT study

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## Abstract

In this work, we synthesized the meso-(aryl) porphyrin derivative 5,10,15,20-tetrakis(4-carboxyphenyl)porphyrin (TCPP) and two meso-(aryl) metalloporphyrins, TCPP-Zn(II) and TCPP-Sn(IV), with reaction yields between 33.91 and 80.4%. The photophysical properties were determined, and the in vitro photodynamic properties were evaluated against *Leishmania* spp in the promastigote stage. The TCPP-Zn(II) reduced the viability of the parasites as shown by the lowest IC<sub>50</sub>, which is even lower than the reference drug glucantime. In general, our results indicate that the beneficial effect related to the lethal capacity of porphyrins was greater in the presence of light irradiation. Furthermore, the inclusion of a diamagnetic metal such as Zn(II) is essential for the biological properties shown by this type of compounds, as it substantially improves their photodynamic activity. The Jablonsky diagrams were proposed using DFT computations, where the decay channels through the ground and excited states were assessed and the feasible generation of singlet oxygen was established, being TCPP-Zn(II) the one that shows a slightly more exothermic process than TCPP-Sn(IV). © 2021, Institute of Chemistry, Slovak Academy of Sciences.

## Author keywords

DFT; *Leishmania* spp; Photodynamic therapy; Porphyrin; Promastigote; Singlet oxygen