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Rational design of porphyin and BODIPY analogues for biomedical applications: further progress and future perspectives

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Over the last two years, considerable further progress has been made in using a rational design approach [1,2] guided by calculations with the Gaussian 09 software package on the Lengau cluster and an application of Michl's perimeter model [3] to prepare novel main group element complexes of porphyrin and boron dipyrromethene (BODIPY) analogues that are suitable for use as photosensitizer dyes in photodynamic therapy against cancer and bacteria [4-8] and as optical limiters in applications relevant to the protection of human eyesight from intense incident laser beams [9-10]. There has been a strong focus on exploring how the lowest energy porphyrin absorption band can be substantially red-shifted into the phototherapeutic window by introducing reduced and confused pyrrole moieties [2,4-7]. Future directions on the use of the Gaussian 09 software package in the context of this research will be described.

References

[1] J. Mack, *Chem. Rev.* **2017**, *117*, 3444-3478.
[2] B. Babu, J. Mack, T. Nyokong, *Dalton Trans.* **2023**, *52*, 5000-5018.
[3] J. Michl, *Tetrahedron* **1984**, *40*, 3845-3934.
[4] R. C. Soy, B. Babu, J. Mack, T. Nyokong, *Molecules* **2023**, *28*, 4030.
[5] S. Dingiswayo, K. Burgess, B. Babu, J. Mack, T. Nyokong, *Photochem* **2023**, *3*, 313-326.
[6] R. C. Soy, B. Babu, J. Mack, T. Nyokong, *Photodiagn. Photodyn. Ther.* **2023**, *44*, 103815.
[7] A. K. May, B. P. Ngoy, J. Mack, T. Nyokong, *J. Porphyrins Phthalocyanines* **2024**, *28*, 88-96.
[8] R. C. Soy, D. Mafukidze, J. Mack, T. Nyokong, *Eur. J. Inorg. Chem.* **2024**, *27*, e202400072.
[9] A. K. May, J. Mack, T. Nyokong, *J. Porphyrins Phthalocyanines* **2023**, *27*, 591-599.
[10] G. Kubheka, J. Mack, T. Nyokong, *J. Porphyrins Phthalocyanines* **2024**, *28*, 61-71.

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