Centre for High Performance Computing 2020 National Conference



Contribution ID: 100 Type: Talk

Rational design of Sn(IV) porphyrins for photodynamic therapy: progress to date and future perspectives

Wednesday, 2 December 2020 14:30 (30 minutes)

In recent years, considerable progress has been made in using a rational design approach [1] guided by calculations with the Gaussian 09 software package on the Lengau cluster and an application of Michl's perimeter model [1,2] to prepare novel Sn(IV) complexes of porphyrin dyes and porphyrin analogues that are suitable for use as photosensitizer dyes in photodynamic therapy [3-9]. Axial ligation results in low levels of aggregation, while the Sn(IV) ion promotes intersystem crossing resulting in relatively high singlet oxygen quantum yields through a heavy atom effect. Relatively low IC50 values have been obtained during *in vitro* studies against MCF-7 breast cancer cells. 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] J. Michl, Tetrahedron 1984, 40, 3845-3934.
- [3] B. Babu, E. Amuhaya, D. Oluwole, E. Prinsloo, J. Mack and T. Nyokong, MedChemComm 2019, 10, 41-48.
- [4] R. C. Soy, B. Babu, D. O. Oluwole, N. Nwaji, J. Oyim, E. Amuhaya, E. Prinsloo, J. Mack and T. Nyokong, J. Porphyrins Phthalocyanines 2019, 23, 34-45.
- [5] B. Babu, E. Prinsloo, J. Mack, T. Nyokong, New J. Chem. 2019, 43, 18805-18812.
- [6] S. Dingiswayo, B. Babu, E. Prinsloo, J. Mack, T. Nyokong, J. Porphyrins Phthalocyanines 2020, 24, 1138-1145.
- [7] B. Babu, J. Mack, T. Nyokong, Dalton Trans. 2020, 49, 9568-9573.
- [8] B. Babu, E. Prinsloo, J. Mack, T. Nyokong, New J. Chem., 2020, 44, 11006-11012.
- [9] B. Babu, J. Mack, T. Nyokong, accepted in Dalton Trans. in 2020. doi: 10.1039/D0DT03296D

Student?

No

Supervisor name

Supervisor email

Primary author: Prof. MACK, John (Rhodes University)

Co-authors: Dr BALAJI, Babu (Rhodes University); Mr DINGISWAYO, Somila (Rhodes University); Ms SOY, Rodah (Rhodes University); Prof. BAPTISTA, Mauricio (University of São Paulo); Prof. TASSO, Thiago (Federal

University of Minas Gerais); Prof. NYOKONG, Tebello (Rhodes University)

Presenter: Prof. MACK, John (Rhodes University)Session Classification: HPC Applications

Track Classification: Computational Chemistry