# Centre for High Performance Computing 2020 National Conference



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

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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

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