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

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Over the last year, considerable further 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 [3-8]. 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 [3-9]. 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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