

# Poster Presentations

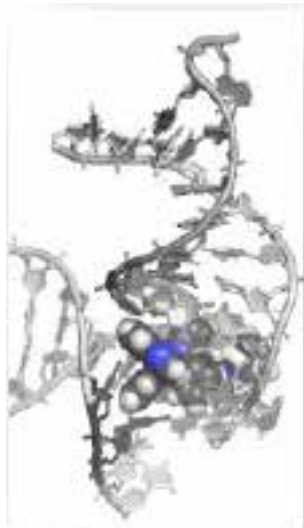
## [MS31-P01] Towards Biophotocrystallography with Photooxidisable Ruthenium Polypyridyl Complexes

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The earliest steps in DNA photodamage are of fundamental importance for an understanding of both the creation of potentially cancer-inducing DNA lesions and of damage repair by photodynamic therapy. It is well established that the DNA base guanine is the most susceptible of the four bases, and that –GG– is a more susceptible sequence than a single G, with 8-oxoguanine the best known oxidation product. The formation of 8oxoguanine leads to subsequent base

mismatching and copying errors.



We recently determined the static structure of the photooxidising complex  $[\text{Ru}(\text{TAP})_2\text{dppz}]^{2+}$  (1) (TAP = tetraazaphenanthrene; dppz = dipyridophenazine bound to the DNA duplex d(TCGGCGCCGA)<sub>2</sub> [1]. The structure showed

the dppz ligand intercalated at the terminal step, with one TAP ligand semi-intercalated at the GG step of an adjacent duplex. A kink of about 50° is introduced at the semi-intercalation step. The combination of these two interactions generates a crystal lattice which suggests great potential for a photocrystallographic study of the excited state. Ultrafast laser solution studies of **1** with

natural DNA or with d(CG)<sub>n</sub> polymer showed that electron transfer (possibly proton –coupled) occurs with a lifetime of 500 ps, yielding one-electron oxidised guanine [2]. Recent preliminary data on the observation of similar transients in the crystal lattice will be presented.

- [1] Hall, J. P.; O’Sullivan, K.; Naseer, A.; Smith, J.A.; Kelly, J.M.; Cardin, C.J. *Proc. Natl. Acad. Sci. USA*, **2011**, *108*, 1761–17614.  
[2] Elias, B.; Creely C.; Doorley G. W.; Feeney M. M.; Moucheron C.; Kirsch -De Mesmaeker A.; Dyer J.; Grills D. C.; George, M.W.; Matousek, P.; Parker, A. W.; Towrie, M.; Kelly, J.M. *Chemistry – Eur. J*, **2008**, *14*, 369-375.

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