

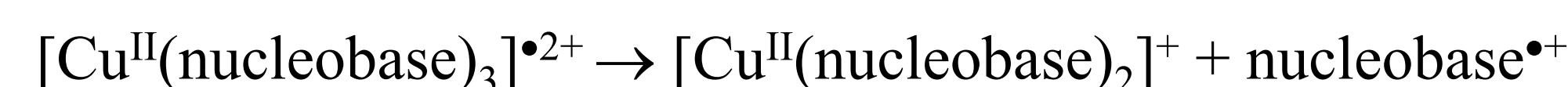
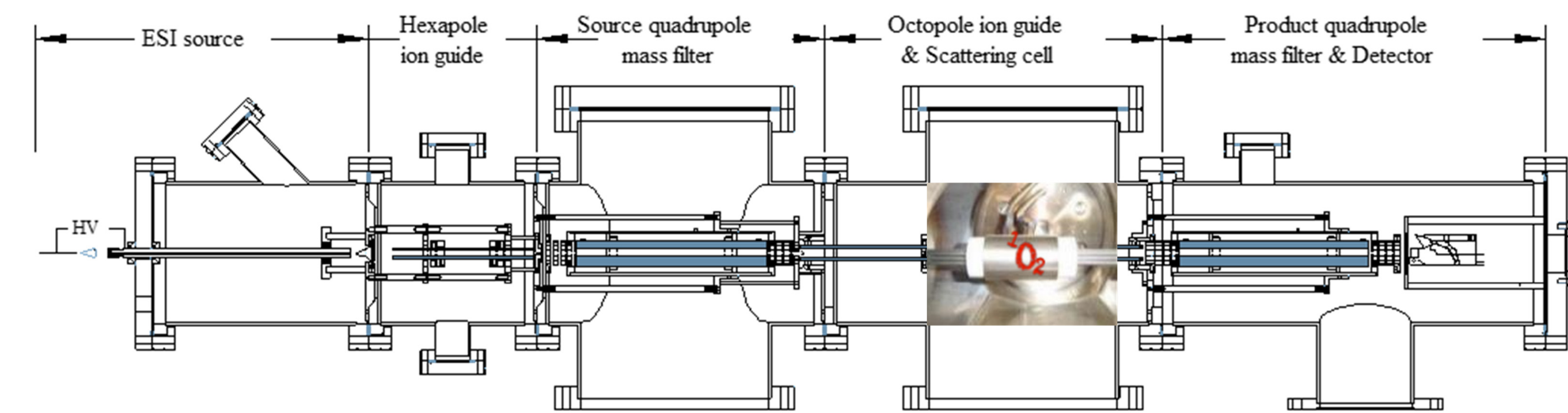
Introduction

Biological significance of oxidatively generated radical cations of guanosine, 8-Oxo-2'-deoxyguanosine, and their 9-methyl analogues by singlet oxygen.

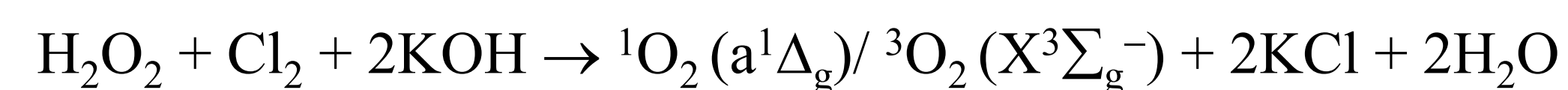
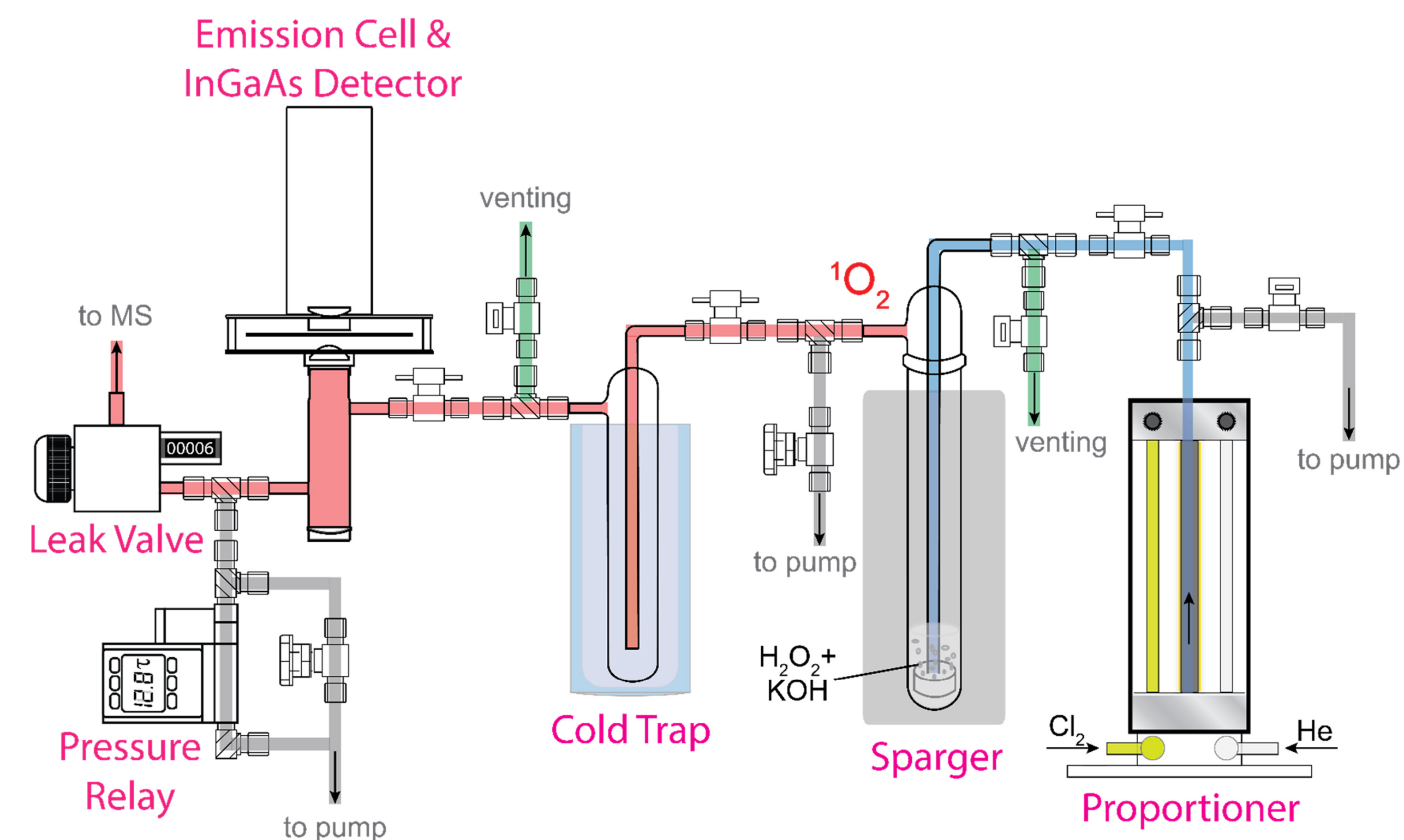
- Mutagenesis and carcinogenesis
- Apoptosis (cell death)
- Biomarker for oxidative stress within cells and tissues
- Singlet oxygen (¹O₂-based photodynamic therapy in cancer treatment)

Instrumentation

1. Guided-Ion-Beam Tandem Mass Spectrometer

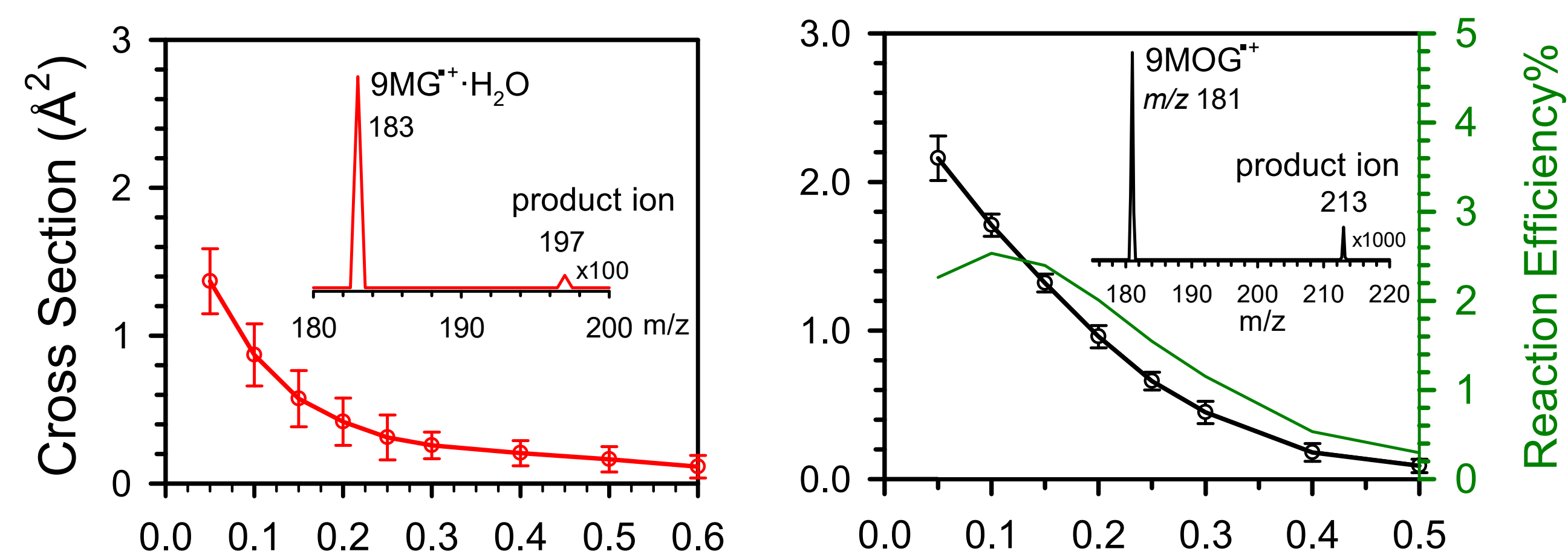


2. Near IR Emission Spectroscopy

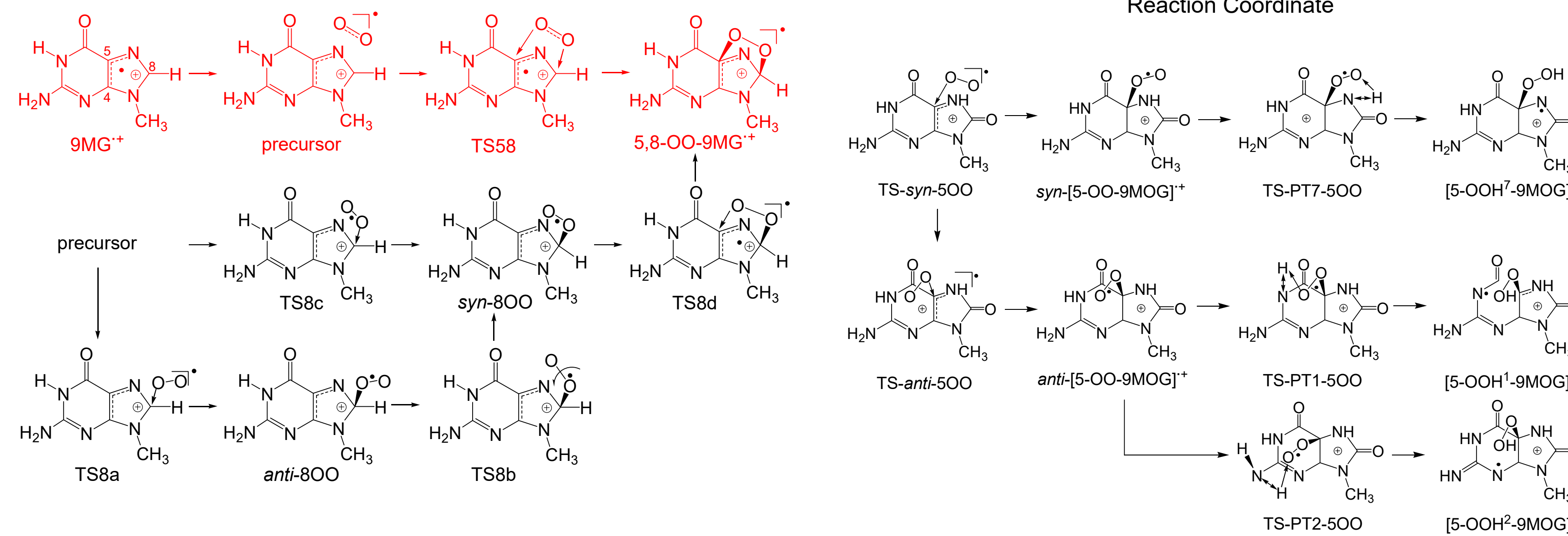
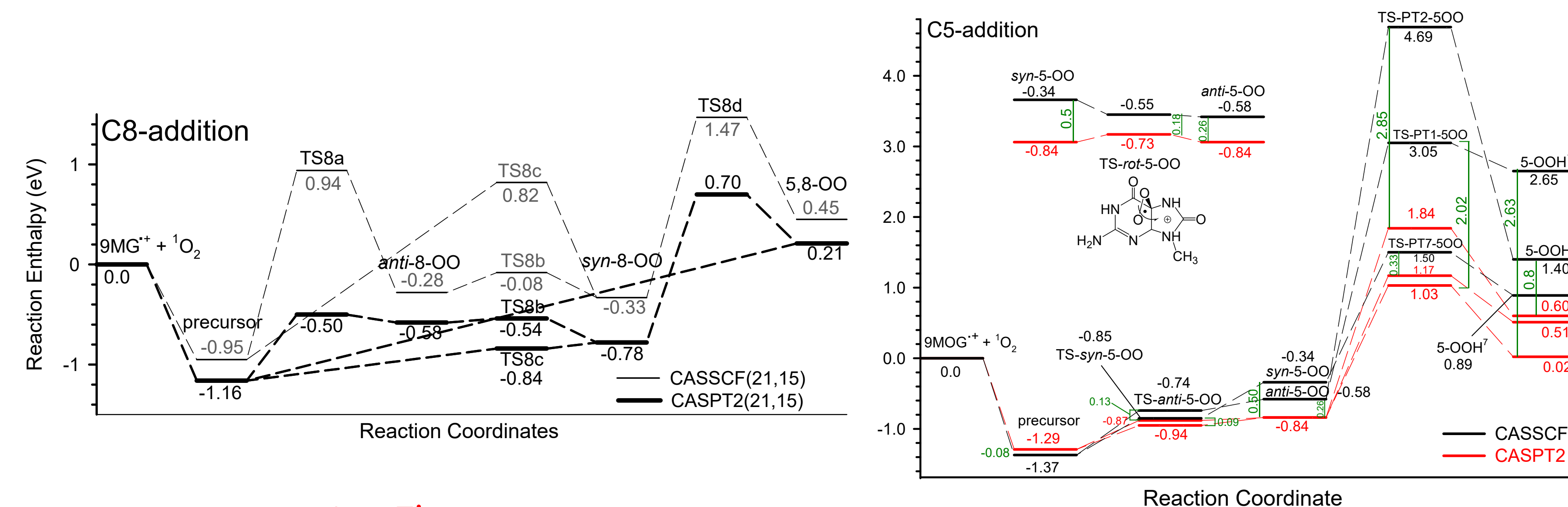


Results

1. Reaction Efficiency of ¹O₂ with 9MG^{•+} and 9MOG^{•+}



2. Reaction Potential Energy Surface of ¹O₂ with 9MOG^{•+} and 9MG^{•+}

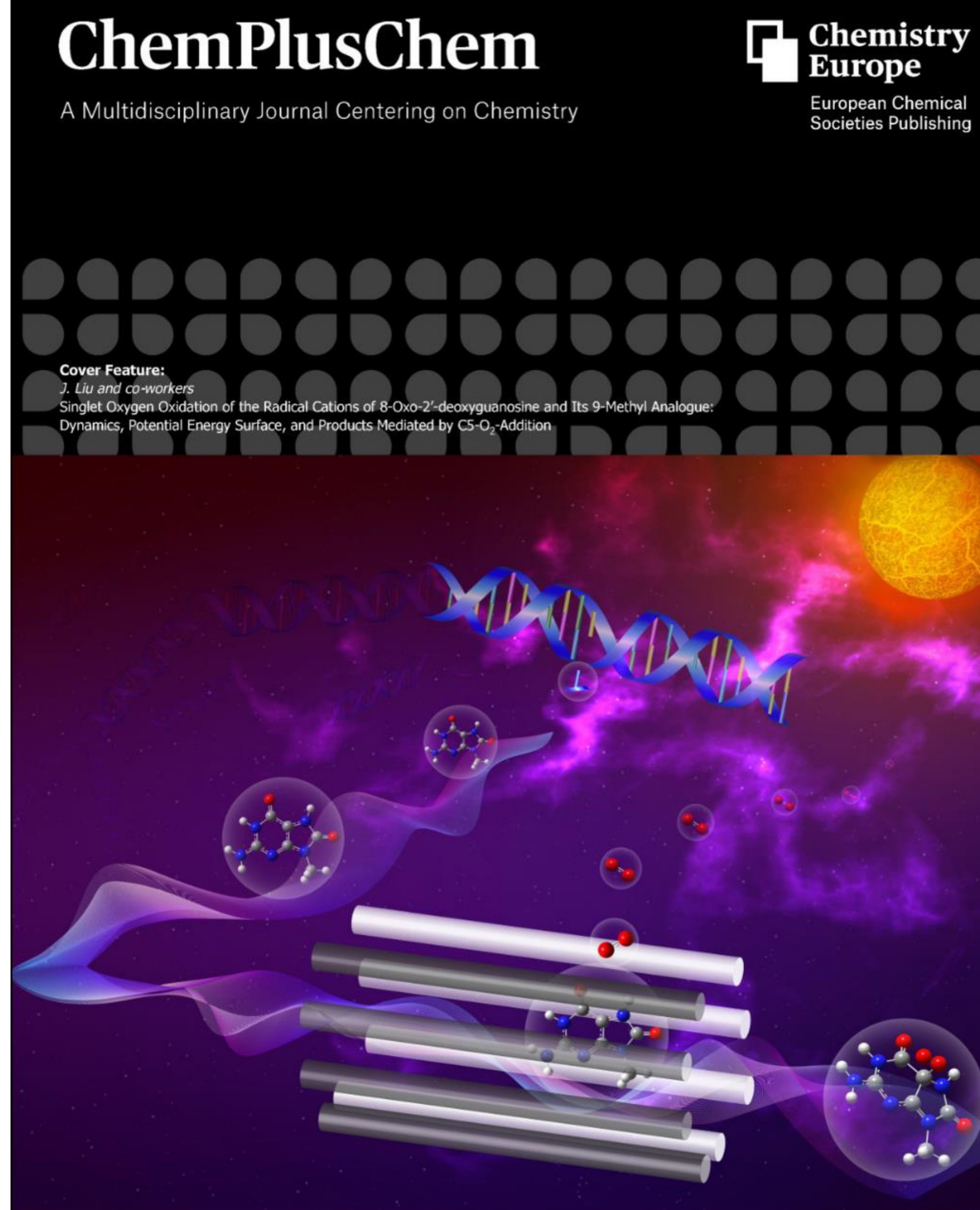


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Conclusions

- In the reaction systems of ¹O₂ with nucleobases, σ increases with decreasing E_{col} from which the reaction thermodynamics is exothermic.
- The reaction efficiency of ¹O₂ with radical cations of 8-oxoguanine nucleobase and nucleosides are twice higher than with radical cations of guanine nucleobases and nucleoside.
- The PES modeling confirmed that the most thermodynamically favorable oxidation product for the radical cations of 9MOG and 9MG are C5-O₂ and C8-O₂ respectively.



References

- Sun, Y.; Tsai, M.; Moe, M. M.; Liu, J. *J. Phys. Chem. A* **2021**, *125*, 1564-1576
- Moe, M. M.; Tsai, M.; Liu, J. *ChemPlusChem* **2021**, *86*, 1243-1254