

## Molecular dynamics insights for DNA lesions in oligonucleotides and nucleosomal DNA

The identification of complex oxidatively-generated DNA lesions involving not only a single-nucleobase but two proximal nucleotides has received much attention over the last years since such lesions are formed with a very low occurrence (typically a few lesions per  $10^9$  nucleotides) but turn out to be highly mutagenic. The structural elucidation of such complex lesions is extremely challenging.

We rely on classical all-atom MD simulations to probe the structures of oligonucleotides featuring a given lesion (abasic sites or intrastrand cross-links). We can monitor the B-helix distortion and the outcome of the initial Watson-Crick pairing: whereas NMR or X-ray structures are not available, our simulation provide a rationale for sequence-dependent repair efficiencies. Another application of all-atom molecular dynamics aspect is the exploration of DNA-photosensitizers interactions.

I will also present our recent efforts towards all-atom simulations of nucleosomal harbouring DNA lesions.

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