Damaged DNA Structures Determination by Means of Molecular Dynamics

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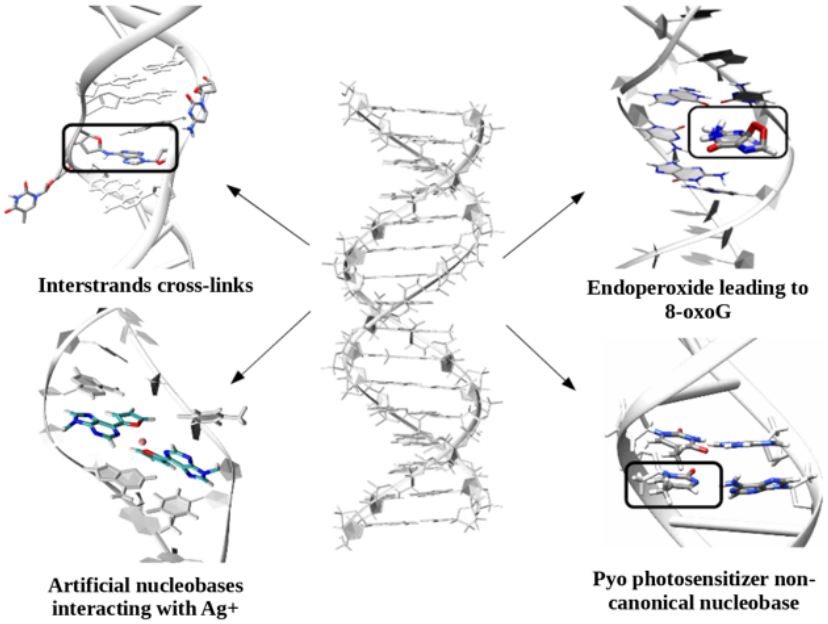
Molecular modelling allows chemical phenomena comprehension at the atomic scale. Nowadays, multi-scale approaches are widely used in the study of lesions formation mechanisms in DNA [1]. The knowledge of this kind of reaction is of capital importance in order to delineate the formation mechanisms of such damages and in a longer perspective, to design novel therapeutics. Molecular modelling can bring information in order to rationalize and characterize phenomena that take place in the DNA double-helix when this latter is the target of agents inducing chemical modifications on nucleobases.



We relied on this powerful tool in order to model the damaged DNA structural behaviour and understand in which manner the lesion can impact the double-helix structure. Molecular dynamics simulations allowed us to study the dynamical behaviour of differents damaged systems, and rationalize such damages formation by structural analysis. We studied many systems, such as the endoperoxide intermediate leading to 8-oxoG, inter-strand crosslinks [2], photo-induced damages on pyrimidine bases [3], and also some artificial systems inducing a metallic atom [4].

References

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