# Benzophenone: Photosensitization routes in DNA

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Benzophenone is a paradigmatic organic molecule for the photosensitization of DNA that exhibited many deleterious pathways[1].
Possible DNA-benzophenone binding modes were firstly investigated by molecular dynamics, minor groove binding and double insertion has been identified as the persistent ones. Subsequently, the photochemistry of benzophenone was investigated by means of extensive non-adiabatic surface-hopping excited-state molecular dynamics and compared with the available experimental and theoretical data. Different mechanisms were found in the femtosecond time scale for population of the low-lying triplet states [2]: direct ($S_1 \rightarrow T_1$) and indirect ($S_1 \rightarrow T_2 \rightarrow T_1$).
Moreover, the feasibility of a competitive process such as hydrogen abstraction was assessed by means of different computational multi-scaling approaches. More in detail, photo-induced hydrogen abstraction from thymine and sugar moieties was considered, and its relevance compared to photo-induced energy transfer discussed[3].

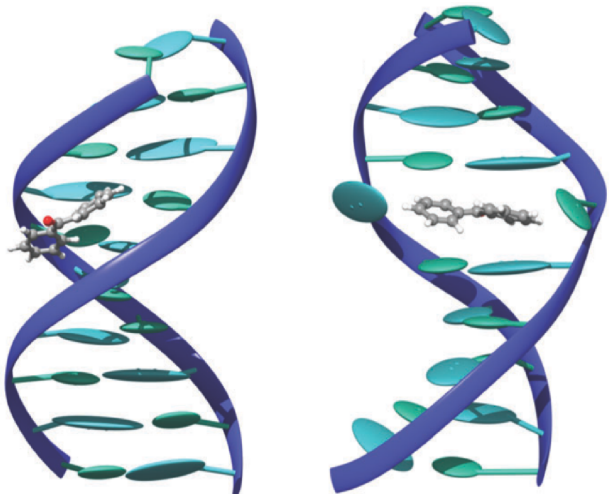

Figure. Minor groove binding (left) and double insertion (right) of benzophenone in DNA.

**References:**

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2. M. Marazzi et al., *J. Phys. Chem. Lett.,* 2016, **7**, 622–626
3. M. Marazzi, et al., *Phys. Chem. Chem. Phys.,* 2016, **18**, 7829–7836