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Carotenoids: from ground-state modelling to access to excited manifold

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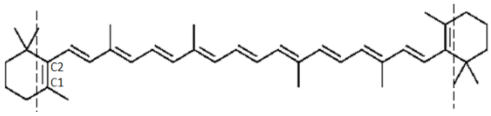
Carotenoid molecules are linear, highly conjugated molecules, with many roles in biology ranging from light-harvesting and photoprotection in photosynthesis, to signaling in fruits and flowers, precursors of plant growth hormones and vitamin A (retinal) or retinol, an essential driver of fetal development.



Structure of β-carotene

Despite their apparent simplicity, carotenoid molecules turn out to be difficult to model with precision, and they actually can be used to benchmark modelling approaches as their electronic and vibrational properties can be easily characterized in detail[1,2]. We are now able to predict with accuracy the properties of quite complex molecules from the carotenoid family[3,4].

Our next goal now resides in modelling carotenoid excited states. Here again, it turns out that the photochemistry of these molecules is much more complex than initially predicted. Only last year were we able to determine with precision the cascade of energy transfers following the photon absorption by these molecules, and we could as well characterize the vibronic properties of each electronic state involved[5]. We aim now to use this information to build-up a comprehensive model of carotenoid electronic properties and photochemistry.

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