

3RD EUROCC VILNIUS WORKSHOP

ON USING HPC

Abstract book

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Modelling Carotenoid Properties

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Carotenoid molecules are essential molecules in all kingdoms of biology. In plants, these llinear, highl conjugated molecules are important constituents of the light-harvesting system, and also play a (photo)protective roles at the level of the photosynthesis apparatus and the chloroplast membranes. They confer their colour to fruits and flowers, and some of their breakdown products control plant growth as hormones or confer them scent. In animals, among other molecules, vitamin A, important for vison and immune system, and retinol, an essential driver of foetal development are produced from carotenoids.



Structure of β-carotene

In the last decade, we have developed computing strategies to model the electronic and vibrational properties of carotenoids, which underlie their biological activity with a dual goal. First we aimed at determining the relationship between the structure and the main electronic properties of these molecules, and this led us to reconsider the conjugation structure of these molecules. Second, we wanted to understand the variety of carotenoid present in Nature: there about many hundreds of different carotenoids present in different organisms, and the reason for such a diversity of molecule is not known. On at least two classes of these molecules, we could determine how additional groups grafted to the conjugated chain could influence their configuration, and thus how they could selectivity for these molecule to their protein binding sites.