

The work deals with the description of carotenoid aggregation in water solutions. The main interactions which are involved in aggregation were analyzed and an efficient way of description of carotenoid aggregation, which leads to a speed up the computation, has been introduced. In addition, two different methods for calculation probability distribution of carotenoids configurations in solutions with variable water concentration were elaborated, and their advantages and disadvantages were discussed. Absorption spectra were calculated from these distributions, and they were compared with the experimental results. The influence of water on formation of different types of aggregates, and its impact on the shape of absorption spectra was also discussed. Results of this study will be used as a base of other, more accurate, description of carotenoids aggregation, which will include other weaker interactions between carotenoids.