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STUDY OF THE ABSORPTION CROSS SECTION TO MEASURE THE DISSIPATIVE CAPACITY OF ANTENNA PROTEINS

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Dissipative structures were first defined by Prigogine in 1973 as structures capable of dissipating an incident external potential in the form of heat. When we talk about an early planetary scenario, this potential will be incident radiation, in particular high energy, i.e. UV (100 nm to 400 nm). The objective of this work is to obtain a methodology to find this type of structures through numerical calculations and chromophores observed in antenna proteins.

In recent years authors (Michaelian et al. 2015) have suggested properties of molecules that show their dissipative capacity, mainly the increase in the global photo-dissipation ratio. In this work, it is suggested to measure the photo-dissipation ratio by calculating the integral cross-section of the molecule of interest. If the existing peptides are suggested as the structures capable of withstanding then the study of the stability and physicochemical interactions of chromophores (e.g. yellow photoactive protein)(Figure 1) and amino acids is of main relevance.

We performed this study obtaining pdb structure of the photoactive yellow protein and edited in order to have an area of interest. Hyperchem software was used to mutate the peptide, then a molecular dynamic was run with the mm+ force field for 3 picoseconds at 298 K to relax the structure. Finally we used a semi-empirical zindo/s method at 10 eV by means of single point method to obtein the electronic spectrum.

The selection of p-coumaric acid as a study model is due to the fact that it has previously been used as a biomarker of the evolution of the solar spectrum on Earth by (Rozema et al. 2001). Experimentally it has been studied the mutations of the yellow photoactive protein and how they affect its absorption spectrum (Imamoto et al. 2001) therefore they could be corroborated with numerical calculations.

For the analysis we use the equation 1 used in (Belay 2010) with the correction for a discrete spectrum, with N=1 and L=1 values.

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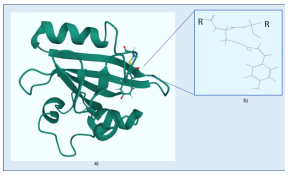

Fig. 1. Photoactive yellow protein and their chromophore (p-coumaric acid)

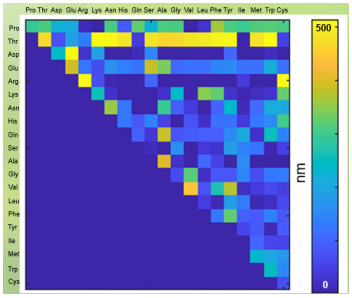

Fig. 2. Symetric results for the 400 configurations of aminoacids.

$$\sigma_t = \frac{1}{NL} \sum_{\lambda=100}^{400} f * \lambda. \quad (1)$$

Where f represents the oscillator force, i.e. the probability of absorption of electromagnetic radiation according to the molecular transition states.

The numerical calculations results are shown in Figure 2, noting that the configurations with the molecules found in nature (Thr and Pro) are the ones with the highest absorption cross-section.

This suggests a selectivity of adjacent aminoacids to maintain or even increase the absorption capacity of chromophore, giving greater resistance to the molecule against UV radiation and energy dissipation. In conclusion, the proposed method can be used and expanded to know the biophysical molecule-scale properties likely to understand the prebiotic molecule selection towards the permanence in early planetary scenarios.

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