

## Theoretical Study on the Nonlinear Optical Responses of Peptide Bonds Created between Alanine and Some Unnatural Amino Acids

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**Abstract :** The Nonlinear optics (NLO) technique is widely used in the field of biological imaging. In fact, grafting biological entities with a high NLO response on tissues and cells enhances the NLO responses of these latter, and ameliorates, consequently, their biological imaging quality. In this optics, we carried out a theoretical study, in the aim of analyzing the peptide bonds created between alanine amino acid and both unnatural amino acids: L-Dopa and Azatryptophan, respectively. Ramachandran plots have been performed for these systems, and their structural parameters have been analyzed. The NLO responses of these peptides have been reported by calculating the first hyperpolarizability values of all the minima found on the plots. The use of such unnatural amino acids as endogenous probing molecules has been investigated through this study. The Density Functional Theory (DFT) has been used for structural properties, while the Second-order Møller-Plesset Perturbation Theory (MP2) has been employed for the NLO calculations.

**Keywords :** biological imaging, hyperpolarizability, nonlinear optics, probing molecule

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