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Original research article

Synthesis of a new cyclic amide derivative: Study its optical nonlinear properties and molecular docking

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ABSTRACT

2-(1,3-dioxoisoindolin-2-yl)-N-(pyrimidin-2-yl) acetamide is synthesized as a new cyclic amide derivative. The structure of this derivative has been characterized by NMR, FTIR, and Mass spectra. The molecular docking calculations of the prepared cyclic amide against (PDB ID: 3PP0) receptor are performed. The prepared compound has the potential to inhibit breast cancer cells, according to molecular docking results. The DFT/B3LYP via 6–311 G(d,p) level was performed to optimize the geometrical structure and the global and local reactivity descriptors of this compound. The calculated values of polarizability and hyperpolarizability of the prepared cyclic amide equal 30.774 $\times 10^{-24}$ esu and 114.678 $\times 10^{-32}$ esu, respectively. The nonlinear optical (NLO) properties of the prepared compound are studied under irradiation with a visible, cw laser beam. The nonlinear refraction index (NLRI), n_2, of the compound is estimated using diffraction patterns (DPs) and the Z-scan techniques, where as high as 2.682 $\times 10^{-11}$ m^2/W are obtained. The optical limiting property of the prepared compound is studied using the same laser beam. An optical limiting threshold of 15 mW is obtained.

1. Introduction

Researchers have been actively seeking new materials with strong and rapid nonlinearities at low-intensity laser beams for applications in light-controlled phase manipulation, optical limiting, optical switching, and refractive index modulation over the past four decades [1–4]. During the past years, we have been studying the nonlinear properties of many available materials [5–10], improving some materials properties by the use of γ-ray [11,12], or by adding number of materials [13–15] or by the synthesize of new materials [16–20]. The measurements of the nonlinear refractive indexes (NLRIs) is the main task for the researchers together with nonlinear absorption coefficients (NLAC), β. The NLRI, n_2, can be easily estimated using a technique known as the spatial self-phase modulation (SSPM) [21] that leads to the generation of diffraction patterns (DPs) at a cw laser beam with low input power. Based on the laser beam of low power input that leads to the DPs with the maximum number of rings, N, n_2 can be estimated. The standard Z-scan technique offers a way to easily obtain n_2 and β. This method relies on the principle of phase transformation, which causes distortions in the beam amplitude while the beam propagates through a nonlinear medium [22,23].

One of the subjects that has attracted substantial attention is light-induced alterations in optical properties, which can be classified

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