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Experimental and theoretical study of two-photon absorption in nitrofuran derivatives: Promising compounds for photochemotherapy

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We report experimental and theoretical studies of the two-photon absorption spectrum of two nitrofuran derivatives: nitrofurantoine, (1-(5-nitro-2-furfurilideneamine)-hidantoine) and quinifuryl, 2-(5′-nitro-2′-furanyl)ethenyl-4-{*N*-[4′-(*N*,*N*-diethylamino)-1′-methylbutyl]carbamoyl} quinoline. Both molecules are representative of a family of 5-nitrofuran-ethenyl-quinoline drugs that have been demonstrated to display high toxicity to various species of transformed cells in the dark. We determine the two-photon absorption cross-section for both compounds, from 560 to 880 nm, which present peak values of 64 GM for quinifuryl and 20 GM for nitrofurantoine (1 GM = 1×10^{-50}cm^4.s.photon^{-1}). Besides, theoretical calculations employing the linear and quadratic response functions were carried out at the density functional theory level to aid the interpretations of the experimental results. The theoretical results yielded oscillator strengths, two-photon transition probabilities, and transition energies, which are in good agreement with the experimental data. A higher number of allowed electronic transitions was identified for quinifuryl in comparison to nitrofurantoine by the theoretical calculations. Due to the planar structure of both compounds, the differences in the two-photon absorption cross-section values are a consequence of their distinct conjugation lengths.

Topics

Density functional theory, **Photon absorption**, **Optical absorption**, **Photodynamic therapy**, **Absorption spectroscopy**, **Oscillator strengths**, **Solvent effect**, **Chemical compounds**, **Radiation therapy**, **Markov processes**

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