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**Structure / Properties Relations in Series of Two-Photon Absorbing Materials for Photodynamic Therapy.** Tatiana V. Timofeeva<sup>1</sup>, Ekaterina V. Bodaeva<sup>1</sup>, Vladimir N. Nesterov<sup>1</sup>, Francis Sena<sup>1</sup>, Sergey Tretiak<sup>2</sup>, <sup>1</sup>Dept. of Natural Sciences, New Mexico Highlands Univ., Las Vegas, NM 87701, <sup>2</sup>Los Alamos National Lab, Los Alamos, New Mexico, 87544.

It was shown that for manifestation of strong two-photon absorption properties molecular structure should contain donor (D) and acceptor (A) groups in a following manner D- $\pi$ -A- $\pi$ -D or A- $\pi$ -D- $\pi$ -A. A large group of molecules (arylidene-piperidones) with such general formula was synthesized and their structure in crystal has been found with X-ray analysis. Experimental spectroscopic investigations have shown significant two-photon absorption activity for representatives with longer  $\pi$ -conjugated bridge. It was found also that some representatives of this group possess anti-tumor activity. Combination of such properties makes these compounds valuable materials for two-photon photodynamic therapy. Structural features of these molecules in crystals, their spectroscopic characteristics (experimental and from quantum mechanical calculations) and their biological activity are discussed.