

OF THE NINTH WORKSHOP ON EXPERIMENTAL MODELS AND METHODS IN BIOMEDICAL RESEARCH WITH INTERNATIONAL PARTICIPATION



JULY 16- 18, 2018
SOFIA, BULGARIA

Oral presentation:

2-CARBAMIDO-1,3-INDANDIONE – A POTENTIAL BIOMARKER AND AN ANTITUMOR AGENT. QUANTUM-CHEMICAL MODELING OF ITS COMPLEXES WITH NUCLEOTIDES OF DNA AND RNA

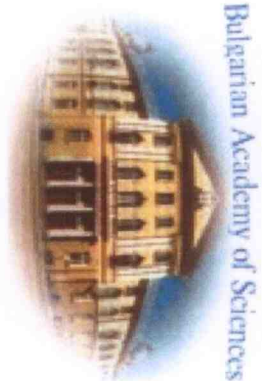
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The 2-substituted 1,3-indanedione derivatives have a wide application in the field of medicine and biology. 2-Carbamido-1,3-indanedione derivatives have potential as antineoplastic agents, and 2-carboxamide-indan-1,3-dione (CAID) itself as biomarker

From a fluorescence-microscopic analysis of CAID in Balb / c 3T3 cell lines, is established its cytotoxicity, its ability to penetrate through cell membranes and also its cellular localization. Fluorescence microscopy data suggests that CAID penetrates into DNA and RNA-containing cell structures, such as nucleus and nucleoli. The in vitro antitumor activity of the compound is determined on different cell lines, with CAID showing good antineoplastic properties. In order to elucidate the affinity of CAID to nucleic acids, quantum chemical B3LYP/6-31+G (d, p) calculations were made. Two ways of binding CAID to the five nucleotides contained in DNA and RNA are discussed - to the nitrogenous base and to the phosphate group. The interaction energies of the complexes formed are calculated to evaluate the binding priority of CAID to nucleotides. It has been found that 2-carboxamide-indan-1,3-dione binds predominantly to the phosphate group in thymidine monophosphate.



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