SUMMARY

Increasing incidence of cancer cases and the negative consequences of chemotherapy, forced to seek new solutions and new therapeutic agents for oncological patients. Unfortunately, pharmacological studies are time-consuming and expensive, which significantly affects the amount of new original drugs appearing on the pharmaceutical market.

This study has been aimed to propose a useful tool, which described selected properties of the compounds in most simple way. Based on computed equations, it will be possible to design a drug's structure which has a desired biological activity. To reach established goals, combined QSRR and QSAR analysis has been utilized. It showed relationship between compound's chemical structure and its retention properties or biological activity, respectively. These relationships are used to be present as non-complicated and well-defined mathematical equations.

The main aim of the study was achieved by chemometric technique (Multiple Linear Regression - MLR). Analysis of such a large amount of chromatographic and molecular modeling data set has been possible by employ particular statistical algorithms and computer programs (Statistica® 10.0 (StatSoft, Tulus, Oklahoma, USA); R® (The R Foundation for Statistical Computing, Auckland, New Zealand); DTClab software (http://dtclab.webs.com/software-tools). MLR methodology allowed to present the relationship between structure and activity as interpretable mathematical equations with linear relationship. This computational method was used to determine acridinones and cytostatics biological activities.

With proposed approach QSAR and QSRR descriptive models have been determined. They allow predict acridinone's ability to the physico-chemical (non-covalent) interactions with DNA helix (stabilize the secondary structure of DNA), acridinone's capacity to form covalent inter-strand DNA cross-links or cytotoxic activity of cytostatic drugs, from different taxonomic groups, diverse in structure and mechanism/s of action. Predictive power of QSAR models and its ability to predict the value of cytostatics activity have been examined. This test was carried out by correlating the activities values calculated with proposed QSAR models, with the actual values of activities obtained by *in vitro* or *in vivo* experiments. All models described in this work have been characterized by good statistical parameters and statistical significance.

Presented results proved, that proposed combined QSAR and QSRR strategy evaluate the biological activity (QSAR model) based on previously predicted set of lipophilicity parameters (QSRR model). Therefore, this approach reduce the amount of chromatographic analyzes and experimental *in vitro* and *in vivo* test, usually performed in new therapeutic agents tests.

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