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The potential of quantitative structure-retention-(Biological) activity relationship (QRAR) investigations in pharmaceutical research

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A large number of compounds can be synthesized during the drug development process, which are then processed and screened for specific properties of interest to obtain the best possible drug candidates. Physical-chemical screenings are increasingly being used during the early stages of drug discovery to provide a more comprehensive understanding of the key properties that affect the biological disposition of promising leads – gastrointestinal absorption and blood brain barrier permeability, distribution in systemic circulation and tissues, metabolism, excretion as well as protein binding, interactions with receptor and toxicity. Lipophilicity parameters *log P* (logarithm of n-octanol–water partition coefficient) and *log D* (distribution coefficient) and dissociation constant *pKa* of a drug candidate are therefore of a primary concern. Determination of those parameters at the early stage of studies can help in eliminating those molecules that are unlikely to become drugs due to their poor pharmacokinetic properties. The reversed-phase liquid chromatography is especially suitable for these kinds of determinations since it was proven that compounds' hydrophobicity measured as a retention factor obtained at different mobile phase compositions and extrapolated to neat water as an eluent, *log kw,* is well correlated with *log P*. Usually, the investigations consist of time/consuming and cost/demanding experimental work as well as animal bioavailability tests. In order to rationalise pharmaceutical research, the mathematical models able to predict chromatographic retention from chemical structure have been introduced (QSRR studies). Likewise, QRAR studies with the possibility to relate the descriptors of the compounds, chromatographic retention and pharmacokinetic properties evaluated *in silico* and/or biological activity measured *in vivo* have been evaluated. The authors have done some effort to prove the usefulness of this concept in investigation of selected antifungal agents and in future of novel potential antibiotics from endophytic fungi.

Biography

Biljana Otašević attended PhD studies at University of Belgrade – Faculty of Pharmacy, where she finished Doctoral thesis in field of pharmaceutical chemistry in the year 2011. Nowadays, she works as an Assistant Professor at the Department of Drug Analysis and participates in the research project financed by the Ministry of Education, Science and Technological Development of the Republic of Serbia (no. 172033). She is the author of 67 scientific publications among which 20 scientific papers were published in the international journals indexed in SCI list. She gave one lecture on an international scientific meeting.

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