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Toward effective synthesis of new drugs and diagnostics

Current drug discovery is multidisciplinary field based on tight collaboration of chemists, biologists and physicians. The part of chemistry plays significant role especially in the beginning of the process, but doesn´t stay apart also during advanced steps of the development. Organic chemistry is a basic tool not only for synthesis of new derivatives, but also for the modification of active species to improve their physico-chemical as well as biological properties, to prepare chemical libraries for structure-activity relationship studies or to derive compounds for molecular target identification or development of drug delivery systems. Modern medicinal chemistry is focused not only on synthesis and modification of low molecular weight compounds, but also synthetic polymers, biopolymers especially in combination with nanochemistry approaches.

The modern drug discovery is based on targeting of defined sites or regulation of molecular processes inside the cells. Recognition of these processes is often performed with use of chemical probes suitable for specific determination of physico-chemical properties of the appropriate environment, like e.g. pH, redox potential, presence of specific ions or for following the processes, in which biomolecules are involved.

With improvement of analytical instrumentation and screening methods for various assays in few past decades and automation of these processes it was necessary to improve also methods of organic synthesis, analyses of reaction mixtures, purification of final compounds to efficiently supplement process of discovery of new active compounds.

The lecture will be focused on synthetic strategy in efficient development of anticancer agents and novel fluorescent probes, in which high throughput synthesis in connection with high throughput analysis is applied. These approaches together with rational design of the target derivatives based on results of biological screening as well as molecular modeling and predictive calculation of compounds properties will be discussed. The application of synthetic methods based on solution-phase chemistry will be compared to solid-phase synthesis and suitable implementation of combinatorial chemistry will be exemplified. The synthetic methods will be illustrated with examples in synthesis of new compounds, including stereoselective synthesis, modification of active compounds to find the molecular target, development of bioavailabile formulations of active species, drug delivery system development, fluorescent pH indicators and novel ion sensitive fluorescent probes synthesis.