## Project summary

General aims of the project are on the borderline between organic and medicinal chemistry with intentions to discover novel classes of anticancer compounds. Our research is based on selected natural products with known biological potential and on the rationally designed heterocyclic compounds. Explored chemical space is defined by privileged structures depicted by natural products and also by further diversification using principles of *biology inspired organic synthesis* (*BIOS*)and *diversity orientated synthesis* (*DOS*). In addition to developing synthetic routes towards novel heterocyclic compounds and their experimental biological profiling, computational chemistry is used as a tool in designing and studying these compounds in more detail.

## Sažetak projekta

Opšti ciljevi projekta nalaze se u granicama organske i medicinske hemije, a okrenuti su pronalaženju novih heterocikličnih jedinjenja sa potencijalnim antikancerogenim osobinama. Istraživanja su zasnovana na studiji odabranih prirodnih proizvoda sa poznatim biološkim potencijalom, ali i na racionalno dizajniranim heterocikličnim strukturama. Proučavani hemijski prostor definisan je privilegovanim strukturama opisanim prirodnim proizvodima i daljoj strukturnoj diverzifikaciji primenom principa organske sinteze inspirisane biologijom(*biology inspired organic synthesis-BIOS*)i diverzitetom usmerene sinteze (*diversity orientated synthesis-DOS*). Paralelno sa razvojem sinteze novih heterocikličnih jedinjenja, računarske metode primenjuju se u cilju proučavanja fizičko-hemijskih i bioloških osobina novih molekula.

## Selected results/Odabrani rezultati

1. M. R. Simic, M. Stankovic, B. M. Mandic, V. V. Tesevic, V. M. Savic

 Synthesis of Novel Tetrahydrobenzazepine Derivatives and Their Cytoprotective Effect on Human Lymphocytes

 ***Arch. Pharm. Chem. Life Sci.*** 2015, **348**, 100-112.

1. G.Tasic, V.Maslak, S.Husinec, N.Todorovic, V.Savic

 Study of the intramolecular Heck reaction: synthesis of the bicyclic core of corialstonidine,

 ***Tetrahedron Lett.*** 2015, **56**, 2529-2532.

1. M. Simic, N. Paunovic, I. Boric, J. Randjelovic, S. Vojnovic, J. Nikodinovic-Runic, M. Pekmezovic, V. Savic

 Functionalised Isocoumarins as Antifungal Compounds: Synthesis and Biological Studies

***Bioorg.Med.Chem.Lett***., 2016, **26**, 235-239.

1. Milena Simic, Ana Damjanovic, Marko Kalinic, Gordana Tasic, Slavica Eric, JelenaAntic Stankovic, Vladimir Savic

 Synthesis, cytotoxicity and computational study of novel protoberberine derivatives

 ***J. Serb. Chem. Soc.*** 2016, **81**, 103-123.

1. M.Petkovic, V. Nasufovic, D.Djukanovic, Z. Tokic Vujosevic, M. Jadranin, R.Matovic, V. Savic

 Cyclative cascades of allenamides derived from aminoacids. Synthesis of annulated indoxyl derivatives.

 ***Eur. J. Org. Chem.*** 2016, 1279-1282.

1. P. Jovanovic,M. Petkovic,M. Simic, B. Ivkovic V. Savic

 A novel thiourea type organocatalyst possessing a single NH functionality

 ***Org.Biomol.Chem***. 2016, **14**, 6712-6719.

1. P. Jovanovic,M. Petkovic,B. Ivkovic V. Savic

 Pyrrolidine derived thioureas as organocatalysts in the Michael reaction of vinyl sulfone. Structure- stereoselectivity study

 ***Tetrahedron Asymm.*** 2016, **27**, 990-997.

1. D. Djukanovic, M. Petkovic, M. Simic, P. Jovanovic, G. Tasic, V. Savic

 Synthesis of 2-unsubstituted imidazolones from bisamides via a one-pot, domino dehydration/base promoted cyclisation process

 ***Tetrahedron Lett.*** 2018, **59**, 914.

1. M. Simic, G. Tasic, P. Jovanovic, M. Petkovic, V. Savic

 Preparation of pyrrolizinone derivatives via sequential transformations of cyclic allyl imides: synthesis of quinolactacide and marinamide

 ***Org.Biomol.Chem***. 2018, **16**, 2125.