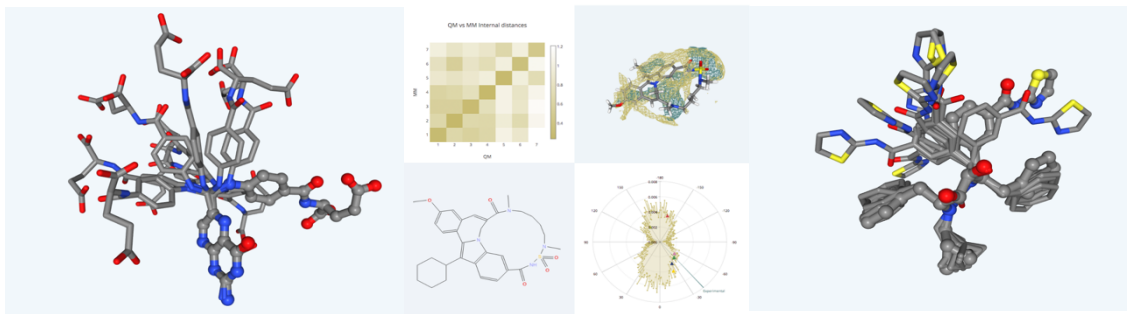


## Hemija budućnosti: računarsko modelovanje i dizajn leka pomoću softvera za predviđanje bioaktivnih konformacija



Uprkos velikom napretku u tehnologiji i nauci i razumevanju mehanizama bioloških sistema, dizajn, razvoj i komercijalizacija leka je iscrpan, dugotrajan i proces velikih troškova. Tipični ciklus razvoja novog leka košta aproksimativno 1 milijardu € i traje do 12 godina. Računarska hemija i bioinformatika, spoj između moderne hemije, farmacije, biologije matematike i informatike, obuhvataju otkrivanje, razvoj i implementaciju računarskih algoritama i softverskih alata u cilju razumevanja bioloških procesa kao i predviđanja ishoda situacije pre pokretanja stvarnog eksperimenta. Ove discipline se primenjuju i u farmaceutskim istraživanjima za identifikaciju ciljnih meta za lekove kao i za optimizaciju celog procesa. Dizajn leka podrazumeva kreiranje malih molekula (drugs, ligands) koji su komplementarni u smislu oblika i naelektrisanja svom biomolekularnom targetu (proteinu). Najvažniji zadatak u otkriću leka je prepoznati da li će protein i određeni inhibitor da inter-reaguju, ali još bitnije je predvideti njegovu konformaciju u trenutku vezivanja (bioaktivna konformacija). Bioaktivna konformacija je geometrija koju molekul mora "prihvatiti" u cilju prepoznavanja od strane proteina i ova konformacija je odgovorna za biološku aktivnost. Istraživanje konformacijskih preferencija malih fleksibilnih molekula igra važnu ulogu u dizajnu leka. Procena relativne slobodne energije molekula u vezanom stanju (bioaktivna konformacija) nužna je za razumevanje postupka molekularnog prepoznavanja i za optimizaciju jačine molekularnog spajanja između proteina i leka.

Predstavljamo multi-level strategiju koja kombinuje tehnike molekularne dinamike za konformacijsku eksploraciju i tehnike kvantne hemije za procenu relativne stabilnosti konformera. Multi-level metod je testiran na više od 200 relevantnih farmaceutskih X-ray kompleksa. Metod je automatizovan, i posle implementacije raznih računarskih algoritama i softverskih alata izrađen je novi programski kod i inovativni softver nazvan "Bioactive Compounds". "Bioactive Compounds" je napredan softver koji omogućava predviđanje 4D bioaktivnih konformacija. Upotreba ovog programa doprinosi ubrzanom procesu otkrića leka i na taj način štedi vreme, novac i broj eksperimenata koji se moraju izvesti kako bi se pronašao novi lek.

U nastavku predavanja će se prezentovati stipendije za doktorske i post-doktorske studije na naučnim institutima u Barseloni kao i stipendije Evropske komisije za master programe na području EU. Prezentacija će biti praćena praktičnim savetima kako uspešno pripremiti aplikaciju za studiranje u inostranstvu.

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# SANJA ZIVANOVIC

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## DETAILS

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08028, Spain  
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### DATE / PLACE OF BIRTH

1900-08-25  
Subotica, Serbia

### NATIONALITY

Croatian, Serbian

### DRIVING LICENSE

Category A and B

## SOCIAL PROFILES

LinkedIn  
<https://www.linkedin.com/in/sanja-zivanovic/>

## SKILLS

Research

Communication

Flexibility

Organisation

Teaching

Leadership

Computing

## LANGUAGES

Serbo-croatian

English

## PROFILE

I am an ambitious young scientist interested in computer aided drug design, innovation and entrepreneurship. My research topic is focused on the study of drug-like molecules and development of software "Bioactive compounds". Bioactive compounds is a platform designed to efficiently generate bioactive conformers and speed up the drug discovery process.

## EMPLOYMENT HISTORY

### PhD Candidate at Institute for Research in Biomedicine (IRB Barcelona), Barcelona, Spain

October 2014 – Present

Final year PhD student at [IRB Barcelona](#) in the group of [prof. Modesto Orozco](#).

- Molecular modelling and bioinformatics field, working on project called "Multy-level strategy for analysis of bioactive conformations" focused on drug design.
- The scientific results were applied for development of software called Bioactive compounds. It is a platform designed to efficiently generate bioactive conformers and speed up the drug discovery process.

### Coordinator of EMA PhD network at Erasmus Mundus Association

June 2017 – Present

The Network aims to improve informal discussion and collaboration between PhD researchers from various disciplines under the [Erasmus Mundus](#) Action 1. EMA PhDNet serve as a platform for the PhD students to share their research and provide a discussion forum to improve communications between PhD students.

- Responsible for leading a network and coordination of the active members
- Working on organisation of workshops, seminars and conferences for PhDs in close collaboration with Marie Curie Alumni Association
- Establish network between PhD senior and students

### Chair of the scientific committee at ENABLE Network, European Commission

July 2016 – November 2017

[ENABLE](#) is a European Union Horizon 2020-funded initiative that brings together four renowned European research institutes (IRB, RIMLS, CPR, SEMM) and an innovative science communication agency (Scienseed), with the aim to promote scientific excellence in biomedicine and active interaction with society. The symposia are organised *by* young researchers and *for* young researchers.

- My main role was to ensure that the whole organisation of the conference is managed effectively
- Involved in coordination of small teams and monitoring tasks
- Responsible for Social media working group and conference promotional campaign
- Organisation of the overall conference program and structure

Spanish

Italian

○ HOBBIES ○

Travelling, Summer outdoor sports,  
Beauty and cosmetics industry

○ Country Representative and PRnet member at Erasmus Mundus Association

May 2016 – December 2017

Occupying different administrative and representative roles:

- Provide overall support to the ongoing projects of the [Erasmus Mundus Association](#). Seek knowledge as to the current problems, wishes and needs of the students and alumni.
- Liaison with EMA elected PRs in order to empower them to become the advocated of course quality. This position involves close collaboration with Internal Affairs team, Vice-president and all the PRs.

○ Tutor at Barcelona International Youth Science Challenge (BIYSC)

February 2016 – May 2017

Tutor at various schools and courses for young talented students:

- [Crazy about Medicine](#), a year-long course directed toward talented students. Giving classes of the theory and practical lessons in the field of computational chemistry.
- [Barcelona International Youth Science Challenge \(BIYSC\)](#), 2 week long course where students acquired the basic knowledge about drug design.

🎓 EDUCATION

○ University of Barcelona, Barcelona, Spain

October 2014 – Present

**Degree: PhD in Molecular Modelling and Bioinformatics**

Molecular Modeling and Bioinformatics

○ University of Valencia and University of Groningen

September 2012 – July 2014

**Degree: Double MSc degree in Theoretical Chemistry and Computational Modelling**

Modelling Chemical Processes in Biological Environments (QM/MM simulations)

GPA: 8.76/10.00

○ University of Novi Sad

September 2009 – June 2012

**Degree: Bsc in Chemistry**

Biochemistry and analytical chemistry

GPA: 9.86/10.00

📖 COURSES

○ How to disseminate your research project in a 60, ESTEVE foundation

February 2018

○ Negotiation Skills Workshop, IRB Barcelona

October 2017

○ From Science to Business, ESADE Business & Law School

May 2017 – June 2017

- ASBTEC Workshops: Keys for bio-entrepreneurship, Fundació Bosch i Gimpera  
May 2017 – May 2017
- ASBTEC Business Workshops: Business Models, Creation of Ideas and Financing, IQS - Chemical Institute of Sarria  
March 2017 – May 2017
- CRG BioBusiness School, Center for Genomic Regulation  
September 2016
- The Scientists with the Media, ESTEVE foundation  
February 2016
- Innovation workshop series, IRB Barcelona  
January 2017 – Present

#### EXTRA-CURRICULAR ACTIVITIES

- Volunteer Work Programme Bio-Europe Spring at EDB group, Barcelona, Spain  
March 2017  
Logical support to the conference's organisation team
- Exhibitor at Institute of Molecular Science (ICMOL), Valencia, Spain  
May 2013 – May 2014  
Presenting molecular modelling to kids

#### AWARDS

- Wiley Outstanding Award for poster presentation, 11th European Conference on Theoretical and Computational Chemistry, Barcelona, Spain  
September 2017
- FEBS Young Researcher fellowship for 17th Young Scientists' Forum and FEBS Congress 2017, Jerusalem, Israel  
September 2017
- Mu.Ta.Lig. COST Action CA15135 award for Trainee at European Workshop in Drug Design, Siena, Italy  
May 2017
- Award for the best oral communication – International Bioscience Conference IBSC, Novi Sad, Serbia  
September 2016
- Full 3 years scholarship of the Catalan Government for making PhD in the leading research center, Barcelona, Spain  
February 2016 – February 2019

- Full 2 year scholarship of Erasmus Mundus Program of Excellence, EU Commission  
September 2012 – August 2014
- Scholarship Dositeja for top 1000 students in Serbia by the Ministry of Youth and Sport, Belgrade, Serbia  
January 2012 – January 2013
- Scholarship of the Government of Serbia for the most successful students in Serbia three years in a row, Belgrade, Serbia  
January 2010 – January 2012
- Awarded as a one of the best students at Faculty of Life Science, Novi Sad, Serbia  
June 2010
- Awarded as one of the best students at University, Novi Sad, Serbia  
May 2010
- Scholarship for the best students of the city, Subotica, Serbia  
January 2010 – March 2018

## REFERENCES

- References available upon request