CURRICULUM VITAE

Assoc. Prof. ANDREJ PERDIH, PhD
Senior Research Fellow

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Member of the Laboratory of Computational Biochemistry and Drug Design, **Theory Department** at the **National Institute of Chemistry**, Slovenia.

RESEARCH INTERESTS:

1. Application of structure-based and ligand-based drug design techniques in virtual screening experiments aimed at identifying and then characterizing novel hit molecules on a range of macromolecular therapeutic targets.

2. Molecular dynamics (MD) simulations of macromolecules to increase the understanding of the target protein molecules structure-function relationships and gain insight into the molecular recognition process of the ligand-target interactions.

3. Modelling of enzymatic and organic reaction mechanisms using quantum chemistry methods

1. EDUCATION

2004-2009 **PhD in MEDICINAL CHEMISTRY**
Faculty of Pharmacy, University of Ljubljana

1999-2004 **MASTER of PHARMACY**
Faculty of Pharmacy, University of Ljubljana

2. RESEARCH POSITIONS

2017- **SENIOR RESEARCH ASSOCIATE**
National Institute of Chemistry, Ljubljana

2013-2017 **Visiting RESEARCH SCHOLAR**
University of Michigan, Ann Arbor, USA
Host: **Prof. ZANETA NIKOLOVSKA-COLESKA** (15 months)

2012-2013 **Visiting POSTDOCTORAL RESEARCHER**
Freie Universität Berlin, Germany
Host: **Prof. GERHARD WOLBER** (12 months)

2012-17 **RESEARCH ASSOCIATE**
National Institute of Chemistry, Ljubljana

2009-2012 **RESEARCH ASSISTANT WITH A PHD**
National Institute of Chemistry, Ljubljana

2008 **Visiting JUNIOR RESEARCHER**
Inte:Ligand, Vienna, Austria
Host: **Prof. GERHARD WOLBER** (4 months)

2004-2009 **JUNIOR RESEARCHER**
Supervisor: **Prof. TOMAŽ ŠOLMAJER**

3. TEACHING

2021- **ASSOCIATE PROFESSOR of Medicinal Chemistry**
University of Ljubljana, Faculty of Pharmacy

2012- **EXTERNAL COLLABORATOR: Structure of Biological Molecules**
Faculty of Mathematics, Natural Sciences and Information Technologies, University of Primorska

2011- 2021 **ASSISTANT PROFESSOR of Medicinal Chemistry**
University of Ljubljana, Faculty of Pharmacy

2006-2011 **TEACHING ASSISTANT for Medicinal Chemistry**
University of Ljubljana, Faculty of Pharmacy

4. HONORS AND AWARDS

2019 **Publons award:** Top peer reviewer

2009 **Krka prize** for Ph.D. Thesis

2004 **Krka prize** for M. Pharm. Thesis

2004 **Faculty of Pharmacy award** for outstanding study achievements

5. FOREIGN LANGUAGE SKILLS

2007 **English Certificate of Proficiency in English** (CPE), Cambridge ESOL
CEFR level C2

2003 **German Zentrale Oberstufenprűfung** (ZOP), Goethe Institut
CEFR level C2

2013 **French Diplôme d'études en langue française** DELF B2, CIEP
CEFR B2 level

6. REVIEWING & EDITORIAL ACTIVITIES

6.1. EDITORAL ROLES

2022 Associate Editor: *Biological Modeling and Simulation*, Frontiers in Molecular Biosciences

2022 Guest Editor/Special Issue: *Pharmaceuticals, MDPI*

6.2. PEER REVIEWER - Scientific Journals*: more than 200 reviews conducted*

WIREs Computational Molecular Science, Chemistry: A European Journal, Communications Biology, Scientific Reports, Journal of Medicinal Chemistry, Drug Discovery Today, Journal of Chemical Information and Modeling, ACS Medicinal Chemistry Letters, European Journal of Medicinal Chemistry, Bioorganic Chemistry, RSC Advances, Chemistry: An Asian Journal, Pharmacological Research, ChemMedChem, Bioorg. & Med. Chem., Bioorg. & Med. Chem. Lett., Journal of Natural Products, Biochemistry, Current Medicinal Chemistry, Chemical Research in Toxicology, Biomedicine & Pharmacotherapy, etc.

EXPERT REVIEWER*: International grant proposals*

Expert evaluator of grant proposals of several European research agencies:
National Science Centre (NCN), Poland. Dutch Research Council (NWO), Nederlands, French National Research Agency's (ANR), France, *Science Fund of the Republic of Serbia*, *Ministry of Science of Montenegro, Autonome Provinz Bozen, Italy*

7. GRANTS AND RESEARCH FUNDING

7.1. PRINCIPAL INVESTIGATOR

2022-2025 **HEAD: ARIS basic research project J1-4402**
Dynamical model of a type II DNA topoisomerase biological nanomachine and design of catalytic inhibitors
Slovenian Research and Innovation Agency

2018-2021 **HEAD: ARRS bilateral US-SI research project BI/US/18-20-068**
Development of inhibitors of human DNA topoisomerase II alpha and Mcl-1 protein as novel anticancer agents
National Institute of Chemistry and University of Michigan
Slovenian Research Agency

2016-2017 **HEAD: ARRS bilateral US-SI research project BI/US/16-17-036**
Development of novel selective small molecule inhibitors of Mcl-1 protein and human DNA topoisomerase II alfa
National Institute of Chemistry and University of Michigan
Slovenian Research Agency

2011-2013 **HEAD: ARRS postdoctoral project Z1-4111**
Design of novel Mur ligase inhibitors and dynamical model of the E. coli MurD enzyme
Slovenian Research Agency

7.2. INNOVATION FUNDING

2023 **NICKI Targeted Proof of Concept funding**
In vivo studies of substituted bithiazoles as anticancer agents
National Institute of Chemistry

2020 **IPBooster: Patent Landscaping and IP evaluation or due diligence**
Patenting of substituted bithiazoles as anticancer agents
META Group

7.3. MEMBER OF THE RESEARCH PROGRAM (STABLE FUNDING)

2013- **MEMBER: ARIS research program P1-0012**
Molecular Simulations, Bioinformatics and Drug Design
National Institute of Chemistry
Head prof. Janez Mavri

7.4. TEAM MEMBER OF THE RESEARCH PROJECTS

2023-2026 **TEAM MEMBER: ARIS basic research project J1-50022**
Enzyme catalysis probably originates from electrostatics: computational study
PI: dr. Jernej Stare
Slovenian Research and Innovation Agency

2021-2024 **TEAM MEMBER: ARRS basic research project J1-3019**
Computational and experimental investigation of senescent cells modulation as a new tool to combat age-related diseases
PI: dr. Jure Borišek
Slovenian Research Agency

2020-2022 **TEAM MEMBER: EU Horizon project EuroCC**
EU Horizon 2020 (WP21)
SI coordinator: dr. Jernej Stare
Horizon Europe

2019-2022 **TEAM MEMBER: ARRS basic research project J1-1709**
Structural insight into the mechanism of Clostridium difficiule surface formation
PI: prof. Dušan Turk
Slovenian Research Agency

2014-2015 **TEAM MEMBER: ARRS bilateral US-SI research project BI/US/14-15-029**
Novel selective small molecule inhibitors of Mcl-1 protein and DNA topoisomerase IIalfa
National Institute of Chemistry and University of Michigan
PI: prof. Tomaž. Šolmajer
Slovenian Research Agency

2009-2011 **TEAM MEMBER ARRS basic research project J1-2151**
Membrane proteins- from static models to structure and transport mechanism
PI: prof. Marjana Novič
Slovenian Research Agency

2009-2011 **TEAM MEMBER: ARRS basic research project J1-0308**
Structure-based design of novel inhibitors of DNA Gyrase
PI: prof. Tomaž Solmajer
Slovenian Research Agency

8. PROFESSIONAL ACTIVITIES

2023-2027 **Member of the Commission for Equal Opportunities in Science**
Ministry of Higher Education, Science and Innovation, Slovenia

2021-2026 **Member of the Committee for Gender Equality in Science**
National Institute of Chemistry, Slovenia

2022 **Member of the Slovenian Chemical Society**

2002 **Member of the Slovenian Pharmaceutical Society**

9. PUBLICATIONS

9.1. ORIGINAL SCIENTIFIC ARTICLES

56. PHUONG, Vu Lan, DIEHL, Claudia J., CASEMENT, Ryan, BOND, Adam G., STEINEBACH, Christian, STRAŠEK, Nika, BRICELJ, Aleša**, PERDIH, Andrej**, SCHNAKENBURG, Gregor, SOSIČ, Izidor. **Expanding the structural diversity at the phenylene core of ligands for the von Hippel–Lindau E3 ubiquitin ligase: Development of highly potent hypoxia-inducible factor-1α stabilizers.** *Journal of medicinal chemistry*, **2023**, 66, 12776–12811.

55. PAVLIN, Matic, HERLAH, Barbara, VALJAVEC Katja, PERDIH Andrej. **Unveiling the Interdomain Dynamics of Type II DNA Topoisomerase through All-Atom Simulations: Implications for Understanding its Catalytic Cycle.** *Computational and Structural Biotechnology Journal*, **2023**, 21, 3746-3759.

54. LJUBIČ, Martin, PRAŠNIKAR, Eva, **PERDIH, Andrej**, BORIŠEK, Jure. **All-atom simulations reveal the intricacies of signal transduction upon binding of the HLA-E ligand to the transmembrane inhibitory CD94/NKG2A receptor.** *Journal of chemical information and modeling*. **2023**, 63, 3486-3499.

53. CVIJETIĆ, Ilija N., HERLAH, Barbara, MARINKOVIC, Aleksandar, **PERDIH, Andrej**, BJELOGRLIC, Snezana K. **Phenotypic discovery of thiocarbohydrazone with anticancer properties and catalytic inhibition of human DNA topoisomerase IIα**. *Pharmaceuticals*. **2023**, 16, [article no.] 341.

52. MEDEN, Anže, KNEZ, Damijan, BRAZZOLOTTO, Xavier, MODESTE, Fabrice, **PERDIH, Andrej**, PIŠLAR, Anja, ZORMAN, Maša, ZOROVIĆ, Maja, DENIC, Milica, PAJK, Stane, ŽIVIN, Marko, NACHON, Florian, GOBEC, Stanislav. **Pseudo-irreversible butyrylcholinesterase inhibitors: Structure–activity relationships, computational and crystallographic study of the N-dialkyl O-arylcarbamate warhead**. *European journal of medicinal chemistry*. **2023**, 247, 115048

51. OGRIZEK, Mitja, JANEŽIČ, Matej, VALJAVEC, Katja, **PERDIH, Andrej**. **Catalytic mechanism of ATP hydrolysis in the ATPase domain of human DNA topoisomerase IIα.** *Journal of chemical information and modeling*. **2022**, 62, 3896–3909.

50. PRAŠNIKAR, Eva, **PERDIH, Andrej**, BORIŠEK, Jure. **What a difference an amino acid makes: an all-atom simulation study of nonameric peptides in inhibitory HLA-E/NKG2A/CD94 immune complexes.** *Frontiers in pharmacology*. **2022**, 13, [article no.] 925427.

49. PRAH, Alja, GAVRANIĆ, Tanja, **PERDIH, Andrej**, SOLLNER DOLENC, Marija, MAVRI, Janez. **Computational insights into β-carboline inhibition of monoamine oxidase A**. *Molecules*. **2022**, 27, [article no.] 6711.

48. HERLAH, Barbara, HOIVIK, Andrej, JAMŠEK, Luka, VALJAVEC, Katja, YAMAMOTO, Norio, HOSHINO, Tyuji, KRANJC, Krištof, **PERDIH, Andrej**. **Design, synthesis and evaluation of fused bicyclo[2.2.2]octene as a potential core scaffold for the non-covalent inhibitors of SARS-CoV-2 3CLpro main protease.** *Pharmaceuticals.* **2022**, 15, [article no.] 539.

47. VITOROVIĆ-TODOROVIĆ, Maja D., CVIJETIĆ, Ilija N., ZLOH, Mire, **PERDIH, Andrej**. **Molecular recognition of acetylcholinesterase and its subnanomolar reversible inhibitor: a molecular simulations study.** *Journal of biomolecular structure & dynamics*. **2022**, 40, 1671–1691.

46. PRAŠNIKAR, Eva, **PERDIH, Andrej**, BORIŠEK, Jure. **All-atom simulations reveal a key interaction network in the HLA-E/NKG2A/CD94 immune complex fine-tuned by the nonameric peptide**. *Journal of chemical information and modeling*. **2021**, 61, 3593-3603.

45. PRAŠNIKAR, Eva, **PERDIH, Andrej**, BORIŠEK, Jure. **Nonameric peptide orchestrates signal transduction in the activating HLA-E/NKG2C/CD94 immune complex as revealed by all-atom simulations**. *International journal of molecular sciences*. **2021**, 22, [article no.] 6670.

44. KENDA, Maša, VEGELJ, Jan, HERLAH, Barbara, **PERDIH, Andrej**, PŘEMYSL, Mladěnka, SOLLNER DOLENC, Marija. **Evaluation of firefly and renilla luciferase inhibition in reporter-gene assays: a case of Isoflavonoids**. *International journal of molecular sciences*. **2021**, 22, [article no.] 6927.

43. STEVANOVIĆ, Strahinja, MARJANOVIC, Djordje S., TRAILOVIC, Sasa M., ZDRAVKOVIC, Nemanja, **PERDIH, Andrej**, NIKOLIĆ, Katarina. **Potential modulating effect of the Ascaris suum nicotinic acetylcholine receptor (nAChR) by compounds GSK575594A, diazepam and flumazenil discovered by structure-based virtual screening approach.** *Molecular and biochemical parasitology*. **2021**, 242, 111350-1-111350-10.

42. BERGANT LOBODA, Kaja, JANEŽIČ, Matej, ŠTAMPAR, Martina, ŽEGURA, Bojana, FILIPIČ, Metka, **PERDIH, Andrej**. **Substituted 4,5'-bithiazoles as catalytic inhibitors of human DNA topoisomerase IIα**. *Journal of chemical information and modeling*, **2020**, 60, 7, 3662–3678.

41. BERGANT LOBODA, Kaja, VALJAVEC, Katja, ŠTAMPAR, Martina, WOLBER, Gerhard, ŽEGURA, Bojana, FILIPIČ, Metka, SOLLNER DOLENC, Marija, **PERDIH, Andrej**. **Design and synthesis of 3,5-substituted 1,2,4-oxadiazoles as catalytic inhibitors of human DNA topoisomerase IIα**. *Bioorganic chemistry*, **2020**, 99, 103828-1-103828-19.

40. PINTAR, Sara, BORIŠEK, Jure, USENIK, Aleksandra, **PERDIH, Andrej**, TURK, Dušan. **Domain sliding of two Staphylococcus aureus N-acetylglucosaminidases enables their substrate-binding prior to its catalysis**. *Communications biology*, **2020**, 3, 178-1-178-9.

39. KUMP, Karson J., MIAO, Lei, MADY, Ahmed S.A., ANSARI, Nurul H., SHRESTHA, Uttar K., YANG, Yuting, PAL, Mohan, LIAO, Chenzhong, **PERDIH, Andrej**, ABULWERDI, Fardokht A., CHINNASWAMY, Krishnapriya, MEAGHER, Jennifer L., CARLSON, Jacob M., KHANNA, May, STUCKEY, Jeanne A., NIKOLOVSKA-ČOLESKA, Žaneta. **Discovery and characterization of 2,5-substituted benzoic acid dual inhibitors of the anti-apoptotic Mcl-1 and Bfl-1 proteins**. *Journal of medicinal chemistry*, **2020**, 63, 2489-2510.

38. VITOROVIĆ-TODOROVIĆ, Maja D., WOREK, Franz, **PERDIH, Andrej**, BAUK, Sonja Đ., VUJATOVIĆ, Tamara B., CVIJETIĆ, Ilija N. **The in vitro protective effects of the three novel nanomolar reversible inhibitors of human cholinesterases against irreversible inhibition by organophosphorous chemical warfare agents**. *Chemico-biological interactions*, **2019**, 309, 108714-1-108714-11.

37. BERGANT LOBODA, Kaja, JANEŽIČ, Matej, VALJAVEC, Katja, SOSIČ, Izidor, PAJK, Stane, ŠTAMPAR, Martina, ŽEGURA, Bojana, GOBEC, Stanislav, FILIPIČ, Metka, **PERDIH, Andrej**. **Structure-guided optimization of 4,6-substituted-1,3,5-triazin-2(1H)-ones as catalytic inhibitors of human DNA topoisomerase IIα**. *European Journal of Medicinal Chemistry*, **2019**, 175, 330-348.

36. SZUTKOWSKI, Kosma, SIKORSKA, Emilia, BAKANOVYCH, Iulia, ROY CHOUDHURY, Amrita, **PERDIH, Andrej**, JURGA, Stefan, NOVIČ, Marjana, ZHUKOV, Igor. **Structural analysis and dynamic processes of the transmembrane segment inside different micellar environments-implications for the TM4 fragment of the bilitranslocase protein**. *International journal of molecular sciences*, **2019**, 20, 4172-1-4172-21.

35. BORIŠEK, Jure, PINTAR, Sara, OGRIZEK, Mitja, TURK, Dušan, **PERDIH, Andrej**, NOVIČ, Marjana. **A water-assisted catalytic mechanism in glycoside hydrolases demonstrated on the Staphylococcus aureus autolysin E**. *ACS catalysis*, **2018,** 8, 4334-4345.

34. BORIŠEK, Jure, PINTAR, Sara, OGRIZEK, Mitja, GOLIČ GRDADOLNIK, Simona, HODNIK, Vesna, TURK, Dušan, **PERDIH, Andrej**, NOVIČ, Marjana. **Discovery of (phenylureido)piperidinyl benzamides as prospective inhibitors of bacterial autolysin E from Staphylococcus aureus.** *Journal of enzyme inhibition and medicinal chemistry*, **2018**, 33, 1239-1247.

33. STEVANOVIĆ, Strahinja, **PERDIH, Andrej**, SENCANSKI, Milan, GLISIC, Sanja, DUARTE, Margarida, TOMÁS, Ana M., SENA, Filipa V., SOUSA, Filipe M., PEREIRA, Manuela M., ŠOLMAJER, Tomaž. **In silico discovery of a substituted 6-methoxy-quinalidine with leishmanicidal activity in *Leishmania infantum***. *Molecules*, **2018**, 23, 1-17.

32. MADY, Ahmed S.A., LIAO, Chenzhong, BAJWA, Naval, KUMP, Karson J., ABULWERDI, Fardokht A., LEV, Katherine, MIAO, Lei, GRIGSBY, Sierrah M., **PERDIH, Andrej**, STUCKEY, Jeanne A., DU, Yuhong, FU, Haian, NIKOLOVSKA-ČOLESKA, Žaneta. **Discovery of Mcl-1 inhibitors from integrated high throughput and virtual screening.** *Scientific reports*, **2018**, 8, 10210-1-10210-15.

31. RIČKO, Sebastijan, MEDEN, Anže, IVANČIČ, Anže, **PERDIH, Andrej**, ŠTEFANE, Bogdan, SVETE, Jurij, GROŠELJ, Uroš. **Organocatalyzed deracemisation of Δ2-pyrrolin-4-ones**. *Advanced Synthesis & Catalysis*, **2017**, 359, 2288-2296.

30. USENIK, Aleksandra, RENKO, Miha, MIHELIČ, Marko, LINDIČ, Nataša, BORIŠEK, Jure, **PERDIH, Andrej**, PRETNAR, Gregor, MÜLLER, Uwe, TURK, Dušan. **The CWB2 cell wall-anchoring module is revealed by the crystal structures of the Clostridium difficile cell wall proteins Cwp8 and Cwp6**. *Structure*, **2017**, 25, 514-521.

29. JANEŽIČ, Matej, POGORELČNIK, Barbara, BRVAR, Matjaž, ŠOLMAJER, Tomaž, **PERDIH, Andrej**. **3-substituted-1*H*-indazoles as catalytic inhibitors of the human DNA topoisomerase II [alpha]**. *ChemistrySelect*, **2017**, 2, 480-488.

28. RIČKO, Sebastijan, SVETE, Jurij, ŠTEFANE, Bogdan, **PERDIH, Andrej**, GOLOBIČ, Amalija, MEDEN, Anže, GROŠELJ, Uroš. **1,3-diamine-derived bifunctional organocatalyst prepared from camphor**. *Advanced Synthesis & Catalysis*, **2016**, 358, 3786-3796.

27. ENIYAN, Kandasamy, KUMAR, Anuradha, RAYASAM, Geetha Vani, **PERDIH, Andrej**, BAJPAI, Urmi. **Development of a one-pot assay for screening and identification of Mur pathway inhibitors in Mycobacterium tuberculosis**. *Scientific reports*, **2016**, 6, 35134-1-35134-12.

26. POGORELČNIK, Barbara, JANEŽIČ, Matej, SOSIČ, Izidor, GOBEC, Stanislav, ŠOLMAJER, Tomaž, **PERDIH, Andrej**. **4,6- substituted-1,3, 5-triazin-2(1H)-ones as monocyclic catalytic inhibitors of human DNA topoisomerase IIα targeting the ATP binding site**. *Bioorganic & Medicinal Chemistry*, **2015**, 23, 4218-4229.

25. AL-ASRI, Jamil, FAZEKAS, Erika, LEHOCZKI, Gábor, **PERDIH, Andrej**, GÖRICK, Cornelia, MELZIG, Matthias F., GYÉMÁNT, Gyöngyi, WOLBER, Gerhard, MORTIER, Jérémie. **From carbohydrates to drug-like fragments: rational development of novel α–amylase inhibitors**. *Bioorganic & Medicinal Chemistry*, **2015**, 23, 6725-6732.

24. POGORELČNIK, Barbara, BRVAR, Matjaž, ŽEGURA, Bojana, FILIPIČ, Metka, ŠOLMAJER, Tomaž, **PERDIH, Andrej**. **Discovery of mono- and disubstituted 1H-pyrazolo[3,4]pyrimidines and 9H-purines as catalytic inhibitors of human DNA topoisomerase IIα** . *ChemMedChem: Chemistry Enabling Drug Discovery*, **2015**, 10, 345-359.

23. **PERDIH, Andrej**, HRAST, Martina, PUREBER, Kaja, BARRETEAU, Hélène, GOLIČ GRDADOLNIK, Simona, KOCJAN, Darko, GOBEC, Stanislav, ŠOLMAJER, Tomaž, WOLBER, Gerhard. **Furan-based benzene mono- and dicarboxylic acid derivatives as multiple inhibitors of the bacterial Mur ligases (MurC-MurF): experimental and computational characterization**. *Journal of computer-aided molecular design*, **2015**, 29, 541-560.

22. MARTINČIČ, Rok, MRAVLJAK, Janez, ŠVAJGER, Urban, **PERDIH, Andrej**, ANDERLUH, Marko, NOVIČ, Marjana. **In silico discovery of novel potent antioxidants on the basis of pulvinic acid and coumarine derivatives and their experimental evaluation**. *PloS one*, **2015**, 10, e0140602.

21. POGORELČNIK, Barbara, BRVAR, Matjaž, ZAJC, Irena, FILIPIČ, Metka, ŠOLMAJER, Tomaž, **PERDIH, Andrej**. **Monocyclic 4-amino-6-(phenylamino)-1,3, 5-triazines as inhibitors of human DNA topoisomerase IIα**. *Bioorganic & Medicinal Chemistry Letters*, **2014**, 24, 5762-5768.

20. **PERDIH, Andrej**, HRAST, Martina, BARRETEAU, Hélène, GOBEC, Stanislav, WOLBER, Gerhard, ŠOLMAJER, Tomaž. **Benzene-1,3-dicarboxylic acid 2, 5-dimethylpyrrole derivatives as multiple inhibitors of bacterial Mur ligases (MurC-MurF)**. *Bioorganic & Medicinal Chemistry*, **2014,** 22, 4124-4134

19. **PERDIH, Andrej**, HRAST, Martina, BARRETEAU, Hélène, GOBEC, Stanislav, WOLBER, Gerhard, ŠOLMAJER, Tomaž. **Inhibitor design strategy based on an enzyme structural flexibility: a case of bacterial MurD ligase**. *Journal of chemical information and modeling*, **2014**, 54, 1451-1466.

18. ROY CHOUDHURY, Amrita, **PERDIH, Andrej**, ŽUPERL, Špela, SIKORSKA, Emilia, ŠOLMAJER, Tomaž, JURGA, Stefan, ZHUKOV, Igor, NOVIČ, Marjana. **Structural elucidation of transmembrane transporter protein bilitranslocase: conformational analysis of the second transmembrane region TM2 by molecular dynamics and NMR spectroscopy**. *Biochimica et biophysica acta, Biomembranes*, **2013**, 1828, 2609-2619

17. ŠKEDELJ, Veronika, **PERDIH, Andrej**, BRVAR, Matjaž, KROFLIČ, Ana, DUBBÉE, Vincent, SAVAGE, Victoria, O'NEILL, Alex J., ŠOLMAJER, Tomaž, BEŠTER-ROGAČ, Marija, BLANOT, Didier, HUGONNET, Jean-Emmanuel, MAGNET, Sophie, ARTHUR, Michel, MAINARDI, Jean-Luc, STOJAN, Jure, ZEGA, Anamarija. **Discovery of the first inhibitors of bacterial enzyme D-aspartate ligase from Enterococcus faecium (Aslfm)**. *European Journal of Medicinal Chemistry*, **2013**, 67, 208-220.

16. MINOVSKI, Nikola, **PERDIH, Andrej**, NOVIČ, Marjana, ŠOLMAJER, Tomaž. **Cluster-based molecular docking study for in silico identification of novel 6-fluoroquinolones as potential inhibitors against mycobacterium tuberculosis**. *Journal of computational chemistry*, **2013**, 34, 790-801

15. **PERDIH, Andrej**, WOLBER, Gerhard, ŠOLMAJER, Tomaž. **Molecular dynamics simulation and linear interaction energy study of D-Glu-based inhibitors of the MurD ligase**. *Journal of computer-aided molecular design*, **2013**, 27, 723-738.

14. BRVAR, Matjaž, **PERDIH, Andrej**, HODNIK, Vesna, RENKO, Miha, ANDERLUH, Gregor, JERALA, Roman, ŠOLMAJER, Tomaž. **In silico discovery and biophysical evaluation of novel 5-(2-hydroxybenzylidene) rhodanine inhibitors of DNA gyrase B**. *Bioorganic & Medicinal Chemistry*, **2012**, 20, 2572-2580.

13. **PERDIH, Andrej**, ŠOLMAJER, Tomaž. **MurD ligase from Escherichia coli: C-terminal domain closing motion**. *Computational and theoretical chemistry*, **2012**, 979, 73-81,

12. BRVAR, Matjaž, **PERDIH, Andrej**, RENKO, Miha, ANDERLUH, Gregor, TURK, Dušan, ŠOLMAJER, Tomaž. **Structure-based discovery of substituted 4, 5`-bithiazoles as novel DNA gyrase inhibitors.** *Journal of medicinal chemistry*, **2012**, 55, 6413-6426.

11. MINOVSKI, Nikola, **PERDIH, Andrej**, ŠOLMAJER, Tomaž. **Combinatorially-generated library of 6-fluoroquinolone analogs as potential novel antitubercular agents: a chemometric and molecular modeling assessment**. *Journal of molecular modeling*, **2012**, 18, 1735-1753.

10. **PERDIH, Andrej**, ROY CHOUDHURY, Amrita, ŽUPERL, Špela, SIKORSKA, Emilia, ZHUKOV, Igor, ŠOLMAJER, Tomaž, NOVIČ, Marjana. **Structural analysis of a peptide fragment of transmembrane transporter protein bilitranslocase**. *PloS one*, **2012**, 7, e38967-1-e38967-14.

9. BRVAR, Matjaž, **PERDIH, Andrej**, OBLAK, Marko, PETERLIN-MAŠIČ, Lucija, ŠOLMAJER, Tomaž. **In silico discovery of 2-amino-4-(2, 4-dihydroxyphenyl)thiazoles as novel inhibitors of DNA gyrase B**. *Bioorganic & Medicinal Chemistry Letters*, **2010**, 20, 958-962.

8. ŠTEFANE, Bogdan, **PERDIH, Andrej**, PEVEC, Andrej, ŠOLMAJER, Tomaž, KOČEVAR, Marijan. **The participation of 2H-pyran-2-ones in [4+2] cycloadditions: an experimental and computational study**. *European journal of organic chemistry*, **2010**, 5870-5883.

7. **PERDIH, Andrej**, KOVAČ, Andreja, WOLBER, Gerhard, BLANOT, Didier, GOBEC, Stanislav, ŠOLMAJER, Tomaž. **Discovery of novel benzene 1, 3-dicarboxylic acid inhibitors of bacterial MurD and MurE ligases by structure-based virtual screening approach**. *Bioorganic & Medicinal Chemistry Letters*, **2009**, 19, 2668-2673.

6. **PERDIH, Andrej**, BREN, Urban, ŠOLMAJER, Tomaž. **Binding free energy calculations of N-sulphonyl-glutamic acid inhibitors of MurD ligase**. *Journal of molecular modeling*, **2009**, 15, 983-996.

5. **PERDIH, Andrej**, HODOŠČEK, Milan, ŠOLMAJER, Tomaž. **MurD ligase from E. coli: tetrahedral intermediate formation study by hybrid quantum mechanical/molecular mechanical replica path method**. *Proteins*, **2009**, 74, 744-759.

4. STENOVEC, Matjaž, ŠOLMAJER, Tomaž, **PERDIH, Andrej**, VARDJAN, Nina, KREFT, Marko, ZOREC, Robert. **Distinct labelling of fusion events in rat lactotrophs by FM 1-43 and FM 4-64 is associated with conformational differences**. *Acta physiologica*, **2007**, 191, 35-42.

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9.3. POPULAR SCIENCE ARTICLES (in Slovene)

5. PRAŠNIKAR, Eva, BORIŠEK, Jure, **PERDIH, Andrej**. **Staranje, celična senescenca in zdravljenje s starostjo povezanih bolezni** *Proteus: ilustriran časopis za poljudno prirodoznanstvo*. **2021**, 83, 314-322.

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1. PAVLI, Matej, **PERDIH, Andrej**. **Ultrazvočno tabletiranje**. *Spatula : glasilo Študentske sekcije Slovenskega farmacevtskega društva*. **2005**, 31, str. 4-7.

9.4. PATENTS

1. PERDIH, Andrej, BERGANT LOBODA, Kaja, BRVAR, Matjaž, JANEŽIČ, Matej. **Substituted 4,5'-bithiazoles as inhibitors of the human DNA topoisomerase II**
European patent EP 3 811 940 B1

10. INVITED TALKS

12. **Dynamic model of a type II DNA topoisomerase and design of catalytic inhibitors as anticancer agents**
Faculty of Chemistry, University of Belgrade, Serbia **7. 9. 2023**

11. **Human DNA topoisomerase IIα revisited: Molecular simulations and design of catalytic inhibitors**
Faculdade de Farmácia, Universidade de Lisboa, Portugal **9. 12. 2019**

10**. Anticancer target human DNA topoisomerase IIα revisited: Design of novel catalytic inhibitors**
Institute of Pharmacy, Freie Universität Berlin, Germany **11. 12. 2017**

9**. Catalytic inhibitors of human DNA topoisomerase IIα: Revisit of an established anticancer target**
***I**nstitute of High-Performance Computing (IHPC), Singapur* **2. 2. 2017**

8**. Human DNA topoisomerase IIα: Atomistic insights and novel catalytic inhibitor design**
Department of Pathology, University of Michigan, Ann Arbor, USA, **29. 12. 2016**

7**. Understanding the MurD enzyme and novel multiple inhibitors of the Mur ligase family**
Department of Pharmaceutical Chemistry, Faculty of Life Sciences, Vienna, **13. 5. 2015**

6**. Computational approaches for designing novel selective small molecule inhibitors of Mcl-1 protein and DNA topoisomerase II**
Department of Pathology, University of Michigan, Ann Arbor, USA **23. 9. 2014**

5. **Computational exploration of the *E. Coli* MurD enzyme and in silico design of novel inhibitors of the Mur ligase family**
Department of Pathology, University of Michigan, Ann Arbor, USA **6. 5. 2013**

4. **An experimental and computational approaches to study the role of 2*H*-Pyran-2-ones in [4+2] cycloadditions**
Institute of Pharmacy, Freie Universität Berlin, Germany **10. 12. 2013**

3. **Novel insights into the dynamic model of the *E. coli* MurD enzyme and identification of multiple inhibitors of the bacterial Mur ligase family**
Institute of Pharmacy, Freie Universität Berlin, Germany **12. 2. 2013**

2. **Computational exploration of the *E. Coli* MurD enzyme and in silico design of novel inhibitors of the Mur ligase family**
Institute of Pharmacy, Freie Universität Berlin, Germany **6. 6. 2012**

1. Dynamical model of the *E. coli* MurD enzyme and in silico design of novel inhibitors
Institute of Pharmacy, University of Innsbruck, Avstrija **26. 11. 2009**

11. SUPERVISION OF STUDENTS AND RESEARCHERS

11.1. POSTDOCTORAL SCHOLARS

2. **Dr. INDRANI BARUAH** *(Cotton University, Assam, India)*
Project: Dynamical model of a type II DNA topoisomerase biological nanomachine and design of catalytic inhibitors (employed within ARIS project: J1-4402)
(November 2023 – February 2024)

1. **Dr. ILIJA CVIJETIĆ** *(University of Belgrade, Serbia)*
Project 1*:* Computational studies of nanomolar reversible inhibitors of human cholinesterases
(May-November 2018)
Project 2: Phenotypic discovery of novel inhibitors of human DNA topoisomerase IIα
(October 2021-April 2022)

11.2. DOCTORAL (PhD) STUDENTS

5. **MARTIN LJUBIČ** (ongoing): Investigation of the immune receptor NKG2A/CD94 and molecular simulation-based design of inhibitors of Src kinases, *University of Ljubljana*
Co-mentor

4. **BARBARA HERLAH** (ongoing): Dynamical model of a type II DNA topoisomerase and in silico design of novel catalytic inhibitors as potential chemotherapeutics, *University of Ljubljana*,
Mentor

3. **Dr. KAJA BERGANT LOBODA:** Design and optimization of catalytic inhibitors of the human DNA topoisomerase IIα as potential anticancer agents. *University of Ljubljana*, **2021**.
Mentor

2. **Dr. EVA PRAŠNIKAR:** Computational and experimental investigation of senescent cell modulation. *University of Ljubljana*, **2023.**
Co-mentor

1. **Dr. BARBARA POGORELČNIK** Structure-based design of novel human DNA topoisomerase IIα inhibitors. *University of Ljubljana*, **2015**.
Co-mentor

11.3. MASTER STUDENTS

14. **GAŠPER TOMŠIČ:** Experimental and computational investigation of the influence of linker heteroatoms in 4,6-substituted 1,3,5-triazin-2(1*H*)-ones on inhibition of human DNA topoisomerase IIα, *University of Ljubljana*, **2023**.
Co-mentor

13. **SARA VOJSKA:** The impact of increased flexibility of disubstituted 1,2,4-oxadiazoles on the inhibitory activity against human DNA topoisomerase IIα, *University of Ljubljana*, **2023**.
Co-mentor

12. **GAŠPER GROŠELJ:** Structure-based design and synthesis of 4,6-substituted 1,3,5-triazin-2(1*H*)-ones as catalytic inhibitors of human DNA topoisomerase IIα, *University of Ljubljana*, **2023**.
Co-mentor

11. **MELITA VELIKANJE**: Synthesis of disubstituted 1,2,4-oxadiazole inhibitors of human DNA topoisomerase IIα, *University of Ljubljana*, **2022**
Co-mentor

10. **ANJA PAVLOVIČ:** Synthesis and evaluation of novel derivatives of 4,6-substitued-1,3,5-triazin-2(1*H*)-ones as catalytic inhibitors of human DNA topoisomerase IIα, *University of Ljubljana*, **2021**.
Co-mentor

9. **KATJA VALJAVEC:** Application of computational methods to investigate the function and inhibition of a type II DNA topoisomerase molecular motor, *University of Trieste*, **2020.**
Co-mentor

8. **MAŠA OCEPEK:** Synthesis of substituted 1H-indazoles and 1H-indoles as potential inhibitors of human DNA topoisomerase IIα, *University of Ljubljana*, **2020**.
Co-mentor

7. **ALJOŠA KOROŠEC**: Optimization and evaluation of 4,6-substitued-1,3,5-triazin-2(1H)-ones as catalytic inhibitors of the human DNA topoisomerase IIα, *University of Ljubljana*, **2019**.
Co-mentor

6. **MOJCA KLEMENČIČ:** Synthesis and evaluation of 4,6-substituted-1,3,5-triazin-2(1*H*)-ones as catalytic inhibitors of human DNA topoisomerase IIα, *University of Ljubljana*, **2018**.
Co-mentor

5. **SANTINA JAZBINŠEK**: Optimization of 3,5-disubstituted 1,2,4-oxadiazoles as human DNA topoisomerase IIα inhibitors, *University of Ljubljana*, **2018**.
Co-mentor

4. **MARUŠA KLEMENČIČ:** Synthesis and evaluation of 4,6-substituted-1,3,5-triazin-2(1*H*)-ones as catalytic inhibitors of human DNA topoisomerase IIα**,** *University of Ljubljana*, **2018**.
Co-mentor

3. **SARA BAVCON:** Synthesis of 3,5-disubstituted 1,2,4-oxadiazoles as potential inhibitors of human DNA topoisomerase IIα, *University of Ljubljana*, **2018**.
Co-mentor

2. **URŠULA GRABNAR**: Prediction of endocrine activity of colours permitted to use in cosmetic products with in silico method, *University of Ljubljana*, **2016.**
Mentor

1. **MATEJ JANEŽIČ:** *In silico* design and evaluation of 1*H*-indazole inhibitors of the human toposiomerase IIα, *University of Ljubljana*, **2016.**
Co-mentor

11.4. BACHELOR STUDENTS

3. **ANA HOJAN** (ongoing): Molecular simulations of inhibitors of the human DNA topoisomerase IIα, *University of Primorska*
Mentor

2. **KATJA VALJAVEC:** Application of molecular modeling methods in design and optimization of inhibitors of the human DNA topoisomerase IIα, *University of Primorska*, **2018**.
Mentor

1. **KATJA PRAČEK**: Homology modeling and molecular simulations of the camelid nanobodies as therapeutic tools in the treatment of sarcoma**,** *University of Primorska*, **2018**.
Mentor

11.5. ERAZMUS PROGRAM STUDENTS

1. **MARTA RAQUEL ERNANDES VICENTE**: Investigation of Flavonoids as inhibitors of human DNA topoisomerase IIα**,** *University of Lisbon*, **2019.**
Mentor