

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 PhD. 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 Oberstufenprüfung (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. EDITORIAL ROLES

- 2025- Editor: *International Journal of Biological Macromolecules*, Elsevier
- 2022- Associate Editor: *Frontiers in Molecular Biosciences*, Frontiers
- 2022- Guest Editor/Special Issue: *Pharmaceuticals*, MDPI

6.2. PEER REVIEWER - Scientific Journals: more than 230 reviews conducted

Science Advances, Journal of the American Chemical Society, 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), Netherlands, French National Research Agency's (ANR), France, Czech Science Foundation (GARČR), Czech Republic, 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. COMPUTATIONAL RESOURCES

- 2024-2025 **Regular research project**
Application of molecular simulations to study the catalytic cycle of type II DNA topoisomerases
Slovenian National Supercomputing Network (SLING)

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 RESEARCH PROJECTS

- 2025-2028 **PROJECT TEAM MEMBER: ARIS basic research project N1-0404**
Computational Insight into the Development of Neurodegeneration following COVID-19 Infection
PI: prof. Janez Mavri
Slovenian Research and Innovation Agency

- 2023-2026 **PROJECT 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 **PROJECT 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 **PROJECT TEAM MEMBER: EU Horizon project EuroCC**
 EU Horizon 2020 (WP21)
 SI coordinator: dr. Jernej Stare
Horizon Europe
- 2019-2022 **PROJECT TEAM MEMBER: ARRS basic research project J1-1709**
Structural insight into the mechanism of Clostridium difficile surface formation
 PI: prof. Dušan Turk
Slovenian Research Agency
- 2014-2015 **PROJECT 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 II α
 National Institute of Chemistry and University of Michigan
 PI: prof. Tomaž Šolmajer
Slovenian Research Agency
- 2009-2011 **PROJECT 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 **PROJECT 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 Commission for Equal Opportunities in Science**
Ministry of Higher Education, Science and Innovation, Slovenia
- 2021-2026 **MEMBER Committee for Gender Equality in Science**
National Institute of Chemistry, Slovenia
- 2022 **MEMBER Slovenian Chemical Society**
- 2002 **MEMBER Slovenian Pharmaceutical Society**

9. PUBLICATIONS

9.1. ORIGINAL SCIENTIFIC ARTICLES

64. STEVANOVIĆ Kristina, HERLAH Barbara, PAVLIN Matic, PERDIH Andrej. **Asymmetric T-segment binding and gate dynamics govern the final stages of the type IIA topoisomerase catalytic cycle.** *International Journal of Biological Macromolecules*. **2025** 270, 147216.
63. LJUBIČ Martin, SOLLNER DOLENC Marija, BORIŠEK Jure, PERDIH Andrej. **Water-based pharmacophore modeling in kinase inhibitor design: A case study on Fyn and Lyn protein kinases.** *Journal of chemical information and modeling*. **2025**, 65, 9747–9761.
62. MEDEN Anže, ŽNIDARŠIČ Neža, KNEZ Damijan, WANG Yuanyuan, XU Ziwei, YANG Huajing, ZHANG Weiting, PIŠLAR Anja, **PERDIH Andrej**, KRANJC BREZAR Simona, GRGUREVIČ Neža, PAJK Stane, SUN Haopeng, GOBEC Stanislav. **Pleiotropic prodrugs for both symptomatic and disease-modifying treatment of Alzheimer’s disease.** *Acta Pharmaceutica Sinica B*, **2025**, 15, 4807-4828.
61. GLISIC, Sanja, STEVANOVIĆ Kristina, **PERDIH Andrej**, BUKREYEVA Natalya, MARUYAMA Junki, PEROVIC Vladimir, LÓPEZ-SERRANO Sergi, DARJI Ayub, RADOSEVIC Draginja, SENCANSKI Milan, VELJKOVIC Veljko, BRUNO Botta, MORI Mattia, PAESSLER Slobodan. **Influenza a Virus Inhibition: Evaluating Computationally Identified Cyproheptadine Through In Vitro Assessment.** *International journal of molecular sciences*. **2025**, 26, [article no.] 5962.
60. LJUBIČ Martin, **PERDIH Andrej**, BORIŠEK Jure. **All-Atom Simulations Reveal the Effect of Membrane Composition on the Signaling of the NKG2A/CD94/HLA-E Immune Receptor Complex.** *Journal of chemical information and modeling*, **2024**, 64, 9374–9387.
59. HERLAH, Barbara, GORIČAN, Tjaša, STRAŠEK BENEDIK, Nika, GOLIČ GRDADOLNIK, Simona, SOSIČ, Izidor, **PERDIH, Andrej**. **Simulation- and AI-directed optimization of 4,6-substituted 1,3,5-triazin-2(1H)-ones as inhibitors of human DNA topoisomerase II α .** *Computational and Structural Biotechnology Journal*. **2024**, 23, 2995-3018.
58. HERLAH, Barbara, JANEŽIČ Matej, OGRIS Iza, GOLIČ GRDADOLNIK Simona, KOLOŠA Katja, ŽABKAR Sonja, ŽEGURA Žegura Bojana, **PERDIH Andrej**. **Nature-inspired substituted 3-(imidazol-2-yl) morpholines targeting human topoisomerase II α : Dynophore-derived discovery.** *Biomedicine & Pharmacotherapy*, **2024**. 175, 116676.
57. HERLAH, Barbara, PAVLIN, Matic, **PERDIH Andrej**. **Molecular choreography: Unveiling the dynamic landscape of type IIA DNA topoisomerases before T-segment passage through all-atom simulations.** *International Journal of Biological Macromolecules*, **2024**, 269, 131991.
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-1 α 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 II α .** *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 II α .** *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 II α .** *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 II α .** *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-COLESKA, 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 II α .** *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.
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 Δ^2 -pyrrolin-4-ones.** *Advanced Synthesis & Catalysis*, **2017**, 359, 2288-2296.

30. USENIK, Aleksandra, RENKO, Miha, MIHELICH, 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-1H-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 II α 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 II α .** *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 II α .** *Bioorganic & Medicinal Chemistry Letters*, **2014**, 24, 5762-5768.

20. **PERDIH, Andrej**, HRAST, Martina, BARRETEAU, H el ene, GOBEC, Stanislav, WOLBER, Gerhard,  SOLMAJER, Toma . **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, H el ene, GOBEC, Stanislav, WOLBER, Gerhard,  SOLMAJER, Toma . **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**,  ZUPERL,  pela, SIKORSKA, Emilia,  SOLMAJER, Toma , JURGA, Stefan, ZHUKOV, Igor, NOVI , 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.  SKEDELJ, Veronika, **PERDIH, Andrej**, BRVAR, Matja , KROFLI , Ana, DUBB EE, Vincent, SAVAGE, Victoria, O'NEILL, Alex J.,  SOLMAJER, Toma , BE TER-ROGA , 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**, NOVI , Marjana,  SOLMAJER, Toma . **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,  SOLMAJER, Toma . **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.
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14. PRAŠNIKAR, Eva, BORIŠEK, Jure, **PERDIH, Andrej**. **Celična senescenca: nova terapevtska tarča pri zdravljenju s starostjo povezanih boleznih = Cell senescence: a new therapeutic target for the treatment of age-related diseases.** *Farmacevtski vestnik*. **2022**, 73, 40 – 53. (in Slovene)
13. PRAŠNIKAR, Eva, BORIŠEK, Jure, **PERDIH, Andrej**. **Senescent cells as promising targets to tackle age-related diseases.** *Ageing research reviews*. **2021**, 66101251-1-101251-33.
12. BERGANT LOBODA, Kaja, JANEŽIČ, Matej, **PERDIH, Andrej**. **Bioassays and in silico methods in the identification of human DNA topoisomerase II α inhibitors.** *Current medicinal chemistry*, **2018**, 25, 3284-3316,
11. BERGANT LOBODA, Kaja, **PERDIH, Andrej**. **Inhibitors and stabilizers of protein-protein interactions.** *Farmacevtski vestnik*, **2017**, 68, 224-233. (in Slovene)
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9. POGORELČNIK, Barbara, **PERDIH, Andrej**, ŠOLMAJER, Tomaž. **Recent advances in the development of catalytic inhibitors of human DNA topoisomerase II α as novel anticancer agents.** *Current medicinal chemistry*, **2013**, 20, 694-709.
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2. **PERDIH, Andrej**, KIKELJ, Danijel. **The application of freidinger lactams and their analogs in the design of conformationally constrained peptidomimetics.** *Current medicinal chemistry*, **2006**, 13, 1525-1556.
1. **PERDIH, Andrej**, PEČAR, Slavko. **Katalitični antioksidanti kot nove zdravilne učinkovine = Catalytic antioxidants as new drugs.** *Farmacevtski vestnik*, **2006**, 57, 24-29. (in Slovene)

9.3. POPULAR SCIENCE ARTICLES (in Slovene)

6. HERLAH Barbara, **PERDIH, Andrej**. Računalniški mikroskop: raziskovanje skrivnosti atomskih svetov z molekulskimi simulacijami *Alternator: Misliti znanost*. **2025**, 7.
5. PRAŠNIKAR, Eva, BORIŠEK, Jure, **PERDIH, Andrej**. Staranje, celična senescenca in zdravljenje s starostjo povezanih bolezni *Proteus*. **2021**, 83, 314-322.
4. VALJAVEC, Katja, **PERDIH, Andrej**. Razvoj zdravilnih učinkovin in metode računalniško podprtega načrtovanja. *Proteus*. **2019**, 81, 339, 350-358
3. VALJAVEC, Katja, BAVCON, Sara, **PERDIH, Andrej**. DNA topoizomeraze pomembne tarče protirakavih zdravilnih učinkovin. *Kemija v šoli in družbi*. **2018**, 1, 1-7.
2. MUNDA, Barbara, **PERDIH, Andrej**. Pogled v svet atomov in molekul s pomočjo računalnika - molekulsko modeliranje. *Spatula* **2013**, 61, 7-11.
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

9.5 EDITORIAL

1. **PERDIH, Andrej**. Topoisomerases as Targets for Novel Drug Discovery. *Pharmaceuticals*. **2025**, 18, [article no.] 1693.

10. INVITED TALKS

14. *International School for Advanced Studies (SISSA), Trieste, Italy* **6. 5. 2025**
Design of Catalytic Inhibitors of Type IIA Topoisomerase: Investigating an Alternative Inhibition Paradigm in Chemotherapy
13. *Faculty of Chemistry, Jagiellonian University, Krakow, Poland* **10. 4. 2024**
Decoding Type II DNA Topoisomerases: Dynamic Molecular Models and Catalytic Inhibitor Design for Optimized Chemotherapy
12. *Faculty of Chemistry, University of Belgrade, Serbia* **7. 9. 2023**
Dynamic model of a type II DNA topoisomerase and design of catalytic inhibitors as anticancer agents
11. *Faculty of Pharmacy, University of Lisbon, Portugal* **9. 12. 2019**
Human DNA topoisomerase II α revisited: Molecular simulations and design of catalytic inhibitors
10. *Institute of Pharmacy, Freie Universität Berlin, Germany* **11. 12. 2017**
Anticancer target human DNA topoisomerase II α revisited: Design of novel catalytic inhibitors
9. *Institute of High-Performance Computing (IHPC), Singapur* **2. 2. 2017**
Catalytic inhibitors of human DNA topoisomerase II α : Revisit of an established anticancer target
8. *Medical School, University of Michigan, Ann Arbor, USA* **29. 12. 2016**
Human DNA topoisomerase II α : Atomistic insights and novel catalytic inhibitor design
7. *Faculty of Life Sciences, University of Vienna, Austria* **13. 5. 2015**
Understanding the MurD enzyme and novel multiple inhibitors of the Mur ligase family
6. *Medical School, University of Michigan, Ann Arbor, USA* **23. 9. 2014**
Computational approaches for designing novel selective small molecule inhibitors of Mcl-1 protein and DNA topoisomerase II
5. *Medical School, University of Michigan, Ann Arbor, USA* **6. 5. 2013**
Computational exploration of the *E. Coli* MurD enzyme and in silico design of novel inhibitors of the Mur ligase family
4. *Institute of Pharmacy, Freie Universität Berlin, Germany* **10. 12. 2013**
An experimental and computational approaches to study the role of 2H-Pyran-2-ones in [4+2] cycloadditions
3. *Institute of Pharmacy, Freie Universität Berlin, Germany* **12. 2. 2013**
Novel insights into the dynamic model of the *E. coli* MurD enzyme and identification of multiple inhibitors of the bacterial Mur ligase family
2. *Institute of Pharmacy, Freie Universität Berlin, Germany* **6. 6. 2012**
Computational exploration of the *E. Coli* MurD enzyme and in silico design of novel inhibitors of the Mur ligase family
1. *Institute of Pharmacy, University of Innsbruck, Austria* **26. 11. 2009**
Dynamical model of the *E. coli* MurD enzyme and in silico design of novel inhibitors

11. SUPERVISION OF STUDENTS AND RESEARCHERS

11.1. POSTDOCTORAL RESEARCHERS

5. Dr. KRISTINA STEVANOVIĆ

Project: Dynamical model of a type II DNA topoisomerase biological nanomachine and design of catalytic inhibitors (employed within ARIS project: J1-4402)
(August 2024 - ongoing)

4. Dr. BARBARA HERLAH

Project: Dynamical model of a type II DNA topoisomerase biological nanomachine and design of catalytic inhibitors (employed within ARIS project: J1-4402)
(November 2024 - February 2025)

3. Dr. INDRANI BARUAH

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)

2. Dr. MATIC PAVLIN

Project: Molecular simulations of yeast type II topoisomerases (*part time*)
(December 2019- December 2021)

1. Dr. ILIJA CVIJETIĆ

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 II α
(October 2021-April 2022)

11.2. DOCTORAL STUDENTS

6. **JAN VAN ELTEREN** (ongoing) Molecular simulation-based investigation of catalytic inhibitors targeting type IIA DNA topoisomerases, *University of Ljubljana*

Mentor

5. **Dr. MARTIN LJUBIČ** Investigation of the immune receptor NKG2A/CD94 and molecular simulation-based design of inhibitors of Src kinases, *University of Ljubljana* **2025**.

Co-mentor

4. **Dr. BARBARA HERLAH:** Dynamical model of a type II DNA topoisomerase and in silico design of novel catalytic inhibitors as potential chemotherapeutics, *University of Ljubljana*, **2024**.

Mentor

3. **Dr. EVA PRAŠNIKAR:** Computational and experimental investigation of senescent cell modulation. *University of Ljubljana*, **2023**.

Co-mentor

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

Mentor

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

Co-mentor

11.3. MASTER STUDENTS

16. **LUKA GOLIČNIK**: Computer-aided optimization, synthesis, and evaluation of 4,6-substituted 1,3,5-triazine-2(1*H*)-ones as catalytic inhibitors of human DNA topoisomerase II α , *University of Ljubljana* **2026**.

Co-mentor

15. **ANA BRENCE**: Synthesis and evaluation of 3,5-disubstituted 1,2,4-thiadiazoles as human DNA topoisomerase II α inhibitors, *University of Ljubljana* **2025**.

Co-mentor

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 II α , *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 II α , *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 II α , *University of Ljubljana*, **2023**.

Co-mentor

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

Co-mentor

10. **ANJA PAVLOVIČ**: Synthesis and evaluation of novel derivatives of 4,6-substituted-1,3,5-triazin-2(1*H*)-ones as catalytic inhibitors of human DNA topoisomerase II α , *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 1*H*-indazoles and 1*H*-indoles as potential inhibitors of human DNA topoisomerase II α , *University of Ljubljana*, **2020**.

Co-mentor

7. **ALJOŠA KOROŠEC**: Optimization and evaluation of 4,6-substituted-1,3,5-triazin-2(1*H*)-ones as catalytic inhibitors of the human DNA topoisomerase II α , *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 II α , *University of Ljubljana*, **2018**.

Co-mentor

5. **SANTINA JAZBINŠEK**: Optimization of 3,5-disubstituted 1,2,4-oxadiazoles as human DNA topoisomerase II α 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 II α , *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 II α , *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 topoisomerase II α , *University of Ljubljana*, **2016**.

Co-mentor

11.4. BACHELOR STUDENTS

3. **ANA HOJAN**: Molecular simulations of triazinone inhibitors of human DNA topoisomerase II α , *University of Primorska*, **2025**

Mentor

2. **KATJA VALJAVEC**: Application of molecular modeling methods in design and optimization of inhibitors of the human DNA topoisomerase II α , *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 II α , *University of Lisbon*, **2019**.

Mentor