Curriculum vitae

AGRIS BĒRZIŅŠ

Laboratory of Molecular Crystals
Faculty of Chemistry
University of Latvia
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Born: September 8, 1986 — Tukums, Latvia
Nationality: Latvian
Languages: Latvian (native), English (C1), Russian (A2)

CURRENT POSITION

University of Latvia, Faculty of Chemistry

Senior researcher	Since 2016
Assistant professor	Since 2018
Head of Chair of Physical Chemistry	Since 2019

EDUCATION

Doctor of Chemistry, University of Latvia, Faculty of Chemistry	2015
Master of Science in Chemistry, University of Latvia, Faculty of Chemistry	2011
Bachelor of Science in Chemistry, University of Latvia, Faculty of Chemistry	2009

RESEARCH EXPERIENCE

University of Latvia, Faculty of Chemistry

- Unofficially Head of Laboratory of Molecular Crystals — Since 2018

Leader of Latvian Council of Science project *Crystal engineering of pharmaceutical multicomponent phases for more efficient crystalline phase design*. Supervisor or 2 PhD students and several Mater and Bachelor students. Results: 1 publication, 5 presentations in international conferences.

- Senior researcher in postdoc position — Since 2017

Research project: Development of method to control the crystallization of selected pharmaceutical molecules using templates and study of the control mechanism. Scientific consultant: Prof. A. Actiņš. Research is performed by collaborating with prof. Sally L. Price, UCL Department of Chemisty, Dr. Matteo Salvalaglio, UCL Department of Chemical Engineering and prof. Joop Ter Horst, Strathclyde Institute Of Pharmacy And Biomedical Sciences. Results: 4 presentations in international conferences.

- Senior researcher and researcher — Since 2014

Research topic: Rationalization of solvate formation, phase transitions and crystal structure diversity of pharmaceutically active molecules. Advisor: Prof. A. Actiņš. Results: 7 publications, 2 presentations in international conferences. Participation in 3 contract works ordered by pharmaceutical companies.

- Doctoral thesis research 2011-2015

Doctoral thesis: "On the rationalization of the formation, stability and phase transitions of pharmaceutically active solid substance solvates". Advisor: Prof. A. Actiņš. Results: 6 publications, 8 presentations in international conferences.

- Undergraduate researcher 2006-2011

Results: 4 publications, 2 presentations in international conferences.

Durham University, Department of Chemistry

- Visiting researcher within the framework of Erasmus student mobility 2013

Study of pharmaceutically active molecules solvates and solvent molecule dynamics using solid-state NMR spectroscopy and theoretical calculations. Advisor: Dr. P. Hodgkinson. Results: 1 publication and 1 presentation in international conference (included in the doctoral thesis).

RESEARCH INTERESTS

- Rationalization of solvate formation and diversity of pharmaceutically active molecules.
- Research and possibilities to control the solid form obtained in the crystallization from solution.
- Rationalization of desolvation mechanism of pharmaceutically active molecule solvates using phase transition, desolvation kinetics, and crystal structure studies as well as theoretical calculations.
- Polymorphism of pharmaceutically active molecules.
- Use of quantum chemistry calculations for studies of organic solids and their stability.
- Rationalization of driving forces leading to the formation of particular crystal structures of pharmaceutically active molecules.

TRAINING

Course "Hands-on Tutorial on Crystal Structure Prediction using the USPEX Code", Montreal, Canada 2014
Course "Tailor-made force fields and dispersion-corrected DFT for crystal structure prediction and other crystallographic applications", Montreal, Canada 2014
Course „Introduction to Gaussian: Theory and Practice", Wroclaw, Poland 2013
Course „MSSC2012 - *Ab Initio* Modelling in Solid State Chemistry", London, UK 2012
Course „Polymorphism and crystal forms", Jyvaskyla, Finland 2010

TEACHING EXPERIENCE

University of Latvia, Faculty of Chemistry
Assistant professor Since 2018
Lecturer 2015-2018
Reader 2012-2014
Structure of Atoms and Molecules (Bachelor of Science program)
Physical Chemistry I (Bachelor of Science program)

Physical Chemistry II (Bachelor of Science program)
Kinetics and Catalysis (Bachelor of Science program)
Physical Chemistry (Master of Science program)
Laboratory assistant 2007-2012
Physical Chemistry I (Bachelor of Science program)
Physical Chemistry II (Bachelor of Science program)

AWARDS

Ludo Frevel Crystallography Scholarship (ICDD) 2014
Bronze medal in 37th International Chemistry Olympiad 2005

SCIENTIFIC PUBLICATIONS

A. INDEXED IN SCOPUS/WOS

1. Kons, A., **Bērziņš, A.**, Actiņš, A., Rekis, T., van Smaalen, S., Mishnev, A. Polymorphism of R-Encenicline Hydrochloride: Access to the Highest Number of Structurally Characterized Polymorphs Using Desolvation of Various Solvates. Cryst. Growth Des. 2019, 19, (8), 4765-4773.
2. Trimdale, A., **Bērziņš, A.** Evaluation of Aspects Controlling Crystallization of Nitrofurantoin. Key Eng. Mater. 2019, 800, 9-13.
3. Filipova, I., Fridrihsone, V., Cabulis, U., Bērziņš, A. Synthesis of Nanofibrillated Cellulose by Combined Ammonium Persulphate Treatment with Ultrasound and Mechanical Processing. Nanomaterials 2018, 8, (9), 640.
4. Rekis, T., **Bērziņš, A.** On the structural aspects of solid solutions of enantiomers: an intriguing case study of enantiomer recognition in the solid state. CrystEngComm 2018, 20, 6909-6918.
5. **Bērziņš, A.**; Zvaniņa, D.; Trimdale, A. Detailed analysis of packing efficiency allows rationalization of solvate formation propensity for selected structurally similar organic molecules. Cryst. Growth Des. 2018, 10.1021/acs.cgd.7b01457
6. Bobrovs, R.; Kons, A.; **Bērziņš, A.**; Rekis, T.; Actinš, A. On the formation and transformations of organic salt hydrates: four encenicline hydrochloride monohydrates and respective isostructural desolvates. Cryst. Growth Des. 2018, 10.1021/acs.cgd.7b01561
7. Rekis, T.; **Bērziņš, A.**; Sarceviča, I.; Kons, A.; Balodis, M.; Orola, L.; Lorenz, H.; Actiņš, A. A Maze of Solid Solutions of Pimobendan Enantiomers: An Extraordinary Case of Polymorph and Solvate Diversity. Cryst. Growth Des. 2018, 18, (1), 264–273.
8. **Bērziņš, A.**; Trimdale, A.; Kons, A.; Zvaniņa, D. On the formation and desolvation mechanism of organic molecule solvates: a structural study of methyl cholate solvates. Cryst. Growth Des. 2017, 17, (11), 5712–5724.
9. Rekis, T.; **Bērziņš, A.**; Džabijeva, D.; Nakurte, I.; Orola, L.; Actinš, A. Structure and stability of racemic and enantiopure pimobendan monohydrates: On the phenomenon of unusually high stability. Cryst. Growth Des. 2017, 17, (4), 1814-1823.
10. Kons, A.; **Bērziņš, A.**; Actinš, A. Polymorphs and hydrates of sequifenadine hydrochloride: Crystallographic explanation of observed phase transitions and thermodynamic stability. Cryst. Growth Des. 2017, 17, (3), 1146-1158.
11. Rekis, T.; **Bērziņš, A.**; Orola, L.; Holczbauer, T.; Actiņš, A.; Seidel-Morgenstern, A.; Lorenz, H. Single enantiomer's urge to crystallize in centrosymmetric space groups: Solid solutions of phenylpiracetam. Cryst. Growth Des. 2017 17, (3), 1411-1418.
12. **Bērziņš, A.**; Actiņš, A., Why Do Chemically Similar Pharmaceutical Molecules Crystallize in Different Structures: A Case of Droperidol and Benperidol. Cryst. Growth Des. 2016, 16, (3), 1643–1653.

13. Kons, A.; Rutkovska, L.; **Bērziņš, A.**; Bobrovs, R.; Actiņš, A.,Three anhydrous forms and a dihydrate form of quifenadine hydrochloride: a structural study of the thermodynamic stability and dehydration mechanism. CrystEngComm 2015, 17, (19), 3627-3635.
14. **Bērziņš, A.**; Skarbulis, E.; Actiņš, A., Structural characterization and rationalization of formation, stability, and transformations of benperidol solvates. Cryst. Growth Des. 2015, 15, (5), 2337-2351.
15. **Bērziņš, A.**; Hodgkinson, P., Solid-state NMR and computational investigation of solvent molecule arrangement and dynamics in isostructural solvates of droperidol. Solid State Nucl. Magn. Reson. 2015, 65, 12–20.
16. **Bērziņš, A.**; Rekis, T.; Actiņš, A., Comparison and Rationalization of Droperidol Isostructural Solvate Stability: An Experimental and Computational Study. Cryst. Growth Des. 2014, 14, (7), 3639–3648.
17. **Bērziņš, A.**; Skarbulis, E.; Rekis, T.; Actiņš, A., On the Formation of Droperidol Solvates: Characterization of Structure and Properties. Cryst. Growth Des. 2014, 14, (5), 2654−2664.
18. **Bērziņš, A.**; Actiņš, A., Effect of Experimental and Sample Factors on Dehydration Kinetics of Mildronate Dihydrate: Mechanism of Dehydration and Determination of Kinetic Parameters. J. Pharm. Sci. 2014, 103, (6), 1747–1755.
19. **Bērziņš, A.**; Actiņš, A., Dehydration of mildronate dihydrate: a study of structural transformations and kinetics. CrystEngComm 2014, 16, (19), 3926–3934.
20. Sutka, A.; Kukle, S.; Gravitis, J.; **Bērziņš, A.** Chemical and physical modification of hemp fibres by steam explosion technology. IOP Conf. Series: Materials Science and Engineering 2013, 49, 012053.
21. Krūkle-Bērziņa, K.; Actiņš, A.; **Bērziņš A.**, A new methodology for the simulation of solid state phase transition kinetics by combination of nucleation and nuclei growth processes. J. Mathem. Chem. 2012, 50, (8), 2120-2129.
22. **Bērziņš, A.**; Krūkle, K.; Actiņš, A.; Kreišmanis, J.P., The relative stability of xylazine hydrochloride polymorphous forms. Pharm. Dev. Technol. 2010, 15, (2), 217-222.
23. **Bērziņš, A.**; Actiņš, A.; Kreišmanis, J.P., Hydration and dehydration kinetics of xylazine hydrochloride. Pharm. Dev. Technol. 2009, 14, (4), 388-399.

B. NOT INDEXED IN SCOPUS/WOS

1. Kons, A.; **Bērziņš, A.**; Krūkle, K.; Actiņš, A., Characterization and Physicochemical Evaluation of Molecular Complexes Formed Between Umifenovir and Dicarboxylic Acids. Latv. J. Chem. 2014, 52, (1-2), 28-40.
2. **Bērziņš, A.**; Actiņš, A., Evaluation of Kinetic Parameter Calculation Methods for Non-Isothermal Experiments in Case of Varying Activation Energy in Solid-State Transformations. Latv. J. Chem. 2012, 51, (3), 209-227.
3. Krūkle-Bērziņa, K.; Actiņš, A.; **Bērziņš A.**, Hydration of Xylazine hydrochloride polymorphic forms A, Z and M. Latv. J. Chem. 2011, 50, (1-2), 73-84.
4. **Bērziņš, A.**; Actiņš, A., Ksilazīna hidrogēnhlorīda kristāliskās formas. Latvijas Ķīmijas Žurnāls 2008, 3, 263-269.

PRESENTATIONS IN INTERNATIONAL CONFERENCES

1. Trimdale, A., **Bērziņš, A.** Computational Study of Association of Dihydroxybenzoic Acids in Solution: Testing the Molecular Self-Association Computational Methodology for Formation of Binary Systems. Materials Science and Applied Chemistry 2019, October 24th, 2019, Riga, Latvia.
2. Saršūns, K., **Bērziņš, A.** An approach for prediction of solid solution formation possibility of chemically similar molecules using calculation of lattice and intermolecular interaction energy. Material Science and Applied Chemistry 2019, October 24th, 2019, Riga, Latvia
3. **Bērziņš, A.**, Actiņš, A. Use of crystal structure prediction to design template crystallization experiments of nitrobenzoic acid derivatives. 32nd European Crystallographic Meeting, August 18 – 23, 2019, Vienna, Austria.

4. Kons, A., **Bērziņš, A.**, Rekis, T. Polymorphism of R-encenicline hydrochloride: access to the highest number of structurally characterized polymorphs using desolvation of various solvates. 32nd European Crystallographic Meeting, August 18 – 23, 2019, Vienna, Austria.
5. **Bērziņš, A.**, Kresse, I., Actiņš, A. Spectroscopic and computational study of association of 2-chloro-4-nitrobenzoic acid in solution. BACG 50th Annual Conference, July 9 – 11, 2019. London, UK.
6. **Bērziņš, A.**, Saršūns, K., Kons, A., Actiņš A. Experimental and computational investigation of solid form landscapes of several nitrobenzoic acid derivatives. 10th Crystal forms at Bologna, June 9 – 11, 2019, Bologna, Italy.
7. Saršūns, K., **Bērziņš, A.** Computational prediction and experimental confirmation of solid solution formation from different nitrobenzoic acid derivatives. 10th Crystal forms at Bologna, June 9 – 11, 2019, Bologna, Italy.
8. Trimdale, A., **Bērziņš, A**. Evaluation of crystallization control in preparation of nitrofurantoin hydrates. 10th Crystal forms at Bologna, June 9 – 11, 2019, Bologna, Italy.
9. Trimdale, A., **Bērziņš, A**. Evaluation of Aspects Controlling Crystallization of Nitrofurantoin. Materials Science and Applied Chemistry 2018, October 26th, 2018, Riga, Latvia.
10. **Bērziņš, A.**, Kresse, I., Bogdanova, E., Actiņš, A. Solid form landscapes and access to polymorphs and solvates of several chlorontrobenzoic acid isomers. 31st European Crystallographic Meeting, August 22 – 27, 2018, Oviedo, Spain.
11. Sala, E., **Bērziņš, A.**, Saršūns, K. Computional studies of droperidol /benperidol solid solution phase formation. 31st European Crystallographic Meeting, August 22 – 27, 2018, Oviedo, Spain.
12. **Bērziņš, A.**; Trimdale, A.; Actiņš, A. Crystallization control of droperidol solid forms using templates and cross-seeding. In 24th Congress and General Assembly of the International Union of Crystallography, August 21–28, 2017, Hyderabad, India.
13. Bogdanova, E.; **Bērziņš A**. Crystal structures and solid form diversity of several chloronitrobenzoic acid isomers. In Paul Walden 10 th Symposium on Organic Chemistry, June 15-16, 2017, Riga, Latvia.
14. Rekis, T.; **Berzins, A.**; Orola, L.; Actins, A.; Seidel-Morgenstern, A.; Lorenz, H. On the formation of phenylpiracetam solid solutions: thermodynamic and structural considerations. BIWIC 2016 - 23rd International Workshop on Industrial Crystallization, September 6 – 8, 2016, Magdeburg, Germany.
15. Rekis, T.; Oša, G.; **Bērziņš, A.**; Orola, L.; Sarceviča, I.; Actiņš, A.; Lorenz, H. The chaos in a solid solution decreased in the presence of a solvent: the case of racemic pimobendan. In 15th European Powder Diffraction Conference, June 12-15, 2016, Bari, Italy.
16. Rekis, T.; **Bērziņš, A.**; Orola, L.; Sarceviča, I.; Oša, G.; Heinmaa, I.; Prekup., R.; Actiņš, A. The chaos in a solid solution decreased in the presence of a solvent: the case of racemic pimobendan. In 8th Crystal Forms@Bologna, June 14-16, 2015, Bologna, Italy.
17. **Bērziņš, A.**; Actiņš, A. Structural characterization and rationalization of formation, stability, and transformations of benperidol solvates. In 13th Annual Pharmaceutical Powder X-ray Diffraction Symposium, May 18–21, 2015, Bad Herrenalb, Germany.
18. **Bērziņš, A.**; Hodgkinson, P. Solid-state NMR and computational investigation of solvent molecule arrangement and dynamics in isostructural solvates of droperidol. In SMARTER 4, September 1–4, 2014, Durham, UK.
19. **Bērziņš, A.**; Actiņš, A. Crystal structures of two molecules with small chemical structure difference. In 23rd Congress and General Assembly of the International Union of Crystallography, August 5–12, 2014, Montreal, Canada. Published in: Acta Cryst. 2014, A70, C1686.
20. **A. Bērziņš**, A. Actiņš. Computational study of the intermolecular interaction energies in droperidol solvates. In 9th European Conference on Computational Chemsitry, September 1-5, 2013, Sopron, Hungary.
21. **A. Bērziņš**, A. Actiņš. Computational study of the dehydration process of mildronate dihydrate. In 9th European Conference on Computational Chemsitry, September 1-5, 2013, Sopron, Hungary.

22. **A. Bērziņš**, A. Actiņš, T. Rēķis, E. Skarbulis, I. Sarceviča. Stability of Isostructural Solvates of Droperidol. In 7th Crystal Forms@Bologna, June 9-11, 2013, Bologna, Italy.
23. Rekis, T.; Oša, G.; Sarceviča, I.; **Bērziņš, A.**; Orola, L.; Actiņš, A. Time dependent systematic unit cell parameter change of pimobendan polymorph. In 7th Crystal Forms@Bologna, June 9-11, 2013, Bologna, Italy.
24. **A. Bērziņš**, E. Skarbulis, A. Actiņš. Preperation and Characterization of Benperidol Solvates and Polymorphs. In XVth Conference on Heterocycles in Bio-organic Chemistry, May 27-30, 2013, Riga, Latvia.
25. Rekis, T.; **Bērziņš, A.**; Actiņš, A. Stability and dehydration kinetics of pemetrexed hydrates. In XVth Conference on Heterocycles in Bio-organic Chemistry, May 27-30, 2013, Riga, Latvia.
26. **A. Bērziņš**, A. Actiņš, T. Rēķis, I. Sarceviča. Desolvation of droperidol isostructural solvates. In 11th Annual Pharmaceutical Powder X-ray Diffraction Symposium, May 15-18, 2012, Fort Myers, USA.
27. **A. Bērziņš**, T. Rēķis, A. Actiņš. Kinetics and mechanism of mildronate dihydrate dehydration. In 12th International Conference on Pharmacy and Applied Physical Chemistry, May 6-9, 2012, Graz, Austria.
28. Ausekle, E.; Priede, M.; Mekss, P.; Klimenkovs, I.; **Bērziņš, A.**; Priksane, A.; Zicmanis, A. Synthesis of long chain symetrical Ethers in Sulfonic Acid-functionalized Ionic Liquids. In 17th international scientific conference "EcoBalt 2012", October 18-19, 2012, Riga, Latvia.
29. Zariņš, A.; Ķizāne, G.; Supe, A.; Baumane, L.; **Bērziņš, A.**; Rašmane, Dz.; Šteins. I. Influence of thermal threatment on radiation stability and radyolysis on nanopowders of Lithium orthosilicate in air atmosphere. In 28th Scientific Conference of Institute of Solid State Physics, University of Latvia, February 8-10, 2012, Riga, Latvia.
30. **A. Bērziņš**, A. Actiņš, E. Skarbulis. Stability and desolvation kinetics of droperidol hydrates and ethanol solvate studied by powder x-ray diffractiometry and differential thermal analysis/thermogravimetry. In 10th Annual Pharmaceutical Powder X-ray Diffraction Symposium, May 16-19, 2011, Liona, France.
31. Zarins, A.; Supe, A.; Kizane, G.; Lescinskis, Br.; Baumane, L.; Steins, I.; **Bērziņš, A**. Accumulation of radiolysis products and defects in nanopowders of lithium orthosilicate. In International Conference on Functional Materials and Nanotechnologies FM&NT 2011, April 5-8, 2011, Riga, Latvia.
32. **A. Bērziņš**, A. Actiņš. Hydration and Dehydration of Xylazine Hydrochloride. In 11th Conference on Pharmacy & Applied Physical Chemistry, February 7-10, 2010, Innsbruck, Austria.

PATENTS

1. T. Reķis, G. Oša, A. Bērziņš, A. Actiņš. A method for preparation of pimobendan crystalline form A. LV patent; Registration number 14737 B; 25.06.2013.

ADDITIONAL PROFESSIONAL INFORMATION

Referee: Crystal Growth & Design, CrystEngComm

Latvian Council of Science expert. Science branch: Chemistry: Physical chemistry

Ludo Frevel Crystallography Scholarship (ICDD), 2014

Bronze medal, 37th International Chemistry Olimpyad, Taipei, Taiwan

09.04.2020 *A.Bērziņš*