INSTITUTUL DE CHIMIE MACROMOLECULARĂ
"PETRU PONI" - IASI
INTRARE
IESIRE Nr. 5070
Ziua 12 luna 11 anul 2026

Anexa 20

MEMORIUL ȘTIINȚIFIC

Subsemnatul Tîrnovan Petru, student doctorand în cadrul SCOSAAR, Școala Doctorală de Științe Chimice, înmatriculat la data de 01.11.2019 în domeniul de studii universitare de doctorat Chimie, la conducătorul de doctorat Prof. Dr. Laaksonen Aatto, autor al tezei de doctorat cu titlul „Studii in silico ale sistemelor dinamice auto-ansamblate în controlul transportului și eliberării principiilor active din medicamente", declar următoarele activități realizate in cadrul stagiului doctoral (se vor păstra doar activitățile realizate):

A. Lista de lucrări științifice

1. Isac, D. L., **Tirnovan, P.**, Nicolescu, A., Fifere, A., Neamtu, A., & Pinteala, M, *Cosolvent effects on the complexation of the antifungal propiconazole nitrate with β-cyclodextrin: A combined molecular dynamics and NMR study*. European Journal of Pharmaceutical Sciences, 213, 107248, 2025, https://doi.org/10.1016/j.ejps.2025.107248;

2. **Tirnovan, P.**, Isac, D. L., Marangoci, N. L., Nicolescu, A., Coroaba, A., Cretu, B., Laaksonen, A., Neamtu, A., & Pinteala, T. (2026). *Supramolecular insights into the complexation of β-Cyclodextrin for alopecia treatment using the mixed cation/anion active principle.* Carbohydrate Polymer Technologies and Applications, 14, 101155, 2026, https://doi.org/10.1016/j.carpta.2026.101155;

3. **Tirnovan, P.**, Isac, D. L., Man, I. C., Puf, R., Dascalu, A., Coroaba, A., Marangoci, N. L., Cibotariu, N., Ciuhodaru, T., Ania, C. O., Pinteala, T. (2026). *Extensive TD-DFT Investigation of the Absorption Wavelength in Single and Multilayer Polycyclic Aromatic Hydrocarbons/Graphene Quantum Carbon Dots*. Surfaces and Interfaces, 98, 110526, 2026, https://doi.org/10.1016/j.surfin.2026.110526.

Baze de date:

1. Isac, D. L., Man, I. C., **Tirnovan, P.**, (2026). Extensive TD-DFT Investigation of the Absorption Wavelength in Single and Multilayer Polycyclic Aromatic Hydrocarbons/Graphene Quantum Carbon Dots. *Zenodo*, https://doi.org/10.5281/zenodo.22525788.

Trimise spre publicare:

1. Bacaita, E. S., **Tirnovan, P.**, Laaksonen, A., Mocci, F. *Toward Reliable LCST Prediction of PNIPAM: The Influence of Water Model and Multi-Chain Interactions.* Journal of Physical Chemistry B, 12.05.2026;

B. Cărți și manuale

1. Nu este cazul

C. Participări la conferințe/workshop-uri

Comunicări orale:

1. *In silico* studies of a novel amphiphilic graft conjugated polymer for biomedical applications; **P. Tirnovan**, F. Mocci, T. Vasiliu, L. Cianga, I. Cianga, M. Pinteala, A. Laaksonen. *MacroYouth 2021*, ICMPP - *Open door to the future scientific communications of young researchers, second edition,* Iași, România; 19 Noiembrie **2021**.

2. Study of Radical Species Formation from Urocanic Acid under UV Irradiation: an Experimental and Theoretical Analysis of its Role in Skin Cancer; **P. Tirnovan**, D. L. Isac, M. Silion, A. Coroaba, T. Rusu, M. Pinteala, A. Laaksonen. *PolyChar'30: PolyChar World Forum on Advanced Materials 30 Edition*, Iași, România, 11-13 Noiembrie **2024**.

3. Unveiling the role or urocanic acid in the formation of skin cancer; **P. Tirnovan**, D. L. Isac, M. Silion, A. Coroaba, A. Laaksonen, M. Pinteala, *MacroYouth 2025, Open door to the future scientific communications of young researchers, 6th edition,* Iași, România, 19 Noiembrie **2025**. (**Premiul III**)

4. BioMat4CAST Multi-Scale *In Silico* Laboratory for Complex and Smart Biomaterials, **P. Tirnovan**, R. Puf, D. L. Isac, *ICUB-IBAR Joint Workshop; Current Topics in Molecular Biosciences*; București, România, 27 Noiembrie **2025**.

Postere

1. *In silico* Investigation of an Amphiphilic Graft Conjugated Polymer. A Comparative Study of Different Solvation Models; **P. Tirnovan**, F. Mocci, T. Vasiliu, R. Puf, T. Rusu, M. Pinteală, A. Laaksonen, *PolyChar'30: PolyChar World Forum on Advanced Materials 30 Edition, Iasi, Romania*, 11-13 Noiembrie **2024**.

2. Urocanic Acid and its Role in skin Cancer Under UV-irradiation. A Combined Experimental and Theoretical Study; **P. Tirnovan**, D. L. Isac, M. Silion, A. Coroaba, T. Rusu, M. Pinteala, F. Mocci, A. Laaksonen, *Recent Advances in Computational Biophysics: Methods and Applications*, Forschungszentrum Jülich, Germania, 3-7 Februarie **2025**.

3. Simulating molecular systems with peculiar fluorescence. A case study of lysine; **P. Tirnovan**, C. M. Carbonaro, L. V. Engelbrecht, A. Laaksonen, T. Rusu, M. Pinteala, F. Mocci, *COST COSY Training School, Exploring Confined Environments with Polymers, Ionic Liquids, and Deep Eutectic Solvents: Predicting Emerging Applications through Modeling and Advanced Experiments*, Iași, România, 8-9 Mai **2025**. (**Premiul III**)

4. Mechanistic insights into the complexation mechanism of an organic salt drug with cyclodextrin; **P. Tirnovan**, D.-L. Isac, N.-L. Marangoci, A. Neamtu, A. Laaksonen, M. Pinteala, *NGMM 2026 Next-Generation Modelling Summer School*, Sardinia, Italia, 27-31 Iulie **2026**.

5. Inclusion of an Organic Salt Drug Formulation with β-Cyclodextrin for the Treatment of Alopecia. A Theoretical and Experimental Investigation; **P. Tirnovan**, D.-L. Isac, N.-L. Marangoci, A. Nicolescu, A. Coroaba, A. Neamtu, B. Cretu, A. Laaksonen, T. Pinteala, *The 5th European Symposium on Chemical Bonding (CBOND2026)*, Bruxelles, Belgia, 8-11 Septembrie **2026**.

D. Brevete

1. Nu este cazul

E. Proiecte

1. Proiectul: „**CORTHOTEC -** Formulation of bio-absorbable class III medical device for local drug delivery", Research agreement no. 5289/09.08.2019 - CORTHOTEC LIMITED, London, UK (2020);

2. Proiectul: „**BioMat4CAST** - "Petru Poni" Institute of Macromolecular Chemistry Multi-Scale In Silico Laboratory for Complex and Smart Biomaterials" Grant Agreement No 101086667 (2024-2026);

3. Proiectul: „Intelligent systems for cancer diagnosis and treatment - **IntelDots**" PNRR-III-C9-2022-I8-291 (2024-2026).

F. Stagii de cercetare/perfecționare

1. Conferința/Seminar RACB (Recent Advances in Computational Biophysics) din Forschungszentrum Jülich, Germania, 3-7 februarie **2025**.

2. Școala de vară NGMM 2026 (Next-Generation Modeling Summer School), Sardinia, Italia, 27-31 Iulie **2026**.

G. Cursuri de perfecționare

1. Training: Advanced in Modern Molecular Modelling, susținut de BioMat4Cast ERA Chair Holder Prof. Aatto Ilmari Laaksonen, Institutul de Chimie Macromoleculară "Petru Poni", Iasi, Romania, 11 și 14 Februarie, 11 și 18 Martie **2025**;

2. Training: Investigating Membrane Proteins by Massively Parallel Quantum-Mechanical/Molecular Mechanics Simulations, susținut de Prof. Paolo Carloni, Iasi, Romania, 17 Martie **2025**,

3. 3rd FemCOSY Virtual Meeting 15 Mai (online)

4. Training: Artificial Intelligence (AI) models used for medical applications susținut de Leonard Gebac (UniBuc) Iasi, Romania, 6 Iunie **2025**,

5. COST COSY Training School: Computational Physics of Confined Systems: From Life to Material Sciences, Kyiv, Ucraina, 24-26 Iunie **2025** (online);

6. Training: In search of the physical chemistry that underlies cell receptor function, Prof. Kalina Hristova, Iasi, Romania, 26-28 Iunie **2025**;

7. Training: Synthetic Molecular Evolution of Membrane-active Peptides Prof. William C. Wimley, Iasi, Romania, 26-28 Iunie **2025**;

7. Training: Qiskit Global Summer School 2025: The Past, Present, and Future of Quantum Computing, Iasi, Romania, 7-22 Iulie, **2025**

8. Training: IBM Qiskit Road to Practitioner, Freeya Mind Campus Iasi, Romania, Aprilie-Iulie **2025**;

9. PRECISEU Personalised MedicineSchool: Advancing Healthcare Innovation, Iasi Romania, 11 Iulie **2025**;

10. Training: Multiscale QM/MM simulations within the MiMiC framework susținut de Prof. Emiliano Ippoliti (Institute of Neurosciences and Medicine (INM) Computational Biomedicine (INM-9) Forschungszentrum Jülich, Germany) Iasi, Romania, 23-25 Septembrie **2025**;

11. Training: Hands-on Training in Constant pH Molecular Dynamics (CpHMD), susținut de Dr. Daniel Kortzak (University of Maryland), Iasi, Romania, 12-15 Ianuarie **2026**;

12. Boosting Frontier Research in Romania, Universitatea Națională de Știință și Tehnologie POLITEHNICA București, 11 iunie **2026** (online).

H. Alte activități

1. Nu este cazul

Student-doctorand

