name of the unit:		symbol:
LABORATORY FOR ISOTOPE EFFECTS STUDIES http://lies.p.lodz.pl Institute of Applied Radiation Chemistry, Lodz University of Technology		I-34 http://mitr.p.lodz.pl
head of the unit:	**potential promoters:**	**contact person:**
Agnieszka Dybała-Defratyka	Agnieszka Dybała-Defratyka Piotr Paneth Michał Rostkowski (as an auxiliary supervisor) Agata Sowińska (as an auxiliary supervisor)	Agnieszka Dybała-Defratyka 31-98 agnieszka.dybala-defratyka@plodz.pl

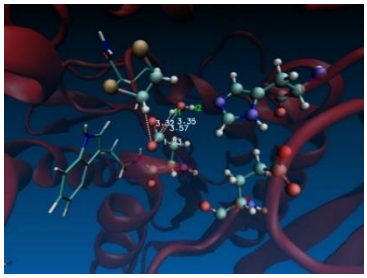
scope of activities:

1. Computations of mechanisms of chemical and enzyme-catalyzed reactions
2. Studies of isotope effects on chemical reactions and processes
3. Carbon, nitrogen, and sulfur isotopic analysis of organic samples
4. Protein-protein and protein-ligand interactions

graphic material:

present activities:

1. Isotopic authentication of products
2. Isotopic composition as marker in cancer diagnostic
3. Combined experiment-theory studies of pharmacologically active substances
4. Computations of isotope effects
5. Protein-ligand interactions in selected dehalogenases
6. Enzymatic degradation of selected halogenated organics
7. Conformational dynamics of selected enzymes
8. Computational (re)design of selected dehalogenases



Future activities:

1. Continuation of isotopic composition as marker in cancer diagnostic
2. Studies of isotope effects on association of drugs with nanostructures
3. Computational design of protein mutations
4. Evolution of enzymes involved in metabolism of persistent organic pollutants
5. Studies of membrane proteins and their interactions with small-molecule ligands with pharmacological potential
6. Development of computational tools for isotope effect calculations

The portfolio of research groups was created as part of the Programme "STER" – Internationalisation of doctoral schools" as part of the realization of the project "Curriculum for advanced doctoral education & taining – CADET Academy of Lodz University of Technology".

Publications/patents, awards, projects:

Selected publications (last 3 yrs)

1. M. Rostkowski, H. Schurner, A. Sowińska, L. Vasquez, M. Przydacz, M. Elsner, A. Dybala-Defratyka, **Isotope Effects on the Vaporization of Organic Compounds from an Aqueous Solution – Insight from Experiment and Computations**, J. Phys. Chem. B, 125 (2021) 13868, DOI: 10.1021/acs.jpcb.1c05574
2. M. Julien, M. Liegeois, P. Hohener, P. Paneth and G. Remaud, **Intramolecular non-covalent isotope effects at natural abundance associated with the migration of paracetamol in solid matrices during liquid chromatography**, J. Chromat. A 1639 (2021) 461932, DOI: 10.1016/j.chroma.2021.461932
3. A. Paneth, P. Paneth, **Isotopic Consequences of Host-Guest Interactions; Noncovalent Chlorine Isotope Effects**, J. Phys. Chem. B 125 (2021) 1874, DOI: 10.1021/acs.jpcb.0c10691
4. L. Chai, H. Zhang, R. Song, H. Yang, H. Yu, P. Paneth, K.P. Kepp, M, Akamatsu, and L. Ji, **Precision Biotransformation of Emerging Pollutants by Human Cytochrome P450 Using Computational–Experimental Synergy: A Case Study of Tris(1,3-dichloro-2-propyl) Phosphate**, Environ. Sci. Technol. 55 (2021) 14037, DOI: 10.1021/acs.est.1c03036
5. "RNA-inspired intramolecular transesterification accelerates the hydrolysis of polyethylene-like polyphosphoesters" Tobias P. Haider, Oksana Suraeva, Ingo Lieberwirth, Piotr Paneth, Frederik R. Wurm Chem. Sci. 12, 16054-16064 (2021)
6. K. Bogusiak, A. Puch, R. Mostowski, M. Kozakiewicz, P. Paneth, and J. Kobos, **Characteristic of Oral Squamous Cell Carcinoma Tissues Using Isotope Ratio Mass Spectrometry**, J. Clin. Med. 9 (2020) 3760, DOI: 10.3390/jcm9113760
7. A. Sowińska, L. Vasquez, S. Żaczek, R. N. Manna, I. Tuñón, and A. Dybala-Defratyka, **Seeking the Source of Catalytic Efficiency of Lindane Dehydrochlorinase, LinA**, J. Phys. Chem. B 124 (2020) 10353, DOI: 10.1021/acs.jpcb.0c08976
8. K. Klajman, A. Dybala-Defratyka, P. Paneth, **Computational investigations of position-specific vapor pressure isotope effects in ethanol toward more powerful isotope models for food forensics**, ACS Omega 5 (2020) 18499, DOI: 10.1021/acsomega.0c02446
9. F. Gelman, A. Dybala-Defratyka, **Bromine Isotope Effects: Predictions and Measurements**, Chemosphere, 246 (2020) 125746, DOI: 10.1016/j.chemosphere.2019.125746
10. S. Kannath, P. Adamczyk, D. Ferro-Costas, D.T. Major, A. Fernandez-Ramos, A. Dybala-Defratyka, **Role of Microsolvation and Quantum Effects in the Accurate Prediction of Kinetic Isotope Effects: The Case of Hydrogen Atom Abstraction in Ethanol by Atomic Hydrogen in Aqueous Solution**, J. Chem. Theory Comput. 16 (2020) 847, DOI: 10.1021/acs.jctc.9b00774
11. S. Kannath, P. Adamczyk, L. Wu, H.H. Richnow, A. Dybala-Defratyka, **Can Alkaline Hydrolysis of γ-HCH Serve as a Model Reaction to Study Its Aerobic Enzymatic Dehydrochlorination by LinA?**, Int. J. Mol. Sci. 20 (2019) 5955, DOI: 10.3390/ijms20235955
12. G. Ciepielowski, B. Pacholczyk-Sienicka, T. Frączek, K. Klajman, P. Paneth, Ł. Albrecht, **Comparison of quantitative NMR and IRMS spectrometry for the authentication of "Polish Vodka"**, J. Sci. Food Agricult. 99 (2019) 263-268, DOI: 10.1002/jsfa.9168
13. M. Pokora, P. Paneth, **Can Adsorption on Graphene be Used for Isotopic Enrichment? A DFT Perspective**, Molecules 23 (2018) 2981, DOI: 10.3390/molecules23112981
14. S. Żaczek, J. Kowalska, A. Dybala-Defratyka, **Ligand-Driven Conformational Dynamics Influences Selectvity of UbiX**, ChemBioChem, 2018, DOI: 10.1002/cbic.201800389
15. L. Vasquez, M. Rostkowski, F. Gelman, A. Dybala-Defratyka, **Can PIMD Make a Good Approximation for Vapor Pressure Isotope Effects Prediction for Organic Solvents? A Comparison to ONIOM QM/MM and QM Cluster Calculation**, J. Phys. Chem. B, 122 (2018) 7353, DOI: 10.1021/acs.jpcb.8b03444
16. A. Drzazga, A. Sowinska, A. Krzeminska, A. Okruszek, P. Paneth, M. Koziołkiewicz, E. Gendaszewska-Darmach, **2-OMe-lysophosphatidylcholine analogues are GPR119 ligands and activate insulin secretion from ßTC-3 pancreatic cells: Evaluation of structure-dependent biological activity**, Biochim. Biophys. Acta 1863 (2018) 91-103, DOI: 10.1016/j.bbalip.2017.10.004,

17. R.N. Manna, A. Grzybkowska, F. Gelman, A. Dybala-Defratyka, **Carbon-bromine bond cleavage – A perspective from bromine and carbon kinetic isotope effects on model debromination reactions**, Chemosphere 193 (2018) 17-23, DOI: 10.1016/j.chemosphere.2017.10.153

Grants (last three years):

1. International Center for Research on Biobased Materials - the International Research Agendas PLUS programme of the Foundation for Polish Science, co-financed by The European Union under the European Regional Development Found
2. SONATA-BIS (UMO-2-14/14/E/ST4/00041) by NCN, Poland, *Revisiting the approaches for isotope effects prediction in condensed phase*
3. Diamentowy Grant Program (0145/DIA/2017/46) by Ministry of Education and Science, Poland, *An investigation regarding biochemical synthesis of styrene and its derivatives*

Keywords:

Computational chemistry, isotope effects, isotopic analysis, computational biochemistry, enzymes, dehalogenation

List of internship proposal in this research team:

- Structural analysis and characterization of intermolecular interactions in protein-ligand systems using computational chemistry tools
- Benchmark studies of various bioinformatic tools for designing protein mutations
- Kinetic studies of selected enzymatic reactions
- Conformational studies of selected membrane proteins
- Benchmarking and testing tools for isotope effect calculations
- Testing tools for visualization and interpretation of intermolecular interactions