



Poster presentations:

1. **Anna J. Kiss-Szemán**
Ligand binding Pro-miscuity of acylpeptide hydrolase
(Presented by: Faculty member/Post-doc)
2. **Szebasztián Szaniszló**
Oxazolidine nature of the pseudoproline moiety
(Presented by: PhD candidate)
3. **Fruzsina Pilhál, Imre Jákli, Ernő Keszei, András Láng, András Perczel**
Investigation of the -AsnGly- isomerization reaction in tetrapeptides by NMR spectroscopy and ab initio calculations
(Presented by: PhD candidate)
4. **Márton Gadanez, Zsolt Fazekas, Dóra K. Menyhárd, András Perczel**
KRAS catalytic intermediates via a new NMR-driven protocol
(Presented by: PhD candidate)
5. **Ádám A. Kelemen, Zsolt Fazekas, Dóra K. Menyhárd, András Perczel, Imre Jákli**
Tracing the signatures of Acid-Catalyzed Amide Cis-Trans Isomerization in Globular Proteins
(Presented by: PhD candidate)
6. **András Gombás, Zsuzsanna Mihálka, Péter Surján, Ágnes Szabados**
The effect of orbital optimalization and correlation correction in spin-unrestricted geminal models
(Presented by: MSc student)
7. **Illés Tamás**
Hygroscopicity changes in the atmospheric aerosol of Budapest on special events
(Presented by: BSc student)
8. **Attila Kardos, Imre Varga**
Synthesis of amine-functionalized responsive nanogel particles
(Presented by: Faculty member/Post-doc)
9. **Nándor Papp, Lilla Csenge Szabó, Fanni Sebák, Andrea Bodor**
ABNMR Research in the Analytical and BioNMR Laboratory
(Presented by: Faculty member/Post-doc)
10. **Fanni Sebák**
Disordered proteins and fuzzy complexes: structural and dynamical characterization by NMR spectroscopy
(Presented by: Faculty member/Post-doc)
11. **Nándor Papp**
The Hateful Five Percent: cis-Pro47 as the Trigger of a Hidden p53–BAX Activation
(Presented by: PhD candidate)
12. **Csenge Lilla Szabó**
Protein diffusion in denaturing media and next to macromolecular crowding
(Presented by: PhD candidate)

13. **Gergő Szentpáli, Zsolt Péter Pákai**
Medicine and NMR spectroscopy - from a student's perspective
(Presented by: MSc student)
14. **Péter Hollósy**
Boundstate Vacuum Polarization
(Presented by: MSc student)
15. **Ayaki Sunaga**
12D vibrational computation of methanol and search for enhanced parity violation effects in substituted methanol compounds
(Presented by: Faculty member/Post-doc)
16. **Ádám Nonn**
Pair corrections to the no-pair Dirac-Coulomb(-Breit) energy of heliumlike systems
(Presented by: MSc student)
17. **Kevin Zsolt Simon**
99m Tc-PYP: a comprehensive investigation of its possible physiologically active structures and a preliminary study of its ATTR amyloid sensitivity
(Presented by: PhD candidate)
18. **Marlene Bosquez**
Rovibrational quantum dynamics of simple van der Waals complexes
(Presented by: PhD candidate)
19. **Barbara Keresztes, Sándor Góbi, Anita Schneiker, György Tarczay**
Cosmic-Ray-Driven Chemistry in the $\text{CH}_3\text{CH}_2\text{OH}$, NH_3 , and $\text{CH}_3\text{CH}_2\text{OH}:\text{NH}_3$ Interstellar Ice Analogs
(Presented by: PhD candidate)
20. **Barbara Keresztes, Sándor Góbi, István Pál Csonka, Gopi Ragupathy, Anita Schneiker, Gábor Bazsó, György Tarczay**
Investigating the $\text{SiH}_4 + \text{H}$ Reaction of Astrochemical Relevance
(Presented by: PhD candidate)
21. **Sándor Góbi, Barbara Keresztes, Anita Schneiker, György Tarczay**
Hydrogen-atom-assisted thione-thiol tautomerization of thiourea derivatives in para- H_2 matrix
(Presented by: Faculty member/Post-doc)
22. **Bence Fejes, Benedek Sajósi**
Laboratory Generation and Spectral Analysis of Interstellar-Relevant Radicals Originating from Isopropanol
(Presented by: BSc student)
23. **Anita Schneiker**
Astrochemical insights into the reaction of alanine and its deuterated forms with hydrogen atoms
(Presented by: PhD candidate)
24. **Khaled Jaradat, Bence B. Mészáros, János Daru**
Elucidating Chemical Reaction Mechanisms through Progressively Refined Quantum Chemical Approaches
(Presented by: Faculty member/Post-doc)
25. **Bence B. Mészáros, Khaled Jaradat, Károly Kubicskó, János Daru**
Understanding Organocatalysis: Computational Protocols for Complex Case Studies
(Presented by: PhD candidate)
26. **Bence B. Mészáros, Noémi Gargya, Ádám Madarász, János Daru**
PIMD-compatible ML Potentials from Classical Reference Simulations
(Presented by: PhD candidate)

27. **Bence B. Mészáros, András Szabó, János Daru**
Short-range Δ -Machine Learning: A cost-efficient strategy to transfer chemical accuracy to condensed phase systems
(Presented by: MSc student)
28. **Máté Kígyósi, János Daru**
Accelerating CCMD: Benchmarking ab initio protocols for high-throughput cluster calculations
(Presented by: MSc student)
29. **Csaba Hegedűs**
Towards exploring protein interaction patterns in Prdx2 and in D27 proteins by crystallography
(Presented by: PhD candidate)
30. **Máté Sulyok-Eiler**
ACWF: exploring hot-spots of organization in polymorphic amyloid fibril structures
(Presented by: PhD candidate)
31. **Márton Németh**
Transition Metal-Catalyzed Ring Opening of [1.1.1]Propellane: Synthesis of 3-Methylenecyclobut-1-ene derivatives
(Presented by: BSc student)
32. **Dávid Papp**
Investigation of Peptide Deamidation Using Cyclic Ion Mobility-Mass Spectrometry
(Presented by: PhD candidate)
33. **Péter Soma Szakály**
Advantages of Alkali Metal Adduct Ion Formation in Cyclic Ion Mobility–Mass Spectrometry of Cyclodextrin Isomers
(Presented by: PhD candidate)
34. **Péter Soma Szakály**
Application of Alkali Metal Adduct Ion Formation in Cyclic Ion Mobility Mass Spectrometric Analysis of Cyclodextrin Isomers
(Presented by: PhD candidate)
35. **Dániel Fülöp, Éva Kiss, Gergő Gyulai**
Fluidic Synthesis of Cationic Carbon Quantum Dots: Investigating Reaction Mechanism and Fluorescence Properties
(Presented by: Faculty member/Post-doc)
36. **Tamás Szidarovszky**
Simulating the strong-field Fourier-transform spectra of cations
(Presented by: Faculty member/Post-doc)
37. **Lizett Fábíán**
Simulation of the vibrational spectra of diatomic cations in SURF spectroscopy
(Presented by: BSc student)
38. **Attila Richárd Herczegh**
Katalitikus átalakítások vizsgálata biotenzid oldatokban
(Presented by: MSc student)
39. **Ádám Kapdos**
Electrochemical decarboxylative borylation
(Presented by: MSc student)
40. **Bálint Nagy**
Functionalized 2-(trifluoromethyl)buta-1,3-dienes derived from HFO gas
(Presented by: PhD candidate)

41. **Rihárd Sisa**
Synthesis of Phenol-, and Tyrosine containing dipeptide-based Diaryloxy-ethenes
(Presented by: PhD candidate)
42. **Krisztina Csörgeiné Kurin, István Szalai, Miklós Orbán**
High-amplitude pH oscillations in the $\text{S}_2\text{O}_8^{2-} - \text{S}_2\text{O}_3^{2-} - \text{Cu}^{2+} - \text{NH}_4\text{OH}$ system
(Presented by: Faculty member/Post-doc)
43. **Luca Szalay, Edina Kiss, Zoltán Tóth**
Research Programme for Public Education Development of the Hungarian Academy of Sciences
(Presented by: Faculty member/Post-doc)
44. **Dávid Péter Jelenfi**
A Novel Approach to Molecular Electron Transport:
Integrating Quantum Chemistry Embedding with the NEGF Framework
(Presented by: PhD candidate)
45. **Zsolt Szakály**
On the Faradaically Active Surface Area of Metal Foam Electrodes
(Presented by: PhD candidate)
46. **Kristóf Ferentzi**
Addressing sustainability challenges in peptide synthesis with flow chemistry and machine learning
(Presented by: PhD candidate)
47. **László Horváth, Tibor Nagy, Tamás Turányi, Máté Papp**
Fast optimization of combustion mechanisms through model and experimental data reduction
(Presented by: PhD candidate)
48. **Ákos Veres-Ravai, István Gyula Zsély, Máté Papp, Tamás Turányi**
Investigating the oxidation of dimethyl ether and dimethyl ether/hydrogen mixtures by chemical kinetic modeling
(Presented by: PhD candidate)
49. **András György Szanthoffer**
Evaluating the performances of recent detailed combustion mechanisms against NH_3 and NH_3/H_2 experimental data
(Presented by: PhD candidate)
50. **János Kóth, Márius Horváth**
Biodegradable composite thin layer for thermal and electrical protection
(Presented by: PhD candidate)
51. **Erzsébet Várnagy, Gergő Tóth, Sándor Hosztafi, Milo Malanga, Szabolcs Béni, Ida Fejős**
Enantioseparation of Xylopinine and Idelalisib by Cyclodextrin-Modified Capillary Electrophoresis and NMR Characterization of Host-Guest Complexes
(Presented by: PhD candidate)
52. **Adila Nazli**
Bioactive metabolites from Chaerophyllum and Anthriscus Species
(Presented by: PhD candidate)
53. **Daniel Bisericar**
Synthesis, Characterization, and Application of Cyclodextrin Derivatives Functionalized with Natural Amino Acids
(Presented by: PhD candidate)