ÚOCHB AV ČR
IOCB PRAGUE

Meeting with Group Leaders

Jan Konvalinka | May 24, 2024

Agenda

- IOCB Most Significant Publications 2023
- Oportunity for Collaboration
- Safety updates
- Miscellanea
  - Czech Academy of Sciences Evaluation 2020-2024
  - Price nominations

IOCB Most Significant Papers 2023

IOCB Most Significant Publications 2023

PHYS	Physical and Theoretical Chemistry
CHEM	Medicinal and Organic Chemistry
BIO	Biochemistry and Molecular Biology

2023: 39 Nominations

- **PHYS** **10** submissions [9 in 2022]
- **CHEM** **15** submissions [10 in 2022]
- **BIO** **14** submissions [9 in 2022]

IOCB Most Significant Publications 2023

- Nominated papers shortlisted by the external members of IOCB Board and trusted independent foreign experts
- The shortlist evaluated by
  - a) IAB members
  - b) external members of IOCB Board and selected outside experts
  - c) subjected to the „popular vote“ by IOCB groupleaders
- Only a) and b) votes taken into account for the award selection
- Director awarded papers highly praised by some expert IAB members or showing extraordinary potential and impact for IOCB future

Nominations 2023 – PHYS

Group	Full Citation
Tomáš Slanina	Dunlop, D., Ludvíková, L., Banerjee, A., Ottosson, H., **Slanina, T.** Excited-State (Anti)Aromaticity Explains Why Azulene Disobeys Kasha's Rule. Journal of the American Chemical Society. 2023, 145(39), 21569-21575. https://doi.org/10.1021/jacs.3c07625
Pavel Jungwirth	Tempra, C., Cruces Chamorro, V., **Jungwirth, P.** Effects of Water Deuteration on Thermodynamic and Structural Properties of Proteins and Biomembranes. Journal of Physical Chemistry B. 2023, 127(5), 1138-1143. https://doi.org/10.1021/acs.jpcb.2c08270
Petr Cígler	Kropáček, J., Maslen, C., van Dijk, B., Iniguez-Rabago, A., Overvelde, J. T. B., Zubov, A., Vrba, J**., Cígler, P.**, Štěpánek, F., Řehoř, I. Hydrogel Microrobots Self-Assembled into Ordered Structures with Programmable Actuation. Advanced Intelligent Systems. 2023, 5(9), 2300096. https://doi.org/10.1002/aisy.202300096
Pavel Hobza	Mallada Faes, B. J., Ondráček, M., Lamanec, M., Gallardo Caparrós, A. J., Jimenez-Martin, A., De La Torre Cerdeño, B., Hobza, P., Jelínek, P. Visualization of pi-hole in molecules by means of Kelvin probe force microscopy. Nature Communications. 2023, 14(1), 4954. https://doi.org/10.1038/s41467-023-40593-3
Petr Bouř	Yang, Q., Bloino, J., Šestáková, H., **Šebestík, J**., Kessler, J., Hudecová, J., Kapitán, J., **Bouř, P**. Combination of Resonance and Non-Resonance Chiral Raman Scattering in a Cobalt(III) Complex. Angewandte Chemie - International Edition. 2023, 62(45), e202312521. https://doi.org/10.1002/anie.202312521
Lubomír Rulíšek	Jaroš, A., Sasar, M., Tučková, L., Bonab, E. F., Badri, Z., **Straka, M.**, Foroutan-Nejad, C. Spinristor: A Spin-Filtering Memristor. Advanced Electronic Materials. 2023, 9(8), 2300360. https://doi.org/10.1002/aelm.202300360
Lubomír Rulíšek	Kipouros, I., Stanczak, A., Dunietz, E. M., Ginsbach, J. W., Srnec, M., **Rulíšek, L.,** Solomon, E. I. Experimental Evidence and Mechanistic Description of the Phenolic H-Transfer to the Cu2O2 Active Site of oxy-Tyrosinase. Journal of the American Chemical Society. 2023, 145(42), 22866-22870. https://doi.org/10.1021/jacs.3c07450
Ivo Starý	Houska, V., Ukraintsev, E., Vacek, J., Rybáček, J., Bednárová, L., **Pohl, R., Stará, I.** G., Rezek, B., Starý, I. Helicene-based π-conjugated macrocycles: their synthesis, properties, chirality and self-assembly into molecular stripes on a graphite surface. Nanoscale. 2023, 15(4), 1542-1553. https://doi.org/10.1039/d2nr04209f
Jiří Kaleta	Perego, J., Bezuidenhout, C. X., Bracco, S., Piva, S., Prando, G., Aloisi, C., Carretta, P., **Kaleta, J.,** Le, T. P., Sozzani, P., Daolio, A., Comotti, A. Benchmark Dynamics of Dipolar Molecular Rotors in Fluorinated Metal-Organic Frameworks. Angewandte Chemie - International Edition. 2023, 62(5), e202215893. https://doi.org/10.1002/anie.202215893
Jiří Kaleta	Lončarić, D., Movahedifar, F., Štoček, J. R., **Dračínský, M., Cvačka, J.,** Guan, S., Bythell, B. J., Císařová, I., Masson, E., **Kaleta, J.** Solvent-controlled formation of alkali and alkali-earth-secured cucurbituril/guest trimers. Chemical Science. 2023, 14(35), 9258-9266), d3sc02032k. https://doi.org/10.1039/d3sc02032k

Nominations 2023 – CHEM

Group	Full Citation
Tomáš Slanina	Žurauskas, J., Boháčová, S., Wu, S., Butera, V., Schmid, S., Domanski, M., **Slanina, T.,** Barham, J. P. Electron-Poor Acridones and Acridiniums as Super Photooxidants in Molecular Photoelectrochemistry by Unusual Mechanisms. Angewandte Chemie - International Edition. 2023, 62(44), e202307550.
Zlatko Janeba	Skácel, J., Djukic, S., Baszczyński, O., Kalčic, F., Bílek, T., Chalupský, K., Kozák, J., Dvořáková, A., Tloušťová, E., Král'ová, Z., Šmídková, M., Voldřich, J., Rumlová, M., Pachl, P., Brynda, J., Vučková, T., **Fábry, M**., Snášel, J., **Pichová, I., Řezáčová, P**., **Mertlíková-Kaiserová, H., Janeba, Z**. Design, Synthesis, Biological Evaluation, and Crystallographic Study of Novel Purine Nucleoside Phosphorylase Inhibitors. Journal of Medicinal Chemistry. 2023, 66(10), 6652-6681. https://doi.org/10.1021/acs.jmedchem.2c02097
Petr Beier	Motornov, V., Klepetářová, B., **Beier, P.** Cu(III) Trifluoromethyl Complexes with 1,3-Diketonate Ligands and Their Versatile Reactivity in C–H Trifluoromethylation. Advanced Synthesis & Catalysis. 2023, 365(17), 2858-2864. https://doi.org/10.1002/adsc.202300695
Tomáš Pluskal	Schmid, R., Heuckeroth, S., Korf, A., Smirnov, A., Myers, O., Dyrlund, T. S., Bushuiev, R., Murray, K. J., Hoffmann, N., Lu, M., Sarvepalli, A., Zhang, Z., Fleischauer, M., Dührkop, K., Wesner, M., Hoogstra, S. J., Rudt, E., Mokshyna, O., Brungs, C., Ponomarov, K., Mutabdžija, L., Damiani, T., Pudney, C. J., Earll, M., Helmer, P. O., Fallon, T. R., Schulze, T., Rivas-Ubach, A., Bilbao, A., Richter, H., **Pluskal, T.** Integrative analysis of multimodal mass spectrometry data in MZmine 3. Nature Biotechnology. 2023, 41(4), 447-449. https://doi.org/10.1038/s41587-023-01690-2
Milan Vrábel	Šlachtová, V., Bellová, S., La-Venia, A., Galeta, J**., Dračínský, M., Chalupský, K.,** Dvořáková, A., **Mertlíková-Kaiserová, H**., Rukovanský, P., Dzijak, R., **Vrábel, M.** Triazinium Ligation: Bioorthogonal Reaction of N1-Alkyl 1,2,4-Triazinium Salts. Angewandte Chemie - International Edition. 2023, 62(36), e202306828. https://doi.org/10.1002/anie.202306828
Pavel Hobza	Civiš, S., Lamanec, M., **Špirko, V**., Kubišta, J., Špeťko, M., **Hobza, P.** Hydrogen Bonding with Hydridic Hydrogen–Experimental Low-Temperature IR and Computational Study: Is a Revised Definition of Hydrogen Bonding Appropriate? Journal of the American Chemical Society. 2023, 145(15), 8550-8559. https://doi.org/10.1021/jacs.3c00802
Eva Kudová	Abramová, V., Leal Alvarado, V., Hill, M., Smejkalová, T., Malý, M., Valeš, K., Dittert, I., Božíková, P., Kysilov, B., Hrčka Krausová, B., Vyklický, V., Balík, A., Fili, K., Kořínek, M., **Chodounská, H., Kudová, E.,** Číž, D., Martinovič, J., Černý, J., Bartůněk, P., Vyklický ml., L. Effects of Pregnanolone Glutamate and Its Metabolites on GABAA and NMDA Receptors and Zebrafish Behavior. ACS Chemical Neuroscience. 2023, 14(10), 1870-1883. https://doi.org/10.1021/acschemneuro.3c00131
Zlatko Janeba	Prener, L., Baszczyński, O., Kaiser, M. M., **Dračínský, M.**, Stepan, G., Lee, Y. J., Brumshtein, B., Yu, H., Jansa, P., Lansdon, E. B., **Janeba, Z.** Design and Synthesis of Novel HIV-1 NNRTIs with Bicyclic Cores and with Improved Physicochemical Properties. Journal of Medicinal Chemistry. 2023, 66(3), 1761-1777. https://doi.org/10.1021/acs.jmedchem.2c01574
Michal Hocek	Brunderová, M., Krömer, M., Vlková, M., **Hocek, M.** Chloroacetamide-Modified Nucleotide and RNA for Bioconjugations and Cross-Linking with RNA-Binding Proteins. Angewandte Chemie - International Edition. 2023, 62(7), e202213764. ISSN 1433-7851. https://doi.org/10.1002/anie.202213764
Michal Hocek	Kuprikova, N., Ondruš, M., Bednárová, L., Riopedre Fernández, M., Poštová Slavětínská, L., Sýkorová, V., **Hocek, M.** Superanionic DNA: enzymatic synthesis of hypermodified DNA bearing four different anionic substituents at all four nucleobases. Nucleic Acids Research. 2023, 51(21), 11428-11438. https://doi.org/10.1093/nar/gkad893
Josef Michl	**Kaleta, J., Dudič, M.,** Ludvíková, L., Liška, A., Zaykov, A., Rončević, I., Mašát, M., Bednárová, L., Dron, P. I., Teat, S. J**., Michl, J.** Phenyl-Substituted Cibalackrot Derivatives: Synthesis, Structure, and Solution Photophysics. Journal of Organic Chemistry. 2023, 88(11), 6573-6587. https://doi.org/10.1021/acs.joc.2c02706
Josef Michl	Magnera, T. F., Dron, P. I., Bozzone, J. P., Jovanovic, M., Rončević, I., Tortorici, E., Bu, W., Miller, E. M., Rogers, C. T., **Michl, J**. Porphene and porphite as porphyrin analogs of graphene and graphite. Nature Communications. 2023, 14(1), 6308. https://doi.org/10.1038/s41467-023-41461-w
Martin Dračínský	Socha, O., Osifová, Z., **Dračínský, M.** NMR-Challenge.com: An Interactive Website with Exercises in Solving Structures from NMR Spectra. Journal of Chemical Education. 2023, 100(2), 962-968. https://doi.org/10.1021/acs.jchemed.2c01067
Ullrich Jahn	Klychnikov, M., Pohl, R., Císařová, I., Hájek, M., **Jahn, U.** Concise Total Syntheses of (+)-Brefeldin A, Diastereomers and Analogs and Their Biological Activity. ChemistryEurope. 2023, 1(2), e202300030. https://doi.org/10.1002/ceur.202300030
Radim Nencka	Mejdrová, I., Dušek, J., Škach, K., Štefela, A., Škoda, J., Chalupský, K., Dohnalová, K., Pavková, I., Kronenberger, T., Rashidian, A., Smutná, L., Duchoslav, V., Smutný, T., Pávek, P., **Nencka, R.** Discovery of Novel Human Constitutive Androstane Receptor Agonists with the Imidazo[1,2-a]pyridine Structure. Journal of Medicinal Chemistry. 2023, 66(4), 2422-2456. https://doi.org/10.1021/acs.jmedchem.2c01140

Nominations 2023 – BIO

Group	Full Citation
Jiří Jiráček	Potalitsyn, P., Mrázková, L., Selicharová, I., Tencerová, M., Ferenčáková, M., Chrudinová, M., Turnovská, T., Brzozowski, A. M., Marek, A., Kaminský, J., **Jiráček, J., Žáková, L**. Non-glycosylated IGF2 prohormones are more mitogenic than native IGF2. Communications Biology. 2023, 6, 863. https://doi.org/10.1038/s42003-023-05239-6
Pavlína Řezáčová	Koutná, E., Lux, V., Kouba, T., Škerlová, J., Nováček, J., Srb, P., Hexnerová, R., Šváchová, H., Kukačka, Z., Novák, P., **Fábry, M.,** Poepsel, S., **Veverka, V.** Multivalency of nucleosome recognition by LEDGF. Nucleic Acids Research. 2023, 51(18), 10011-10025. https://doi.org/10.1093/nar/gkad674
Tomáš Slanina	Wohlrábová, L., Okoročenkova, J., Palao, E., Kužmová, E., Chalupský, K., Klán, P., **Slanina, T**. Sulfonothioated meso-Methyl BODIPY Shows Enhanced Uncaging Efficiency and Releases H2Sn. Organic Letters. 2023, 25(36), 6705-6709. https://doi.org/10.1021/acs.orglett.3c02511
Evžen Bouřa	**Šilhán, J.**, Klíma, M., Otava, T., Škvára, P., Chalupská, D., Chalupský, K., Kozic, J., **Nencka, R., Bouřa, E.** Discovery and structural characterization of monkeypox virus methyltransferase VP39 inhibitors reveal similarities to SARS-CoV-2 nsp14 methyltransferase. Nature Communications. 2023, 14(1), 2259. https://doi.org/10.1038/s41467-023-38019-1
Lenka Maletínská	Freitas-Lima, L. C., **Pačesová, A.,** Staňurová, J., **Šácha, P., Marek, A., Hubálek, M**., Kuneš, J., Železná, B., **Maletínská, L.** GPR160 is not a receptor of anorexigenic cocaine- and amphetamine-regulated transcript peptide. European Journal of Pharmacology. 2023, 949(June), 175713. https://doi.org/10.1016/j.ejphar.2023.175713
Tomáš Pluskal	**Kouba, P.,** Kohout, P., Haddadi, F., Bushuiev, A., Samusevich, R., Sedlář, J., Damborský, J., **Pluskal, T.,** Sivič, J., Mazurenko, S. Machine Learning-Guided Protein Engineering. ACS Catalysis. 2023, 13(21), 13863-13895. https://doi.org/10.1021/acscatal.3c02743
Pavel Jungwirth	Ticháček, O., Mistrík, P**., Jungwirth, P.** From the outer ear to the nerve: A complete computer model of the peripheral auditory system. Hearing Research. 2023, 440(December), 108900. https://doi.org/10.1016/j.heares.2023.108900
Eva Kudová	Solntseva, E. I., Bukanova, J. V., Kondratenko, R., **Kudová, E.** Corticosteroids as Selective and Effective Modulators of Glycine Receptors. ACS Chemical Neuroscience. 2023, 14(17), 3132-3142. ISSN 1948-7193. E-ISSN 1948-7193. https://doi.org/10.1021/acschemneuro.3c00287
Michal Hocek	Kuba, M., Khoroshyy, P., **Lepšík, M., Kužmová, E.,** Kodr, D., Kraus, T., **Hocek, M**. Real-time Imaging of Nascent DNA in Live Cells by Monitoring the Fluorescence Lifetime of DNA-Incorporated Thiazole Orange-Modified Nucleotides. Angewandte Chemie - International Edition. 2023, 62(38), e202307548. https://doi.org/10.1002/anie.202307548
Michael Mareš	Buša, M., **Matoušková, Z**., Bartošová-Sojková, P., Pachl, P., **Řezáčová, P.,** Eichenberger, R. M., Deplazes, P., Horn, M., Štefanić, S., **Mareš, M.** An evolutionary molecular adaptation of an unusual stefin from the liver fluke Fasciola hepatica redefines the cystatin superfamily. Journal of Biological Chemistry. 2023, 299(3), 102970. https://doi.org/10.1016/j.jbc.2023.102970
Michael Mareš	Martins, L. A., Buša, M., Chlastáková, A., Kotál, J., Beránková, Z., Stergiou, N., Jmel, M. A., Schmitt, E., Chmelař, J., **Mareš, M.,** Kotsyfakis, M. Protease-bound structure of Ricistatin provides insights into the mechanism of action of tick salivary cystatins in the vertebrate host. Cellular and Molecular Life Sciences. 2023, 80(11), 339. https://doi.org/10.1007/s00018-023-04993-4
Sebastian Zoll	Sülzen, H., Began, J., Dhillon, A., Kereiche, S., Pompach, P., Votrubová, J., Zahedifard, F., Šubrtová, A., Šafner, M., **Hubálek, M.,** Thompson, M., Zoltner, M., **Zoll, S.** Cryo-EM structures of Trypanosoma brucei gambiense ISG65 with human complement C3 and C3b and their roles in alternative pathway restriction. Nature Communications. 2023, 14(1), 2403. https://doi.org/10.1038/s41467-023-37988-7
Robert Hanus	Macháček, S., Tupec, M., Horáček, N., Halmová, M., Roy, A., Machara, A., Kyjaková, P., **Lukšan, O., Pichová, I., Hanus, R**. Evolution of Linoleic Acid Biosynthesis Paved the Way for Ecological Success of Termites. Molecular Biology and Evolution. 2023, 40(4), msad087. https://doi.org/10.1093/molbev/msad087
Radim Nencka	Inniss, N. L., Kozic, J., Li, F., Rosas-Lemus, M., Minasov, G., Rybáček, J., Zhu, Y., Pohl, R., Shuvalova, L., **Rulíšek, L.,** Brunzelle, J. S., Bednárová, L., Štefek, M., Kormaník, J. M., Andris, E., **Šebestík, J**., Li, A. S. M., Brown, P. J., Schmitz, U., Saikatendu, K., Chang, E., **Nencka, R.,** Vedadi, M., Satchell, K. J. F. Discovery of a Druggable, Cryptic Pocket in SARS-CoV-2 nsp16 Using Allosteric Inhibitors. ACS Infectious Diseases. 2023, 9(10), 1918-1931. https://doi.org/10.1021/acsinfecdis.3c00203

IOCB Most Significant Publications 2023 – PHYS

- Dunlop, D., Ludvíková, L., Banerjee, A., Ottosson, H., Slanina, T. **Excited-State (Anti)Aromaticity Explains Why Azulene Disobeys Kasha's Rule.** *Journal of the American Chemical Society.* 2023, 145(39), 21569-21575.

- Tempra, C., Cruces Chamorro, V., Jungwirth, P. **Effects of Water Deuteration on Thermodynamic and Structural Properties of Proteins and Biomembranes.** *Journal of Physical Chemistry B.* 2023, 127(5), 1138-1143.

- Yang, Q., Bloino, J., Šestáková, H., Šebestík, J., Kessler, J., Hudecová, J., Kapitán, J., Bouř, P. **Combination of Resonance and Non-Resonance Chiral Raman Scattering in a Cobalt(III) Complex.** *Angewandte Chemie - International Edition.* 2023, 62(45), e202312521.

IOCB Most Significant Publications 2023 – CHEM

- Civiš, S., Lamanec, M., Špirko, V., Kubišta, J., Špeťko, M., Hobza, P. **Hydrogen Bonding with Hydridic Hydrogen–Experimental Low-Temperature IR and Computational Study: Is a Revised Definition of Hydrogen Bonding Appropriate?** *Journal of the American Chemical Society.* 2023, 145(15), 8550-8559.

- Magnera, T. F., Dron, P. I., Bozzone, J. P., Jovanovic, M., Rončević, I., Tortorici, E., Bu, W., Miller, E. M., Rogers, C. T., Michl, J. **Porphene and porphite as porphyrin analogs of graphene and graphite.** *Nature Communications.* 2023, 14(1), 6308.

- Šlachtová, V., Bellová, S., La-Venia, A., Galeta, J., Dračínský, M., Chalupský, K., Dvořáková, A., Mertlíková-Kaiserová, H., Rukovanský, P., Dzijak, R., Vrábel, M. **Triazinium Ligation: Bioorthogonal Reaction of N1-Alkyl 1,2,4-Triazinium Salts.** *Angewandte Chemie - International Edition.* 2023, 62(36), e202306828.

Director's Award

- Schmid, R., Heuckeroth, S., Korf, A., Smirnov, A., Myers, O., Dyrlund, T. S., Bushuiev, R., Murray, K. J., Hoffmann, N., Lu, M., Sarvepalli, A., Zhang, Z., Fleischauer, M., Dührkop, K., Wesner, M., Hoogstra, S. J., Rudt, E., Mokshyna, O., Brungs, C., Ponomarov, K., Mutabdžija, L., Damiani, T., Pudney, C. J., Earll, M., Helmer, P. O., Fallon, T. R., Schulze, T., Rivas-Ubach, A., Bilbao, A., Richter, H., Pluskal, T. **Integrative analysis of multimodal mass spectrometry data in MZmine 3.** *Nature Biotechnology.* 2023, 41(4), 447-449.

- Socha, O., Osifová, Z., Dračínský, M. **NMR-Challenge.com: An Interactive Website with Exercises in Solving Structures from NMR Spectra.** *Journal of Chemical Education.* 2023, 100(2), 962-968.

IOCB Most Significant Publications 2023 – BIO

- Koutná, E., Lux, V., Kouba, T., Škerlová, J., Nováček, J., Srb, P., Hexnerová, R., Šváchová, H., Kukačka, Z., Novák, P., Fábry, M., Poepsel, S., Veverka, V. **Multivalency of nucleosome recognition by LEDGF.** *Nucleic Acids Research.* 2023, 51(18), 10011-10025.

- Kuba, M., Khoroshyy, P., Lepšík, M., Kužmová, E., Kodr, D., Kraus, T., Hocek, M. **Real-time Imaging of Nascent DNA in Live Cells by Monitoring the Fluorescence Lifetime of DNA-Incorporated Thiazole Orange-Modified Nucleotides.** *Angewandte Chemie - International Edition.* 2023, 62(38), e202307548.

- Šilhán, J., Klíma, M., Otava, T., Škvára, P., Chalupská, D., Chalupský, K., Kozic, J., Nencka, R., Bouřa, E. **Discovery and structural characterization of monkeypox virus methyltransferase VP39 inhibitors reveal similarities to SARS-CoV-2 nsp14 methyltransferase.** *Nature Communications.* 2023, 14(1), 2259.

Director's Award

- Ticháček, O., Mistrík, P., Jungwirth, P. **From the outer ear to the nerve: A complete computer model of the peripheral auditory system.** *Hearing Research.* 2023, 440(December), 108900.

IOCB Most Significant Publications 2023 – Popular vote*

- Dunlop, D., Ludvíková, L., Banerjee, A., Ottosson, H., Slanina, T. **Excited-State (Anti)Aromaticity Explains Why Azulene Disobeys Kasha's Rule.** *Journal of the American Chemical Society.* 2023, 145(39), 21569-21575.

- Mallada Faes, B. J., Ondráček, M., Lamanec, M., Gallardo Caparrós, A. J., Jimenez-Martin, A., De La Torre Cerdeño, B., Hobza, P., Jelínek, P. **Visualization of pi-hole in molecules by means of Kelvin probe force microscopy.** *Nature Communications.* 2023, 14(1), 4954.

- Koutná, E., Lux, V., Kouba, T., Škerlová, J., Nováček, J., Srb, P., Hexnerová, R., Šváchová, H., Kukačka, Z., Novák, P., Fábry, M., Poepsel, S., Veverka, V. **Multivalency of nucleosome recognition by LEDGF.** *Nucleic Acids Research.* 2023, 51(18), 10011-10025.

- Kuba, M., Khoroshyy, P., Lepšík, M., Kužmová, E., Kodr, D., Kraus, T., Hocek, M. **Real-time Imaging of Nascent DNA in Live Cells by Monitoring the Fluorescence Lifetime of DNA-Incorporated Thiazole Orange-Modified Nucleotides.** *Angewandte Chemie - International Edition.* 2023, 62(38), e202307548.

- Šilhán, J., Klíma, M., Otava, T., Škvára, P., Chalupská, D., Chalupský, K., Kozic, J., Nencka, R., Bouřa, E. **Discovery and structural characterization of monkeypox virus methyltransferase VP39 inhibitors reveal similarities to SARS-CoV-2 nsp14 methyltransferase.** *Nature Communications.* 2023, 14(1), 2259.

***Popular vote:** publications which received >50 % of internal votes

IOCB Most Significant Publications 2023 – Results

2023: 39 nominations

- CHEM 15 submissions → 3 Awards + 2 Director's Awards
- BIO 14 submissions → 3 Awards + 1 Director's Award
- PHYS 10 submissions → 3 Awards

The corresponding author(s) of the awarded publications receive 300 000 CZK each.

Opportunity for Collaboration

National Taiwan University, Taipei, Taiwan

國立臺灣大學
National Taiwan University

- The foreign partner is very interested in cooperation with IOCB. They first propose to organize a bilateral one-day meeting in Taipei on **Friday**, **4 October 2024**, which would be attended by those interested in cooperation from both the Czech and Taiwanese sides.
- They suggest (30 min talks + 5 min discussion of 5-7 CZ & TW PIs) on the following topics:
  - **Supramolecular chemistry**
  - **NMR**
  - **Photophysics**
  - **Novel aromatics**
  - **Organic materials**
  - **Bioorganic chemistry**
  - **Chemical biology**
- It is an excellent opportunity to attract well-educated Taiwanese PhD students/Exchange students

- The accommodation for the Czech delegates will be provided by Taiwanese partner
- There is a promise that the Institute would contribute to the travel costs (CZK 10K), the estimated price of a return ticket (direct flight) is ca CZK 23K (price valid at the beginning May 2024)
- If are interested in attending the meeting contact Dr. **Irena G. Stará** by **June 7**, 2024 at stara@uochb.cas.cz

- From 10-14 June, **Prof. Ken-Tsung Wong**, the contact person at the Taiwanese side, will visit Prague and IOCB, so if you want to discuss anything with him, it is possible.

Safety updates

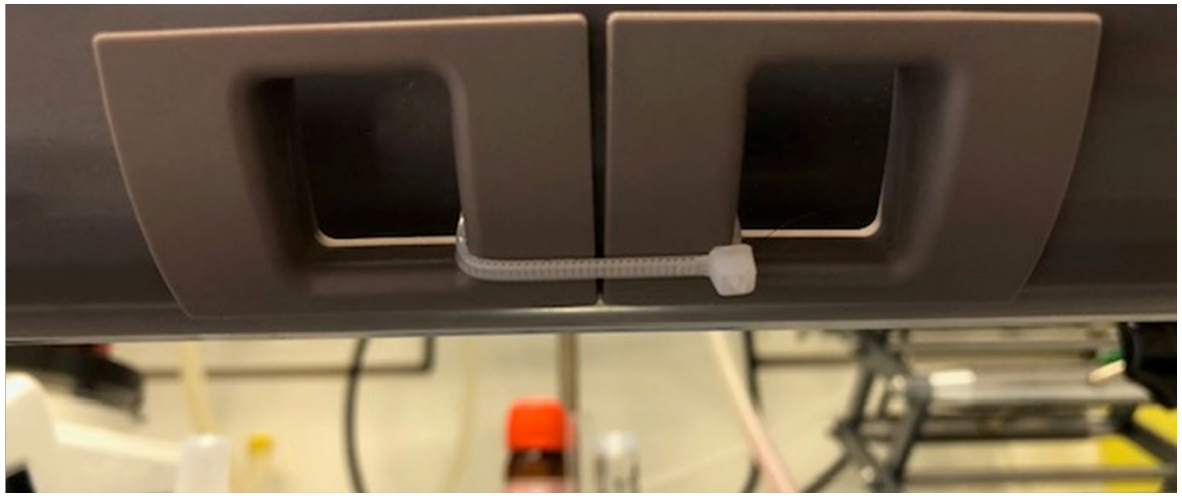
Children and Pets

- Children are not allowed to enter the laboratories.
- Children can enter only offices or common places
- The only opportunity for children to enter the lab is during the Excursions organized by the Institute when the preventive safety measures are taken care of.
- The same is valid for pets.

Safety of the Fume Hoods

Do-it-yourself Solutions to Eliminate Safety Functions

- Some solutions are more or less sophisticated, but nearly all hoods are equipped with this Auxiliary
- This is a safety feature: that the sash is blocked in a position, when secure exhaust is guaranteed. Above this position the hood should not be used.
- Very similar situation with the sensors which are “blinded” by the duck tape
- The hood which costs 600.000 CZK is safe. When the incident happens, do you believe that the State Labor Practice Inspection would consider this practice safe?



Waste Handling

This is CONTAMINATED GLASS CONTAINER

- No plastic allowed
- Only contaminated glass – we aim to minimize the amount (dispose only glass that cannot be rinsed, washed or evaporated in a hood)

This is NEW Organic/Aqueous Container

- disposal of aqueous phase containing organic or inorganic impurities.
- put the canister inside the blue box
- containers are located on a waste collection points

Miscellanea

Czech Academy of Sciences Evaluation 2020-2024

HR EXCELLENCE IN RESEARCH

- evaluations of CAS institutes every 5 years, interlinked with the Methodology 17+
- two-phase process (during 2025):

  Phase I: evaluation of the individual selected outputs of the research activities of CAS institutes and their teams, using international panels and independent external evaluators

  Phase II: evaluation of the institutes as a whole and their teams according to the specified criteria using international commissions

- upcoming evaluation now in a preparatory stage
- CAS: To ensure a high-quality evaluation, it is essential to establish a sufficiently robust pool of **experts**. These experts will be selected either as **commissioners**, who conduct the evaluations of the institutes; or as **reviewers**, who remotely assess assigned selected outputs in the first phase.
- CAS is inviting us to recommend suitable external (international) experts for these roles
- **you will receive a link to the corresponding table via email - your timely cooperation is highly appreciated!**

Call for Prizes nominations

Nadání Josefa, Marie a Zdeňky Hlávkových

Due 30 June 2024 (IOCB Board by 15 June 2024)

- **Josef Hlávka Award:** for early career researchers up to 33 years
- **Josef Hlávka Medal:** an outstanding personality of Czech science

ČESKÁ HLAVA

Due 12 July 2024

- **Award Doctorandus – Natural sciences:** PhD students and postdocs (Czech nationality only)

BADER PHILANTHROPIES, INC.

Due 15 June 2024

- **Alfred Bader prize for organic chemistry 2024:** for Czech researchers up to 35 years

More information on intraweb

IOCB events Code of Conduct

HR EXCELLENCE IN RESEARCH

1. We appreciate everyone's time and attention.
   Be present, both physically and mentally.
2. We value each other's perspectives and input. Say what you think, not what others might want to hear.
3. We use wisely the provided break time. Do not get distracted with your PCs and mobiles during the sessions.
4. We encourage everyone to participate in the discussions. There are no stupid questions.
5. We'll ensure a respectful and inclusive environment. Do not tolerate harassment or aggressivity.
6. Please, drink responsibly – plenty of water, minimum of alcohol.
7. We are committed to making the IOCB events collaborative, supportive and enjoyable.
   Have a great time!

IOCB Events 2024

27–31/5	IOCB Retreat (Valeč u Hrotovic)
30/5–1/6	Science Fair (EXPO Letňany)
5/6	Science at the Prague Castle: Tomáš Cihlář
6/6	Meeting with candidates for the President of the CAS
7/6	Career Workshop: Darlene Solomon
19/6	ScienceFest (Vítězné náměstí)
20/6	IOCB Family Day (Ladronka)
27/6	Lecture: Jules Hoffmann – Evolutionary perspectives on immune defences
28/ 6	Sounds of Science - Public scientific lecture by French Nobelists: Jean-Marie Lehn, Jules Hoffmann, Alain Aspect (Stavovské divadlo)
22/8	Happy Hours
2–6/9	10th Prague-Weizmann Summer School (NTK)
11/9	IOCB Invited Lecture: Leo Gross – Chemical Reactions and Synthesis by Atom Manipulation
18–20/9	IAB Visit & Evaluation of Research Groups
26/9	Happy Hours
27/9	European Researchers‘ Night
1-3/10	Nencki-IPHYS-IOCB meeting, Liblice
7–10/10	PhD Bootcamp (Dolní Malá Úpa)
15/10	IOCB Invited Lecture: Henrik Ottosson – Excited State Aromaticity and Antiaromaticity: From Pitfalls to Scopes
31/10	IOCB Invited Lecture: Hiroyuki Isobe – Synthesis-Driven Chemistry of Nanocarbon Molecules
4–10/11	Week of the CAS & Openhouse Days
28/11	IOCB Invited Lecture: Connor W. Coley – Artificial Intelligence for Synthetic Organic and Analytical Chemistry
13/12	Christmas gathering

Mtgs with GLs – Schedule

2024

- June 21
- October 4
- November 1
- December 6

Thank you!