



ÚOCHB ^{AV}
IOCB PRAGUE

Meeting with Group Leaders

Zdenek Hostomský | March 27, 2017

AGENDA



- Most significant publications 2016
- TEA update – Milan Drahoňovský
- OP VVV update – Iva Pichová
- HR update – Aranka Rozinková
- ITS update – Jiří Polách
- Miscellanea
- Important reminders

Most significant publications in 2016



- Physical and Theoretical Chemistry
- Medicinal and Organic Chemistry
- Biochemistry and Molecular Biology
- Interdisciplinary (within IOCB)

Each group may submit 1 most significant paper published in 2016 per category, but no more than 2 papers total. Semi-autonomous units within larger groups may submit their own paper if the group leader is not listed as co-author. The papers will be pre-screened internally before they are sent to the external panel (IAB members, *ad hoc* reviewers) as well as to an internal IOCB panel (group leaders and management). 2 – 4 papers in each category will be awarded prizes in the form of group money.

Most significant results 2016

Physical and Theoretical Chemistry

- **8** submitted results

Medicinal and Organic Chemistry

- **7** submitted results

Biochemistry and Molecular Biology

- **7** submitted results

Interdisciplinary (within IOCB)

- **11** submitted results

Most significant results 2016

Physical and Theoretical Chemistry

- **P. Junwirth** - A Non-Exploding Alkali Metal Drop on Water: From Blue Solvated Electrons to Bursting Molten Hydroxide
- **P. Hobza** - The SQM/COSMO filter: reliable native pose identification based on the quantum-mechanical description of protein–ligand interactions and implicit COSMO solvation
- **L. Rulíšek** - Accurate Prediction of One-Electron Reduction Potentials in Aqueous Solution by Variable-Temperature H-Atom Addition/Abstraction Methodology
- **P. Bouř** - Diamagnetic Raman Optical Activity of Chlorine, Bromine, and Iodine Gases
- **M. Hocek** - A Rotational BODIPY Nucleotide: An Environment-Sensitive Fluorescence-Lifetime Probe for DNA Interactions and Applications in Live-Cell Microscopy
- **D. Šaman** - Uncovering Key Structural Features of an Enantioselective Peptide-Catalyzed Acylation Utilizing Advanced NMR Techniques.
- **J. Cvačka** - Thin-Layer Chromatography/Desorption Atmospheric Pressure Photoionization Orbitrap Mass Spectrometry of Lipids
- **J. Vondrášek** - Sequence-Specific Recognition of DNA by Proteins: Binding Motifs Discovered Using a Novel Statistical/Computational Analysis

Medicinal and Organic Chemistry

- **I. Rosenberg** - 4-Toluenesulfonyloxymethyl-(H)-phosphinate: A Reagent for the Introduction of O- and S-Methyl-(H)-phosphinate Moieties
- **P. Majer** - Discovery of 6-Diazo-5-oxo-L-norleucine (DON) Prodrugs with Enhanced CSF Delivery in Monkeys: A Potential Treatment for Glioblastoma
- **E. Kudová** - Neurosteroid-like Inhibitors of N-Methyl-D-aspartate Receptor: Substituted 2-Sulfates and 2-Hemisuccinates of Perhydrophenanthrene
- **F. Teplý** - Structural revisions of small molecules reported to cross-link G-quadruplex DNA *in vivo* reveal a repetitive assignment error in the Literature
- **M. Hocek** - 2-Substituted dATP Derivatives as Building Blocks for Polymerase-Catalyzed Synthesis of DNA Modified in the Minor Groove
- **J. Konvalinka** - Specific Inhibitors of HIV Capsid Assembly Binding to the C-Terminal Domain of the Capsid Protein: Evaluation of -Arylquinazolines as Potential Antiviral Compounds
- **P. Cigler** – Benchtop fluorination of fluorescent nanodiamonds on a preparative scale: Toward unusually hydrophilic bright particles

Most significant results 2016

Biochemistry and Molecular Biology

- **J. Jiráček** - Rational steering of insulin binding specificity by intra-chain chemical crosslinking
- **I. Valterová** - Gene Expression Dynamics in Major Endocrine Regulatory Pathways along the Transition from Solitary to Social Life in a Bumblebee, *Bombus terrestris*
- **I. Pichová** - Myristoylation drives dimerization of matrix protein from mouse mammary tumor virus
- **P. Řezáčová** - Oligomeric interface modulation causes misregulation of purine 5'-nucleotidase in relapsed leukemia
- **E. Curtis** - Altered biochemical specificity of G-quadruplexes with mutated tetrads
- **E. Boura** – Structural insights and *in vitro* reconstitution of membrane targeting and activation of human PI4KB by the ACBD3 protein
- **P. Cigler** – Imaging of transfection and intracellular release of intact, nan-labeled DNA using fluorescent nanodiamonds

Interdisciplinary (within IOCB)

- **L. Rulíšek** - Copper(II) and Zinc(II) Complexes of Conformationally Constrained Polyazamacrocycles as Efficient Catalysts for RNA Model Substrate Cleavage in Aqueous Solution at Physiological pH
- **J. Jiráček** - Probing Receptor Specificity by Sampling the Conformational Space of the Insulin-like Growth Factor II C-domain
- **I. Valterová** - Regulation of Isoprenoid Pheromone Biosynthesis in Bumblebee Males
- **D. Nachtigalová** - Solvatochromic fluorene-linked nucleoside and DNA as color-changing fluorescent probes for sensing interactions
- **E. Kudová** - Distributions of therapeutically promising neurosteroids in cellular membranes
- **F. Teplý; P. Bouř** - Intense chirality induction in nitrile solvents by a helquat dye monitored by near resonance Raman scattering
- **H. Macíčková Cahová** - 5-Substituted Pyrimidine and 7-Substituted 7-Deazapurine dNTPs as Substrates for DNA Polymerases in Competitive Primer Extension in the Presence of Natural dNTPs
- **J. Konvalinka** - iBodies: Modular Synthetic Antibody Mimetics Based on Hydrophilic Polymers Decorated with Functional Moieties
- **D. Šaman** - Tunable Push-Pull Interactions in 5-Nitrosopyrimidines.
- **R. Nencka** - Single-Step Formation of Pyrimido[4,5-d]pyridazines by a Pyrimidine-Tetrazine Tandem Reaction
- **J. Vondrášek** - Artificial proteins as allosteric modulators of PDZ3 and SH3 in two-domain constructs: A computational characterization of novel chimeric proteins

Internal Pre-selection



- Pre-selection panel is composed of the external members of IOCB Board and the director:

Tomáš Obšil
Petr Slavíček
Petr Svoboda
Zdeněk Hostomský

- Typically, only papers with principal or corresponding author from IOCB should be submitted.
 - Papers not meeting these criteria may still be submitted, but only work done at IOCB will be judged.
 - Print version date counts
- Assignment to categories will be scrutinized
- Clarification re Interdisciplinary vs. Collaborative
- Interdisciplinary: Chemistry - Biology
Computational – Experimental
- Question re analytical techniques component (NMR, MS, x-ray structure analysis)



- Iva Pichová,
Vice-director for Science



- Milan Drahoňovský,
Head of TEA.

Sick Days (Indispoziční volno)

- **Basic principles**

- 3 days per year.
- Covering 100 % of personal cost.
- Cost allocation according to donators' rules (based on official requests):
 - Deductible costs – grant resource;
 - Non-deductible cost – „VEJ“ resource.
- Registration – Albína (new position).
- Using Sick Days before or after an official holiday/vacation not desirable.
- Employee has to announce the Sick Day via email / phone to supervisor immediately – registration in Albína as soon as possible.
- No year-to-year transfer possible.
- „Docházka“.

- **Status**

- Testing (end of March).
- Update of collective agreement.
- Employee communication.
- **Official start May 1st** (2 sick days till end of 2017).

Planning of costs

Plánování nákl. grantů

Personal Costs

- According to the rules of GAČR 2018 the capacity of head scientist shall be allocated (recommended 30%).
- In GAČR within the co-financing it is possible to allocate the personal costs of head from grant or non-grant funds (VEJ), according to his financial strategy.

Overhead

- It is still valid the scientist has to required maximum of overhead costs enabled by the provider.
- In the case of applications for projects GAČR for 2018 it is allowed to claim overhead directed only in the amount of previously applicable rules, GAČR, 20 % from eligible costs (80+20) from grant funds, not 20 % from all eligible costs as currently possible based on the new GAČR rules for 2018.

Personální náklady

- Dle pravidel GAČR pro rok 2018 musí být alokována kapacita řešitele (dop. 30%).
- U GAČR je možné financovat (kofinancování) plat vedoucího jak z nedotačních tak i dotačních prostředků, dle finanční strategie vedoucího (VEJ).

Režie

- I nadále platí, že řešitel je povinen při podání návrhu projektů nárokovat v položce režijní náklady maximální výši umožněnou poskytovatelem.
- V případě žádostí o projekty GAČR na rok 2018 umožňuje pracoviště nárokovat režii pouze ve výši doposud platných pravidel, GAČR, tj. 20% uznaných nákladů (80+20) z dotované části projektu, nikoli 20% celkových uznaných nároků projektu, jak nově pravidla GA ČR umožňují.

More for GAČR 2018 grant conditions: Personal Costs – page 17, point 3, 4; Overhead Costs – page 20, point 6.



- Aranka Rozinková,
Head of HR

Ph.D. Boot Camp 2017



Date - 6.10.2017 - 8.10.2017 (Friday - Sunday)

Place - Malá Úpa (IOCB Cottage)

Submitting list of students (name + email address) - 30.6.2017





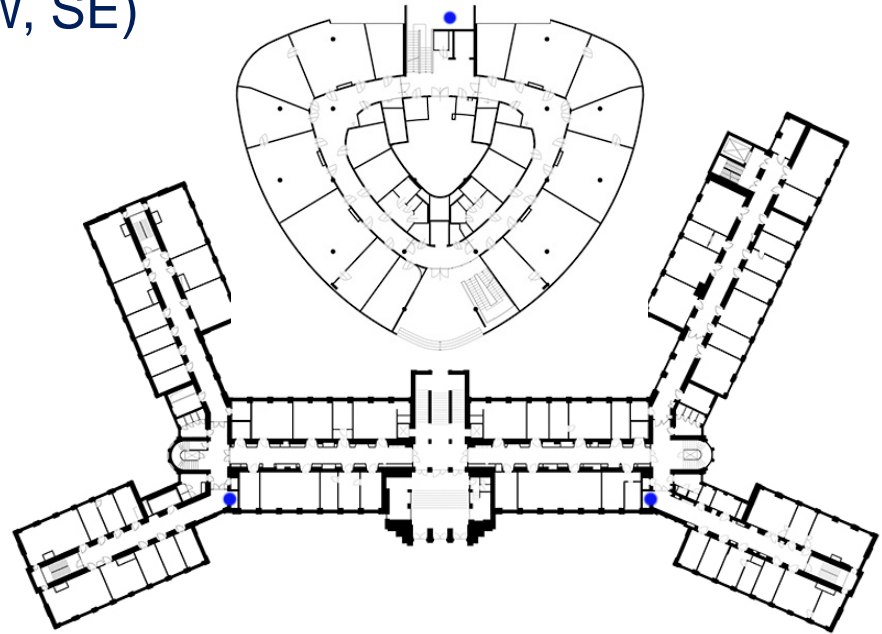
- Jiří Polách,
Head of ITS.

Printing



- **A3 printers Konica-Minolta c258 – 5 pcs**

- A: 1PP (SW, SE), 2NP (SW, SE)
- B: 2/3NP (N), somewhere



- **poster plotter broken**

- new plotter purchase process started (~ 2 months)
- printing on canvas considered
- meanwhile - repro Fetterle, Na Santince 5

Storage server / Library



- **large scientific data storage server**
 - discussed with some group leaders in 2016
 - preparing technical specification – **survey**
- **new chemTK library web pages – April 3**
 - www.chemtk.cz
 - access to electronic resources
 - catalogue search, article search, ILS, ASEP, ...
 - will replace library.uochb.cas.cz
- **Google scholar & IOCB library**
 - direct access to articles - results of a query



Miscellanea



Mtgs w GLs - 2017 Schedule



- January 23
- February 27
- March 27
- April 24
- May 22
- June 26
- September 4
- October 2
- November 6
- December 18

Always on Mondays at 10:00 am in the Director's Boardroom

Important Reminders



- Labor union committee election
Wednesday, March 29 10 am – 2pm
- Bernard Feringa lecture
Wednesday, March 29 3 pm
- Next meeting with Group Leaders
April 24, 2017

Important Reminders



March 31 deadlines:

- Neuron Award for contribution to science
- Neuron Award for promising young scientists
- Otto Wichterle Award
- Praemium Academiae
- Jaroslav Heyrovský Medal
- The honorary medals of science
- The Jan Patočka honorary medal
- The CAS Award for young scientists