Meeting with Group Leaders:

Most significant 2014 publications

June 1 , 2015

Zdenek Hostomský

Agenda

- Most significant 2014 publications results
- (Post)doc seminars
- Summer School 2015

- Miscellanea

Most significant publications

- Physical and Theoretical Chemistry
- Analytical Chemistry, Spectroscopy and other analytical methods
- Medicinal and Organic Chemistry
- Biochemistry and Molecular Biology
- Interdisciplinary (within IOCB)

Each team may submit 1 most significant paper published in 2014 for each category. The papers are judged by an external panel (IAB members, *ad hoc* reviewers), as well as by an internal IOCB panel (team leaders and management). Top 1/3 od the submitted papers in each category (listed in the following slides alphabetically by first author) will be awarded a cash prize for the group.

Most significant publications 2014

- Physical and Theoretical Chemistry

  (11) 12* submissions → **4** awards

- Analytical Chemistry, Spectroscopy and other analytical methods

  7 submissions → **3** awards

- Medicinal and Organic Chemistry

  (10) 12* submissions → **4** awards

- Biochemistry and Molecular Biology

  11 submissions → **4** awards

- Interdisciplinary (within IOCB)

  (15) 10* submissions → **3** awards

Most significant publications in 2014

Lessons learned

- Preselection of submission will be done by IOCB management before evaluation by international panel, based on explicit rules:
  - 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.
- Assignment to categories will be scrutinized
- Clarification re Interdisciplinary vs Collaborative
- Interdisciplinary: Chemistry - Biology
  Computational - Experimental
- Question re analytical techniques component

Most Significant Publications 2014

Physical and Theoretical Chemistry part 1

Listed alphabetically by first author

- Chalupský J, Rokob TA, Kurashige Y, Yanai T, Solomon* EI, Rulíšek* L, and Srnec* M

Reactivity of the Binuclear Non-Heme Iron Active Site of Δ^9 Desaturase Studied by Large-Scale Multireference *Ab Initio* Calculations

J Am Chem Soc 2014, 136, 15977-15991

- Pospíšil *L, Bednárová L, Štěpánek P, Slavíček P, Vávra J, Hromadová M, Dlouhá H, Tarábek J, and Teplý* F

Intense Chiroptical Switching in a Dicationic Helicene-Like Derivative: Exploration of a Viologen-Type Redox Manifold or a Non-Racemic Helquat

J Am Chem Soc 2014, 136, 10826-10829

Most Significant Publications 2014

Physical and Theoretical Chemistry part 2

Listed alphabetically by first author

- Savolainen J, Uhlig F, Ahmed S, Hamm* P, and Jungwirth* P

Direct observation of the collapse of the delocalized excess electron in water

Nature Chemistry 2014, 6, 697-701

- Vazdar K, Kunetskiy R, Saame J, Kaupmees K, Leito* I, and Jahn* U

Very Strong Organosuperbases Formed by Combining Imidazole and Guanidine Bases: Synthesis, Structure and Basicity

Angew Chem Int Ed 2014, 53, 1435-1438

Most Significant Publications 2014

Physical and Theoretical Chemistry part 1

External

- Chalupský J, Rokob TA, Kurashige Y, Yanai T, Solomon* EI, Rulíšek* L, and Srnec* M

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J Am Chem Soc 2014, 136, 10826-10829

Internal

- [redacted]

- [redacted]

Physical and Theoretical Chemistry part 2

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- Savolainen J, Uhlig F, Ahmed S, Hamm* P, and Jungwirth* P

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Very Strong Organosuperbases Formed by Combining Imidazole and Guanidine Bases: Synthesis, Structure and Basicity

Angew Chem Int Ed 2014, 53, 1435-1438

Internal

- Famfrlík J, Přáda A, Padělková, Pecina, Macháček, Lepšík, Holub, Růžička* A, Hnyk* D, and Hobza* P

The dominant role of chalcogen bonding in the crystal packing of 2D/3D aromatics

Angew Chem Int Ed 2014, 53, 10139-10142

Analytical Chemistry, Spectroscopy, etc.

- Šebestík* J, and Bouř* P

Observation of Paramagnetic Raman Optical Activity of Nitrogen Dioxide

Angew Chem Int Ed 2014, 53, 9236-9239

- Buděšínský* M, Vaněk V, Dračínský M, Pohl R, Poštová-Slavětínská L, Sychrovský V, Pícha J, and Císařová I

Determination fo the configuration in six-membered saturated heterocycles (N, P, S, Se) and their oxydation products using experimental and calculated NMR chemical shifts

Tetrahedron 2014, 70, 3871-3886

- Růžička M, Čížková M, Jirásek M, Teplý F, Koval D, and Kašička* V

Study of deoxyribonucleic acid-ligand interactions by partial filling affinity capillary electrophoresis

J Chromatogr A 2014, 1349, 116-121

Most Significant Publications 2014

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J Chromatogr A 2014, 1349, 116-121

Internal

- [redacted]

- Horká P, Vrkoslav V, Hanus R, Pecková K, and Cvačka* J

New MALDI matrices based on lithium salts for the analysis of hydrocarbons and wax esters

J Mass Spectrom 2014, 49, 628-638

- Tykvart J, Navrátil V, Sedlák F, Corey E, Colombatti M, Fracasso G, Koukolík F, Bařinka C, Šácha P, and Konvalinka* J

Comparative analysis of monoclonal antibodies against prostate-specific membrane antigen (PSMA)

J The Prostate 2014, 74,1674-1690

Medicinal and Organic Chemistry part 1

Listed alphabetically by first author

- Kafka F, J, Holan M, Hidasová D, Pohl R, Císařová I, Klepetářová B, and Jahn* U

Oxidative Catalysis Using the Stoichiometric Oxidant as a Reagent: An Efficient Strategy for Single-Electron-Transfer-Induced Tandem Anion-Radical Reactions

Angew Chem Int Ed 2014, 53, 9944-9948

- Opekar S, Pohl R, Beran P, Rulíšek L, and Beier* P

Diethyl Fluoronitromethylphosphonate: Synthesis and Application in Neutrophilic Fluoroalkyl Additions

Chem Eur J 2014, 20, 1453-1458

Medicinal and Organic Chemistry part 2

Listed alphabetically by first author

- Řehoř I, Macková H, Filippov SK, Kučka J, Proks V, Šlegerová J, Turner S, Van Tendeloo G, Ledvina M, Hrubý* M, and Cígler* P

Fluorescent Nanodiamonds with Bioorthogonally Reactive Protein-Resistant Polymeric Coatings

ChemPlusChem 2014, 79, 21-24

- Vaníková Z and Hocek* M

Polymerase Synthesis of Photocaged DNA Resistant against Cleavage by Restriction Endonucleases

Angew Chem Int Ed 2014, 53, 6734-6737

Medicinal and Organic Chemistry part 1

External

- Kafka F, J, Holan M, Hidasová D, Pohl R, Císařová I, Klepetářová B, and Jahn* U

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Diethyl Fluoronitromethylphosphonate: Synthesis and Application in Neutrophilic Fluoroalkyl Additions

Chem Eur J 2014, 20, 1453-1458

Internal

- Chercheja S, Klívar J, Jančařík A, Rybáček J, Salzl S, Tarábek J, Pospíšil L, Vacek Chocholoušová J, Vacek J, Pohl R, Císařová I, Starý* I, and Stará* IG

The use of Cobalt-mediated cycloisomerization of Ynedinitriles in the Synthesis of Pyridazinohelicenes

Chem Eur J 2014, 20, 8477-8482

Medicinal and Organic Chemistry part 2

External

- Řehoř I, Macková H, Filippov SK, Kučka J, Proks V, Šlegerová J, Turner S, Van Tendeloo G, Ledvina M, Hrubý* M, and Cígler* P

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Angew Chem Int Ed 2014, 53, 6734-6737

Internal

- Tykvart J, Schimer J, Bařinková J, Pachl P, Poštová-Slavětínská L, Majer P, Konvalinka J, and Šácha* P

Rational design of urea-based glutamate carboxypeptidase II (GCPII) inhibitors as versatile tools for specific drug targeting and delivery

Bioorg Med Chem 2014, 22, 4099-4108

- [illegible]

Medicinal and Organic Chemistry part 3

Director's honorary mention

- Krečmerová* M, Pohl R, Masojídková M, Balzarini J, Snoeck R, and Andrei G

N^4-Acyl derivatives as lipophilic prodrugs of cidofovir and its5-azacytosine analogue, (*S*)-HPMP-5-azaC: Chemistry and antiviral activity

Bioorg Med Chem 2014, 22, 2896-2906

Biochemistry and Molecular Biology part 1

Listed alphabetically by first author

- Bäumlová A, Chalupská D, Różycki B, Jović M, Wiśniewski E, Klíma M, Dubánková A, Kloer DP, Nencka R, Balla T, and Bouřa* E

The crystal structure of the phosphatidylinositol 4-kinase IIa

EMBO reports 2014, 1-8

- Čermáková K, Těšina P, Demeulemeester J, El Ashkar S, Méreau H, Schwaller J, Řezáčová P, Veverka* V, and De Rijck*J

Validation and Structural Characterization of the LEDGF/p75-MLL Interface as a New Target for the Treatment of MLL-Dependent Leukemia

Cancer Res 2014, 74, 5139-5151

Biochemistry and Molecular Biology part 2

Listed alphabetically by first author

- Jílková A, Horn M, Řezáčová P, Marešová L, Fajtová P, Brynda J, Vondrášek J, McKerrow JH, Caffrey CR, and Mareš* M

Activation Route of the *Schisostoma mansoni* Cathepsin B1 Drug Target: Structural Map with a Glycosaminoglycan Switch

Structure 2014, 22, 1786-1798

- Zoll S, Stanchev S, Began J, Škerle J, Lepšík M, Peclinovaká, Majer P. and Stříšovský* K

Substrate binding and specificity of rhomboid intramembrane protease revealed by substrate-peptide complex structures

The EMBO Journal 2014, 33, 2408-2421

Most Significant Publications 2014

Biochemistry and Molecular Biology part 1

External

- Bäumlová A, Chalupská D, Różycki B, Jović M, Wiśniewski E, Klíma M, Dubánková A, Kloer DP, Nencka R, Balla T, and Bouřa* E

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Validation and Structural Characterization of the LEDGF/p75-MLL Interface as a New Target for the Treatment of MLL-Dependent Leukemia

Cancer Res 2014, 74, 5139-5151

Internal

- Kielkowski P, Famfrlík J, and Hocek*M

7-aryl-7-deazaadenine 2'deosyribonucleoside triphosphates: Better substrates for DNA polymerases than dATP in competitive incorporations

Angew Chem Int Ed 2014,53, 7552-7555

Biochemistry and Molecular Biology part 2

External

- Jílková A, Horn M, Řezáčová P, Marešová L, Fajtová P, Brynda J, Vondrášek J, McKerrow JH, Caffrey CR, and Mareš* M

Activation Route of the *Schisostoma mansoni* Cathepsin B1 Drug Target: Structural Map with a Glycosaminoglycan Switch

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Substrate binding and specificity of rhomboid intramembrane protease revealed by substrate-peptide complex structures

The EMBO Journal 2014, 33, 2408-2421

Internal

- P

- P

Interdisciplinary (within IOCB)

- Kožíšek M, Lepšík M, Grantz Šašková K, Brynda J, Konvalinka* J, and Řezáčová* P

Thermodynamic and structural analysis of HIV protease resistance to darunavir – analysis of heavily mutated patient-derived HIV-1 proteases

FEBS Journal 2014, 281, 1834-1847

- Snášel J, Nauš P, Dostál J, Hnízda A, Fanfrlík J, Brynda J, Bourderioux A, Dušek M, Dvořáková H, Stolaříková J, Zábranská H, Pohl R, Konečný P, Džubák P, Votruba I, Hajdúch M, Řezáčová P, Veverka V, Hocek* M, and Pichová* I

Structural Basis for Inhibition of Mycobacterial and Human Adenosine Kinase by 7-Substituted 7-(Het)aryl-7-deazaadenine Ribonucleosides

J Med Chem 2014, 57, 8268-8279

- Šimák O, Pachl P, Fábry M, Buděšínský M, Jandušík T, Hnízda A, Skleničková R, Petrová M, Veverka V, Řezáčová P, Brynda* J, and Rosenberg* I

Conformationally constrained nucleoside phosphonic acids – potent inhibitors of human mitochondrial and cytosolic 5‘(3‘)-nucleosidases

Org Biomol Chem 2014, 12, 7971-7982

Physical and Theoretical Chemistry

- Excellent and improving quality

Analytical Chemistry, Spectroscopy, etc.

- Do we want to support it prominently?

Biochemistry and Molecular Biology

- Improved quality
- Prominence of Structural Biology
- Challenge: it‘s a tool, even if sofisticated. What to use it for?
  - Address fundamental biological questions
  - Structure-guided drug design

- Emerging themes:
  - Membrane biology
  - Metabolic signaling peptide network

Medicinal and Organic Chemistry

- True medicinal chemistry papers appear underappreciated by both external and internal reviewers.

Interdisciplinary (within IOCB)

- This is what we definitely want to support
- But, the category devolved into a depository of second best or additional shots on goal.

General issues

- How to discourage submission of weaker papers? (pushing boundaries of science vs. filling in with incremental progress)
  - Anti-contest for least significant paper?
  - Pay a modest entrance fee which the contestants would be willing to do only if they are convinced their paper has a serious chance of scoring well?
- How to divide submissions?
  - One big category
  - Biology – Chemistry
  - Theoretical – Experimental (at IOCB only in the Chemistry area)

A true reviewer's comment

- … Although a change could be politically difficult (and depending upon the goal you hope to achieve), it might be an interesting experiment (strictly within the Board) to consider listing only those manuscripts that members feel will have a "lasting impact". At least for the "experiment", it would remove a specific number of rankings needed in each category and give a sense of work that is conceptual or ground breaking (lasting) versus good quality but incremental.

Summer School

PRELIMINARY PROGRAMME

August 31st	**arrival** and welcome party
September 1st	**Lectures 9 AM – 5 PM**
September 2nd	**Lectures 9 AM – 3 PM, city tour, beer party**
September 3rd	**Lectures 9 AM – 5 PM**
September 4th	**Lectures 9 AM – 1 PM**, departure

http://www.praguesummerschool.cz/programme.php

SELECTED SPEAKERS

- Markus Zettl, *Boehringer Ingelheim, DE*
  Topic: **Biologics - immunomodulatory antibody therapeutics**
- Berndt Joost, *FHNW Basel, CH*
  Topic: **Modern ways to drug nanoformulations**
- Jeroen Bokhoven, *ETH Zurich , CH*
  Topic: **Heterogeneous catalysis**
- Andrzej Marek Brzozowski, *Department of Chemistry University of York, UK*
  Topic: **Structural endocrinology and medicinal chemistry**
- Richard Mackman, *Gilead Sciences, Foster City, USA*
  Topic: **Discovery and development of novel virostatics**
- Peter Sebo, *Institute of Microbiology, ASCR Prague, CZ*
  Topic: **Next generation of vaccines for prevention and therapy of important pathologies**
- Bruno Martoglio, *Novartis Institutes for BioMedical Research, Basel, CH*
  Topic: **Integrated Drug Discovery**
- Gert De Wilde, *Galapagos NV, Mechelen, BE*
  Topic: **Target discovery for orphan diseases at Galapagos**

(Post)doc seminar series

- Jiří Kaleta presented an idea to have regular short seminars for PhD students and postdocs, to practice their presentation skills and and to make colleagues aware of what they are working on.
- He volunteered to organize and coordinate the series.
- It could start this fall, with the availability of the refurbished main seminar hall.

Upcoming dates

- Museum night - June 13, 2015
- Happy Hours in June (18 or 25) on the roof of B
- Next Meeting with Group Leaders June 29, 2015
- IAB evaluation of Junior Groups – September 4-5, 2015
- Science Fair - September , 2015