

Meeting with Group Leaders:

IOCB most significant publications in 2015

May 23, 2016

Zdenek Hostomský

Agenda



- New official name of IOCB
- IOCB most significant publications in 2015
 - Results
- GSRC-3
- Miscellanea

New official name of IOCB



Based on the information from the Czech Academy of Sciences (Foundation Deed), the name of the institute in English should be:

**The Institute of Organic Chemistry and
Biochemistry of the Czech Academy of Sciences**

The IOCB of the CAS

(no v.v.i. should be used in English, only in the Czech name, which remains: Ústav organické chemie a biochemie Akademie věd České republiky, v.v.i.)

Most significant publications 2015



- Physical and Theoretical Chemistry

(11 for 2014) **8** submissions → **7** preselected → **3** awards

- Medicinal and Organic Chemistry

(10 for 2014) **7** submissions → **7** preselected → **4** awards

- Biochemistry and Molecular Biology

(11 for 2014) **6** submissions → **5** preselected → **3** awards

- Interdisciplinary (within IOCB)

(15 for 2014) **8** submissions → **4** preselected → **2** awards

Physical and Theoretical Chemistry part 1

Listed alphabetically by first author



- Mason P E, Uhlig F, Vaněk V, Buttersack T, Bauerecker S, and Jungwirth * P

Coulomb explosion during the early stages of the reaction of alkali metals with water

Nature Chemistry 2015, 7, 250-254

- Wen J, Havlas Z, and Michl * J

Captodatively Stabilized Biradicaloids as Chromophores for Singlet Fission

J Am Chem Soc 2015, 137, 165-172

Most Significant Publications 2015

Physical and Theoretical Chemistry part 2



Listed alphabetically by first author

- KC Wu* T, Kapitán* J, Mašek V, and Bouř* P

Detection of Circularly Polarized Luminescence of a Cs-Eu-III Complex in Raman Optical Activity Experiments

Angew Chem Int Ed 2015, 54, 14933-14936

External

- Coulomb explosion during the early stages of the reaction of alkali metals with water,

- Wen J, Havlas Z, and Michl J

Captodatively Stabilized Biradicaloids as Chromophores for Singlet Fission

J Am Chem Soc 2015, 137, 165-172

Internal

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Planning a
 Reaction
 Reactivity of
 Heme Iron
 Oxidation
 Multireference
 Calculations
- 

Planning a
 Synthesis
 Intense Chiro
 Dicationic Hel
 Derivatives
 A Mologen-Type Redox Manifold or
 Non-Racemic Helical

Physical and Theoretical Chemistry part 4



External

Internal

- Wu T, Kapitán J, Mašek V, and Bouř P
Detection of Circularly Polarized Luminescence of a Cs-Eu-III Complex in Raman Optical Activity Experiments

Angew Chem Int Ed 2015, 54, 14933-14936



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Organic and Medicinal Chemistry part 1

Listed alphabetically by first author



- Amatov T, Pohl R, Císařová I, Jahn* U

Synthesis of Bridged Diketopiperazines by Using the Persistent Radical Effect and a Formal Synthesis of Bicyclomycin

Angew Chem Int Ed 2015, 54, 12153-12157

- Kaletová E, Kohutová A, Hajduch J, Kaleta J, Bastl Z, Pospíšil L, Stibor I, Magnera T F, and Michl* J

The Scope of Direct Alkylation of Gold Surface with Solutions of C₁-C₄ *n*-Alkylstannanes

J Am Chem Soc 2015, 137, 12086-12099

Organic and Medicinal Chemistry part 2

Listed alphabetically by first author



- Šámal M, Chercheja S, Rybáček J, Vacek Chocholoušová J, Vacek J, Bednářová L, Šaman D, Stará* I G, and Starý* I

An Ultimate Stereocontrol in Asymmetric Synthesis of Optically Pure Fully Aromatic Helicenes

J Am Chem Soc 2015, 137, 8469-8474



Director's Award

- Petrová* M, Páv O, Buděšínský M, Zborníková E, Novák P, Rosenbergová Š, Pačes O, Liboska R, Dvořáková I, Šimák O, and Rosenberg* I

Straightforward Synthesis of Purine 4'-Alkoxy-2'-deoxynucleosides: First Report of Mixed Purine-Pyrimidine 4'-Alkoxydeoxyoligonucleotides as New RNA Mimics

Org Lett 2015, 17, 3426-3429

Organic and Medicinal Chemistry part 4



External

Internal

- Amatov T, Pohl R, Císařová I, Jahn* U
Synthesis of Bridged Diketopiperazines by Using the Persistent Radical Effect and a Formal Synthesis of Bicyclomycin

Angew Chem Int Ed 2015, 54, 12153-12157

- Kaletová E, Kohutová A, Hajduch J, Kaleta J, Bastl Z, Pospíšil L, Stibor I, Magnera T F, and Michl * J

The Scope of Direct Alkylation of Gold Surface with Solutions of C₁-C₄ *n*-Alkylstannanes

J Am Chem Soc 2015, 137, 12086-12099

- P. Kaleta, A. Kohutová, I. Císařová, D. Pohl, R. Amatov, T. F. Magnera, T. Stibor, and U. Jahn
Stoichiometric Oxidative Radical C–C Coupling Using the Stoichiometric Oxidant as a Reagent: An
Angew Chem Int Ed 2014, 53, 9914–9918



Organic and Medicinal Chemistry part 5



External

Internal

- Šámal M, Chercheja S, Rybáček J, Vacek Chocholoušová J, Vacek J, Bednářová L, Šaman D, Stará* I G, and Stary* I

An Ultimate Stereocontrol in Asymmetric Synthesis of Optically Pure Fully Aromatic Helicenes

J Am Chem Soc 2015, 137, 8469-8474

- J. Vaníček, S. Chercheja, I. M. Stary, M. Šámal, J. Vacek, L. Bednářová, D. Šaman, J. Chocholoušová, J. Rybáček, I. G. Stará
Polymer-Induced Asymmetric Synthesis of
Photocatalytic Helicenes Resistant
against Photobleaching by
Restriction of Helicene Nucleases



Angew Chem Int Ed 2014, 53, 6731-6737

Biochemistry and Molecular Biology part 1



Listed alphabetically by first author

- Buček A, Matoušková P, Vogel H, Šebesta P, Janh U, Weissflog J, Svatoš* A, and Pichová* I

Evolution of moth sex pheromone composition by a single amino acid substitution in a fatty acid desaturase

Proc Natl Acad Sci USA 2015, 112, 12586-12591

- Těšina** P, Čermaková** K, Hořejší M, Procházková K, Fábry M, Sharma S, Christ F, Demeulemeester J, Debyser Z, De Rijck* J, Veverka* V, Řezáčová* P

Multiple cellular proteins interact with LEDGF/p75 through a conserved unstructured consensus motif

Nature Communications 2015, 6, 1-14



Director's Award

- Tykvart J, Bařinka C, Svoboda M, Navrátil V, Souček R, Hubálek M, Hradílek M, Šácha P, Lubkowski J, and Konvalinka*J

Structural and Biochemical Characterization of a Novel Aminopeptidase from Human Intestine

J Biol Chem 2015, 290, 11321-11336

Biochemistry and Molecular Biology part 1



External

- Buček A, Matoušková P, Vogel H, Šebesta P, Jahn U, Weissflog J, Svatoš A, and Pichová I

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Multiple cellular proteins interact with LEDGF/p75 through a conserved unstructured consensus motif

Nature Communications 2015, 6, 1-14

Internal



The crystal structure of the phosphatidylinositol 4-kinase IIa



Elife 2015, 4, 1-15



Interdisciplinary (within IOCB) part 1

- Mejdrová**I, Chalupská**D, Kögler**M, Šála M, Plačková P, Baumlová A, Hřebabecký H, Procházková E, Dejmek M, Guillon R, Strunin D, Weber J, Lee G, Birkus G, Mertlíková-Kaiserová H, Bouřa*E, and Nencka*R

Highly Selective Phosphatidylinositol 4-Kinase III β Inhibitors and Structural Insight into Their Mode of Action

Journal of Medicinal Chemistry 2015, 58, 3767-3793

- Schimer J, Pávová M, Anders M, Pachi P, Šácha P, Cígler P, Weber J, Majer P, Řezáčová P, Kräusslich H-G, Müller*B, Konvalinka*J

Triggering HIV polyprotein processing by light using rapid photodegradation of a light-binding protease inhibitor

Nature Communications 2015 Mar 9;6:6461. doi: 10.1038/ncomms7461.

Interdisciplinary (within IOCB) part 2



External

- Mejdrová I, Chalupská D, Kögler M, Šála M, Plačková P, Baumlová A, Hřebabecký H, Procházková E, Dejmek M, Guillon R, Strunin D, Weber J, Lee G, Birkus G, Mertlíková-Kaiserová H, Bouřa E, and Nencka R

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Triggering HIV polyprotein processing by light using rapid photodegradation of a light-binding protease inhibitor

Nature Communications 2015 :6461.

doi: 10.1038/ncomms7461.

Internal

Pharmlova J, Rozycki B, Baumlová A, Křimová M, Hřebabecký H, Křivánek P, Svoboda E, Procházková E, Guillon R, Strunin D, Weber J, Lee G, Birkus G, Mertlíková-Kaiserová H, Bouřa E, and Nencka R
The crystal structure of the phosphatidylinositol 4-kinase IIa



Pharmlova J, Pávová M, Anders M, Pachi P, Šácha P, Cígler P, Weber J, Majer P, Řezáčová P, Kräusslich H-G, Müller B, Konvalinka J



General Comments



- Excellent quality of all submissions noted - dramatic improvement from the last year
- Preselection was helpful and commented on positively
- Each submitted paper was scored at least in the third place by at least one of the judges

Gilead Sciences Research Center



- GSRC-3 new format:
- Interdisciplinary collaboration
- Program concept

Gilead Sciences Research Center



- The second 5-year Donation Agreement between Gilead and IOCB will expire on July 14, 2016.
- Gilead has decided to extend the funding support for GSRC by additional 5 years.
- The support will increase from \$1.15M to \$1.35M per calendar year.
- The application for membership in GSRC is open to all IOCB research groups.



GSRC3 – Fund Allocation

- Multidisciplinary programs in biology, synthetic and medicinal chemistry, pharmacology, and structural and computational research. (4 to 8)
- Up to 2 larger collaborative programs involving multiple IOCB groups focusing on chronic hepatitis B infection – aiming at HBV cure.
 - Biology, virology and structural research related to HBV
 - Identification and screening of novel HBV targets
 - Design, synthesis and pharmacological profiling of novel HBV inhibitors and immunomodulators. Seeking external collaborations is encouraged.
- Internship programs at Gilead for IOCB PhD students. 1 to 2 students selected to spend up to 3 months at Gilead.



GSRC3 - Timeline

- June 30, 2016 - submission of GSRC applications to IOCB leadership
 - 1. Summary, rationale and benefits of project proposal
 - 2. Principal Investigator's background
 - 3. Size, organization and expertise of the groups
- July 15, 2016 - Feedback from Gilead provided to IOCB leadership
- July 30, 2016 - Selection of GSRC members, Advisory Board and Steering Committee
- August 15 - Execution of the amendment to the Gilead-IOCB Donation Agreement
- September 2016 - introductory GSRC meeting in Prague attended by Gilead and GSRC members

Upcoming dates

- Museum night - June 11, 2016
- **Happy Hours** - June 16 on the roof of B
- Next Meeting with Group Leaders June 27, 2016 ?
- Audits
 - Internal audit concluded May 20, 2016
 - Audit from Ministry of Interior June 2, 2016
 - Audit from the CAS June 20, 2016
- IAB Strategy Session- September 9-10, 2016
- GSRC-3 meeting in Prague, September
- Science Fair - September 2016