

Meeting with Group Leaders:

Scientific output update
Most significant publications

May 12 , 2014

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Output of Research Groups



- Group Efficiency Factor
- More explicit rules needed
- Work of current members of a group done before they joined the group should not be included (even when it was published during the time of current group membership)
- New groups: previous postdoc work of the group leader - should it be included?

Probably not

Group Evaluation

Group	Award (CZK)	Numerator per Year	GEF (A)	GEF (B)	Group	Award (CZK)	Numerator per Year	GEF (A)	GEF (B)
Hobza	403 886	171,96	41,034	31,809	Pichová	49 041	20,88	13,882	8,575
Hocek	254 625	108,41	106,733	60,125	Jiráček	48 525	20,66	11,678	6,879
Jungwirth	254 037	108,16	52,537	30,421	Jahn	47 867	20,38	14,023	8,287
Bouř	220 075	93,7	43,489	29,261	Rosenberg	44 226	18,83	8,821	5,471
Michl	217 186	92,47	41,784	27,902	Majer	38 895	16,56	17,814	9,275
Šaman	131 646	56,05	42,337	29,811	Krečmerová	34 667	14,76	22,563	10,341
Valterová	122 627	52,21	19,16	13,604	Mareš	25 977	11,06	9,556	5,37
Rulíšek	82 323	35,05	52,497	20,501	Mertlíková Kaiserová	24 474	10,42	11,3	9,185
Janeba	78 518	33,43	89,554	26,548	Nencka	22 853	9,73	23,071	9,55
Konvalinka	67 455	28,72	17,211	11,169	Vondrášek	21 702	9,24	38,517	14,2
Kašička	62 030	26,41	35,452	19,593	Šrogl	12 331	5,25	6,168	3,084
Maloy Řezáčová	60 174	25,62	34,33	22,714	Weber	10 053	4,28	9,921	4,234
Beier	54 655	23,27	33,408	17,296	Havlas	7 164	3,05	3,508	2,186
Cvačka	53 081	22,6	26,733	18,191	Total	2 500 000			
Stary	49 910	21,25	7,424	5,162					

Most significant publications



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

Each team may submit 1 most significant paper published in 2013 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 of 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 2013



- Physical and Theoretical Chemistry

(15) 11* submissions → 4 awards

- Medicinal and Organic Chemistry

(8) 7* submissions → 3 awards

- Biochemistry and Molecular Biology

(10) 6* submissions → 2 awards

- Interdisciplinary (within IOCB)

10 submissions → ~~4~~ 5 awards

Most significant publications 2013

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

Physical and Theoretical Chemistry part 1



Listed alphabetically by first author

- Gutten O, and Rulíšek* L

Predicting the Stability Constants of Metal-Ion Complexes from First Principles

Inorg Chem 2013, 52, 10347-10355

- Kessler J, Dračínský M, and Bouř* P

Parallel Variable Selection of Molecular Dynamics Clusters as a Tool for Calculation of Spectroscopic Properties

J Comput Chem 2013, 34, 366-371

Physical and Theoretical Chemistry part 2



Listed alphabetically by first author

- Kolář M, Hobza P, and Bronowska* AK

Plugging the explicit σ -holes in molecular docking

Chem Commun., 2013, 49, 981-983

- Stirnemann G, Wernersson E, Jungwirth* P, and Laage* D

Mechanisms of Acceleration and Retardation of Water Dynamics by Ions

J Am Chem Soc 2013, 135, 11824-11831

Medicinal and Organic Chemistry



Listed alphabetically by first author

- Dadová J, Orság P, Pohl R, Brázdová M, Fojta M, and Hocek* M

Vinylsulfonamide and Acrylamide Modification of DNA for Cross-linking with Proteins

Angew Chem Int Ed 2013, 52, 10515-10518

- Jančařík A, Rybáček J, Cocq K, Chocholoušová JV, Vacek J, Pohl R, Bednářová L, Fiedler P, Císařová I, Stará* IG, and Starý* I

Rapid Access to Dibenzohelicenes and their Functionalized Derivatives

Angew Chem Int Ed 2013, 52, 9970-9975

- Mucha M, Kaletová E, Kohutová A, Scholz F, Stensrud ES, Stibor I, Pospíšil L, von Wrochem F, and Michl* J

Alkylation of Gold Surface by Treatment with C₁₈H₃₇HgOTs and Anodic Hg Stripping

J Am Chem Soc 2013, 135, 5669-5677



Director's honorary mention

- Keough DT, Špaček P, Hocková* D, Tichý T, Vrbková S, Slavětínská L, Janeba Z, Naesens L, Edstein MD, Chavchich M, Wang T-H, de Jersey J, and Guddat* LW
Acyclic Nucleoside Phosphonates Containing a Second Phosphonate Group Are Potent Inhibitors of 6-Oxopurine Phosphoribosyltransferases and Have Antimalarial Activity
J Med Chem 2013, 56, 2513-2526

Biochemistry and Molecular Biology



Listed alphabetically by first author

- Sedlák F, Šácha P, Blechová M, Březinová A, Šafařík M, Šebestík J, and Konvalinka J

Glutamate Carboxypeptidase II Does Not Process Amyloid- β Peptide

FASEB J 2013, 27, 000-000

- Selicharová* I, Kořínek M, Demianová Z, Chrudinová M, Mládková J, and Jiráček J

Effects of Hyperhomocysteinemia and Betaine-Homocysteine S-methyltransferase Inhibition on Hepatocyte Metabolites and the Proteome

Biochem Biophys Acta 2013, 1834, 1596-1606

Interdisciplinary (within IOCB) part 1



Listed alphabetically by first author

- Brynda J, Mader P, Šícha V, Fábry M, Poncová K, Bakardiev M, Grüner B, Cígler P, and Řezáčová* P

Carborane-Based Carbonic Anhydrase Inhibitors

Angew Chem Int Ed 2013, 52, 13760-13763

- Fanfrlík J, Brahmshatriya PS, Řezáč J, Jílková, Horn M, Mareš, Hobza* P, and Lepšík* M

Quantum Mechanics-Based Scoring Rationalizes the Irreversible Inactivation of Parasitic *Schistosoma mansoni* Cysteine Peptidase by Vinyl Sulfone Inhibitors

J Phys Chem B 2013, 117, 14973-14982



- Lagoutte R, Šebesta P, Jiroš P, Kalinová B, Jirošová A, Straka J, Černá K, Šobotník J, Cvačka J, and Jahn U

Total Synthesis, Proof of Absolute Configuration, and Biosynthetic Origin of Stylopsal, the First Isolated Sex Pheromone of *Strepsiptera*

Chem Eur J 2013, 19, 8515-8524

- Vávra J, Severa L, Císařová I, Klepetářová B, Šaman D, Koval D, Kašička V, and Teplý* F

Search for Conglomerate in Set of [7]Helquat Salts: Multigram Resolution of Helicene-Viologen Hybrid by Preferential Crystallization

J Org Chem 2013, 78, 1329-1342

- Žáková L, Kletvíková E, Veverka V, Lepšík M, Watson CJ, Turkenburg JP, Jiráček* J, and Brzozowski* AM

Structural Integrity of the B24 Site in Human Insulin Is Important for Hormone Functionality

J Biol Chem 2013, 288, 10230-10240

Lanny S. Liebeskind

New member of IAB

Emory University, Atlanta, Georgia, USA

Office of University Science Strategies

Senior Advisor to the Provost

Samuel Candler Dobbs Professor

Associate Editor, *Organometallics*

Degrees

PhD, University of Rochester, 1976

BS, State University of New York at Buffalo

Specific Research Area

Molecular Synthetic Science, Catalysis

Liebeskind-Šrogl coupling



IOCB Library



- Library of compounds synthesized at IOCB
- AKA Antonin Holy Library (AHL)
- Coordinated by Radim Nencka
- Status of the project will be presented in Harrachov

Chemické Listy



- Big Thank you to Petr Holý and all contributors for the fantastic issue dedicated to 60th Anniversary of IOCB

Upcoming dates

- Thank you to Petr Holy and all participants (Chemické listy)
- Invited speaker series - NTK Balling Hall
 - May 27, 2014 C. Dale Poulter
 - June 5, 2014 Van der Donk
- Museum night June 14, 2014
- Building B Opening June 19 + Happy Hours
- Next Meeting with Group Leaders June 19 at 10 am, 2014
- Science Fair September 10, 2014
- Open House (Dny otevřených dveří) November 6 - 8, 2014
-

Science Fair 2014

Wednesday, September 10, 2014, Vítězné náměstí

- VĚDA NÁS BAVÍ, o.p.s.,
- Institute of Organic Chemistry and Biochemistry
- The Institute of Chemical Technology
- Czech Technical University in Prague

Special thanks to: Groups of Petr Bouř, Filip Teplý and NMR.



Prague Museum Night 2014

Saturday, June 14, 2014, Museum of Police CR
7pm - 1.00 am, Free admission and transport





Discussion

Evaluation of scientific output



A component of team financing

- Team efficiency factor (TEF) quantitative aspect

$$\text{TEF} = \frac{\text{J+B+C+D+P+T+S+L}}{\text{IS (Institutional Salaries)}}$$

Completed

- Most significant publications qualitative aspect

Completed

Team Efficiency Factor -



„faktor výkonnosti týmu -FVT“

Director's order 3/2008

TEF: period of 2010, 2011 and 2012, normalized for one year

- Version A (excl. Team Leader salary and over limit parts) *„ bez mzdy vedoucího a nadlimitních složek“*
- Version B (incl. Team Leader salary and over limit parts) *„ včetně mzdy vedoucího a nadlimitních složek“*
- Numerator of the TEF (=J+B+C+D+P+T+S+L)



Team efficiency factor (TEF) - Numerator vs. Most significant papers in 2012

