



ÚOCHB AV
IOCB PRAGUE

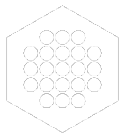
Meeting with Group Leaders

April 24, 2020

Zdenek Hostomsky

Agenda

- Quantitative evaluation of IOCB groups
- IOCB most significant papers 2019
- Evaluation of the IOCB Research-service groups



- Miscellanea
 - ITS update
 - Heyrovsky Institute mtg
 - CryoEM update
 - Valeč retreat

The Quantitative Evaluation - rules



- Directive S2018-01:
- Only such outputs can be included in the evaluation which have been entered in the ASEP [Automated System for Publication Index] database
- A group's performance is numerically evaluated by means of the group performance index (GPI) based on the formula

$$\text{GPI} = J + B + C + D + P + T + S + L$$

J - articles published in a high-impact journal

B = specialized books

C = chapters of a book

D = article in a collection

P = patent granted

T = operation on a semi-industrial scale, attested technology

S = prototype, implemented methodology, functional sample, authorized software, utility and industrial design

L = income from license fees and other income from the application of IP

The Quantitative Evaluation 2017-2019



Group	GPI per year	Award (CZK)	Group	GPI per year	Award (CZK)
Jungwirth	135,346	278 234	Rosenberg	25,924	53 292
Hocek	128,414	263 983	Cvačka	24,664	50 702
Hobza	110,816	227 807	Vondrášek	23,840	49 009
Konvalinka	71,526	147 037	Nencka	22,755	46 778
Michl	68,023	139 836	Mertlíková Kaiserová	21,967	45 159
Maletínská	64,815	133 241	Yushchenko	21,799	44 813
Beier	61,652	126 738	Čeřovský	20,198	0
Majer	58,934	121 152	Stříšovský	18,323	37 668
Šaman	58,461	120 179	Pichová	16,386	33 686
Bouř	51,498	105 866	Vrábel	14,683	30 183
Cígler	49,367	101 484	Weiss	13,293	27 327
Rulíšek	47,133	96 891	Havlas	12,855	26 426
Starý	39,108	80 394	Hanus	11,128	22 875
Janeba	38,302	78 738	Curtis	8,600	17 680
Kudová	35,530	73 040	Mareš	7,650	15 727
Řezáčová	33,943	69 778	Weber	6,593	13 554
Rejman	29,602	60 852	Matějková	5,870	12 068
Bouřa	28,797	59 199	Birkuš	4,831	9 932
Jiráček	27,793	57 134	Marek	4,299	8 838
Jahn	26,175	53 808	Macíčková Cahová	2,711	5 572
Kašička	25,937	53 318			3 000 000

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Junior
Research
Groups
highlighted

The Quantitative Evaluation 2017-2019



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Research-
Service
Groups
highlighted

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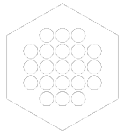
Targeted
Research and
Service Groups
highlighted

The Quantitative Evaluation 2017-2019



Group Leader	J	B	C	D	P	T	S	L	GPI	GPI per year
Beier	84,955				100,000				184,955	61,652
Birkuš	14,494								14,494	4,831
Bouř	149,270	5,000		0,225					154,495	51,498
Bouřa	86,391								86,391	28,797
Cígler	121,900		6,000	0,200	20,000				148,100	49,367
Curtis	25,801								25,801	8,600
Cvačka	72,092			1,900					73,992	24,664
Čeřovský	10,595				50,000				60,595	20,198
Hanus	33,383								33,383	11,128
Havlas	37,897		0,667						38,564	12,855
Hobza	332,449								332,449	110,816
Hocek	184,742		0,500		200,000				385,242	128,414
Jahn	68,525				10,000				78,525	26,175
Janeba	59,820			0,086	55,000				114,906	38,302
Jiráček	45,778			0,100	37,500				83,378	27,793
Jungwirth	406,039								406,039	135,346
Kašička	73,610		2,000	2,200					77,810	25,937
Konvalinka	77,077				137,500				214,577	71,526
Kudová	36,590				70,000				106,590	35,530
Macíčková Cahová	7,632		0,500						8,132	2,711
Majer	64,303				112,500				176,803	58,934
Maletínská	54,445				140,000				194,445	64,815
Marek	10,898		2,000						12,898	4,299
Mareš	22,951								22,951	7,650
Matějková	17,511			0,100					17,611	5,870
Mertlíková Kaiserová	16,752		0,250		48,900				65,902	21,967
Michl	200,069		4,000						204,069	68,023
Nencka	68,265								68,265	22,755
Pichová	48,959		0,200						49,159	16,386
Rejman	14,203				45,000				59,203	29,602
Rosenberg	25,772		2,000		50,000				77,772	25,924
Rulišek	141,398								141,398	47,133
Řezáčová	89,330				12,500				101,830	33,943
Starý	115,323	2,000							117,323	39,108
Stříšovský	50,303		4,667						54,970	18,323
Šaman	167,983		2,000	0,400	5,000				175,383	58,461
Vondrášek	71,521								71,521	23,840
Vrábel	43,048		1,000						44,048	14,683
Weber	19,780								19,780	6,593
Weiss	37,879		2,000						39,879	13,293
Yushchenko	65,198			0,200					65,398	21,799

IOCB Most Significant Publications 2019



Most significant publications in 2019



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

Each group may submit 1 most significant paper published in 2019 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). 3 to 5 papers in each category will be awarded prizes in the form of group money.

Most Significant Publications - 2019



- **PHYS** (9 for 2018) **11** submissions
- **CHEM** (6 for 2018) **8** submissions
- **BIO** (7 for 2018) **8** submissions

Did everyone who sent the nomination for the most significant publication get the answer from the secretariat?

Internal pre-Selection



- Pre-selection panel is composed of the external members of IOCB Board, an Adjunct Professor and the Director:

Tomáš Obšil

Petr Slavíček

Petr Svoboda

Pavel Kočovský

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 checked

Change of rules for 2020 !

Most significant publications in 2020

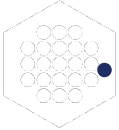


- **PHYS** Physical and Theoretical Chemistry
- **CHEM** Medicinal and Organic Chemistry
- **BIO** Biochemistry and Molecular Biology

Each group may submit **up to two significant papers** published in 2020 **regardless of category**.

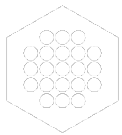
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Internal evaluation of Research- Service Groups

- IOCB Research-Service Group Annual Report
 - Completed by group leaders
 - Deadline: January 2020
- Evaluation — early 2020
 -  Service part – evaluated by **Board of Users** – 2 per group (14 total)
 - Nominate responsible users – in coordination with RSG leaders
 - Science part – evaluated by the IOCB Board at a dedicated meeting

Board of Users – call to nominate

- | | |
|---|-----|
| • NMR | • X |
| • Mass spectrometry | • X |
| • Electromigration methods | • X |
| • Drug discovery | • X |
| •  Biochem. Pharmacology | • X |
| • Bioinformatics | • X |
| • Virology | • X |



Miscellanea



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Meeting with Group Leaders

ITS Update

Jiří Polách | Apr 24, 2020

Optibrium StarDrop



A modular suite of software with a range of plug-in modules

The core features of StarDrop™ can be extended with a comprehensive range of predictive modelling, 3D SAR analysis and *de novo* design approaches.

[Learn more about the plug-in modules for StarDrop™ >](#)



Optibrium StarDrop



StarDrop Plan

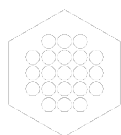
Step 1	Installing the temporary computing and license server.
Step 2	Testing the software - one month trial period.
Step 3	Obtaining the feedback, optimizing the number and the type of licenses to buy and setting the financing scheme.
Step 4	Purchasing / installing server (if needed), purchasing licenses.

Number of licenses	1	2	3
StarDrop	825	1,545	2,155
Additional cost for optional modules (StarDrop required)			
ADME QSAR Module	300	565	785
P450 Module	750	1,405	1,960
Auto-Modeller Module	750	1,405	1,960
Nova Module	625	1,170	1,635
MPO Explorer Module	750	1,405	1,960
BIOSTER Module	500	935	1,305
SeeSAR View Module	250	470	655
SeeSAR Affinity Module	750	1,405	1,960
SeeSAR Pose Module	500	935	1,305
torch3D Module	250	470	655
Derek Nexus Module	400	795	1,190

To take part in the testing apply by email to
lukas.svoboda@uochb.cas.cz

price / year in £ without VAT

- Joint Meeting with Heyrovsky Institute of Physical Chemistry



CryoEM update

- Two competitors: **ThermoFisher** and **JEOL**
- CryoEM Task Force:
Evžen Bouřa, Michal Hocek, Zdeněk Hostomský, Jiří Polách, Pavlína Řezáčová,
Kvido Stříšovský, Karel Šobíšek, Sebastian Zoll
-  Facility: 200 keV for screening and microED + 300 keV instrument
- New underground construction - bunker
- Next steps: Market research with concrete floorplan of the new facility



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GA ČR Calls 2021 – deadlines postponed

conditions remain unchanged

- **Mon 4 May 2020** - the new deadline
- **Wed 1 April 2020** - inform the Project Office about the intention to submit (email or the IOCB request form)
- **Wed 29 April 2020** - IOCB internal deadline



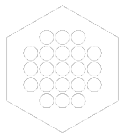
Intraweb: Calls + Apply
(documentations, templates, presentations)

Contact us at: projectoffice@uochb.cas.cz

IOCB Retreat - Valeč

23

- Moved to May 2021





Mtgs w GLs - 2020 Schedule

- January 17
- February 14
- March 25
- April 24
- May 22
- June 26
- September 11
- October 16
- November 13
- December 11

Always (almost) on Fridays at 10:00 am in the Director's Boardroom A4.01