



ÚOCHB AV
IOCB PRAGUE

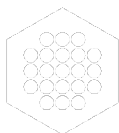
Meeting with Group Leaders

April 29, 2022

Zdenek Hostomsky

Agenda

- Quantitative evaluation
- Most significant publications 2021 update
- The Elegance of the Molecule Symposium
- Pete Schultz' visit
- Valeč update



- Miscellanea
 - Up-coming events
 - Recruiting Jr.GL – organic synthesis

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 - 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
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The Quantitative Evaluation – rules 2022



- **Directive S2022-05:**
- 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

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

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C = chapters of a book

D = article in a collection

P = patent granted

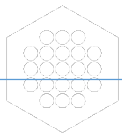
T = operation on a semi-industrial scale, attested technology

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

P = Patent granted

The numerical value **P** is determined using the equation:

old	$P = \sum 5 \times (\text{contribution of the authors})$ $P = \sum 50 \times (\text{contribution of the authors})$	national patent (with the exception of USA and Japan) international patent, patent from USA and Japan,
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new	$P = \sum 1 \times (\text{contribution of the authors})$ $P = \sum 10 \times (\text{contribution of the authors})$ $P = \sum 20 \times (\text{contribution of the authors})$	national patent (with the exception of USA and Japan) international patent, patent from USA and Japan, licensed patent,
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The Quantitative Evaluation 2019-2021



Group Leader	J	B	C	D	P	T	S	GPI	GPI per year
Beier	103,330		2,000		31,000			136,330	45,443
Birkuš	36,576				22,600			59,176	19,725
Bouř	200,880	5,000	14,000	0,200				220,080	73,360
Bouřa	139,048						1,000	140,048	46,683
Cígler	113,143		2,000	0,200	13,250	7,500	3,750	139,843	46,614
Curtis	62,954							62,954	20,985
Cvačka	110,316			1,000	1,000			112,316	37,439
Dračínský	194,675	2,500	2,000		1,100			200,275	66,758
Hanus	38,065							38,065	12,688
Havlas	70,566			0,200				70,766	23,589
Hobza	315,645							315,645	105,215
Hocek	207,094				50,000			257,094	85,698
Jahn	79,057				2,000			81,057	27,019
Janeba	80,643				21,330			101,973	33,991
Jiráček	64,057							64,057	21,352
Jungwirth	277,146							277,146	92,382
Kaleta	61,641							61,641	20,547
Kašička	110,058		2,000	1,800				113,858	37,953
Kečkéšová	12,701							12,701	4,234
Konvalinka	155,887		2,000		57,000		2,500	217,387	72,462
Kudová	64,854				18,000			82,854	27,618
Macíčková Cahová	37,622		0,500					38,122	12,707
Majer	59,492	5,000	0,200		56,000			120,692	40,231
Maletínská	80,544				39,000			119,544	39,848
Marek	29,755							29,755	9,918
Mareš	41,122		6,000					47,122	15,707
Matějková	31,043							31,043	10,348
Mertlíková Kaiserová	23,893							23,893	7,964
Nencka	133,260				4,400		0,500	138,160	46,053
Pichová	92,329							92,329	30,776
Pluskal	0,745							0,745	0,745
Rejman	27,552	2,500			9,900			39,952	13,317
Rulíšek	224,510							224,510	74,837
Řezáčová	174,470				0,250			174,720	58,240
Slanina	40,778							40,778	20,389
Starý	75,088		2,000					77,088	25,696
Stříšovský	45,695				7,000			52,695	17,565
Vondrášek	110,828							110,828	36,943
Vrábel	34,301		1,000					35,301	11,767
Weber	50,364							50,364	16,788
Zoll	2,420							2,420	1,210

The Quantitative Evaluation 2019-2021



Group	GPI per year	Award (CZK)	Group	GPI per year	Award (CZK)
Beier	45,443	96 496	Macíčková Cahová	12,707	26 983
Birkuš	19,725	41 886	Majer	40,231	85 427
Bouř	73,360	155 775	Maletínská	39,848	84 615
Bouřa	46,683	99 128	Marek	9,918	21 061
Cígler	46,614	98 982	Mareš	15,707	33 353
Curtis	20,985	44 560	Matějková	10,348	21 972
Cvačka	37,439	79 498	Mertlíková Kaiserová	7,964	16 911
Dračínský	66,758	141 757	Nencka	46,053	97 791
Hanus	12,688	26 943	Pichová	30,776	65 352
Havlas	23,589	50 089	Pluskal	0,745	1 582
Hobza	105,215	223 417	Rejman	13,317	28 278
Hocek	85,698	181 974	Rulíšek	74,837	158 911
Jahn	27,019	57 373	Řezáčová	58,240	123 669
Janeba	33,991	72 178	Slanina	20,389	43 295
Jiráček	21,352	45 341	Starý	25,696	54 563
Jungwirth	92,382	196 167	Stříšovský	17,565	37 298
Kaleta	20,547	43 630	Vondrášek	36,943	78 446
Kašička	37,953	80 590	Vrábel	11,767	24 987
Kečkéšová	4,234	8 990	Weber	16,788	35 649
Konvalinka	72,462	153 869	Zoll	1,210	2 569
Kudová	27,618	58 645			3 000 000

The Quantitative Evaluation 2019-2021



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Konvalinka	72,462	153 869		Zoll	1,210	2 569
Kudová	27,618	58 645				3 000 000

Junior
Research
Groups
highlighted

The Quantitative Evaluation 2019-2021



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Beier	45,443	96 496	Macíčková Cahová	12,707	26 983
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Research-
Service
Groups
highlighted

The Quantitative Evaluation 2019-2021



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Targeted
Research and
Service Groups
highlighted

IOCB Most Significant Publications - 2021



PHYS

Physical and Theoretical Chemistry

CHEM

Medicinal and Organic Chemistry

BIO

Biochemistry and Molecular Biology

	2019	2020	2021
• PHYS	11	9	10
• CHEM	8	9	12
• BIO	8	11	10

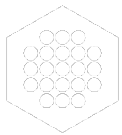
Most Significant Publications - 2021



Most Significant Publications 2021					
No.	Category	Authors	Laboratory	Article / Publication	Journal
1	CHEM	Filip Kalčík, Michala Zgarbáková	Z. Janeba	Discovery of Modified Amidate (ProTide) Prodrugs of Tenofovir with Enhanced Antiviral Properties	J. Med. Chem. 2021, 64, 16425–16449
2	CHEM	Athanasios Markos, a, b, c, d, e, f, g, h, i, j, k, l, m, n, o, p, q, r, s, t, u, v, w, x, y, z	P. Beier	Haloalkenyl Imidoyl Halides as Multifacial Substrates in the Stereoselective Synthesis of N-Alkenyl Compounds	Advanced Synthesis & Catalysis
3	CHEM	Terezie Pániková, Katarína Štefániková	J. Jiráček	Insulin Analogues with Altered Insulin Receptor Isoform Binding Specificities and Enhanced Aggregation Stabilities	J. Med. Chem. 2021, 64, 14848–14859
4	CHEM	Rastislav Džijak, Juraj Gašparík	M. Vrábel	Structurally Redesigning Bioorthogonal Reagents for Mitochondria-Specific Prodrug Activation	JACS Au 2021, 1, 23–30
5	CHEM	Denise-Liu' Leone, Martine L. H. de Azevedo	M. Hocek	1,3-Diketone-Modified Nucleotides and DNA for Cross-Linking with Arginine-Containing Peptides and Proteins	Angew. Chem. Int. Ed. 2021, 60, 17383–17387
6	CHEM	David Kodr, + Cansu Pinar	M. Hocek	Carborane- or Metallocarborane-Linked Nucleotides for Redox Labeling. Orthogonal Multipotential Coding of all Four DNA Bases for Electrochemical Analysis and Sequencing	J. Am. Chem. Soc. 2021, 143, 7124–7134
7	CHEM	Petr Šimon, [a] Markéta Šimonová	M. Dračinský	Phosphate-Based Self-Immolative Linkers for Tuneable Double Cargo Release	Chem. Eur. J. 2021, 27, 12763–12775
8	CHEM	Thi Phuong Le, Igor Rončević	J. Kaleta	Polyhalogenated Bicyclo[1.1.1]pentane-1,3-dicarboxylic Acids	J. Org. Chem. 2021, 86, 10303–10319
9	CHEM	Tomáš Otava, Michal Šalanda	R. Nencka	The Structure-Based Design of SARS-CoV-2 nsp14 Methyltransferase Ligands Yields Nanomolar Inhibitors	ACS Infect. Dis. 2021, 7, 2214–2220
10	CHEM	Markéta Pimková Polidová	G. Birkuš	Synthesis and Biological Evaluation of Phosphoester and Phosphorothioate Prodrugs of STING Agonist 3',3'-c-Di(2'F,2'dAMP)	J. Med. Chem. 2021, 64, 7596–7616
11	CHEM	Katerina Svehlova, Ondřej Štěpánek	E. Curtis	Supernova: A Deoxyribozymethat Catalyzes a Chemiluminescent Reaction	Angew. Chem. Int. Ed. 2022, 61, e20210934
12	CHEM	Robin Kryštof, Pavel Šácha, Jana Starková	J. Konvalinka	Re-emerging Aspartic Protease Targets: Examining Cryptococcus neoformans Major Aspartyl Peptidase 1 as a Target for Antifungal Drug Discovery	J. Med. Chem. 64 (10), 6706–6719
13	BIO	Miroslava Kacířová, Blažena Jílková, A., Horn, M., Farah	Lenka Maletinská	Aging and high-fat diet feeding lead to peripheral insulin resistance and sex-dependent changes in brain of mouse model of tau pathology THY-Tau22	Journal of Neuroinflammation
14	BIO	Jílková, A., Horn, M., Farah	L. Marešová	Azantrile inhibitors of the SmCB1 protease target are lethal to Schistosoma mansoni: structural and mechanistic insights into chemotype reactivity.	ACS Infectious Diseases, 7, 189–201.
15	BIO	Natalie Ben Abu, 1,2,5, Philip E. Mason 3,5.	P. Jungwirth	Sweet taste of heavy water	COMMUNICATIONS BIOLOGY
16	BIO	Pavel Dostalík, a Petra Králová	E. Bouřa	Structural Analysis of the OC43 Coronavirus 29-O-RNA Methyltransferase	Journal of Virology / jvi.asm.org
17	BIO	Cermakova K, Demeuler	P. Řezáčová	A ubiquitous disordered protein interaction module orchestrates transcription elongation	Science. 2021 Nov 26;374(6571)
18	BIO	Eva Dolejší, a, Nikolai Chumachenko	E. Kudová	Neuroactive steroids, WIN-compounds and cholesterol share a common binding site on muscarinic acetylcholine receptors	Biochemical Pharmacology 192 (2021) 114699
19	BIO	Eva Dolejší, a, Eszter Szabó	E. Kudová	Neurosteroids and steroid hormones are allosteric modulators of muscarinic receptors	Neuropharmacology 199 (2021) 108798
20	BIO	Tereza Streckerová, 1,2, Jaroslav Kurf, 1,2,3	E. Curtis	Single-round deoxyribozyme discovery	Nucleic Acids Research, 2021, Vol. 49, No. 12 6971–6981
21	BIO	Kristýna Blazková, 1,2, Jana Beranová, 1,3, Zuzana Hejdankova, Václav Vanek,	J. Konvalinka	The development of a high-affinity conformation-sensitive antibody mimetic using a biocompatible copolymer carrier (iBody)	J. Biol. Chem. 297, 101342
22	BIO	Zuzana Hejdankova, Václav Vanek,	P. Cigler	Lipid Nanoparticles for Broad-Spectrum Nucleic Acid Delivery	Adv. Funct. Mater. 2021, 2101391
23	PHYS	Philip E. Mason, 1,12, H. C.	P. Jungwirth	Spectroscopic evidence for a gold-coloured metallic water solution	Nature
24	PHYS	Miroslav Smola, Ondřej Rulíšek	L. Rulíšek	Ligand Strain and Its Conformational Complexity Is a Major Factor in the Binding of Cyclic Dinucleotides to STING Protein	Angew. Chem. Int. Ed. 2021, 60, 10172–10178
25	PHYS	Das, M.; Gangopadhyay,	P. Bouř	Chiral detection by induced surface-enhanced Raman optical activity	Chem. Commun. 2021, 57, 6388–6391
26	PHYS	Kurochka, A.; Průša, J.; K.	P. Bouř	α-Synuclein conformations followed by vibrational optical activity. Simulation and understanding of the spectra	Phys. Chem. Chem. Phys. 2021, 23, 16635–16645
27	PHYS	J. Chalupský, M. Srnec	Z. Havlas	Beyond the Classical Contributions to Exchange Coupling in Binuclear Transition Metal Complexes.	Journal of Physical Chemistry A. Roč. 125, č. 11 (2021), s. 2276–2283
28	PHYS	J. Chalupský, M. Srnec, T.	Z. Havlas	Interpretation of Exchange Interaction through Orbital Entanglement.	Journal of Physical Chemistry Letters. Roč. 12, č. 4 (2021), s. 1268–1274
29	PHYS	Martin Dračinský, Carina Santos Hurtado.	J. Kaleta	Stuffed pumpkins - Mechanochemical synthesis of host-guest complexes with cucurbit uril	Chem. Commun., 2021, 57, 2132
30	PHYS	Rabindranath Lo, Il Deba	P. Hobza	Addition Reaction between Piperidine and C60 to Form 1,4- Disubstituted C60 Proceeds through van der Waals and Dative Bond Complexes-Theoretical and Experimental Study	J. Am. Chem. Soc. 2021, 143, 10930–10939
31	PHYS	B. Mallada, 1,2,3†, A. Gallardo	P. Hobza	Real-space imaging of anisotropic charge of s-hole by means of Kelvin probe force microscopy	Science 374, 863–867 (2021)
32	PHYS	Benjamin Mallada, † Bruni	D. Nachtigallová	On-Surface Strain-Driven Synthesis of Nonalternant Non-Benzenoid Aromatic Compounds Containing Four- to Eight-Membered Rings	J. Am. Chem. Soc. 2021, 143, 14694–14702

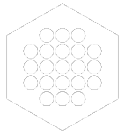
Appeal to participate

- External votes are pouring in
- Only two internal votes were received so far
- Do people care?
- A new link will be sent
- Deadline extended till May 6, 2022
- Results announced on May 20, 2022
- Posters displayed in Valeč



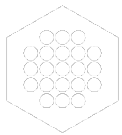
Pete Schultz' visit

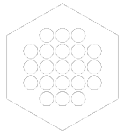
- Director of the Scripps Research
- Visit on September 8-9, 2022
- Tony Holy Lecture
- IOCB-Scripps collaboration



The Elegance of the Molecule Symposium

- Leuven - September 7-8, 2022
- Joint action with Rega Institute of KU Leuven
- Dejvické divadlo – Dejvice theater
- Czech presidency of EU

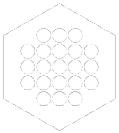




Miscellanea

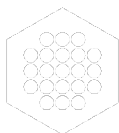
Upcoming events

- Off-site meeting at Valeč **May 23-26, 2022**
- IAB in Prague **June 24-25, 2022**
- Tony Holy Lecture **Sept 8-9, 2022**



Recruitment of Jr. GL – organic synthesis

- Deadline May 16, 2022
- 12 applications so far





Mtgs w GLs - 2022 Schedule

- January 28
- February 18
- March 31
- April 29
- May 20
- June 17
- September 16
- October 21
- November 18
- December 16

Always on Fridays at 10:00 am in the Director's Boardroom A4.01 (and/or via ZOOM)