Evaluation of research and professional activity of research-oriented institutes of the Czech Academy of Sciences for the period 2015–2019

Final Report

Name of the Institute:

Institute of Organic Chemistry and Biochemistry of the CAS, v. v. i.

Evaluated teams and their leaders:

1. Molecular modeling and spectroscopy in chemistry and biology (Lubomír Rulíšek)
2. Spectral analytical methods and separations (Josef Cvačka)
3. Bioorganic and medicinal chemistry (Michal Hocek)
4. Synthetic organic, materials and nano chemistry (Ivo Starý)
5. Molecular interactions in biomedicine (Jan Konvalinka)
6. Chemical biology for life and diseases (Pavlína Maloy Řezáčová)

Part A: Evaluation of the institute

Strengths:

- A modern research institute performing at a high international standard.
- Efficiency and success oriented directing team.
- Flat structure of research management.
- Research groups are basic organisational units reporting directly to the Director.
- Two types of research groups (tenure track): Junior and Senior.
- Meritocracy-based selection process.
- A high number of new PhD studentships each year.
- Internal annual evaluation of groups' scientific output.
- Regular evaluation of research groups by International Advisory Board.
- Fast staff and economic consequences of the evaluation for the groups.
- A very intense and fruitful partnership with companies in the chemical and pharmaceutical sector.
- Substantial income stream from royalties.
- Tradition and expertise in drug development together with pharma industry.
- A practical and easy to navigate webpage.

Weaknesses:

- Too rigid hiring system to get key researchers.
- Strong gender imbalance with too few female group leaders.
- Only few highly valued key European grants like ERC.
- Service departments are mixed with fundamental research, requiring that highly experienced researchers have to spend some of their time by performing routine analytics that could be done by skilled technicians.

Opportunities:

- Increase research reputation further by using the scientific expertise of researchers in Team 2 to full extent: Split departments into "research" and "service" groups and apply IOCB evaluation rules to the resulting research groups. The service group should report to a service manager without the expectation to undertake research.
- Hire junior researchers holding ERC grants.

Threats:

- Too few women in leadership positions is viewed unfavourably by research institutions in other European countries, putting the Institute at a disadvantage when applying for European projects.
- The tough recruitment and evaluation system could deter excellent candidates, who may choose other institutions over the IOBC that offer more job security.
- Having analytical groups alongside research groups implies two yardsticks that could lead to a dissimilar evaluation system and lower scientific performance.

Main criterion: 1. Quality of results (H1.1-H1.5)

H1.1	Quality of selected outputs of Phase I
Good to very good.	
H1.2	**Contribution of workers on the outputs reached**
All researchers, PhD students, researchers and group leaders are contributing. About 75% of the publications originate from research carried out (almost fully) at IOCB, with the first and/or corresponding author having IOCB affiliation.	
H1.3	**Quality of all outputs and results**
Good to very good.	
H1.4	**The most valuable discoveries and findings in the fields, their importance for the field**
Medicinal chemistry group with mix of fundamental and applied research; molecular mo delling and simulations in the physical chemistry group.	
H1.5	**Contribution of the participation of the authors in large collaborations**
The IOCB has major collaborations with internationally renowned institutions, such as John Hopkins University, Weizmann Institute of Science, The University College London or the biopharmaceutical company Gilead Sciences, among others, that is due to the researchers of and research performed in the IOCB.	

Main criterion: 2. Societal relevance (H2.1-H2.5)

H2.1	Societal relevance of outputs and results pursuant to CAS and institute mission
The Institute has a long-standing history based on research performed by Antonin Holý, whose influence in the current research activity of the Institute is noticed in all its research areas, but very particularly in medicinal chemistry, computer modelling, and somehow less in synthetic organic, materials and nano chemistry that are in their turn more related with energy. Holý cooperated in the development of important antiretroviral drugs used in the treatment of HIV and hepatitis B, that have certainly benefited society.	
H2.2	**System functionality for knowledge transfer into practise, its usefulness for society. The impact of the institute´s activity on proper practice in society in the area of social sciences and humanities**
See H2.1. Possible industrial application of compounds made by the team of synthetic organic, materials and nano chemistry, in particular the research on singlet fission, which could be of interest for the energy industry (solar cells). The IOBC has a spin-off company for licencing inventions and managing a large portfolio of patents, which create significant income through royalties.	
H2.3	**Relation to practice**
The institute's research profile spans from fundamental to applied research, depending on the individual	

groups; it is not enforced to undertake applied research, which provides the group with maximum freedom in the research activities (and creativity). Despite this, several drugs are already applied as antivirotics, analogues of hormones, cancerostatics or dermatologics. In the area of energy steps are done ahead although the application seems to be far or may never take place, but it is necessary to be done.

H2.4	**Participation in AV21 strategy**
The institute contributes to the AV21 strategy through the topics “Diagnostic Methods and Techniques”, “Wellbeing in Health and Disease” and “Molecules and Materials for Life”.	

H2.5	**Cooperation with regions of the Czech Republic**
Good.	

Further criterion: 1. Position in international and national context (D1.1-D1.3)

D1.1	**Comparison of the teams and the institute with similar international and national institutes**
This Institute clearly is a player in the top international league.	

D1.2	**Scope and quality of international and national cooperation and the role of the institute in such cooperation; engagement in broad international cooperation**
Excellent. Wide collaborative network, both nationally and internationally, where IOBC often seems to take the lead/initiative.	

D1.3	**Participation of the workers in scientific community activities (organizing of conferences and workshops, invited lectures, awards)**
High.	

Further criterion: 2. Vitality, sustainability and strategy (D2.1-D2.9)

D2.1	**Direction in line with the perspective of the planned research directions**
The Institute's management aims to achieve its scientific objectives and to maintain its high status.	

D2.2	**Assessment of the previous research objectives and their achievement**
The management of the IOBC has a consistent approach to the objectives pursued.	

D2.3	**Assessment of implementation of recommendations from past evaluation**
The management of the institute implemented the recommendations made previously, except those suggested for the bioorganic and medicinal chemistry team as the panel did not have the scientific expertise in this research area (this lack of expertise has been admitted by the commission in an ensuing exchange of rebuttals, however, no late change to the recommendations was made). In addition to the CAS reviews, every	

group is evaluated every 5 years by the IAB to provide feedback on their progress and future research strategies.	
D2.4	**Success in receiving grants**
The success is high but should enforce the value of successful applications for ERC grants. The lack of considerable European funding is a weak point of the IOCB.	
D2.5	**Adequacy of instrumental equipment**
Adequate, however, some major investments will be required in the nearer future. There is excellent technical support staff.	
D2.6	**Effectiveness of management**
Management is very good to excellent, very efficient through the flat organisational structure. It's just the institute director, and each research group leader (senior and junior) reports directly to them without any additional layers. This management model is recommended for each CAS institute. However, the hiring process could be improved (see D2.7).	
D2.7	**Assessment of professional structure, development strategy and the strategy of keeping best scientists, age structure, career and qualification growth**
There are clearly problems in obtaining good young people, so that the age structure reflects the part-time employment of retirees very strongly. The gender balance in leading position is currently very poor and bringing more women into leadership positions should be one of the top priorities for the Institute's management (see also D2.8).	
D2.8	**Creating work-life balance conditions, assessment of approach towards possible gender issues**
See D2.7. The poor gender balance in leading positions should be addressed by identifying and recruiting excellent female researchers as junior/senior group leaders (national and international).	
D2.9	**Relation of the institute with regard to the integration, development and sustainability of the research centre funded by the National Programme of Sustainability II.**
The institute is very viable.	

Further criterion: 3. Cooperation with universities and participation in education (D3.1-D3.6)

D3.1	**Scope of cooperation with universities on national and international level**
Good. Joint or adjunct appointments of IOCB research group leaders (Med chem, physical chemistry, amongst others) with various CZ universities; numerous collaborations with international universities but details on the area of research were mostly not disclosed.	
D3.2	**Effectiveness of joint research centres**
Not much detail was provided, however a collaboration with Gilead Sciences established in 2006, with ongoing close collaboration; also, collaboration with Novo	

Nordisk on prolactin-releasing peptide (PrPR) analogues active in treatment of obesity and type 2 diabetes (this research group was not reviewed by this commission).	
D3.3	**Success rate in supervision of PhD students**
Good to excellent.	
D3.4	**Participation of PhD students in the outputs**
Good.	
D3.5	**Participation of the institute in master or bachelor studies**
Good.	
D3.6	**Assessment of cooperation intensity with universities in the form of teaching**
Good, particular positive is that it's not only the same few engaged with these tasks but that many researchers take the opportunity to engage with universities through teaching.	

Further criterion: 4. Outreach activities (D4.1-D4.3)

D4.1	**Sufficiency of media strategy and activities in the area of research popularisation**
Could be improved, as there appear to be some inconsistencies. While the website is very homogeneous and it is easy to find what one is looking for, which is an indication of complacency towards scientific competitors. However, there is no website for dissemination of results to the general public. It is suggested that an office be created to combine both efforts.	
D4.2	**Publishing activities and its quality**
Could be improved.	
D4.3	**Participation in professional organisations in the area of research and development**
Not too many details were provided.	

Other comments of the commission:

The Institute has a flat structure with junior and senior groups all reporting directly to the management. This scheme has proven to be very efficient. The management is supported by various evaluation panels and follows their recommendations; however, the final decision-making lies in the hands of the management.

However, this committee believes that the groups performing both research and services should be restructured into research groups (which should be evaluated similar to the other research groups) and a clearly defined service department headed by a scientific director (which is not expected to undertake research). This suggestion is based on the commission's impression that the 'mixed' research/service groups had a disadvantage over the pure research groups with regards to the clarity of their research direction as well as research funding/output, as a highly variable fraction of their time is spent by providing service to other groups of the Institute (or even outside the IOBC).

Research outcomes and research collaborations within the centre, nationally and internationally are at a very high level. Protection of IP and research commercialisation is identified and managed by a dedicated team.

The hiring process of the IOBC is very rigorous and avoids inbreeding, which the commission has noticed to occur frequently in other institutes. However, the fact that in three years they have not been able to identify and recruit a junior team leader in the area of organic chemistry poses the question whether the selection process is too ambitious or whether suitable candidates do not apply (if this is the case it would be interesting for the Institute to explore the reason and work towards rectifying this issue). Furthermore, at current the Institute's gender balance with regards to female group leaders is poor. Recruitment strategies such as targeting suitable women scientists or women-only positions should be considered.

The commission noted a mixed approach with regards to the Institute's visibility to the public. At the scientific level it is very easy to get to know the groups and their research through an efficient website. However, information of the IOBC's research that is tailored to the general public is less available, and it is therefore recommended to establish an outreach office that could form a unit with the website service.

Part B: Evaluation of teams

1. Molecular modelling and spectroscopy in chemistry and biology

Strengths:

- Strong leadership.
- Highly innovative and complementary research areas at the international forefront.

Weaknesses:

- Poor gender balance with not a single woman research group leader.
- In some cases, computational research appears to be too distant from experimental research.
- A too strong focus on fundamental research.

Opportunities:

- Increase alignment with experimentation, where possible.
- Dedicate more effort into investigating currently less well understood biological processes.

Threats:

- Competition with groups with large computing centres.
- Potential segregation between theoretical and experimental work.

Main criterion: 1. Quality of results (H1.1-H1.5)

H1.1	**Quality of selected outputs of Phase I**
Very good.	
H1.2	**Contribution of workers on the outputs reached**
Good.	
H1.3	**Quality of all outputs and results**
Very good.	
H1.4	**The most valuable discoveries and findings in the fields, their importance for the field**
Pavel Hobza group. A new quantum mechanics-based scoring function has been developed and has been tested on a large dataset of diverse protein-ligand complexes. Its performance has been compared with other scoring functions from academia and industry finding that the IOCB protocol outperforms the standard functions. This approach is currently focused on insulin analogs and mimetics using the structures of the insulin receptor. It is also proposed for general use in computer-aided drug design. Pavel Jungwirth Group. By using molecular dynamics simulations and quantum chemical methods they attempt to understand the ion-protein interactions responsible for the Hofmeister series. Subjects as important as protein aggregation, precipitation, denaturation	

and controlling enzymatic activity in the presence of ions are studied, particularly the action of calcium ions involved in membrane fusion and cationic cell penetrating peptides. Related research activities concern electron solvation pertinent to radiation chemistry and the Birch reduction process. Zdeněk Havlas Group. This groups works on biradicals and transition metal compounds as main topics. They propose new chromophores as suitable candidates for the singlet fission process using modern multi-reference electronic structure methods. Lubomír Rulíšek Group. This group works on metalloproteins as catalysts facilitating reactions that would not occur under physiological conditions. The presence of metal ions is key for electron transfer processes fundamental in respiration and photosynthesis. Their research is focused into understanding the structure and function of metalloproteins. The theoretical calculations complement observable structural data so that the reaction mechanisms of bioinorganic systems can be elucidated.
H1.5 Contribution of the participation of the authors in large collaborations
Average, should be improved.

Main criterion: 2. Societal relevance (H2.1-H2.5)

H2.1	**Societal relevance of outputs and results pursuant to CAS and institute mission**
Considerable: The research of the groups in this Team is focused on interpreting mechanisms of action of biological materials, to assist the drug design process and the development of energy materials.	
H2.2	**System functionality for knowledge transfer into practise, its usefulness for society. The impact of the team´s activity on proper practice in society in the area of social sciences and humanities**
The theoretical research groups provide important insight that supports the development/design of new materials (drugs, energy materials, etc.), which cannot be or only with difficulty obtained through other approaches. Commercialisation is therefore not a priority and it should not be one. In fact, it is the nature of fundamental research that commercialisation may only occur many years (even decades) after the discovery was made.	
H2.3	**Relation to practice**
See H2.2.	
H2.4	**Participation in AV21 strategy**
Their research will benefit the practical applications mentioned in AV21 in the longer term.	
H2.5	**Cooperation with regions of the Czech Republic**
Average.	

Further criterion: 1. Position in international and national context (D1.1-D1.3)

D1.1	Comparison of the team with similar international and national institutes
Outstanding, an internationally highly competitive team.	
D1.2	**Scope and quality of international and national cooperation and the role of the team in such cooperation; engagement in broad international cooperation**
High.	
D1.3	**Participation of the workers in scientific community activities (organizing of conferences and workshops, invited lectures, awards)**
High.	

Further criterion: 2. Vitality, sustainability and strategy (D2.1-D2.9)

D2.1	Direction in line with the perspective of the planned research directions
Good to very good.	
D2.2	**Assessment of the previous research objectives and their achievement**
Good to very good.	
D2.3	**Assessment of implementation of recommendations from past evaluation**
Very good.	
D2.4	**Success in receiving grants**
Good, although no ERC grant.	
D2.5	**Adequacy of instrumental equipment**
Good.	
D2.6	**Effectiveness of management**
The groups are successful.	
D2.7	**Assessment of professional structure, development strategy and the strategy of keeping best scientists, age structure, career and qualification growth**
The science and scientists are at the highest level, who are working in an excellent scientific environment. Good age distribution but lack of female leaders.	
D2.8	**Creating work-life balance conditions, assessment of approach towards possible gender issues**
The research group leader's influence on hiring female research group leaders is limited (this is a task for the IOBC management). The gender balance in research groups itself is generally much better.	

D2.9	Relation of the team with regard to the integration, development and sustainability of the research centre funded by the National Programme of Sustainability II.
No information provided.	

Further criterion: 3. Cooperation with universities and participation in education (D3.1-D3.6)

D3.1	Scope of cooperation with universities on national and international level
Good, team members give lectures on their areas of expertise at Charles University, South Bohemica and Palacky University	
D3.2	**Effectiveness of joint research centres**
Most of the members of the team are involved as external faculty members either as Full Professor or Associate Professor with Czech universities, e.g. Palacky, or Charles University.	
D3.3	**Success rate in supervision of PhD students**
Good to very good.	
D3.4	**Participation of PhD students in the outputs**
Good to very good.	
D3.5	**Participation of the team in master or bachelor studies**
Good to very good.	
D3.6	**Assessment of cooperation intensity with universities in the form of teaching**
Very good, the university's teaching programs clearly benefits from the expertise of the team members.	

Further criterion: 4. Outreach activities (D4.1-D4.3)

D4.1	Sufficiency of media strategy and activities in the area of research popularisation
Mixed level of contributions (a particular mention of Jungwirth and Lazar).	
D4.2	**Publishing activities and its quality**
Excellent.	
D4.3	**Participation in professional organisations in the area of research and development**
Very good. Hobza, Jungwirth, Rulisek, Lazar participate in several societies, are members of scientific and editorial boards as well as grant agencies panels.	

Other comments of the commission:

2. Spectral analytical methods and separations

Strengths:

 Large expertise in spectroscopy, and separations, alongside with computational studies and data processing.

 Excellent facilities with a wide range of spectrometers; some not so common in synthetic laboratories, dedicated to chirality studies.

Weaknesses:

 Mixing genuine research with service function.

 Expert researchers dedicating part of their time to routine experiments.

 Some equipment appears to be outdated.

Opportunities:

 Collaborations between researchers in complementary fields when synergy is needed.

 Highly qualified researchers in spectroscopy and separations are available to solve uncommon problems.

 Separation of services from spectroscopy research to increase research focus.

Threats:

 Underutilisation of the expertise of highly qualified personnel by requiring them to perform routine work.

Main criterion: 1. Quality of results (H1.1-H1.5)

H1.1	Quality of selected outputs of Phase I
Good.	
H1.2	**Contribution of workers on the outputs reached**
Excellent.	
H1.3	**Quality of all outputs and results**
Very good.	
H1.4	**The most valuable discoveries and findings in the fields, their importance for the field**
Petr Bour group. This group uses organic synthesis, spectroscopy and theory as tools to understand the functioning of biologically relevant molecules. The overall aim is to use the knowledge of the structure and properties of molecules to change them to use their functions more efficiently. To this end, they develop new spectroscopic techniques, e.g., chiroptical methods that require quantum chemistry and computational modelling. Typical applications include peptide folding, behaviour of nucleic acids, and biomolecular imaging. Josef Cvačka group. This group uses mass spectrometry as a tool to retrieve structure information, and the identification and quantification of small molecules to large biomacromolecules. They collaborate in improving the performance of the equipment	

through new methods, applications and devices such as the development of new ion sources. They analyse lipids in the vernix caseosa, their structural analysis and MALDI imaging of lipids, and the study of proteins. They participate through their services in the research of other IOCB groups.

Martin Dračínský group. This group participates very actively with other groups in the IOBC, being a group of fundamental importance, but has few projects of its own, its research being mainly of support to the other groups in the IOBC.

Václav Kašička Group. This group is dedicated to capillary electromigration (CE) and its application in the separation, analysis, micropreparation and physicochemical characterisation of (bio)molecules. Methodological developments include all major CE techniques: zone electrophoresis, affinity electrophoresis, isotachophoresis, isoelectric focusing, electrokinetic chromatography and electrochromatography. They are developing new devices for one- and two-dimensional CE methods but, although the groups produces interesting publications, many are supportive to other groups.

H1.5	Contribution of the participation of the authors in large collaborations

Very active. All groups participate in large collaborations, e.g., Both the Bouř group and the Cvačka group are involved in a large collaborative project of the European Regional Development Fund entitled Chemical biology for drugging undruggable targets. The Kašička group participates in the COST Action CA16215: European network. The Martin Dračínský formerly the Šaman group of NMR Spectroscopy participated in InterBioMed project supported by the National Programme for Sustainability I of Ministry of Education, Youth and Sports.

Main criterion: 2. Societal relevance (H2.1-H2.5)

H2.1	Societal relevance of outputs and results pursuant to CAS and institute mission

Considering the social relevance of the research of the IOBC, and considering how much intertwined is the research of team 2 with the other research groups at the institute the conclusion is that the outputs are of societal relevance.

H2.2	System functionality for knowledge transfer into practise, its usefulness for society. The impact of the team´s activity on proper practice in society in the area of social sciences and humanities

See H2.1.

H2.3	Relation to practice

See H2.1.

H2.4	Participation in AV21 strategy

No information provided.

H2.5	Cooperation with regions of the Czech Republic

The Team cooperates with other institutes in the country mostly by providing analytical and spectroscopic services.

Further criterion: 1. Position in international and national context (D1.1-D1.3)

D1.1	Comparison of the team with similar international and national institutes
Due to the dual research and service characteristics of the teams no clear assessment can be provided. However, the Bour that has international research collaboration.	
D1.2	**Scope and quality of international and national cooperation and the role of the team in such cooperation; engagement in broad international cooperation**
See D1.1.	
D1.3	**Participation of the workers in scientific community activities (organizing of conferences and workshops, invited lectures, awards)**
Very good. The 6th Czech Lipidomics Conference, June 14-15, 2018, Prague; Galaxy Proteomics workshop, October 4-6, 2018, 45th International Symposium on High-Performance Liquid Phase Separations and Related Techniques, HPLC 2017, 18-22.6.2017, Prague, Czechia, ca. 1350 participants. EUROMAR2015, Prague, July 5-10, 2015, were organized by these teams.	

Further criterion: 2. Vitality, sustainability and strategy (D2.1-D2.9)

D2.1	Direction in line with the perspective of the planned research directions
All groups in this Team are principally research active. However, they are required to provide service to other research groups, which negatively impacts on their own research progress.	
D2.2	**Assessment of the previous research objectives and their achievement**
It appears that all major aims outlined in the section “Assessment of the activity plan of the team for the period of 2015-2019" have been successfully met.	
D2.3	**Assessment of implementation of recommendations from past evaluation**
For the Kašička group the general recommendation was that “the group is a valuable resource for the Institute and its share of internal collaborations with scientists should be encouraged”. This recommendation has been implemented since 2018 by changing the status of the group from the Senior Research Group to the Research-Service Group. The commission feels that the target is good, but should be implemented more strongly.	
D2.4	**Success in receiving grants**
Good, the Team is recipient of Czech Science Foundation grants; Participation in the IOCB-wide European Regional Development Fund project (ChemBioDrug; Bouř and Cvačka groups); Participation in the COST Action (Kašička group); InterBioMed Project of MEYS (Dračínský group).	
D2.5	**Adequacy of instrumental equipment**
Adequate for the services they are providing.	
D2.6	**Effectiveness of management**
Good.	

D2.7	**Assessment of professional structure, development strategy and the strategy of keeping best scientists, age structure, career and qualification growth**
Balanced, apart from a gender imbalance at the research group leader level.	
D2.8	**Creating work-life balance conditions, assessment of approach towards possible gender issues**
The research group leader's influence on hiring female research group leaders is limited (this is a task for the IOBC management). The gender balance in research groups itself is generally much better.	
D2.9	**Relation of the team with regard to the integration, development and sustainability of the research centre funded by the National Programme of Sustainability II.**
No information provided.	

Further criterion: 3. Cooperation with universities and participation in education (D3.1-D3.6)

D3.1	**Scope of cooperation with universities on national and international level**
Most of the leaders of the Team do teach at the Charles University.	
D3.2	**Effectiveness of joint research centres**
The Team is not involved in joint research centres with universities.	
D3.3	**Success rate in supervision of PhD students**
There is a notable difference between groups that do their own research and those providing service to other groups. It has been difficult for this commission to assess from the available data whether the student is member of a group in this Team or whether they are from other research groups. From our reading of the report and presentations, it seems that the more research-focused Bour group has its own PhD students whereas the more service-focused groups have PhD students from other institutions that spend time in the premises of the IOCB.	
D3.4	**Participation of PhD students in the outputs**
Good.	
D3.5	**Participation of the team in master or bachelor studies**
Good.	
D3.6	**Assessment of cooperation intensity with universities in the form of teaching**
Active.	

Further criterion: 4. Outreach activities (D4.1-D4.3)

D4.1	**Sufficiency of media strategy and activities in the area of research popularisation**

Very good by giving lectures and providing mentoring for high school students, with the Open House Days, through funfairs, lectures, articles. The commission highlights the fact that members of the MS group founded, maintain and operate a unique Czech Mass Spectrometry Museum.	
D4.2	**Publishing activities and its quality**
Active, by publishing popularization articles (in the Czech language).	
D4.3	**Participation in professional organisations in the area of research and development**
All group members have good conditions for further professional development, they participate in variable courses, workshops, and national and international conferences and symposia.	

Other comments of the commission:

3. Bioorganic and medicinal chemistry

Strengths:

- Excellent previous history in the area that leads to a unique expertise in chemistry of nucleos(t)ides, nucleic acids, peptides, steroids, prodrugs etc.
- Excellent know-how in drug discovery and development.
- Adequate environment/facilities with excellent research groups within IOCB and outside.

Weaknesses:

- Medicinal chemistry requires time-consuming synthesis, large series of compounds for SAR studies and delays due to confidentiality and patenting; the publication output is therefore usually slower compared with other teams in the IOCB more related to Computation or Analytical methods. Performance metrics need to take this fact into account.

Opportunities:

- Highly transferable research with immediate applications in the Pharmaceutical Industry, and income through licensing royalties.
- Emerging viral diseases (COVID-19), cancer, neurodegenerative or metabolic diseases has stimulated interest in new drugs, providing new research avenues for the Team.
- Area of diagnostics and imaging could provide opportunities for complementary work between chemical biology and theory to gain better understanding of biological processes.

Threats:

- Nature of this type of research provides few opportunities for the development of new synthetic methodology as synthesis of new pharmaceutically active compounds is highly target-oriented and usually employs well-established protocols.
- High competition in emerging targets.
- Difficulty to find and recruit talented and highly-trained synthetic chemists.

Main criterion: 1. Quality of results (H1.1-H1.5)

H1.1	**Quality of selected outputs of Phase I**
Good.	
H1.2	**Contribution of workers on the outputs reached**
Excellent.	
H1.3	**Quality of all outputs and results**
Very good.	
H1.4	**The most valuable discoveries and findings in the fields, their importance for the field**
Michal Hocek Group Bioorganic and Medicinal Chemistry of Nucleic Acids This group is doing synthetic, bioorganic and medicinal chemistry of nucleic acids and their components. Basic developments of methodology for the synthesis of these modified	

biomolecules are performed largely using modern methods (including metal- or enzyme-catalysed reactions). Biological activity (antitumor, antiviral etc.) of the novel nucleobases, nucleosides and nucleotides is systematically studied in collaboration with groups both in academia and in pharmaceutical industry. Enzymatic synthesis is developed and the modified oligonucleotides or nucleic acids are applied in bioanalysis**.**

Zlatko Janeba Group Medicinal Chemistry of Nucleotide Analogues

The research of the group deals with development of inhibitors of enzymes involved in the metabolism of nucleosides and nucleotides. The design of novel types of modified nucleosides and nucleotides, is based on the previous SAR done in the group. Target structures are designed based on inhibition of key enzymes.

Radim Nencka Group Drug Design and Medicinal Chemistry

The objective is the design and synthesis of new molecules as potential therapeutics and as tools for chemical biology, particularly to decipher biological processes connected with viral replication. Their major target are RNA viruses
from *Flaviviridae*, *Picornaviridae* and *Togaviridae* families. They have invented highly selective chemical probes based on inhibition of phosphatidylinositol 4-kinase IIIβ. Also, they aim at discovery of novel inhibitors of enzymes involved in pathology of neurodegenerative diseases and liver diseases or injury.

Milan Vrábel Group Chemistry of Bioconjugates

This group combines modern organic chemistry with chemical biology tools and combinatorial library synthesis to create hybrid biological systems with improved features and unique functions. They aim at developing small molecule-biomolecule conjugates as the next generation of therapeutics and bioanalytic.

The Yushchenko group

This group works on the development of chemical tools for modulating and studying biological processes. They synthetized caged signalling lipids that can be selectively delivered to specific cellular compartments, activated by a UV light pulse, and induce Ca-signalling at desired moment. The group also developed new environment-sensitive fluorescent dyes and labels to study interactions of amyloidogenic proteins. They found a new approach to inhibit misfolding of Parkinson's disease related protein α-synuclein.

Pavel Majer Group Drug Discovery

The Drug Discovery group is dedicated to the design and synthesis of biologically active compounds. They collaborate with the Drug Discovery Group at Johns Hopkins University (JHU) in Baltimore, USA, developing prodrugs of glutamine antimetabolite 6-Diazo-5-oxo-L-norleucine (DON), inhibitors of Glutamate Carboxy Peptidase II (GCPII), Decitabine and Mebendazole. The prodrugs target cancer cells and selectively deliver the active drugs, thus lowering their toxicity. Some of these compounds have been patented, and some of them are currently undergoing preclinical testing.

Eva Kudová Group Neurosteroids

Neurosteroids are endogenous steroids that are synthesized from cholesterol and produce rapid effects on neuronal excitability and synaptic function that involve direct or indirect modulation of neurotransmitter-gated ion channels. The effects of neurosteroids are mediated by interactions with ligand-gated ion channels such as glutamate, GABAA, glycine, nicotinic acetylcholine receptors, etc. The group research tries to find novel potentially beneficial drugs to treat neurological damage/neurodegeneration. To this target this group designs, synthesizes and screens SMART Steroids
– Steroidal Molecules As Rapid-acting Therapeutics. It aims at treating diseases like epilepsy, neuropathic pain, ischemia, neuropsychiatric disorders, and others.

Dominik Rejman Group Antimicrobial Compounds

This group is dedicated to attack bacterial strains resistant to known antibiotics and to develop new antibiotics. They work on three main projects: Lipophosphonoxins – antibacterial compounds acting via disrupting bacterial cell membrane. Pyrrolidine inhibitors of hypoxanthine-guanine-xanthine phosphoribosyl transferase as potential antimalarials and/or antituberculotics. Study on bacterial stringent response as a potential antibiotic drug target.

Ivan Rosenberg Group Nucleotides and Oligonucleotides

The group's research is directed towards basic research in the area of nucleoside phosphonic acids (NPAs) as potential antimetabolites, building units for solid phase synthesis of chimeric antisense oligonucleotides as compounds capable of interfering with gene expression, and regulatory oligonucleotides (2',5'-linked oligoadenylates and CpG oligonucleotides).

H1.5	Contribution of the participation of the authors in large collaborations

The groups of Hocek, Nencka, Majer cluster are involved in the European Regional Development Fund; OP RDE (Title: Chemical biology for drugging undruggable targets; No. CZ.02.1.01/0.0/0.0/16_019/0000729). The groups of Janeba, Nencka are involved in the "Personalized Medicine – Diagnostics and Therapy" (TN01000013 from programme NCK for years 2019-2020) supported by Technology Agency of the Czech Republic.

Main criterion: 2. Societal relevance (H2.1-H2.5)

H2.1	Societal relevance of outputs and results pursuant to CAS and institute mission

High. The medicinal chemistry research of this Team has applications in the pharmaceutical industry and health sector.

H2.2	System functionality for knowledge transfer into practise, its usefulness for society. The impact of the team´s activity on proper practice in society in the area of social sciences and humanities

See H2.1.

H2.3	Relation to practice

See H2.1.

H2.4	Participation in AV21 strategy

No details provided.

H2.5	Cooperation with regions of the Czech Republic

Adequate.

Further criterion: 1. Position in international and national context (D1.1-D1.3)

D1.1	Comparison of the team with similar international and national institutes

Good to excellent.

D1.2	Scope and quality of international and national cooperation and the role of the team in such cooperation; engagement in broad international cooperation
Examples of cooperations are with Gilead Sciences IOCB Research Center Hocek, Janeba, Nencka, Vrábel, Majer. Johns Hopkins University (US) Nencka with 8 patent applications, 3 licenses to companies and many publications. Weizmann Institute, Nencka. Practically all groups participate in international cooperations as well as within the Czech Republic.	
D1.3	**Participation of the workers in scientific community activities (organizing of conferences and workshops, invited lectures, awards)**
The Team is recipient of many awards, and has given many lectures. Particularly awarded are the groups of Hocek, Janeba, and Nencka, although all groups are highly celebrated.	

Further criterion: 2. Vitality, sustainability and strategy (D2.1-D2.9)

D2.1	Direction in line with the perspective of the planned research directions
Fully in agreement.	
D2.2	**Assessment of the previous research objectives and their achievement**
The Hocek, Rosenberg, Janeba and Nencka groups have fulfilled the proposed goals. The other groups (Kudova, Vrabel, Majer, Rejman, Yushchenko) have not been evaluated or have not even existed at that time.	
D2.3	**Assessment of implementation of recommendations from past evaluation**
According to the report, the Chemistry panel at that time did not have expertise in bioorganic and medicinal chemistry but was critical on all three medicinal chemistry groups evaluated because they criticized the lack of development of new reactions. This commission does not agree at all with the opinion of the previous commission, and this point is highlighted in the SWOT analysis of this Team. Drug discovery and development requires excessive synthetic chemistry, using mostly established methodology. The primary goal is the drug itself and not the pathway of its synthesis.	
D2.4	**Success in receiving grants**
Very high.	
D2.5	**Adequacy of instrumental equipment**
Good.	
D2.6	**Effectiveness of management**
Good.	
D2.7	**Assessment of professional structure, development strategy and the strategy of keeping best scientists, age structure, career and qualification growth**
Appears to be balanced.	

D2.8	Creating work-life balance conditions, assessment of approach towards possible gender issues
The research group leader's influence on hiring female research group leaders is limited (this is a task for the IOBC management). The gender balance in research groups itself is generally much better. One junior group is led by a woman.	
D2.9	**Relation of the team with regard to the integration, development and sustainability of the research centre funded by the National Programme of Sustainability II.**
No information provided.	

Further criterion: 3. Cooperation with universities and participation in education (D3.1-D3.6)

D3.1	Scope of cooperation with universities on national and international level
Strong commitment with Charles University, Univ. Of Chemistry and Technology in Prague, Palacky University mostly by Hocek, Janeba, Nencka, Chodounska and Rejman.	
D3.2	**Effectiveness of joint research centres**
The Hocek group is an official Joint Laboratory of Bioorganic and Medicinal Chemistry of Nucleic Acids of IOCB and Charles University (CU). Michal Hocek is a Full Professor at the Department of Organic Chemistry, Faculty of Science, Charles University and at the same time a Senior Group Leader at IOCB. The major lab space of the Hocek group is at IOCB, but the group also runs a lab at the CU. Students, postdocs and staff scientists are members of the Joint Laboratory.	
D3.3	**Success rate in supervision of PhD students**
Excellent. The research groups have good sizes providing ample opportunity for young scientist to be trained in cutting-edge synthetic, bioorganic and medicinal chemistry. The Hocek group has currently 20 PhD students from 8 different countries. The Janeba group has currently 6 PhD students from 2 countries. The Nencka group has currently 5 PhD students, the Yushchenko group has currently 4 PhD students. In the groups of Bioorganic and Medicinal Chemistry team, 37 PhD students are currently supervised and working on their theses and during the evaluation period, 23 PhD students successfully graduated.	
D3.4	**Participation of PhD students in the outputs**
Very good, PhD students participated on almost all publications and patents of the teams.	
D3.5	**Participation of the team in master or bachelor studies**
Very good, particularly Hocek, Janeba, Nencka, Chocounska and Rejman.	
D3.6	**Assessment of cooperation intensity with universities in the form of teaching**
Very good.	

Further criterion: 4. Outreach activities (D4.1-D4.3)

D4.1	Sufficiency of media strategy and activities in the area of research popularisation
Hyde Park Civilizace (Czech TV), comments on Nobel prize winners of 2018, short spots for Czech TV or Czech Radio, popularization articles, short presentation for students from Czech Universities and from abroad, mostly by Hocek, Vrabel and Majer.	
D4.2	**Publishing activities and its quality**
Very good.	
D4.3	**Participation in professional organisations in the area of research and development**
Ver good with memberships on different societies.	

Other comments of the commission:

An excellent team that knows how to combine research, teaching and dissemination of their findings to both scientists and the general public.

4. Synthetic organic, materials and nano chemistry

Strengths:

 Experts in synthetic methodology development (small molecules) and development of new reagents.

 Strong expertise in organic and polymer chemistry, which is developed on demand to access new materials, for example nanoparticles and interfaces.

 Total synthesis of complex natural products of either methodology-oriented or biology-driven targets molecules.

 Unique expertise, experience and methodology in electrochemistry, computation, physical chemistry, physics and various aspects of chirality.

Weaknesses:

 Team does not have a unique target but is combining several renowned scientists with different research focus under one umbrella.

Opportunities:

 Identification of compounds with useful biological activities.

 Development of effective in vivo delivery nanosystems for nucleic acids (applications in vaccines, RNA interference and gene editing).

 Exploration of new chemical space around natural products.

 Emerging practical applications (organic photovoltaics, display technology, organic electronics, batteries, catalysis, etc.)

Threats:

 Subjects tackled by this Team are facing rapidly growing international competition in chemistry and physics and their applications in physics and technology.

Main criterion: 1. Quality of results (H1.1-H1.5)

H1.1	**Quality of selected outputs of Phase I**
Good.	
H1.2	**Contribution of workers on the outputs reached**
Excellent.	
H1.3	**Quality of all outputs and results**
Very good.	
H1.4	**The most valuable discoveries and findings in the fields, their importance for the field**
Petr Beier Group Organic Chemistry of Fluorine and Main Group Elements Their target research is in the development of new, selective and convenient synthetic reagents and methods towards novel organic molecules, which can find applications in crop protection, drug design and in materials. They focus on new reactions and their	

mechanisms. They are focusing on organic chemistry of the main group elements such as fluorine, phosphorus, silicon, sulfur and iodine. They have made substantial progress in fluorinated phosphonates, pentafluorosulfanyl (SF5) containing compounds, fluoroalkylations, transfer of tetrafluoroethyl and tetrafluoroethylene fragments, bioconjugations, and the chemistry of fluorinated azides, heterocycles, enamines and enamides.

Petr Cígler Group Synthetic Nanochemistry

They study new types of nanoparticles for use in therapeutics, imaging and diagnostics of diseases. These nanomaterials are based either on bioorganic or inorganic cores and include virus-like particles, fluorescent nanodiamonds and plasmonic systems. Importance is given to the biocompatibilization of nanoparticles, their targeting to cells and on non-invasive, remote control of nanoparticles' action in cells by external stimuli.

Ullrich Jahn Group Chemistry of Natural Products

Their research focus on the total synthesis of natural products and their biological investigation. They attempt to establish and confirm the structures of natural products, and then to find good yield approaches for biological investigations. The interest spans from complex indole and bridged diketopiperazine alkaloids via terpenoid and steroid natural products to lipid metabolites. Also, they explore new pathways in transition metal catalysis using unconventional ligand architectures, photochemistry and -catalysis, radical reactions, the chemistry of reactive intermediates, and electron transfer chemistry.

Josef Michl Group Organic Chemistry

This group encompasses organic, inorganic, physical, electrochemistry, and theoretical chemists, which combines chemical synthesis with spectroscopic and other physical measurements. The current research consists of four main projects: *Singlet fission*, *Alkylation of gold surfaces*, *Regular arrays of artificial molecular rotors*, and *Porphene – a 2-dimensional polymer*.

Ivo Starý Group Chemistry of Functional Molecules

Their research is focused on the non-conventional π-electron architectures, which are attractive for applications to chemistry and physics. Particularly to the synthesis of helically chiral aromatics (helicenes) that are enantiopure and properly functionalised. They investigate systematically their (chir)optical properties, self-assembly in crystals or at interfaces, charge/spin transport properties and on-surface reactivity at nanoscale. They are also active in the general synthetic methodology development and enantioselective catalysis.

H1.5	Contribution of the participation of the authors in large collaborations

The Cígler group is involved in the large collaborative project, the European Regional Development Fund; OP RDE (Title: Chemical biology for drugging undruggable targets; No. CZ.02.1.01/0.0/0.0/16_019/0000729). No data about the other groups were provided.

Main criterion: 2. Societal relevance (H2.1-H2.5)

H2.1	Societal relevance of outputs and results pursuant to CAS and institute mission

Substantial. While the research of the groups in this Team is fundamental in nature, they are pursuing innovation that could benefit society in the area of healthcare and energy.

H2.2	System functionality for knowledge transfer into practise, its usefulness for society. The impact of the team´s activity on proper practice in society in the area of social sciences and humanities
See H2.1.	
H2.3	**Relation to practice**
See H2.1.	
H2.4	**Participation in AV21 strategy**
No information was provided.	
H2.5	**Cooperation with regions of the Czech Republic**
Some cooperation with CAS institutes is provided but not sufficient to enable assessment.	

Further criterion: 1. Position in international and national context (D1.1-D1.3)

D1.1	Comparison of the team with similar international and national institutes
Good to excellent.	
D1.2	**Scope and quality of international and national cooperation and the role of the team in such cooperation; engagement in broad international cooperation**
All groups cooperate at international level. Examples are: The Beier group has ongoing collaboration with S. Prakash (USC, LA, US) funded by MŠMT INTEREXCELLENCE; The Cígler group collaborates with a high-tech company NVision (Ulm, Germany) focused on application of quantum technology in imaging. The Jahn group collaborates with the Durand group (University of Montpellier, FR) in the area of the identification and biological investigation of autoxidatively formed lipid metabolites. The Michl group has ongoing international collaborations in the individual research topics. E.g. in Singlet Fission: The development of singlet fission into a practical tool for increasing the efficiency of solar cells: MacQueen at the Humboldt-Zentrum Berlin; Germany, Kaupp at the Technical University, Berlin, Germany; The Starý group continues its international cooperation with experts in chiroscience, physics, and surface science: J. Crassous (University of Rennes 1, France; chiroptical properties of helicenes), K.-H. Ernst (EMPA & University of Zurich, Switzerland)	
D1.3	**Participation of the workers in scientific community activities (organizing of conferences and workshops, invited lectures, awards)**
All members of the team have participated in many scientific community activities, many, but outstanding is the number of invited lectures by J. Michl. Incredible, where does he find the time?	

Further criterion: 2. Vitality, sustainability and strategy (D2.1-D2.9)

D2.1	Direction in line with the perspective of the planned research directions
Fully in agreement.	

D2.2	Assessment of the previous research objectives and their achievement
All groups indicate and it can be verified that „Based on the plans for the period 2015–2019, the group's goals were met".	
D2.3	**Assessment of implementation of recommendations from past evaluation**
The Evaluation committee recommended the Beier group to do efforts towards publishing in top-ranked chemical journals, and this group has done so. The Jahn group was very positively evaluated during the period 2010-2014 with the recommendation to encourage to continue to develop its creative research. The Starý group was suggested to establish strong and fruitful collaborations with established groups of physicists and engineers for the helical aromatics subject. The group has followed this recommendation.	
D2.4	**Success in receiving grants**
It seems so, but no specific section for grants in the report.	
D2.5	**Adequacy of instrumental equipment**
Good.	
D2.6	**Effectiveness of management**
Good.	
D2.7	**Assessment of professional structure, development strategy and the strategy of keeping best scientists, age structure, career and qualification growth**
Seems to be balanced but the commission was slightly surprised by the decision to employ a very senior and internationally highly regarded research group leader instead of providing younger scientists with an opportunity to develop their own research group.	
D2.8	**Creating work-life balance conditions, assessment of approach towards possible gender issues**
The research group leader's influence on hiring female research group leaders is limited (this is a task for the IOBC management). The gender balance in research groups itself is generally much better.	
D2.9	**Relation of the team with regard to the integration, development and sustainability of the research centre funded by the National Programme of Sustainability II.**
No information was provided.	

Further criterion: 3. Cooperation with universities and participation in education (D3.1-D3.6)

D3.1	Scope of cooperation with universities on national and international level
Good, particularly with Charles University and Boulder University (due to the link between Prof Michl and Boulder)	
D3.2	**Effectiveness of joint research centres**
No information provided.	

D3.3	Success rate in supervision of PhD students
Good to excellent.	
D3.4	**Participation of PhD students in the outputs**
PhD students participated in most or all publications and patents of the group.	
D3.5	**Participation of the team in master or bachelor studies**
Excellent.	
D3.6	**Assessment of cooperation intensity with universities in the form of teaching**
Lecturing at universities at Boulder Michl and at Charles University by Starý.	

Further criterion: 4. Outreach activities (D4.1-D4.3)

D4.1	Sufficiency of media strategy and activities in the area of research popularisation
Good use of various types of media: Twitter, radio show, science café, radio show „Metero“, popularization articles in portal iDnes.cz, News magazine of the German Chemical Society Nachrichten aus der Chemie, Chemienotizen, lectures for high school students and for The Learned Society, appearances in Czech TV or Czech Radio Hyde Park Civilizace, Traditional High School Modřany, "Jedna molekula stačí", radio show “Meteor” (Czech Radio) The Learned Society of the Czech Republic.	
D4.2	**Publishing activities and its quality**
High.	
D4.3	**Participation in professional organisations in the area of research and development**
Members of this Team participate in many societies, editorial boards, committees. Examples include: Czech Chemical Society Materials Research Society Committee for evaluation of results of science Royal Society of Chemistry European Photochemical Association, Chemistry Olympiad of the Czech Republic, editorial advisory boards, Chemistry Olympiad of the Czech Republic, American Chemical Society, Czech Chemical Society, Fluorine Division of the American Chemical Society, Evaluation Committee in Chemistry Panel of the Czech Science Foundation.	

Other comments of the commission:

An excellent team with a very diverse research portfolio that provides superb training opportunities for young scientists.

Top 10 publications for the 4 evaluated teams
Team 1: Molecular modelling and spectroscopy in chemistry and biology

Papers were ranked #1-#3(or -#2 in the case of the Havlas group, to get closer to 10) within each group: Hobza, Jungwirth, Havlas, and Rulíšek, by the group leaders, but not ranked within the team, i.e. comparing papers between different groups was avoided, therefore ranking 1.- 4.; 5.-8.; 9.-11.)

1.-4. Kolar M.H.; Hobza P.: Computer Modeling of Halogen Bonds and Other sigma-Hole Interactions. *Chem. Rev.* **2016***, 116,* 5155*.*

Description of a new type of noncovalent interactions playing important role in bio- and material sciences. 334 citations.

1.-4. Allolio C., Magarkar A., Jurkiewiczf P., Baxová K., Javanainen M., Mason P.E., Sachl R., Cebecauer M., Hof M., Horinek D., Heinz V., Rachel R., Zieglerg C.M., Schrofel A., Jungwirth P.: Arginine-rich cell-penetrating peptides induce membrane multilamellarity and subsequently enter via formation of a fusion pore. *Proc. Natl. Acad. Sci.* **2018**, *115*, 11923.

A new mechanism of cell penetration of cationic peptides with potential for drug delivery suggested. 38 citations.

1.-4. Bím, D.; Maldonado-Domínguez, M.; Rulíšek, L.; Srnec, M.: Beyond the Classsical Thermodynamic Contributions to Hydrogen Atom Abstraction Reactivity. *Proc. Natl. Acad. Sci.* **2018**, *115*, E10287.

New concept in understanding hydrogen transfer reactions and non-Bell-Evans-Polanyi processes. 25 citations.

1.-4. Wen, J.; Havlas, Z.; Michl, J.: Captodatively Stabilized Biradicaloids as Chromophores for Singlet Fission. *J. Am. Chem. Soc.* **2015**, *137*, 165.

It has been shown that captodatively stabilized biradicaloids might have T1 (triplet) state half- way between S0 and S1 states and might be optimal c andidates for the singlet-fission chromophores. 28 citations.

5.-8. de la Torre, B.; Švec, M.; Hapala, P.; Redondo, J.; Krejčí, O.; Lo, R.; Manna, D.; Sarmah, A.; Nachtigallová, D.; Tuček, J.; Blonski, P.; Otyepka, M.; Zbořil, R.; Hobza, P.; Jelínek, P.: Non- covalent control of spin-state in metal-organic complex by positioning on N-doped graphene. *Nat. Comm.* **2018**, *9*, Art. No. 2831.

Theoretical and experimental study on the modulation of the spin state in Fe(II)-porphyrines in different phases. 36 citations.

5.-8. Okur H. I., Hladílková J., Rembert K. B., Cho Y., Heyda J., Dzubiella J., Cremer P. S., Jungwirth P.: Beyond the Hofmeister Series: Ion Specific Effects on Proteins and Their Biological Functions. *J. Phys. Chem. B* **2017**, *121***,** 1997.

Summary of our contributions to molecular understanding of ion-specific effects on proteins and beyond. 230 citations

5.-8. Jaroš, A.; Bonab, E. F.; Straka, M.; Foroutan-Nejad, C.: Fullerene-Based Switching Molecular Diodes Controlled by Oriented External Electric Fields *J. Am. Chem. Soc.* **2019**, *141*, 19644.

New molecular electronic component – molecular memristor – has been designed. 22 citations.

5.-8. Zaykov, A.; Felkel, P.; Buchanan, E. A.; Jovanovic, M.; Havenith, R. W. A.; Kathir, R. K.; Broer, R.; Havlas, Z.; Michl, J.: Singlet Fission Rate: Optimized Packing of a Molecular Pair. Ethylene as a Model. *J. Am. Chem. Soc.* **2019**, *141*, 19644.

A procedure is described for unbiased identification of all p***-electron chromophore pair geometry choices that locally maximize the rate of conversion of a singlet exciton into a singlet biexciton (triplet pair), using a simplified version of the diabatic frontier orbital model of singlet fission (SF).*** 8 citations.

9.-11. Holá, K.; Sudolská, M.; Kalytchuk, S.; Nachtigallová, D.; Rogach, A.; Otyepka, M.; Zbořil, R.: Graphitic Nitrogen Triggers Red Fluorescence in Carbon Dots. *ACS Nano* **2017**, *11*, 12402.

A combined experimental (XPS, FT-IR, Raman spectroscopy) - computational (DFT) study reveals a crucial factor which cause a significant red-shift of the CD photoluminescence. 175 citations.

9.-11. Mason, P.; Uhlig, F.; Vanek, V.; Buttersack, T.; Bauerecker, S.; Jungwirth, P.: Coulomb Explosion during the Early Stages of the Reaction of Alkali Metals with Water. *Nature Chem.* **2015**, *7*, 250.

An unexpected explanation of a textbook problem why alkali metals explode in water. 56 citations.

9.-11. Straka, M.; Andris, E.; Vícha, J.; Růžička, A.; Roithová, J.; Rulíšek, L.: Spectroscopic and Computational Evidence of Intramolecular Au···H^+–N Hydrogen Bonding. *Angew. Chem. Int. Ed.* **2019**, *58*, 2011.

New and unexpected gold(I)...hydrogen bond was proved experimentally and computationally. 21 citations.

Team 2: Spectral analytical methods and separations

Papers were ranked within each group (Bouř, Cvačka, Dračínský, and Kašička) by the group leaders; they were not ranked within the team to avoid comparing papers between the groups.

1.-4. Li, G.; Kessler, J.; Cheramy, J.; Wu, T.; Poopari, M. R.; Bouř, P.; Xu, Y., Transfer and Amplification of Chirality within the 'Ring of Fire' Observed in Resonance Raman Optical Activity Experiments." *Angew. Chem Int. Ed.*, 58 (2019) 16495-16498.

Selected as Best IOCB paper, winning also international P. Stephens's prize, it describes experiment and theory of a transfer of chirality to achiral organic solvents in ROA experiments.

1.-4. Dračínský, M.; Buchta, M.; Buděšínský, M.; Vacek-Chocholoušová, J.; Stará, I. G.; Starý, I.; Malkina, O. L., Dihydrogen contacts observed by through-space indirect NMR coupling. *Chem. Sci.* 9 (2018) 7437-46.

We demonstrated that, contrary to many textbooks, J-coupling interaction can be observed between hydrogen atoms not connected by covalent bonds.

1.-4. Kalužíková, A.; Vrkoslav, V.; Harazim, E.; Hoskovec, M.; Plavka, R.; Buděšínský, M.; Bosáková, Z.; Cvačka, J., Cholesteryl esters of ω-(O-acyl)-hydroxy fatty acids in vernix caseosa, *J. Lip. Res*. 58 (2017) 1579-1590.

We discovered a new lipid class in vernix caseosa and developed a unique method for structure elucidation of these lipids using mass spectrometry.

1.-4. Šolínová, V.; Žáková, L.; Jiráček, J.; Kašička, V., Pressure assisted partial filling affinity capillary electrophoresis employed for determination of binding constants of human insulin complexes with serotonin, dopamine, arginine, and phenol. *Anal. Chim. Acta*, 1052 (2019) 170-178.

The strength of noncovalent interactions of important protein hormone, human insulin, with its biologically relevant ligands was quantified.

5.-8. Keiderling, T. A.; Bouř, P. Theory of Molecular Vibrational Zeeman Effects as Measured with Circular Dichroism. *Phys. Rev. Lett*. 121 (2018) 073201.

We developed a theory for calculation of MVCD molecular spectra; this spectroscopy was discovered in 1984, but not understood in terms of molecular properties so far.

5.-8. Dračínský, M.; Čechová, L.; Hodgkinson, P.; Procházková, E.; Janeba, Z, Resonance- assisted stabilisation of hydrogen bonds probed by NMR spectroscopy and path integral molecular dynamics. *Chem. Commun*. 51 (2015) 13986-13989.

We developed a methodology for including nuclear quantum effects, such as nuclear delocalization or proton tunneling, into computations of NMR parameters and applied it for an investigation of short strong hydrogen bonds.

5.-8. Rejšek, J.; Vrkoslav, V.; Vaikkinen, A; Haapala, M. ; Kauppila, T.J. ; Kostiainen, R. ; Cvačka, J., Thin-Layer Chromatography/Desorption Atmospheric Pressure Photoionization Orbitrap Mass Spectrometry of Lipids, *Anal. Chem*. 88 (2016) 12279-12286.

We developed a new analytical method (device) for detecting and identifying compounds from TLC plates using photoionization mass spectrometry.

5.-8. Konášová, R.; Koval, D.; Jaklová Dytrtová, J.; Kašička, V: Comparison of two low flow interfaces for measurement of mobilities and stability constants by affinity capillary electrophoresis–mass spectrometry, *J. Chromatogr. A* 1568 (2018) 197-204.

The new interfaces allowed hyphenation of home-made capillary electrophoretic device with electrospray ionization mass spectrometry detection with minimized dilution of analytes.

9.-10. Procházková, E.; Čechová, L.; Kind, J.; Janeba, Z.; Thiele, C. M.; Dračínský, M., Photoswitchable intramolecular hydrogen bonds in 5-phenylazopyrimidines revealed by in situ irradiation NMR spectroscopy. *Chem. Eur. J.* 24 (2018) 492-498.

We designed, prepared and investigated a new class of orthogonal photoswitches, where two different structural changes can be induced by different wavelength of irradiation. Selected as the Best IOCB Paper.

9.-10. Kessler, J.; Kapitán, J.; Bouř, P., First-principles predictions of vibrational Raman optical activity of globular proteins, *J. Phys. Chem. Lett*. 6 (2015) 3314-3319.

We developed and applied a computational method to simulate and thus interpret ROA spectra of large proteins (~10000 atoms) with exceptional accuracy.

Team 3: Bioorganic and medicinal chemistry

1. Vaníková, Z.; Janoušková, M.; Kambová, M.; Krásný, L.*; Hocek, M.* Switching transcription with bacterial RNA polymerase through photocaging, photorelease and phosphorylation reactions in the major groove of DNA. *Chem. Sci.* **2019**, *10*, 3937–3942.

   the first chemical regulation of transcription through reactions in major groove of DNA

2. Zawada, Z.; Tatar, A.; Mocilac, P.; Buděšínský, M.; Kraus, T.* Transport of Nucleoside Triphosphates into Cells by Artificial Molecular Transporters. *Angew. Chem. Int. Ed.* **2018**, *57*, 9891–9895.

   the first synthetic transporter for nucleoside triphosphates through cell membrane

3. Dziuba, D.; Jurkiewicz, P.; Cebecauer, M.; Hof, M.*; Hocek, M.* A Rotational BODIPY Nucleotide: An Environment-Sensitive Fluorescence-Lifetime Probe for DNA Interactions and Applications in Live-Cell Microscopy. *Angew. Chem. Int. Ed.* **2016**, *55*, 174–178.

   viscosity sensitive fluorescence lifetime-probe for DNA sensing protein-DNA binding

4. Rais, R.; Jančařík, A.; Tenora, L.; Nedelcovych, M.; Alt, J.; Englert, J.; Rojas, C.; Le, A.; Elgogary, A.; Tan, J.; Monincová, L.; Pate, K.; Adams, R.; Ferraris, D.; Powell, J.; Majer, P.*; Slusher, B. S.* Discovery of 6-Diazo-5-oxo-l-norleucine (DON) Prodrugs with Enhanced CSF Delivery in Monkeys: A Potential Treatment for Glioblastoma. *J. Med. Chem.* **2016**, *59*, 8621–8633.

   new prodrug of DON for delivery into brain and treatment of glioblastoma

5. Vázquez, A.; Dzijak, R.; Dračínský, M.; Rampmaier, R.; Siegl, S. J.; Vrabel, M.* Mechanism- Based Fluorogenic trans-Cyclooctene-Tetrazine Cycloaddition. *Angew. Chem. Int. Ed.* **2017**, *56*, 1334–1337.

   new fluorogenic bioconjugations of different isomers of trans-cyclooctene

6. Matyašovský, J.; Perlíková, P.; Malnuit, V.; Pohl, R.; Hocek, M.* 2-Substituted dATP Derivatives as Building Blocks for Polymerase-Catalyzed Synthesis of DNA Modified in the Minor Groove. *Angew. Chem. Int. Ed.* **2016**, *55*, 15856–15859.

   the first polymerase synthesis of DNA modified or labelled in minor groove

7. Krausova, B.; Slavikova, B.; Nekardova, M.; Hubalkova, P.; Vyklicky, V.; Chodounska, H.; Vyklicky, L.*; Kudova, E.* Positive Modulators of the N-Methyl-d-aspartate Receptor: Structure-Activity Relationship Study of Steroidal 3-Hemiesters. *J. Med. Chem.* **2018**, *61*, 4505–4516.

   discovery of allosteric modulators of NMDA receptors

8. Špaček, P.; Keough, D. T.; Chavchich, M.; Dračínský, M.; Janeba, Z.; Naesens, L.; Edstein, M. D.; Guddat, L. W.*; Hocková, D.* Synthesis and Evaluation of Asymmetric Acyclic Nucleoside Bisphosphonates as Inhibitors of Plasmodium falciparum and Human Hypoxanthine-Guanine- (Xanthine) Phosphoribosyltransferase. *J. Med. Chem.* **2017**, *60*, 7539–7554.

   discovery of new type of inhibitors of HGPRP with antiparasitic activity against malaria

9. Mejdrová, I.; Chalupská, D.; Plačková, P.; Müller, C.; Šála, M.; Klíma, M.; Baumlová, A.; Hřebabecký, H.; Procházková, E.; Dejmek, M.; Strunin, D.; Weber, J.; Lee, G.; Matoušová, M.; Mertlíková-Kaiserová, H.; Ziebuhr, J.; Birkus, G.; Boura, E.*; Nencka, R.* Rational Design of Novel Highly Potent and Selective Phosphatidylinositol 4-Kinase IIIβ (PI4KB) Inhibitors as Broad-Spectrum Antiviral Agents and Tools for Chemical Biology. *J. Med. Chem.* **2017**, *60*, 100–118.

   discovery of nanomolar inhibitors of PI4KB with broad spectrum antiviral activity

10. Tichý, M.; Smoleň, S.; Tloušťová, E.; Pohl, R.; Ožd ian, T.; Hejtmánková, K.; Lišková, B.; Gurská, S.; Džubák, P.; Hajdúch, M.; Hocek, M.* Synthesis and Cytostatic and Antiviral Profiling of Thieno-Fused 7-Deazapurine Ribonucleosides. *J. Med. Chem.* **2017**, *60*, 2411–2424.

    discovery of novel type of fused deazapurine nucleosides with potent cytostatic effect

Team 4: Synthetic organic, materials & nano chemistry

5 independent groups: Petr Beier, Petr Cígler, Ullrich Jahn, Josef Michl, Ivo Starý

Chronologically ordered (2 most important papers for each group), because they are all good and significant. A brief description of these key achievements will be provided during the live presentations.

1. The Scope of Direct Alkylation of Gold Surface with Solutions of C1–C4 *n*-Alkylstannanes J. Michl & co-workers • *J. Am. Chem. Soc*. **2015**, *137*, 12086–12099
   IF: 14.612, WoS: 9 citations
2. An Ultimate Stereocontrol in Asymmetric Synthesis of Optically Pure Fully Aromatic Helicenes I. Starý, I.G. Stará & co-workers • *J. Am. Chem. Soc*. **2015**, *137*, 8469–8474
   IF: 14.612, WoS: 53 citations

3. Synthesis of Bridged Diketopiperazines by Using the Persistent Radical Effect and a Formal Synthesis of Bicyclomycin U. Jahn & co-workers • *Angew. Chem. Int. Ed*. **2015**, *54*, 12153–12157 IF: 12.959, WoS: 20 citations
4. Expanding the Scope of Hypervalent Iodine Reagents for Perfluoroalkylation: From Trifluoromethyl to Functionalized Perfluoroethyl
   P. Beier, A. Togni & co-workers • *Chem. Eur. J.* **2016**, *22*, 417–424
   IF: 4.857, WoS: 46 citations
5. Azidoperfluoroalkanes: Synthesis and Application in Copper(I)–Catalyzed Azide–Alkyne Cycloaddition P. Beier & co-workers • *Angew. Chem. Int. Ed*. **2017**, *56*, 346–349 IF: 12.959, WoS: 22 citations
6. Optical Imaging of Localized Chemical Events Using Programmable Diamond Quantum Nanosensors P. Cígler, Z. Chu & co-workers • *Nat. Commun*. **2017**, *8*, 14701 IF: 12.121, WoS: 52 citations
7. From Helical to Planar Chirality by On-Surface Chemistry
   I. Starý, P. Jelínek & co-workers • *Nat. Chem.* **2017**, *9*, 213–218 IF: 21.687, WoS: 48 citations
8. Supported Lipid Bilayers on Fluorescent Nanodiamonds: A Structurally Defined and Versatile Coating for Bioapplications P. Cígler & co-workers • *Adv. Funct. Mater*. **2018**, *28*, 1803406 IF: 16.836, WoS: 5 citations
9. Photochemical C-H Amination of Ethers and Geminal Difunctionalization Reactions in One Pot U. Jahn & co-workers • *Angew. Chem. Int. Ed*. **2019**, *58*, 12440–12445 IF: 12.959, WoS: 4 citations
10. Singlet Fission Rate: Optimized Packing of a Molecular Pair. Ethylene as a Model J. Michl & co-workers • *J. Am. Chem. Soc*. **2019**, 141, 17729–17743
    IF: 14.612, WoS: 8 citations

5. Molecular interactions in biomedicine – BIO 1 – Team 5

Strengths:

BIO 1 – team 5 brings together similar themes, assessed together for this evaluation. BIO 1 – team 5 comprised 5 groups led by Senior PIs, 2 research services & a more focused targeted research team. Their main strengths are (i) to target common questions of major interest (viruses and enzymes for therapeutic developments), and this with extreme efficiency, (ii) to have cutting-edge methodologies at the international level (structural biology, chemical biology and medicinal biology). The team has excellent publications and strong links with the industry (11 patents, an impressive number).

Weaknesses:

The seven groups are highly diverse in terms of themes and methodologies. They are often among the best teams on their theme at the international level and therefore have a good number of national and international collaborations. The links between the different groups are somewhat limited. Similarly, with their strong interactions with companies, their publications are specialized and sometimes do not have a high number of citations.

Opportunities:

At the quantitative view of publication data, an adequate policy to better design the publications policy to reach more basic research articles with more citations can be considered. Likewise, stronger local joint actions can bring about this better result.

Threats:

The main weakness is one of their strengths, BIO 1 – team 5 has a large number of facilities which must be maintained and possibly upgraded in the future. Access to dedicated grants can become problematic.

Main criterion: 1. Quality of results (H1.1-H1.5)

H1.1	Quality of selected outputs of Phase I
Very good quality with ~ 1/5 of them being in the top journals (first decile or first quartile).	
H1.2	**Contribution of workers on the outputs reached**
They are highly diverse, but on the 150 publications made by BIO 1 – team 5, a significant number have members at strategic positions in the author list.	
H1.3	**Quality of all outputs and results**
Impressive in terms of scientific results, and also in terms of patents.	
H1.4	**The most valuable discoveries and findings in the fields, their importance for the field**
Every group of BIO 1 – Team 5 had highly pertinent discoveries published during the evaluated period. The Konvalinka group works on a large variety of human viruses, and some cancers. They handled a large set of methodologies (organic synthesis, molecular modelling, medicinal chemistry, enzymology, X-ray and NMR structure, transgenic mice,	

...). Their most striking results were on analysis of mutations inducing drug resistance, an essential point to design pertinent new drugs, and the realisation of DIANA assay for screening. The Pichová group research analyses life cycles of some human pathogens such as retroviruses, Hepatitis B virus, *Mycobacterium tuberculosis* and especially their interaction with host cells. They have made fruitful collaborations that led to structure protein resolution useful for future drug design purposes. The Mareš group had developed cathepsin inhibitors as chemotherapeutics. They underlined a novel structural mechanism of allosteric regulation of aspartic peptidases via an evolutionarily conserved exosite. The Bouřa group has expertise in structural and molecular biology of membrane associated proteins. They have been interested in numerous protein structures implicated in virus and virus lifecycle. For instance they recently provided high resolution SARS-CoV-2 methyltransferase (composed of nsp10 and nsp16), an interesting target again COVID infection. The Strisovsky group had analysed the structure of rhomboid proteases, and designed first specific and biocompatible inhibitors of these enzymes, leading to potential efficient applications. Mertlíková group (research- service organization unit - Biochemical Pharmacology) support other IOCB teams in their research activities, but also have their own centres of interest. They show expertise in the assessment of inhibitors against e.g. adenylate cyclase toxin, transports of compounds, e.g. antileukemic and viral compounds, or even nanodiamonds. The Weber research-service group works on different nanoparticles applied to virus. The Birkus targeted research group is specialized in drug discovery and more precisely tries to master the entire process from design to production using computational approaches coupled with *in vivo* and *in vitro* tests. Nearly all the groups have published their researches in excellent journals. Another essential output is the impressive number of patents.
To summarize, BIO 1 – Team 5 had analysed a large number of proteins associated to pathologies, often parasites and cancers, proposed mechanisms of actions using structure information for a large number of them and also drive design and production of novel inhibitors and drugs against them.

H1.5	Contribution of the participation of the authors in large collaborations

Every laboratories of BIO 1 – team 5 collaborates with multiple laboratories in the Czech Republic, Europe and USA. They are supported by national and industrial grants, i.e. European structural funds (OPPK, NPUI, OP VVV) and Gilead Research Centre.

Main criterion: 2. Societal relevance (H2.1-H2.5)

H2.1	Societal relevance of outputs and results pursuant to CAS and institute mission

Societal relevance of the research of BIO 1 is obvious as their researches are clearly driven by pathologies and the design of potential drugs. Their results are so highly interesting for multiple types of cancers and infections issues and multiple different cancers.

H2.2	System functionality for knowledge transfer into practice, its usefulness for society. The impact of the team´s activity on proper practice in society in the area of social sciences and humanities

With the total number of patents obtained during this period, it worked well for BIO 1 – team 5.

H1.3	Relation to practice

11 patents have been obtained by BIO 1 – team 5. IOCB had the knowledge and the human resource to deal with complex issues of patenting and licensing. Interactions with industrial companies are numerous and excellent. This strategy is clearly fruitful.

Further criterion: 1. Position in international and national context (D1.1-D1.3)

D1.1	Comparison of the team with similar international and national institutes
The groups are often of limited size with a correct number of students. In comparison to similar international team they are, for most of them, in direct competition with other excellent teams. Some groups are more at the national level in terms of publication quality.	
D1.2	**Scope and quality of international and national cooperation and the role of the team in such cooperation; engagement in broad international cooperation**
Very decent number of national and international co-operations. They are engaged in co-operation with recognized specialists.	
D1.3	**Participation of the workers in scientific community activities (organizing of conferences and workshops, invited lectures, awards)**
BIO 1 – team 5 had a good communications in terms of symposiums and could be improved for workshop. Number of invited lectures is excellent for most of the group leaders.	

Further criterion: 2. Vitality, sustainability and strategy (D2.1-D2.9)

D2.1	Direction in line with the perspective of the planned research directions
The direction is fully in line with the planned research direction.	
D2.2	**Assessment of the previous research objectives and their achievement**
Previous recommendation was to continue their research, they have done it. Production rate was excellent.	
D2.3	**Assessment of implementation of recommendations from past evaluation**
The recommendations have been effectively followed up.	
D2.4	**Success in receiving grants**
The funding level of the BIO 1 – team 5 is very good. It comprises very good success rate to national grant, some international and excellent links to the private sectors.	
D2.5	**Adequacy of instrumental equipment**
Excellent and highly diverse.	
D2.6	**Effectiveness of management**
Management is excellent.	

D2.7	**Assessment of professional structure, development strategy and the strategy of keeping best scientists, age structure, career and qualification growth**
The selection system is quite competitive. During the period, two young groups have been evaluated and promoted to Senior group.	
D2.8	**Creating work-life balance conditions, assessment of approach towards possible gender issues**
The age and gender balance are very good.	
D2.9	**Relation of the team with regard to the integration, development and sustainability of the research centre funded by the National Programme of Sustainability II.**
Excellent.	

Further criterion: 3. Cooperation with universities and participation in education (D3.1-D3.6)

D3.1	**Scope of cooperation with universities on national and international level**
Group leaders are teaching in different Universities. It is done at a correct level in regards to international standard.	
D3.2	**Effectiveness of joint research centres**
The development of the service laboratories is excellent both in securing funding for the future and in providing technological platform for their own research laboratories.	
D3.3	**Success rate in supervision of PhD students**
Number of PhDs per scientists is very good, management is well done. They have a good future as post-docs as they have good publication rates and also excellent implications of interactions with industry.	
D3.4	**Participation of PhD students in the outputs**
Author list are generally containing PhD students reflecting their active participation in the research outputs. They have a good average number of publications.	
D3.5	**Participation of the team in master or bachelor studies**
PIs are implicated in different masters.	
D3.6	**Assessment of cooperation intensity with universities in the form of teaching**
They are implicated in teaching at the nearby universities.	

Further criterion: 4. Outreach activities (D4.1-D4.3)

D4.1	Sufficiency of media strategy and activities in the area of research popularisation
Excellent. As many researches have societal impacts, group leaders have used multiple media.	
D4.2	**Publishing activities and its quality**
More than 150 publications are concerned, an excellent ratio per scientists. Moreover, some are in good to excellent journals. Number of citations is a little more limited, and could be discuss in the future for some groups. The service groups have very good materials and therefore are implicated in a high number of publications. In the future, it is necessary to differentiate specifically for these groups their own research from the “service” research to facilitate a fair evaluation with the other team.	
D4.3	**Participation in professional organisations in the area of research and development**
Group leaders are well connected with various private sectors	

Other comments of the commission:

6. Chemical biology for life and diseases - BIO 2 – Team 6

Strengths:

BIO 2 groups have all researches with very high societal implications, links to various pathologies. They managed to handle a large number of recent technologies, being internationally very competitive. They have published a high number of publications with a very good number in excellent journals; their grant success rate is also very good. They are very active in translating their research results with companies.

Weaknesses:

The research choices led to the number of papers with zero citations being higher than expected. This raises questions about impact.

Opportunities:

BIO 2 - TEAM 6 has a good number of junior groups. This youth will allow them to expand their areas of expertise by bringing in the latest techniques. Similarly, certain themes should be able to take advantage of high-throughput sequencing data, phylogeny and computational approaches to increase the quality of the targeted journals.

Threats:

The number of facilities is impressive, their maintenance and evolution are always a challenge, as grant policies are difficult to evaluate in a few years. This is probably the major threats for BIO 2 - TEAM 6.

Main criterion: 1. Quality of results (H1.1-H1.5)

H1.1	Quality of selected outputs of Phase I
Excellent quality with ~ 2/3 of them being in the top journal (first decile or first or second quartile).	
H1.2	**Contribution of workers on the outputs reached**
All teams have publications in best journal with corresponding authorship from the team.	
H1.3	**Quality of all outputs and results**
288 published papers is an excellent number. Globally, outputs are mostly published in reviewed journals indicating the high standard of the performed research. Number of patents is more limited. Particularly useful web services freely provided for the scientific community must be noticed.	
H1.4	**The most valuable discoveries and findings in the fields, their importance for the field**
The team Chemical biology for life and diseases (BIO 2 - TEAM 6) consisted of 10 independent research groups. The Maloy Řezáčová group (Senior group) developed and characterized series a large series of inhibitors of human carbonic anhydrase based on sulfamides and sulphonamides incorporating carborane clusters lading to different	

patents as they reduced tumour size in mice. Their research elegantly linked molecular and cellular approaches with experimental structures analysis and computational approaches.
The Jiráček group (Senior group) is interested in all aspects of insulin and insulin-like growth factors 1 and 2 (IGF-1/2) physiology. They successfully designed and analysed modified insulin and insulin-like growth factors leading to effective and selective ones; they were patented.
The Maletínská group (Senior group) is expert on peptides involved in the regulation of food intake links obesity, diabetes and neurodegeneration. They have characterized anorexigenic neuropeptides (PrRP, CART). They have industrial cooperation to look for development of anti-obesity agents.
The Cahová group (Junior group) studies function, biogenesis and biodegradation of viral RNA modifications. They identified nine new caps covalently attached to bacterial RNA based on unmethylated or methylated NpnNs, and for the first time, they propose mechanism of action in the RNA capping.
The Curtis group (Junior group) focussed on G-quadruplexes, they applied with efficiency artificial evolution to identify DNA and RNA molecules with interesting and potentially useful functions. It is most basic research group of BIO 2 - TEAM 6.
The Hanus group (Junior group) is the most exotic group of BIO 2 - TEAM 6 as they study the biology and chemistry of social insects. However, they are using a large series of chemical and biochemical approaches as the other groups. They described asexual reproduction (parthenogenesis) via unfertilized eggs, to produce harems of replacement queens.
The Weiss group (Junior group) was interested in voltage-gated-calcium channels with approaches ranging from genetics to biophysics; they had underlined the link of some mutations with chronic pain and absence seizures. As it was not promoted during evaluations held in year 2019 and thus this group was dissolved.
The Kečkéšová group (Junior group established in 2018) focuses on cancer biology and tumour suppressors. They characterized on of these genes, called LACTB (Lactamase B-like) that acts through reprogramming of cancer lipid metabolism implicated in differentiation of cancer stem cells.
The Vondrášek group (Research Service Group) had a strong computational axis (molecular modelling, molecular simulations, computational chemistry, bioinformatics analysis and mathematical statistics methods) and also an experimental axis dedicated to production of designed proteins. Their works led to essential theoretical development such as the impact and evaluation of phosphorylation on macromolecules, series of different webservers highly useful to scientific community, e.g. protein stability and protein-protein and protein-DNA interactions.
Most of the findings presented here are breakthrough researches in their fields; they are always associated to very good to excellent journal publications and sometimes patents.

H1.5	Contribution of the participation of the authors in large collaborations

The team members participated in numerous international collaborative efforts. They are associated to European ELIXIR and other collaborative projects.

Main criterion: 2. Societal relevance (H2.1-H2.5)

H2.1	Societal relevance of outputs and results pursuant to CAS and institute mission

Excellent fit of BIO 2 - TEAM 6 research outputs with the general societal goal of the IOCB, all teams focus on various pathologies. They produced both applied and fundamental results on the various topics they are interested in.

H2.2	System functionality for knowledge transfer into practise, its usefulness for society. The impact of the team´s activity on proper practice in society in the area of social sciences and humanities
Knowledge transfer is good with two series of patents (insulin analogues, inhibitors of human carbonic anhydrase). Interactions with some companies are also pretty good with various subcontracts. Impact in the area of social sciences and humanities is not applicable.	

H1.3	Relation to practice
It follows general IOCB strategy and is of good quality. The current research is of high quality, but often just before the parts that may be of definite interest to industry. These activities will be naturally expended in the future.	

Further criterion: 1. Position in international and national context (D1.1-D1.3)

D1.1	Comparison of the team with similar international and national institutes
BIO 2 - TEAM 6 teams are very competitive with similar institutes for most of the groups. They are very dynamic and have accessed to a large series of facilities that made them clearly competitive at international level. This number and diversity of methodologies can be complex to handle within the short time frame of the received grants (3 years).	

D1.2	Scope and quality of international and national cooperation and the role of the team in such cooperation; engagement in broad international cooperation
Every groups of BIO 2 - TEAM 6 had excellent international collaborations with experts in their field. They also have a large number of national collaboration of a very high standard. Most of this cooperation concerns technologies or expertise that are not present in the neighbourhood.	

D1.3	Participation of the workers in scientific community activities (organizing of conferences and workshops, invited lectures, awards)
Most group leaders are members of international association at various levels (chairman, members and auditors), they have been invited in numerous seminars and oral presentations. They (co-)organized 9 conferences/work-shop during the last 5 years. Youngest scientists have less visibility.	

Further criterion: 2. Vitality, sustainability and strategy (D2.1-D2.9)

D2.1	Direction in line with the perspective of the planned research directions
The direction is fully supportive of the planned research projects.	

D2.2	Assessment of the previous research objectives and their achievement
Two senior groups were evaluated positively with no specific objectives. IOCB International Advisory Board regularly evaluates installation of Junior groups, research group, and even senior groups.	
D2.3	**Assessment of implementation of recommendations from past evaluation**
See before.	
D2.4	**Success in receiving grants**
The different groups are very successful in acquiring grants with an average of 2-3 grants per laboratory composing BIO 2 - TEAM 6.	
D2.5	**Adequacy of instrumental equipment**
Outstanding. It is very clear that the ensemble is particularly competitive at the international level.	
D2.6	**Effectiveness of management**
The management seems effective and the research is of high quality. The good follow-up of the grants policy has allowed the service groups to have very good materials and therefore an excellent valorisation. In the future, it is necessary to manage the difference between own research and service.	
D2.7	**Assessment of professional structure, development strategy and the strategy of keeping best scientists, age structure, career and qualification growth**
Excellent. One Senior group was established in 2015, and the Junior groups more recently. This shows the dynamics of BIO 2 - TEAM 6 within the Institute. The junior groups were successful in gathering funding and published nice outputs. These groups should be positively reviewed in the coming years to switch their status to Senior groups.	
D2.8	**Creating work-life balance conditions, assessment of approach towards possible gender issues**
No gender issues or biases have been observed, i.e. maternity leaves are well managed in many groups. Work-life balance appears respected.	
D2.9	**Relation of the team with regard to the integration, development and sustainability of the research centre funded by the National Programme of Sustainability II.**
Excellent.	

Further criterion: 3. Cooperation with universities and participation in education (D3.1-D3.6)

D3.1	Scope of cooperation with universities on national and international level
Most of the group leaders are regularly teaching at the nearby Universities.	

D3.2	Effectiveness of joint research centres
The development of the service laboratories for most the groups and access to external facilities is excellent. Similarly, funding was good, but can be a threat for the future.	
D3.3	**Success rate in supervision of PhD students**
They supervised more than 40 PhD students indicating that approximately each group enrolled 1 to 2 PhD student(s) every year, which is an excellent ratio.	
D3.4	**Participation of PhD students in the outputs**
Most of the papers with a group leader as corresponding author are co-signed with PhD students. They have well to excellent records in terms of publications at the end of their studies.	
D3.5	**Participation of the team in master or bachelor studies**
PIs are in their majority teaching at the various University levels.	
D3.6	**Assessment of cooperation intensity with universities in the form of teaching**
Collaboration seems good. They include lecturing at all levels (Bachelor and Master).	

Further criterion: 4. Outreach activities (D4.1-D4.3)

D4.1	Sufficiency of media strategy and activities in the area of research popularisation
Excellent. The different teams of BIO 2 - TEAM 6 are actively participating in numbers of outreach activities ranging from Open Days, Science Festival to TV or radio interviews.	
D4.2	**Publishing activities and its quality**
Science popularization is represented by some intervention in Czech language and in classical journals.	
D4.3	**Participation in professional organisations in the area of research and development**
Nothing is précised.	

Other comments of the commission:

Final report was elaborated by:

Commission 3.2 - Chemical sciences
Evaluated teams No.: 1, 2, 3, 4

Commission Chair: Professor Bengt Norden
Commission Deputy Chair: Alexander Čegan
Commission Members:
- Teresa Bandosz
- Timothy Clark
- Vladimir Sepelak
- Francesc Teixidor
- John Tsibouklis
- Hans-Achim Wagenknecht
- Uta Wille

Commission 5.2 - Biological sciences A
Evaluated teams No.: 5, 6

Commission Chair: Professor Bryan Cullen
Commission Deputy Chair: Marcela Chmelařová
Commission Members:
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- Josef Glössl
- Michael Hausmann
- Stéphanie Robert
- Didier Stainier
- Martin Teichmann
- Stéphane Thore
- Jianlong Wang
- Alexandre G. de Brevern