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

Summary Final Report

Name of the Institute:

Institute of Chemical Process Fundamentals of the CAS, v. v. i.

Evaluated teams and their leaders:

1. Department of Membrane Separation Processes (Pavel Izák)
2. Department of Aerosols Chemistry and Physics (Vladimír Ždímal)
3. Department of Catalysis and Reaction Engineering (Olga Šolcová)
4. Department of Multiphase Reactors (Marek Růžička)
5. Department of Analytical Chemistry (Jan Sýkora)
6. Department of Environmental Engineering (Michal Šyc)
7. Department of Molecular and Mesoscopic Modelling (Martin Lísal)
8. Department of Laser Chemistry (Radek Fajgar)
9. Group of Advanced Materials and Organic Synthesis (Jan Storch)
10. SuperCritical Technologies Group (Marie Sajfrtová)
11. Department of Bioorganic Compounds and Nanocomposites (Tomáš Strašák)

Part A: Evaluation of the institute

Overall evaluation of the institute elaborated in agreement of all commissions' chairs, who evaluated the institute.

Strengths:

- Good training programs in place for PhD students
- Six H2020 projects
- The research of the institute has a highly interdisciplinary character and is performed by experienced and internationally recognised experts.
- The six engineering departments combine fundamental with applied research. A strong focus is laid on knowledge transfer to the practise and on international collaboration. The research topics are of societal relevance and are well embedded in the AV21 strategy.
- The institute hosts several centres of competence. It is well managed and has a good Human Resources policy resulting in motivated employees.

Weaknesses:

- In the five chemistry departments the vertical organisational structure is assumed to be inflexible.
- In the age distribution the fraction of young researchers should be increased.
- Apparent poor scientific interaction between engineering and chemistry departments
- The gender balance varies along the departments. It is good in the engineering departments (3 out of 6 has women in leader position and balanced gender in workforce), while gender is unbalanced in the 5 chemistry departments.
- Although there was a serious reorganisation of the institute to concentrate on promising research directions during the evaluation period, fragmentation is still visible which leads partially to internal duplication of research.
- The institute has a strong international network, however, participation in international projects especially in the role as a coordinator should be expanded. More attempts on the diversification of funding sources is therefore needed.
- The mobility of researchers for short-term research stays abroad is still low although special mobility programmes were installed.
- The institute reports for some departments limitations of resources for infrastructure, including key equipment and instrumentation. These departments can easily fall behind other departments across Europe, which will make it more difficult to obtain high-impact results and publications as well as competitive grants.

Opportunities:

- Introduce tenure-track for junior group leaders.
- A new, flat organisational structure would be desirable for the chemistry departments. In engineering this demand is not obvious.
- Rationalise and focus service departments.
- Since the department is active and successful in national grant applications and has an excellent international network, the commission recommends to strengthen the applications for international grants. This requires a clear strategy, training and incentives by the CAS.
- Further specialisation in relevant research areas will allow even more collaborations with industry with the benefits of access to exciting and relevant problems, industrial infrastructure, as well as budget for the development of staff, infrastructure and dissemination activities.

Threats:

- Staffing difficulties might be caused by retirement or by leaving key scientists, especially in one small group.

- Research areas are in part redundant because they are duplicated by other CAS institutes. It is only problem if all use the same method (and not complementary).
- The relative low level of salaries makes it unlikely to attract scientists from western European countries and makes it more difficult to keep the best Czech scientists at the CAS. A starting point to create more international exchange is hosting master level and PhD students from abroad for short-term research stays (strategy required) as well as seeking opportunities to participate in more doctoral commissions abroad. This openness will create new contacts and consequently a higher likelihood to join EU projects as partner. Optimal is establishing new bilateral programmes with regular exchange of students and staff.

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

H1.1	Quality of selected outputs of Phase I
The quality of the majority of selected outputs is good or average. Detailed information is given in Part B.	
H1.2	**Contribution of workers on the outputs reached**
The share of researchers' of the institute differs between the evaluated departments. Detailed information is given in Part B.	
H1.3	**Quality of all outputs and results**
The quality of all outputs is good or average.	
H1.4	**The most valuable discoveries and findings in the fields, their importance for the field**
Due to the various departments working in different field it is difficult to determine the most valuable discoveries. Therefore, more general remarks will be given and more detailed information can be found in Part B. During the evaluated period the institute contributed to: • The waste treatment methodology. • Improve the understanding and the modelling of hydrodynamics, mass and heat transfer and/or reaction processes at various scales and in different devices such as membrane separators and chemical reactors. • Develop processes for the cleaning of exhaust gases and water, for the separation of gases from gas mixtures and of bioactive substances from natural products, as well as for biorefineries, circular economy and waste-to-x, • Enhance the knowledge of aerosols including their behaviour in the atmosphere as well as indoor environments.	
H1.5	**Contribution of the participation of the authors in large collaborations**
Not applicable.	

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

H2.1	Societal relevance of outputs and results pursuant to CAS and institute mission
Moderate, no breakthroughs that have become mainstream.	

The societal relevance of the institute arises mainly from two aspects. On the one hand, the institute contributes to the development of apparatus, technologies and processes aiming on the decarbonisation of industry and society, the establishment of a circular economy, and the removal of pollutants from the environment. These developments are enabled by combining fundamental and applied research in the fields of chemical engineering, environmental engineering, chemical sciences, new materials and biotechnologies. On the other hand, the institute contributes to enhance the competitiveness of the national economy through applied research in cooperation with various industrial partners.

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

Average, some processes have been transferred into the private sector.

The engineering part of the institute demonstrates excellent engagement to transfer knowledge into practical applications. In the evaluation period, 33 TACR projects in collaboration with industry and contractual research of nearly 800,000 Euro was performed by the members of the institute. Further indicators for an efficient transfer into practise are several applications and granting of national and international patents as well as their exploitation by partners, e.g. patents and licenses were sold worth nearly 500,000 Euro. The fast implementation of research aiming on protective equipment against viruses such as COVID-19 underlines the institute's strength to rapidly adopt emerging societal relevant topics.

H2.3	Relation to practice

Remains to be seen. Are, for instance, the microwave techniques practicable?

The institute efficiently links fundamental research to industrial applications. The strong ties with practise are documented through various collaborations with national and international companies as explained before.

H2.4	Participation in AV21 strategy

Some parts it is "Passive cooperation".

Other parts of the institute contribute to the programmes of Efficient Energy Conversion and Storage, Foods for the Future, Water for life, as well as Natural Hazards.

H2.5	Cooperation with regions of the Czech Republic

Good to average

The institute intensively cooperates with other universities (e.g. Prague: UCT and Charles, Ostrava, Ústí nad Labem), companies, and municipalities in Czech Republic. Furthermore, the institute adequately demonstrates the capability of leading national consortia, e.g. BIORAF, BIOCIRTECH. This supports the cross-linking of research institutes, educational organisations, as well as enterprises along various value chains.

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

Lower midrange.

The institute's performance is similar to other national and international research institutes in the same field. The involvement in a smaller number of European Consortia and EU projects underlines the reputation and research quality.

D1.2	Scope and quality of international and national cooperation and the role of the institute in such cooperation; engagement in broad international cooperation

Quality varies strongly.

The scope and quality of international and national cooperations is very good for several departments. On a national level, the initiation and leading of Centres of Competence in the fields of biorefineries (BIORAF), circular economy (BIOCIRCTECH), waste-to-energy (WtE) will increase the competiveness of Czech Republic in emerging and social relevant fields. On an international level, the departments are integrated into collaborate research, e.g. ACTRIS, with up to 30 partners (EU projects, NATO projects). Besides there are good bilateral collaboration of the departments with universities and companies mainly from Europe but also from other continents.

This broad and multifaceted network should be used more intensively to apply for international funds. Furthermore, the institute should also take leading roles in such projects because of its reputation, scientific excellence and multidisciplinary. It is suggested to further strengthening organisational structures supporting applications and project management.

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

Low in some departments.

However, 6 international conferences, 8 national conferences and several workshops were organised by members of the institute (between 2015 and 2019). Additionally, scientists of the departments join boards of several conferences, are invited regularly for giving lectures, and received awards for their scientific outcome (mainly on a national level).

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 continues its mission combining fundamental and applied research to solve current and emerging research challenges in engineering. Current directions are aerosols, membrane separation, waste-to-x, circular economy, NMR metabolomics. It seems that the institute convinces its departments to develop appropriate research strategies depending on their strengths and the given opportunities. It is suggested to further develop the areas in which the institute and its departments can have a leading role in Europe.

However, the weaknesses pointed out in the last evaluation have not been removed completely and the chemistry departments would need sweeping organisational changes. If anything, the structure of the chemistry units is more fragmented and less directed than before the 2018 changes.

D2.2	Assessment of the previous research objectives and their achievement

There is a strong element of "maintain the status quo" within the Institute. This may result in a moderate-to-below-average level of research quality and originality in chemistry if „as little change to the existing structure as possible" is targeted.

On the other hand, a strategy plan of the institute is also seen, which aimed on improvement of quality of basic research, of implementation of applied research, and

presentation of the institute. In this context, the institute was restructured into smaller better-profiled departments, a new wage and award system was implemented also considering scientific excellence, a system for exploiting intellectual property rights was installed, and a new visual identity was formed and realised on web pages and social media channels. According to the institute's report, this lead to a significant increase of sold licenses and also to a spin-off company, which provides a backflow of money to improve the analytical and experimental equipment. Furthermore, the quantity of publications only slightly decreased but shifts constantly to more quality.

D2.3	Assessment of implementation of recommendations from past evaluation

The recommendations of the last evaluation were taken very seriously and lead to corresponding actions. One major concern in the last assessment was the historical accumulation of scientifically unrelated sub-groups within the scientific departments. It is good that the institute dissolved the existing departments and formed new departments around experts in the fields. In consequence, the previous 6 departments were turned into 10 smaller departments.

However, the reorganisation of the chemistry departments has not sufficiently solved any of the original problems. Here the changes have been made but apparently reluctantly and with little effect. For instance, the policy of requiring young people to spend one year abroad before returning to the Institute only has alibi function. Such acquisition of experience that is brought back home is regarded a useful step in engineering.

D2.4	Success in receiving grants

The success with H2020 has been significant.

The institute is also successful in receiving grants from national funding bodies. The main funding sources are GARC and TACR as well as programmes established by Czech Ministries. Additionally, around 10% of the external funding origin from intellectual properties' commercialisation and from the private sector. On an international level, the institute solicited a good amount of grants from funding sources such as H2020, NATO, US ARL, COST. However, more efforts are needed to achieve higher amounts of cash-flow per researcher from competitive EU grants for original research at the highest level.

D2.5	Adequacy of instrumental equipment

The adequacy of instrumental equipment is difficult to analyse and evaluate because there were no on-sight visits. Information from, for instance, the web pages suggests that instrumentation is old but functional. However, at some stage major investments will be necessary.

The written reports express an institutional underfunding which is compensated by an institutional structure-fund financed by the revenues of licences etc. The impression from the presentations regarding up-to-date instrumentation in the engineering departments and in information technology was positive.

D2.6	Effectiveness of management

Effectiveness of management can only be assesed indirectly from the results based on the vision how the structure of the institute should be formed. A vision of „flat organizational structure" (see Opportunities) would have required courage from the management to break out the established pattern. However, from the point of view of engineering departments (where the vertical structure seems to be appropriate) steps of management look more positive. Structural changes of the institute were well planned, implemented and monitored. Furthermore, special funds for purchase of instruments were established as well as a reward system to improve quality of publications was implemented.

D2.7	Assessment of professional structure, development strategy and the strategy of keeping best scientists, age structure, career and qualification growth

The institute developed and implemented an elaborate Human Resources policy, which includes, for example, a good strategy for recruitment, career development, and evaluation of researchers. In 2018, a performance-based wage system replaced the age-based system to motivate and keep talented scientists.

Even though, there are clearly problems in obtaining good young people, so that the age structure reflects the part-time employment of retirees very strongly.

No active intervention strategies for the recruitment of more female researchers are apparent and it is reflected in the lack of elaborating this problem in the presentations explicitly. The gender balance is very poor in major part of the institute, especially in leading positions. However, there are also good examples in the engineering departments. Women are the chairs in 2 of the 6 departments and the deputy chair is a woman in a third. In 3 of the 6 departments the gender balance is good.

D2.8	Creating work-life balance conditions, assessment of approach towards possible gender issues

Please see D2.7!

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.

Not applicable.

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

Average.

The institute has close collaborations with most Czech universities in the field of chemistry and chemical engineering and a good amount of collaborations with universities from abroad. The cooperation is based on joint projects as well as the exchange of a small number of master and PhD students which is supported by mobility funds.

D3.2	Effectiveness of joint research centres

The effectiveness of joint research centres is convincingly demonstrated. The ICPF participates in platforms for joint research with universities and companies such as the Centre of Competence for Biorefinery Research (BIORAF), the National Centre of Competence on Circular Economy (BIOCIRTEC), and Centre of Competence on Waste to Energy (WtE).

D3.3	Success rate in supervision of PhD students

Average-to-good. Strong efforts have been made.

Between 2015 and 2019, 23 PhD were successfully defended in which the evaluated departments of the institute were involved. A PhD success rate of 80% is reported. Considering the size of the institute, it is suggested to increase the number of supervised PhD students which will contribute to a further increase in scientific outputs (publications), awards and visibility.

D3.4	Participation of PhD students in the outputs
Good. PhD students participate in all outputs of the departments, for example, as authors in papers, as poster and lecture presenters at conferences, or as inventors in utility models and patents.	
D3.5	**Participation of the institute in master or bachelor studies**
Good. It is important to notice that the level of activities significantly varies between the departments. For example, some departments, especially those with small teaching activities, claim that the recruitment of students is challenging. This gives direct guidance to potential improvements through more teaching activities.	
D3.6	**Assessment of cooperation intensity with universities in the form of teaching**
Good. The cooperation intensity with higher engineering education in the Czech Republic is very good and several good activities exists with universities from abroad.	

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

D4.1	Sufficiency of media strategy and activities in the area of research popularisation
Poor. All in all, the institute organises regularly events for the public (Science Fairs, Open Lab Days, Week of Science) as well as invites children and high school students to the CAS to inspire them for science and technology. Additionally, members of the institute join television debates and radio programs. The institute hosts an attractive up-to-date website as well as a Facebook and a Twitter channel.	
D4.2	**Publishing activities and its quality**
Poor The members of the institute participate in publishing brochures, articles, and books for non-scientific audiences. The activities are mainly at national level.	
D4.3	**Participation in professional organisations in the area of research and development**
Not strong Scientists of the institute hold leading positions in international research networks and committees, professional organisations, and evaluation panels.	

Other comments of the commission:
The commissions were hampered by not having a complete overview of the Institute. What is even more important, different situations were experienced in the chemistry departments and in the engineering departments and that led to different conclusions and suggestions for the two groups of departments. That is why the comments (recommendations) of the two Committees are also presented separately.

The comments of Committee 7.1- Engineering and technology are the following:

The commission recommends to maintain the efforts to improve the exchange of students and researchers with other countries as well as to deepen and expand the network to universities, research institutes, and companies from abroad. This will strengthen the basis to obtain grants from EU and other international funding organisations. It is suggested to establish institutional positions (or to hire freelancer that possess necessary skills) that support the researchers with training and hands-on support in grant applications, design thinking, and project management. The institute and its departments should define if global trends in process industry such as advanced automation, digitalisation and robotics among others are relevant in their field and may set-up a strategy to include these topics into the research programs. The CAS should be informed about these trends and funding needs, to keep the pace with institutions from abroad. The institute may consider to extend the external advisory board by industrial experts to learn about industrial trends and challenges as well as customer needs.

Comments of Commission 3.2 - Chemical sciences follow

Structure and direction of the Institute

The commission was disturbed by the lack of structure and purpose of the chemistry departments within this Institute. The 2018 reforms have obviously had little or no effect, or maybe even an adverse one. The root evil is the vertical structure, which provides very little flexibility and favours inbreeding. A flat structure with tenure-track for young researchers is absolutely essential, even at the expense of downsizing the Institute.

From the commission's view of the departments reviewed, the Institute has little coherent structure or purpose. It is striking that:

- The individual departments pursue separate and unrelated research directions with no discernible strategy.
- It is difficult to see why much of the research presented is located in an "Institute of Chemical Process Fundamentals", or even what it has to do with the formal names of the departments
- There is much overlap with Institutes such as Microbiology, Macromolecular Chemistry and Organic Chemistry and Biochemistry. Much of the research carried out would be better situated in a more focussed Institute.

The integration of many of the departments reviewed within the Institute as a whole was either not evident or, in one case explicitly non-existent.

Suggestions of the Commission: Institute structure

As in other Institutes evaluated by the chemistry commission, the rigid vertical structure of the Institute is hampering changes in research focus, improving the quality of the Institute, supporting young researchers, establishing gender equality and preventing inbreeding.

The commission regards the flat structure and the tenure-track procedure implemented in IOCB as an ideal model for Institutes such as ICPF, in particular as the cosmetic changes made previously did not improve the situation and the Institute's standing.

The commission does not find combined service/research departments (i.e., Departments 5 Analytical Chemistry and 8 Laser Chemistry) to be effective, and it was not evident how the scientific output of those researchers with dual functions was evaluated relative to opportunity. Overall, the research conducted in these departments appears to be unfocussed (likely due, at least in part, to the burden from the split activities of these departments) and

has little to do with the direction of the Institute itself. We recommend that both departments become 100% service departments.

The commission was unable to see the need for the research components of Departments 5 (Analytical Chemistry), 8 (Laser Chemistry), 9 (Advanced Materials and Organic Synthesis) and 11 (Bioorganic Compounds and Nanocomposites) to be situated in ICPF. The research interests of these Departments bear little relation to the formal names of the Departments, thus negating any effect of the 2018 reforms, and essentially represent individual, localized research interests. The research directions of these groups are largely already covered by other CAS-Institutes.

Department 7 (Molecular and Mesoscopic Modelling) is a special case. The members of this department conduct high-level research that is of obvious relevance to the engineering departments within ICPF. However, they are, as far as the commission can judge, not integrated at all into the research of the Institute. Furthermore, other modelling and simulation (M&S) groups exist within the engineering Departments not reviewed by the Chemistry Commission. Department 7, together with these other M&S groups, represents a major untapped resource that would benefit ICPF immensely. The commission therefore recommends establishing a single M&S group within ICPF that can cover a range of scales and include all the M&S activities of the Institute “under one roof”.

This reorganisation would entail recruiting young researchers on a tenure-track basis to cover missing or underrepresented scales and would necessarily require that the existing Department 7 be strengthened to give it the capacity for extensive intra-Institute cooperations.

Part B: Evaluation of teams

1. Department of Membrane Separation Processes

Strengths:
The team members show a broad expertise in their fields of research and use interdisciplinary approaches to tackle problems. The departments collaborate intensively with scientists on national and international level in the fields of fundamental and applied research. The latter incorporates various research and innovation projects with companies. A unique characteristic of the team is the ability to develop not only at material level but also at system level up to TRLs of 7-8.

Weaknesses:
The members of the department are comparably less involved in teaching. This less intense contact with undergraduate and graduate students limits options to find and integrate the most talented students into research projects and careers in research. The commission agrees that own manufacturing capabilities for membranes would allow to extent tests under a much broader range of conditions as well as at higher TRLs.

Opportunities:
European grants and more collaborative research with industry will provide access to additional scientific infrastructure, access to a broader range of technical problems as well as additional budget to invest in people and equipment, including software.

Threats:
Although the department was quite successful in incorporating undergraduate and PhD students from abroad, it remains difficult to attract researchers from all western European countries because of the wage differences. Therefore, it is more difficult to join research consortia and to incorporate new knowledge from outside.

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

H1.1	Quality of selected outputs of Phase I
The department performs internationally recognized research in the field of membrane separations. The research is related to the determination of phase equilibria, the study of intermolecular interactions, as well as molecular modelling and covers applications in the separation of gases (gas/gas and vapour/gas) and liquid mixtures. The quality of the outputs of Phase I are above the average in the field and demonstrate a solid advancements of the field.	
H1.2	**Contribution of workers on the outputs reached**
The outputs divide equally into outputs with less than 50% contribution in collaborated research and into outputs with more than 50% contribution of CAS researchers.	
H1.3	**Quality of all outputs and results**
The quality of all outputs was evaluated by analysing the categorisation according to the journal ranking. Four outputs of the selected outputs were in the first quartile by journal ranking whereas all outputs are equally distributed within second, third and fourth quartile.	

Overall, the quality of all outputs and results is good. It is suggested to further specialise in promising research direction to obtain results of higher impact.

H1.4	The most valuable discoveries and findings in the fields, their importance for the field
Valuable discoveries cover the development of processes for the single-step purification of biogas, the determination and modelling of phase equilibria and mass transport in membranes. Furthermore, racemic mixtures were successfully separated by nanofibrous composite membranes which opens broad application areas.	

H1.5	Contribution of the participation of the authors in large collaborations
Not applicable.	

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

H2.1	Societal relevance of outputs and results pursuant to CAS and institute mission
The research of the department follows the institute‘s mission and has a certain level of research activities in areas of societal relevance such as decarbonisation of the industry, capture of CO2, removal of pollutants, and effective production of pharmaceuticals.	

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 knowledge transfer into the practise is good and documented by projects together with industry leading to process validation also on pilot scale. Some knowledge is transferred through granted patent licenses to industry.	

H2.3	Relation to practice
During the evaluation period, the department has demonstrated a strong commitment to translate its research into technological innovations, which is supported by the joint research with companies such as Czech head, Veolia, and Atrea.	

H2.4	Participation in AV21 strategy
The department participates in AV21 strategy in the programmes Natural Hazards and Water for Life.	

H2.5	Cooperation with regions of the Czech Republic
The department corporates with universities, research institutions and companies in various regions of Czech Republic.	

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 scientists of the department perform very good research focusing on fundamental knowledge as well as on industrial application which is comparable with other international teams in this field.	

D1.2	Scope and quality of international and national cooperation and the role of the team in such cooperation; engagement in broad international cooperation
The department cooperates on national and international (North America, Europe) level in form of joint projects and joint publications. The main tasks in such cooperations are the testing of membranes in advanced, self-fabricated devices including the modelling of the processes as well as the experiment- and model-based optimisation of membrane separation processes.	
D1.3	**Participation of the workers in scientific community activities (organizing of conferences and workshops, invited lectures, awards)**
The researchers of the department are very active in the scientific community in terms of organizing conferences (CHISA), joining boards of institutions and conferences, and were invited 15-times for lectures at conferences and advanced schools.	

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 followed directions are aligned with emerging trends on providing novel energy-efficient processes for purification of exhaust gases and wastewater, providing pure CO2-streams needed to reduce the consumption of fossil fuels, or separation of enantiomers.	
D2.2	**Assessment of the previous research objectives and their achievement**
The previous research objectives were of good quality and mainly achieved. It is suggested to further link the research directions with societal relevant problems to enhance the impact.	
D2.3	**Assessment of implementation of recommendations from past evaluation**
The recommendations have been taken seriously and there were actions to implement them. In detail, activities in the field of career development were intensified. For example, the department employed more bachelor, master, and PhD students as well as Postdocs also from different countries.	
D2.4	**Success in receiving grants**
The department is very successful in acquiring grants mainly from GACR and partially from MEYS and TACR. In total about 1.3 Mio. Euro were received in the considered period.	
D2.5	**Adequacy of instrumental equipment**
The department owns adequate state-of-the-art equipment. In this context, the commission admires the capability to build advanced and custom-made equipment to study specific processes.	
D2.6	**Effectiveness of management**
The department is efficiently managed, creating a good environment for performing research. Specific attention is laid on the qualification of team members in management of projects.	

D2.7	Assessment of professional structure, development strategy and the strategy of keeping best scientists, age structure, career and qualification growth
The age structure of the department is well balanced enabling senior researchers to pass their knowledge and experience to the younger generation. The department can attract young researchers from Czech Republic and abroad validating its efficient career and qualification strategy.	
D2.8	**Creating work-life balance conditions, assessment of approach towards possible gender issues**
The work-life balance conditions are very good and gender issues are appropriately taken into account. The department actively supports parental leave and part-time jobs. The researchers on a parental leave are involved into current developments to foster their connection to the department. The team is well gender balanced (55% man and 45% women).	
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.**
Not applicable.	

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
The department is well engaged in joint research projects together with national as well as international universities, research institutions. There is a less pronounced interaction with universities on a national level.	
D3.2	**Effectiveness of joint research centres**
The department is involved in a joint research centre together with the Technical University of Ostrava which led to one joint publication. Furthermore, one team member is head of one unit in the BIORAF consortium.	
D3.3	**Success rate in supervision of PhD students**
In the examination period, five PhD thesis were successfully defended.	
D3.4	**Participation of PhD students in the outputs**
PhD students are well engaged in the output of the department and are co-authors of four publications.	
D3.5	**Participation of the team in master or bachelor studies**
Several bachelor and master students were incorporated into the research.	
D3.6	**Assessment of cooperation intensity with universities in the form of teaching**
The team is adequately involved in student education at Universities in Ústí nad Labem and Prague. The researcher gave lectures 13 semestrial lectures/courses on bachelor level, as well as 5 lectures on master and PhD level.	

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

D4.1	Sufficiency of media strategy and activities in the area of research popularisation
The department frequently shows various activities in public outreach for audiences with different backgrounds from Czech Republic and abroad, e.g. open lab days and exhibitions. The homepage gives general information on the team, research fields, latest results (2018 and 2019), and ongoing projects. These outreach activities might be intensified to attract more students and scientists from other institutions.	
D4.2	**Publishing activities and its quality**
There are no publishing activities detailed that focus on popularisation of research and informing the general public about activities and outcomes.	
D4.3	**Participation in professional organisations in the area of research and development**
The staff of departments holds leading positions in international research networks and committees, professional organisations, and evaluation panels.	

Other comments of the commission:

The commission recommends to maintain the efforts in attracting students and researchers from other countries. The teaching activities should be expanded, e.g. also in form of guest lectures at Czech universities as well as universities from abroad. The members of the department should focus to publish their results in higher ranked journals. In order to reduce the dependency on others in terms of the membrane material, collaborations with other departments and companies should be intensified and extended.

2. Department of Aerosols Chemistry and Physics

Strengths:
The research of the well-managed department is well-focussed and the motivated team members show a broad expertise and know how enabling to perform excellent research in traditional fields but also in emerging, highly interdisciplinary fields. The laboratories are excellently equipped with partially unique equipment. The committee is impressed by the very intense collaboration with scientists on national and international level and the activities within ACTRIS ERIC. The institute fast adopts societal needs shows in measurement related to the COVID pandemic.

Weaknesses:
The department is integrated in a strong vital international network, however, projects in the role as a coordinator may be expanded. Although the department is able to publish in top-level journals, a significant amount is published in lower ranked journals. As in all eastern countries, it is difficult to attract scientists from western European partners because of the wage difference. The report claims the need for improvement on the data and knowledge management which cannot be evaluated by the commission due to the missing on-sight visits.

Opportunities:
Since the department is very active and successful in grant applications and has an excellent international network, the commission recommends to strengthen the applications for international calls besides ACTRIS. The excellent infrastructure and human resources favour to expand contractual research on a national and international level.

Threats:
The excellent equipment may also be a burden because there are difficulties to acquire money for maintenance and repair. The relative low level of salaries complicates to attract scientists from western European countries. This might be overcome by establishing further bilateral programmes with regular exchange of students and staff.

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

H1.1	Quality of selected outputs of Phase I
The department substantially enhanced the fundamental understanding on aerosol formation and transformation as well as how they interact with different environments. In this context, novel and original data on distribution and composition are presented which are important to evaluate the impact on workers and humans in general. The productivity of the department in terms of world-leading and excellent outputs is significantly above the average of this field.	
H1.2	**Contribution of workers on the outputs reached**
About 50% of the evaluated outputs had a full or major contribution of researchers from CAS whereas around 10% had a contribution of less than 50%. The outputs with less contributions are caused by projects in larger consortia or by highly interdisciplinary research.	
H1.3	**Quality of all outputs and results**
The quality of all outputs was analysed according to the journal ranking. Around 100 papers have been published in journals with IF from which 3 belong to the top decile and 11 to the top quartile. The rest of publications is uniformly distributed around the third quartile.	

H1.4	The most valuable discoveries and findings in the fields, their importance for the field
The most valuable discoveries are related to aerosol formation and transformation, highly resolved measurements on aerosol composition in urban and indoor environments as well as interaction between in- and outdoor as well as to the source apportionment and interaction with clouds of atmospheric aerosols. Additionally, sophisticated laboratory methods to constantly generate nanoparticles for inhalation studies were developed.	
H1.5	**Contribution of the participation of the authors in large collaborations**
Not applicable.	

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

H2.1	Societal relevance of outputs and results pursuant to CAS and institute mission
The outputs and results are highly relevant to the mission of CAS and the institute and have a significant societal relevance. The understanding how aerosols in several environments, such as indoors, in the atmosphere, etc., behave and are composed is important to ensure human health as well as to protect the environment. In this context, the contribution to build-up a is a pan-European research infrastructure for short-lived atmospheric constituents such as aerosol, clouds and trace gases must be highlighted that will significantly improve Earth observation and provide important knowledge for sustainable development of society.	
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 group is active in the knowledge transfer into practise. The department contributes to the development of apparatus and technologies in order to enhance the competitiveness of the national economy through applied research in cooperation with various industrial partners (drug inhalers, filtering facepiece respirators, ionic liquids for various applications, etc.).	
H2.3	**Relation to practice**
The department has good relations to the practise in form of collaborative projects but also to some extend in form of contractual work. In this context the collaboration with scientists from the medical field should be mentioned in order to elucidate the impact of aerosols on health of organisms.	
H2.4	**Participation in AV21 strategy**
The department is involved in the AV21 strategy focusing on current societal challenges. In particular, the institute contributes to the programme of Efficient Energy Conversion and Storage and Natural Hazards.	
H2.5	**Cooperation with regions of the Czech Republic**
There is close cooperation with a number of Czech institutions, e.g. Czech Hydrometerological Institute, Masaryk University, Global Change Research Institute.	

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 department is a worldwide recognised team in the fundamentals of aerosol physics but also on aerosol in different environments such as atmospheric aerosols, as well as indoor and outdoor aerosols. The department is partner of several EU projects also with larger consortia. This further underlines its reputation as well as research quality and originality.	
D1.2	**Scope and quality of international and national cooperation and the role of the team in such cooperation; engagement in broad international cooperation**
The commission is impressed by the high-quality of national and international collaborations. On an international level, the activities in the pan-European Research Infrastructure ACTRIS (The Aerosols, Clouds and Trace Gases Research Infrastructure) should be highlighted with more than 100 European partners. On a national level, the departments collaborates with 3 partners within the ACTRIS-CZ project as well as with National Atmospheric Observatory Košetice.	
D1.3	**Participation of the workers in scientific community activities (organizing of conferences and workshops, invited lectures, awards)**
The researchers of the department are very active in the scientific community in terms of organizing meetings and conferences (e.g. Annular Conference of the Czech Aerosol Society, Special Symposium within the IUPAC Congress), workshops and training schools, joining boards of conferences, more than 10 times for giving lectures. The department received several awards of the Czech Aerosol Society in the Young Scientist competition as well as of the CAS.	

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 commission appreciates that the department continues to perform research in traditional fields, e.g. formation, transformation, and composition of aerosols or nucleation kinetics but also adopts other emerging fields, e.g. aerosol-cloud interaction, source apportionment, indoor and workplace aerosols.	
D2.2	**Assessment of the previous research objectives and their achievement**
The previously planned research objectives were assessed and the main research directions are followed as well as partially intensified or extended for very promising research directions/areas. The department's vitality is exemplarily visible in the fast adoption of societal need due to the current pandemic by testing personal protective equipment.	
D2.3	**Assessment of implementation of recommendations from past evaluation**
In the report, there are three recommendations mentioned from the last evaluation which led to some actions for implementation. In this context, the cooperation with other institutes of the CAS and other Czech universities was intensified or newly started. Additionally, collaborations with other meteorological groups such as with the Institute of Atmospheric Physics and Thermomechanics at CAS and the National Atmospheric Observatory Košetice were initiated and resulted in several joint papers. The commission agrees that joining another large-scale funded European programme besides ACTRIS.	
D2.4	**Success in receiving grants**

The department is very successful in acquiring grants mainly from MEYS, GACR and partially from EU and MC. In total about 3.7 Mio. Euro were raised between 2015 and 2019.	
D2.5	**Adequacy of instrumental equipment**
The department was able to acquire many new aerosol instruments during the last evaluation period. Additionally, home-made instrumentation can be designed and built according to the needs of the research. The report claims that the department is the best equipped aerosol lab in Central and Eastern Europe hosting very good instrumental equipment. However, difficulties in financing repairs of the expensive equipment are reported. Therefore, the repairs are usually done by members of the department.	
D2.6	**Effectiveness of management**
The management seems to be very effective because the teams is highly productive and works in national and international consortia as well as recommendations from the last evaluation were fast implemented.	
D2.7	**Assessment of professional structure, development strategy and the strategy of keeping best scientists, age structure, career and qualification growth**
The age structure of the department lists 19 people between 25 and 45 years, 5 people between 45 and 65 years, and 4 people above 65 years. During the evaluation period, the department was able to increase the amount of researchers.	
D2.8	**Creating work-life balance conditions, assessment of approach towards possible gender issues**
The team employs an appropriate Human Resources policy which includes various aspects of personal training and development. A fraction of females of about 40% was estimated from the members list given on the webpage.	
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.**
Not relevant.	

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**
There is a good cooperation with universities mainly on a national level.	
D3.2	**Effectiveness of joint research centres**
The department is involved in a number of national and international research consortia which is an indicator for its effectiveness.	
D3.3	**Success rate in supervision of PhD students**
The department shows a high success rate in the supervision of PhD students. Within the evaluation period, 8 PhD theses were successfully defended.	
D3.4	**Participation of PhD students in the outputs**

PhD students are seen as important members of the team. They participated by performing experimental campaigns, analysing and interpretation of the experimental data, as well as to write publications. Each PhD student is expected to publish at least one paper as first author and one paper as co-author in an impacted journal.

D3.5	Participation of the team in master or bachelor studies

Bachelor and master students are engaged within the research of the department. From 2015 to 2019, 4 bachelor and 3 master thesis were completed.

D3.6	Assessment of cooperation intensity with universities in the form of teaching

There is a good cooperation with universities in Prague. Members of the department teach at the Charles University and the Institute of Chemical Technology Prague in the fields of Meteorology, Climatology, Aerosol Engineering and physical Chemistry on bachelor, master and doctoral level.

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

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

The department is very active in activities as public outreach for audiences with different backgrounds. The members of the department regularly give courses and participate in fairs and exhibitions for the general public of all age categories. Additionally, the department is involved in several outreach videos resulting from projects and participated in the science popularisation theatrical play.

D4.2	Publishing activities and its quality

Members of the department are active in publishing scientific results, about 100 papers in journals with IF. There are no special publishing activities listed in the reports in terms of research polarisation.

D4.3	Participation in professional organisations in the area of research and development

The staff of departments holds leading positions in different national and international research networks and committees, professional organisations, and evaluation panels.

Other comments of the commission:

The commission recommends to maintain the efforts in deepening and expanding the network to universities, research institutes, and companies. The initiation and implementation of mobility programmes might improve the mobility of Czech scientists. The department has an excellent reputation and hosts special equipment which enables to apply for further grants from the EU also in the role as a coordinator as well as for projects from other international funding organisations. Additionally, the department should intensify the efforts to expand contractual research. This further diversification and less restricted financial resources might help to overcome difficulties in financing maintenance and repair of expensive equipment. The researchers of the department should publish their results in higher ranked journals which will further improve the international visibility as well as citation score.

3. Department of Catalysis and Reaction Engineering

Strengths:
The department combines a strong expertise in the fields of catalyst preparation, chemical process design as well as characterisation and modelling of complex processes which forms a solid fundament for holistic developments in the fields of biorefineries, circular economy and others. The collaboration activities are excellent and comprise research projects with scientists from universities, research institutes, and national and international companies as well as joint research centres. Additionally, the media strategy and outreach activities are excellent.

Weaknesses:
The members of the department are very active in publishing papers, book chapters and books. However, most of the scientific papers were published in lower ranked journals with low numbers of citations. This indicates that the reported results are less relevant in the scientific community.

Opportunities:
More EU grants and industrial collaboration can bring additional budget as well as access to infrastructure and committee positions to shape the research directions in Europe.

Threats:
The department express concerns about a future lack of PhD students. The commission agrees that a project funding quote of 60% may create some instabilities in periods with less success in obtaining projects resulting in leaving of young workers. However, the this is a regular funding quote within CAS and also on international level.

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

H1.1	Quality of selected outputs of Phase I
The scientific publications of the department have importantly contributed to the body of scientific knowledge in fundamental research as well as applied research in the area of catalysed processes in the field of environmental technologies and renewable resources. The quality of outputs of Phase I is below the average of this field.	
H1.2	**Contribution of workers on the outputs reached**
About 75% of the evaluated outputs had a full or major contribution of researchers from CAS. The other outputs result from projects in larger consortia with involvement of the department.	
H1.3	**Quality of all outputs and results**
The quality of all outputs and results is fair. The analysis revealed that the majority of outputs was in the third and fourth quartile or in the category n.a.	
H1.4	**The most valuable discoveries and findings in the fields, their importance for the field**
The most valuable discoveries include novel, very active and selective catalysts and/or corresponding processes for fuel cells, biorefineries, and exhaust gas cleaning. In this context, it must be emphasized that the department efficiently combines its expertise in all touched disciplines such as surface science, chemistry, chemical reaction engineering among others to design tailored catalysts and reactors.	

H1.5	Contribution of the participation of the authors in large collaborations
Not applicable.	

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

H2.1	Societal relevance of outputs and results pursuant to CAS and institute mission
The department‘s research is in line with the mission of the institute. Society benefits from significant developments in the following fields: decarbonisation of the industry and society, the establishment of a circular economy, as well as the removal of pollutants from the environment.	
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 transfer the knowledge into practise is very good. This is validated by leading of national consortia (BIORAF, BIOCIRTECH) and several cooperations with industrial partners.	
H2.3	**Relation to practice**
Within the evaluation period, the combination of innovative strength and practical orientation has led to an intense collaboration with industry in form of contract work in analysis of properties of solids as well as joint projects in various technical applications funded by TACR.	
H2.4	**Participation in AV21 strategy**
The themes of Efficient Energy Conversion and Storage, Foods for the Future, and National Hazards of the AV21 strategy are well embedded in the research of the department.	
H2.5	**Cooperation with regions of the Czech Republic**
The department cooperates with universities, research institutions and companies in nearly all regions of Czech Republic.	

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 scientists of the department perform very good fundamental as well as applied research. Two EU projects and one NATO project were funded which confirms its reputation and research quality within Europe and beyond.	
D1.2	**Scope and quality of international and national cooperation and the role of the team in such cooperation; engagement in broad international cooperation**
The department cooperates very intensively on national and international (Europe: Belgium, Bulgaria, Finland, France, Germany, Hungary, Italy, Turkey, United Kingdom, America: Peru) level in form of joint projects and joint publications. The main tasks in such	

cooperation are the synthesis, testing and optimisation of catalysts as well as the development of corresponding processes.
D1.3 **Participation of the workers in scientific community activities (organizing of conferences and workshops, invited lectures, awards)**
The researchers of the department are very active in the scientific community in terms of organizing conferences (CHISA), workshops, joining boards of institutions and conferences, and were invited for giving lectures. Three researchers of the department received several and high-ranked prices from Czech organisations.

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

D2.1	**Direction in line with the perspective of the planned research directions**
It is highly appreciated that the department works in the significant and emerging fields in order to develop novel materials for modern technologies as well as novel sustainable processes.	
D2.2	**Assessment of the previous research objectives and their achievement**
The previously planned research objectives were assessed and partially extended for promising research directions in terms of scientific depth as well as application.	
D2.3	**Assessment of implementation of recommendations from past evaluation**
The recommendations of the last evaluation were fully implemented and led to several actions. The efforts to get involved into EU or other international funding have been extended, i.e. 3 proposals for EU funding have been submitted applications for EU projects. One of them was successful. Furthermore, NATO funds were acquired. In the context of internationalisation, closer contact to French universities were established, i.e. exchange of students and scientists from both institutions.	
D2.4	**Success in receiving grants**
The department is very successful in acquiring grants mainly from GACR and TACR and partially from EU, MEYS, MI, MIT and NATO. In total about 3.6 Mio. Euro were received in the investigated period, which is very good.	
D2.5	**Adequacy of instrumental equipment**
The department owns adequate equipment for its research. However, some analytical systems and experimental rigs need investments to reach the state-of-the-art and to ensure the creation of new knowledge as a leading department in Europe.	
D2.6	**Effectiveness of management**
The department involves the traditional units for an experimental-based research team and is well managed.	
D2.7	**Assessment of professional structure, development strategy and the strategy of keeping best scientists, age structure, career and qualification growth**
The age structure of the department inhibits 16 people between 25 and 45 years and 4 people between 60 and 65 years out of 27 members, i.e. the group with ages below 25 years and between 45 and 60 years is less incorporated. During the evaluation period more and more PhD students and young researchers were employed. The department	

should continue this development. The department is able to attract young researchers from Czech Republic and abroad validating its efficient career and qualification strategy.	
D2.8	**Creating work-life balance conditions, assessment of approach towards possible gender issues**
The department actively supports parental leave and part-time jobs. The researchers on a parental leave are involved into current developments to foster their connection to the department. The team is well gender balanced.	
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.**
Not relevant.	

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**
The department collaborates very intensively with universities on a national and international level. The cooperation is based on joint projects as well as the exchange of master and PhD students.	
D3.2	**Effectiveness of joint research centres**
The department takes a leading role in joint research centres, such as the centres of competence for Biorefinery Research BIORAF and circular economy BIOCIRTECH. These centres are a virtual platform for exchange and joint research which is documented by publications in high impact journals.	
D3.3	**Success rate in supervision of PhD students**
The success rate of PhD students is about 80%.	
D3.4	**Participation of PhD students in the outputs**
PhD students are considered as full team members and participate in all outputs of the department, i.e. in publications, utility models, and patents. Within the examination period, 33 publications, 8 utility models, and 6 patents have to be mentioned.	
D3.5	**Participation of the team in master or bachelor studies**
Several bachelor and master students were incorporated into the research. 6 bachelor and 9 master thesis were defended in the examination period.	
D3.6	**Assessment of cooperation intensity with universities in the form of teaching**
The team is to a large extend involved in student education at a national level (UCT, CU, UJEP) as well as on the international level (University of Maribor, Slovenia and University of KwaZulu-Natal, South Africa). The courses cover courses for bachelor, master, as well as PhD students.	

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

D4.1	Sufficiency of media strategy and activities in the area of research popularisation
The commission is impressed by the excellent outreach activities of the department. The members of the department regularly participate in running courses and lectures, publishes brochures and popularizations articles and books, as well as present their research on open lab days and science fairs for audiences with different backgrounds. Additionally, the researchers take part in television debates and radio programmes in order to reach a variety of people.	
D4.2	**Publishing activities and its quality**
Members of the department are very active in popularisation of science, e.g. publishing of brochures, articles, and books fur various audiences as expressed in the reports of the individual departments.	
D4.3	**Participation in professional organisations in the area of research and development**
The staff of departments holds leading positions in international research networks and committees, professional organisations, and evaluation panels.	

Other comments of the commission:

The commission recommends to maintain the efforts in attracting students and researchers from other countries as well as to deepen and expand the network to universities, research institutes, and companies. This will form a solid basis to participate in grants from the EU and other international funding organisations. This diversification in project funding resources will reduce the feared fluctuation in projects leading to leaving young scientists. Strategic partnerships with universities may be an opportunity to minimize the risk of lacking in PhD students because of the missing right to confer doctoral degrees. The members of the department should focus to publish their results in higher ranked journals which will further improve the international visibility. Furthermore, social media and mutual contacts may be extended to inform the scientific community about reported research results which might also increase the number of citations per publication.

4. Department of Multiphase Reactors

Strengths:
The department has a long history and deals with research on the important topic of multiphase flows. It has a unique position within Czech Republic which is combined with an excellent international reputation. The spectrum of research covering theory, experiments, simulation, and application gathers experts with different skills enabling to tackle various problems dealing with multiphase flows on a high scientific level. The department uses and further develops a large toolbox of theoretical and experimental methods to elucidate multiphase flow phenomena and the interplay with the reactor, process and value chain.

Weaknesses:
The department inhibits a professional diversity which origins from the merging of three smaller groups in the past. Furthermore, the department performs research in various fields such as gas-liquid flows, gas-solid flows, micro reactors, and bioreactors. These directions are united under the umbrella of multiphase flows. However, this thematic diversification makes it difficult to dominate on field of research in Europe. There is a comparable small amount of young talent and researchers.

Opportunities:
The broad appearance of multiphase flow phenomena creates diverse collaboration opportunities as already partially utilized by the department. Further specialisation in emerging areas of application such as wastewater treatment, bio feedstock processing and chemical specialities can result in a leading position in topics of high societal relevance. In this context, the department should continue its activities to build-up and establish international collaborations.

Threats:
The multi-facetted appearance of multiphase flows opens broad collaboration opportunities. On the other hand, this may lead to an even further fragmentation of the research directions. A strong focus on the fundamentals of multiphase flows and the alignment with societal needs might be a compromise to ensure international visibility and simultaneously to transfer the knowledge into the practise.

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

H1.1	Quality of selected outputs of Phase I
The department majorly contributed to the fundamental understanding of multiphase flows such as gas-liquid or gas-solid flows as well as to an improved design and operation of micro reactors and bioreactors based on a better understanding of the occurring phenomena. The quality of the outputs of Phase I is very good and above the average of this field.	
H1.2	**Contribution of workers on the outputs reached**
About 70% of the evaluated outputs had contributions with a work fraction of 50% and above, which is very good. Outputs with a lower fraction are mainly the result of research collaboration in form of internships at other institutions as well as the using of the multiphase competence in non-classical fields such as in food and pharmaceutical application or biotechnology.	
H1.3	**Quality of all outputs and results**

The quality of all outputs was evaluated by analysing the categorisation according to the journal ranking. The majority of items is equally distributed across the second to fourth quartile with a fraction of about 5% in the top quartile. Overall, the quality is good but attention should be given to further improve the impact and quality of research results, mainly through choosing emerging fields with societal relevance.

H1.4	The most valuable discoveries and findings in the fields, their importance for the field
The most valuable research contributes to a better understanding of bubble dynamics in bubble columns as well as granular mixing on different length scales as well as in the advanced manufacturing and design of micro reactors. Profound results were obtained but they cannot be considered as ground-breaking since it is rather a step by step continuation than real paradigm shift.	

H1.5	Contribution of the participation of the authors in large collaborations
Not applicable.	

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

H2.1	Societal relevance of outputs and results pursuant to CAS and institute mission
The department‘s research supports the mission of the institute. The better understanding of the multiphase phenomena may support more atom and energy efficient contacting devices. Also parts of the research focus on optimised downstream processing of microalgae in the context of renewable carbon sources.	

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
There is a considerable transfer of knowledge into the practise, documented by collaborate research projects with industry as well as contractual research.	

H2.3	Relation to practice
There are strong ties with industry in form of joint projects funded by TACR or by the companies themselves.	

H2.4	Participation in AV21 strategy
The department works on topics mainly relating to the theme Water for Life.	

H2.5	Cooperation with regions of the Czech Republic
The department cooperates intensively within the Institute of Chemical Process Fundamentals at CAS as well as with national universities, e.g. Ostrava, Prague, Ústí nad Labem, research institutes, e.g. ASCR or AVCR, and companies, e.g. Synthomer.	

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 performance of the department is on a similar level as other international research institutes. The department successfully joined one EU project which is an indicator for its reputation and research 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**
There is an intense international collaboration with universities and companies from Belgium, Brazil, Finland, France, Germany, Italy, Japan, Poland, United Kingdom, department cooperates intensively on national and international (Europe: Belgium, Bulgaria, Finland, France, Germany, Hungary, Italy, Norway, Portugal, and Spain) level in form of joint projects and joint publications. The scope covers the exchange of students, the transfer of knowledge, as well as joint projects.	
D1.3	**Participation of the workers in scientific community activities (organizing of conferences and workshops, invited lectures, awards)**
The researchers of the department are very active in the scientific community in terms of organizing conferences (CHISA 2016 and 2018), workshops for students, joining boards of conferences, and were invited 8 times for giving lectures. The department received awards for a best paper of the Czech Chemical Society as well as a poster award of CHISA.	

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 department planned to follow research in 3 new directions such as unsteady phenomena in multiphase systems, generic analogies in different systems, and scale-up of multiphase systems. Two of them were pursued resulting in corresponding research outputs. Additionally, the members worked on side issues with context to multiphase flows.	
D2.2	**Assessment of the previous research objectives and their achievement**
The performed research resulted in progress in most of the fields. The outcome was positively assessed in the report. Further potential emerging fields with challenges of multiphase flows were identified.	
D2.3	**Assessment of implementation of recommendations from past evaluation**
The department mentions three main recommendations from the last evaluation in the actual report, reorganisation of the internal structure considering the critical mass for each unit, internal programs to stimulate actions according to the strengths and weaknesses, and identification of new research topics. The department continued its efforts to seek foreign partners for joint research projects. The other recommendations were not seen relevant for the research team.	
D2.4	**Success in receiving grants**
The department is successful in acquiring grants mainly from GACR (4) and TACR (2) as well as partially from EU (1) and MEYS (1). In total about 650 thousand Euro were received in the evaluation period. This is below the average considering the amount of FTE.	

D2.5	Adequacy of instrumental equipment
The department owns state-of-the-art hardware and software tools for its research as reported in the provided documents. Nevertheless, further investments in infrastructure and instruments are needed to keep the pace with the leading groups in Europe. Clear and intentional specialisation will help guiding potential investments in high-impact directions.	
D2.6	**Effectiveness of management**
It seems that the department is well managed. The report states that potential conflicts arise from the leadership and responsibilities in different technical subunits (theory, experimentation, and simulation), in different fields (multiphase flows, micro reactors and bioreactors), as well as in different projects. However, it is mentioned that conflicts are easily solved. Special attention is laid on an effective communication strategy within the department.	
D2.7	**Assessment of professional structure, development strategy and the strategy of keeping best scientists, age structure, career and qualification growth**
The department employs 3 members below 30 years, 14 members with ages between 35 and 50, and 3 between 55 and 60 years. Additionally, there are two emeriti. The small amount of young researchers is related with the comparably small amount of external funds. The report lists several options for the development of individuals which rather depends on the person itself and not on a strategy of the department.	
D2.8	**Creating work-life balance conditions, assessment of approach towards possible gender issues**
The female and male genders are well balanced. There are no information on activities creating a harmful work life-balance or related issues.	
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.**
Not relevant.	

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
The department is very active in cooperation with universities on a national and international level. The scope is very good.	
D3.2	**Effectiveness of joint research centres**
The department participates in joint research centres with universities in Prague (UCT, Charles) and Ústí nad Labem.	
D3.3	**Success rate in supervision of PhD students**
One PhD-thesis was defended in the evaluation period, which is too little for an ambitious group. There are no information of the success rate given.	
D3.4	**Participation of PhD students in the outputs**

There are 4 supervised and 2 consulting PhD students in the department. They contributed to a significant amount to scientific output of the department.	
D3.5	**Participation of the team in master or bachelor studies**
Seven bachelor and master students worked in the group and were incorporated into the research within the evaluation period.	
D3.6	**Assessment of cooperation intensity with universities in the form of teaching**
Dr. Havlica is involved to very large extend in student education at UJEP Ústí nad Labem on Bachelor, Master and PhD level. Dr. Stavárek, Dr. Zedníková, Dr. Tihon, and Dr. Vejražka are minor involved in lectures at universities in Ostrava and Prague.	

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

D4.1	**Sufficiency of media strategy and activities in the area of research popularisation**
The members of the department regularly participate in courses, fairs and exhibitions for the general public, e.g. lessons and lab-courses for high-school students as well as open lab days at Festival of Science, Science and Technology week etc.	
D4.2	**Publishing activities and its quality**
There are no special publishing activities in terms of research polarisation.	
D4.3	**Participation in professional organisations in the area of research and development**
The staff of departments are active members of several working parties, scientific societies as well as committees and advisory boards.	

Other comments of the commission:

The holistic approach is good, which combines the advance of knowledge by fundamental research with its application to improve specific multiphase contact apparatus. The broad expertise in various multiphase flows may be useful in many disciplines. The commission recommends to maintain the activities to expand the collaboration with other European universities, research institutes and companies as well as to exchange students of different levels and staff. This larger network will create further opportunities to apply for international funds and may lead to more contractual research. This diversification in project funding will reduce the feared fluctuation in projects leading to unplannable research and the leaving young scientists. Partially, the research appears fragmented and overlapping with the research of other departments in the institute and beyond (e.g. Fluid Mechanics Group, Department of Catalysis and Reaction Engineering).

5. Department of Analytical Chemistry

Strengths:
- NMR-omics, in particular in metabolomics as competitive research area, and airosolomics as new research area

Weaknesses:
- Research topics are diverse and unfocussed
- No outstanding ideas

Opportunities:
- Separate service and research, move research to more appropriate CAS Institutes or Departments within ICPF

Threats:
- Loss of identity from conflict between service and research
- Instrumentation becomes outdated

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

H1.1	**Quality of selected outputs of Phase I**
Average	
H1.2	**Contribution of workers on the outputs reached**
Average	
H1.3	**Quality of all outputs and results**
Average	
H1.4	**The most valuable discoveries and findings in the fields, their importance for the field**
NMR-omics for aerosols	
H1.5	**Contribution of the participation of the authors in large collaborations**
Average	

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

H2.1	**Societal relevance of outputs and results pursuant to CAS and institute mission**
Potentially important contribution to aerosol research.	
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**
One spinoff.	
H2.3	**Relation to practice**

Moderate.	
H2.4	**Participation in AV21 strategy**
Average	
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**
The individual research projects are at an intermediate level. The service in the area, for instance of aerosols is possibly higher rated.	
D1.2	**Scope and quality of international and national cooperation and the role of the team in such cooperation; engagement in broad international cooperation**
International cooperation with Graz and Florence. It is laudable that the team chose to learn about NMR-omics in Florence**.**	
D1.3	**Participation of the workers in scientific community activities (organizing of conferences and workshops, invited lectures, awards)**
Average	

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

D2.1	**Direction in line with the perspective of the planned research directions**
Only the NMR-omics is 100% compatible with the needs of the Institute. The team complains of a “lack of projects in metabolomics”	
D2.2	**Assessment of the previous research objectives and their achievement**
No improvement since the 2018 reforms is discernible	
D2.3	**Assessment of implementation of recommendations from past evaluation**
See D2.2	
D2.4	**Success in receiving grants**
Local	
D2.5	**Adequacy of instrumental equipment**
Apparently currently adequate but an update to 600 Mhz NMR is part of the planning.	
D2.6	**Effectiveness of management**
Doing their best under difficult conditions.	
D2.7	**Assessment of professional structure, development strategy and the strategy of keeping best scientists, age structure, career and qualification growth**

No discernible strategy	
D2.8	**Creating work-life balance conditions, assessment of approach towards possible gender issues**
Gender-balance poor	
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.**
n/a	

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**
Graz and Florence	
D3.2	**Effectiveness of joint research centres**
n/a	
D3.3	**Success rate in supervision of PhD students**
Some success	
D3.4	**Participation of PhD students in the outputs**
Students sometimes first authors	
D3.5	**Participation of the team in master or bachelor studies**
Below average	
D3.6	**Assessment of cooperation intensity with universities in the form of teaching**
Below average	

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

D4.1	**Sufficiency of media strategy and activities in the area of research popularisation**
Low activity	
D4.2	**Publishing activities and its quality**
Low activity	
D4.3	**Participation in professional organisations in the area of research and development**
Some conference organisation etc.	

Other comments of the commission:
See also comments made in Part A (Evaluation of the institute).
The department suffers, like many such Departments in CAS Institutes, under the combination of service tasks with original research. Particularly the latter appears uncoordinated and corresponds to the personal interests of the researchers involved. With the exception of NMR-omics, the research projects of the Department have little to do with the aims and direction of the Institute as a whole. It is difficult to find any justification for the Department being part of ICPF except for its service function. We suggest that it, together with Laser Chemistry services, be converted into a 100% service Department and that the research activities would be more appropriate in other CAS Institutes. The NMR-aerosolomics research can be moved to, for instance, Department 2, which the commission did not evaluate.

6. Department of Environmental Engineering

Strengths:
The department is well-focussed and, in spite of the applied research topics, capable to publish research results on an excellent level. It is well equipped with laboratories and well connected to industry. Also, it is well embedded within the national research landscape as it is involved in two national competence centres.

Weaknesses:
The success rate related to international project proposals, such as Horizon 2020, is rather low. Correspondingly, there is a lack of international projects within the department.

Opportunities:
Since the department is very active in writing project proposals and also publishes on a high academic level, it should be possible to strengthen the success rate in international project calls and to strengthen international cooperations.

Threats:
Among the team members, five members are close to retirement and might leave gaps behind. The department also heavily relies on project funding. This might become a threat in times of lower acquisition rates, even though the department currently is very successful in this respect.

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

H1.1	Quality of selected outputs of Phase I
Compared to other teams of CAS, the quality of selected outputs of Phase I is very high with a significant portion of output being located in the first and second quality group.	
H1.2	**Contribution of workers on the outputs reached**
About one third of the output of Phase I was created by members of the department only. The majority of the output was produced within collaborations, with most publications written by a majority of members of the department. Therefore, contributions of the team members to the scientific output are solid and significant.	
H1.3	**Quality of all outputs and results**
Overall, the quality of all outputs is comparatively high. The department manages to place publications in journals that are ranked in the first quartile, including those within the first decile. Additionally, the productivity of teams in excellent outputs is highest if compared to other teams of the same institute.	
H1.4	**The most valuable discoveries and findings in the fields, their importance for the field**
The department focusses on two field, first the treatment of flue gas and flues and second on new technologies for treatment or recycling of wastes and waste material. A judgement of the results obtained in these field depends on whether one focusses more on the fundamental or more on the applied aspects. One should certainly mention the success of the department in developing actual technology, such as for the recycling of composite packaging materials which has been patented and licensed to a private company.	
H1.5	**Contribution of the participation of the authors in large collaborations**
None.	

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

H2.1	Societal relevance of outputs and results pursuant to CAS and institute mission
The reduction of pollutants and the recycling of wastes and waste materials is of a high relevance for modern and industrial societies. Therefore the conducted research is along the mission of CAS and the institute.	
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 department manages to link fundamental to applied research and to turn research results into working technology. Combined with the relevant research topics the usefulness for society is out of the question. In the long run, a positive impact towards proper practice in society can be expected as well.	
H2.3	**Relation to practice**
As mentioned above, the research of the department relates very well to industrial processes in practice.	
H2.4	**Participation in AV21 strategy**
The department is involved in the AV21 strategy and occupied with several tasks in the related „Efficient Energy Conversion and Storage programme“.	
H2.5	**Cooperation with regions of the Czech Republic**
Apart from the excellent links of the department to national industry one should also mention the participation of the department in the „Waste-to-energy Competence Centre“ and the „National Centre for Energy“.	

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 effectiveness of this team is very high and it also manages to combine fundamental and applied research. Therefore the team can be considered as close to excellence, if compared to teams in similar institutes.	
D1.2	**Scope and quality of international and national cooperation and the role of the team in such cooperation; engagement in broad international cooperation**
The department cooperates well on a national and international level, even though in view of broad international cooperations there seems to be room for improvement. It should be mentioned that the department took part in a couple of Horizon 2020 project applications, indicating a solid network of international partners, but only one has been successful. This might be due to the typically low success rate in this European program, though.	
D1.3	**Participation of the workers in scientific community activities (organizing of conferences and workshops, invited lectures, awards)**
A number of about five team members is quite active in scientific communities and engages in several committees, scientific boards, and in the organization of international	

congresses and workshops. One member occasionally receives invitations to lectures but earned awards are limited to one scholarship only.

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

D2.1	Direction in line with the perspective of the planned research directions
During the last evaluation period, the department successfully got more focussed on a lesser number of research topics. Based on the resulting research directions the department intends to continue and extend its main research directions and this is meaningful and should be considered as promising.	
D2.2	**Assessment of the previous research objectives and their achievement**
Among the four topics envisaged for the period 2015-2019, one was abandoned while the others were successfully continued, leading to the afore mentioned high quality journal publications and technological applications. Therefore the former period 2015-2019 has been a successful one.	
D2.3	**Assessment of implementation of recommendations from past evaluation**
As recommended in the past evaluation, the department became more focussed and this led to good success. The efforts to become more involved in international collaborations have not been very successful, yet, but should be further pursues.	
D2.4	**Success in receiving grants**
The department is very successful in the acquisition of national grants, leading to sufficiently external funds to be successful in applied research and to maintain sufficient laboratory equipment.	
D2.5	**Adequacy of instrumental equipment**
The instrumental equipment is adequate and, as stated by the department head, sufficient for the needs of the department.	
D2.6	**Effectiveness of management**
Compared to other teams of the same institute, the department efficiently creates high quality research output such that it can be concluded that the management must be very effective as well to achieve these goals.	
D2.7	**Assessment of professional structure, development strategy and the strategy of keeping best scientists, age structure, career and qualification growth**
The age structure of the department exhibits a somewhat typical age gap in the age interval 45 to 60. There are younger but experienced researchers and there is a notable number of 6 PhD students. In particular, the involvement of PhD students seems to be a good strategy to support career and qualification growth.	
D2.8	**Creating work-life balance conditions, assessment of approach towards possible gender issues**
The department follows a Human Resources policy which supports each individual researchers in terms of guidance and supervision. PhD students are encouraged to participate in international exchanges and internships. There are no particular measures in relation to possible gender issues mentioned.	

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.
Not applicable.	

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
While cooperation with international universities could be improved, the cooperation with national universities is very good and quite intense, as becomes evident from the following points D3.2 to D3.6.	
D3.2	**Effectiveness of joint research centres**
As seen from the evaluated literature of Phase I, about two thirds of important scientific output is created from collaborations which include joint research in corresponding centres. Therefore these activities can be considered as effective and successful.	
D3.3	**Success rate in supervision of PhD students**
Compared to the size of the team, the success rate in supervision of PhD students is satisfying, in 2015-2019 two PhD theses were successfully defended. More PhD theses are under way.	
D3.4	**Participation of PhD students in the outputs**
The involvement of PhD student in scientific outputs appears as rather intense, well-structured and supported by the department head and its deputy. This is positively acknowledged.	
D3.5	**Participation of the team in master or bachelor studies**
A very good participation can be observed, as 11 master and 8 bachelor theses were successfully completed in 2015-2019.	
D3.6	**Assessment of cooperation intensity with universities in the form of teaching**
Three team members hold regular lectures at two national universities and, obviously, attract a good number of students to eventually work and do research in the department.	

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

D4.1	Sufficiency of media strategy and activities in the area of research popularisation
Activities in the area of research popularisation seem to be sufficient and flawless, as the team also publishes in popular journals, organizes workshops for the public and takes part in public talks and discussions.	
D4.2	**Publishing activities and its quality**

The overall publishing activities are very good, of a high quality, and also aim towards popularization, as stated above. Publishing activities in the popular sector are difficult to judge, though, but happen on a regular basis.	
D4.3	**Participation in professional organisations in the area of research and development**
The leading scientists of the department are well connected in their corresponding scientific communities, mostly on a national level. International involvement is reasonably well but perhaps not outstanding.	

Other comments of the commission:

7. Department of Molecular and Mesoscopic Modelling

Strengths:
- High-level research using techniques that are not generally represented in mainstream M&S
- Very high potential relevancy to the engineering Departments

Weaknesses:
- Department exists within a vacuum in the Institute. Projects are centred on external funding and interests

Opportunities:
- Establish a high-level and broader M&S Department including M&S groups from the engineering Departments

Threats:
- Inability to establish communication with the engineering groups
- Poor internal funding forces reliance, and thus concentration, on external projects of little use to ICPF
- Reliance on US-Army funding and research on fracking can potentially lead to adverse publicity.

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

H1.1	**Quality of selected outputs of Phase I**
High quality modelling	
H1.2	**Contribution of workers on the outputs reached**
The younger members of the Department still work with their postdoc supervisors	
H1.3	**Quality of all outputs and results**
High quality modelling	
H1.4	**The most valuable discoveries and findings in the fields, their importance for the field**
None of importance for ICPF	
H1.5	**Contribution of the participation of the authors in large collaborations**
N/a	

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

H2.1	**Societal relevance of outputs and results pursuant to CAS and institute mission**
Potentially very large if coupled to the engineering Departments if ICPF. Currently defined by external project definitions (fracking, explosives, earthquakes)	

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
N/a	
H2.3	**Relation to practice**
Important potential support function for practical research but currently not realised	
H2.4	**Participation in AV21 strategy**
N/a	
H2.5	**Cooperation with regions of the Czech Republic**
moderate	

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
High international standard, not least because of the simulation techniques used.	
D1.2	**Scope and quality of international and national cooperation and the role of the team in such cooperation; engagement in broad international cooperation**
Internationally well networked	
D1.3	**Participation of the workers in scientific community activities (organizing of conferences and workshops, invited lectures, awards)**
Low, no conferences organised	

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

D2.1	Direction in line with the perspective of the planned research directions
Potentially extremely high relevance if the leadership of the Institute and the Department can bundle and integrate all M&S activities within ICPF.	
D2.2	**Assessment of the previous research objectives and their achievement**
Determined by external funding and cooperations.	
D2.3	**Assessment of implementation of recommendations from past evaluation**
n/a department was founded in 2018.	
D2.4	**Success in receiving grants**
Adequate	
D2.5	**Adequacy of instrumental equipment**
Currently adequate. In the long term, a mid-range compute cluster will become necessary.	

D2.6	Effectiveness of management
Has failed completely to integrate the Department into ICPF as a whole.	
D2.7	**Assessment of professional structure, development strategy and the strategy of keeping best scientists, age structure, career and qualification growth**
Two young and promising researchers, no females.	
D2.8	**Creating work-life balance conditions, assessment of approach towards possible gender issues**
No females in research positions. Not unusual for a modelling department but needs attention	
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.**
N/a	

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.	
D3.2	**Effectiveness of joint research centres**
N/a	
D3.3	**Success rate in supervision of PhD students**
Adequate	
D3.4	**Participation of PhD students in the outputs**
Students participate well	
D3.5	**Participation of the team in master or bachelor studies**
Average	
D3.6	**Assessment of cooperation intensity with universities in the form of teaching**
Quite high	

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

D4.1	Sufficiency of media strategy and activities in the area of research popularisation
None.	
D4.2	**Publishing activities and its quality**
None	

D4.3	Participation in professional organisations in the area of research and development
None	

Other comments of the commission:

See also comments made in Part A (Evaluation of the institute).
The M&S resources within ICPF are being wasted. Not only has Department 7 no real connection to ICPF but M&S groups in the engineering Departments also have no direct relationship to Department 7.

The commission recommends that all M&S activities within ICPF be bundled in one group that bridges all modelling scales and that this group be given the specific capacity to

(a) Cover simulation scales not currently treated by the existing groups
(b) Provide the manpower to support the engineering groups with interpretational and predictive simulations

In order to establish this group, the leadership of both the M&S activities and of ICPF itself must grasp the importance of a powerful simulation capability within the Institute and proactively work towards establishing such a group.

The commission notes that the suggested flat organisational structure with tenure track for young researchers would be ideal for Department 7.

8. Department of Laser Chemistry

Strengths:
- Laser-based services

Weaknesses:
- Research topics are diverse and unfocussed
- No outstanding ideas

Opportunities:
- Separate service and research, move research to more appropriate CAS Institutes

Threats:
- Loss of identity from conflict between service and research
- Instrumentation becomes outdated

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

H1.1	**Quality of selected outputs of Phase I**
Adequate: Specialised subjects generally published in specialist journals	
H1.2	**Contribution of workers on the outputs reached**
Variable: ICPF researchers seldom play a leading role	
H1.3	**Quality of all outputs and results**
Adequate, in specialist journals	
H1.4	**The most valuable discoveries and findings in the fields, their importance for the field**
Fenton chemistry, if at all.	
H1.5	**Contribution of the participation of the authors in large collaborations**
None	

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

H2.1	**Societal relevance of outputs and results pursuant to CAS and institute mission**
Adequate in a service context	
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**
Adequate in a service context	
H2.3	**Relation to practice**
Adequate in a service context	

H2.4	Participation in AV21 strategy
N/a	
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
Very low profile.	
D1.2	**Scope and quality of international and national cooperation and the role of the team in such cooperation; engagement in broad international cooperation**
Adequate	
D1.3	**Participation of the workers in scientific community activities (organizing of conferences and workshops, invited lectures, awards)**
Adequate	

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

D2.1	Direction in line with the perspective of the planned research directions
Unfocussed.	
D2.2	**Assessment of the previous research objectives and their achievement**
Unfocussed.	
D2.3	**Assessment of implementation of recommendations from past evaluation**
The 2018 reforms have not improved the situation	
D2.4	**Success in receiving grants**
Adequate	
D2.5	**Adequacy of instrumental equipment**
Apparently functional	
D2.6	**Effectiveness of management**
Poor	
D2.7	**Assessment of professional structure, development strategy and the strategy of keeping best scientists, age structure, career and qualification growth**
Poor	
D2.8	**Creating work-life balance conditions, assessment of approach towards possible gender issues**
Poor	

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.
N/a	

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
Nationally good, internationally at a minimal functional level	
D3.2	**Effectiveness of joint research centres**
n/a	
D3.3	**Success rate in supervision of PhD students**
Low activity	
D3.4	**Participation of PhD students in the outputs**
Low	
D3.5	**Participation of the team in master or bachelor studies**
None	
D3.6	**Assessment of cooperation intensity with universities in the form of teaching**
None	

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

D4.1	Sufficiency of media strategy and activities in the area of research popularisation
Poor, only open days	
D4.2	**Publishing activities and its quality**
Low, only refereeing	
D4.3	**Participation in professional organisations in the area of research and development**
Low	

Other comments of the commission:

See also comments made in Part A (Evaluation of the institute).
The department suffers, like many such Departments in CAS Institutes, under the combination of service tasks with original research. Particularly the latter appears uncoordinated and corresponds to the personal interests of the researchers involved. The research projects of the Department have little to do with the aims and direction of the Institute as a whole. It is difficult to find any justification for the Department being part of ICPF except for its service function. We suggest that it, together with Analytical Chemistry services, be converted into a 100% service Department and that the research activities would be more appropriate in other CAS Institutes.

9. Group of Advanced Materials and Organic Synthesis

Strengths:
- Competent synthesis capacity

Weaknesses:
- Unfocussed applications
- Reliance on external biological and medical testing

Opportunities:
- Move to a more compatible environment than ICPF

Threats:
- Isolation within a predominantly engineering environment
- Diffuse application goals lead to even more loss of identity

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

H1.1	**Quality of selected outputs of Phase I**
Average: No highlights but solid results	
H1.2	**Contribution of workers on the outputs reached**
Variable: ICPF researchers seldom play a leading role	
H1.3	**Quality of all outputs and results**
Average: No highlights but solid results	
H1.4	**The most valuable discoveries and findings in the fields, their importance for the field**
Advances in helicene chemistry	
H1.5	**Contribution of the participation of the authors in large collaborations**
Only a COST action	

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

H2.1	**Societal relevance of outputs and results pursuant to CAS and institute mission**
Difficult to see any high relevance: The research is still very fundamental	
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**
N/a	
H2.3	**Relation to practice**
Very indirect	

H2.4	Participation in AV21 strategy
N/a	
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
Solid synthesis in a niche area	
D1.2	**Scope and quality of international and national cooperation and the role of the team in such cooperation; engagement in broad international cooperation**
Low activity and visibility	
D1.3	**Participation of the workers in scientific community activities (organizing of conferences and workshops, invited lectures, awards)**
Low	

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

D2.1	Direction in line with the perspective of the planned research directions
Research directed by the methodology and compound-type with which the group feels comfortable, rather than allowing the research goals to dictate the methodology. (i.e. No research driven by an inspirational end-goal).	
D2.2	**Assessment of the previous research objectives and their achievement**
N/a The Department was formed in 2018	
D2.3	**Assessment of implementation of recommendations from past evaluation**
The 2018 reform has produced a Department that is struggling. It is difficult to see the purpose of the 2018 reform.	
D2.4	**Success in receiving grants**
Too low	
D2.5	**Adequacy of instrumental equipment**
Low level of financing	
D2.6	**Effectiveness of management**
They are doing their best under difficult conditions.	
D2.7	**Assessment of professional structure, development strategy and the strategy of keeping best scientists, age structure, career and qualification growth**
The department seems to be in survival mode.	

D2.8	Creating work-life balance conditions, assessment of approach towards possible gender issues
As throughout ICPF, serious issues and no modern gender-equality strategy.	
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.**
N/a	

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
Adequate	
D3.2	**Effectiveness of joint research centres**
N/a	
D3.3	**Success rate in supervision of PhD students**
Adequate	
D3.4	**Participation of PhD students in the outputs**
Adequate	
D3.5	**Participation of the team in master or bachelor studies**
None to low	
D3.6	**Assessment of cooperation intensity with universities in the form of teaching**
Low	

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

D4.1	Sufficiency of media strategy and activities in the area of research popularisation
Only open days	
D4.2	**Publishing activities and its quality**
None	
D4.3	**Participation in professional organisations in the area of research and development**
Moderate	

Other comments of the commission:

See also comments made in Part A (Evaluation of the institute).
The commission saw little connection between the research carried out by the group and the aims and goals of ICPF. Other CAS Institutes have interests far closer to those of the Department than ICPF. This leads to apparent isolation and lack of purpose. Note that the commission considers this to be an organisational weakness that is probably evident elsewhere within CAS. A complete review of the research carried out by CAS as a whole and of that situated in the individual Institutes is needed. This cannot be achieved within the current review process as the individual commissions often, as in the present case of the ICPF, do not even have a complete overview of the activities of the Institute. If it continues in its current form, the Department must receive adequate funding unless it is to remain crippled. It has not been successful enough in receiving external funding.

10. SuperCritical Technologies Group

Strengths:
The young team has a broad expertise in high pressure applications ranging from fundamental research in modelling extraction processes to applied research in development of extraction procedures for specific compounds as well as their downstream processing. The lab is well equipped and collaborates with national and international universities and research institutes. The outreach activities are very good, especially in the field of popularisation.

Weaknesses:
Currently, the group is too small to form a critical mass of knowledge which is needed to lead the research in one field in Europe. Scientific leadership and project management qualities are not sufficiently represented in the current structure. The group is only minor involved in teaching.

Opportunities:
The research addresses emerging fields such as bioactive substances from natural products or the use of environmental-friendly solvents. More collaborations with industry are possible due to the well-suited experimental unique equipment.

Threats:
The output of the team is dependent on few leading individuals. Maternity leaves or professional reorientation of team members might be a serious threat for the successful continuation of the group. The group may grow with further projects, however, these less long-term projects may hinder to keep experienced junior researchers in the group. The small contact with students may cause a lack of bachelor and master students as well as graduated students interested in starting a PhD and working at the department.

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

H1.1	Quality of selected outputs of Phase I
The group performs internationally visible research in the field of supercritical technology with focus on using scCO2 for extraction and fractioning processes as well as extract conditioning. The quality of the outputs of Phase I are good and in the average of this field.	
H1.2	**Contribution of workers on the outputs reached**
The members of the group mainly contributed to the outputs reached, i.e. 4 of the 5 evaluated papers have a share of 67% and above. Therefore, the contribution is good.	
H1.3	**Quality of all outputs and results**
The quality of all outputs was evaluated by analysing the categorisation according to the journal ranking. In this evaluation, three out of five selected outputs were in the second quartile whereas the average of all outputs is uniformly distributed around the third quartile. The quality of the outputs is good.	
H1.4	**The most valuable discoveries and findings in the fields, their importance for the field**
Valuable discoveries cover the development of methods and procedures for extraction of bio-active substances from plants including the processing of extracts as well as new routes to manufacture nanostructured metal oxides as well as polymer foams.	

H1.5	Contribution of the participation of the authors in large collaborations
Not applicable.	

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

H2.1	Societal relevance of outputs and results pursuant to CAS and institute mission
The research of the group follows the institute's mission and has a very good level of societal relevance with contributions in the following fields: botanical pesticides, environmentally friendly solvents, as well as novel materials from plant waste.	
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 group well transfers its knowledge into practise in terms of collaborations with industry. In this context, the team members perform custom extractions or optimise extraction conditions for various substances.	
H2.3	**Relation to practice**
The group is partly able to transfer its research into practical applications leading to at least one patent and several projects with companies such as ASIPO, MikroChem LKT, Kanebos, xMed21, Algamo among others.	
H2.4	**Participation in AV21 strategy**
The research of the group fits into the programmes Foods for the Future of the AV21 strategy. One researcher is part of the popularisation group of AV21 strategy.	
H2.5	**Cooperation with regions of the Czech Republic**
The department is active in selected regions of Czech Republic.	

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 scientists of the group perform solid research focusing on fundamental knowledge in terms of process understanding and modelling as well as on industrial application in terms of process optimisation as well as new products. The performance is good in comparison with similar international and national institutes.	
D1.2	**Scope and quality of international and national cooperation and the role of the team in such cooperation; engagement in broad international cooperation**
Respecting the size of the group, the group is rather active on an international level. In this context joint projects, exchange of staff, and teaching with groups in Austria, Bulgaria, Germany, Slovenia, Portugal as well as coordinating one subgroup of a cost action with partners in 21 countries is applauded by the commission. The role in these projects are of theoretical as well as experimental nature. Overall, scope and quality are good.	

D1.3	Participation of the workers in scientific community activities (organizing of conferences and workshops, invited lectures, awards)
The researchers of the group participate in activities of the scientific community by organizing specialised symposia in the frame of CHISA in 2016 and 2018 and gave lectures at a European summer school or after invitations from three different institutions.	

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 activity plan of the group involves the process development for the complex processing of valuable natural materials containing health promoting substances or biological active compounds. Together with the experience in downstream processing of the extracts, this forms a promising niche of research with emerging industrial and societal impact.	
D2.2	**Assessment of the previous research objectives and their achievement**
Not applicable.	
D2.3	**Assessment of implementation of recommendations from past evaluation**
Not applicable.	
D2.4	**Success in receiving grants**
Respecting the small size, the group is rather successful in acquiring grants mainly from GACR, MIT and partially from TACR. In total about 450 thousand Euro were received in the considered period. However, the impact of contractual research is rather small (7 thousand Euro) which should be exploited more intensively also in the context of future applied research projects funded by TACR.	
D2.5	**Adequacy of instrumental equipment**
The group owns and runs adequate and comparably rare state-of-the-art equipment. It is suggested to further invest in technology to obtain a leading position in Europe.	
D2.6	**Effectiveness of management**
Although maternity leaves of the team leader and researchers, the group managed to be effective in research and publication.	
D2.7	**Assessment of professional structure, development strategy and the strategy of keeping best scientists, age structure, career and qualification growth**
The group consists only of researchers with ages below 45 except one emeritus. It is suggested to support the group with professional mentoring in scientific leadership, career development and project management as well as design thinking.	
D2.8	**Creating work-life balance conditions, assessment of approach towards possible gender issues**
Parental leave and part-time jobs are elementary parts of the gender-balanced group. However, this creates also risks in the continuity of research because of the small size of the group. The group could hold a former PhD as postdoc after graduation which might be an indicator for a harmonious work-live-balance.	

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.
Not applicable.	

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
The group is engaged in teaching at UCT Prague as well as was actively supporting an European summer school.	
D3.2	**Effectiveness of joint research centres**
The group joins the COST Action of Green Chemical Engineering Network towards upscaling sustainable processes. It is not possible to evaluate the effectiveness.	
D3.3	**Success rate in supervision of PhD students**
In the examination period, one PhD finished his thesis and other plans to finish in 2020.	
D3.4	**Participation of PhD students in the outputs**
PhD students intensively participate in the outputs of the department, e.g. articles, conference contributions, function samples, and proven technologies.	
D3.5	**Participation of the team in master or bachelor studies**
Only, two bachelor students joined the research team during the examination period which could be caused also by the limiting teaching activity of the group.	
D3.6	**Assessment of cooperation intensity with universities in the form of teaching**
The team is only minor involved in student education at UCT Prague within Czech Republic.	

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

D4.1	Sufficiency of media strategy and activities in the area of research popularisation
The department frequently shows various activities in public outreach for audiences with different backgrounds from Czech Republic and abroad, e.g. open lab days also for kids from kindergarten as well as students from high school besides attending and supporting events such as Science Festival, Science Expo, Week of Science among others.	
D4.2	**Publishing activities and its quality**
Besides the intense popularisation activities for kids and young students, there are no publication activities mentioned aiming on the popularisation of research.	
D4.3	**Participation in professional organisations in the area of research and development**

The head of the group is one Czech representative of the EFCE Working Party on High Pressure Technology, which is excellent.

Other comments of the commission:

The commission recommends to expand the collaborations with industry. The available unique state-of-the-art equipment is seen as an excellent starting point to work to attract research grants and industry funds. The teaching activities of the group should be expanded to attract potential bachelor, master and PhD students for this rather small field of research. The team is comparably small which makes it difficult to form a critical mass needed to dominate a specific area of research within Europe. The extraction of health-promoting or biological active substances might be one promising direction that should be further strengthened.

11. Department of Bioorganic Compounds and Nanocomposites

Strengths:
- Competent synthesis capacity
- Expertise in dendron chemistry

Weaknesses:
- Lack of definition within ICPF

Opportunities:
- Move to a more compatible environment than ICPF

Threats:
- Isolation within a predominantly engineering environment
- Diffuse application goals lead to even more loss of identity

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

H1.1	**Quality of selected outputs of Phase I**
Average: Competent synthesis as the Department's major contribution	
H1.2	**Contribution of workers on the outputs reached**
See H 1.1	
H1.3	**Quality of all outputs and results**
Average: Competent synthesis as the Departments major contribution	
H1.4	**The most valuable discoveries and findings in the fields, their importance for the field**
Providing candidate molecules to medical/biological teams elsewhere	
H1.5	**Contribution of the participation of the authors in large collaborations**
ICPF researchers seldom play a leading role.	

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

H2.1	**Societal relevance of outputs and results pursuant to CAS and institute mission**
Possibly important as part of large medical/biological teams	
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**
Probably depends largely on the cooperation partners	
H2.3	**Relation to practice**
Probably depends largely on the cooperation partners	

H2.4	Participation in AV21 strategy
N/a	
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
Solid synthetic group but without highlights	
D1.2	**Scope and quality of international and national cooperation and the role of the team in such cooperation; engagement in broad international cooperation**
ICPF researchers seldom play a leading role	
D1.3	**Participation of the workers in scientific community activities (organizing of conferences and workshops, invited lectures, awards)**
Low activity	

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

D2.1	Direction in line with the perspective of the planned research directions
Research directed by the methodology and compound-type with which the group feels comfortable. Planned research directions are those that fit the type of compound available, rather than being goal-oriented.	
D2.2	**Assessment of the previous research objectives and their achievement**
Compounds have been made and tested but the goals should be higher.	
D2.3	**Assessment of implementation of recommendations from past evaluation**
The 2018 reform has brought together researchers from three different previous Departments. It has not produced a focussed and relevant team within ICPF. The current team would be far more comfortable in other CAS Institutes.	
D2.4	**Success in receiving grants**
Average	
D2.5	**Adequacy of instrumental equipment**
Apparently adequate	
D2.6	**Effectiveness of management**
Poor: No unified Departmental direction is discernible.	
D2.7	**Assessment of professional structure, development strategy and the strategy of keeping best scientists, age structure, career and qualification growth**

The Department seems to be in survival mode.	
D2.8	**Creating work-life balance conditions, assessment of approach towards possible gender issues**
As throughout ICPF, serious issues and no modern gender-equality strategy.	
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.**
N/a	

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**
Adequate	
D3.2	**Effectiveness of joint research centres**
n/a	
D3.3	**Success rate in supervision of PhD students**
Adequate	
D3.4	**Participation of PhD students in the outputs**
Low activity	
D3.5	**Participation of the team in master or bachelor studies**
Masters low; bachelors higher	
D3.6	**Assessment of cooperation intensity with universities in the form of teaching**
Adequate	

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

D4.1	**Sufficiency of media strategy and activities in the area of research popularisation**
Low activity	
D4.2	**Publishing activities and its quality**
Low activity	
D4.3	**Participation in professional organisations in the area of research and development**
Some conferences organised and some refereeing/editing activity	

Other comments of the commission:

The commission saw little connection between the research carried out by the group and the aims and goals of ICPF. Other CAS Institutes have interests far closer to those of the Department than ICPF. This leads to apparent isolation and lack of purpose. Note that the commission considers this to be an organisational weakness that is probably evident elsewhere within CAS. A complete review of the research carried out by CAS as a whole and of that situated in the individual Institutes is needed. This cannot be achieved within the current review process as the individual commission often, as in the present case of the ICPF, do not even have a complete overview of the activities of the Institute.

Top 10 Publications of the evaluated teams

5. Department of Analytical Chemistry (5)

1. BLECHTA, Vratislav, SÝKORA, Jan. Proton Detection of Carbon-Carbon Couplings in Symmetrical Molecules: Analytical Explanation, SYMONA Pulse Sequence. *Journal of Magnetic Resonance* **2019**, *298*(JAN 2019), 107-114. 10.1016/j.jmr.2018.12.002 (Q2, 1 citation)

   This is our first publication devoted to the measurement of one-bond indirect spin-spin coupling constants between equivalent nuclei.

2. BLECHTA, Vratislav, SÝKORA, Jan. STRONG INADEQUATE, an Experiment for Detection of Small J(C,C) Couplings in Symmetrical Molecules. *Magnetic Resonance in Chemistry* **2019**, *57*(12), 1107-1120. 10.1002/mrc.4897 (Q2, 3 citations)

   This publication is the second in a row dedicated to the determination of the NMR couplings between equivalent carbon atoms, mainly focused on small interactions between atoms separated in the molecule by several bonds.

3. MICHÁLKOVÁ, Lenka, HORNÍK, Štěpán, SÝKORA, Jan, HABARTOVÁ, L., SETNIČKA, V. Diagnosis of Pancreatic Cancer via 1H NMR Metabolomics of Human Plasma. *Analyst* **2018**, *143*(24), 5974-5978. 10.1039/c8an01310a (Q1, 6 citations)

   This is our first publication on metabolomics. This is a pilot study performed on a very small cohort. Encouraged by the results, further study is ongoing. The publication was prepared solely by the team. However, the correspondence stayed in the team which provided the blood plasma samples.

4. CUŘÍNOVÁ, Petra, DRAČÍNSKÝ, Martin, JAKUBEC, Martin, TLUSTÝ, M., JANKŮ, K., IZÁK, Pavel, HOLAKOVSKÝ, R. Enantioselective Complexation of 1-Phenylethanol with Chiral Compounds Bearing Urea Moiety. *Chirality* **2018**, *30*(6), 798-806. 10.1002/chir.22855 (Q3, 4 citations)

   The investigation of urea-based receptors with special effort to chiral ones is a target of Dr. Cuřínová for almost 15 years. This publication is providing insight into the internship between the structure of the solvating agent and its ability to form diastereomeric complexes with sufficiently distant signals.

5. CUŘÍNOVÁ, Petra, HÁJEK, P., JANKŮ, K., HOLAKOVSKÝ, R. 5. Method for Determination of Optical Purity of 2-Arylpropanoic Acids Using Urea Derivatives Based on a 1,1′-Binaphthalene Skeleton as Chiral NMR Solvating Agents: Advantages and Limitations Thereof. *Chirality* **2019**, *31*(5), 410-417. 10.1002/chir.23067 (Q3, 3 citations)

   In this publication, the previously used design of the NMR shifting agent was extended to a series of receptors capable of controlling the enantiomeric purity of aryl propanoic acids (profens). Profens, widely known as nonsteroidal anti-

inflammatory drugs, are mostly used in racemic mixtures, despite their target pharmacological effect residing in the (S)-enantiomer only.

6. CUŘÍNOVÁ, Petra, KRUPKOVÁ, Alena, ČERVENKOVÁ ŠŤASTNÁ, Lucie, MÜLLEROVÁ, Monika, ČERMÁK, Jan, STRAŠÁK, Tomáš. ESI-TOF Mass Spectrometry of Cationic Carbosilane Dendrimers: a Potent Tool for Characterization of Structural Defects. *Journal of Mass Spectrometry* **2018**, *53*(10), 986-996. 10.1002/jms.4269 (Q3, 1 citation)

   This method was originally developed as a part of our service activities as the synthesis and testing of dendrimers is one of the topics in ICPF. As this method provided a potent tool to find even minor levels of the corresponding defect as well as to trace the quality of anion exchange, we found it to be useful for common use.

7. HEJTMÁNEK, Vladimír, DRAČÍNSKÝ, Martin, SÝKORA, Jan. A Preview of a Construction of a Crystal Lattice Based on Intermolecular Interactions. *Crystals* **2019**, *9*(3), 159. 10.3390/cryst9030159 (Q2, 0 citation)

   This publication describes a general procedure of crystal packing reconstruction using a certain number of intermolecular interactions that can be provided by solid-state NMR spectroscopy. This is an alternative approach to crystal structure elucidation when standard crystallographic techniques cannot be applied. This approach could be an alternative to NMR crystallography which used brutal computational force to solve the crystal structure.

8. DRAČÍNSKÝ, Martin, STORCH, Jan, CÍRKVA, Vladimír, CÍSAŘOVÁ, I., SÝKORA, Jan. Internal dynamics in helical molecules studied by X-ray diffraction, NMR spectroscopy and DFT calculations. *Physical Chemistry Chemical Physics* **2017**, *19*(4), 2900-2907. 10.1039/c6cp07552e (Q1, 14 citations)

   This paper brings a unique description of the dynamic properties of [6]helicene molecules. The original idea of molecular dynamics study and X-ray part was done here. Therefore, one of the paper correspondences belongs to the team member.

9. JAKUBEC, Martin, BERÁNEK, Tomáš, JAKUBÍK, Pavel, SÝKORA, Jan, ŽÁDNÝ, Jaroslav, CÍRKVA, Vladimír, STORCH, Jan. 2-Bromo[6]helicene as a Key Intermediate for [6]Helicene Functionalization. *Journal of Organic Chemistry* **2018**, *83*(7), 3607-3616. 10.1021/acs.joc.7b03234 (Q1, 12 citations)

   The data sorting, analysis, and direction of the final experiments was done here as well as a logical structure and a final shape of the publication. Therefore, the paper correspondence belongs to the team member.

10. CÍRKVA, Vladimír, JAKUBÍK, Pavel, STRAŠÁK, Tomáš, HRBÁČ, J., SÝKORA, Jan, CÍSAŘOVÁ, I., VACEK, J., ŽÁDNÝ, Jaroslav, STORCH, Jan.

Preparation and Physicochemical Properties of [6]Helicenes Fluorinated at Terminal Rings. *Journal of Organic Chemistry* **2019**, *84*(4), 1980-1993. 10.1021/acs.joc.8b02870 (Q1, 9 citations)

The data sorting, analysis, and direction of the final experiments was done by the team member. Besides the discussion of NMR and X-ray data, the final shape of the publication was also done here. Therefore, one of the paper correspondences belongs to the team member.

7. Department of Molecular and Mesoscopic Modelling

1. MALIJEVSKÝ, Alexandr, PARRY, A.O. Modified Kelvin Equations for Capillary Condensation in Narrow and Wide Grooves. *Physical Review Letters* **2018**, *120*(13), 135701. 10.1103/PhysRevLett.120.135701 (Q1*, 5 citations)
2. LÍSAL, Martin, LIMPOUCHOVÁ, Zuzana, PROCHÁZKA, Karel. *Physical Chemistry Chemical Physics* **2016**, *18*(JUN 28), 16127-16136. 10.1039/c6cp00341a (Q1, 24 citations)
3. MOUČKA, Filip, SVOBODA, Martin, LÍSAL, Martin. Modelling Aqueous Solubility of Sodium Chloride in Clays at Thermodynamic Conditions of Hydraulic Fracturing by Molecular Simulations. *Physical Chemistry Chemical Physics* **2017**, *19*(JUL 7), 16586-16599. 10.1039/c7cp02121f (Q1, 14 citations)
4. SVOBODA, Martin, MOUČKA, Filip, LÍSAL, Martin. Saturated aqueous NaCl solution and pure water in Na- montmorillonite clay at thermodynamic conditions of hydraulic fracturing: Thermodynamics, structure and diffusion from molecular simulations. *Journal of Molecular Liquids* **2018**, *271*(DEC 1), 490-500. 10.1016/j.molliq.2018.08.144 (Q1, 8 citations)
5. MALIJEVSKÝ, Alexandr, PARRY, A.O., POSPÍŠIL, M. Scaling Behavior of Thin Films on Chemically Heterogeneous Walls. *Physical Review E* **2017**, *96*(3), 032801. 10.1103/PhysRevE.96.032801 (Q1, 6 citations)
6. MALIJEVSKÝ, Alexandr. Geometry-induced Interface Pinning at Completely Wet Walls. *Physical Review E* **2019**, *99*(4), 040801. 10.1103/PhysRevE.99.040801 (Q1, 4 citations)
7. SVOBODA, Martin, MALIJEVSKÝ, Alexandr, LÍSAL, Martin. Wetting Properties of Molecularly Rough Surfaces. *Journal of Chemical Physics* **2015**, *143*(10), 104701. 10.1063/1.4930084 (Q2, 18 citations)
8. REZLEROVÁ, Eliška, ZUKAL, Arnošt, ČEJKA, Jiří, SIPERSTEIN, F.R., BRENNAN, J.K., LÍSAL, Martin. Adsorption and Diffusion of C1 to C4 Alkanes in Dual-Porosity Zeolites by Molecular Simulations. *Langmuir* **2017**, *33*(42), 11126-11137. 10.1021/acs.langmuir.7b01772 (Q2, 14 citations)
9. LÍSAL, Martin, LARENTZOS, J.P., SELLERS, M.S., SCHWEIGERT, I.V., BRENNAN, J.K. Dissipative Particle Dynamics with Reactions: Application to RDX Decomposition. *Journal of Chemical Physics* **2019**, *151*(11), 114112. 10.1063/1.5117904 (Q2, 6 citations)
10. DOČKAL, J., MOUČKA, F., LÍSAL, Martin. Molecular Dynamics of Graphene-Electrolyte Interface: Interfacial Solution Structure and Molecular Diffusion. *Journal of Physical Chemistry C* **2019**, *123*(43), 26379-26396. 10.1021/acs.jpcc.9b07487 (Q2, 5 citations)

8. Department of Laser Chemistry

1. CHERNEV, I.M., SHEVLYAGIN, A.V., GALKIN, K.N., STUCHLÍK, Jiří, REMEŠ, Zdeněk, FAJGAR, Radek, GALKIN, N.G. On the way to enhance the optical absorption of a-Si in NIR by embedding Mg2Si thin film. *Applied Physics Letters* **2016**, *109*(4), 043902. 10.1063/1.4960011 (Q1, 9 citations)

   The paper is a result of a broad cooperation with Institute of Physics, CAS, and Russian Academy of Sciences in the field of preparation of photovoltaic materials with increased absorption in near infra-red region.

2. JANDOVÁ, Věra, POKORNÁ, Dana, KUPČÍK, Jaroslav, DYTRYCH, Pavel, CUŘÍNOVÁ, Petra, FAJGAR, Radek, POLA, Josef. Infrared Laser Radiation-Produced TiO-doped Si/SiOx/SiO2 Nanocomposite – Entry to TiO- containing Materials. *Journal of Photochemistry and Photobiology A-Chemistry* **2017**, *332*(JAN 1), 376-383. 10.1016/j.jphotochem.2016.09.019 (Q2, 7 citations)

   Novel type of photocatalysts is introduced, activity is demonstrated by Vis decomposition of methylene blue dye.

3. DŘÍNEK, Vladislav, KLEMENTOVÁ, Mariana, FAJGAR, Radek, DYTRYCH, Pavel. Silicon Nanowires Grown on Metal Substrates via Self-Catalyst Mechanism. *Materials Letters* **2015**, *160*(DEC 1), 109-112. 10.1016/j.matlet.2015.07.098 (Q2, 4 citations)

   Our first publication on formation of Si NW growth. Unique self-catalyst mechanism is described.

4. BAKARDJIEVA, Snejana, MAREŠ, Jakub, FAJGAR, Radek, ZENOU, Victor Y., MALEČKOVÁ, Michaela, CHATZISYMEON, Efthalia, BIBOVÁ, Hana, JIRKOVSKÝ, Jaromír. The relationship between microstructure and photocatalytic behavior in lanthanum-modified 2D TiO2 nanosheets upon annealing of a freeze-cast precursor. *RSC Advances* **2019**, *9*(40), 22988-23003. 10.1039/c9ra03940f (Q2, 1 citation)

   The complex study of photochemical behavior of TiO2/La nanostructured material. Broad range of technics were applied to describe the material and UV photochemical study was accomplished in our Department.

5. DŘÍNEK, Vladislav, KLEMENTOVÁ, Mariana, PALATINUS, Lukáš, DYTRYCH, Pavel, FAJGAR, Radek, JANDOVÁ, Věra, KOŠTEJN, Martin, KUPČÍK, Jaroslav. Synthesis and characterization of nanostructured molybdenum oxynitride films fabricated by sub-atmospheric chemical vapor deposition. *Journal of Alloys and Compounds* **2019**, *808*(NOV 5), 151470. 10.1016/j.jallcom.2019.07.182 (Q2, 1 citation)

   Molybdenum oxynitride nanostructures were deposited, characterized and photochemical splitting of water was demonstrated by photoelectrochemical measurements.

6. DŘÍNEK, Vladislav, REMEŠ, Zdeněk, KLEMENTOVÁ, Mariana, PALATINUS, Lukáš, JAROŠOVÁ, Markéta, LUGSTEIN, A., SISTANI, M., KOŠTEJN, Martin, JANDOVÁ, Věra, FAJGAR, Radek. Ytterbium silicide nanostructures prepared by pulsed laser ablation in oven: Structural and electrical characterization. *Materials Letters* **2019**, *246*(JUL 1), 17-19. 10.1016/j.matlet.2019.03.032 (Q2, 0 citation)

   The first paper on preparation of Si/Yb. The single nanostructure was successfully,electrically contacted and conductivity measurements were performed.

7. KOŠTEJN, Martin, FAJGAR, Radek, DYTRYCH, Pavel, KUPČÍK, Jaroslav, DŘÍNEK, Vladislav, JANDOVÁ, Věra, HUBER, Š., NOVOTNÝ, F. Characterization of thin MnSi and MnGe Layers Prepared by Reactive UV Pulsed Laser Deposition. *Thin Solid Films* **2016**, *619*(NOV 30), 73-80. 10.1016/j.tsf.2016.10.035 (Q3, 2 citations)

   PLD is demonstrated as a technique for preparation of highly concentrated Mn nanoparticles in silicon or germanium matrix. Unique ferromagnetic properties were presented here.

8. JANDOVÁ, Věra, FAJGAR, Radek, DYTRYCH, Pavel, KOŠTEJN, Martin, DŘÍNEK, Vladislav, KUPČÍK, Jaroslav. Reactive laser-induced ablation as approach to titanium oxycarbide films. *Thin Solid Films* **2015**, *590*(SEP 1), 270-275. 10.1016/j.tsf.2015.07.052 (Q3, 2 citations)

   Unique approach to thin titanium oxycarbide layers was demonstrated – frozen titanium ethoxide target was ablated in presence of gaseous methane.

9. MAMOŇ, Filip, FAJGAR, Radek, JANDOVÁ, Věra, KOČÍ, Eva, JAKUBEC, Ivo, ZHIGUNOV, Alexander, BROVDYOVÁ, T., BAKARDJIEVA, Snejana. TiO2 microrods with stacked 3D nanovoids for photoelectrochemical water splitting. *Pure and Applied Chemistry* **2019**, *91*(11), 1733-1747. 10.1515/pac- 2018-1116 (Q3, 0 citation)

   Unique TiO2 nanostructures were fixed on a FTO glass electrodes based on zeta-potential measurements. The material was demonstrated as efficient, low-cost and promising for water splitting.

10. DŘÍNEK, Vladislav, KŘENEK, Tomáš, KLEMENTOVÁ, Mariana, FAJGAR, Radek, POLA, Michal, SAVKOVÁ, Jarmila, MEDLÍN, Rostislav, NOVOTNÝ, Filip. Formation of Cu1-xGex Nanoplatelets Using LPCVD of Ge2Me6 or Ge2Me6/Et4Pb Mixture. *NANO: Brief Reports and Reviews* **2015**, *10*(4), 1550061. 10.1142/S1793292015500617 (Q4, 0 citation)

    Novel unique, extremely flat nanoplatelets were grown and characterized. Recently we have focused on the material due to optical properties and ability to reduce CO2 to form C2-C3 organic molecules.

9. Group of Advanced Materials and Organic Synthesis

1. STORCH, Jan, ŽÁDNÝ, Jaroslav, STRAŠÁK, Tomáš, KUBALA, M., SÝKORA, Jan, DUŠEK, Michal, CÍRKVA, Vladimír, MATĚJKA, P., KRBAL, M., VACEK, J. Synthesis and Characterization of a Helicene-Based Imidazolium Salt and Its Application in Organic Molecular Electronics. *Chemistry - A European Journal* **2015**, *21*(6), 2343-2347. 10.1002/chem.201405239 (Q1, 42 citations)

   In terms of significance, this is our first publication of helicene application in the field organic molecular electronics. The prepared racemic 1-butyl-3-(2-methyl[6]helicenyl) imidazolium bromide was immobilized onto a SiO2 substrate and used for the construction of a fully reversible humidity sensor. These findings have enabled us further applied research in the field of humidity sensor exploitation.

2. KALACHYOVA, Y., GUSELNIKOVA, O., ELASHNIKOV, R., PANOV, Illia, ŽÁDNÝ, Jaroslav, CÍRKVA, Vladimír, STORCH, Jan, SÝKORA, Jan, ZÁRUBA, K., ŠVORČÍK, V., LYUTAKOV, O. Helicene-SPP Based Chiral Plasmonic Hybrid Structure: Toward Direct Enantiomers SERS Discrimination. *ACS Applied Materials and Interfaces* **2019**, *11*(1), 1555-1562. 10.1021/acsami.8b15520 (Q1, 20 citations)

   The initial study concerns on fabrication of chiral plasmon substrates based on surface plasmon-polariton- supported structure coupled with optically active helicene enantiomers. The work is essential in the field of helicene based plasmon sensors. Method allows enantioselective detection with detection limits below the limits of standard spectral techniques and serves as a proof-of-concept for further applications. Based on these results we have successfully received grant funding (2021 – 2025) from Ministry of Interior.

3. VACEK, J., HRBÁČ, J., STRAŠÁK, Tomáš, CÍRKVA, Vladimír, SÝKORA, Jan, FEKETE, Ladislav, POKORNÝ, Jan, BULÍŘ, Jiří, HROMADOVÁ, Magdaléna, CRASSOUS, J., STORCH, Jan. Anodic Deposition of Enantiopure Hexahelicene Layers. *ChemElectroChem* **2018**, *5*(15), 2080-2088. 10.1002/celc.201800565 (Q2, 8 citations)

   The study deals with electrochemical preparation of polymeric layers of carbo[n]helicenes (n=5,6,7) using cyclic voltammetry. The benefit is that the anodic deposition of chiral P and M enantiomers of [6]helicene leads to the formation of enantiopure polymeric layers on ITO glass as confirmed by CD. The new electrodeposited layers are being used in our group for further development of materials applicable in organic electronics and sensing technologies.

4. HRBÁČ, J., STRAŠÁK, Tomáš, FEKETE, Ladislav, LADÁNYI, V., POKORNÝ, Jan, BULÍŘ, Jiří, KRBAL, M., ŽÁDNÝ, Jaroslav, STORCH, Jan, VACEK, J. Potential-Driven On/Off Switch Strategy for the Electrosynthesis of [7]Helicene-Derived Polymers. *ChemElectroChem* **2017**, *4*(12), 3047-3052. 10.1002/celc.201700441 (Q2, 6 citations)

This work relates to electropolymerization of 3-([7]helicen-9-yl)-thiophene using cyclic voltammetry. The main success was the preparation of conductive and non-conductive polymers by a potential-driven on/off switch strategy. The new electrodeposited layers are being used in our group for further development of materials applicable in organic electronics and sensing technologies.

5. JAKUBEC, Martin, BERÁNEK, Tomáš, JAKUBÍK, Pavel, SÝKORA, Jan, ŽÁDNÝ, Jaroslav, CÍRKVA, Vladimír, STORCH, Jan. 2-Bromo[6]helicene as a Key Intermediate for [6]Helicene Functionalization. *Journal of Organic Chemistry* **2018**, *83*(7), 3607-3616. 10.1021/acs.joc.7b03234 (Q1, 12 citations)

   This is our fundamental study in the field of helicene chemistry dealing with the functionalization of 2- bromo[6]helicene. A library of 17 different carbon, boron, nitrogen, phosphorus, oxygen and sulfur substituted derivatives were prepared. Also, the racemization barrier of 2-bromo[6]helicene was determined, and the use of enantiomers in the synthesis of optically pure helicenes was rationalized. Results are widely used not only in our group.

6. CÍRKVA, Vladimír, JAKUBÍK, Pavel, STRAŠÁK, Tomáš, HRBÁČ, J., SÝKORA, Jan, CÍSAŘOVÁ, I., VACEK, J., ŽÁDNÝ, Jaroslav, STORCH, Jan. Preparation and Physicochemical Properties of [6]Helicenes Fluorinated at Terminal Rings. *Journal of Organic Chemistry* **2019**, *84*(4), 1980-1993. 10.1021/acs.joc.8b02870 (Q1, 9 citations)

   This is the pilot study on the first racemization-stable [6]helicene derivatives fluorinated at terminal ring. In addition to the synthetic part, the physicochemical properties of fluorinated helicenes were also obtained. The results are of high interest for further development of n-type semiconducting materials for OFET applications that are ongoing in our group.

7. STORCH, Jan, KALÍKOVÁ, K., TESAŘOVÁ, E., MAIER, V., VACEK, J. Development of Separation Methods for the Chiral Resolution of Hexahelicenes. *Journal of Chromatography A* **2016**, *1476*(DEC 9), 130-134. 10.1016/j.chroma.2016.10.083 (Q1, 10 citations)

   This is our key publication in the field of chiral helicene separations using HPLC or SFC into single enantiomers. The results are widely used in our group for further research.

8. DRAČÍNSKÝ, Martin, STORCH, Jan, CÍRKVA, Vladimír, CÍSAŘOVÁ, I., SÝKORA, Jan. Internal dynamics in helical molecules studied by X-ray diffraction, NMR spectroscopy and DFT calculations. *Physical Chemistry Chemical Physics* **2017**, *19*(4), 2900-2907. 10.1039/c6cp07552e (Q1, 14 citations)

   This work, although mostly performed by Jan Sýkora group (Dep. 5), deals with the conformational behavior of [6]helicene and fluorinated[6]helicene in solution (variable-temperature NMR experiments) and the solid state (X ray).

The obtained results were confirmed by DFT calculations. The publication is considered as an important for our further study in the field of optoelectronic – OFET.

9. ROTH, A., SCHAUB, T.A., MEINHARDT, U., THIEL, D., STORCH, Jan, CÍRKVA, Vladimír, JAKUBÍK, Pavel, GULDI, D.M., KIVALA, M. p-Doping of Graphene in Hybrid Materials with 3,10-Diazapicenium Dications. *Chemical Science* **2017**, *8*(5), 3494-3499. 10.1039/c7sc00533d (Q1, 1 citation)

   This excellent work relates to the first application of N,N'-didodecyl-substituted 3,10-diazapicenium salts as novel p-dopants to produce hybrid materials with exfoliated graphene sheets. We hope that the newly synthetized salts will be the highly promising candidates for the fabrication of functional graphene materials with tailored properties.

10. VRBA, J., ROUBALOVÁ, L., CÍRKVA, Vladimír, STORCH, Jan, VACEK, J. Cytotoxicity of hexahelicene and its effect on the aryl hydrocarbon receptor pathway. *Toxicology in Vitro* **2019**, *57*(June 2019), 105-109. 10.1016/j.tiv.2019.02.020 (Q2, 2 citations)

    This is an ongoing study on helicene toxicity. If helicenes were to be used in molecular electronics, it is good to know their toxicity. [6]Helicene and 1-butyl-3-(2-methyl[6]helicenyl) imidazolium bromide were studied as model substances. The activity of the aryl hydrocarbon receptor (AhR) and expression of cytochrome P450 1A1 (CYP1A1) in human hepatoma HepG2 cells have been examined, concluding that [6]helicene may exhibit low carcinogenic properties.

11. Department of Bioorganic Compounds and Nanocomposites

1. TSENG, H.-H., WANG, Ch.-T., ZHUANG, G.-L., UCHYTIL, Petr, ŘEZNÍČKOVÁ ČERMÁKOVÁ, Jiřina, SETNIČKOVÁ, Kateřina. Enhanced H2/CH4 and H2/CO2 Separation by Carbon Molecular Sieve Membrane Coated on Titania Modified Alumina Support: Effects of TiO2 Intermediate Layer Preparation Variables on Interfacial Adhesion. *Journal of Membrane Science* **2016**, *510*(JUL 15), 391-404. 10.1016/j.memsci.2016.02.036 (Q1*, 33 citations)
2. KONONOVA, S.V., KREMNEV, R.V., SUVOROVA, E.I., BAKLAGINA, Y.G., VOLCHEK, B.Z., UCHYTIL, Petr, SHABSELS, B.M., ROMASHKOVA, K.A., SETNIČKOVÁ, Kateřina, ŘEZNÍČKOVÁ ČERMÁKOVÁ, Jiřina. Pervaporation Membranes with Poly(γ-Benzyl-L-Glutamate) Selective Layers for Separation of Toluene - n-Heptane Mixtures. *Journal of Membrane Science* **2015**, *477*(MAR 1), 14-24. 10.1016/j.memsci.2014.11.047 (Q1*, 18 citations)
3. BARTOŠÍK, M., KOUBKOVÁ, L., KARBAN, Jindřich, ČERVENKOVÁ ŠŤASTNÁ, Lucie, HODÍK, Tomáš, LAMAČ, Martin, PINKAS, Jiří, HRSTKA, R. Electrochemical Analysis of a Novel Ferrocene Derivative as a Potential Antitumor Drug. *Analyst* **2015**, *140*(17), 5864-5867. 10.1039/c5an00958h (Q1, 10 citations)
4. SETNIČKOVÁ, Kateřina, ŠÍMA, Vladimír, PETRIČKOVIČ, Roman, ŘEZNÍČKOVÁ ČERMÁKOVÁ, Jiřina, UCHYTIL, Petr. Separation of Gas

Mixtures by New Type of Membranes – Dynamic Liquid Membranes. *Separation and Purification Technology* **2016**, *160*(FEB 29), 132-135. 10.1016/j.seppur.2016.01.025 (Q1, 10 citations)

5. LIEGERTOVÁ, M., WRÓBEL, D., HERMA, R., MÜLLEROVÁ, Monika, ČERVENKOVÁ ŠŤASTNÁ, Lucie, CUŘÍNOVÁ, Petra, STRAŠÁK, Tomáš, MALÝ, M., ČERMÁK, Jan, SMEJKAL, J., ŠTOFIK, M., MALÝ, J. Evaluation of Toxicological and Teratogenic Effects of Carbosilane Glucose Glycodendrimers in Zebrafish Embryos and Model Rodent Cell Lines. *Nanotoxicology* **2018**, *12*(8), 797-818. 10.1080/17435390.2018.1475582 (Q1, 5 citations)
6. LOIMER, T., SETNIČKOVÁ, Kateřina, UCHYTIL, Petr. Consideration of the Joule-Thomson Effect for the Transport of Vapor through Anodic Alumina Membranes under Conditions of Capillary Condensation. *Separation and Purification Technology* **2019**, *215*(MAY 15), 548-556. 10.1016/j.seppur.2019.01.051 (Q1, 2 citations)
7. HERMA, R., WRÓBEL, D., LIEGERTOVÁ, M., MÜLLEROVÁ, Monika, STRAŠÁK, Tomáš, MALÝ, M., SEMERÁDTOVÁ, A., ŠTOFIK, M., APPELHANS, D., MALÝ, J. Carbosilane dendrimers with phosphonium terminal groups are low toxic non-viral transfection vectors for siRNA cell delivery. *International Journal of Pharmaceutics* **2019**, *652*(MAY 1), 51-65. 10.1016/j.ijpharm.2019.03.018 (Q1, 2 citations)
8. UCHYTIL, Petr, SETNIČKOVÁ, Kateřina, TSENG, H.-H., ŠÍMA, Vladimír, PETRIČKOVIČ, Roman. Description of the Gas Transport through Dynamic Liquid Membrane. *Separation and Purification Technology* **2017**, *184*(AUG 31), 152-157. 10.1016/j.seppur.2017.04.014 (Q1, 1 citation)
9. KURFIŘT, Martin, ČERVENKOVÁ ŠŤASTNÁ, Lucie, DRAČÍNSKÝ, Martin, MÜLLEROVÁ, Monika, HAMALA, Vojtěch, CUŘÍNOVÁ, Petra, KARBAN, Jindřich. Stereoselectivity in Glycosylation with Deoxofluorinated Glucosazide and Galactosazide Thiodonors. *Journal of Organic Chemistry* **2019**, *84*(10), 6405-6431. 10.1021/acs.joc.9b00705 (Q1, 1 citation)
10. HORNÍK, Štěpán, ČERVENKOVÁ ŠŤASTNÁ, Lucie, CUŘÍNOVÁ, Petra, SÝKORA, Jan, KÁŇOVÁ, K., HRSTKA, R., CÍSAŘOVÁ, I., DRAČÍNSKÝ, Martin, KARBAN, Jindřich. Synthesis and in Vitro Cytotoxicity of Acetylated 3-Fluoro,4-Fluoro and 3,4-Difluoro Analogs of D-glucosamine and D-galactosamine. *Beilstein Journal of Organic Chemistry* **2016**, *12*(Apr 20), 750-759. 10.3762/bjoc.12.75 (Q2, 11 citations)

Final report was elaborated by:

Commission 3.2 - Chemical sciences
Evaluated teams No.: 5, 7, 8, 9, 11

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 7.1 - Engineering and technology
Evaluated teams No.: 1, 2, 3, 4, 6, 10

Commission Chair: Dr. János Lábár
Commission Deputy Chair: Jan Dusza
Commission Members:
- Tobias Bauer
- Frank Gronwald
- Stefan Haase
- Oliver Kastner
- Vladislav Musil
- Ryszard Pohorecki