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Chemistry Community Roadmap 2024

Update of Swiss Community Needs for Research Infrastructures 2029–2032

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Content

1 Executive summary

Chemical innovation impacts nearly every aspect of daily life, from food and clothing to travel, energy production, and healthcare. Switzerland is a global leader in chemical research due to the strong collaboration between top universities and a thriving chemical and pharmaceutical industry. This sector generates over 50% of Swiss exports and employs more than 75,000 people. The industry is drawn to Switzerland by world-class research and education institutions.

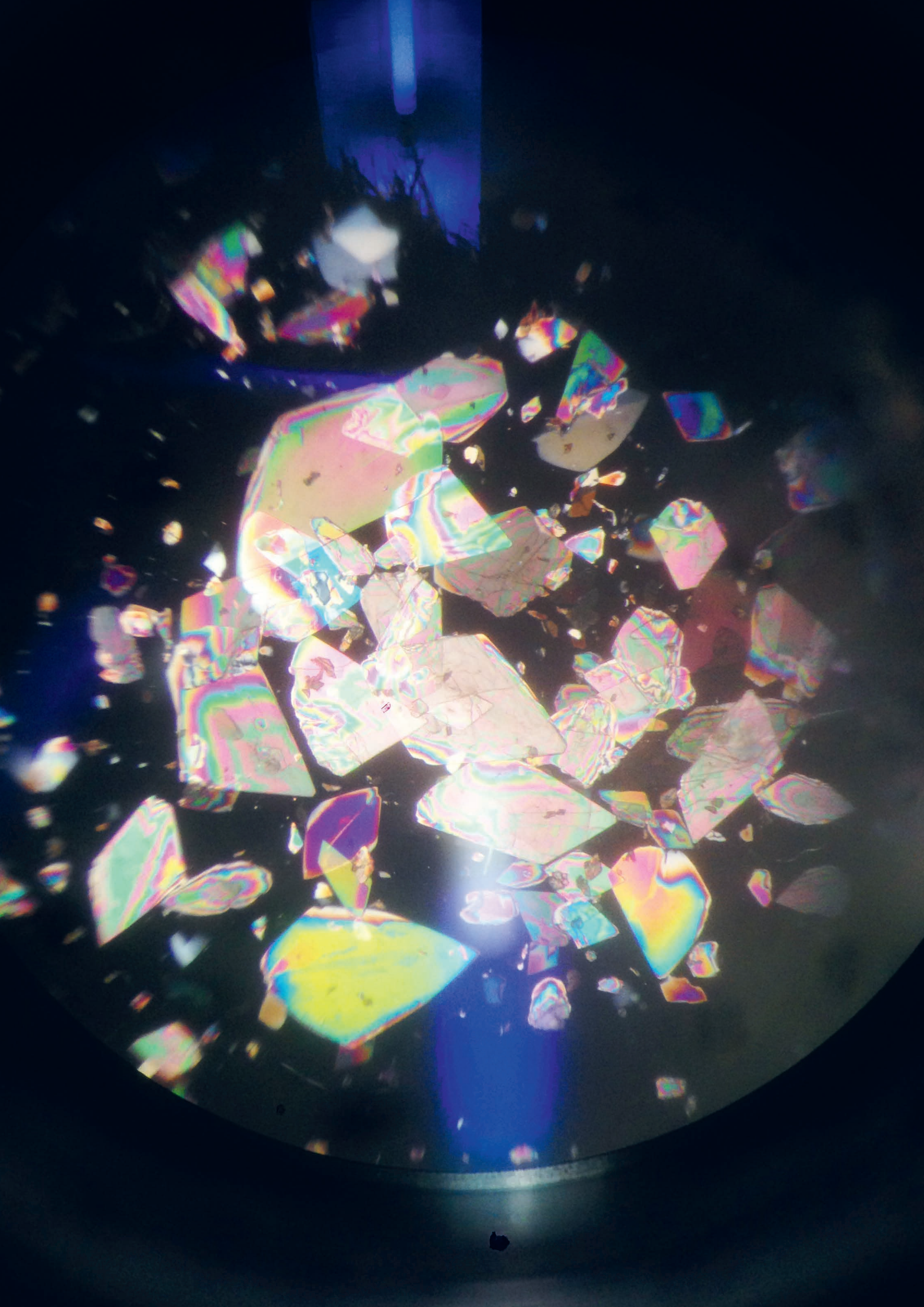
Academic research in the chemical sciences is undergoing a profound transition. Characterised by studies carried out at the single laboratory level in the past, research is increasingly oriented towards multi-laboratory collaborative endeavors in decentralised networks; it also requires access to more advanced tools at highly specialised facilities and across disciplinary expertise. This transition is propelled by the increasing scope and complexity of chemical problems which today require exchanges across classical disciplinary boundaries together with the need for research infrastructures that provide state-of-the-art instrumentation and expertise at the edge and beyond the classical boundaries of chemistry. Therefore, national hubs are needed to provide researchers with state-of-the-art infrastructure, keeping Switzerland at the forefront of chemical research.

This update of the Chemistry Community Roadmap proposes establishing or strengthening nine national infrastructures, categorised as discovery-driven, challenge-driven, or network-driven.

2 Foreword

This document is an update to the Chemistry Community Roadmap published in 2021.[1] It presents the needs of the Swiss chemistry community in terms of future national and international research infrastructures. Together with similar community roadmaps in other disciplines, it is an important element of the four-year process leading to the development of the Swiss Roadmap for Research Infrastructures 2027 to be written by the State Secretariat for Education, Research and Innovation (SERI) in view of the ERI Dispatch 2029–2032 to the Federal Council. The role of these 'bottom-up' inputs is to serve as an important basis for the strategic planning of the higher education institutions in terms of new or major upgrades to national infrastructures, as well as to inform and support SERI during its decision-making process on Swiss participation in international research infrastructure networks and organisations.

SERI has formally mandated the Swiss Academy of Sciences (SCNAT) to update the seven community roadmaps previously published in the disciplines of biology, chemistry, geosciences, astronomy, particle physics, photon science and neutron science. SCNAT engaged its network of member societies and commissions to reach out to the scientists willing to get involved. It encouraged diversity of the participating scientists and provided the needed support for the collaborative writing, the layout, the publication and printing of this document.



3 Introduction

Chemical innovation affects almost every aspect of our daily life: it affects, for instance, what we eat and wear, the structures we live in, how we communicate, how we go to work and travel around the world, how we produce and store energy and how we diagnose and cure disease. Consequently, chemical innovation is key to improving our health and protecting the environment. It will contribute to the reduction of our carbon footprint and to the discovery of virtuous resource and energy cycles, paving the way towards a truly sustainable economy and society. Chemical innovation is only possible with detailed insights into chemical structures and processes. This is what then opens the possibility to design novel compounds and materials and to access sustainable production processes.

Regarding chemical research, Switzerland is among the leading nations of the world. This remarkable success results from the interplay and mutually beneficial relationship between top ranking universities and a strong chemical and pharmaceutical industry. The Swiss chemical and pharmaceutical industry generated roughly 50% of total Swiss exports selling over CHF 100 billion in chemical and pharmaceutical products abroad.[2] This economic sector directly employs more than 75,000 people in Switzerland with another 203,000 jobs in associated branches. This industry is attracted to Switzerland and is retained here because of the world class academic research and education environments arising from the Swiss universities of applied sciences, and the renowned Swiss universities and federal institutes of technology (ETH domain).

For decades, essential infrastructures for chemistry research could be provided at single university, institute or even laboratory level. However, frontier instrumentation is no longer affordable to single institutions. Not only does cost become prohibitive, but the expertise required to develop and operate the instrumentation is rare. Furthermore, the complexity of the data generated, from acquisition to interpretation, also requires novel approaches, which is being propelled by the ongoing digital revolution where chemistry applications emerge among the most demanding today. Consequently, a set of national hubs/centres are needed to provide state-of-the-art infrastructure to all Swiss researchers across the chemical sciences and, thereby, maintain Switzerland at the forefront of chemical research and innovation.

Following established models, these infrastructure-hubs can either be organised as central national facilities, for instance around the synchrotron radiation sources today offered at PSI, or as distributed networks linking multiple sites that host complementary instrumentation and expertise. All the hubs are expected to be open and accessible to researchers across Switzerland and to develop as international centres. Since frontier instrumentation requires specific skills for operation as well as specialised expertise for data analysis, these hubs will provide both frontier tools and expert staff to the broad user community.

Moreover, the proposed infrastructures should foster multinational scientific exchange and collaboration. Presently, Switzerland is a member of several international research organisations, including the European Council for Nuclear Research (CERN), the European Synchrotron Radiation Facility (ESRF) comprising the Swiss-Norwegian Beamline (SNBL), the European X-Ray Free Electron Laser (European XFEL), the European Spallation Source (ESS) and the European Life Science Infrastructure for Biological Information (ELIXIR). This international connectedness is crucial for the high quality of chemistry research in Switzerland. The national infrastructures proposed in this roadmap will continue to pursue an international vision, that will also help to attract further international talent, foster exchange at the international level and develop the international competitivity of the Swiss research environment.

This roadmap recommends to set-up or consolidate nine national infrastructures classified as **discovery-driven**, **challenge-driven** or **network-driven** infrastructures.

Building on the Chemistry Roadmap published in 2021, the community has confirmed the continued need for all seven infrastructures proposed in 2021, and suggested two additional initiatives to be included. Two of the original infrastructures (EM-Frontiers, IMPACT) were featured in the Swiss Roadmap for Research Infrastructure 2023,[3] and are reiterated in the current document to underscore the communities' persisting need. Overall, the updated Chemistry Community Roadmap recommends to set-up or consolidate infrastructures grouped into two pillars of discovery- and challenge driven infrastructures and including a network-driven initiative.

A first group of **discovery-driven infrastructures** will provide essential capabilities for characterisation at different temporal and spatial resolutions and to study fundamental structure-function relationships under relevant conditions, which is at the basis for rational development and innovation. This first group comprises:

1. An electron microscopy and diffraction hub (included in the Swiss Roadmap for Research Infrastructures 2023, EM-Frontiers);

2. A magnetic resonance and magnetism hub;

3. A centre for *operando* synchrotron studies.

The second group of infrastructures builds on the insights from fundamental structure-function relationship studies to tackle major social challenges. These **challenge-driven infrastructures** are oriented to screen, discover, generate and develop lead chemicals and materials for specific applications related to energy, health and sustainability. This second group comprises:

1. A facility to produce Terbium radionuclides for diagnostics and treatment of disease (included in the Swiss Roadmap for Research Infrastructures 2023, IMPACT);

2. A mass spectrometry-based screening platform for (bio)catalysts and environmental samples;

3. A centre providing state-of-the-art instrumentation for translational chemistry and managing a national library of compounds synthesised in academic laboratories across Switzerland;

4. A catalysis hub (SwissCAT+) to discover and develop catalysts and catalytic processes;

5. A pilot plant to upscale chemical and bioprocesses (new).

In addition, a **network-driven infrastructure** is proposed:

1. A consortium to foster Swiss heritage science (new).

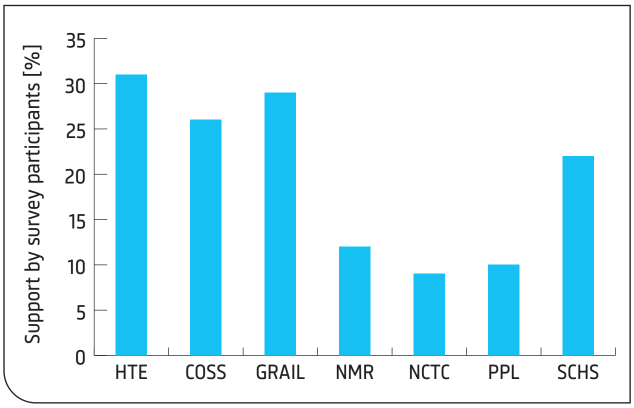
4 Findings and recommendations

4.1 General findings and recommendations

Finding: Frontier instrumentations can often no longer be accommodated at a single university or institution, due to both cost and the requirements to have highly specialised personnel with advanced skills for operation and data analysis. While the user groups have expertise in their specific fields of application, they often lack access to the most advanced instrumentation and are short on the comprehensive skills required to run such instruments and fully process and analyse the data obtained. Consequently, research groups in chemistry now require state-of-the-art research infrastructures with well-trained staff.

Recommendation: It is recommended to develop national infrastructures accessible to all researchers in Switzerland, as well as in other nations, to provide access to advanced instrumentation and expertise. Trained permanent staff should support and advise users regarding data acquisition as well as data analysis and exploitation.

The updated list of the proposed infrastructures has been identified in the course of a 9-month process starting in early 2024. All public institutions conducting chemistry research were represented throughout the process. Moreover, the input from chemists (group leaders, professors) across Switzerland was collected in an online survey conducted by the SCNAT Platform Chemistry and organised in close collaboration with the Swiss Chemical Society. The elaboration of this roadmap constitutes an important first step towards long-term strategic consultation and planning within the Swiss chemistry community.



Overview of survey results showing the support for the proposed infrastructures by the Swiss Chemistry Community. (Note: survey results for TATTOOS and EM-Frontiers are not shown as the infrastructures are featured in the Swiss Roadmap for Research Infrastructure 2023).
HTE: High Throughput Experimentation (Catalysis Hub),
COSS: A Center for *Operando* Synchrotron Studies,
GRAIL: High-throughput Screening Hub for Chemical Biology,
NMR: Magnetic Resonance and Magnetism,
NCTC: National Centre for Translational Chemistry,
PPL: Pilot Plant, SCHS: Swiss Cultural Heritage Science.
Source: SCNAT, Platform Chemistry

4.2 Specific findings and recommendations

Catalysis hub

Finding: High Throughput Experimentation (HTE) facilities have now been created at University (UZH), Institute (Empa) or even at the national level (SwissCat+) since the Chemistry Roadmap 2021, highlighting the need of such platforms where both frontier instrumentations and expert personnel enable faster discovery and development of catalysts or materials. However, challenges due to economics and reforms in Swiss research and education are emerging; maintaining these facilities and allowing them to grow in a highly competitive international environment are under clear threat, endangering the leading role of Switzerland in the development of sustainable processes.

Recommendation: Strengthen these open-access national facilities, offering frontier capabilities and expertise, i.e. maintain high level investments, in terms of instrumentation and expert personnel position at the interface of data-science automation and chemistry/biology.

A Center for *Operando* Synchrotron Studies

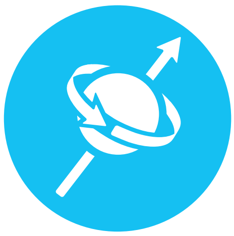
Finding: The Swiss chemistry and material science communities have a continuously increasing need for (fast access to) multiple-technique beamlines at synchrotron light sources for operando studies. These beamlines provide information rich large datasets that need data analysis experts.

Recommendation: A Center for *Operando* Synchrotron Studies (COSS) localised at two complementary synchrotrons (the Swiss Light Source and the European Synchrotron Radiation Facility) and centred around multi-technique beamlines is proposed. The new center will exploit synergies between multi-technique beamlines and provide a gateway to the highly specialised beamlines at both state-of-the-art synchrotron facilities. Moreover, the center will provide an inter-disciplinarily educational and analysis platform enabling research groups to fully exploit their datasets.

High-throughput Screening Hub for Chemical Biology

Finding: The success of Swiss academia and chemical industry builds on powerful catalysts and their resource-saving implementation in syntheses and manufacturing processes. In Switzerland, the development of sustainable (bio)catalysts, environmentally safe chemicals and biomolecular therapeutics is currently hampered by the lack of a screening hub providing fast handling and analysis of samples at miniaturised scale.

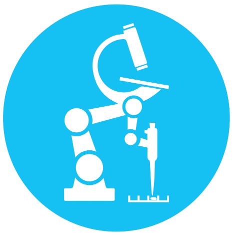
Recommendation: We recommend to create an open access high-throughput screening hub to accelerate the development of new (bio)catalytic entities and safe and sustainable by design substances. In addition, the hub will allow to screen intact proteins and environmental samples by building on cutting-edge high-throughput screening technology, in particular micro-fluidics and acoustic mist ionisation coupled to mass spectrometry.



Magnetic resonance and magnetism

Finding: Switzerland is a global leader in magnetic resonance. Infrastructure in electron paramagnetic resonance (EPR), magnetic measurements, and high-field nuclear magnetic resonance (NMR) is essential for the community across the whole of chemistry, from chemical biology to materials chemistry. Our capacity in this area will no longer meet the international standards in five years from now. Single institutions or local consortia can no longer meet this need.

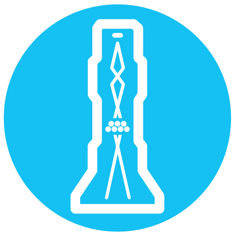
Recommendation: There is the need for the creation of a new distributed infrastructure serving the whole Swiss community. The infrastructure will maintain international leadership in magnetic resonance and support academic and industrial research across the chemical sciences.



National Centre for Translational Chemistry

Finding: Switzerland is lacking a centralised national infrastructure for academic drug discovery. The National Centre of Competence in Research (NCCR) Chemical Biology created and developed screening platforms at the EPFL and UNIGE to harness chemistry research to respond to societal changes, particularly public health. The number of projects submitted from most of the major Swiss academic institutions to these platforms has steadily increased over the years, especially for translational projects.

Recommendation: We recommend to build on the foundations of the EPFL and UNIGE platforms a National Centre for Translational Chemistry (NCTC) to accelerate academic drug discovery in Switzerland. Investments are required to significantly upgrade existing platforms, broaden their scope, building synergies with specialised complementary platforms across the country and assure that the top standards applied serve the whole Swiss community. Through the envisaged NCTC, Switzerland may also play a critical role at the European level.



Electron microscopy and diffraction

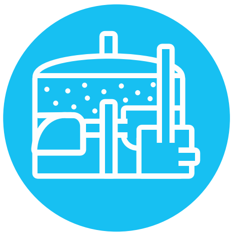
Finding: Electron microscopy (EM) is a powerful analytical method that can simultaneously provide structural, compositional and chemical information for complex structured materials at atomic resolution. In situ and operando capabilities allow the observation of materials under application-relevant conditions, including the study of dynamic chemical and structural processes. EM is key for advancing technologies which strongly affect our society with challenges such as net zero emission, quantum computing or drug design.

Recommendation: To establish EM-Frontiers, a decentralised electron microscopy facility. Each of the participating units provides a station offering support, expertise and innovative EM infrastructure specifically configured for specialised applications covering both, life and physical sciences. EM-Frontiers synergises interdisciplinary EM expertise in Switzerland and ensures that Switzerland stays at the forefront of EM research in order to be able to tackle current and future societal challenges.

Targeted Alpha Tumour Therapy and Other Oncological solutions

Finding: Nuclear medicine uses radionuclides for the diagnosis and/or treatment of disease. Today, radionuclides of highest purity are made available at PSI for preclinical and first in-human clinical studies. However, some of the desired radionuclides (such as ^{149}Tb and ^{152}Tb) are difficult to produce by currently available means, but can be produced via Isotope Separation On-Line (ISOL) techniques proven at CERN.

Recommendation: A facility at PSI should be extended to produce additional radionuclides, in particular the extremely promising radionuclides ^{149}Tb and ^{152}Tb. The extended facility will allow for performing the entire process onsite, comprising spallation, collection and chemical separation of these radionuclides, followed by the production of radiopharmaceuticals. Through this facility novel radiopharmaceuticals will be made available and enable world-first clinical studies throughout the country.



Pilot plant

Finding: Switzerland excels in chemistry and life sciences with world-class research institutions and a strong industrial sector, leading to numerous discoveries. However, a key challenge is translating these innovations into commercial products due to limited infrastructure for scaling up processes from lab to market. Smaller entities, like start-ups and research groups, particularly struggle with this gap. The lack of facilities for process scale-up in academic institutions prevents many promising discoveries from reaching industrial application and commercialisation.

Recommendation: To create a national open-access pilot plant hub to bridge academic research and industry, enabling the scale-up of chemical processes and accelerating innovations to market. Embedded at a central location for chemistry, with expansion into biotech entities, the hub will have trained permanent staff to support users regarding scale-up and exploitation. Upgrades with advanced data tools, Process Analytical Technologies (PAT), and process intensification equipment, along with added bioprocessing, will foster agility and sustainable productions.

Cultural heritage

Finding: Cultural Heritage Science is a transdisciplinary research field aimed at promoting a better/more efficient/sustainable preservation of our vast cultural heritage. It includes natural sciences, art conservation and humanities. Through the European Research Infrastructure for Heritage Science (E-RIHS), soon to be implemented as a European Research Infrastructure Consortium (ERIC), the European Union is embracing the continuous growth of heritage sciences. While Switzerland's contributions to heritage science research are internationally acknowledged, an official Swiss node is currently missing.

Recommendation: We propose to create a distributed Cultural Heritage Science (CHS) network to 1) consolidate specialised competences available across Switzerland and 2) strengthen Switzerland's position as a strategic stakeholder in national, European and international research programmes and 3) provide access to instrumentation and data, as well as training opportunities in heritage science.

5 Infrastructures

5.1 Catalysis hub – High Throughput Experimentation

Recent developments

The national/international context
With the urgent global environmental need to discover and optimise sustainable chemical processes and materials within the next few decades, speeding up research and development has never been as important. Besides climate change, our world also faces geopolitical challenges that impact our accessibility to critical resources, causing the need to develop alternative catalysts, based for instance on earth-abundant elements, to fulfil current and future societal energy and chemical demands. In parallel, machine learning (ML) and artificial intelligence (AI) algorithms are being developed at a startling pace, and are being used to accelerate discovery in various field of chemistry, and biology (2024 noble prizes in chemistry and physics). In that context, numerous (mega)large-scale initiatives have appeared worldwide, e.g. in Canada, Germany, and the US. In Switzerland, several HTE infrastructures have been launched, focusing on the development of molecular systems and materials for catalysis and energy conversion/storage, e.g. SwissCat+ (ETH domain) and other facilities at UZH and Empa. Finally, the NCCR Catalysis clearly indicates the commitment to push towards digital chemistry (data-driven development of catalytic and sustainable processes). On the European level, the large-scale, long-term research initiative Battery2030+ is promoting the use of data-driven approaches for battery materials and cell chemistry research.

Major successes
Major initiatives have been launched to set-up (data-driven)-HTE platforms in Switzerland (SwissCat+) that are now open to the public, in conjunction with major public and private sector efforts towards digitalisation and automatisation of chemistry (e.g. NCCR Catalysis, ETH Board Open Research Data (ORD) program PREMISE,[4] IBM, Chemspeed recently acquired by Bruker). Similar efforts have been directed to Battery research (Empa). Finally, while there is currently no open HTE infrastructure in biocatalysis, efforts have been made in that direction (e.g. ZHAW).

Description and development prospects
While Switzerland was clearly ahead, major initiatives have appeared across the world with orders of magnitudes larger funding (e.g. CAD 500 million in Canada). In parallel, funding equipment and infrastructure have become challenging in Switzerland due to recent national reforms (e.g. disappearance of R'Equip) and global economic challenges. Despite this complex situation, there is no doubt that with these newly available HTE platforms, the 2nd phase of NCCR Catalysis and the 3rd phase of Battery2030+ in place, as well as major initiatives in AI ideally position Switzerland at the forefront in data-driven HTE, provided these infrastructures can reach a critical mass and remain ahead to serve best the Swiss scientific community.

Future needs – Scientific need and urgency

The few infrastructures in place are facing challenges in terms of identifying new funding sources for capital investments and to cover operational expenditures. For instance, implementation of self-driving labs, handling of more complex reaction systems (multi-step syntheses and catalytic processes), and incorporation modern activation processes, e.g. photo- and electrochemistry, remain grand scientific and technology challenges. Fast characterisation techniques also remain a main bottle-neck in HTE-driven research. In addition, the implementation of data analysis and management, curation and analysis software represent a major, often underestimated effort, and remains one of the important challenges in data-driven science. While integration of experimental and computational data should in principle speed up discovery, these approaches remain treated as mostly separate targets. Among important future points will be 1) the development of ontologies to better communicate across platforms, 2) the implementation of ways to facilitate data-sharing and implement FAIR principles and approaches to guarantee data-quality, standardisation, and safety, and 3) the integration of modern artificial intelligence algorithms to suggest new hypotheses and insights gathered from the generated data. All these challenges can only be addressed when pursued within infrastructures wherein all expertise is present in one place.

Impact
SwissCat+ and related HTE infrastructures for catalyst and battery materials research are fully operational and validated. However, further investments are needed to enhance their accessibility for the broader scientific community, as well as to improve automation, data management, AI integration, and interoperability. As these platforms become more widely available, the demand for

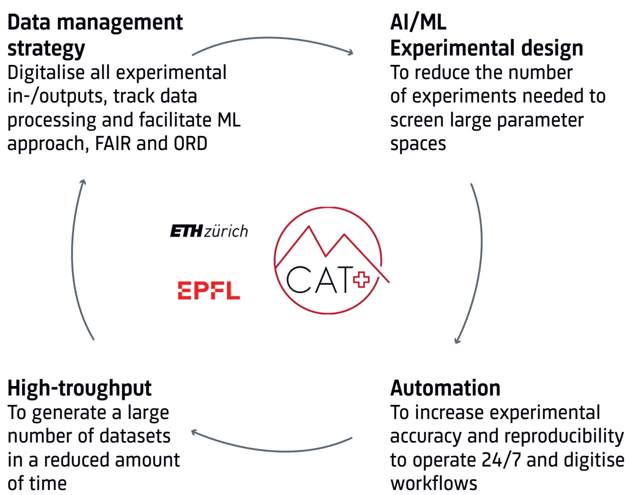
their use is steadily increasing. It is clear that expanding this approach is crucial to addressing current challenges. These developments not only strengthen Switzerland's leadership in research but also address an existing gap in advanced technological platforms. As previously mentioned, data-driven HTE platforms are designed with a focus on sustainable development and energy research but have the potential to expand into other fields, such as functional materials and drug discovery. Swiss chemical companies have already invested in or shown strong interest in these platforms. The development of high-end HTE platforms for both academic and industrial applications is poised to play a pivotal role in driving innovation within the chemical sector. This will, in turn, enhance the global attractiveness and competitiveness of the Swiss chemical industry.

Community

These infrastructures have just opened and have attracted great interest from the catalysis, organic/inorganic and battery materials research communities. The recently opened SwissCat+ have already users across many of the Swiss academic Institutions, and numbers are rapidly increasing as novel state-of-the-art equipment and expertise are offered to the users. Empa's Aurora HTE battery research platform is embedded into the large-scale long-term European battery research initiative Battery2030+, and have several projects with academic and industrials partners. There is also a clear interest of national and international companies to have access to these infrastructures, few contracts have already been signed directly with the infrastructure or through professorships. This will be a key point of the coming phase as large (competitive) international initiatives have just started.

Vision for the future

The launch of the first Swiss HTE infrastructures triggered much interest from the national and international academic and industrial community. These infrastructures clearly address a pressing challenge for the chemical and material scientific community, across academia and industry and need to maintain state-of-the-art high-end equipment and provide expertise in data-science.



ETHZ SwissCAT+ (East Hub) EPFL SwissCAT+ (West Hub)

Left: Major steps of the closed-loop data-driven automated and high-throughput experimentation strategy at SwissCAT+.
Right: ETHZ SwissCAT+ high-throughput and automated fixed-bed reactors and synthesis units. Source: SwissCAT+

5.2 Center for *Operando* Synchrotron Studies

Recent developments

The national/international context

Both the ESRF with Swiss participation and the Swiss Light Source (SLS) have been or are being upgraded to new generation diffraction limited light sources. Both sources host unique multi-scale beamlines for *operando* studies in chemistry and material science which entail a higher experimental complexity with much increased information content. The proposed COSS will enable users to fully exploit the information content generated by these beamlines by providing an education and data analysis service platform, further strengthening the leading position by Swiss chemists and material scientists and fostering exchange at the international level.

Major successes

In the 2025–2028 roadmap COSS was introduced, consisting of the following backbone:

1. Synchrotron instruments dedicated to *operando* X-ray diffraction and spectroscopy,
2. X-ray techniques and their combinations focused on obtaining crystal, molecular, atomic and electronic structures,
3. Setups for *in situ* and *operando* experimentation compatible with synchrotron instrumentation,
4. Data management and data analysis tools facilitating effective use of synchrotron beamtime,
5. Direct beamtime allocation, rapid access, mail-in service and remote access models.

The need for *operando* synchrotron techniques is well established in the chemistry community, as shown for example by its prominent presence within the NCCR catalysis or the fact that about 80 Swiss research groups use these facilities. Establishing COSS in the Swiss research landscape to support the chemistry and material science research communities is therefore even more urgent for the 2029–2032 period.

Part of this backbone of COSS has been implemented: The Debye beamline at the SLS has been added to the portfolio, doubling the capacity of state-of-the-art facilities for combined *operando* X-ray spectroscopy, diffraction, and scattering studies. SNBL's BM31 beamline now provides a unique facility combining multi-edge X-ray absorption fine structure (XAFS), diffraction and total scattering in a single *operando* experiment.

Description and development prospects

With respect to the 2025–2028 roadmap, COSS was not established due to a lack of funding. Furthermore, operation funding of SNBL at ESRF is not guaranteed past 2028; where the current operation costs are being provided by paid access established only for ETH, EPFL and the University of Geneva. This model precludes broad Swiss access. The Debye beamline at SLS is understaffed, therefore limited currently to using only one third of its capacity. In order to make optimal use of both multi-technique beamlines and have the Swiss chemistry community branch out efficiently to single technique beamlines at both synchrotron facilities, national funding through COSS is essential.

Another trend observed is that the datasets acquired during time-resolved multi-modal operando experiments have developed to such an extent that analyzing the datasets needs experts. Such competences are not available at the individual research group level. To democratise the highly sought for operando synchrotron techniques, an enhanced 4th pillar is therefore proposed: namely the establishment of an inter institutional educational and analysis platform within COSS with strong involvement of experts from Swiss universities/ETH domain.

Future needs – Scientific need and urgency

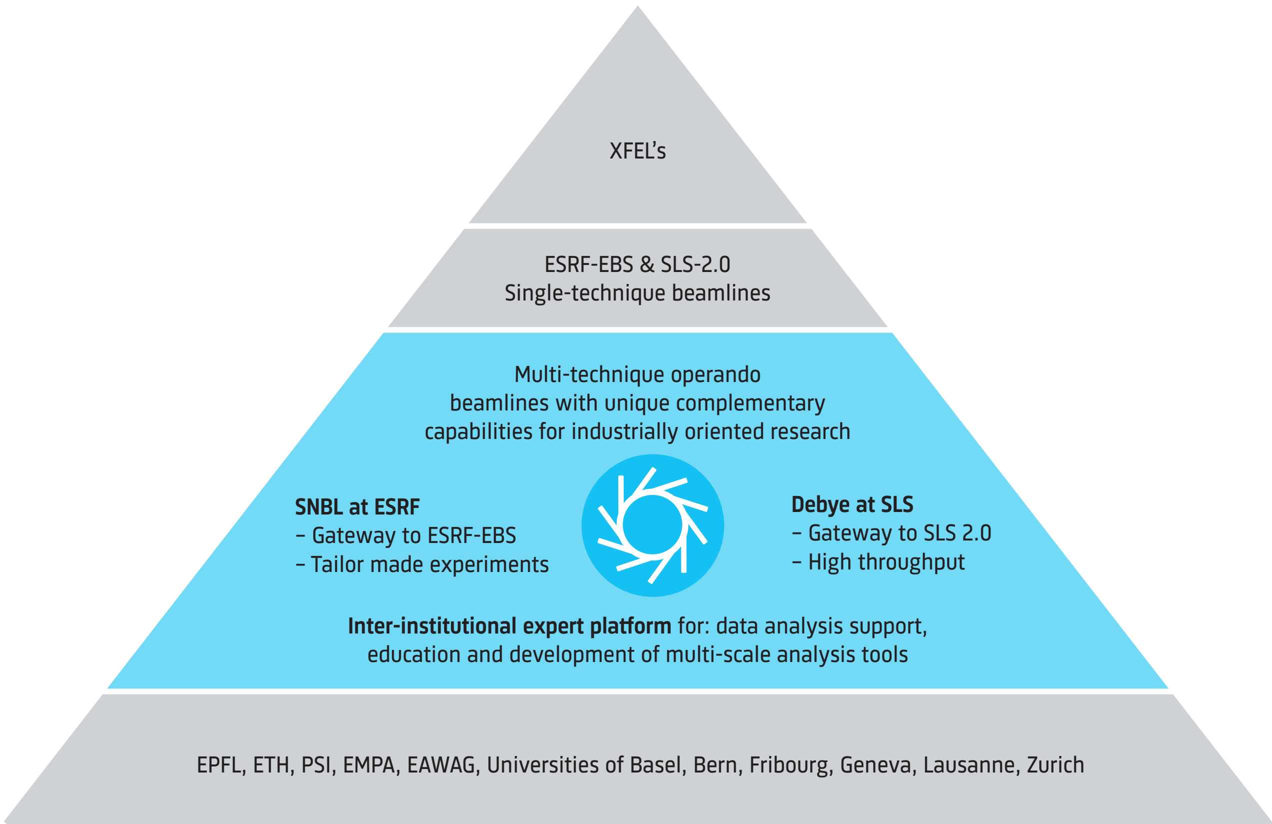
COSS will allow a multi-modal and multi-scale approach to determine structure-performance (activity, selectivity) relationships of functional materials e.g. catalytic reactors and batteries. Such an approach is essential for the rational design of new functional materials or the optimisation of functional devices and existing (industrial) chemical processes.

COSS will: 1) help mature the combination of the most widely used and combined operando synchrotron techniques (X-ray absorption spectroscopy (XAS), X-ray diffraction (XRD), total scattering) including the development of dedicated experimental operando cells, 2) push automation of measurements and data analysis, and 3) provide an expert support and education structure. Individual research groups will be able to focus on their main research questions thus providing Swiss research groups with a competitive edge.

Impact

The facilities offered at COSS will significantly improve the strength and competitiveness of Swiss chemistry and material science research.

Synchrotron instrumentation is advancing fast compared to commercial home lab instrumentation creating a tech-



Centre for operando synchrotron studies (COSS) embedded in the Swiss landscape. Source: Wouter van Beek, SNBL at ESRF

nological and know-how gap impossible to close at the individual research group level. COSS will close this gap by establishing Swiss summer schools, workshops and integration with Swiss university curricula also creating direct synergies with the photon science landscape.

This research infrastructure is mostly used by chemists that address several globally relevant challenges, such as climate change, clean water, clean energy production, energy storage and conversion and other issues coupled to future sustainability.

Community

The research community that benefits strongly from COSS consists of researchers in chemistry/material science, engineering and physics, consisting of about 80 research groups distributed over all Swiss universities and the ETH domain. Many of these groups work with industrial partners. COSS has synergies with three other large research infrastructure (LRI) roadmaps: photon science, biology and geoscience.

Switzerland owns 4% of the beamtime at the ESRF and 50% of the beamtime at the SNBL. European collaborations are indispensable for Switzerland as they facilitate knowledge, technology transfer and skills development. ESRF and SNBL are prime success stories in this respect, both should be maintained and consolidated.

Vision for the future

Swiss scientists are among the leading scientists for materials and chemistry research which is increasingly based on *operando* studies that allow a rational design of new functional materials and catalytic processes. The advent of 4th generation synchrotrons will be providing researchers with state-of-the-art capabilities and applications including AI-based analysis tools. COSS will enable Swiss chemists and material scientists to make maximum use of these unique instruments.

5.3 High-throughput Screening Hub for Chemical Biology

Recent developments

The national/international context

The High-throughput Screening Hub for Chemical Biology is based on ultrafast mass spectrometry and microfluidics which will make it possible to generate large amounts of data in the context of the development of biocatalysts, protein therapeutics and environmental analysis addressing urgent societal needs in our rapidly changing world. The biocatalysts and proteins developed will be used in sustainable chemical production, can serve as tailor-made biomolecular therapeutics and can be applied in medicinal chemistry to identify specific and powerful active ingredients, complementing the capabilities of the Catalysis Hub (SwissCat+, ETHZ/EPFL). The use of the High-Throughput Screening Hub for Chemical Biology in the field of environmental sciences will allow for large-scale analysis of the occurrence, behavior and effects of organic pollutants in the environment. The platform opens an analytical window onto the increasing number of new chemicals and chemical mixtures, and will cover groups of substances discussed in the European Partnership for the Assessment of Risks from Chemicals (PARC) initiative, as well as respond to EU Initatives like the Zero Pollution Action Plan or the Water Framework Directive. It provides an important platform for national and international researchers and companies working on the development of 'safe and sustainable by design' chemicals and processes.

The central element of the infrastructure is the provision of the generated data, both in the area of the structure-function relationship of (bio)catalysts and proteins as well as in in the area of environmental analysis under uniform conditions. In the context of the envisioned Open Data Strategy, a strong positive impact on the application and further development of machine learning algorithms for experimental research is expected.

Major successes

High throughput experimentation and screening has emerged as an essential and powerful tool in chemical biology. In a global context, several high-level biofoundries have been established with the aim to provide powerful enzymatic catalysts as well as cell factories and to harness the synergies between chemical biology, machine learning, and automation (US, South Korea, China, Japan, EU).

Description and development prospects

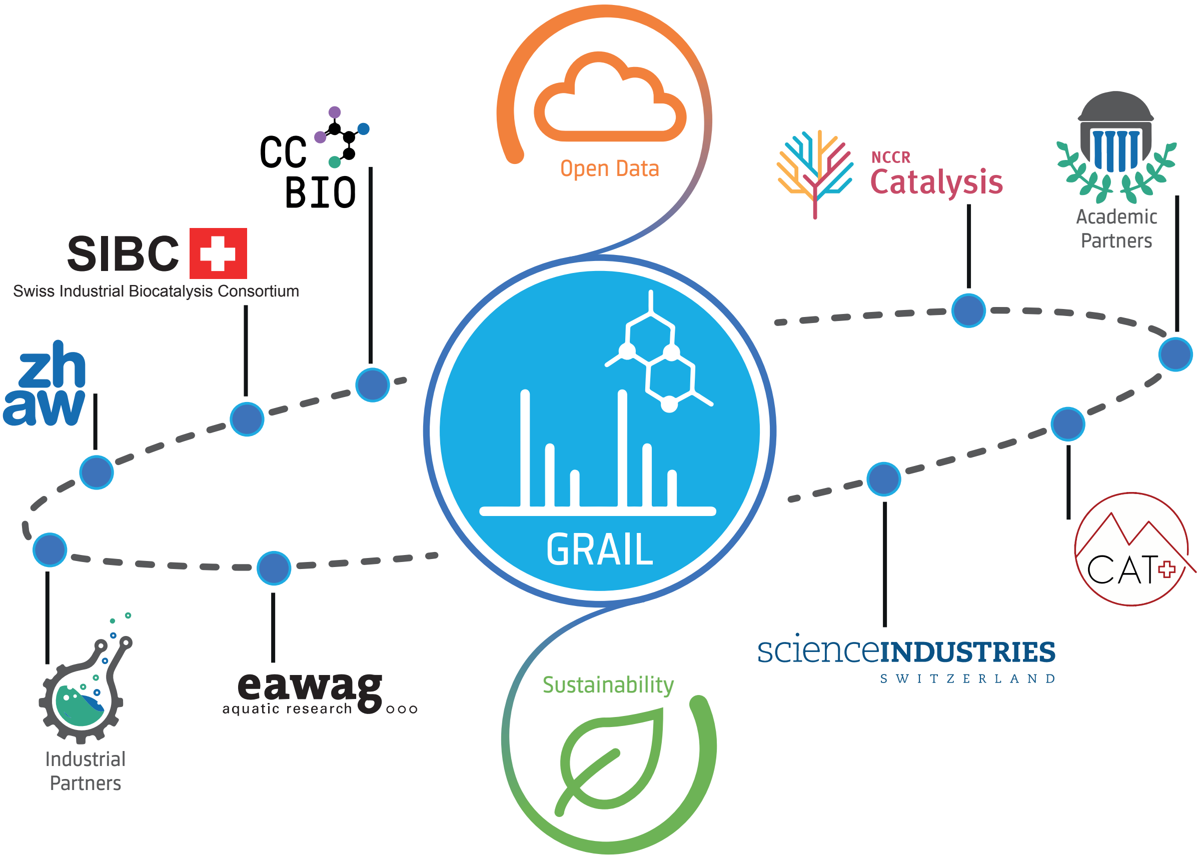
The following recent developments reinforce the need to implement a High Throughput Screening Hub for Chemical Biology in Switzerland:

1. **Biocatalysis:** Advances in algorithm-assisted enzyme engineering and protein design increases demand for the generation of sequence-function data. Achieving the goal of net zero carbon emission requires the rapid discovery, development and implementation of environmentally benign (bio)catalysts.
2. **Environmental Sciences:** The per- and polyfluoroalkyl substances (PFAS) Regulation (addressing persistent per- and polyfluoroalkyl substances), the EU Urban Waste Water Treatment Directive and the Chemicals Strategy for Sustainability, as well as European initiatives such as PARC or Zero Pollution, increase the need for the rapid screening of environmental samples. 'Safe and Sustainable by Design' initiatives are gaining momentum and will support the goal of a circular.
3. **Protein Modifications:** Advances in non-canonical amino acid (ncAA) incorporation and protein modifications increase the need to determine the mass of intact proteins in HT mode.

Future needs – Scientific need and urgency

In contrast to more comprehensive facilities abroad, current complementary Swiss automated platforms are primarily dedicated to specific aspects of (bio)catalyst design (Automated Enzyme Design Platform at ZHAW;[5] SwissCat+ at the ETHZ/EPFL,[6] High-Throughput Experimentation Laboratory at UZH,[7] Laboratory Automation Facility at ETHZ in Basel.[8] A subsequent integration of a label-free, low-volume and high-throughput analysis of reaction samples via mass spectrometry is currently a bottleneck in Switzerland and hampering (bio)catalyst and protein therapeutic development as well as environmental sample analysis and the design of environmentally safe chemicals. Implementation of the High Throughput Screening Hub for Chemical Biology will allow for the:

1. Development of an open-access and integrated high-throughput experimentation platform to rapidly design, build and test (bio)catalysts, to analyze intact (modified) proteins and to process and test environmental samples and substances of concern at miniaturised scale.
2. Discovery of chemo-enzymatic catalytic processes for the synthesis of complex molecules in a sustainable and efficient way.
3. Establishment of a customised database infrastructure operating via the FAIR data principles and interfaceable with machine learning algorithms.



Embedding of the High-throughput Screening Hub for Chemical Biology in the Swiss academic and industrial community highlighting key stakeholders. Through the infrastructure, powerful novel catalyst will drive a sustainable chemical industry and its open data policy will facilitate the synergistic co-development of theoretical and experimental disciplines in chemical sciences. Source: Rebecca Buller, ZHAW

Impact

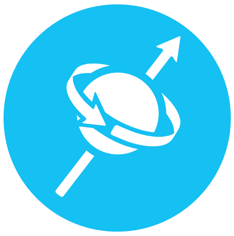
Climate change, chemical pollution, population growth and the simultaneous dwindling of natural resources and biodiversity anticipated for the next decades will enforce the development of sustainable manufacturing routes and chemical products. In this context, biocatalysis and protein design are anticipated to play an important role: These open up new and particularly resource-conserving paths in the conversion of raw materials into basic chemicals and high-quality derivatives as well as protein therapeutics. To protect human health, the environment and biodiversity, it is essential to understand the sources, distribution and effects of chemicals released into the environment and to select benign and recyclable substances in the development process. High-throughput chemical analysis tools that can be combined with flexible effect-based tools are needed to obtain the necessary data to guide the safe and sustainable by design process.

Community

The community consists of groups active in chemical biology, biocatalysis, catalysis, environmental science, data science and machine learning consisting of > 40 groups situated at all Swiss universities and the ETH domain. In addition, the availability of the infrastructure is a very important asset to groups working with industrial partners.

Vision for the future

Internationally, ‘synthetic biology’ is a critically important corner stone for the development of safe and sustainable processes, which will be key to achieve a zero waste and carbon emission society by 2050. A holistic view, comprising the design of benign catalysts and chemicals and the analysis of their subsequent environmental fate, will be essential to guide ‘safe and sustainable by design’ efforts. The High-Throughput Screening Hub for Chemical Biology will provide the analytical tools needed to enable this important transformation in Switzerland.



5.4 Magnetic Resonance and Magnetism

Recent developments

The national/international context

Strategic research foci in the field of chemistry for sustainability, and for health sciences, including materials, devices, and drug discovery, are growing faster and faster. These include materials development in the fields of construction, energy technologies, CO_2 capture and release, catalysis and polymers. The growth in these strategic areas makes high-performance atomic-level characterisation techniques an increasingly critical need. As one consequence of these strategic targets, NMR facilities are experiencing an exponential increase in requests for advanced characterisation by solid-state NMR. The same applies to EPR spectroscopy.

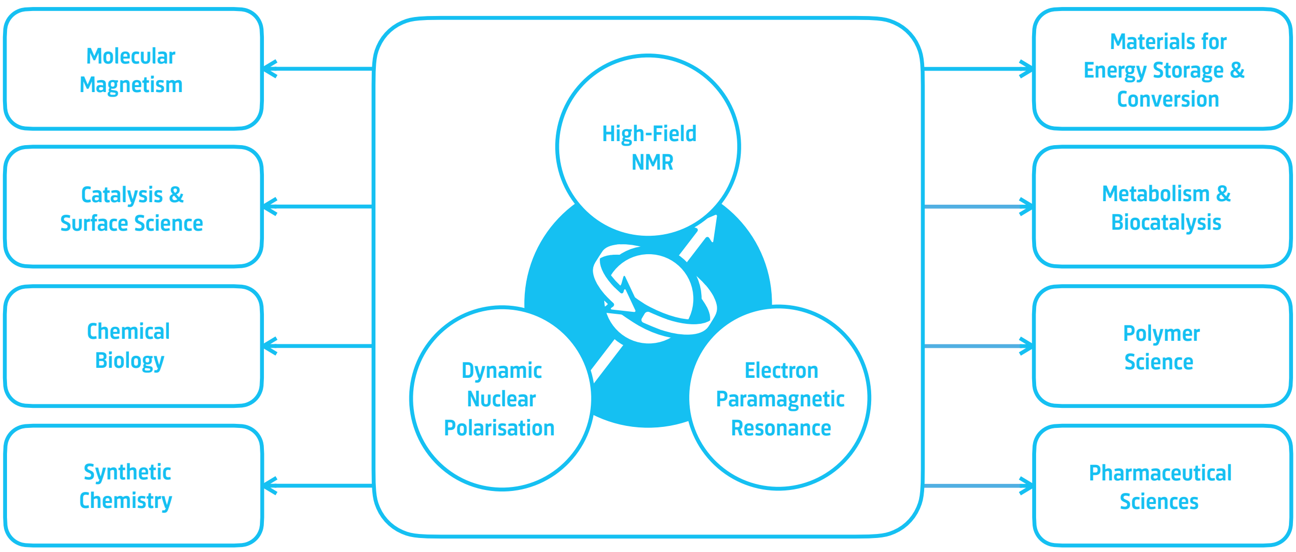
The most important development in the field of MR instrumentation since the publication of the last roadmap is the rapid growth in the number of 1.2 GHz NMR spectrometers installed internationally. Following the installation of the world's second 1.2 GHz NMR spectrometer at ETH Zürich in 2020, there are now 18 GHz-class NMR spectrometers installed in 2024 across the world. In 2024, delivery is expected for a second 1.2 GHz spectrometer in Switzerland, for use in solution NMR, at the UZH. This system, with a configuration directed towards applications in structural biology, was first included in the 2019 roadmap, and will be the flagship instrument in a facility jointly funded and operated by UZH and UNIBAS, together with the ETHZ: SwissNMR.[9]

Major successes

The installation of a second 1.2 GHz spectrometer in Switzerland is a major success. Nevertheless, infrastructures at the national level have not yet been implemented in either NMR or EPR.

Description and development prospects

Bruker has now announced 1.3 GHz NMR spectrometers, and developments towards 1.5 GHz NMR are envisaged on the 5–10 year horizon. In parallel there are cutting edge developments in small extremely high field HTS magnets operating above 45 Tesla. Microwave components and fast arbitrary waveform generators developed for communications technology have improved performance of advanced EPR spectrometers in the 30–34 GHz range, and in parallel automation is lowering the barrier for non-specialist users. In order to best leverage these advancements achieved at Swiss Universities, a coordinated infrastructure for magnetic resonance at the national level for broad chemistry research, from molecules to materials, is more pertinent than ever in order to maintain investment and Swiss leadership at the highest magnetic fields, to fund expert resident staff, and to maintain operation and repair of instrumentation. These costs are too high to bear by single groups or institutions.



Schematic representation of the core techniques in the magnetic resonance infrastructure, and the connection to some of the key users communities that will directly benefit from the facility. Source: Lyndon Emsley, EPFL

Future needs – Scientific need and urgency

As stated in the chemistry roadmap 2021, and as highlighted above, the complexity of biochemical systems and materials under investigation at the forefront of chemical sciences continuously increases. This development can only be supported in the longer run if techniques for the characterisation of atomic-level structure and dynamics keep pace. In NMR this has notably been the driving force for the push to higher and higher magnetic fields. We see today that especially for solids and for biochemistry/chemical biology, NMR and EPR still have a great potential for further developments and applications, for example to understand microscopic processes occurring in solid state materials and devices such as phase transformations, degradation phenomena, interface transformation, to observe catalytic processes by operando spectroscopy, and to observe conformational equilibria in intrinsically unfolded proteins and in cellular environments.

In this context the proposed MR infrastructure is more pertinent and urgent than ever, in particular to allow access to these essential characterisation methods to the largest possible community of untrained users from areas not directly related to MR research.

Impact

As outlined above, the needs for a coordinated national MR infrastructure have significantly increased, both in terms of the scientific needs, and the strategic nature of a coordinated national infrastructure to fulfil these needs. The impact of the infrastructure will be through, for example, the characterisation of pharmaceutically relevant molecules to understand and treat human diseases, or the study of catalytic materials to improve industrial efficiency, including energy efficiency and the reduction of carbon emissions.

Community

The infrastructure will directly benefit a large part of the chemistry R&D in Switzerland from academia to industry, in particular start-up companies that have no access to such state-of-the-art technology. There are several thousand potential users. For example, the local NMR facilities at EPFL or ETHZ alone serve more than 500 users each.

As described previously in the roadmap, MR infrastructures provide solutions across the breadth of academic and industrial R&D in chemistry and to materials and molecular problems across disciplines, from medicine (metabolism, drug design) to civil engineering (building materials). Also, development of state of the art MR instrumentation relies on industry, with Switzerland home to the international leader (Bruker), and leads to new innovations driving startups and small business around new technology.

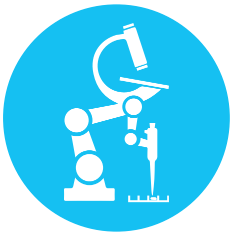
Swiss NMR research groups are already embedded in EU infrastructure initiatives, e.g. PANACEA.[10]

Vision for the future

The underlying driving force justifying the creation of a national infrastructure in MR, as previously set out in the roadmap, has not changed. It is simply more relevant than ever.

Advanced NMR and EPR are today state-of-the-art characterisation techniques for all fields of research in chemistry, biology and materials sciences. However, to cover the full scope of NMR and EPR experiments, a large variety of instrumentation is needed. The development of an MR hub giving open access to a complete range of advanced NMR and EPR equipment across Switzerland will be of colossal benefit to local NMR facilities, to research groups in the fields of NMR and EPR, and to non-specialist users. The infrastructure will have the capacity to acquire NMR spectrometers operating at 1.3 GHz and above, but will also provide access to specialised probes at different field strengths, high-throughput automation, and systems capable of sensitivity-enhanced NMR through hyperpolarisation or unique cryo-probes, among others.

Filling this gap will help Switzerland to expand its role as a powerhouse in fundamental molecular and materials research, for health sciences and the chemical industry.



5.5 National Centre for Translational Chemistry

Recent developments

The national/international context

We propose to build a national multidisciplinary centre to provide the scientific community in Switzerland with: chemical diversity, screening platforms at the EPFL and the University of Geneva, know-how in chemical genetics and in medicinal chemistry for drug discovery and chemical biology projects. The scope includes screening large chemical libraries for other application areas such as sustainable chemistry. NCTC will give access to a national repository of chemical collections, composed of a unique collection of molecules synthesised in Swiss labs and more than 100,000 commercially available compounds.

Major successes

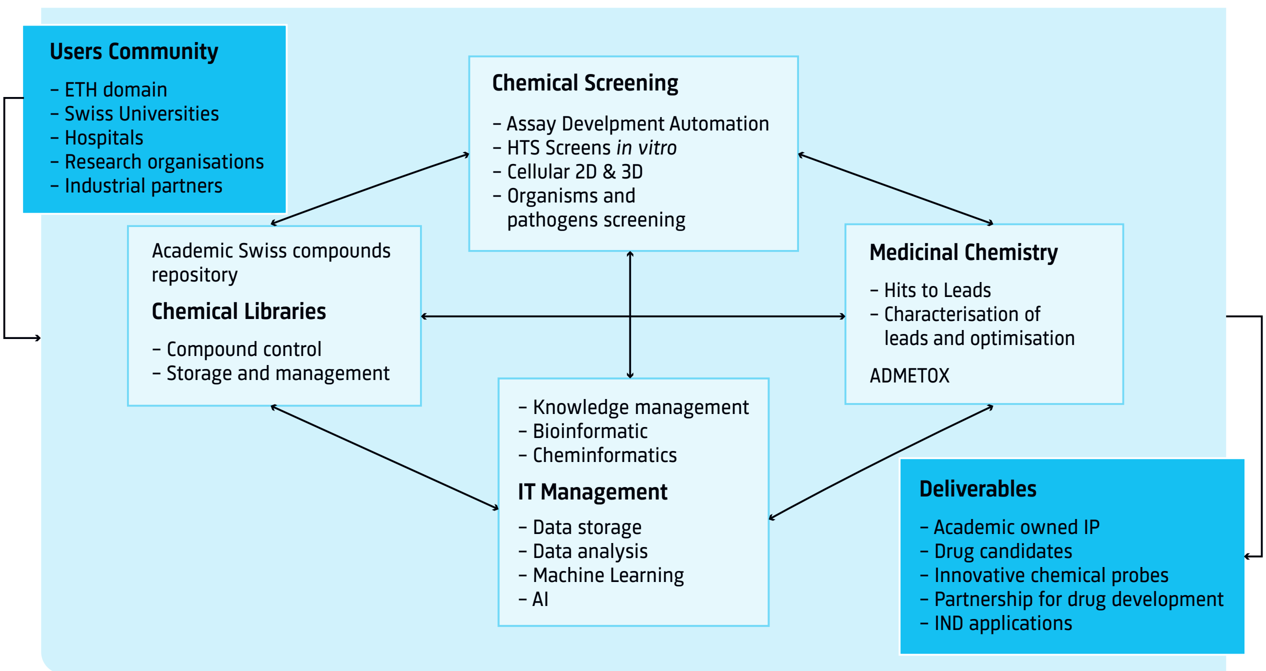
The infrastructures developed during the NCCR Chemical Biology are currently applying operating models aiming at further generating impactful developments for sustainably fulfil the mission of a county-wide coverage of academic drug discovery activities. Since the 2021 thematic roadmap publication, the two platforms at EPFL and UNIGE have been progressing in terms of equipment acquisition, know-how and successfully achieved projects that can be considered as important developments for the National Centre we are envisioning.

Description and development prospects

Recent significant innovations result in a paradigm shift in drug discovery with emerging potential applications of these developments in the field relying in some major evolutions: New chemical diversity needed beyond the traditionally defined drug-like small molecules for difficult-to-address targets and for new screening applications. This includes the generation of libraries of more complex molecules able to modulate protein-protein interactions such as macrocycles collections or specific libraries for targeting protein degradation using proteolysis targeting chimeras (PROTAC) technology and molecular glues approaches. A major evolution in screening assays arise from the development of 3D (organoids, spheroids) cellular assays better recapitulating physiological states aiming at reduce the animal models experimentation and consequently shortening the process of discovery of molecules for therapeutic use.

Future needs – Scientific need and urgency

The main scientific questions to be addressed are directed towards a better understanding of diseases at the molecular level, to provide active compounds (hits) detected through physiologically-relevant chemical screenings



The NCTC plans a complete infrastructure for academic early drug discovery comprising a centralised repository of chemical libraries, screening facilities performing in vitro biochemical assays, cellular assays including 3D multicellular models (organoids), model organisms and Med Chem for hits to leads and leads optimisation. Source: NCTC and further optimised molecules (leads) using Medicinal Chemistry for selecting drug candidates with appropriate potency and absorption, distribution, metabolism and excretion and toxicity (ADME-Tox) properties. Drug discovery for certain disease areas is currently neglected by the pharmaceutical industry. Therefore, it is urgent that through a national infrastructure for translational chemistry, academic research takes the lead for addressing these important public health issues.

Impact

The increasing number of requests at the EPFL and UNIGE platforms from Swiss universities to perform a large variety of screens illustrates a certain national coverage and is reflecting the need of a Swiss-wide structure for academic drug discovery. Constructing a translational center for projects targeting various therapeutic areas will clearly improve Swiss research by providing research groups with a centralised national repository of chemical libraries (commercial and collected from Swiss chemistry labs) and with screening infrastructures. These facilities will cover assays from in vitro biochemical target-based assays to phenotypic screening using automated fluorescence microscopy for a variety of cellular models (i.e. 3D multicellular organoids), model organisms (i.e. C. elegans, zebra fish embryos) and pathogens up to P3 safety level. Moreover, the medicinal chemistry activities planned will contribute to move forward promising projects for translating the academic discoveries into potential drug developments leading to new therapies.

The vision of the NCTC will focus on translational research through the development of existing infrastructures towards a complete national academic drug discovery setting. The centre will address public health challenges in various therapeutic areas not necessarily addressed by the pharmaceutical industry related for instance to infectious diseases including antibiotic resistance, autoimmunity syndromes and rare diseases. The capabilities offered will be beneficial for chemical biology and life science research in general as well as investigations in other fields, including studies on environmental sustainability.

Community

This project proposes the creation of a centre that will provide access to state-of-the-art instrumentation and expertise for translational chemistry research to the Swiss community. Currently, many projects treated at the screening platforms at the EPFL and UNIGE come from external institutions demonstrating the Swiss-wide need. The community of users is to be further enlarged through a centralised National Translational Centre that will federate efforts, resources and centralised investments for further development. We are also handling several projects coming from industrial partners. For these mainly small- and medium-sized Enterprises (SMEs) biotech companies, having access to the infrastructure proposed represents a clear advantage for their projects of drug discovery or screening technologies development. It is expected that a national infrastructure will be open to establish interactions with the industry sector for collaborative projects according with our missions and goals. Early drug discovery is a multidisciplinary endeavor. Synergies with chemistry and medicinal chemistry are essential for the generation of chemical diversity, approaches designed for new mode of action of drugs and improving the molecules detected. The interactions with life sciences researchers are critical since they bring their knowledge in biology, chemical biology and medicine concerning diseases, molecular targets or pathways for the design and development of screening assays. We also expect synergies with bioengineers in the field of assay design, miniaturisation and automation as well with bio-informaticians for the development and application of machine learning approaches in particular for interpreting large sets of image analysis data from high content screens. The EPFL screening facility is in contact with the EU-OPENSCREEN[11] consortium and the European Federation of National Academic Chemical Collections (EUFNACC) association, with the aim of federating and sharing unique academic compounds collected from chemistry groups In Europe.

Vision for the future

A national public drug discovery infrastructure will benefit all Swiss academic settings for efficiently contribute in advancing translational research to be performed in the ETH domain, Swiss Universities, hospitals and in collaboration with the industry sector. A vast domain of disease areas will be covered including those not sufficiently investigated areas such as autoimmune inflammatory, rare and other neglected diseases.

5.6 Electron microscopy and diffraction

Recent developments

The national/international context

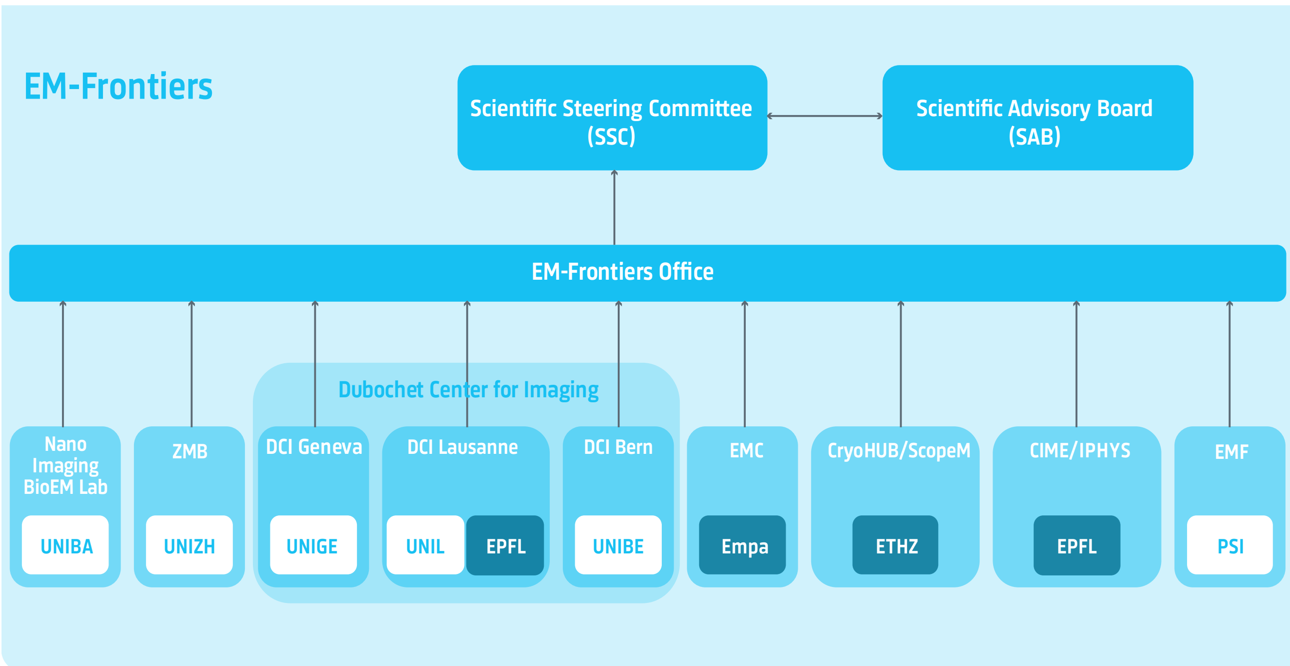
The worldwide market for electron microscopy (EM) is expected to increase by more than 120% from 2022 to 2032, i.e. from about USD 3.9 billion to 8.7 billion.[12] Most of the field is driven by high tech sectors such as semiconductors, photonics and catalysis with 30% in life sciences, especially in structural biology and drug development. This trend reveals that EM experiences a rapid growth in industry, and thus reflects the fast technological advancements in EM modalities. Switzerland hosts a unique expertise in EM, covering life, materials, chemical and physical sciences. Several Swiss companies are leading in specific areas of developing devices for EM (see below). To maintain the leadership position in EM, access to new technologies are needed for academic and industrial research in Switzerland. Specific EM applications often require sophisticated high-end equipment, which is costly and should not be duplicated without need. Specialised EM instruments should therefore be hosted at specific sites and made available to users of other institutions. Networking is thus essential. This allows for an economic operation of the instruments while benefiting from the local expertise.

Major successes

In the previous Chemistry Roadmap 2025–2028 (2021) it was proposed to establish a decentralised research infrastructure (RI). At Swiss research institutions, specialised, but complementary electron microscopes should have been realised which benefit from the synergetic expertise by combining different research fields of EM. A similar effort was suggested in the Biology Roadmap. While independent research proposals were submitted to the corresponding funding institutions, ETH board and SERI asked to consolidate the two initiatives, which led to EM-Frontiers, an interdisciplinary, decentralised RI involving four ETH institutions (ETHZ, EPFL, PSI and Empa) and five Swiss Universities (UNIBAS, UNIBE, UNIGE, UNIL and UZH) including the recently established Dubochet Center for Imaging, see figure. EM-Frontiers was added to the ETH board's and SERI's roadmap for 2025 – 2028. Due to federal budget cuts, beginning of 2024, it was decided to postpone a funding decision for one year. Nevertheless, the inclusion of EM-Frontiers in the RI roadmaps 2025 – 2028 highlights the urgent need to enhance these capabilities in Switzerland. Moreover, the fact that a life-science initiative and an initiative in the physical sciences were successfully merged, underlines the need for an interdisciplinary RI, where methodologies and expertise of both disciplines can synergise.

Description and development prospects

Since the last roadmap, further fields and materials have been identified to be critical to research and the tech-



EM-Frontiers: institutions involved in EM-Frontiers and its management structure. Each institution operates a specific EM instrument as part of the research infrastructure. Source: EM-Frontiers nological development in Switzerland (e.g. metal-halide perovskite quantum dots, metal organic frameworks (MOFs), self-assembled nanomaterials). These growing fields are critical to both academics and companies situated in Switzerland. National efforts in catalysis research (NCCR Catalysis – SwissCat+) require additional efforts to monitor, e.g. details about individual atoms under function while on the other hand infrastructures are meant to address large numbers of samples for high throughput experimentation. This includes experimentation at liquid He temperature or measurements at ultra-short time scales. Additionally, the Federal Council created the Swiss Quantum Initiative in 2022 to consolidate Switzerland's excellent position in the field of quantum technology. These and other emerging fields rely on state-of-the-art equipment for materials characterisation and similarly important, on expert teams to support their application.

Future needs – Scientific need and urgency

Impact

The findings from the Chemistry Roadmap 2021 still hold as the most important strategic directions in EM. Three areas were in focus: operando experiments, dynamic and ultrafast effects and crystal structure determination. The growing interest in quantum materials, batteries, catalysis or protein crystals, to mention a few, requires world-class dedicated equipment. Advanced EM characterisation is pivotal to understand these material systems, which are expected to strongly affect our society with challenges such as net zero emission, quantum computing or drug design. It is thus pivotal to have local access to infrastructures able to support the development of such materials and substances in order to realise the technologies that advance our society. The need for realizing new EM technologies is reflected by the success of several Swiss companies active in this area, e.g. ELDICO Scientific (diffractometers),[13] Dectris Ltd. (detectors),[14] condenZero (cryo technology)[15] or attolight (CL spectroscopy).[16] In addition, due to the big data often recorded with these new technologies, data handling, analysis and local storage has become challenging. Solutions are needed for automation, possibly leveraging our progress in AI assisted techniques. OpenEM,[17] a Swiss Open Research Data Grants (CHORD) project funded by ETH and SwissUniversities, is a first initiative to address this emerging challenge. Democratisation of high-end EM instrumentation has become a key aspect. We thus propose to establish a national system similar to ESTEEM3[18] or to Microscopy Australia[19] that 1) logistically facilitates access to specialised instruments nationwide, 2) provides educational support and 3) enables financial means for realizing cross-institutional projects and instrument access.

Community

While EM for life science is covered in the Biological Imaging chapter of SCNAT's Biology roadmap, there is a significant and increasing overlap between both fields. As an example, development and instrumentation for ultra-fast EM and diffraction-based structure determination benefit both material and life sciences. It is thus important to synergise with the bioimaging community to coordinate RIs as has been done with the EM-Frontiers initiative. EM facilities benefit already thousands of students and researchers as well as several industries in key sectors such as photonics, microtechnology, advanced manufacturing and drug development. However, equipment limitations in Switzerland often causes researchers to depend on infrastructures abroad. Without a clear structure and without financial support allowing Swiss researchers to build cross-institutional research projects, access to high-end EM proves to be difficult in Switzerland.

Vision for the future

To address the above discussed scientific challenges, the establishment of a Swiss EM network, as targeted by EM-Frontiers, is more important than ever. Making specialised EM instrumentation available to the relevant communities benefits researchers in academia and industry. It is highly critical to ensure that these facilities have the human resource to support nationwide needs.

5.7 Radiochemistry: Targeted Alpha Tumour Therapy and Other Oncological Solutions

Recent developments

The national/international context

Research needs towards radiopharmaceutical development for theragnostic application, using relevant radionuclides for cancer imaging and therapy, is on the increase. The nuclear medicine industry looks to benefit from research and development, resulting in pressure on radiochemistry research to come up with new ideas to combine new nuclides with new ligands being developed towards radioligand therapy. New clinical trials are coming into play (^{161}Tb in Switzerland) along with interest in other difficult-to-produce alpha emitters (e.g. ^{212}Pb).

Major successes

No new infrastructures have been implemented, however, new results of ^{149}Tb development as part of the PSI/ISOLDE collaboration have been published[20] and presented at international radiopharmacy/nuclear medicine conferences. The development of this novel nuclide is as a result of optimizing the collection thereof, along with its mass isobars and impurities using the ISOL concept. The yield of the collection, as a result, substantially increased. This, along with an optimised chemical separation method ensured radionuclidically and chemically pure product for use in preclinical therapeutic experiments.

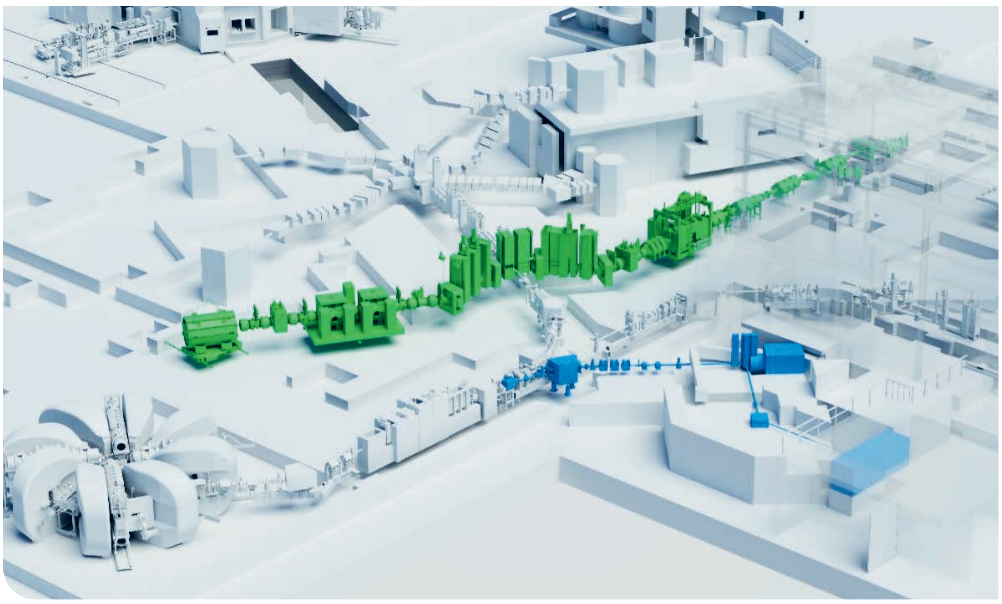
Description and development prospects

The IMPACT (Isotope and Muon Production using Advanced Cyclotron and Target technologies) project aims to produce and fully exploit unprecedented intensities and quantities of muons and radionuclides at the High Intensity Proton Accelerator (HIPA) for advancements in particle physics, chemistry, materials science, life sciences, medicine, and clinical research. Two new target stations, one for High-Intensity Muon Beams (HIMB), and one for TATTOOS online isotope separation facility, will significantly extend the existing infrastructure. TATTOOS will provide unrivalled quantities of a wide range of previously unobtainable radionuclides.

There has been a timeline change within IMPACT, where TATTOOS will begin two years later than the HIMB part of the project. This is due to financial and manpower issues, as the people involved will have to complete another large-scale project, creating some overlap. This was agreed with the ETH Board and TATTOOS will be expected to have first beam on target in 2030, instead of 2028.

Future needs – Scientific need and urgency

ISOL-produced radionuclides for radiopharmaceutical application requires basic physics, radiochemistry and radiopharmaceutical research, all of which could lead to clinical theragnostic application. The infrastructure is urgent, as initial basic research in this field has already raised the point/desire of clinical need from clinicians.



The proposed IMPACT (Isotope and Muon Production using Advanced Cyclotron and Target technologies) project to be implemented at PSI's HIPA facility, consisting of HIMB (in green) and TATTOOS (in blue), respectively. Source: PSI

Impact

TATTOOS will one of only three facilities of its kind worldwide dedicated to this form of radiochemical/radiopharmaceutical/physics research towards potential nuclear medicine/clinical application. The only other facility in Europe that will focus on similar research is MYRRHA at SCK CEN[21] (Belgium), however, the initial energy used for their research will be vastly different. The other facility, currently under construction, is ARIEL at TRIUMF[22] (Canada).

The use of the TATTOOS facility addresses a health need: the diagnosis and therapy of cancer.

Community

The community consists of radiochemists, radiopharmacists, nuclear/accelerator physicists, nuclear medicine physicians, medical physicists and engineers. The community is constantly growing.

The facility and its use will be of interest to industry, particularly pharma, as well as the potential for industry to utilise the technology developed towards other facilities of its kind to be built in future.

Switzerland is involved in PRISMAP[23] – a European network for medical radionuclides. It is expected to continue in this vein in the long term and TATTOOS is greatly anticipated.

Vision for the future

TATTOOS will substantially extend the capabilities that can be extracted from HIPA as a large research facility, thus, enhancing its value for the Swiss and international user base. Radiochemistry and radiopharmaceutical facilities at UZH and USZ will optimally leverage this potential to spur clinical research with novel radiopharmaceuticals for targeted tumour therapy, a rapidly developing field with outstanding potential for personalised medicine. An upgrade of PSI's neutron spallation source facility SINQ is proposed for 2033–2036 (SINQ++), which is discussed in the Swiss Neutron Science Roadmap. This would exploit an increased neutron flux for the development of neutron-rich radionuclides towards potential cancer therapy.

In the longer term, researchers far beyond the initial core user groups could benefit from IMPACT, specifically in astrophysics, materials science and radiochemistry. The facility will continuously engage with the research base in order to continue maximising its potential for research and innovation in Switzerland.

5.8 New: Pilot plant for chemical- and bioprocesses

Context (national and international), scientific rationale, and challenges

Switzerland has long held a prominent position in the global scientific community, particularly in the fields of chemistry and life sciences. Known for its world-class research institutions and thriving industrial sector, Switzerland has been responsible for numerous groundbreaking discoveries. However, a persistent challenge remains: the translation of these discoveries into commercially viable products. One of the key barriers to this progression is the lack of access to infrastructure capable of scaling up chemical and biotechnological processes from the lab to market. This transition is particularly challenging for smaller entities like start-ups and research groups, which often lack the resources and facilities to produce materials in quantities sufficient for commercialisation. While innovation thrives in Swiss universities and research centers, the lack of scale-up infrastructure causes many promising discoveries to stagnate before reaching industrial application. The absence of such infrastructure in most academic institutions leaves research groups unable to bridge the gap between laboratory-scale experiments and the quantities required for proof-of-market applications.

The HEIA (Haute Ecole d'Ingénierie et d'Architecture of the HES-SO in Fribourg) is home to the only atmospheres explosibles (ATEX) fully equipped pilot plant in Switzerland, providing a critical solution to this infrastructure gap. This facility is unique within the Swiss academic landscape, offering reactors up to 630L and purification equipment capable of processing large amount of material. While some universities of applied sciences have smaller-scale reactors and distillation columns, they lack the comprehensive suite of equipment needed for full-scale production. The facility has already attracted industry partners like Firmenich, Straumann, Deasyl or Metalor, fostering collaborations that push the boundaries of chemical research and development. Participation in Innosuisse projects and several European initiatives further highlights the plant's role as a leader in chemical process innovation. For start-ups like Bloom Biorenewables, Seprify, and various projects at the Adolph Merkle Institute and at the University of Fribourg, this facility has been essential in navigating the 'valley of death' that so often derails innovative projects.

This limitation is not only felt in Switzerland but is common throughout Europe. On an international level, the HEIA pilot plant represents a unique asset in academia, offering significant opportunities to advance chemical research and industrial applications. Potential users of the facility include Swiss and European universities, applied universities, and federal institutes of technology, as well

One of the three 100L glass-lined reactors at HEIA-FR. Source: HEIA-FR/HTA-FR as start-ups and SMEs. These institutions and companies span a wide array of industries, from pharmaceuticals and materials science to biotechnology and environmental sustainability. The pilot plant is particularly well-suited for research groups that require large quantities of specialised compounds, such as therapeutic molecules, gels, pesticides, polymers, nanoparticles, or single-atom catalysts, to continue their research or to move closer to commercialisation. Such infrastructure will also serve technology transfer offices at the various research institutions (e.g. Alliance) and other organisations that supports business creation (e.g. Fri Up).

Aims of the proposed infrastructure

The HEIA, faculty has seen a sharp increase (3 times more) in demands for scale-up within the last 10 years. Half of these are from start-ups, the rest from SME and universities. This is most probably because more start-ups are being created in healthtech, cleantech, material sciences and pharmaceutics (1.9 billion CHF invested in 2022). In addition, universities are increasingly encouraged to add value to their discoveries by bringing them to market or creating start-ups, for example. To meet these growing demands for new-generation processes and to service Swiss and European academic and industrial partners, the aim is to create a LRI for scale-up by improving the existing assets at HEIA and complementing them with external biotech infrastructures from other universities.

The primary goal of this LRI is to establish a high-performance, open-access hub that bridges the gap between academic research and industrial application. By providing a collaborative environment and state-of-the-art equipment, the facility will enable research groups, universities, start-ups, and small companies to scale up their laboratory processes to pre-industrial volumes. This infrastructure is vital for producing multi-kilogram quantities of compounds necessary for further testing, optimisation, and market validation. By offering this platform, the pilot plant will play a pivotal role in fostering innovation and contributing to Switzerland's economic growth.

Significant efforts and investments have been made to establish the current pilot plant at HEIA, focusing primarily on batch chemistry. 20–30 years ago, processes were developed almost exclusively in batch chemistry and the target molecules were relatively simple. In the last 10–15 years, research scope changed, new materials emerged, target molecules are more complex, production technologies have improved, and new tools appeared. To stay at the forefront of chemical research and industry needs, the existing capabilities must evolve by integrating equipment for continuous reactions and intensified processes. Thus, another aim is to expand the existing infrastructure by investing in cutting-edge technologies for process intensification to accommodate new and emerging chemical processes, such as continuous flow reactions, photochemistry, and electrochemistry. The facility will also integrate data management, process control, and Process Analytical Technologies (PAT) to improve precision and efficiency. The future plant will focus on incorporating more sustainable processes, aligning with the global shift towards greener chemical production methods. Thus, another aim is to complement the facility of HEIA for chemical processes with external biotech infrastructures for bioprocesses, for example through partnerships with FHNW, ZHAW, HES-SO/VS and BCC (Biofactory Competence Center).

In conclusion, by continually upgrading its capabilities, the plant will ensure that Switzerland remains at the forefront of chemical and biotechnological research, capable of responding to emerging challenges in these rapidly evolving fields. This LRI serves as a critical resource for scaling up chemical processes and bioprocesses, ensuring that innovative discoveries can move beyond the laboratory and into the marketplace. The goals of this infrastructure are:

- Offering an open-access hub bridging academic research and industry: the pilot plant offers a platform for collaboration, enabling researchers and industry to scale up bioprocesses and chemical processes. By supporting knowledge transfer and practical application, it accelerates innovations from lab to market.

- Upgrading the HEIA pilot with advanced data treatment and process intensification equipment. The plant will modernise its capabilities with real-time data tools, PAT systems, and new equipment to improve process efficiency and address sustainability challenges in response to evolving industry and academic needs.

- Integrating bioprocessing to meet growing biotech demand: by expanding the chemical infrastructure of HEIA to include bioprocessing. This will create a multidisciplinary hub that caters to both chemical and biotech partners.

5.9 New: Cultural heritage science consortium

Context (national and international), scientific rational and challenges

Cultural heritage science is an transdisciplinary field combining natural sciences, humanities, and engineering to study and preserve our significant historical and artistic legacy. It addresses questions about ancient techniques, uncovering artists' secrets, material histories of objects and buildings, including their management and preservation. Analytical chemistry plays a crucial role in this field, determining composition, alteration mechanisms, age, origin, etc. and includes development of conservation strategies and materials to protect the world's multifaceted heritage.

In a global context, several European countries have well established research programs to support their cultural heritage science community and to enable connections among researchers from the different disciplines involved. To cite one example, the Netherlands Institute for Conservation+Art+Science+ (NICAS)[24] has successfully federated both museums, cultural heritage institutions and academics. Europe is at the forefront of this emerging field of research as the E-RIHS[25] is entering the final stage of its implementation phase (2022-2024) before the creation of the European Research Infrastructure Consortium (ERIC). This is a strong signal from the European Union, that is embracing the continuous growth of heritage sciences to preserve testimony to our cultural past, and which is becoming an increasingly complex task.

Across Switzerland, numerous researchers are active in the field of heritage science with complementary skills, state of the art equipment and expertise distributed among existing research infrastructures, universities, and heritage institutions. As such a wide panel of objects/materials are studied conveying painting, glass, metal, stone, ceramic, stucco, wall paintings, concrete, plastics, paper, textile, wood, foodstuffs, electronic media and restoration materials. While Switzerland's contributions to heritage science research are internationally acknowledged, Switzerland is not yet part of the E-RIHS network as an official Swiss node is missing.

Analytical expertise available among Swiss research institutions include:

— Physical-mechanical properties analysis (BFH-HKB, HESSO-HE-Arc CR, SUPSI)

— Material characterisation/identification
  - Portable devices for non-invasive investigations (ESC-UNIL, HESSO-HE-Arc CR, PSI, SNM, SUPSI)
  - Spectroscopy (BFH-HKB, ESC-UNIL, HESSO-HE-Arc CR, PSI, SNM, SUPSI, Natural History Museum of Geneva)
  - Ion beam analysis (ETHZ-LIP)
  - Chromatography (ESC-UNIL, BFH-HKB, HESSO-HEIA)
  - Elemental analysis (BFH-HKB, ESC-UNIL, HESSO-HE-Arc CR, PSI, SUPSI)
  - Imaging, surface and stratigraphic analysis (BFH-HKB, ESC-UNIL, SIK-ISEA, SNM, PSI)

— Radiocarbon dating (ETHZ-LIP) and compound specific radiocarbon analysis (HESSO-HEIA)

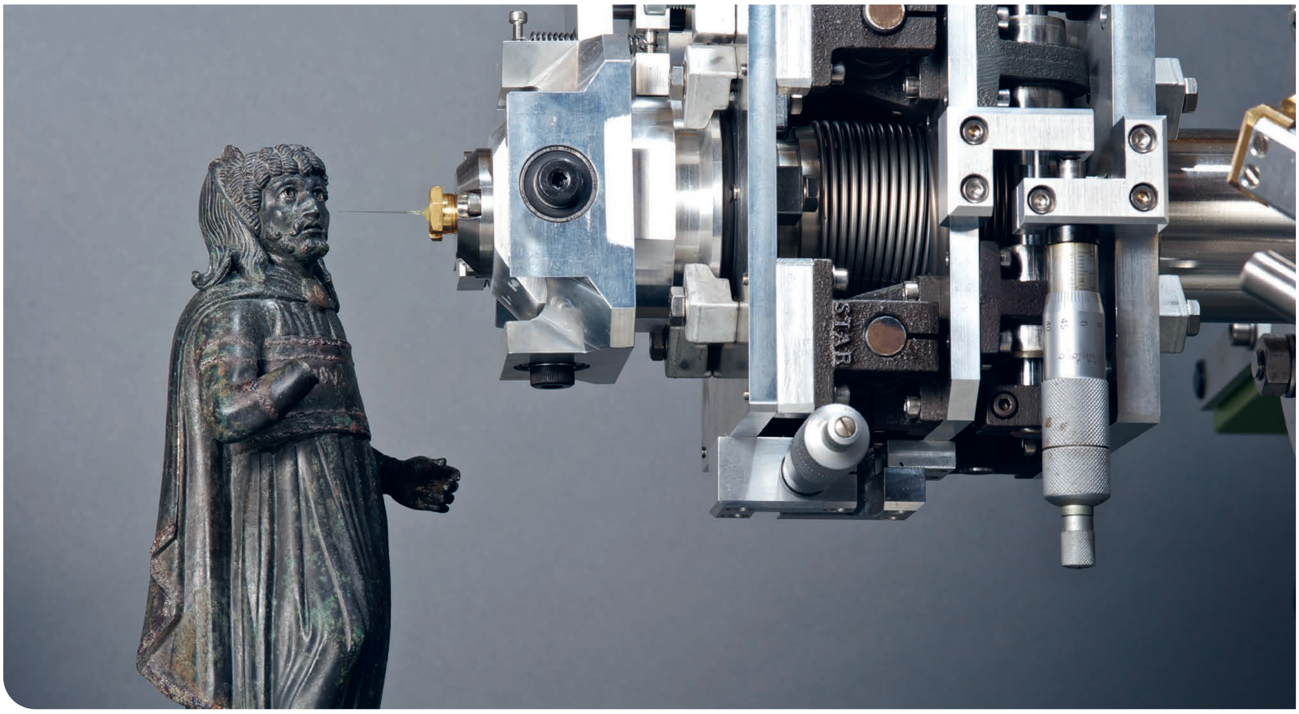
— Imaging and scattering techniques with (synchroton) X-rays, muons and neutrons (PSI)

— Authentication (BFH-HKB, ESC-UNIL, SIK-ISEA)

Aims of the proposed infrastructure

Today, Swiss heritage scientists want to grow as a community, because unity creates strength. In order to support the growing heritage science community, we therefore propose to build a distributed analytical chemistry-based CHS network to 1) consolidate specialised competences available across Switzerland, 2) strengthen Switzerland's position as a strategic stakeholder in national, European and international research programs and 3) provide access to instrumentation and data, as well as awareness and training opportunities in heritage science. While humanistic expertise is more easily shared, the establishment of a formal analytical chemistry network is essential. With scientific research at its core, our aim is to bring together different sites that host and develop complementary instruments/know-how and leading expertise to study cultural heritage from all angles to provide necessary knowledge and to guarantee conservation.

The Swiss Conservation Restoration Campus (BFH-HKB, HESSO-HE Arc CR, SUPSI) is intended to take the lead, building the bridge between art conservation practice, natural sciences and the humanities. Additional institu-



Investigation of a roman quaternary alloy figurine composition, known as the 'Tragic Actor', using ion beam analysis at the Laboratory of Ion Beam Physics (LIP) at ETH Zurich. Object owner: Site et Musée romains d'Avenches SMRA, inventory number 1864/01286a. Source: H. Hostettler, ETHZ

tions with key capabilities to this end are listed below and will be associated partners, bringing their specific expertise, methods and equipment to the table.

Together we will provide expertise and facilitate access to analytical infrastructure for (inter)national research and service activities, as well as inter- and trans-disciplinary collaborations. From the humanities, the social and the natural sciences, advanced knowledge on some of the most intricate, complex and fascinating problems in cultural heritage will be gained and shared. The proposed consortium will contribute to academic education and work towards a sustainable future of our cultural heritage legacy, making highly specialised know-how among the Swiss Institutions accessible to many users (non-exhaustive lists):

– Academic research institutions: BFH-HKB, HESSO-HE-Arc CR, HESSO-HEIA, SUPSI, ETHZ LIP, Archaeometry of Ancient Metals group (UNIFR), School of Criminal Justice (ESC-UNIL), UZH, Swiss Art Research Infrastructure (SARI), Cultural Heritage & Innovation Center (EPFL), Durability of Engineering Materials Group (ETHZ) and Construction Heritage and Preservation Group (ETHZ), Applied Materials Group (PSI), TOMCAT synchrotron X-ray imaging group (PSI), Muon Spin Spectroscopy Lab (PSI), ISA Accademia di Architettura Mendrisio (USI)

– Heritage institutions: Swiss Institute for Art Research (SIK-ISEA), Swiss Research Centre for Stained Glass and Glass Art (Vitrocentre), Abegg-Stiftung Riggisberg, Swiss National Museum (SNM) – The collection centre, Musée d'ethnographie de Genève (MEG) , Natural History Museum of Geneva.

– Customers gaining from infrastructure know-how, research and services: museums, cantonal monument preservation, cantonal archaeology departments, historic building architecture, public and private conservator restorers.

6 Conclusions

This Update of the Chemistry Community Roadmap proposes the discovery-driven and challenge-driven research infrastructures (RI) that are required to keep the Swiss chemistry community in academia and in industry at the forefront of international research in the chemical sciences. The proposed infrastructures will enable scientists to translate knowledge into solutions for the current global challenges in energy, environment, health and sustainability.

The Swiss chemistry community has realised the necessity to join forces and to collectively install frontier instrumentation, open to all, at a higher level than is possible by individual university units. The community underlines the need for national infrastructures in order to enable access to state-of-the-art large instrumentation and expertise that can no longer be hosted by single institutions. Moreover, these facilities should provide inter- and transdisciplinary support and expertise to users to improve data acquisition and analysis, one of the key challenges in chemical research and a necessary step toward improving scientific quality and in moving towards quality open data.

Nine key enabling infrastructures have been identified and updated, three discovery-driven research infrastructures and five challenge-driven research infrastructures and a network-driven infrastructure:

Discovery-driven research infrastructures

→ Discovery RI-1: An electron microscopy and diffraction hub

→ Discovery RI-2: A magnetic resonance and magnetism hub

→ Discovery RI-3: A Centre for *operando* synchrotron studies

Challenge-driven research infrastructures

→ Challenge RI-1: A facility to produce Terbium radionuclides for diagnostics and treatment of disease

→ Challenge RI-2: A mass spectrometry-based screening platform for (bio)catalysts and environmental samples

→ Challenge RI-3: A centre that provides state-of-the-art instrumentation for translational chemistry and manages a national library of compounds synthesised in academic laboratories across Switzerland

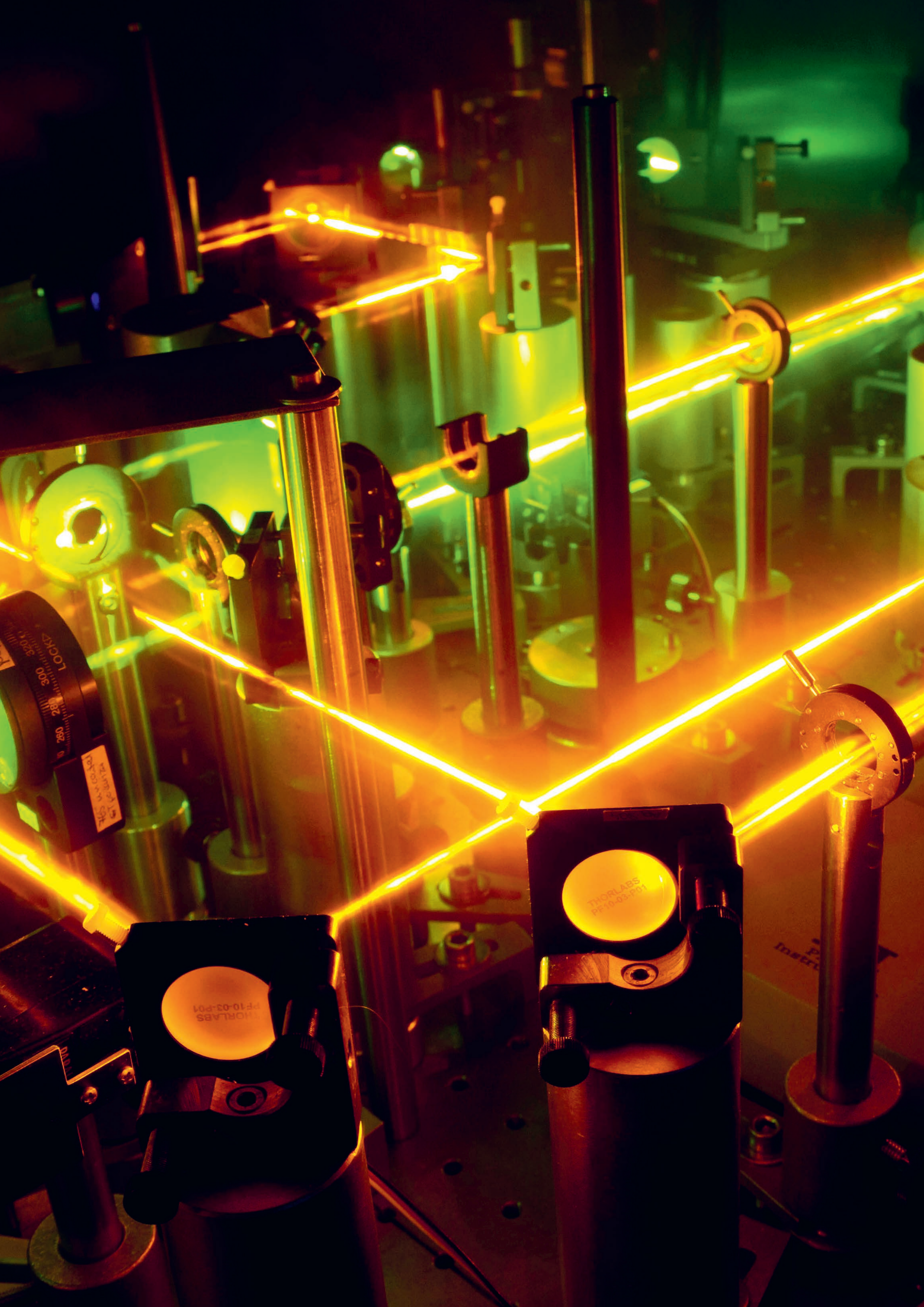
→ Challenge RI-4: A catalysis hub (SwissCAT+) to discover and develop catalysts and catalytic processes towards a sustainable society

→ Challenge RI-5: A pilot plant to upscale chemical and bioprocesses (new)

Network-driven research infrastructures

→ Network RI-1: A consortium to foster Swiss heritage science (new).

The infrastructures proposed in this Chemistry Roadmap for Research Infrastructures will build on existing Swiss expertise and aim to be tightly linked to other community roadmaps, namely the Photon Science Community Roadmap, the Neutron Science Community Roadmap, the Biology Community Roadmap and the Geosciences Community Roadmap. The ultimate goal is to provide unique world class facilities to the Swiss and international science community. As a result, Switzerland will remain attractive and innovative in chemical sciences, one of the key assets of Switzerland at the international level, and an essential component for a sustainable development of Switzerland.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7 Links

1 https://zenodo.org/records/4572642

2 https://www.eda.admin.ch/aboutswitzerland/en/home/wirtschaft/taetigkeitsgebiete/chemie-und-pharma.html

3 https://www.sbfi.admin.ch/dam/sbfi/en/dokumente/2023/06/roadmap_forschungsinfrastrukturen_2023_teil_1.pdf.download.pdf/Roadmap_Forschungsinfrastrukturen_2023_Teil_1_EN.pdf

4 https://ord-premise.org

5 https://www.zhaw.ch/ccbio

6 https://catplus.ch

7 https://www.chem.uzh.ch/en/research/services/htel.html

8 https://bsse.ethz.ch/laf

9 https://swissnmr.ch

10 https://panacea-nmr.eu

11 https://www.eu-openscreen.eu

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20 https://www.nature.com/articles/s41598-024-53610-2

21 https://www.sckcen.be/en/infrastructure/myrrha

22 https://www.triumf.ca/ariel-advanced-rare-isotope-laboratory

23 https://www.prismap.eu

24 https://www.nicas-research.nl

25 https://www.e-rihs.eu

8 Acronyms

2D, 3D	Two-dimensional, three-dimensional
ADME-Tox	Absorption, Distribution, Metabolism, Excretion and Toxicity
AI	Artificial Intelligence
ARIEL	Advanced Rare Isotope Laboratory at TRIUMF
ATEX	Atmospheres Explosibles
Battery2030+	European large-scale, long-term research initiative
BCC	Biofactory Competence Center
BFH	Berner Fachhochschule, University of Applied Sciences Bern
BFH-HKB	Hochschule der Künste Bern, University of the Arts Bern
CERN	Conseil Européen pour la Recherche Nucléaire, European Council for Nuclear Research
CHS	Cultural Heritage Science
CO_2	Carbon dioxide
COSS	Center for Operando Synchrotron Studies
COST	European Cooperation in Science and Technology
CRC	Conservation Restoration Campus
ELIXIR	European Life Science Infrastructure for Biological Information at ESRF
EM	Electron microscopy
EM-Frontiers	Electron microscopy Frontiers
Empa	Eidgenössische Materialprüfungsanstalt, Swiss Federal Laboratories for Materials Science and Technology
EPFL	École Polytechnique Fédérale de Lausanne
EPR	Electron paramagnetic resonance
ERIC	European Research Infrastructure Consortium
E-RIHS	European Research Infrastructure for Heritage Science
ERI	Education, Research and Innovation
ESC-UNIL	Ecole des Sciences Criminelles, School of Criminal Justice of UNIL
ESRF	European Synchrotron Radiation Facility
ESS	European Spallation Source
ETHZ	Eidgenössisch Technische Hochschule Zürich, Swiss Federal Institute of Technology Zurich
EU	European Union
EUFNACC	European Federation of National Academic Chemical Collections
FAIR Principles	Principle for research data, standing for Findable, Accessible, Interoperable, and Reusable
FDFA	Federal Department of Foreign Affairs
FHNW	Fachhochschule Nordwestschweiz, University of Applied Sciences and Arts Northwestern Switzerland
GHz	Gigahertz
GRAIL	High Throughput Screening Hub for Chemical Biology
HEIA-FR	Haute Ecole d'Ingénierie et d'Architecture de Fribourg, part of the University of Applied Sciences and Arts of Western Switzerland HES-SO
HES-SO	Haute école spécialiseée de Suisse Occidentale, University of Applied Sciences and Arts of Western Switzerland
HESSO-HE-Arc CR	Haute Ecole Arc Conservation-Restauration
HIMB	High-Intensity Muon Beams
HIPA	High Intensity Proton Accelerator
HT	High Throughput
HTE	High Throughput Experimentation
IBM	International Business Machines Corporation
IOR Bellinzona	Institute of Oncology Research
IMPACT	Isotope and Muon Production using Advanced Cyclotron and Target technologies
ISA	Istituto di storia e Teoria dell-arte e dell'architettura, Institute of the History and Theory of Art and Architecture at USI
ISOL	Isotope Separation On-Line
ISOLDE	Isotope Separator On-Line Device Radioactive Ion Beam Facility
LIP	Laboratory of Ion Beam Physics at ETHZ
MEG	Musée d'ethnographie de Genève, Ethongraphic museum Geneva
ML	Machine Learning
MOF	Metal organic frameworks
MR	Magnetic resonance
MYRRHA	Multi-purpose hYbrid Research Reactor for High-tech Applications at the Belgian Centre for Nuclear Research
ncAA	Non-canonical amino acid
NCCR	National Centres of Competence in Research
NCTC	National Centre for Translational Chemistry
NICAS	Netherlands Institute for Conservation+Art+Science+
NMR	Nuclear magnetic resonance
OPENSCREEN	European Research Infrastructure Consortium on chemical biology tools
ORD	Open Research Data
PANACEA	Pan-European solid-state NMR Infrastructure for Chemistry-Enabling Access

PARC	European Partnership for the Assessment of Risks from Chemicals initiative
PAT	Process Analytical Technologies
Pb	Lead (chemical element)
PFAS	Per- and polyfluoroalkyl substances
PREMISE	ORD program of the ETH Board
PRISMAP	European network for medical radionuclides
PROTAC	Proteolysis targeting chimeras
PSI	Paul Scherrer Institute
R&D	Research & Development
R'Equip	Research Equipment funding scheme of the SNSF
REA	European Research Executive Agency
RI	Research infrastructure
SARI	Swiss Art Research Infrastructure
SCHS	Swiss Cultural Heritage Science
SCNAT	Swiss Academy of Sciences
SERI	State Secretariat for Education, Research and Innovation
SIK-ISEA	Swiss Institute for Art Research
SCK CEN	Studiecentrum voor de Toepassingen van den Kernenergie, Belgian Nuclear Research Centre
SLS	Swiss Light Source
SME	Small- and medium-sized Enterprises
SNBL	Swiss Norwegian Beamline at ESRF
SNFS	Swiss National Science Foundation
SNM	Swiss National Museum
SwissCAT+	Swiss Catalysis Hub – a data-driven HTE platform located at EPFL and ETHZ
SUPSI	Scuola universitaria professionale della Svizzera Italiana, University of Applied Sciences and Arts of Southern Switzerland
SUPSI-DACD	Department of Environment Constructions and Design at SUPSI
TATTOOS	Targeted Alpha Tumour Therapy and Other Oncological Solutions
Tb	Terbium (chemical element)
TOMCAT	Syncrotron X-ray Imaging Group
Tox	Toxicity
TRIUMF	TRI-University Meson Facility, Canada's particle accelerator centre
UNIBAS	University of Basel
UNIBE	University of Berne
UNIFR	University of Fribourg
UNIGE	University of Geneva
UNIL	University of Lausanne
USI	Università della Svizzera Italiana
USP	Universitätsspital Zürich, University hospital Zurich
UZH	University of Zurich
Vitrocentre	Swiss Research Centre for Stained Glass and Glass Art
XAFS	X-ray absorption fine structure
XAS	X-ray absorption spectroscopy
XFEL	European X-Ray Free Electron Laser (at ESRF)
XRD	X-ray diffraction
ZHAW	Zürcher Hochschule für angewandte Wissenschaften, Zurich University of Applied Sciences

SCNAT – network of knowledge for the benefit of society

The **Swiss Academy of Sciences (SCNAT)** and its network of 35,000 experts works at regional, national and international level for the future of science and society. It strengthens the awareness for the sciences as a central pillar of cultural and economic development. The breadth of its support makes it a representative partner for politics. The SCNAT links the sciences, provides expertise, promotes the dialogue between science and society, identifies and evaluates scientific developments and lays the foundation for the next generation of natural scientists. It is part of the association of the Swiss Academies of Arts and Sciences..