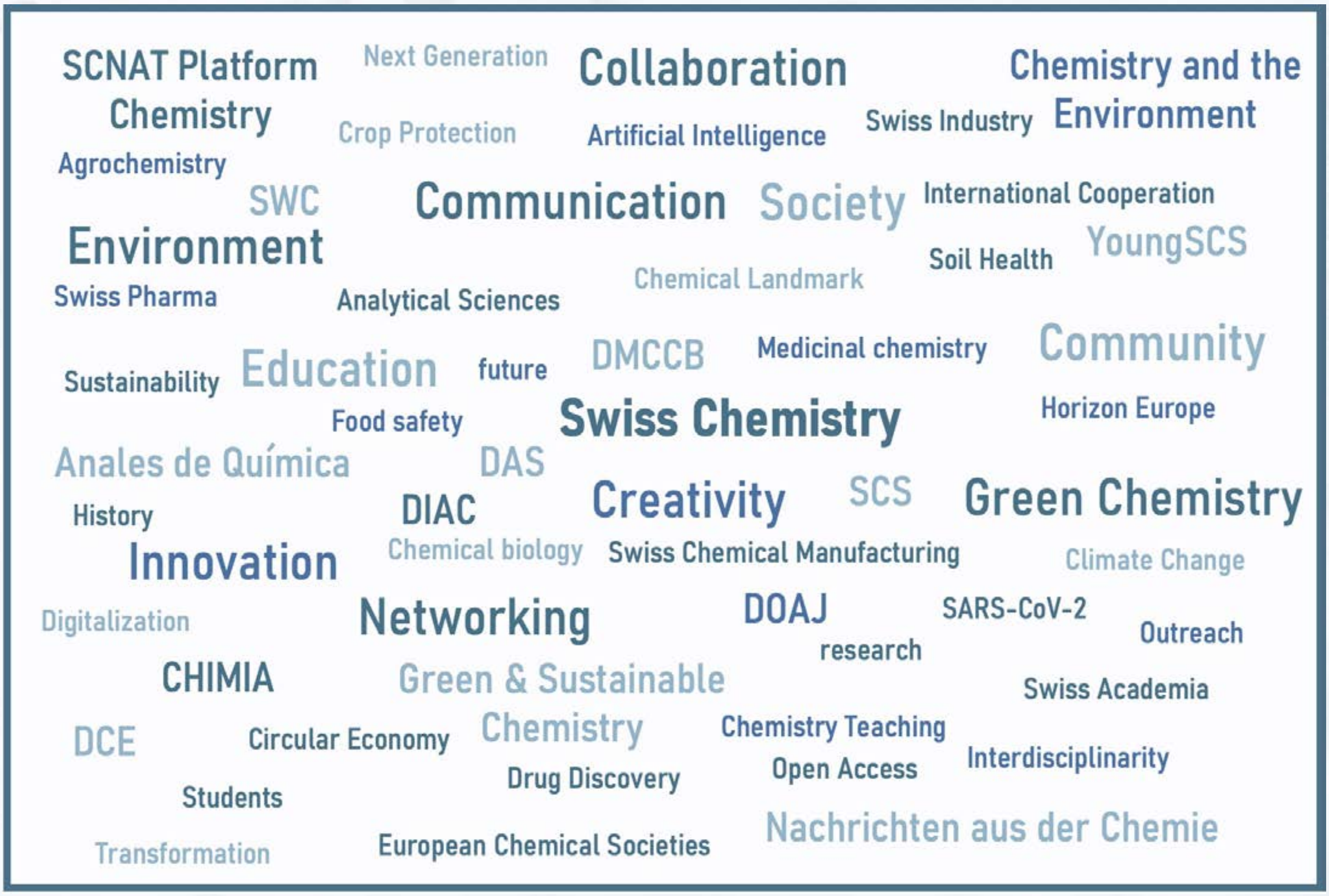
CHIMIA 2021, vol. 75

CHIMIA

75 ANNIVERSARY

Perspectives on Chemistry and Society on the Occasion of the 75th Anniversary of CHIMIA



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Swiss Chemical Society

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Perspectives on Chemistry and Society on the Occasion of the 75th Anniversary of CHIMIA

In 2021, CHIMIA published its 75th volume, after being called into life in 1947. To celebrate this milestone, throughout the year, we published short opinion pieces by invited authors on wide-ranging topics including science, industry, the environment, education, society, and politics under the title 'A Perspective on Chemistry and Society'. We asked the authors to look forward rather than back and address current and future prospects for chemistry and society.

The authors are experts in their fields and represent the Divisions and Sections of the Swiss Chemical Society, universities, industry, and many other fields and we hope that you were able to take the opportunity to read and enjoy these articles and that they provided much food for thought.

In this special open access issue, which is available online, we present all twenty-two 75th Anniversary articles so that they can be enjoyed once more as a whole.

We would like to thank all the authors who generously and enthusiastically contributed their insightful thoughts and took the time to write these articles.

We look forward to many more volumes of CHIMIA while developing and improving both in print and online and thank the Swiss Chemical Society for the constant support and encouragement.

CHIMIA Editorial Board

Perspectives on Chemistry and Society on the Occasion of the 75th Anniversary of CHIMIA

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A Perspective on Chemistry and Society

A Column on the Occasion of the 75th Anniversary of CHIMIA

The President of the Swiss Chemical Society

75th Anniversary of CHIMIA, the Essential Communication Link of the Swiss Chemical Society

Alain De Mesmaeker*

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Alain De Mesmaeker was born in Brussels, Belgium (1955). He earned his licence and PhD in Chemistry (1983), Catholic University of Louvain-La-Neuve, Belgium (Synthesis/thermal isomerisation of capto-dative cyclopropanes, Prof. H. G. Viehe). He undertook post-doctoral research (1983–1985), at the Weizmann Institute of Sciences, Israel (Total synthesis of carba-clavulanic acid, Prof. M. D. Bachi). He then became Group Leader in the Central Research Laboratories, Ciba-Geigy, Basel, Switzerland (1985–1996: Natural Products synthesis, Radical Chemistry, Carbohydrates, Nucleic Acids, Combinatorial Chemistry), followed by Head of Research Chemistry, Novartis Crop Protection (1997–2000), Global Head of Research Chemistry, Syngenta (2000–2008), Principal Chemistry Expert, Principal Syngenta Fellow (2008–2020). He and his team were awarded the Sandmeyer Award (2018) and he has served as President of the Swiss Chemical Society from 2016 to 2021.

This year we have the pleasure to celebrate the 75th anniversary of CHIMIA and I take the opportunity to underline the essential roles that this journal plays and will continue to play in the future for the Swiss Chemical Society (SCS).

CHIMIA is the official journal of the SCS and, consequently, is the main communication channel with our members, partners and with the international scientific community. The second journal of the SCS is *Helvetica Chimica Acta*, edited in collaboration with Wiley-VHCA, which is exclusively focusing on original research articles.

CHIMIA publishes very high-quality scientific articles mainly in thematic issues covering a broad range of very relevant topics, which are actively worked on internationally and in the academic and industrial Swiss organizations. I would like to thank here the excellent work achieved by the CHIMIA editorial board together with the editors-in-chief who have served during many years to the success of the journal. There is no doubt that CHIMIA belongs to the leading journals of its kind. We have retained the full control of CHIMIA in order not only to secure its content according to the SCS needs but also to retain and develop our expertise in the field of scientific publishing. This has some financial consequences that we are endorsing for the benefit of our members and partners.

CHIMIA has major contributions in addition to the scientific articles of the thematic issues. We welcome also notes and scientific articles of high-quality not covered by the thematic issues and we would like to encourage our members to take this opportunity to disclose their scientific results to the Swiss community and beyond.

As important are all the other topics covered by CHIMIA, such as the Swiss Science Concentrates, the Highlights of the various Divisions and Sections, the Conference Reports, the Community News including the Events in Switzerland. We have the possibility to disclose and promote our numerous activities from our core Divisions, as well as new initiatives and Sections which are covering an increasing part of Chemistry performed in Switzerland. For example, we have launched new Divisions and Sections such as Chemical Education, Chemistry and the Environment, Green and Sustainable Chemistry, Chemistry in Flow, and very importantly the Women in Chemistry Network. CHIMIA welcomes all contributions from our core Divisions/ Sections as well as from the emerging ones. Two additional Sections will be launched this year on Materials Chemistry and on Chemical Ecology, which will be presented soon in CHIMIA. CHIMIA is also instrumental in calling for nominations and for reporting on the Laureates of our spectacular SCS Awards program.

Our strategic Institutional Members have also the possibility to write reports on their company in CHIMIA. These reports are not only very valuable for the companies, which can underline their new strategy and development but also to the entire chemistry community, including students who think of their future career and potential attractive employers.

For all these reasons, CHIMIA is a unique and essential communication tool for the SCS, which is highly appreciated by our members and partners. According to numerous feedbacks we received, we are convinced that the paper version of CHIMIA complements perfectly the electronic one.

A very important decision has been taken in 2020 to move to the Platinum Open Access version of CHIMIA. This has again some financial consequences that we agreed to take over because we are convinced that CHIMIA should be freely accessible to the entire scientific community. In addition, we expect to enjoy an even broader visibility of the SCS journal.

In the future, we are convinced that CHIMIA will remain an essential communication tool for the SCS and for the chemistry community in Switzerland and internationally. Each of us will have even more possibilities to collect information through existing and new technologies. However, the selection of the most relevant information will remain challenging. CHIMIA should provide to the Chemistry community the most relevant information in a high-quality form. The content of CHIMIA could be even further improved and broaden due to your active contribution and participation. There is no doubt that Chemistry will remain a core scientific discipline to help the world for a better future. Unfortunately, the immensely positive roles that Chemistry is and will play are not obvious for a large part of the population. CHIMIA has to play an increasingly active role to provide the scientific information needed to base opinion and decisions. This will only be feasible with your active support. I am confident that the long tradition and experience gained over the past 75 years by the CHIMIA and the SCS Teams will contribute to our success in the difficult future that we will have to face.

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A Perspective on Chemistry and Society

A Column on the Occasion of the 75th Anniversary of CHIMIA

The History of CHIMIA

The 75th Anniversary of CHIMIA

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Gillian Harvey completed her chemistry education in the UK (BSc, University of East Anglia; Norwich, PhD, University of Aberdeen). After a year on a Royal Society Fellowship at the Zentralinstitut für Anorganische Chemie, Akademie der Wissenschaften der DDR, Berlin, in 1986, she moved to the ETH as a postdoc in the Institute for Crystallography and Petrography (1986–1988) and then as Oberassistentin at the Institute for Technical Chemistry (1989–1996). Since 2000, she has worked as the Technical Editor for CHIMIA and since 2019 she has also taken over the Chair of the Editorial Board.

CHIMIA was published for the first time in 1947 by the Schweizerischer Chemiker-Verband (SChV). To celebrate the 75th volume of CHIMIA, the Swiss Chemical Society (SCS) and the Editorial Board are presenting, throughout 2021, opinion pieces by authors in science, industry, education, and society. To start this celebration, a history of CHIMIA from 1946 to the present day is given here.

Prof. Hans-Jürgen Hanssen (Professor and Director of the Organic Chemistry Institute, University of Zurich) wrote an Editorial[1] in issue 12/1995 on the eve of the 50th anniversary of CHIMIA. That Editorial covered the beginnings of CHIMIA and subsequent milestones during the first 50 years. The first part of this article is based on Hans-Jürgen Hanssen's Editorial.

Beginnings and the first 25 Years

The Annual General Meeting of the Schweizerischer Chemiker-Verband (SChV, Swiss Chemists' Association) on 19. October 1946 voted to publish a new journal with the name of CHIMIA to replace the *Schweizer Chemiker-Zeitung & Technik-Industrie*. In 1947, an Editorial Commission with representatives from academia and industry, under the lead of the President of the SChV, PD Dr. Hermann Mohler, was called into action to supervise the publication of the new journal. The declared objectives of the new journal:[2] to aid in the training and further education of chemists, to inform them of scientific and technological advances, to inform on the economy, patent law, careers and politics, to publish scientific articles and reports, were ambitious and reflected the hope of new beginnings in the post-war era.

The articles in the first volume of CHIMIA (Fig. 1), which began with an article by Paul Karrer (Professor for Organic Chemistry, University of Zurich, Nobel Prize for Chemistry 1937, 1889–1971[3]). This article, 'Vitamine als Bausteine von Fermenten' – 'Vitamins as Building Blocks in Fermentation,[4] reflects the enthusiasm with which the new Editorial Commission went about its work and the willingness with which authors responded. Selected articles are:

- A report of the celebrations of the 80th birthday of Hans Rupe[5] (Professor of Organic Chemistry, University of Basel, 9.10.1866–12.1.1951),
- H. Pallmann and H. Deuel of the Agricultural Institute of ETH Zurich on the chemistry and physics of pectins,[6]
- C. Rubin, Schweizerische Sprengstoff AG, Liestal-Isleten, 'Über die Entwicklung von Chloratsprengstoffen' – 'Developments in Chlorate Explosives',[7]
- H. Mohler and P. Giger, Zurich Chemical Laboratory, 'Absorptionsspektrosopische Untersuchungen von Sonnenschutzmitteln' – 'Absorption Spectroscopy of Sun Protection Agents,[8]
- H. Deringer, Gaswerk Winterthur, 'Über ein Absorptionsmittel zur Auswaschung und Gewinnung von Kohlenoxyd aus Gasgemischen' – 'Absorbents for the Extraction and Recovery of Carbon Oxide from Gas Mixtures',[9]
- R. Haller, Reihen, a historical review of 'Die Färberei als wissenschaftliches Problem' – 'Dyeing as a Scientific Problem',[10]
- The lecture entitled 'Old Dyestuffs and New Textiles and New Dyestuffs and Old Textiles' given by H. E. Fierz-David, Organic Institute, ETH Zurich, at the 11th International Congress for Pure and Applied Chemistry, was reprinted in its entirety, in English,[11]
- Frey-Wyssling, Plant Physiology Institute, ETH Zurich, reported on the 'Feinbau des Zytoplasmas' – 'The Detailed Structure of the Cytoplasm',[12]
- E. P. Hauser, 'Andreas Siegmund Marggraf und zweihundert Jahre Rübenzucker' – 'Andreas Siegmund Marggraf and Two Hundred Years of Sugar Beet'.[13]
- H. Mohler gave an extensive review of the University of Basel dissertation in political science by R. Baumgartner, 'Die wirtschaftliche Bedeutung der chemische Industrie in Basel' – 'The Economic Significance of the Chemical Industry in Basel',[14] a subject that, after 75 years, has lost none of its significance.

The range of different contributions in this first volume of CHIMIA, comprising 250 pages, is impressive and earns great respect. It also confirms the importance of the chemical industry to the chemical community. This is additionally reflected in the vast number of advertisements, the revenue from which would today go a long way to cover the production costs.

At the time, there was a second chemical society in Switzerland, Schweizerische Chemische Gesellschaft (Swiss Chemical Society SCG), which published *Helvetica Chimica Acta*. The driving force behind the decision to create a Swiss journal of chemistry in 1917 was Karl Friedrich Rudolf Fichter (1869–1952), Professor of Inorganic Chemistry at the University of Basel.[15] He was a native of Basel, and became known for having prepared beryllium for the first time in highly purified form, and especially for his fundamental work on organic electrochemistry. In his efforts to found what was to become *Helvetica Chimica Acta* (*HCA*), he was actively supported by Philippe-Auguste Guye (1862–1922),[16] Professor of Physical Chemistry at the University of Geneva, who was president of the Swiss Chemical Society during 1917 and 1918. (the Swiss Chemical Society came into existence on August 6th, 1901, with Alfred Werner as its first president.) Before the creation of


CHIMIA

1. Jahrgang / Année · Nº 1 · 15. Januar 1947

HERAUSGEBER: SCHWEIZERISCHER CHEMIKER-VERBAND
EDITEUR: ASSOCIATION PROFESSIONNELLE SUISSE DES CHIMISTES
EDITORE: ASSOCIAZIONE PROFESSIONALE SVIZZERA DEI CHIMICI

Inhalt / Sommaire / Sommario

CHIMIA Vol. I · Fasc. 1 1947 · Pag. 1–26

Fig. 1. The cover of the first issue of CHIMIA in 1947.

HCA, Swiss chemists had to rely almost exclusively on foreign periodicals, mainly German and French, for the publication of their scientific results. Only the physical chemists had their own Swiss journal, the *Journal de Chimie Physique* founded in 1903 by Guye. In addition, the *Schweizerische Apothekerzeitung* and the *Mitteilungen aus dem Gebiet der Lebensmitteluntersuchung und Hygiene* accepted contributions from the specialists. For his efforts in creating *HCA*, Fichter was awarded the Paracelsus Medal by the Swiss Chemical Society in 1948. A detailed history of the first 75 years of *Helvetica Chimica Acta* can be found in ref. [17]. *HCA* is now published by Wiley-VHCA AG but the Swiss Chemical Society is still involved and it continues to be perceived as a Swiss journal of chemistry. CHIMIA was never intended to be a competition to *HCA*, which was reflected in the emphasis on review articles in CHIMIA compared to the original research articles in *HCA* and this complementary relationship has been maintained over the years.

A large number of very well-known chemists published review articles and lectures in CHIMIA. For example, in 1950, Thaddeus Reichstein (Professor of Organic Chemistry, University of Basel, 1897–1996) published in two parts the lecture he had held at the Schweizerische Naturforschende Gesellschaft on Sept. 9, 1949, on 'Chemie der Nebennierenrinden-Hormone' – 'The Chemistry of the Adrenal Cortex Hormones'.[18] In the November issue of the same year there was a report of the award of the Nobel Prize in Physiology or Medicine to T. Reichstein, together with P. S. Hench and E. C. Kendall, for their discoveries relating to the hormones of the adrenal cortex, their structure and biological effects.[19]

In 1966, an extensive issue was devoted to a colloquium in honour of the 70th birthday of Prof. Robert Wizinger. The colloquium was on the subject of organic dyes and sponsored by Ciba, Geigy and Sandoz, reflecting the strong position of dye research and production in Switzerland at that time.[20]

An additional feature was introduced that proved to be very popular: 'Kurze Mitteilungen' or 'Notes', short contributions on experimental chemistry that could be submitted by the 20th of the previous month to be published in the following month's issue.

The early years of CHIMIA also contained pages of information as a service to their readers and the members of the SChV, including notifications of lectures, conferences, book reports, new Swiss patents, and other communications. One communication[21] contained a detailed description of emigration possibilities with very strong recommendations and warnings to, *e.g.* Australia, Belgian Congo, USA, Belgium, *etc.* This may appear strange to today's readers but it reflects the awareness of the SChV of the yearning for wider horizons in the post-war period and thereby providing the necessary information as food for thought.

25 to 50 Years of CHIMIA

Hermann Mohler remained the chairman of the Editorial Commission of CHIMIA until 1953, followed by Prof. Hans Amman (1953–1955), Prof. Wilhelm Busser (1956–1959†), and Prof. Hans Nitschmann (1960–1984). In his review of '25 Jahre *CHIMIA*' – '25 Years of *CHIMIA*' (Fig. 2), the President of the SChV, Dr. Max Lüthi[22] (for whom the SCS Dr. Max Lüthi Award for outstanding degree theses completed in a chemistry department of a Swiss University of Applied Sciences was named) explained that the original objectives had been reassessed to move away from an association journal to a scientific one. Emphasis would be given, in the section 'Wissenschaft – Forschung' – 'Science – Research', to review articles as before, transcriptions of lectures given in Switzerland, and Notes. A new section: 'Praxis – Technik – Industrie' – 'Practice – Technology – Industry', for which Max Lüthi was directly responsible, was aimed at the practical chemist and the workers of other disciplines in the chemical industry. The continued large number of advertisements were considered a service to the reader. The commitment of the Swiss Chemical Industry to CHIMIA was reflected in the financial support given to the journal *via* the 'Zeitschriftenfonds' – 'Publication Fund', which continued until 1969. The years that followed showed that publishing a journal of CHIMIA's format was becoming more and more difficult, not only with respect to the workload for the Editorial Commission to attract submissions but also with regard to the financial costs. The Schweizerische Chemische Gesellschaft (SCG, Swiss Chemical Society) as the publisher of *Helvetica Chimica Acta* was experiencing similar problems. For both journals, different options were tried: The SChV created a publishing company for CHIMIA which did not last more than


25. Jahrgang · Nº 1 · 15. Januar 1971

CHIMIA

Chimia Vol. 25 · Fasc. 1-1971 · Pag. 1–40

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Herausgeber: Schweizerischer Chemiker-Verband
Edition: Association Suisse des Chimistes
Edizione: Associazione Svizzera dei Chimici
Edition: Swiss Chemists' Association

Fig. 2. Issue 1, 1971, of the 25th anniversary volume of CHIMIA.

a few years, while a full-time editor (Dr. M. Volkan Kisakürek) was appointed for *HCA* to lower print and distribution costs in collaboration with Verlag Birkhäuser AG.

1984 became the final year that CHIMIA was produced by the Editorial Commission, still led by Hans Nitschmann. The effort involved for the members of the commission became too much in addition to their professional activities and it was decided to employ a full-time editor from 1985. An Advisory Board, chaired by Prof. Dieter Seebach (ETHZ), was created to support the editor. In 1985 the new Editor, Dr. O. Smrekar, took up his new assignment and an Editorial in the first issue by Seebach described that the Advisory Board had been extended to include scientists from biosciences, material and engineering sciences with the intention to stimulate authors to submit their articles to CHIMIA and to identify possible subjects for special topic issues.[23]

Five years later, in 1990, the experiment with a full-time Editor was abandoned, CHIMIA was again redesigned and published by the Verlag Helvetica Chimica Acta, and the two societies, SChV and SCG began a process of amalgamation to form the 'Neue Schweizerische Chemische Gesellschaft' (official foundation 14. Feb 1992, renamed the Swiss Chemical Society in 2001). Prof. Camille Ganter (Organic Chemistry Institute, ETHZ) was appointed as Editor-in-Chief, responsible for the content and Dr Kisakürek took over the technical editing together with that of *HCA*. The reorganisation resulted in an improvement of the financial situation for CHIMIA, which was declared to be both a scientific journal in the chemical sciences and the official society journal of the NSCG.

In 1994, the appointment of a newly created new Editorial Board, an Advisory Board with representatives of the four sections of the NSCG, and new CHIMIA regulations secured the publication of CHIMIA in its new form for the foreseeable future. Already at this time there was a tendency to thematic issues, often based on international conferences that had taken place in Switzerland. Camille Ganter took this idea and developed it to become the main scientific content of the journal: thematic issues on subjects of current interest to the chemical community in Switzerland. At the same time, individual articles on a range of chemistry subjects and from the 'Ingenieur Schulen', later the Fachhochschulen or Universities of Applied Sciences, and often opinion pieces on matters of interest for chemists were published. Most articles up to this point were published in German, with fewer in French and English. Authors were generally based in Switzerland with the exception of transcriptions of lectures by international scientists held at conferences in Switzerland.

Also in 1994, the Verlag Helvetica Chimica Acta AG was founded by the NSCG, with the Society holding 54% of the shares with two partners Birkhäuser + GBC AG and VCH Verlagsgesellschaft mbH Holding, Weinheim (24% each), to cover all publishing activities (*HCA*, CHIMIA and books). In 1999, the NSCG sold its shares in the company to Wiley-VCH whilst retaining the rights to the name *Helvetica Chimica Acta*. By the end of 1999 it became clear that Wiley-VCH would no longer undertake the technical editing of CHIMIA and a Technical Editor was employed.

Looking back over the first 50 years of CHIMIA, the support it enjoyed from professors from the Swiss universities can be seen from the large number of excellent review articles. What is fascinating is the number of articles, commentaries and communications that give an insight into the wider societal history of Switzerland. The emigration information for Swiss chemists has been mentioned above. In 1981, Prof. H. Zollinger, wrote an essay on 'Logik, Psychologie und Zufall in der Entwicklung wissenschaftlicher Erkenntnisse' – 'Logic, Psychology and Chance in the Development of Scientific Knowledge', encouraging the reader to expand their thinking far beyond the mere reporting of experimental results.[24] In 1985, after a Federal popular initiative to ban vivisection (animal testing) had been decisively rejected, Prof. G. Patzig wrote an commentary on 'Ethische Aspekte von Tierversuche' – 'Ethical Aspects of Animal Testing', appealing for a return to a rational and ethical discussion of animal testing, away from the aggression and emotional initiative campaigns of both camps.[25] In 1986, just a few weeks after the fire at a Sandoz storage facility in Schweizerhalle caused widespread air pollution and devastating ecological damage to the Rhine from the runoff of the water used to extinguish the fire, Dr. Bruno Böhler, Director of the Bundesamt für Umweltschutz (Federal Office for the Environment), wrote an Editorial Commentary 'Umweltkatastrophen – Lehren ziehen' – 'Learning from Environmental Catastrophes' in which he argues strongly for the need for a higher valuation of human life and the environment over the needs of the economy: "*Wir haben uns viel zu wenig Rechenschaft darüber gegeben, dass wir bezogen auf die Umwelt auf Pump leben, und dass wir vom Umweltkapital kommender Generationen zehren.*" "*We have held ourselves far too little accountable for the fact that we have been living off the environment at the cost of future generations*." He had held a lecture at that year's Annual General Meeting of the Schweizerische Gesellschaft für Chemische Industrie (Swiss Society of the Chemical Industry) in June where he had been optimistic that the Federal environmental laws were fit for purpose, a view that he acknowledges in his commentary, had received quite a blow.[26]

50th Anniversary

In 1996, the 50th anniversary of CHIMIA was celebrated by a series of leading articles by invited authors on scientific, industrial, technological, environmental, political and economic aspects. Alexander von Zelewsky, President of the NSCG, addressed the importance of chemistry in society. CHIMIA was described as fulfilling a triple function:[27]

1) Official publication channel of the NSCS, sections and member societies;
2) Information to all NSCS members and a wider chemical public (300 subscribers in 1996);
3) Scientific articles on scientific and industrial developments (Fig. 3).

Fig. 3. The 50th anniversary cover of CHIMIA.

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The past 25 Years

In 1997, the New Swiss Chemical Society went online for the first time. All CHIMIA scientific articles, backdated to 1990, are online (presently at *Ingentaconnect.com*) and are open access.

Camille Ganter remained the driving force behind CHIMIA for many years and his influence is reflected in the structure of of the journal to this day. He was responsible for producing 16 years of content in CHIMIA before retiring as Editor-in-Chief in 2006 and becoming chairman of the Editorial Board until 2009. He was also responsible for the finances and the general running of the journal. He introduced recurring issues dedicated to New Professors, Hot Topics, SCS Prizewinners (issue 4, containing articles by the Junior Laureates of the previous year's Fall Meeting, was introduced in 2004) and ensured that the thematic issues covered areas of current interest and significance to Swiss chemistry.

Special topic issues featuring 'classical' chemistry subjects such as analytical chemistry, organic chemistry, physical chemistry and computational chemistry were published many times, but also related disciplines like biotechnology, food science, material science, environmental sciences appeared at an ever-increasing rate. Topics have evolved over the years to reflect the increasingly interdisciplinary nature of the chemical sciences.

Fig. 4. Front cover of issue 10, 2016, 'Malaria Vector Control' as an example of the excellent cover pictures provided by the guest editors: in this case Paul Dyson and Peter Maienfisch.

Industry continued to be strongly featured with issues such as '100 Years of Progress with Lonza',[28] 'The First 100 Years of the Roche Group',[29] 'Safety and Environmental Protection in Chemistry',[30] 'Bauchemie' – 'Chemistry for Construction',[31] 'Outsourcing',[32] 'Industrielle Produktion mit Hochreaktiven Stoffen' – 'Industrial Production with Highly Reactive Materials',[33] 'Fluorine in the Life Science Industry',[34] 'Quality Aspects in Industrial Chemistry'.[35]

Other topics were presented for a general readership: 'Art and Chemical Sciences',[36] including 'Arts and Sciences. A Personal Perspective of Tibetan Painting', by Prof. Richard Ernst (Nobel Prize for Chemistry, 1991), which contained wonderful colour photos of the artworks that presented quite a challenge to the printers.[37] This issue was followed in 2001 by Conservation of Cultural Heritage.[38] Other issues covered areas that held particular significance at the time: 'Intellectual Property',[39] 'Analytical Chemistry at Forensic Institutes',[40] covered doping controls, and 'REACH: Registration, Evaluation, and Authorization of CHemicals',[41] described in detail the consequences arising from the planned EU new chemicals legislation, which came into force in June, 2007.

The Swiss National Science Foundation (SNSF) projects National Centres of Competence in Research (NCCR) and Swiss Competence Centres (SCCER) in the chemical sciences have also been featured regularly in CHIMIA, giving the project leaders the opportunity to present the range and progress of the research: NCCR MUST,[42] NCCR Chemical Biology,[43] SCCER BIOSWEET,[44] SCCER Heat Energy Storage,[45] NCCR Molecular Science Engineering,[46] NCCR Bio-Inspired Materials,[47] and NCCR RNA & Disease.[48]

Women authors were increasingly represented in the articles, and also, with time, as professors and senior scientists but the first issue to contain articles exclusively with women group leaders was published very recently in 2020, 'Innovative Tools in Organic / Organometallic Chemistry' guest edited by Prof. Cristina Nevado.[49]

By 2006, it was recognised that the many tasks undertaken by Camille Ganter were too much for one person and new roles on the Editorial Board were created. The Editor-in-Chief is responsible for the scientific content and thematic issues are organised by Swiss University professors (Philippe Renaud, University of Bern, 2006–2010; Jerome Lacour, University of Geneva, 2011–2013; Paul Dyson, EPFL, 2014–2017; E. Peter Kündig, University of Geneva 2018–2020; Catherine Housecroft, University of Basel 2021). The thematic issues are collated by guest editors who invite authors to submit their review articles. Roland Kunz, University of Zurich, took over the role as Chairman of the Editorial Board and Associate editor and was instrumental in guiding CHIMIA's development from 2003 to 2018. Each new Editor-in-Chief brought and continues to bring his or her own expertise and professional interests to the role. The other roles on the Editorial Board: Chairperson, Managing Editor, Associate Editor, News Editor, Technical Editor, Treasurer, Web Editor, Swiss Science Concentrates Editor, Advisory Board contact, Universities of Applied Sciences contact, have developed over the years and reflect the large amount of work that is necessary to produce a quality scientific journal ten times a year. The only employed (part-time) person is the Technical Editor, the other EB members work as volunteers or receive a small honorarium. The Managing Director of SCS (currently David Spichiger) is also a member of the EB and contributes in particular to the Community pages and the CHIMIA Report.

In 2020, the journal became a platinum open access journal (no page charges to author and free to the reader, under license CC BY, copyright retained by the author) as a proactive move to the widespread recognition of open science. Over previous years, the number of external subscribers had been falling steadily, reflecting the difficulty of a small independent publisher to maintain subscribers in the face of the large publishing houses offering journal packages. For the past 15 years, advertising revenue also became increasingly difficult to access in the print media in general, which also reduced the overall income for CHIMIA. The review articles in CHIMIA present the research that is being undertaken in Swiss Institutions funded by the public purse and therefore should be accessible to all who are interested. It was also acknowledged that the main resource of CHIMIA are the contributing authors and guest editors, who, it is hoped, would be more willing to write for an open access journal. Therefore, the SCS agreed to take over the full costs of producing CHIMIA, financed mainly through the membership fees. The print version

Fig. 5. Issue 11, 2020, showing the new cover design of CHIMIA.

continues to be produced and is distributed to the SCS membership.

Current Role of CHIMIA

As the society journal of the Swiss Chemical Society, CHIMIA will continue to represent and inform the wider chemistry community in Switzerland: in academia, industry, education.

The Swiss Chemical Society is seeking to evolve and grow and expand its contacts to related scientific fields: Chemistry and the Environment, Material Chemistry, Flow Chemistry, AI/Computational Chemistry, *etc.* Where possible the activities of the Society are reflected in the content of CHIMIA, *e.g.* Green and Sustainable Chemistry issue[50] coincided with the same topic at the SCS Forum at ILMAC, or Chemistry and the Environment issue[51] to mark the launch of the new SCS section Chemistry and the Environment and the Spring Meeting in 2021 on the same subject. All divisions have the right to produce short columns featuring innovations in their fields.

Information for the SCS membership is included in the Community News and Events sections.

The layout and front cover design of CHIMIA has been updated over the past two years. The cover retains the CHIMIA font and therefore is still recognisable, but without the previously used 'Saarland green' (Fig. 5).

In the immediate future, the plan is to host the journal entirely on one online platform, which is scheduled to be completed in mid-2021. This will enable one-stop access from submission through to online publication and all articles, columns and information will be visible and directly available for download. This is made possible by the move to open access in 2020, and the objective is to improve the visibility of CHIMIA online, far beyond the borders of Switzerland. CHIMIA is listed in the most important databases: Current Contents/Physical, Chemical and Earth Sciences, Chemical Abstracts, Science Citation Index, Research Alert, Scisearch, Index Chemicus, Chemistry Citation Index, Current Chemical Reactions, Reaction Citation Index, Biological Abstracts, and the Directory of Open Access Journals.

The Swiss Chemical Society and the Editorial Board are working to ensure that CHIMIA will continue to thrive and evolve to its 100th anniversary and beyond. For this to happen, we can quote the words of Hans-Jürgen Hanssen, in the conclusion of his Editorial in 1995: "*Let us not forget that the publication of CHIMIA can only succeed as a society effort of the NSCG (now SCS) and its members and a willing pool of authors from all parts of Switzerland. For CHIMIA, let us wish for the coming 50 years, wise, forward-looking Presidents of the Society, intelligent, well-informed authors, and a supportive readership*".[1]

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A Perspective on Chemistry and Society

A Column on the Occasion of the 75th Anniversary of CHIMIA

SCS Division of Medicinal Chemistry and Chemical Biology

Medicinal Chemistry and Chemical Biology in the Age of the Pandemic

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The authors represent the board of the Division of Medicinal Chemistry and Chemical Biology (DMCCB) of the Swiss Chemical Society. The board is composed of representatives from Swiss universities, and Swiss pharmaceutical and agrochemical industries. Activities of the DMCCB include the organization of schools and scientific events and fostering an international network between scientists of different expertise.

In this perspective, we argue that the complexification of medicinal chemistry and the rise of chemical biology over the last 40 years, which has been a necessary step to produce better and safer drugs, has created the framework for a rapid and effective response to the challenge of the SARS-CoV-2 pandemic. Scientific societies such as ours have played an essential role in this process by cultivating information exchange and networking within and across disciplines and generations of scientists from multiple backgrounds. They must continue to do so in the future.

Why is it so hard?

Scientific understanding strives for simplicity and elegance.[1] The natural world might indeed have seemed simple at the age of the scientific revolution, however since then we have learned to appreciate its extraordinary complexity, especially with regard to human health and disease and the action of drugs. While their chemical structure may be deceptively simple, how drugs act is often, if not always, extremely complex. This has been shown by the analysis of biological processes down to the molecular level, revealing not only multiple sites of action for any drug but also differential responses among patients.

One Health

It has also been realized that our health is closely related to the health and well-being of our environment. When the animals and plants in our ecosystem fare badly, it impacts us directly. In a globalized world with a population soon exceeding eight billions, these aspects, known under 'One Health',[2] become ever more important as is well illustrated by the recent corona virus pandemic.

Providing safe food and water to the growing population is a global imperative, considering that 600 million people still suffer every year from food-borne illnesses.[3] Food safety must be ensured at all stages of the farm-to-fork path, starting from preventing crops from being contaminated by pathogens and potential toxins sources.

Crop science innovation is key for the reliable production of healthy food, but also to address threats to global agriculture such as deforestation, desertification, soil erosion and weather extremes. The international collaboration established to ensure food security on the planet in the current crisis, sets an example to address with a joint action other global issues such as climate change or biodiversity protection. This is the world we live in, which cannot be meaningfully understood and acted upon unless by large and interdisciplinary teams.

Fig. 1 highlights the importance of interdisciplinary approaches to address emerging diseases such as SARS-CoV-2, including wildlife health as a critical element of global disease prevention and management.

Creative Scientists

In our globalized culture of scientific publishing, conferences, and the internet, the scientific community operates at unprecedented scale almost as one very large team. As such, we can easily afford to not always follow the most probable path and to also explore daring hypotheses and ideas. These ideas are shared, critically evaluated, and further developed, feeding a reservoir of opportunities waiting for their day to shine. The fast response of the international scientific community to the SARS-CoV-2 pandemic exemplifies this inherent strength. For instance, mRNA and DNA-based vaccines were deemed an exotic, far too complex and costly technology until the change of tide triggered by the pandemic.[4,5] Similarly, until a few years ago cryo-electron microscopy was considered a curiosity in front of X-ray crystallography, until it suddenly supplanted it as the workhorse of structural biology.[6] Cryo-EM now enables rapid structural understanding of the SARS-CoV-2 and opens the door to discovering drugs that might soon emerge as first line of treatment.[7]

The Role of Scientific Societies

Research organizations benefit from sharing their findings globally not only because they cannot compete in isolation, but because the world is changing so fast that individual researchers must constantly challenge themselves. Scientific societies play a key role by providing the framework for this global exchange and continuing education in form of journals, conferences and workshops. The DMCCB and EFMC have recently intensified communication and created virtual events, mentoring programs and online symposia, to counteract the difficulty of maintaining active networks in this period of physical distancing. These events are of prime importance for all scientists, as the development of new concepts and technologies has markedly increased the remit of life sciences and drug discovery. In particular, the growing interest for multifunctional molecules, such as degraders and antibody-drug conjugates, has reshaped the understanding of what a drug actually looks like, and opened the path to completely new treatment modalities.

The value of the medicinal chemistry and chemical biology network is particularly important in the fight against SARS-CoV-2. The management of the current pandemic pins high hopes on vaccines, but these do not address all issues and might fail to treat emerging variants of the virus. In this sense, a multi-pronged approach drawing on the expertise of well-networked research groups is critical. Those have the best chance to discover drugs against conserved viral targets, with the potential to treat future pandemic-causing coronavirus infections, such as the COVID-19 main protease (Mpro).[8]

Finally, scientific societies must provide multiple networking and training opportunities for the next generation of scientists. These facilitate integration in the global community and provide exposure to the broad range of disciplines required for excellence in medicinal chemistry and chemical biology. Likewise, they facilitate academia-industry collaborations and active scientific exchange, minimizing the gap between academic and industrial research as well as encouraging international collaborations.

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A Perspective on Chemistry and Society

A Column on the Occasion of the 75th Anniversary of CHIMIA

SCS Division of Industrial and Applied Chemistry

Passion and Perspectives for Swiss Chemical Manufacturing

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Dr. Bernhard Urwyler studied organic chemistry at the Organic Institute of the University of Basel and obtained his doctorate 1990 at the Physical Chemistry Institute of University of Basel with research in Photochemistry. He started his career at Ciba-Geigy AG 1990 in the research labs in Klybeck and moved 1995 as team leader of a chemical development lab of Novartis AG to the Agro chemical development centre in Münchwilen. With the formation of Syngenta, he took in 2000 the role of a production manager in the production at Syngenta crop protection, Monthey SA. He then held several leading positions within chemical production at Syngenta crop protection, as site manager at Syngenta Aigues-Vives in France and from 2012 as head of production at the largest production site of Syngenta in Monthey. In his current position, since 2020, he is Integration Manager at the newly acquired Syngenta production plant at Muttenz. From 2004 to 2020 he was a member of the SCS DIAC board and from 2016 to 2020 president. Bernhard Urwyler will retire on 1.4.2021 but continue to work part-time in his own company 'Urwyler ChemPro GmbH'. Since 2020 he also became a member of the board of directors of Dottikon Exclusive Synthesis Holding AG.

MEGA Trends

Chemical production in Switzerland has been significantly shaped by time-changing MEGA trends over the last decades. These trends have strongly influenced the strategy of decision-makers in large and medium-sized chemical companies and will continue to do so in the future.

Is it therefore sufficient to analyse these mega trends of the past to make long-term predictions about the industrial development of tomorrow, *e.g.* for upcoming siting decisions with associated investments?

The demand for chemicals is growing proportionally with the rapidly growing and aging population. It triggers the aspiration to get access to more food diversity, but also to more pharmaceuticals and consumer commodities.

Overall, the chemical manufacturing industry shows a steady growth with a significant increase in imports and exports from 2016 onwards. Main driver is the pharma industry (Fig. 1).

The shaping trends of yesterday, today, and tomorrow do not have the same impact on all chemical production sectors and should therefore be interpreted in a differentiated manner. Nevertheless, the major changes in industrial chemistry have also had a strong impact on the SCS (Swiss Chemical Society), and especially on the DIAC (Division of Industrial and Applied Chemistry). If we split MEGA trends of past 30 years into yesterday's, today's and tomorrow's trends, the following pictures appear:

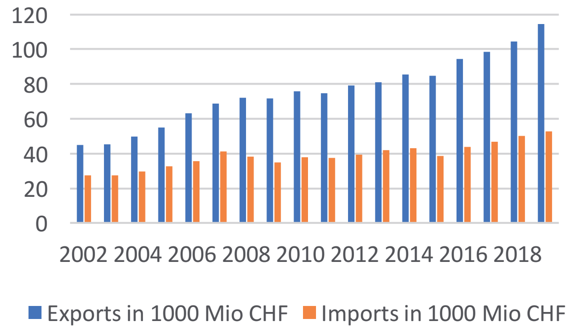

Fig. 1. CH import and export of chemical-pharmaceutical products 2002–2019. (Source: www.bfs.admin.ch)

Trends of the Recent Past

In the period 1990–2010, globalisation was in full swing. India, then China and Russia gained interest among Western investors.

Markets for chemical products grew at double-digit rates, especially in China, where important state subsidies led to an aggressive pricing strategy with corresponding growth in China.

In parallel the flow of goods was optimised further thanks to the World Trade Organisation (WTO), and thanks to bilateral, or regional commercial agreements. This facilitated the trade of raw materials and intermediate products, including patented active ingredients.

Large Western chemical companies shifted large parts of their production to the East ('go east strategy'), mainly to China and India. Finished products, such as antibiotics or pesticides, were increasingly produced only at a few locations for the global market. This led to a concentration of chemical manufacturing to fewer locations producing at lowest costs. Large volume productions of basic chemicals in Switzerland and Europe dropped dramatically, as illustrated by the example of chlorine production in Switzerland. Consequently, chlorine and caustic soda producers planned to reduce capacity. Both commodities were and remain important basic chemicals for 60–70% of all chemical processes. Their availability is the backbone of all chemistry, as is widely acknowledged. In 2019, European capacity was 9.4 million tonnes of chlorine but demand fell as a large proportion of PVC and other fine chemicals were relocated to Asia. The withdrawal of chlorine and caustic soda production in CH came very quickly after the start of the new millennial.

The Oslo-Paris-Commission (OSPARCOM)[1] had already recommended at the beginning of the 1990s to shut down all chlorine production facilities in Europe that produced with the amalgam process, or to replace them with membrane processes by the end of 2010. Without coordination within the EuroChlor group or the production companies in Switzerland, production units were closed, one after the other; Syngenta Monthey in

2002 and the 'Schweizerische Sodafabrik' (Solvay) by 2004. Only CABB Chemicals adapted their chlorine production to membrane technology to comply with the new standards and environmental requirements, however, they only produce for their own use and their required capacity. Chlorine now had to be sourced from Germany and France *via* two main ports of entrance; Basel and/ or Geneva.

The issue of transport safety for dangerous goods, especially chlorine, triggered a violent controversy with the consequence that only ten years later, *i.e.* in 2015, the canton of Geneva submitted a 'Standesinitiative' to stop all chlorine transports in CH.[2]

The withdrawal of production volumes had a significant impact on the exchange of know-how and caused a reduction in the number of innovations in applied and industrial chemistry.

DIAC was affected by this and experienced a reduction in its membership. In parallel, the EPFL, for example, has increasingly invested its resources for education and research in biotechnology instead of chemical engineering. At the same time, more and more finished products in the field of plastics, dyestuffs, active ingredients, or drugs that had lost patent protection, moved to India or China.

Current Trends

The loss of know-how accelerated with the departure of Western chemical production to China or India. Their chemical manufacturing has become progressively better and, in many cases, even reached Western standards.

Already by 2010, public pressure increased for a proper remediation of contaminated soil and no longer usable areas, caused by the chemical industries.

With this growing pressure from the public, investors began to evaluate the sustainability of a company, also because environmental remediation requires a lot of capital. Several environmental scandals accelerated this trend. Another trend was that bigger pharmaceutical companies, *e.g.* Novartis, Roche, Astra Zeneca, *etc.*, were gradually separating themselves from conventional 'small molecules' production, so that they can focus more on biological macromolecules and invest more in research and development,

Environmental organisations were gaining more influence on political decision-makers, as shown by the example of chlorine transports, where the canton of Geneva has launched its initiative to 'Stop the transport of chlorine to protect the population and the construction of housing'. Negotiations with the SBB and the Federal Government are still underway and the outcome is uncertain, but for the chemical manufacturing this represents a further factor of uncertainty and is not a promising development.

Trends of Tomorrow

The five megatrends 2020–2030 mentioned in *www.thegeniusworks.com* in 2019 were:[3]

1. Economic power shift (from G7 to emerging economies E7), with increasing polarisation between USA and China.
2. Climate change impact and natural resource capacity, *e.g.* increasing scarcity of oil or drinking water
3. Increase in technological breakthroughs with 'Artificial Intelligence'.
4. Demographic and social transformation.
5. Increased urbanisation.

A new, sixth, emerging trend, is the growing risk of pandemics, such as the current Covid-19 pandemic. Together, these trends will contribute to a significant slowdown in globalisation and, at the same time, accelerate socio-political pressure for more sustainability and 'greener' chemistry, also in industry.

New market protectionist demarcation is also taking place in safety and environmental protection requirements (such as the REACH regulation, which has been in force for some time, where now the Chinese variant: 'Order No. 7' (MEP) and the new 'Order No. 12' (MEE China), represent similar regulations. The aim is to improve the protection of human health and the environment from the risks that can arise from chemicals and at the same time to increase the competitiveness of its own chemical industry, *i.e.* in the EU and in China. All these directions are leading to more regulation and to an increasing influence of the government on the economy.

The trend towards complete globalisation has reached its limits. Thus, global production, sourced from one location, bears high risk in the event of conflicts (*e.g.* in the case of further polarisation between China and USA).

> ***Remark***: China MEP Order 7 was issued in Jan 2010 by the Chinese Ministry of Environmental Protection (MEP) and came into force on 15. Oct 2010. This regulation is comparable to EU REACH regulations and is also known as 'China REACH'. In mid-Dec. 2020 it was changed to China MEE Order 12 – The Measures for the Environmental Administration Registration of New Chemical Substances. The Chinese Ministry of Ecology and Environment (MEE) issued Order 12.[4]

As long as production is not able to be more sustainable and in compliance with environmental and safety guidelines, social and political pressure from environmental organisations will further increase, also in China and India, and there is a risk that entire industrial regions will be shut down, as was recently the case in China (see the consequences of the explosion disasters in Tianjin in 2015[5] and the severe explosion in the Chinese chemical factory of Jiangsu Tianjiayi Chemical Co in the city of Yangchen in 2019[6]). Both are among the worst industrial catastrophes in China and caused the closures of many chemical industry parks in the province.

Western chemical manufacturing was suddenly cut off from the supply chain of important raw materials, intermediates, and actives from one day to the next, which triggered a change in the trend.

New Opportunities

The need for process research and development capacity in Switzerland increased rapidly, to the advantage of agile, flexible, and fast-acting chemical productions.

In addition, research and development of new molecules for pharma and crop protection, but also new innovations in speciality chemistry are tending toward more complex and higher active molecules. More chemical steps are required for the finished product, in smaller volumes, as they become more effective in the case of pharmaceutical and crop protection active ingredients. In other words, where 4 to 6 steps were sufficient in the past, 10 to 25 steps or more will be required tomorrow.

The example of Dottikon Exclusive Synthesis, as a 'Specialist for Hazardous Reactions' offers exactly in this segment chemical development and first production volumes. Together with the demand for agility, flexibility and reliability, this market segment is growing in a way that compensates for the decline in production activity of the large pharmaceutical companies.

Even Syngenta, which belongs to Chem China, is investing in new production facilities in Switzerland, such as the Monthey (VS) plant and the newly acquired Muttenz plant. The latter was taken over by Syngenta after a production relocation at Novartis. This takeover led to a sustainable win-win situation for both companies, where thanks to the continuation of a well-maintained production facility at the Pratteln BL plant, jobs and assets could be preserved. The owner's logo has changed from Novartis to Syngenta, but the assets and people have remained (Fig. 2)

Fig. 2. The logo has changed but the assets remain the same. A good example of sustaining assets.

Even the large volume producing chemical industries have good chances in these new trends as long as they can score with sustainability, better environmental protection and safety as the examples DSM (vitamin production), Ems Chemie (speciality plastics), Lonza (specialities and biologics), Firmenich (flavours and fragrances), Givaudan (flavours and fragrances), *etc.,* show.

Companies that did not identify the trends of the time, or saw them too late, had to close or were taken over, for example, CIBA in 2008, or Rohner in Pratteln in 2019.

New Stars in the Sky

Good research and development at our Federal Institutes of Technology, universities and other institutes with applied chemistry, bring new innovations to applications in close collaboration with industry. Many start-ups have emerged from research at our institutes, some of them inventing highly specialised new chemicals or processes to meet the growing demand for sustainability. Almost all private equity is now focusing on sustainability. And there are good cases in point, such as novoMOF, AVA Biochem BSL AG, or other examples described in CHIMIA 10/2020, 'The Swiss Startup Ecosystem: Innovation in Chemistry and the Life Sciences'.[7]

I am convinced that the following conditions will guarantee the preservation of applied chemistry and chemical industry in Switzerland:

1. Production facilities must be designed sustainably, with a high standard in safety and environmental protection.
2. Benefit from close collaboration with R&D institutes and open access to manufacturing-related and applied development.
3. Ensure good education in chemical research and development and in chemical engineering, including general technical apprenticeships in the field of applied chemistry (laboratory technicians and chemical and pharmaceutical operators).
4. Assure optimized plant maintenance by maintaining a balance between preventive and curative maintenance, leading to maximum reliability in production for the benefit of customers.
5. Maintain agile and flexible production facilities that can adapt rapidly to changes and thus to the fast-changing market.
6. Digitalization and usage of new technologies to increase efficiency.
7. Never give up on 'continuous improvement'.

I am sure that the vast majority of chemical producing companies in Europe and Switzerland produce on average much more sustainability than is the case in the E7. Every year the pressure for more sustainability will increase and, as recently proven by China's authorities, this leads to decisions that could strongly destabilise the market and unexpectedly interrupt supply chains.

Future Vision for the Role of the SCS DIAC

Where DIAC contributes significantly, and must continue to do so, is in providing the network for the manufacturing industry.

The DIAC brings together a network of applied and industrial chemistry and organises symposia, lectures, and plant visits to link applied innovations from R&D with production to make them available and inspire new innovations.

What has always been practiced in research and development has been applied only sparsely in chemical manufacturing, or hardly at all because of intellectual property restrictions.

Understandably, there was a lack of open exchange of new innovations in production. Newly developed technologies in applied chemistry are rarely patented and therefore not published.

This is unlikely to change in the short term. But through a network and the associated looking over the fence or the exchange among different related disciplines, this often results in the determining key for the vital new innovations in production. *e.g.* in Operational Excellence (OpEx), Industry 4.0, BigData or SusChem, *etc*.

New ideas and innovation only deliver added value if they are brought to commercial application. The DIAC must drive the passion for an extended network across the individual disciplines to generate this high added value in industrial and applied chemistry.

In a first step, this will be realised at the next Freiburg Symposium in April 2021 with the promising title: 'Industry 4.0, Current and Future Trends in Chemical Production'.[8]

Sharing best practice and knowledge in the symposia lectures across the network will keep the interest high, (Fig. 3). This guarantees the sustainable existence of our industrial chemistry in Europe and thus of Switzerland and finally the DIAC.

Fig. 3. DIAC's annual meeting held at Metalor Technologies SA in Marine Epagnier in 2019.

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A Perspective on Chemistry and Society

A Column on the Occasion of the 75th Anniversary of CHIMIA

YoungSCS

The Young Swiss Chemical Society Empowering Young Chemists in Switzerland for 20 Years

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Introduction

Young scientists are key drivers for innovation and intellectual progress. They will become the future professional and scientific leaders. Tomorrow's science will only be as strong as our pool of diverse young talents today.[1] In our knowledge-driven economy, nurturing a well-educated, connected, and organised academic youth is the determining factor for future success.[2,3] Therefore, the question arises on how to best support, connect and empower young scientists with a set of professional skills that will be key in advancing their career development.[4,5]

Collaborative networks stimulate professional and personal development.[6–10] Hence, the young Swiss Chemical Society (youngSCS) aims to provide such a network for young chemists all over Switzerland (Fig. 1). This is achieved through various events by which young chemists can develop meaningful competences. Soft-skills are enhanced in symposia and seminars. Networks are expanded through career-path-focused events, organised as industrial or academic visits, which lead to better informed decisions about future endeavours. Furthermore, professional and personal views are broadened thanks to the diversity of our members. The youngSCS supports chemists at different career stages, from various backgrounds and aims to represent all areas of chemistry across Switzerland.

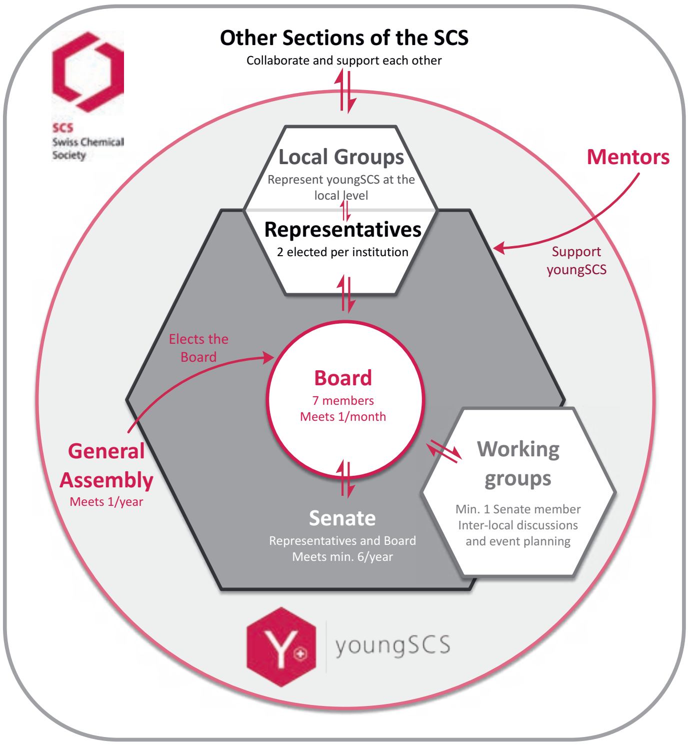

Fig. 1. The youngSCS is a subgroup of the SCS directed to young chemists. At the yearly general assembly the members of youngSCS elect the board. The youngSCS members are organised into local groups and every institution sends two representatives to the senate. These representatives act as linkers between the local groups and the board. Events are organised and planned in working groups, which are set up by the senate. These are generally open to any member that might be interested.

In addition to a historical glance, this article is intended to inform the reader about the past and future activities of the recently rebranded youngSCS, along with details concerning our community as well as our mission.

youngSCS

- How can I become an active youngSCS member?
- By joining SCS on the new SCS-website;
- By following youngSCS on Linkedln and/or Twitter to share your passion for chemistry and not miss any chemistry-related event and career advancement opportunity;
- By participating in the events organized by youngSCS and spreading the word around you to benefit others as well.

History of the youngSCS

Founded in 2001 under the name of 'Swiss Young Chemists' Committee', 'Club des Jeunes Chimistes Suisses' or 'Schweizer Jungchemikerforum', respectively, a group of PhD students from the University of Basel intended to initiate a platform for young scientists inspired by the German Jungchemikerforum. With the sponsorship of the Swiss Chemical Society and the support of the Basler Chemische Gesellschaft & KGF, its main focus was to provide PhD and PostDocs with a platform for networking and to give rise to regional groups in Swiss universities.

Back then, the communication between the Chemical Institutes of the University in Basel was predominantly informal. The activities consisted of monthly board meetings, a football tournament and presentations by young researchers. In addition to that, the country's first career fair exclusively for chemists was held in Basel in 2002 and the next year in Lausanne. The Swiss Snow Symposium – a tradition held up to this day – was first organised in 2003. It combines a scientific conference with snow sports and quickly grew from less than 10 to more than 60 participants in 2006. A group photo of the first Swiss Snow symposium is shown in Fig. 2.

Over the course of time, the young association 'grew organically', as the former president Dr. Ellie Piper (née Shardlow) recalled: in 2003, the first official board reformed the network into an association by law and decided to become a body to foster national events, with first seminars held in Basel. In the SCS

Fig. 2. Participants at the first Swiss Snow Symposium, held in March 2003.

Spring meeting on March 10th 2005, it was formally integrated into the Division of Chemical Research of the SCS.[10,11] The JCF changed its name into 'Swiss Young Chemists' Association' (SYCA) to reflect the multilingualism of Switzerland. In 2020, the SYCA was rebranded as 'youngSCS' to express the close connection to its mother organisation, the SCS.

Mission and Activities of the youngSCS

The youngSCS ***represents, connects***, and ***empowers*** young scientists in chemistry-related fields all across Switzerland.

Young chemists are ***represented*** both nationally, *i.e.* in the SCS board, local universities, Swiss career fairs, and internationally. The youngSCS board currently includes up to two representatives from each university and institute in Switzerland (Fig. 1, Fig. 3). The youngSCS collaborates closely with the European Young Chemists' Network (EYCN[12]) and the International Young Chemists' Network (IYCN[13]) and has one delegate in each of these organisations. A recent example of an international collaboration is the Young Chemists' Summit, organised in September 2020. This hybrid conference was initiated by the Austrian Young Chemists as a mixture of virtual talks and local hubs and offered participants a rare opportunity for face-to-face scientific exchange in the pandemic-stricken year 2020. The youngSCS represented Switzerland in this conference and set up local hubs in Fribourg and Zurich.

A picture of the plenary session by Prof. Giese is shown in Fig. 4. Moreover, the youngSCS committed to support the Young Chemists' sustainability guidelines in collaboration with the German and Austrian young chemists' associations, JCF and Jungchemiker, respectively.[14] As their representative body, the youngSCS aims to advocate for rising chemists and communicates their interests towards the general public, industry, and academia.

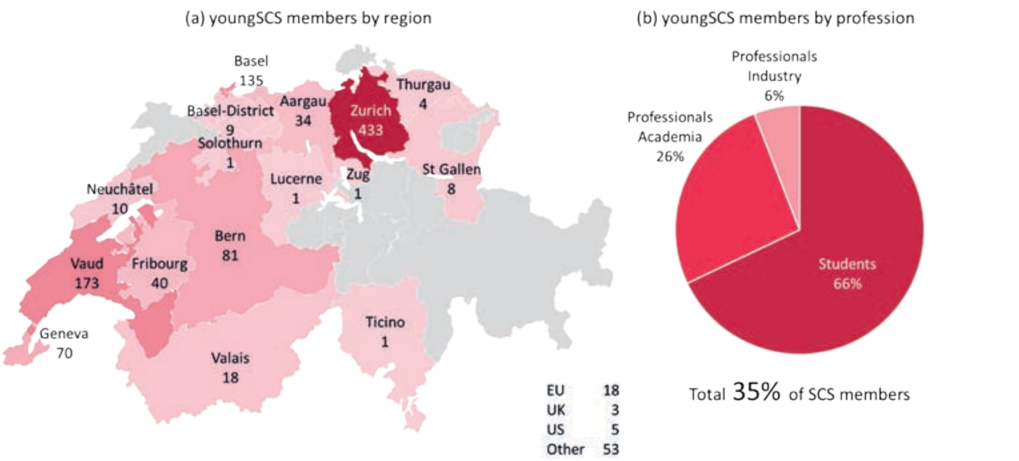

Fig. 3. youngSCS statistics of 2020 (a) youngSCS members by region illustrates the location of youngSCS members. Most members were based in canton Zurich, followed by the cantons Vaud and Basel. 'Other' includes members outside the annotated regions or with unknown locations. (b) youngSCS members by profession shows that in 2020, 66% of youngSCS members were students, 26% senior scientists in academia and 6% employed in industry. In total, youngSCS counted 1098 members, and contributed to 35% of all SCS members.

Fig. 4. The youngSCS has established four event tracks to empower young chemists. A comparison between different career tracks was virtually organised to provide students new perspectives. Innovative research was presented at one of the plenary lectures of the young chemists summit in Fribourg, in collaboration with the Austrian Young Chemists. The Swiss snow symposium (group picture from January 2020) connects young chemists all over Switzerland and members are encouraged to enhance their presentation skills by annual awards.

- Are you a chemist or chemistry-related scientist in Switzerland?
- Are you studying chemistry or a chemistry-related science and/or working in a swiss-based academic institution or industry?
- Are you interested in the swiss-wide chemistry community?
  If you answered 'YES!' to any of the above questions, the Swiss Chemical Society (SCS) is the scientific organization you should be member of.
- Are you a member of the SCS and less than 35 years old?
  Then, you automatically belong to the youngSCS.

To ***connect*** young chemists, the division supports the exchange of scientific and technical know-how and offers networking possibilities with academia, industry, and public relations. The focus of the youngSCS is to connect students, young professionals and staff from all Swiss universities and research institutions. A multitude of youngSCS events offer networking opportunities. Here, we only highlight a few of them. 'Visit each other' is an event where youngSCS members visit chemistry departments of Swiss-based universities. This strengthens the ties between universities and provides students with a broader picture of the chemical research in Switzerland. Furthermore, the youngSCS organises company visits, *e.g.* a virtual tour at IBM Research Europe in Zurich (March 2021), to provide youngSCS members with insights into possible career paths. Another highlight is the aforementioned annual Swiss Snow Symposium. The deliberately small venue of the Snow Symposium fosters not only intense exchange among the youngSCS members, but also with external partners from industry and academia. Thanks to industry sponsors and the SCS, the youngSCS is able to offer the Swiss Snow Symposium at an affordable fee for students. This relates to another core value of the youngSCS: the youngSCS is an advocate for diversity. It supports chemists at different career stages, from various social and cultural backgrounds and minority groups.

The youngSCS ***empowers*** young chemists by providing unique opportunities to train and strengthen their skills. Early career chemists are ***informed*** *via* its freshly-established newsletter and social media channels of webinars and relevant events. Recent examples include a webinar about insights into academic publishing by Richard J. Smith (February 2021) and a comparison between an academic and an industrial career path in the outreach event 'Chemistry Degree and Now?' by Prof. Dr. Christof Sparr and Dr. Amandine Kolleth-Krieger (December 2020), shown in Fig. 4. In addition, the youngSCS and the SCS provide multiple platforms for enhancing ***presentation and communication skills***. Members are encouraged to present their work at the SCS Fall Meeting and/or the Swiss Snow Symposium, opportunities that, at other conferences, are often limited to more advanced or senior researchers. Another key asset for young researchers is ***international competence***. The youngSCS supports international exchange via their network and traveling grants are provided by the SCS. Last but not least, becoming an active youngSCS member and taking over responsibilities in the board fosters one's ***leadership skills***. Board members advance their teamwork ability, learn to organise events as well as to communicate efficiently to large groups and build competences in how-to-moderate a meeting and lead a team.

In summary, these events and opportunities are all aimed to provide all youngSCS members with the information and skills they need to get noticed in their field or just find their next job.

Acknowledgements

We would kindly like to thank Dr. Ellie Piper, Lukas Scherer, as well as Thomas Haefele-Racin, who led the SYCA board from 2003-2006, for an interview and information about the youngSCS' early years. We would also like to thank David Spichiger for providing the membership statistics. Special thanks to Marie Perrin, Marie-Désirée Scheidt, Iluc Farrera-Soler, and Melanie Gut for the elaboration of the youngSCS structure figure. We would also like to thank our board members Benjamin Ries, Patrick W. Fritz, Ahmed Elabd, and Amin Hodaei.

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A Perspective on Chemistry and Society

A Column on the Occasion of the 75th Anniversary of CHIMIA

Division of Analytical Sciences of the Swiss Chemical Society

Perspectives and Future Directions of the Division of Analytical Sciences of the Swiss Chemical Society

Eric Bakker*[a], Davide Bleiner*[b], and Ksenia Groh*[c]

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From left to right: Eric Bakker, Davide Bleiner and Ksenia Groh.

Happy 75th birthday, CHIMIA! Switzerland is a traditional powerhouse in the analytical sciences and has been at the forefront of X-ray and magnetic resonance spectroscopy and imaging, mass spectrometry, chemical sensing, microfluidics, separation science, environmental trace analysis and bioanalytics, to name but a few examples. The instrumentation developed and the scientific insights obtained within these fields have had a profound impact on our understanding of the world and brought tremendous advantages to society as a whole. Of course, most natural sciences absolutely rely on the routine use of analytical tools to make progress. The 2020 IUPAC survey states that as much as 50% of the top ten emerging technologies in Chemistry are related to the measurement sciences, including nanosensors, rapid diagnostics for testing, liquid gating, and aggregation-induced emission.[1]

A sizable community has made the invention and further development of analytical methodologies and their practical application a core aspect of their professional passion. The Division of Analytical Sciences (DAS) of the Swiss Chemical Society (SCS) counts over 500 members and is the place where analytical science in Switzerland finds a united voice. It is a highly diverse division because analytical science has become a core component of many disciplines including chemistry, biology, health science, environmental science, food science, and process control. The DAS unites actors from traditional universities and universities of applied sciences, national research institutes and centers, and industry organizations. It is a stimulating and diverse environment to be part of. However, this diversity also makes it a challenge to forge a sense of community. This latter point is a primary motivation behind many activities of the DAS and the SCS as a whole.

The core tasks of the DAS are performed by a board that consists of an active group of more than a dozen representatives from a wide range of scientific organizations and fields. The main missions of the DAS team involve networking, education, dissemination and recognition. This column is authored by the current DAS president, Eric Bakker (University of Geneva), and the two newest additions to the DAS board, Davide Bleiner (Empa) and Ksenia Groh (Eawag). While Walter Giger just in 2017 recounted the history of the DAS on the occasion of its 25th anniversary,[2] we aim here to discuss the opportunities and challenges facing us in the future.

Together We Are Stronger: A Unifying Effort of the SCS

A major development within the Swiss Chemical Society has been to aim for a more unified presentation toward a wide range of potential stakeholders, and the DAS is playing a significant role in this development. Relationships with industrial partners are now increasingly sought at the SCS level, which allows their voice to be heard while also providing for recurring support of various activities and events held by different divisions. Most awards, including the METAS prize in metrology, are now selected by an SCS awards committee, with the exception of the bi-annual Simon Widmer Award given by DAS, which is handled by an international committee. Another major change involves the continuing education program (see below), which is being topically broadened and rebranded, and its administration newly integrated into the SCS head office. The reader may have also already seen the new face of the SCS website, which has been set up to allow for an easier navigation by reducing the traditional compartmentalization by each SCS division. The result of this modification is a fresh, modern appearance of the DAS that projects to be a core part of the SCS while serving its own community as effectively and professionally as possible.

Nurturing Networks of Analytical Scientists

In this (hopefully finite) period of Covid-19 and endless online meetings, building new connections has become so much harder, especially for young researchers. The most important recurring event organized by the DAS is *CH*analysis, which for the coming years will be under the main responsibility of Davide Bleiner. It is an annual spring meeting that specifically aims for Swiss-based researchers in the analytical sciences to get to know each other. This conference is traditionally held in Beatenberg, Bernese Oberland, and features high-quality invited speakers and contributed talks. However, the major emphasis is placed on poster presentations and informal discussions, because the main goal of this recurring meeting is to build a strong sense of community and facilitate the exchange of scientific ideas, while showcasing the amazing diversity of the analytical science landscape in Switzerland. In the first few years, *CH*analysis was mainly cross-financed by the continuing education program of the DAS, but by now the event benefits from company sponsors and thus has sufficiently matured for it to become cost neutral. The next meeting is scheduled for spring 2022. While this decision might evolve, we currently feel that the networking aspect is central to this event so that we will only hold it as an in-person meeting. Please join us!

The DAS is also actively involved with the annual Fall Meeting of the SCS, with Eric Bakker, Ksenia Groh, and Hanspeter Andres (METAS) playing organizing roles. The aim is complementary to *CH*analysis, *i.e.* to have a stronger representation for the dissemination of advanced analytical impact. A major draw for students is the possibility of receiving a prize for best poster or oral presentation and, of course, the broad exposure to other fields of science.

As the representing body of the analytical scientists in Switzerland, DAS is well positioned to organize major events hosted in Swiss cities, as it has done in the past decade with ANAKON 2011 (in Zurich), IMSC 2014 and HPLC 2015 (both in Geneva). The next such major event will be Euroanalysis 2023, again in Geneva, with Franka Kalman (HES Sion), Bodo Hattendorf (ETH) and Eric Bakker as chairpersons. Such events also showcase the connection of DAS to European organizations, in this case the Division of Analytical Chemistry of the European Chemical Society (EuChemS), where Franka Kalman is our representative.

We mention here also the Highlights in Analytical Chemistry column in CHIMIA, tirelessly put together by the DAS board member Veronika Meyer. These 1-page descriptions appear in most CHIMIA issues and offer stimulating insights into analytical problems and discoveries. Please use this opportunity to highlight your research and support the continuation of this column. It is a citable item that speaks to non-specialists and is therefore a great addition to your typical research paper.

Education and the Future of Analytical Science in Switzerland

Analytical science is everywhere, but where is it in the educational curricula? An observed trend is that analytical experts tend to be increasingly single-method specialists while the present challenges in industry and society require a much broader analytical expertise. To fill this gap, a sub-committee of the DAS has been working since 1999 to offer vocational training courses on broad subjects in the analytical sciences, with an emphasis on a wide range of analytical techniques as well as regulatory education, for example in quality control. As already mentioned above, a major ongoing development of the training program of the DAS is its integration into a new SCS-wide platform, termed SCS Academy. This will allow one to find programs of a much broader topical diversity, all marketed in a unified manner by the SCS. To assist the SCS, the DAS has moved the education office (Esther Wolff) away from Dübendorf to the SCS head office, with a unified email and billing address. For DAS, like other SCS divisions, this will allow us to place more focus on content rather than administration. Importantly, this development also eliminates financial risk to our division. The DAS is quite excited about this structural optimization and confidently looks into the future of our continuing education program.

As for the future of education in analytical science at Swiss Universities, it seems that we are now experiencing both very rich and rather poor times simultaneously. Analytical science in general is flourishing and many new hires in Switzerland are in fact active analytical scientists. Most of them, however, are not hired as pure analytical scientists but rather as bioengineers, environmental scientists, microbiologists, or organic, physical or biological chemists. So, while the research landscape remains very active, the branding of our discipline has become less identifiable. Is this part of our success, with the measurement sciences becoming such an integral part of making scientific progress that we no longer need to worry about promoting it as a separate discipline of its own? Yet, one could also argue that we need to maintain this identity because, compared to some other scientific branches, analytical science requires a different, more holistic way of thinking about, first, quantifying and then interpreting the collected measurement data. Maintaining and further developing an analytical science identity becomes particularly important in the face of the rapid developments and novel challenges that have presented themselves in the recent years. Modern analytical sciences struggle to accommodate divergent trends fueled by diverse societal demands, not infrequently standing in opposition to each other. For example, the current trends towards miniaturization, portable devices and mobile laboratories may not always be able to simultaneously provide for the highest standards of analytical selectivity and sensitivity. Thus, certain tradeoffs may need to be accepted in exchange for the ability to gain a better spatial and temporal resolution of obtained monitoring data. The growing demand for a more sustainable, greener chemistry, with minimized use of hazardous substances and maximized safety for both the workers and the environment, may on the one hand be supported by the ongoing developments towards miniaturization. On the other hand, certain innovations, such as those based on nanotechnology, still need to be evaluated and properly managed with regard to their environmental risks. As yet another example of opposing demands, the increasing complexity of analytical instruments and measurement workflows often requires extensive training on the part of operators, resulting in an ever-narrowing specialization. This in turn might hamper answering the simultaneously ongoing call for more collaborations and open sharing of research results and even raw data. The latter should ideally be presented in formats understandable and usable by scientists from other fields or even by non-specialists. Apropos the research data, the ever-increasing volumes created by sophisticated analytical platforms generate a unique need for broader involvement of data scientists, able to foster artificial intelligence to help collect, curate, mine, and interpret the analytical data, as well as to enable seamless data sharing across platforms and disciplines.

The utilization of large shared user facilities and their increasing openness to the broader community provides a host of new opportunities. The Swiss Roadmap for Research Infrastructures is updated every four years: the State Secretariat for Education, Research and Innovation (SERI) is strengthening the view of the research community throughout the process leading to the Swiss roadmap. Therefore, SERI gave a mandate to the Swiss Academy of Sciences (SCNAT) to produce discipline specific roadmaps by March 2021.[3] These disciplinary roadmaps will provide insights for decision-making on the allocation of university and federal funding for costly research infrastructures over the period 2025–2028. The future of discovery hinges on the innovation of today's measurement tools.

Whatever the future brings, a community organization such as the DAS continues to realize an important mission of helping to define an analytical science identity, able to unite a diverse array of researchers scattered across various disciplines. This unifying effort is likely the most important challenge that we face. So please join our ranks and make us strong.

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A Perspective on Chemistry and Society

A Column on the Occasion of the 75th Anniversary of CHIMIA

The Division of Chemical Education of the Swiss Chemical Society

The Division of Chemical Education Supporting Teachers throughout Switzerland

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Jan Cvengros was born in Slovakia and studied organic chemistry at Comenius University in Bratislava and completed his PhD thesis in organic chemistry at University of Cologne (Prof. H.-G. Schmalz). After postdoctoral stints at University of Milan (Prof. C. Gennari) and at ETH Zurich (Prof. Antonio Togni) and a short employment as a process chemist at Syngenta, he established an independent research as an SNSF Ambizione fellow. His interests gradually shifted towards teaching leading him to his current position as a lecturer at ETH Zurich. In 2020 he became the president of the Division of Chemical Education of the Swiss Chemical Society.

Switzerland might be known for cheese, chocolate or watches, but chemistry is certainly, albeit not obviously, contributing to the positive reputation of this country. It is only seldom recognized by people that a broad palette of Swiss chemical companies, some of them worldwide leaders, specialize in a variety of fields and offer products and solutions for a broad community.[1] Similarly, numerous research groups at Swiss universities and institutes develop innovative ideas in basic and applied chemistry leading to valuable results of wide interest. Eight Nobel prizes were awarded to Swiss chemists so far, three of them in the last 30 years. Such endeavours would certainly not be possible without a quality education and training. The efforts and the dedication of all teachers, lecturers or mentors are thus highly appreciated. Interestingly, unlike in a variety of European countries, *chemical education* as the study of teaching and learning chemistry in a coordinated and structured manner receives in Switzerland much less attention than expected.[2] This statement should not degrade the efforts of the individuals but rather point to the fact that academic positions dedicated to chemical education are in Switzerland basically non-existent. Furthermore, a Division, which would focus on this matter, has been only relatively recently added to the portfolio of the Swiss Chemical Society.[3]

Division of Chemical Education

The importance of such a division was recognized by Antonio Togni, Markus Müller, and Hans Peter Lüthi from ETH Zurich and following their initiative, the Swiss Chemical Society established the Division of Chemical Education (DCE) in April 2017. Right from the outset the activities were aimed at establishing a platform for the exchange of educational know-how at all levels (horizontal integration) and also between educational levels (vertical integration). An essential task was to identify suitable and dedicated individuals across Switzerland active in different fields related to chemical education. The first impression that this may include high school chemistry teachers and lecturers at universities only is quite inaccurate. To a certain extent, it was rather unexpected even for the board members to witness, how broad the network could be, once we cast our net wide. Accordingly, it was just recently that the composition of the Board of the Division was finalized.[4] The members representing high schools, secondary schools with vocational training, universities and universities of applied sciences stem basically from every corner of Switzerland. We hope that with such a broad coverage we will be able to address a vast majority of those dealing with chemical education. Albeit four years may seem to be a rather long period, the Division of Chemical Education is still young and we intensively work on identifying, establishing and developing the future ventures. It is important to stress that we are aware of a variety of activities offered by the independent associations (*e.g.* Zentralkürse organized by the Swiss-German Committee on Chemistry[5]) and the Division has absolutely no intention of competing for the same audience. Our goal is to support and to contribute to any event aimed at improving chemical education or promoting chemistry. The symposia organized by the Division will primarily focus on filling thematic gaps not covered by others.

Professor Antonio Togni, one of the initiators and first president of the Division of Chemical Education, during a presentation at the 'Future of Chemical Education' symposium, 2019.

We would like to also encourage any individuals, schools or institutes to approach the Division of Chemical Education, if they feel that we might be the right partner for their endeavors. Recently, we have been contacted by the organizers of the Chemistry Olympiad (a chemistry competition mainly for high school students), who seek opportunities to promote this event between students and teachers.[6] The Board of the Division discussed our possible involvement in this matter and agreed to use our communication channels to advertise the abovementioned contest. The Division will also help to find volunteers willing to mentor the students, especially as the International Chemistry Olympiad in 2023 will take place at ETH Zurich.[7]

Chemistry Education and COVID-19

The events organized by the division were collectively entitled ‘Future of Chemical Education’, whereas the word future was intended to illustrate our intention to constantly contribute to the improvement of the teaching process, *e.g.* by introducing new methods or technologies. In other words, we offered a glimpse at how teaching chemistry might look in the future. Back in 2019 when initiating the first steps towards the next ‘Future of Chemical Education’ event we had no clue how close the future is and that these efforts may actually help to sustain the teaching and enable further education without calling off lectures, skipping the exams or even cancelling the entire school year during the corona pandemic.

The leitmotif of the symposium focused on problems and challenges related to teaching chemistry for a large and typically very heterogeneous body of students in the first year at the universities. The event was originally scheduled to take place in August 2020 in Muttenz, but for obvious reasons it was rescheduled to April 2021. Although, to our dismay, traditional personal encounters were still not possible, the online symposium turned out to be a motivating and stimulating event. Speakers primarily described their strategies, how they deal with a task that is already quite difficult and demanding, yet their abilities were challenged even more in the last year. The sudden change in the teaching process forced the lecturers to find alternative solutions – solutions, which were maybe foreseen for the future but had to be applied almost immediately. Certainly, a further optimization is still necessary in many cases, but obviously this challenging situation prompted all of us to modify our teaching methods – something we probably wouldn’t have done under normal circumstances. There is hardly anyone who does not look forward to a return to the traditional way of teaching, but the experience gathered during the current difficult situation should have a positive effect on our lectures in the future.

A screenshot of the ‘Future of Chemical Education’ event 2021, organized as an online Zoom conference.

CHIMIA and Chemical Education

Cover pages of both CHIMIA issues dedicated to Chemical Education.

There is no doubt that any chemistry journal is a source of valuable information, which might be used in the teaching process. And there is also a decent number of journals dedicated specifically to chemical education. Yet it is great that *CHIMIA* continues to offer space for teachers and lecturers to share their knowledge, methods or experience within the Swiss community, thus enabling an efficient networking between those involved in the educational processes in chemistry. This includes, in particular, a regular *CHIMIA* Chemical Education column – a short 1–2 page contribution dealing with a chosen topic relevant to teaching chemistry.[8] Furthermore, two entire issues were dedicated to chemical education helping to increase the awareness of the Division.[9] The Division of Chemical Education also seeks other opportunities to further promote chemistry and chemical education *via* contributions to the journal with an outreach to the entire Swiss chemical community. We sincerely believe that the future cooperation will remain equally fruitful and we wish *CHIMIA* all the best for the forthcoming years.

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b) Website of the Austrian Educational Competence Centre Chemistry at the University of Vienna: https://aeccc.univie.ac.at/; Education website of the Royal Society of Chemistry: https://edu.rsc.org/.
[3] a) Website of the Division of Chemical Education of the German Chemical Society: https://en.gdch.de/main-navi/network-structures/divisions/chemical-education.html;
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[4] Website of the Division of Chemical Education of the Swiss Chemical Society: www.scg.ch/dce.
[5] Activities of the Swiss-German Committee on Chemistry: http://www.vsn.ch/DCK/DCK.html.
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[7] International Chemistry Olympiad 2023 at ETH Zurich: https://chab.ethz.ch/en/news-and-events/icho2023.html
[8] List of all Chemical Education columns: https://chimia.ch/component/content/article/1773.
[9] a) *CHIMIA*, **2018**, *72*, issue 1-12;
b) *CHIMIA*, **2021**, *75*, issue 1/2: www.chimia.ch

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A Perspective on Chemistry and Society

A Column on the Occasion of the 75th Anniversary of CHIMIA

Division of Fundamental Research of the Swiss Chemical Society

Fundamental Research in Chemistry and the SCS: Past, Present, Future

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Stefan Willitsch graduated from ETH Zurich in 2000 and received his PhD from the Laboratory of Physical Chemistry at ETH in 2004. From 2004–07, he held a Junior Research Fellowship at the University of Oxford. He was appointed lecturer in physical chemistry at University College London in 2007 and joined the faculty at the Department of Chemistry at the University of Basel in 2008. His research interests focus on translationally cold molecules and ions and their applications in chemistry, spectroscopy and quantum technologies. Since 2020, he acts as the president of the Division of Fundamental Research of the Swiss Chemical Society.

The 75th anniversary of CHIMIA offers not only an opportunity to reflect on the colourful history of the journal itself,[1] but also on its publisher, the Swiss Chemical Society (SCS), and the venerable scientific discipline it represents. Like CHIMIA, chemistry has evolved enormously over the past three quarters of a century and has advanced its scope, its methods, its relationship to other scientific disciplines and its role in society. In the middle of the past century, chemistry still broadly articulated into three core domains inorganic, organic and physical chemistry. For sure, these disciplinary categories have always been fluid and always needed to be taken with a grain of salt. Nonetheless, the topical diversity into which chemistry has expanded over the past decades is remarkable. Although chemistry departments at many universities are still largely organised along the traditional sub-disciplinary lines, the scope of topics covered has broadened significantly and now includes chemical biology, material science, computational chemistry, nanoscience, energy research, molecular physics and biophysics, to name only a few. Much of the scientific progress in modern chemistry occurs at the boundaries to other disciplines like biology, physics, computer science, materials science and even mathematics. Chemistry has become one of the most interdisciplinary academic disciplines. In the economic domain, many traditional Swiss chemical companies have transformed and merged into pharmaceutical companies. Classical chemical industries have largely relocated to Asia.[2] These paradigm shifts also did not leave the SCS unaffected, as a glance at its new website confirms. Today, the SCS branches into an increasing variety of divisions, sections and thematic networks which form its atomic constituents and are a reflection of the broad thematic scope of modern chemistry.

Quo vadis, Chemistry ?

An outside spectator might get a bit dizzy in the face of all this diversity and may well ask us: "What is chemistry today?" In fact, I had to address this question many times myself during my tenure as my department's study counselor when I tried to explain to prospective students why studying chemistry is a worthwhile enterprise to build a career on. Clearly, it is the duty of every academic discipline to constantly question and renew itself in order to find its role in a changing environment of scientific questions, societal challenges and evolving technologies. It is thus rewarding to every now and then reflect on what defines us and on what can be undertaken to foster our community and advance our discipline.

Modern definitions of chemistry often refer to the 'science of molecules'. Indeed, it is molecular concepts that have radiated out into other disciplines and have led to their 'molecularisation'. Biology, material science and the modern nanosciences are maybe among the most prominent examples. This development is a success story for chemistry which has put it centre stage within the canon of sciences. However, this also means that for everyone aiming to unravel molecular phenomena, in whatever discipline, a solid education in the core chemistry subjects is, and remains, indispensable in order to be able to understand the structure, properties and transformations of molecules. I would thus argue that teaching chemistry has lost nothing of its topicality over the past 75 years. On the contrary, it has gained importance in a much wider context.

The Role of the DFR

Within the SCS, the Division of Fundamental Research (DFR) has traditionally represented the voice of academic science in the core chemistry disciplines. It constitutes the largest division of the SCS comprising around 1300 members. Its role is to promote and support chemistry and its community in Switzerland. It does so with a wide range of initiatives.

The DFR organises the annual Spring and Fall Meetings. The former is a focused event on varying topics held at a different Swiss institution every year. The latter represents the largest recurring chemistry conference in Switzerland with close to a thousand participants. Both meetings serve as focal points for the Swiss chemistry community spanning both academia and industry. Another important function of the Division is the financial support of scientific conferences related to chemical topics in Switzerland. These are typically international meetings of sizes varying from small workshops to large signature congresses which are held in Switzerland on a one-term basis. These events form an important element for showcasing Swiss chemistry on the world stage and for strengthening the international ties of the Swiss community. On the order of five such meetings are supported every year, including leading events like the 'Bürgenstock Conference'. Moreover, in recent years the DFR introduced the 'SCS Lectureship Awards' inaugurated by the late Prof. Thomas Bally. Within this framework, internationally renowned chemists, usually from overseas, are invited each year on a one-week lecture tour to Swiss universities and companies. The lecturers are nominated and selected in a democratic process by the entire Swiss community. This programme not only further strengthens our exchange with the international chemistry scene, but it also fulfils an important function in offering our young generation of chemists[3] teaching and networking opportunities with outstanding scientists which they otherwise would not have the chance to meet. The scheme has been an outstanding success, as the vivid participation from all over Switzerland demonstrates.

I would argue that it is precisely thanks to the momentous changes which chemistry has witnessed over the past 75 years that the discipline thrives and remains as vibrant as ever in Switzerland. The SCS, and the DFR as one of its central parts, May 21, 2021 take it as their mission to ensure that this success story will continue. It will do so by fostering our human capital, by promoting the education of our next generation of scientists, by nurturing scientific exchange within Switzerland and on the international level and by providing a focal point for our community. CHIMIA will continue to play an integral part in this endeavour, and it will be fascinating to see where the journal, and indeed chemistry in Switzerland, will stand at its next big anniversary.

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A Perspective on Chemistry and Society

A Column on the Occasion of the 75th Anniversary of CHIMIA

Swiss Academy of Sciences - Platform Chemistry

SCNAT Platform Chemistry

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Abstract: The Platform Chemistry of the Swiss Academy of Sciences SCNAT is a small component in the Swiss network of education and research. The platform board analyses the education and research scene in Switzerland in order to identify issues that can be addressed by projects or initiatives or by coordinating efforts of others.

Keywords: Chemistry · Research · Education · Outreach · Switzerland

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Leo Merz is the head of the Platform Chemistry. He studied chemistry in Basel and moved to the physics department for his PhD on scanning tunnelling microscopy. He went to Japan for a Post-doc at the Tokyo Institute of Technology and back to Switzerland for research at Empa in the Molecular Surface Science lab. After a five-year journey on a sailboat, he joined the Swiss Academy of Sciences.

What is the SCNAT Platform Chemistry?

The Swiss Academy of Sciences ('SCNAT' from SCientia NATuralis) was founded 1815 as the 'Schweizerische Naturforschende Gesellschaft' (SNG). In 1901 the chemists of this society founded the Swiss Chemical Society as a section of the SNG.[1] And to this day the Swiss Chemical Society is a member organisation of the SCNAT with an excellent collaboration. The SCS is the only member society that has its head office at the House of the Academies in Bern.

The Swiss Academy of Sciences is one of the institutions in the area of 'promotion of research' with a mandate from the state. The federal law on the Promotion of Research and Innovation defines the funding of the Swiss National Science Foundation (SNSF), the Academies, Innosuisse, the Swiss Science Council, and the institutions of the ETH domain.

There, the academies are tasked with (a) early recognition of relevant topics in education, research and innovation, (b) ethics with respect to research and innovation, and (c) encouraging dialogue between science and society including politics. This includes promotion of (inter-)national collaboration, promotion of young scientists, and anything to keep the scientific disciplines healthy.

About 13 years ago, the SCNAT reorganised its structure into disciplinary platforms, one of which is the Platform Chemistry (for the other organisational units of SCNAT see scnat.ch). The SCNAT member societies in the Platform Chemistry are the Swiss Chemical Society, the Swiss Society for Food Chemistry (SFC), and the Verein Schweizerischer Naturwissenschaftslehrerinnen und -lehrer (VSN). The member societies are represented in the board of the platform to facilitate a close collaboration between them.

Projects of the Platform Chemistry

To illustrate the role of the Platform Chemistry, we take a look at some recent projects and initiatives.

The SCNAT provides support for CHIMIA, helping the journal reach as wide a chemical community as possible.

In 2018, a potential shortage of radiochemistry experts became apparent, and the platform assembled a group of experts to compile a whitepaper on education in radiochemistry in Switzerland.[2] Even the preliminary stages of the preparation of the report helped to raise the awareness of the topic and the ETH board established a radiochemistry professorship. The final white paper has been published online: chem.scnat.ch/radiochemie

Another major effort focusing on science policy has been the preparation of the Roadmap for Research Infrastructures in Chemistry 2025–2028.[3] This project was initiated by a mandate from the State Secretariat for Education, Research and Innovation (SERI). SCNAT was asked to assemble the research communities from different disciplines to elaborate roadmaps for research infrastructures similar to the earlier ones in astronomy and particle physics. This community roadmap is one of the major inputs for the universities planning and discussions with regards to national (inter-institutional) research infrastructures. This roadmap is also a basis for the national roadmap which is being prepared by SERI. The national roadmap offers a way forward for collaborative research within Switzerland, thereby facilitating partnerships and moving away from an introverted research projects.

Over the past few years, the board of the Platform Chemistry recognised the need for ethics education in the chemistry curriculum. This initiated the SCNAT Ethics Series (chem.scnat.ch/ELT) and is offered to chemistry departments across Switzerland. SCNAT invites one or several international experts on a range of topics around ethics in chemistry to tour Swiss universities. Together with the local hosts, an evening of discussions in a format like a 'world cafe' is organised and participants from master students to senior professors address issues including publishing, dual use, and scientific integrity. The next series is planned for January 2022 with Lee Penn from University of Minnesota (USA) and will address the topic of 'implicit bias'. Our aim is for the Platform Chemistry Ethics Series to serve as a catalyst, and we very much hope that universities across Switzerland will eventually integrate ethics education into their own curricula, as, for example does the NCCR MSE.

While the Platform is too small to organise major outreach activities, it has found a niche in several activities, for example, the annual Chemical Landmark which raises awareness of important historical events and sites relevant to chemistry in Switzerland. Chemistry is one of the important foundations of Switzerland's wealth. Last year, more than half of the Swiss exports were in the area of chemistry and pharma! The Chemical Landmark is awarded to sites where important milestones were achieved, or where famous chemists worked. Awards include the first chemical factory in Switzerland,[4] the workplaces of many Nobel laureates,[5,6] Kekule's laboratory in Reichenau (he worked as assistant there),[7] atmospheric chemistry and Max Perutz's work on ice crystals at the Jungfraujoch research station,[8] the invention of Ovomaltine in Bern,[9] and the discovery of the elements Yb and Gd in Geneva.[10] The next celebration will be the Chemical Landmark 2020 (postponed to November 2021); the Pharmaziemuseum Basel will be awarded a Chemical Landmark plaque as the workplace of Paracelsus. Nominations for chemical landmarks are welcome at any time: chemicallandmarks.ch

Additionally, the platform supports activities such as the VSN's experiments for schools, or exceptionally this year the 125th anniversary celebrations of HES-SO Fribourg: 125.heia-fr.ch/?cat_id=36

Apart from supporting many conferences, seminars and symposia of the member societies, the platform organises the annual Young Faculty Meeting (chem.scnat.ch/YFM). The YFM brings together young research group leaders (from senior post-doctoral associates with their own group to young professors) from Swiss institutions to network, and to exchange and discuss concepts and ideas. The one-day meeting consists of scientific talks by participants, and talks and discussions focused on, for example, fundraising, science communication, group management, outreach topics. The focus is on topics not usually covered in depth during the course of chemistry educational programs, nor in doctoral and postdoctoral training.

Apart from the YFM, the platform organises the Chemistry Travel Award together with the SCS (chem.scnat.ch/travel_award). Excellent PhD students receive support to present their work at an international conference. Currently, the Travel Award scheme has been adapted the needs of the Covid-19 pandemic and the option to visit another research group for a short project has been added. To compensate for the missed conferences in 2020, the EYCN meeting in Fribourg is also supported in January 2022.

A further highlight of the promotion of young scientists is the Prix Schläfli. The Prix Schläfli is awarded annually in the disciplines of the SCNAT platforms for 'the best Swiss PhD in natural sciences' (scnat.ch/prixschlaefli). The Prix Schläfli is one of the oldest prizes of its kind in Switzerland and is highly prestigious. Currently it consists of CHF 5,000 with a trophy, and awardees in chemistry are also invited to present their research at several Swiss institutes.

The Platform Chemistry also represents Switzerland in the IUPAC and financially supports SCS's membership in EuChemS.

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A Perspective on Chemistry and Society

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Syngenta Crop Protection AG

Crop Protection Chemistry: Innovation with Purpose

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Jérôme Cassayre was born in Nancy, France (1973). He graduated from the Ecole Polytechnique (Palaiseau, FR, 1995) and obtained his PhD in chemistry at the Institut de Chimie des Substances Naturelles (ICSN, Gif-Sur-Yvette, FR, 1999, Prof. S. Z. Zard). He joined Novartis Crop Protection (which became Syngenta) as chemistry lab lead (Basel, CH, 2000). He became group leader (2008), then head of insecticide and seed care chemistry (Syngenta Stein, CH, 2011), followed by head of new active ingredient process technology (Münchwilen, CH, 2016). In 2018 he was appointed head of global research chemistry, Syngenta Crop Protection, Stein, Switzerland.

The SARS-CoV-2 pandemic crisis has put food security back at the center of the debate, with our western societies rediscovering the tremendous effort required to grow and supply food while other parts of the world already suffering from hunger and malnutrition before the virus became even more vulnerable during and likely will remain so after this crisis.[1] As the adage goes "every cloud has a silver lining", we can only welcome that the vital role of agriculture has been duly recognized, as well as society becoming more aware of the multiple challenges faced by farmers around the world including climate change, pest pressure, soil degradation, and the urgency to achieve greater sustainability and biodiversity. We may only wish that a similar awareness is drawn towards the recognition of science achievements which enabled agriculture to continuously improve productivity until today and the urgent need to accelerate innovation to secure future food security. In this perspective, I advocate for chemistry being part of the solution for sustainable agriculture but also explore how crop protection research may reinvent itself to better respond to growers' needs and restore the damaged but not broken link between agrochemical innovation and society.

Accelerate Innovation: Necessity Rather than Choice

Agricultural research has been the main contributor to the 60% increase of global agricultural output during the past 40 years while cropland has only increased by 5% during the same period.[2] Besides the rationalization of agronomical practices, crop protection products have played a major role in the productivity gains by preventing yield losses due to pest.[3] Crop protection chemists have been continuously innovating with the discovery of molecules acting at lower rate (a 10-fold decrease in average in the last 50 years) and displaying a much more favorable human and environmental safety profile.[4] However, a recent study confirmed and quantified that anthropogenic climate change has slowed global agricultural growth, an effect even more pronounced in the southern hemisphere.[5] With the impact of climate change expected to accelerate, it poses a serious threat to the delicate balance which exists between the constant development of pest shift and resistance, and our ability to innovate at a pace required for agriculture to sustain food production for a world population projected to reach *ca.* 10 billion by 2050.[6]

Accelerating innovation to help farmers become more resilient to the consequences of climate change while limiting its causes (food production represents 26% of anthropogenic greenhouse gas emissions)[7] is the great challenge for the next decade. The urgency to respond to the food security question in a world impacted by climate change should wind up the sterile debate between man-made or nature-made solutions, and encourage us to explore the complementarity and synergies between crop protection chemistry, biological control and modern agronomical practices.

Less is more: Expanding the Chemistry Toolbox

Modern farming techniques[8] enable the use of crop protection products at the right time (through sensing technologies), at the right place (through precision application) and at the right dose (through informed management systems), contributing to reduce the agrochemical input while optimizing output. This evolution also opens new territories in the chemical space so far largely uncharted in crop protection for cost limitations. Applying less product more precisely indeed allows for more diverse and complex chemistry to meet more stringent performance, safety and sustainability criteria while continuing to reduce the cost of application *per* hectare (Fig. 1). This will also unleash opportunities for synthetic modalities beyond small molecules following the trend observed in drug discovery in the last decade:[9] natural products already proved as a reliable source of agrochemical leads and novel modes of action,[10] peptides are emerging as promising agrochemical entities,[11] RNA interference technology has been explored for insect biocontrol,[12] and protein degraders (PROTAC technology) may also find their place in the crop protection toolbox.[13]

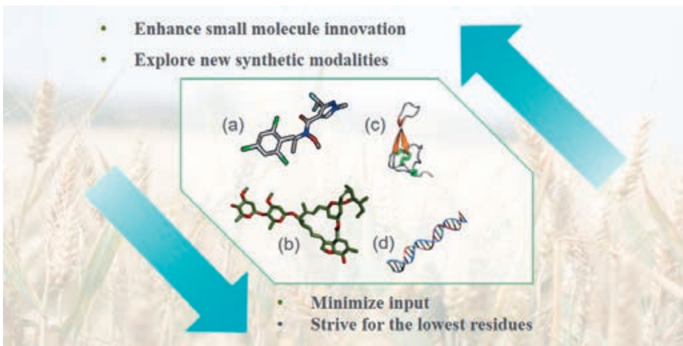

Fig. 1. Rate reduction expands the chemistry toolbox in crop protection: (a) small molecules (b) natural products, (c) peptides (d) RNA-based biocontrols.

The crop protection industry is thus committed to promote agricultural practices with less chemical input, and for chemists this is a chance to enhance and diversify small molecule innovation.

More is less: Greener Labs for Greener Products

Rethinking agrochemical innovation comes with the imperative to embed the sustainability principles in the design and synthesis of new active ingredients. Our 'sustainable design' framework, inspired by the circular economy,[14] embeds the entire lifecycle of an agrochemical product in molecular design (Fig. 2). Upstream considerations include synthetic feasibility from a cost and an environmental standpoint taking advantage of advances in synthetic tractability methods[15] and chemical complexity metrics.[16] There is also an opportunity to exploit renewable starting materials in discovery programs as alternatives to fossil-based feedstock; peptides fall naturally into this category but other options exist such as terpenes[17] and more generally through the valorization of biomass using chemo- or bio-catalysis. Downstream considerations on the other hand aim at designing compounds for optimal efficacy/selectivity ratio while considering the environmental fate of the active ingredient itself as well its metabolites.

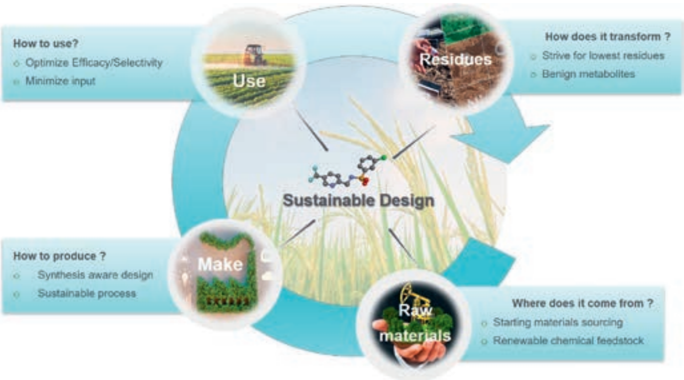

Fig. 2. A chemical design framework for sustainable crop protection innovation.

The 12 principles of green chemistry[18] provide an excellent framework to guide chemists in this quest for more sustainable innovation.[19] The change, however, starts at the laboratory doorstep: while the lab culture of safety and environmental risk assessment continuously improves, we may consider whether some hazards could be *avoided* before being *managed* thus creating a virtuous circle for adoption of more sustainable methods. We could show at Syngenta[20] that a drastic reduction in the use of seven of the most hazardous solvents (including the commonly used dichloromethane and dimethylformamide) was possible by raising awareness and promoting alternatives,[21] for example in the amide coupling reaction where effective substitutes exist[22] for the most usual solvents (DMF and CH_2Cl_2) and reagents (EDC and HATU) but wider adoption of these more sustainable solutions still requires a deliberate effort.

Hence, by consciously adopting more virtuous practices in our laboratories, we also promote innovation towards more sustainable crop protection products.

Digital Chemistry: Embracing Complexity

The design of modern agrochemicals in an enlarged chemical space and their optimization against more diverse criteria does obviously come with increased complexity for crop protection chemists. However, they find in the ongoing digital transformation a precious ally on their journey. The digitalization of the Design-Synthesis-Test-Analysis cycle,[23] at the heart of our agrochemical innovation model, can indeed transcend the usual boundaries of reductionist approaches and embrace the complexity of biological systems and chemical space to increase both quality and speed (Fig. 3). The collection of downstream data from R&D (*e.g.* field trials, product safety) but more importantly from customers (*e.g.* real-use data, agroecological biomarkers) can improve their translation into robust target functional properties, which themselves can serve as a basis for generative chemistry and multi-parameter optimization. This inverse design[24] paradigm shift brings the requirements from the customers, the regulators, and the society closer to the scientists thus increasing the quality of their research. At the same time, the convergence of technologies such as microfluidics, robotics, and artificial intelligence allow for more robust design of experiment and greater automation of chemical synthesis and biological testing thus significantly speeding up the optimization and selection of new active ingredients and ultimately accelerating the delivery of products to our customers.

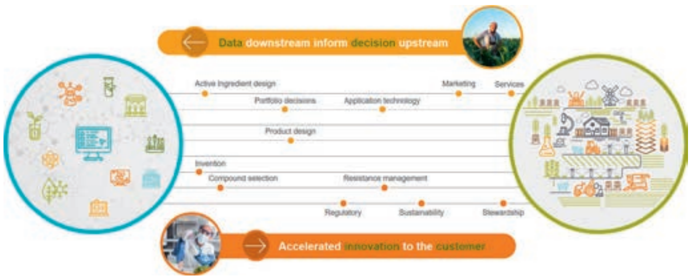

Fig. 3. Customer-centric accelerated innovation model enabled by digital chemistry.

Innovation with Purpose

The necessity to accelerate innovation in agriculture to support the growing demand for food is accentuated by climate change. While the evolution of agronomical systems and the emergence of biological solutions will contribute, chemists will continue to play the key role through the discovery of new molecules to prevent crop losses from pest, abiotic stress and more generally to improve plant and soil health. This chemical innovation imperative requires a delicate triangle balance between customer needs, regulatory standards, and society expectations. Driven by the meaningful purpose of sustainable agriculture, crop protection chemists are ready to take up this challenge and benefit from a growing innovation ecosystem both from a technology and a collaboration standpoint.

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A Perspective on Chemistry and Society

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ETH Zurich

Chemie versus Chemie

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The title of this essay in the 75th volume of Chimia is intentionally the same as that for the antecedent essay written by Jakob Nüesch for the 50th volume in 1996,[1] because the fundamental issue remains the same: the Chemistry of tomorrow against the Chemistry of yesterday. We represent a field with a long and glorious history, and it is incumbent on the leaders today to seek the path forward so that we do not dwell too long in places where we could simply stagnate, and then decline. While it is easy to quote statistics on how useful Chemistry is, and Chemistry is indeed useful if one simply pauses to consider all of the materials around us, all of the active pharmaceutical ingredients, all of the components in our electronics, the catalysts, and so forth, the statistics themselves do not tell us where we need to go. Moreover, Chemistry has become an indispensable part of Life Sciences, for example, delivering, among other things, tools and methods for Biology, upon which Jakob Nüesch elegantly commented. It would be a mistake, however, and I think Jakob Nüesch would agree, to reduce Chemistry to its utility, either in commercial applications, or to other scientific fields. We are grateful that Chemistry is useful – we appreciate the generous support from State and Industry – but when Chemistry becomes merely useful (bloss nützlich), a 'Department of Chemistry' becomes, in the words of my late Doktorgrossvater, Bill Doering, just a 'Department of Chemicals,'[2] which is an altogether different beast. Every vital, growing intellectual endeavor needs its own internal logic, and its own internal motivation (motivator?), or else it ceases to attract the best and most ambitious minds. What from the past applies still, and what needs to change? How can we conceptualize where Chemistry needs to go, and how do we need to educate the next generation of Chemists?

At the risk of being accused of dwelling on the past, I do want to use one particular episode from the history of Organic Chemistry to exemplify the unique way in which Chemistry had worked and continues to work, even today; it gives us a certain intellectual continuity. While the chemical problem in the particular episode is closed, the narrative nevertheless points to where Chemistry can and will make unique contributions to the solution of new problems. Let's look at August Kekulé (1829–1896), Jacobus Henricus van't Hoff (1852–1911), Victor Meyer (1848–1897), and Emil Fischer (1852–1919), and the classical theory of chemical structure. Marcellin Berthelot, a French chemist, wrote about Chemistry in 1860, 'La chimie crée son objet,'[3] emphasizing the central role of synthesis of new entities. Richard Feynman expressed (curiously in the present context of a discussion of Chemistry because he was a physicist) a similar sentiment in 1988, "What I cannot create, I do not understand."[4] With due respect to analytical chemistry, theory, and even my own area of reaction mechanisms, I would postulate that the hard core of Chemistry is synthesis; we understand something by making it. There is a curious, and curiously deep, logic to the claim. At the most superficial level, one sees why Chemistry is so useful. We always make new things. Our society needs things, and industry sells things. We will always need chemists. But what shall we make? What does this logic imply about the areas into which the Chemistry of the future must go?

Flipping back to the particular episode I would highlight, I would point to a remarkable publication that Don Hilvert brought to my attention. In an illuminating study of Emil Fischer's progression to the structural proof of glucose by synthesis, for which Fischer received the Nobel Prize in 1902, Catherine Jackson, a science historian, highlights the role of chemical experimentation in 19th century organic chemistry.[5] A bit under-emphasized in the narrative, however, is the oddly ambiguous relationship of this landmark achievement in organic chemistry with the theory of chemical bonding. Today, we teach chemical bonding at the very beginning of the Chemistry curriculum, with the electron pair bond, and even molecular orbitals providing a physics-based explanation for the forces holding molecules together, and, furthermore, the ultimate rationale for the three-dimensional structures that the molecules take. Structure, with lines and wedges, Fischer projections, Neumann projections, and even stereochemistry, is taught as the classical representation of the underlying quantum mechanics. It is perhaps sobering to consider that Thomson's identification of electrons as the negative charge carrier in cathode rays came only in 1897,[6] Rutherford's experiment indicating a dense, positively charged atomic nucleus in 1911,[7] and even Lewis' proposal of the electron pair bond only in 1916.[8] The Heitler-London valence bond picture of covalent bonding in H_2 was published in 1927;[9] the molecular orbital model by Mulliken[10] and Hund[11] followed shortly thereafter. Classical structure theory, usually considered to begin with work by August Kekulé, starting in 1857,[12] and A. S. Couper in 1858,[13] preceded any physical model by which one could describe a chemical bond. While Kekulé reportedly fabricated molecular models with tetrahedral carbon atoms as lecture aids, as early as 1867, he referred to the models as heuristics rather than representations of actual physical structure, given the absence of any consistent physical theory. Van't Hoff and LeBel pointed out that the model explained the otherwise unexplainable phenomenon of optical activity,[14] and the pictures of tetrahedra sharing vertices, edges, or faces as representations of single, double, and triple bonds appear in van't Hoff's 1874 publication even though the models are most often ascribed to G. N. Lewis a half-century later. By 1877, Kekulé was attributing the structural models with more physical reality, even talking about vibrations of the atoms along the bonds, but the viewpoint was fiercely opposed by some, for example, Hermann Kolbe,[15] who criticized structural theory, in the words of Alan Rocke,[16] as simultaneously "too empirical and too speculative," there having been no physical basis for the chemical bond beyond vague attributions of affinities. Nevertheless, Victor Meyer postulated what we now call stereoisomerism in 1888,[17] and used the new theory as a framework for the assignment of structure to a wide range of natural products.[18] Fischer, originally no great proponent of a structure theory that lacked a solid basis in physics, nevertheless combined consistently the speculative, even fanciful, ideas of structure theory, with the solidly established tradition of chemical experimentation, in work done between 1884[19] and 1890,[20] to produce a rigorously executed and logically flawless structure elucidation and rational synthesis of glucose. Even against our infinitely better tools and theory, Fischer's proof of the structure of glucose stands today as a landmark of classical structure determination. Turning Kolbe's criticism around, a certain "speculative empiricism" seems, in retrospect, to characterize some of the greatest achievements of 19th century chemistry.

The episode, overlaid with the chronology, illustrates a key characteristic of Chemistry that proved historically so important in the evolution of the science. Not only did chemists rationally produce complex structures in a systematic, step-by-step manner prior to the development of rigorous physical theory, *e.g.* quantum mechanics, they did so even prior to the experimental proof that electrons and nuclei, or indeed, atoms, exist. Chemists have dealt with complexity by making ever more complicated molecular entities and objects before they could be 'derived' from first principles. I do not mean to imply that theory was absent, but rather that fruitful chemical practice could be done with speculative, incomplete, and even fanciful or not-completely-consistent theoretical concepts. The synthesis of these molecules was intertwined with the development of the analytical tools to detect, characterize, and quantify them, which should not be underestimated – see Jackson's description of the historical importance of oximes and hydrazones[5] – as well as the ultimate elaboration of theory which transforms initially murky heuristics into respectable physics. The successes of the heuristic approaches imply deeper, physical regularities of varying obscurity, and it is a task of theory to dig those out. The latter enterprise typically follows the synthesis, though, by up to many decades.

Taking the leap from the past to the future, and considering what has made Chemistry unique, as well as uniquely useful, consider that the problem of describing and working with complexity in the material world is still with us. The challenges today are immeasurably more difficult than those faced by Kekulé, van't Hoff, Meyer, and Fischer in the 19th century, even when viewed from the standpoint of our present technical and technological capability, but I wonder whether we are bold enough to treat large interacting systems far beyond the safety net of established theory. To apply a metaphor, if molecules are like words, Chemistry has spent the last century-and-a-half working out the rules of spelling, and those who see a Department of Chemistry as nothing more than a Department of Chemicals, reduce mastery of a language to possession of a large vocabulary. Mastery of words, however, says nothing about grammar, and even mastery of grammar means that one could, for example, write an understandable, information-rich, and most certainly useful instruction manual for a toaster. One could also write poetry, and therein lies a difference. Within the language metaphor, this is what complexity means.

Returning from the metaphor to the more practical question of what we need to teach the Chemistry students who may be our future poets, it is clear that the education must be broad, with strong foundations in mathematics, and physics, plus the very important laboratory work which, among other things, should be structured so as to teach students to expect surprises. Experimental work in new areas is perhaps the best antidote for scientific overconfidence and intellectual complacency. While the acquisition of skills in experimental research requires students to learn to work reliably and reproducibly – and here Jackson's discourse on experimental work in Fischer's laboratory is still valid – it would be a mistake to teach students that the best experiment is one that always produces the expected result. The experiment never quite goes as predicted, and the skilled experimentalist keeps an eye open for systematic discrepancies. I shudder at suggestions made prior to, but also during, the coronavirus-mandated shutdowns, that laboratory courses might be run sensibly in virtual simulation. In terms of curriculum, too much specialization, too early, promotes the unhelpful idea that scientific work is the acquisition and application of a canon or dogma. Students also need a healthy sense of the process by which innovation arises, why new ideas come to this person, at that place, in that time? How can I be that person, in this place, in this time? Last of all, Chemistry must push forward, understanding the material world by making functional objects, not just molecules. I think of Don Hilvert's nucleocapsids, which assemble a structurally well-defined, regular object from 240 engineered and artificially evolved protein subunits that work like natural analogs even if they may be structurally quite different. They spontaneously recognize and encapsulate their coding DNA suspiciously like the way by which a virus puts itself together.[21] I think of Roeland Nolte's (Nijmegen) molecular machine that reads and writes binary information encoded stereochemically on a chiral polymer chain.[22] The functions described above may occur in Nature, but the constructs themselves are not natural. I think of hybrid organic/inorganic perovskites, whose internal motions on different time scales and different length scales, wholly unanticipated at the time of their original synthesis, and, moreover, different from those in their simpler, purely inorganic antecedents precisely because of the much larger structural diversity in the hybrids, apparently provide the physical basis for their extraordinary properties in connection to photovoltaic and other charge/hole-transport-based devices.[23] Thinking ahead, can we build, for example, a catalyst that disproportionates N_2 to ammonia and nitrite under mild conditions, which would be the microscopic reverse of the primary metabolic process in anammox bacteria?[24] While still a bit endothermic, the catalytic cycle would be, in principle, an energetically more efficient alternative to the Haber-Bosch reduction of N_2 to ammonia, followed by re-oxidation of ammonia to nitrate, but it would be primarily a most elegant case of construction of a very complicated assembly of interacting molecules. Who makes these things? Chemists make them. We do then need analytics and theory. With regard to the former, one wonders if the new imaging methods with atomic resolution,[25] for example, unimaginable just decades before, will change how we work in the coming generation as much as NMR and X-ray diffraction had done in the generation prior to ours. For the latter, the statistical mechanics of non-equilibrium systems,[26] open or dissipative systems, is still growing, as are better and faster electronic structure methods. The intuition we learn from the present Chemistry curriculum teaches us to think about molecules at equilibrium, but, at the risk of sounding flippant to illustrate why out-of-equilibrium systems are so interesting, one could say that living things which reach a state of equilibrium can be generally described as dead. We therefore need a different intuition. We still need more and better ways to build molecules, and then hook them together. To highlight just one methodological direction among many, CLICK chemistry gives us a glimpse of what a truly universal ligation reaction could achieve, even with CLICK's (not small number of) limitations.[27] Just think of how much of Chemical Biology comes from the CLICK reaction. Where is the universal, traceless ligation reaction with which we can confidently assemble large constructs without worrying (too much) about the particulars of what we want to hook together? The only two synthetic reaction classes which even come close to the ideal of 'robust' chemistry are formation of amide bonds and the formation of phosphodiester linkages, respectively the basis for automated peptide and nucleic acid synthesizers. If we had a universal, traceless ligation making, for example, aliphatic C–C bonds, what could we build up in a modular way? How would we conceive of a search in chemical space if we had such a robust, universal ligation reaction? Consider that we prove mastery of chemical transformations by synthesis of complex molecules. This logic applies equally well for even more complex systems. Chemistry today faces issues of immense complexity, but we should embrace the complexity as the essential feature that makes Chemistry interesting rather than a hurdle to be avoided, and we will master the complexity by making the objects.

In this essay, I had hoped to review retrospectively the essay by Jakob Nüesch from 1996,[1] and turn the view to the future. After a quarter-century, much of what he wrote still applies in the larger sense. With the views expressed in the present essay, I would highlight two bits of the 1996 essay: "Die erfolgreiche Weiterentwicklung der Chemie hängt nicht zuletzt davon ab, ob es ihr gelingt, die selbst gesetzten Grenzen der eigenen Wissenschaft immer wieder zu überwinden," and "Sie verlangt nach einem fortlaufenden Überdenken des eigenen Tuns und einem verantwortungsbewussten Umgang mit ihrem Ergebnisse." Especially with regard to Nüesch's recognition that any scientific field, not just Chemistry, must constantly reinvent itself, I try in this essay to find in past successes the spirit of exploration that will set our feet on the path to future success.

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A Perspective on Chemistry and Society

A Column on the Occasion of the 75th Anniversary of CHIMIA

Chemistry and the Environment & Green and Sustainable Chemistry

A Roadmap Towards Sustainable Chemical Products and Processes for Switzerland

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Pollution of the environment with man-made chemicals is an issue of increasing concern with scientists, society and legislators. Environmental chemistry and (eco-)toxicology research provide evidence for the disruptive effects that many synthetic compounds have on ecosystem and human health. Involved scientists also point out that problems recognized some 30 years ago (*e.g.* with persistent organic pollutants) continue, while the market is flooded with new chemicals that exhibit similar properties or even raise new concerns.[1–3] In light of this, one may question the impact the '12 principles of green chemistry' have had, which John Warner and Paul Anastas had formulated in 1998 to guide chemical research and industry towards greener chemical processes and products.[4]

More recently, however, the sense of urgency has increased, with society by large recognizing and agreeing on the fact that chemical industry must move towards sustainable business and consumption models that are significantly more environmentally benign, and that it must do so fast as consumption and hence use of chemicals continues to speed up.[5] An increasing number of industry commitments towards green and sustainable chemistry, either as part of corporate social responsibility programs or large initiatives (*e.g.* Innovative Medicines Initiative (IMI) research projects iPiE, ChEM21,[6] PREMIER) has, finally, been matched with clear agenda setting at the EU political level in 2020. Most prominently, the 'Chemicals Strategy for Sustainability Towards a Toxic-Free Environment' of the European Commission[7] formulates a new framework for how chemical risk should be dealt with in the future. One of its core aspects is the 'toxic-free hierarchy' of actions to protect health and the environment and to encourage innovation (Fig. 1). While the 'toxic-free hierarchy' recognizes that there is obviously still much need to assess, reduce or eliminate existing pollution problems, it clearly puts the development and use of safe and sustainable chemicals, as well as clean production processes for those chemicals, on top of the hierarchy of priorities for action.

Fig. 1. The toxic-free hierarchy, adapted from ref. [6].

Switzerland has been at the forefront of chemical product discovery and production, witnessing such milestone compounds as DDT, benzodiazepine or cyclosporin, which revolutionized our understanding of how chemicals could impact our life, both positively and negatively. Switzerland has been and remains a landmark for chemistry, home to many of the biggest chemical, agrochemical and pharmaceutical companies worldwide. We would like to take the opportunity of the 75th anniversary of CHIMIA, the journal who has witnessed and communicated most of that development in Switzerland, to highlight the unique opportunity and obligation we have as a scientific community to reflect on how the specific Swiss industrial and academic environment could be leveraged to move towards more sustainable chemical products and processes, and what immediate next steps need to be taken to move into that direction.

Current Practice in Chemical Product and Process Design

Chemical product design, particularly for new active ingredients for medical and agricultural purposes, two key areas of chemical industry in Switzerland, is a highly targeted and time-consuming process that requires significant investments. Its primary goal is to discover and refine new chemical principles that have highest possible intrinsic activities to fulfill their purpose, *i.e.* a specific activity on a target disease, pest, or health outcome. These goals are increasingly challenged by growing resistance to currently used classes of bioactive compounds, most widely known by the example of resistance to antibiotics in human pathogens, but also observed, for instance, as emerging resistance of target pests in agriculture to currently used plant protection products.

Typically, the development of a new agrochemical product takes over 10 years and costs over 200 Mio Euros.[8] In the research phase, which takes up about one third of time and costs of the whole R&D process, hundred thousands of candidate structures are screened and finally reduced down to 1–2 lead structures that are taken into development, registration, and ultimately commercialization. Up to far in the development process, limited characterization of potential adverse environmental fate properties or ecotoxicological effects required for ultimate potential market registration of those lead structures will have taken place, at least for agrochemicals.

For active pharmaceutical ingredients, because of the importance of excluding severe side effects, hit-to-lead and lead optimization of potential scaffolds during the late stages of the research phase do consider human toxicity through a number of bioassays (*e.g.* genotoxicity P450 inhibition, hERG assay *etc.).* However, also for pharmaceuticals, consideration of potential environmental health outcomes takes place only late in the development process.

In both cases, when it comes to chemical process development, the conceptual steps that routinely take place are as follows:

1. Route design: elaboration of sequence of events from commodities to desired targets; manually or *via* computer-aided approach (rule- or AI-based)
2. Decision on better options commonly driven by economic, intellectual property, scalability, robustness, safety, process readiness and developability, technologies, regulatory, productivity/expediency aspects; might optionally go through feedstock considerations or consider overall environmental impact of project
3. (Semi)-automation to identify the optimal choice of reagents, solvents; some process simulation is utilized to increase productivity and identify the best solution; time allowing, optimization to improve overall process intensification with one or the other technology incorporated (*e.g.* flow, robot…)
4. Process understanding to optimize process design; time allowing, typically conducted in parallel to previous activities to minimize risks of discarding wrong options
5. Waste management, and potential life cycle activities to reduce waste (*via* recycling, waste valorization)
6. Optionally, if time allows and for some industries, full revisit of the overall process in a holistic manner to streamline solvent or purification strategies and maximize overall throughput.

Environmental fate, *e.g.* biodegradability, and ecotoxicological properties of the process wastewater are typically considered relatively late in process development and based on measured data. They can therefore only be generated for already advanced campaigns, thus reducing the chances to change in a meaningful way a process if undesirable outcomes are observed. Also, there is hardly any opportunity for process design to feed back into the early stages of product research, such as the smart integration of relevant (bio-)feedstock or valorized materials within syntheses and processes.

Major Obstacles Impeding Change towards more Sustainable Chemical Products and Processes

The development of new chemical products is highly challenging and complex due to the many requirements and boundary conditions imposed by the targeted application itself. Additional requirements for the products and processes to be more environmentally benign and sustainable top those with a plethora of new requirements that may exhibit complex interdependencies or may not be very well defined (*e.g.* they may be subject to change depending on how the system boundaries are defined). Also, requirements on the application side may stand in contradiction to requirements on the environmental safety side. Organofluorine compounds, for instance, are constantly rising in products for both medical and agrochemical applications due to their advantageous properties for fine-tuning physico-chemical properties, increased stability and ease of synthesis.[9] Yet many of these compounds containing aliphatic C–F-bonds – the most stable chemical bond known –are close to impossible to being broken down by any environmental degradation process available. As a consequence, environmental pollution by highly persistent (per)fluorinated compounds is increasingly being recognized as major environmental threat.[10]

Yet, while we agree that these problems are challenging, we believe that they should be and can be solved, particularly in a country as rich in know-how, skillsets and talent pool as Switzerland. However, success will require processes and conditions that are adequate to tackle the complexity of the problem, which, in our opinion, is not the case for at least five reasons: First, the complexity of the agrochemical and pharmaceutical business has led to fragmentation of activities. A lot of responsibilities are split in organizations, creating silos, short-term visions, missed opportunities or the pursue of sub-optimal leads. Second, at least up until recently, there was limited recognition of the environmental agenda, and a lack of appropriate incentive systems in companies. In most industries, even when committed to sustainability, decisions tend to be taken on purely financial grounds, rather than value creation. For instance, the notion of fairness inherent in conducting the production in one or the other location alters the assessment of a process. Neglecting it may lead to the wrong decisions being taken (*i.e.* typically more 'polluting' standard chemistry, intensive in human work, being preferred over innovative and capital-intensive fine chemistry, although scalable for the next projects), and thus prevent significant environmental improvements and economic savings. A related aspect is short-term financial accounting, with the amortization, in case of capital investment, being calculated project per project. Instead, allowing amortization to be spread out over multiple projects would allow for a more long-term planning of capital-intense but sustainable modifications in production processes and facilities. Third, the incentive problem is aggravated by a lack of flexibility and speed in the regulatory acceptance of, *e.g.* 2nd generation synthesis processes. With current regulatory constraints, very few organizations take the efforts to go through re-registration of a new synthesis and/or process, although much improved alternatives may have already been demonstrated. As a consequence, it is estimated that only a small fraction of the commercial syntheses and processes in the pharmaceutical industry are optimal, both from an economical and environmental perspective. Fourth, there is a lack of tools such as models or high-throughput assays that are fast and accurate enough to consider the environmental risk of chemicals early in the research process. Also, tools that quickly match lead structures to the feasibility and sustainability of synthesis routes are still in their infancy. Fifth, we notice a striking lack of education of chemistry students, and even chemistry practitioners in large, in green chemistry and related topics such as life-cycle analysis, environmental chemistry, ecotoxicology, system design *etc.* throughout most Swiss universities. Prominent examples have been the loss of chemical safety and environmental technology programs at key Swiss institutions.

Roadmap towards Change in Switzerland and the Potential Role of SCS

To take full advantage of the unique Swiss research ecosystem, we suggest the following actions enhancing collaboration and science for the acceleration of best practices in sustainable chemical product and process design (see Fig. 2).

Fig. 2. Roadmap towards best practice in sustainable chemical product and process design in Switzerland.

Align the community: An overview of actors in academic and industrial research across Switzerland in the broad area of sustainable chemical product and process design should be gained. Thematically, this should go well beyond current efforts in catalysis research, such as in the frame of NCCR Catalysis, and broadly include research on chemical-intense products and processes, such as, for instance, new energy technology materials. Drawing this map of actors is necessary, but requires manpower and resources not currently available at any one institution. This raises the question whether there could be a role for the SCS, potentially in collaboration with the chemistry platform of SCNAT, in supporting such a future-oriented endeavor?

Educate the next generation: Considerable efforts are needed to mainstream green and sustainable chemistry (GSC) education into classical chemistry education, including gathering and disseminating best practices.[11] Teaching materials supporting such activities are starting to emerge.[12,13] In line with the call for considering environmental aspects early in product and process design, basic GSC principles should already be taught at the bachelor level. As chemistry bachelor programs are typically densely packed with theoretical classes and laboratory courses teaching traditional, disciplinary chemistry knowledge, finding space and the best format for introducing GSC principles requires concerted action at the level of curriculum design and hiring strategies. Respective endeavors are also an important part of the ongoing NCCR Catalysis.

Educate leaders: We need to raise the awareness of those who take decisions in our organizations, whether industrial, governmental or regulatory, about their social duty. This should best be achieved through communicating real-life examples of product and process improvements that have had real impacts on their environmental footprint, the companies' reputation, and/or for society. Such success stories should be communicated internally and externally, *e.g.* through road shows *etc*.

Generate action: We should jointly take all efforts needed to foster a community focusing on sustainable chemical product and process design that is in intense exchange and that profits from and maintains the competitive advantage of the Swiss chemistry research ecosystem. These goals can be partly achieved by defining joint actions between the SCS Sections on 'Green & Sustainable Chemistry' and on 'Chemistry and the Environment'. Yet, as a community, we should also aim to initiate ambitious, pre-competitive national collaborative projects on the subject, *e.g.* by exploiting the NCCR and NRP formats offered by the Swiss National Science Foundation. The map of actors will be an important basis upon which such initiatives can be built. We hope that the SCS will play an important role in these actions.

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A Perspective on Chemistry and Society

A Column on the Occasion of the 75th Anniversary of CHIMIA

Syngenta Crop Protection AG

Chemical Innovation for Sustainable Agriculture by Investing in Soil Health

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Claudio Screpanti is an agronomist working in Syngenta R&D organization in Switzerland. He has several years of experience in agricultural research. He obtained his PhD in agronomy from the University of Bologna, Italy in 2003. He carried out additional studies in molecular biology and genetic engineering at the University of Louvain-la-Neuve, Belgium. Later, Claudio joined the Syngenta R&D organization, covering different scientific roles always in relation to soil biology. In 2018 he became a Syngenta Fellow, a company award recognizing outstanding scientific achievements. In his current role, Claudio leads the Soil Health Centre in Stein (Switzerland) and acts as Syngenta soil expert looking at the behavior and effects of new small molecules in the soil-crop systems. The aim is to support the discovery and development of new and more sustainable crop protection solutions.

Agriculture and Current Challenges

There is an increasing urgency for a more resilient and sustainable way to produce food, feed and fibers. Science and technologies can play a pivotal role in these endeavors. A broad array of new promising technologies is steeply growing in the farming area spanning from precision agriculture techniques, advanced modeling and predictive approaches to optimize inputs, new crop breeding programs up to microbiome harnessing to improve crop performance and resilience against the major climatic and pest threats.[1,2]

Beside this technological panoply, there is an emergent trend towards new and exciting opportunities to support sustainable agriculture using chemical innovation. In the following paragraphs, new perspectives on how chemistry can contribute and support food production in the context of some of the major challenges of this century will be presented.

Soil Health and Priorities for the Global Challenges

More than 95% of food comes from soil. However, there is an increasing concern about the rapid degradation of soil resources. New actionable programs have been put in place to preserve this non-renewable resource.[3] Soil health, as an emerging concept, has gained increasing attention in several scientific, social, and political areas in recent years. Soil health can be defined as "the capacity of a living soil to function, within natural or managed ecosystem boundaries, to sustain plant and animal productivity, maintain or enhance water and air quality, and promote plant and animal health".[4] New policies aiming at preserving soil were promoted in several geographies like Switzerland, EU and beyond.[5–7]

Using soil health as criterion to drive innovation in agriculture requires a solid evaluation framework to profile any new and promising technology.[8–10] Identifying the best approach to measure soil health is still a matter of debate,[8–11] here, a framework suitable for crop protection R&D is presented. Three major priorities reflecting the global challenges are considered: promote soil biodiversity, preserve soil from major threats and mitigate climate changes (as indicated in Fig. 1). These priorities enable to identify eight targets to evaluate the impact of new technologies.

Several enabling technologies and agronomical management practices have been disclosed as impactful to support and improve the soil health addressing one or more of the highlighted targets,[4,11,12] yet in this context, the potential role of chemical-based technologies has been often neglected and discounted, even though a tremendous role is played by natural small molecules on a multitude of processes below ground.[13–15] It is worth mentioning the striking and not yet

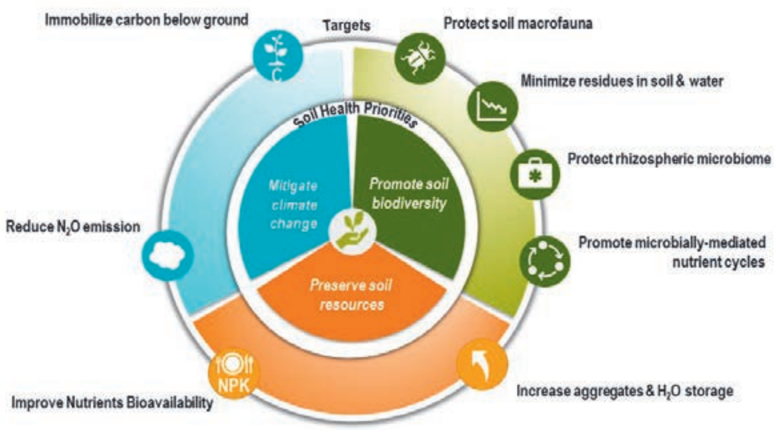

Fig.1. Framework with soil health priorities and associated targets.

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fully uncovered chemical diversity that can be found below ground with thousand different chemical features isolated from the roots of different plant species.[14,16] The next section aims to provide a historical perspective of the role of chemistry in the soil and crop sciences and how it evolved in the last centuries. Such perspectives will help to highlight possible trajectories for the chemical innovation for future agriculture.

Soil and Chemistry: A Historical Perspective.

The importance of chemistry in soil and the relevance for crop production goes back to the nineteenth century with the first attempts by von Thaer in Germany,[17] Davy in England,[18] and Boussingault in France[19] to shed light on the essential role of soil to support plant growth by providing nutrients. Later Way unveiled the ability of soil to exchange ions and the underlying the ion-sorption processes;[20] and then together with Liebig's work[21] they set up the foundations for the soil fertilization and ultimately contributed to the soil fertility concept. Other milestones followed in the twentieth century and marked the contribution of the chemical innovation in the agriculture particularly with the Haber-Bosch process through which it became possible to synthesize ammonia from atmospheric nitrogen with the help of iron-based catalyst, paving the way for modern agriculture and use of synthetic fertilizer.[22]

From the 1950s onwards chemical innovation sustained a growing crop protection industry with many – among others – soil-applied agrochemicals.[23] This innovation led to a significant increase in labor and land productivity[24] as well as in food security.[25,26]

Whilst the past technological efforts were devoted to more abundant and safer foods, the future emerging direction points to the urgent needs of more sustainable food production addressing the major interconnected global challenges like climate change[27] and biodiversity and soil losses.[3] Thus, this historical perspective leads to enquiry how chemical innovation can support sustainable agriculture by targeting soil health?

Chemical Innovation Targeting Soil Health

As indicated in Fig. 1, the framework for implementing soil health science in crop protection R&D identified eight major targets. For succinctness purpose, only a few of them will be discussed in this section.

Minimizing residues of future chemical crop protection solutions is one of the highest priorities to support soil health. To this end, information about the environmental degradability of early chemical leads should be available as early as possible and drive a rational chemical design. Therefore, new alternative predictive approaches able to provide swiftly and in a high-throughput manner indications about degradation are highly valuable.[28,29] A few recent investigations harvested some encouraging results, the published approach hinged on the fast evaluation of the degradation kinetics of a wide range of compounds on activated sludge systems and used this to predict soil half-lives from studies with a regulatory setting. Satisfactory predictions across a wide range of agrochemicals were observed and were superior to other approaches relying on other available predictive models.[28]

Protecting the soil microbial community and promoting the microbial nutrient cycles hold great potential. In this respect the naturally occurring below-ground chemicals particularly in the rhizosphere – the thin interface between plant roots and near soil – represents unique and fascinating examples of 'Chemistry-in-action' underpinning a vast range of biological interactions and biogeochemical processes with a fundamental ecological relevance and exceedingly important agronomical implications. Plants strongly contribute to such a 'Chemical parade' by deploying up to 50% of their photosynthates in the rhizosphere[14] as primary or secondary metabolites (Fig. 2). They regulate several interactions as plant-plant; microbes-plant, plant-pest and nutrient assimilation.

Chemical signals like flavonoids are involved in the plant-microbe interactions and the recruitment of beneficial N-fixing rhizobial bacteria by the leguminous plants. Benzoxazinoids are multifunction molecules acting as phytosiderophores for iron assimilation and also mediate the recruitment of other beneficial microorganisms[30] or attract herbivore insects.[31]

Similarly, soil microorganism use signals to communicate and coordinate growth and other behavior features like competitions, symbiosis, or diseases. Several recent studies showed that rhizosphere microorganisms can produce antimicrobials like DAPG (2,4-diacetylphloroglucinol), PHZ (phenazines) and PRN (pyrrolnitrin) which can be active against pathogens causing different soil borne-diseases.[13,32] Soil microorganisms release also other classes of molecules acting as phytohormone compounds (*i.e.* auxins, gibberellins, and cytokinins) which influence the development and other physiological processes in plants.

If an anthropomorphic consideration would be allowed here, it could be stated that plants speak chemistry and use small molecules to call for food, cry for help and compete for space.

Understanding the hidden language of crops particularly below ground can be a way forward to synthetize natural

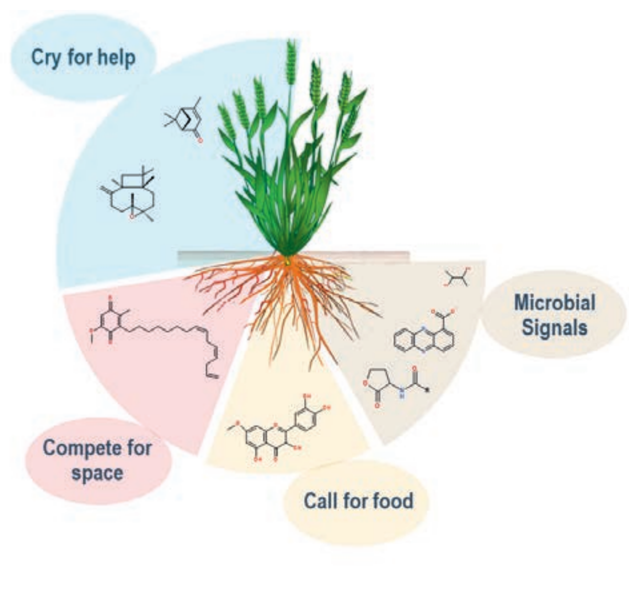

Fig. 2. Naturally above- and below-ground chemicals produced by plants and microbes and controlling several processes.

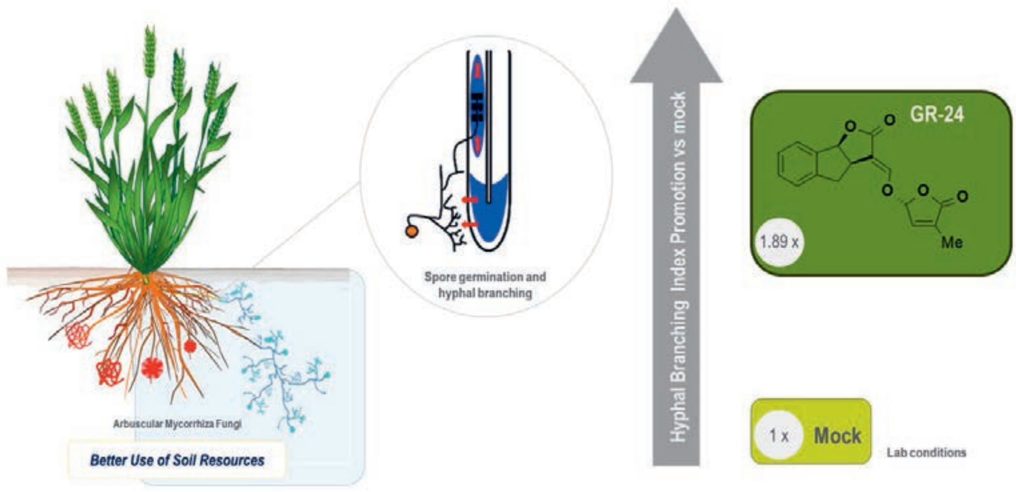

Fig. 3. Strigolactones derivatives induce hyphal branching in mycorrhizae, an important step in the establishment of the symbiosis between the fungus and the root of the plant host.

molecule or invent and optimize new compounds inspired by the natural chemical signals.

An example of innovation in this area is represented by strigolactones. Strigolactones are terpenoid-derived natural molecules acting as phytohormones and controlling several physiological and development processes in planta. They act also as potent rhizosphere signals with many potential applications in modern agriculture.[33] Interestingly, they are involved in the establishment of relevant symbiotic interactions between crops and arbuscular mycorrhizae and/or rhizobium. Moreover, new evidence suggests that strigolactones can influence the composition of the root microbiome.[34] The role of strigolactones on the promotion of mycorrhization is particularly relevant for soil health. Arbuscular mycorrhizae are considered keystone taxa supporting many important ecosystem processes like carbon, nitrogen and phosphorus cycles, biodiversity soil structure promotion.[35,36] Recent studies showed how synthetic mimics of strigolactones are active to promote key steps in the symbiotic relationship (Fig. 3).[37,38]

Successful total synthesis of natural strigolactones like sunflower-specific heliolactone[39,40] and orobanchol in rice[41] represent interesting chemical leads to promote soil health.

In the context of climate change, reducing greenhouse gas emission is an unavoidable challenge requiring the involvement of public and private organizations. According to a recent ICPP report[42] about 23% of greenhouse emissions derive from agriculture and other land uses. Nitrogen fertilization is of massive importance for crop production at farm level and it is associated with nitrous oxide release. This is a potent greenhouse gas accounting for about one third of the total agriculture and other land use greenhouse emissions.[43] The current consensus is that fertilization practices and other interventions are the most effective approaches to control the soil N-cycle and reduce greenhouse gas emissions.[27] However, small molecules can have profound and specific effects on different steps of the soil N-cycle. A broad range of natural or synthetic compounds – encompassing several agrochemicals – have been shown to interact directly with different steps of the soil N-cycle.[44–46] The soil N-cycle is a multi-step process mediated by microbes.[46] Any shift in one step will also have indirect consequences on N pools' partitioning and thus on other cycle steps. To manage the soil N-cycle effectively, it is necessary to consider the processes' holistic nature and control N availability, leaching, and emissions.

Conclusive Remarks

Since the inception of the agriculture sciences in the nineteenth century, chemistry has been at the cornerstone of crop productivity, nutrients, and soil fertility concepts. Chemical innovation supported almost two centuries of exceptional development in agriculture securing access to food, feed and fibers.

Yet, today climate change and other global challenges are threating our food production system. Therefore, a more resilient and sustainable agriculture is urgently needed. A way forward is through the promotion of soil health. Although the concept is open to many definitions and interpretations, three clear priorities can be used to drive the innovation: promoting soil biodiversity, preserving soil resources from major threats and mitigating climate change. New chemical solutions can address these targets. An exciting and very promising venue for innovation lies with new non-cidal molecules miming rhizosphere signals controlling important biogeochemical processes with a tremendous agronomical relevance. Knowing and mastering the chemical lexicon of the plants can support a healthy crop by promoting a healthy soil.

To build the future using wisdom gained from the past, the following quote from Liebig sounds timely "Perfect Agriculture is the true foundation of all trade and industry – it is the system of Agriculture cannot be formed without the application of scientific principles; for such a system must be based on an exact acquaintance with the means of nutrition of vegetables , and with the influence of soils and action of manure upon them . This knowledge we must seek from chemistry".[21]

The Swiss Chemical Society is leading the way with many new and thrilling initiatives.[47] For instance, by establishing and promoting new thematic communities like Chemistry and the Environment, Green & Sustainable Chemistry and Chemical Ecology; without doubt important steps to reap future benefits.

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A Perspective on Chemistry and Society

A Column on the Occasion of the 75th Anniversary of CHIMIA

Nachrichten aus der Chemie, German Chemical Society (GDCh)

The 'Burden' of the Member Magazines

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Christian Remenyi, Editor in-chief *Nachrichten aus der Chemie*

A few years ago, Chemistry Europe (then called ChemPubSocEurope), the European publishing organization of 16 chemical societies including SCS and GDCh, invited the editors of its member journals to a meeting. This was a wonderful opportunity to get to know the many different – and in some respects very similar – member journals. And for me, it also was the first opportunity to talk about our two journals with Gillian Harvey, the technical editor in charge of the production of *CHIMIA*.

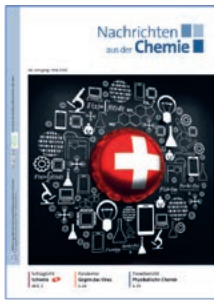
It is the typical *déformation professionnelle* of the magazine editor: just reading for fun is not possible. You are constantly comparing, looking for things that others have solved better and smiling when you discover tiny mistakes (which you would never make yourself, of course...).

What member magazines have to do

The challenges facing us member magazines of the European chemical societies are similar. There are many tasks to be fulfilled at the same time: We have to be the newsletter of the respective society, keep an eye on the balance between members and interests from industry and academia, and offer lots of services to our readers – they want to know about meetings, birthdays, and book reviews. And the science must always be correct, too. Although we are not purely professional journals, there is no tolerance zone. But one of the most important tasks of our journals is to give readers the feeling that they are part of a large community of like-minded people, the chemistry community, beyond the boundaries of their special disciplines.

Shoulder to shoulder in the magazine rack: *Nachrichten aus der Chemie* and *CHIMIA* (and some other not so important journals…)

CHIMIA and *Nachrichten aus der Chemie* are about the same age (well, *Nachrichten aus der Chemie* is the younger sister of *CHIMIA*, which is six years older...). But while *CHIMIA* still very much emphasizes its character as a professional chemistry journal, *Nachrichten* defines itself more as magazine style and has become steadily more colorful over the years (some would even say more like a tabloid).



Focus issue 'Switzerland' of Nachrichten aus der Chemie 5/2020[1]

International Impact

For me it is impressive how *CHIMIA*, despite not having a major publisher in the background, is among the frontrunners in modern publishing developments – be it electronic publishing or open access. The journal thus directs its focus far beyond the limited readership in Switzerland and addresses a worldwide audience.

For this, *CHIMIA* is a great role model for us in terms of internationalization. Whereas one of the unique selling points of *Nachrichten aus der Chemie* is its German-language content, which makes sense with a target group of more than 30,000 German-speaking GDCh members, *CHIMIA* is the only member journal of a European chemical society to rely fully on English as the international language of science. (A magazine in the national language would also be associated with difficulties in multilingual Switzerland; the Belgian colleagues solve the problem by having their own Flemish-language and French-language chemistry societies...).

But it is clear that if you want to make an international impact, you have to do it in the lingua franca of chemistry, even if it may be comfortable in the national corner. *CHIMIA* succeeds exceptionally well in this art – preserving the national identity of its "own" chemical society while addressing the global chemistry community.

I wish *CHIMIA* continuing success for the next 75 years and its readers much pleasure with the journal!

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A Perspective on Chemistry and Society

A Column on the Occasion of the 75th Anniversary of CHIMIA

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Open – An Obvious Concept!

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Open – an obvious concept!

For me it all started in 2000 when I, as Director of Libraries at Lund University, Sweden, was approached by a young researcher, who just had quit the university and got a job at one of the many spin-off companies at the university's Science Park. He came to me and was very annoyed and disappointed: suddenly he was no longer an authorized user, and his access to the 10.000+ digital journals was cut off. He was supposed to develop new products in his company, and suddenly he had lost access to the research results, which were mostly generated by taxpayer money.

For my part this was also an eye-opener. It suddenly became clear that instead of providing information to users, we as librarians and libraries are, in fact, blocking relevant users from access to the information they need to be able to do innovation, product development, *etc.*

For our societies to benefit from research results, these must be available for those who can transform the knowledge into innovative products and services, without barriers.

Why have our societies ended up in this mess?

In Western Europe and North America, it has become the norm that academia outsourced the dissemination of research results based on research funded by public money, to corporate companies. These companies are then able to turn these research results into a commodity priced in a way that only university libraries (hardly) can afford to make it available to institutional users. Users not affiliated to universities cannot afford access. (Please note, that I do not blame the publishers. They are doing what they are supposed to do; creatively exploit the conditions offered to them from academia).

In other parts of the world (particularly in Latin America) the tradition has been that not only the research is publicly funded (upfront), but also the dissemination of the research results as they appear in academic journals with no subscription charges. In fact Latin America invented Open Access before we began discussing it!

Open is the future

Initially – with the Budapest Open Access Initiative[4] from 2002 – it was primarily about providing access to academic journals and provide the "*free availability on the public internet, permitting any users to read, download, copy, distribute, print, search, or link to the full texts of these articles, crawl them for indexing, pass them as data to software, or use them for any other lawful purpose, without financial, legal, or technical barriers*".

The Open Access concept was met with broad skepticism from academia and resistance from the dominant publishers. A lot of misinformation had to be dealt with. But now, nearly two decades later, the open agenda has broadened to encompass academic monographs, research data and peer-review. We have the open science agenda supported by the leaders of universities, research funders, governments, and international organizations. Today it is difficult to find a university president or a president of a research funder who would dare say that the open agenda is wrong.

So, we should be happy, we have won the discussion. But there is apparently quite a distance between what decision-makers say they want to see happen, and what they actually do, what kind of behavior they actually reward!

Strong forces are delaying the implementation of open.

Academic Freedom – Academic Responsibility!?

In the discussions about Open Access the question about the freedom to decide where to publish has been central! The core of the problem is Research Assessment and Career Development for researchers. Unfortunately, academia has not only outsourced the dissemination of research but also the tools to support research assessment to third parties. The abuse of the Journal Impact Factor and other journal metrics has developed the practice of assessing research not based on the actual research but rather on where the results are published!! This has had (and still has) a lot of damaging consequences. Fortunately, we can see that more and more funders and universities are slowly moving away from this and adopting and most importantly actually implementing the Declaration on Research Assessment (DORA) principles.[5] But progress is too slow.

The concept of the Academic Freedom was quickly picked up by not only researchers (being subject to research assessment based on journal metrics), their institutions (involved in the global competition for research grants, based on university rankings (which in turn to some extent also are based on misleading journal metrics)) and of course the dominant publishers. Pushing for Green Open Access[6] with embargo could for a time allow researchers to publish in their favorite journals, while at same time accommodate first-generation soft open-access mandates. Later came the invention of the Hybrid journals,[6] again allowing researchers to accommodate Open Access mandates by paying specifically for open access to their results.

We all know the history of this: The publishers creatively lobbying against open access, claiming to protect the Academic

Freedom of researchers, and thus allowing hesitant decision makers in academia to avoid taking tough decisions.

Open advocates have stressed that Academic Freedom has nothing to with where you publish, but with how to do your research (methods, *etc*.). Instead, the concept of Academic Responsibility should carry weight: You should publish your research, your data and your software in the open. This should be considered responsible researcher behavior and should be rewarded.

However, inertia in academia makes progress very slow.

Who can change the system?

It is up to the decision makers to change the system, to introduce incentives for researchers to do the right thing – accommodating the open principles.

University managers and research funders have for more than a decade introduced open access mandates, at first as rather soft mandates, like recommendations – later more strong mandates, like requirements, have been issued. Unfortunately, the follow-up has not been very strong.

But strong mandates and concrete incentives are needed to bring about change in researcher behavior.

Universities and research funders should also promote the APC-free Open Access model by subsidizing the dissemination of the research they fund!

Open (access) is inevitable

Much progress has been made over the last two decades. Universities, research funders, governments and international organizations have all realized that access to research results, research data and the software associated with this should be open. Open benefits innovation, speeds up development of new products and treatments, thus benefitting our societies and people.

For two decades, we have come quite far in advocating for open access to research results and it is generally estimated that between 30–50% of results are published in Open Access in one form or another.

Open Access is inevitable. It will come in several forms. But much more determined decisions and actions from the decision makers are needed, or else we will see the access crisis develop into a participation crisis. Less privileged countries and their researchers might have access to more information, but due to high publication charges they will not be able to participate in the global scholarly discussion. This will harm all of us, just like we are now reproducing the global divide in access to Covid-19 vaccines!!

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A Perspective on Chemistry and Society

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University of Bern

Swiss Science: Quo Vadis after Exclusion from the European Framework Program?

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Keywords: Horizon Europe · International cooperation · International funding · Research and Education · Student exchange

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Christian Leumann graduated in organic chemistry from the Federal Institute of Technology (ETH) Zurich in 1986. After a post-doc stay at the University of California in Berkeley and five years of research at the Federal Institute of Technology (ETH) Zurich, he became Professor of Bioorganic Chemistry at the University of Bern in 1993. In addition to his teaching and research activities, Christian Leumann has also held a number of other positions. For example, he was a member of the research council and President of the Division for Mathematics, Natural Sciences and Engineering of the Swiss National Science Foundation (SNF). Since 2011 he is member of the Executive Board of the University of Bern, serving first as Vice-Rector for research and as of August 1, 2016 as Rector of the University.

Introduction

On July 14, 2021, it became official that Switzerland was dropped from the list of non-EU countries which are to engage in negotiations with the European Community for association to the European research network Horizon Europe and the student exchange program Erasmus+. The reason being the unilateral abandonment of the framework contract between Switzerland and the EU by the Swiss government. Switzerland with its internationally very competitive, world-class research capacities has been associated since 2004 to the European framework programs. With the degradation to third country status, it has lost its access to the prestigious grants of the European Research Council (ERC), it has only very limited access to the Marie Sklodowska-Curie actions (MSCA) for young researchers and it can no longer lead cooperation projects and only participate in such projects in a limited way. What does this mean for the future of academic research and education at Swiss universities?

Current Situation

Unfortunately, this situation is not new. Already in 2014, after the Swiss people accepted the initiative against mass immigration, Switzerland was excluded completely for a short period of time from the previous program *Horizon 2020*. By intervention of the Federal Council for Economy, Research and Education, the Swiss National Science Foundation (SNSF) was mandated to set up a temporary backup scheme to fund Swiss projects that were positively evaluated by the scientific panels of the ERC. In 2016, full association of Switzerland could be re-established. An evaluation by the SNSF four years after exclusion showed that the Swiss scientific community did not fully recover from the negative consequences of the lock-out as its participation in projects dropped from 3.2% to 2.4% relative to the previous funding period, and fewer Swiss scientists obtained invitations to join cooperation projects.[1]

Today we are facing a very similar situation in which it is expected that the State Secretariat for Education Research and Innovation (SERI) will mandate again the SNSF to introduce a similar temporary backup scheme. What is now different? The trust of our European partners in having Swiss groups reliably integrated in cooperation projects is already damaged. This will have a potentiating effect on the known negative consequences from the 2014 exclusion.

Switzerland with its very innovative scientific contributions to areas such as climate science, space science, biomedical science or chemical and material sciences is dependent on the possibility to be part of large, international research consortia, as those funded by the Horizon program, to maintain or further strengthen its world class position in research. Such programs are based on longstanding commitments of its partners and severely suffer from stop-and-go politics that we have faced now twice since 2014.

Reactions of our European Research Partners

Already in 2018, the SNSF warned about the consequences of a renewed exclusion of Switzerland from *Horizon Europe*.[1] Earlier this year, Swissuniversities, the roof organization of all Swiss higher education institutions, also expressed its concern, just before the Swiss-EU framework agreement was abandoned.[2] But what is the view of the European research community?

Fortunately, there is overwhelming support by the European University organizations offered to Switzerland, despite the political differences in Swiss-EU relations. In an open letter of June 7, 2021,[3] no fewer than 15 European science organizations expressed their concern about the exclusion of Switzerland, pointing to the strength and competitiveness of the Swiss science landscape and the lose-lose situation the exclusion would create for the whole European Research Area (ERA). Not to forget the open statement of April 23 of five research-intensive university groups, namely the German U15, the Russell Group, the UDICE, the LERU and The Guild, that even urged the EU commission to reconsider its stance in the context of restricting access of UK, Switzerland and potentially other countries to certain parts of the ERA.[4] In addition, the exclusion of Switzerland gained a lot of attention in the scientific press as can be seen by articles in *ChemistryWorld*,[5] *Science Business*,[6] *University World News*,[7] and others. This support clearly highlights the negative impact that the exclusion of Switzerland has for both Switzerland and the EU.

Alternatives

It is a paradox that Switzerland, being geographically at the heart of Europe and culturally and economically strongly connected to the EU, should no longer be part of the European research network. By speaking to persons in Swiss politics or economy, one often hears the question on why not instead associate with countries outside the EU. Very often these questions originate from a negative view of Europe's capabilities to become a game changer in research and innovation in the future. Typically, the US and the southeast Asian countries, including China and India are mentioned here as potential partners.

One of the strengths of the Swiss academic system is its openness and its strong connections worldwide, including all relevant countries. This is reflected by our academic staff and our PhDs and post-docs in which the degree of internationality is close to or above the 50% level in many of our universities. Fact is, however, that there does not exist a similar network. The Horizon Europe program is with € 95.5 billions the largest financed, international research network in the world. Its instruments in funding basic research and innovation in a competitive way, in all societally relevant fields respecting the freedom of academic research, committed to open science and inclusiveness are unparalleled. The same holds true for the student exchange program Erasmus+. Participation is essential for a small country like Switzerland being a big international player in science. Thus, there is no alternative with similar impact available.

Consequences

If the exclusion of Switzerland from the European research network persists it will have severe negative consequences for the quality and the competitiveness of the Swiss academic system. These consequences will not be visible today or next year, but they will gradually become apparent over the next 10 years.

In the previous program Horizon 2020, the University of Bern, for example, has gained 175 projects (2014–2020) with a total financial volume of 120 MCHF. Amongst these projects were 37 ERC starting, consolidator or advanced grants, 66 Marie Sklodowska Curie grants as well as 72 collaboration projects. For many of the latter, we were the leading institution. If this is compared to the total funding of UniBE by the SNSF in the same period of time of 688 MCHF, this corresponds to 16.5% of total competitive funding for basic research. Thus, it becomes evident that the financial loss is severe, but will not be the game changer, given that the SERI and the SNSF will cover most of the financial losses by their projected backup schemes.

The real threat is the loss of reputation and attractiveness of the Swiss academia. Roughly half of all 12 Swiss universities are among the top 150 Universities worldwide in the Times Higher Education (THE) or the Quacquarelli Symonds (QS) ranking. These rankings parametrize not only scientific output and citations, but also international staff and scientific reputation. If we are now excluded from the European research community, we will lose attractivity for foreign staff and partnership in collaborations. Thus, it will only be a question of time when this will be reflected negatively in the rankings.

As just mentioned, being excluded from the ERC program will reduce the attractiveness of the research location Switzerland for the best European talents. Why should a researcher who earned a prestigious ERC starting, consolidator or advanced grant be attracted to Switzerland? Even if this researcher gets financial reimbursement by the SNSF, he or she will be excluded from other funding possibilities of the Horizon network. And why should a young investigator be attracted to a Swiss University if he or she cannot apply for a Marie Sklodowska Curie grant? Especially for young investigators, this highly competitive reward is important for their future academic career.

The same is also true the other way round. Why should a Swiss young or advanced scientist remain in Switzerland if his or her career opportunities are brighter at the research-intensive European Universities?

Being excluded from the Erasmus+ program will also lead to a loss of attractiveness on the level of Bachelor and Master students. Already in Horizon 2020, Switzerland was excluded from this program, but could still be associated *via* the Swiss-European Mobility Program (SEMP). The mutual recognition of academic credits between European and Swiss institutions is at risk in the future, as the European academic system is constantly evolving its policy on university cooperation. In other words, the future of SEMP is not guaranteed at all.

The mobility of students, however, is important for their future professional careers. Swiss students can take advantage to become integrated in international scientific networks at the best European institutions and the European students have the possibility to become integrated in the Swiss research environment, becoming optimally prepared for an academic or professional career in Switzerland, thus alleviating the skilled workers shortage in the high-tech Swiss economic environment.

Conclusions

For ten years now, Switzerland is the Champion in the ranking of the global innovation index. This has been mainly achieved *via* high investments in research and development and with the high quality of Swiss universities attracting human capital. Why put this at risk by the exclusion of Switzerland from the world's largest academic research and education network Horizon Europe? The mutual political understanding between Switzerland and the EU is currently at odds, yet this understanding is necessary to establish long-lasting, stable relations. This in turn is needed to keep the Swiss academic system fit for the future challenge to maintain and even improve its scientific quality and competitiveness. Therefore, the only option for the Swiss academic system is to get associated to Horizon Europe as soon as possible. For this to happen the political authorities are asked to provide the corresponding framework.

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EPFL

Society and Chemistry They Are a-Changin'

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Nicolai Cramer joined EPFL in 2010 and is the director of the Institute of Chemical Sciences and Engineering since 2020. Paul J. Dyson joined the Institute of Chemical Sciences and Engineering at EPFL in 2002. Between 2008 and 2016 he served as the Director of the Institute.

Need for Change

As we write this article over the summer the extreme weather events around the globe are difficult to ignore. In several parts of the world record temperatures have been witnessed for prolonged periods, resulting in massive wildfires as well as countless premature deaths. Closer to home unprecedented flooding has also resulted in extensive damage and loss to life. These events have been linked to anthropogenic climate change, a phenomenon known for decades,[1] and yet where politics and economics largely overrule scientific recommendations. The latest scientific report from the Intergovernmental Panel on Climate Change (IPCC) underscores the urgency of strong, sustained cuts in greenhouse gas emissions.

Graffiti by Banksy, a street artist and political activist. Photo by Matt Brown, https://www.flickr.com/photos/londonmatt/4203327856/in/photostream/. License: CC_BY 2.0.

The Past and the Present

Chemistry has no doubt transformed the world we live in for the better. The Haber-Bosch process coupled with other agrochemicals feed the burgeoning population of the planet, pharmaceuticals and other chemical products contribute significantly to increased life-expectancies and quality of life, and chemical fuels largely power the planet. However, nearly all these molecular products we take for granted are derived from petrochemicals, and it is the uncontrolled use of petrochemicals that is the greatest contributor to the anthropogenic increase in the global temperature. Over the last century modern chemistry has been developed around transforming relatively simple petrochemical feedstocks into a wealth of complex and valuable molecules. Switzerland has been particularly successful at discovering ingenious routes to agrochemicals, food supplements, pharmaceuticals and performance polymers, which correspond to a major part of the economy.[2] This chemistry has taken many decades to develop and specific advances are far too many to mention. However, catalysis, combined with developments in modern analytical techniques, may be attributed as being principal drivers.

The Future

To avert further global warming, we must rapidly transition to a carbon neutral or even a carbon negative society. Such a transition is highly challenging, and requires efforts from many sectors, with energy and chemistry having a major role to play. A considerable increase in energy demand is required beyond merely switching fossil-based energy sources to renewable sources. Chemistry has a key role to play here, *e.g.* with the development of the next generation of photovoltaics, efficient (solar driven) green hydrogen production, *etc*.[3] Moreover, the broad introduction of smaller footprint mobility will not be feasible without basic research in chemistry. Key topics in this respect include the development of inexpensive high capacity batteries, fuel cells based on non-precious metal catalysts for hydrogen-based mobility and synthetic renewable based hydro-carbon fuels.[4] On another axis, the use of petrochemical feedstocks by the fine/specialty chemical industries must be phased out and all our chemical products must be derived from renewable feedstocks such as biomass and carbon dioxide, *etc*.[5] Non-organic feedstocks are also diminishing and landfill sites are increasingly overflowing – this waste also represents a valuable future resource and at some point the word waste should be confined to the history books. All waste must be considered a resource/feedstock for a sustainable, circular and carbon neutral economy.

The transition to a circular economy is pressing and we do not have the luxury of another century to invent the chemistry required for this major undertaking. To achieve this goal, *i.e.* transforming renewable feedstocks and waste streams into useful products, catalysis remains the key to success, potentially with an even greater role compared to today as synthetic fuels will have to replace fossil fuels. Although continued improvements in instrumentation may be expected, in order to achieve the development of new catalysts that transform these alternative feedstocks, which relies on selectively decreasing complexity, at least in the first instance, it will be necessary for chemists to increasingly embrace robotic high-throughput experimentation with the generation of large data sets. Armed with this data, machine learning methods and artificial intelligence will likely become accelerators for the game-changing discoveries in new sustainable catalytic transformations. Eventually, quantum computing will start to play a significant role for more accurately predicting the properties of molecules and materials, and consequently facilitating the search for the optimal catalysts needed drive the transition to a circular economy.

Swiss academia has taken up this challenge. At the EPFL, one of our core tasks is to anticipate such megatrends and chairs with a focus on renewable energy, solar fuels, biomass conversion, and most recently in digital chemistry, have been strategically created over the years. Of equal importance is the training of the next generation of chemists – beginning with Bachelor studies and progressing all the way to our doctoral program. New courses covering these topics are constantly implemented and hands-on expertise in cutting-edge research topics is fostered. The scientific challenges are manifold and call for synergistic collaborative approaches. In this respect, EPFL together with ETHZ created a National Center of Competence in Research (NCCR) in Catalysis headed by Javier Perez-Ramirez and Jerome Waser, and primarily funded by the Swiss National Science Foundation.[6] Its core mission is to establish Switzerland as international leading center for sustainable chemistry research, education and innovation.

The Catalysis Hub CAT+ initiated by Christophe Copéret and Nicolai Cramer is a cutting-edge technology platform for catalyst discovery and optimization embracing automated experimentation and artificial intelligence and machine learning tools.[7] While localized at EPFL and ETHZ, it aims to be an open-access facility serving the entire Swiss scientific community. Moreover, the Swiss Chemical Society also launched SusChem Switzerland that bridges academia and industry and is a testament to the interests and efforts of Swiss industry in transitioning to carbon neutrality.[8]

Concluding Remarks

This is without doubt an exciting time to be a research chemist and we should feel confident about solving the challenges facing society. Chemistry has transformed the world for the better, and in recent years chemistry has come to the rescue at short notice, showing the power of the theories and tools available to us today. We expect that robotic-based high throughput experimentation, machine learning, artificial intelligence and quantum computing will gain rapidly further significance for chemists and become key tools to tackle the challenges we face. Despite these advances, the need for creative and imaginative chemists with a firm foundation in the chemical sciences will remain important.

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A Perspective on Chemistry and Society

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Anales de Química de la Real Sociedad Española de Química

Anales de Química, la Revista de la Real Sociedad Española de Química – The Magazine of the Spanish Royal Society of Chemistry

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Abstract: Anales de Química de la Real Sociedad Española de Química is the flagship journal of the Spanish Royal Society of Chemistry (RSEQ). *Anales* currently publishes different types of articles including essays, interviews, opinion, and review articles written for readers (scientists and teachers) who are not specialists in the field. The journal has a special focus in didactics and history of chemistry. A substantial part of its content is directed towards high school chemistry teachers. An overview of the history of the journal together with its current activities, as well as a brief history of the RSEQ are presented.

Miguel A. Sierra obtained his PhD in Organic Chemistry at the Complutense University of Madrid (UCM), Spain in 1987. He was an Assistant (UCM, 1987), Associated (UCM, 1990) and Full Professor by 2005. He was a member of the Scientific Advisory Board of the Organization for the Prohibition of Chemical Weapons (OPCW) (2003–2009). He is the General Editor of *Anales de Química* (RSEQ) and a member of the Editorial Board of the *Eur. J. Org. Chem*. He was awarded (2003) the Military Cross with white ribbon, the Ignacio Ribas and Felix Serratosa Excellence Awards (Organic Section, RSEQ, 2013, 2019). Prof. Sierra's research interests focus on the synthesis of functional bio-organometallic compounds, the production of hydrogen using hydrogenase mimics, the mechanisms of Fe-capture by plants and the design and synthesis of novel energetic materials.

1. *Anales de Química de la Real Sociedad Española de Química*

Anales de Química de la Real Sociedad Española de Química (analesdequimica.es), colloquially known in Spain as *Anales*, is the flagship magazine of the Spanish Royal Society of Chemistry (RSEQ, rseq.org). *Anales* currently publishes different types of articles including essays, interviews, opinion, and review articles written for scientists and teachers not specialists in the field. The journal has a special focus on didactic and history of chemistry. A substantial part of its content is directed towards high school chemistry teachers. The four issues of *Anales de Química* published every year are exclusively written in Spanish. *Anales* is fully electronic, published as an open access journal, and it can be printed on demand. Around 350-400 pages are published annually.

2. History

The history of *Anales* is long and complicated. It is intimately bound to the history of the RSEQ and by extension to the history and development of science in Spain. The journal was born as *Anales de la Sociedad Española de Física y Química* (Anales of the Spanish Society of Physics and Chemistry) in 1903 and is approaching its 120th anniversary, which for a Spanish journal is not only remarkable but exceptional.

The first issue of *Anales* was published in March of 1903 (Fig. 1), as a consequence of the initiative of the recently founded Sociedad Española de Física y Química (Spanish Society of Physics and Chemistry). The aim of this new scientific journal was "*To disseminate among the specialists the work of Spanish and, to the limit of our possibilities, foreign scientists…and to spread to the general public interested in Science the scientific information available to the Society*".


AÑO PRIMERO TOMO PRIMERO

ANALES DE LA SOCIEDAD ESPAÑOLA DE FÍSICA Y QUÍMICA

NÚMERO 1.- MARZO 1903.

MADRID

Fig. 1. The front cover of the first issue of *Anales de la Sociedad Española de Física y Química* (March 1903).

This declaration of good intentions collided with the lack of a scientific tradition in Spain. The difficulty of publishing original contributions in *Anales* forced the journal to widen its scope. The publication of (translated into Spanish) articles extracted from the German and French scientific literature was fundamental for the survival of the journal during its early childhood. The years of WWI were especially critical due to the shortage of paper and the skyrocketing costs of production (printing and distribution). The IUPAC meeting in Madrid in 1934 (the first after the WWI) was carefully and joyfully collected in *Anales*. This attempt to internationalize *Anales* ended abruptly with the military coup that took place in July 1936.

Anales was published again in 1941 as a journal from the Spanish Scientific Council (CSIC) and the RSEFyQ. Interestingly, this version of *Anales* is the first to contain the *nihil obstat* signed by the censor and the *imprimatur* from the ecclesiastic (catholic) authority, in this case the vicar general of Spain. *Anales* was split in two series, A and B, for Physics and Chemistry respectively, in 1948. This was also the first clue for the future excision of the Societies of Physic and Chemistry, which became effective in 1976. The year 1965 marked the separation of *Anales de Física y Química* in *Anales de Química* and *Anales de Física*.

Since 1965 *Anales de Química* (Fig. 2) began a long and painful journey. The journal published articles in Spanish written by Spanish authors when, at that moment, science and particularly chemistry was published in English. The beginning of democracy in Spain exacerbated the problems in *Anales*. Spanish research experienced an explosive growth. The number and quality of scientific publications in chemistry in Spain placed the country in the 8th position of the world in a few years. The consequence was that *Anales* lost most of its most prestigious contributors which, obviously, preferred to publish articles in English in international journals.

Fig. 2. The front cover of the *Anales de Química* after the separation from the *Anales de Física y Química.*

To counteract this language handicap, the RSEQ decided in 1996 to publish the journal in English. *Anales de Química* was renamed *Anales de Química International Edition* (Fig. 3). The slight increase in impact factor (from 0.12 to 0.3) at the expense of unaffordable costs for the RSEQ did not justify the continuity of the journal.

Fig. 3. The front cover of the first issue of *Anales Química International Edition*.

These years witnessed an exceptional, difficult, and unprecedented effort of various European societies that decided to amalgamate their flagship journals. Nine European societies published *Chemistry – A European Journal* in 1995. The sentimental cost of this unification for the different societies was immense. The negotiations that ended with the foundation of ChemPubSoc Europe, were memorable, but this is a different story. The condition to participate in ChemPubSoc was to end the publication of original research articles in the national journals. Therefore, *Anales de Química International Edition* ceased publication in 1998.

Upon the disappearance of *Anales de Química International Edition* due to its incorporation in the European consortium, the RSEQ decided to recover the old name *Anales de la Real Sociedad Española de Química* as the Society magazine (Fig. 4). The goals of this new *Anales* (marked as the 2nd epoch on the cover page) were to be a vehicle for communication between the members of the Spanish society, as well as to publish teaching materials for high school education and history of chemistry. The publication of scientific reviews by Spanish authors to disseminate the highlights of their research fields and their personal contributions remains the backbone of the magazine. This may appear as a longing for old times, but these reviews fulfil the role to provide in a concise and state of the art fashion, high level informative reviews to the Spanish speaking community. Incorporation of interviews, essays, and in general different articles to promote communication between Spanish-speaking scientists widened the scope of the journal.

Fig. 4. The front cover of the *Anales de Química* after its incorporation to ChemPubSoc Europe.

It should be highlighted that *Anales* provides great support and information to the international Spanish-speaking chemistry community. In fact, during the last years around 50–65% of our readers are from Central and South America. Three of our twelve Associate Editors are from America (Mexico, Argentina and Chile). One of the priorities of the magazine is to attract publications from foreign Spanish-speaking authors.

Currently, *Anales* is completing a complete renewal initiated in 2014. This renewal has included a new submission system (based on OJS), new design of the magazine, new structure for contributions, and the formalization of integration into scholarly databases. The future of the magazine is the full digitalization of its archives and the integration as a reference in the Spanish-speaking scientific and teaching communities (Fig. 5).

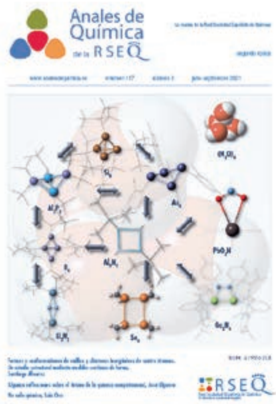

Fig. 5. The front cover of the latest issue of *Anales de Química*.

3. La Real Sociedad Española de Química – The Spanish Royal Society of Chemistry

The Spanish Society of Physics and Chemistry (SEFyQ) was established on January 23, 1903, in Madrid. The first president was José Echegaray (interestingly he was awarded the Nobel Prize for Literature in 1904). The history of the Spanish Society of Physics and Chemistry is as turbulent as the history of Spain in the 20th century.

From the beginning the Society's fundamental goal was to promote the equalization of the poor and retarded Spanish science with that of the European scientific powers (especially Germany, England, and France). This was the longstanding and unfulfilled objective of the SEFyQ during the next 30 years, even if its work was recognized with the title of 'Real' by King Alfonso XIII in 1928. During these initial years the claim of the Society for funds to improve science in Spain met with little success. The Spanish Civil War (1936–1939) followed by the 40 years of Franco's dictatorship did not help to advance science and by extension the Society (now Royal Society). Lack of funding together with the forced emigration of republican scientists after the Civil War were a permanent handicap for the recovery and development of the Science in Spain during these years.

Nevertheless, the generation of chemists born after the Civil War began the revitalization of chemistry in Spain during the 1960s. The separation of the Physics and Chemical Societies in 1976 coincided with the difficult path of Spain to democracy, and with the strong recovery of Spanish science (especially chemistry). The so-called 'Spanish Miracle' that put Spanish chemistry in the 8th position of the world ranking was not matched by the fortunes of the RSEQ. Economic and political problems marked the life of the Society until the end of the first decade of the 21st century. Since then, the RSEQ has experienced a superb recovery. The incorporation of *Anales de Química* to ChemPubSoc Europe (now Chemistry Europe) alleviated the economic problems of the Society. This fact, together with the hard work of the last presidents of the Society has resulted in a sensational recovery of the Society, that is now the first (based on the number of members and activities) scientific society of Spain.

The RSEQ has currently around 4800 members, and its structure is federal, with 22 Territorial Sections (closely matching the autonomous communities of Spain). The RSEQ is divided in Specialized Sections (26), according to the different areas of specialization of its members. Following this structure, the RSEQ holds a Biennial General Scientific Meeting that attracts around 1000 participants. The Scientific Meetings are organized by the different Territorial Sections. The next meeting is scheduled for 2022 in Granada. The Groups celebrate their meetings every two years alternating with the General Meetings.

The current goals of the RSEQ are the representation against the state scientific agencies of scientists and docents working in chemistry, the dissemination of chemistry to the people, and, as the priority issue, the attraction of scientific vocations. The organization of the Chemistry Olympics (national and international), as well as support for high school teachers are main actions of this society.

Finally, the defense of initiatives to prevent the degradation of the environment as well as the equality of opportunities define the spirit of the RSEQ.

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A Perspective on Chemistry and Society

A Column on the Occasion of the 75th Anniversary of CHIMIA

Givaudan

Fragrance Molecules Need Chemical Biology

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Since 2014, ***Dr. Agnes Bombrun*** has been in charge of the Ingredients Research in the Fragrance & Beauty division of Givaudan, based in Kemptthal, Switzerland. Her main responsibilities are to drive dynamically a rich and competitive pipeline of sustainable innovation for the perfumers, which consists of delivering the best fragrance molecules and processes by green chemistry and biotechnology. Agnes started out her career in the pharmaceutical industry. By training she is a chemical engineer (Lyon, France) and an organic chemist with a PhD (Emory University, Atlanta). Agnes was Director of Medicinal Chemistry for Merck Serono and also worked for GSK and Affymax.

With over 30 years' experience in the Fragrance and Flavours industry, ***Jeremy Compton*** has had a diverse global career with significant management positions in commercial, development and research functions across the businesses. Passionate about the positive impact fragrance can have on consumer's lives and how research into new materials, formulations, methods and forms of delivery can make this true. In addition to the UK he has lived and worked in Brazil, Indonesia, France, the United States and Singapore and is now based in Kemptthal, Switzerland where he has been running Fragrance Science and Technology since 2016.

Controversial Origin and Use of Fragrance Molecules

In the fragrance industry, perfumers use a plethora of odorant molecules to create perfumes. Historically the first family of odorant molecules was the Naturals. Extraction and distillation of raw materials coming from plants (flowers, roots, leaves, …) or animals (deer, civet cat, beaver …) gave access to the first used odorant molecules. At the end of the nineteenth century and at the beginning of the twentieth century, perfumers were given the opportunity of multiplying their options by adding synthetic molecules to their creations. A first example is the industrial synthesis of coumarin, which was developed in 1868. Coumarin is present in tonka beans and found up to 50% in Fougère Royale (1884). Another famous illustration is probably Chanel 5 (1921) with the first use of synthetic aldehydes. Since 1980s calone has been used for new olfactive marine notes (New West 1988, Eau D'Issey 1992), and ethyl maltol in the gourmand family (Angel 1992).

Such synthetic molecules, which became available, could be used directly or turned into a more valuable molecule using simple and efficient chemical transformations, inspired by Nature. Interestingly these synthetic molecules were not made for perfumery in the first instance but at the end of the nineteenth century, the exploitation of petroleum gave a unique opportunity to provide feedstocks for liquid fuels, solvents, waxes and the production of many common materials of the modern world. Many synthetic molecules, feedstocks, intermediates or commodities became available on the market for multiple usage, up to an amazing dependence as of today. Approximatively 92%[1] of organic chemical products are produced from petroleum, that is fossil, or mineral oil, and gas. In addition, these same resources are generally used to provide the large quantities of process heat and power needed by the industry. And therefore, reducing greenhouse gas (GHG) emissions and finding alternative renewable sources of feedstocks have been clear targets in the fragrances houses like in many other industry sectors.

Ambition

The industry of perfumery may not be the most impactful but taking into account the urgency and the complexity of the challenge, at Givaudan, in 2019 we launched the FiveCarbon Path™, a new ambition that will drive Givaudan's fragrance molecule developments while delivering on our environmental commitments (Fig. 1). For scientists, the ambition formalises the use of the latest and emerging scientific disciplines to meet the future demands of our industry and consumers' expectations around the world. Odorant molecules may contain heteroatoms but the most predominant atom is Carbon. Consequently, the vital role that carbon atoms play in our industry is at the centre of our FiveCarbon Path™ ambition. Every fragrance that perfumers create is a complex mixture of ingredients, including naturals, which are all based on carbon elements, often as the core backbone. Our new vision concretely implements our approach to innovating responsibly, which considers the potential impact of our processes and products on the environment, by designing ingredients following our unique FiveCarbon Path™. It focuses on:

1. Increasing the use of renewable Carbon,
2. Increasing Carbon efficiency in synthesis,
3. Maximizing biodegradable Carbon,
4. Increasing the 'odour per Carbon ratio' with high impact material and
5. Using upcycled Carbon from side streams.

Such an approach allows us to focus on the different aspects of the challenge and importantly, gives opportunities to deliver various solutions immediately and consolidate the future with innovation. The 12 green chemistry principles are also used and now embrace the whole life cycle of a molecule in perfumery, from the feedstock to its final use or re-use in Fragrances.

There is a necessity to substitute fossil carbon with renewable alternatives – and the three main sources are: biomass, CO_2, and recycling. The 'Renewable Carbon Initiative' (RCI) initiated by the nova-Institute is supporting the transition from fossil to renewable carbon for all organic chemicals and materials (Fig. 2). Givaudan has recently joined the board of RCI, and one year after inauguration, the initiative has already more than 30 member companies. The industry working on chemicals and derived materials is dependent on carbon and with the increasing population the need for many daily products made out of carbon will increase and decarbonisation is not an option. New

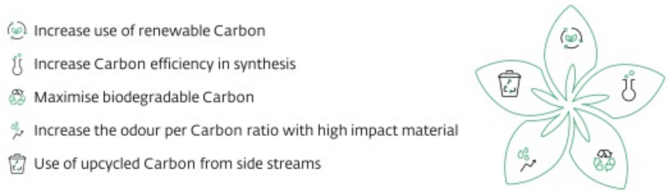

Fig 1. The FiveCarbon Path™.

innovations are on the rise that allow us to tackle the challenge from various angles while having one common goal to reduce the use of virgin petrochemicals and transition to the use of renewable feedstock, to become more circular. Using biomass from wood, CO_2 from fossil power plants and recycled carbon from plastic waste is already a reality and there are many more opportunities. While there are still many hurdles to overcome to achieve a circular carbon management including a supportive policy framework – the journey to become more renewable in perfumery and to play a leading role in this industry is part of our purpose.[2]

Fig. 2. The vision of RCI. It addresses the main cause of anthropogenic climate change by facilitating the transition from fossil C to renewable C for all organic chemicals and materials. Members of the RCI are pioneers who support the urgently needed acceleration and increase of volume of this transformation.

Applications

Being eco minded, the FiveCarbon™ Path is embedded in all research programs. Nevertheless, given that the access and production of iconic molecules, which are biodegradable and powerful, are key assets for the creations of the perfumers, it is of the utmost importance that scientists implement the correct changes to increase the chance of success. Such ambitions are molecule- and process-dependent. Chemistry and biotechnology (fermentation and biocatalysis) have never been so fusional. This can be illustrated by a first example of one of the most used ambery molecules, Ambrofix™ (Fig. 3). Traditionally the feedstock is the diterpene sclareol, currently isolated from clary sage (*Salvia sclarea*), which is then modified and cyclized by classical chemistry steps into Ambrofix™. The availability of a new feedstock farnesene, a diesel and jet fuel precursor produced through fermentation opened new pathways to precursors and derivatives made by green chemistry, for a final biotransformation using a Squalene Hopene Cyclase enzyme. The new biotechnology process of Ambrofix™ is implemented and requires 100 times less land to produce 1 kg of Ambrofix™ compared to the old route based on clary sage. Years of optimization and extensive tests proved that the two processes are giving the same quality with no olfactive impact on the final fragrance. The second example, Ebelia™ (Fig. 4) illustrates the move to a new renewable feedstock, namely furfural, used to make a key intermediate for a fresh fruity cassis note. Ebelia™ can replace cassis molecules traditionally made from intermediates of the petrochemical industry. But the access of such new feedstocks remains limited. The challenge of exploiting biomass, waste gas and recycled feedstock continues to be a challenge.

Furthermore, new molecules combine both higher performance and improved sustainability. This is possible and measured by increasing the 'odor per Carbon ratio' with high impact material.

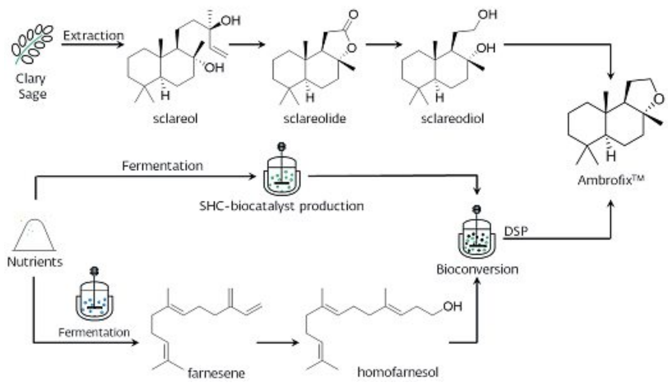

Fig. 3. Synthesis of Ambrofix™. Traditional route ex clary sage and the most recent biotech route to Ambrofix™.

Nympheal™ delivers 13 times more odor per carbon than Lilial. The odor per carbon is measured by a proprietary formula taking into account the number of Carbon of the molecule and the odor threshold, the lowest concentration of a component that can be perceived by the human nose. Ultimately this leads to compacted fragrances, a clear trend in fragrance design and key part of the sustainability journey

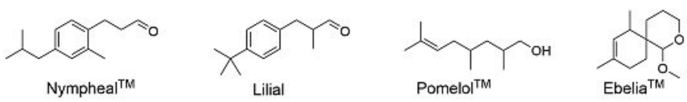

Fig. 4. Chemical structure of fragrance molecules.

Additional Challenges and Solutions

More examples of switching chemistry steps by biotransformations and alternatives feedstocks are coming. The speed and opportunities should increase as many industries as well as the fragrance industry have embarked on this journey for more sustainability. There is a strong need for affordable alternatives. In the beginning of the twenty-first century, establishing new processes based on biomass is shown to face considerable technical and economical obstacles to reaching a scale that can contribute valuable emissions reductions.

At Givaudan, human safety is also part of our purpose. Through our Safe by Design™ initiative, we are leading industry efforts to replace animal testing, while at the same time speeding up the testing process. Scientific innovation centred around early testing of molecules without animals have a wide range of benefits: For consumers by ensuring safety for use on human skin, for customers by bringing products faster to market, and for the environment by creating eco-friendly ingredients. These new approaches are based around an understanding of how biochemical processes can help us to develop and understanding of chemical impact on humans. In 2016 Nympheal™ (Fig. 4) was introduced to replace Lilial, in the white floral olfactive space. Nympheal™ prevents a critical metabolism observed in Lilial.[3] Nympheal™ was launched successfully as a safe replacer.[4] This shows the essential need for a combined approach of chemistry and biochemistry. Recently, a platform for PBT screening without animal testing was established (PeBiToSens™) which is key in the Givaudan Safe by Design™ approach to develop safer and environmentally friendly fragrance ingredients. The determination of persistence (P), bioaccumulation (B) and toxicity (T) plays a central role in the environmental assessment of fragrance chemicals. While P assessment is a standard microbial degradation test, the determination of B (*i.e.* bio concentration in fish) and T (fish acute toxicity) classically involves vertebrate testing. At Givaudan we use the OECD standardised *in vitro* assays based on fish liver cells[5] or liver S9 fractions[6] to determine biotransformation rates. Biotransformation increases excretion from the body and reduces bioaccumulation. The impact on the viability of a gill cell line from rainbow trout as a recently adopted OECD test is used as a surrogate for acute fish toxicity. The environmental profile of the recently launched Pomelol™,[7] a green citrus floral note, was assessed completely without vertebrate testing using the PeBiToSens™[8] platform. Our own laboratories were involved in the validation studies for both these two non-animal test methods ultimately leading to OECD acceptance. By this we helped to make this approach available to the whole chemical industry globally.

Growth with Purpose

The necessity to accelerate innovation in the fragrance industry to support the growing demand in multiple applications while improving sustainability is key. Chemical biology in various optimised combinations is also an essential asset to design, develop, test and understand new solutions. Givaudan chemists, biotechnologists and process experts together are engaged in revolutionary innovation to support our perfumers to create for happier and healthier lives with love for nature.

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doi:10.2533/chimia.2021.1085 Chimia 75 (2021) 1085–1087

A Perspective on Chemistry and Society

A Column on the Occasion of the 75th Anniversary of CHIMIA

Idorsia Pharmaceuticals Ltd.

Organic Chemistry: At the Core of Idorsia's Business

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Stefan Abele received his PhD in chemistry at the ETH Zurich (Prof. D. Seebach) in 1999. He joined Carbogen-Amcis where he held positions of growing responsibility in R&D and GMP manufacturing of Drug Substances. In 2006, he set up a fully integrated Chemistry Process R&D department at Actelion where he received the 2015 Sandmeyer Award[1] with his teams. Since the inception of Idorsia in 2017, Stefan is responsible for drug substance R&D and manufacturing from the preclinical phase to launch and commercial supplies. As Head of Chemical Development and Commercial Manufacturing (CDCM) he is part of the Idorsia Leadership Team.

'Organic Chemistry – Where Now?', the title of a review by Prof. D. Seebach in 1990[2] has not lost its rigor and relevance. Over the last decades, there has been a stunning array of innovations in fields like photo-redox chemistry, electrochemistry, flow chemistry, C-H activation, as well as gene technology and molecular biology. These advances have brought forth new solutions to some key global challenges like new drugs for devastating diseases, new materials for batteries, and catalysts for green technologies. Simultaneously, the resources and energy required to produce target molecules are more and more under scrutiny driven by the need to develop sustainable and environmentally benign processes. Moreover, cost pressure from health systems and the need to deliver affordable drugs have increased. More than ever organic chemists are pivotal players to solve these challenges. Advanced chemistry combined with state-of-the art manufacturing technology are key capabilities that remain the undisputed strength of our innovation-oriented society. The following perspective highlights the impact and significance of organic chemistry at Idorsia, with a focus on process chemistry and manufacturing, embedded both in the Swiss science ecosystem and a global supply network.

Idorsia – Small Molecules and Organic Chemistry

Idorsia Pharmaceuticals Ltd started operations after demerging from Actelion[3] following its acquisition by Johnson & Johnson in 2017. In addition to over 650 highly skilled employees, a rich early-stage pipeline was transferred to Idorsia. Over just four years, the clinical pipeline has progressed and six compounds are now in late-stage development. We expect two product launches in major markets in the first half of 2022, subject to regulatory approval. With now over 1'000 professionals, Idorsia covers all disciplines required for drug discovery and development ranging from Molecular Biology, Biochemistry, Structural Biology, Research Information Management and Modelling, Pharmacology, to Medicinal Chemistry, and Chemistry Process R&D.

At Idorsia, it's a strategic choice to focus on small molecules, and the design and synthesis of small molecules of increasing complexity is the turf of organic chemists. This particular 'Idorsia DNA' is promulgated publicly by the founder and CEO, Jean-Paul Clozel, who is convinced that small molecule drugs will remain well-poised to treat many diseases where there is an unmet need, whilst also fulfilling important criteria such as ease of administration and affordability.[4] The percentage of new molecular entities approved by the FDA that were small molecules was between 70–75% over the last five years.[5] Idorsia's clear focus allows for a differentiation from peer companies who are betting on diversifying into large molecules like biologics, oligonucleotides, or peptides. Our focus on small molecules is an asset for attracting highly talented organic chemists amidst global competition. Medicinal chemists are the 'drug hunters', equipped with state-of-the-art technologies, including artificial intelligence tools to more quickly design and identify molecules for further preclinical development. Process chemists, the 'process hunters', then begin to design and develop innovative, scalable, robust and cost-efficient processes. From finding the right molecule as part of drug discovery to synthesizing and physically delivering the drug substance at every step of the development and commercialization lifecycle, chemistry is indeed at the core of our company, and contributes significantly to each of Idorsia's five strategic priorities (Fig. 1). The process chemists' additional privilege and motivation are to have a sizable impact on the Cost of Goods by developing new chemical routes for the drug substance, which can ultimately translate into higher profits for the company.

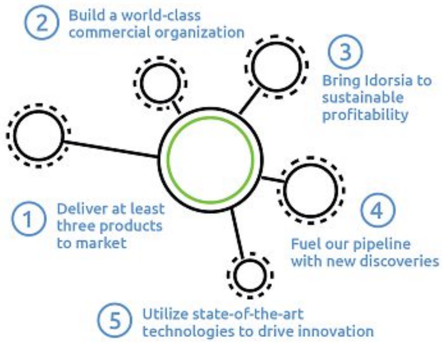

Fig. 1. Organic Chemistry plays a key role in each of Idorsia's five strategic priorities.

Chemical Development and Commercial Manufacturing

At Idorsia, our highly productive Discovery unit produces an average of two candidates per year for entry-into-human studies. Together with the large number of late-stage assets, this creates formidable challenges for our two teams of chemists who play crucial roles in delivering high-quality drug substance: the Process R&D team and the Development and Manufacturing team (Fig. 2).

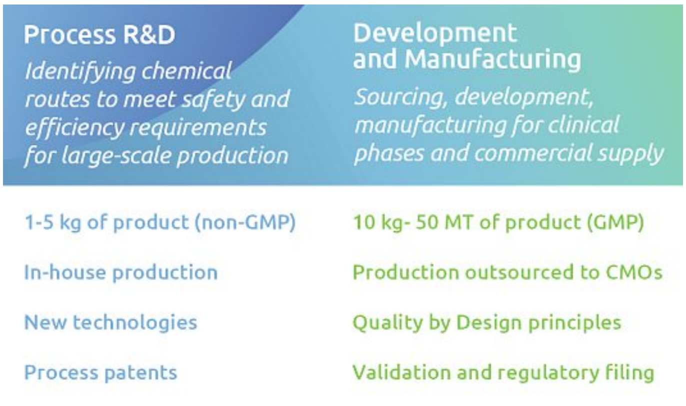

Fig. 2. Chemical Development and Commercial Manufacturing at Idorsia: Drug substance from grams to tons, from discovery to market.

The Process R&D chemists have the great challenge and opportunity to present innovative solutions to intricate synthesis problems. They are scouting for new chemical routes that allow for an expeditious and safe production of first kilogram quantities (produced in-house in the non-GMP kilo lab) for toxicology studies and formulation trials. In addition, process chemists are designing and developing so-called '2nd generation routes' for the late-stage clinical assets that qualify for registration, validation and future commercial large-scale manufacturing. They also bolster our company's intellectual property by filing process patent applications.

Sharing the results of Process R&D with the scientific community is an added benefit to our work, beyond the pride we take in helping to bring new treatments to patients in need. In addition to the genuine motivation of sharing and gauging our own research in a peer-reviewed setting, Idorsia is able to attract talented chemists by spotlighting the quality of science at Idorsia. Ultimately, publishing is used more and more as a tool to secure freedom-to-operate.[6] Organic chemistry is at the core of these activities, with a broad skill set required, ranging from keeping abreast of recent new methodologies published in literature to producing multi-kg amounts in a small plant. Deep knowledge in thermokinetics, mass-transfer phenomena, process safety, and a holistic view of the scalability and feasibility on the larger scale is essential. Concepts like Quality by Design (QbD) are applied to develop robust crystallization protocols for the drug substance, supported by online analytical tools. Physical attributes of the drug substance such as particle size and density are critical parameters for the successful formulation of the final drug product.

In parallel, the Development and Manufacturing chemists have the challenge to scale up organic chemical reactions in a highly regulated cGMP environment. At Idorsia, we manage GMP manufacturing through a global network of suppliers, called Contract Manufacturing Organizations (CMO). It is essential to ensure a seamless transfer of knowledge from the first kilo-batches to final commercial batches. The know-how accumulated during the process development and non-GMP production serves as a basis for the first outsourced GMP batch. This is followed by process development, scale-up, registration, and validation of the manufacture of commercial supplies in line with cGMP and regulatory guidelines. An additional role of the Development and Manufacturing chemists includes the coordination of further functions, including formulation and drug product development, Quality Control, Quality Assurance, packaging and distribution, clinical trial supply, and Regulatory Affairs, all of which make up Chemistry Manufacturing & Controls (CMC). Thorough process understanding is primordial in controlling impurities and securing consistent quality of the API (Active Pharmaceutical Ingredient) at scale and over time. In the end, the CMC data accumulated during development are an important part of the dossiers filed with health authorities to seek market approval.

Identifying and selecting the right partner companies for these activities[7] are key to both supply security and to reach the financial goals for our Cost of Goods. The success of outsourced API manufacturing is built on trustful supplier relationships, recognizing the added value of in-time delivery and enhanced process know-how. CMO performance is monitored with emphasis on quality, timelines, and cost efficiency. This is best realized by visits and on-site audits to control the cGMP status. Relying on external suppliers is associated with risks that need proper mitigation to secure the supply chain, as witnessed during the COVID-19 pandemics when our industry was under particular scrutiny for vaccine shortages.

Supply Chain in the Headlines

The convoluted supply chain for mRNA and other vaccines has ruthlessly revealed bottlenecks, be it a shortage of glass vials or filter aids, custom-made nanolipids, delayed shipments or the sheer lack of enough manufacturing capabilities and trained staff. A further backlog and surge of demand in 2021 has created significant shortages and delays in logistics, as well as some massive increases of the costs of commodities such as solvents. The supply chain for a small molecule API comprising several registered starting materials and half a dozen steps to produce the final API is not trivial. Not only must the quality of all intermediates, solvents and reagents be guaranteed, but we must also ensure the timely availability of the ingredients and raw materials to deliver enough API for the patients enrolled in clinical studies or, after approval, for the commercial supply. Several levers are used to set-up and nurture a resilient supply chain of API, such as dual sourcing or stockpiling strategic intermediates for expedited manufacture of API. Purely local sourcing of complex APIs is challenging for two reasons: first, for commercial large-scale supply, the higher costs of western CMOs could lead to a negative business case. Second, since a decade, it proves more and more difficult to secure enough capacity in European CMOs. Additionally, large pharma companies are increasingly outsourcing API manufacturing. CMOs in India and China are offering a larger volume and flexibility of capacity. However, accelerated by the lessons learnt by shortages of drugs during the pandemic, there is a general trend for onshoring, or repatriation of at least parts of API production. This will inevitably come with a price increase that has to be absorbed by all market players.[8] China is forcefully implementing its environmental regulations and the recent shortage of coal and gas has led to the sudden closure of whole industrial parks.[9] This is a trend with two benefits: first, running environmentally benign processes in all parts of the world is a boon for our planet. Second, the onshoring of manufacturing and R&D into European countries will require many well-trained chemists and engineers: a bright outlook for young scientists!

Manufacturing in Switzerland

Gratifyingly, the Swiss CMO landscape is reacting to the increased demand of their services with – for local standards – massive CAPEX investments. Over the next few years, five large Swiss CMOs are investing over CHF 1 billion into plant extensions.[10,11] While raising their profiles as drivers of innovation, they will also benefit from a stable socio-economic, innovation-friendly environment. Whereas countries like the US have very few manufacturing capabilities left, Europe has maintained higher levels of manufacturing in countries like Italy, Spain, Germany, and Switzerland. The impact of manufacturing cannot be underestimated: it attracts large-scale investments, requires a skilled workforce, is based on adjacent disciplines like civil engineering, craftsmen, electronics, and spurs the development of efficient and 'green' processes that can be run profitably in high-cost countries. And, it is the biggest asset in reducing dependency on other countries for the supply of life-saving drugs.

Swiss Chemistry Ecosystem

Idorsia is well embedded in the Swiss chemistry ecosystem. Some of the most renowned global institutes and universities are located in Switzerland. There is a strong organic chemistry heritage: several Nobel prizes in Organic Chemistry have been awarded to chemists from the ETH, the universities of Zurich and Basel. The Basel region, where three countries meet, with its strong chemistry and pharma history is preparing for the next wave of investments. Idorsia is in close vicinity to the Switzerland Innovation Park Basel Area,[12] which is being built to create several thousand work spaces for scientists, further strengthening Basel's role as science hub and magnet for talent from across the globe. Idorsia is profiting from this vivid and highly productive local environment on several levels: by attracting the best scientists and tapping into the global talent pool; and by exchanging perspectives with the exceptionally high density and quality of scientific peers from neighboring companies. The Swiss Chemical Society and its flagship journal *CHIMIA* play an active role in strengthening the Swiss chemical science community. Idorsia is proud of our role in this community. Through activities such as maintaining close relationships with nearby universities, hosting students and training apprentices, we hope to further the growth of future co-workers in organic chemistry.

Conclusion

Organic chemistry, with its impact on the efficiency of drug development, on manufacturing costs and on the reduction of our ecological footprint, is at the heart of the biopharmaceuticals industry. It is an essential discipline for companies like Idorsia to find, develop and manufacture new drugs for the benefit of patients. It will be interesting to see which innovations from organic chemistry will unfold to master future challenges: 'Organic Chemistry – What's Next?'

Acknowledgements

The author is indebted to Jean-Paul Clozel for his daunting vision and thanks the entire Chemical Development and Commercial Manufacturing department for their brilliant work.

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A Perspective on Chemistry and Society

A Column on the Occasion of the 75th Anniversary of CHIMIA

Swiss Women in Chemistry (SWC)

Swiss Women in Chemistry – Two Years Later …

Maud Reiter, Rachel Hevey, Rebecca Buller, and Inga Shybeka*

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Abstract: The SCS Swiss Women in Chemistry network was launched in September 2019. Under the umbrella of the Swiss Chemical Society, its aim is to create visibility, facilitate networking and provide a supportive community for female chemists in Switzerland across all career stages both in industry and academia. The current article provides an overview on the platform's activities over the past two years.

Dr. Maud Reiter is the Director of New & Renewable Ingredients in the corporate R&D Division of Firmenich S.A. in Geneva (Switzerland). Maud received her undergraduate degree from Imperial College, London in 2002, followed by her DPhil with Professor Véronique Gouverneur at the University of Oxford. After postdoctoral work with Professor David MacMillan at Caltech/Princeton University, Maud joined Merck & Co. in 2008 in Rahway, NJ, USA as a medicinal chemist. In 2011, Maud moved to Firmenich, where she is overseeing the discovery of novel & sustainable perfumery ingredients and since October 2020, the implementation of renewable versions of existing ingredients. She is a core team member of the SCS Swiss Women in Chemistry & Suschem.ch networks and joined the SCS board of directors in June 2021.

Prof. Dr. Rebecca Buller is a biological chemist and Professor for Biotechnological Methods, Systems and Processes at the Zurich University of Applied Sciences. Rebecca Buller studied chemistry at the Westfälische-Wilhelms Universität Münster (D) and the University of California Santa Barbara (US). After completing her PhD with a focus on enzyme engineering at the ETH in Zurich (CH), Rebecca Buller accepted a position as laboratory head at the flavour and fragrance company Firmenich (CH). In 2015 she relocated to the Zurich University of Applied Sciences where she founded the Competence Center for Biocatalysis (CCBIO). Rebecca Buller serves as an expert on numerous panels, among them the steering board of the NCCR Catalysis, the working group 'Biotransformations' of the DECHEMA/VAAM, the European Section of Applied Biocatalysis (ESAB) and she is founding board member of the SCS Swiss Women in Chemistry. Research in Rebecca Buller's laboratory focusses on the expansion of the biocatalytic toolbox by sourcing and engineering enzymes for synthetic applications.

Dr. Rachel Hevey is a Research Associate at the University of Basel. After completing degrees in both Chemistry and Biological Sciences, she undertook her PhD studies with Prof. Chang-Chun Ling at the University of Calgary (Canada). In 2013, she joined the group of Prof. Beat Ernst in Switzerland as a postdoctoral researcher, and in 2015 was promoted to a Research Associate at the University of Basel. Her main research interests involve glycan synthesis and the development of carbohydrate-based pharmaceuticals. Her research and teaching have been recognized through several awards, including the J.B. Hyne Research Innovation Award and recent selection for the IUPAC centenary 'Periodic Table of Younger Chemists' highlighting emerging chemistry leaders under age 40. Rachel is a co-founder and core member of the SCS Swiss Women in Chemistry.

Inga Shybeka is a PhD candidate in the group of Professor Stefan Matile at the University of Geneva since 2018, where she is working on cellular uptake. Inga obtained her MSs degrees following a double diploma program. Firstly, she carried out her master thesis project in green chemistry with Professor Michele Baltas at the Université Toulouse III – Paul Sabatier in Toulouse, France in 2018. Afterward, Inga completed her 2nd MSs in chemistry of natural compounds from Taras Shevchenko National University of Kyiv, Ukraine in 2019. Inga is a student ambassador of the SCS Swiss Women in Chemistry network for the Swiss Romandy area.

Introduction

It has been two years already since the official launch of the SCS Swiss Women in Chemistry (SWC) platform. The network was created, in part, as an initiative to increase participation of female speakers at SCS chemistry conferences and scientific advisory boards within Switzerland. Typically, over the past years, women comprise from 20–30% of the SCS conference audience, but this percentage is not reflected in the speakers' program, with several recent Swiss meetings lacking any female speakers.

Social Media

SWC social media accounts highlight local events, celebrate award recipients, and share recent publications either first- or senior-authored by Swiss female scientists to increase awareness of work currently being done in Switzerland. In addition, SWC will soon launch a 'Meet the Members' campaign to further highlight the achievements of our members.

The SWC network has been highly active on social media. Compared to the first year after launch, the SWC network has increased by 2.5 times and today includes:

- ~400 members within its LinkedIn group
- ~570 followers on @SwissWomenChem on Twitter
- ~200 followers on Instagram (swisswomenchem)

Events

SWC has been organising several yearly events:

- Corporate Insights
- Mentor program dinners
- IUPAC Global Women's breakfasts
- Career round tables

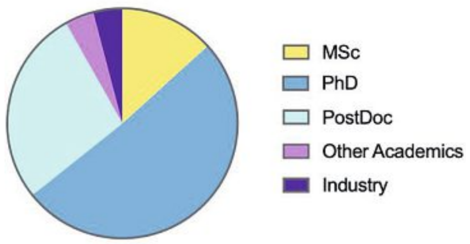
Corporate Insights

Two events have been held, namely at Novartis and Firmenich, both in an online format. During these Insights events, students had the opportunity to learn more about the career path of junior or senior industrial scientists, as well as interact more directly with female industrial scientists through workshops in small groups.

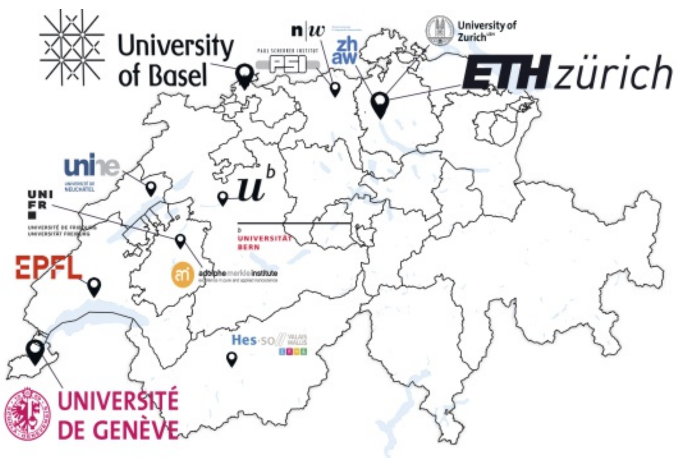
Novartis Round Tables

Organised in collaboration with Novartis, the Round Table events covered the topic of careers in chemistry. The two events already held were online due to the pandemic but we are hoping to move to an in-person format in 2022.

The two sessions attracted approximately 100 ***participants*** each. For the second event, half of the participants (51%) were PhD students, another 27% were PostDocs and 13% were master students, with the remaining percentage corresponding to established academic or industrial members.



Among the students, more than half of attendees were from larger universities: University of Basel (22%), ETH Zurich (17%) and University of Geneva (16%). Other participants attend EPFL (11%), University of Bern (11%), University of Fribourg (4%) and University of Zurich (3%). In addition, there were several participants from Adolphe Merkle Institute, FHNW, HES-SO Valais, Paul Scherrer Institute, University of Neuchatel, ZHAW, one academic from outside Switzerland, and several specialists from industry (4%).



The round table discussion was split into different topical rooms, covering Analytical Chemistry, Automated & High-Throughput Experimentation, Materials Science, Medicinal Chemistry, Biotechnology, Process Chemistry, and Computational Chemistry, with a final room being dedicated to Pursuing a PostDoc. The latter was introduced in the 2nd series, as per survey outcome, stating that students were interested in learning more about the different options of postdoctoral studies in industry versus academia. Various topics were covered during the round table discussions, such as job search strategies and tools, importance of personalised cover letters, networking, what a classic workday looks like, and the evolution of responsibilities while progressing up the career ladder.

Mentor Program

Each year, the SWC network matches up local mentees with established mentors in both academia and industry across the three regions. The Mentor Program was initiated in 2019 and has helped to support over 25 mentees per year. Currently, the 3rd round of mentoring is ongoing and consists of more than 30 Mentor/Mentee pairs. As there is no better way to provide you with feedback on the program, we would like to give the word to the participants themselves.

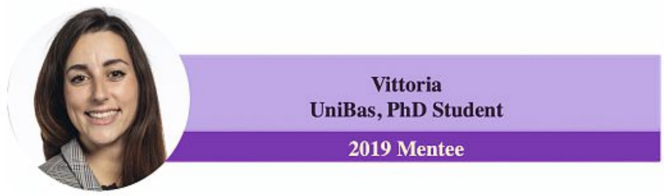
"Just as my master studies in chemical engineering at EPFL were coming to an end, I learned about the SWC mentoring program. I saw this as an opportunity to receive much-needed guidance and support for the transition between university and an industrial career, so I decided to join the program. As the program spans across several months, it was able to cover all important steps during my transition, starting with job applications and finishing with my first months as a new Lonza employee. My mentor's advice was always empowering, and our regular meetings helped me evaluate my progress and prepare for the next big step. The insights of an experienced professional, as well as personal contact with another colleague were very valuable to me in this period."

"[…] I believe SWC mentoring program offers excellent support to recent graduates of all levels, as it can be tailored to personal needs of each participant and their career goals, whether it be in academia or industry. I joined this program since I'm convinced that the exchange of needs, expectations and experiences between generations is beneficial to both the mentee and the mentor. Different times and periods in own's lives require different solutions for both, professional and private lives. But there is a convergence in needs, probably more specially for women, about making choices and progressing in their careers while maintaining a harmonious social life…."

"The SWC mentorship program has given me a lot of guidance and confidence for important steps in my academic career. Above all, it has encouraged me to go further than I would have on my own."

"The SWC mentoring program provides a unique networking platform to connect with female role models in academia and industry that empowered me to make confident decisions on my next career steps. I am truly grateful to my mentors for openly sharing their personal views, struggles, keys to success and the invaluable knowledge that can only be gained through experience."

"I joined the SWC network in my last year of doctoral studies by participating as a mentee in the SWC mentoring program. At that time, I was unsure if I wanted to pursue postdoctoral studies or go directly into industry. I felt like there was a considerable gap between where I was then and where I was supposed to be the following year. This transition to the 'real working world,' as I used to call it, raised many questions. With my mentor, we could discuss career choices and opportunities. We also talked about the importance of work–life balance. I could benefit from her past experiences and unbiased guidance. We shared our respective journeys, the highs and the lows, the success, and the challenging situations. We may have the best relationship with our PIs, colleagues, friends, or family, but it is always helpful to have someone outside of our circle who has been through a similar path and whom we can trust, who listens, understands, and supports us. I am grateful to have met my mentor through this program, as well as other great scientists, at some of SWC's networking events."



"I would say that the mentoring program taught me to take up space and stand my ground. My mentor taught me that communication and mediation is fundamental, but so it is to be seen, heard and understood."

Conclusions

Connecting virtually allowed us to continue our activities during the pandemic, however, we look forward to transitioning back to in-person meetings as soon as it is safe, in order to benefit most from networking opportunities within the SWC community.

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We would like to thank all mentors, who since 2019 have kindly supported our mentees in their professional development, as well as the principal coordinators for the Career round tables organized with Novartis, Cara Brocklehurst and Lucie Lovelle. Finally, we would also like to thank Melanie Vanberghem for serving as seed crystal and Alain De Mesmaeker as a sponsor of the Swiss Women in Chemistry network.

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A Perspective on Chemistry and Society

A Column on the Occasion of the 75th Anniversary of CHIMIA

Novartis

Perspectives and Opportunities in Medicinal Chemistry: A View from the Novartis Institute for BioMedical Research in Basel, Switzerland

Yves P. Auberson* and Martin Missbach

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Abstract: An opinion on changes and opportunities for the pharmaceutical industry in Switzerland, as seen from the Global Discovery Chemistry platform of the Novartis Institutes for BioMedical Research in Basel.

Keywords: Digitalization · Drug discovery · Medicinal chemistry · Synthesis

Yves P. Auberson is an Executive Director in Global Discovery Chemistry at the Novartis Institute for BioMedical Research (NIBR) in Basel, Switzerland. He is the past president of the European Federation for Medicinal chemistry and Chemical Biology (EFMC) and vice-president elect of the Swiss Chemical Society.

Martin Missbach is the NIBR Basel Site Head for Global Discovery Chemistry. He has a long experience in drug discovery in the area of autoimmunity, inflammation and transplantation. Both have a 30-year record of scientific leadership in drug discovery.

1. Introduction

Medicinal chemistry in Switzerland is a very dynamic area of research. Basel is the home of many leading international companies and hosts a growing number of innovative biotech companies, many in the Switzerland Innovation Park Basel Area. The latter serves as a catalyst for innovation, offering co-working spaces and shared research facilities across four locations, including the Novartis Campus.[1]

In this article, the authors discuss the recent evolution of drug discovery, and the opportunities they create for Novartis and the pharmaceutical industry in Switzerland.

2. A Strong Commitment

Novartis is a medicine-focused company, with research and development being at the heart of its activities. In early 2022, it will open a fully renovated building on the Basel campus (Fig. 1) hosting a large part of the Global Discovery Chemistry activities in Basel. This investment will facilitate cooperation and synergies, reinforcing the quality and effectiveness of drug discovery and optimization programs. Medicinal chemists, analytical chemists and several advanced technology groups will benefit from these state-of-the-art facilities.

Fig. 1. The new Global Discovery Chemistry building (left, with wall painting from Swiss artist Claudia Comte) on the Novartis campus in Basel.

Besides updated chemical and analytical laboratories, pilot-sized bioreactors in the lower floor of the new building will enable to access larger amounts of biologically produced natural products and custom-made enzymes. The latter will enable the exploration of chemical spaces that are difficult to reach synthetically, as well as the development of greener processes for building block synthesis, chemical production, or late-stage functionalization of complex molecules.

3. A New Research Environment

The Sars-Cov-2 pandemic has profoundly influenced scientific research, temporarily limiting lab-based operations and preventing face-to-face interactions. It had strong consequences on medicinal chemists and their working environment, forcing many scientists to work remotely. It fundamentally changed the perception of the workplace and the dynamics of professional interactions. Most scientific meetings became virtual, from informal coffee breaks to large scientific symposia. This led to permanent changes in the way people perceive their work, creating new ways to communicate independently of physical meetings, commuting and international travel. While it took time to get used to it, most people now agree that a combination of physical and virtual presence has become the most effective way to work and share information. This change was enabled by the deployment of more efficient group collaboration software, in a direct response to the situation caused by the pandemic.

Novartis has implemented a flexible working model to adapt to a diversity of work requirements. It allows any option, from working remotely to being exclusively on site for lab-based scientists. This added flexibility provides a powerful means to optimize the time usage of all associates, on both a personal and professional basis, improving quality of life and scientific productivity.

In parallel, efforts are ongoing to increase work force diversity, to enhance the quality of research by contrasting and synergizing different approaches, experiences and thought processes. Diversity is a broad concept embracing education, gender and cultural diversity, and provides the basis to adapt to changing societal trends. Equal opportunity was discussed extensively over the last few years, and led to significant efforts to remove historical career obstacles, *e.g.* for women in leading scientific positions. These discussions had a clear impact on our society and brought about much-needed change. A challenge for the future will be to maintain the diversity of opinions and scientific approaches in the novel cultural environment of our community, which comes with its own norms and expectations.

4. Opportunities

The scientific continuum across chemical biology and medicinal chemistry evolves rapidly.[2] As borders between scientific specialities dissolve, drug discovery exploits synergies to take on a variety of therapeutic approaches. Most striking has been the progress achieved by the integration of new technologies into the practice of drug discovery, including activity-based synthesis of chemical probes[3] and novel screening technologies (*e.g.* cryo-electron microscopy[4] or DNA-encoded synthesis[5]), as well as protein degraders[6] and imaging agents.[7] Beyond these technological advances, some fundamental changes are taking place in the practice of medicinal chemistry, as illustrated by the increasing role of chemical biology, the upcoming wave of computer-driven applications and, interestingly, the re-emergence of enzymatic-driven chemical transformations.

4.1 *The Impact of Digitalization*

Artificial intelligence (AI) and machine learning become increasingly important technologies in drug discovery. Despite the scientific complexity of their application to medicinal chemistry, AI begins to show impact in some important aspects, including in predicting the three-dimensional structure of proteins.[8] Machine learning also proves very helpful in scrutinizing and analysing large sets of data, including from massive databases such as ChEMBL or PubChem, and in developing predictive models. Beyond classical compilation and analysis, the development of generative chemistry applications also provides suggestions for novel molecules, by combining partial structure-activity relationships, profiling data and predictive models.[9] To accelerate the development of such tools, Novartis announced in 2019 a multi-year research and development alliance with Microsoft, the AI Innovation Lab. It focuses on AI empowerment, bringing AI applications to the desktop of every medicinal chemist, as well as AI exploration. The lab will tackle some of the hardest computational challenges within life sciences, including several aspects of chemical optimization.

4.2 The Promise of Automation

At first sight automation sounds like a process that should only be applied to highly repetitive tasks, which do not need regular attention or human intervention. However, while the art of drug discovery is far from an engineering process that can be automated easily, some individual steps are amenable to automation. It starts with, but is not limited to, the handling of the many individual data points generated during the synthesis and analytical characterization of a molecule, even prior to tests in biological assay systems. Automating workflows, data capture and interpretation frees up a lot of time for more creative activities for medicinal chemists.

Furthermore, the combination of data digitalization and automation enables the delegation of repetitive tasks – not to service labs but to computers and robotic systems. For instance, integrated drug discovery platforms, which utilize micro-scale chemistry, real-time biological and physicochemical characterization as well as machine learning driven compound design, can take over the tedious task of chemical space exploration around specific scaffolds. By accelerating the optimization of specific properties through automated, iterative exploration, they also allow medicinal chemists to focus on the most innovative aspects of drug discovery.

4.3 The Potential of Biotransformations

The exquisite ability of enzymes to enable site- and stereospecific transformations makes enzymatic catalysis an attractive tool in synthesis. The use of such reagents was however historically limited by the biotransformations achieved by natural enzymes, and by their substrate specificity. Recently, the engineering of novel enzymes optimized for specific reactions[10] enabled the extension of their application range, including unconventional biotransformations such as stereo-controlled halogenations[11] (Fig. 2).

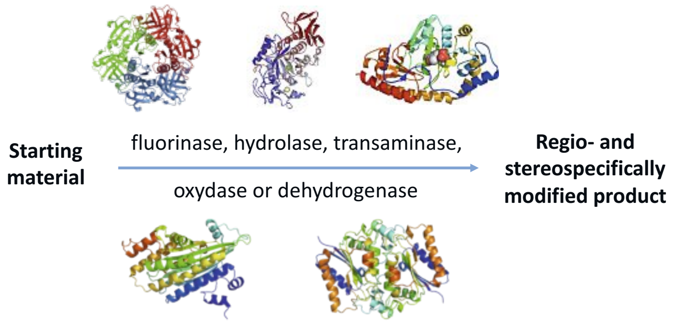

Fig. 2. Some enzyme classes useful for regio- and stereospecific chemical transformations.

With such tools in hand, biocatalysis can be used to prepare synthetically challenging molecules, and to explore chemical space regions that might otherwise be neglected during drug discovery programs. Custom enzymes evolved to enhance specificity and enable efficient transformations can be produced in large amounts, to support both chemical optimization and production,[12] making them particularly valuable. The increased availability of such reagents also opens the door to late-stage functionalization of drug candidates. This provides innovative molecules, with unique intrinsic properties and potential for further modification. Biotransformations are also an efficient method for metabolite synthesis. They allow the evaluation of potential drug liabilities resulting from metabolic products, arising from intrinsic activities, or from an interference with the pharmacological effect of the parent compound. Finally, the application of enzymatic transformations to specific steps of building block or drug candidate synthesis often leads to a reduced consumption of organic solvents and energy. Enzymatic reactions usually perform well in aqueous media at room temperature or slightly above. They hold the potential for more environmentally friendly chemistry, especially at large scale.

4.4 *The Value of Outsourcing*

A judicious use of outsourcing also helps scientists focus on complex issues and creative solutions, by providing additional, external resources for standard synthetic and profiling activities. Far from replacing experienced medicinal chemists, it allows them to focus on scientific challenges rather than operational needs. Typically, novel entities, unprecedented targets and technologies such as radioligand therapies or targeted protein degradation will be pursued internally, while library synthesis, building block production, and the standard activities of drug optimization programmes may be outsourced.

5. Opening the Framework

Opportunities related to collaborations with academic partners in Switzerland were discussed recently.[13] They are not the only source of external innovation for Novartis and other pharmaceutical companies, which look for innovative techniques, targets and drug candidates worldwide. Indeed, collaborations between academic centres, small and large pharmaceutical companies create a number of mutual benefits. These go from sharing biological tools with a larger community to study a disease at the cellular and atomic level, to developing new technologies or sharing risk for larger endeavours.

Interactions with the members of the chemical biology and medicinal chemistry community across the world are important, and no pharmaceutical company conducts research in complete isolation. In Switzerland, several learned societies regroup the medicinal chemistry, chemical biology and related scientific communities (Fig. 3). By organizing conferences and courses, as well as providing incentives for high quality research, they play an important role in fostering exchanges and the pursuit of new ideas within the scientific community. The participation in the activities of learned societies plays an important role in exploring new ideas and scientific challenges, and in revealing areas of innovation at the intersection of scientific disciplines.

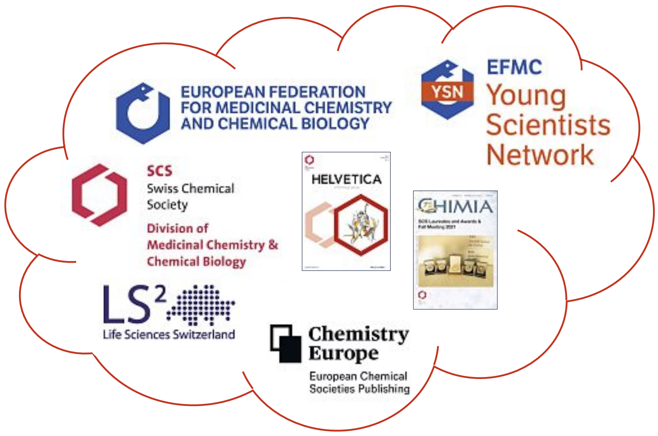

Fig. 3. The Swiss Chemical Society, the European Federation for Medicinal chemistry and Chemical biology, as well as Life Sciences Switzerland represent the medicinal chemistry and chemical biology community in Switzerland.

6. The Challenges that Remain

While drug discovery made impressive scientific progress over the last decades and identified drugs that changed the lives of millions of patients, many challenges remain. Despite improved success rates in late-stage phases, many drug candidates fail in the course of clinical development. Indeed, the rate of success in the pharmaceutical industry has hardly improved over time.[14] This is in part due to the difficulty of identifying therapeutically relevant targets, the complexity of some of the novel targets pursued, and a limited ability to predict dose, safety and efficacy in patients.

The identification of therapeutic targets heavily relies on high-throughput biology, including screens based on CRISPR/Cas9 gene editing, single cell RNA sequencing, or affinity proteomics. Medicinal chemists contribute to this effort by providing optimized, tailored tools to explore cellular biology. The principle of such tools, or chemical probes,[15] is to influence a specific cellular pathway and observe the effect of this perturbation on a disease-relevant parameter. Unfortunately, it is not easy to ensure that such molecules are perfectly selective, and even when they are, that their study in artificial or isolated systems is relevant. In addition, many disease models in animals are insufficiently validated or have intrinsic limitations,[16] leaving scientists with a limited ability to predict efficacy in human patients. The fundamental assumptions at target selection, that underlie otherwise successful medicinal chemistry programs, can end up being a major cause for failure in clinical settings.

Predicting the pharmacokinetic behaviour of drug candidates in patients has made significant progress, and drug candidates rarely fail in the clinic due to inadequate absorption or elimination.[17] In contrast, improper prediction of target engagement remains a frequent source of failure in the clinic,[18] especially for indications where preclinical models are poorly predictive of efficacy in humans.[19] A more systematic use of target engagement assays, both in animals and patients, *e.g.* imaging agents for positron emission tomography (PET), can however help address this issue. Similarly, the ability to tailor the route of administration, and to exploit diverse formulations to modulate the duration of action of drugs, has created novel opportunities. Extending the half-life of short acting drugs by different mechanisms (ligation to fatty acids to modulate duration of action, encapsulation in nanoparticles or embedding in slowly degrading matrices) proved successful in many different applications.[20] In addition, long-acting depot formulations, which by their nature prevent missing a dose, can help address the issue of poor patient compliance.

In contrast, predicting toxicology still remains difficult, and many drug candidates fail due to safety issues, or lack of efficacy related to doses limited by safety. Despite significant efforts, the investigative toxicology[21] of both oral and topically-administered drugs[22] remains a challenge. In the future, the use of integrated databases and computational tools to support the translational safety assessment of new drugs might facilitate their assessment, and the prediction of toxicological liabilities.[23]

Finally, the art of translating preclinically optimized candidates into clinically efficacious drugs remains a challenge in drug development. Further improvements are required for the prediction of human efficacious doses, and for refining the use of clinical biomarkers for patient selection and demonstration of efficacy. Likewise, the development of efficient clinical protocols to study chronic diseases or address new indications quickly and with good predictability remains difficult. A close collaboration between translational medicine and preclinical research experts fosters progress on this front, and this dialog should start at an early stage in a drug discovery project. Such challenges, often combined with pressure on costs, may lead to sluggish progress in the development of classical drugs as much as of innovative approaches, including cell-based or gene therapies.[24]

7. What Will Not Change

The quality and inter-disciplinarity of drug discovery science, across the chemical biology and medicinal chemistry continuum, are fundamental requirements for success. They result from the collaboration of highly educated and creative scientists, whose open-mindedness and curiosity is the basis of innovation. Novartis heavily invests in both technical and cultural aspects of drug discovery, striving for continuous improvement of its research activities.

The development of novel methods in organic chemistry enables many new technologies, and synthetic proficiency remains a critically important expertise. DNA-encoded libraries, miniaturized automatic synthesis systems, the exploration of new modalities, radioligand therapies as well as the optimization of ligands for classical drug targets rely on the synthesis of complex molecules. They often require the synthesis and functionalization of novel scaffolds, which frequently include a high level of structural complexity. During the drug discovery process, these molecules are modified to optimize multiple parameters, and ultimately must be prepared in large amounts for *in vivo* testing and clinical development. While people far afield sometimes entertain the misperception that organic chemistry is a mature science, it remains an area where constant progress is critical. In parallel, the need for more sustainable and environmentally friendly processes adds another level of scientific complexity. Sophisticated organic chemistry is thus required to make such drug development projects possible, with optimal use of the latest technological developments.

8. Conclusions

Medicinal chemistry in drug discovery is a dynamic science. It strives to integrate the latest developments brought about by progress in digitalization, automation, and a better understanding of cellular pathways and human diseases. Over the last few years, medicinal chemists explored many innovative therapeutic opportunities such as new modalities or chemically modified biologics, as well as novel technologies to take advantage of advances in hit generation, synthetic methods, as well as data capture and processing. Medicinal chemists show remarkable flexibility and adaptability, and have the courage to explore concepts that require multi-disciplinary skills. Breaking down barriers to further enrich collaborations with drug discovery partners will be the key of their future success. Partnerships with cell biology, physics, medicine and related sciences are necessary to take on the current challenges of drug discovery. It is good to see medicinal chemists embracing and often leading this change, steadily improving science and communication, and taking up new therapeutic challenges.

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