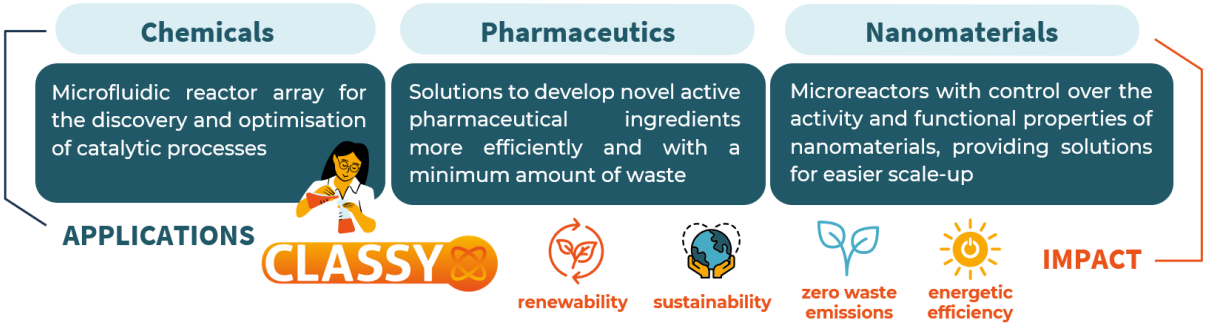
European research and innovation to emulate living cells in the design of self-regulating chemical reaction processes

Over more than four years, the multidisciplinary CLASSY research and innovation action which has been funded under the Horizon 2020 FET programme addressed the need for new technologies that have the potential to constitute an advancement towards sustainability and limited waste production of modern industrial synthetic processes. Inspired by the elegance with which living cells synthesise a large variety of complex components, CLASSY envisioned using the compartmentalisation strategy of cells to regulate chemical synthesis in a metabolic way. This strategy would allow synthetic methods to be more environmentally friendly by being more efficient and limiting the amount of generated waste. We are thrilled to share CLASSY's contributions to the development of a microfluidic platform of microreactors and significant progress in the areas of molecular synthesis dynamics, advancements in self-replication, microfluidic systems, biocatalysis, chemical biology, and supramolecular chemistry.



New advances in systems chemistry and chemical networks

The project coordinator, Prof. Andrés de la Escosura (Universidad Autónoma de Madrid, Spain), and Prof. Gonen Ashkenasy (Ben-Gurion University of the Negev, Israel) achieved new insights into the dynamic self-organisation of multi-component synthetic systems. At the same time, the groups of Prof. Helma Wennemers (ETH Zürich, Switzerland) and Prof. Wolfgang Kroutil (Universität Graz, Austria) joined mutual efforts to investigate the efficiency of enzymes in the presence of peptide catalysts. The Wennemers group has successfully demonstrated the use of peptides as efficient catalysts that are robust and versatile in applications and together with the group of Prof. Kroutil they were able to show that a combination of peptide- and biocatalysts in a single pot-reaction, can complete a two-step biocatalytic process. The work of Prof. Wilhelm Huck (Radboud University, Netherlands) instead focused on the study of chemical reaction networks and led research efforts on microfluidic production of catalytic reactors, supported by Micronit Micro Technologies B.V., a company based in Netherlands specialised in the development of microfluidic chips.

New EU initiatives to revolutionise research of self-thinking molecular systems

Complimentary to the ongoing CLASSY project, Prof. Huck has received a contribution of 97 million euro from the Dutch government's National Growth Fund, to develop an autonomous robot lab. His scientific project—*Robotlab: the revolution of self-thinking molecular systems*—will build a fully automated robotic laboratory that can devise complex molecular systems with the use of artificial intelligence. As Prof. Huck has explained in his interview "We humans have to formulate the problem, the robot lab works out the solution that we can then refine". This

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technology aims to bring a huge acceleration of scientific research to find answers to the questions we face due to the climate crisis, developing green and energy-efficient products.

Research highlights and wide-ranging collaborations

The most recent CLASSY findings were highlighted in the project's final Scientific Symposium event—*"Catalysis in chemical networks and supramolecular assemblies: New advances in systems chemistry"*—held online on 15 March 2024 and attracting over 50 participants from 42 organisations. The Symposium was key in disseminating the outcomes of the project both within the consortium and to external participants from academic institutions and research companies. The partners had the opportunity to share their latest discoveries with a wider audience on the topics with the view of four external experts in catalysis and compartmentalisation strategies in the context of systems chemistry. All members also shared insights on the importance of facing challenges to revolutionise the methodologies in which we synthesise chemical molecules. The event marked a successful end to this ambitious and multidisciplinary project, achieving not only significant develops in the fundamental understanding of molecular synthesis, but also strong collaborations between internal and external partners of the CLASSY consortium.

New partnerships, originating from CLASSY, brought about several new Horizon Europe funded projects, such as CORENET (EIC Pathfinder Open), DarChemDN (MSCA Doctoral Network), and MiniLife (ERC Synergy Grant). As one of the successful projects, CORENET launched in April 2022 under the coordination of Prof. de la Escosura. The inspiration for the project originated from the brain, being one of the world's most amazing computers that runs entirely on chemical reactions. CORENET's vision is to construct a brain-mimicking computing device that utilises networks of chemical reactions as molecular information processing systems. These networks will then convert input molecules into a pattern of product molecules based on different environmental conditions. The patterns will be monitored by a combination of analytical methods, cheminformatics and artificial intelligence (AI) tools. CORENET's future goal is to apply this innovative computing device in applications such as brain-machine interfaces, personalised medicines and implantable devices.

On the lookout for new funding opportunities

As with any scientific project, CLASSY faced many challenges along its journey, from an on-set of the pandemic to scientific methodology and overview changes. The CLASSY partners never put their hands down and battled through any challenge facing their way. We are delighted to see how well it worked out and how much all of the members were able to achieve as a team of multidisciplinary research groups. As one of the CLASSY partners specialised in European research, development and innovation support initiatives, accelopment Schweiz AG is facilitating the lookout for new funding opportunities that would finance future research ideas. The future looks bright and new opportunities and ideas are emerging to bring the fundamental findings of CLASSY to the next step in its research development stage.

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The CLASSY consortium pictured during the 10th General Assembly at Graz in 2023

Besides five leading research groups with expertise in systems chemistry, biocatalysis, chemical biology and microfluidics, the team also includes two companies specialized in microfluidic technology and project management, communication, dissemination and exploitation.

Seven project partners from five different countries:

- Biohybrid Materials and Systems Chemistry Group, Universidad Autónoma de Madrid, Spain (coordinator)
- accelopment Schweiz AG, Switzerland
- Laboratory for Systems Chemistry, Ben-Gurion University of the Negev, Israel
- Laboratory of Organic Chemistry, ETH Zürich, Switzerland
- Physical-Organic Chemistry Research Group, Radboud University Nijmegen, Netherlands
- Biocatalytic Synthesis Group, Universität Graz, Austria
- Micronit Micro Technologies B.V., Netherlands

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