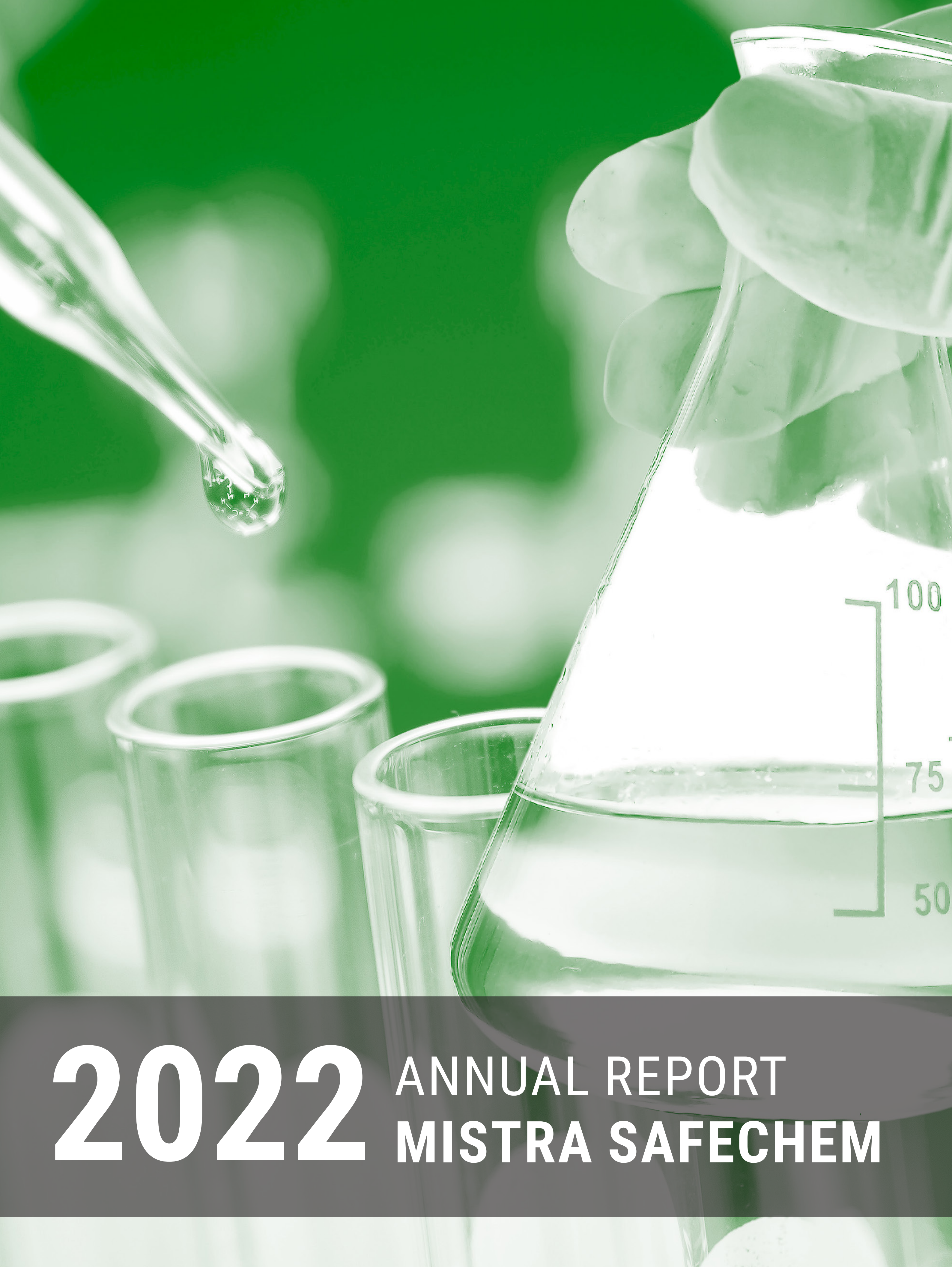

2022 ANNUAL REPORT MISTRA SAFECHEM

MISTRA
The Swedish Foundation for
Strategic Environmental Research

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SAFECHEM

CONTENT

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This is the annual report for 2022 from Mistra SafeChem,
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(pages 6-7), Alejandro Valiente (page 14), Ragnhild Berglund (page 20).

MISTRA

SAFECHEM

ANNUAL REPORT FOR 2022

This is the third annual report from Mistra SafeChem, in which we can report much progress from the programme.

In the first half, you can read in-depth interviews with researchers, representing successful work within each work package (pages 6-11).

Much of the work in the programme is done by the research students. You meet most of them on pages 12-13.

The latter part of the annual report includes concentrated facts on programme results and structure, especially the texts on the key achievements of the work packages during 2022 (pages 15-19).

We hope you enjoy reading about our work!

The vision of Mistra SafeChem is to enable and promote the expansion of a safe, sustainable and green chemical industry

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ABOUT MISTRA SAFECHEM 2022:

An extensive collaboration for a safe, sustainable and green chemistry

Mistra SafeChem is based on the concept of green chemistry and has the overarching vision to enable and promote the expansion of a safe, sustainable, and green chemical industry in Sweden.

Through research and development, the programme aims to contribute to a reduction of hazardous chemical exposure in the human population and the environment.

In the programme, we put chemists, toxicologists, ecotoxicologists, and life cycle assessment experts side-by-side with the task of making chemical development right from the start.

The toolbox in practical use

The work will result in a toolbox. During the year this toolbox has been set to practical use in case studies on substitution and in the assessment of new chemicals, materials and processes. Through interactions between research groups within the programme we increase our understanding of each other's requirements and challenges, as well as knowledge about what can be learnt regarding safety and sustainability already in the design phase of a chemical or material.

By the end of 2022, with Mistra SafeChem being more than halfway through its 4.5 years, we in the programme lead are happy to see that these interactions have fallen well into place and that results from these collaborations will result in publications in 2023.

Looking outside the programme we saw several research calls, both in Sweden and on the EU level, that requested the inclusion of safety and sustainability in the design of chemicals and materials. Delightfully we saw proposals from programme partners being accepted to some of these calls, giving rise to new projects that strengthen the network activity in the programme further.

Also, in the light of strengthening the programme collaboration further, we saw the green chemistry symposium and programme conference hosted by Astra Zeneca in Mölndal as a real milestone of the year (more on pages 6-7).

New chemicals, materials, processes

Textile recycling, metal and enzyme catalysis, the use of forestry residues and particle recovery and reuse are fields in focus in work package 4, Design and management of chemicals, materials and processes. Read about the achievements on pages 9 and 17, and in the report "Chemical synthesis – half-time achievements and outlook" (one of the deliverables we list on pages 22-23).

The optimization of these new processes has been integrated into the development of the toolbox system in the programme, testing and further advancing several of the tools for environmental and human health assessment.

Safe and Sustainable by Design

As we have the intention to create a research and innovation platform for the expansion of green and sustainable chemistry – in Sweden, the EU and on a global level – continuous external analysis and interactions are key.

One example is the EU Commission's recommendation for establishing a European assessment framework for *Safe and Sustainable by Design* (SSbD) chemicals and materials. The Mistra SafeChem toolbox system aims to contribute to its operationalisation by considering SSbD in toolbox assessment and further development.

During the year the Swedish start-up EnginZyme joined the programme. The company, based in Solna, has the vision to replace traditional fossil-based manufacturing with a cell-free technology platform to unlock the potential of enzymes. This makes EnginZyme a great fit for Mistra SafeChem, especially in our enzyme catalysis work stream.

Richard Lihammar,
IVL Swedish Environmental Research Institute, Programme Director

Hanna Holmquist,
IVL Swedish Environmental Research Institute, Programme Manager

2022 in numbers

For those of you who like numbers the following list can in part summarize Mistra SafeChem in 2022:

97
researchers and industry representatives active in the programme

40
appearances at scientific conferences and meetings (at least!)

22
scientific articles published

28
news articles published on the website

11
active case studies

3
external seminars on synthetic methods, programme tools and case studies

3
programme forums

3
research student group meetings

1
programme symposium on green chemistry

CHAIRMAN OF THE BOARD:

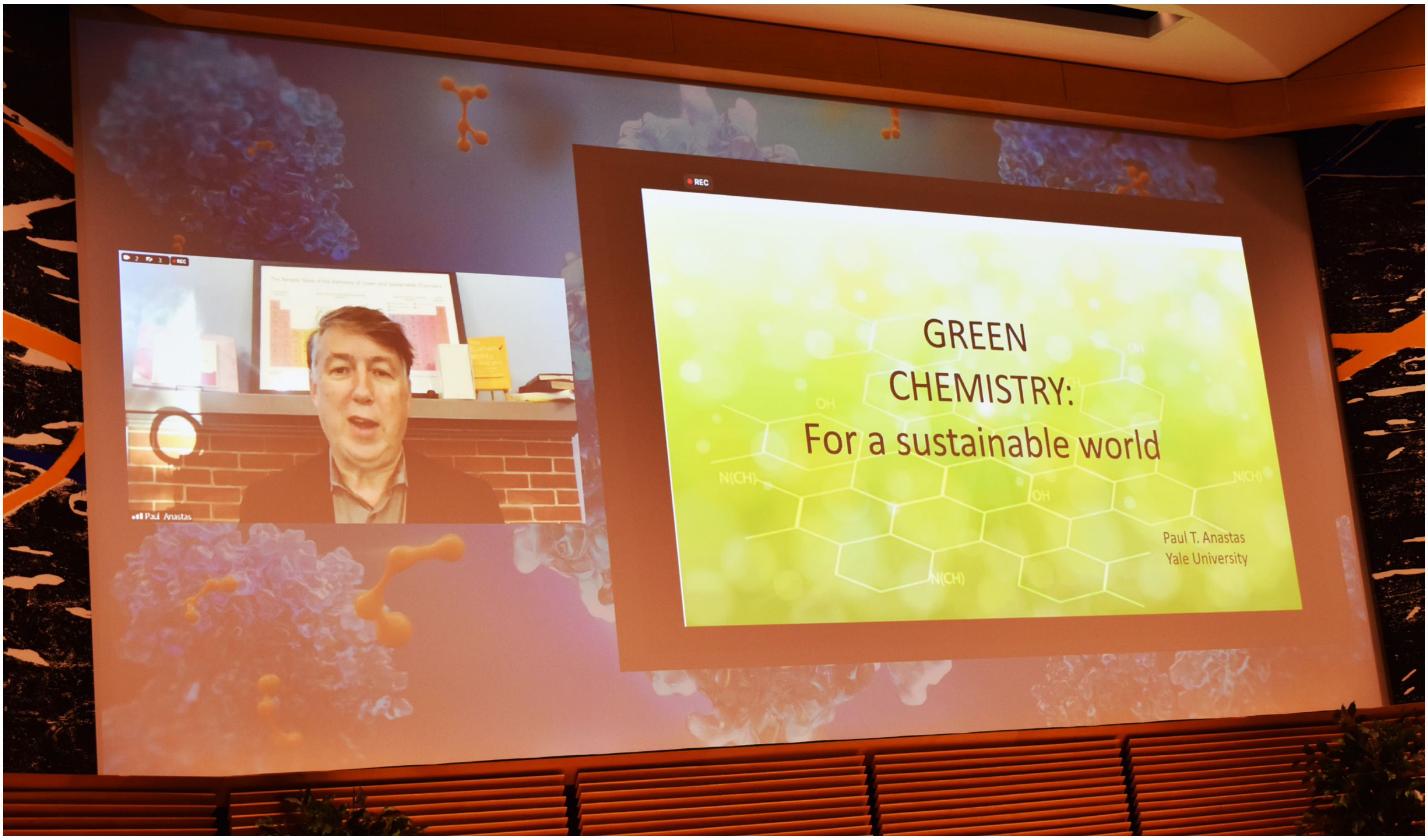
Go green or go broke!

Mistra SafeChem's ambition, to promote safe and sustainable chemical production, is a timely one. Every serious chemical company and most users of chemicals are now aware of the environmental and safety aspect of their products. They also know that environmentally benign chemicals are what the market – at the end the customer – wants today. "Go green or go broke" was launched some time ago as a slogan among environmentally concerned politicians.

The attitude towards environmental issues has changed rapidly and we have not seen the end of it. When REACH was launched in 2007 the European chemicals industry was afraid that their business would suffer and that competitors outside the EU would have an advantage. Now we see that this has not been the case. The industry is healthy and other countries, in particular the US and Japan, are also implementing strict regulations.

"Go green or go broke" has become a business reality and Mistra SafeChem is well-positioned to contribute to the transition.

Krister Holmberg
Professor emeritus, Chalmers, Chairman of the Mistra SafeChem board



Professor Paul Anastas gave his speech from his library in the USA. The fact that he had covid couldn't stop him from taking part in the Mistra SafeChem symposium.

HIGHLIGHT FROM WP2: A VISION AND AGENDA FOR GREEN AND SUSTAINABLE CHEMISTRY

Enabling meetings and opportunities for a green and sustainable chemistry

In line with the title of this work package, work has continued with the long-term goal to set a vision and agenda for green and sustainable chemistry.

A main task in 2022 was to investigate potential opportunities and obstacles in the transformation to a green and sustainable chemistry. In addition, work was started on assessing how on-going policy processes on chemicals would affect industry and society. Both research tasks are to a large extent influenced by the on-going work to implement the EU Chemicals Strategy for Sustainability and the many activities started up in the research community, industry and authorities.

A main event was the Mistra SafeChem symposium on green and sustainable chemistry, held at AstraZeneca in Mölndal on September 26, 2022. The question in focus was how to reduce people's and the environment's exposure to hazardous substances. About 100 persons attended on-site and 150 digitally.

Anastas: "We need a change of thought"

The symposium was opened by keynote speaker Professor Paul Anastas, Yale University, who gave an inspiring lecture (albeit remotely) on green chemistry for a sustainable world.

He highlighted that hundreds of man-made chemicals are accumulating in our bodies. But he also noted the possibility of creating new chemicals, or entirely new materials and products, fulfilling the intended function but without the hazards and risks involved. He concluded that we need to change how we think about chemistry.

❶ Around 100 persons were on-site at AstraZeneca in Mölndal. ❷ Lennart Bergström, Stockholm University, was one of the moderators. ❸ Richard Lihammar, IVL, talked about his superpowers. ❹ Many of the Mistra SafeChem students showed posters with their work.

After this, presentations focused on the innovative research in Mistra SafeChem including Ian Cotgreave, RISE, on the utility of computational tools, which are inexpensive and can quickly generate new data for decision-making. Per-Olof Syrén, KTH, declared his love for enzymes and described his research to find enzymes that are adapted to the higher temperature and harsher conditions used in chemical production and thus suitable for replacing current synthesis steps. Aji Mathew, SU, presented her research on textile recycling to produce cellulose nanocrystals from cotton or mixed fabric with very high purity. These nanocrystals can be used as building blocks for a wide range of high-value-added applications.

An invited lecture followed by Professor Lutz Ackermann, Georg-August-University Göttingen, on sustainable molecular synthesis by catalyzed C-H activation with potential applications in the late-stage functionalization of drug candidates, enabling chemists to make several variants from one common scaffold.

The last invited speaker, Stewart Owen, Principal Environmental Scientist at AstraZeneca, highlighted the anniversary of the book *Silent Spring* by Rachel Carson (published in 1962) and concluded that while we are on our way to fixing climate change, we will still be dealing with pollution.

"A superhero with superpowers"

The next speaker was Richard Lihammar, IVL, programme director of Mistra SafeChem. He ended the symposium on a more positive note and with the statement:

– I am a chemist, which means I am a superhero with superpowers! Chemistry is needed in so many fields. But we need to see already in the design phase what the effect might be. Would we have used DDT, PFAS or fossil fuels if they were invented today?

Richard Lihammar emphasized how persons in Mistra SafeChem learn from each other and that the whole value chain is represented among the industry partners.

Finally, it was concluded that the future of green chemistry is bright, judging by the skills of the research students who displayed their results on posters during the symposium.

HIGHLIGHT FROM WP3: HAZARD AND RISK SCREENING – EARLY WARNING AND PROACTIVITY

Developing machine learning models for toxicity prediction

Ziye Zheng, a postdoc working at Mistra SafeChem partner Cytiva, is developing a toxicity prediction toolbox based on machine learning models.

What is the focus of your research in Mistra SafeChem?

I am a member of the *in silico* team in work package 3. In this team, our goal is to develop a toolbox of computational models for chemical toxicity prediction, and my focus is to develop toxicity models based on traditional machine learning algorithms.

Why do you want to develop this toolbox?

When I was a PhD student, my research focus was to use computational models for the selection of less hazardous chemical alternatives. In 2021, I heard that my current employer, Cytiva, was collaborating with Mistra SafeChem to hire a postdoc and develop an *in silico* toolbox for their chemical alternative selection. I believe this is the perfect opportunity for me to continue my research in the field and directly combine my research with real industrial challenges, so I applied and work with Mistra SafeChem ever since.

How does your research contribute to the Mistra SafeChem vision of a safe, sustainable and green chemical industry?

If industries want to be greener in the chemical aspect, the first thing they need to know is whether the chemicals they plan to produce or use are toxic or not. However, many chemicals, especially novel ones, lack experimental toxicity data, and toxicity testing is both expensive and time-consuming. Computational toxicity models can provide reliable toxicity predictions for a large number of chemicals in a very short time, and they are very easy to use. They are excellent tools for industries to identify potentially toxic chemicals and narrow down their chemical alternatives list.

What are the results?

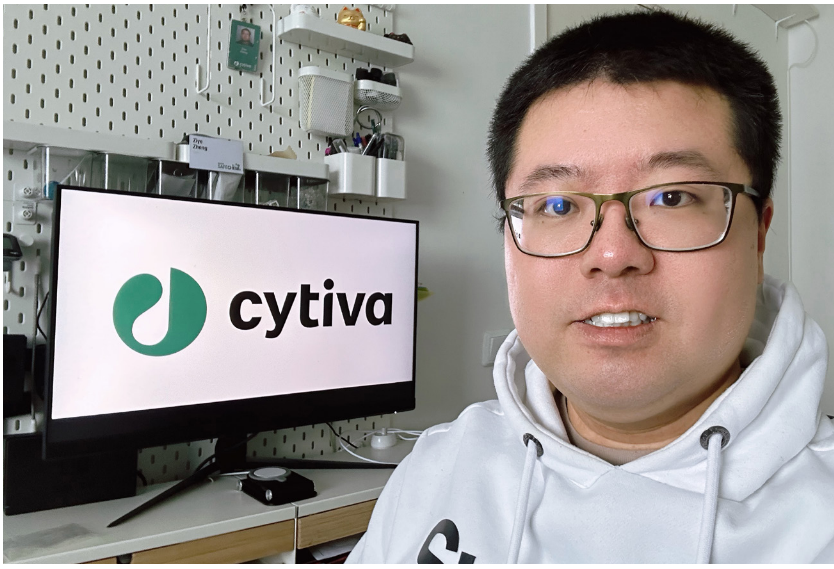
So far, I have developed machine learning models for the prediction of mutagenicity, carcinogenicity, reproductive toxicity, skin sensitization, eye irritation and corrosion, as well as endocrine disruptions. The models have good prediction reliability. Also, I have developed these models into computer software with an easy-to-understand graphical user interface.

How have you collaborated with others within Mistra SafeChem in your work?

In my work package, I work closely with Ian Cotgreave and Swapnil Chavan from RISE and Ulf Norinder from Stockholm University. We share our knowledge of chemistry, toxicology and computational modelling. We also work on developing different models for the same toxicity endpoints with different modelling approaches. My colleagues in Cytiva also give me a lot of suggestions for developing the software and help me to test the tool.

What further research is needed in this field?

There are many needs, one of the most important is that more high-quality experimental toxicology data are needed for the development of high-quality models. This requires closer collaboration between *in silico* and experimental toxicologists. Also, to have the models better used, collaborations are needed between modellers and other people in the green chemistry field, such as life cycle assessment experts and industrial partners. Mistra SafeChem provides a good platform for these collaborations.

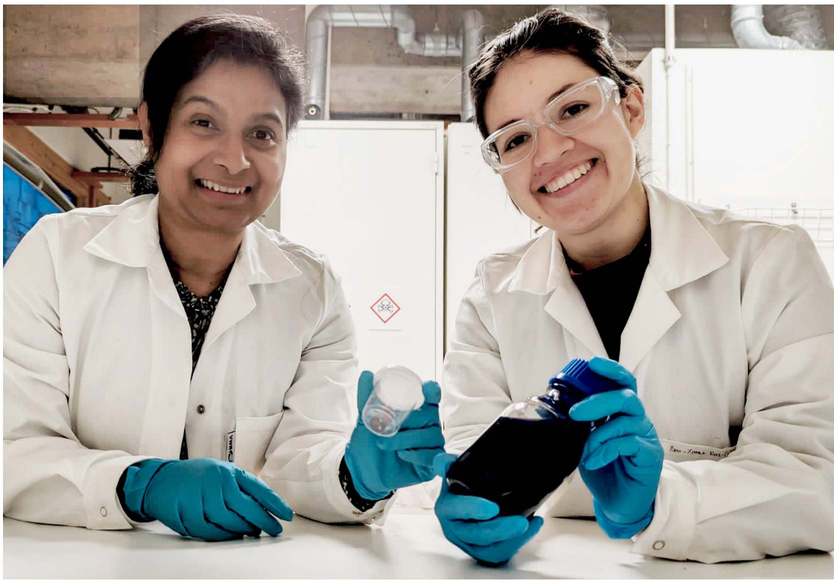


– So far, I have developed machine learning models for the prediction of mutagenicity, carcinogenicity, reproductive toxicity, skin sensitization, eye irritation and corrosion, as well as endocrine disruptions, Ziye Zheng says.

HIGHLIGHT FROM WP4: DESIGN AND MANAGEMENT OF CHEMICALS, MATERIALS AND PROCESSES

Successfully finding processes to recycle post-consumer textiles

Aji Mathew, Professor at Stockholm University, is finding solutions to upcycle used textiles of both cotton and synthetic fibres.



Aji Mathew (left) works with PhD student Maria-Ximena Ruiz-Caldas on developing sustainable processes for recycling post-consumer textiles.

What is the focus of your research?

The research focuses on upcycling of cotton in post-consumer textiles into high-value products such as nanocellulose. The processes also allow the recovery and use of non-cellulosic parts of the textiles, such as synthetic fibers.

Why are you doing this study?

The textile industry has one of the highest environmental impacts among industry sectors globally. As much as 63 percent of all textiles are made of fossil-based resources with high climate impact. 30 percent comes from cotton cultivation with water depletion, intensive use of pesticides and fertilizers and toxic air and water pollution during industrial processing. As a consequence, interest is growing from the textile and fashion industry, decision-makers and academia to reduce the negative social and environmental impacts of textiles.

How does the research of your group contribute to the Mistra SafeChem vision of a safe, sustainable and green chemical industry?

We look for solutions to upcycle and ”cascade use” textile waste into valuable additives and materials following the principles of green chemistry. The use of water-based reactions and the reduction of waste are some of the key guiding principles. We also contribute to sustainability by evaluating the chemical fate during the recycling process and finding solutions to improve the processes to decrease the chemical and carbon footprint.

What are the results?

We have successfully developed water-based processes using mineral acid and organic acids to convert cotton-based textiles into nanocellulose and recover non-cellulosic polymers such as polyester, acrylics, elastane etc.* The nanocellulose from textiles showed similar properties as conventional nanocellulose but also has colour originating from the dyes in the starting material. The project has contributed to a startup, CelluCircle AB, which can produce 3D printable materials from recycled cellulose.

How have you collaborated with others within Mistra SafeChem in your work?

We collaborate closely with the analytical chemistry team in work package 3 (Professor Ulrika Nilsson’s group) for non-targetted screening of the nanocellulose and the process water which provided new insight into the fate of chemicals as dyes during the process. The life cycle assessment team at RISE evaluated the environmental footprint of the process under work package 5 which provided useful feedback for process improvement and increased recycling of chemicals used in the process.

What further research is needed in this field?

We have to find a road map for utilizing the additives and polymers recovered from post-consumer textiles in high-value products and applications. The scalability of the developed processes needs to be evaluated. It is also important to evaluate the chemical and carbon footprint during upcycling and cascading use to ensure that the proposed road map is sustainable and safe.

* See Ruiz-Caldas et al, Scientific publications, WP4, page 22.

HIGHLIGHT FROM WP5: LIFE CYCLE ASSESSMENT AND MANAGEMENT

Bridging the worlds of digitalization and sustainability assessment

Kerstin von Borries, PhD student at DTU, is investigating machine learning tools to advance life cycle toxicity characterization and chemical substitution.

What is the focus of your research?

I focus on applying digitalization methods to advance assessment methods that quantify the toxicity impacts of chemicals emitted along entire material and product life cycles. This is essential to evaluate the impacts of chemicals in consumer products and industrial processes. Unfortunately, data are unavailable for millions of chemical-product combinations. To address this, my project focuses on exploring the potential of machine learning techniques to close the most relevant data gaps.

Why are you doing this project?

I want to contribute to reducing the impact of chemicals on humans and the environment. To find out where we can do it most effectively, we need to make assessments along the entire life cycle. But the lack of data makes it difficult. I see great potential in digital methods for more and faster assessments. The fact that I can combine my passion for both chemistry and data science in this project makes it simply a perfect fit for me.

How does this contribute to the vision of a safe, sustainable and green chemical industry?

To create a sustainable chemical industry, it is necessary to know what is sustainable. Life cycle based assessments can answer this without risking burden shifting between different types of impacts, locations, or life cycle stages. Digital tools can speed up the assessment process and allow assessing chemicals even before creating them. This will be essential in a *Safe and Sustainable by Design* approach for newly designed chemicals, materials, and products.

What are the main results of your work?

As we need to assess pretty much all of the roughly 350,000 chemicals on the global market, we want to evaluate how significant the potential of machine learning methods is. Based on our analysis, we can prioritize parameters where the scientific community should focus their efforts to develop machine learning methods that can provide predictions for chemicals that can currently not be characterized at all. We have also identified parameters where we need to generate more data to develop widely applicable models.

How have you collaborated within the programme?

Mistra SafeChem provides a great platform to exchange ideas across scientific disciplines and between academia and industrial partners. In the practical parts of my project, where I am developing my own models, we are tightening collaborations with the *in silico* experts from work package 3. Once the models are in place, the Mistra SafeChem case studies provide great opportunities to apply and test them in practice.

What further research is needed in this field?

The lack of chemical data will require research to extract information by, for example, automatic data curation, optimizing algorithm performance, and creating informative predictors. Another major field will be how to use new approach methods for data generation and integrate them into the assessment frameworks. Based on such research, life cycle based assessments will become more robust, cover a wider range of real-life chemicals and products, and ultimately help move toward a sustainable chemical industry.

Kerstin von Borries, Technical University of Denmark, can combine her passion for both chemistry and data science in this project.

HIGHLIGHT FROM WP6: CASE STUDIES

Promising findings of alternatives to silicones and siloxanes in cosmetics

Lisa Skedung, RISE, is leading a case study about silicones and siloxanes in cosmetics which can be considered an alternatives assessment and substitution case.

Lisa Skedung and her case study partners have found over 170 possible alternatives to silicones and siloxanes in cosmetics, and have narrowed them down to about 30 for further assessment.

What is the focus of your case study?

The first part of the study has been to better understand the concerns with silicones considering production, use phase and end-of-life by doing a qualitative life-cycle mapping. We are now applying an SSbD approach (*Safe and Sustainable by Design*) to evaluate possible alternatives to silicones in selected cosmetic products, where the assessment tools from Mistra SafeChem are used.

Why are you doing this study?

Silicones provide unique functions in cosmetics. But some of them, such as cyclic siloxanes, have been raised as a possible concern due to exhibiting PBT properties (persistent, bioaccumulative and toxic). The cyclic siloxane D4 is prohibited in all cosmetic products and the use of D5 in wash-off cosmetic products shall not be greater than 0.1 percent by weight. The European Chemicals Agency is planning to further restrict the use of D5 and D6. Cyclic siloxanes can be used either as such or as precursors to a wide range of linear, branched and crosslinked silicones that are all widely used in cosmetics and personal care products.

How does your research contribute to the Mistra SafeChem vision of a safe, sustainable and green chemical industry?

While we are trying to find safer and more sustainable alternatives, we also want to contribute to developing a methodology to assess the safety and environmental impact of ingredients and formulations early on in the design phase. We do that by considering a life cycle perspective, where the proposed SSbD approach is used as inspiration.

What are the results?

So far, we have found over 170 possible alternatives that could theoretically deliver relevant functions. They have been narrowed down to about 30 prioritised substances after a first hazard screening. We have also summarised concerns about siloxanes and silicones from a health and environmental perspective in an internal report. In summary, the production of silicones is energy-demanding and an ozone-depleting substance is emitted. Cyclic siloxanes have shown some toxicity potential where the main exposure from cosmetics is through the skin or inhalation. Silicones are potentially bioaccumulative in the environment and very persistent under certain conditions.

How have you collaborated within Mistra SafeChem in your case study?

We have a strong collaboration between work packages 3, 5 and 6 and with the industry partner H&M.

What further research is needed in this field?

We are now in the process of further assessing the safety of prioritised alternatives with tools from Mistra SafeChem such as predictions of human toxicity, skin sensitization, eye irritation, bioaccumulation, biodegradation and assessment of what degradation products may be formed in the environment. The alternatives will be benchmarked against silicones and an LCA will be performed on the most promising alternatives. Performance testing of ingredients and simple formulations will also be done to ensure similar functions, such as good spreadability and a smooth, non-tacky, non-greasy feel.

RESEARCH STUDENTS:

Major contributors to the work of Mistra SafeChem

Research students make major contributions to the work of Mistra SafeChem. Their areas of expertise range from organic chemistry, inorganic chemistry and ecotoxicology to environmental chemistry, life cycle assessment and programming.

Many PhD students and post-docs are working in the programme. Here you can learn more about most of the persons engaged in the research student group of Mistra SafeChem.

Cedric Abele, PhD student

Stockholm University, Department of Environmental Sciences, and SciLifeLab. **Supervisor:** Oskar Karlsson. **WP connection:** WP3.

Project: Multiplexed high-content screening of chemical toxicity in aquatic test organisms.

I am aiming for an image-based high-content screening method to assess the toxicity of newly designed chemicals, using *Daphnia magna* as a model organism. The application of molecular dyes combined with fluorescence microscopy and image analysis software provides information about the health status of the organism and consequently the toxicity of the test compound. This will be used to get a better understanding of toxic mechanisms within an organism.

Background: Bachelor in environmental sciences, master in ecotoxicology (both in Germany). Applied fluorescence microscopy during master's project at Environmental Research Center (UFZ), Leipzig.

Kerstin von Borries, PhD student

Technical University of Denmark, Department of Environmental and Resource Engineering. **Supervisor:** Peter Fantke. **WP connection:** WP5, WP3.

Project: The aim of my PhD project is to contribute to introducing different digitalization and machine learning tools in order to advance the fields of life cycle toxicity characterization and chemical substitution in different industrial product and process applications.

Background: Environmental engineer with a focus on environmental chemistry and a passion for data science. My PhD project combines these aspects by exploring the use of machine learning and other digital tools to support the sustainability assessment of chemicals, focusing on toxicity and ecotoxicity impacts.

Josefine Carlsson, PhD student

Stockholm University, Department of Materials and Environmental Chemistry. **Supervisor:** Ulrika Nilsson. **WP connection:** WP3.

Project: The aim is to develop analytical methods for skin-close garments, such as a greener screening method, based on thermal desorption of the garments and online connection to a gas chromatograph/mass spectrometry. Chemicals migration from textiles and their potential for causing health effects will be investigated. Peptide reactivity assays will identify possible protein-reactive species in garments, using commercially available reconstructed human epidermis and a bottom-up proteomic approach, which might lead to the discovery of skin peptide adducts.

Background: Bachelor in chemistry and master's degree in analytical chemistry, Stockholm University. Diploma thesis in the division of analytical chemistry.

Joy Ngozi Onwumere, PhD student

Stockholm University. **Supervisor:** Adam Slabon. **WP connection:** WP4.

Project: Development of photoactive hybrid materials for efficient removal of pollutants.

Since it is a "green" technology for converting water into hydrogen and oxygen, inactivating viruses, and/or eliminating all types of contaminants under the illumination of sunlight, semiconductor photocatalysis has garnered much attention.

Background: A background in materials chemistry. My research focuses on photocatalysis and the synthesis of semiconductors. Interested in the removal of pollutants from the wastewater as water bodies have been contaminated by industrialisation.

Amira Pérez Liñán, PhD student

Stockholm University, Department of Environmental Science. **Supervisor:** Magnus Breitholtz. **WP connection:** WP3.

Project: High content screening as a tool to predict adverse effects on growth and reproduction in *Daphnia magna*.

The overall aim is to develop high content screening (HCS) as a tool that can be used to estimate the hazard properties of chemicals and to predict adverse ecotoxicological effects on growth and reproduction in *Daphnia*. The objective is to establish a staining toolbox for images based on HCS and help to apply HCS in *Daphnia magna* to visualize and detect the toxicity effect of chemicals of industrial interest.

Background: Biologist specialising in molecular and cell biology, MSc in Integrated water management. Interested in the emerging pollutants, how anthropogenic activity is impacting the aquatic ecosystem and in developing risk assessments.

May Britt Rian, PhD student

Stockholm University, Department of Environmental Science, SciLifeLab. **Supervisor:** Jonathan Martin. **WP connection:** WP3.

Project: Nontarget analysis of organic micropollutants in Swedish waters.

We are developing workflows for the analysis of polar and semi-polar organic micropollutants in various water matrices. We combine liquid chromatography and high-resolution mass spectrometry with computational tools for molecular characterizations. The methods will be applied for nontarget analysis of organic micropollutants in groundwaters, surface waters, drinking waters, and wastewaters, collected with a wide geographical distribution within Sweden.

Background: Master's degree in environmental analytical chemistry and teacher education from the Norwegian University of Science and Technology. Research interests: environmental pollution, analytical chemistry and chemometrics.

Maria-Ximena Ruiz-Caldas, PhD student

Stockholm University, Department of Materials and Environmental Chemistry. **Supervisor:** Aji Mathew. **WP connection:** Mainly WP4.

Project: Valorization of post-consumer cotton fabrics into cellulose nanocrystals.

We aim to develop scalable routes to generate high-added value chemicals and nanostructures from post-consumer cotton fabrics. These routes will be based on the principles of green chemistry and aim to minimize the waste and generation of toxic chemicals.

Background: Chemical engineer from Colombia. Master's degree in chemical engineering at McMaster University, Canada, where I studied the application of cellulose nanomaterials as colloidal stabilizers for metallic nanoparticles. Research interests: polymer chemistry, surface and interface science, and the synthesis and functionalization of nanomaterials.

Elisabeth Söderberg, PhD student

KTH, Division of Coating Technology. **Supervisor:** Per-Olof Syrén. **WP connection:** WP4, WP3, WP5.

Project: Safe and sustainable by design by biocatalytic amide-bond coupling.

We have analysed thousands of potential starting materials with *in silico* tools. A pool of safe building blocks for amide bond synthesis was generated, whose structures we have matched against known accepted substrates of characterized amide bond synthesizing enzymes. Thus, we could select the most suitable starting family of biocatalysts for the targeted transformation. Bioinformatic tools have improved the enzyme's thermostability and substrate promiscuity.

Background: Civil engineer in biotechnology, Uppsala University.

Pedro Tortajada, PhD student

Stockholm University, Department of Organic Chemistry. **Supervisor:** Belén Martín-Matute. **WP connection:** WP4, also WP5 and WP3.

Project: Development of greener synthetic methodologies with transition-metal catalysts.

Hydrogenation frequently employs noble metal catalysts in combination with hydrogen gas. Our work presents an alternative method for the hydrogenation of alkenes: electrochemical conditions with nickel foam and water as proton sources. Environmental and hazard aspects are assessed to determine its potential in comparison with the traditional method using palladium on carbon and hydrogen gas.

Background: From Barcelona, Spain, where I did my bachelor's and master's studies.

Vu Duc Ha Phan, PhD student

Stockholm University, Department of Organic Cemistry. **Supervisor:** Belén Martín-Matute. **WP connection:** WP4.

Project: Using CO_2 as a one-carbon building block in organic synthesis.

Development of heterogeneous catalysts for conversion of CO_2 to value-added products.

Background: Chemical engineering, material science, organic chemistry.

Ziye Zheng, postdoc

Cytiva, in collaboration with RISE. **Supervisor:** Ismet Dorange, Cytiva. **WP connection:** WP3.

Project: Development of toxicity prediction toolbox.

The development of the toolbox will be based on machine learning models for selecting more sustainable chemical alternatives.

Background: Postdoc in computational chemistry. PhD in environmental chemistry.

Tim Åström, PhD student

Stockholm University, Materials and Environmental Chemistry. **Supervisor:** Ulrika Nilsson. **WP connection:** Mainly WP3, also WP4.

Project: Development of targeted and non-targeted screening tools to identify textile pollutants in clothing textiles, laundry waste and textile manufacturing processes.

We develop analytical methods for textile pollutants with toxic effects or suspected impacts. We have identified several hundred, such as azo dyes, possibly mutagenic and allergenic arylamines and the carcinogen quinoline. I also develop a fast and solvent-free screening method for semivolatile pollutants in textiles.

Background: Got interested in chemistry in high-school. As a PhD student, I can contribute to a better society for people worldwide.

We asked a couple of the Mistra SafeChem industry partners why they decided to join the programme.

MISTRA SAFECHEM INDUSTRY PARTNER

EnginZyme

We at EnginZyme have the ambition to play a crucial role in tackling climate change by enabling new enzyme technologies in existing industrial infrastructure and thereby disrupting unsustainable chemical markets. We strive to produce low-cost and green chemistry products by replacing traditional fossil-based manufacturing with cell-free synthetic biology.

EnginZyme, who joined the programme in 2022, is eager to collaborate with the members of Mistra SafeChem, where we see synergies with their technology and opportunities to apply green and efficient solutions.

We hope our participation will lead to fruitful combinations of the academic and industrial expertise in Mistra SafeChem, and thereby to significant contributions to the green chemistry field.

Karim Engelmark Cassimjee
CEO and co-founder, EnginZyme

MISTRA SAFECHEM INDUSTRY PARTNER

H&M

H&M Group is committed to making fashion and design accessible to the many, in a way that is good for people, the planet, our industry and our business. With the aim of reducing our impact on the environment, we have set a goal for all our materials to be either recycled or sourced in a more sustainable way by 2030. Our main product offerings are apparel and textiles, but cosmetics are also a significant product category for our customers.

Mistra SafeChem is one of the cooperations we take part in to work towards our goals for our cosmetic products. It is important to identify and understand the environmental impact of cosmetic ingredients, such as silicones.

Currently, there are regulatory restrictions on cyclic siloxanes, but our attention was drawn also to other silicones which are widely used as ingredients due to their superior functional properties. For this reason, we need to have a good understanding of their potential environmental risks.

Mistra SafeChem is a good platform for gathering different experts in the field and understanding the environmental properties of silicones. Life cycle assessment of identified sustainable alternatives is also an important part of the project, and H&M Group sees the opportunities to develop and apply these tools for other cosmetic ingredients.

Haiyan Chen Gällstedt
Global Product Compliance Specialist,
Cosmetic & Chemical Products,
H&M

KEY ACHIEVEMENTS IN 2022: WORK PACKAGE 2

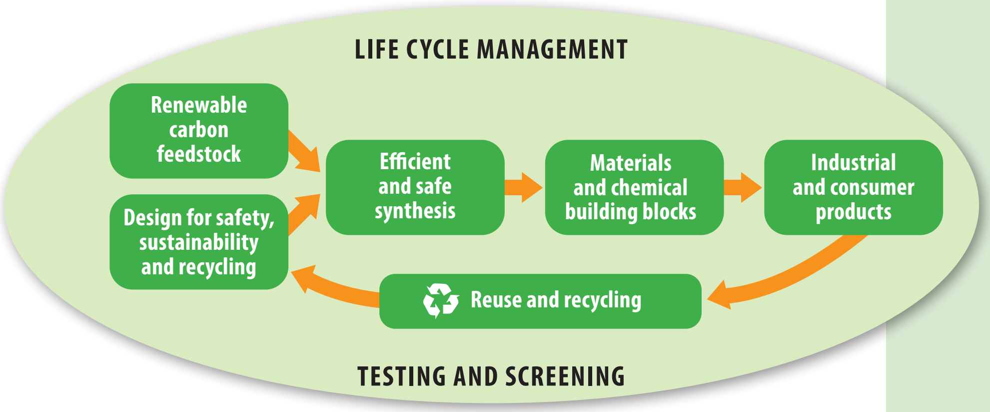
A vision and agenda for green and sustainable chemistry

● A compilation of information on the Swedish chemical industry, data on import, export and use of selected chemicals as well as interviews with representatives of the chemical industry has been made. This information is used to formulate opportunities and obstacles to enable a green and sustainable chemistry.

● A policy lab approach has been used to evaluate the industry's views and response to new regulatory initiatives on hazardous chemicals in complex products.

● The Mistra SafeChem symposium on green and sustainable chemistry was arranged at AstraZeneca, Mölndal, on September 26.

● The Master's Program in Sustainable Chemistry at Stockholm University completed its first full curriculum for first- and second-years students in 2022. Teachers from the departments of Materials and Environmental Chemistry, Organic Chemistry and Environmental Science at Stockholm University and from IVL Swedish Environmental Research Institute contribute to the programme.



A simple concept for safe, sustainable and green chemistry. It is also a framework to illustrate how the research performed in Mistra SafeChem contributes to that and a foundation for formulating a vision and agenda for green and sustainable chemistry in Sweden.

FACTS ABOUT WP2

Objectives

- To define a conceptual structure for green chemistry in Sweden.
- To assess opportunities and obstacles in markets and policies for expanding green chemistry in Sweden.
- To identify and assess novel evaluation criteria in the legal framework.
- To create a vision and agenda for green chemistry in Sweden.
- To prepare for establishment of a permanent platform for research and implementation of green chemistry.
- Competence development, education and communication.

Participants

AstraZeneca, IKEM, IVL Swedish Environmental Research Institute, KTH, Perstorp, RISE, Stockholm University and Volvo Cars.

WP leaders

John Munthe, IVL Swedish Environmental Research Institute

Lennart Bergström, Stockholm University

KEY ACHIEVEMENTS IN 2022: WORK PACKAGE 3

Hazard and risk screening – early warning and proactivity

In silico tools

● Traditional machine learning, deep learning transfer and AI-based (artificial intelligence) approaches now give wide operational coverage of important physical-chemistry properties and hazards such as carcinogenicity, mutagenicity and reprotoxicity, eye irritation, skin sensitization, hormone disruption and fate. During 2022 the methods have been adapted to include uncertainty quantification and toxicophore identification. Two dashboard interfaces are now in use and training of programme partners has been initiated.

● *In silico* predictive support to prioritization/alternatives assessments in ongoing case studies is exemplified by the selection of safe chemicals for enzymatic amide synthesis and alternatives identification in the siloxane case study. A new case study with Perstorp has started using *in silico*-based compound hazard profiling and potential Classification, Labelling and Packaging (CLP, H-phrase) classification for REACH.

● Interactions with work package 5 has been intensified, both in terms of the flow of digital information from hazard screening to the digital LCA tools, as well as in specific case study work with Renfuel.

In vitro tools

● Ecotoxicological testing in *Daphnia magna* is now operational. Methods for mutagenesis screening, Ames-test, and a variety of human toxicological endpoints using cell painting are near to operational. Initial use of *in vitro* models in the siloxane and textile processing case studies is being planned.

Analytical chemistry tools

● Tools for prediction of biodegradation and transformation have been developed, validated and applied to alternatives assessment in plasticizer and siloxane case studies.

● A suspect screening workflow for upcycling of textiles has been established (SU), including both a new, solvent free automated thermal desorption GC/MS method and LC/HRMS. Information on chemical identity (and quantity where possible) has been integrated into ongoing alternatives assessments, with a particular focus on carcinogenicity, mutagenicity and reprotoxicity and skin sensitization hazards feeding into risk and LCA analyses.

● A nontarget screening tool for organic micropollutants in water has been developed. The methods link screening protocols and suspect identification with computational hazard tools to greatly facilitate digital information flow into alternative assessments and will be offered sustainably through the National Facility for Exposomics at SciLifeLab.

Defined approach

● Workflows integrating Mistra SafeChem *in silico* and *in vitro* tools into defined approaches for various hazards of regulatory significance are being defined.

FACTS ABOUT WP3

Objectives

WP3 will construct and maintain a framework of capabilities and competencies providing a workflow moving through the following steps:

• Initial mitigation planning for hazard identification, exposure estimations and risk assessment, from both the human and environmental perspectives.

• *In silico* screening of available human and ecotoxicological/environmental fate data, read-across data by structural QSAR (quantitative structure-activity relationship) and application of other predictive computational toxicological tools.

• *In vitro* screening for critical human and ecotoxicological adversities relevant for risk assessment, including for combinatorial exposures.

• Development and application of analytical methodologies and techniques, including non-target analyses of exposures and bio-stability, particularly from the ecosystem perspective.

• Integrated hazard and risk assessments which are fit for purpose in appropriate material/process developments and case studies.

Participants

AstraZeneca, ChemSec, Cytiva, IVL Swedish Environmental Research Institute, RISE, Stockholm University. Four PhD students and one postdoc.

WP leaders

Ian A Cotgreave, RISE

Magnus Breitholtz, Stockholm University

KEY ACHIEVEMENTS IN 2022: WORK PACKAGE 4

Design and management of chemicals, materials and processes

● On the design of sustainable by design catalytic processes towards zero waste:

- A carbon-hydrogen amination method was developed using high-throughput experimentation. The miniaturization to a nanomolar scale enabled sustainable screening with decreased material consumption.
- A method to access non-natural chiral amino acids, important as small-molecule drugs or in peptide therapeutics, using a recyclable iridium catalyst, was disclosed. Quantitative yields were obtained, thus having an outstanding atom economy.
- A highly selective method to prepare enantiomerically pure allenes, important motifs in biologically active compounds by a first-row catalyst (nanocopper on microcrystalline cellulose) was developed.
- Electrochemical methods were developed for the direct use of CO_2 as a one-carbon synthon for synthetic organic chemistry, biomimetic electrochemical oxidation, and reduction of organic compounds using a nickel catalyst and water as the H_2 source. In collaboration with work packages 3 and 5, the latter reduction reaction was compared to the traditional reduction technique using H_2 gas and palladium on charcoal.
- Sequence-based protein engineering pipeline for the generation of biocatalysts with enhanced robustness was successfully developed and implemented in collaboration with work packages 3 and 5 that provided toxicity based screenings and basis for later LCA studies.
- Green chemoenzymatic routes to valorize biomass-derived molecules into added-value sustainable building blocks were generated.
- *Safe and Sustainable by Design* approach and a multidisciplinary collaboration have resulted in a set of building blocks that are safe from a toxicology point of view.

● On catalytic fractionation of forest residues and recycled textiles to generate materials and chemicals:

- Developed a value chain from beetle-infected spruce to textile fiber and biofuel, including a sustainability assessment by LCA.
- Developed a value chain from tops and branches to textile fiber and fuel.
- A new family of renewable thermosets was developed from Kraft lignin.
- Developed novel hydrolysis processes using organic acid for the recycling of cotton textiles to nanocellulose and performed LCA to identify hot spots in collaboration with work package 5.
- Developed a route to yield nanocellulose from recycled textiles with new surface chemistry and established methodologies to recover and recycle the chemicals used in the process.
- Non-targeted screening of process water to understand the fate of chemicals and potential toxicity. Collaboration with work package 3.
- Reductive electrochemical depolymerization of lignin was developed, opening the pathway for customised bio-derived molecules for either bio-based coatings or green substitutes for lubricant additives.

FACTS ABOUT WP4

Objectives

- Optimize material use, re-use and recycling for maximum benefits for resource efficiency and sustainability.
- Develop green chemistry industrial processes aiming at replacing/minimizing the use of toxic chemicals and minimizing waste.
- Rational design of first-row transition metal and enzyme catalysts, upscaling of green catalytic processes towards industrial scale.
- Development of methods to define and quantify resource efficiency and circularity of value chains.
- Providing data for evaluation and understanding toxicology determinants of the developed processes.

Participants

AC2T Research, AstraZeneca, Holmen, Krahnen, KTH, Perstorp, RenFuel, Stockholm University, Wargön Innovation.
Six PhD students and four postdocs.

WP leaders

Belén Martin-Matute, Stockholm University

Per-Olof Syrén, KTH

KEY ACHIEVEMENTS IN 2022: WORK PACKAGE 5

Life cycle assessment and management

● Further development of the life cycle based chemicals assessment toolbox:

- Following the methodological framework and global recommendations for advancing near-field/far-field exposure and human toxicity characterization,[1] USEtox has been developed and made available as beta-stage version 3, which can be accessed at usetox.org.
- A methodological framework and global recommendations have been developed for advancing USEtox for characterizing freshwater ecotoxicity impacts of chemical emissions and chemicals in products.[2]
- A ProScale case study on indoor wall paint to showcase the applicability of ProScale in product environmental footprint (PEF) was published (see Neuwirth et al. (2022), page 22).
- In collaboration with work package 3 an initial guidance for how to make possible ProScale assessments for new chemicals, not yet assessed under EU classification regulation, was developed, and tested by use of the work package 3 *in silico* toolbox.

● LCA experts in work package 5 have contributed to the transdisciplinary case studies in work packages 4 and 6:

- Cradle-to-gate screening LCAs were performed to assess the environmental impacts of processing routes to isolate cellulose nanocrystals (CNC) from post-consumer cotton and to hydrogenate alkenes over a nickel foam. In addition to the Environmental Footprint 3.0 impact assessment, the work package 5 toolbox was applied to assess indirect (far-field) exposure (USEtox 2.1) and direct exposure (ProScale). These screening LCA results are included in manuscripts intended for scientific publication. Prospective assessment in a theoretical case was reported by Appiah-Twum (2022), see page 23. We show how early screening LCA studies can be useful for understanding and improving the environmental performance of lab-scale routes, important information for potential future scale-up.
- Guidance on the inclusion of life cycle thinking was given in the two substitution case studies. Initial life cycle considerations were included by risk mapping covering production, use and end-of-life.

● The PhD project "Advancing life cycle based chemical toxicity characterization through digitalization":

- A prioritization framework has been developed to assess the potential of developing machine learning based approaches to fill input data-related gaps in human and ecosystem toxicity characterization.

● The life cycle based chemicals assessment toolbox was presented on several occasions, for example in Mistra SafeChem webinars.

FACTS ABOUT WP5

Objectives

- To develop and provide a life cycle based chemicals assessment toolbox.
- To develop a tool for high throughput alternatives assessment for chemical substitution.
- To develop a model fit-for-purpose for estimating near-field human exposure for different product application contexts for integration into life cycle assessment and alternatives assessment.
- To provide ProScale/ProScaleE and USEtox LCIA characterization factors for human toxicity and eco-toxicity for all case study relevant chemicals that are within the scope of the included methods.
- To build a database compiling all relevant information from LCA carried out from case studies.
- To deliver guidelines and training on how to apply life cycle approaches/assessment in case studies and along the design process.

Participants

AstraZeneca, BASF, Cytiva, DTU, IVL Swedish Environmental Research Institute, Perstorp, RISE, Volvo Cars. One PhD student.

WP leaders

Hanna Holmquist, IVL Swedish Environmental Research Institute

Anna-Karin Hellström, RISE

1. Fantke, P., W. A. Chiu, L. Aylward, R. Judson, L. Huang, S. Jang, T. Gouin, L. Rhomberg, N. Aurisano, T. McKone and O. Jolliet (2021). Exposure and Toxicity Characterization of Chemical Emissions and Chemicals in Products: Global Recommendations and Implementation in USEtox. *Int J Life Cycle Assess*, 26(5), 899-915.
2. Owsianiak, M., M. Z. Hauschild, L. Posthuma, E. Saouter, M. G. Vijver, T. Backhaus, M. Douziech, T. Schlekat and P. Fantke (2023). Ecotoxicity characterization of chemicals: Global recommendations and implementation in USEtox. *Chemosphere* 310: 136807

KEY ACHIEVEMENTS IN 2022: WORK PACKAGE 6

Case studies

In work package 6 of Mistra SafeChem, the tools and workflows developed in the other work packages are brought together and evaluated with the use of real scenario challenges. Feedback is collected on how they perform, how they match the needs of the industry and how they can be developed further

● In the case study on the indoor environment of cars, the focus has been on performing the first sampling campaign and analyzing the data, listing potential alternatives, collecting *in silico* data on the substances of interest, and planning the alternatives assessment using the LCAA (Life cycle based alternatives assessment) framework published by Fantke et al (2020).

● In the case study on personal care products, the focus has been on mapping possible alternatives to silicones. A list of over 170 alternatives has been screened for hazards using the suggested SSbD step 1 criteria (*Safe and Sustainable by Design*). Based on the screening results, 19 alternatives came out as safer and further screening using the *in silico* toolbox has been initiated. The qualitative life-cycle mapping showing the concerns with silicones from a health and environmental perspective has been summarized in an internal report.

● During the year the third large case study, focusing on the possibility of incorporating green chemistry and environmental assessment in the production scale-up of a specialty chemical, has started. A simulation model of a future production process has been made and the output from this model will now be linked to an LCA. By adjusting the production process in the simulation, change in LCA output can be recorded and an optimization of the process, based on minimizing the potential environmental impacts, can be made.

● The additional case studies developed with work package 4 have been rounded up. In most cases, they have achieved their purpose of being able to contribute to the work from work package 4 by adding additional components towards a sustainability assessment of the methods. Their results will be summarized in a short internal report that will be published in the first half of 2023. This report will also be part of the overall summary of work package 6.

● Aside from the case studies, work package 6 has focused on mapping the tools available within Mistra SafeChem and making those participating in the programme more aware of what each tool could be used for and who could be contacted for more support regarding a specific tool. This toolbox was presented both at breakfast seminars as well as at internal workshops.

FACTS ABOUT WP6

Objectives

- To coordinate the interaction between the case studies and the various tools and methods generated in WP3, WP4 and WP5.
- To transform industrial challenges into cases fit for the programme and for evaluation of the tools.
- To formulate the results from the case studies into general conclusions with respect to efficiency and reliability of the toolbox.

Participants

AstraZeneca, H&M, IVL Swedish Environmental Research Institute, KTH, Perstorp, RISE, Stockholm University, Volvo Cars.

WP leaders

Dämien Bolinius, IVL Swedish Environmental Research Institute

Lisa Skedung, RISE

SHORT FACTS

This is Mistra SafeChem

Organisation

The research programme is constituted by a consortium of six research partners and fourteen industry partners.

The consortium, funded by Mistra and the partners, is led by IVL Swedish Environmental Research Institute and reports to the Programme board.

Research partners

- International Chemical Secretariat (ChemSec)
- Technical University of Denmark (DTU)
- IVL Swedish Environmental Research Institute
- Royal School of Technology (KTH)
  Fibre and Polymer Technology
  SciLifeLab
- RISE Research Institutes of Sweden
- Stockholm University
  Department of Computer and System Sciences
  Department of Environmental Science
  Department of Materials and Environmental Chemistry
  Department of Organic Chemistry

Industry partners

- AC2T Research GmbH
- AstraZeneca
- BASF
- Cytiva
- EnginZyme
- Holmen
- H&M
- IKEM
- Krahnen GmbH
- Perstorp
- RenFuel
- Stockholm Vatten och Avlopp
- Volvo Cars
- Wargön Innovation

Running time

December 2019 – June 2024

Financier and budget

In total 103 MSEK

- 70 MSEK from Mistra
- 4.25 MSEK as cash contribution from industry partners
- 29 MSEK as in-kind contribution from research and industry partners

Work packages

- **WP1: Programme management, WP coordination and communication**

WP leaders:
Richard Lihammar, IVL Swedish Environmental Research Institute
Hanna Holmquist, IVL Swedish Environmental Research Institute

- **WP2: A vision and agenda for green and sustainable chemistry**

WP leaders:
John Munthe, IVL Swedish Environmental Research Institute
Lennart Bergström, Stockholm University

- **WP3: Hazard and risk screening – early warning and proactivity**

WP leaders:
Ian Cotgreave, RISE
Magnus Breitholtz/Jonathan Martin, Stockholm University

- **WP4: Design and management of chemicals, materials and processes**

WP leaders:
Belen Martín-Matute, Stockholm University
Per-Olof Syrén, KTH

- **WP5: Life cycle assessment and management**

WP leaders:
Hanna Holmquist, IVL Swedish Environmental Research Institute
Anna-Karin Hellström, RISE

- **WP6: Case studies**

WP leaders:
Dämien Bolinius, IVL Swedish Environmental Research Institute
Lisa Skedung, RISE

Programme board

Presented as standing in the picture to the right

Sara Brosché, Senior Advisor, IPEN (International Pollutants Eliminations Network)

Krister Holmberg, Professor Emeritus, Chalmers (Chair)

Anna Wiberg, Celluxtreme

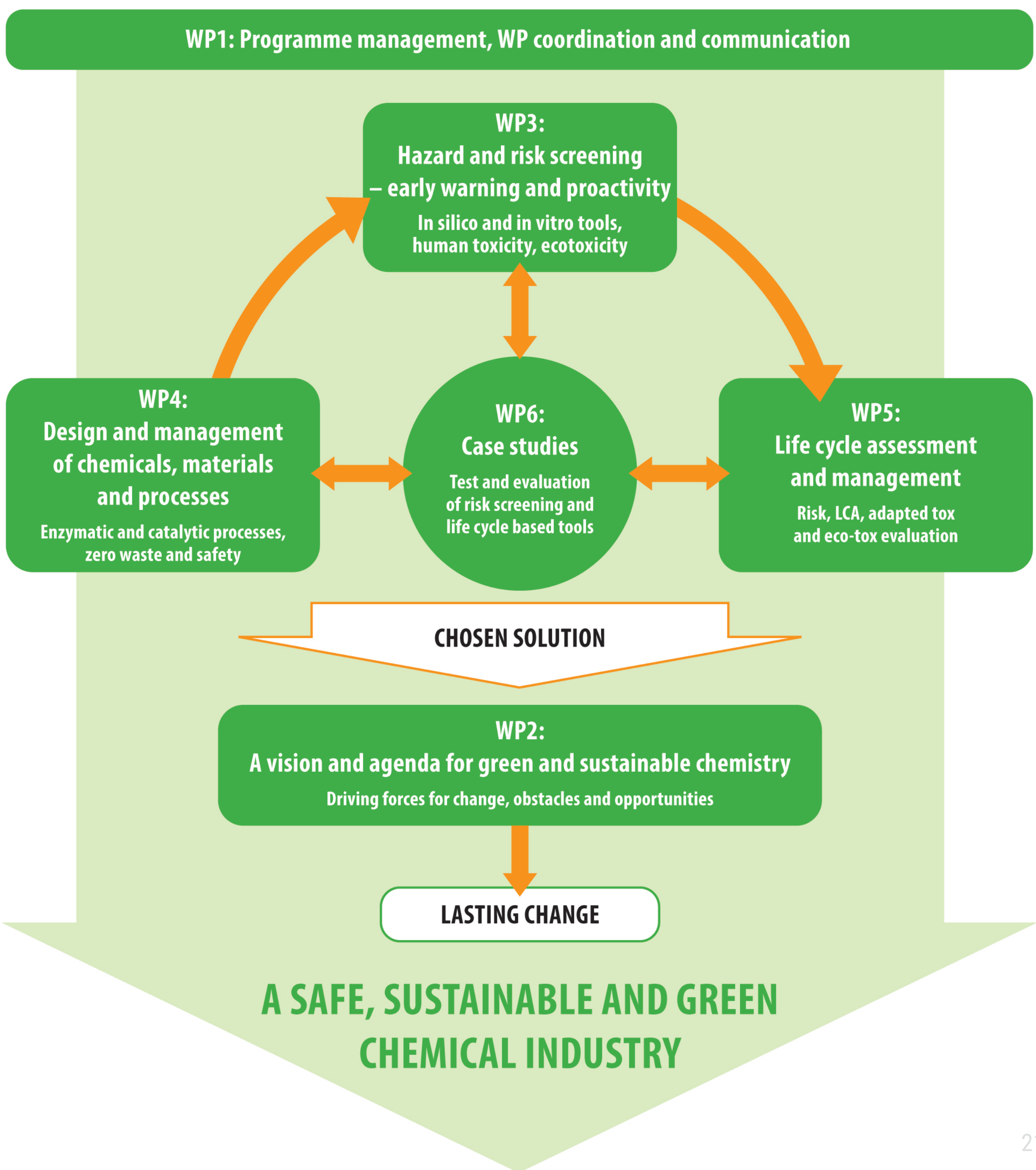
Per Ängquist, Director General, Swedish Chemicals Agency

Malin Lindgren, Programmes Director, Mistra (co-opted)

Patrik Andersson, Professor, Umeå University

ORGANISATION OF MISTRA SAFECHEM

WORK PACKAGES AND COOPERATION



DELIVERABLES 2022

You find links to all publications on the page Deliverables on our website mistrasafechem.se

SCIENTIFIC PUBLICATIONS

WP3: Hazard and risk screening – early warning and proactivity

Carlsson, J., Astrom, T., Ostman, C., & Nilsson, U. (2022). Disperse azo dyes, arylamines and halogenated dinitrobenzene compounds in synthetic garments on the Swedish market. *Contact Dermatitis*, 87, 315

Carlsson, J., Iadaresta, F., Eklund, J., Avagyan, R., Östman, C., & Nilsson, U. (2022). Suspect and non-target screening of chemicals in clothing textiles by reversed-phase liquid chromatography/hybrid quadrupole-Orbitrap mass spectrometry. *Analytical and Bioanalytical Chemistry,* 414, 1403

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Posevins, D., & Bäckvall, J.-E. (2022). Iron-catalyzed cross-couplings of propargylic substrates with Grignard reagents. *Journal of Organometallic Chemistry*, 964, 122304

Ruiz-Caldas, M.-X., Carlsson, J., Sadiktsis, I., Jaworski, A., Nilsson, U., Mathew, A. P. (2022) Cellulose Nanocrystals from Postconsumer Cotton and Blended Fabrics: A Study on Their Properties, Chemical Composition, and Process Efficiency. *ACS Sustainable Chemistry & Engineering* 2022 10, 3787

Valencia, M. S., Ruiz-Caldas, M.-X., Li, J., & Mathew, P. A. (2022). Cellulose nanocrystals (CNCs) derived from dyed and bleached cotton-based textile waste. *Current Applied Polymer Science*, 5, 1

Valiente, A., Martínez-Pardo, P., Kaur, G., Johansson, M. J., & Martín-Matute, B. (2022). Cover Feature: Electrochemical Proton Reduction over Nickel Foam for Z-Stereoselective Semihydrogenation/deuteration of Functionalized Alkynes. *ChemSusChem*, 15, e202102221

Valiente, A., Martínez-Pardo, P., Kaur, G., Johansson, M. J., & Martín-Matute, B. (2022). Electrochemical Proton Reduction over Nickel Foam for Z-Stereoselective Semihydrogenation/deuteration of Functionalized Alkynes. *ChemSusChem*, 15, e202102221

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WP5: Life cycle assessment and management

Aurisano, N., & Fantke, P. (2022). Semi-automated harmonization and selection of chemical data for risk and impact assessment. *Chemosphere,* 302, 134886

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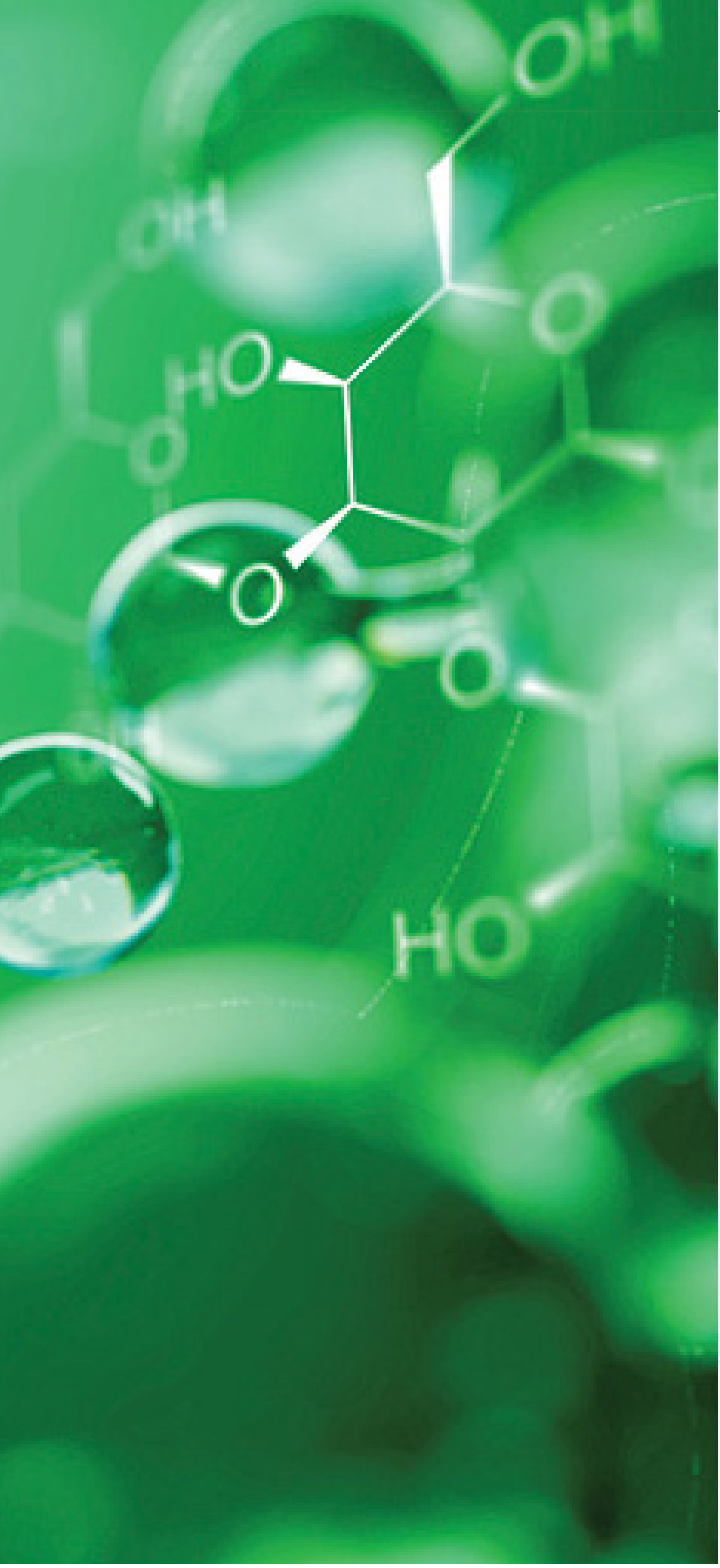

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Li, Z., Xiong, J., & Fantke, P. (2022). Screening of pesticide distributions in foods of animal origin: a matrix-based approach for biotransfer factor modeling of grazing mammals. *Environmental Science: Processes & Impacts*, 24, 609

Mainka, A., & Fantke, P. (2022). Preschool children health impacts from indoor exposure to PM2.5 and metals. *Environment International*, 160, 107062

REPORTS AND BRIEFS

Aji Mathew, Joseph Samec, Belén Martín-Matute, Jan-Erling Bäckvall, Per-Olof Syrén and Adam Slabon (2022). Chemical synthesis – half-time achievements and outlook

Josefin Neuwirth, Marie Gottfridsson, Tomas Rydberg and Lisa Hallberg (2022). A ProScale case study on indoor wall paint

PhD THESES

Erik Weis (2022) Iridium-Catalyzed C-H Activation Methods for Late-Stage Functionalization of Pharmaceuticals (Stockholm University, Department of Organic Chemistry)

Aitor Bermejo López (2022) Iridium-Catalyzed carbon-heteroatom bond forming reaction via hydrogen transfer. Method Development and Mechanistic elucidations (Stockholm University, Department of Organic Chemistry)

MASTER THESES

Appiah-Twum, H. (2022) Prospective Life Cycle Assessment of an Electrochemical Hydrogenation Process Over a Nickel Foam Cathode. (Uppsala University, Disciplinary Domain of Science and Technology, Earth Sciences, Department of Earth Sciences)

Salvador Aranibar (2022) Cellulose nanocrystals (CNCs) derived from dyed and bleached cotton-based textile waste through acid-catalysed hydrolysis (Stockholm University, Department of Materials and Environmental Chemistry)

Swarna Baddigham (2022) Use of cellulose nanocrystals from textile waste as support for iridium catalysts (Stockholm University, Department of Organic Chemistry and Department of Materials and Environmental Chemistry)

OUTREACH ACTIVITIES IN 2022

- Breakfast webinars:
  Sustainable chemistry – from catalysis to materials
  – February 8, 65 participants
  A life cycle based chemicals assessment toolbox
  – March 23, 95 participants
  Mistra SafeChem's toolbox in practice, highlights from case studies – May 24, 66 participants
- **The Mistra SafeChem symposium on green and sustainable chemistry** – September 26, AstraZeneca, 100 participants on-site, 150 online
- 40+ appearances at scientific conferences and meetings
- **Kemisk tidskrift** (the Swedish Chemical Journal) 4/2022: Interview with Programme Director Richard Lihammar

MISTRA SAFECHEM

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