

DATA SCIENCE

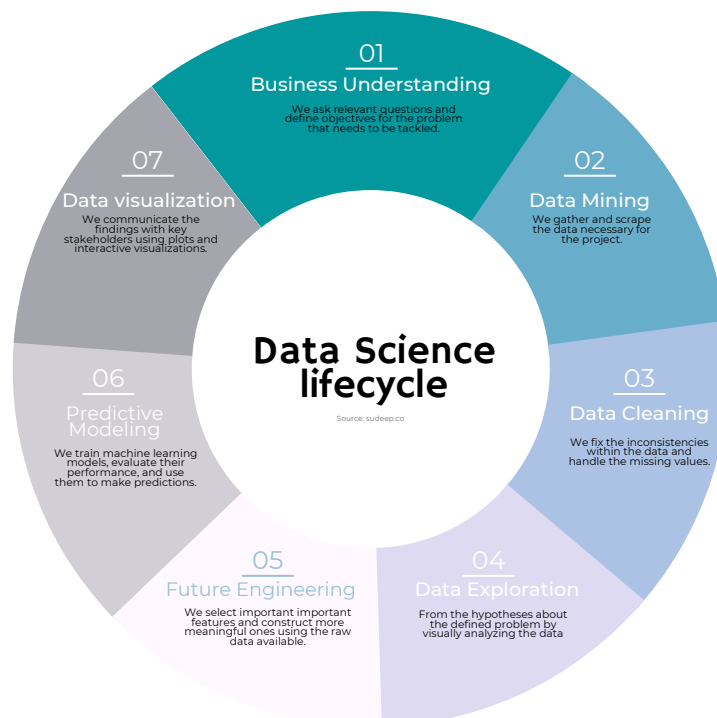
at SaferWorldbyDesign

Coordinated by: [EdelweissConnect](#)

Our packages are designed to support the early stage risk assessment of chemicals across a variety of concerns, such as systemic and organ toxicity, neurotoxicity, skin irritation and sensitization, endocrine disruption, and environmental endpoints. Our computational approach incorporates the following:

- Integrating data on physical and chemical properties such as solubility, reactivity, volatility, biodegradability etc.
- Integrating (eco)toxicological data from standardized or non-standardized tests.
- Integrated *in silico* approaches where we apply machine learning algorithms to evaluate compounds based on combinations of chemical and biological features
- Read across for a compound grouping (based on best practices as developed under EU-ToxRisk and interactions with OECD/ECHA).

Therefore, it is important to consider several main elements throughout the data processing workflow and to have a clear management of data and knowledge life cycle. This includes the definition of how the data should be structured; for example, data inputs can be defined over the input panels of a software application where it is made clear what data is necessary to be given as input to be able to further process it. There are several methods to import data and it has to be evaluated in each case what method should be used to be able to process it as efficiently as possible. Data can directly be processed by accessing it from a database or by importing it from a template file into the corresponding data analysis tools.



What is Data Science?

Data science is the science of data management based on computer science and mathematical, statistical, machine learning and artificial intelligence methods supporting the use of *in silico* approaches to guide decision making and strategic planning. We practice such approaches in the development of applications supporting product design, predictive toxicology and risk assessment.

A typical workflow we pursue consists of:



Data collection

During this step, data is collected. Data might be collected out of databases, documents, real time streaming or from ongoing research processes and exist in a lot of different formats including image files, raw data, processed data and results.



Data storage and processing

This step includes the processing of data by data management teams which set the standards for data storage. Data is stored in repositories where it can be organized, searched and accessed.



Data Analysis

During data analysis, data is retrieved from repositories and integrated with analysis procedures, machine learning, artificial intelligence and other algorithms so that it can be used for predictive modeling and risk assessment.



Reporting

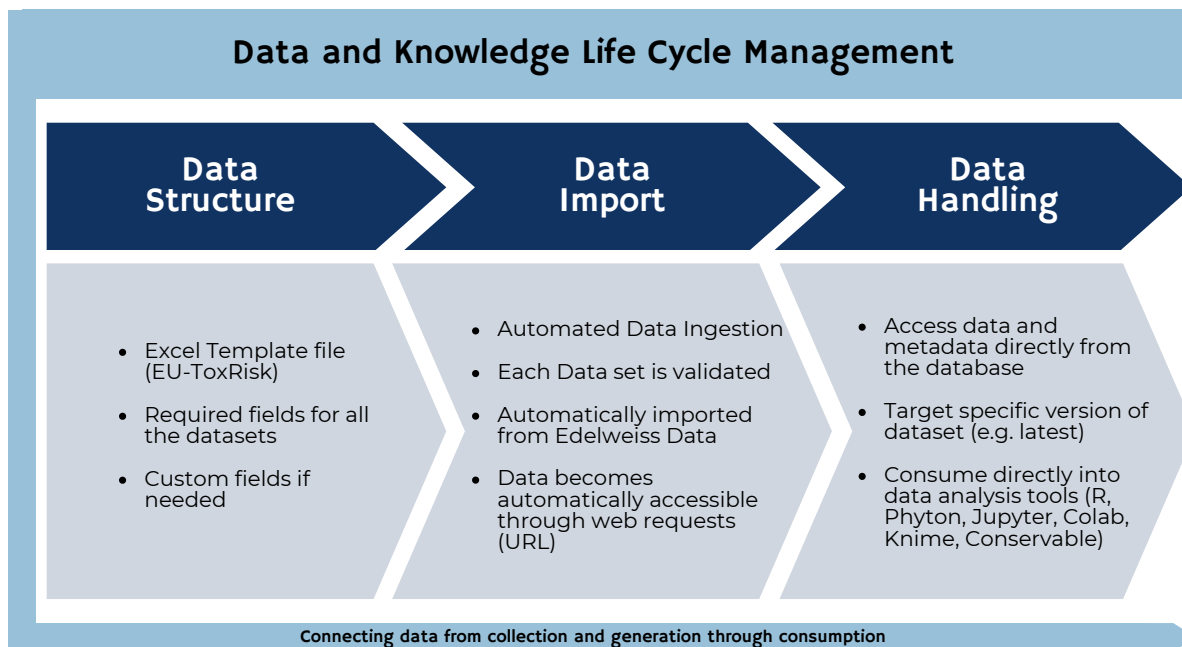
In the final step an analysis or assessment report is generated with explanations and visualization of the analysis supported by referenced protocols and data sources of high integrity.

Data Science constitutes the interface between three main pillars:
Domain knowledge, Computer Science and the applied mathematical aptitude.

- The domain knowledge includes features such as client requirements and the explanation of the technical concepts.
- The mathematical applications are the basics for understanding data science processes, building *in silico* models, the development of machine learning and deep learning algorithms and the description of the statistics needed to interpret the data.
- Computer science is the tool with which the domain knowledge and the mathematical methods are integrated to what we call data science.

Our Data Science Expertise

Our data management is driven by EdelweissData™. This approach organizes your data into a single location, which makes it easy to be found and used for various purposes: browsing, modelling and end-user applications. The graphic below shows an overview of our solutions and activities supporting the design and assessment of safer, greener products.



Source: EdelweissConnect, Barry Hardy, Slide 9, 2023.

EdelweissConnect

SaferWorldbyDesign excels in the field of Data Science by adopting a holistic approach that combines technical expertise with strategic thinking.

Along with our expert team of data scientists, we identify key data sources relevant to our clients to analyze and interpret the data. We use data analytics tools such as data visualization software, statistical analysis software, and machine learning platforms to identify patterns and trends that may signal potential risks present in formulations.

We also develop predictive models that use machine learning techniques to identify and mitigate potential chemical risks.

Similarly, we ensure robust data privacy measures to protect the sensitive information we collect from clients and other sources. We continuously review and refine our data science processes to ensure we are using the latest techniques and tools to generate insights for our clients.

SaferWorldbyDesign integrates data insights into the design of safer products and services. This approach helps our clients take appropriate actions to mitigate risks and make the world a safer place with better and safer products.



Applied to our integrated solutions

Application of our data services using our integrated solutions include:

**Safer Neuron**

The SaferNeuron is an application developed using advanced modeling techniques to analyze and predict how potential drugs interact with the brain's BBB (blood-brain barrier), helping to increase safety and effectiveness by identifying target and off-target interactions.

**Safer Skin**

The SaferSkin Solution is developed through data science using a technique called Bayesian Network-based IATAs to help determine the potency of potential skin irritants, ensuring that our clients' products are safe and effective for use on the skin.

**Safer Endocrine**

This solution uses advanced techniques like QSARs, species-distributions, and EATS models to assess the safety of potential endocrine disruptors, ensuring that our clients' products are free from harmful effects on hormone systems.

**Safer Liver**

SaferLiver is a comprehensive solution that uses techniques to construct and implement tiered strategies and models, helping to identify potential liver problems like cholestasis, steatosis, and DILI, ensuring our clients' products are safe and effective.

[Learn about other solutions](#)

Partner contributions

Our partners can provide you with a wide variety of services including computational toxicology, the most up-to-date in vitro assays, Toxicokinetic methods, consumer testing, and regulatory toxicology assessments.



We offer various solutions in collaboration with a broad range of expert knowledge partners to improve risk assessment processes. Our partners include organisations like Kreatis, IRFMN, Euclia, Maieutix, Multicase, Phenaris, SafeDose Ltd., SBX Corporation, SciLicium, The Vertex laboratories, Edelweiss Connect and EdelweissData Solutions.

These partners provide expertise in areas such as QSAR data modeling, computational predictive toxicology, multi-omics data analysis, machine learning, deep learning, and more. The solutions provided by these partners aim to develop predictive models, offer decision support, and provide innovative technologies to improve risk assessment processes.

By building on our expertise, we effectively search through existing databases, public knowledge sources and document repositories - a process that leads to safer, greener, and more coherent products.

Contact us



email



website



1-to-1 demo



webinar