

Eco-design of energetic materials

Romain Kerdoncuff - AI Project Manager - Alysophil

GTPS Technical days 2025

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REFRESHING THE
CHEMICAL INDUSTRY





INTELLIGENT FLOW CHEMISTRY

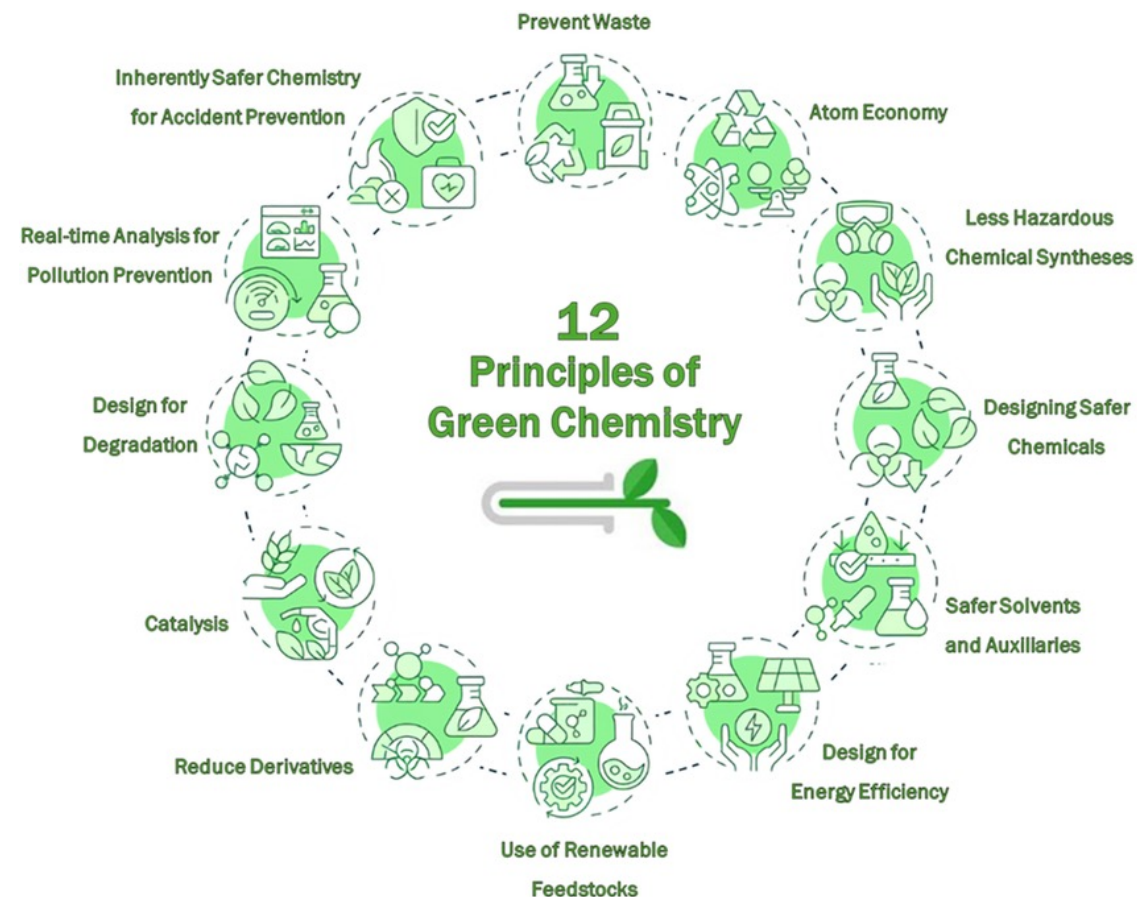
12 principles of Green Chemistry

Alysophil's goal is to help create chemistry that meets the challenges of the 21st century

The 12 principles bring together the main levers for action to develop more virtuous chemical syntheses

To meet these challenges, two major technologies are used side by side :

- Flow chemistry
- Artificial intelligence



Source: Mah et al., 2025, ChemSusChem

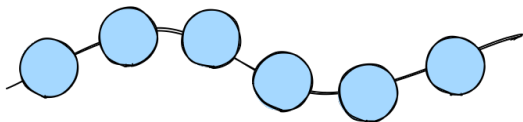
AI for efficient screening with increased novelty of energetic materials

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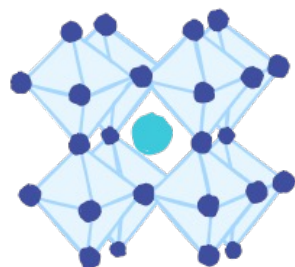
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INTELLIGENT FLOW CHEMISTRY

Starting point: Specifications

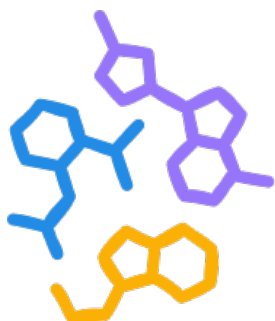
Polymers



Inorganic structures



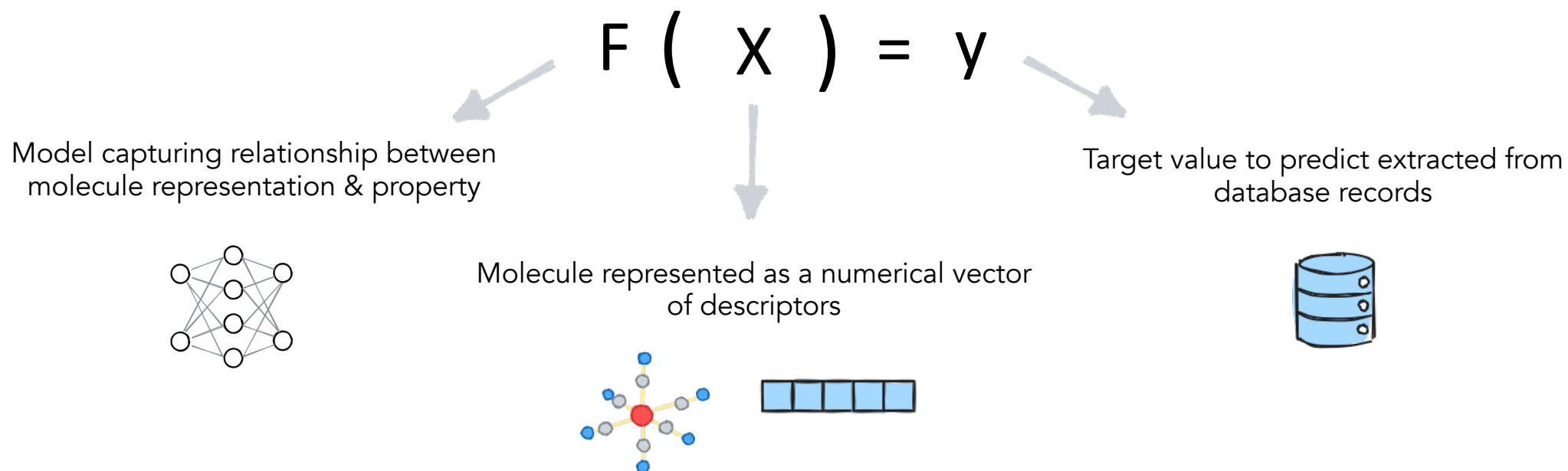
Organic molecules



- **Must Have**
 - Density
 - Pyrotechnic properties
 - ...
- **Nice to Have**
 - No CMR activities
 - ...
- **Bonus**
 - Bio-based materials
 - ...
- **No Go**
 - No halogens
 - ...

How to predict molecular properties

Quantitative Structure-Property Relationship (QSPR)

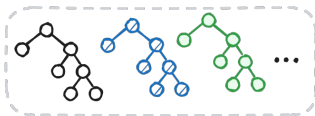


QSPR : details

$$F(x)=y$$

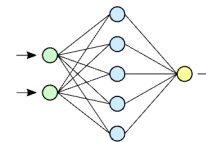
Models:

Machine Learning



or

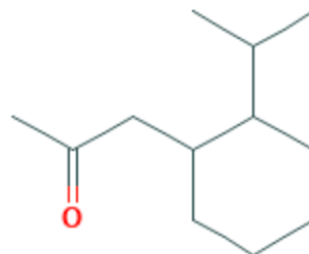
DeepLearning



$$F(x)=y$$

Descriptors:

- SMILES
- SELFIES
- Graphs
- Molecular properties
- Electronic distribution
- DFT-calculated descriptors
- Combinations of above



CC(=O)CC1CCCCC1C(C)C

MW	Ncarbon	Noxygen	Ncycles
182,3	12	1	1

$$F(x)=y$$

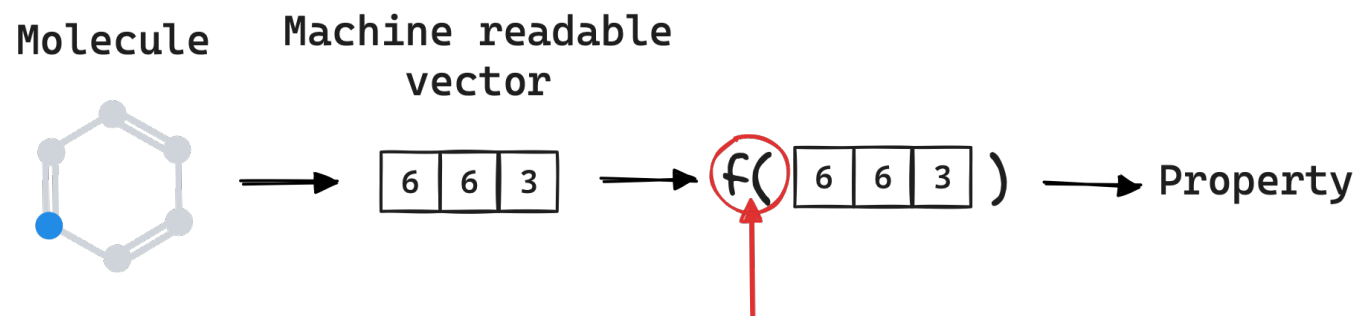
Experimental properties

Toxicity, Boiling Point, Sensitivity, etc...



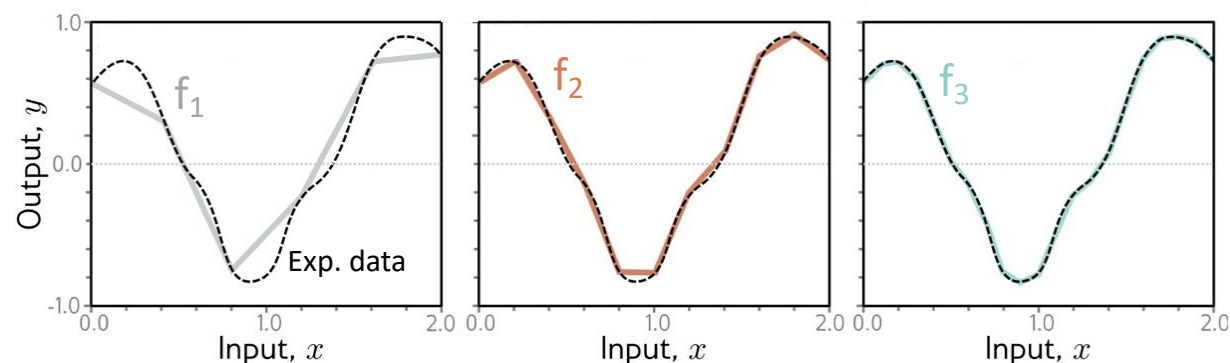
QSPR : Training process

AI models learn structure-property relationships through iterations



The algorithm will learn iteratively through the samples from the dataset to find the best estimation of the property from the structure

Here, the algorithm will propose a first estimation f_1 , then learn from mistakes to obtain f_2 , until it reaches f_3 where the property is perfectly modeled



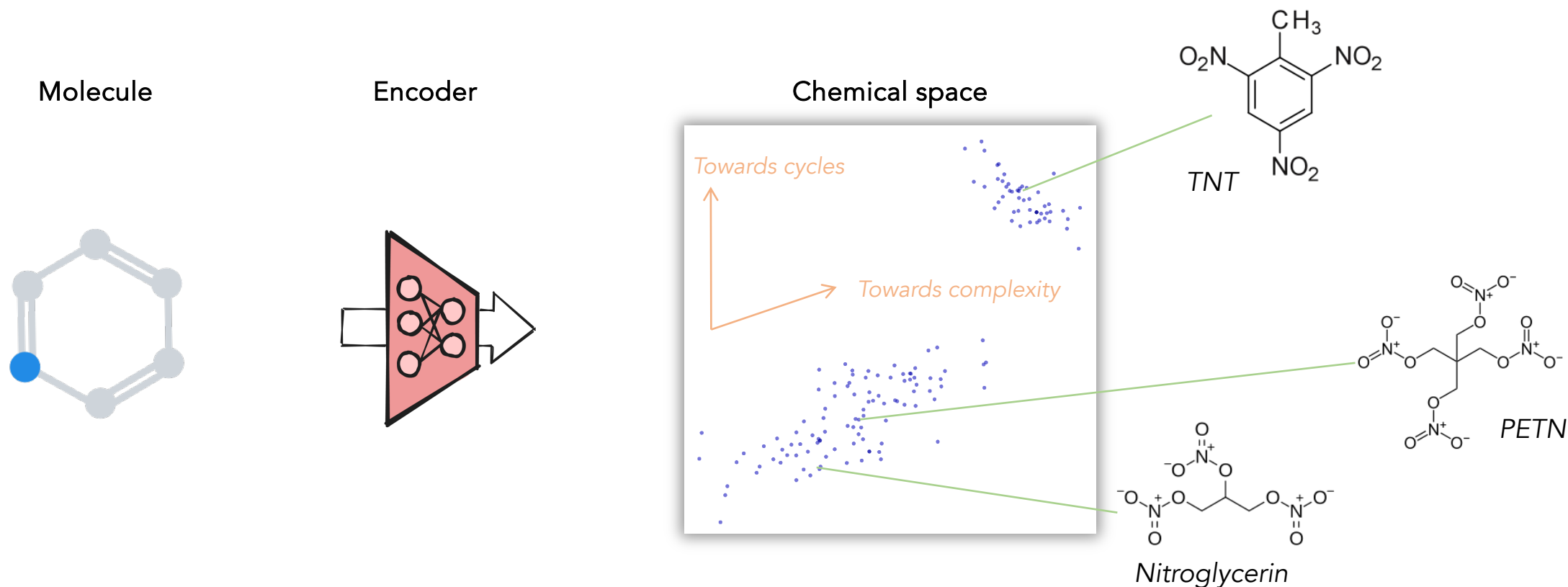
Simon J. D. Prince, Understanding Deep Learning, MIT Press, 2023

Finding new materials: Chemical Space

Through algorithms, a chemical space can be created

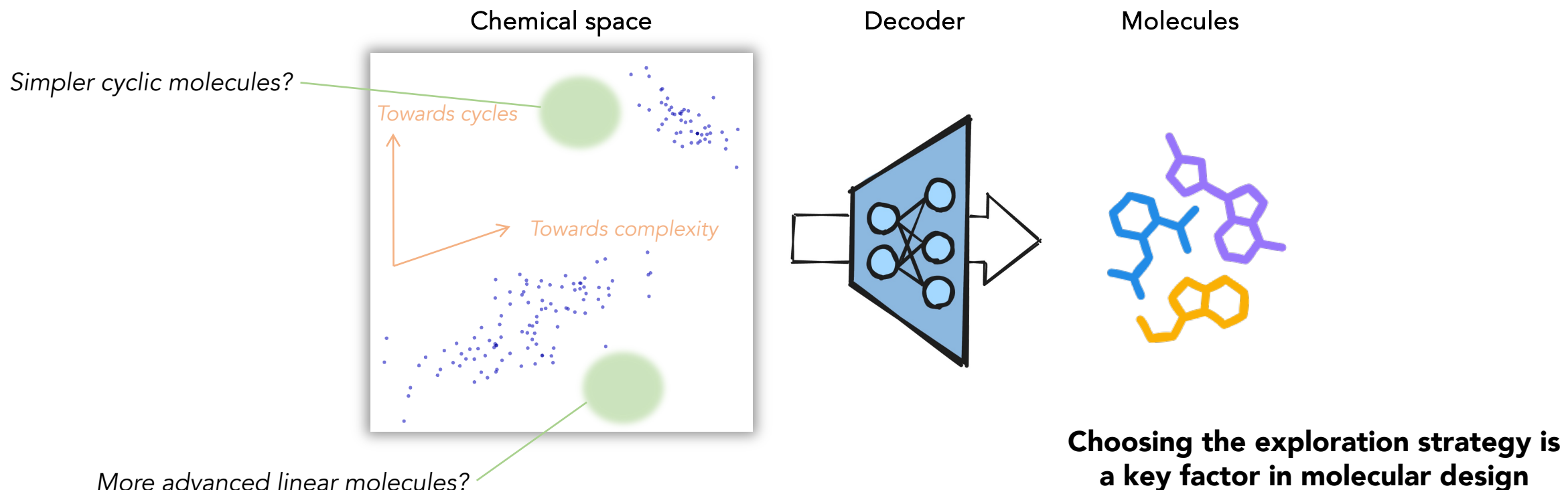
This multidimensional space embeds the diversity of chemical structure in a mathematical space

Similar molecules are located closely in the chemical space



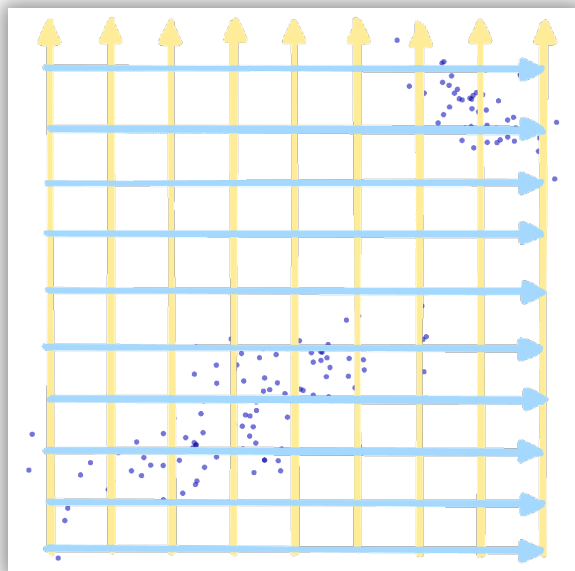
Exploration of the chemical space

The chemical space is continuous. One can generate molecules from any vector of this space, including from unexplored areas, leading to potentially unknown materials

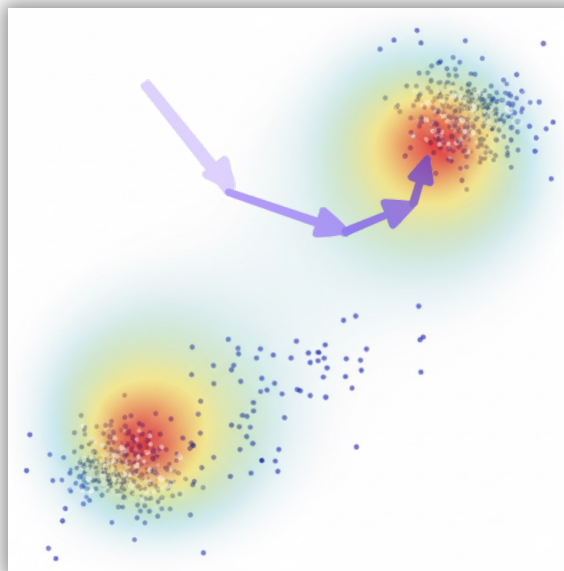


Exploration strategies

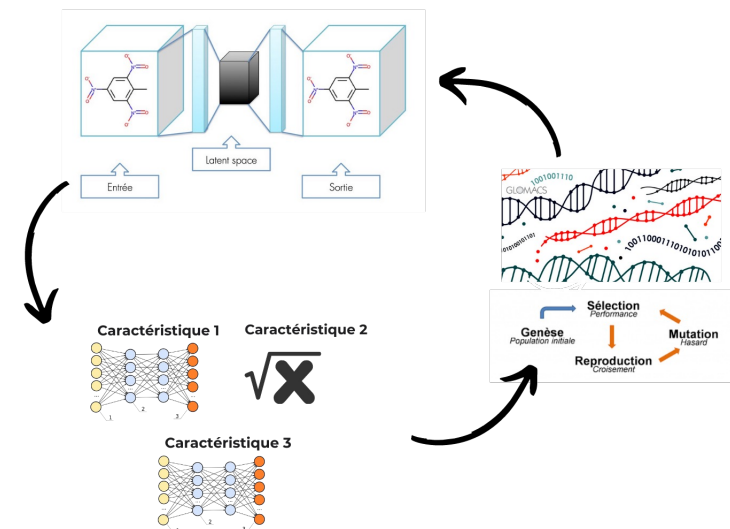
Grid search strategy



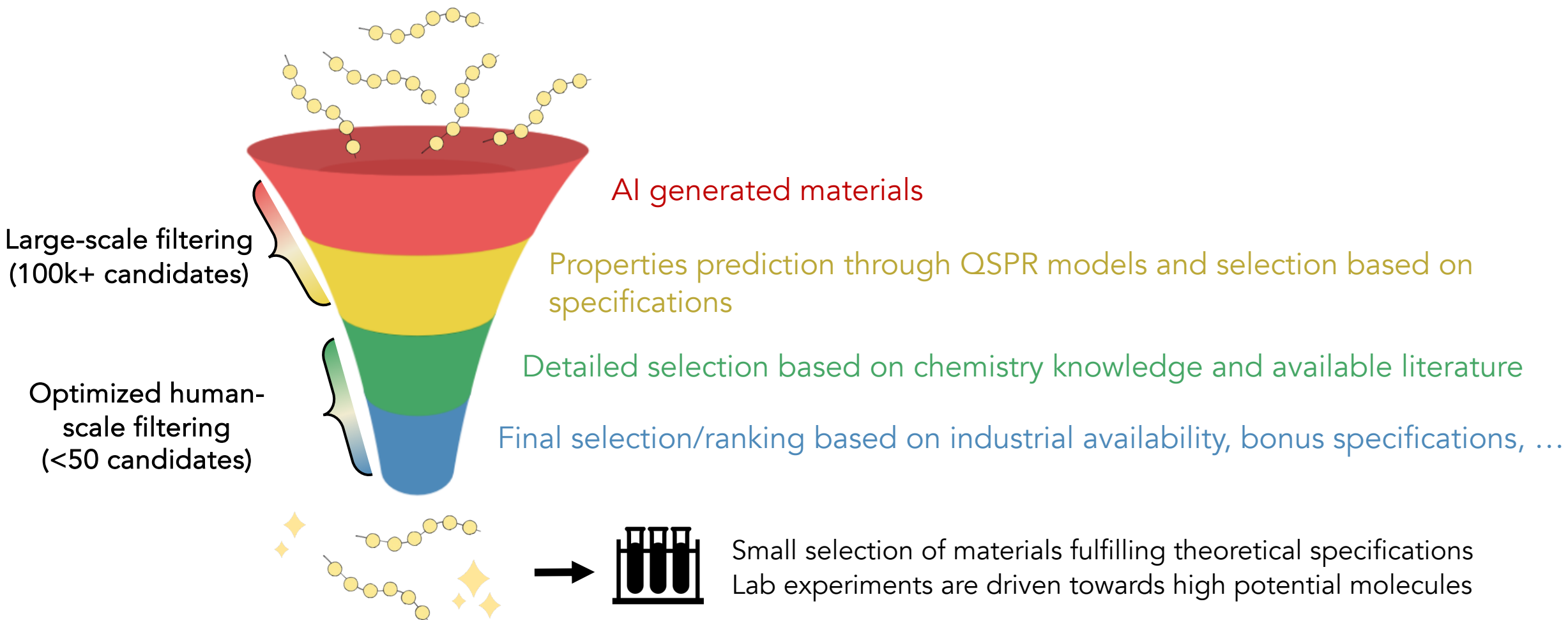
Simple conditional exploration



Genetic algorithm



Selection of the best candidates



Unique selling point



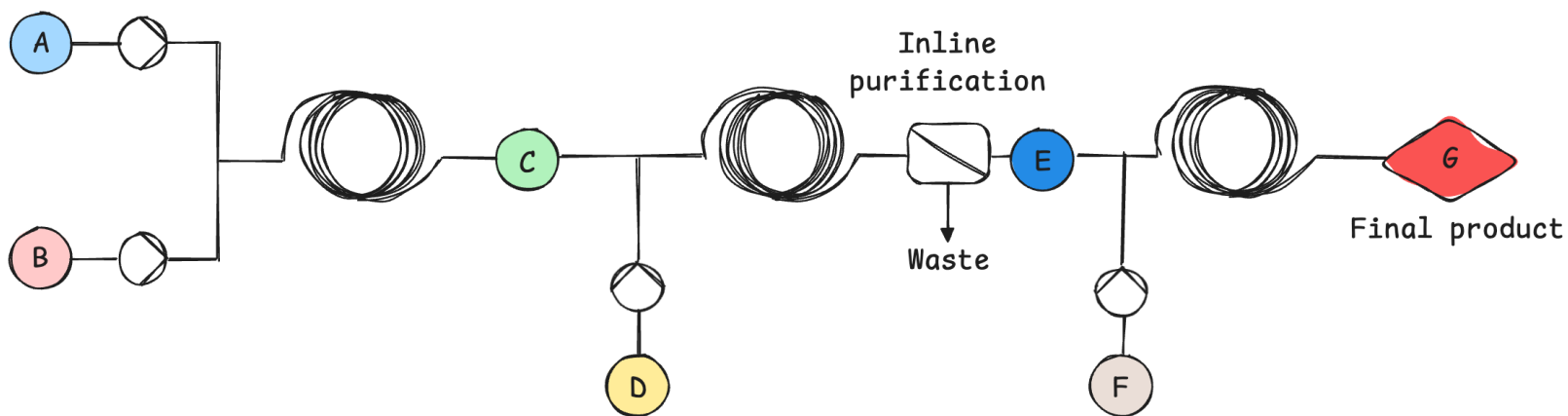
Create in Silico – Realize in our lab

Flow chemistry to fasten scale-up with increased efficiency and safety

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General concepts of flow chemistry

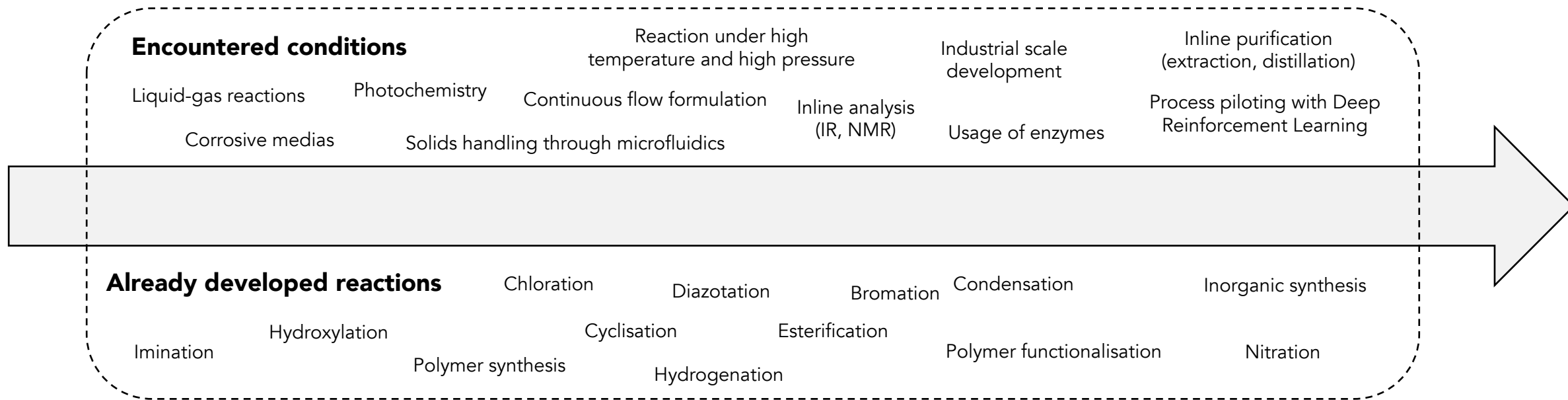


- Reactants are continuously pushed into small pipes
- Reaction occurs during all the contact phase inside the reactor
- Total reactor capacity doesn't exceed several liters for high production rates
- Surface/Volume ratio is favored leading to more efficient heating and cooling
- Intermediate molecules can be handled without isolating them



- + Efficiency
- + Safety
- + Production rate
- + Compacity
- + Scale-up

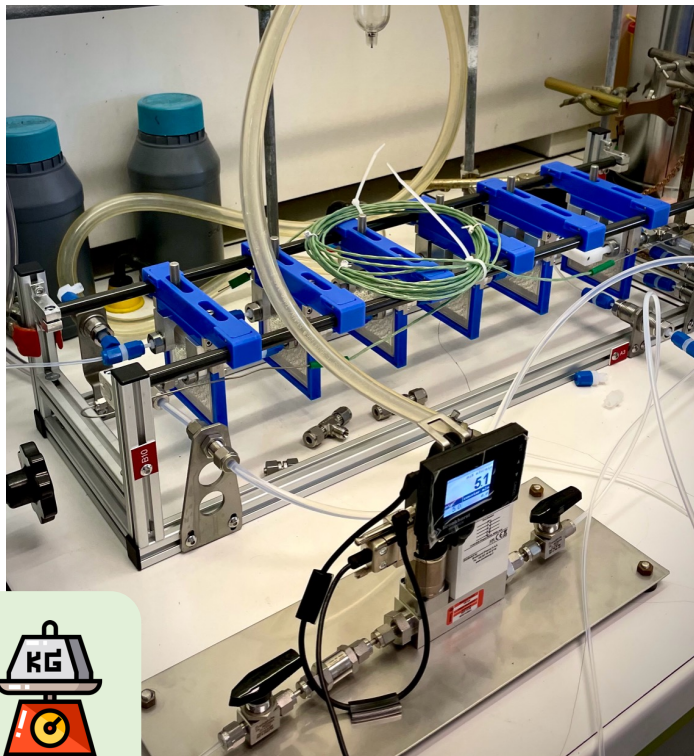
Diversity of reactions in FC



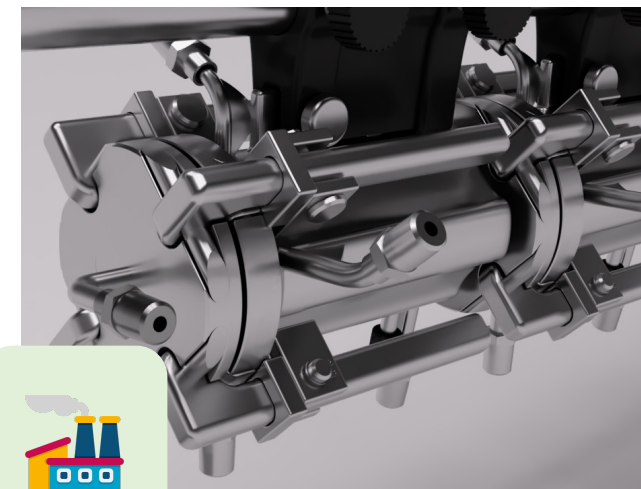
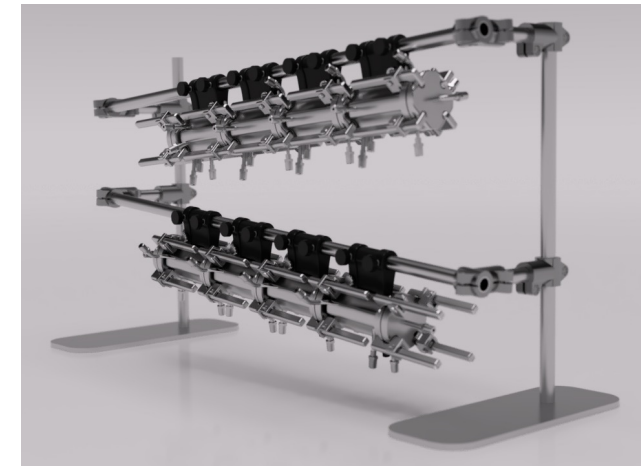
Our flow chemistry equipment



Basic approach to identify characteristics of the reaction in flow chemistry

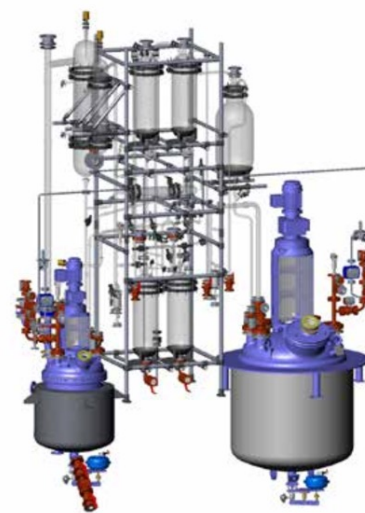
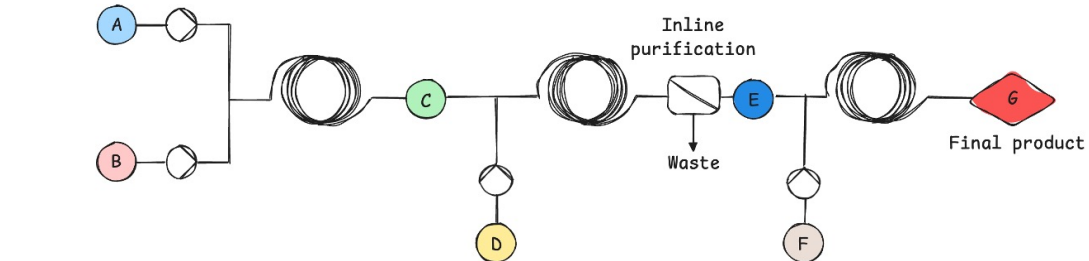
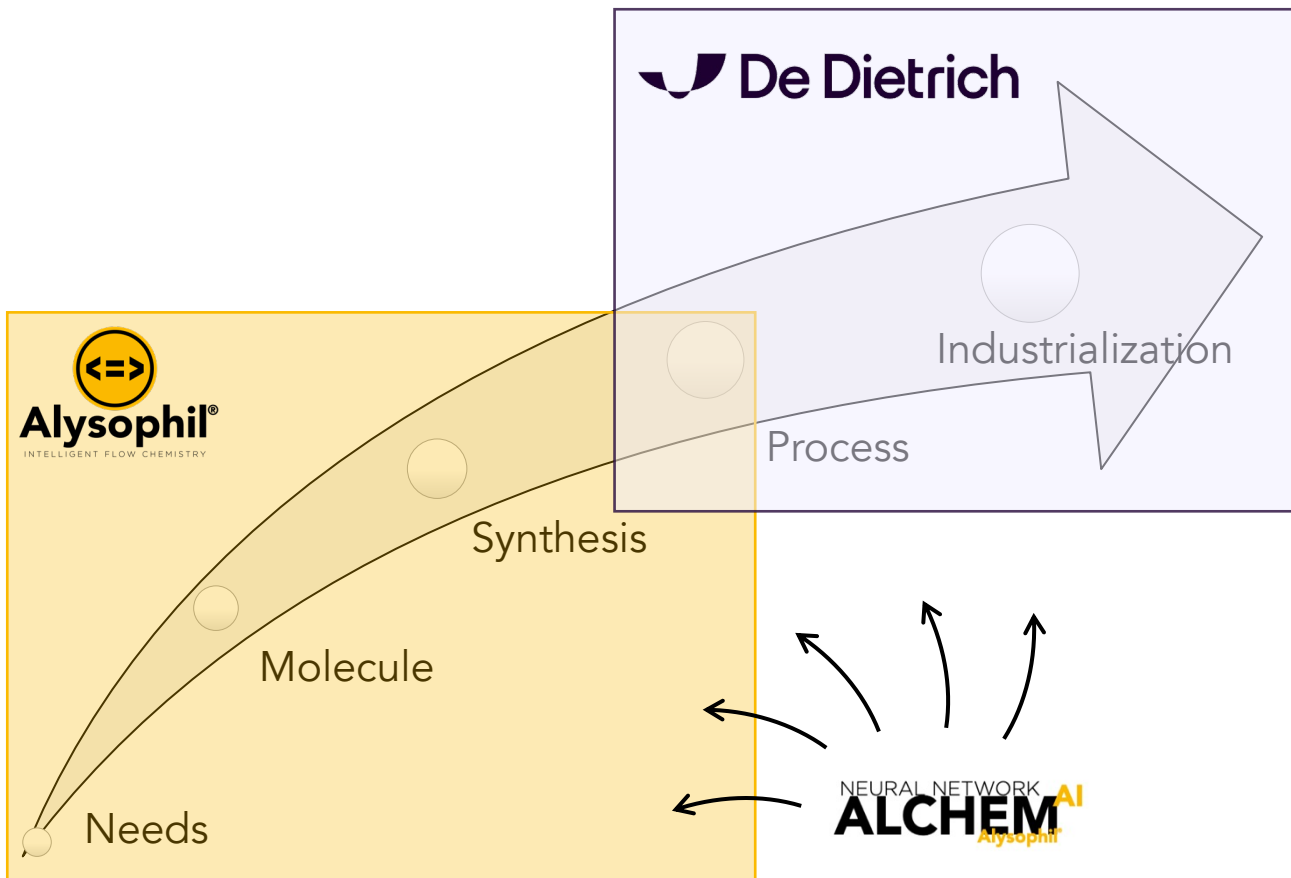


Sophisticated equipments to model the industrial process at lab-scale



Highly specific 3D-printed reactors to adapt the reactor to the reaction

One stop shop

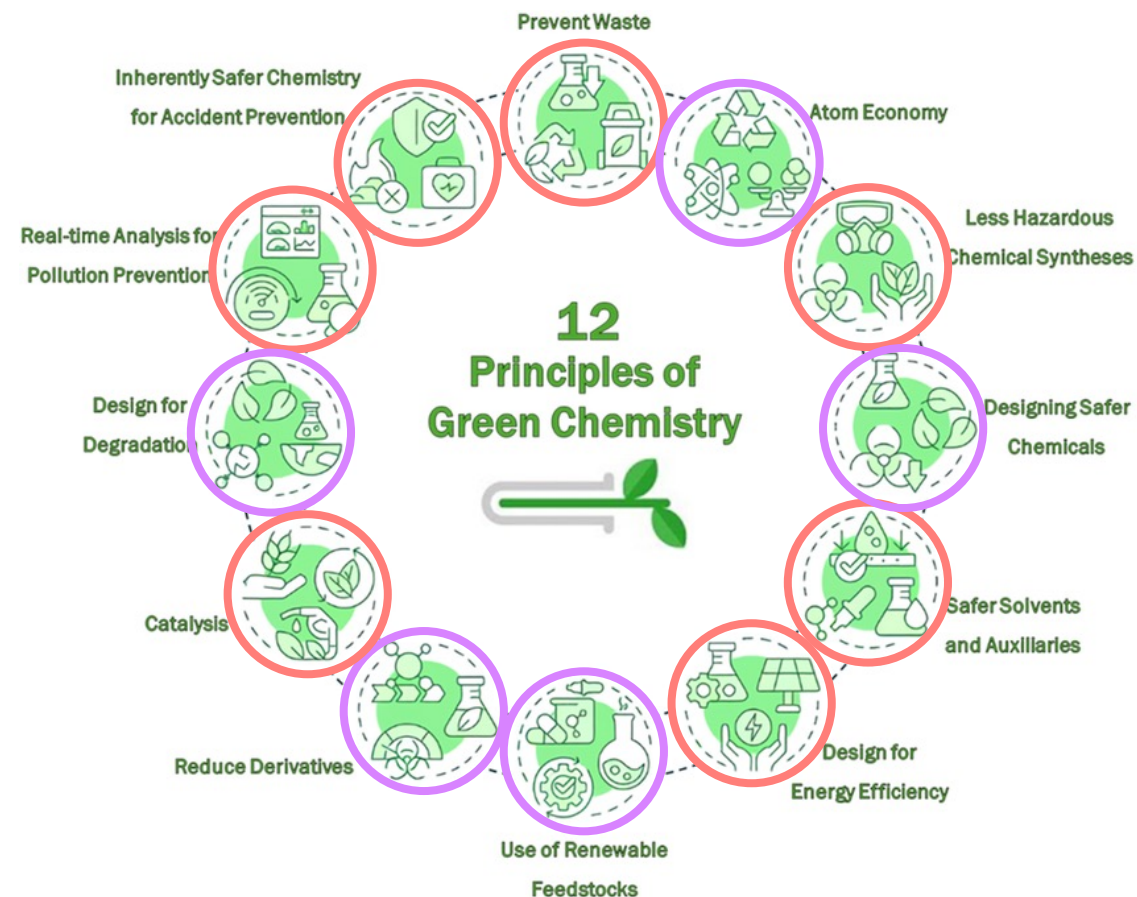


12 principles of Green Chemistry

Alysophil interacts with 12 principles of green chemistry through flow chemistry and during the selection of molecules and their synthesis

AI can provide valuable insights to identify novel candidates and optimize lab experiment by predicting their potential properties

Flow chemistry sets up more efficient and safer process from reaction development to high-scale production



Source: Mah et al., 2025, ChemSusChem

Contacts:

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what do we want for the 21st century?

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