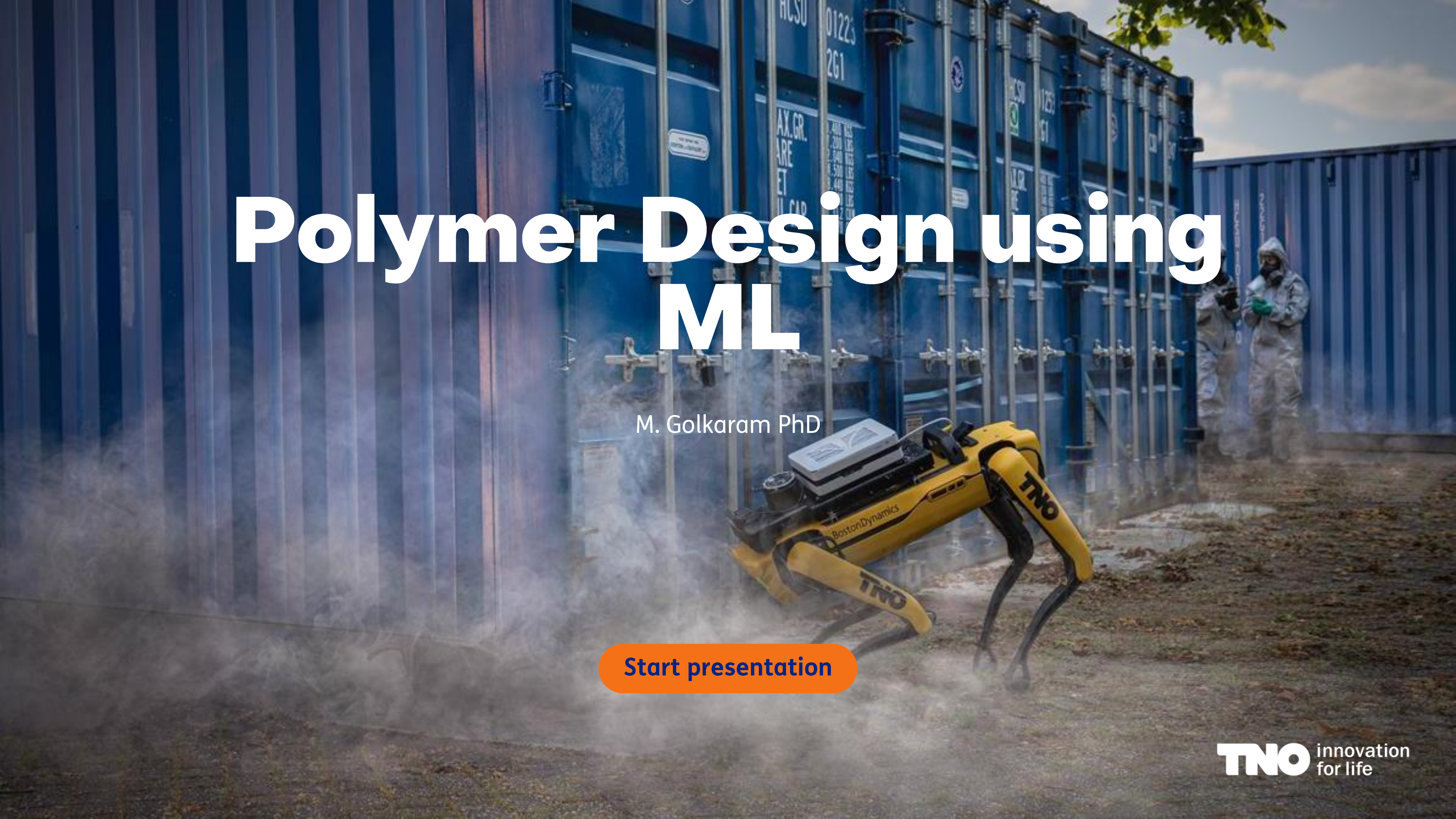
Polymer Design using ML

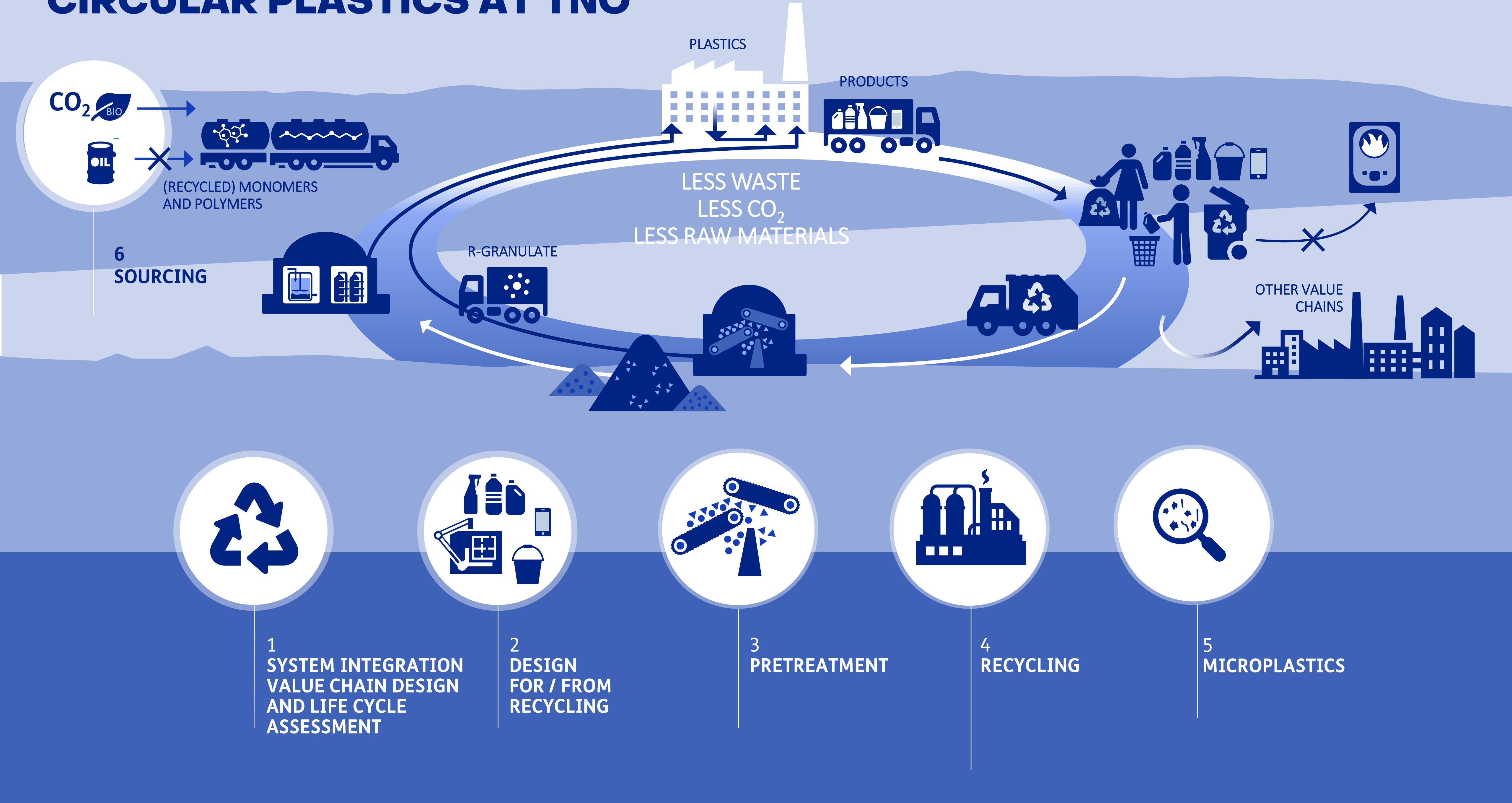
M. Golkaram PhD

Start presentation



TNO innovation for life

CIRCULAR PLASTICS AT TNO



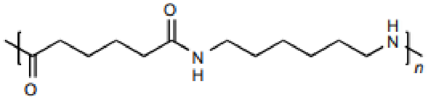
Polymer innovations over the past two centuries

a **Selected milestones of polymer science**

- **1833:** Berzelius coins the term 'polymer'
- **1844:** Goodyear patents the vulcanization of rubber
- **1846:** Schonbein synthesizes nitrocellulose
- **1856:** Parkes patents the first thermoplastic
- **1892:** Cross, Bevan and Beadle patent 'viscose'
- **1907:** Baekeland creates the first synthetic plastic
- **1912:** Klatte invents the production process of PVC
- **1920:** Staudinger publishes 'uber polymerization'
- **1933:** Fawcett and Gibson discover LDPE
- **1937:** Bayer discovers polyurethane
- **1938:** Carothers patents nylon, i.e., Polyamide 6.6, and Plunkett discovers Teflonane
- **1944:** McIntire discovers polystyrene
- **1954:** Ziegler–Natta catalyst discovered for polypropylene production
- **1965:** Kwolek creates Kevlar
- **1977:** Heeger, MacDiarmid and Shirakawa develop polyacetylene, the first conductive polymer
- **2011:** Launch of Materials Genome Initiative
- **2020:** 100-year anniversary of modern polymer science

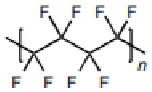
b **Typical deployment progress of some notable polymers**

Nylon



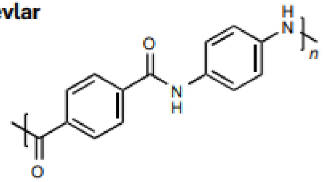
- **1927:** Started development
- **1935:** The first nylon synthesized
- **1938:** Patented
- **1940:** Went to department store

Teflon



- **1938:** Discovered
- **1945:** Trademark registered
- **1948:** Mass production

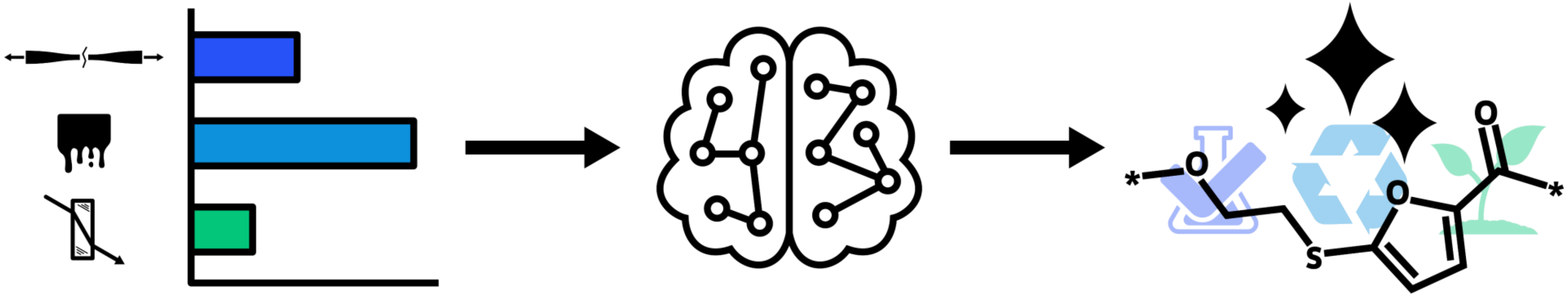
Kevlar



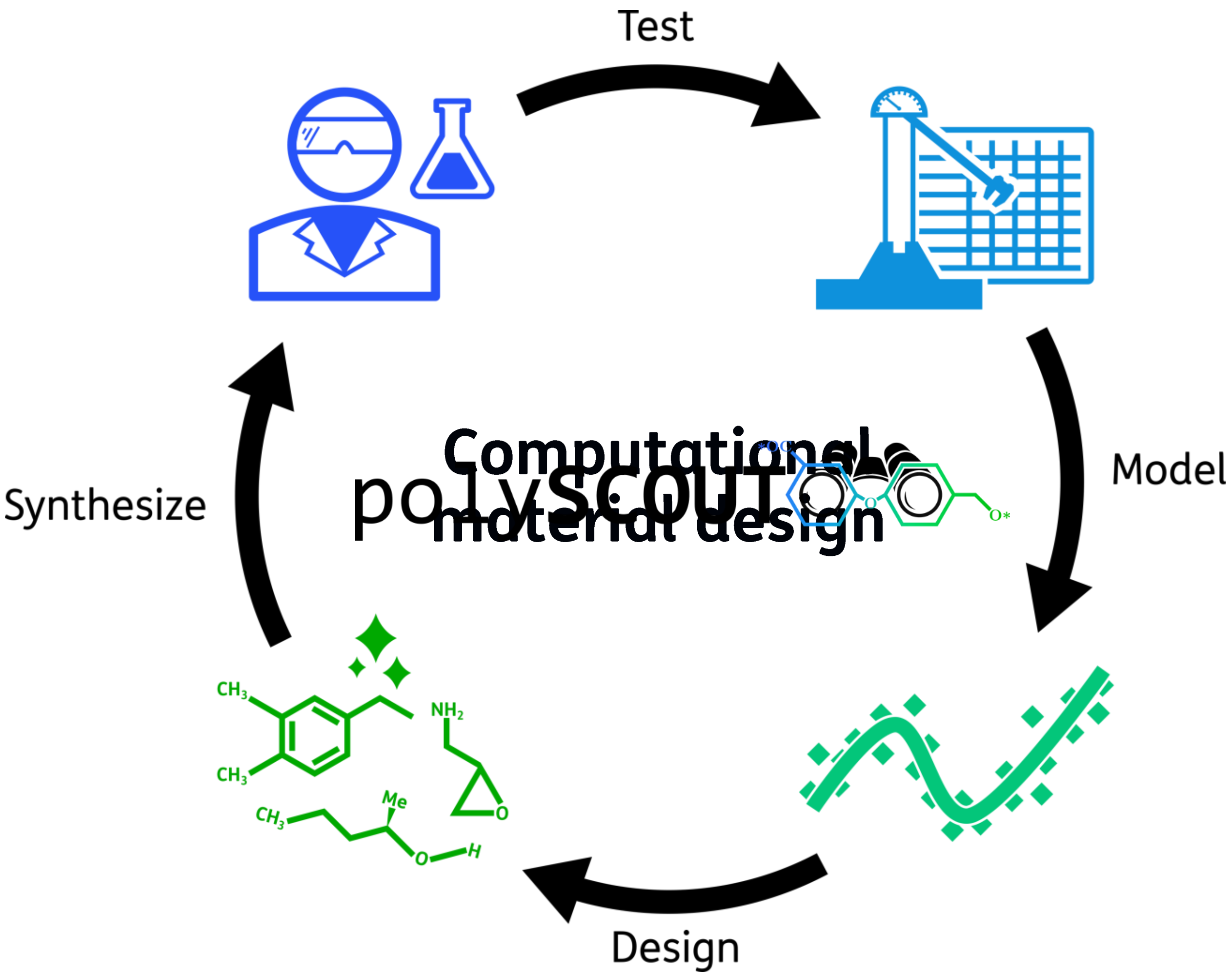
- **1965:** Developed
- **1971:** Introduced to the market

polySCOUT

Goal: Develop fast **machine learning-based** methods that realistically **capture the complexity** of polymers to **design novel candidates** matching with requirements for **future-proof plastics**



Polymer Informatics @TNO



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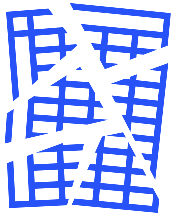
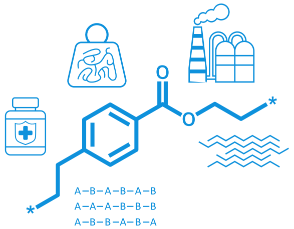
Addressing the challenges

Fragmentation



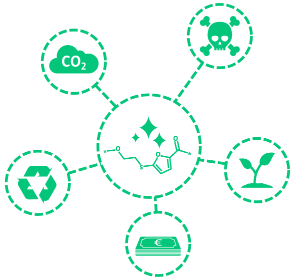
- Collecting and curating published data
- Creating our own data in the lab

Representation



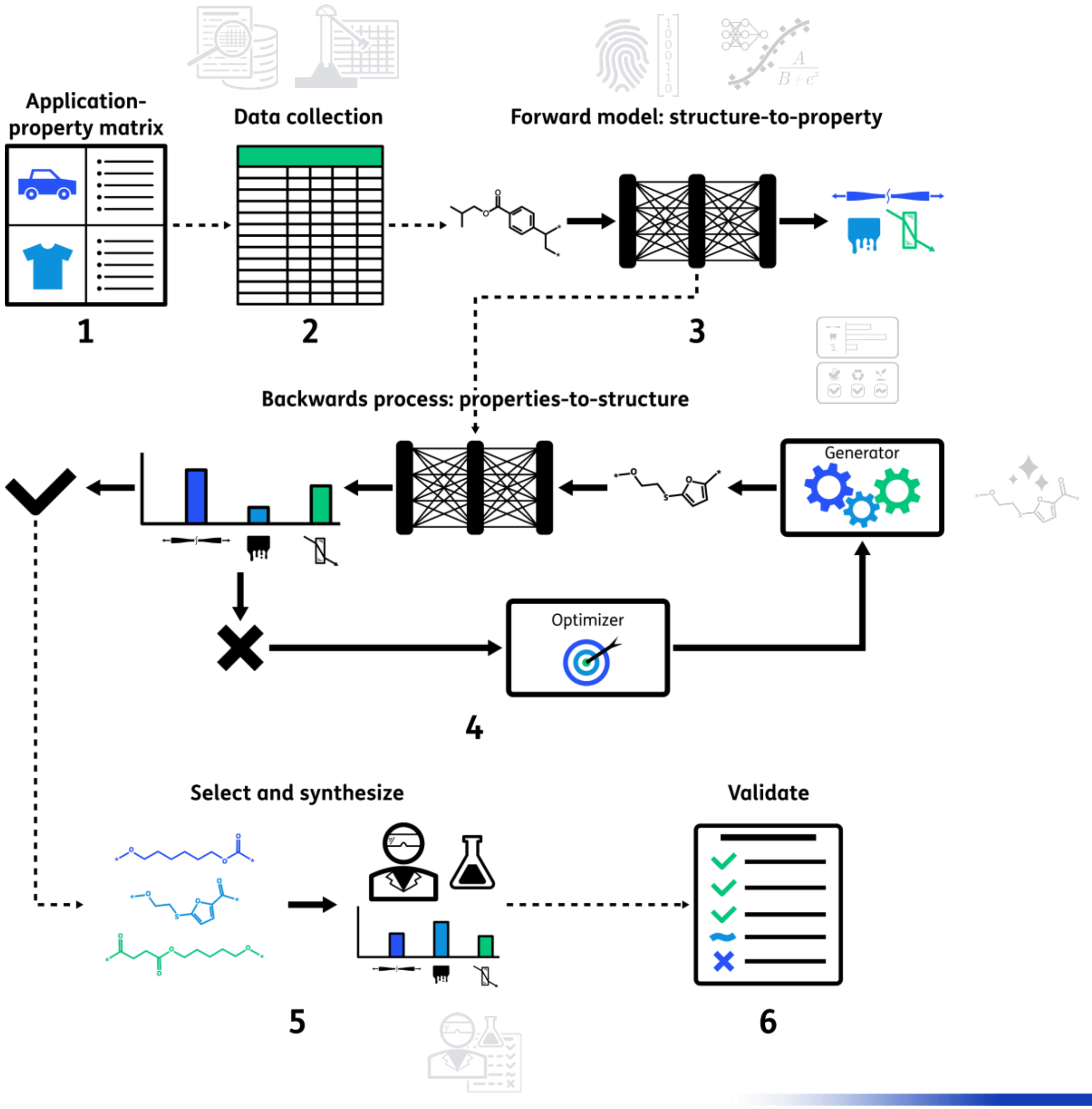
- Developing comprehensive (co)polymer fingerprints
- Exploring hybrid modelling approaches

Validation



- Predicting properties and viability
- Designing from the bottom up
- Testing outcomes and incorporating results

Our workflow



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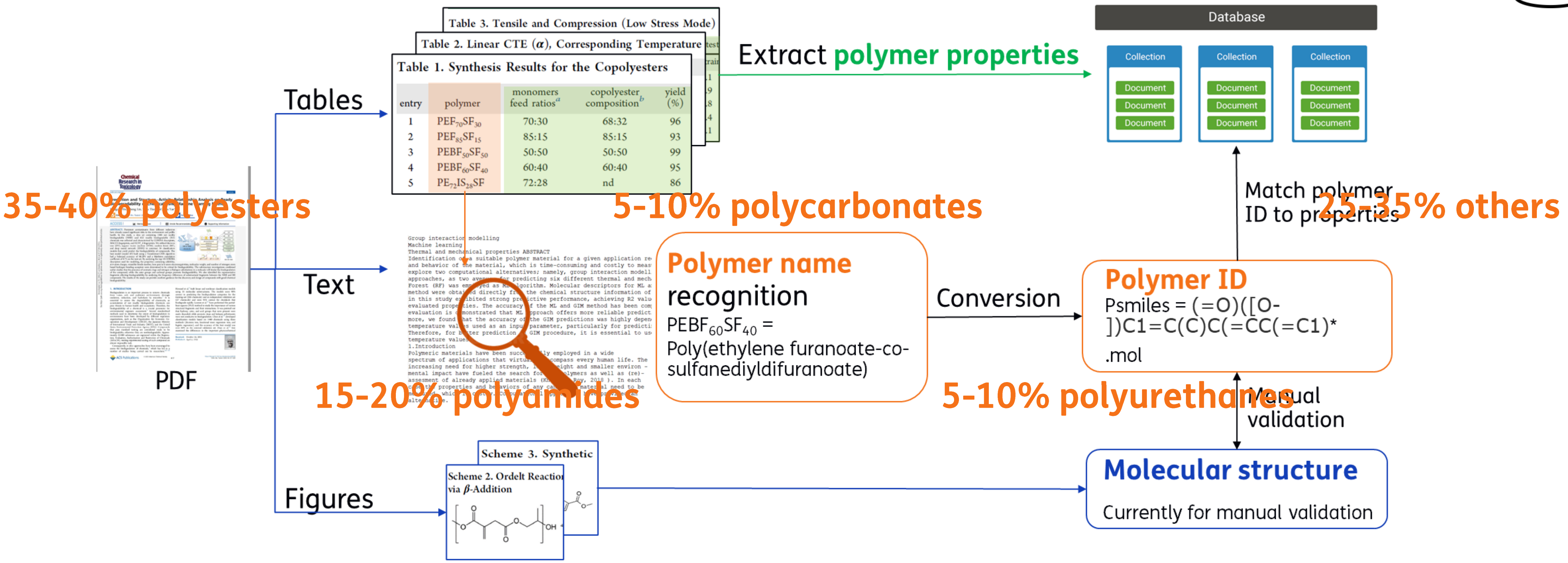
Application-property matrix

Overview of conventional polymer types and applications

Literature study on existing biopolymers

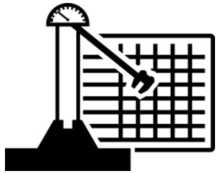
Textile and packaging identified as first targets

Data curation



Currently properties for ~6000 polymers (and counting) in database

Data creation



High-throughput screening of 8 properties:

- compression modulus
- hardness
- yield strength
- scratch resistance
- storage and loss modulus
- glass transition temperature
- impact strength

To be incorporated in active learning loop with data-driven models

Experimental work: Filling the data base

- Initial materials that will be assessed:

  - PET – high IV
  - PET – medium IV
  - PET – low IV
  - PA6.6
  - PBS
  - PBAT
  - PHA
  - PLA
  - Polytetrahydrofuran
  - Polypropyleneglycol
  - Polyethyleneoxide
  - Polyethyleneglycol
  - PA6
  - PA11
  - PA12
  - PA66
  - Polyglycolic acid
  - Polylactic acid-L
  - Polylactic acid-D
  - Polylactic acid-L/D
  - Polyethylene succinate
  - Polyethylene adipate
  - Polybutylene adipate
  - Polybutylene terephthalate
  - Polypropylene (8x)
  - Polyethylene (2x)
  - Polystyrene
  - PMMA
  - ASA
  - ABS
  - PC

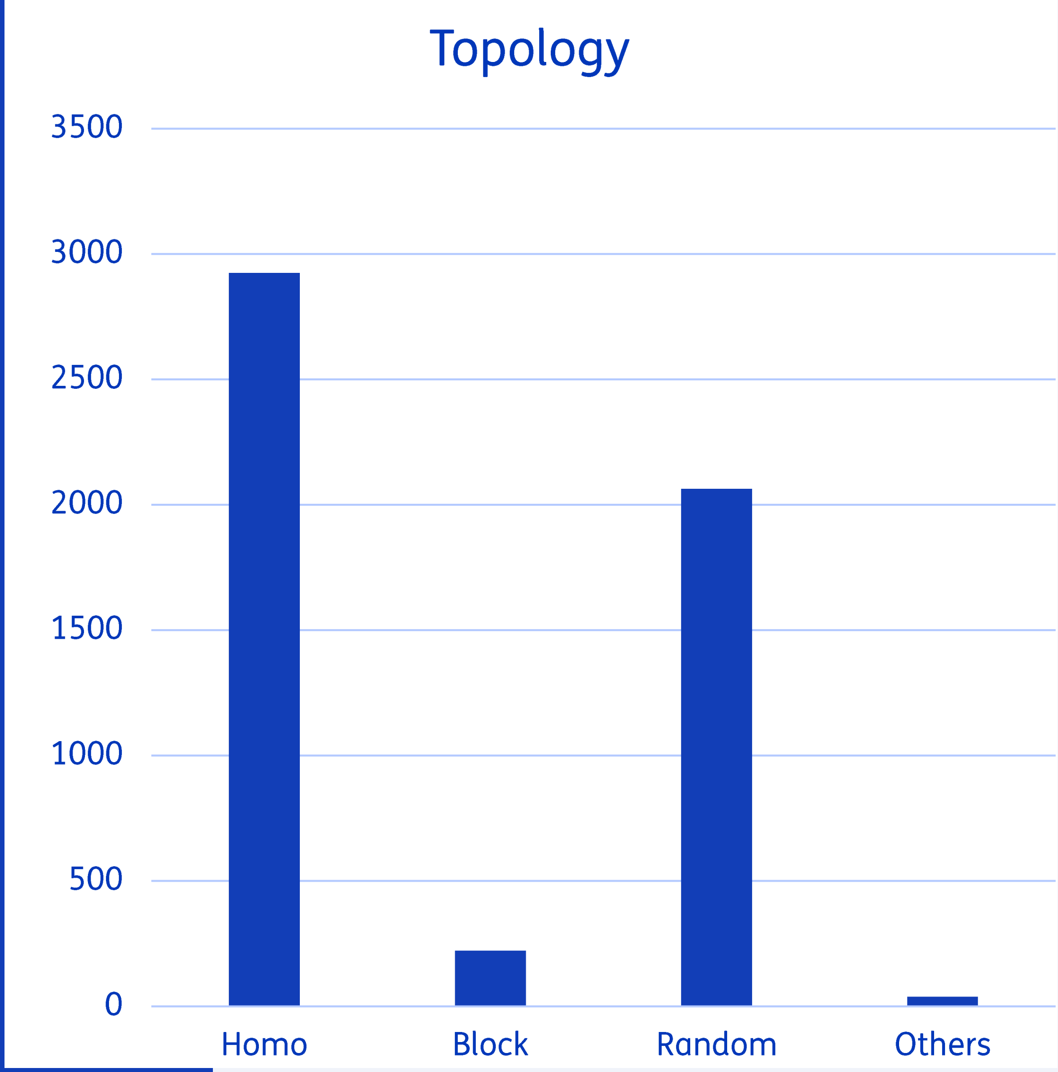
10 of these polymers have been assessed to develop a protocol for **melt strength**

10 of these polymers have been assessed to develop a protocol for measuring **crystallization rate**

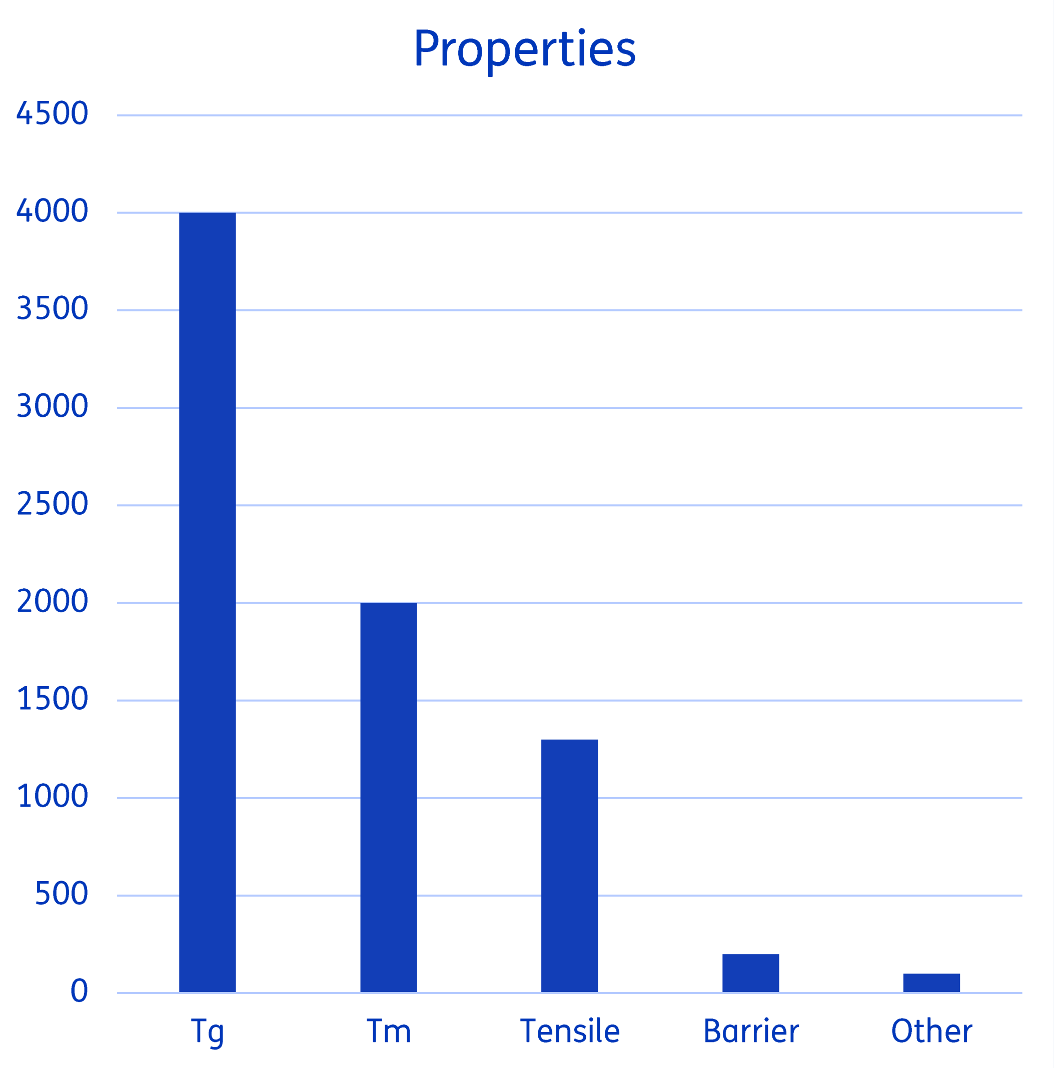
45 of these polymers have been tested for **hardness**

PolyScout database

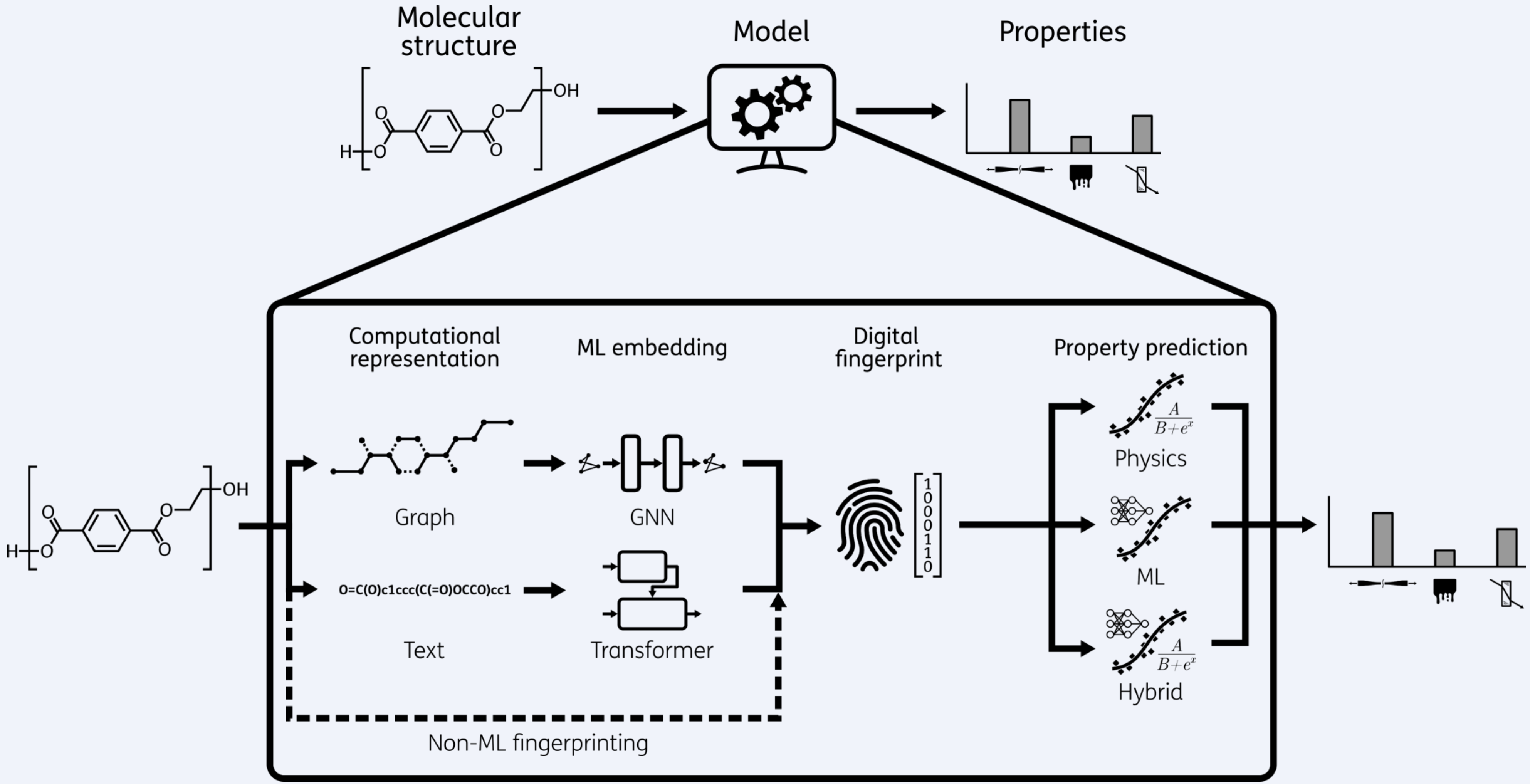
polySCOUT



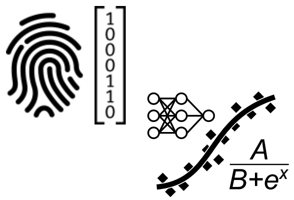
PolyScout database



Fingerprint + Artificial Neural Network

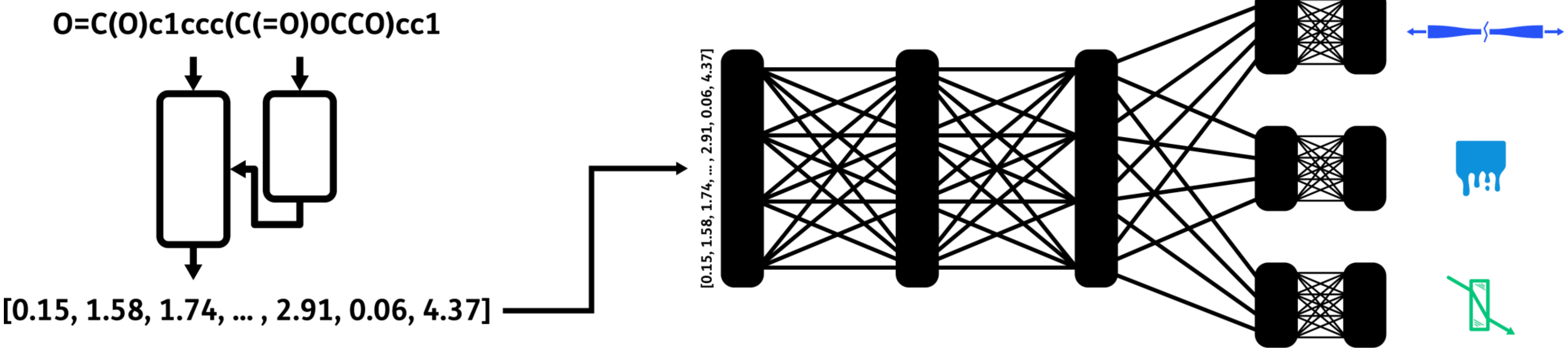


Property prediction



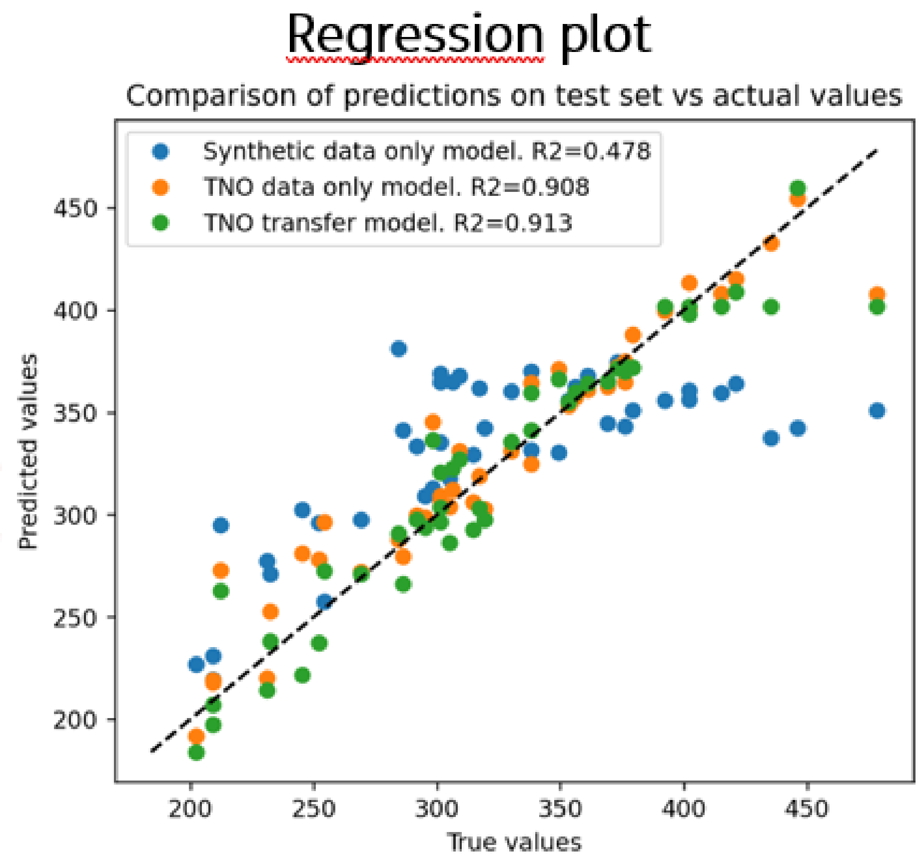
Transformer-based fingerprinting

Multi-task property prediction



Extended copolymer representation in progress

PolyScout database



Rule-based polymerization mechanism

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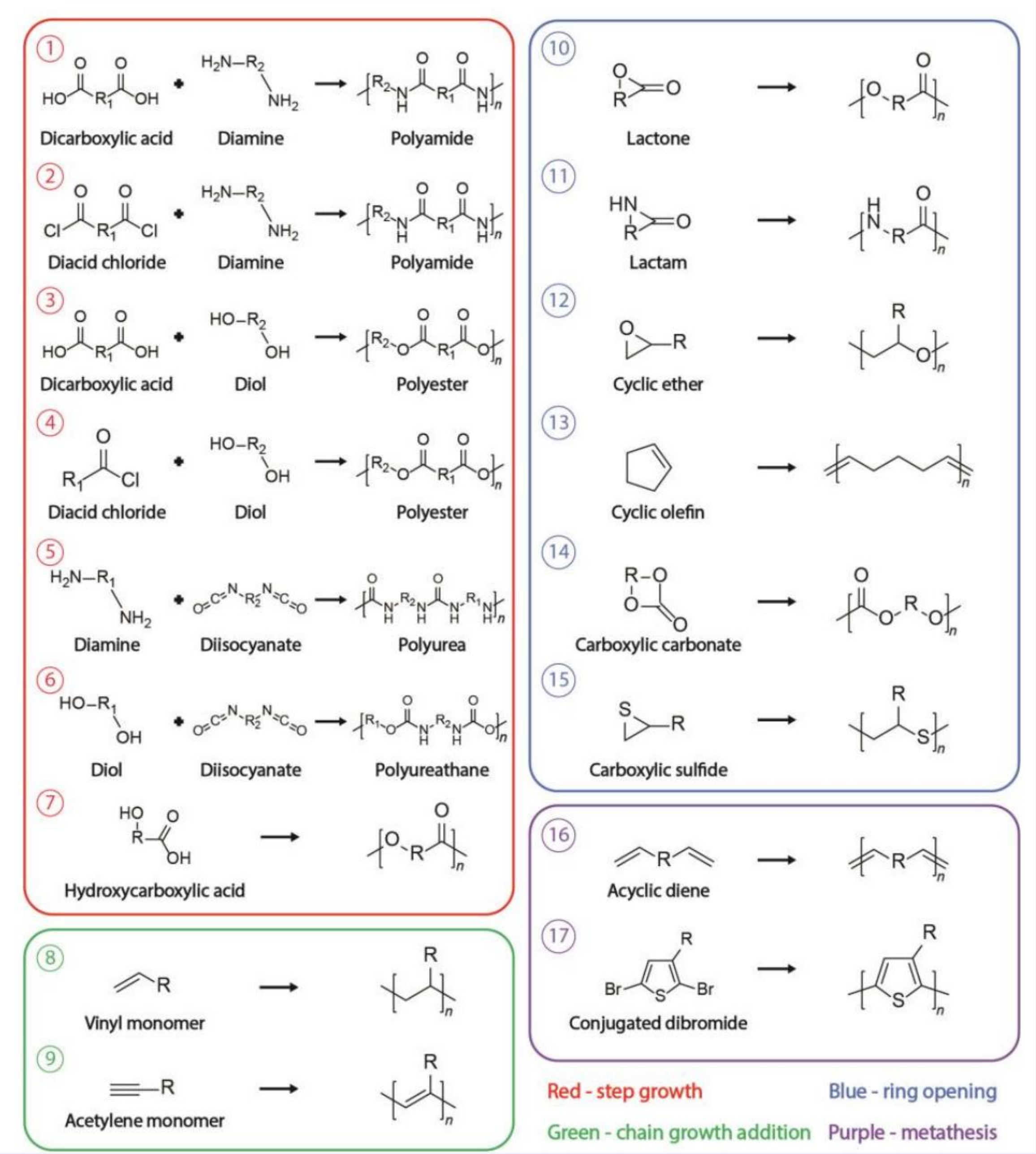
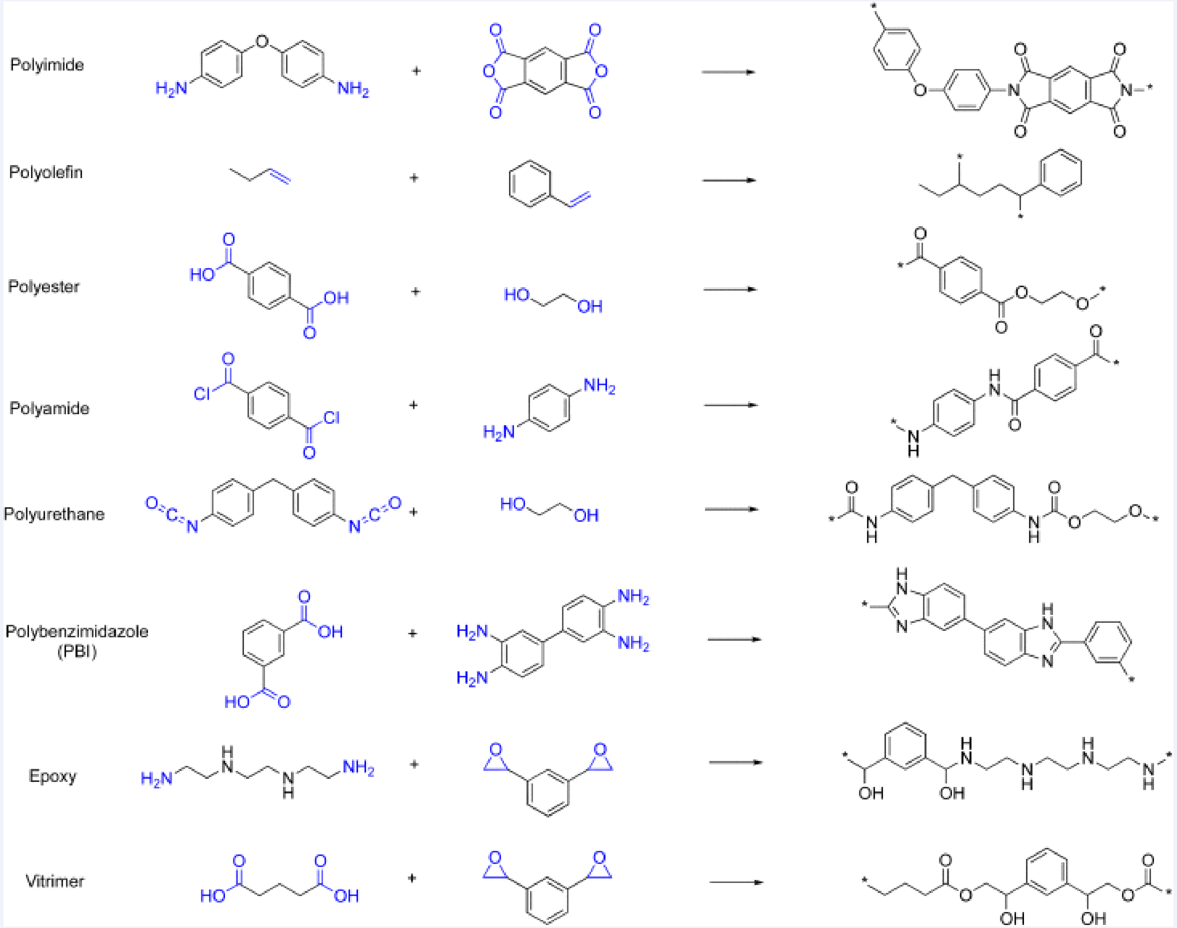
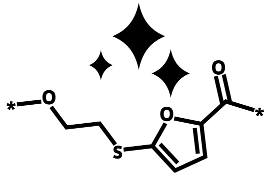
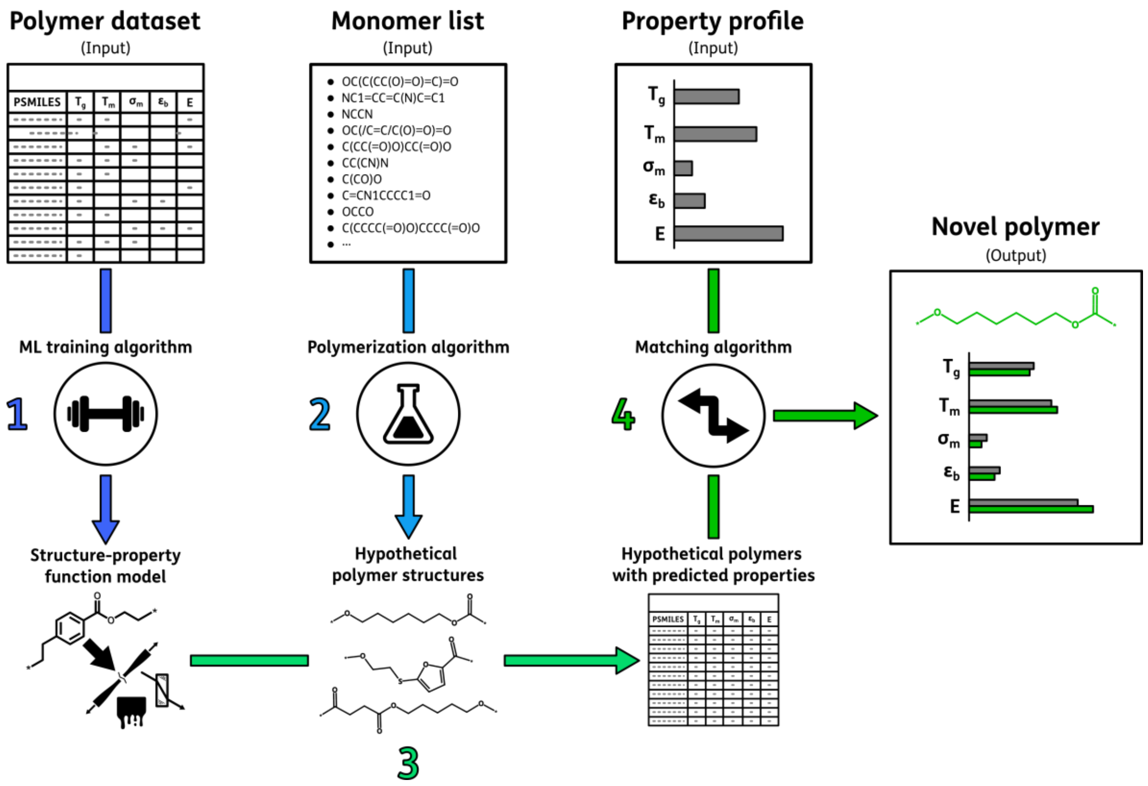




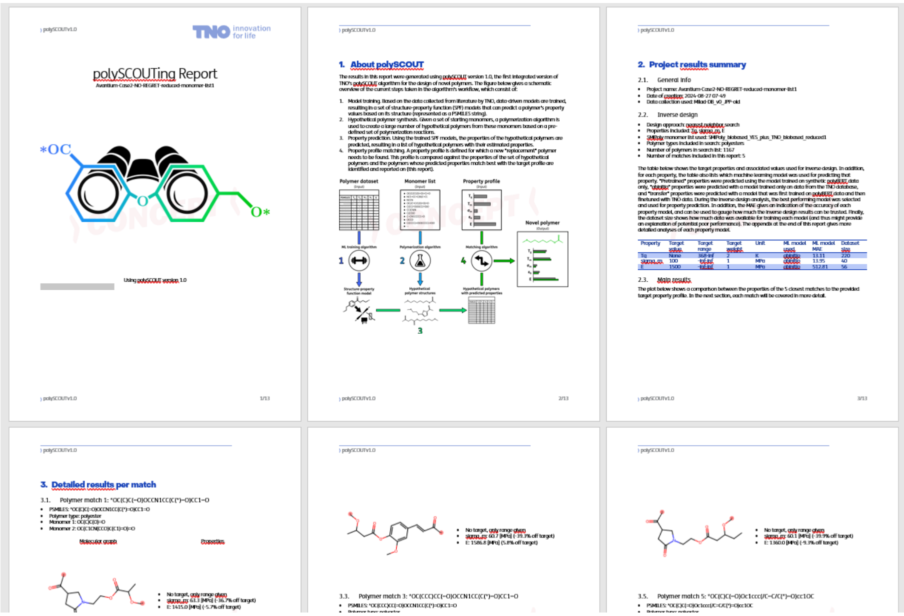
Inverse polymer design



High-throughput virtual screening approach

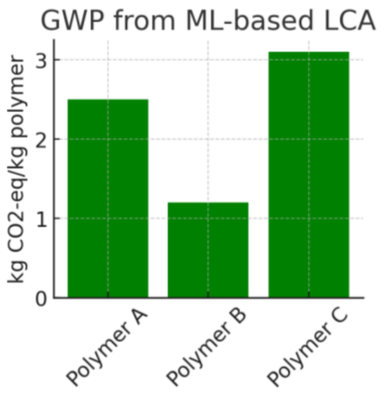


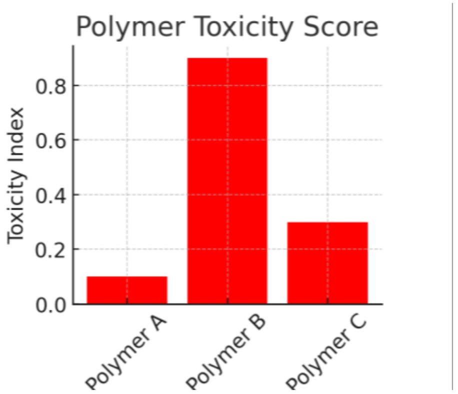
Automated reporting of results

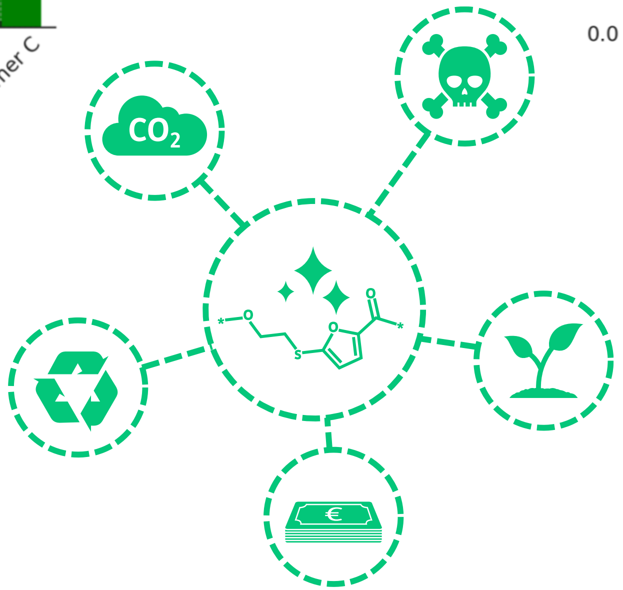


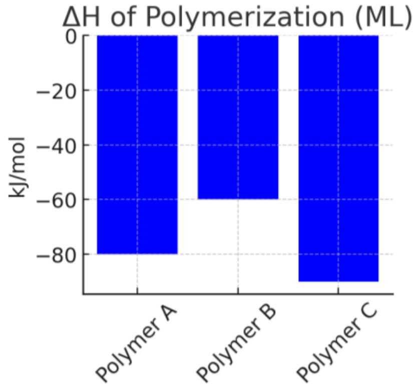
SSbD

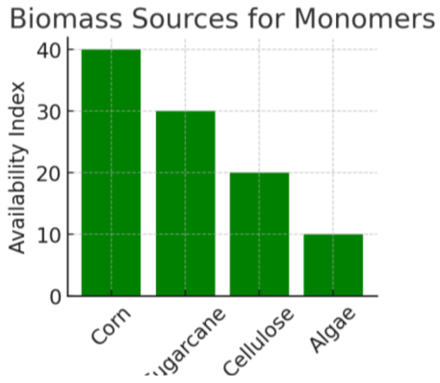
1. **CO_2 (Life Cycle Assessment):** Global Warming Potential (GWP) estimated via machine learning models.
2. **Toxicity:** toxicity scores of different polymers, highlighting Polymer B as the most toxic.
3. **Cost (Aspen modeling):** Energy consumption for polymerization, modeled conceptually using Aspen—Polymer B is most energy-intensive.
4. **Recyclability (Enthalpy of Polymerization):** Negative enthalpy values predicted by ML show thermodynamic favorability for recyclability.
5. **Resource Availability:** Biomass feedstock availability (e.g., corn, sugarcane, cellulose, algae) shown as potential monomer sources.

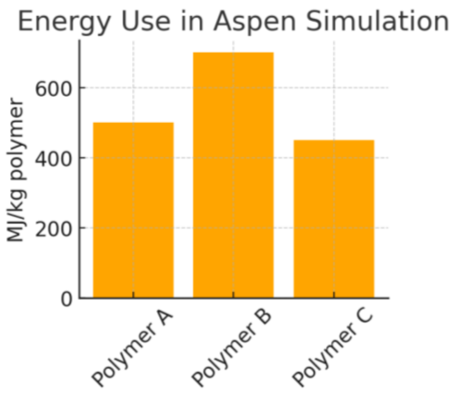




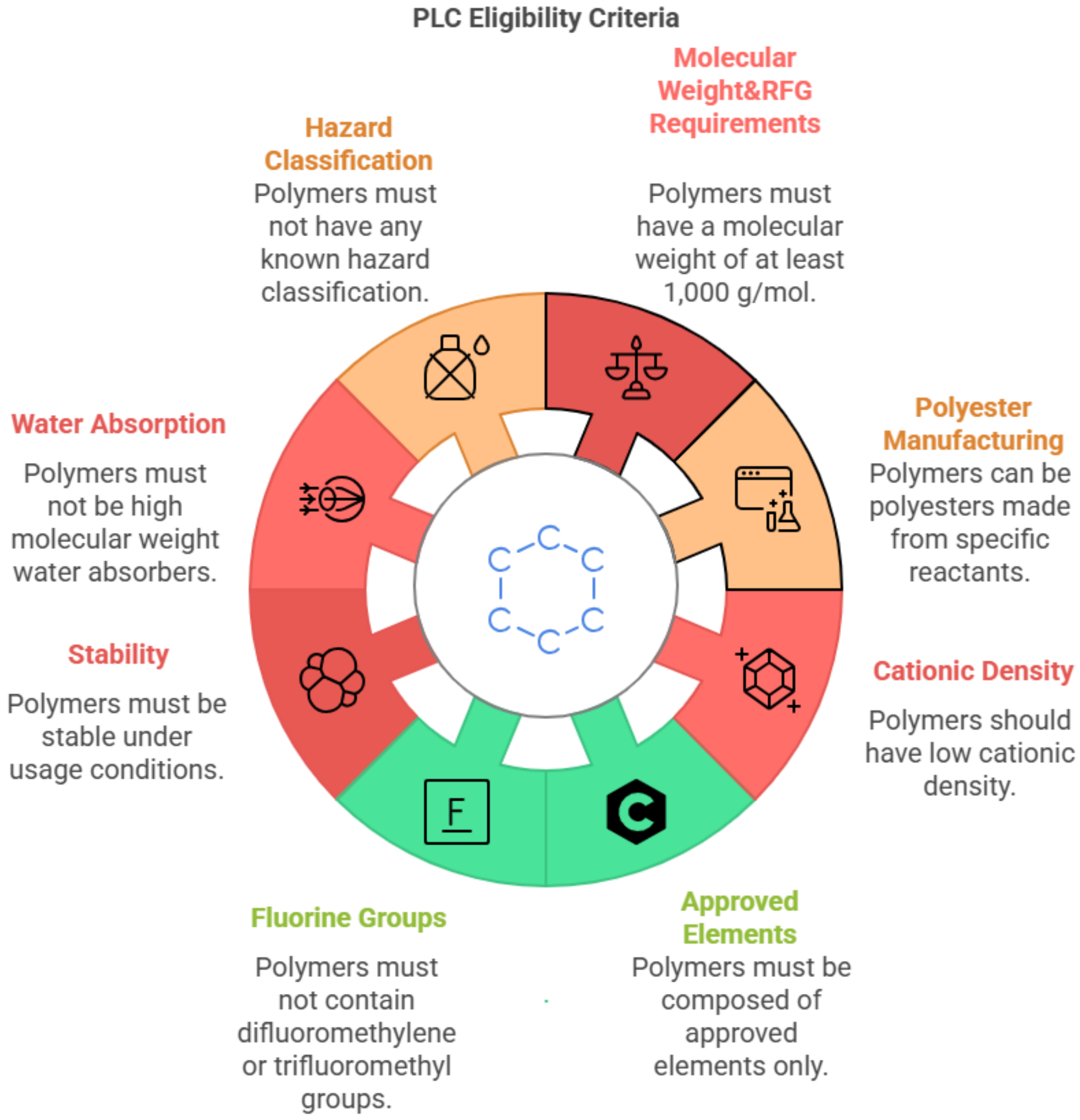




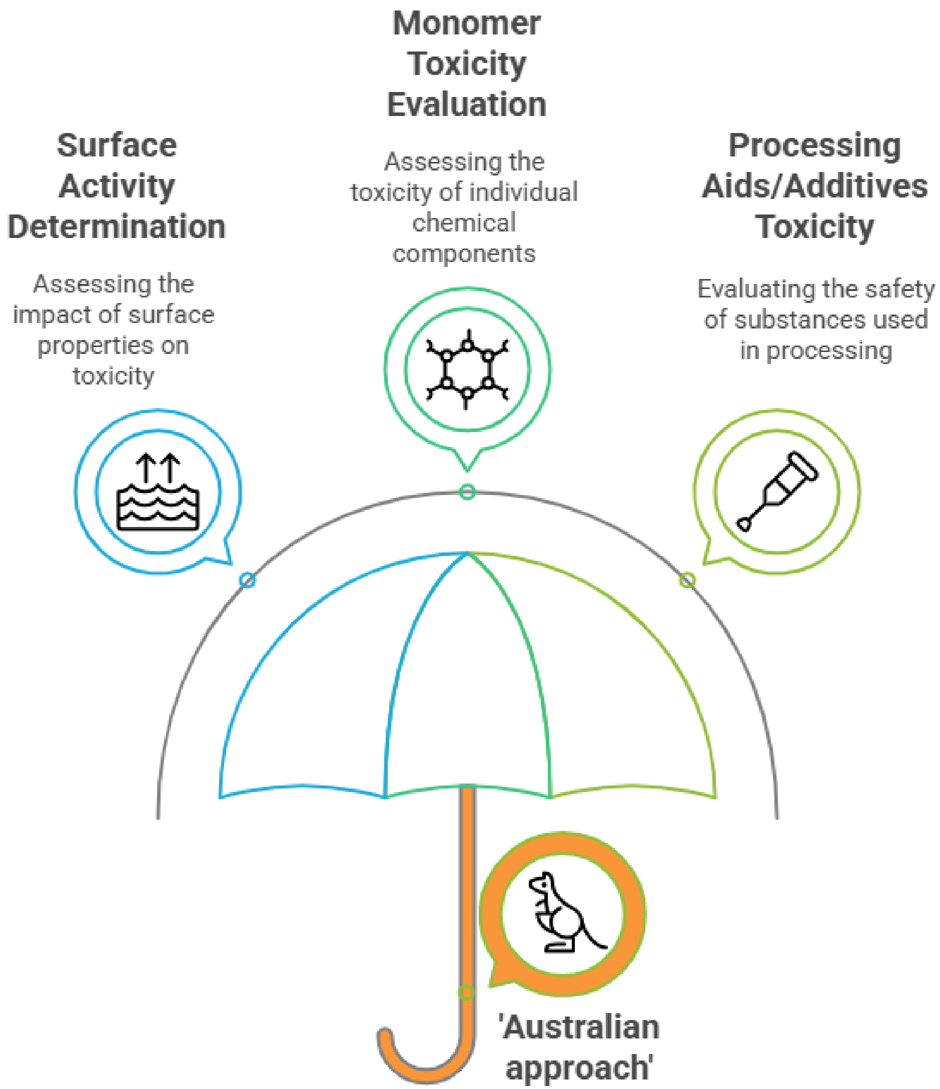




SSbD

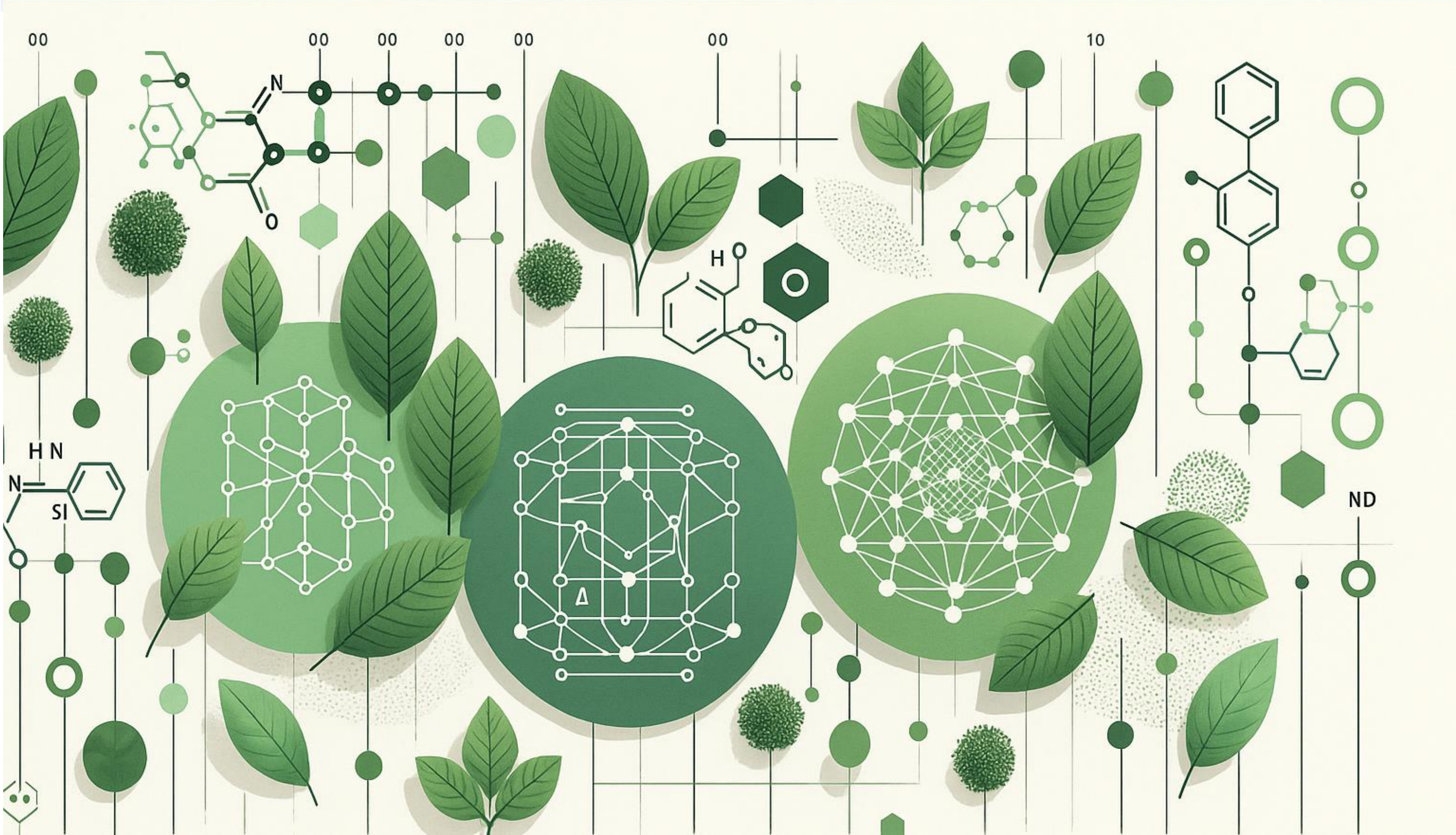


PLC Eligibility Criteria
Molecular Weight&RFG Requirements
Polymers must have a molecular weight of at least 1,000 g/mol.
Polyester Manufacturing
Polymers can be polyesters made from specific reactants.
Cationic Density
Polymers should have low cationic density.
Approved Elements
Polymers must be composed of approved elements only.
Fluorine Groups
Polymers must not contain difluoromethylene or trifluoromethyl groups.
Stability
Polymers must be stable under usage conditions.
Water Absorption
Polymers must not be high molecular weight water absorbers.
Hazard Classification
Polymers must not have any known hazard classification.



Surface Activity Determination
Assessing the impact of surface properties on toxicity
Monomer Toxicity Evaluation
Assessing the toxicity of individual chemical components
Processing Aids/Additives Toxicity
Evaluating the safety of substances used in processing
'Australian approach'

Let's collaborate to drive innovation in biobased polymers!



Thank you!

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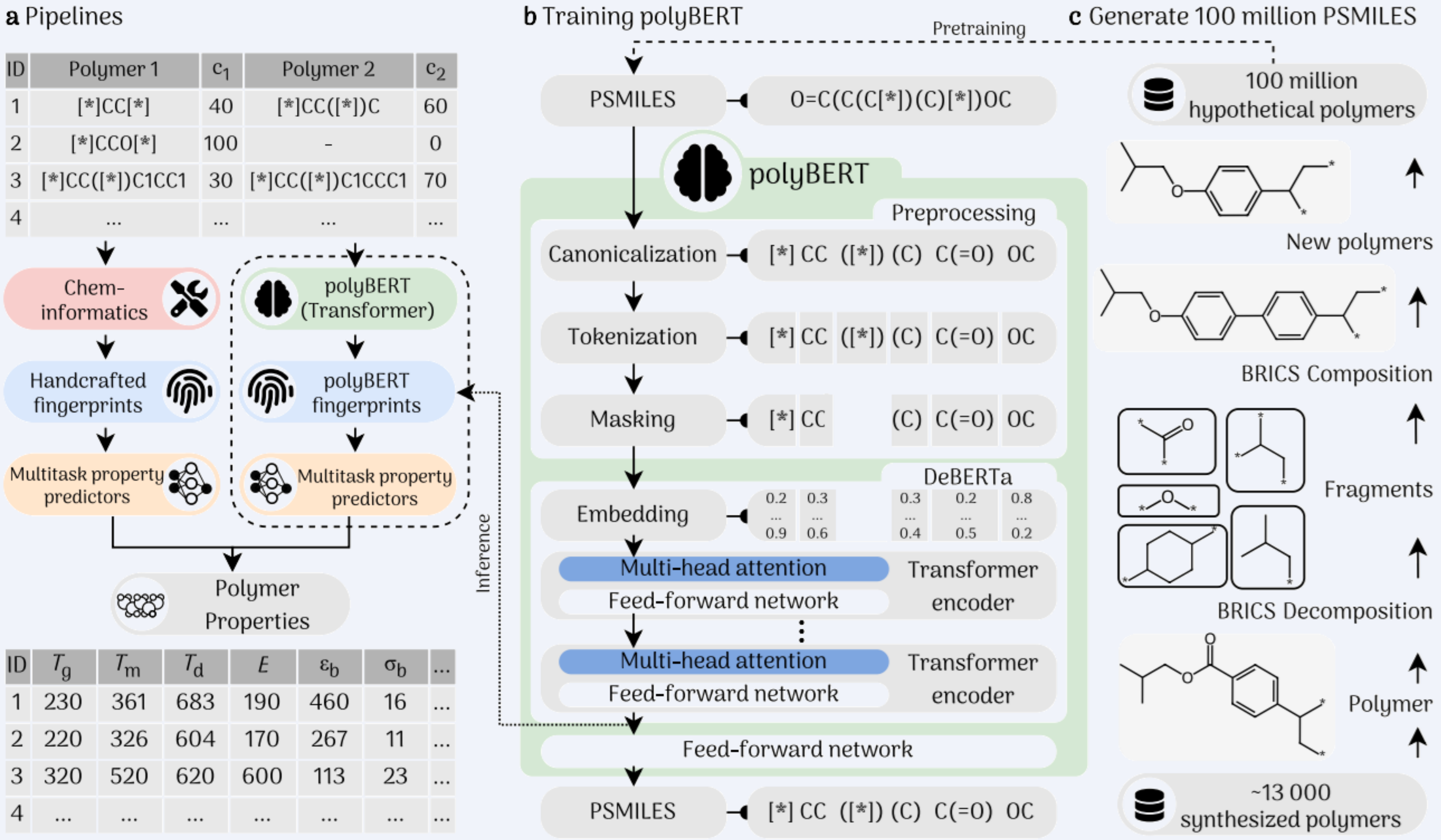
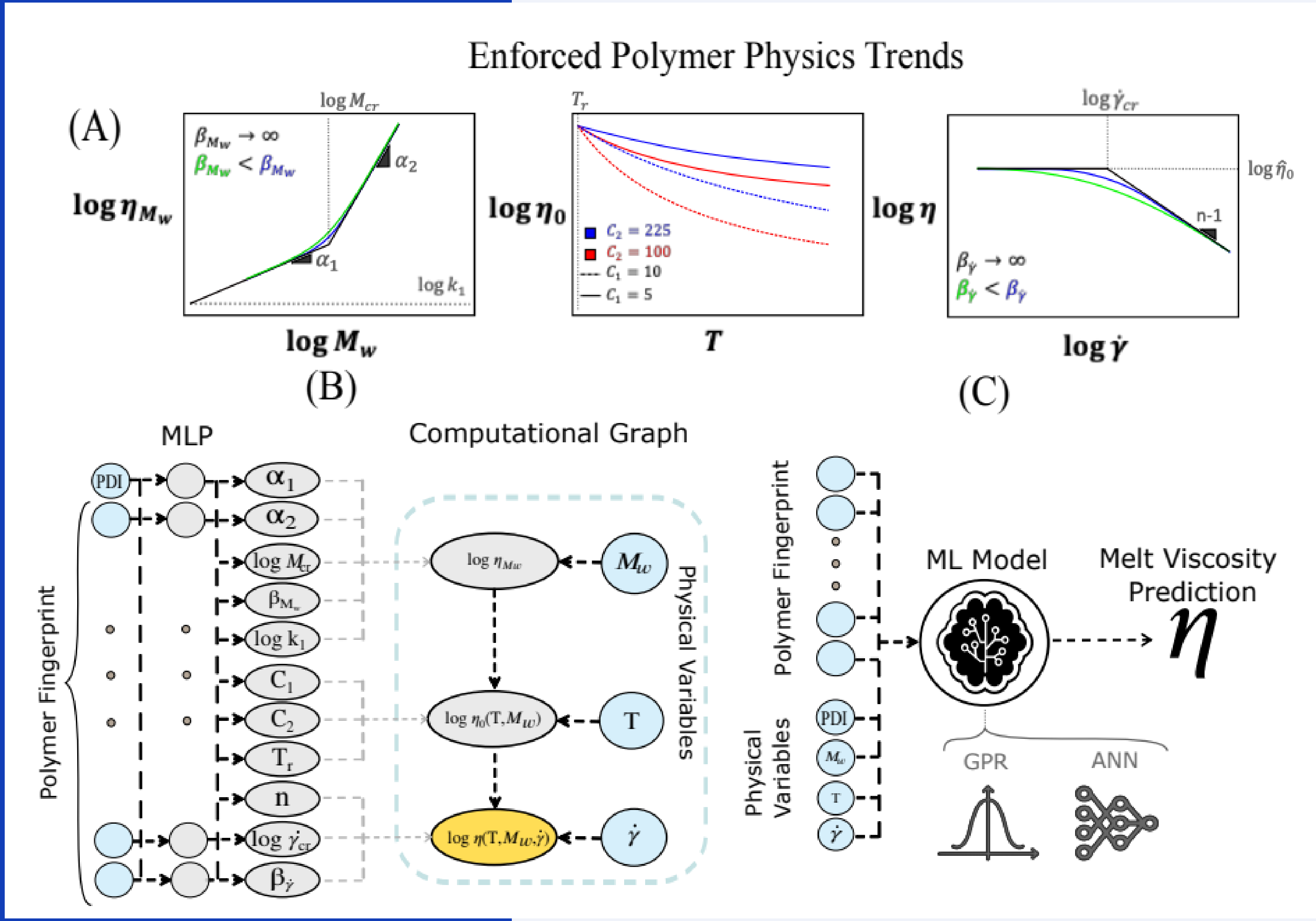
Machine learning approach



Kuenneth, C. and R. Ramprasad. 2023. polyBERT: a chemical language model to enable fully machine-driven ultrafast polymer informatics. Nature Communications 14(1): 4099. https://doi.org/10.1038/s41467-023-39868-6.

Hybrid models

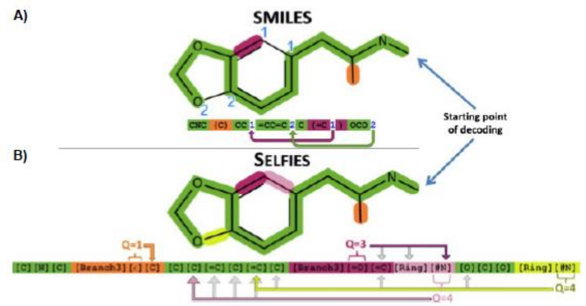
- Physics-informed, physics-guided

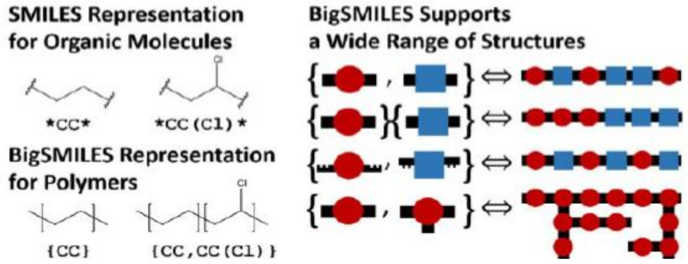


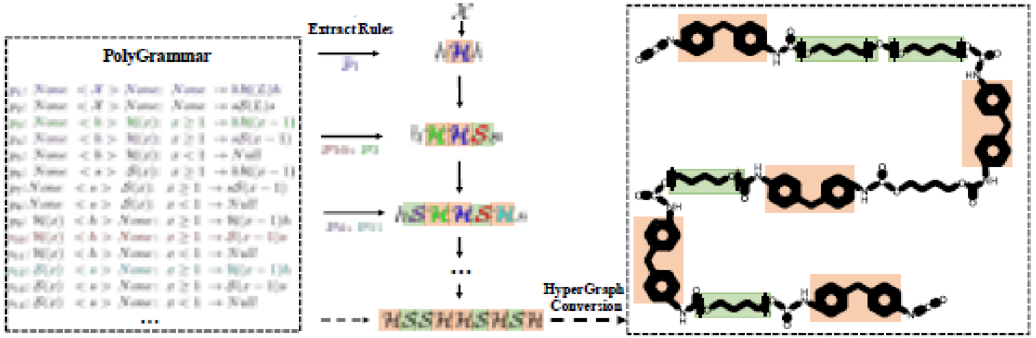
Reference: 2409.05240

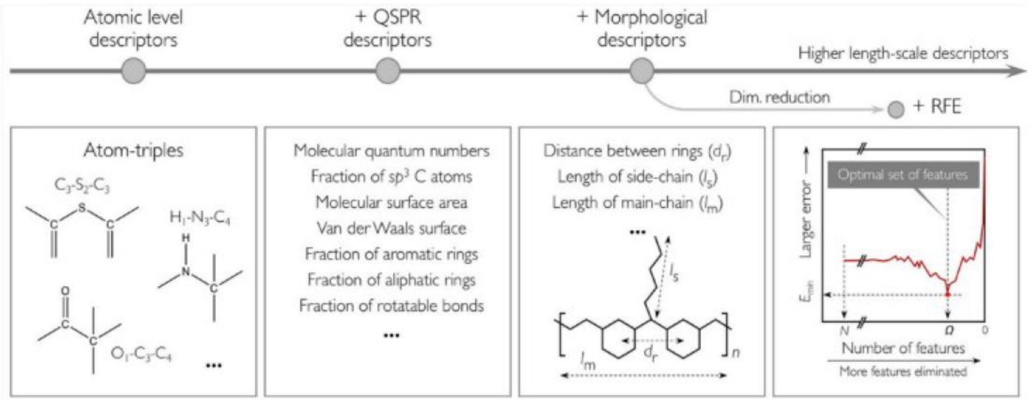
Polymer complexity

- Various representations, polyBERT uses PSMILES
- BigSMILES[1] provide better options to represent complexity of polymers (topology)









[1]BigSMILES: A Structurally-Based Line Notation for Describing Macromolecules | ACS Central Science