

# InverseESA - Inverse Design of Industrial Catalysts for Sustainable Epoxide Manufacture



**José Ferraz-Caetano**

jose.caetano@fc.up.pt

Supervisors: Filipe Teixeira<sup>1,2</sup>, M. Natália D. S. Cordeiro<sup>1</sup>

1. LAQV-REQUIMTE – Department of Chemistry and Biochemistry – Faculty of Sciences, University of Porto – Rua do Campo Alegre, S/N, 4169-007 Porto, Portugal

2. Centro de Química, Universidade do Minho, Campus de Gualtar, 4710-057 Braga, Portugal

MIT Portugal

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### The Chemistry

Jacobsen's Catalyst

R-CH=CH-R1 + O -> R-CH(O)-CH(O)-R1

R = aryl, alkenyl, alkynyl, alkyl  
R1 = bulky alkyl group

Catalytic Epoxidation of Small Alcohols and Alkenes provides valuable industrial intermediates

such as

Ethylene Oxide

### The Economics

- \$20 billion industry
- 22 million ton/year
- High CO<sub>2</sub> footprint

Essential for the production of

Pesticides Flavourings Plastics Fine Drugs

### The Problem

Fossil raw materials condition economic and environmental sustainability.

Production costs and pollution emissions are increasingly high.

## The Solution

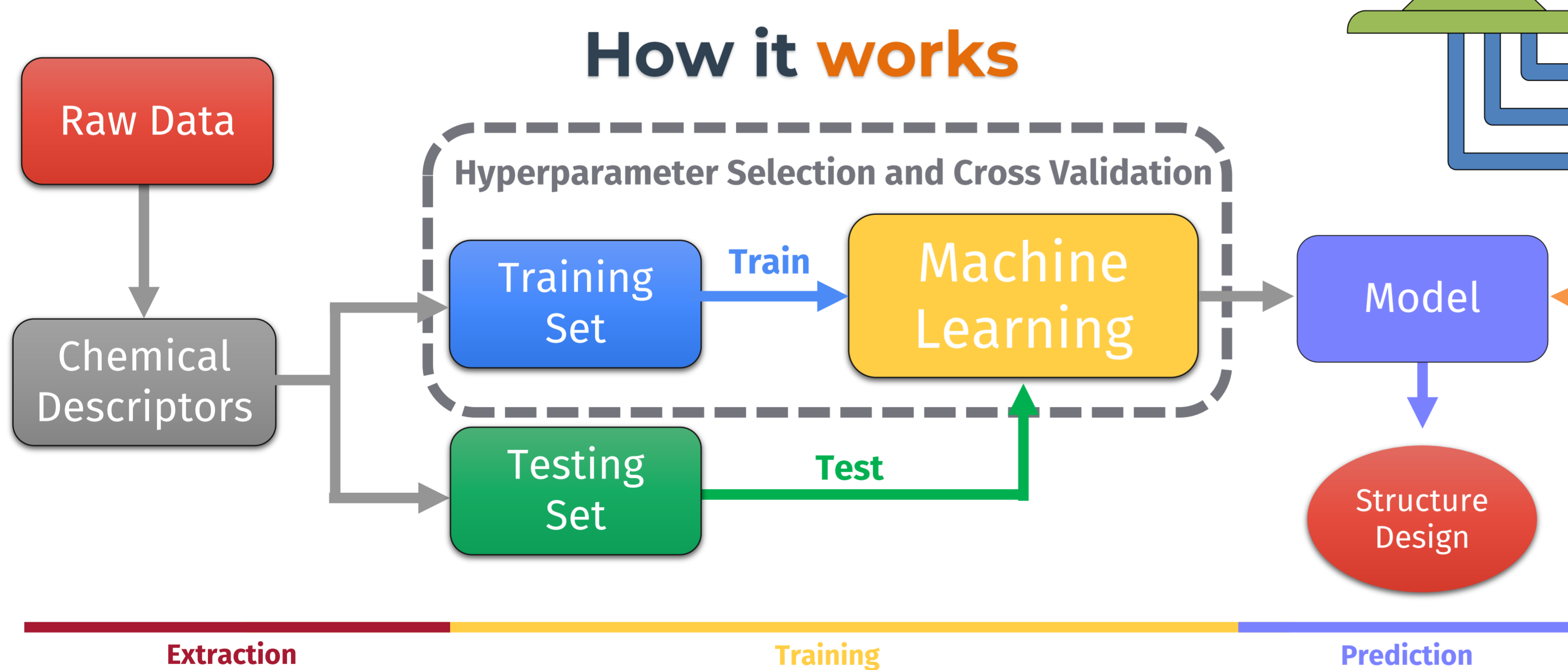
Computational models to design new catalytic solutions for epoxidation from biomass sources.

**Sustainable Data Driven**

## Our Model

- In-house developed framework
- Team of experienced computational chemists
- Funded with competitive Grant Projects

Using large data sets of catalytic activity from industry and academia, through models based on iQSAR design, it will provide new chemical structures.



By combining data science with computational chemistry, these models will assist on predicting new catalysts with unprecedented speed and accuracy.

Tested on our

### Proof of Concept

- Complex Thermodynamic Properties
- Prediction Accuracy: 99%
- estimated \$10k - \$20k Savings/batch

### Proprietary Algorithm

We design catalysts that can convert biomass into epoxides

### Major Project Outputs

Beyond PhD Project: 2-4 years

- Production of valuable and cost-effective catalysts
- Creating value from industry data
- Fast and economic production of high-end chemicals

### Where are we now?

And in 5 years ...

**30%** Progress: On Track

Tailor-Made Licensing Framework

**B2B Commercial Software**

Funded by: