

How Many Substances

*Are Regulated
Worldwide?*

How Many Substitutes

...And What Are Their Structures?

regulated
Worldwide?

NGI



Empa

Materials Science and Technology



TZW

Technologiezentrum
Wasser



Sivani Baskaran



Hans Peter Arp



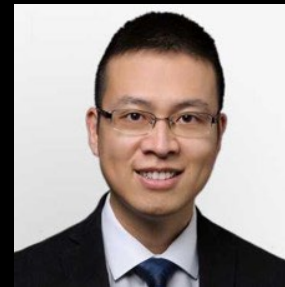
Emma Palm



Emma Schymanski



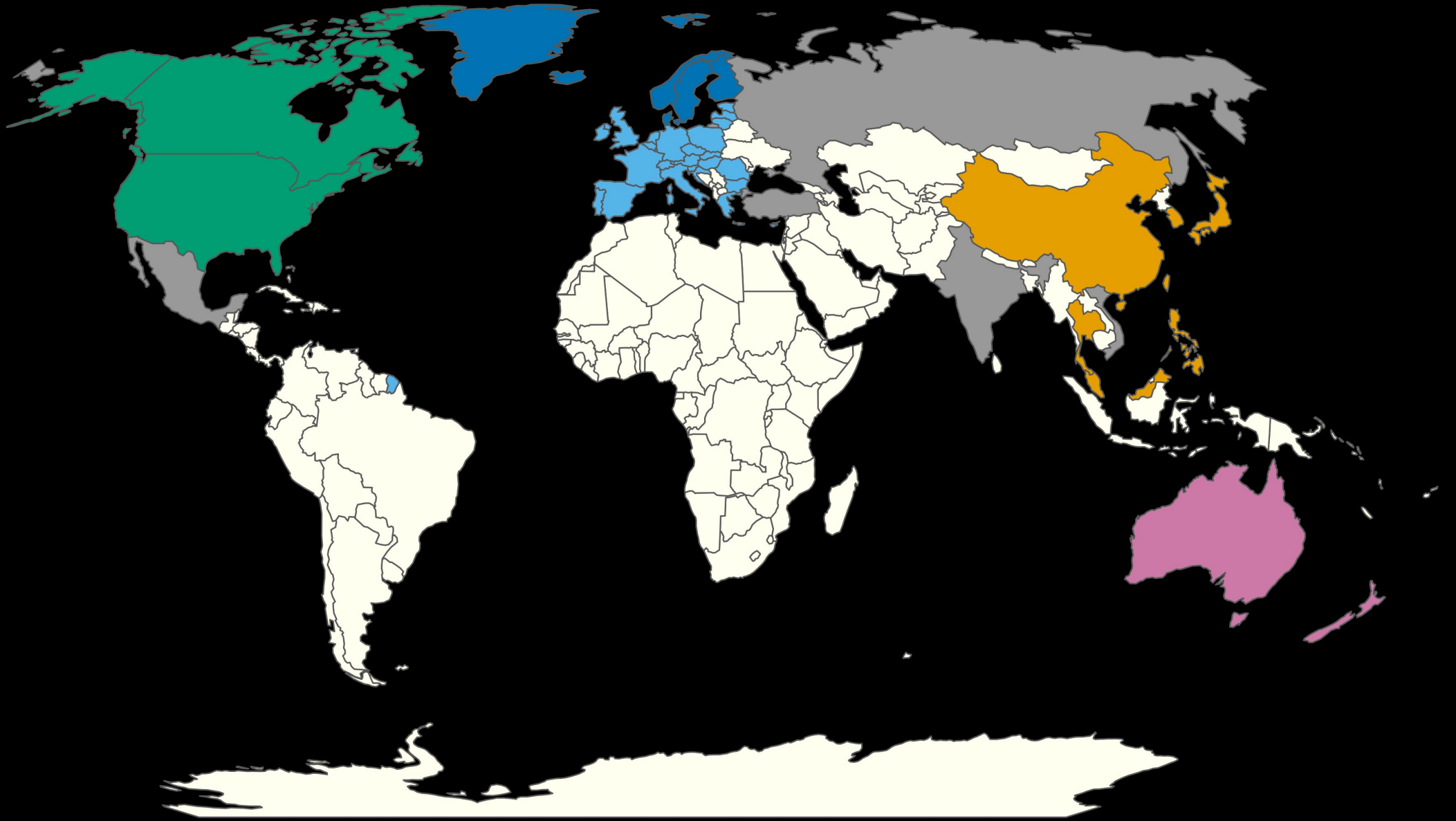
Parviel Chirsir



Zhanyun Wang



Sarah Hale

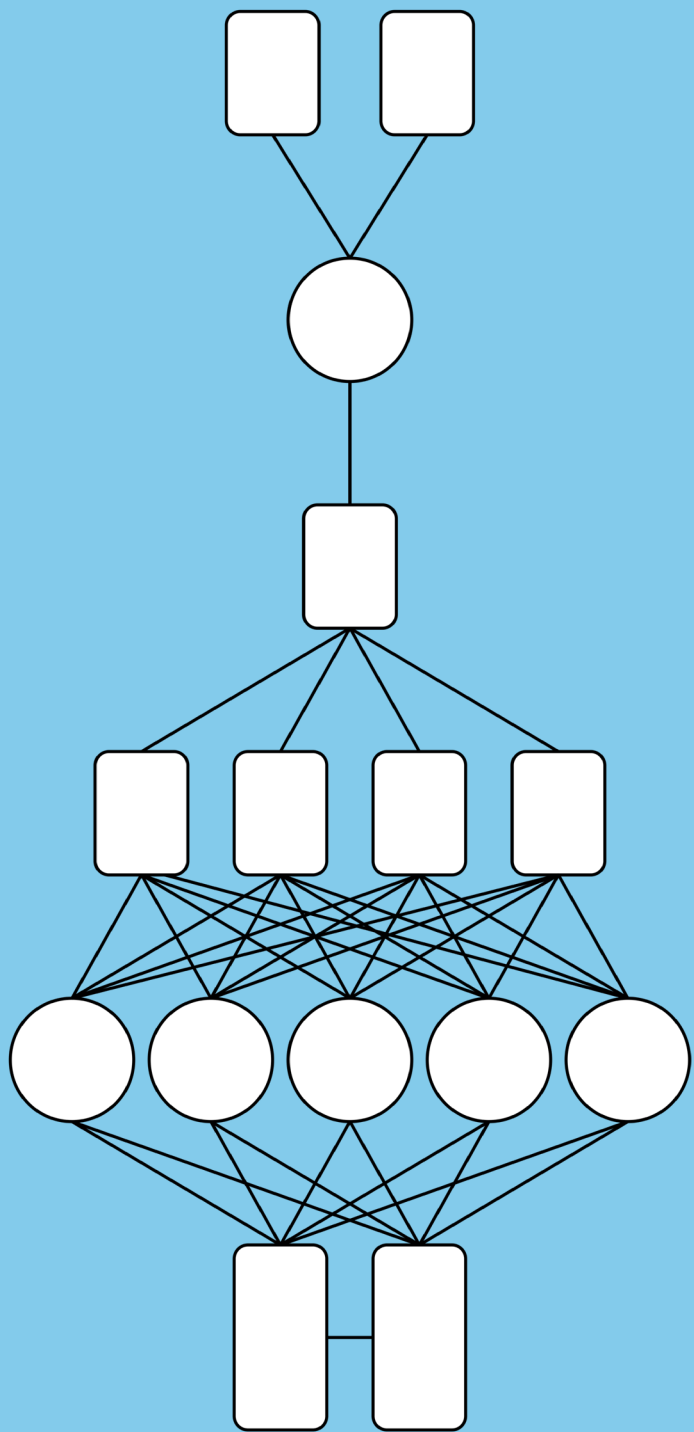


A few words about “chemical” data

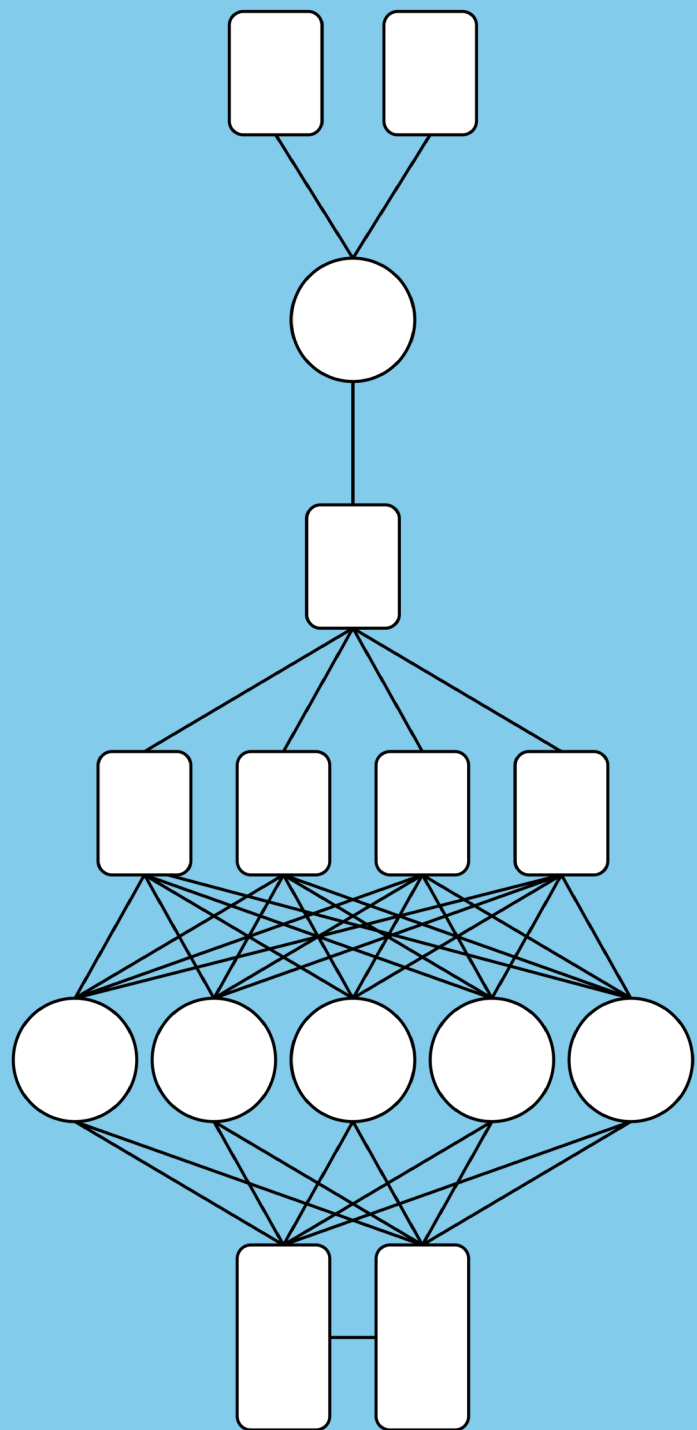
FAIR

clean

Global Chemical Inventory

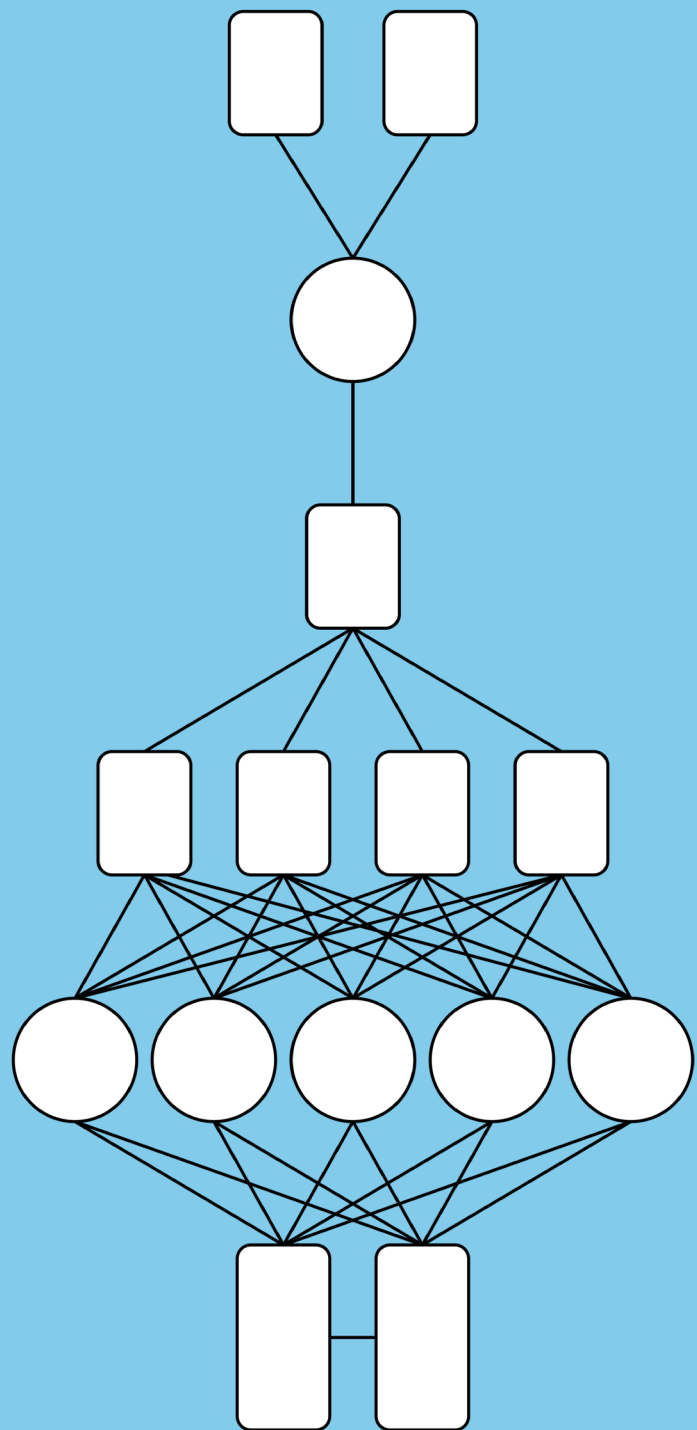


The
cleanventory
Approach



Input information

CAS Registry Numbers, chemical names, EC numbers, abbreviations, ...

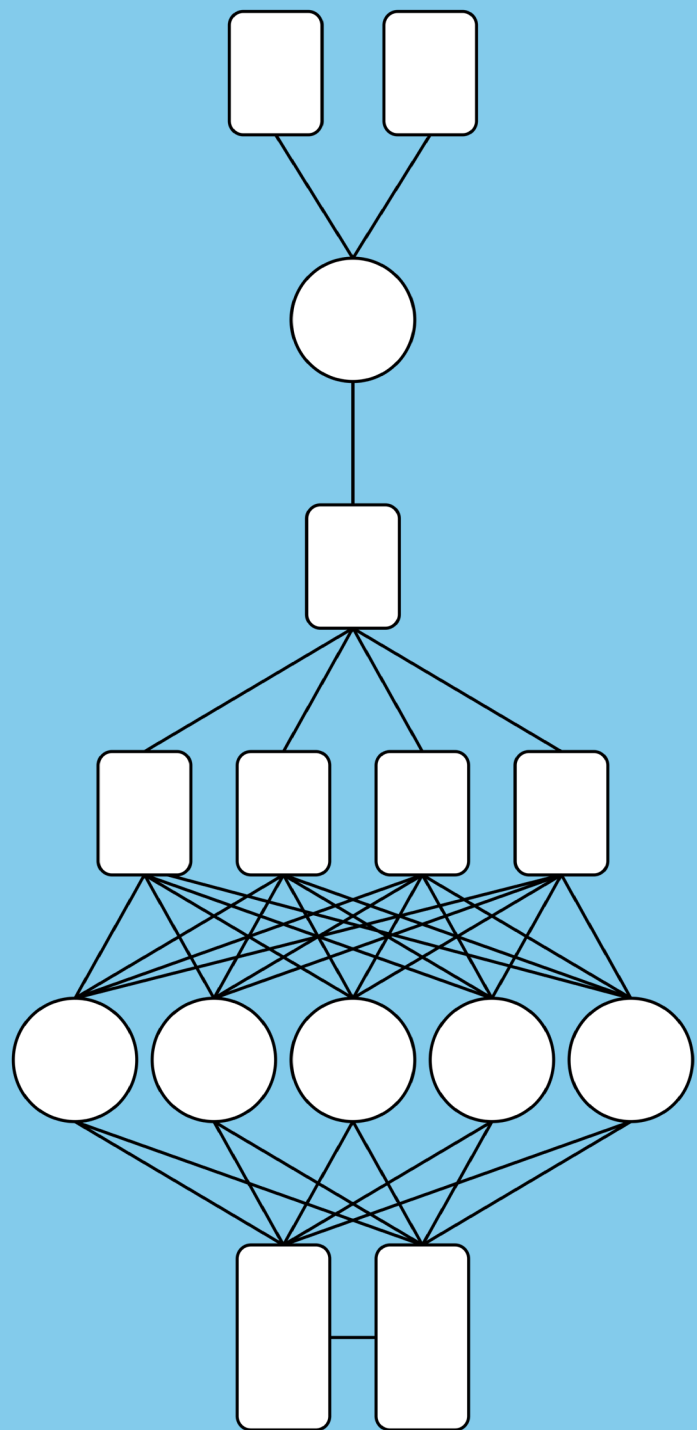


API Services

PubChem, CompTox, CAS Common Chemistry, CACTVS

Input information

CAS Registry Numbers, chemical names, EC numbers, abbreviations, ...



Candidate Structures

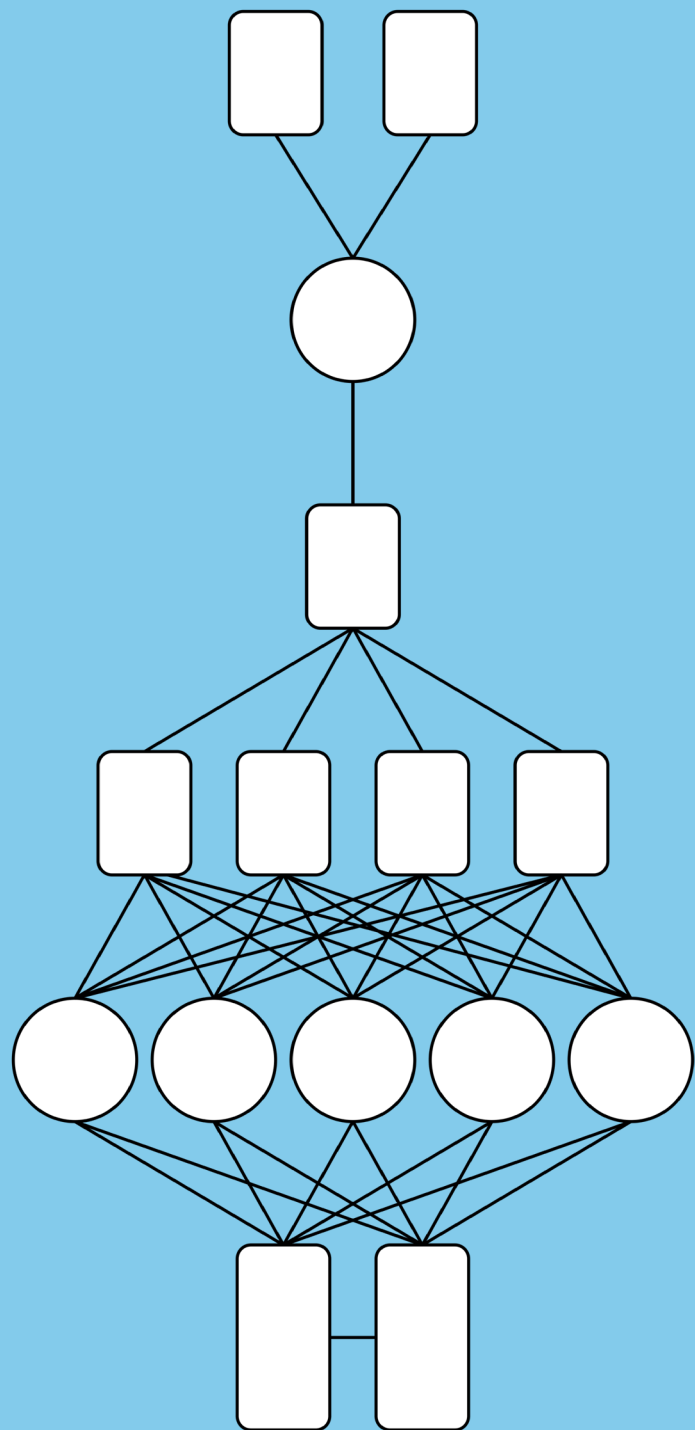
Ranked API results, InChI

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Input information

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Most-Likely Structure

Based on highest consensus rank

Candidate Structures

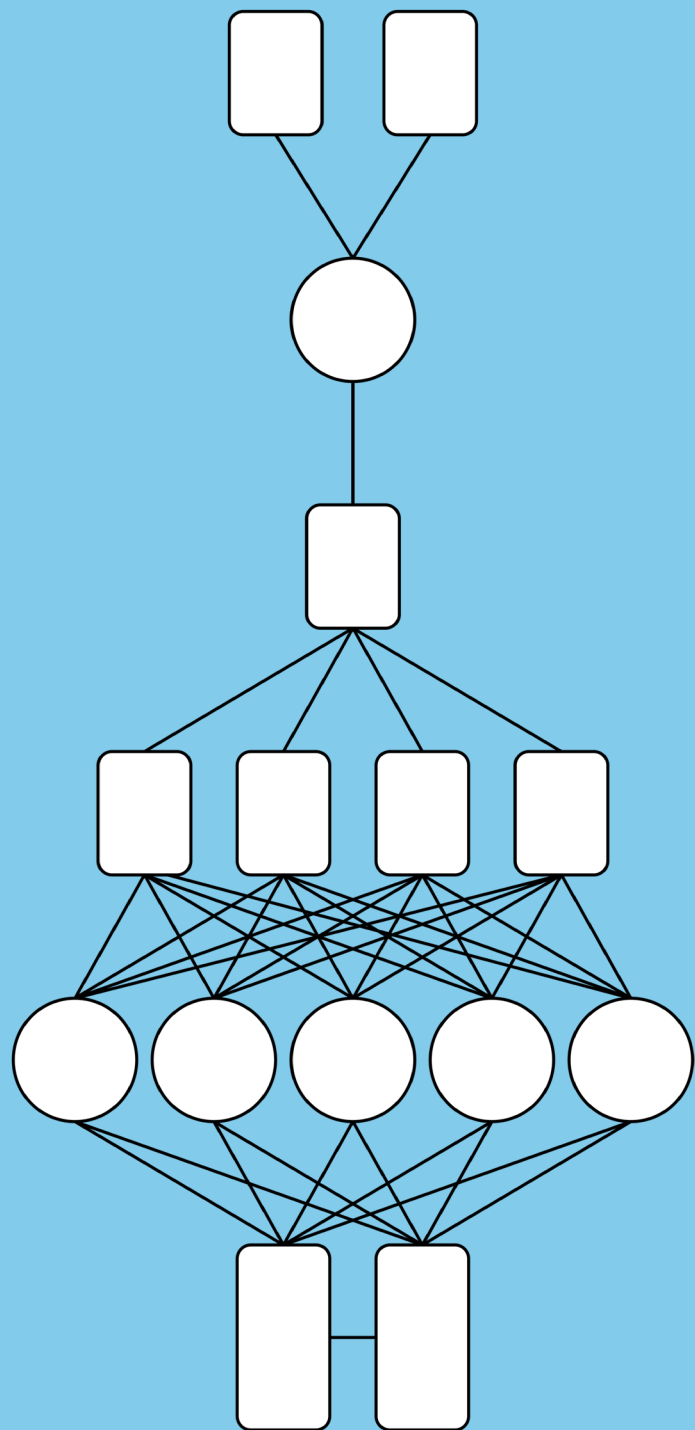
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OpenBabel

Splitting of multi-component structures

Most-Likely Structure

Based on highest consensus rank

Candidate Structures

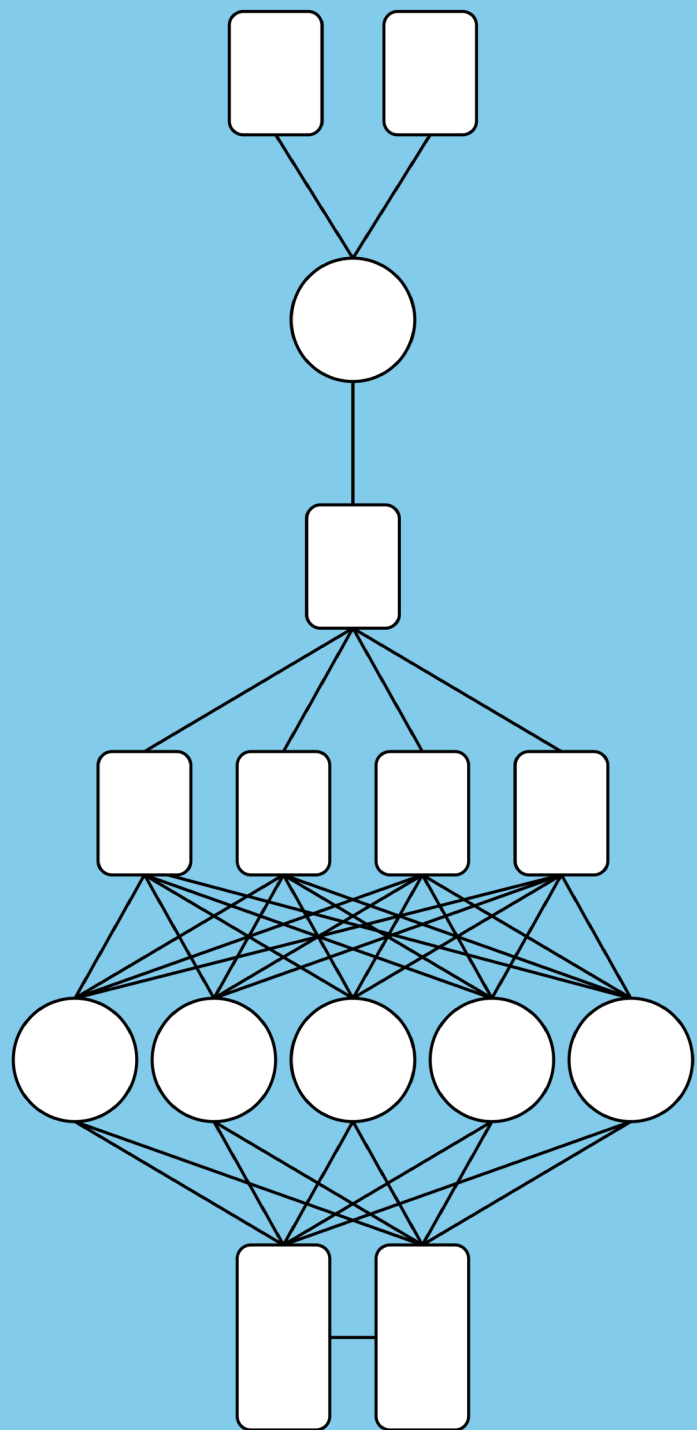
Ranked API results, InChI

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Individual Structures

Single-component structures

OpenBabel

Splitting of multi-component structures

Most-Likely Structure

Based on highest consensus rank

Candidate Structures

Ranked API results, InChI

API Services

PubChem, CompTox, CAS Common Chemistry, CACTVS

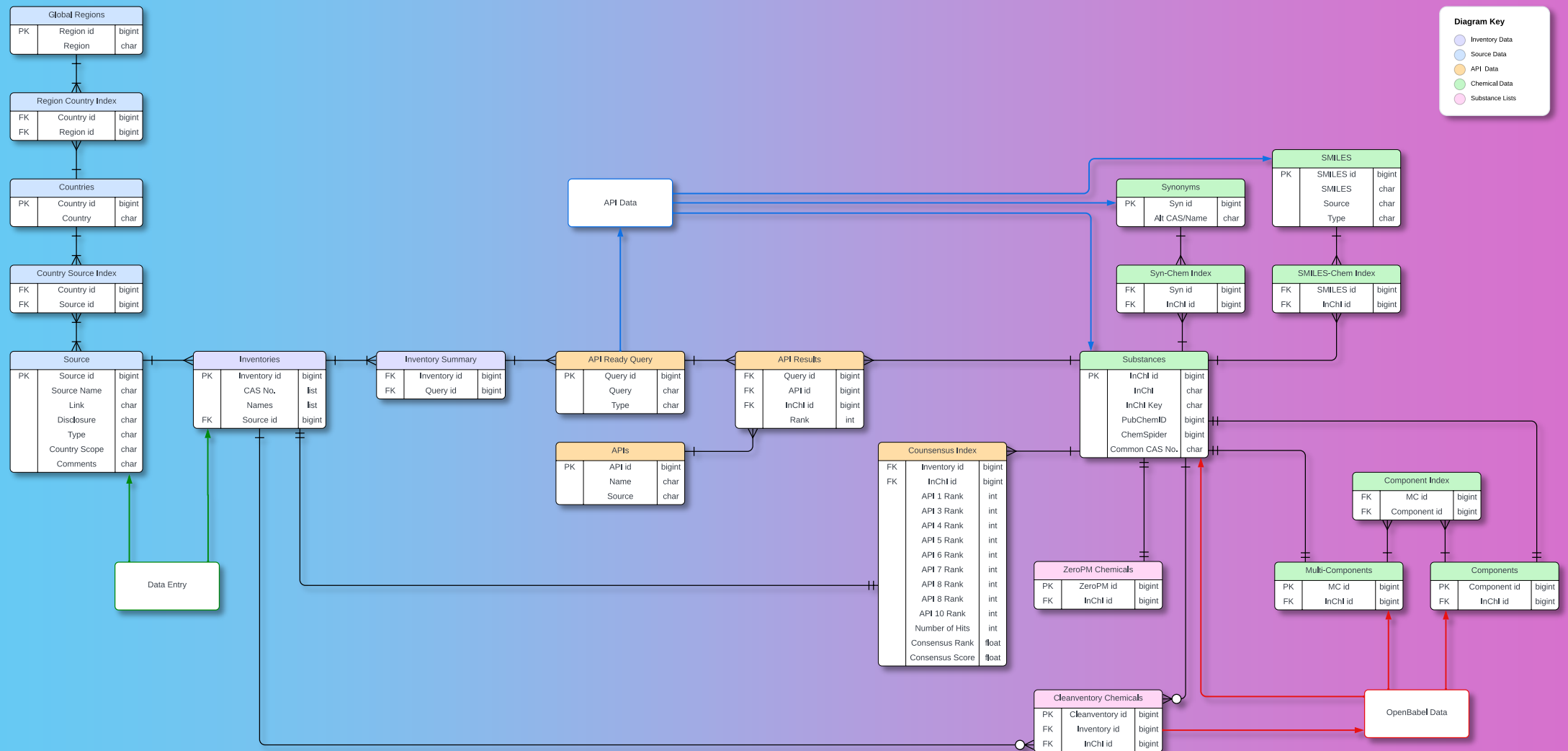
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The ZeroPM Database



The ZeroPM Database



25 Inventories

25 Inventories

> 500 000 Entries*

25 Inventories

> 500 000 Entries

> 1 500 000 Search Terms

25 Inventories

> 500 000 Entries

> 1 500 000 Search Terms

> 400 000 Potential Structures

25 Inventories

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140 123 Zero  PM Substances

140 123 Zero  PM Substances

140 123 Zero  PM Substances

Inventory Information

Regions

Countries

...

140 123 Zero PM Substances

Inventory Information

Regions

Countries

...

Identifiers and Structures

Provided Identifiers

Consensus Structure

...

140 123 Zero PM Substances

Inventory Information

Regions

Countries

...

Identifiers and Structures

Provided Identifiers

Consensus Structure

...

Assessments

Persistence

Mobility

...

<https://database.ZeroPM.eu>

<https://github.com/ZeroPM-H2020>

<https://zenodo.org/communities/zeropm-h2020>

<https://pubchem.ncbi.nlm.nih.gov/source/25168>

ZeroPM

ZeroPM: Zero pollution of
Persistent, Mobile substances

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