

How Many Chemicals

*Are Regulated
Worldwide?*

How Many Chemicals

...And What Are Their Structures?

Are They Regulated
Worldwide?

So FAIR, so *clean*

How the *cleanventory* Approach Provides
Reliable Data for Chemical Structures
Regulated in Global Trade Markets

Raoul Wolf, Senior Scientist, Norwegian Geotechnical Institute (NGI)

ZeroPM

ZeroPM: Zero pollution of
Persistent, Mobile substances

This project has received funding from the
European Union's Horizon 2020 research
and innovation programme under grant
agreement number 101036756



Work Package 5

Substance Grouping

NGI



Materials Science and Technology



TZW
Technologiezentrum
Wasser



Sivani Baskaran



Hans Peter Arp



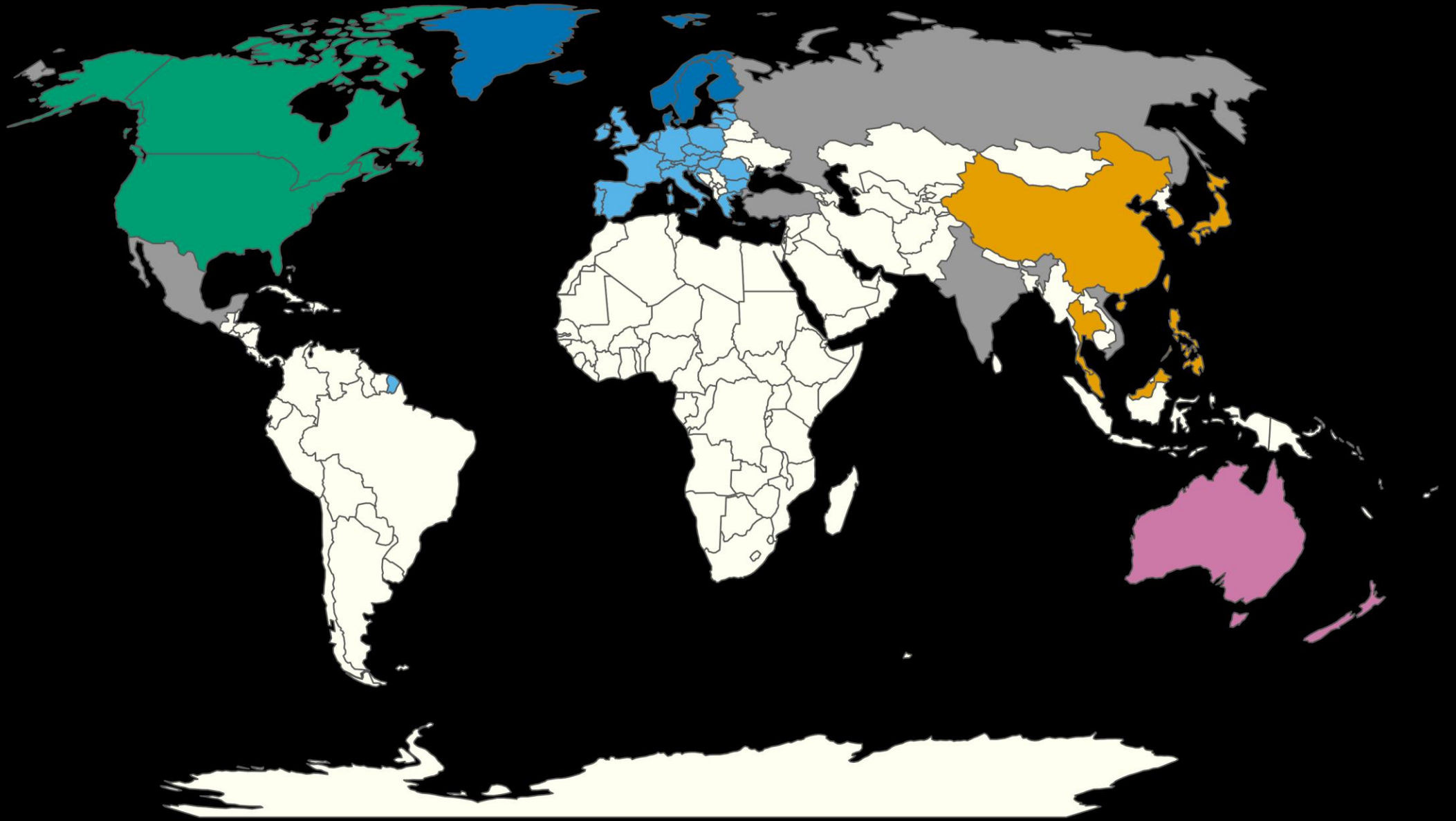
Emma Schymanski



Zhanyun Wang



Sarah Hale

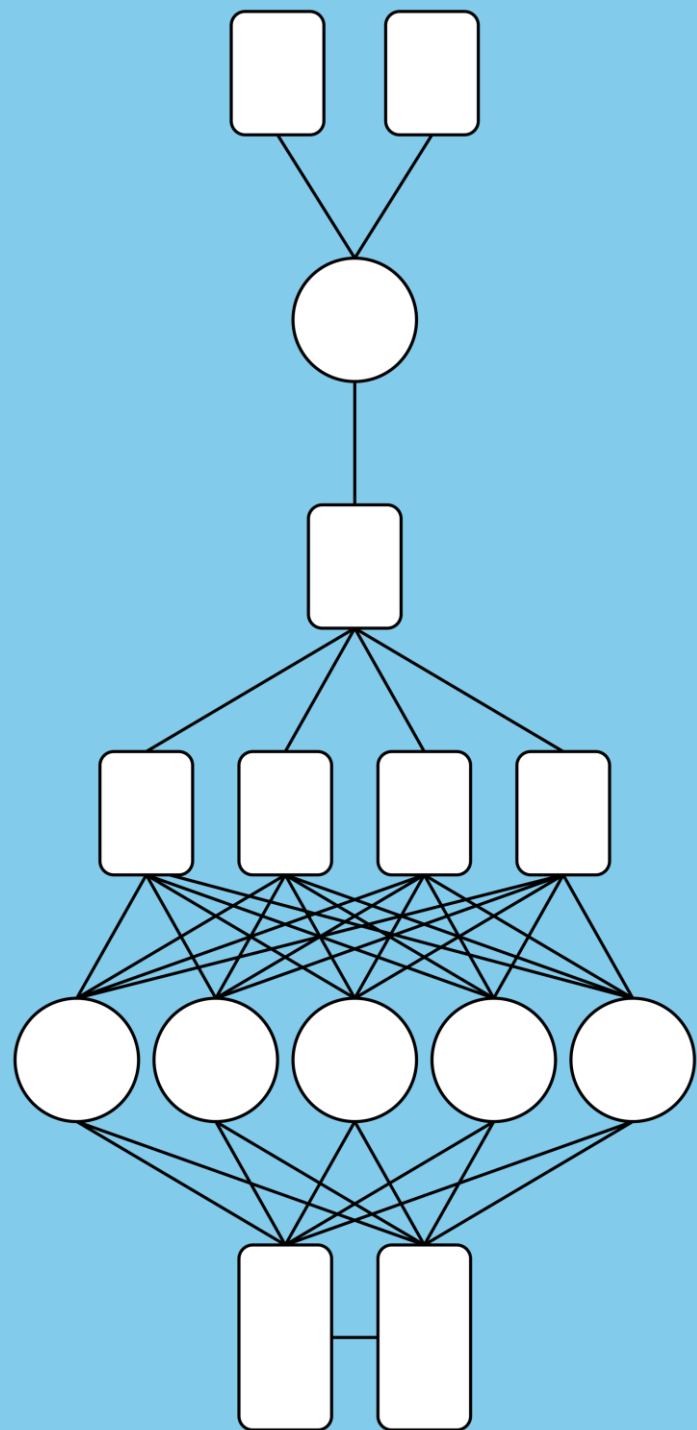


A few words about chemical data quality

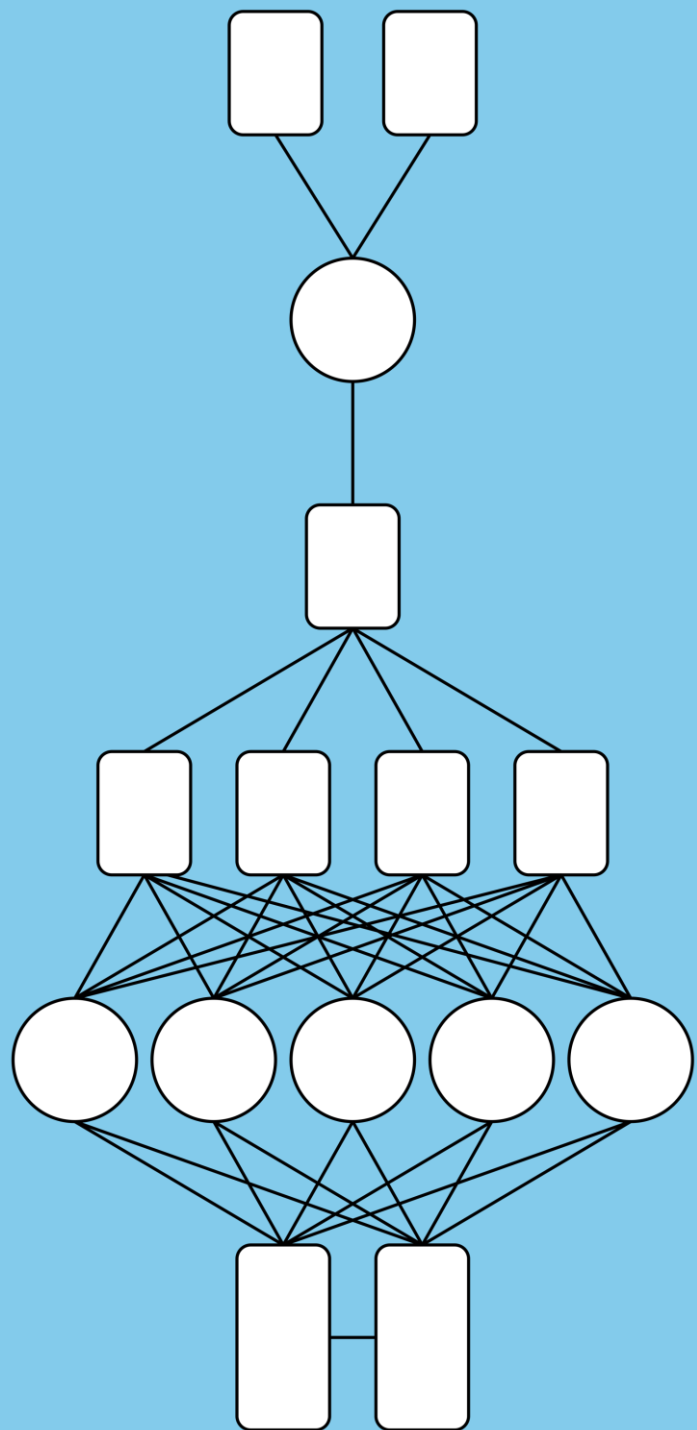
FAIR

clean

Global Chemical Inventory

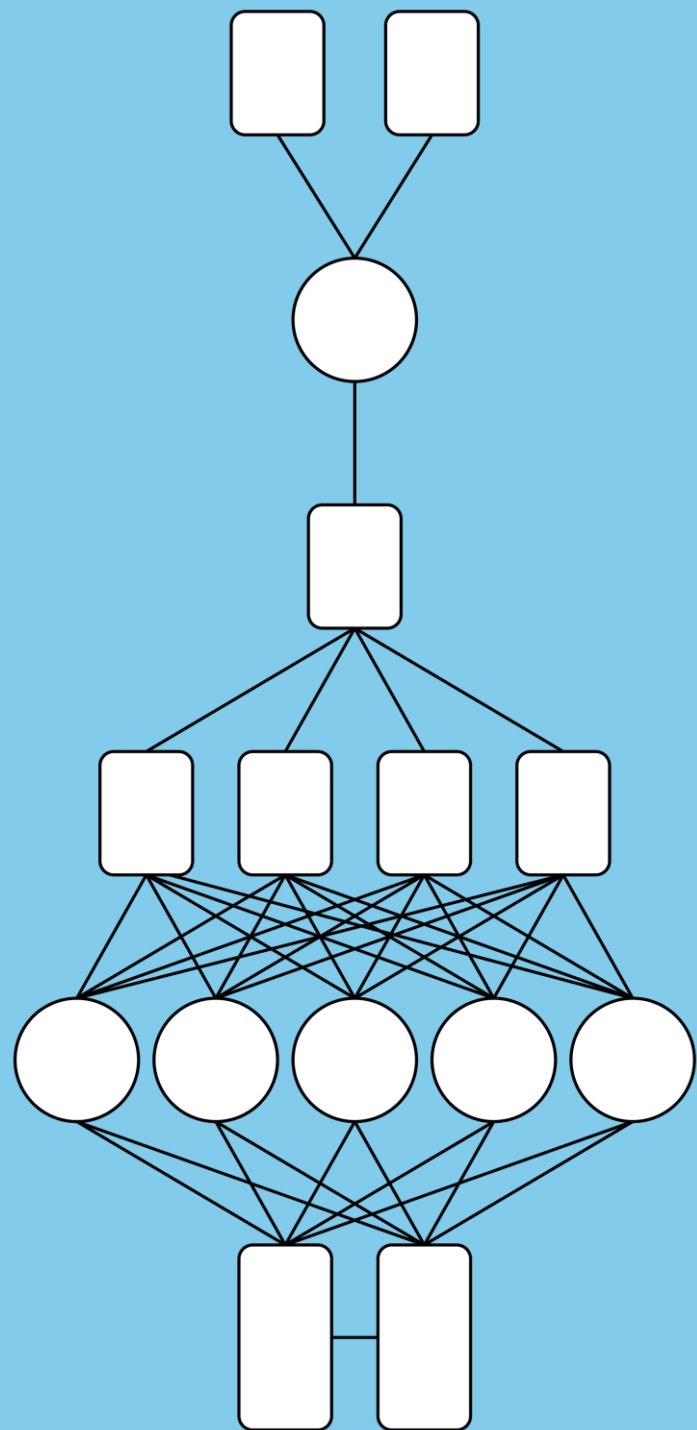


The *cleanventory* Approach



Input information

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

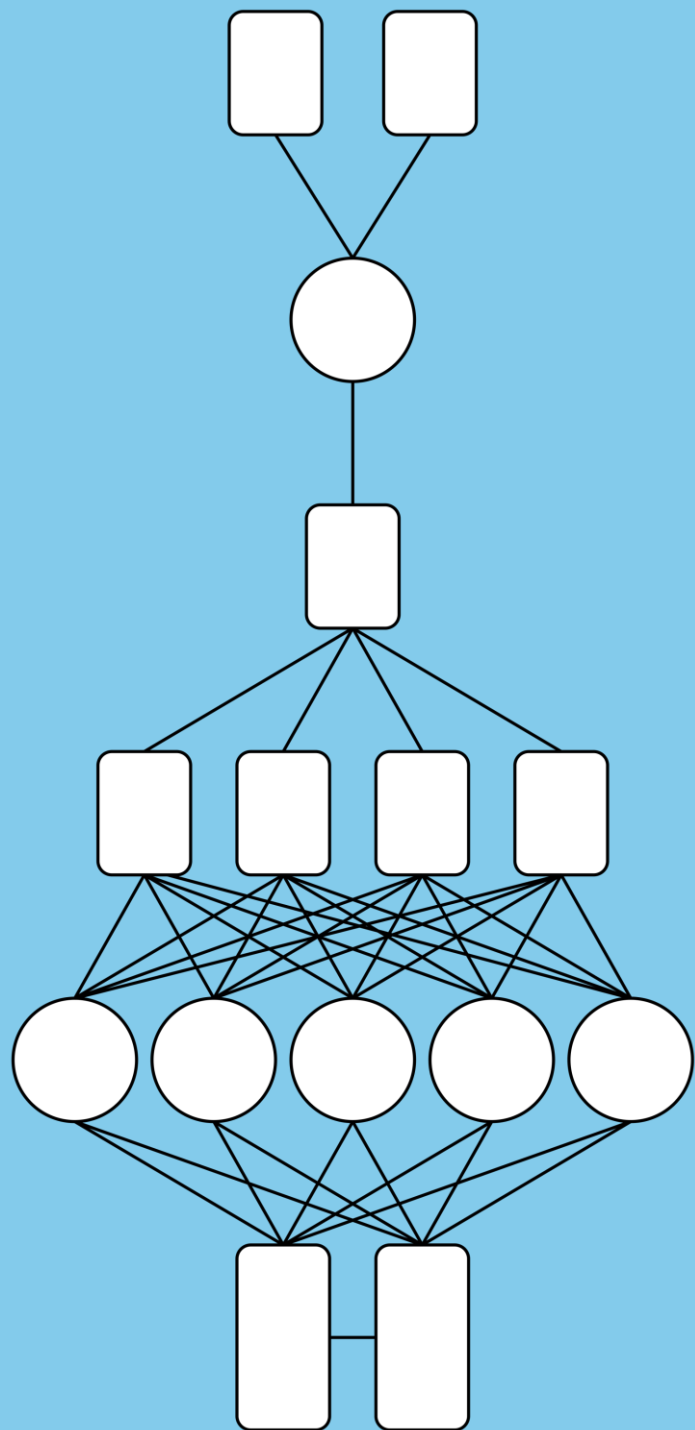


API Services

PubChem, CompTox, CAS Common Chemistry, CACTVS

Input information

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



Candidate Structures

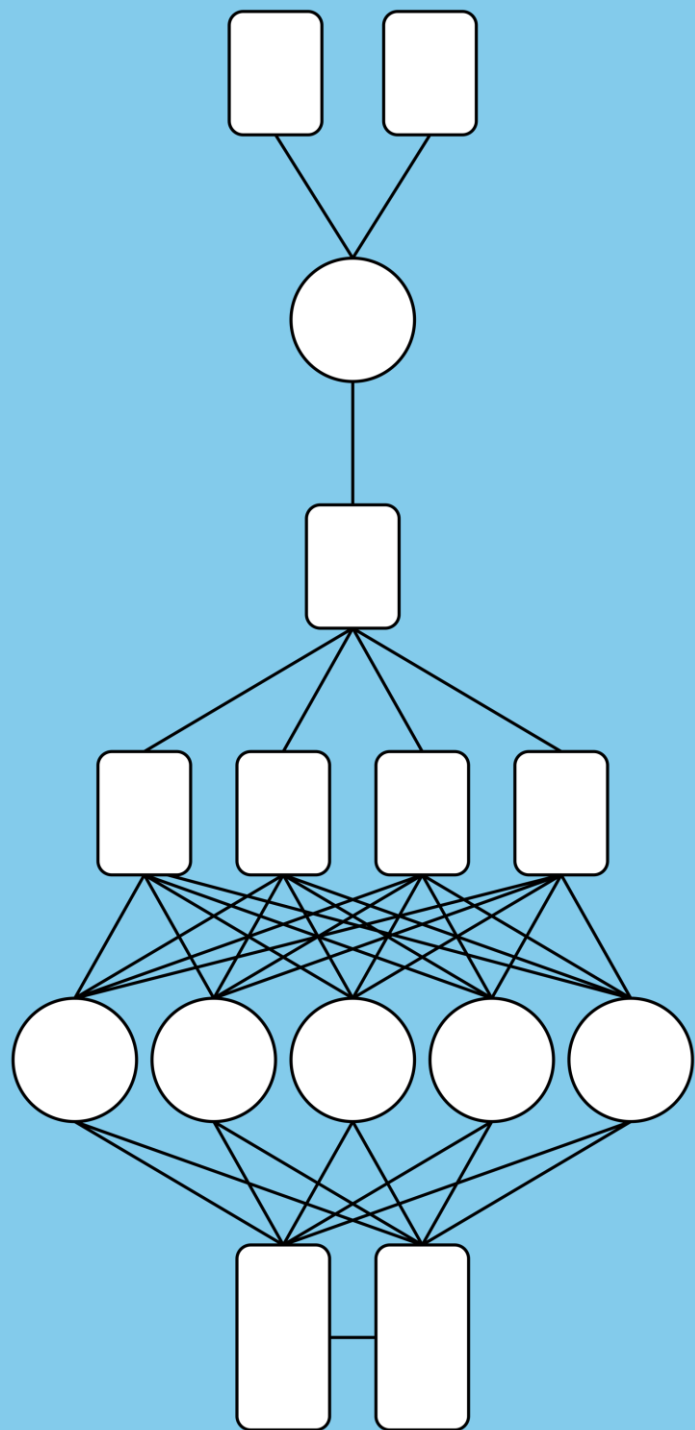
Ranked API results, InChI

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Most-Likely Structure

Based on highest consensus rank

Candidate Structures

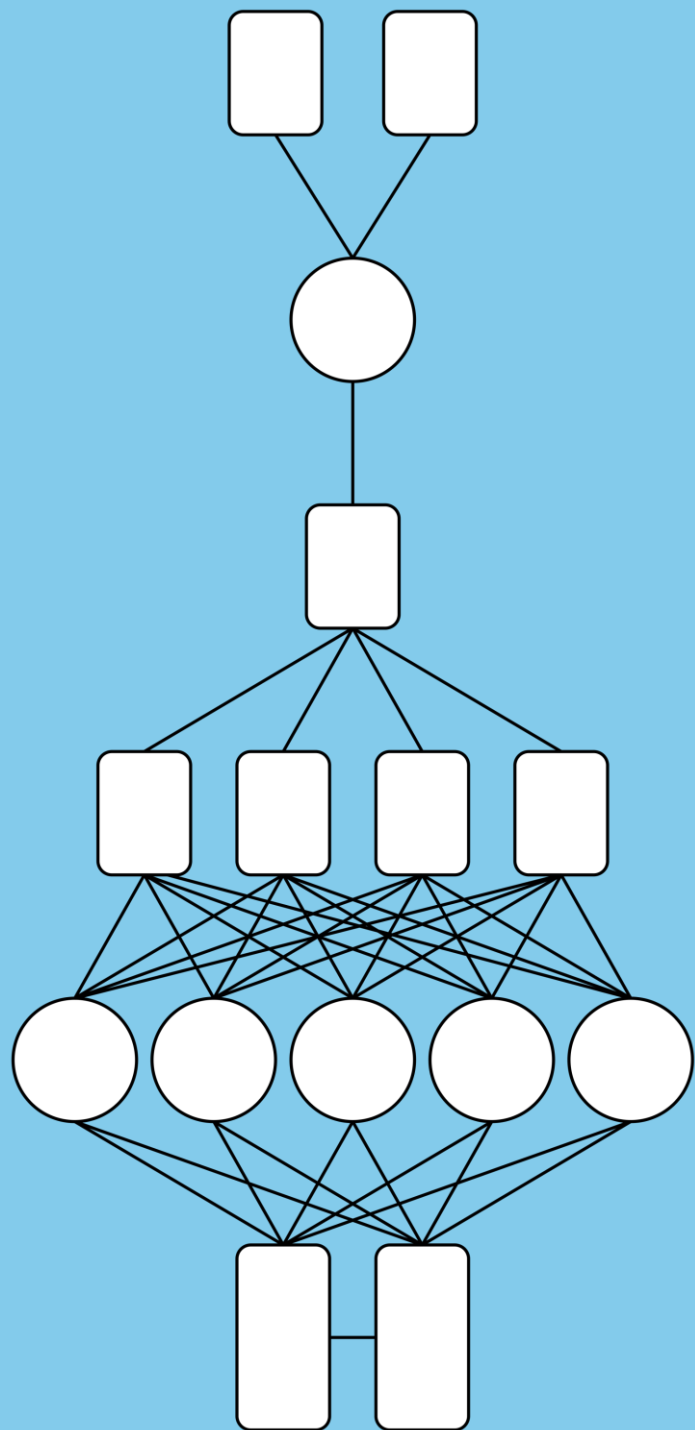
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OpenBabel

Splitting of multi-component structures

Most-Likely Structure

Based on highest consensus rank

Candidate Structures

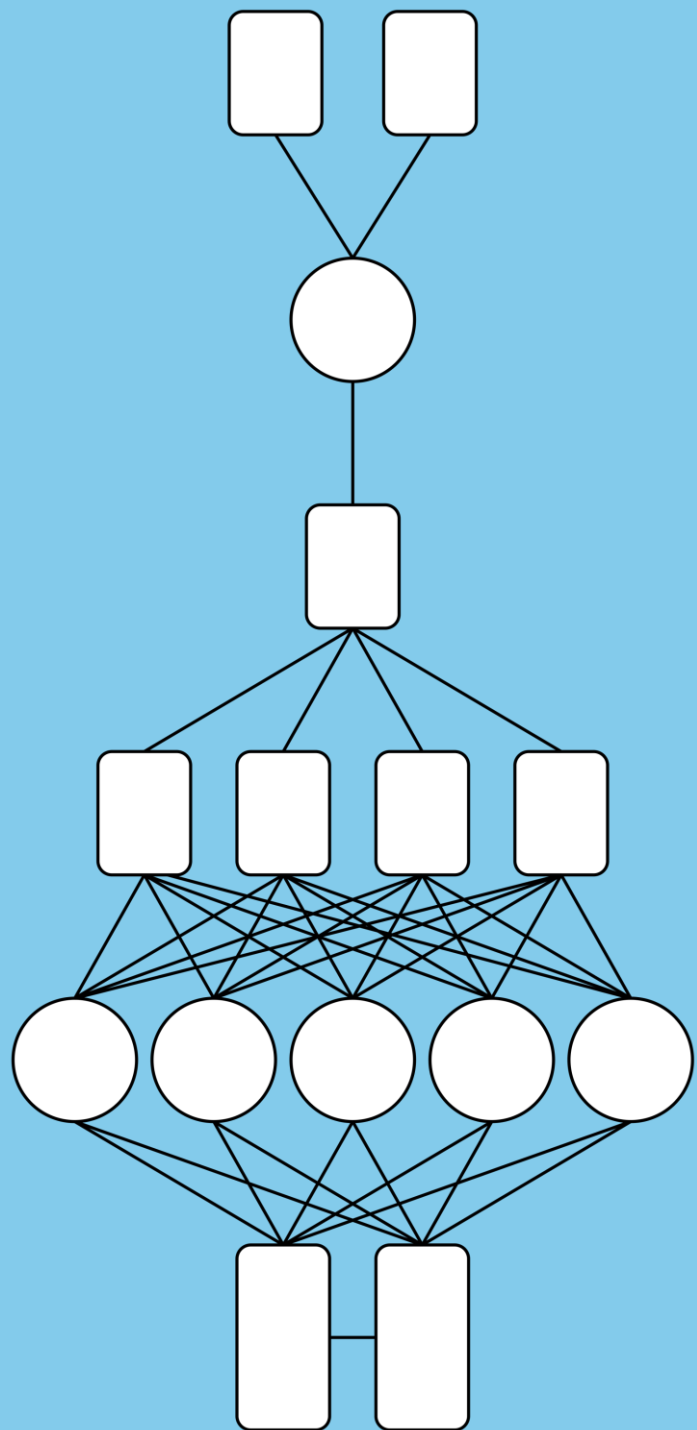
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Individual Structures

Single-component structures

OpenBabel

Splitting of multi-component structures

Most-Likely Structure

Based on highest consensus rank

Candidate Structures

Ranked API results, InChI

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32 Inventories

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> 500 000 Entries*

32 Inventories

> 500 000 Entries

> 1 500 000 Search Terms

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> 400 000 Potential Structures

32 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 ZerO₂PM 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

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