

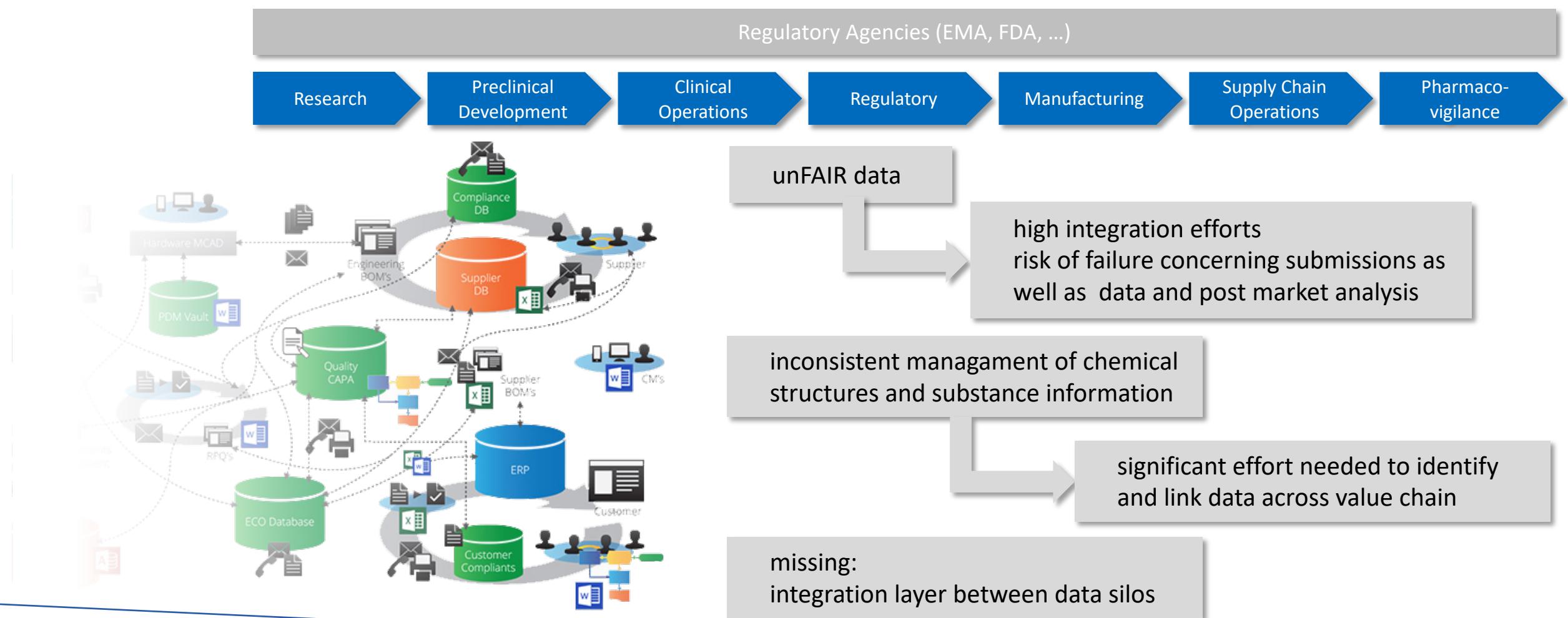
Semantic Chemical Data Management

From FAIR to IDMP Compliance

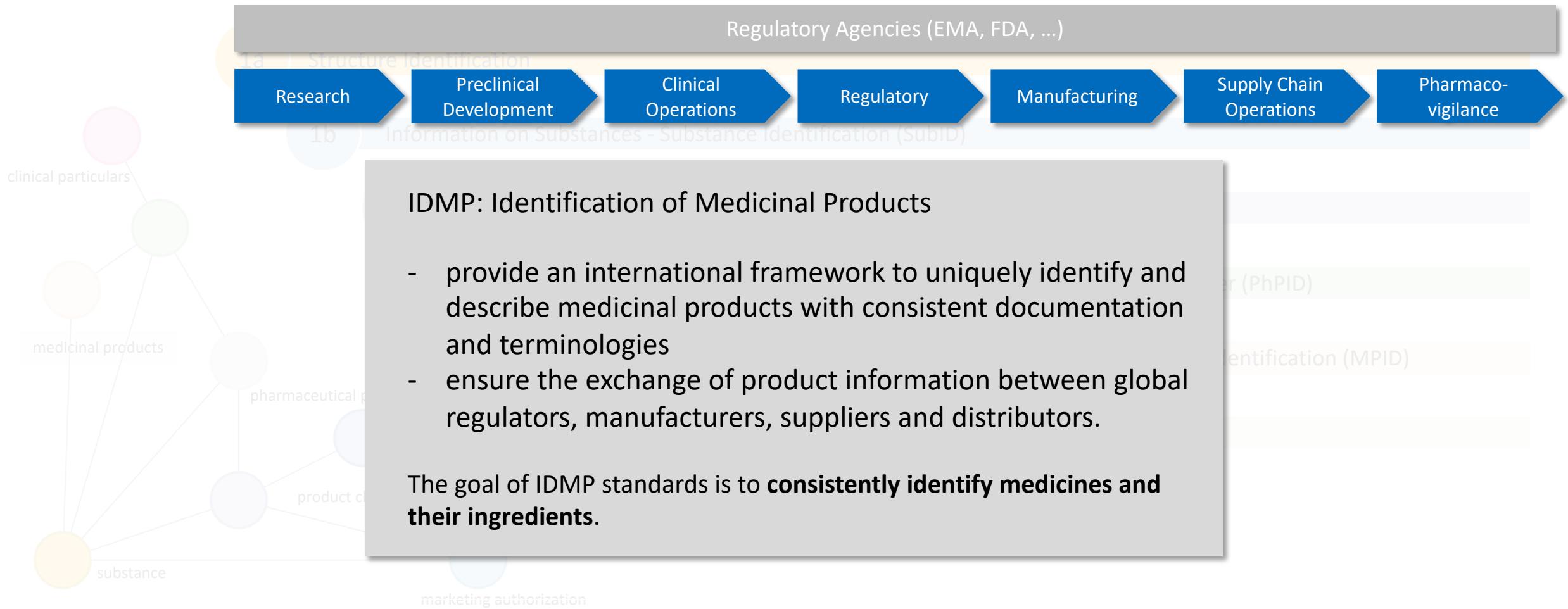
Dr. Matthias Nolte

matthias.nolte@chemantics.com

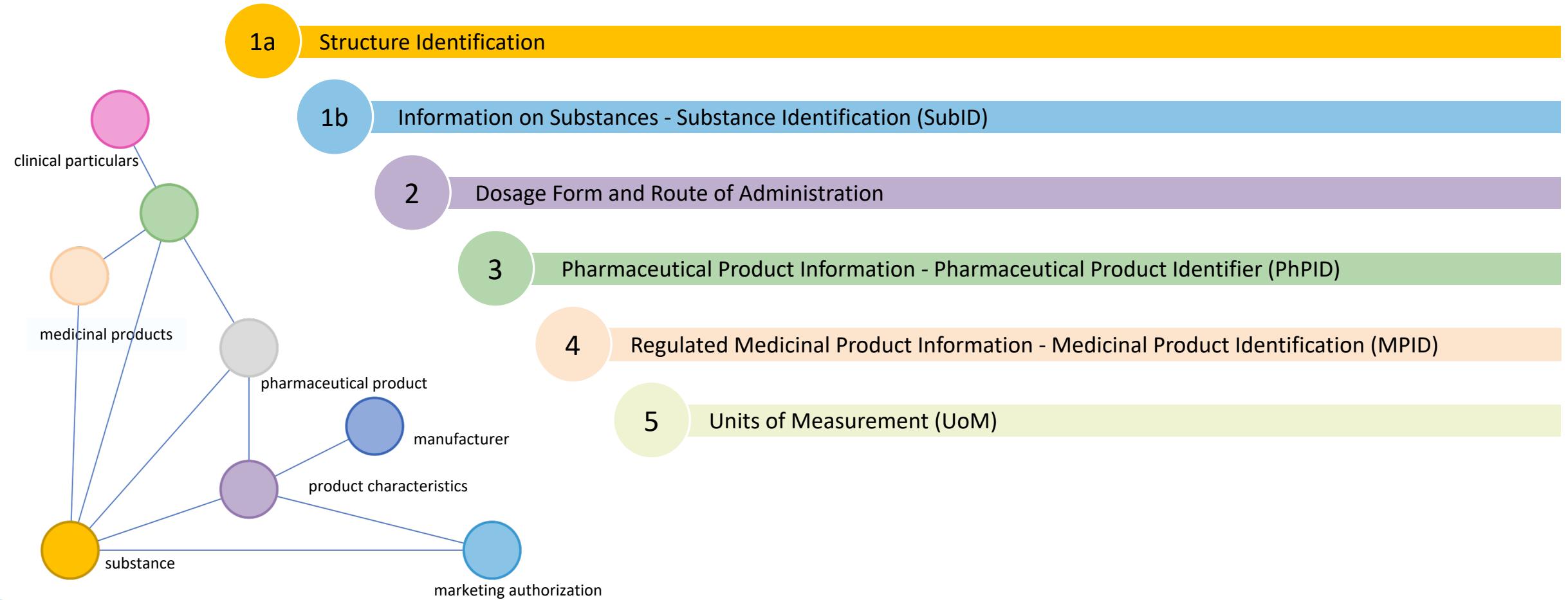
Chemical Data Management Across the Pharmaceutical Value Chain



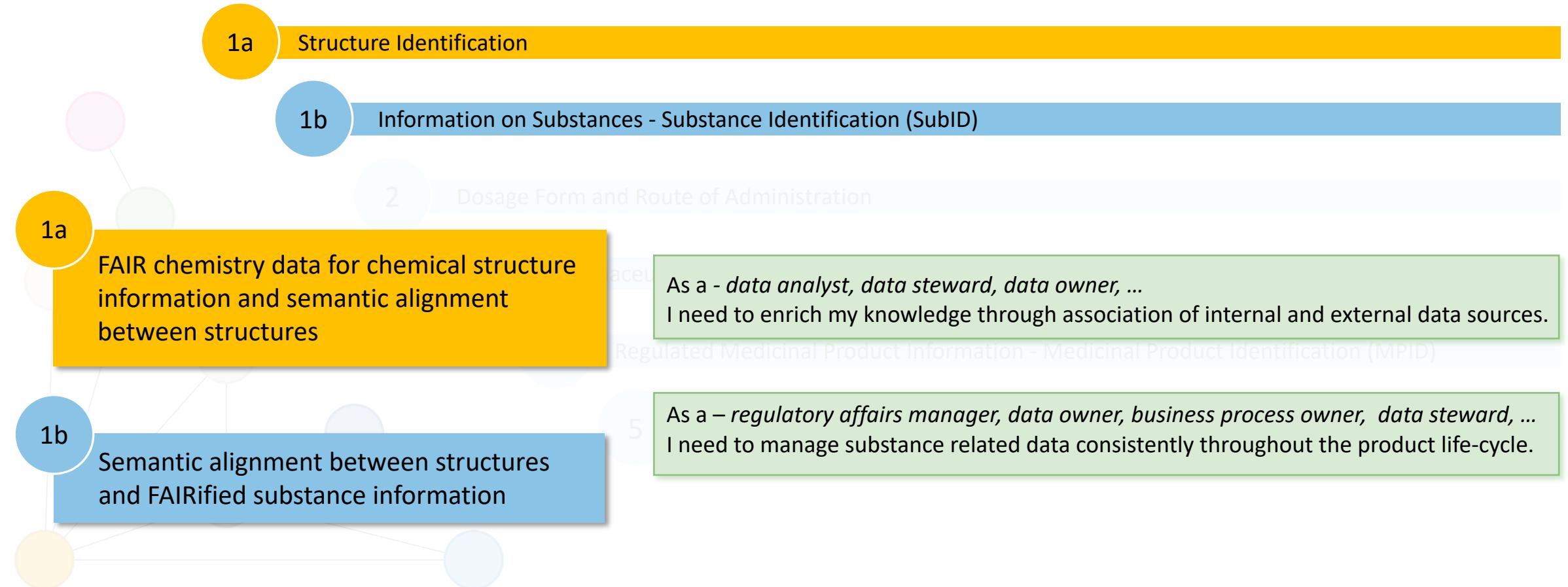
The Pistoia IDMP Core Ontology Project



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FAIR Chemistry (and FAIR Biology)



Registration

- generate normalized structure representation, PID
- generate structure/structure relationships

Organisation

- maintain source level database organization,
- categorize data sources via semantic relationships

Annotation

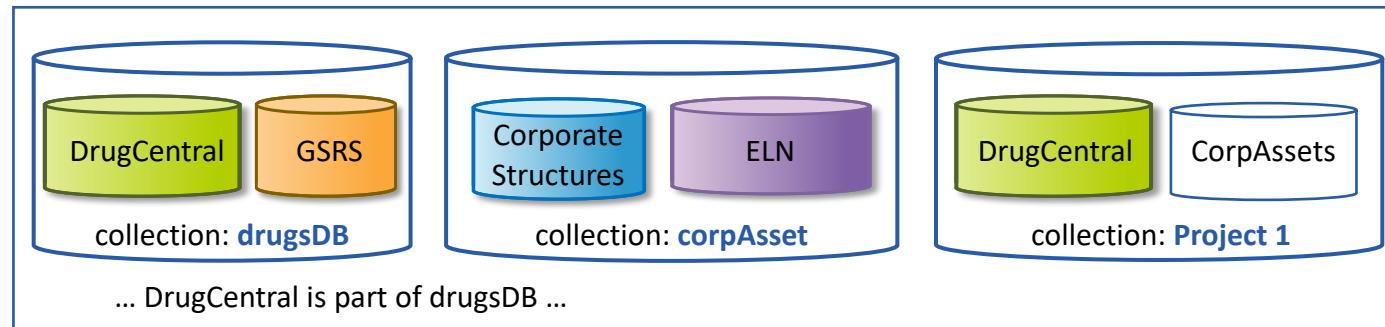
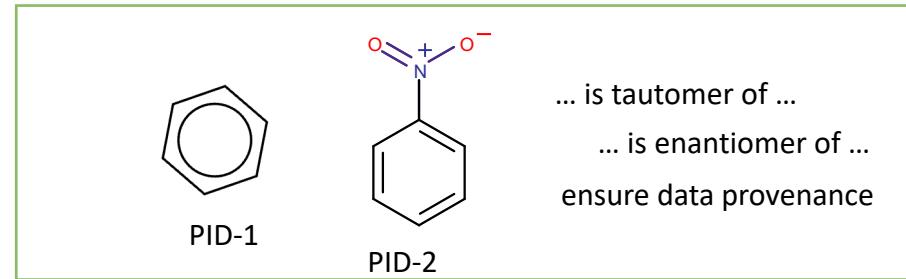
- annotate chemical entities through generation of multi-level abstractions and subsystem identification

Classification

- classify chemical structures based on chemical structure classes

Integration

- API to access any data entity in the Chempacts eco system
- API to calculate structure based properties



... is an alcohol ...
... contains amino acid ...
... is a hydrocarbon ...
~ 2500 classifications

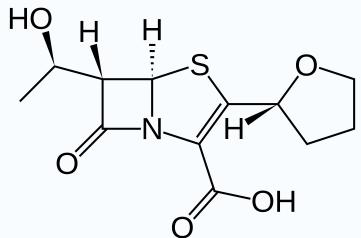
... has ring ...
17 annotation types / relationships

... create a new database collection
... register new compounds
... get calculated attributes
... search specific structure collections

Structure Graph: faropenem

Integration
access

Faropenem is an orally active beta-lactam antibiotic belonging to the penem group.[\[WIKI\]](#)



The **PubChem** database contains chemical molecules and their activities against biological assays.

The **DrugBank** database contains information on drugs and drug targets

The **Human Metabolome Database** (HMDB) contains detailed information about small molecule metabolites found in the human body.

The **Norman** Suspect List Exchange collects data relevant for environmental monitoring purposes.

PubChem

DrugBank

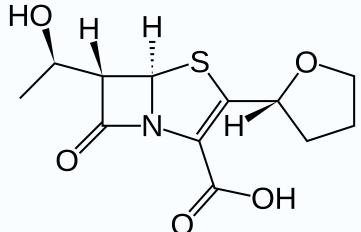
Human...

NORMAN

Structure Graph: faropenem



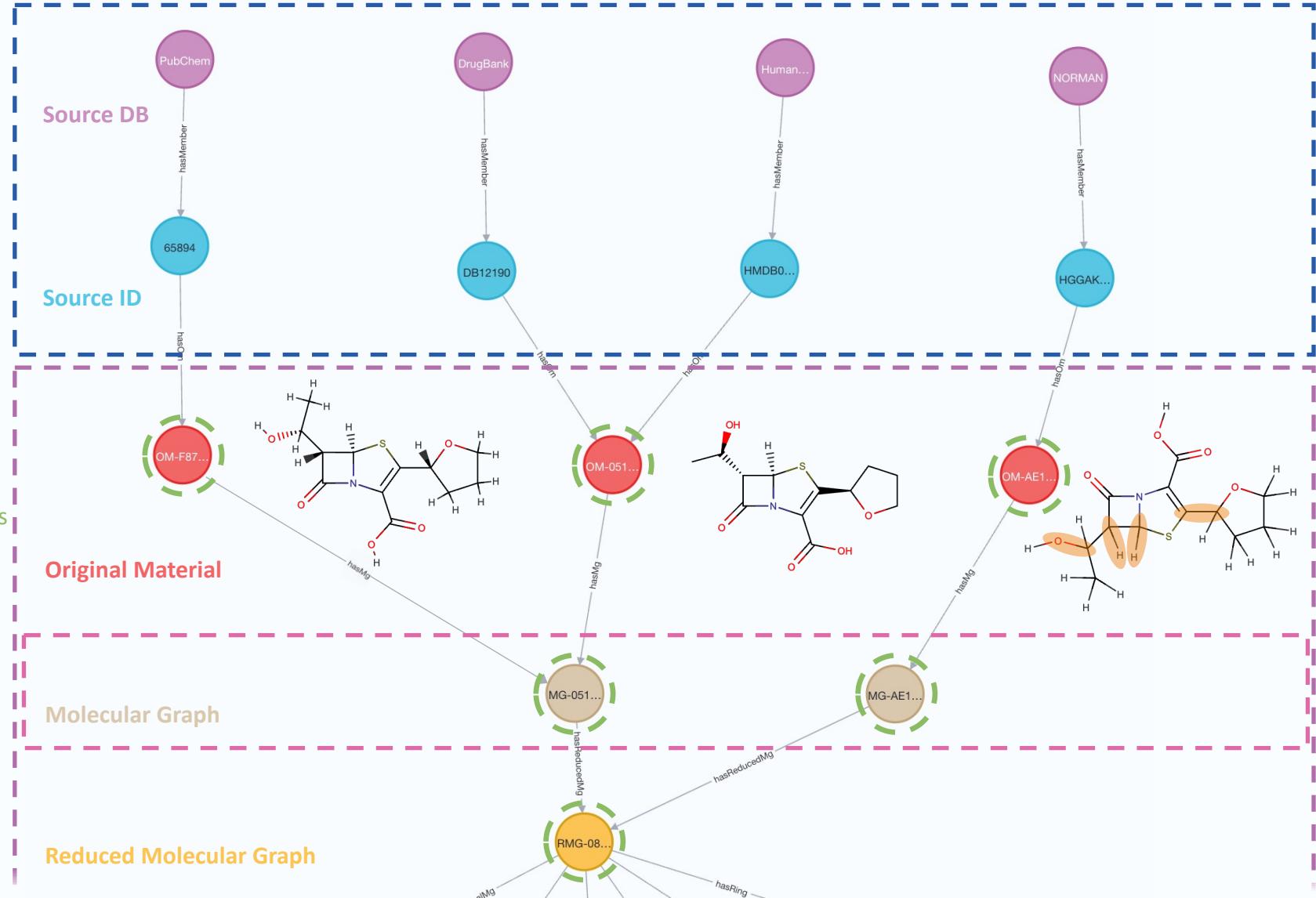
Integration
access



Organisation
provenance

Annotation
enrichment
Registration
structure PIDs

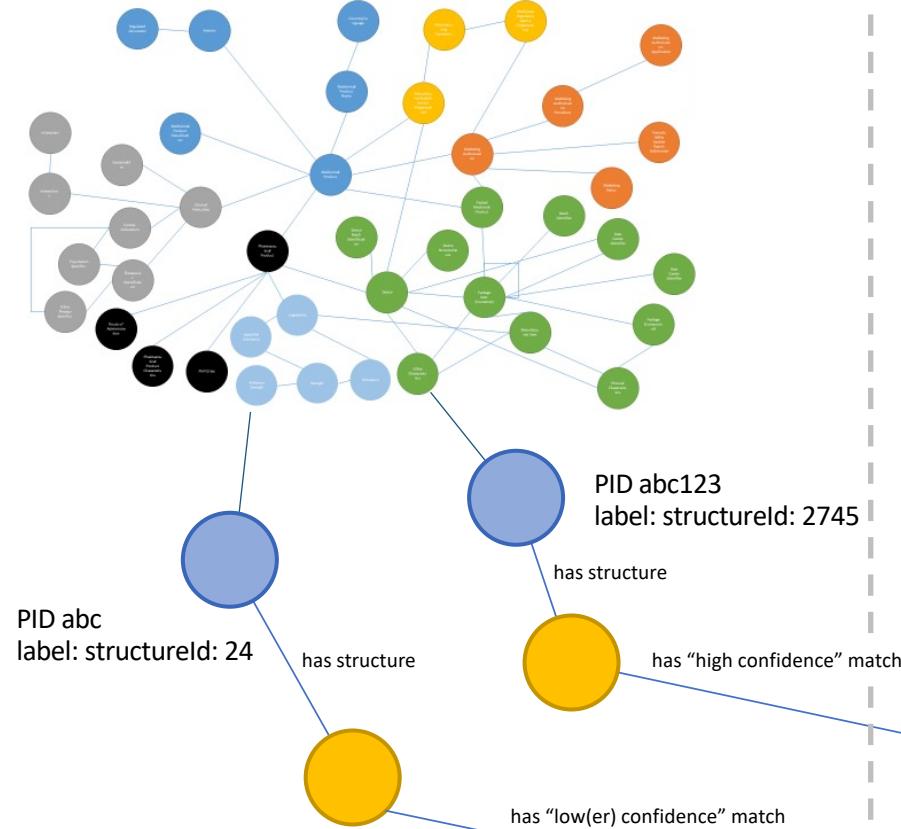
Classification
metadata



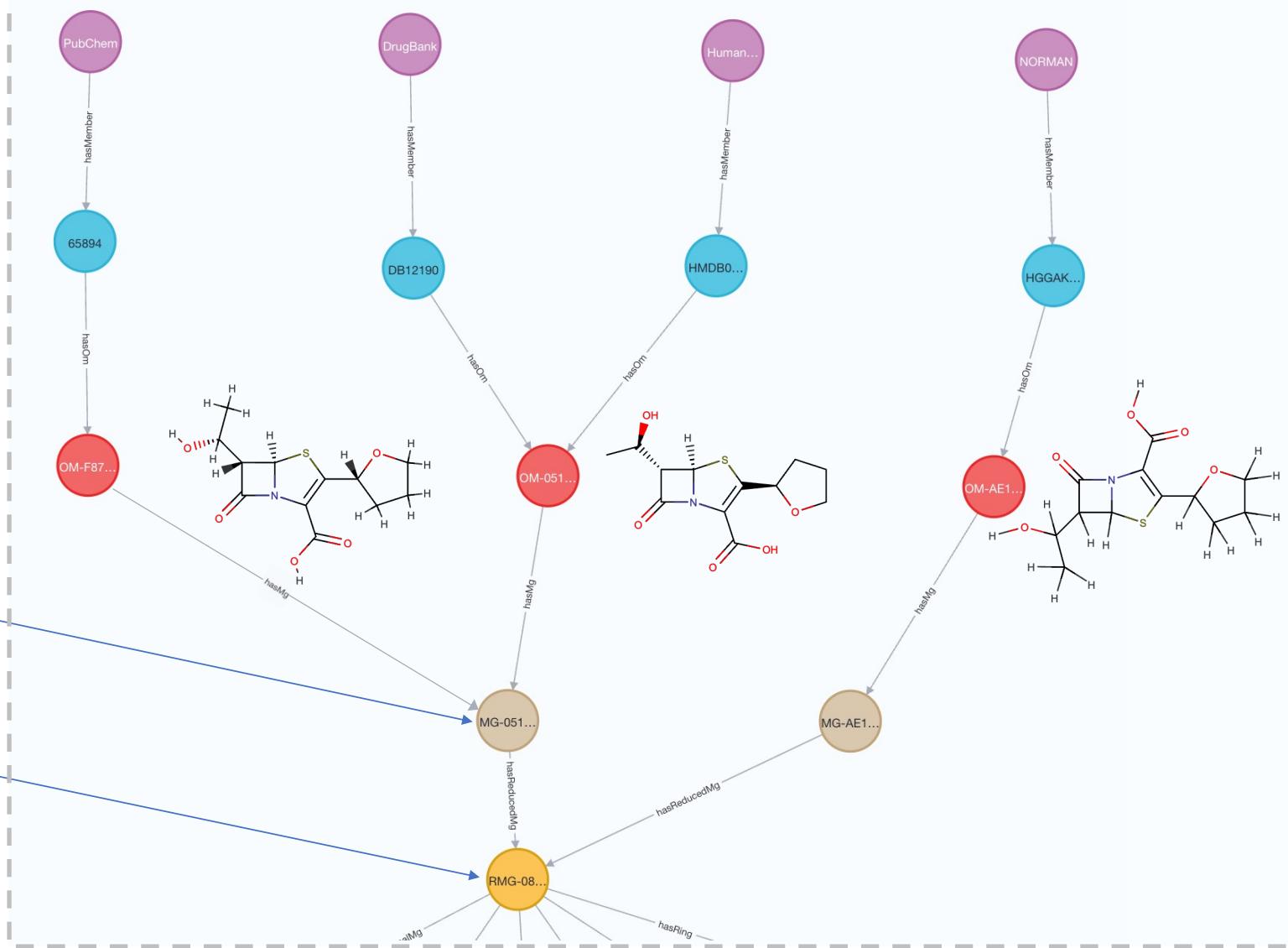
IDMP Core Ontology

How the Structure Graph Solves the Substance Identification Issue

Substance Graph



Structure Graph



Summary

- FAIR principles can be applied to chemistry representations in an automated and consistent manner through accurate identification and alignment of identical structures.
- Once FAIR Chemistry is implemented, the knowledge graph enables structure based data matching/linking with high accuracy.

Now, as a - *data analyst, data steward, data owner, ...*

I **can** enrich my knowledge through association of internal and external data sources.



Now, as a – *regulatory affairs manager, data owner, business process owner, data steward, ...*

I **can** manage substance related data consistently throughout the product life-cycle.



- The Pistoia's Alliance IDMP project integrates the combined capabilities

- open core ontology
- FAIR Chemistry

to support the implementation of IDMP standards as mandated by European Submissions office by 2023.



Questions