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KGs in the Era of LLMs: Neurosymbolic AI for Medicine

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The Academy of Medical Sciences

Network on Neurosymbolic AI for Medicine

- **Network grant:** March 2024 - March 2025
- **Team**:
  - Lead: **University of Zurich and City St Georges, University of London**
  - Partners: US, Ireland, Germany, France, Netherlands, India, Portugal, Austria, Australia, Canada, Norway, Italy, China, Spain, UK (including **St George's** *Prof. Franklyn Howe*).

Janna Hastings
University of Zurich

- **Network KPIs:**
  - Joint project bids for larger grants (EU and UKRI).
  - A **white paper** on challenges, opportunities and solutions of Neurosymbolic AI for medicine.
  - Shared repository of **use cases**, datasets and tools.
  - Gathering relevant teaching material.

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Repository: https://github.com/neuro-symbolic-ai-medicine

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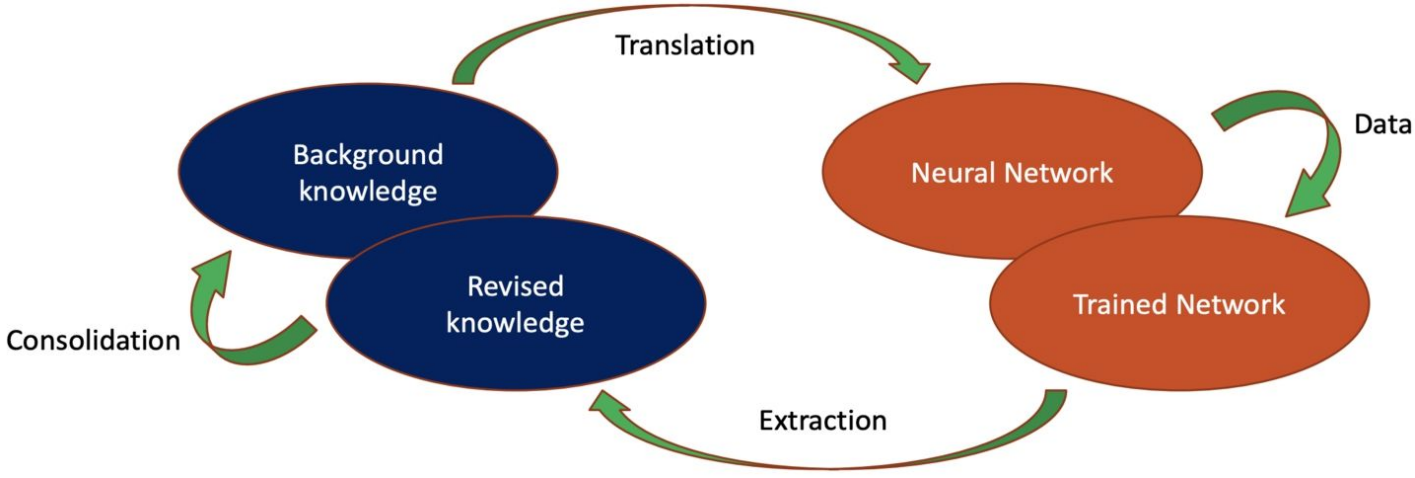
Neurosymbolic: data and knowledge driven learning (and reasoning)

More generally → Hybrid AI system



Neurosymbolic Cycle extracted from *A neurosymbolic approach to AI alignment*. NAI Journal. 2024

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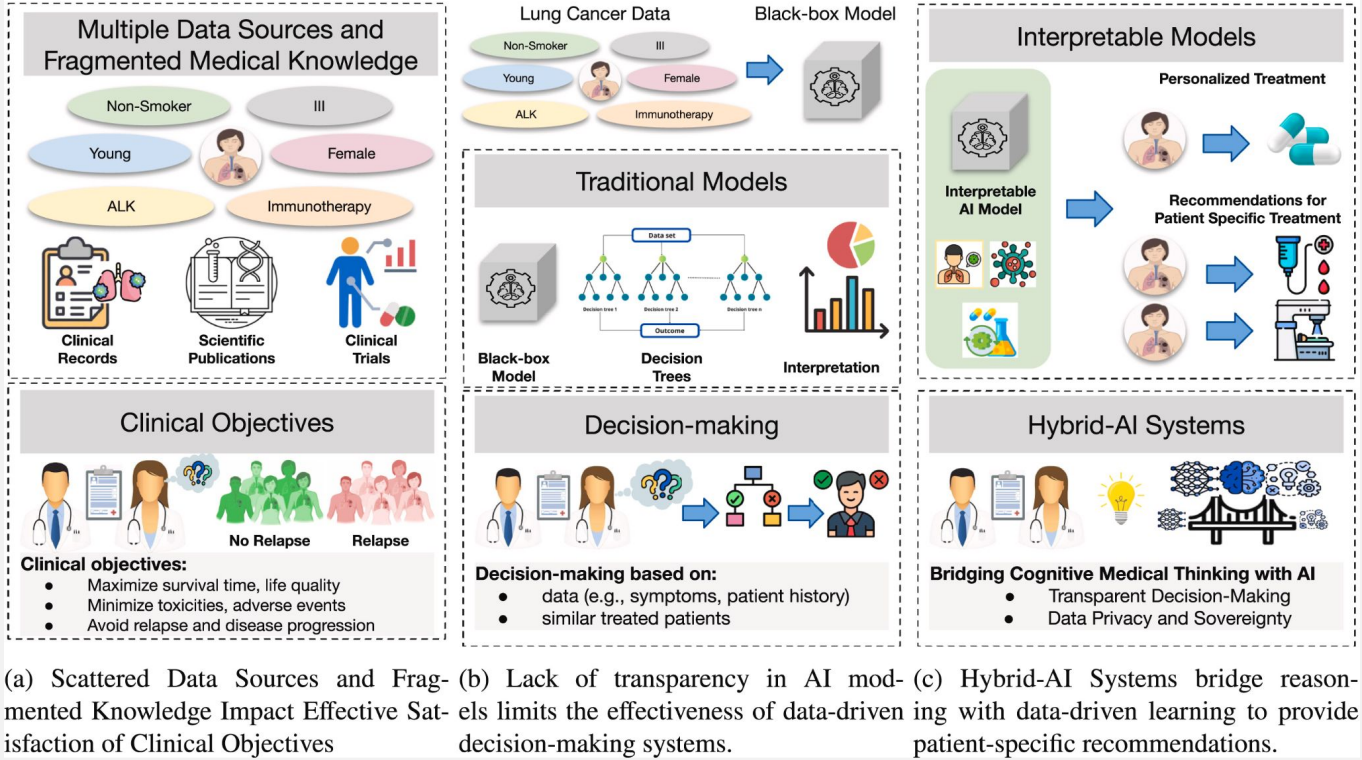
Need for NeSy/Hybrid AI Systems in Medicine



(a) Scattered Data Sources and Fragmented Knowledge Impact Effective Satisfaction of Clinical Objectives

(b) Lack of transparency in AI models limits the effectiveness of data-driven decision-making systems.

(c) Hybrid-AI Systems bridge reasoning with data-driven learning to provide patient-specific recommendations.

Extracted from *Integrating Knowledge Graphs with Symbolic AI: The Path to Interpretable Hybrid AI Systems in Medicine*. Journal of Web Semantics 2025.

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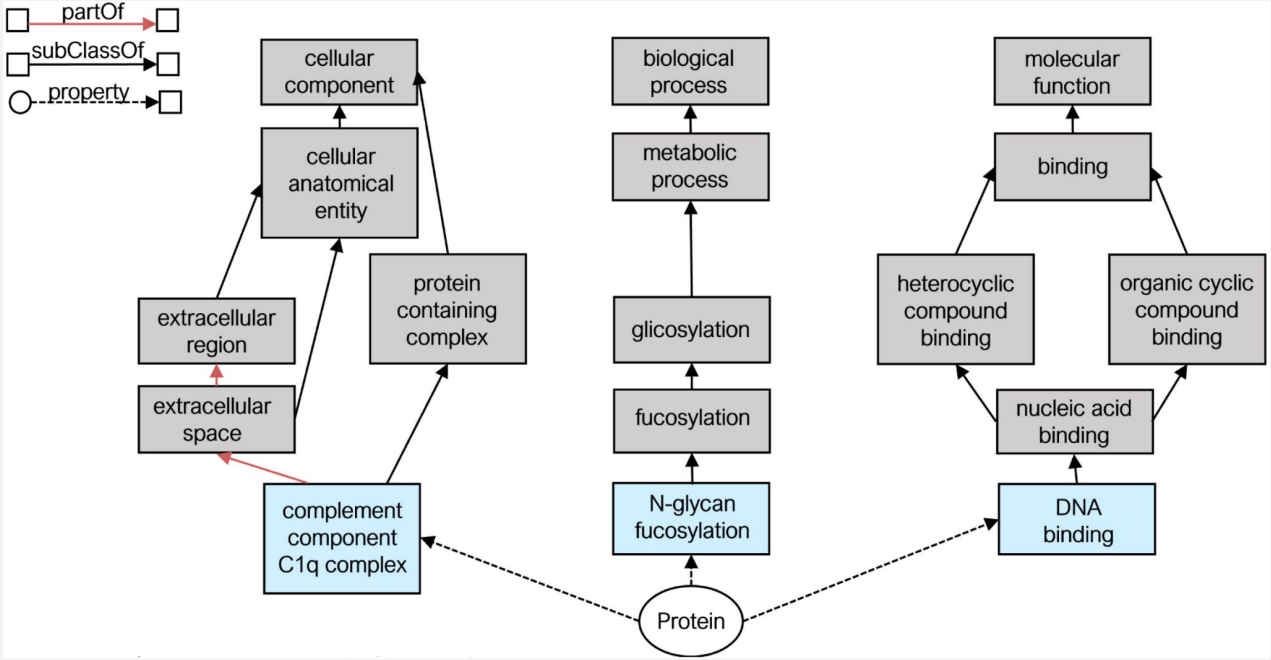
Symbolic side (Knowledge)



Fragment of the **Gene Ontology (GO)** extracted from *Explaining protein–protein interactions with knowledge graph-based semantic similarity*. Computers in Biology and Medicine 2024.

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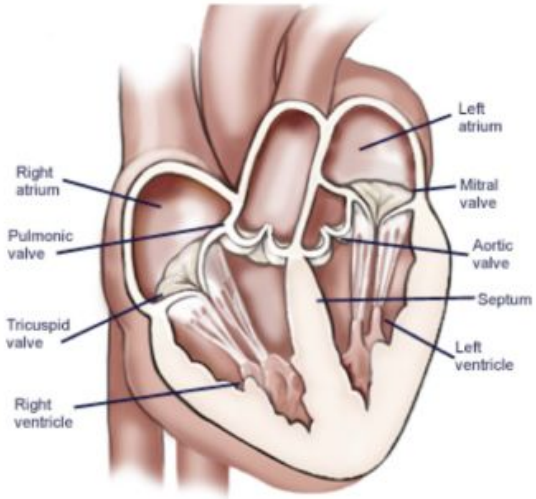
Ontologies as domain models

Simplified (abstract) **representation** of a domain

- include **vocabulary** relevant to a domain (*e.g.*, with RDF and IRIs)
- specify meaning (**semantics**) of terms (*e.g.*, with OWL)
  - Heart is a muscular organ that is part of the circulatory system
- are **formalised** using a suitable logic language (*e.g.*, with OWL)
  - Heart SUBCLASSOF MuscularOrgan AND (isPartOf SOME CirculatorySystem)



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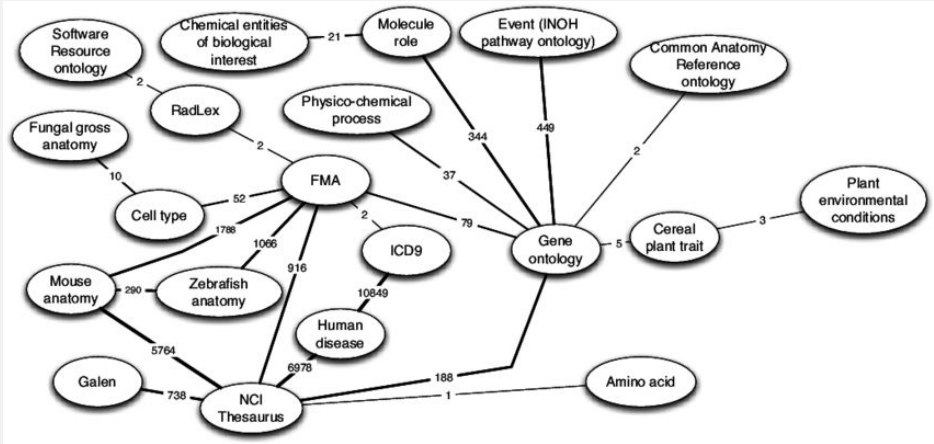
Ontologies and Knowledge Graphs

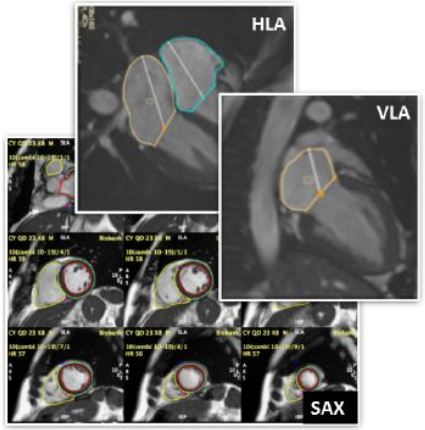
BioPortal (https://bioportal.bioontology.org/)

- A repository of more than >1,100 ontologies



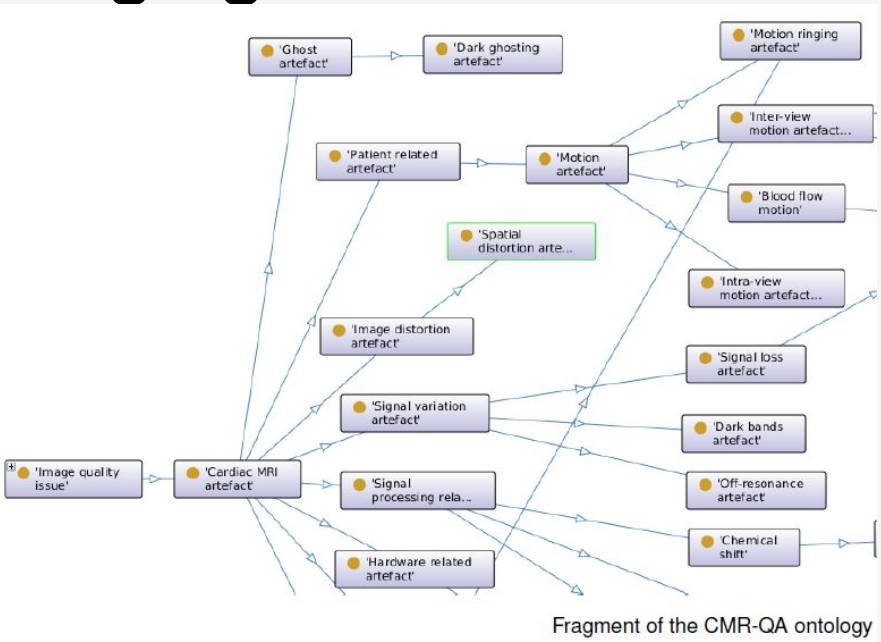
Fragment of the **BioPortal Ontology Network** extracted from *Collecting Community-Based Mappings in an Ontology Repository.* ISWC 2008.

A Knowledge Graph for the Quality Assessment of CMR Imaging Data

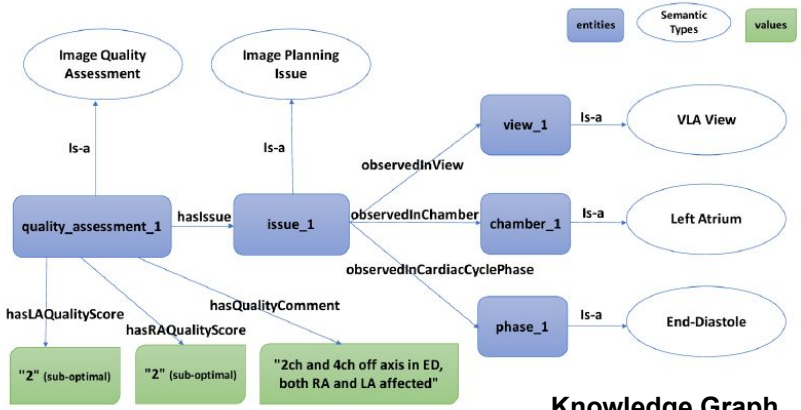


Free text comment (example)			
Motion artefact in SAX stack, affects LV. HLA off axis. VLA with technical issue.			
LV-score	RV-score	LA-score	RA-score
2	1	3	2

Quality issue	Sub-comment associated	Manual annotation
Issue_1	Motion artefact in SAX stack, affects LV	Motion_Artefact
Issue_2	HLA off axis	Image_Planning_Issue
Issue_3	VLA with technical issue	Unspecified



Fragment of the CMR-QA ontology



Knowledge Graph

Project Ontology Paper

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Towards a Personalised KG

Image from *Clinical Knowledge Graph:* https://ckg.readthedocs.io/en/latest/INTRO.html

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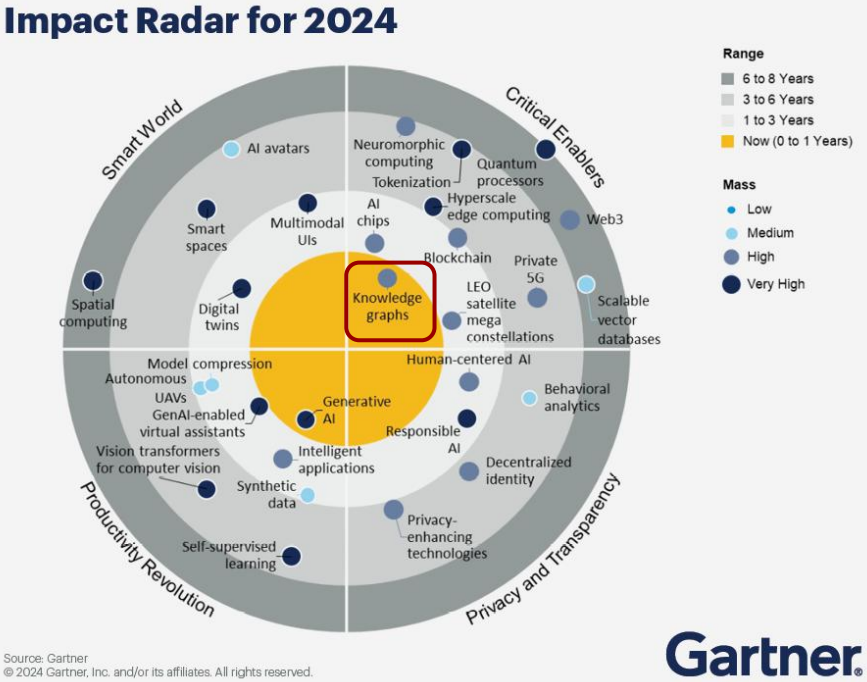
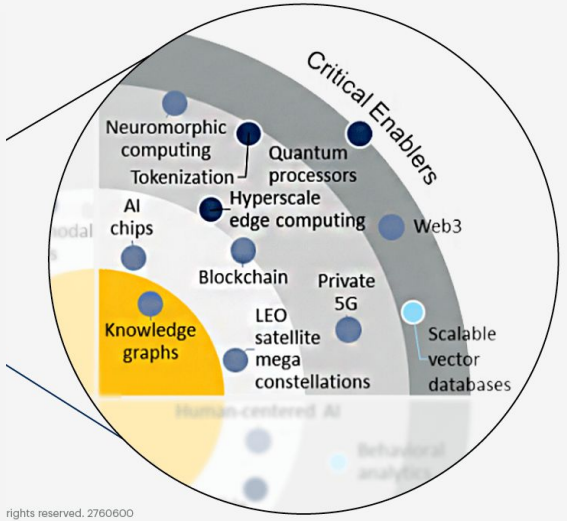
Knowledge Graphs as Critical Enablers





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Applications

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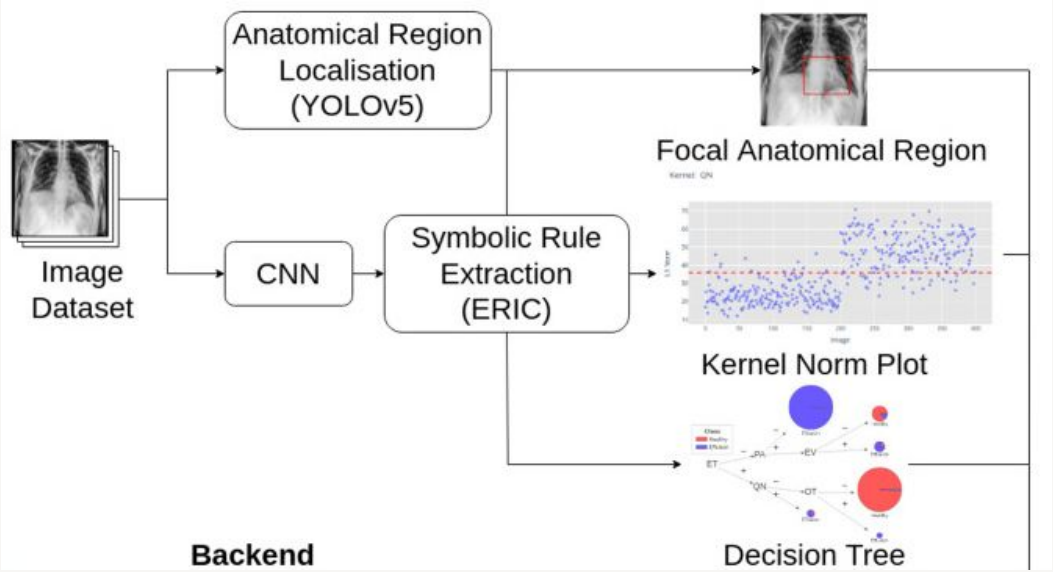
Explaining Chest X-Rays AI-based diagnoses

Explaining AI-based diagnoses (i)

- **AI systems can provide the right answer for the wrong reason!**
- **Healthy/Unhealthy AI-based triage from chest X-rays** is explained by extracting logical rules from Convolutional Neural Networks (CNN)



K Ngan, E Mansouri-Benssassi, J Phelan, J Townsend, A d'Avila Garcez. From explanation to intervention: Interactive knowledge extraction from Convolutional Neural Networks used in radiology, Plos one 19 (4), 2024.

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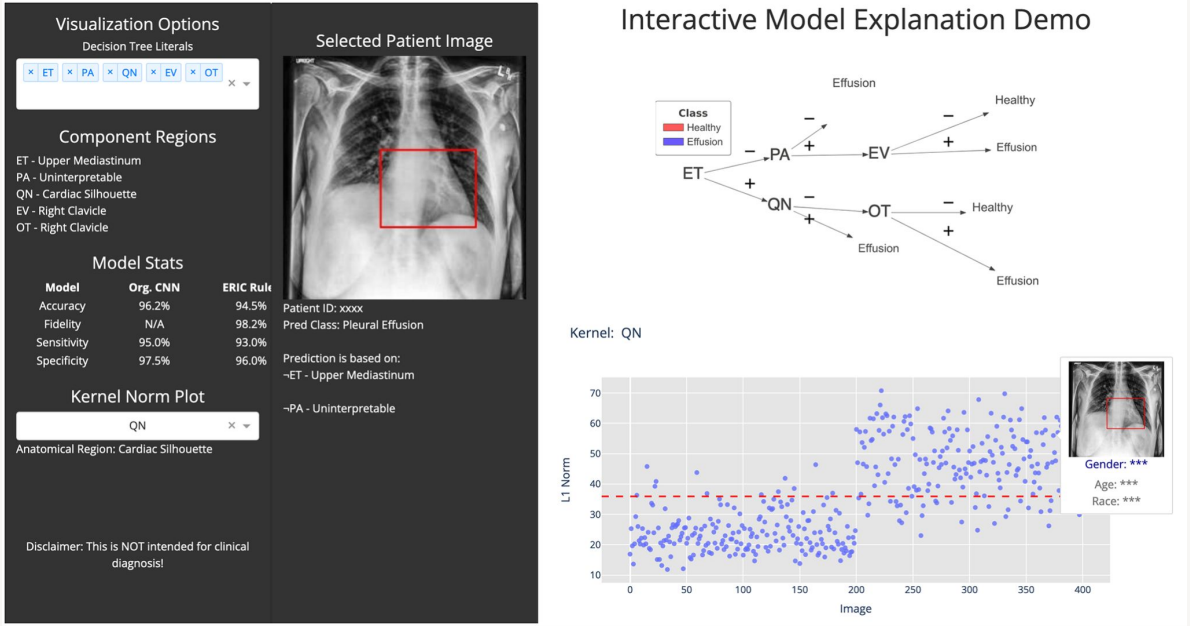
Explaining AI-based diagnoses (ii)

- **Matching/Labelling activated CNN kernels with anatomical regions**
- **Detection of relevant kernels and their impact**



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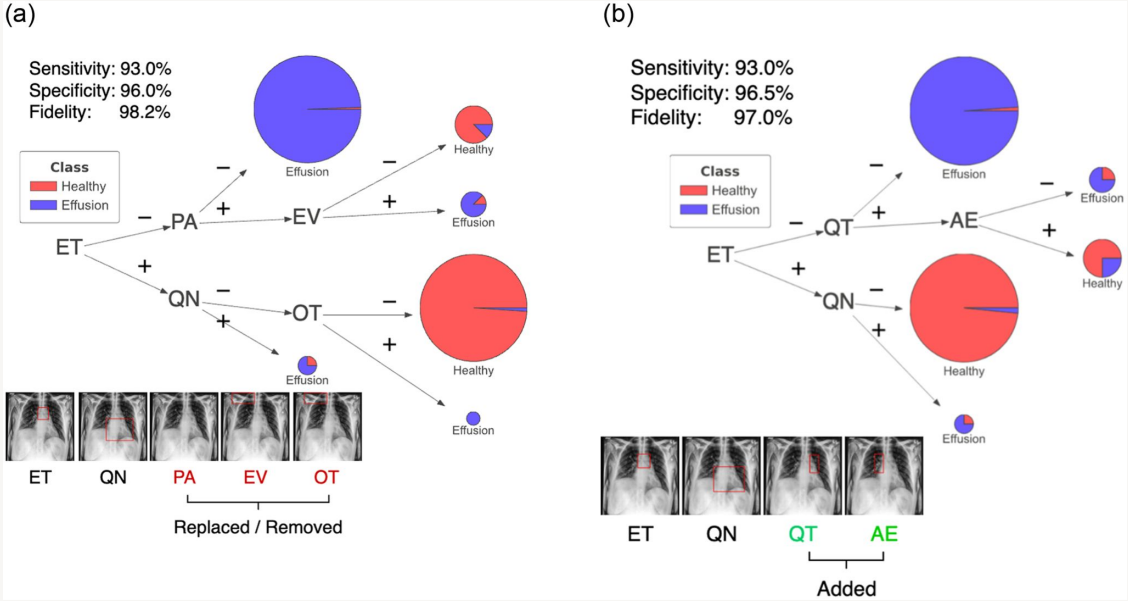
Explaining AI-based diagnoses (iii)

- **Detection of relevant kernels and their impact**
  - Upper Mediastinum (ET), Left Hilar (QT), Right Hilar (AE) and Cardiac Silhouette (QN)



K Ngan, E Mansouri-Benssassi, J Phelan, J Townsend, A d'Avila Garcez. From explanation to intervention: Interactive knowledge extraction from Convolutional Neural Networks used in radiology, Plos one 19 (4), 2024.

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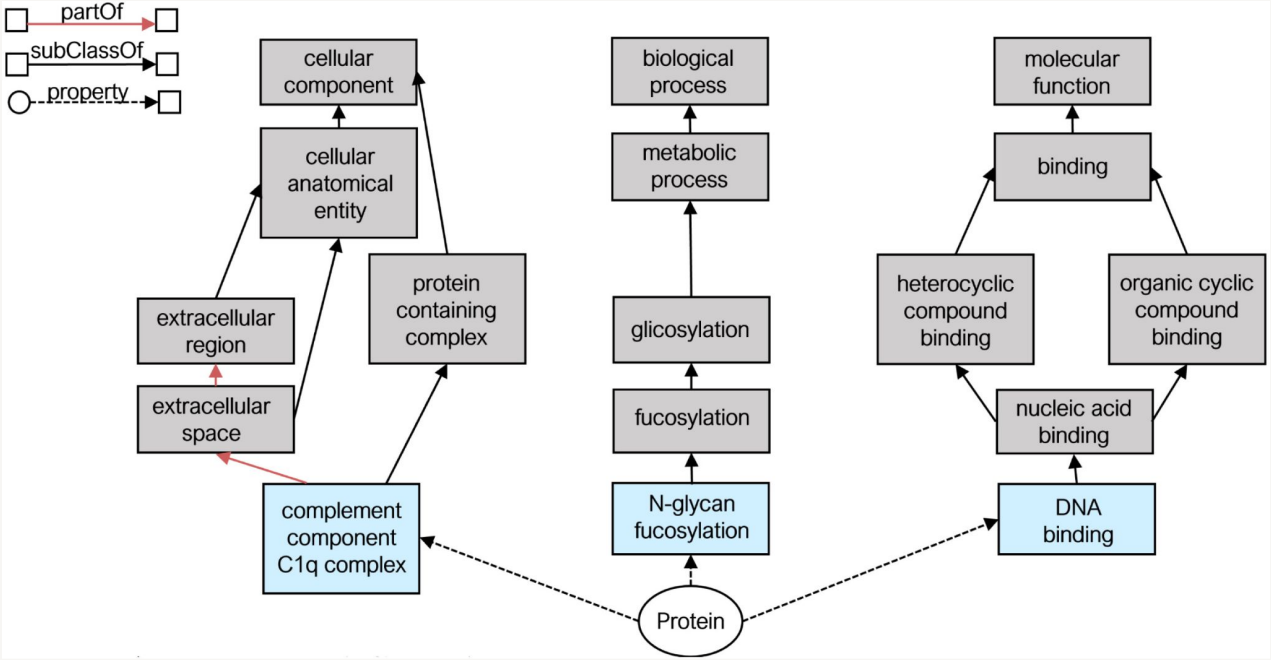
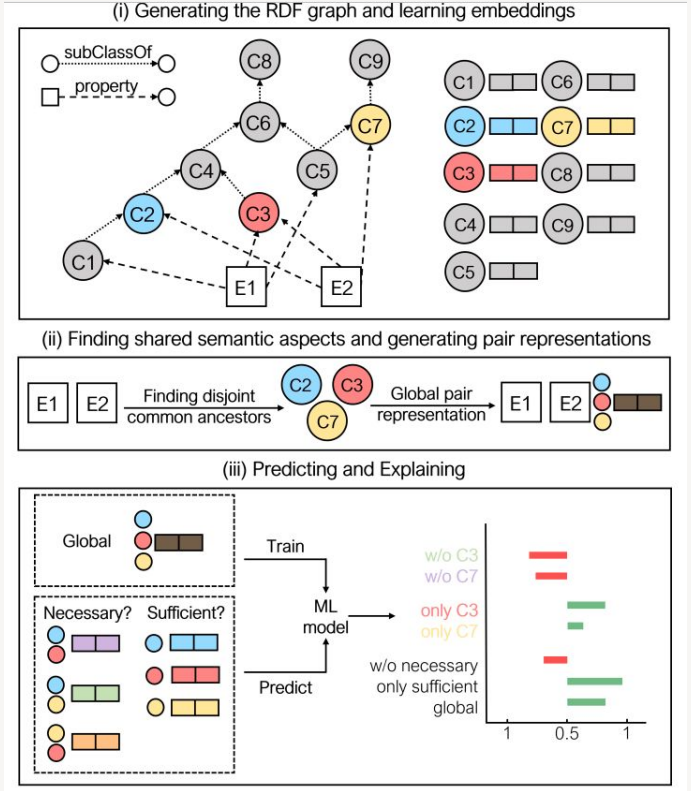
Exploiting KGs in NeSy AI

KGs to explain protein-protein interactions (i)



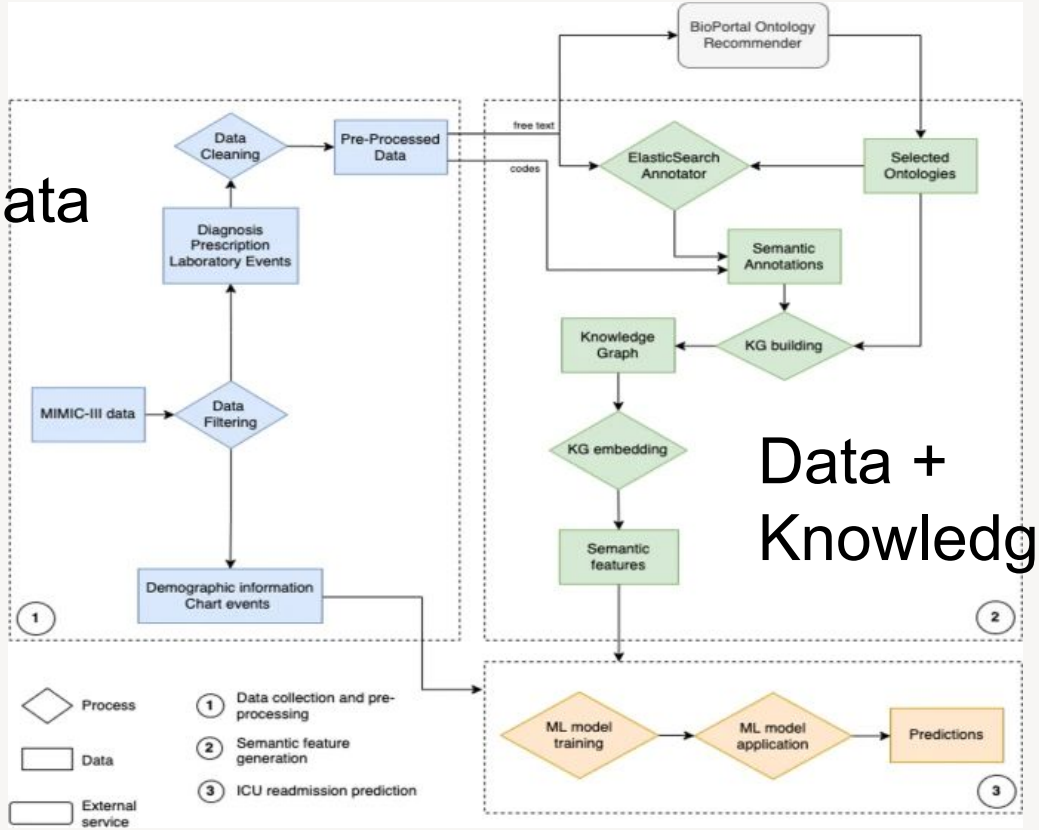
Fragment of the **Gene Ontology (GO)** extracted from *Explaining protein–protein interactions with knowledge graph-based semantic similarity*. Computers in Biology and Medicine 2024.

KGs to explain protein-protein interactions (ii)



*Explaining **protein–protein interactions** with knowledge graph-based semantic similarity*. Computers in Biology and Medicine 2024.

KGs for ICU readmission prediction



Extracted from *Knowledge Graph Embeddings for ICU readmission prediction.* BMC Medical Informatics and Decision Making 2023

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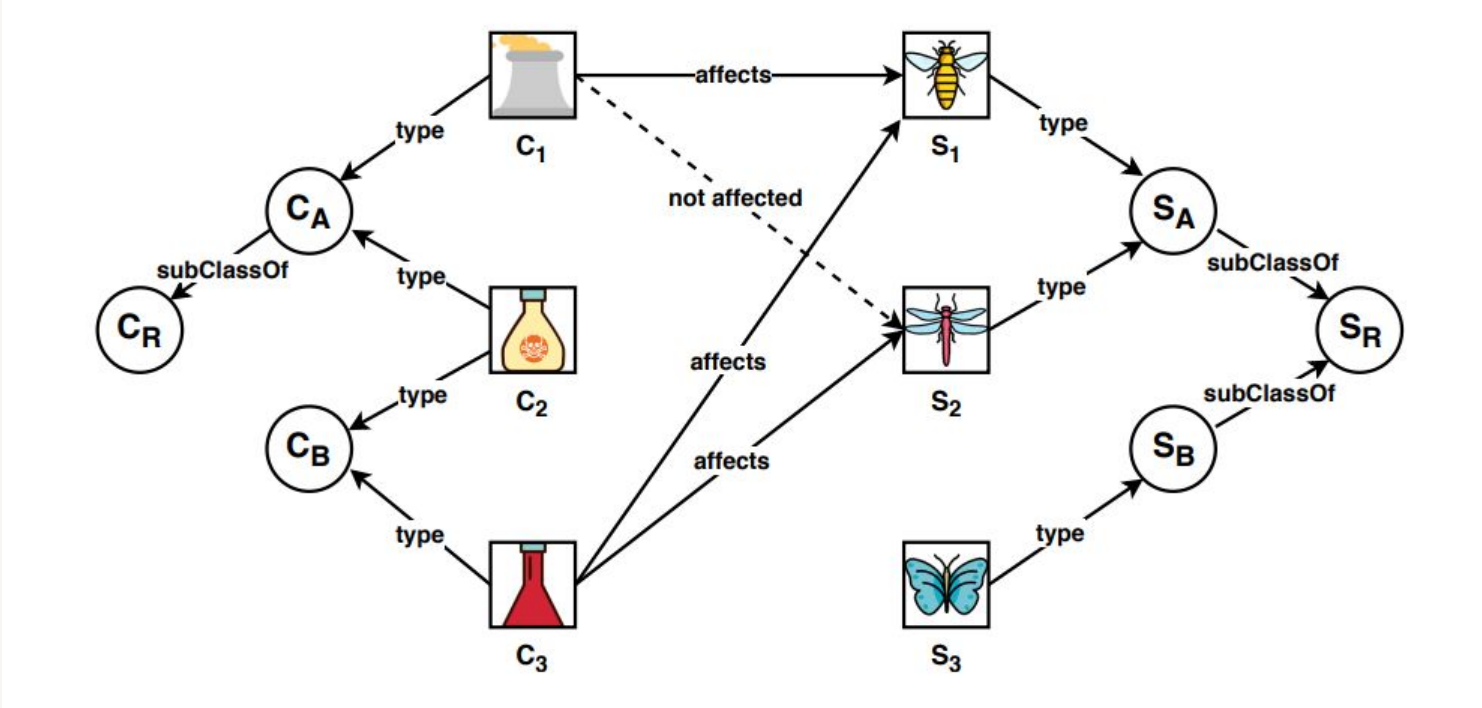
KGs for Prediction in Ecotoxicology



Extracted from *Prediction of Adverse Biological Effects of Chemicals Using Knowledge Graph Embeddings.* Sem Web. 2022.

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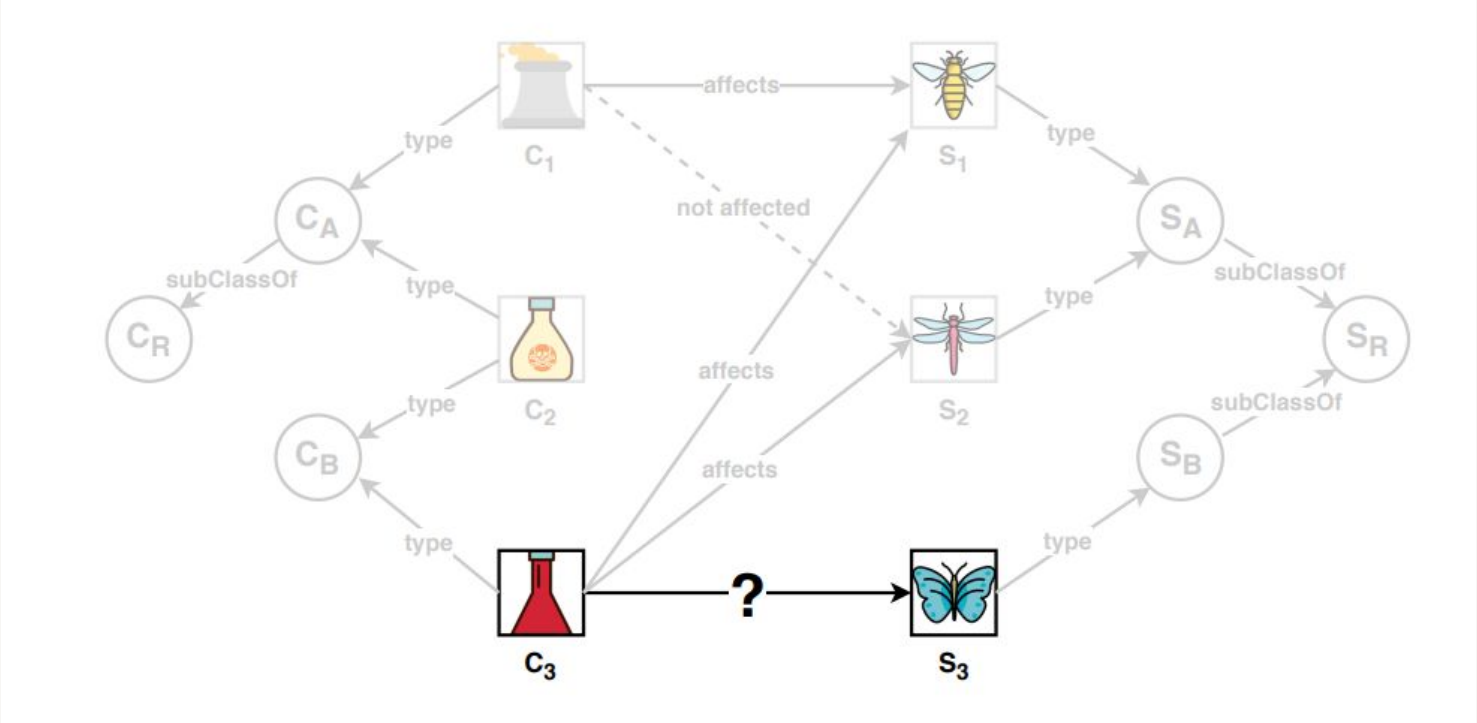
KGs for Prediction in Ecotoxicology



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