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Motivation: ONTOX Meta

- ❖ ONTOX is Horizon2020 project to deliver Ontology-driven and artificial intelligence-based repeated dose toxicity testing of chemicals for next generation risk assessment
- ❖ ONTOX Meta is a meta database within ONTOX HUB knowledgebase for the following:
 - To establish a data repository ready for analysis and modeling
 - To expand the domains to genes, proteins, assays beyond current chemistry-focused databases
 - To update the current public QSAR databases (e.g., JRC legacy reposit) to be relevant to NAM approaches (OECD QSAR Assessment Framework)

User Requirements: Content

- ❖ In Silico data
 - QSAR models with QMRF (JRC database)
 - Rulebase knowledge
 - PBK models
- ❖ Compound Properties, predicted and measured
 - Molecular, physicochemical, ADME
- ❖ AOP pathways
- ❖ Biological assays to support AOP pathways and enable / support dose-response modeling
- ❖ Omics data to link to chemistry

User Requirements

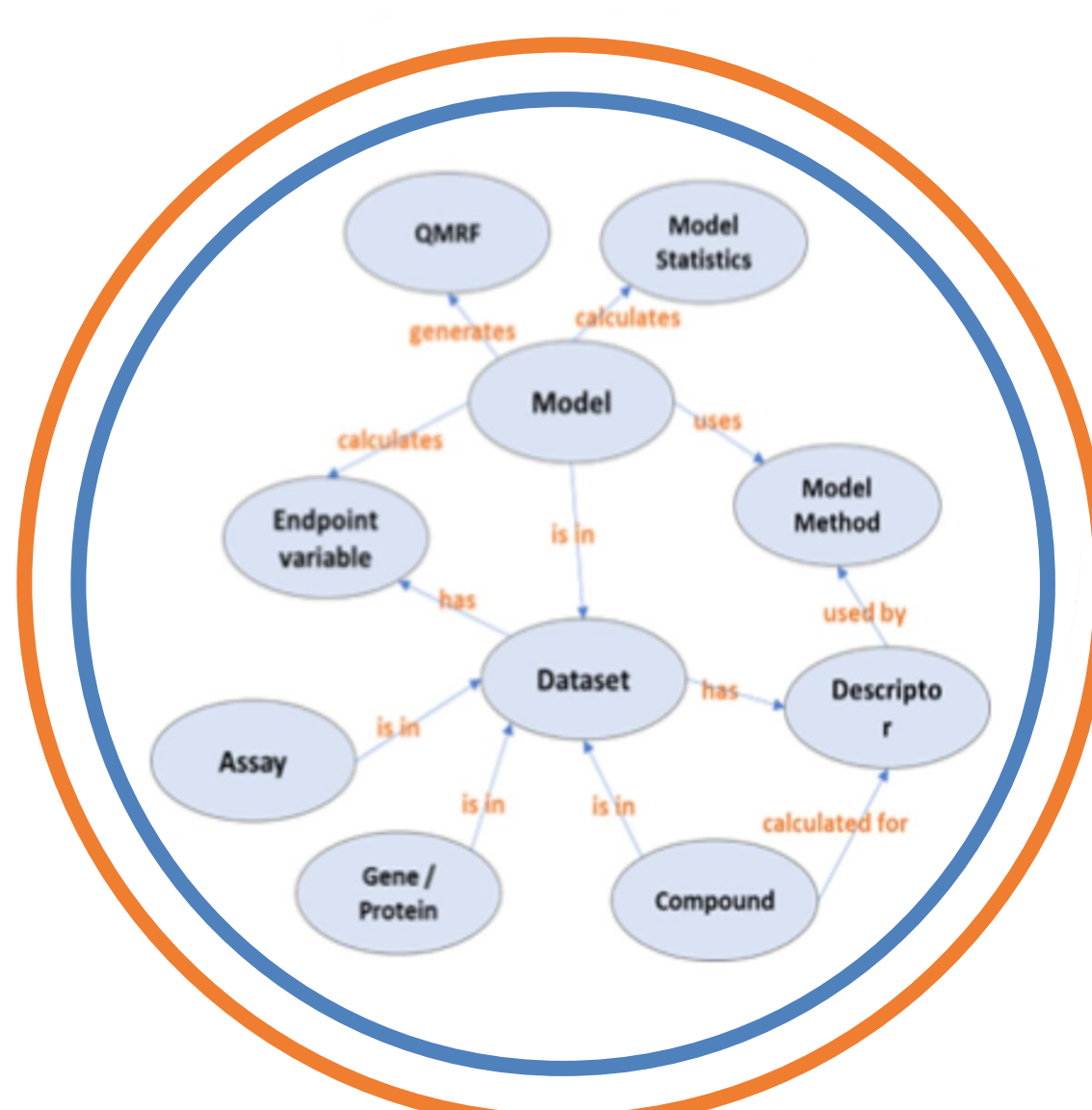
- ❖ House definitions and processing rules to represent a set of objects to deliver knowledge
 - Provide actionable data for immediate analysis
 - Enable calculations within the database
- ❖ Resources for *automatic processes* to interface with other knowledgebases and eventually with AI systems
- ❖ Accommodate OECD QAF approaches

DEVELOPMENT PROCESS ONTOX Meta

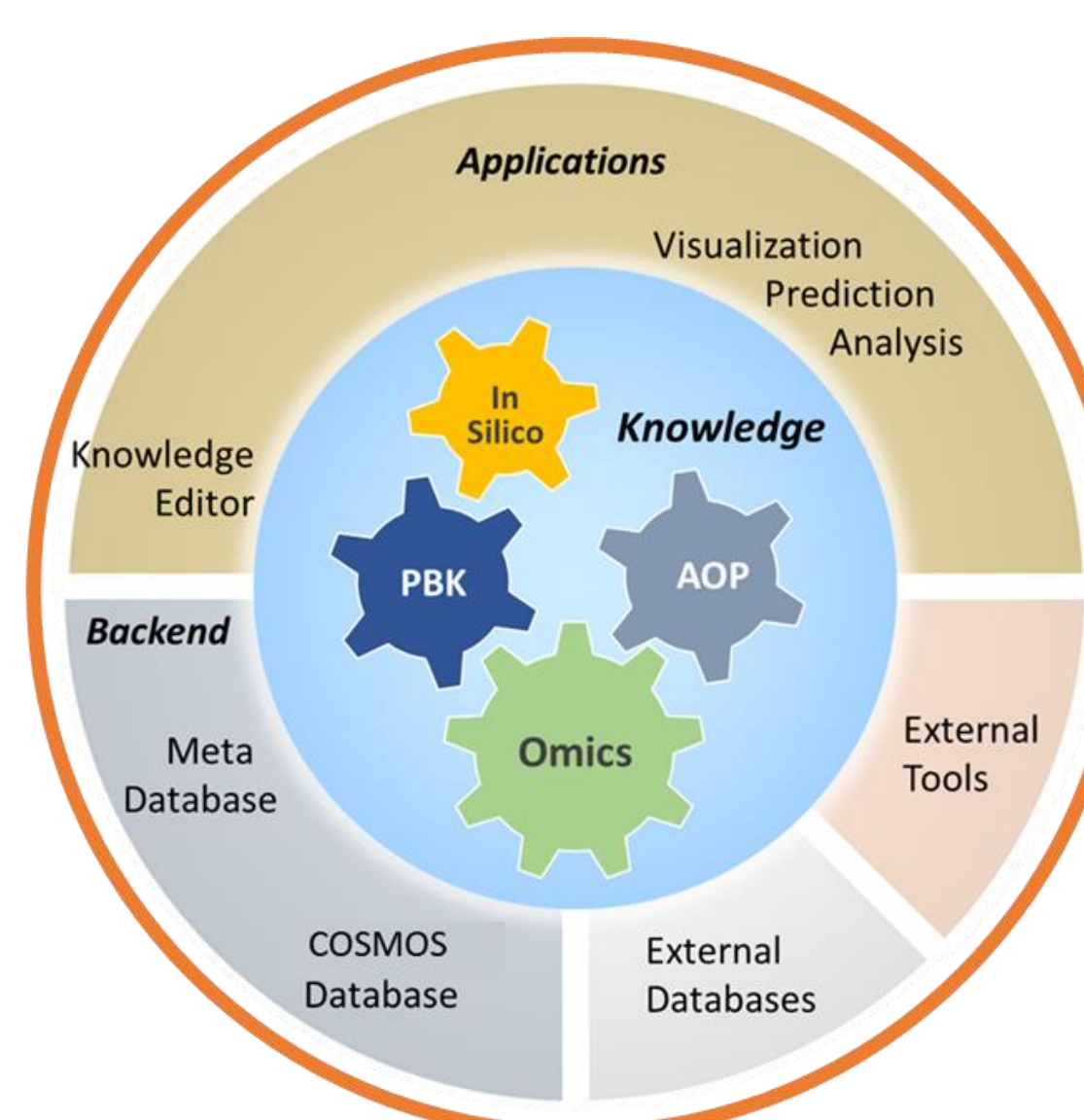
Chemical Registration & Study Locations



Compound – Data Relationships



Knowledge from ONTOX Hub



ONTOX-COSMOS

- ❖ Technology base
- ❖ COSMOS chemical registration system
- ❖ Toxicity & NAM data, partner data
- ❖ Select knowledge and tools from both public and commercial systems.

BioBricks Tox Track

- ❖ Empower COSMOS compound registration
- ❖ Establish compound-study space in chemical safety
- ❖ Global data locator

ChemTunes•ToxGPS®

- ❖ Database
- ❖ QSAR models
- ❖ TTC
- ❖ Read-Across
- ❖ Properties
- ❖ Chemotype profiling
- ❖ Chemotype editor and ToxPrints

ProtoQSAR

- ❖ Toxicity
- ❖ ADME models
- ❖ Transporters

VEGA

- ❖ QSAR Models – 95 prediction endpoints (physicochem / bioavailability properties, toxicity, ER/AR binding assays)
- ❖ Read-Across

ONTOX HUB

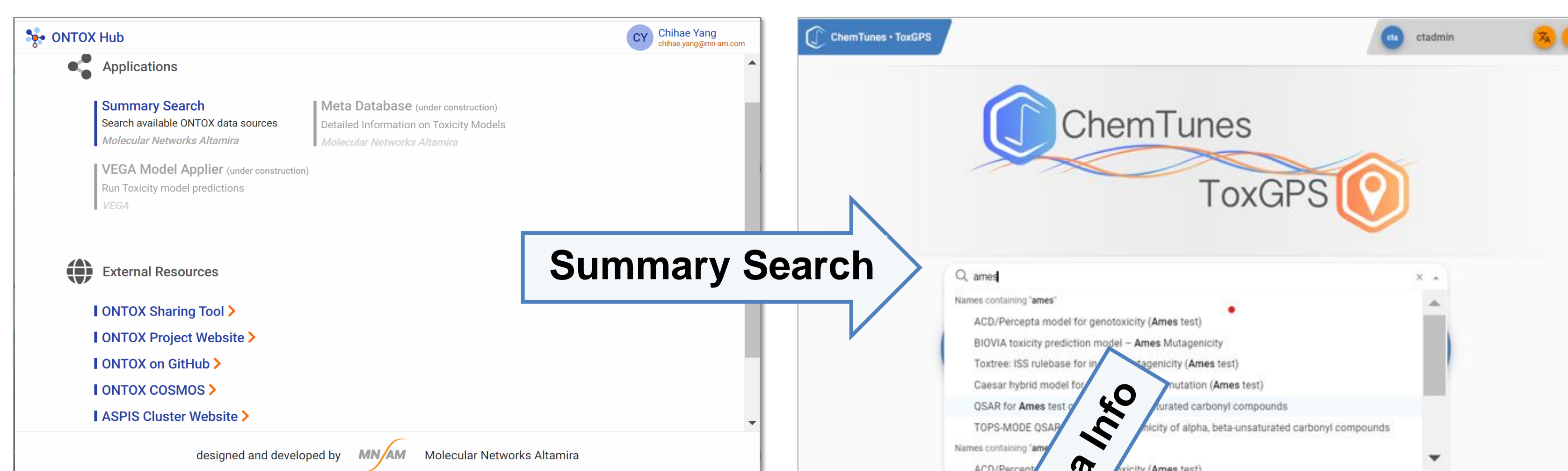
- ❖ **Backend components:**
- ❖ **Applications:** ONTOX View (hub-wise searching for summary view), tools (RASAR, VEGA, COSMOS properties & profilers)
- ❖ **User Preparatory Tools:** SysRev, Chemotype Editor, Meta DB template, external tools

<https://test.hub.ontox.eu/home>

RESULTS

ONTOX HUB: Landing Page

- ❖ Summarization view of ONTOX data sources
- ❖ Modern and easy-to-use interface
- ❖ Builds on work from a previous EU funded project

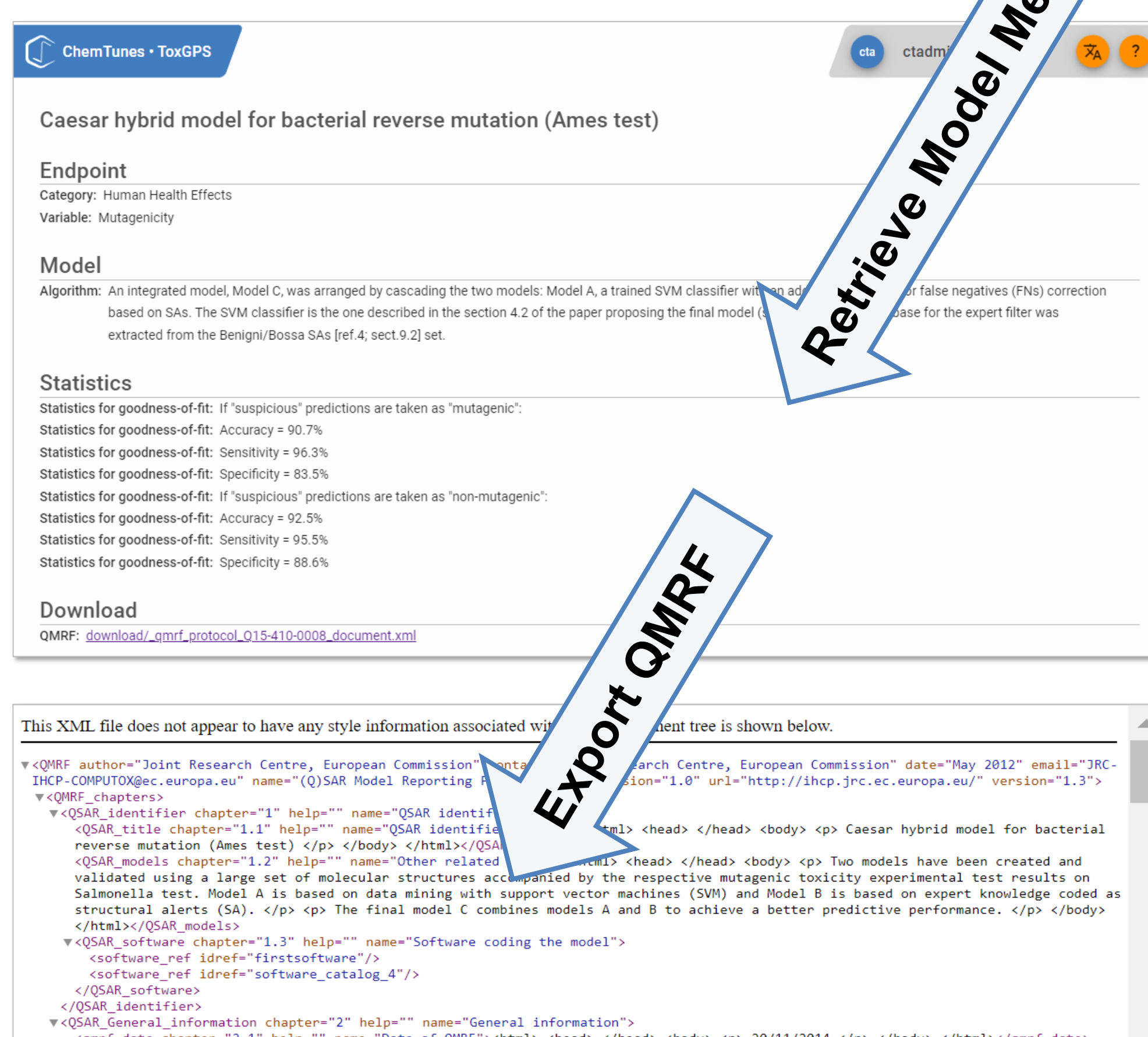


ONTOX Meta Query & Retrieval: Summary Search

- ❖ Retrieve the database data in a structure easy to be used in data analysis
- ❖ Provide data and meta information that are consumable from AI/ML approaches

ONTOX Knowledge Hub Contribution Requirements

- ❖ All data contributions to ONTOX Hub will be interfaced through a registry system.
- ❖ In silico software components will communicate via defined API.
- ❖ Software components can be integrated through a containerized environment or via connection to external web services.



Prediction data are federated within the ONTOX Hub based on data compiled from the ONTOX project

CONCLUSIONS

- ❖ ONTOX Hub v1 was released in May 2023.
- ❖ The content data includes COSMOS database, additional chemical data from BioBricks, the new ONTOX Meta database.
- ❖ ONTOX Meta prototype includes QMRFs from JRC QSAR database, ONTOX partners (Vega and ProtoQSAR).
- ❖ ONTOX Meta prototype also includes OPERA training sets, additional measured values of physicochemical properties and ADME data from ChemTunes•ToxGPS®.