AILANI™ version 3.1 Release Notes (RC)

Artificial Intelligence LANguage Interface

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Version Information AILANI version 3.1

These release notes are current as of April 2023.

AILANI version 3.1 is a full public release.

AILANI is based on the BioXM Semantic Core platform version 264.7.

Supported client platforms and operating systems

The AILANI semantic search platform version 3.1 is a zero-footprint Web application. No additional software is required beyond one of the supported Web Browsers.

Supported Web Browsers are:

- Microsoft Edge 84, or later
- Google Chrome 84, or later
- Apple Safari Version 14 or higher

Support for Mozilla Firefox has been deprecated and will be removed April 1st, 2023.

Note that usage of a Chromium/Blink-based Browser (Chrome, Edge) or a WebKit-based Browser (Safari) is recommended. The JavaScript Performance of Mozilla Firefox significantly lags behind those browsers, resulting in an inferior user experience.

Note that usage of the Microsoft Edge compatibility mode with Internet Explorer 11 (IE Mode) is not supported. In addition, Legacy Edge mode emulating the EdgeHTML engine instead of Chromium is also not supported.

Supported Operating Systems are:

- Microsoft Windows 11 (recommended)
- Microsoft Windows 10
- Apple macOS 13 Ventura (recommended)
- Apple macOS 12 Monterey
- Apple macOS 11 Big Sur

Note that usage on small mobile devices (mobile phones) is not yet fully supported.

Main Features

Next generation search for Key Opinion Leaders (KOL)

Currently one can search across 15 million world-wide experts based on ORCID IDs. These authors are part of a big author network consisting of 73 million co-author relationships. To identify experts or knowledgeable people in your field of research you enter a disease, a drug, a technology, an organism or any other relevant term in the main search box.

Within the KOL Tab Panel an author-centric result list is returned. The list can be further refined for additional expertise, number of publications, publication activity or type.

New Refiners

New refiners associated with the employment of authors have been introduced (Figure 1), such as

- **Countries** (associated with the affiliation ORCID user enter when filling in or updating their records at orcid.org)
- **Most recent Country** (Country associated with the most recent affiliation in orcid.org)
- **Most recent Role** (Most recent Employment ORCID user filed in orcid.org)
- **Start Year** (associated with the Employment entry in orcid.org)

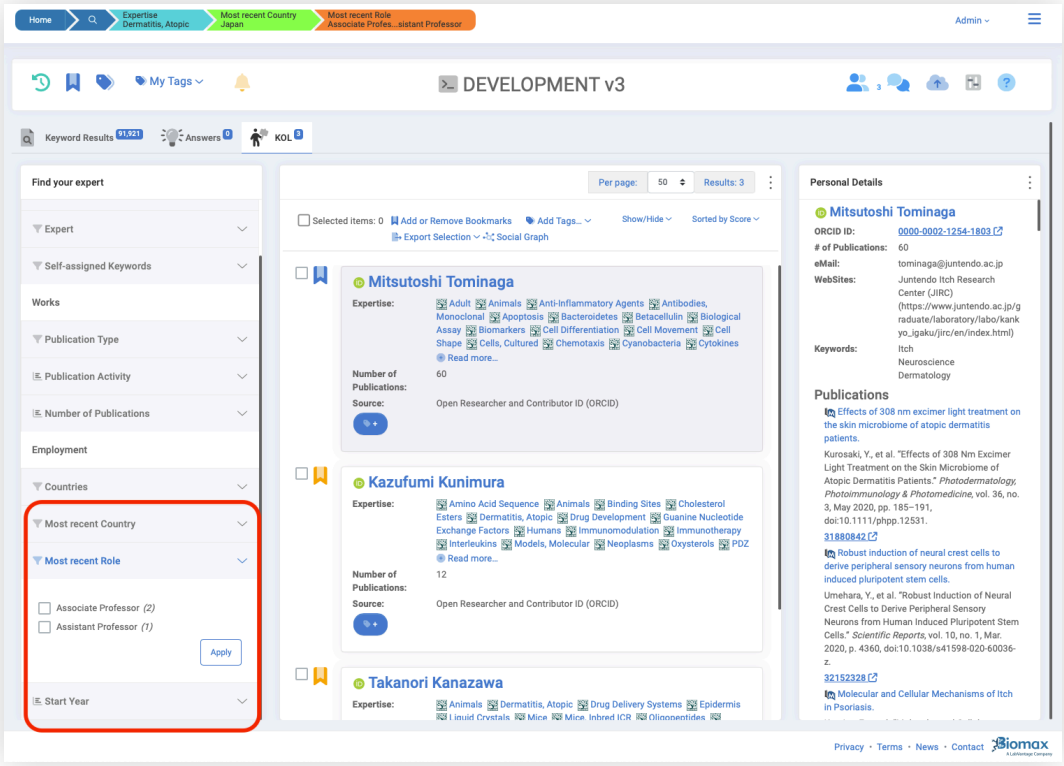

Figure 1: KOL result page with "Employment refiners"

Updated Social Graph Visualization

A refined set of authors can be selected (Figure 2) and visualized by an optimized Social Graph. The social graph calculates and visualizes a network of authors that connects the selected ones finding the shortest paths between them.

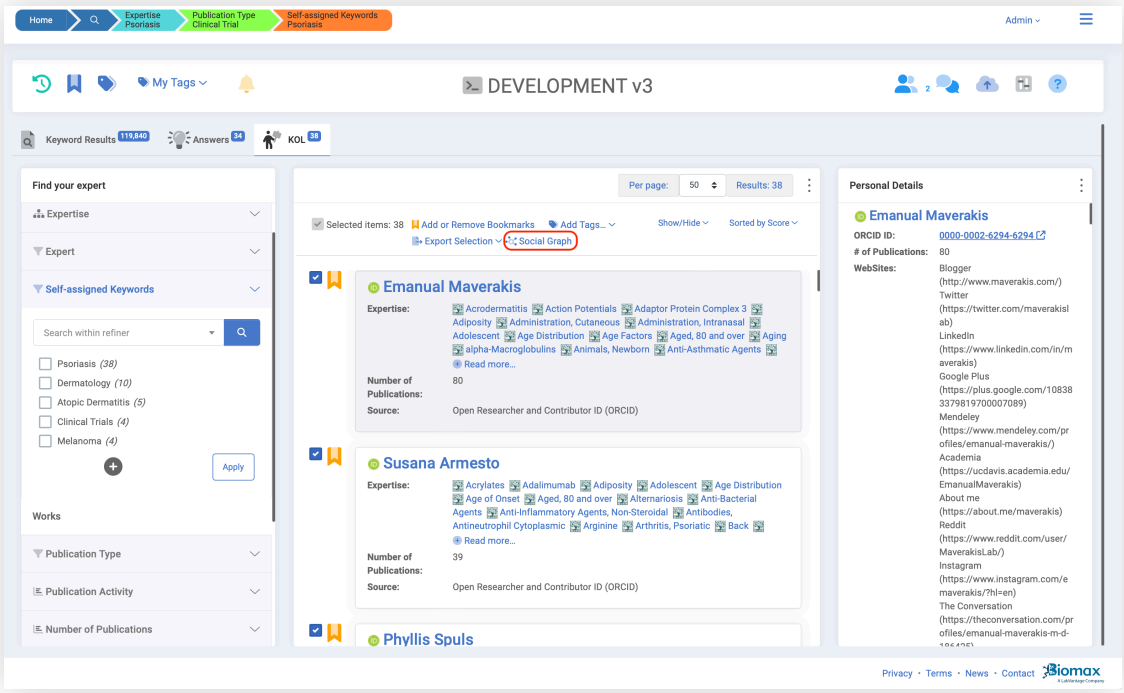

Figure 2: Selection of refined authors for Social Graph

Search within the Social Graph Viewer

Authors can now be searched for within the network using the search box on top of the network (Figure 3)

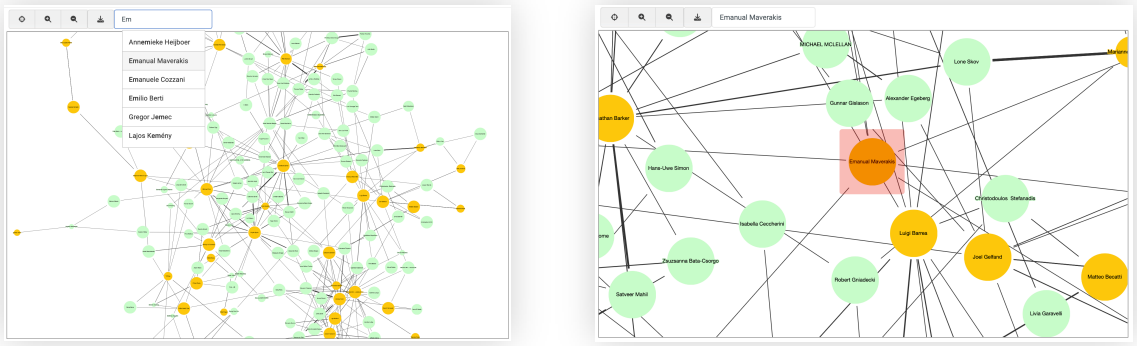

Figure 3: Search for authors in Social Graph

Authors highlighted in yellow are “bookmarked” authors, the size of the author node is proportional to the number of authored publications. The thickness of the edges is proportional to the number of co-authored publications.

More Entry Points allow visualizing the Social Graph

The Social Graph can also be accessed from the Author Report within the 3rd panel in the two Tabs “Coauthors” and “Similar Authors” (Figure 4)

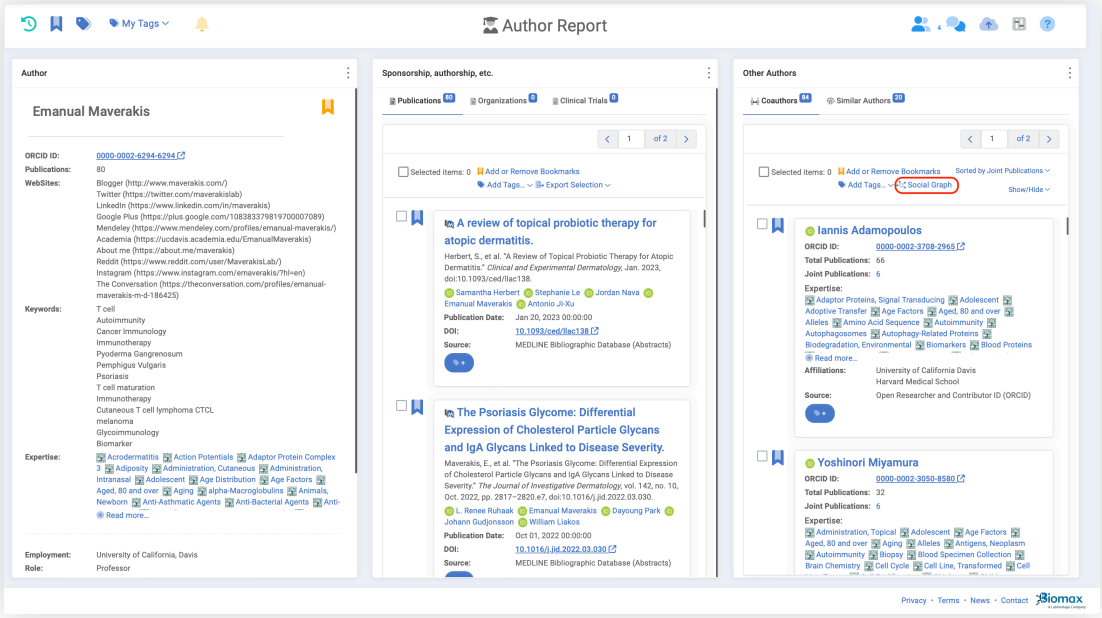

Figure 4: Access to the Social Graph from the Author Report

Clinical Trials Search

Within the specialized search for Clinical Trials accessible via the Quick Link buttons below the main search box two additional refiners have been introduced:

- Actual Enrollment
- Anticipated Enrollment

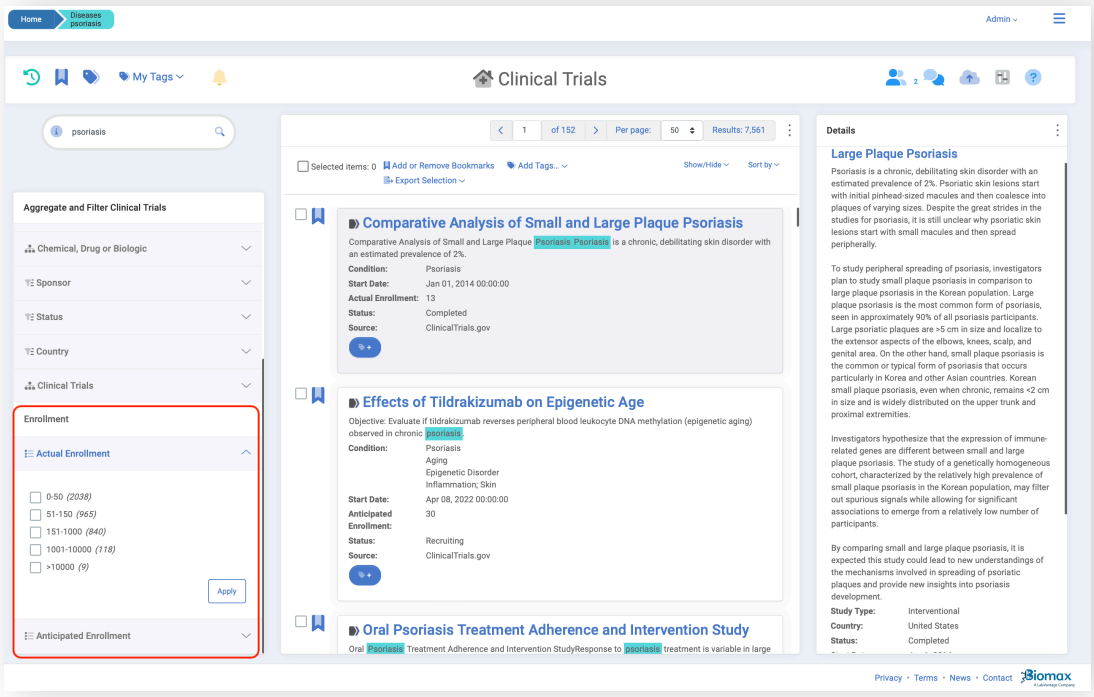

Figure 5: New Enrollment refiner for Clinical Trials search

Food Product Search

Note that the Food Product Search is only available for subscribers of the “Food, Nutrition & Health” Persona.

- Additional Refiners for aggregation and filtering of food nutrition facts have been added (Figure 6).

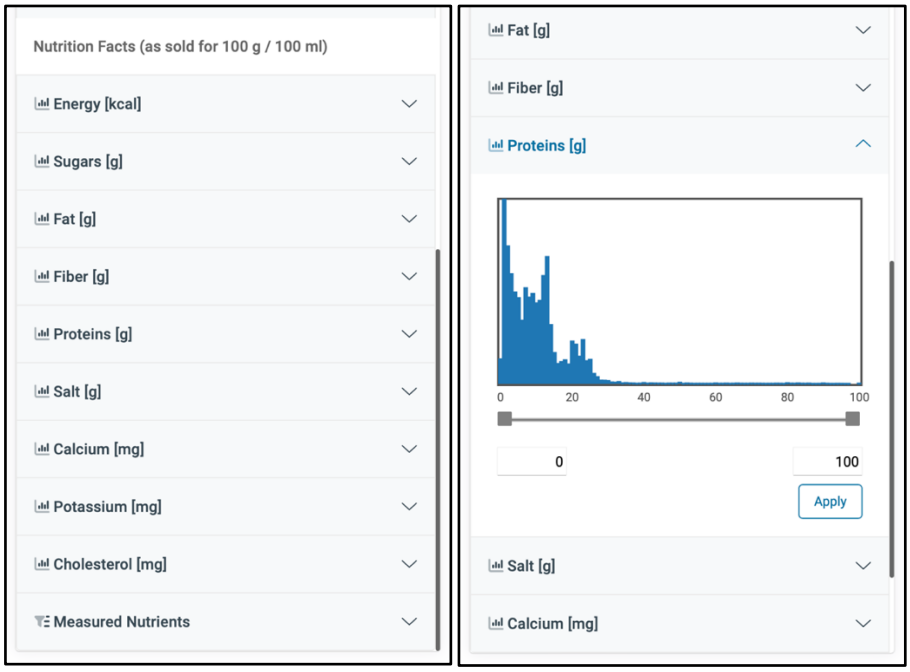

Figure 6: Refiners for Nutrition Facts

Additional Export Options

- Export for Authors in KOL Search
- Export for Rare Diseases in Rare Disease Search

Answers are ranked by relevance

Answers are ranked automatically by relevance based on journal impact factor and up-to-dateness. Answers derived from publications with a high impact factor and published most recently are ranked higher.

Redirect from Chemical Report to all patents referencing chemical structure of interest

Within Chemical reports cross referenced databases including patents are listed in the left panel in the section “Sources” (Figure 7). If a chemical structure of interest is mentioned within a patent the respective link with the InChI Key and a patent icon can be used to be redirected to a report listing all additional patents mentioning the chemical structure of interest as well as patents mentioning similar structures to the chemical structure of interest (Figure 8)

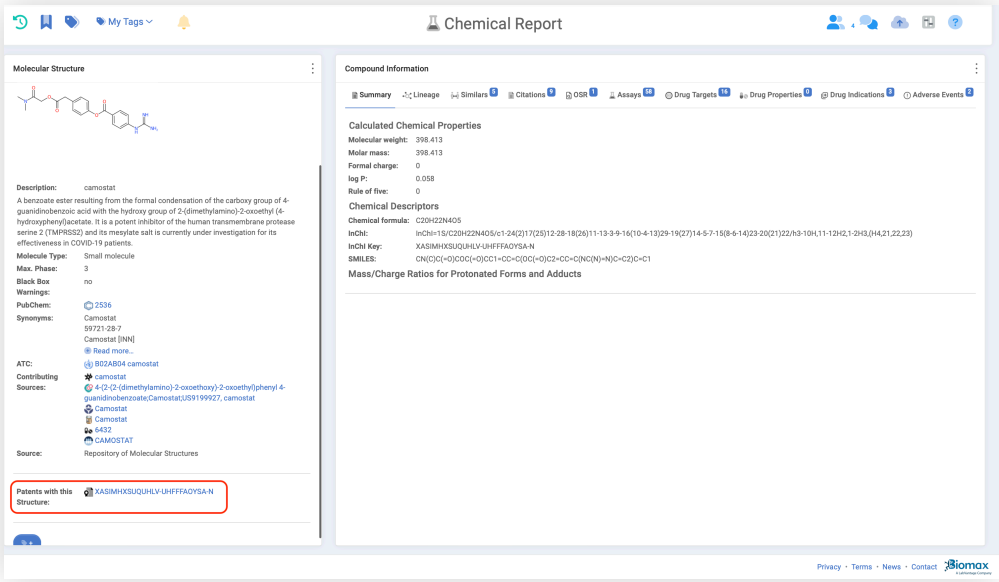

Figure 7: Chemical report of Camostat with cross reference to additional USPTO patents

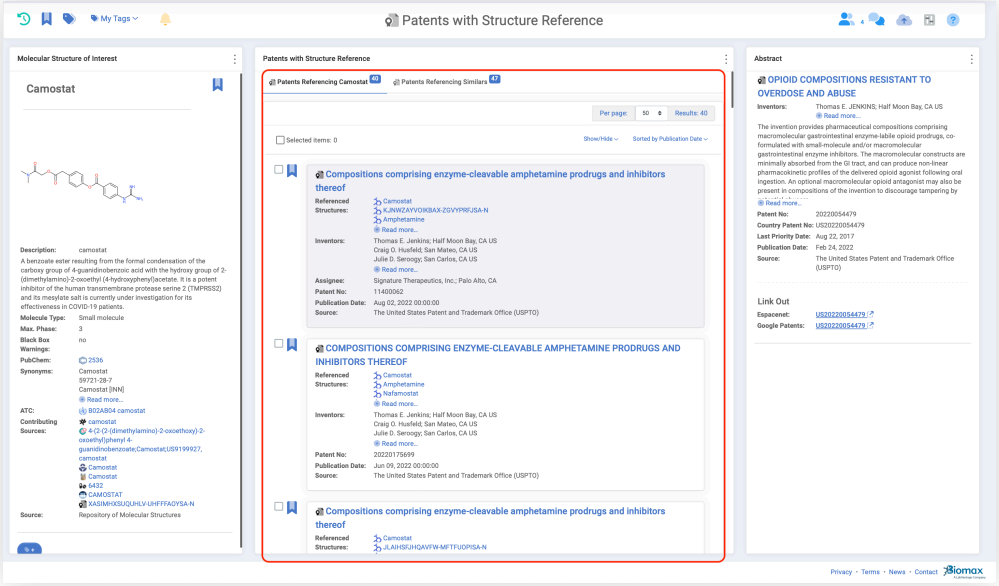

Figure 8: Chemical Report listing all patents mentioning structure of interest (Camostat)

Other Changes

Chemistry

Chemistry Editor

The Chemistry Editor "Chem Composer" from Kekule.js (Figure 9) has been updated to the latest release version 1.0.

Kekule.js is an open source cheminformatics toolkit that provides a 2D diagram editor for molecules and other chemical objects (License: MIT; DOI: 10.1021/acs.jcim.6b00167).

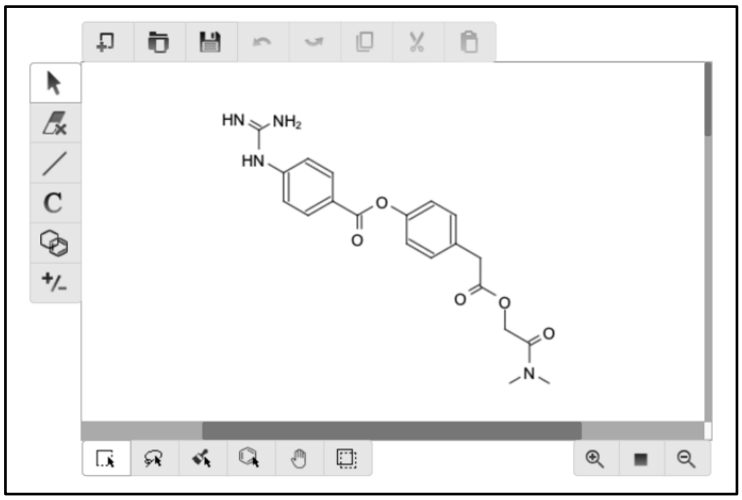

Figure 9: Kekule.js Chem Composer chemistry editor

Chemical Search Algorithms

- The chemical search algorithms are now more robust in case one or multiple chemical structures that are similar have stereo-chemical (3D) information attached.
- The chemical search algorithms now work reliably with ionic compounds as query structures.

User Interface/User Experience

Concept selectors below sunburst refiner ranked by number of hits

Concepts displayed below the sunburst control are now ranked by the frequency of concepts identified within documents. The number of hits across all documents is displayed after the concept name.

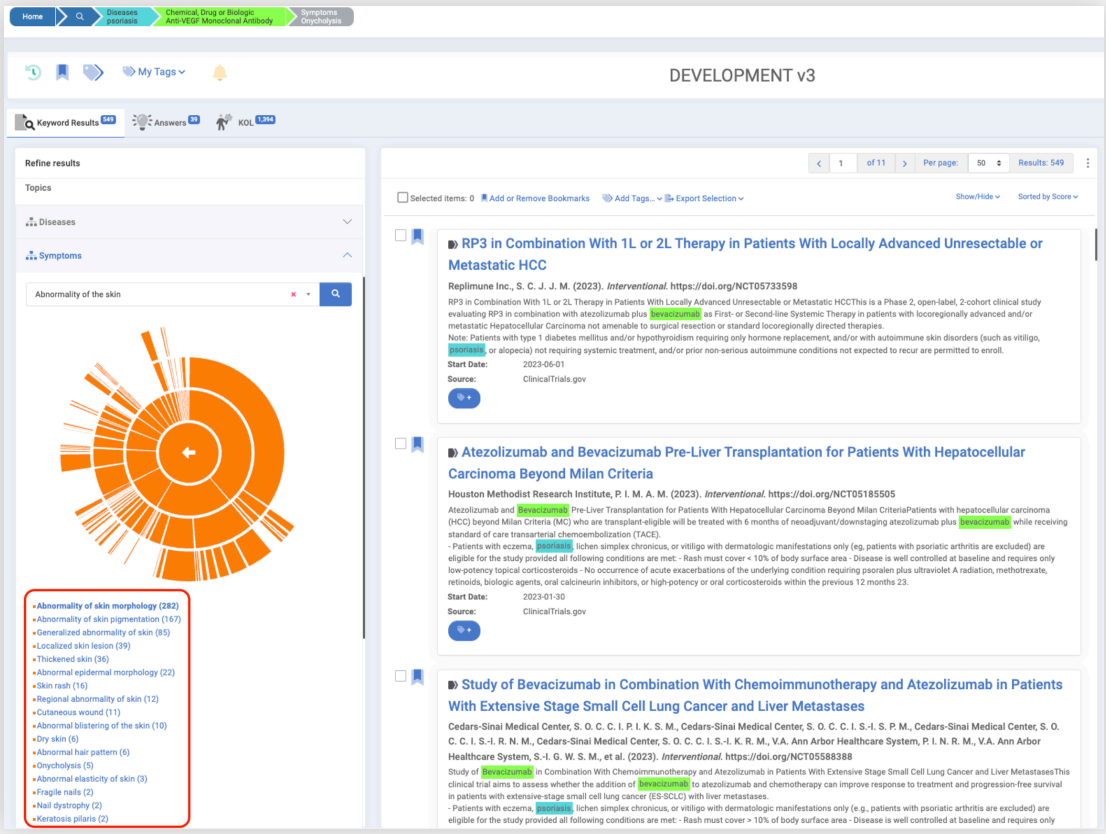

Figure 10: Concepts ranked by occurrence below sunburst control

User Preferences Dialog allows List Size Customization

The user preferences dialog (Figure 11) has been extended to allow changing the default list size for all list views. In addition to the default list size of 25 items, list sizes of 10, 50 or 100 items are supported.

Note, that increasing the list size may slow down the loading time of result lists.

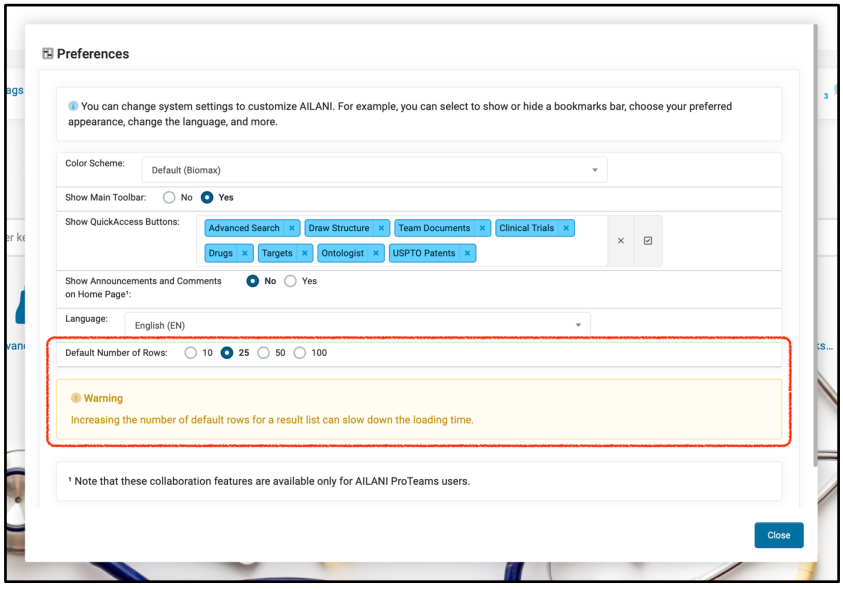

Figure 11: Extended User Preferences Dialog

Updated Typography and Imagery

The AILANI Portal now uses Font Awesome Pro 6, introducing new symbols and images.

Displaying Maps within Lists of Organizations

Lists within AILANI of research organizations have been updated to show a zoomed-in map of the location (Figure 12).

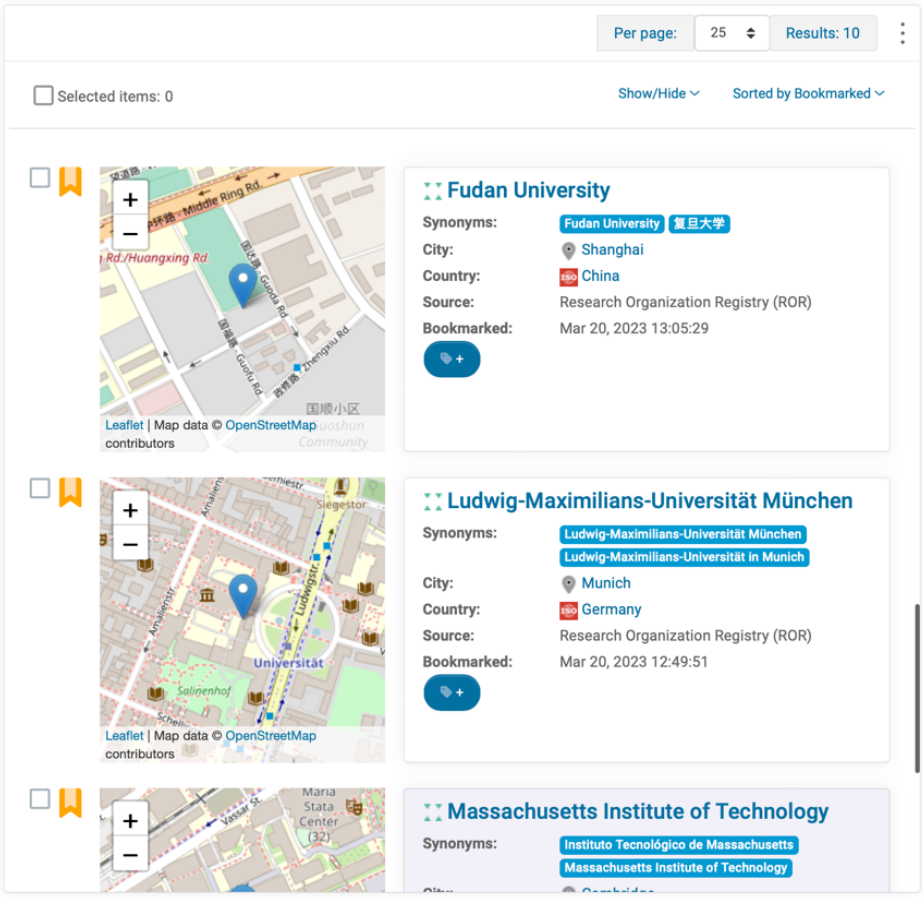

Figure 12: Lists of Research Organizations with Map

Redesigned Organization Reports

The Organization Reports have been redesigned (Figure 13), now providing information about the organization structure (parent and child organizations, related organizations), known current and previous staff, and a large map (Figure 14) providing an overview of the organization of interest and all its child organizations.

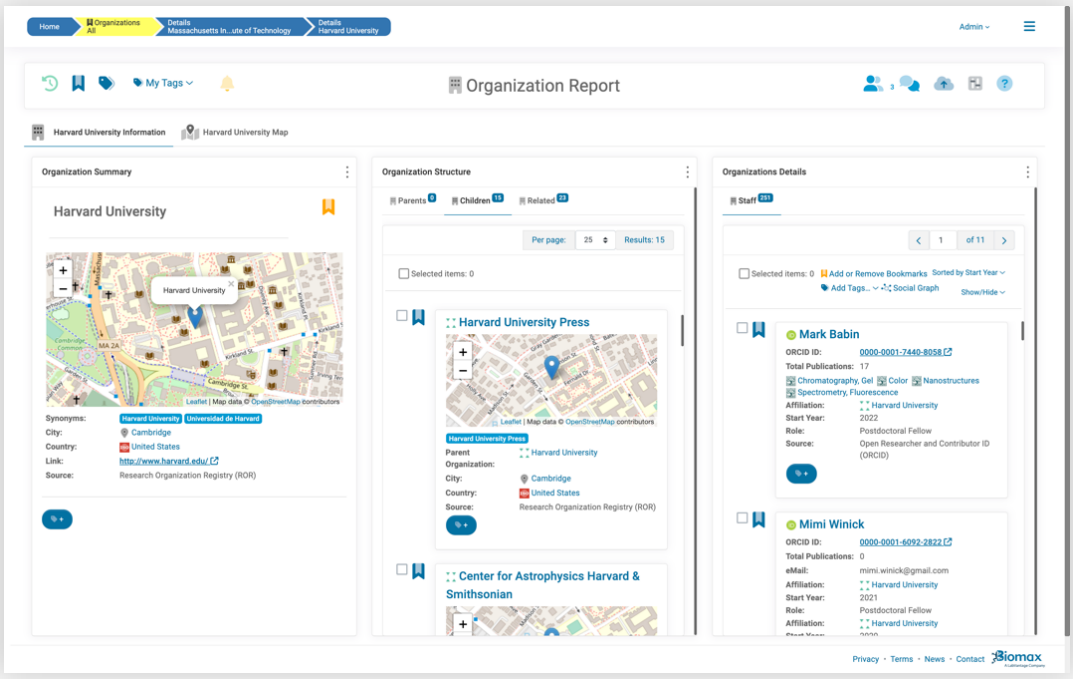

Figure 13: Redesigned Organization Report

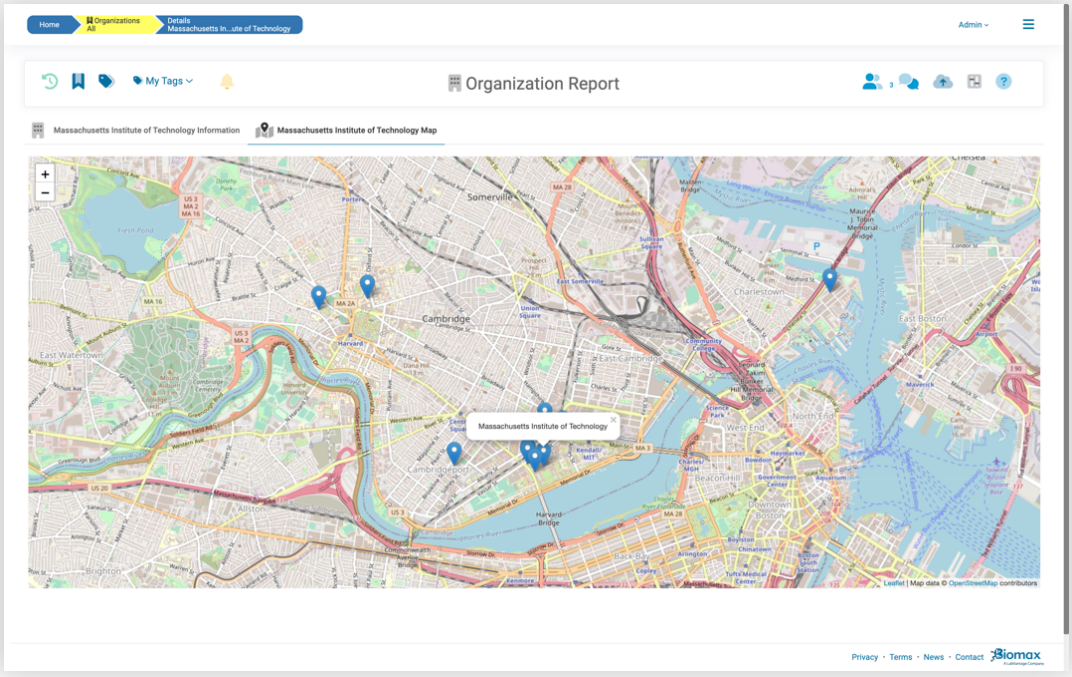

Figure 14: Overview Map of Organization and its Children

Search Field User Query Parsing

The query parser that interprets user search requests (Figure 15) is now more forgiving of unintentional user input. For example, multiple spaces between words previously prevented successful matching of concepts, resulting in a pure keyword search as a fallback.

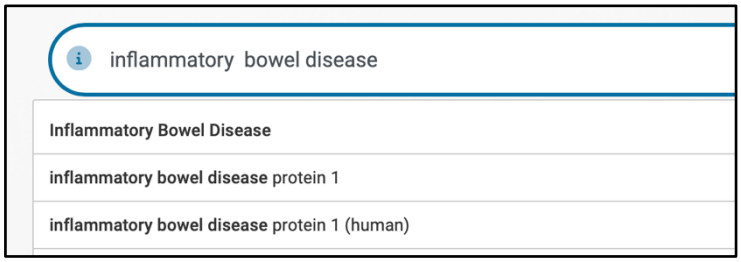

Figure 15: Main Search Field

Knowledge Graph Updates

Linked Data

Patent Data

- **Patents (USPTO):** The number of patents (public domain information, source: United States Patent and Trademark Office) maintained by AILANI increased to 12.8 million. Note: Only 3 million are currently accessible in AILANI. The full set will be available with the next release.

Food Products

- **Open Food Facts (OFF):** Open Food Facts data (License: ODbL) increased from 2.4 to 2.8 million food products, updated to a current snapshot (March 2023).

Chemistry Data

Molecular Structures: The central repository of molecular structures has been updated to a total number of 7.2 million unique chemical structures.

The repository is built and updated on a regular schedule (weekly to monthly, specific to the source) based on the following resources:

- **ChEMBL** — ChEMBL is a manually curated database of bioactive molecules with drug-like properties. It brings together chemical, bioactivity and genomic data to aid the translation of genomic information into effective new drugs. (License: CC BY-SA 3.0; DOI: 10.1093/nar/gky1075)
- **ChEBI** — Chemical Entities of Biological Interest are molecular entities focused on 'small' chemical compounds, referring to any constitutionally or isotopically distinct atom, molecule, ion, ion pair, radical, radical ion, complex, conformer, etc. (License: CC BY 4.0; DOI: 10.1093/nar/gkv1031)
- **DSSTox** — The U.S. EPA Distributed Structure-Searchable Toxicity (DSSTox) Database provides a high-quality public chemistry resource for supporting improved predictive toxicology. (License: CC0 1.0; DOI: 10.1016/j.comtox.2019.100096)
- **SwissLipids** — SwissLipids is an expert curated resource that provides a framework for the integration of lipid and lipidomic data with biological knowledge and models. (License: CC BY 4.0; DOI: 10.1093/bioinformatics/btv285)
- **GtoPdb Ligands** — The IUPHAR/BPS Guide to PHARMACOLOGY is an expert-curated resource of ligand-activity-target relationships, the majority of which come from high-quality pharmacological and medicinal chemistry literature. (License: CC BY-SA 4.0; DOI: 10.1093/nar/gkab1010)
- **UNII** — The Unique Ingredient Identifier is linked to a substance's molecular structure or descriptive information and is generated by the Global Substance Registration System (GSRS) of the FDA.
- **USPTO** — Compounds in Chemical Patents in United States Patent and Trademark Office (USPTO)

PubChem — Open chemistry database at the NIH (License: Public domain; DOI: 10.1093/nar/gkac956)

- **FDA Drug Labels** — Prescription drug/biological products

Geographical Information

- **Geolocations:** Based on the GeoNames database (License: CC BY 4.0), the number of geolocations has been updated to 13 million worldwide geolocations covering Cities, Villages, Buildings, Farms, Mountains, Forests, Lakes, Parks, etc.

Ontologies

Primary Ontologies

No changes have been introduced to the primary domain ontologies. Larger updates are planned for the next release of AILANI (Summer 2023):

- **Open Biomedical Master Ontology (OBMO)** (© LabVantage – Biomax GmbH)
- **Open Food and Nutrition Master Ontology (OFMO)** (© LabVantage – Biomax GmbH)

Secondary Ontologies

- **Research Organization Registry Ontology (ROR):** A Biomax-generated ontology based on the content of the Research Organization Registry (License: CC0 1.0) has been updated to its latest version (March 2023), increasing the number of supported research organizations to 105 thousand organizations.
- **Chemical Entities of Biological Interest (ChEBI):** The ChEBI ontology (License: CC BY 4.0) has been updated to the official release version 218.

Revision History

Version	Date	Comment	Author
1.0	March 30th 2023	Release Candidate	Angela Bauch

About AILANI

AILANI is a state-of-the-art semantic search and discovery platform designed to revolutionize information access and knowledge management in the life sciences and pharmaceutical sectors. Powered by advanced AI, natural language processing, and knowledge graph technology, AILANI enables users to quickly uncover relevant insights, promote interdisciplinary collaboration, and drive innovation. With its intuitive interface, AILANI supports organized serendipity by connecting disparate data sources and fostering the discovery of hidden relationships, helping researchers make informed decisions and accelerate the development of groundbreaking solutions in their respective fields.

About LabVantage – Biomax

LabVantage - Biomax is a leading provider of cutting-edge solutions designed to empower organizations in the life sciences and pharmaceutical industries. Combining LabVantage's expertise in laboratory informatics with Biomax's deep understanding of semantic technology and knowledge management, LabVantage - Biomax offers a comprehensive suite of innovative solutions, including the AILANI semantic search and discovery platform. By leveraging advanced technologies like AI, natural language processing, and semantic search, LabVantage - Biomax enables organizations to accelerate R&D, streamline workflows, and foster innovation by harnessing the power of organized serendipity through interconnected data and insights.

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