

ONTOFORCE and ChemAxon facilitate linked chemical data search

10 October 2018 – Ghent, Belgium – Budapest, Hungary – Semantic search company ONTOFORCE and cheminformatics and bioinformatics software solution provider ChemAxon; have set up a collaboration to make it easier to search for linked chemical data. ChemAxon's web-based molecule drawing and editing tool Marvin JS will be integrated in ONTOFORCE's DISCOVER platform. As such, researchers and others will be able to take advantage of an easier way to describe a chemical – by drawing it – combined with more advanced search capabilities.

DISCOVER is a web-based platform where you can search and navigate across multiple internal, third party and public data sources. It's mainly used in life sciences. A typical search starts with entering one or multiple keywords or 'strings' that quickly retrieve results from different data sources. This is a convenient way to start exploring information about diseases, publications, clinical trials, patents, genes, genetic variants, proteins, active substances or chemicals amongst others. DISCOVER is now including the capability of performing a chemical search by drawing a molecule or molecular fragment.

How it works

A plug-in architecture has been created in DISCOVER and a first application includes ChemAxon's web-based molecule drawing and editing browser component Marvin JS. Users of DISCOVER will be able to switch between the classical 'string' search and the new 'chemical' search, from the moment the Marvin JS plugin is configured on their version of DISCOVER.

- Users can now draw a molecule or molecular fragment in Marvin JS and select a search action which is sent to a third-party service.
- The results are sent back to DISCOVER, where the user can continue to navigate the linked data.

The advantages

This setup will make it much easier for chemists to solve several use cases, like:

- Searching for chemicals similar to a drawn structure and find where they are stored internally, or continue the search by looking at related publications, patents, etc.
- Searching for information about a drawn molecule in public and/or local data sources.

Eufrozina Hoffmann, Product Owner of Marvin JS: "I am glad to see how seamlessly ONTOFORCE integrated and configured Marvin JS to fit their current workflows, while understanding the possibilities of our API also."

Hans Constandt, CEO of ONTOFORCE: "The new DISCOVER plugin architecture combines chemical structure search with semantic search linking internal and external data instantly. This collaboration with Chemaxon allows us to bring a solution to an unsolved problem in the chemistry space."

The collaboration between ONTOFORCE and ChemAxon allows both companies to expand their activities in medicinal chemistry in pharma and biotech and other chemistry related life science niches. In the near future, ONTOFORCE also intends to include these new chemical search capabilities in the public version of DISCOVER.

About ONTOFORCE

ONTOFORCE is a Belgian company, with offices in Ghent, Belgium and Cambridge Massachusetts, USA that develops breakthrough semantic search technology. Its user-friendly search platform DISCOVER builds intelligent links between data sources and facilitates access to valuable information with only a few clicks. ONTOFORCE is acknowledged by and collaborates with world renowned research institutes and communities such as IMEC, ELIXIR, EIT, UCSD, MIT and Harvard Catalyst Group.

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About ChemAxon

ChemAxon is a leading cheminformatics and bioinformatics software provider for the chemistry, biotechnology, pharmaceutical, food & fragrance, petrochemical and agrochemical industries. ChemAxon creates innovative cross platform solutions that power modern cheminformatics activities. ChemAxon's headquarters are in Budapest, Hungary, and to support their global customers they have offices in Europe, the Asia-Pacific region, and North America.

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