DOME 4.0 Showcases – User Guide

1. Showcases List

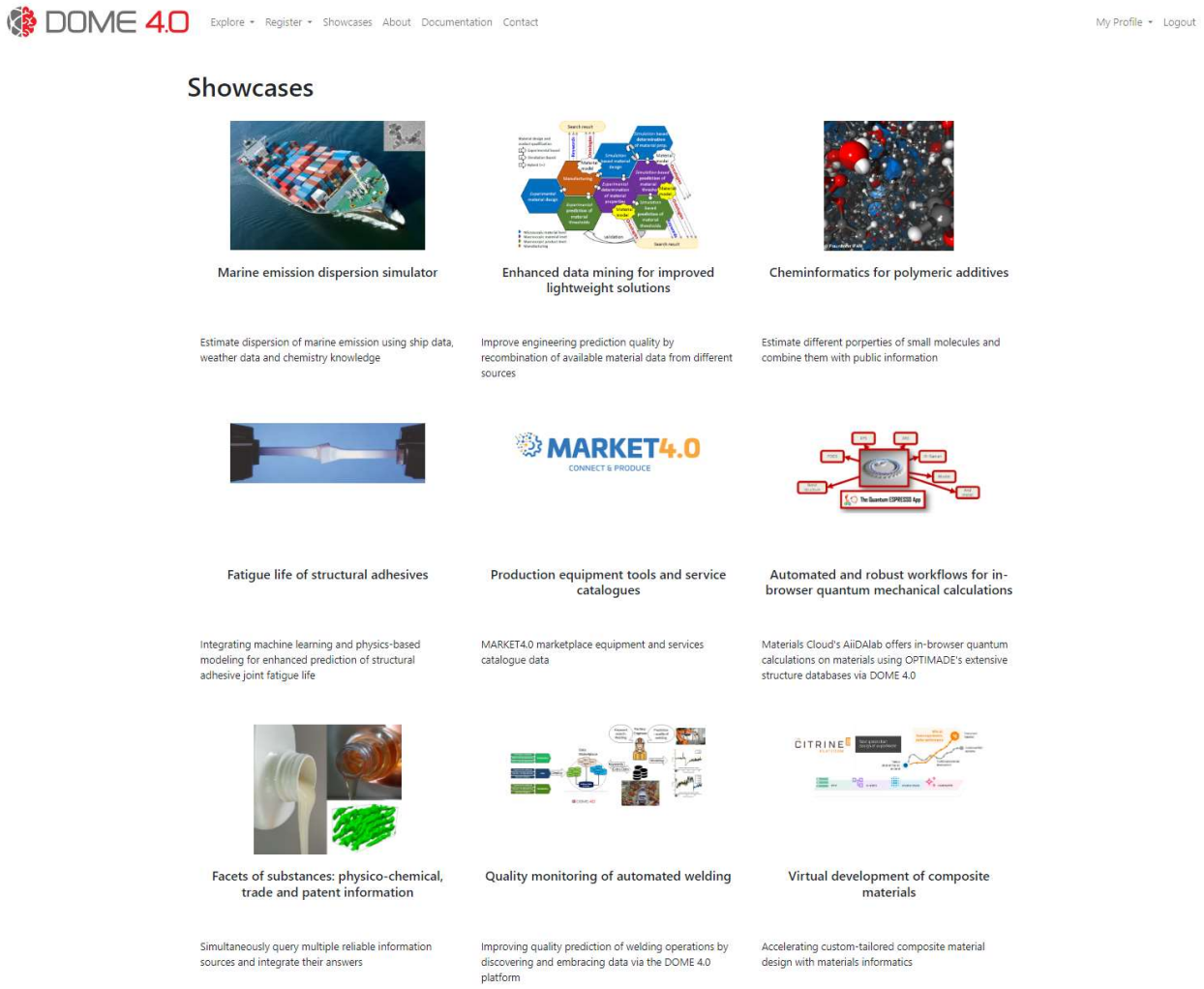

Figure 1 - Showcases Page on the DOME 4.0 Platform

Figure 1 illustrates the Showcases Page on the DOME 4.0 platform, which features a mosaic of the nine B2B showcases that span various industry sectors, including marine, materials, and manufacturing. For a detailed overview, **Error! Not a valid bookmark self-reference.** lists the nine B2B showcases along with their respective industry sectors. The diversity of these showcases highlights the platform's versatility and its potential to drive innovation across multiple domains. Clicking on one of the tiles navigates to a page dedicated to that specific showcase, which is explained in the following section of this document.

Table 1 - DOME 4.0 B2B Showcases

SC #	B2B SC	Sector	Owner(s)
SC 1	Chemistry Knowledge Graph – marine, air quality and nanoparticles	MARINE, ENVIRONMENTAL, NANOPARTICLES	CMCL
SC 2	Lightweight construction – fibre reinforced plastics	PLASTICS	FRAUN, BOSCH
SC 3	Polymer additives for corrosion protection	POLYMERS	FRAUN, SISW
SC 4	Structural adhesives: fatigue behaviour	ADHESIVES	FRAUN, SISW
SC 5	Production equipment tools and service catalogues (metals, plastics, high-tech) – MARKET4.0	MANUFACTURING	INTRA
SC 6	Turnkey services & custom workflows integrating simulations and data	MATERIALS	EPFL
SC 7	Formulated consumer products	CHEMICAL PROCESSES, MATERIALS	UKRI
SC 8	Semantic analytics of manufacturing assets	SMART MANUFACTURING	BOSCH
SC 9	Virtual development of composite materials	COMPOSITE MATERIALS	SISW

2. Showcases Details

2.1 Showcase 1 – Chemistry Knowledge Graph – Marine, Air Quality and Nanoparticles

Showcase 1 features CMCL's Chemistry Knowledge Graph (KG), offering a robust framework to intelligently store, access, and interpret the rapidly expanding datasets on chemical information, marine emissions, location, and air quality. Utilising the DOME 4.0 ecosystem, it ensures semantic interoperability across diverse data sources, including ship location/positioning databases, marine nanoparticle emissions software, air quality dispersion modeling software, and data-based surrogate model generation software. This facilitates a comprehensive analysis of local air quality which can support informed decision-making in urban planning and manufacturing.

Showcase 1 benefits significantly from the DOME 4.0 platform in several ways. Firstly, the platform allows users to initiate new simulations by incorporating external data, such as ship locations, into the modeling workflow of Showcase 1. An example is shown below.

After logging in to the DOME 4.0 platform, users may search for ship location data by the keyword “AIS”. On the page of individual result compatible with the simulation tool of Showcase 1, a button allows user to pass the ship location data to Showcase 1, as shown in Figure 2.

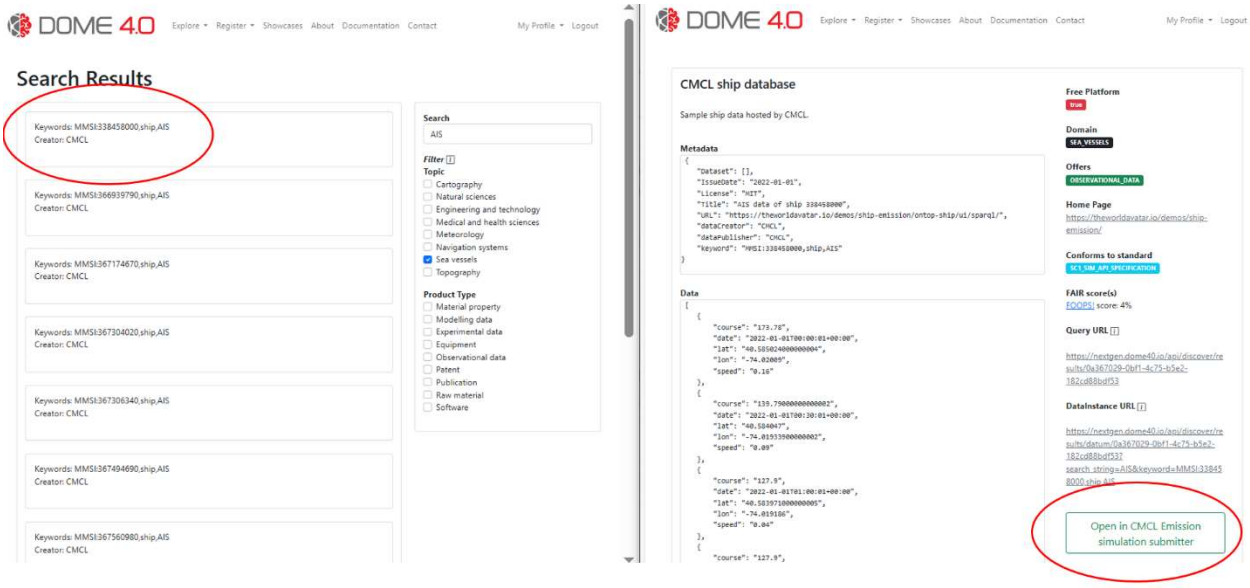

Figure 2 - Ship location data can be searched on the DOME 4.0 Platform

Users will be redirected to the simulation submitter interface as shown in Figure 3, where they can inspect the ship location data, configure the simulation and submit the simulation request to the remote server.

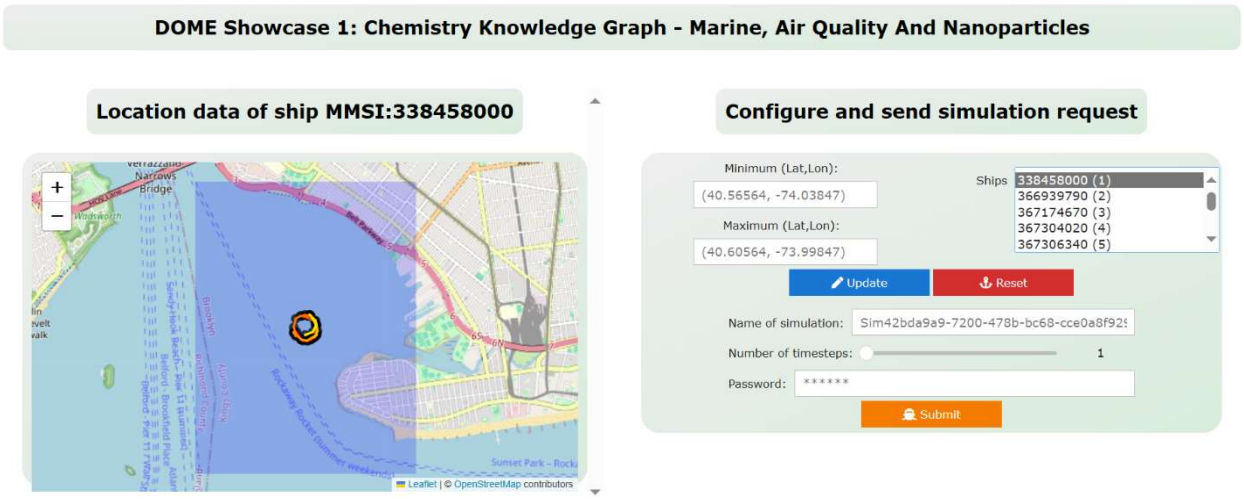

Figure 3 - Simulation submitter for SC1

Once the simulations are completed, the modeling results are made available through the DOME 4.0 platform. Users may search with the keyword ”ship” for available simulation data, as shown in Figure 4. A button will appear to allow users to view the simulation data with the visualisation tool, which is also embedded on the showcase page as shown in Figure 5. This user-friendly access ensures that stakeholders can easily interpret and utilise the data for informed decision-making.

Additionally, the platform offers the potential for further processing of these results using other tools available within the DOME 4.0 ecosystem. This capability allows for more comprehensive analyses and the development of more sophisticated models, ultimately supporting better outcomes in urban planning, environmental monitoring, and other related fields.

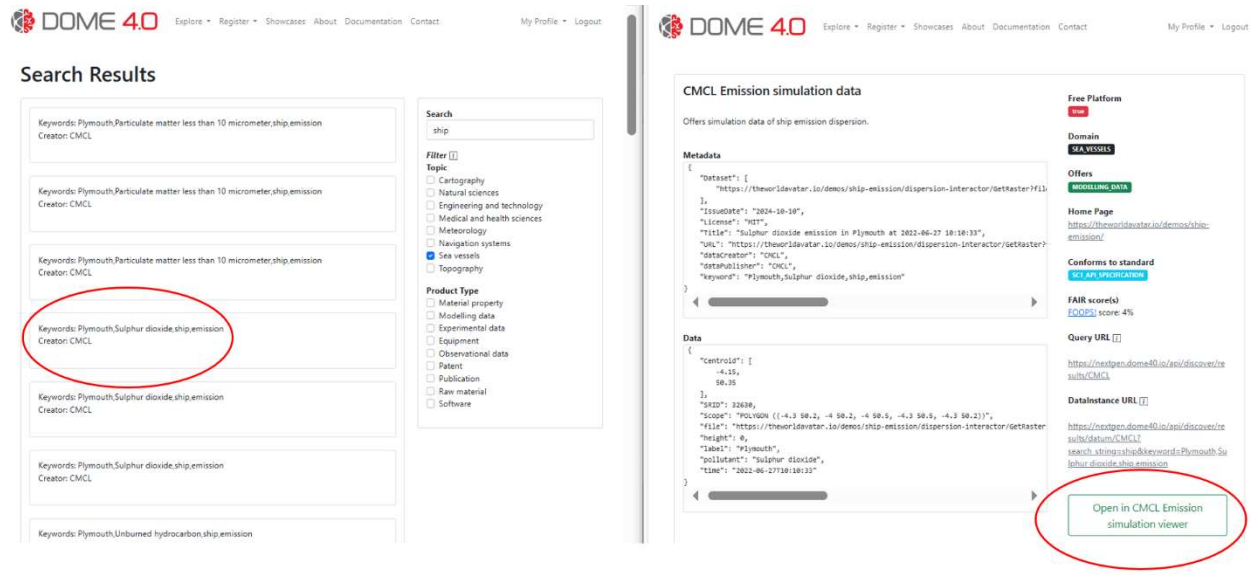

Figure 4 - Simulation output of SC1 can be searched on the DOME 4.0 Platform

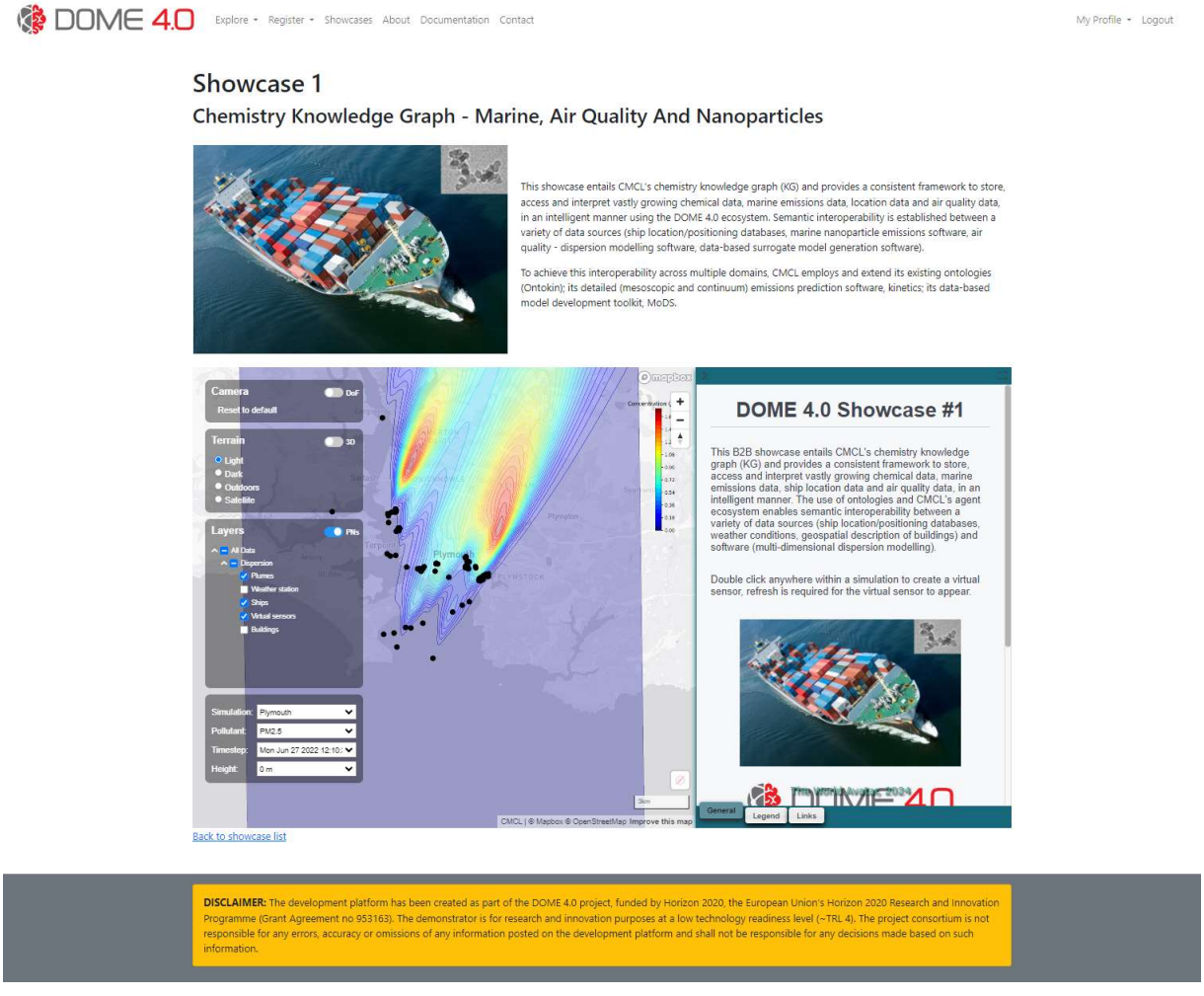

Figure 5 - SC1 Page on the DOME 4.0 Platform

2.2 Showcase 2 – Lightweight Construction – Fiber Reinforced Plastics

Showcase 2 is related to the material data exchange for engineering simulations concerning fiber reinforced polymeric materials. Fiber reinforced polymeric materials especially of the short fiber reinforced type have several special features requiring a significant effort for material parameter determination, including a disordered, spatially varying microstructure, complex temperature dependence across the glass transition of the matrix, strong humidity effects as well as a strong tendency towards creep deformation, aging and other long-term effects.

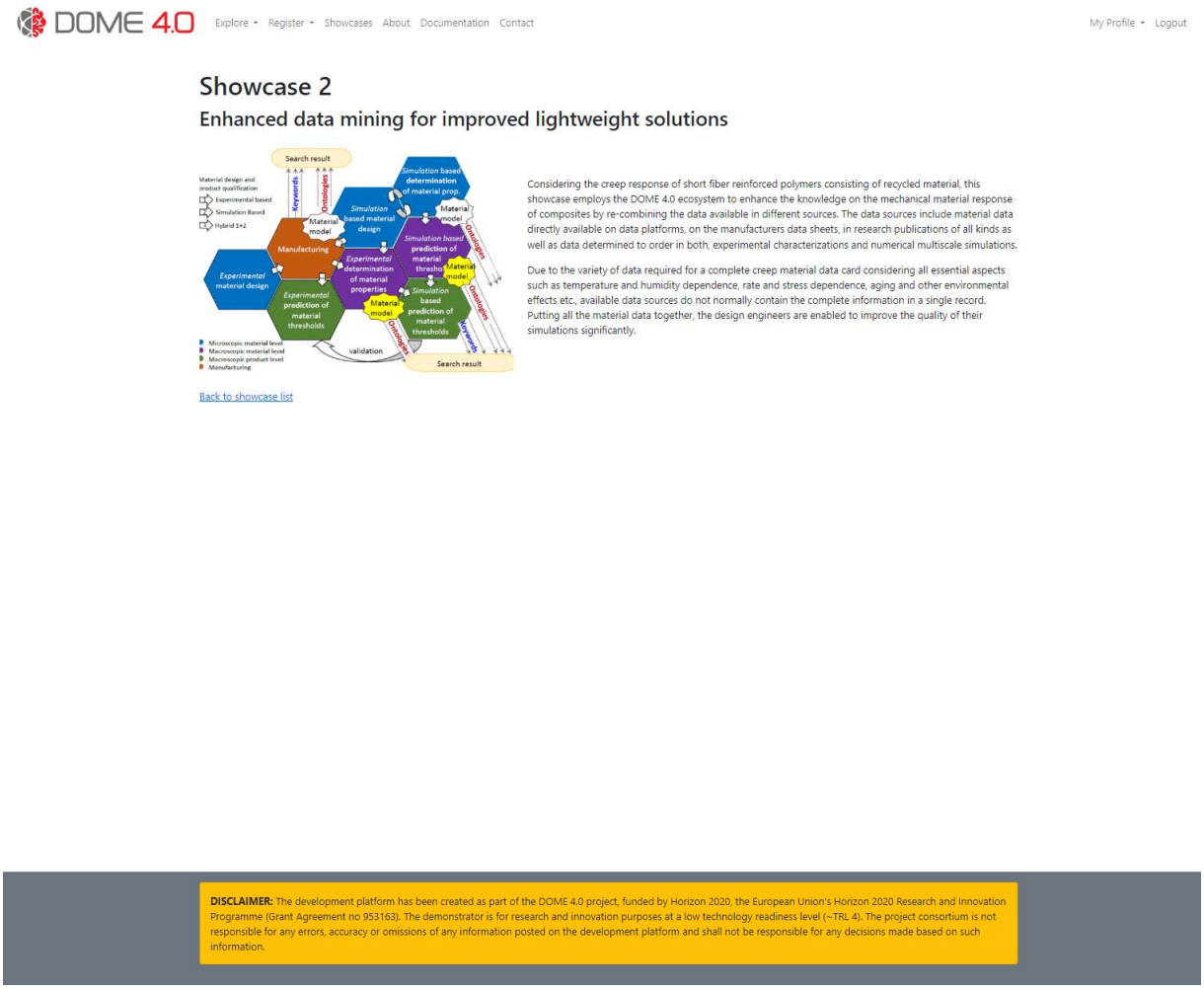

Figure 6 - SC2 Page on the DOME 4.0 Platform

In this showcase the DOME4.0 platform is employed to enrich the usually limited data available for the long-term response – here the creep response – of short fiber reinforced plastics by using pre-existing data from a variety of different sources. These may include experimental data sets for the same material or similar materials made readily available by different data providers on DOME4.0 or other data exchange platforms registered to the DOME4.0 platform, information from material manufacturers available on the

Web, numerical data from various multiscale studies or analyses made-to-order as well as material data and other information from the vast body of scientific literature in the field. Recombination of all these data helps to significantly improve the prognosis quality of engineering simulations, thereby reducing the required (own) experimental effort to a minimum, reducing unnecessary conservatisms, enhancing the utilization of the material, and not least reducing the time-to-market.

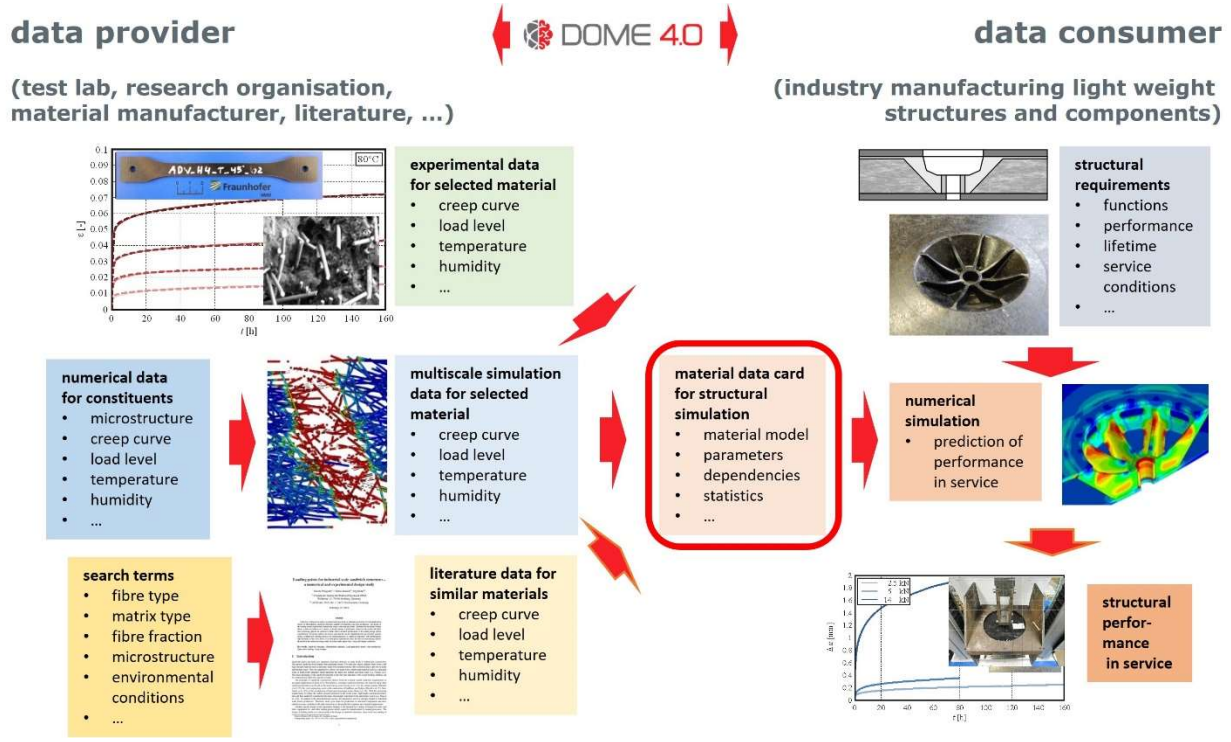

Figure 7: Data flow and re-combination in Showcase 2.

Using the DOME4.0 platform, the data providers can easily register their data sets using the "register catalog data" option of the platform by providing keywords and some related information on the data together with a URL through which the data is available. The data set itself remains on the data providers platform (or a third party data exchange/marketplace platform) with no need to transfer the data to the DOME4.0 platform. By this means, the data providers may also restrict the access to the provided data sets to specific users or users from specific regions using the password protection capabilities of their own platform. By this means business models to provide available data on a pay-per-view or pay-per-download basis are also possible. Although the data preferably is provided in interoperable formats like .json it may also be in other formats as well. In the same manner, articles from the scientific literature may be registered by their DOI leading the data consumer to the publisher's repository together with the respective subscription requirements of their choice without violation of copyright requirements.

The data consumers can simply search the DOME4.0 platform for availability of material data for their specific materials. DOME4.0 then returns all relevant hits providing all information the data providers have provided when registering their catalog data.

2.3 Showcase 3 – Polymer additives for corrosion protection

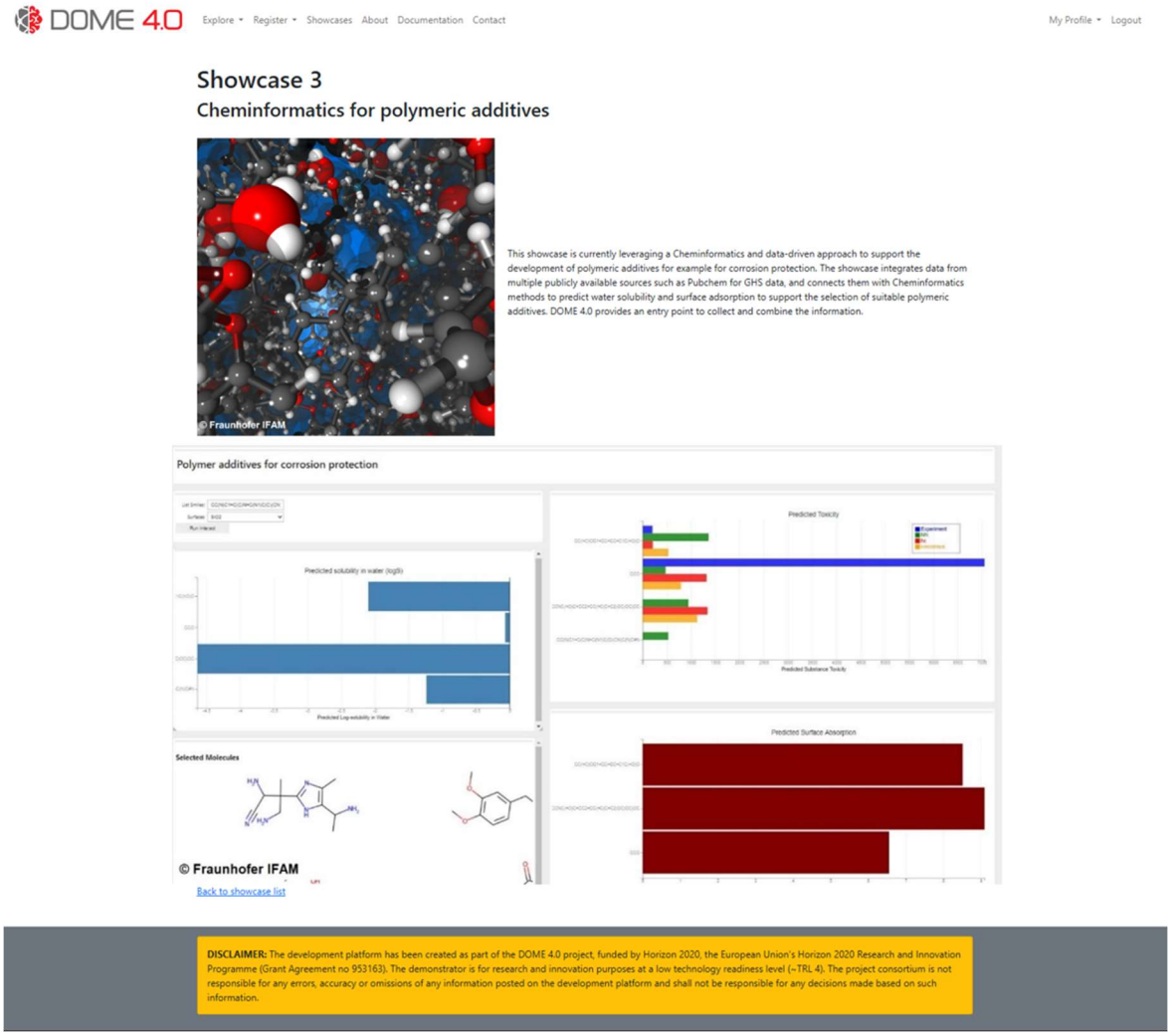

Figure 8 - SC3 Page on the DOME 4.0 Platform

In showcase 3 Cheminformatics and data-driven approaches are combined to expedite the development of polymeric additives for corrosion protection. The showcase integrates data from multiple publicly available sources, such as Pubchem, and connects them with Cheminformatics methods. Figure 8 shows a screenshot of the showcase 3 page and interactive application.

The information is presented as dashboard with individual cells for different types of information, e.g. hazard data, water solubility or toxicology. The individual cells are draggable and resizable.

The molecules that shall be analyzed are specified in the top, left cell (see Figure 9). The molecules are specified a list of SMILES (comma separated). The SMILES (Simplified Molecular Input Line Entry System)

is a specification for describing the structure of chemical species using short ASCII strings[1]. The drop-down menu below allows to specify a surface used for the calculation of the surface adsorption. The button starts the analysis.

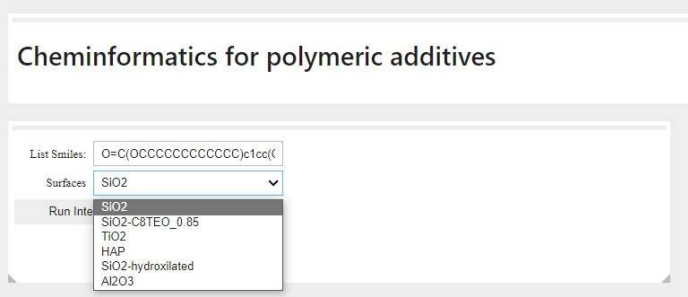

Figure 9 - Top left cell of the dashboard used for specification of molecules and surfaces.

After starting the analysis, the top, right cells will depict the molecules selected. The remaining cell will subsequently populated when the results were calculated or collected from the public sources. The cells will show:

- calculated water solubility (logS), based on a model derived from experimental solubilities (Figure 10 top left),
- predicted surface adsorption, estimated as distance between the molecule and the surface in the Hansen Solubility Parameter space (Figure 10 top right),
- predicted toxicity, calculated by the WebTEST[2] service of the EPA. Shown are the oral rat LD_{50} values calculated using different QSAR Methodologies, e.g. hierarchical clustering or group contribution (Figure 10 bottom),
- documented GHS data (Globally Harmonized System of Classification and Labeling of Chemicals) requested from Pubchem. For each molecule the tables will, if the data is available, show the H-Code and the respective source.

For all calculations the numerical data is also shown as a table in separate cells.

[1] For the generation of SMILES based on 2D structures see e.g. PubChem Sketcher https://pubchem.ncbi.nlm.nih.gov/edit3/index.html

[2] https://www.epa.gov/comptox-tools/users-guide-webtest-version-10-web-services-toxicity-estimation-software-tool

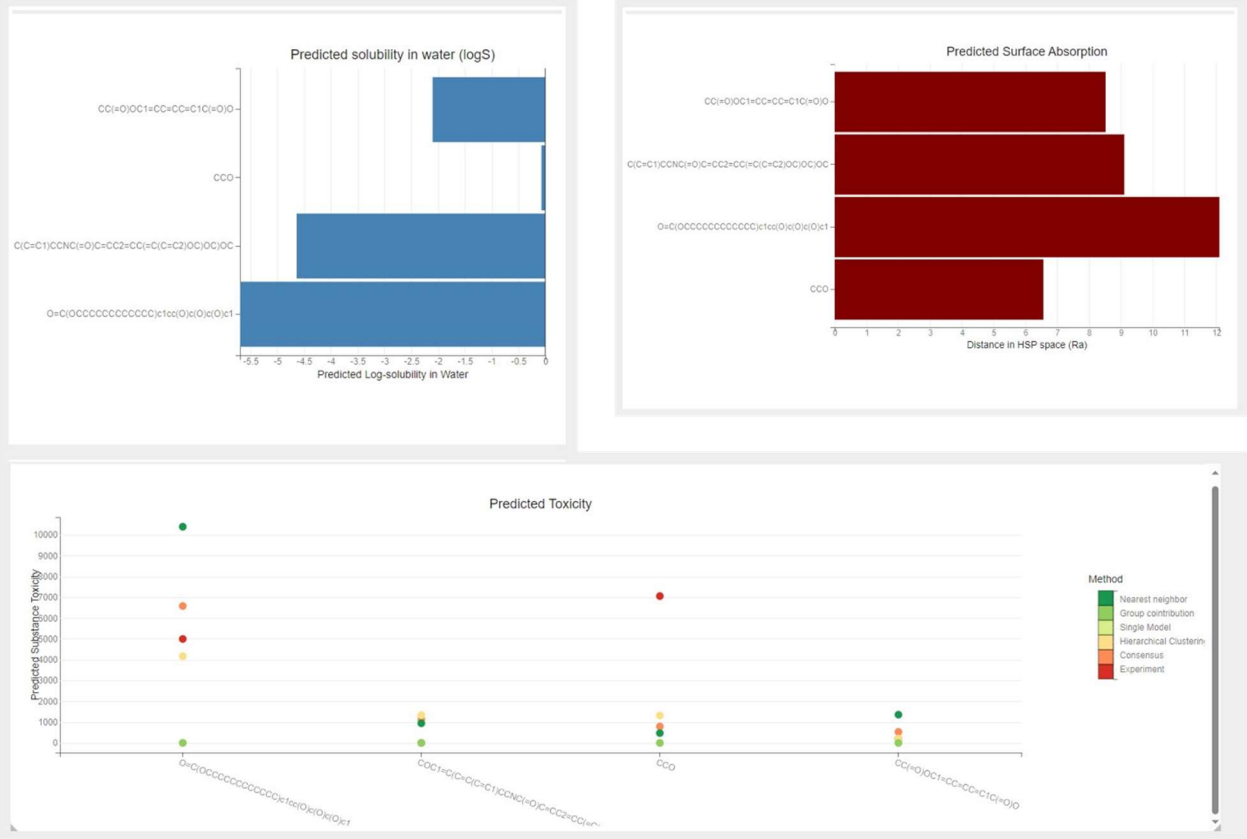

Figure 10 - Exampes for the predicted results (water solubility, surface adsorption, toxicity)of showcase 3 APP.

2.4 Showcase 4 – Fatigue life of structural adhesives

Showcase 4 presents a workflow designed to streamline the fatigue life prediction of adhesives through the utilization of machine learning (ML) models. Its aim is to assist customers in the selection of the appropriate adhesive for adhesively bonded structures, considering specific geometrical and material attributes, as well as usage conditions. This objective is realized through a collaborative effort involving data-provider Fraunhofer and Citrine Informatics, which specializes in materials-aware AI for advancing next-generation materials and chemicals. The showcase caters to a range of industry sectors, including material manufacturers, product manufacturers, software and service providers, and data providers.

For a deeper dive into the industrial context of this showcase, please read our blog post titled "Advancements in predicting the fatigue lifetime of structural adhesive joints".

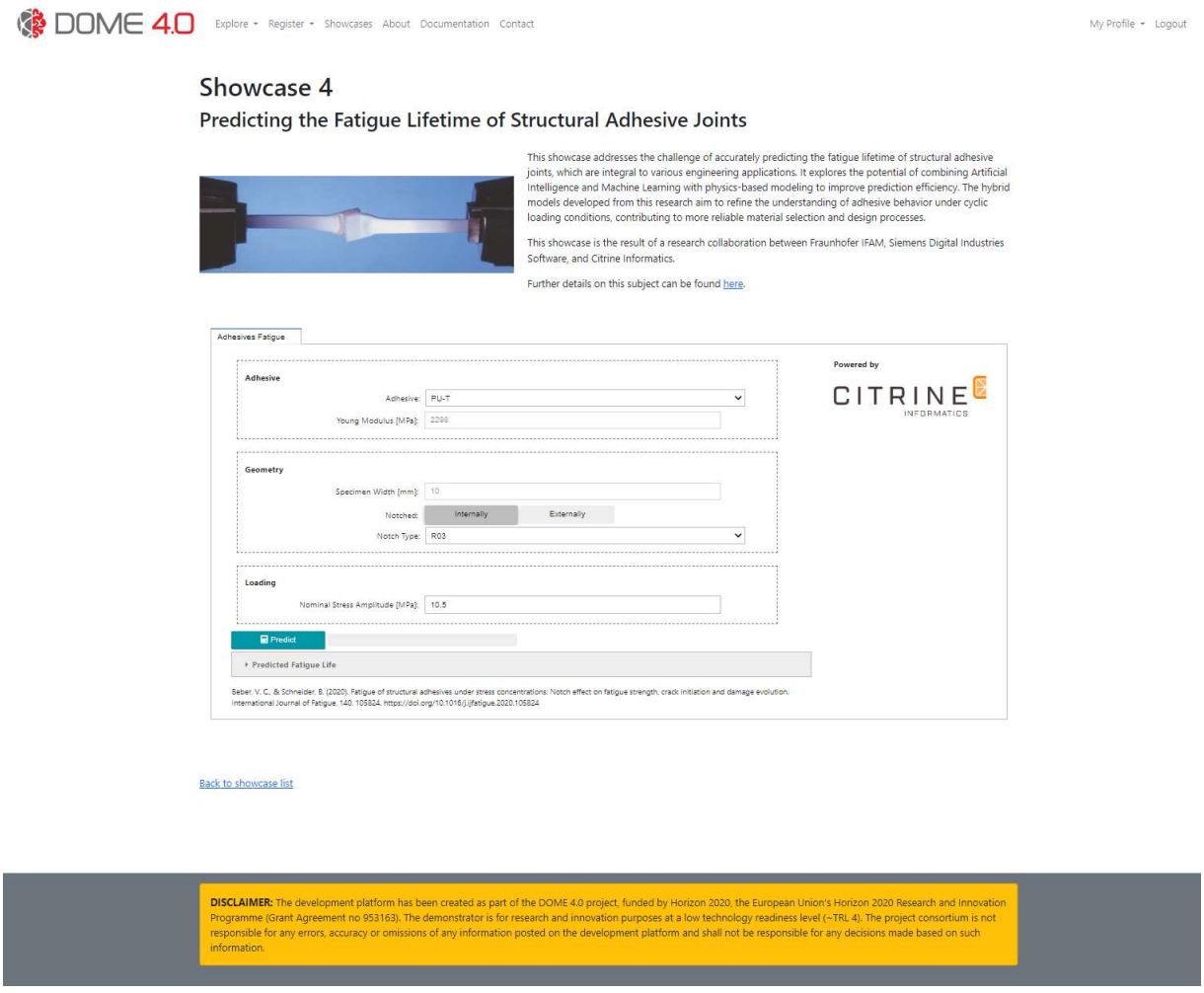

Figure 11 - SC4 Page on the DOME 4.0 Platform

Figure 11 depicts the showcase page for SC4, featuring a brief description of the showcase along with an embedded iframe containing the interactive tool at its core.

A detailed view of the interactive tool is presented in Figure 12. Here, users can select the type of adhesive they are interested in, with the corresponding Young's modulus updating automatically. Additionally, users can input geometric details related to specimen and notch sizes, as well as the nominal stress amplitude applied. By clicking the "Predict" button, the input data is sent to the trained Machine Learning (ML) model on the Citrine platform, which then returns the expected fatigue life of the selected adhesive under the specified conditions, expressed in both the number of cycles until failure and its logarithmic value. The tool also provides the auxiliary quantity, Length of Highly Stressed Region, for additional context.

For further technical details about the quantities and the fatigue dataset used to train the ML model that powers this tool, please refer to the scientific publication: Beber, V. C., & Schneider, B. (2020). Fatigue of structural adhesives under stress concentrations: Notch effect on fatigue strength, crack initiation and damage evolution. International Journal of Fatigue, 140, 105824. https://doi.org/10.1016/j.ijfatigue.2020.105824.

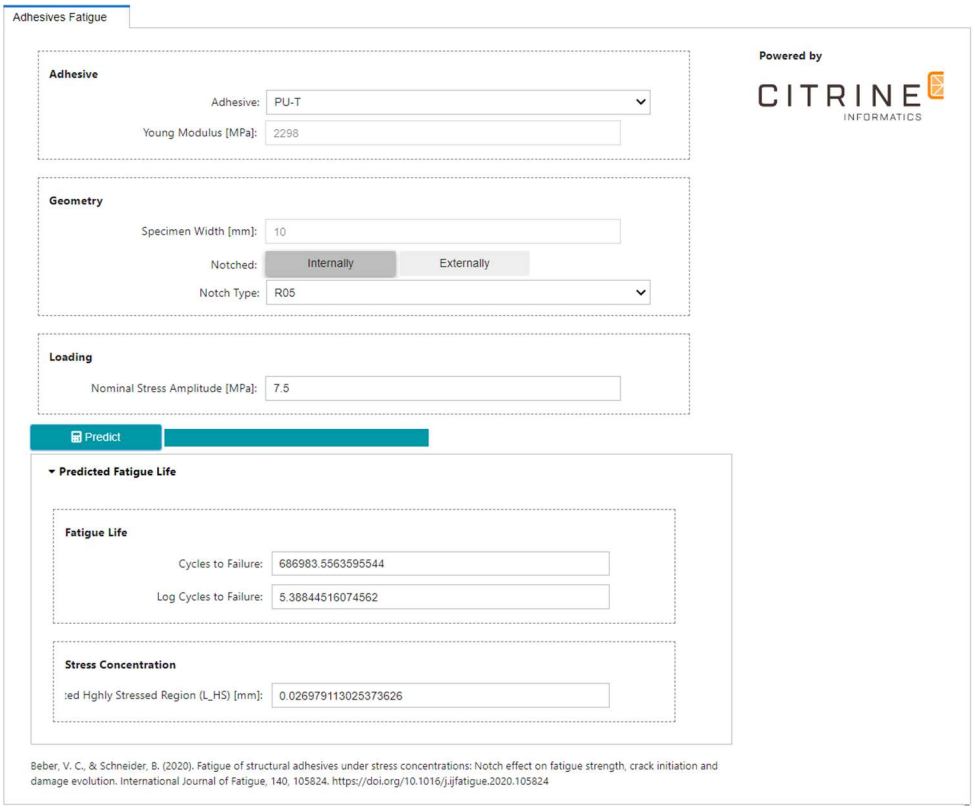

Figure 12 - SC4 Prediction Tool

In addition to the described showcase page and interactive tool, datasets related to the fatigue life of structural adhesives and adhesive joints have been registered on the DOME 4.0 platform, complete with detailed metadata and keywords to facilitate search and retrieval. Users are notified that these datasets are related to SC4 through the "SC4 API Specification," which indicates an associated tool by displaying a green button in the right panel. This button directs users to the SC4 showcase page. An example demonstrating the association between a dataset and the tool can be seen in Figure 13.

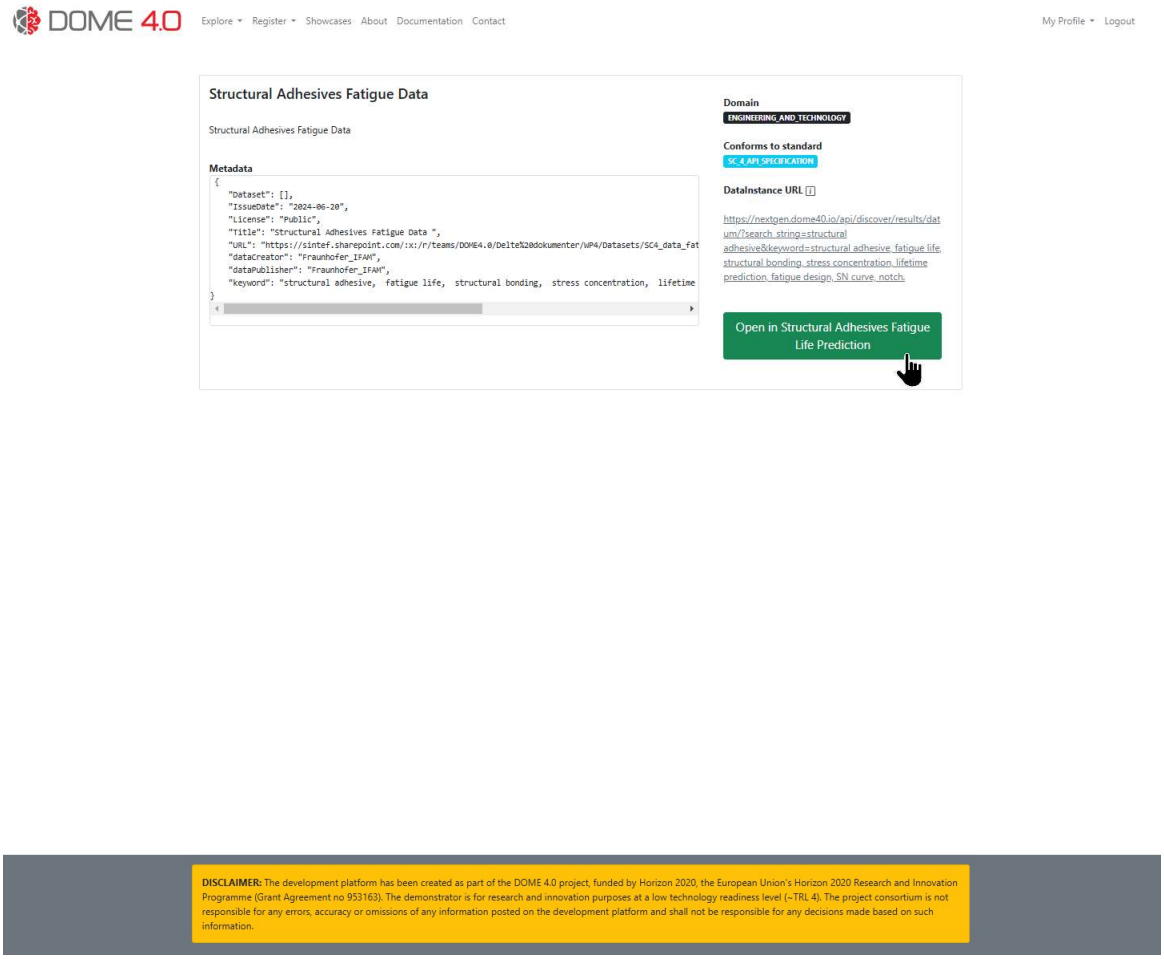

Figure 13 - Example of a dataset associated to SC4

2.5 Showcase 5 – Production equipment tools and service catalogues (metals, plastics, high-tech) – MARKET4.0

Showcase 5 deals with the integration of the MARKET4.0 marketplace with the DOME 4.0 platform. Showcase 5 has enriched the DOME 4.0 platform with data coming from the production equipment procurement domain.

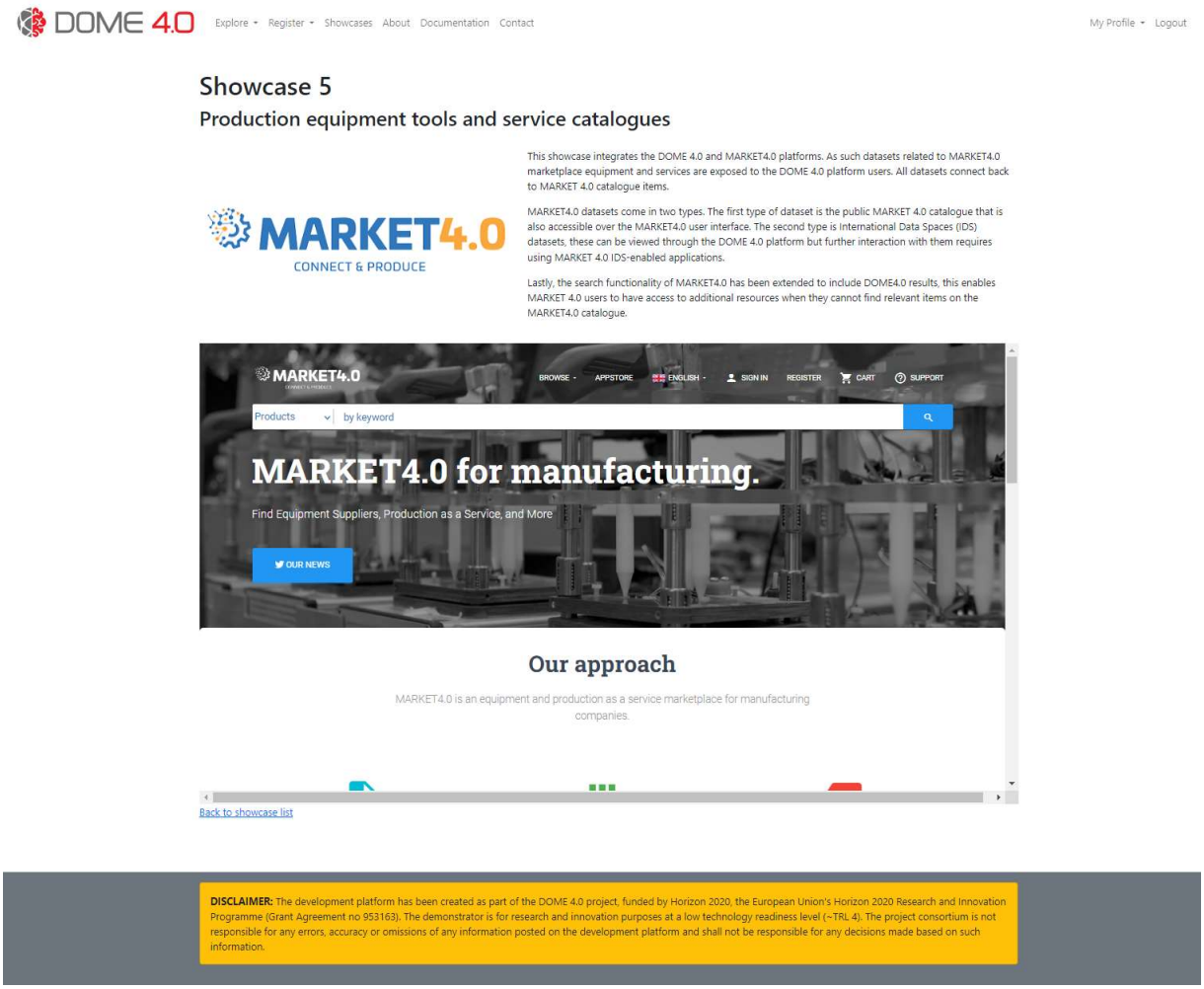

Figure 14 - SC5 Page on the DOME 4.0 Platform

Due to the nature of the MARKET4.0 platform two kinds of data sources were integrated in the DOME 4.0 platform. The public catalogue data that are available over a typical HTTP API and private supplier data that are available over IDS. Both types are seamlessly integrated and are available for querying over the platform's search functionality. In Figure 15 one dataset is presented for using the keyword 'copper'. This dataset will lead back to the MARKET4.0 platform where the users may further interact with the supplier of the equipment.

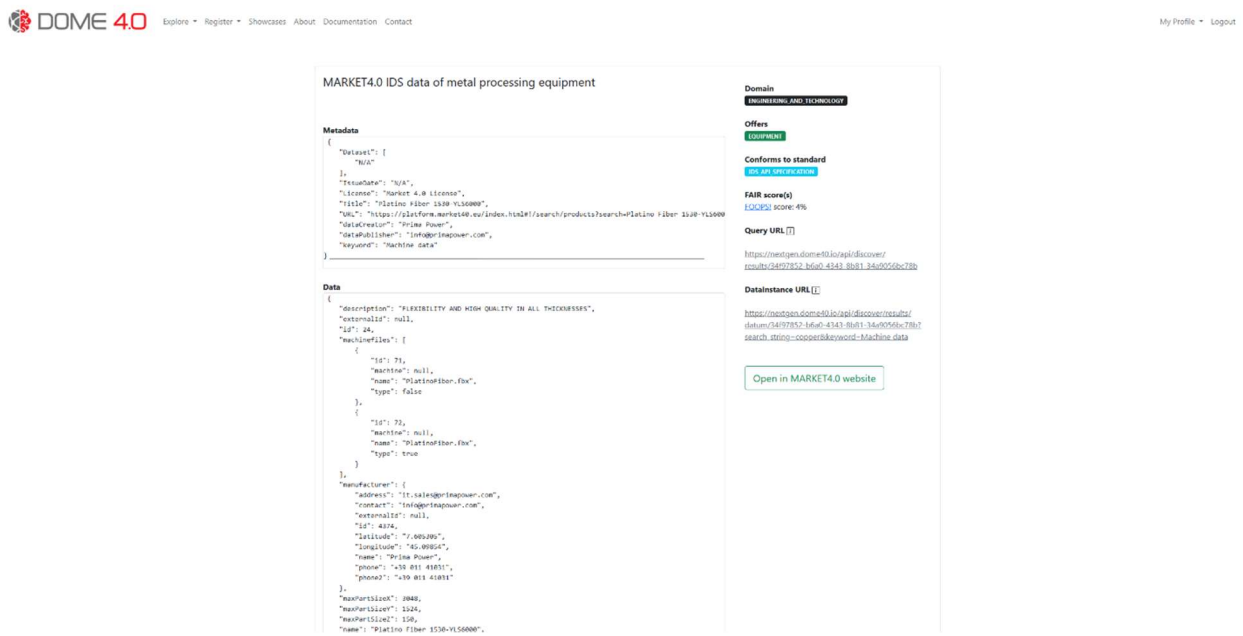

Figure 15 MARKET4.0 dataset for keyword 'copper'

However, when searching for data in DOME4.0 different sectors results will appear which provides an opportunity to the users to explore combinations of different information. For example, equipment supplier information in combination with material information. Lastly, DOME4.0 data are also accessible over the MARKET4.0 platform. For example, see Figure 16 results for keyword 'Digitoxin'. Showcase 5 acts as two-way gateway between the DOME4.0 and MARKET4.0 platforms enabling both platforms to take advantage of the other user base.

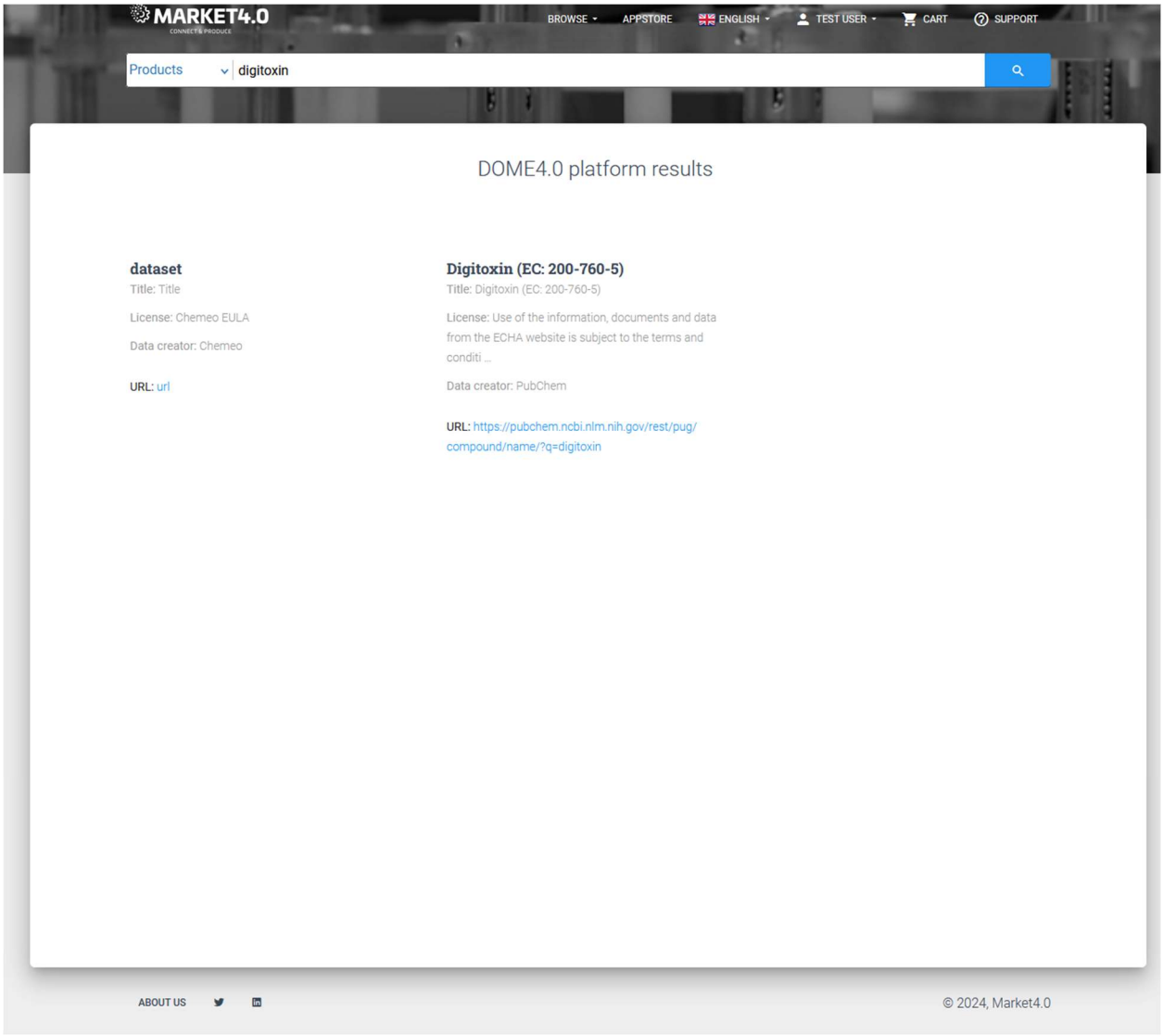

Figure 16 DOME 4.0 dataset for keyword 'digitoxin'

2.6 Showcase 6 – TITLE

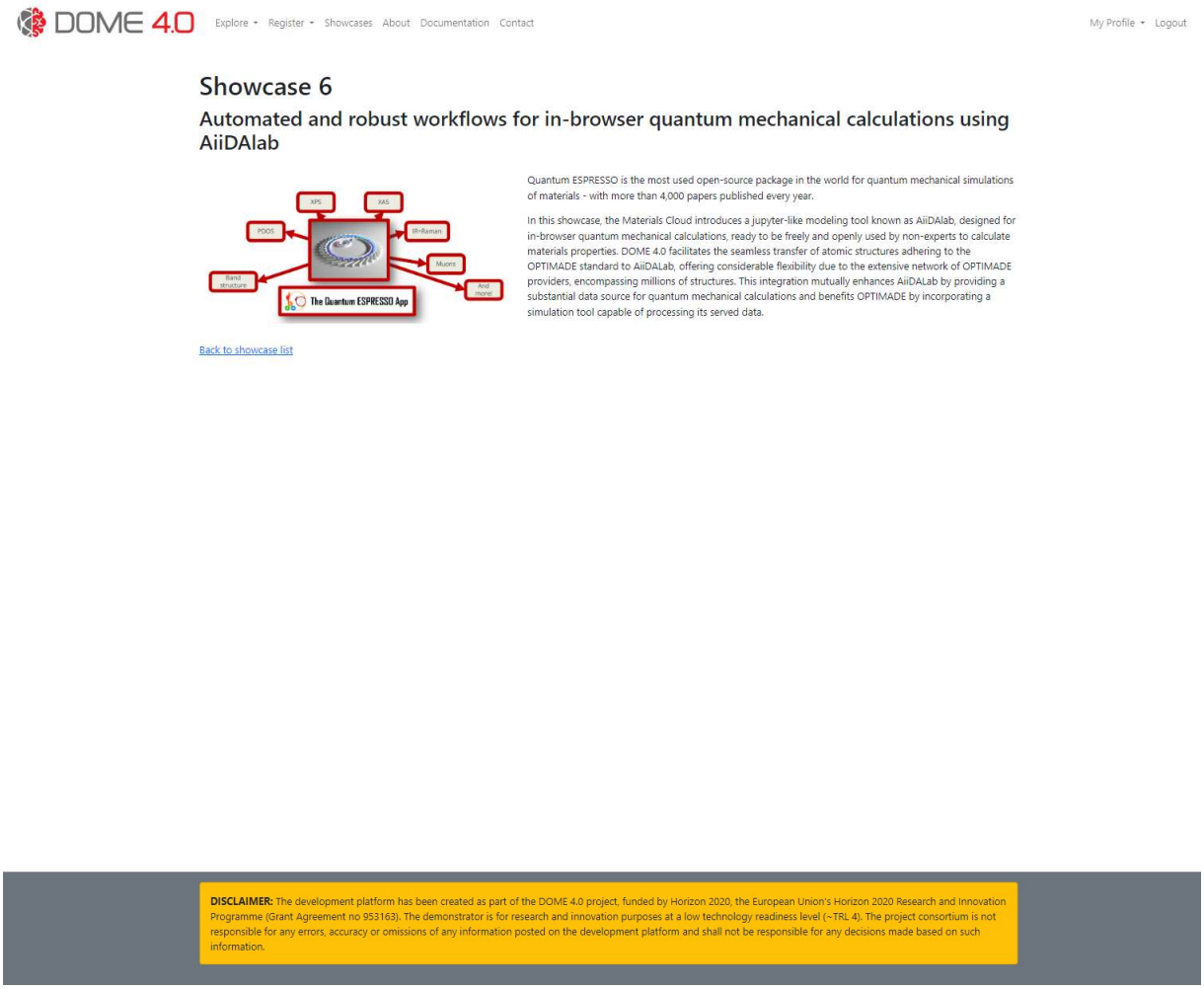

Figure 17 - SC6 Page on the DOME 4.0 Platform

2.7 Showcase 7 – Consumer-formulated products. Facets of substances: physico-chemical, trade and patent information

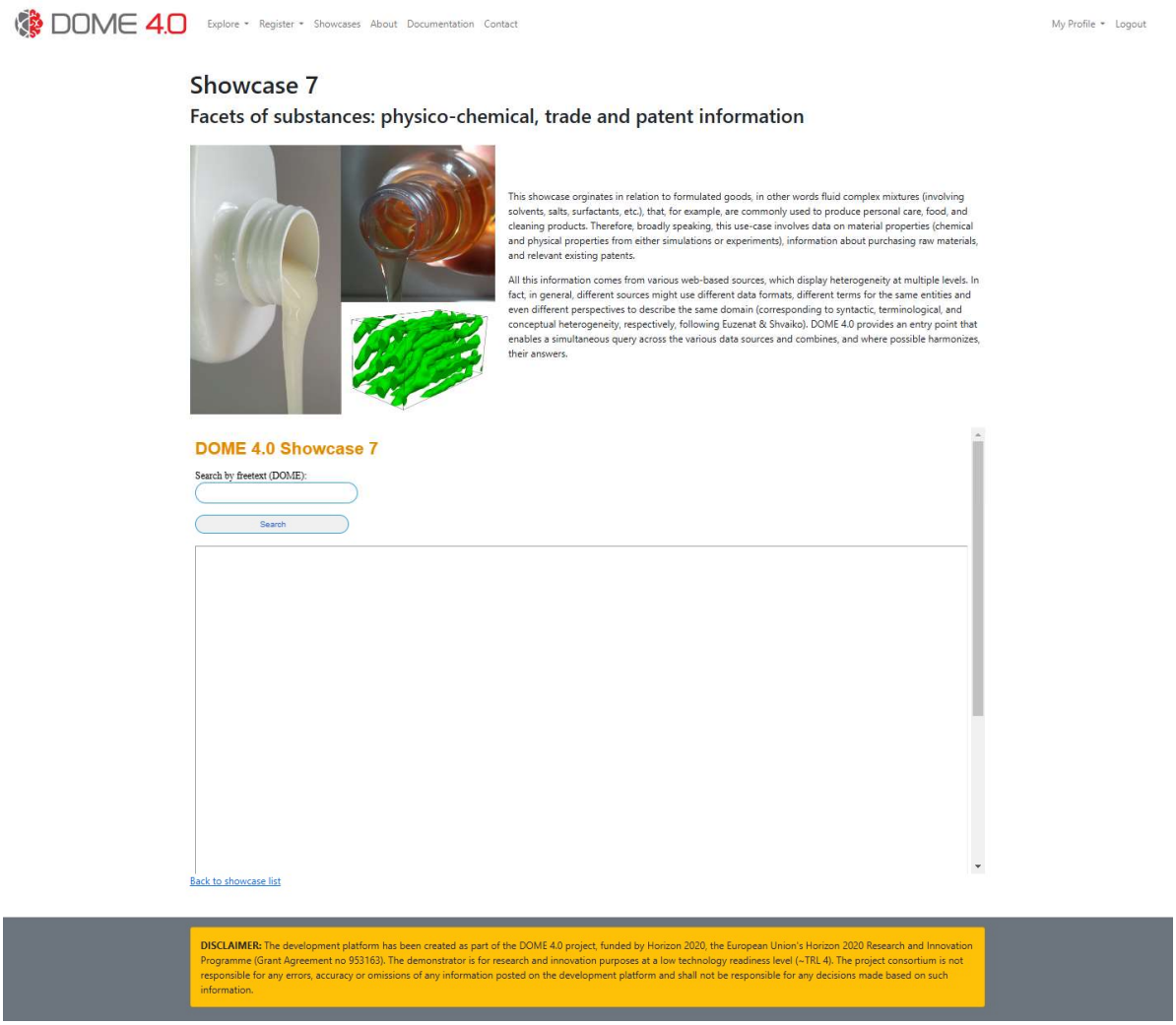

Figure 18 - SC7 Page on the DOME 4.0 Platform

Context

Showcase #7 is about *formulated goods*, in other words fluid complex mixtures (involving solvents, salts, surfactants, etc.), that, for example, are commonly used to produce personal care, food, and cleaning products. Broadly speaking, this use-case involves data on chemical and physical *material properties*, information about purchasing *raw materials*, and relevant existing *patents*. All this information comes from various web-based sources, which display heterogeneity at multiple levels. DOME 4.0 showcase #7 allows to simultaneously query these reliable information sources and combine their answers, providing a unified view of information (see Figure 19).

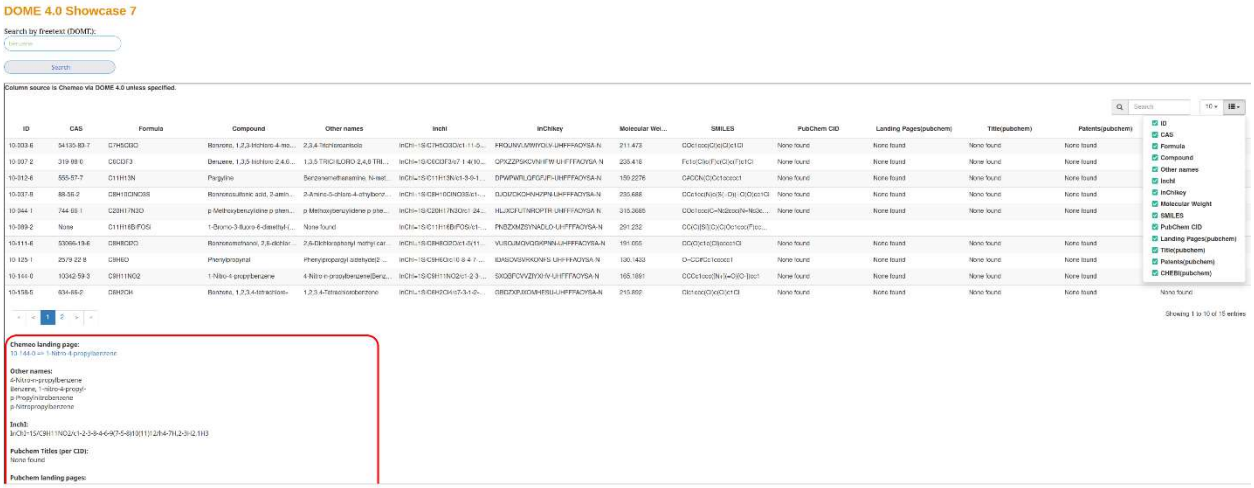

Figure 19 - SC7 Interactive Tool

Brief description

This is a website allowing the user to search a string literal on the data provided by the Chemeo API service. The matching records will then be used to fetch more data from other sources behind the scenes. All data will be sorted as a dynamic table (as depicted). The table will act as client-side storage. A row can be clicked to show a better view of the information harvested.

The results are paginated according to the numeric top right combo box (default is 10). The visibility of the columns can be also adjusted. To search the visible table cells the top right input box may be used to search a string literal dynamically on the data. The columns are sortable by clicking either alphanumerically or numerically according to the current configuration file.

How it works

The user will search all available internal and external APIs by using a string literal on the input box and pressing submit. Depending on the number of records fetched (hits) and the number of IDs of interest in their data payload, it may take a while (A limit can be configured).

Currently, for each row (aka record) different PubChem APIs will be queried to obtain associated pieces of information and expand what we know. There will be a strict one-to-one correspondence to the record taking the CAS registry number as the initial ID to find more unique IDs of use, particularly PubChem CIDs.

The initial columns of the table are based on what a Chemeo reponse (JSON payload) will provide consistently. (the columns can be configured/expanded) More information is added thereafter. It is fully configurable.

A red infobox is used to highlight one record, or make it more readable, adding more information stored. It also provides links to the data sources (created out of IDs) to ease navigation.

Below the infobox there are dropdown web widgets with further information and references.

Conclusion

All the information to create a subgraph of the Knowledge Graph related to the searched string is available. The emphasis here is on the usability and accessibility afforded by the web UI.

2.8 Showcase 8 – TITLE

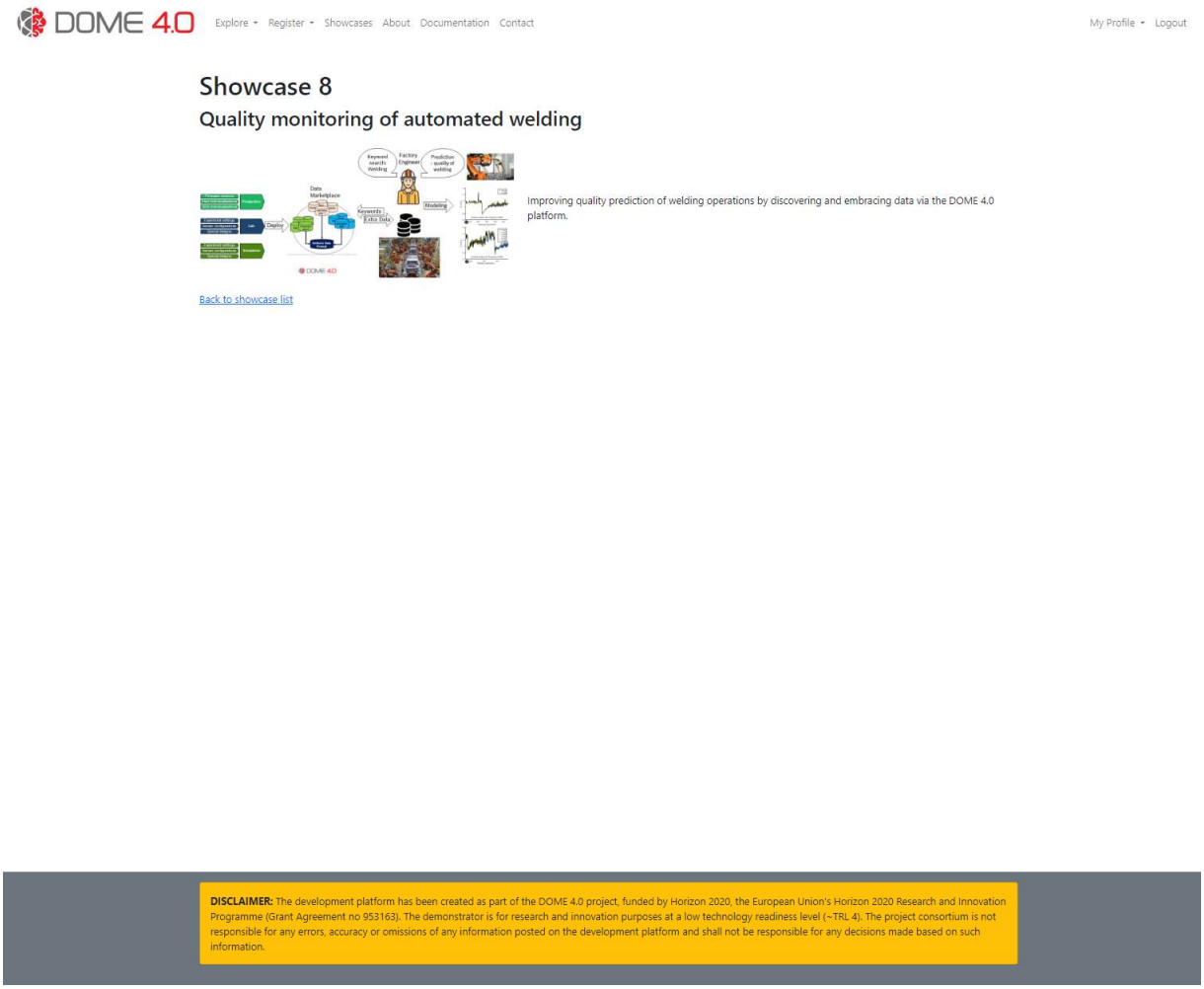

Figure 20 - SC8 Page on the DOME 4.0 Platform

2.9 Showcase 9 – Virtual development of composite materials

Showcase 9 presents a comprehensive workflow for virtual composite material development, leveraging a machine learning (ML) framework integrated with the DOME 4.0 environment. The primary commercial objective is to empower material manufacturing companies to assist their customers in identifying optimal mixing ratios for open-compound material systems based on specific requirements. This objective is realized through collaborative efforts involving data-provider SABIC, a chemical company, and Citrine Informatics, a specialist in materials-aware AI for advancing next-generation materials and chemicals. The showcase caters to various industry sectors, including material manufacturers/chemical companies, product manufacturers, software and service providers, and data providers.

For a deeper dive into the industrial context of this showcase, please read our blog post titled "Materials informatics accelerates customer tailored composite material design".

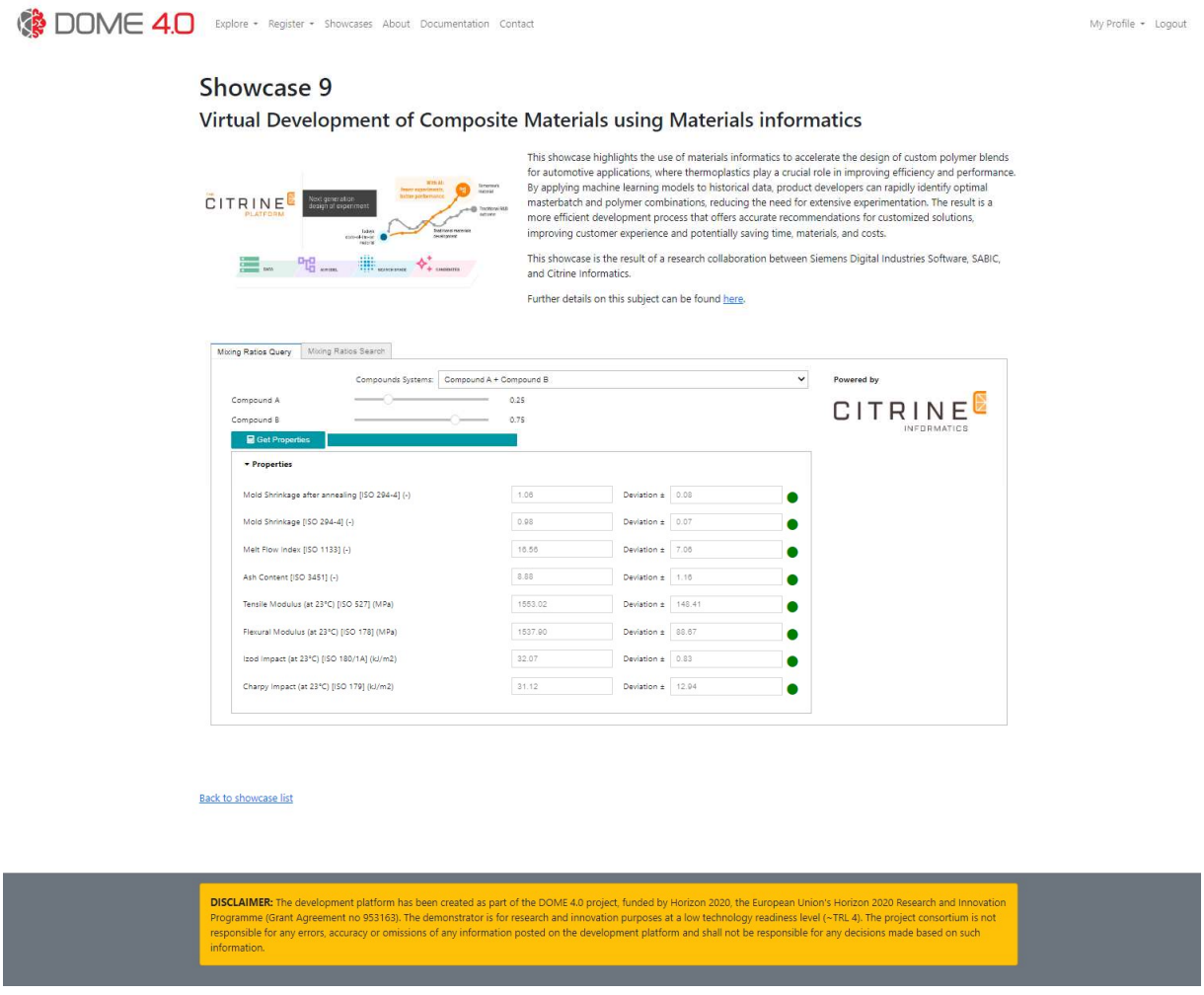

Figure 21 - SC9 Page on the DOME 4.0 Platform

Figure 21 depicts the showcase page for SC9, featuring a brief description of the showcase along with an embedded iframe containing the interactive tool at its core.

This tool offers two distinct functionalities: (i) Mixing Ratio Query, detailed in Figure 22, and (ii) Mixing Ratio Search, illustrated in Figure 23.

Mixing Ratio Query: Users can specify a pair of open compounds (commercial names redacted) and the intended mixing ratio. By clicking the "Predict" button, this data is sent to the trained Machine Learning (ML) model on the Citrine platform, which then forecasts the resulting mechanical properties. Within a few seconds, the results are displayed in the lower box.

Mixing Ratio Search: Users can specify the desired mechanical properties, such as Mold Shrinkage, for a chosen pair of open compound systems. The inputs are sent to the Citrine platform, and after a few minutes, the suggested mixing ratios and the predicted mechanical properties are returned to the user.

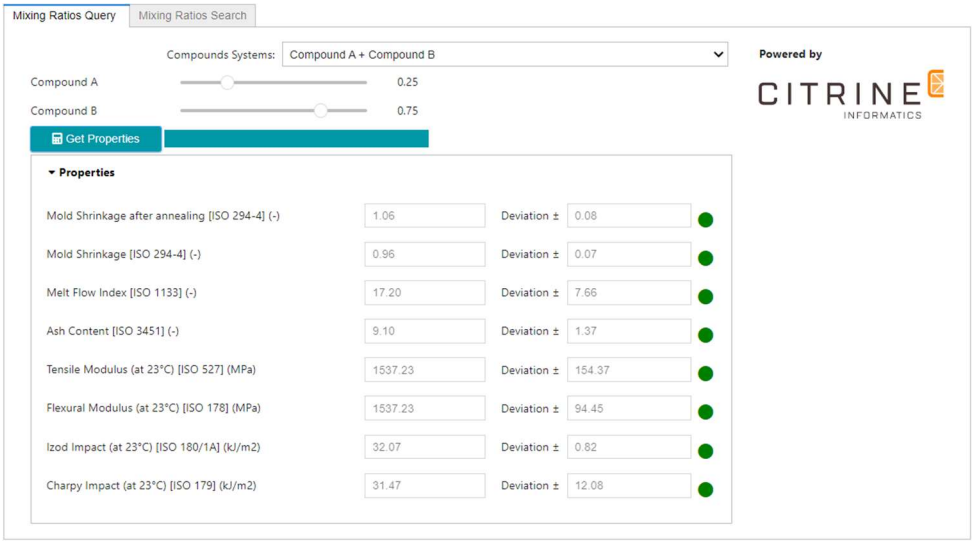

Figure 22 - SC9 Prediction Tool – Query

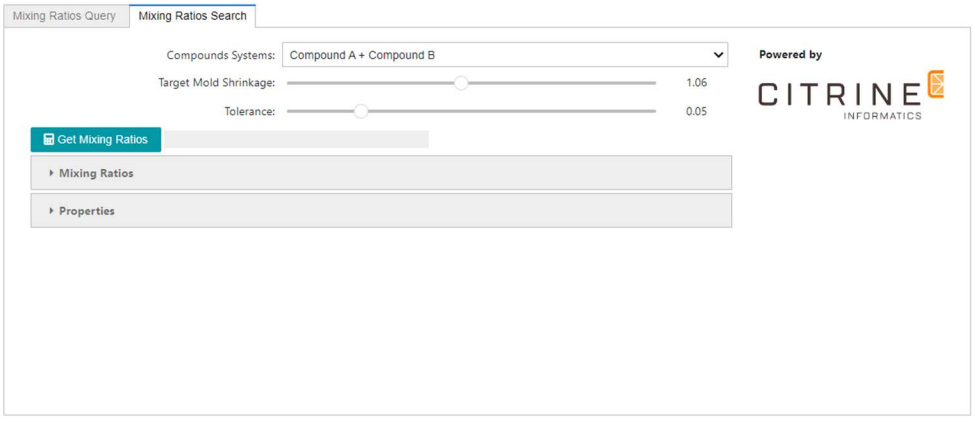

Figure 23 - SC9 Prediction Tool – Search

In addition to the described showcase page and interactive tool, datasets pertinent to this showcase, such as the list of open compounds, have been registered on the DOME 4.0 platform. These datasets come with detailed metadata and keywords to facilitate search and retrieval. Users are informed that these datasets are related to SC9 through the "SC9 API Specification," which highlights an associated tool by displaying a green button in the right panel. This button directs users to the SC9 showcase page. An example demonstrating the association between a dataset and the tool can be seen in Figure 24.

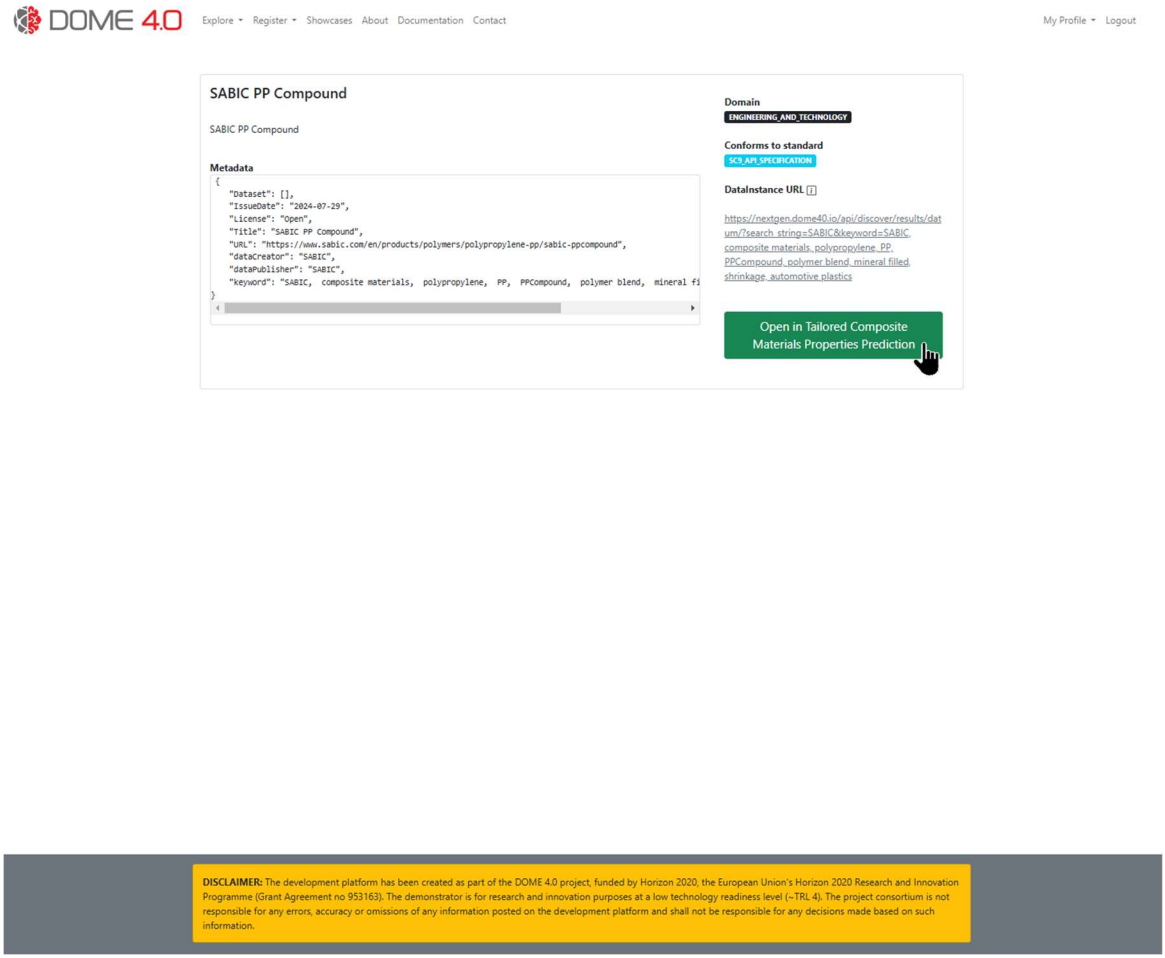

Figure 24 - Example of a dataset associated to SC9