AsedaSciences® Partners with Chemspace to Visualize 13 Billion Compounds on 3RnD® Cloud Platform

The world's largest synthesizable chemical library to be visualized in the 3RnD Compound Universe, enabling easy nearest neighbor identification and ordering

April 23, 2025 – Schindellegi, Switzerland, Schwyz – AsedaSciences, an innovator in advanced chemical analysis and visualization solutions, is excited to announce its collaboration with Chemspace to integrate their unparalleled collection of over 13 billion compounds into AsedaSciences' 3RnD cloud platform. This partnership will simplify and enhance how researchers, chemists, and drug developers interact with chemical structures, making the process of searching, selecting, and ordering similar compounds easier and more efficient than ever before.

Through this collaboration, AsedaSciences will leverage its innovative Compound Universe visualization tool to enable users to cluster and select the nearest neighbor chemical structures of interest and seamlessly order them from Chemspace via the 3RnD platform. This integration allows scientists to upload their compound structures and compare them against the largest commercially accessible chemical library, which includes over 13 billion compounds offered by Chemspace. Now, this extensive library of synthesizable compounds will be visualized and accessible directly within the 3RnD interface, enabling users to search for compounds and their nearest neighbors with ease. By streamlining the complex task of compound selection, this integration allows scientists to rapidly identify novel chemical entities to include in their research and development activities.

AsedaSciences' Compound Universe tool offers an intuitive and robust platform for visualizing vast chemical libraries, providing interactive and dynamic representations of compounds that aid in understanding molecular relationships. By integrating Chemspace's comprehensive dataset into the 3RnD platform, users gain access to the largest collection of synthesizable compounds globally, with the ability to select and order compounds based on proximity and other relevant chemical properties.

"We are excited to collaborate with Chemspace to bring this groundbreaking visualization of the world's largest commercial chemical library to scientists globally," said Brad Calvin, CEO of AsedaSciences. "By integrating the immense library offered by Chemspace into the 3RnD platform, we are enabling a more efficient and streamlined research experience for scientists around the world. This collaboration is a key step in our mission to empower researchers with the tools they need to make faster, more informed decisions earlier in drug discovery."

"We believe this partnership with AsedaSciences will provide our users with unprecedented access to the largest set of synthesizable compounds available globally," said Olga Tarkhanova, PhD, CEO of Chemspace. "With AsedaSciences' advanced visualization capabilities, users can now explore our library in a more intuitive and effective way, enhancing the research process and speeding up the discovery of new compounds with high therapeutic potential."

The integration of Chemspace's library into AsedaSciences' 3RnD platform provides a powerful, user-friendly solution for accessing a vast array of compounds, selecting optimal chemical structures, and facilitating seamless compound ordering. This collaboration is poised to accelerate the pace of innovation in various sectors, including pharmaceutical research, materials science, and more.

About AsedaSciences

AsedaSciences integrates non-animal testing methods, machine learning, and cloud-based data analysis and visualization for earlier prediction of toxicity risk to support safer compound design across the chemical-producing industries. Through its innovative, cloud-based, AI-enabled 3RnD® platform, AsedaSciences empowers scientists to rapidly understand the relationship between chemical structures and their biological effects to support the selection, prioritization and progression of compounds that are safer for human health and the environment.

About Chemspace

Chemspace is the world's largest catalog of synthesizable chemical compounds, offering over 13 billion compounds from various suppliers. Chemspace's platform is a critical resource for researchers and companies involved in drug discovery, materials science, and other chemical research fields, providing access to a vast array of compounds for screening, selection, and ordering. Chemspace is also a global provider of drug discovery services. They streamline hit finding by integrating Computational Chemistry tools, Bioinformatics, and Machine Learning-based services for smarter drug discovery. Their integrated projects combine hit identification and biological validation, offering a seamless path through early-stage drug discovery.

For more information, visit https://chem-space.com

For media inquiries, please contact:

For Chemspace

Olga Tarkhanova, Ph.D.

Email: o.tarkhanova@chem-space.com

https://chem-space.com

For AsedaSciences

Brad Calvin info@asedasciences.com

https://www.asedasciences.com/