

FOR IMMEDIATE RELEASE

Machine Learning of Better Physical Property Relationships

Frankfurt, Germany (August 22, 2022) – Molecular Knowledge Systems (MKS) debuted their new machine learning software module atACHEMA 2022. The software discovers new physical property relationships by combining molecular structure manipulation algorithms, physical property estimation techniques, and multiple regression analysis with a library of example model templates. This combination enables chemical companies to quickly develop tailored physical property relationships, thus enhancing their process optimization and product innovation, by just adding their own proprietary data.

The new machine learning module is available in both Cranium 5.0, MKS’s physical property estimation software, and Synapse 4.0, MKS’s chemical product design software. Incorporating the module into these software products enables users to easily manage hundreds or even thousands of physical property models, add their own physical property data for both pure chemicals and mixtures, estimate the physical properties of new chemicals and mixtures, and design new, innovative chemical products.

“The release of our new machine learning module is very exciting not only because it enables chemical companies to capitalize on their proprietary physical property data, which was often obtained at significant time and expense, but it also gives us here at MKS a content-rich method for distributing our three decades of expertise in developing physical property relationships,” said Dr. Kevin Joback, president of Molecular Knowledge Systems, Inc and a recognized expert in physical property estimation methods. “The ultimate goal of our new machine learning module is to enable users to develop estimation methods just as well as we can.”

Molecular Knowledge Systems, Inc. is a leading provider of computer software and consulting services that enable companies to develop new, improved chemical products by understanding and exploiting the relationships between chemical structure and physical properties. The company will be exhibiting in Hall 9.1, Booth D85 atACHEMA in Frankfurt, Germany from August 22 through August 26, 2022.

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<https://www.molecularknowledge.com/news/2022-08-22-ACHEMA/MachineLearning.html>.

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