

May 9, 2017

## MilliporeSigma Acquires Grzybowski Scientific Inventions to Expand Chemical Synthesis Offering

- **Revolutionary computer-aided retro-synthesis software optimizes productivity, organic synthesis**
- **Complements MilliporeSigma's leading e-commerce platform and chemistry portfolio of more than 400,000 building blocks, catalysts and reagents for chemical synthesis**

Billerica, Massachusetts, May 9, 2017 — [MilliporeSigma](#) today announced the acquisition of Grzybowski Scientific Inventions (GSI), a company that developed the revolutionary computer-aided retro-synthesis tool, Chematica. Chematica uses advanced reaction rules and proprietary algorithms to identify synthesis pathways that meet user-defined constraints. Financial details of the transaction were not disclosed.

"With a 350-year legacy in the pharmaceutical and chemistry business, we recognize the attractiveness of the chemical synthesis and cheminformatics market and how it complements our existing leadership position in chemicals and reagents" said Udit Batra, CEO, MilliporeSigma.

Virtual synthesis significantly reduces the time between chemical target conception and route evaluation by using a lab's preferences to filter millions of data points. The tool quickly and efficiently provides optimized routes, providing significant benefit to all researchers, especially those working in medicinal chemistry and drug discovery.



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GSI's knowledge base of tens of thousands of expert-defined rules of chemical reactivity, combined with proprietary algorithms, enables the program to scrutinize millions of synthetic pathways and to choose the routes that lead to desired targets in the most cost-effective way.

"As chemists who grew up with Sigma-Aldrich and Millipore in the lab, we couldn't be more proud to be acquired by a company with such a long legacy and sincere interest in chemistry," said Bartosz Grzybowski, founder of GSI and inventor of Chematica. "Combining our revolutionary planning tool with MilliporeSigma's large number of available starting materials and its industry leading e-commerce platform will provide immense value to our customers."

The Chematica tool is available now through a limited release for users in academia and in industry.

### **About Grzybowski Scientific Inventions (GSI)**

Grzybowski Scientific Inventions (GSI) is a start-up company with exclusive licensing, development, marketing and sales rights to the revolutionary chemistry decision-making and synthetic planning software product Chematica. Since its establishment in December 2013, GSI has successfully engaged a clientele composed of a wide range of industries as well as academic and government institutions from all over the world. Today, Chematica is widely recognized as the first computer program capable of "chemical thinking" and the only expert system able to design chemically viable synthetic pathways for complex targets -- including drugs, natural products as well as theoretical molecules -- within seconds.

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### **About the Life Science Business of Merck KGaA, Darmstadt, Germany**

The life science business of Merck KGaA, Darmstadt, Germany, which operates as MilliporeSigma in the U.S. and Canada, has 19,000 employees and 65 manufacturing sites worldwide, with a portfolio of more than 300,000 products enabling scientific discovery. Udit Batra is the global chief executive officer of MilliporeSigma.

Merck KGaA, Darmstadt, Germany completed its \$17 billion acquisition of Sigma-Aldrich in November 2015, creating a leader in the \$125 billion global life science industry.

Merck KGaA, Darmstadt, Germany is a leading company for innovative and top-quality high-tech products in healthcare, life science and performance materials. The company has six businesses – Biopharmaceuticals, Consumer Health, Allergopharma, Biosimilars, Life Science and Performance Materials – and generated sales of €15.0 billion in 2016. Around 50,000 employees work in 66 countries to improve the quality of life for patients, to foster the success of customers and to help meet global challenges.

Merck KGaA, Darmstadt, Germany is the world's oldest pharmaceutical and chemical company – since 1668, the company has stood for innovation, business success and responsible entrepreneurship. Holding



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an approximately 70 percent interest, the founding family remains the majority owner of the company to this day. The company holds the global rights to the name and the trademark "Merck" internationally except in the United States and Canada, where the company operates as EMD Serono, MilliporeSigma and EMD Performance Materials.