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Computational Chemistry and AI in Chemistry Conference at Merck KGaA, Darmstadt, Germany

- **RDKit conference with more than 300 participants**
- **Applications of open-source cheminformatics and machine learning tool expand from small molecules to oligonucleotides, peptides and quantum chemistry**
- **Conference celebrates 20th birthday of RDKit and highlights examples of scientific expertise being turned into applications**

Darmstadt, Germany, September 21, 2026 – Merck KGaA, Darmstadt, Germany, a leading science and technology company, has hosted one of the largest conferences focusing on computational chemistry and AI in chemistry, bringing together a global community of chemists, data scientists and software developers. All attendees share the common goal of making precompetitive molecular research faster, more reliable and more collaborative. Around 300 participants met in Darmstadt, half of them in person, the other half virtually.

“RDKit is a powerful example of how chemistry, data and software can come together to accelerate scientific innovation. We are proud to welcome the RDKit community to Darmstadt and to support the shared foundations that help turn scientific expertise into impact,” said Philipp Harbach, Chief Science and Technology Officer at Merck KGaA, Darmstadt, Germany.

The [agenda](#) for the 2026 meeting of prestigious digital chemistry experts shows that the applications of [RDKit](#), originally developed to handle small molecules, have expanded to include promising modalities such as oligonucleotides and peptides as





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well as quantum chemistry. Contributions from Novartis, Bayer, Sanofi, and AbbVie, among others, highlight the importance of RDKit as a key toolkit for pharmaceutical research. “RDKit helps our research and development scientists within our Healthcare business sector turn chemical data into AI-ready representations and actionable insights for faster, better-informed molecular design. By supporting its open-source community, we help advance shared tools that enable us to bring more medicines to more patients, faster,” said Arvind Rajpal, Head of Discovery & Development Technologies at Research and Development within the Healthcare business sector of Merck KGaA, Darmstadt, Germany.

RDKit is an important open-source cheminformatics and machine learning tool that has more than 100,000 users worldwide. The open-source software helps scientists represent, analyze and compare molecules in a computer – giving digital tools a common language for chemical structures. Researchers can use it to check molecular structures, look for similarities between compounds and prepare chemical data for modeling.

The software is now an important building block in many chemistry- and life science-focused AI workflows. It helps turn the rich but complex information contained in molecular structures into data that models can use – supporting scientists as they identify promising molecules, estimate properties and design the next experiments.

Examples of digital science projects at Merck KGaA, Darmstadt, Germany, using RDKit are:

- **Predictive Modeling Platform**, a tool for AI-driven design of drug-like molecules for the Healthcare business sector, recently recognized with an in-house award at Merck KGaA, Darmstadt, Germany
- **Protein Design Platform**, a suite of protein AI tools developed at the Science & Technology Office at Merck KGaA, Darmstadt, Germany, recognized with an award by Merck KGaA, Darmstadt, Germany in 2025
- **BayBE**, a [Bayesian optimization tool](#) by the Science & Technology Office at Merck KGaA, Darmstadt, Germany, that helps teams choose informative follow-up experiments, recognized with a Merck KGaA, Darmstadt, Germany in-house award in 2025



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- **Synthia®**, an externally available retrosynthesis [product](#) from the Life Science business sector of Merck KGaA, Darmstadt, Germany, that helps chemists explore practical routes for synthesizing a target molecule

These tools address different scientific questions, from deciding which experiment to run next to planning how a molecule could be made or can show how drug candidates interact with proteins.

However, RDKit is used much more broadly in digital tools. Pharmaceutical and chemical companies also use RDKit to develop digital tools in-house. Google (Patents) and Google DeepMind (AlphaFold), Amazon Web Services and NVIDIA use RDKit alongside chemical supplier Enamine and software provider Schrödinger.

RDKit began with its first open-source publication in 2006 as a company-developed project and has grown into a widely used open-source toolkit with almost 4 million downloads per month and an expanding international community. Google Scholar had more than 4,500 hits for “RDKit” in 2024 alone. Its value is in the software and community itself, and in the way it enables scientists in academia, technology companies and the pharmaceutical industry to learn from one another. When companies share methods, code and experience responsibly, the wider scientific community moves faster.

Merck KGaA, Darmstadt, Germany has been part of the RDKit community since its earliest days. The first and then still very small RDKit User Group Meeting was in 2012 with Merck KGaA, Darmstadt, Germany employees contributing. In 2014, Merck KGaA, Darmstadt, Germany hosted the third User Group Meeting in Darmstadt with several contributions. By welcoming this community to Darmstadt for the 20th anniversary, Merck KGaA, Darmstadt, Germany is celebrating the RDKit community’s open-source progress and helping shape the next generation of digital chemistry. “Hosting this community at our headquarters offers a valuable opportunity to exchange ideas and strengthen collaboration across industry, academia and open-source contributors. We are proud to support this spirit of openness and innovation – because the future of science depends on connecting people, data and technology,” said Jérémie Eblé, Head of Digital Center of Excellence at the Life Science business sector of Merck KGaA, Darmstadt, Germany.



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About Merck KGaA, Darmstadt, Germany

Merck KGaA, Darmstadt, Germany, a leading science and technology company, operates across life science, healthcare and electronics. More than 62,000 employees work to make a positive difference to millions of people's lives every day by creating more joyful and sustainable ways to live. From providing products and services that accelerate drug development and manufacturing as well as discovering unique ways to treat the most challenging diseases to enabling the intelligence of devices – the company is everywhere. In 2025, Merck KGaA, Darmstadt, Germany, generated sales of € 21.1 billion in 65 countries.

The company holds the global rights to the name and trademark "Merck" internationally. The only exceptions are the United States and Canada, where the business sectors of Merck KGaA, Darmstadt, Germany, operate as MilliporeSigma in life science, EMD Serono in healthcare and EMD Electronics in electronics. Since its founding in 1668, scientific exploration and responsible entrepreneurship have been key to the company's technological and scientific advances. To this day, the founding family remains the majority owner of the publicly listed company.

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