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Merck KGaA, Darmstadt, Germany, Collaborates with Acceleration Consortium on Open-Sourcing AI-Driven Experimentation Planner

- **Bayesian optimization engine that already powers dozens of use cases at Merck KGaA, Darmstadt, Germany, now open sourced to foster adoption**
- **Close partnership to enable the self-driving labs of tomorrow**

Darmstadt, Germany, December 6, 2022– Merck KGaA, Darmstadt, Germany, a leading science and technology company, and the [Acceleration Consortium](#), based at the University of Toronto, Canada, today jointly announced that their AI-driven experimentation planner Bayesian Back End (BayBE) is now available open-source on [GitHub](#), with an unrestricted Apache 2.0 license. The joint open-source initiative combines the Merck KGaA, Darmstadt, Germany, portfolio of use cases with the Acceleration Consortium’s world-leading excellence in self-driving labs.

“The release and maintenance of open-source code for scientific discovery is imperative for the advancement of self-driving labs. This collaboration moves the needle of multi-stakeholder work in the area of self-driving labs. I am thrilled about our collaboration with Merck KGaA, Darmstadt, Germany on developing and publishing software for AI-assisted experimental planning. As society faces ever-growing challenges, we have no time for science as usual. With this software, we can revolutionize the way experiments are designed and conducted, accelerating discoveries and driving progress in ways we have never imagined before,” said Alán Aspuru-Guzik, Professor of Chemistry and Computer Science at the University of Toronto, and Director of the Acceleration Consortium, which recently launched a



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seven-year program worth CA\$ 200 million, supported by the Canada First Research Excellence Fund.

“This development is a great outcome of our focus on ‘innovation powered by data and digital’. Together with our partners at the Acceleration Consortium, we continue to push productivity with digital tools such as BayBE. Our company continues to invest in digital technologies that can disrupt the healthcare, life science and electronics industries,” said Laura Matz, Chief Science and Technology Officer at Merck KGaA, Darmstadt, Germany. “BayBE unites several advanced technologies under one umbrella and focuses on making them useful for industrial purposes. While it already has many internal use cases, we are excited to share it with a wider community through open source. What started out as a cross-sectorial advancement can now become a cross-industrial one,” Matz continued.

BayBE was built jointly across all three business sectors of Merck KGaA, Darmstadt, Germany. It is a general-purpose toolbox for smart iterative experimentation with emphasis on important add-ons for chemistry and materials science. It enables a more systematic approach by providing recommendations for the next best experiment, leading to better results faster. BayBE can also act as the “brain” for automated equipment, enabling entirely closed-loop self-driving laboratories.

The traditional approach for design of experiments is largely based on intuition and experience of the experimentalist. This can lead to considerable variation between different labs and is particularly challenging for complex campaigns that aim to optimize numerous properties simultaneously. Merck KGaA, Darmstadt, Germany, faces these challenges on an every-day basis, for instance as part of experimental optimization campaigns in research, product development and operations. Artificial intelligence (AI) enables novel ways of tackling these problems and reducing the time needed and money spent as well as increasing sustainability.

The BayBE software already powers dozens of use-cases at Merck KGaA, Darmstadt, Germany, for instance:

- *VRP ExcipientFinder*: Part of the [viscosity reduction platform service](#) of the Life Science business sector of Merck KGaA, Darmstadt, Germany; a tool to accelerate selection of viscosity reducing excipients

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- *BayChem*: Self-service experimental planner available to everyone at Merck KGaA, Darmstadt, Germany, directly enabling our lab users
- *Self-driving autonomous flow chemistry at Merck KGaA, Darmstadt, Germany*: closed-loop platform in the R&D of the Life Science business sector that optimizes chemical reactions fully autonomously

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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 64,000 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 2022, Merck KGaA, Darmstadt, Germany, generated sales of € 22.2 billion in 66 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.