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Applying machine learning to challenges in the pharmaceutical industry

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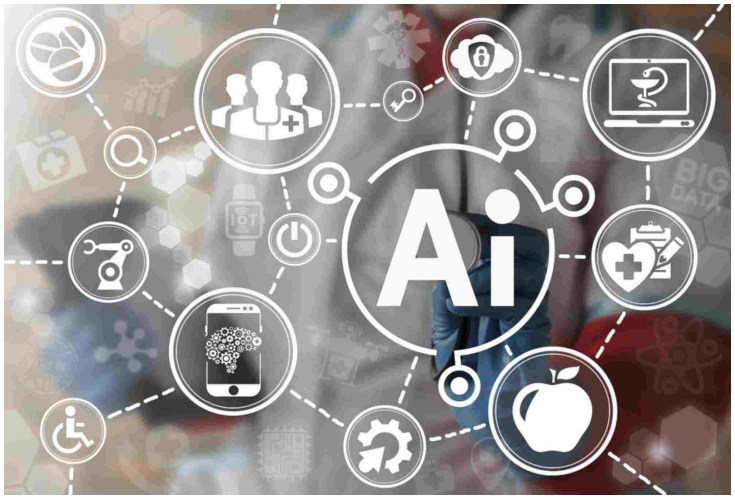
MIT researchers and industry form new consortium to aid the drug discovery process.



MIT continues its efforts to transform the process of drug design and manufacturing with a new MIT-industry consortium, the Machine Learning for Pharmaceutical Discovery and Synthesis.

The new consortium already includes eight industry partners, all major players in the pharmaceutical field, including Amgen, BASF, Bayer, Lilly, Novartis, Pfizer, Sunovion, and WuXi.

A large number of these have a research presence in Cambridge or the surrounding areas, allowing for close cooperation and the creation of a center for artificial intelligence (AI) applications in pharmaceuticals.

The drug discovery process can often be exceedingly expensive and time-consuming, but machine learning offers tremendous opportunities to more efficiently access and understand vast amounts of chemical data — with great potential to improve both processes and outcomes.

The consortium aims to break down the divide between machine learning research at MIT and drug discovery research; bringing MIT researchers and industry together to identify and address the most significant problems.

As part of the broader initiative to bring together machine learning and drug research, in April, MIT hosted a summit led by Regina Barzilay, the Delta Electronics Professor of Computer Science, and Dina Katabi, the Andrew and Erna Viterbi Professor of Electrical Engineering and Computer Science.

The summit gathered MIT researchers with leaders of technology, biotech, and regulatory agencies to engage in ways digital technologies and artificial intelligence can help address major challenges in the biomedical and health care industries.

The earliest seeds for the consortium began with software and technology funded by the Defense Advanced Research Projects Agency (DARPA) “Make-It” program, which has the goal of integrating machine learning with automated systems for chemical synthesis.

MIT researchers discussed the potential for a consortium with pharmaceutical industry contacts, initially meeting with company representatives in May 2017 and again in September 2017 at which time there was great interest from both industry and MIT researchers in working together.

Since then, through work with the MIT Office of Sponsored Programs (OSP) and the MIT Technology Licensing Office (TLO), the consortium has been officially formed. A consortium meeting on May 3 brought together industry members and MIT researchers.

“The enthusiasm of the member companies and the potential of machine learning create a tremendous opportunity for advancing the toolbox for medical scientists in the chemical and pharmaceutical industries,” says Klavs Jensen, the Warren K. Lewis Professor of Chemical Engineering and professor of materials science and engineering.

The May 3 meeting aimed to introduce the industry members to fundamentals of machine learning through tutorials and joint research projects. Toward this goal, Barzilay taught the first tutorial on the basics of supervised learning; the tutorial covered neural models and focused on representation learning with the goal of preparing participants for technical presentations in the afternoon.

“The application of machine learning tools provides an opportunity to augment and accelerate drug discovery and development — and get new medicines to patients more quickly,” says Shawn Walker, director of process development of pivotal drug substance technologies at Amgen.

“We are excited to participate in this MIT machine learning consortium, along with our other industry partners,” says José Duca, head of computer aided drug discovery in global discovery chemistry at the Novartis Institutes for BioMedical Research.“This consortium will tackle the challenge of efficient and targeted route-planning using state-of-the-art machine learning approaches. Ultimately, we hope this accelerates our ability to make safer, more potent drugs against human disease.”