



NovAliX partners with Chemical.AI to develop artificial intelligence toolkit for drug discovery

Partnership will accelerate development of AI tools and enhance industry-available services such as next generation Computer-Aided Synthesis Planning (CASP)

Strasbourg, France, and Wuhan, China, January 25, 2021 - NovAliX, a drug discovery-focused contract research organization (CRO), and Chemical.AI, an artificial intelligence company leveraging human expertise and cutting-edge AI technology for chemistry and pharmaceuticals, today announce a strategic collaboration in artificial intelligence applied to drug discovery. In the years to come this dynamic affiliation between a leading European CRO and a growing artificial intelligence company will help create the most relevant AI solutions for drug developers.

NovAliX brings 20 years of industry experience and know-how in drug discovery to the collaboration. Combined with Chemical.AI's innovations in artificial intelligence, this will enable the partners to jointly develop an AI toolkit for drug discovery. The advanced toolkit will be integrated into NovAliX's drug discovery services whilst commercial release will be available at Chemical.AI.

Through the collaboration, NovAliX will have access to a customized and enhanced AI toolkit ahead of the market. Chemical.AI, on the other hand, will be able to rely on NovAliX's experienced scientists and unique in-house, high-quality data to develop the most relevant AI tools. The first joint program focuses on enhancing Chemical.AI's Computer-Aided Synthesis Planning (CASP) system, in order to be at the forefront of the industry for next generation predictive retrosynthesis.

CASP is a promising area of research, with the potential to have a tremendous impact on pharmaceutical and fine chemistry industries, by significantly reducing the attrition of synthetic chemistry and increasing efficiency and productivity; it helps to accelerate the process by which chemists decide how to synthesize small molecule compounds. The ideal CASP program would take a molecular structure as input, and then output a sorted list of detailed reaction schemes that each connect a target to purchasable starting materials via a series of chemically feasible reaction steps.

"We are thrilled to collaborate with Chemical.AI at this significant and impactful time for us," said Denis Zeyer, PhD, CEO of NovAliX. "With this collaboration, NovAliX and Chemical.AI have launched a research program aimed at demonstrating the performance of Chemical.AI's CASP system. As a result of this teamwork, NovAliX clients will benefit from cutting-edge AI solutions for their research projects. For example, the most advanced version of Chemical.AI's CASP is already used by NovAliX chemists in discovery chemistry and process research services."

"The decision to collaborate with NovAliX was a natural move for us," said Ning Xia, PhD, CEO of Chemical.AI. "First, we wanted to team up with scientists who need to solve very complex synthetic challenges. Second, we were seeking exposure to scientists who embrace the variety of preclinical drug discovery projects that enhance the development of the relevant AI solutions for the pharmaceutical industry."



This partnership meets critical and growing industry needs and demands. The global artificial intelligence in drug discovery market was valued at \$473.4 million (€395.3M) in 2019 and is expected to grow at a compound annual growth rate ([CAGR](#)) of 28.8% from 2020 to 2027. In today's business world, multiple pharmaceutical and biotechnology companies embrace artificial intelligence and big data technology in order to accelerate drug discovery and development.

About Chemical.AI

Chemical.AI is an artificial intelligence company leveraging both human expertise and AI technology. The company empowers chemists to accelerate their innovation; helping shape the future of chemistry. Chemical.AI has developed a customizable platform to plan synthetic routes in anything from a few seconds to a couple of minutes. Based on advanced machine-learning and big-data technologies, the computer-aided synthesis route design is gaining much research attention in developing it into a practical tool for chemists. Chemical.AI's system is designed, used and proven by chemists. The system notably displays the following characteristic features: (i) predicting the synthesis route for unreported molecules, (ii) finding new routes for reported molecules, (iii) sorting or filtering routes by cost, steps, green score, etc. (iv) generating multiple synthesis routes in one click, (v) finding more adaptable conditions for a clients' reaction, (vi) potentially integrating clients' Electronic Lab Notebook (ELN) data to provide reaction procedures and (vii) installing on a local server for security. With customers including leading CROs and big pharma, and looking at user feedback, Chemical.AI provides one of the best CASP solutions in its sector.

www.chemical.ai

About NovAliX

Founded in 2002 and based in Strasbourg, France, NovAliX is a drug discovery-focused CRO with several unique technologies. It employs 170 researchers, with capabilities combining chemistry and biophysics. NovAliX offers its clients original collaborative models and extensive services within the framework of research programs dedicated to drug discovery. Its ambition is to continue its development by both strengthening its internationalization and extending and integrating the new capabilities essential to the success of its clients' therapeutic research projects into its technologies and base of expertise.

www.novalix.com

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