# Simulations Plus Enters Partnership to Apply AI/ML Technologies to Design Novel Compounds

***Promising intellectual property resulting from the collaboration with Polish Academy of Sciences will be jointly owned for further development opportunities***

LANCASTER, Calif.--([BUSINESS WIRE](http://www.businesswire.com))-- [Simulations Plus, Inc.](https://cts.businesswire.com/ct/CT?id=smartlink&url=https%3A%2F%2Fwww.simulations-plus.com%2F%3Futm_source%3DIssuerDirect%26utm_medium%3Dpressrelease%26utm_campaign%3Dai-ml_mar2023&esheet=53362404&newsitemid=20230315005427&lan=en-US&anchor=Simulations+Plus%2C+Inc.&index=1&md5=606564e7ee716eff88fc53426336207a) (Nasdaq: SLP), a leading provider of modeling and simulation software and services for pharmaceutical safety and efficacy, today announced that it entered into a collaborative research agreement with the Institute of Medical Biology of the Polish Academy of Sciences (IMB PAS) to jointly design new compounds for the RORγ/RORγT nuclear receptors using its cutting-edge artificial intelligence (AI) / machine learning (ML) technology in the [ADMET Predictor®](https://cts.businesswire.com/ct/CT?id=smartlink&url=https%3A%2F%2Fwww.simulations-plus.com%2Fsoftware%2Fadmetpredictor%2F%3Futm_source%3DIssuerDirect%26utm_medium%3Dpressrelease%26utm_campaign%3Dai-ml_mar2023&esheet=53362404&newsitemid=20230315005427&lan=en-US&anchor=ADMET+Predictor%26%23174%3B&index=2&md5=b14eb44d77db1b87777dffa9c65306b1) software platform.

Per the terms of the collaboration, Simulations Plus will deploy the [AIDD Module](https://cts.businesswire.com/ct/CT?id=smartlink&url=https%3A%2F%2Fwww.simulations-plus.com%2Fsoftware%2Fadmetpredictor%2Fai-driven-drug-design-aidd%2F%3Futm_source%3DIssuerDirect%26utm_medium%3Dpressrelease%26utm_campaign%3Dai-ml_mar2023&esheet=53362404&newsitemid=20230315005427&lan=en-US&anchor=AIDD+Module&index=3&md5=f9a2697e53395edaada05c76877cfe08) in ADMET Predictor® to create predictive models of inhibition and activation for the human RORγ/RORγT nuclear receptors. The computational and medicinal chemists at Simulations Plus will then interact with researchers at the IMB PAS to define the multi-objective parameters against which the lead molecule(s) will be optimized. The generative chemistry approaches within the AIDD Module will produce novel libraries of virtual compounds with desired combinations of the properties chosen, and the IMB PAS will synthesize and test promising analogs. Emerging intellectual property, in the form of encouraging lead compounds, will be jointly owned by Simulations Plus and IMB PAS for further development opportunities.

“Many organizations continue to explore the use of AI algorithms to complement the drug design and lead optimization process with human interaction,” said [Dr. Rafal Bachorz](https://cts.businesswire.com/ct/CT?id=smartlink&url=https%3A%2F%2Fwww.simulations-plus.com%2Fpeople%2Frafal-bachorz%2F%3Futm_source%3DIssuerDirect%26utm_medium%3Dpressrelease%26utm_campaign%3Dai-ml_mar2023&esheet=53362404&newsitemid=20230315005427&lan=en-US&anchor=Dr.+Rafal+Bachorz&index=4&md5=2fc3f5716c6b7e9965185292e3eb34fc), Senior Cheminformatics Scientist II at Simulations Plus and project lead. “We are excited to work with the IMB PAS to apply our cheminformatic toolkits with the AIDD Module to generate novel chemical matter for the human RORγ/RORγT nuclear receptors.”

“Simulations Plus is an organization that has the AI-based drug discovery technology and computational/medicinal chemistry skills which are unique in a partner,” added Professor Jarosław Dziadek, director of the IMB PAS. “Our goal is to combine our expertise with RORγ/RORγT receptor biology, which many pharmaceutical companies are targeting as it may be involved in the progression of certain types of cancer, and relevant assays of receptor activity with all that Simulations Plus offers to accelerate the design and optimization of novel lead molecules.”

[John DiBella](https://cts.businesswire.com/ct/CT?id=smartlink&url=https%3A%2F%2Fwww.simulations-plus.com%2Fpeople%2Fjohn-a-dibella%2F%3Futm_source%3DIssuerDirect%26utm_medium%3Dpressrelease%26utm_campaign%3Dai-ml_mar2023&esheet=53362404&newsitemid=20230315005427&lan=en-US&anchor=John+DiBella&index=5&md5=9a1abef466dbd538378703335f9c57ae), SLP Division President, said: “This collaboration is another in a long line of ‘win-win’ situations, although this time with a twist. Both Simulations Plus and the IMB PAS will be making meaningful contributions in areas where each organization is strongest, and we will share equally the promising outcomes which are generated. We are highly motivated to explore where this will take us in terms of identifying the next generation of compounds that could help in the treatment of cancer. Simulations Plus continues to invite future collaborations which benefit organizations and, most importantly, the global communities we serve.”

**About Simulations Plus, Inc.**

Serving clients worldwide for more than 25 years, Simulations Plus is a leading provider in the biosimulation market providing software and consulting services supporting drug discovery, development, research, and regulatory submissions. We offer solutions that bridge machine learning, physiologically based pharmacokinetics, quantitative systems pharmacology/toxicology, and population PK/PD modeling approaches. Our technology is licensed and applied by major pharmaceutical, biotechnology, and regulatory agencies worldwide. For more information, visit our website at [www.simulations-plus.com](https://cts.businesswire.com/ct/CT?id=smartlink&url=https%3A%2F%2Fwww.simulations-plus.com%2F&esheet=53362404&newsitemid=20230315005427&lan=en-US&anchor=www.simulations-plus.com&index=6&md5=f7947404c22c5296d89ec03ff20e07d7) . Follow us on [LinkedIn](https://cts.businesswire.com/ct/CT?id=smartlink&url=https%3A%2F%2Fwww.linkedin.com%2Fcompany%2Fsimulations-plus%2Fmycompany%2F&esheet=53362404&newsitemid=20230315005427&lan=en-US&anchor=LinkedIn&index=7&md5=a92d9e1b1e7544df935587cfa35d8a30) | [Twitter](https://cts.businesswire.com/ct/CT?id=smartlink&url=https%3A%2F%2Ftwitter.com%2FSimulationsPlus&esheet=53362404&newsitemid=20230315005427&lan=en-US&anchor=Twitter&index=8&md5=1aae3da7617e1ed5b42483f484afd2a4) | [YouTube](https://cts.businesswire.com/ct/CT?id=smartlink&url=https%3A%2F%2Fwww.youtube.com%2Fc%2FSimulationsPlusInc&esheet=53362404&newsitemid=20230315005427&lan=en-US&anchor=YouTube&index=9&md5=59a1f937c8d4270206fdb81d273217fb) .

**About the Institute of Medical Biology at the Polish Academy of Sciences**

Established in 1951, the Polish Academy of Sciences is a Polish state-sponsored institution of higher learning. Headquartered in Warsaw, it is responsible for spearheading the development of science across the country by a society of distinguished scholars and a network of 68 research institutes.

**Safe Harbor Statement Under the Private Securities Litigation Reform Act of 1995** – With the exception of historical information, the matters discussed in this press release are forward-looking statements that involve a number of risks and uncertainties. Words like “believe,” “expect” and “anticipate” mean that these are our best estimates as of this writing, but that there can be no assurances that expected or anticipated results or events will actually take place, so our actual future results could differ significantly from those statements. Factors that could cause or contribute to such differences include, but are not limited to: our ability to maintain our competitive advantages, acceptance of new software and improved versions of our existing software by our customers, the general economics of the pharmaceutical industry, our ability to finance growth, our ability to continue to attract and retain highly qualified technical staff, our ability to identify and close acquisitions on terms favorable to the Company, and a sustainable market. Further information on our risk factors is contained in our quarterly and annual reports and filed with the U.S. Securities and Exchange Commission.

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