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IPN Applies Artificial Intelligence to Discover New Treatments for Rheumatoid Arthritis

- **AI opens up possibilities to identify, among thousands of molecules, those best suited to combat this autoimmune disease, explains IPN researcher**
- **Various algorithms are used to run detailed simulations with candidate molecules, reducing both research time and costs**

To help relieve the pain and inflammation in joints caused by rheumatoid arthritis, Edgar Eduardo Lara Ramírez, researcher at the Instituto Politécnico Nacional (IPN), is using Artificial Intelligence (AI) to search for new treatment options against this chronic-degenerative condition, which significantly impacts patients' quality of life and can become disabling in advanced stages.

Lara Ramírez, who is affiliated with the Pharmaceutical Biotechnology Laboratory at the Center for Genomic Biotechnology (CBG) and holds Level II membership in Mexico's National System of Researchers (SNII), pointed out that AI tools make it possible to reduce research time and costs significantly.

"The progress we've made in just one year with AI would have otherwise taken at least a decade and much higher investment," he stated. Based on his experience treating severe cases of rheumatoid arthritis in a public hospital, Lara Ramírez believes AI offers an effective alternative for identifying new treatments with fewer side effects, which could substantially improve patients' quality of life.

He explained that current treatments for this incurable autoimmune disease include nonsteroidal anti-inflammatory drugs (NSAIDs) and steroids, both of which can cause adverse side effects. Additionally, biologic therapies used in treatment may suppress the immune response, making patients vulnerable to opportunistic infections.

"AI applications such as machine learning make it possible to select, from a vast number of options, molecules already approved by the U.S. Food and Drug Administration (FDA) that may be repurposed for a different use—in this case, for treating rheumatoid

arthritis," he explained.

The biotechnology PhD added that with this information, statistical algorithms can be used to predict the activity of the selected molecules, and computer simulations allow researchers to study in detail how they interact with a protein's active site.

For example, Lara Ramírez highlighted peptidylarginine deiminase 4 (PAD4), a protein expressed in neutrophils (immune cells), whose abnormal production is closely linked to the pathogenesis of rheumatoid arthritis by triggering the excessive production of these cells.

"In the first stage of the research, using AI, we screened 16,000 candidate drug molecules, and confirmed that two of them inhibit PAD4: one is currently used as an antimalarial, and the other is in clinical trials with anticancer properties. Through computational simulations, we demonstrated that both are ideal candidates to inhibit this protein."

The researcher expressed confidence that the progress made in these trials will help lay the groundwork for future treatments that not only alleviate symptoms, but also permanently halt the damage caused by this autoimmune disease.

For more information, visit www.ipn.mx

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