Release no. 043
Mexico City, April 11th, 2023

IPN obtains patent for design of anticancer compound

- **IMPI issues patents because it overcame the effect of the drug that is currently used as an antiproliferative in cervical and breast cancer cells.**
- **This compound opens expectations for a new, more specific, and less toxic treatment for these neoplasms in the future.**

The Instituto Politécnico Nacional (IPN) obtained a patent from the Instituto Mexicano de la Propiedad Industrial (IMPI) for the design and synthesis of a compound derived from valproic acid (an anticonvulsant drug), which proved to be antiproliferative of HeLa cells (cervical cancer) and breast cancer.

The patent was obtained after 12 years of work by the team headed by José Correa Basurto, a scientist from the Escuela Superior de Medicina (ESM), who pointed out that this compound opens expectations for a new, more specific and less toxic treatment for these neoplasms in the future.

Behind this scientific contribution, which received an honorable mention in the Basic Research category of the 2021 Research Award granted by the IPN, is the design of more than a thousand molecules in silico (made by computer).

"The molecules were analyzed using chemoinformatics tools, sequence bioinformatics (analysis of nucleic acid and protein sequences) and structural bioinformatics, protein folding, molecular dynamics studies, and docking (molecular docking)," explained Correa Basurto.

In addition, they were subjected to a virtual screening to choose the most promising ones according to their Admet properties (absorption, distribution, metabolism, excretion, toxicity) and protein-ligand affinity, to choose the ones with the best response at the computational level.

The scientist, who is a member of the Sistema Nacional de Investigadores (SNI) Level III, pointed out that previous preclinical studies determined that the new compound has greater potency and less toxicity than valproic acid since it was designed using theoretical-computational tools to act selectively (only on malignant cells and without causing damage to healthy cells).

Humans have proteins called histone deacetylases (HDAC) that are overexpressed in the presence of cancerous processes. "Because they play an important role in the origin and development of cancer, especially isoforms 1, 6, and 8, we studied them in depth, determined their structure at a three-dimensional level, and evaluated the best ligands derived from valproic acid that fit with them," the specialist explained.

Based on these results, the five most promising molecules were selected and their chemical synthesis was carried out. In vitro studies in cervical and breast cancer cells determined that the compound called HO-AAVPA had the best antiproliferative response in cancer cells. The compound inhibits the proliferation of HDACs, which causes cell death by apoptosis, which is like generating a bio-directed cell death.

This line of research has generated more than 20 scientific articles in prestigious international journals. Five bachelor's degree theses associated with the project, five master's degree theses, three doctoral theses, and two more doctoral theses are in process.

The results of the research have been presented at 10 national and international congresses; the patent of three more HDAC inhibitors is in process.

===000===