

## **Title: Artificial Intelligence Approaches for Antibiotic Discovery**

### **Abstract**

Artificial intelligence (AI) has the potential to outperform humans and revolutionize our world. In this talk, I will describe our efforts using AI to develop computational approaches for antibiotic design and discovery. Computers can already be programmed for superhuman pattern recognition of images and text. In order for machines to discover novel antibiotics, they have to first be trained to sort through the many characteristics of molecules and determine which properties should be retained, suppressed, or enhanced to optimize antimicrobial activity. Said differently, machines need to be able to understand, read, write, and eventually create new molecules. I will discuss how we trained a computer to execute a fitness function following a Darwinian algorithm of evolution to select for molecular structures that interact with bacterial membranes, yielding the first artificial antimicrobials that kill bacteria both *in vitro* and in relevant animal models. My lab has also developed pattern recognition algorithms to mine the human proteome, identifying throughout the body thousands of antibiotics encoded in proteins with unrelated biological function, and has applied computational tools to successfully reprogram venoms into novel antimicrobials. Computer-generated designs and innovations at the intersection between machine and human intelligence may help to replenish our arsenal of effective drugs, providing much-needed solutions to global health problems caused by infectious diseases.

### **Presenting author details**

Full name: Prof. Cesar de la Fuente

Contact number: +1-215-746-6083

Twitter account: [@delafuenteupenn](https://twitter.com/delafuenteupenn)

LinkedIn account: <https://www.linkedin.com/in/cesardelafuentenunez/>