

THE USE OF AI AND ADVANCED COMPUTER SYSTEMS TO DEVELOP DRUGS AGAINST NEW EMERGING THREATS

Disruptive Technology To Design Broad-spectrum Countermeasures And Vaccines

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Rapid design of Medical Countermeasures (MCM) against new and emerging threats is desired. Currently, the capability to use computer modeling and Machine Learning (ML) technologies to identify effective therapeutics is largely ineffective. One key to help unlock this capability is high quality data on biological systems that can be rapidly obtained and analyzed at reasonable costs. Obtaining high quality data on biological systems is hard because the majority do not form crystals that are amenable to interrogation by X-ray diffraction methods. In fact the success rate of structure determination of small molecules (drugs) by x-ray crystallography is less than 20%.

Over the past decade we have developed a new method in the field of cryoEM called Microcrystal Electron Diffraction, or MicroED for short. Samples that are a billionth the size which is required by X-ray crystallography can be interrogated by MicroED and high quality structures determined rapidly. In fact the success rate of MicroED in determining small molecule structures is a whopping >95%.

Our effort will focus on developing a prototype capability to rapidly provide large volumes of biological data that will be useful in designing MCMs and vaccines. Our system will be fully automatic and capable to deliver a structure a minute – a capability currently unmet by any structural biology method and one which will propel our countermeasure capabilities 10,000x and help guide AI and ML efforts in the future.

This study was supported by the National Institutes of Health P41GM136508. Portions of this research or manuscript completion were developed with funding from the Department of Defense grants MCDC-2202-002. Effort sponsored by the U.S. Government under Other Transaction number W15QKN-16-9-1002 between the MCDC, and the Government. The US Government is authorized to reproduce and distribute reprints for Governmental purposes, notwithstanding any copyright notation thereon. The views and conclusions contained herein are those of the authors and should not be interpreted as necessarily representing the official policies or endorsements, either expressed or implied, of the U.S. Government. The PAH shall flowdown these requirements to its subawardees, at all tiers. The Gonen laboratory is supported by funds from the Howard Hughes Medical Institute