Oncology: Prostate Cancer

AI Drug Discovery

Tulane and Atomwise: Using AI to Develop the Next Generation of Prostate Cancer Drugs

Castration resistant progression of metastatic prostate cancer is a major cause of prostate cancer death, and spliced isoforms of the androgen receptor are critically involved in this process. These androgen receptor isoforms can effectively activate their downstream targets independent of androgen signaling, as they lack the androgen-binding domain and can dimerize and become active without androgen. **Yan Dong and Oliver Sartor** are working in collaboration with the AI drug-development company **Atomwise** to develop molecules that can inhibit the dimerization of these splice variants. These molecules will be invaluable in studying the biology of these important proteins in prostate cancer biology and could one day be leveraged as the next-generation of prostate cancer treatments.

Using AI to Shorten Drug Discovery Time

Screening drugs for activity against a given protein target, even using high-throughput methods, could be a lengthy and costly process. While traditional *in silico* screening can shorten the list of possible small molecules, in theory reducing time spent screening, it has several shortcomings. Most notably, it is still dependent on human input and judgment, impacting both impartiality of potential hits and time spent. Additionally, in the case of the Dong Lab, the necessary small molecule is supposed to disrupt a protein-protein interface, one of the most notoriously difficult targets in drug design. Thus, the lab needed a way to reduce the time spent on screening and also to shorten a list of many hundreds of potential inhibitors to a testable handful.

Atomwise uses Artificial Intelligence (AI) to find small molecules that may bind to a given area on a protein.

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Using AI… (Continued)

This technology is ideally suited to help the Dong Lab narrow down its list of possible inhibitors, as it can rapidly screen them for best fit, significantly improving the odds of identifying effective molecules and condensing what could be years of research into months. Additionally, this narrower list will save the lab significant resources, allowing them to focus more effort on those fewer molecules identified in the AI screen. It is of note that Atomwise's AI is particularly adept at finding fits for those difficult-to-target protein-protein interfaces, making this approach useful in a way unmatched by the more conventional screening methods.

A Model for Innovative Collaboration

The collaboration between the Dong Lab at Tulane and Atomwise is emblematic of the novel types of activities Tulane is looking to forge with corporate counterparts. We bring our unique and specialized expertise, in this case in the field of prostate cancer (which Tulane is internationally recognized for) and marry it to an outside entity in a way that both parties can advance science and possible treatments for diseases – all with minimal red tape. At Tulane, the goal with our collaborations is always to move the science forward first. We anticipate that the relationship between Atomwise and Tulane, which already reaches beyond the Dong Lab to multiple other investigators at earlier stages, will be among the first of many over the years to come.

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