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Microenvironment-controlled 3d Cell Systems with Super-resolution Optics and Intelligent Computation for Effective Drug Screening

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Abstract

Due to the high cost for developing new drugs, it is of central importance to develop tissue and quasi-organ in vitro 3D models that are based on human cells to effectively screen new chemical molecules from a large library of drug-like compounds. To achieve this goal, it is essential to be able to control the microenvironment of the cell culture systems in high definition. With focused-ion beam scanning electron microscopy (FIB/SEM), we can now obtain the structural information over volumes of tens of thousands of cubic micrometers, revealing complex microanatomy of patient tissues at subcellular resolutions, and such information can be used to corroborate the in vitro 3D models constructed for drug screening. The recent advancement of super-resolution optics provides a new opportunity for visualizing the spatial distribution and the temporal order of subcellular events and biomolecular interactions in unprecedented details, which provides the basis for checking the quality of the cell culture systems with direct visual evidences in high resolution. Recently, we demonstrated with tumor spheroids formed with the human hepatocellular carcinoma cells (HepG2) that the actions of drugs are significantly different when testing with the 2D culture systems and with the 3D spheroids, which exemplifies the need to move on the more realistic 3D cell system. I will also talk about our computational drug discovery platforms that can perform virtual screenings of more than millions of compounds within a few weeks with structure- and dynamics-based docking and molecular dynamics simulations. In particular, I will describe how the recent development of artificial intelligent techniques, in particular, the convolutional neural networks (CNN), can be incorporated in the virtual drug screening platform to achieve better accuracy and better efficiency. By combining the high-definition experimental system and the efficient computational approaches, we anticipate that new drug discovery can be expedited with higher success rates.

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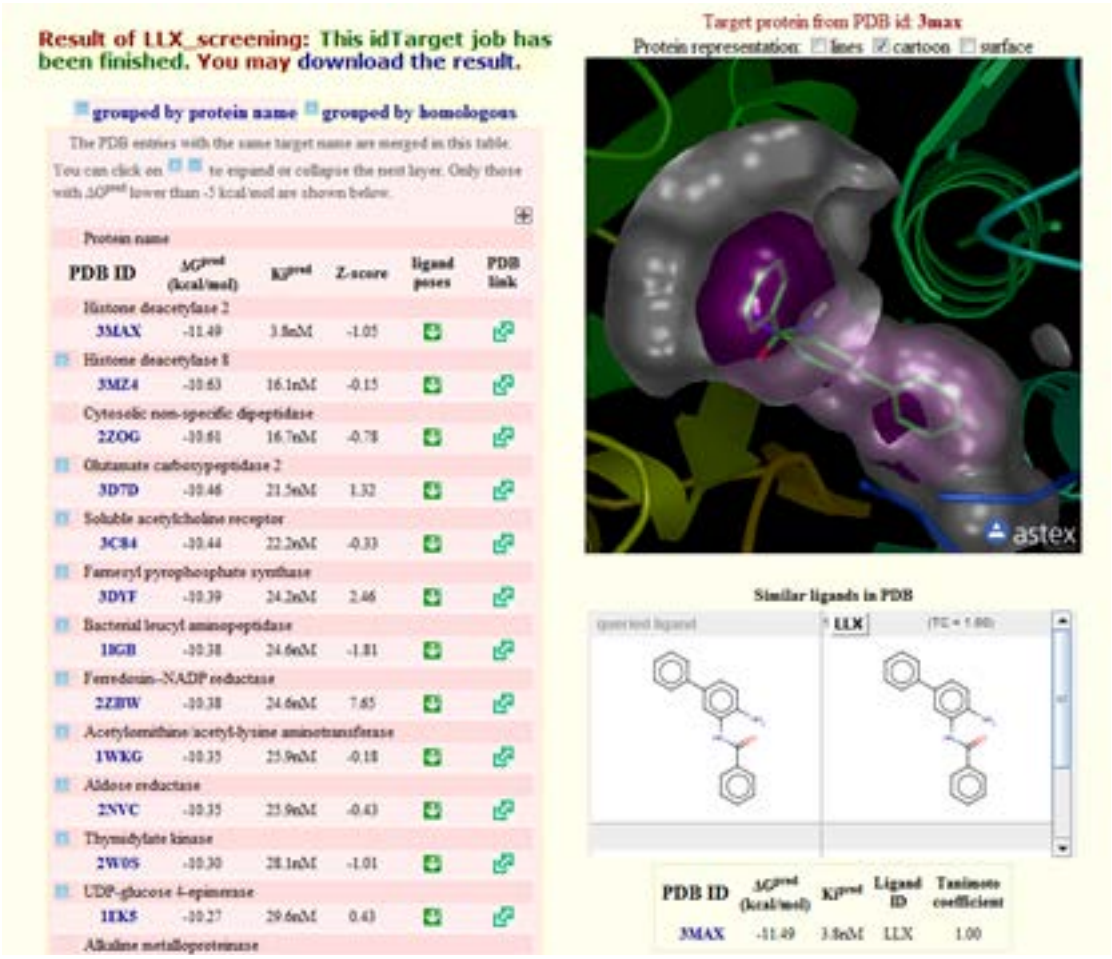

Figure: Predicted target for a given small molecule reported by idTarget.

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