Machine Learning to Predict Multicellular Dynamics Driven by Concentrated Polymer Brush-Modified Cellulose Nanofibers
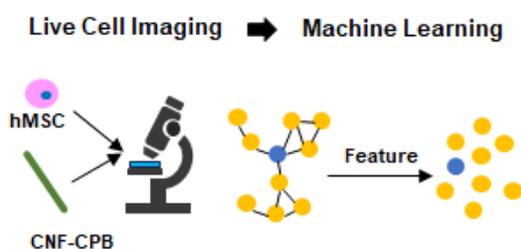
Chiaki Yoshikawa[1] and Hiroshi Mamitsuka[2]

[1]*Research Center for Functional Materials, National Institute for Materials Science (NIMS), Tsukuba, 305-0047 Ibaraki, Japan*
[2]*Bioinformatics Center, Institute for Chemical Research, Kyoto University, Uji, 611-001 Kyoto, Japan*

Abstract

Manipulating the three-dimensional (3D) structures of cells is important for facilitating tissue repair and regeneration. We developed a self-assembly system for human mesenchymal stem cells (hMSCs) using cellulose nanofibers (CNFs) surface modified with concentrated polymer brushes (CPBs) to fabricate various cell 3D structures.[1] To further generate tissues at an implantable level, it is necessary to carry out a large number of experiments using different cell culture conditions and material properties; however, this is too complex on a practical level. To address this issue, we

Figure 1. Schematic illustration of the machine leaning.

present a graph neural network-based simulator (GNS) that can be trained using assembly process images to predict the assembly status of future time steps (figure 1).[2] A total of 24 (25 steps) time-series images were recorded (four repeats for each of the six conditions), and each image was transformed into a graph by regarding the cells as nodes and the connecting neighboring cells as edges. Using the obtained data, the performances of the GNS were examined under three scenarios (i.e., changing a pair of the training or test data) to verify the possibility of using the GNS as a predictor for further time steps. It was confirmed that the GNS could reasonably reproduce the assembly process, even under the toughest scenario wherein the experimental conditions differed between the training and test datasets. This result could reduce the number of experiments required to find the optimal conditions required for generating cells with desired 3D structures. Ultimately, such systems could accelerate progress in regenerative medicine.

Biography

Dr. C. Yoshikawa received the Ph. D. degree in 2006 from Kyoto University in polymer chemistry. She worked for one year as a postdoctoral researcher in Institute for Chemical Research, Kyoto University before she became a Researcher with National Institute for Materials Science (NIMS) in 2007. She has been a Team Leader of Polymer Surface and Devices Team at Research Center for Macromolecules and Biomaterials, NIMS, since April 2024. Her research interests are the interdisciplinary topics of biomaterials, regenerative medicine and biosensors, focusing on the control of interactions between material surfaces and biomolecules, cells, and tissues.

References

1. Nonsuwan, P.; Nishijima, N.; Sakakibara, K. Nakaj-Hirabayashi, T.; Yoshikawa, C. *J. Mater. Chem. B* **2022**, *10(14)*, 2444-2453.
2. Yoshikawa, C.; Nguyen, D. A.; Nakaji-Hirabayashi, T.; Takigawa, I.; Mamitsuka, H. *ACS Biomaterials Science & Engineering* **2024,** 10(4), 2165-2176.