Analysis of Correlation between Physicochemical Properties of Self-Assembled Monolayers and Protein Adsorption Using Artificial Neural Network

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Material design based on informatics has been attracting many interests, since they are expected to cut cost and time compared with the conventional trial-and-error-based approaches. Material informatics has already been successfully applied in the fields of battery, catalysis, etc. In this work, for the first time, we attempt to design biomaterial to exhibiting desired responses to biomolecules and cells.

Artificial Neural Network (ANN) is a strong machine learning method that has been applied in material science to analyze correlation between material properties and functions. It predicts an output of a system and evaluate correlation between input and output using large data set. In our study, we employ ANN to statistically analyze the correlation between physicochemical properties of self-assembled monolayers (SAMs) and adsorption of protein (fibrinogen). We set the physicochemical properties and the amount of the adsorbed protein molecules as the inputs and outputs of the ANN, respectively (Figure 1). We performed the machine learning by using more than one hundred date sets of the experimental results for the SAMs' physicochemical properties (chemical structure, water contact angle, lateral packing density of SAMs, etc.) and adsorbed protein mass on the SAMs to develop our ANN. Our results showed that most of the data was well predicted with relatively small error (about 19%). In addition, we carried out the analysis of the "importance" of each physicochemical property of SAMs to determine the amounts of the adsorbed proteins (Figure 2), and we found good agreement with general consensus for the requirements for protein-resistance. Based on these results, we concluded that the ANN has a strong potential for the design of biomaterials with desired functions.

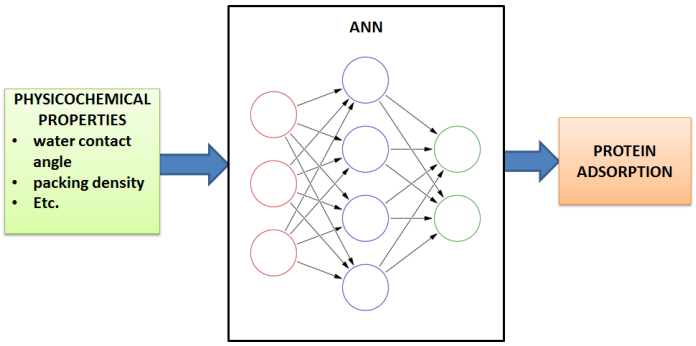

Fig. 1: Our ANN model to predict protein adsorption

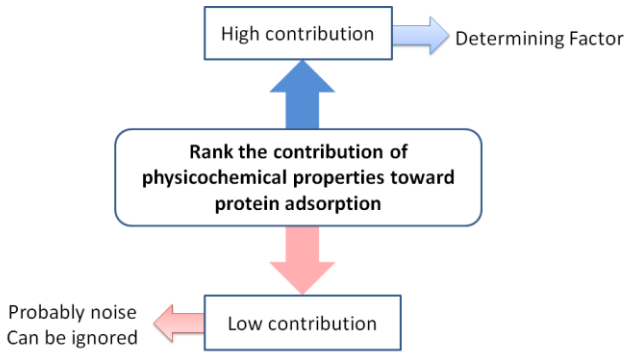

Fig.2 Procedure for the analysis of contribution of each physicochemical property