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Machine learning based prediction of layer-by-layer coating thickness

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Introduction: Layer-by-layer film coatings are an effective technique for surface modification, particularly in the biomedical industry. Despite the large number of papers on LbL assembly, prediction of LbL coating thickness, as a functional property, is a challenging and time consuming task from the aspect of experiment. Machine learning (ML) approaches that are already being developed have the potential to speed up and improve novel coating development thus reducing time and material consumption.

Materials and methods: The data used represented a combination of the literature and experimental data generated in-house using a Quartz Crystal Microbalance with dissipation monitoring (QCM-D). The whole dataset for coating thickness [nm] prediction included the 22 input features (Polycation, Polyanion, Polycation unit MW, Polyanion unit MW, Polycation MW, Polyanion MW, Number of the bilayer, Ending polymer etc.). In total, there were 98 instances from the literature and 33 from the in-house experiments. Proposed methodology included several preprocessing steps (such as outlier removal and missing data imputation) and machine learning techniques for coating thickness prediction (Linear regression, Logistic regression, Support Vector Regressor, Random Forest Regressor, and Extra Tree Regressor). SMOGN was used to deal with skewed data.

Results and discussion: The results show that Extra Tree Regressor outperformed other algorithms when combined with optimal hyperparameters and missing data imputation. Relevant metrics achieved were R2 =0.980, MSE = 46933.204, RMSE = 216.64 and MAE = 111.414 on the test dataset. The 6 best predictors of coating thickness were identified, with top three being Polyanion, Number of the bilayer and Ending polymer, which can be used to predict coating thickness without the need for numerous parameter measurements.

Conclusions: Further research will focus on outputs associated with antibacterial, anti-inflammatory, and antiviral capabilities, allowing researchers to respond to real-world biomedical issues like as antibiotic resistance, implant rejection, and COVID-19 outbreaks.

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