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הפקולטה להנדסה כימית
ע״ש וולפסון
The Wolfson Department of Chemical Engineering

Wolfson Department of Chemical Engineering Seminar

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Room 6

Optimising Liposome Sizing Through Active Learning and Automated Liquid Handling (LiHa)

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MSc Seminar

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The application of liposomes in targeted drug delivery has had a major impact on the medical world and continues to show promising results for the future of medicine. The current research practices for formulating liposomes are based upon previous literature, intuition, knowledge, and trial-and-error. Rapidity and precision of new formulations are becoming increasingly important in the medical industry whilst maintaining cost effectiveness. There is no single solution to these challenges, but rather a combination of automation, cheminformatics and computer science will be required. This project aims to combine automated liquid handling technology with machine learning to leverage available liposome formulation data for the prediction of future formulation characteristics. Incorporating prior knowledge to machine learning models can allow users to gain insight on potential liposome formulations, whether it be the size of the formulated particles, aggregation, homogeneity, or other important characteristics. This in turn can guide researchers on selecting the optimal liposomal formulation and accelerate the optimisation process. A common approach to 'teaching' machine learning models is with large amounts of training data. However, there is a lack of available liposome data that is standardised. Therefore, this project focussed on utilising an active learning approach with an automated liquid handler (LiHa). The LiHa provided considerable and standardised control for the ethanol injection method that is not possible during manual liposome formulation. The active learning approach is a machine learning method where the models select which formulation the researcher must produce and analyse to improve the models learning and validation. During the project we compared this approach with a random learning approach, a method of choosing random formulations that are completed and provided to the models. Both approaches were done iteratively, feeding the machine learning method with ten new formulated liposome data points for each iteration. After completion of ten iterative loops of selecting formulations, the active learning approach showed promising results compared to the random learning approach. Importance of the liposome formulation features were also assessed at each iterative loop, and at the tenth iteration, the active learning approach produced a more stable scaling of feature importance. Based on our results, we predict that moving forward, an active learning approach will improve liposome predicting models more rapidly while reducing the required number of experiments to be completed.