



COLLEGE OF PHARMACY
PHARMACEUTICAL SCIENCES
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Pharmaceutical Sciences Seminar

Wednesday, November 18, 2020

Join Zoom Meeting

<https://umich-health.zoom.us/j/96037906837>

4:00-5:00 pm

“Machine Learning Methods for Antibody Optimization”

Presented by:

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Abstract: In the last thirty years, antibodies have become intensely studied as therapeutics for treatment of a diverse range of diseases due to the possibility of an extremely favorable combination of biophysical properties. However, achieving this favorable combination has proven difficult due to the closely interrelated nature of these properties: often exhibited with strict tradeoffs that arise from overlapping molecular determinants. Recent advances in sequencing technology have facilitated the acquisition of extensive datasets consisting of primary protein sequences, however, failure to extract features that accurately describe the exhibition of biophysical properties has left these datasets severely underutilized. In this work, a trained recurrent neural network (UniRep) was used to extract features from thousands of labeled primary protein sequences. Linear discriminant analysis algorithms were trained to predict property exhibition which were shown to accurately reflect two closely and inversely related biophysical properties: affinity and specificity. Pareto optimization facilitated the accurate prediction and isolation of several antibody variants with tunable exhibition of these properties and minimized tradeoff. Prediction and evaluation of novel mutations testing the generalizability of the feature extraction method and model demonstrated promise for further improvements to properties such as specificity. Overall, a novel feature extraction method was validated for the robust co-optimization of antibody biophysical properties, that is generalizable to novel mutations.

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