Experimental validation of the predictions of a mathematical model for protein purification and tag selection

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To improve downstream processing, protein engineering can be used to modify particular properties of a protein, such as specific affinity, charge, or hydrophobicity. The most common modification involves the peptide tags fusion to the protein. Nevertheless, the selection of both the optimal peptide tag and the right purification system to use is not trivial. The aim of this work is to experimentally validate our previous mathematical model based on MINLP models. This model was modified to find the minimum number of chromatographic operations, and the ideal tag for obtaining a required level of purification. A weighted linear combination of the number of purification steps and the target protein purity obtained after the last step was used as the objective function. The chromatographic steps suggested by the model were carried out using an example based on two mutated cutinases. The results show that average deviations between experimental data and those predicted by the model, for yiel