



The Best of BIOT Awards: October 25, 2017

Date	Area	Time	Presenter	Institution
Wednesday, October 25th	Biomolecular and Biophysical	12:00-12:30 PM	Marieke Klijn	Karlsruhe Institute of Technology
			Multidimensional data visualization and data mining for characterization of long term protein phase behavior	
	Peterson Award	12.30 -1:00 PM	TBD	TBD
		TBD		

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“Multidimensional data visualization and data mining for characterization of long term protein phase behavior”

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The characterization of protein phase behavior for formulation and long term storage of biopharmaceuticals is essential to identify stable storage conditions. A widely used approach is to store proteins for prolonged periods (40 days up to 2 years) under varying solution conditions. Afterwards, samples are optically scored as stable or instable, where aggregation in the form of precipitation, crystallization or phase separation is considered instable. This procedure is time consuming and has a trail-and-error nature, where experience is required for selecting solution conditions. Therefore, it is desired to reduce development time and costs via rational design of characterization experiments and protein phase behavior prediction. To achieve this goal, understanding of the underlying protein-protein and protein-solvent interactions is required. These interactions are dependent on protein properties, which are in turn influenced by multiple physical and chemical parameters of the solution and the protein itself. This system can therefore be defined as multidimensional. Many studies have investigated this subject, but its multidimensionality is only partially (or not at all) taken into account.

This study aims to describe the effects of varying solution conditions on hydrophobicity, charge, secondary and tertiary structure as well as temperature induced aggregation propensity of lysozyme via empirical determination. Advanced multidimensional data visualization and data mining is used to correlate these protein properties to long term stability experiments to investigate underlying protein-protein and protein-solvent interactions. This involves careful experimental design and processing raw data for the extraction of novel features to represent the desired protein properties. These

features will subsequently be used to generate empirical phase diagrams for multidimensional data visualization, which allows for easy identification of alterations in protein properties as a function of changes in solution pH, salt type and concentration and protein concentration. This will lead to a more detailed understanding of underlying protein-protein and protein-solvent interactions responsible for observed protein phase behavior.

“TBD”

Peterson Awardee

Peterson Awardee abstract