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POS-53 Effects of native state topology vs. sequence in protein folding

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Most small single-domain proteins spontaneously organize into essentially unique three-dimensional structures determined by their amino acid sequence. While much has been learned about this folding process from experiment and theory, open questions remain. Here we use an intermediate-level coarse-grained model with 7 atoms per amino acid to explore the interplay of two factors in the folding process, namely (1) the amino acid sequence and (2)the topological complexity of the native fold. To this end, we first design three different 35-54 amino acid model sequences that fold into 3alpha, 4beta+alpha and beta barrel structures, respectively, and hence exhibit varying fold complexities. The folding free energy landscapes of these three sequences are determined using Monte Carlo simulations. We thereafter employ a novel multisequence algorithm to determine the folding thermodynamics of large numbers of mutants of the three proteins. Effects of the mutations on the folding free energy landscapes within and between the folds are compared.

Author: WALLIN, Stefan (Memorial University of Newfoundland)

Presenter: WALLIN, Stefan (Memorial University of Newfoundland)

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