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Folding and Aggregation of Mucin Domains. BRIGITA URBANC, RAMA BANSIL, Boston University, BRADLEY TURNER, Harvard Medical School — Mucin glycoproteins consist of tandem repeating glycosylated regions flanked by non-repetitive protein domains with little glycosylation. These non-repetitive domains are involved in polymerization of mucin via disulfide bonds and play an important role in the pH dependent gelation of gastric mucin, which is essential to protecting the stomach from autodigestion. We have examined the folding and aggregation of the non-repetitive sequence of von Willebrand factor vWF-C1 domain (67 amino acids) and PGM 2X (242 amino acids) using Discrete Molecular Dynamics (four-bead protein model with hydrogen bonding and amino acid-specific hydrophobic/hydrophilic and electrostatic interactions of side chains). Simulations of vWF C1 show 4-6 β-strands separated by turns/loops with more loops at lower pH. A simulation of several vWF C1 proteins at low pH shows aggregates still with a high content of β-strands and enhanced turn/loop regions. For the PGM 2X simulation the contact map shows several salt bridges enclosing hairpin turns. The implications of these simulations for describing the aggregation/gelation of PGM will be discussed.

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