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Molecular Dynamics Study of the Solubility Curve of Polyglutamine for the PLUM Model.[1] SONGUL KUTLU, JASON HAAGA, JAMES D. GUNTON, Lehigh University — A recent study by Crick et al [1,2] determined the saturation (solubility) curve for polyglutamine (PolyQ) for several different repeat lengths, n, of Qn, and for different flanking sequences, such as K2. The degree of supersaturation S, (S=ln(Co/Ce), where Co and Ce are the metastable and equilibrium saturation monomer concentrations, respectively) plays a crucial role in the kinetics of aggregation of misfolded proteins containing polyQ. Thus the degree of supersaturation is an important factor in diseases such as Huntington's disease for which polyQ is a major component. We present here preliminary results of a molecular dynamics study for the solubility curve for a PLUM model of Q10. (An extensive study of the kinetics of aggregation for this model is being carried out in a separate study [3]) Our results display a normal solubility curve behavior, with the saturation concentration increasing with increasing temperature. This is only in partial qualitative agreement with the experimental results, which show a retrograde behavior at low temperatures. We are extending this study to other repeat lengths, including Q40. \\ \\1. PhD Thesis, S. Crick, Jan (2011), Washington University. 2. S.L. Crick, K. M. Ruff, K. Garai, C. Frieden, and R. V. Pappu, PNAS 2013 110 (50) 20075-20080. 3. J. Haaga, C. N. Buckley and J. D. Gunton, unpublished (2016).

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