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Dimer model for Tau proteins bound in microtubule bundles[1]
NATALIE HALL, ALEXANDER KLUBER, N. ROBERT HAYRE, RAJIV SINGH, DANIEL COX, University of California, Davis — The microtubule associated protein tau is important in nucleating and maintaining microtubule spacing and structure in neuronal axons. Modification of tau is implicated as a later stage process in Alzheimer's disease, but little is known about the structure of tau in microtubule bundles. We present preliminary work on a proposed model [1] for tau dimers in microtubule bundles (dimers are the minimal units since there is one microtubule binding domain per tau). First, a model of tau monomer was created and its characteristics explored using implicit solvent molecular dynamics simulation. Multiple simulations yield a partially collapsed form with separate positively/negatively charged clumps, but which are a factor of two smaller than required by observed microtubule spacing. We argue that this will elongate in dimer form to lower electrostatic energy at a cost of entropic "spring" energy. We will present preliminary results on steered molecular dynamics runs on tau dimers to estimate the actual force constant.

[1] Rosenberg, K. J. Ross, J. L. Feinstein, H. E., Feinstein, S. C. Israelachvili, J., PNAS (USA) 105, 2008, 7445-50.

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