WAKATE INITIATIVE SPECIAL SEMINAR

演題：β–**Amyloid GNNQQNY Fibres: Thermodynamic, Mechanics and a *bit of Kinetics***

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会場：Room 311, Sogo-kenkyu (Building D)

要旨：Ranges of debilitating human diseases are associated with protein misfolding events that result in the formation of amyloid fibres and small toxic oligomers. These include Alzheimer's and Parkinson's, all of which are progressive disorders associated with high morbidity.

The most remarkable property of the amyloid fibres, which has no equal in molecular biology science, is the outstanding stability and resistance to degradation. They have been described as having a similar strength to steel, a property that they share with their structural cousin, silk. As a consequence, the outstanding mechanical properties together with the capacity to produce amyloid fibres under mild conditions, make real the opportunity to synthesize a new class of biocompatible materials with unique strength and flexibility.

The central aim of this study is to understand and characterize at the molecular level the thermodynamic and mechanical properties of amyloid fibres.

Free energy simulations show that single peptides are less stable than fibrils giving rise to a fast elongation of the amyloid fibres with a small lag phase. The mechanical properties (stress/strain relation) of the amyloids have been studied by constraining two pulling groups at the two end-to-end fiber extremities and by applying a force to the center of mass of the pulling groups. The value at which the fibril fracture represent the ultimate strength (0.23-0.25 GPa) whereas the slope of the stress/strain curve represent the Young modulus (9.18 GPa). Both values are within the experimental errors [1, 2].

Our work suggests that a fibril 10 *μm* in length breaks spontaneously on average 1-10 min and therefore internal fracturing can contributes in the proliferation of amyloid fibrils.

References

[1] J.F. Smith, T.P. Knowles, C.M. Dobson, C.E. Macphee, M.E. Welland, Characterization of the nanoscale properties of individual amyloid fibrils, Proc Natl Acad Sci USA 103(43) 15806-15811 (2006).
[2] T.P. Knowles, A.W. Fitzpatrick, S. Meehan, H.R. Mott, M. Vendruscolo, C.M. Dobson, M.E. Welland, Role of Intermolecular Forces in Defining Material Properties of Protein Nanofibrils, Science 318:1900 (2007).

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