中国科学院数学与系统科学研究院
Academy of Mathematics and Systems Science, CAS

生物信息学研究中心

Center of Bioinformatics

学术报告

题　　目： Numerical approach to structure and folding of protein and microRNA

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时　　间： 4 月 1 日（星期五）下午 14:00

地　　点： 思源楼 712 室

摘　　要：

In this talk, I briefly review some recent developments in numerical approach to structure and folding of proteins and microRNA. The topics under discussion include: (1) developments of algorithms and computer packages for all-atom simulations of proteins [1], (2) development of algorithm to compute volume V, surface area A, and cavity of proteins by analytic equations [2], (3) unfolding and refolding of immunoglobulin domain I27 and ubiquitin [3], and (4) TAROKO: a webserver for microRNA 3D structures and folding thermodynamics [4].

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(2) S. Hayryan, C.-K. Hu, J. Skvrivanek, E. Hayrjan, I. Pokorny. J. Comp. Chem. 26, 334 (2005); J. Busa, J. Dzurina, E. Hayryan, S. Hayryan, C.-K. Hu, J. Plavka, I. Pokorny, J. Skrivanek, and M-C. Wu. Comp. Phys. Commun. 165, 59 (2005); J. Busa,, S. Hayryan, C.-K. Hu, J. Skrivanek, and M.-C. Wu, J. Comp. Chem. 30, 346-357 (2009) and Comp. Phys. Commun. 181, 2116 (2010).
(3) M.-S. Li, C.-K. Hu, D. K. Klimov, and D. Thirumalai, Proc. Natl. Acad. Sci. USA 103, 93 (2006); M.-S. Li, M. Kouza and C.-K. Hu. Biophysical J. 91, 547(2007). M. Kouza, C.-K. Hu and M. S. Li, J. Chem. Phys 128, 045103 (2008).
(4) S. Harryan, M.-C. Wu, F. Ding, D. Tsao, N. V. Dokholyan and C.-K. Hu, submitted for publication.