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등과학원), 이승종(수원대), 이주영(고등과학원) We introduce a novel method for the second structure prediction of proteins, PREDICT(PRofile Enumeration DICTionary). This method uses a concept of distance between patterns. For a given protein sequence, this method uses PSI-BLAST to generate profiles, which define patterns for amino acid residues. This pattern is compared with the pattern database generated from PDB, and the pattern closest to a query profile is selected to determine the secondary strucutre of the query residue. This method combines the idea of the nearest-neighbor method of Yi and Lander with the profile generating technology of PHI-BLAST which proved to be very powerful in recent years. We tested the method on the set of 513 non-homologous proteins CB513, and applied it to the CASP5 targets for blind test. The performance on the CB513 set is at least comparable to the state of art methods such as neural networks.

F-P021 **The Unbiased Global Optimization of Lennard-Jones Clusters using Conformal Space Anealing Method** 이주련, 이인호, 이주영(고등과학원) By applying the newly-developed Conformal Space Annealing (CSA) method to the Lennard-Jones cluster, we find all the known lowest energy conformations, up to 201 atoms, without using any information on the symmertry of the known global minima of the system. In particular, based on 10 seperate optimizations of upto 183 atoms, we demonstrate that the CSA finds the lowest energy conformations more efficiently than existing methods.

F-P022 **A Monte Carlo study on protein-folding dynamics** 김승연,이주련,이주영(고등과학원) Folding dynamics of small peptides and proteins, such as Betanova, 1fsd, HP-36, and Protein A, has been studied by Monte Carlo simulations. We have used UNRES potential as the fundamental interaction. In particular, the parameters of UNRES potential have been optimized simultaneously for Betanova, 1fsd, HP-36, and Protein A. Monte Carlo results demonstrate that, starting from random conformations, these macromolecules fold into their native-like conformations at appropriate temperatures. Estimates for glass temperatures are also obtained. Overall features of these folding folding dynamics are consistent with two state folding.

F-P023 **Global Effect of Transverse Bifurcations in Coupled Chaotic Systems** 임우창, 김상윤(강원대) We investigate the global effect of transverse bifurcations in symmetrically coupled one-dimensional maps. A transition from strong to weak synchronization occurs via a first transverse bifurcation of a periodic saddle embedded in the synchronous chaotic attractor (SCA). For the case of a supercritical transverse bifurcation, a soft bubbling transition occurs. On the other hand, a subcritical transverse bifurcation leads to a hard transition. It is found that the global effect of such subcritical hard bifurcations depends on whether they may or may not induce a "contact" between the SCA and its basin boundary. For the case of a "contact" bifurcation, an absorbing area, surrounding the SCA and acting as a bounded trapping vessel, disappears, and hence basin riddling occurs. However, for the case of a "noncontact" bifurcation such an absorbing area is preserved, and hence hard bubbling takes place. Through a detailed numerical analysis, we obtain the phase diagram for chaos synchronization and give explicit examples for all kinds of transverse bifurcations. Dynamical transitions following the first transverse bifurcations are also discussed.

F-P024 **Jamming Transition in a Highly Dense Granular System under Vertical Vibration** 김기범, 문종균, 박종진, 김형국, 박혁규(부산대) The dynamics of the jamming transition in 3D