2P28

分子スペクトル計算による小ペプチド分子の立体配座解析

○後藤仁志[1]、中山尚史[1,2]、鎌倉寿行[1]
[1]豊橋技術科学大学（〒441-8580 豊橋市天伯町雲雀ヶ丘 1-1）
[2]科学技術振興機構（〒332−0012　埼玉県川口市本町 4−1−8）

INTRODUCTION

Short peptides that have well-defined tertiary structure, offer outstanding systems for detailed conformational analyses, both experimental and computational studies of protein folding and biological function. In this meeting, we propose our computational approach to prediction for a folding process of a short peptide by using combination of an exhaustive conformational space search and conformation clustering technique, which are accelerated with both general parallel processing and Grid technology.　A folding process of a 12-residue peptide (1LE0, Fig. 1) known as a stable beta-hairpin tryptophan zipper, is predicted as an example. Theoretical CD spectra (Fig. 2) assigned to some conformers of the peptide were calculated and compared with the experimental data (Fig. 3).

COMPUTATIONS

Target Molecule	Tryptophan Zipper 1: a stable, β-hairpin mini-protein (1LE0-model 1, 12 residues)
Force Field	MMFF94 force field and dielectric constant=78.4 for water condition
Conformational Space Search	Totally, 22,897 conformers found by using parallel CONFLEX search with 16 workers (7.2 days)
Conformation Clustering	Single linkage method and conformational (torsional) distance matrix approach used
Pathway Prediction	Our original method

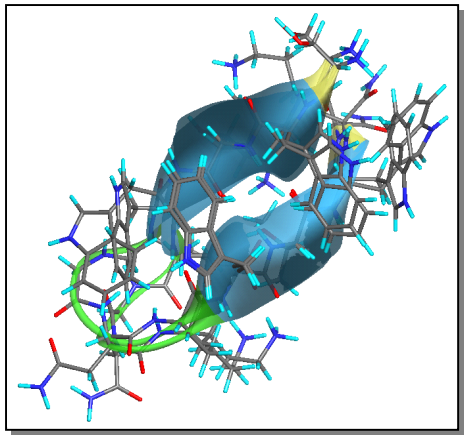

Fig.1　Superimposed image of NMR(AMBER) and MMFF94 optimized structures (RMSD=0.647A)

RESULTS

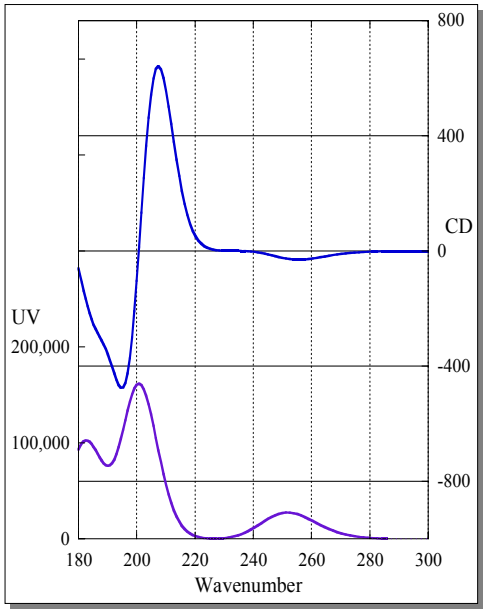

Fig.2　Calculated CD spectrum

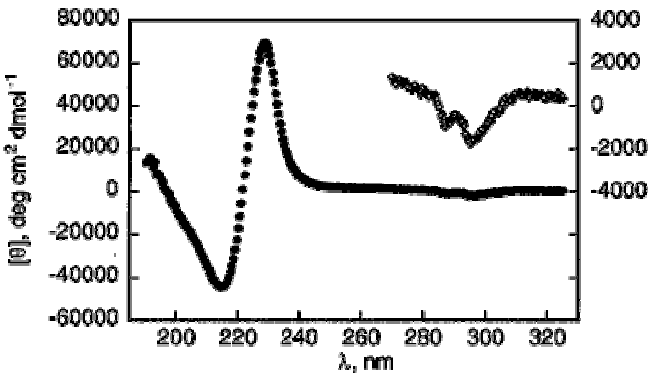

Fig.3　Experimental CD spectrum

[A.G.Cochran, et. al, PNAS, 98, 2001, 5578-5583]