Computational Chemistry as a Key to Structural Bioinformatics

Young Kee Kang
Department of Chemistry, Chungbuk National University
Cheongju, Chungbuk 361-763, Korea

Abstract

Computational chemistry is a discipline using computational methods for the calculation of molecular structure, properties, and reaction or for the simulation of molecular behavior. Relating and turning the complexity of data from genomics, high-throughput screening, combinatorial chemical synthesis, gene-expression investigations, pharmacogenomics, and proteomics into useful information and knowledge is the primary goal of bioinformatics. In particular, the structure-based molecular design is one of essential fields in bioinformatics and it can be called as structural bioinformatics. Therefore, the conformational analysis for proteins and peptides using the techniques of computational chemistry is expected to play a role in structural bioinformatics.

There are two major computational methods for conformational analysis of proteins and peptides; one is the molecular orbital (MO) method and the other is the force field (or empirical potential function) method. The MO method can be classified into ab initio and semiempirical methods, which have been applied to relatively small and large molecules, respectively. However, the improvement in computer hardwares and softwares enables us to use the ab initio MO method for relatively larger biomolecules with up to ~100 atoms or ~800 basis functions.

In order to show how computational chemistry can be used in structural bioinformatics, I will present on (1) cis-trans isomerization of proline dipeptide and its derivatives, (2) positional preference of proline in α-helices, and (3) conformations and activities of Arg-Gly-Asp-containing tetrapeptides.

Curriculum Vitae

Name: **Young Kee Kang**

Title: Professor of Chemistry

Birthplace: Seoul, Korea

Birthday: July 24, 1953

Present Address: Department of Chemistry, Chungbuk National University,
Cheongju, Chungbuk 361-763, Korea

Education: B.S., Chemistry, February 1977,
Yonsei University, Seoul, Korea

M.S., Physical Chemistry, February 1980,
Korea Advanced Institute of Science and Technology,
Seoul, Korea

Ph.D., Physical Chemistry, February 1983,
Korea Advanced Institute of Science and Technology,
Seoul, Korea

Academic Experiences: Assistant Professor, March 1983 - September 1987,
Associate Professor, October 1987 - September 1992,
Professor, October 1992 - Present,
Department of Chemistry, Chungbuk National University,
Cheongju, Chungbuk 360-763, Korea

Postdoctoral Research Associate,
March 1985 - February 1987,
Baker Lab. of Chemistry, Cornell University,
Ithaca, NY 14853, USA

Visiting Scientist, June 1987 - August 1987,

June 1989 - August 1989,
March 1990 - February 1991,
Visiting Professor, June 1994 - August 1994,
July 1996 - August 1996,
July 1997 - August 1997,
July 1998 - August 1998,
July 1999 - August 1999,
July 2000 - August 2000,
Baker Lab. of Chemistry and Chmical Biology, Cornell University,
Ithaca, NY 14853, USA

Visiting Scientist, June 1993 - August 1993,
December 1993 - February 1994,
Institute for Molecular Science,
Okazaki 444, Japan

Membership: Korean Chemical Society, Biochemical Society of the Republic of Korea, American Chemical Society, Korean Biophysical Society, The Protein Society, American Peptide Society, Korean Peptide Society

Research Interests:
1. Theoretical Studies on the Conformation and Hydration of Peptides and Proteins
2. Development of Potential Parameters Used in Conformational Analysis of Peptides and Proteins
3. Molecular Modeling of Bioactive Molecules