



# International Society of Quantum Biology and Pharmacology

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## ISQBP Election Results

In January elections were held for the offices of Vice President and Councilor. Richard Lavery, Institut de Biologie Physico-Chimique, Paris, France was elected Vice President. He will continue as Vice President for the remainder of 2006 and assume the office of President of the ISQBP on January 1, 2007. A major part of his duties will involve organizing the 2008 ISQBP President's Meeting. Lennart Nilsson was elected as ISQBP Councilor. He assumes the position immediately, where he will act in an advisory role, facilitating decisions of the ISQBP president and other elected officers.

The next elections will be held in Winter 2007 for the offices of Vice President, Secretary and Councilor. The election for Vice President is being performed in consecutive years to allow the President and Vice President to work together over the full two years of the President's term. Nominations for of individuals for the above offices may be sent to [Alex MacKerell](#)

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## 2006 ISQBP President's Meeting

### ISQBP 2006 President's Meeting Website

The 2006 ISQBP President's meeting, June 24-27, involved 117 participants from 16 countries (Austria, Belgium, Cyprus, Czech Republic, Denmark, France, Germany, Italy, Norway, Poland, Portugal, Spain, Sweden, Switzerland, UK, USA). The meeting was held on the Université Louis Pasteur campus in Strasbourg, France. The campus is within walking distance of the animated and impressive city center, located in a beautiful setting close to the botanical garden and the old Observatory. The registration, held in the late afternoon of July 23, included a welcome reception featuring Alsatian wines and beer, tasty elegant sandwiches and pastries. This was an excellent ice-breaking activity, helping to develop an atmosphere that was warm and collegial, facilitated by the rather warm weather in Strasbourg.

The meeting was held in the Atrium building of the ULP campus. The Atrium offered a bright hall, where the posters were displayed for the duration of the meeting. Adjacent to the hall was a long terrace for coffee breaks and informal discussions. After an initial attempt to use the auditorium on the same level as the poster room, the lectures were delivered in the (better) air-conditioned upper auditorium of the Atrium.



The lectures were organized based on four main topics; Large scale Conformational Changes in Biological Molecules, Computer-aided Drug Design/Molecular Recognition, QM/MM, and Protein-Nucleic Acid Interactions. In each session a number of leading scientists in the field (for detailed information refer to the meeting schedule at the meeting website) presented their latest achievements. Harold Scheraga, as the recipient of the 2006 Gilda Loew Lectureship, presented a seminar entitled "The Two Aspects of the Protein Folding Problem", explaining his novel method, based on the united residue model (UNRES), to increase the time scale of MD so as to be able to simulate protein folding and unfolding (JPCB 2005, 109, 13785–13810). After the lecture Alex MacKerell presented Prof. Scheraga with a plaque commemorating the occasion.

On Monday, July 26, stimulating late afternoon lectures were delivered by Jean-Marie Lehn (the 1987 Nobel Prize Laureate in Chemistry as well as a native of Alsace and a Strasbourg graduate) and Arie Warshel (the 2006 ISQBP President's Award winner). Jean-Marie Lehn, in an ample fresco, described the dynamic properties of a wide number of self-assembling organic materials. A prolonged and exciting discussion followed his intriguing talk. Arie Warshel, who at the end of his talk received a plaque from the President commemorating his award, highlighted the numerous accomplishments of his scientific career dedicated to the elucidation of the function of biological molecules with emphasis on what remains to be accomplished in the ever-growing field of computational chemistry.

The seminar schedule included the "ABC" DNA presentation of David Beveridge and the ISQBP annual meeting. At the meeting a number of topics were discussed, including the role of the society in facilitating the organization of workshops oriented toward graduate student training. Any individuals interested in organizing such events are welcome to contact the ISQBP president.

Following the final seminar on Tuesday July 27, the ISQBP President made a number of closing remarks and announced the winners of the awards for best posters. Each winner, listed below, received \$300 based on a generous donation from the Molecular Graphics and Modeling Society.

**Conformation and catalysis in lysozyme**, Ian M. Grant, Anna L. Bowman, Adrian J. Mulholland, School of Chemistry, University of Bristol

**EADock a multiobjective evolutionary framework for the docking of small molecules into protein active sites,**

Aurélien Grosdidier, Vincent Zoete and Olivier Michielin, Swiss Institute of Bioinformatics - Molecular Modeling Group - Quartier Sorge - Batiment Genopode - CH-1015 Lausanne – Switzerland

**Atomistic molecular dynamics simulations of DNA minicircles**,

Filip Lankaš<sup>1</sup>, Richard Lavery<sup>2</sup> and John H. Maddocks<sup>1</sup>, <sup>1</sup>Laboratory for Computation and Visualization in Mathematics and Mechanics, Institut de Mathématiques B, Ecole Polytechnique Fédérale de Lausanne, Station 8, CH-1015 Lausanne, Switzerland, <sup>2</sup>Laboratoire de Biochimie Théorique, CNRS UPR 9080, Institut de Biologie Physico-Chimique, 13 rue Pierre et Marie Curie, Paris 75005, France

**Target RNA in complex with antisense PNA studied by MD simulations**,

Boel Nyström and Lennart Nilsson, Department of Biosciences and Nutrition at Novum, Karolinska Institutet, Huddinge, Sweden

The afternoon of Tuesday July 27 was free time. Attendees had the choice of two social events that included a walking tour of Strasbourg and a vineyard tour. In the evening, the conference dinner was held at the Maison Kammerzell, a restaurant located in an ancient Renaissance mansion on Cathedral Square. The “Coq au Riesling” menu perfectly matched the old mansion atmosphere. Brief comments by the President to the attendees, who applauded him and all the meeting organizers, concluded the dinner.



Maison Kammerzell



One of the frescoes in the dining room of Maison Kammerzell

Special thanks goes out to the local organizers, Roland Stote, CNRS, Strasbourg and Annick Dejaegere, Université Louis Pasteur along with their postdoctoral fellows and students, to the Symposium Secretary Christine Guibert of the Université Louis Pasteur, to Laurent Buhl for technical assistance, to Rémy Louis, Director Institut de Chimie and to Babeth Vacarro, Secretary to the Director. These individuals laid the ground work for a enjoyable and intellectually stimulating meeting that will be remembered for years to come. Please go to the meeting website for more information on the meeting as well as pictures of meeting participants. In addition we would like to thank the meeting sponsors including Université Louis Pasteur and the Institut de Chimie, Strasbourg, Chemcomco LLC, Fujitsu/FQS Poland, Schrödinger Inc, Région Alsace, Syngenta, Strasbourg Communauté Urbaine, Molecular Graphics and Modeling Society and the University of Maryland Computer-Aided Drug Design Center.

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## ISQBP Website

<http://isqbp.umaryland.edu/ISQBP>

The site contains a variety of information about the ISQBP including a somewhat fragmented history of the organization. Please visit the site and let us know your thoughts on the site as well as the types of information you would like to see on the site. In the future we hope to add an interactive job forum to the site. Email comments to [Alex MacKerell](#)



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## Membership Information

**Annual Dues:** Annual dues for the ISQBP are now \$30 US. It is now possible to pay dues via Paypal.com or via check. Please visit the ISQBP website for more information. As all governance and organizational efforts of the ISQBP are performed by volunteers, dues are used to support society-sponsored events including the various workshops and meetings that are supported by the ISQBP.

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## ISQBP Leadership

President	Alex MacKerell	2005 - 2006
Vice President	Richard Lavery	2006*
Secretary	Caterina Ghio	2005 - 2007*
Past- President	Nigel Richards	2005 - 2006
Treasurer	Jane Murray	2004 - 2006
	Nigel Richards	2007 - 2009
Councilors	Lennart Nilsson	2006 - 2009
	Tim Clark	2004 - 2006*
	Modesto Orozco	2005 - 2007
*Indicates up for election in 2006/2007		