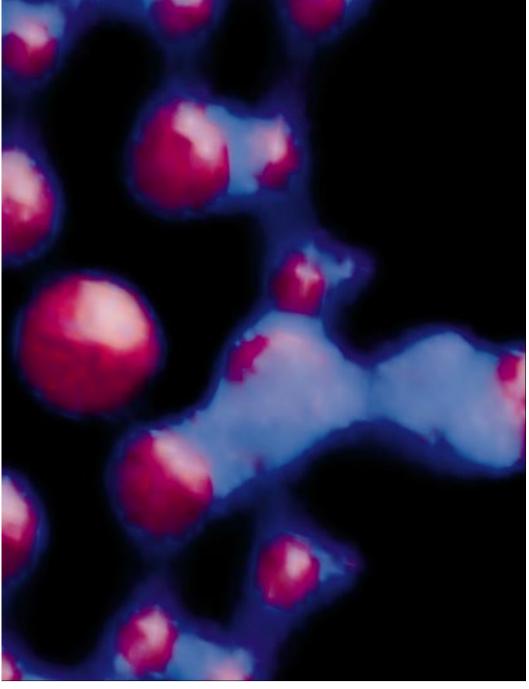
ISCB NEWSLETTER





volume 5. issue 1. spring 2002

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A NOTE FROM ISCB PRESIDENT

Phil Bourne

EXECUTIVE COMMITTEE

Philip E. Bourne, Ph.D., *President*Michael Gribskov, Ph.D., *Vice President*Anna Tramontano, Ph.D., *Vice President*David Rocke, Ph.D., *Treasurer*Barbara Bryant, Ph.D., *Secretary*

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Cathy H. Wu, Ph.D. SOCIETY STAFF

Kim Baldridge, Staff Oversight
Cassie Ferguson, Writer
Stephanie Hagstrom,
Conference Coordinator
Jennifer Matthews, Design
BJ Morrison McKay,
Administrative Officer
Josh Polterock, Webmaster
Chris Smith, Finance
Tracy Zhao, Programming

On January 21, I officially took over the ISCB Presidency from Russ Altman and I am looking forward to fulfilling a demanding agenda as well as setting new long-term goals. Our science is in a tremendous state of expansion, and the agenda for this year centers around serving the society's rapidly growing and diverse membership.

Let me begin by introducing the other elected members of the 2002 ISCB Executive Committee:

- Michael Gribskov (USA) Vice President (gribskov@sdsc.edu)
- Anna Tramontano (Italy) Vice President (Anna. Tramontano@uniroma1.it)
- Barbara Bryant (USA) Secretary (bryant@mpi.com)
- David Rocke (USA) Treasurer (dmrocke@ucdavis.edu)

Accompanying rapid growth is a more diversified science and the need for special interest groups (SIGs) to affiliate with the Society in ways not dissimilar to regional groups. SIGs are an active and vital part of the Society's official conference, Intelligent Systems in Molecular Biology (ISMB), and a variety will be represented at this year's meeting in Edmonton, Canada (www.ismb02.org). I have asked Barbara Bryant to foster the development of formal relationships between the SIGs and ISCB. Clearly, these efforts require a professional and well-organized Society office, beyond that provided by the Executive Committee, who are all volunteers with extremely demanding scientific jobs. A professional office requires funds, and I have asked David Rocke to explore fund raising opportunities, particularly through interactions with corporate partners.

I recently attended the International Conference on Bioinformatics 2002 in Bangkok to understand the needs of this area and how ISCB can foster regional groups. The ISCB has a role to play in fostering regional group development while doing everything it can to have our science be represented in a

unified way to governments and society worldwide. What is clear is that there is a huge future for bioinformatics in the Asian region, but research organizations there have some of the same problems that plague



all geographic areas—most notably insufficient trained personnel and a large number of scientists wishing to be trained in bioinformatics.

I've had a chance to contact representatives from the Japanese Society for Bioinformatics (JSBi), which shares common goals with us. JSBi has generously offered to inform its membership of what's happening within the ISCB. I sincerely hope this is the beginning of a long and fruitful interaction between the two organizations. On behalf of the Executive Committee, the Board and our membership, I look forward to this interaction and encourage the membership of JSBi to contact the ISCB with ideas for joint programs.

This speaks to a general program of regional affiliation. In coming months, we will be proposing initiatives to assist regional groups to get established and to flourish, as well as instituting a more active educational program. I have asked Anna Tramontano to lead our regional affiliates effort and Michael Gribskov to begin work on an educational program. The first step, in both cases, is to understand the scope of what has previously been done. The improved ISCB Web site at www.isch.org will include details of these and other efforts as they begin to unfold. Suggestions on the Web site and on the Society in general can be sent via email to admin@isch.org.



ISCB WELCOMES BJ, NEW ADMINISTRATIVE OFFICER

The ISCB is pleased to welcome BJ Morrison McKay as our new full-time administrative officer. Based at the University of California, San Diego, McKay succeeds Stanley Jacob at Stanford, who has served as administrator for the past two years. BJ has some big shoes to fill, but she is equipped to take us to new levels in our growth as the predominant scholarly society for computational biologists.

McKay's previous management experience has been based in the corporate world of hotels, hospitality and conference administration. With 20 years of sales experience behind her, she has managed staffs ranging from five to 15, and run the business development division of a California consulting firm with a national clientele. Her employers have included Four Seasons Hotels and Marriott, medical conference organizers AM Medica Communications, and a hospitality-consulting firm, The Karro Group, Incorporated.

It was her understanding of association management that attracted the ISCB to McKay, and McKay to the ISCB. She has spent years on the boards of local chapters of San Diego Women in Travel (SWIT), Meeting Professionals International (MPI) and Society of International Travel Executives (SITE). For those non-profit organizations, she upgraded the quality of MPI and SWIT's membership directories, served as SWIT's Newsletter Editor and Membership Director, acted as a board of

directors parliamentarian and chapter support liaison for MPI, and served on the education committee of SITE. Most recently she has tackled the task of creating San Diego MPI's Chapter of the Year submission, creating a 400 page document on the goals, accomplishments and activities for the fiscal year, which the international headquarters will judge among other entries from its 20,000-member organization.

When she's not busy with Society business, McKay heads for the great outdoors. She enjoys hiking the California mountains and deserts with her husband, Jim, and their dog Whiskey, a Queensland Heeler, and is currently training for a three-day, 60 mile walk to raise funds for breast cancer research. She's also a dedicated swimmer with a preference for outdoor lap pools, rain or shine, swimming an average of 5000 meters a week.

McKay says that organizational skills and the ability to get things done are essential to the success of her role. Her initiative and an entrepreneurial spirit are the elements that can help the ISCB to grow and thrive as a vibrant community of scientists, providing excellent services and benefits to its members. McKay can be reached at *admin@iscb.org*.

ISCB NOMINATIONS SOLICITED

Nominations are now being solicited for the officers and board of directors of ISCB. Please send nominations with a justifying rationale to Toni Kazic toni@athe.cecs.missouri.edu.

POST AND VIEW JOBS ON ISCB's WEBSITE

ISCB is proud to announce a new service for its members. As the fields of bioinformatics and computational biology grow in scope and scale, employers and job seekers in these fields will be able to benefit from ISCB's newly created job posting page.

To post or edit a job posting, members may go to ISCB's membership page, (www.iscb.org/membership.html), login using their membership ID numbers and email addresses, select "post/edit jobs" from the left hand tool bar then fill in the required fields. Postings may be viewed at www.iscb.org/jobs.

CONTact information Questions, comments, and suggestions may be posted to.

ISCB c/o San Diego Supercomputer Center University of California, San Diego 9500 Gilman Drive La Jolla, CA 92093-0505 USA

phone: +1.858.822.0852
email: admin@iscb.org
internet: www.iscb.org

For specific queries, please refer to the following.

Membership: membership@iscb.org

Corporate: corporate@iscb.org

Sponsorship: sponsorship@iscb.org

TRANSITIONS

ISMB02 SPONSORSHIP OPPORTUNITIES

Sponsors receive access to 1700 bioinformaticians representing hundreds of companies, from over 40 countries worldwide.

Sponsorship packages are designed for different levels of exposure: From exhibiting on the trade show floor to major conference sponsorship packages which include corporate exposure throughout the conference and on collateral materials.

Sponsorship opportunities include:

- · Exhibit Booths
- Software Demos
- Job Fair
- Student Travel Fellowships Visit www.ismb02.org/ corporate.html

REQUEST FOR PROPOSALS TO HOST THE ISMB 2004 AND 2005 CONFERENCES

ISCB is now accepting proposals from potential organizing committees to host future ISMB conferences. Submissions must be received by July 19, 2002. For more information, please access the ISCB website conference page (www.iscb.org/conferences.html) or contact Stephanie Hagstrom: shagstro@iscb.org.

The ISCB office has traditionally moved with the President of the Society. Thus, over the past two months we have transitioned the office from Stanford University to the San Diego Supercomputer Center (SDSC), an organized research unit of the University of California San Diego (UCSD). Thanks to Stanley Jacob for his administrative support and to Jon Dugan for his duties as Webmaster while the office was at Stanford.

SDSC and UCSD have made commitment to support the Society while it is here and offer significant resources, both human and machine, on an as-needed basis to support the membership of the Society. Central to this effort is the hiring of BJ Morrison McKay the Society's Administrative Officer (see p.3). McKay is available at admin@isch.org to help with any problems related to ISCB. Web support includes Jennifer Matthews and Joshua Polterock. Web updates sent to admin@iscb.org will be added to the ISCB Web site, www.iscb.org within 24 hours.

With the move of the membership database to SDSC, the website was redesigned to improve functionality and to implement it using the free software MySQL. Future stewards of the site will not need to have a Sybase license to operate the ISCB membership database. The revised schema permits better tracking of membership and enables the production of monthly reports on membership activity. Tracy Zhao serves as our database administrator.

Matthews has also produced the template for this newsletter as well as an ISCB poster to display at meetings and membership flyers to distribute at major conferences. Thanks also go to Kim Baldridge for overseeing these staff efforts and to Chris Smith who interfaces the ISCB to UCSD's HR and finance departments.

As the Society becomes more established, moving the office with each new President becomes impractical. We will explore the use of a management company or an organization like the Federation of American Societies for Experimental Biology (FASEB) and their equivalents in Europe and Asia to help represent the membership and to provide a single voice in support of our science to government and society at large. This will allow the next President to hit the ground running with new programs and activities from which the Society can benefit.

ISCB Extends Gratitude to Stanley Jacob

ISCB wishes to acknowledge and thank Stanley Jacob for his dedication as the Society administrator for the past two years. March 31 2002 marked Jacob's final day. For the past two years, Stanley Jacob has played an integral role in the Society. Jacob's management of the ISCB's membership, newsletter, book keeping, and administrative tasks required of a non-profit, has kept well apace with the Society's rapid growth since 2000. During his tenure as administrator, Jacob has seen the ISCB membership more than double, in that same time, participation at ISCB's primary conference, ISMB has grown from about 580 to over 1300.

Thank you Stanley. You will be missed.

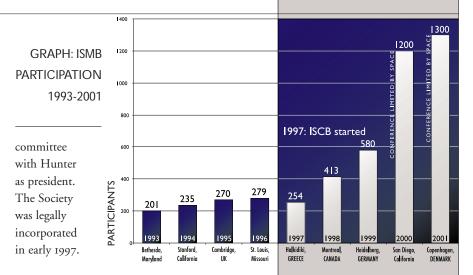
ISCB IN REVIEW

Computational biology—the unique mix of molecular biology and computer science—has come of age in recent years, earning status as a scientific discipline in its own right. The development of the field and the high demand for qualified professionals have given rise to the International Society for Computational Biology (ISCB), an organization dedicated to the advancement of scientific understanding of living systems through computation.

Since its founding in 1997, the Society has grown to over 1300 members and looks to sustain strong membership growth in the near future. Current ISCB president, Philip E. Bourne of the San Diego Supercomputer Center at the University of California San Diego, says, "This is a critical time in bioinformatics and biology. The science is booming and we're here to bring the benefits of a professional society to the world of computational biology."

In 1993, the Society's founder, Larry Hunter, now at the University of Colorado, started the first Intelligent Systems in Molecular Biology (ISMB) conference, held in Washington DC. During that meeting and the ISMBs that followed, members of what would become the Society's board of directors had discussed the formation of a formal group related to the emerging discipline of computers in biological science. Ultimately, the need to house the funds for the ISMB conference spurred the formation of the Society.

At the 1996 ISMB in St. Louis, a union of all of the previous years' conference steering committees, serving as the Society's inaugural board of directors, encouraged the formation of the new society and elected an executive



After four one-year terms, including a four-month break from September 1997 until January 1998, when Chris Rawlings at SmithKline Beecham served as acting president, Hunter resigned. In 2000, the board elected Russ Altman at Stanford as the second president. Altman's track record included salvaging the 1994 ISMB conference when it unexpectedly wound up moving from Seattle to Palo Alto and he campaigned with a two-sentence platform, "We need more members. Without members, it's a waste of time."

During Altman's tenure, the board instituted the initial legal and administrative scaffolding of the Society. He also developed a mechanism for the election of officers rather than the board making the appointments. In transferring responsibility to his successor, Altman remarks that Bourne now has the challenge of figuring out what to do with the rapidly expanding society. "Phil is the perfect next president. He's going to now take the basic building blocks and push them in new directions," he says.

MEMBERSHIP RECORD MAINTENANCE

Members who move, change email addresses, or simply wish to check their record for personal information, may now do so with ease. Visit www.isch.org, select Membership, then select Member Login. From there members may use their membership ID numbers and email address used for initial registration to read and review their records.

Members who change their street and/or email addresses and have journal subscriptions, MUST send notice to thomsonp@oup.co.uk at Oxford University Press for their subscription to Bioinformatics, and pmasi@liebertpub.com at Mary Ann Liebert, Inc. for subscription to the Journal of Computational Biology.



Edmonton, Canada

EDUCATION COMMITTEE

ISCB's education committee, co-chaired by Michael Gribskov and Winston Hide, solicits member input on issues in education and bioinformatics. The committee's immediate plans are to establish a clearinghouse of courses and curricula in bioinformatics and computational biology, with the aim that this information will be useful to institutions starting or considering training programs in bioinformatics. The committee also hopes to develop a repository of sharable materials for conventional and virtual courses. The committee welcomes the participation and input of members who share an interest in education. For more information, contact Michael Gribskov, gribskov@sdsc.edu.

THE 2003 ISMB CONFERENCE GOES TO AUSTRALIA

The University of
Queensland, Brisbane has
been selected to host
ISMB03 to be held
June 29-July 3, 2003.
Conference Chairs Mark
Ragan of the University of
Queensland and Gene
Meyers of Celera encourage
members to mark their calendars now and watch for
announcements on the ISCB
Website.

This year the 10th Intelligent Systems for Molecular Biology (ISMB 2002) conference will be held in Edmonton, Alberta, Canada from August 3-7. The ISMB conference is the world's largest bioinformatics symposium and has become the flagship conference of the International Society for Computational Biology (ISCB). This year it is expected that more than 1700 scientists from nearly 50 countries will attend. An additional 700-800 registrants will be attending ISMB SIG meetings on Aug. 1, 2, and 8. The ISMB 2002 host city, Edmonton, is noted for its affordability, safety, numerous summer festivals, and wide-ranging recreational opportunities. August daytime temperatures average 25°C (80°F) with approximately 18 hours of sunlight. The conference will be held in the Shaw Conference Centre, a tiered glass, state-of-the-art conference facility that overlooks the beautiful North

Saskatchewan River valley. An outstanding selection of eight invited speakers along with 42 podium presentations from an equally impressive group of scientists promises to make this year's ISMB conference one of the best ever. Modern, spacious facilities for internet access, dining, vendor exhibits, poster displays, tutorials and software demos should make the entire conference experience both educational and enjoyable. More information about the conference, registration, accommodations and travel can be found at www.ismb02.org This year we would like to invite everyone to come to Edmonton—to see the sights and become part of ISMB 2002.

**Register early (www.ismb02.org) as previous ISMB conferences have sold out within weeks of the registration cut-off date. Online registration will be available mid-April 2002.

EVENTS AND OPPORTUNITIES OF INTEREST

Center for Discrete Mathematics and Theoretical Computer Science (DIMACS) Special Focus on Computational Molecular Biology

DATE: September 2000-August 2003 UPCOMING EVENTS:

- Workshop on Complexity in Biosystems: Innovative Approaches at the Interface of Experimental and Computational Modeling: *April* 8-10, 2002; DIMACS Center, Rutgers University, Piscataway, New Jersey; URL: dimacs.rutgers.edu/ Workshops/Complexity
- DIACS-National Chiao Tung University
 Conference on the Interconnections Among
 Codes, Designs, Graphs and Molecular Biology:
 May 24-26, 2002; National Center of Theoretical
 Science, National Chiao Tung University,
 Hsinchu, Taiwan; URL: dimacs.rutgers.edu/
 Workshops/Chiaotung
- Protein Domains: Identification, Classification and Evolution Dates: February 27-28, 2003, DIMACS Center, Rutgers University, Piscataway, New Jersey; URL: dimacs.rutgers.edu/Workshops/ index-compmolecbiol.html

CALL FOR SUBMISSIONS: **Methods in Functional Genomics (A Special Issue of** *Machine Learning Journal*)

DEADLINE: May 15, 2002 URL: www.genomethods.org/mlj CONTACT: Paola Sebastiani (sebas@math.umass.edu)

ABOUT: *Machine Learning Journal* invites submissions to a Special Issue devoted to machine learning advances in functional genomics. The special issue seeks contributions of significant methodological content and high potential impact on the functional genomics research community.

Second Annual RECOMB Satellite meeting on DNA Sequencing and Characterization

DATE: May 18-19, 2002 LOCATION: Stanford University, Palo Alto, California

URL: robotics.stanford.edu/~serafim/ra2002/ra2002.htm

ABOUT: Genome sequencing has flourished the past several years, with genomes such as the *C.elegans, D.melanogaster*, the human, mouse, and rat either complete, or currently being sequenced and

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assembled. Computational assembly has been an essential part of sequencing since the conception of the sequencing technology. Recent sequencing achievements have become possible due to advances in lab techniques, computational power, and algorithms and software. This meeting will bring together many people working on algorithms and systems for genome-scale sequencing and analysis.

SHORT COURSE: **Bioinformatics: Methods and Techniques**

DATE: June 18-20, 2002 LOCATION: Stanford University, Palo Alto, California

URL: proed.stanford.edu/bioinformatics

ABOUT: An introduction to fundamental problems in genomics and bioinformatics. Topics include DNA and protein sequence and structure analysis, structure prediction and the impact of new technologies such as mRNA expression arrays and proteomics techniques. CONTACT: Jody Gladstein, 650-723-9041 (scpd_proed@forsythe.stanford.edu)

Bioinformatics

DATE: June 19-21, 2002 LOCATION: Boston, Massachusettes URL: www.LifeScienceSolutions.com

ABOUT: Conference synopsis: This information-intensive conference will bring together the industry's most forward-thinking computational biologists to examine diverse bioinformatics strategies and applications. Key components of this event include open-source industry collaboration and integration, computational proteomics, post-genomic bioinformatics and drug discovery. Focused pre-conference tutorials will offer hands-on experience with leading bioinformatics tools.

CONTACT: Ann Pendleton, 312.894.6418 (conferences@marcusevansch.com)

NETTAB 2002 Second International Workshop on Agents in Bioinformatics

DATE: July 12-14, 2002

LOCATION: Bologna, Italy (Ex scuola Ercolani, Mura Anteo Zamboni, 2b)

URLs: www.nettab.org,

www.nettab.org/2002/progr.html

ABOUT: This workshop aims to bring together researchers working toward the vision of a genome analysis and annotation using agents-based systems. NETTAB2002 aims to strength-

en the relationships within the bioinformatics community, to activate cooperation between bioinformatics and computer science communities, to collect the latest ideas, achievements and proposals in the application of agents and multiagent systems to the bioinformatics area.

CALL FOR PAPERS, DEADLINE: April 30, 2002 CALL FOR PAPERS, TOPICS:

- Co-operation between intelligent agents to improve information retrieval in bioinformatics
- Multi-agent systems to support eScientists during their daily research
- · Agents applications in bioinformatics
- Multi-agent systems that improve the data resources integration
- Bioinfomatics agent-based decision support systems
- Information agents that gather, compile and organize biological knowledge available on Internet
- · Biological data and knowledge modeling tools
- Ontologies, Databases and Applications of Semantics in Bioinformatics
 APPLICATION URL:

www.nettab.org/2002/progr.html

The Third International Conference on Bioinformatics of Genome Regulation and Structure (BGRS2002)

DATE: July 14-20, 2002 LOCATION: Novosibirsk, Russia URLs: www.bionet.nsc.ru/meeting/ bgrs2002/index_local.html

ABOUT: BGRS2002 will provide a forum for the accumulation, analysis, and recognition of genomic regulatory sequences. Experimental biologists are also encouraged to attend—BGRS2002 aims to be a stimulating event to facilitate an application of computational biology to experimental research.

WABI 2002: 2nd Workshop on Algorithms in BioInformatics

DATE: September: 16-21, 2002 LOCATION: Faculty of Engineering, University of Rome "La Sapienza" (Italy) URL: www.dis.uniroma1.it/%7Ealgo02/wabi02

ABOUT: WABI2002 will cover research in algorithmic work in bioinformatics and computational biology. The emphasis is on discrete algorithms that address important problems in molecular biology, genomics and genetics that are founded on sound models, computationally efficient, and have been implemented and tested

in simulations and on real datasets.
CALL FOR PAPERS, DEADLINE: April 26, 2002
CALL FOR PAPERS, TOPICS:

- Exact and approximate algorithms for genomics, genetics, sequence analysis, gene and signal recognition, alignment, molecular evolution, phylogenetics, structure determination or prediction, gene expression and gene networks, proteomics, functional genomics, and drug design.
- Development of methods, software and dataset repositories to develop and test such algorithms and their underlying models.
- High-performance computing approaches to computationally hard problems in bioinformatics, particularly optimization problems.
 APPLICATION URL: www.dis.uniromal.it/ %7Ealgo02/wabi02/wabi02-cfp.txt

Invitation to the 3rd International Conference on Systems Biology — The Logic of Life

DATE: December 13-15, 2002 LOCATION: Karolinska Institutet, Stockholm, SWEDEN

URL: www.icsb2002.org

ABOUT: ICSB 2002 will feature experimental, computational and theoretical advances in the rapidly advancing fields of gene expression acquisition technologies, gene expression data analysis, functional analysis of biological control systems, proteinomics, modeling and analysis of kinetic networks, metabolomics, signal transduction, morphogenesis, and much more.

EVENT REPORTS

First O'Reilly Bioinformatics Technology Conference Built Bioinformatics Bridges

SUMMARY: O'Reilly and Associates' first Bioinformatics Technology Conference took place January 28-31, 2002. Over 700 scientists, researchers, programmers and bioinformaticians came together to examine the state of computational biology and learn from each other's study and practice. O'Reilly and Associates will post news on future conferences as they become available on their website: conferences.oreilly.com/biocon

To recommend a conference for inclusion in the ISCB Newsletter, please write to admin@iscb.org

New ISCB Website!

The ISCB has launched a redesigned and upgraded version of its website, which can be found at www.iscb.org. The site, housed at the San Diego Supercomputer Center in La Jolla, California, provides a wealth of information for researchers interested in computational biology as well as an online gathering place for Society members. Features include a jobs board, conference calendar, the Society's newsletter, a "members only" section, and a secure online registration system offered through Verisign. The entire site also received an updated look and feel that should make it easier for members and other people interested in the Society to navigate the site.

How are We Doing?

Please email ISCB staff at *admin@sdsc.edu* with any comments, questions, or concerns regarding the website *(www.iscb.org)*, this newsletter, or any other ISCB effort. The ISCB staff aims to meet the needs of ISCB's membership—member advice goes a long way toward helping the staff meet their objectives.

Resource. Staffing for ISCB promotions and publications has been provided by the National Biomedical Computation Resource.



www.iscb.org

About the Cover Image

The role of dynamics in the biological function of proteins and enzymes has been a topic of intense debate for decades. The use of vibrational spectroscopy, the most direct method to study dynamics, has been limited by the congestion of the protein vibrational spectrum. Floyd Romesberg, assistant professor of chemistry at the Scripps Research Institute, and his colleagues use cytochrome c as a model system to demonstrate that individual protein vibrations may be directly observed by the incorporation of an isotopically labeled amino acid, and that those labeled vibrations are sensitive probes of the protein environment. This volume-rendered image shows a model that was investigated with computational quantum chemical methods, for the Fe (II)- and Fe (III)- cytochrome c prosthetic group, revealing the structure and specific vibrational properties of the FeP (DMS) complex, which were then compared to experimentally generated data.