

# The QSAR and Modelling Society

*Chair:* Yvonne Martin

*Officers:* Hugo Kubinyi (advisor to the chair), Lowell Hall (treasurer)  
Han van de Waterbeemd (secretary/editor)

*Board:* Antonia do Amaral, Marvin Charton, Gabriele Cruciani, Rainer Franke, Toshio Fujita, Klaus Gundertofte, Osman Guner, Lemont B. Kier, David Livingstone, James McFarland, Tudor Oprea, Oleg A. Raevsky, Joachim K. Seydel, Bernard Testa, Herschel Weintraub

*Honorary chair:* Corwin Hansch *Past chairs:* Phil Magee, Hugo Kubunyi

## NEWSLETTER

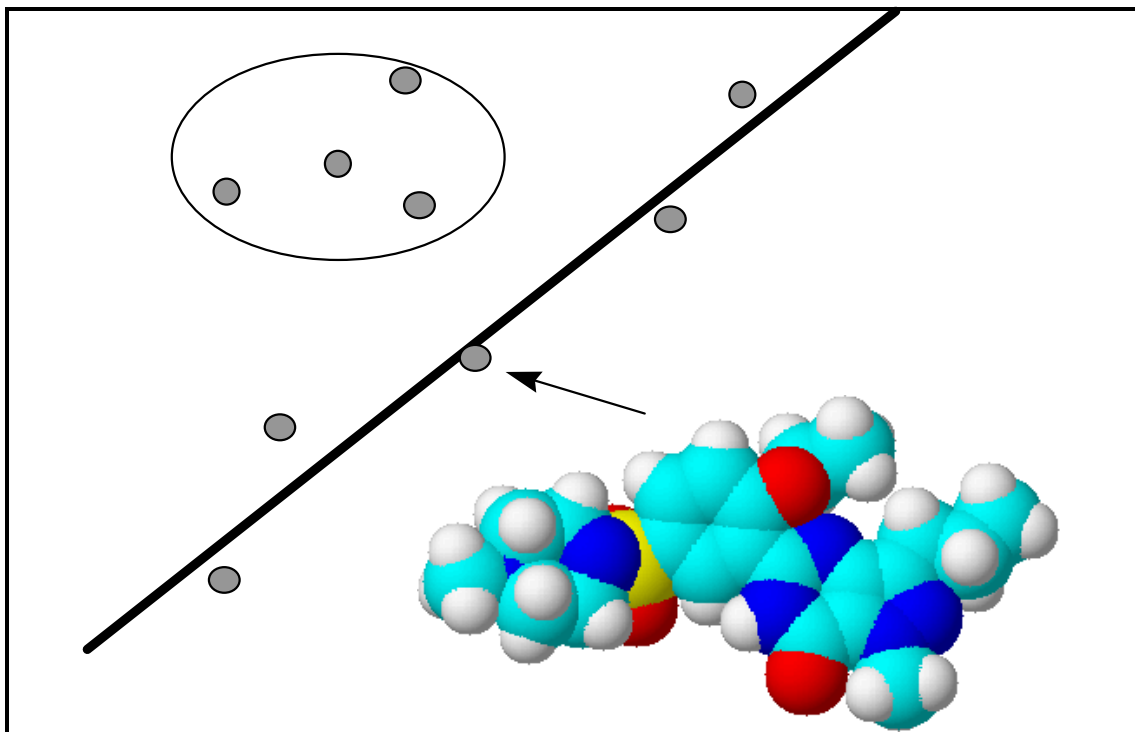
[http://www.ndsu.nodak.edu/qsar\\_soc/](http://www.ndsu.nodak.edu/qsar_soc/)

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Issue No. 11

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## **Editorial**

I wish to extend my thanks to the vote of confidence of the membership who selected me as the next chair. I will do my best to live up to your expectations. Although it will certainly be difficult to follow Hugo and Phil, with the help of the membership, we will continue the work of the society.

One of the Society's biggest successes is the support of young people to attend meetings. This is necessary for the continuation of the discipline. The awarding of the Corwin Hansch award is another way that we promote the discipline and recognize the work of emerging researchers. Both of these activities will continue.

Our biggest concern is that the membership is so quiet. We wonder why the e-mail system is not flooded with messages. Certainly you have questions or concerns that you would like to share with your colleagues. The other e-mail lists for which I am registered generate several messages a day: contrast that with the QSAR list, which generates that many only in a year!

We have discovered that many "members" have not paid their dues. In order to make this easier, we are looking into the feasibility of accepting credit cards. We also suggest that you consider paying dues for multiple years so that you don't have to be bothered so often. Although the dues are modest, they support our work bringing young people to meetings and recognizing researchers with the Corwin Hansch Award.

*Yvonne Martin*

## **Thanks of the past Chair**

First, and most important:

### **Congratulations to Yvonne C. Martin,**

elected by our members as the new Chair of The QSAR and Modelling Society, for the years 2001-2005. As a tradition, the past chair steps down after the conference, where the results of the election are announced. Thus, I would like to thank all of you who supported my activities in the past five years. I am sure that Yvonne Martin, who already was the Advisor to the Chair, and Han van de Waterbeemd, who continues to serve as the Secretary and Newsletter Editor, will lead the Society in the same spirit as Phil Magee, our first Chair, and I did. In addition, Yvonne Martin decided to pick me as her Advisor to the Chair. Thus, there should be no major changes in the direction into which the Society develops! Many thanks go to James King, who served as our treasurer for the past 11 years. Lowell Hall will follow up.

Looking back to the 1995-2000 period, I see a significant increase in the activities and the importance of our Society. The number of members is now more than twofold, as compared to summer 1995, and the Society still grows continuously. We have local

groups in Italy, Hungary, Rumania, Russia, and the UK. We support students to attend QSAR conferences and we created the Corwin Hansch Award for young scientists, in 2000. Since 1995, we have a well-structured Website and since a few years an E-mail list. What still should be improved, is the active participation of our members in the life of our Society, in two respects: first of all, by paying the annual membership dues, to allow us to provide support to people who desperately need it, and second, to contribute information and messages to our Newsletter, the Website and the E-mail list. It's not just our Society, it is your Society!

It is my duty and my pleasure, to thank all candidates for the Chair and the Board for their active engagement, as well as the former Board Members who decided not to continue.

**Best wishes**

*Hugo Kubinyi*

## **Report of the (past) Chair**

In the past five years, the number of our **members** increased from

August 1995	346 members
August 1996	463 members
July 1997	549 members
July 1998	599 members
July 1999	660 members to
August 2000	725 members.

In the following countries we have more than three members:

Austria	7	
Belgium	10	
Brasil	6	
Bulgaria	7	
Canada	12	
Czech Republic	5	
Denmark	4	
France	20	
Germany	35	
Hungary	22	
Italy	41	
Japan	33	
Romania	21	
Russia	70	(about 10 %)
Slovenia	4	
Spain	11	
Sweden	18	

Switzerland	20	
The Netherlands	10	
Turkey	6	
Ukraine	4	
United Kingdom	37	
USA	277	(about 40 %)

(45 members in 23 other countries)

According to the result of our election, the **Board Members 2001-2005** are (in alphabetical order)

Antonia T. do Amaral  
 Marvin Charton  
 Gabriele Cruciani  
 Rainer Franke  
 Toshio Fujita  
 Klaus Gundertofte  
 Osman Guner  
 Lemont B. Kier  
 David Livingstone  
 Jim McFarland  
 Tudor Oprea  
 Oleg Raevsky  
 Joachim Seydel  
 Bernard Testa  
 Hershel Weintraub

Lowell Hall, Hugo Kubinyi and Han van de Waterbeemd, who were elected as Board members but were selected by Yvonne Martin to join the Board of Officers, are not listed. Instead of these persons, three additional candidates joined the Board.

According to our (past) Treasurer, James King, the **budget of our Society** is:

June 30, 1999	US-\$	8,932.31
September 01, 1999	US-\$	9,382.31
<u>Income</u> from dues	US-\$	730.--
<u>Expenses:</u>		
Support of Bourgas QSAR Conference	US-\$	600.--
Support of Duesseldorf QSAR Conference	US-\$	750.--
Corwin Hansch Award	US-\$	1,000.--
Bank charges, etc.	US-\$	42.52
<u>Balance</u> (08.08.2000)	US-\$	7,719.89

The next **QSAR Gordon Research Conference** will take place in Tilton, NH, U.S.A., August 5-10, 2001,

Chair: Kate Holloway, kate\_holloway@merck.com  
Programme Chair: John van Drie, john.h.vandrie@am.pnu.com

The **14th European QSAR Conference** will be organised by Martyn Ford, University of Portsmouth, in the very south of England, in late summer 2002.

According to a decision of the Chairs of the former European QSAR conferences, in a meeting in Duesseldorf, the 15th European QSAR Conference, in 2004, will be organised by Prof. Esin Sener and her colleagues, in Turkey.

*Hugo Kubinyi,*  
Chair 1995-2000

## **The Corwin Hansch AWARD**

In 1999 the society decided to present the Corwin Hansch award to an outstanding young scientist. The award consists of a citation and \$1000. The committee chose Hua Gao to be the first recipient of this award. The following summarizes the nomination:

Hua Gao is a truly outstanding scientist. His potential was clearly recognized early on when he was awarded a scholarship from the Boehringer Ingelheim Foundation in Germany so that he could come to the US. for graduate work. Here, he obtained his Ph.D. in Medicinal Chemistry at the University of Southern California working with Professor E.J. Lien.

From 1995-1998 he was a post-doc in Hansch's group. During that time he wrote, or was co-author on nine papers, three of which were published in Chemical Reviews. These papers were a sideline from his major job of helping build a large computerized database of QSAR. He added 1,442 biological QSAR to the system. In the vast majority of these reports, the authors had made no attempt to formulate any kind of QSAR. During this period he also uncovered 2,745 QSAR on the subject of physical organic chemistry and entered these into our system too, sometimes improving what the authors had done.

Dr. Gao's review on radical reactions was the first serious attempt by anyone to cover physical chemical and biochemical examples of radical reactions. This review and his review of the QSAR of estrogens provided the foundation needed to develop a truly remarkable QSAR model for the estrogenic and

carcinogenic activity of phenols. This covers simple phenols as well as Bisphenol A, diethylstilbestrol and the female hormones estradiol, estriol, equilin and equilenin. In preparation is a co-authored review on biological QSARs that lack hydrophobic terms and contain an electronic term that can be related to an electronic term in a QSAR from physical organic chemistry.

Dr. Gao left Pomona to work for MDS Panlabs, then joined Pharmacia and Upjohn in 1999. At these two companies he has done novel work in binary QSAR, BCUT descriptors, library design, and 3D database searching. A list of his publications follows:

H. Gao. Application of BUCT descriptors in binary QSAR analysis of carbonic anhydrase inhibitors and estrogen receptor ligands. *J. Chem. Inf. Comput. Sci.* (submitted).

J.H. van Drie, D.C. Rohrer, J.R. Blinn, and H. Gao. 3D database searching and related methods for the structure-based design of combinatorial libraries. Book chapter In: *Modern Methods of Drug Discovery*, Hilgenfeld and Jillich (eds.), (submitted).

R. Garg, S.P. Gupta, H. Gao, M.S. Babu, A.K. Debnath, and C. Hansch. Comparative quantitative structure-activity relationship studies on anti-HIV drugs. *Chem. Rev.* 1999, 99:3525.

L. Xue, J. Godden, H. Gao, J. Bajorath. Identification of a preferred set of molecular descriptors for compound classification based on principal component analysis. *J. Chem. Inf. Comput. Sci.* 1999, 39:699.

H. Gao, and J. Bajorath. Comparison of binary and 2D-QSAR analyses using inhibitors of human carbonic anhydrase II as a test case. *Mol. Divers.* 1999, 4:115.

H. Gao, R. Garg, and C. Hansch. Comparative QSAR analysis of estrogen receptor ligands. *Chem. Rev.* 1999, 99:723.

H. Gao, C. Williams, P. Labute, and J. Bajorath. Binary QSAR analysis of estrogen receptor ligands. *J. Chem. Info. Comput. Sci.* 1999, 39:164.

L. Zhang, H. Gao, C. Hansch, and C.D. Selassie. Molecular orbital parameters and comparative QSAR in the analysis of phenol toxicity to leukemia cells. *J. Chem. Soc. Perkin trans 2.* 1998, 2553.

H. Gao, W.A. Denny, R. Garg, and C. Hansch. Quantitative structure-activity relationships (QSAR) for 9-anilinoacridines: a comparative analysis. *Chem.-Biol. Interact.* 1998, 116:157.

C.D. Selassie, T.V. De Soyza, M. Rosario, H. Gao, and C. Hansch. Phenol toxicity in leukemia cells: a radical process? *Chem.-Biol. Interact.* 1998, 113: 175.

C. Hansch and H. Gao. A generalized approach to comparative QSAR. In: *Comparative QSAR*. J. Devillers (ed.) Taylor & Francis, Washington, D.C. 1998, pp. 285-368.

C. Hansch and H. Gao. Comparative QSAR: Radical reactions of benzene derivatives in chemistry and biology. *Chem. Rev.* 1997, 97:2995.

- H. Gao and C. Hansch. QSAR of P450 oxidation: On the value of comparing  $k_{cat}$  and  $K_m$  with  $k_{cat}/K_m$ . *Drug. Metab. Rev.* 1996, 28:513.
- C. Hansch, D. Hoekman, and H. Gao. Comparative QSAR: Toward a deeper understanding of chemico-biological interactions. *Chem. Rev.* 1996, 96:1045.
- H. Gao, F.Z. Wang, and E.J. Lien. Hydrophobic contribution constants of amino acids to hydrophobicities of oligopeptides. *Pharm. Res.* 1995, 12:1279.
- E.J. Lien and H. Gao. QSAR Analysis of Skin Permeability of various Drugs in Man as compared in vivo and in vitro Studies in Hairless Mouse. *Pharm. Res.* 1995, 12:583.
- E.J. Lien and H. Gao. Structure-System-Activity relationship analysis of drug disposition. In: *QSAR and Molecular Modeling: Concepts, Computational Tools and Biological Applications*. Giraldo, S.J. and Manaut, F. (eds.) Prous Sciences Publishers. 1995, pp. 94-100.
- E.J. Lien, H. Gao, and F.Z. Wang. Dipolarity and partition coefficient of solvents, drugs and chemicals. *Q.S.A.R.* 1994, 12:158.
- H. Gao, E.J. Lien and F.Z. Wang. Hydrophobicity of oligopeptides having un-ionizable side chains. *J. Drug Targeting* 1993, 1:59.
- E.J. Lien and H. Gao. Physical factors contributing to the partition coefficient and retention time of 2',3'-dideoxynucleoside analogues. *J. Pharm. Sci.* 1991, 80:517.
- P. Nandy, S. Banerjee, H. Gao, M.B. Hui, and E.J. Lien. Quantitative structure-activity relationship analysis of combretastatins: A class of novel antimitotic agents. *Pharm. Res.* 1991, 8:776.
- P.H. Wang, M.B. Hui, P. Nandy, S. Banerjee, H. Gao, and E.J. Lien. QSAR analysis of the cytotoxicities of aminohydroxyguanidine derivatives and their antiviral activities. *Pharm. Res.* 1991, 8:1006.
- H. Gao, F.Z. Wang, E.J. Lien, and M.D. Trousdale. Immunostimulating polysaccharides from *Viola yedoensis*. *Int. J. Orient. Med.* 1996, 21:1.
- E.J. Lien and H. Gao. New applications of spectroscopic methods in biomedical and pharmaceutical analysis: A survey. *J. Food Drug Anal.* 1995, 3:431.
- E.J. Lien, H. Gao and L.L. Lien. In search of ideal antihypertensive drugs: Progress in five decades. *Prog. Drug Res.* 1994, 43:43.
- A.Y. Shen, M.I. Tsai, H. Gao and E.J. Lien. Antifungal activities of naphthol derivatives. *Acta Pharm.* 1994, 44(2):109.
- H. Gao and E.J. Lien. Analysis of natural products against HIV. *Int. J. Oriental Med.* 1991, 17:1
- H. Gao and E.J. Lien. Natural products and cancer prevention. *Int. J. Oriental. Med.* 1991, 16:55.
- E.J. Lien, H. Gao, and F.Z. Wang. Stepping-Down (SDA) and Stepping-Up (SUA) approach in new drug design. *Med. Chem. Res.* 1991, 1:173.
- H. Gao and E.J. Lien. Chemistry and pharmacology of *Salvia miltiorrhizae*

radix. Int. J. Oriental Med. 1991, 1:173.

E.J. Lien and H. Gao. Higher plant polysaccharides and their pharmacological activities. Int. J. Oriental Med. 1990, 15:123.

H. Gao and E.J. Lien. Chemistry and pharmacology of Bupleurum species. Int. J. Oriental Med. 1990, 15:206.

H. Gao, and E.J. Lien. Biochemistry and SAR analysis of Scutellaria baicalensis. Int. J. Oriental Med. 1990, 15:70.

H. Gao, T.M. Zhang. Prevention of atherosclerosis with heparin extracted from bovine and sheep lung tissues. J. Pharm. Bulletin. 1987, (4):34.

H. Gao, T.M. Zhang. Physicochemical properties and biological activities of heparin extracted from different tissues. Acta Academiae Med. Shandong. 1987, (2):41.

H. Gao and T.M. Zhang. Advances in search of new types of heparin. J. Biochem. Pharm. 1987, (1):64.



**From the Secretary**



Total number of members (1-October-2000): **737**.

### **Distribution of the Newsletter**

Starting with this issue, an alert will be sent to all members via our Mailbox that the Newsletter is available in pdf format at our website. No printed copies will be sent to save costs.

### **Update of e-mail addresses**

Please support our work, especially for the distribution of messages, by regularly updating e-mail addresses. If you detect a wrong address in the members list in our Web page, please inform [han\\_waterbeemd@sandwich.pfizer.com](mailto:han_waterbeemd@sandwich.pfizer.com)

### **Lost members**

We have no address of the following members. Does anyone know where these people are now?

<b>Dietrich</b>	Stephen
<b>Gange</b>	David
<b>Jonsson</b>	Jörgen
<b>Namboodiri</b>	Krishnan
<b>Robson</b>	Barry
<b>Sapegin</b>	Alexey M.
<b>Sauchet</b>	Michael
<b>Shimomura</b>	Satoshi
<b>Space</b>	Brian
<b>Spears</b>	Colin P. / Lucy Ann
<b>Wohl</b>	Ronald

### Lost email addresses

Although we all work with computers, still some email addresses are missing. Can you help finding them?

<b>Allen</b>	Mark	Novartis Pharma UK	UNITED KINGDOM
<b>Araki</b>	Koichi	Mitsubishi Petrochem. Co.	JAPAN
<b>Ashman</b>	William P.	U.S. Army Chem. Res.Dev.	USA
<b>Ashton</b>	Michael	Rhône Poulenc Rorer Ltd	UNITED KINGDOM
<b>Barlett</b>	Bob	834 Estates St.	USA
<b>Basak</b>	Subjash C.	Natural Resources Research Institute	USA
<b>Bauman</b>	Norman	Innapharma	USA
<b>Bellott</b>	Emile M.	Pharm-Eco Laboratories	USA
<b>Berner</b>	Heinz	Novartis	AUSTRIA
<b>Biagi</b>	Gian Luigi	Istituto di Farmacologia	ITALY
<b>Blaschke</b>	Heinz	CI Pharma AG	AUSTRIA
<b>Blum</b>	Diane J. W.	112 Clwyd Road	USA
<b>Bolton</b>	Evan	American Cyanamid Company	USA
<b>Boulu</b>	Laurent	Sanofi Recherche	FRANCE
<b>Boxall</b>	Alistair	WRC	UNITED KINGDOM
<b>Bradley</b>	Prudence K.		USA
<b>Brannigan</b>	Lawrence H.	9411 Cimarron Court	USA
<b>Burgot</b>	Jean Louis	Laboratoire Chimie Analytique	FRANCE
<b>Burgot</b>	Gwenola	Maitre de Conférences	FRANCE
<b>Can</b>	Hatice	Mersin Universitesi	TURKEY
<b>Cativiela Marin</b>	Carlos	Dpto. Quimica Organica	SPAIN
<b>Cato</b>	Stephen, J.	Chemical Design Inc.	USA
<b>Caumel</b>	Yves	SANOFI Recherche	FRANCE
<b>Chau</b>	Pak-Lee	University of Cambridge	UNITED KINGDOM
<b>Cherkasov</b>	Artem	University of Saskatchewan	CANADA
<b>Cholinski</b>	Jacek	Instytut Farmaceutyczny	POLAND
<b>Cipriano</b>	Robyn	SciVision	USA
<b>Coats</b>	Joel	Iowa State University	USA
<b>Coe</b>	Chris	BioTeknik Rational Drug	UNITED KINGDOM

<b>Colombo</b>	Lino	Design	ITALY
<b>Cossement</b>	E. R.	University of Pavia	BELGIUM
<b>Csorvasi</b>	Istvan	UCB Pharm. Sector	HUNGARY
<b>Darvas</b>	Ferenc	Alkaloida Rt.	HUNGARY
<b>De Paulis</b>	Tomas	ComGenex Inc.	USA
<b>Dietrich</b>	Stephen	Vanderbilt University	USA
<b>Donescu</b>	Alexandrina	Universitatea Bucuresti	ROMANIA
<b>Dragos</b>	Dan	University of Medicine and Pharmacy	ROMANIA
<b>Dross</b>	Karl	Inst. Brain Research	GERMANY
<b>Elenes</b>	Florin	Institutul de Chimie al Academeie	ROMANIA
<b>Eng</b>	George	University District of Columbia	USA
<b>Engle</b>	Thomas	Rhône-Poulenc AG Products	USA
<b>Escobar</b>	Jose-Luis	College of Pharmacy 4.214	USA
<b>Evans</b>	Suzanne	Anaquest, Inc	USA
<b>Fadhil</b>	G. F.	Chemistry Department	IRAQ
<b>Farahi</b>	Asgar Kh.	Drug Design Center	IRAN
<b>Fisanick</b>	William	Chemical Abstracts Service	USA
<b>Fukami</b>	Harukazu	Suntory Limited Research Center	JAPAN
<b>Gange</b>	David		USA
<b>Gao</b>	Ying-Duo	Pharm-Eco Lab, Inc.	USA
<b>Geiss</b>	Kevin T.	GeoCenters Inc.	USA
<b>Golender</b>	Valery	DCL Systems International Ltd.	ISRAEL
<b>Goncharenko</b>	Ludmila V.	NRC BAC	RUSSIA
<b>Gorbunov</b>	Sergey	Arbuzov Institut of Organic and	RUSSIA
<b>Govers</b>	H.	Dept of Environmental & Toxicological Chem.	THE NETHERLANDS
<b>Hadzi</b>	Dusan	Boris Kidric Institute	SLOVENIA
<b>Helmes</b>	C. Tucker	ETAD	USA
<b>Hillenbrand</b>	Mihaela	Universitatea Bucuresti	ROMANIA
<b>Hoeschele</b>	James D.	6865 Montfort Dr.	USA
<b>Holzgrabe</b>	Ulrike	Universität Bonn (Poppelsdorf)	GERMANY
<b>Howe</b>	W. Jeffrey	Pharmacia & Upjohn	USA
<b>Izumi</b>	Keiichi	Sumitomo Chemical Co. Ltd.	JAPAN
<b>Jerman-Blazic</b>	Borka	Institut Josef Stefan	SLOVENIA
<b>Jonsson</b>	Jörgen		SWEDEN
<b>Kamoshita</b>	Katsuzo	Sumitomo Chemical Co. Ltd.	JAPAN
<b>Khambay</b>	B. P. S.	Crop & Environ. Protection Div.	UNITED KINGDOM
<b>Kido</b>	Masaru	Otsuka Pharmaceutical Ind.	JAPAN
<b>Kint</b>	Saima	USDA	USA
<b>Knjasev</b>	Boris Ananjevich	Lenin Street 30, 63	RUSSIA
<b>Kuchar</b>	Miroslav	Research Institute Pharmacy & Biochemistry	CZECH REPUBLIC
<b>Kuchcaev</b>	Boris Irikovich	Molodesznaya Street 9, 27	RUSSIA

<b>Kumita</b>	Izumi	Nippon Soda Co.	JAPAN
<b>Kurbatova</b>	Svetlana	Samara State University	RUSSIA
<b>Kuyper</b>	Lee	Burroughs Wellcome Co.	USA
<b>Ladner</b>	David W.	American Cyanamid Co.	USA
<b>Lämmerhofer</b>	Michael	University of Vienna	AUSTRIA
<b>Lau</b>	Wan	Bristol-Meyers Squibb	USA
<b>Lee</b>	On	School of Pharmacy	TAIWAN
<b>Lehmann</b>	Pedro A.	Depto. Farmacologia y Toxicologia	MEXICO
<b>Leonardi</b>	A.	Recordati S.p.A	ITALY
<b>Luca</b>	Costantino	Dip. di Scienze Farmaceutiche	ITALY
<b>Mager</b>	Harry	Bayer AG, Bldg. 470	GERMANY
<b>Makino</b>	Kenzi	Central Research Institute	JAPAN
<b>Matova</b>	Mariana	Faculty of Medicine	BULGARIA
<b>Mattie</b>	Renee	AstraZeneca Pharmaceuticals	USA
<b>Miller</b>	Joseph	Universidade Federal da Paralba	BRAZIL
<b>Moser</b>	Peter	Gempengasse 71	SWITZERLAND
<b>Moyer-Zirpoli</b>	Susan	Slippery Rock University	USA
<b>Mracec</b>	Mioara	Institutl de Chimie al Academiei	ROMANIA
<b>Murcko</b>	Mark	Vertex Pharmaceuticals	USA
<b>Namboodiri</b>	Krishnan		USA
<b>Natcheva</b>	Roumiana	Faculty of Pharmacy	BULGARIA
<b>Naylor</b>	Adel	Merck Sharp & Dohme Research Laboratories	USA
<b>Negrié</b>	Cristina	Lacer SA, R&D Dept.	SPAIN
<b>Nurgabylova</b>	Aigul	Moscow Medical Academy I.M. Secherov	KAZAHKSTAN
<b>O'Connor</b>	Mary V.	Exxon Biomedical Sciences, Inc.	USA
<b>Oda</b>	Kengo	Mitsui Toatsu Chemicals, Inc.	JAPAN
<b>Ohtaka</b>	Hiroshi	Kanebo Ltd	JAPAN
<b>Omata</b>	Kenzo	Mitsubishi Kasei Corporation	JAPAN
<b>Ordukhanian</b>	A. Ashot	GRICC	RUSSIA
<b>Pallakoff</b>	Pamela A.	SRI International	USA
<b>Parodi</b>	Silvio	Inst.Nat. Ricerca Sul Cancro	ITALY
<b>Parton</b>	Richard	Eastman Kodak	USA
<b>Passino-Reader</b>	Dora R.	U.S. Fish and Wildlife Service	USA
<b>Phillips</b>	Richard B.	975 California Ave.	USA
<b>Pillan</b>	Antonio	Pharmacia R&D	ITALY
<b>Potashnikov</b>	Piotr	Altufievskoye shosse 40, Apt.219	RUSSIA
<b>Pouplana Sole</b>	Ramon	Universitat de Barcelona	SPAIN
<b>Profeta, Jr.</b>	Salvatore	Monsanto	USA
<b>Ramsden</b>	C. A.	Department of Chemistry	UNITED KINGDOM
<b>Rejholec</b>	Valcav	Research Institute	CZECH REPUBLIC
<b>Ren</b>	Shijng	University of Southern California	USA

<b>Robson</b>	Barry		UNITED KINGDOM
<b>Roy</b>	Timothy	Mobil Oil Corp	USA
<b>Rozenblit</b>	Anatoly	Latvian Institute Organic Synthesis	LATVIA
<b>Sahini</b>	Victor Emanuel	Universitatea Bucuresti	ROMANIA
<b>Salama</b>	Zoser	L.A.B. GmbH & Co	GERMANY
<b>Sapegin</b>	Alexey M.		RUSSIA
<b>Sauchet</b>	Michael		
<b>Seclaman</b>	Eduard	Institutul de Chimie al Academeie	ROMANIA
<b>Shimomura</b>	Satoshi		JAPAN
<b>Shorter</b>	John	29 Esk Terrace	UNITED KINGDOM
<b>Siegel</b>	Sidney	Office Hazardous Substances Information	USA
<b>Singh</b>	Bupinder	Institute Pharmaceutical Sciences	INDIA
<b>Singh</b>	Suresh B.	Wyeth-Ayerst Research	USA
<b>Smith</b>	Eric W.	School of Pharmacy	SOUTH AFRICA
<b>Southwick</b>	Rett	Philip Morris USA	USA
<b>Spears</b>	Colin P. / Lucy Ann		
<b>Speece</b>	R. E.	Civil & Environmental Engineering Dept.	USA
<b>Stein</b>	Mark M.	ICI Americas, Inc.	USA
<b>Stein</b>	Reinhardt	Wyeth-Ayerst Research	USA
<b>Szabadaï</b>	Zoltan	Department Organic Chemistry	ROMANIA
<b>Szalkowski</b>	Mary B.	Prisma Corp.	
<b>Tosato</b>	Maria Livia	Embassy of Italy	USA
<b>Turner</b>	James E.	Health and Safety Research Division	USA
<b>Umeda</b>	Yoshihisa	Takara Shuzo Co., LTD.	JAPAN
<b>Vassiliev</b>	Pavel	SPC SPLINE	RUSSIA
<b>Volanschï</b>	Elena	Universitatea Bucuresti	ROMANIA
<b>Vorpagel</b>	Erich, R.	Biosym Technologies, Inc	USA
<b>Weber</b>	Hans-Peter	Nova Research Services	SWITZERLAND
<b>Weinberg</b>	Josette	Universitatea Bucuresti	ROMANIA
<b>Wipf</b>	Hans-Kaspar	Dr.R. Maag AG, Agrochemical Research	SWITZERLAND
<b>Wohl</b>	Ronald		USA
<b>Wolters</b>	Fred	Clorox Technical Center	USA
<b>Wong</b>	Rosalind Y.	USDA Western Regional Research Center	USA
<b>Xie</b>	Qian	Laboratory of Computer Chemistry	P.R.CHINA
<b>Yamakawa</b>	Masumi	Shionogi Pharmaceutical Co.	JAPAN
<b>Yoshimura</b>	Yoshinobu	Takeda Chemical Industries	JAPAN
<b>Yoshioka</b>	Hirosuke	Bioregulator Design & Synthesis Laboratory	JAPAN
<b>Yuta</b>	Kohtaro	Fujitsu Makuhari Systems Laboratory	JAPAN

## **New webmaster**

After many years serving as webmaster Didier Rognan moved on to a new job at the University of Strasbourg in France. We thank Didier very much for keeping the site up and contribution to it's image. The new webmaster will be Stefan Balaz at North Dakota University (stefan\_balaz@ndsu.nodak.edu). The new URL is in the heading of this Newsletter.

## **Contributions to the Newsletter and our web site**

All members are invited to contribute our Newsletter and to our web site. This Newsletter shall not be a one-man show, it gains from your experience. Our publishing policy will not allow us to accept scientific contributions which better should be sent to a reviewed journal. However, tips and tricks, key references, conferences, books, shareware, even the announcement of new commercial software, are welcome. We depend on your active participation!

Please send your comments and contributions to



Han van de Waterbeemd  
c/o Pfizer Global Research and Development  
Sandwich Laboratories  
Dept. Drug Metabolism  
Sandwich, Kent CT13 9NJ, UK  
FAX +44-1304-656433  
E-MAIL han\_waterbeemd@sandwich.pfizer.com



## FROM OUR BRANCHES



### Russia

Contact: Oleg Raevsky  
<http://www.ibmh.msk.su/qsar/>

### Italy

Contact: Sergio Clementi

### UK

Contact: Iain McLay (chairman) or Patrick Barton (Newsletter)  
<http://www.iainm.demon.co.uk/>

### Hungary

Contact Antal Lopata (lopata@chemicro.hu)

Hungarian Section of the Society 2000. We are pleased to announce that in 1999 we formed the QSAR and Modelling group of the Hungarian Chemical Society. We have got altogether 30 members, 20 of which wished to join The QSAR and Modelling Society, so our group can be considered as the Hungarian Section of the Society.

Our members represent various universities, academic institutions, and pharmaceutical companies, as well as various areas of science such as medicinal chemistry, biochemistry, protein NMR spectroscopy, theoretical chemistry, and chemometrics.

We plan to organize meetings where our members give lectures about their work in the field of QSAR and molecular modelling. In this way we can promote the collaboration between Hungarian scientists working in these fields.

In the first meeting held on April 19, 1999, Dr. Antal Lopata was elected to be the first chair of our group. Since then we have organized three meetings where the following lectures were given:

G. G. Ferenczy (Chinoin Ltd, Budapest):

*Protein-Ligand Interaction Energies by the LIE method*

B. Bordás (Plant Protection Institute, Hung. Acad. Sci., Budapest):

*Comparative 3D QSAR Study of Safeners and Herbicides*

A. Lopata (CheMicro Ltd, Budapest):

*Investigation of the Nucleophilicity and Electrophilicity of Radicals Using CoMFA*

P. Nagy (University of Toledo, Toledo, USA):

*Development of a Selective Muscarinic M<sub>1</sub> Agonist Using Computer-Aided Modelling*

T. Veszprémi (Technical University of Budapest):

*How to Design Stable Silylenes?*

I. Lukovits (Institute of Chemistry, Chem. Res. Center, Hung. Acad. Sci., Budapest):

*Relationships Between the Electronic Structure and the Efficiency of Corrosion Inhibitors*

G. M. Keserü (Gedeon Richter Ltd, Budapest):

*In Silico Predictions of Membrane Penetration Using High Throughput Methods*

A. Perczel (Eötvös Loránd University, Budapest):

*Main Factors Influencing the Conformation of the Hydrophobic Core of Proteins*

Z. Bikádi (Institute of Chemistry, Chem. Res. Center, Hung. Acad. Sci., Budapest):

*Investigation of the O–H Bond Stretching Vibration in 2,6-Diisopropyl-Phenol*

Our next meeting will be held in Szeged, Hungary on November 15-16, 2000.

We hope this sort of collaboration will be very useful for each of us.

Dr. Antal Lopata

CheMicro Research & Development Co. Ltd.

Hegedüs Gyula u. 6, H-1136 Budapest, Hungary

Tel: +36-1-3493847

Fax: +36-1-3398730

E-mail: lopata@chemicro.hu

## **Romania**

Contact: Zeno Simon & Tudor Oprea

### **The Romanian Branch of the QSAR and Modeling Society**

**1999-2000**

Over the past year, the QSAR and Quantum Chemistry Group in Timișoara has continued to have regular meetings, hosted bimonthly by Professors Zeno Simon and Adrian Chiriac in the Pestalozzi building of the [Faculty of Chemistry-Biology-Geography](#), University of West, Timisoara. These meetings are intended not only for the scientists that report ongoing activities, but also for PhD and Master-degree students in chemistry, which have the opportunity to present their work to a wider audience. Last year, our facilities were improved by a network of twelve Pentium computers (linked to an IBM Netfinity 3000 server), computers that were kindly donated by [AstraZeneca](#) R&D Mölndal (Sweden), with help from Dr. Nils-Åke Bergman. These computers are used to teach molecular modelling, QSAR and cheminformatics to the postgraduate students that are enlisted in the M.Sc. programme. Our QSAR group has also been making extensive use of the multivariate statistical analyses packages SIMCA 8.0 and Modde 5.0, donated by [Umetrics](#) (Umeå, Sweden), courtesy of Dr. Erik Johansson.

As of May 2000, Professor Mircea Mrovec is the new director of the Institute of Chemistry of the Romanian Academy in Timișoara. The Computational Chemistry Department was officially recognised in this Institute, after more than a decade of informal existence. Along with its previous lines of research, especially QSAR studies of dye-fibre interaction, a novel research direction was initiated – modeling of saline bond interactions in connection with more theoretical aspects of specific interactions (Ludovic Kurunczi, Zeno Simon, Cristian Bologna, Magdalena Banda, Valentin Careja). A review concerning QSAR-

type studies for dye-cellulose fibre interactions, especially from our group, is to appear in "Dyes and Pigments" (Simona Timofei, W. Schmidt, L. Kurunczi, Z. Simon). A PLS-version of MTD related to scoring functions for receptor-ligand interactions, was submitted to "SAR and QSAR in Environmental Chemistry" (Tudor I. Oprea, Marius Olah, L. Kurunczi, Z. Simon). With assistance from several members of our group, Speran• a Avram (Faculty of Biology, University of Bucharest) has performed several CoMFA studies on HIV protease inhibitors, as part of her Ph.D. thesis. At the recent EUCCO-CCC3 Quantum Chemistry Conference in Budapest, Valentin Careja presented a poster with preliminary results of our saline bond modeling studies. Due to financial difficulties, there was no Romanian participant at this year's European QSAR Symposium in Düsseldorf, Germany.

Concerning members from other Romanian cities, Dr. O. Ivanciuc (from Bucharest) is now at the Texas A&M University at Galveston, where he joined Professor Alexandru Balaban. Dr. Ivanciuc continues to publish an interesting series of contributions to the design of new topological indices for QSAR, in *Revue Roumaine de Chimie*.

Since the scientific literature on QSAR and molecular modelling, in Romanian, is far from abundant, we also note the book "Course in Molecular Drug Design", co-authored by Tudor Oprea, Ludovic Kurunczi and Oana Martin (Mirton Publishing House, December 1999). The book covers topics ranging from macromolecular structures (proteins and nucleic acids) to bioisosterism, and includes sections dedicated to molecular mechanics and dynamics, cheminformatics and cytochrome P450s. An extremely interesting section covers chemical and legal aspects regarding patents of chemical structures for therapeutic use. Another book, "Accuracy in Molecular Biologic Recognitions" co-authored by Z. Simon, A. Chiriac and V. Ostafe, appeared recently (Mirton Publishing House, September 2000).

The organization of a summer school on Chemometrics and Applications, by the Institute of Chemistry and our department of Chemistry is intended next year, for participants from Romania and neighbouring countries.

Z. Simon

**University of West of Timisoara  
Department Chemistry**



## MEETING REPORTS



### **QSAR and QSPR at the ACS Meeting, August 2000**

The American Chemical Society's National Meeting in Washington DC had four full days of symposia and papers devoted to QSAR and QSPR. Most of the papers were in the Division of Computers in Chemistry. Symposia topics included "Current Status of Molecular Force Fields," QSAR *in vivo*," "Computational ADME," and "Molecular Connectivity."

A highlight was seeing and listening to Corwin Hansch describe his huge database of QSAR equations and how data mining software can pick out relationships that might not be obvious by visual inspection. People interested in Corwin's work with his database should consult his recent papers.

Many of the papers were using QSAR and QSPR with libraries to identify pharmacophoric groups that would have desirable ADME (absorption, distribution, metabolism and excretion) properties. As anyone knows who works in the field pharmaceuticals knows, these are complex phenomena with a variety of mechanisms affecting the drug's fate. Whereas several years ago, multivariate statistics was the way to analyze large data sets from which large numbers of variables are generated, many of the papers now describe the use of neural networks and genetic algorithms.

Another group of papers applied the same techniques used with "drug libraries" to very large toxicological databases. The end point usually was death, but death was caused by a variety of mechanisms. The problem to be solved was how to locate common toxicological mechanisms among very diverse structure sets.

Unique to this ACS meeting was the 25<sup>th</sup> anniversary symposia on Molecular Connectivity. It was very international in scope and featured both the developers of the technique and some of the younger investigators. A nice feature was a round table discussion at the end of the formal talks that encouraged audience participation. Much of the conversation revolved on how to interpret the connectivity values in physicochemical terms and how can one use a connectivity relationship to design additional active compounds.

The tentative program for symposia sponsored by the Division of Computers in Chemistry at the April ACS meeting in San Diego promises to be as provocative as the Washington meeting. Workers in the field of QSAR should seriously consider attending these meetings. They definitely are QSAR and QSPR focused.

***John Block***

### **13<sup>th</sup> European Symposium on Quantitative-Structure-Activity Relationships and Molecular Modelling in Duesseldorf, Germany**

350 scientists from academia and pharmaceutical industry gathered in Duesseldorf from August 27 through September 1, 2000 for the 13<sup>th</sup> European QSAR Symposium. The conference under the subtitle "Rational Approaches to Drug Design" took place at the Heinrich-Heine Universität. The program was opened on Sunday evening by an inaugural lecture given by Prof. Camille Wermuth (Strasbourg). His talk entitled "The Impact of QSAR and CAMD Methods on Drug Design" was based on his own experiences from thirty years of scientific work in medicinal chemistry and focussed on the synergistic effects of theoretical and experimental methods in the search for new and active drug molecules. The conference programme was divided into eight sessions which each was opened by an invited lecture delivered by an internationally well renowned expert in the particular field:

-Protein Modelling, Rebecca Wade, EMBL Heidelberg

-Knowledge-based Methods in Bioinformatics, Manfred Sippl, Universität Salzburg

- QM/MM Embedding Methods, Tim Clark, Universität Erlangen
- Superposition and Alignment Strategies, Christian Lemmen, Dupont Pharmaceutical Research Labs, San Diego
- New Developments and Applications in Chemometrics, Gabriele Cruciani, Università di Perugia
- Synthesis Planning and Combinatorial Libraries, Andrew Leach, Glaxo Wellcome Research and Development, Stevenage
- High-Throughput Structure-Based Design, Hans-Joachim Böhm, Hoffmann-LaRoche Basel
- Data Mining, Johann Gasteiger, Universität Erlangen

In addition 30 selected short oral communications were given, scanning a large part of the actual problems encountered in theoretical drug design. 140 posters presented in two poster sessions completed the program. The discussion after the lectures, in the coffee breaks or in front of the posters set a lively frame for an extremely interesting and scientifically dense meeting. In the exhibition organised with the symposium eight software and hardware vendors were giving an overview on their newest products.

The social program featured an organ concert, an Italian style open air reception and an excursion to the remnants of the heavy industry of the famous Ruhr district. The conference dinner which as always was the highlight of the non-scientific part of the program took place with a view on the river Rhine and did benefit as all other events from the pleasant weather situation.

***Hans-Dieter Höltje***

Chairman, 13.Eur. QSAR Symposium

## OPINIONS

None this time!



# CONTRIBUTIONS



## CAN NEW ACTIONS BE FOUND FOR OLD PHARMACEUTICALS THROUGH COMPUTER PREDICTION OF BIOLOGICAL ACTIVITY?

V. Poroikov, D. Filimonov, D. Akimov

**Institute of Biomedical Chemistry of Russian Academy of Medical Sciences;  
10, Pogodinskaya Street, Moscow, 199832, Russia; E-mail: vvp@ibmh.msk.su**

Each biologically active compound possesses a number of biological activities. Its specificity of action is defined by the peculiarities of object, dose, route, and other terms & conditions of the experiment. On the contrary, biological potential of compound includes all activities, which can be discovered under any specific experimental conditions. This biological potential is called the biological activity spectrum and can be predicted on the basis of structure-activity relationships found by the analysis of the known data from the training set. Based on the analysis of large training set consisting of tens thousands of biologically active compounds, computer program PASS [1-3] provides the means to evaluate the biological activity spectrum of any compound.

Computer program PASS is the product of ideas originated more than 25 years ago within the framework of the National Registration System of New Chemical Compounds organized in the USSR in 1972 [4]. It was V. Avidon who suggested that many kinds of biological activity could be predicted on the basis of structural formulae of chemical compounds [5]. Similar approach was under development by V. Golender and A. Rozenblit [6]. In 1985, when we (V.P and D.F) joined in the project, previous experience was taken into account. The only published example of a comparable approach developed and applied outside the Soviet Union was the U.S. National Cancer Institute's Drug Information System [7]. In that time possibilities for cooperation with scientists from Western countries were restricted and our team had to follow its own way. It was the way of trial and error, but due to this the team developed an innovative concept of biological activity spectra according to which the compound's biological action is considered as an intrinsic property of the structure [8], an original mathematical algorithm [9], new universal chemical descriptors [10], reasonable training set (3). The program, which predicts more than 500 kinds of biological activity, was created on this basis.

In the past years computer program PASS was reconstructed several times and its current version 1.41 is rather different even from the product which was available several years ago [8, 11]. During this evolution the accuracy and robustness of predictions has been increased substantially.

Mean accuracy of PASS prediction in LOO cross-validation for the total training set, including ~35,000 compounds with 565 kind of activity, equals to about 85% [3]. PASS testing in a blind mode by 9 scientists from 8 countries on the heterogeneous set of 118 compounds having 138 activities has demonstrated the mean accuracy of prediction 82.6% [12]. Using MDDR database [13] to create heterogeneous training

and evaluation sets it was recently demonstrated that the predictions are robust despite excluding up to 60% of information [14].

PASS uses MOL or SD-files [13] as input. The results of prediction (output) can be obtained as CSV, TXT or SD-files. Since the prediction of biological activity spectra for 1,000 compounds in usual PC takes about 1 minute, PASS can be effectively applied both to predict biological potential of separate compounds and to analyze large chemical databases [15].

Here we present the results of PASS application to the pharmaceuticals from TOP200 list [16], which are especially significant for the nowadays healthcare. Finding a new "lead" among the launched drugs (probable new indications) is more attractive because the safety of such compounds is already proved, in many cases, by previous clinical practice. Predicted biological activities, while being compared with those experimentally established, give an additional evidence for the reliability of computer program PASS. On the other hand, novel activities found due to the computer-aided predictions may open new horizons in the study of widely used pharmaceuticals.

Results of biological activity spectra prediction for 132 compounds from the list of TOP200 drugs (duplicates, mixtures, peptides etc. are excluded) coincide with the experimental data in 96.6% [17]. Examples of new activities which are predicted with high probability for some of these compounds are presented in the table below.

<b>Pharmaceutical</b>	<b>Predicted Activities</b>	<b>• • *</b>
Fluticasone	<b><u>Anti-inflammatory</u></b> **	<b>0.991</b>
	Angiogenesis inhibitor	0.651
Divalproex	<b><u>Anticolvulsant</u></b>	<b>0.348</b>
	Angiogenesis inhibitor	0.679
Amlodipine	<b><u>Antihypertensive</u></b>	<b>0.742</b>
	Antineoplastic enhancer	0.584
Quinapril	<b><u>Angiotensin-converting enzyme inhibitor</u></b>	<b>0.629</b>
	Antiarthritic	0.521
Ramipril	<b><u>Antihypertensive</u></b>	<b>0.548</b>
	Multiple sclerosis treatment	0.595
Oxaprozin	<b><u>Antiinflammatory</u></b>	<b>0.844</b>
	Bone formation stimulant	0.785
Sertraline	<b><u>Antidepressant</u></b>	<b>0.436</b>
	Antiparkinsonian	0.609
Omeprazole	<b><u>Antisecretory (Gastric)</u></b>	<b>0.974</b>
	TNF-alpha release inhibitor	0.658
Lisinopril	<b><u>Antihypertensive</u></b>	<b>0.500</b>
	Corneal wound healing stimulator	0.598
Cisapride	<b><u>Stimulant (Peristaltic)</u></b>	<b>0.601</b>
	Irritable Bowel syndrome therapy	0.720
Alprazolam	<b><u>Sedative</u></b>	<b>0.896</b>
	Platelet activating factor antagonist	0.853
Hydrochlorothiazide	<b><u>Diuretic</u></b>	<b>0.821</b>
	Anticoccidial	0.606

Fluoxetine	<b><u>Antidepressant</u></b> Urinary incontinence treatment	<b>0.830</b> 0.647
Verapamil	<b><u>Anti-arrhythmic</u></b> Urinary incontinence treatment	<b>0.753</b> 0.705
Lansoprazole	<b><u>Anti-ulcerative</u></b> Urinary incontinence treatment	<b>0.915</b> 0.568
Amitriptyline	<b><u>Antidepressant</u></b> Antitoxic	<b>0.966</b> 0.813
Fluvastatin	<b><u>Antihyperlipidemic</u></b> Platelet adhesion inhibitor	<b>0.861</b> 0.541
Salmeterol	<b><u>Bronchodilator</u></b> Antiobesity	<b>0.680</b> 0.659
Albuterol	<b><u>Bronchodilator</u></b> Antiobesity	<b>0.688</b> 0.659
Levothyroxine	<b><u>Thyroid hormone agonist</u></b> Dopa decarboxylase inhibitor	<b>0.638</b> 0.748
Fexofenadine	<b><u>Antihistaminic</u></b> Choleretic	<b>0.534</b> 0.627
Cetirizine	<b><u>Histamine H1 antagonists</u></b> Spasmolytic	<b>0.553</b> 0.559
Metformin	<b><u>Antidiabetic</u></b> Hypertensive	<b>0.818</b> 0.824
Tramadol	<b><u>Analgesic</u></b> Hypotermic	<b>0.882</b> 0.733

\*Pa is the probability to have the appropriate activity. Its values vary from 0.000 to 1.000, the most probable biological activities have the highest Pa values.

\*\*Activities known from the experiment are marked in bold.

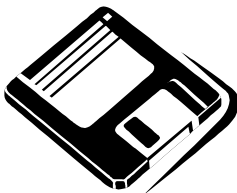
As one may see from this table, new biological activities are predicted with high probabilities for compounds which are already in medical use, e.g., Angiogenesis inhibitor (Fluticasone, Divalproex), Antiarthritic (Quinapril), Bone formation stimulant (Oxaprozin), Multiple sclerosis treatment (Ramipril), etc. Being confirmed by the experiment, these activities may provide the reason for a new drug indications.

If one which to obtain the results of prediction for any drug from TOP200 list, such information will be provided free on request via E-mail.

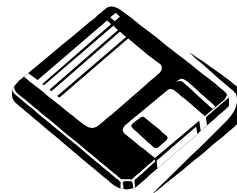
Similar prediction can be performed for any other launched pharmaceutical. Investigation of lead compound and drug-candidate is limited by the firm's research strategy and test standards for drug safety assessment, therefore, the information on their biological activity is always incomplete. Since it is practically impossible to study each compound in all available tests, computer-aided prediction with PASS is the "method of choice" to evaluate the biological potential of compounds and to establish the priorities in biological testing.

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# SOFTWARE



- **TRITON release announcement**

The graphical program TRITON has been developed for modelling protein mutants and assessment of their activities. Protein mutants are modelled from the wild type structure by homology modelling using the external program Modeller. Chemical reactions taking place in the mutants active site are modelled using the semi-empirical quantum mechanic program MOPAC. Semi-quantitative predictions of mutants activities can be achieved by evaluating the changes in energies of the system and partial atomic charges of active site residues during the reaction. The program TRITON offers graphical tools for the preparation of the input data files, for calculation and for the analysis of the generated output data. Implementation ensures the overall integrity of consecutive steps in the modelling of mutants and calculation of reaction coordinates, but the program can also be used simply for combinatorial generation of multiple mutants by homology modelling. The program functionality has been validated by the modelling of activities of haloalkane dehalogenase mutants.

Availability: The program TRITON can run under operating systems IRIX, Linux and NetBSD. The software is FREE for academic users and is available at <http://www.chemi.muni.cz/lbsd/triton.html>.

Dr. Jiri Damborsky  
Laboratory of Biomolecular  
Structure and Dynamics  
Masaryk University  
Kotlarska 2, 611 37 Brno  
Czech Republic

Phone +420-5-41129377  
FAX +420-5-41129506  
e-mail: [jiri@chemi.muni.cz](mailto:jiri@chemi.muni.cz)  
<http://www.chemi.muni.cz/~jiri/index.html>

- **MIPSIM 1.1.1 Release Announcement**

MIPSIM is a computational system developed by the Grup de Recerca en Informatica Medica at IMIM/UPF in order to automatically explore the similarities between biomolecules on the basis of molecular interaction potentials (MIP). It is based on the ideas behind the MEPSIM program, developed in our group during the last decade. The goal of the old program MEPSIM was the automatic evaluation of the molecular electrostatic potential (MEP) features and similarities within series of compounds.

The old MEPSIM program has been completely rewritten in a more modular and sophisticated program called MIPSIM. The latter can be used as an standalone program for the automatic analysis of biomolecular similarities but it can also make use of its interfaces to well-known external programs: a quantum mechanics package (GAMESS), a package for the computation of molecular interaction potentials (GRID), the statistical analysis tools developed by the Laboratorio di Chemiometria of the Universita di Perugia, and visualization packages (INSIGHT(MSI), gOpenMol).

MIPSIM includes the following main modules:

**MIN:** A module which allows to find automatically the MIP minima of a molecular system. It supplies the cartesian coordinates of these minima, their values and all the geometrical relationships between them (distances, angles and dihedral angles). This module may use on the quantum mechanical definition of MEP (computed with the GAMESS package), or MIPs as computed by the program GRID.

**COMP:** This module computes a similarity coefficient between the MIP distributions of pairs of molecules and finds their relative position that maximizes this MIP-based similarity. The program can handle up to 100 molecules and build the corresponding pairwise similarities matrix.

The current version of the MIPSIM software runs under the Linux and IRIX operating systems.

The program is free for academia and can be obtained at

<http://www1.imim.es/mipsim>

MIPSIM has been created at the

Grup de Recerca en Informatica Medica  
Institut Municipal d'Investigacio Medica, IMIM  
Dep. de Ciències Experimentals i de la Salut  
Universitat Pompeu Fabra  
Barcelona (Spain)

- **DRAGON (version 1.0) for the calculation of 853 theoretical molecular descriptors is now free downloadable from Website.**

This software has been produced by us, coherently to the Handbook of Molecular Descriptors, by Roberto Todeschini and Viviana Consonni, edited in these days by WILEY - VCH, in the Series of Methods and Principles in Medicinal Chemistry, Vol. 11 (Editors: R.Mannhold, H.Kubinyi, H.Timmerman); pp.680.

We have also activated a bibliographic reference service about molecular descriptors at our Website and a special e-mail address

(moldes@disat.unimib.it) for the exchange of information of the researchers in this field.

Roberto Todeschini and Viviana Consonni

- Relibase: a program for searching protein/ligand databases (<http://relibase.ebi.ac.uk/>).



## NEW BOOKS



- **Evolutionary Algorithms in Molecular Design**, Ed. David E. Clark, Methods and Principles in Medicinal Chemistry, Vol.8. Wiley-VCH, Weinheim, Germany.

The book comprises 12 chapters

from experts in the application of EAs to molecular design problems

- 1 Introduction to Evolutionary Algorithms - Dr. Abby L. Parrill
- 2 Small-molecule Geometry Optimization and Conformational Search - Dr. Ron Wehrens
- 3 Protein-Ligand Docking - Dr. Garrett M. Morris, Prof. Arthur J. Olson and Dr. David S. Goodsell
- 4 De Novo Molecular Design - Dr. Valerie J. Gillet
- 5 Quantitative Structure-Activity Relationships - Dr. Sung-Sau So
- 6 Chemometrics - Dr. Ron Wehrens and Prof. Lutgarde M. C. Buydens
- 7 Chemical Structure Handling - Prof. Peter Willett
- 8 Molecular Diversity Analysis and Combinatorial Library Design - Dr. Lutz Weber
- 9 Evolutionary Algorithms in Crystallographic Applications - Prof. Kenneth D.M. Harris
- 10 Structure Determination by NMR Spectroscopy - Dr. Bryan C. Sanctuary
- 11 Protein Folding - Dr. Jan T. Pedersen
- 12 New Techniques and Future Directions - Dr. Andrew Tuson and Dr. David E. Clark

For more information, please visit the Wiley-VCH web site:

<http://www.wiley-vch.de/books/tis/eng/3-527-30155-0.html>

- **Combinatorial Chemistry**, Eds. W. Bannwarth and E. Felder, Methods and Principles in Medicinal Chemistry, Vol.9. Wiley-VCH, Weinheim, Germany (2000).

- **Virtual Screening for Bioactive Molecules**, Eds. H.-J. Boehm and G. Schneider, *Methods and Principles in Medicinal Chemistry*, Vol.10. Wiley-VCH, Weinheim, Germany (2000).
- **Handbook of Molecular Descriptors**, R. Todeschini and V. Consonni, *Methods and Principles in Medicinal Chemistry*, Vol.11. Wiley-VCH, Weinheim, Germany (2000).
- **REVIEWS IN COMPUTATIONAL CHEMISTRY**. Volume 14 contents:
  - The tutorials and reviews in this volume cover:
  - Mapping atomic charges to electrostatic potentials.
  - Coupled cluster theory.
  - Zeolite modeling.
  - More accurate intermolecular potentials for organic molecules.
  - Nonequilibrium molecular dynamics.

The featured authors are: Ken Bagchi, Sundaram Balasubramanian, Lisa Emily Chirlian, T. Daniel Crawford, Michelle Miller Francl, Mehran Jalaie, Michael L. Klein, K. B. Lipkowitz, Glenn J. Martyna, Christopher J. Mundy, Swie Lan Njo, Sarah L. Price, Henry F. Schaefer, Konstantin S. Smirnov, Mark E. Tuckerman, and Bastiaan van de Graaf.

Volume 14 also presents an essay on the history of the Gordon Research Conferences on Computational Chemistry. Also included is a large compendium of published force field parameters for molecular mechanics, molecular dynamics, and Monte Carlo simulations.

K. B. Lipkowitz and D. B. Boyd are the editors. The ISBN of this Wiley book is (xxiii + 525 pages) is 0-471-35495-3.

- **REVIEWS IN COMPUTATIONAL CHEMISTRY**, Volume 15.

The tutorials and reviews in this volume cover:

- Understanding chemistry with Kohn-Sham density functional theory
- Computational strategy for organic photochemistry
- Predicting enthalpies of formation for gaseous compounds
- Development of computational chemistry in Canada

The featured authors are: Evert Jan Baerends, Fernando Bernardi, F. Matthias Bickelhaupt, Russell J. Boyd, Larry A. Curtiss, David J. Frurip, Marco Garavelli, Massimo Olivucci, Paul C. Redfern, and Michael A. Robb.

More information about the books can be found at

- **Topological Indices and Related Descriptors in QSAR and QSPR.** Devillers, J. and Balaban, A. T. (1999).

Gordon and Breach Science Publishers, The Netherlands, Hardcover, p. 811, ISBN 90-5699-239-2, US\$ 198.

Preface.

Chapter 1: No-free-lunch molecular descriptors in QSAR and QSPR (J. Devillers).

Chapter 2: Historical development of topological indices (A. T. Balaban and O. Ivanciuc).

Chapter 3: The graph description of chemical structures (O. Ivanciuc and A. T. Balaban).

Chapter 4: Vertex- and edge-weighted molecular graphs and derived structural descriptors (O. Ivanciuc, T. Ivanciuc, and A. T. Balaban).

Chapter 5: Matrices and structural descriptors computed from molecular graph distances (O. Ivanciuc and T. Ivanciuc).

Chapter 6: The detour matrix and the detour index (S. Nikolic, N. Trinajstic, and Z. Mihalic).

Chapter 7: Molecular connectivity Chi indices for database analysis and structure-property modeling (L. H. Hall and L. B. Kier).

Chapter 8: Overall connectivity and topological complexity: A new tool for QSPR/QSAR (D. Bonchev).

Chapter 9: Novel strategies in the search of topological indices (E. Estrada).

Chapter 10: The Kappa indices for modeling molecular shape and flexibility (L. B. Kier and L. H. Hall).

Chapter 11: The electrotopological state: Structure modeling for QSAR and database analysis (L. B. Kier and L. H. Hall).

Chapter 12: Information theoretic indices of neighborhood complexity and their applications (S. C. Basak).

Chapter 13: Autocorrelation descriptors for modeling (eco)toxicological endpoints (J. Devillers).

Chapter 14: DARC site topological correlations: Ordered structural descriptors and property evaluation (J. E. Dubois, J. P. Doucet, A. Panaye, and B. T. Fan).

Chapter 15: A hierarchical approach to the development of QSAR models using topological, geometrical, and quantum chemical parameters (S. C. Basak, B. D. Gute and G. D. Grunwald).

Chapter 16: Molecular graph descriptors used in neural network models (O. Ivanciuc).

Chapter 17: Algorithms and software for the computation of topological indices and structure-property models (O. Ivanciuc and J. Devillers).

Index.

- **Oral Drug Absorption. Prediction and Assessment,** Eds. J.B. Dressman and H. Lennernaes, Marcel Dekker, New York (2000).



## BOOK REVIEW



none



## POSITIONS



none



## JOURNALS



- **Quantitative Structure-Activity Relationships**

This VCH journal is considered to be the "home" journal of THE QSAR AND MODELLING SOCIETY. Editors are Prof. Michael Wiese, University of Bonn, and Prof. Gerd Folkers, ETH Zurich.

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Pharmazeutisches Institut  
Pharmazeutische Chemie  
An der Immenburg 4  
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Germany  
Tel. +49-228-73 5212  
Fax +49-228-73 7929  
Email [mwiese@uni-bonn.de](mailto:mwiese@uni-bonn.de)

and consider that a publication in this journal will reach your audience of QSAR and modelling colleagues much better than a publication in JACS, JCICS, JMC, Biochemistry, etc.

Of course, Ferenc Darvas remains the Editor of the Abstracts Section. Please consider also to subscribe personally to the QSAR journal. It's good and it's cheap, extremely cheap for members of our Society (call VCH, phone +49-6201-6060, for the current price).

Of course, the publisher Wiley-VCH would also like to encourage you to order a personal copy of this important journal. First of all, it has a relatively high impact factor, as compared to many other journals, and second, an incredibly low price for personal subscriptions is offered to our members:

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***Preview Quantitative Structure-Activity Relationships, 19/5 (2000)***

The accepted manuscripts for issue 5 are:

QSAR study of antimalarial activities and artemisinin-heme binding properties obtained from docking calculations

S. Tonmunphean, V. Parasuk, S. Kokpol

The electron-conformational approach to QSAR study in series of benzodiazepine derivatives

Y. Chumakov, A. Terletskaia, A. Dimoglo, S. Andronati

Experimental Validation of a Structure-Activity Relationship Model of Skin Irritation by Esters

J.S. Smith, O.T. Macina, N.B. Sussman, M.H. Karol, H.I. Maibach

Three-Dimensional Structure-Activity Relationships of Synthetic Pyrethroids: 2. Three-Dimensional and Classical QSAR Studies

H. Chuman, S. Goto, M. Karasawa, M. Sasaki, U. Nagashima, K. Nishimura, T. Fujita

• **Journal of Computer-Aided Molecular Design**

Kluwer Academic Publishers is pleased to offer members of The QSAR and Modelling Society a special individual subscription rate to the Journal of Computer-Aided Molecular Design. Further information, including Instructions for Authors and Tables of Contents can be found at the Journal's homepage:

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Table of Contents  
Volume 14, Issue 7, October 2000

Steroid binding by antibodies and artificial receptors: Exploration of theoretical methods to determine the origins of binding affinities and specificities  
Sandra Handschuh, Bernd Goldfuss, Jiangang Chen, Johann Gasteiger, K.N. Houk  
pp. 611-629

Localization and quantification of hydrophobicity: The molecular free Energy density (MolFESD) concept and its application to sweetness recognition  
Robert Jäger, Friedemann Schmidt, Bernd Schilling, Jürgen Brickmann pp. 631-646

3D-QSAR using 'Multiconformer' alignment: The use of HASL in the analysis of 5-HT<sub>1A</sub> thienopyrimidinone ligands†  
Salvatore Guccione, Arthur M. Doweyko, Hongming Chen, Gloria Uccello Barretta, Federica Balzano

pp. 647-657

Hydration of  $\beta$ -cyclodextrin: A molecular dynamics simulation study  
R.G. Winkler, S. Fioravanti, G. Ciccotti, C. Margheritis, M. Villa  
pp. 659-667

Classical QSAR and comparative molecular field analyses of the  
host-guest interaction of organic molecules with cyclodextrins  
Takahiro Suzuki, Masaru Ishida, Walter M.F. Fabian, pp. 669-678

Indices of differences of path lengths: Novel topological descriptors  
derived from electronic interferences in graphs  
Jorge Gálvez, Ramón Garcia-Domenech, Carolina de Gregorio-Alapont  
pp. 679-687

Conformational properties of amphotericin B amide derivatives – impact  
on selective toxicity  
Haluk Resat, F. Aylin Sungur, Maciej Baginski, Edward Borowski, Viktorya  
Aviyente  
pp. 689-703

- Special issue of the **Journal of Molecular Graphics and Modelling (Vol. 18, No. 2)** features advances in the molecular modelling of carbohydrates.

The following articles were organized by Prof. J. Raul Grigera, Guest Editor.

Constructing and evaluating energy surfaces of crystalline disaccharides.  
Alfred D. French, Anne-Marie Kelterer, Glenn P. Johnson,  
Michael K. Dowd, and Christopher J. Cramer

Single-coordinate-driving method in molecular docking. Application to  
modeling of guest inclusion in cyclodextrin.  
Jaroslav K., Martin Ludin, Serge Perez, and Anne Imberty

Hydration of T-antigen Gal- $\beta$ (1-3)GalNAc and the isomer Gal- $\beta$ (1-3)GlcNAc  
by molecular dynamics simulations.  
Ernesto R. Caffarena and Paulo M. Bisch

Glycosylation of prions and its effect in protein conformation relevant to  
amino acid mutations.  
Nicky K. C. Wong, D. V. Renouf, S. Lehmann, and E. F. Hounsell

Studies on the solution conformation and dynamics of the polysaccharide from  
*Sinorhizobium fredii* hh103 and its monosaccharide repeating unit.  
Miguel A. Rodriguez-Carvajal, Manuel Bernabe, Jose L. Espartero,  
Pilar Tejero-Mateo, Antonio Gil-Serrano, and Jesus Jimenez-Barbero

Diffusion of water molecules in crystalline  $\beta$ -cyclodextrin hydrates.

K. Braesicke, T. Steiner, W. Saenger and Ernst Walter Knapp

Investigation on the mobility of the glycosidic linkage in sucrose through the study of the phase space structure of a two-degrees of freedom model.

G. Longhi, M. Malandrino, and Sergio Abbate

Online versions of these articles are at [www.chemweb.com](http://www.chemweb.com).

The News and Views section of this issue includes contributions from David Goodsell, Bruce Gaber, Ken Lind, Gustavo Arteca, Jurgen Bajorath, Rebecca Rone, Leo Caves, and Klaus Schulten.

• Perspectives in Drug Discovery and Design

<http://www.wkap.nl/journals/pd3>

Table of Contents Volume 20, 2000

<http://www.wkap.nl/issuetoc.htm/0928-2866+20+1+2000>

Virtual Screening: An Alternative or Complement to High Throughput Screening?

Preface

Gerhard Klebe

Combination of molecular similarity measures using data fusion

Claire M.R. Ginn, Peter Willett, John Bradshaw

pp. 1-16

Optimization of the drug-likeness of chemical libraries

Jens Sadowski

pp. 17-28

Generating consistent sets of thermodynamic and structural data for analysis of protein-ligand interactions

Thomas G. Davies, Jeremy R.H. Tame, Roderick E. Hubbard

pp. 29-42

Multiple molecular superpositioning as an effective tool for virtual database screening

Christian Lemmen, Marc Zimmermann, Thomas Lengauer

pp. 43-62

A recursive algorithm for efficient combinatorial library docking

Matthias Rarey, Thomas Lengauer

pp. 63-81

Modifications of the scoring function in FlexX for virtual screening

applications  
Martin Stahl  
pp. 83-98

A knowledge-based scoring function for protein-ligand interactions:  
Probing the reference state  
Ingo Muegge  
pp. 99-114

Predicting binding modes, binding affinities and 'hot spots' for  
protein-ligand complexes using a knowledge-based scoring function  
Holger Gohlke, Manfred Hendlich, Gerhard Klebe  
pp. 115-144

Hydrophobicity maps and docking of molecular fragments with solvation  
Nicolas Majeux, Marco Scarsi, Catherine Tenette-Souaille, Amedeo  
Caflisch  
pp. 145-169

Virtual screening with solvation and ligand-induced complementarity  
Volker Schneck, Leslie A. Kuhn  
pp. 171-190

Similarity versus docking in 3D virtual screening  
Jordi Mestres, Ronald M.A. Knegtel  
pp. 191-207

Discovering high-affinity ligands from the computationally predicted  
structures and affinities of  
small molecules bound to a target: A virtual screening approach  
Tami J. Marrone, Brock A. Luty, Peter W. Rose  
pp. 209-230

In vitro and in silico affinity fingerprints: Finding similarities  
beyond structural classes  
Hans Briem, Uta F. Lessel  
pp. 231-244

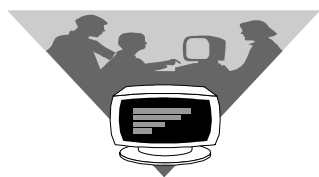
Computer-assisted synthesis and reaction planning in combinatorial  
chemistry  
Johann Gasteiger, Matthias Pförtner, Markus Sitzmann, Robert Höllering,  
Oliver Sacher, Thomas Kostka, Norbert Karg  
pp. 245-264

Evaluation of reactant-based and product-based approaches to the design  
of combinatorial libraries  
Valerie J. Gillet, Orazio Nicolotti  
pp. 265-287

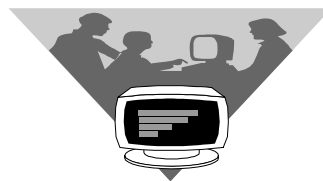
- *Perspectives in Drug Discovery and Design* is included with a subscription to Journal of Computer-Aided Molecular Design.

Society members might be especially interested in a series of issues, edited by Yvonne Martin and Robert S. DeWitte, on the topic of *Including Solvation in the Prediction of Binding Affinity*. The collection brings together a broad spectrum of expertise into a frank and direct treatise on the state of present day understanding of the desolvation phenomena as they relate to drug discovery. Chapters are authored by Corwin Hansch and Albert Leo; Frank Eisenhaber; Dudley Williams and Ben Bardsley; Paul Ruelle; Greg Hura, Jon Sorenson, Robert Glaeser, and Teresa Head-Gordon; Raimund Mannhold and Roelof Rekker; Albert Leo and David Hoekman; Christian Laurence and Michel Berthelot; Paul Ruelle, America Farina-Cuendet and Ulrich Kesselring; Irina Massova and Peter A. Kollman; Ulf Norinder and Thomas Osterberg; Peter Buchwald; Renxiao Wang, Ying Gao, and Luhua Lai; William M. Meylan and Philip H. Howard; Vellarkad N. Viswanadhan, Arup K. Ghose, and John J. Wendoloski; Alanas A. Petrauskas and Eduard A. Dolovanov; James Devillers; Roustem D. Saiakhov, Liliana R. Stefan and Gilles Klopman; Stefan Balaz; Bernard Testa, Patrizia Crivori, Marianne Reist, and Peirre-Alain Carrupt. More are in the works!

A volume soon to appear will include papers presented at the March, 15 - 18, 1999 Schloß Rauischholzhausen meeting on virtual screening.



## Meetings /Courses



### 2000

- Molecular Graphics and Modelling Society Meeting "Structure-based Drug Design" honoring Peter Goodford's scientific contributions to the field. December 13-15, 2000 at St. Catherine's College, Oxford.

Sessions cover: Principles and applications of structure-based drug design, advances in computational and experimental methods, new drug targets, combinatorial chemistry, genomics and proteomics.

Confirmed invited speakers are: Hans-Joachim Boehm (Basel), Gabriele Cruciani (Perugia), Philip Dean (Cambridge), Peter Goodford (Oxford), Wim Hol (Seattle), Rod Hubbard (York), Gerhard Klebe (Marburg), Andrew Martin (Reading), Jenny Martin (Queensland), Yvonne Martin (Abbott Park), Jon Moore (Boston), Graham Richards (Oxford), Dave Stammers (Oxford), Dave Stuart (Oxford)

Further details can be found at: <http://www.mgms.org/oxford2000>.  
Contact: Rebecca Wade: [wade@embl-heidelberg.de](mailto:wade@embl-heidelberg.de)

- Pacificchem 2000, December 14 - 19, 2000 Honolulu, Hawaii

The many symposia will concentrate on Bioscience and Technology including Pharmaceutical Chemistry, Environmental Chemistry, Macromolecules, Medicinal Chemistry, Organic Chemistry, and Physical and Theoretical Chemistry. Web site: <http://www.acs.org/meetings/pacific2000/>

## 2001

- New Approaches to Drug Design and Discovery, Schloss Rauischholzhausen, near Marburg, Germany, March 19-22, 2001. Contact: H.J.Boehm ([hans-joachim.boehm@roche.com](mailto:hans-joachim.boehm@roche.com)). See <http://pc1664.pharmazie.uni-marburg.de/workshop2001/>
- The Chemical Structure Association and the Molecular Graphics and Modelling Society Second Joint Sheffield Conference on Chemoinformatics: Computational Tools for Lead Discovery. Stephenson Hall, University of Sheffield, UK from 9th to 11th April 2001.

Sessions will cover: 3D databases, including docking and pharmacophore analysis, assay QC and its influence on data mining, chemical data mining, descriptor validation, design of leadlike combinatorial libraries, design of screening collections, e-business to facilitate lead discovery, novel software and hardware systems for lead discovery, selective compound acquisition from in house and commercial suppliers, similarity and clustering methods, structure-activity methods for lead identification and early optimisation, structure-based design for lead identification and early optimisation, virtual screening, and case histories.

- Spring Meeting of the American Chemical Society, San Diego, April 1-5, 2001 ([www.acs.org](http://www.acs.org))

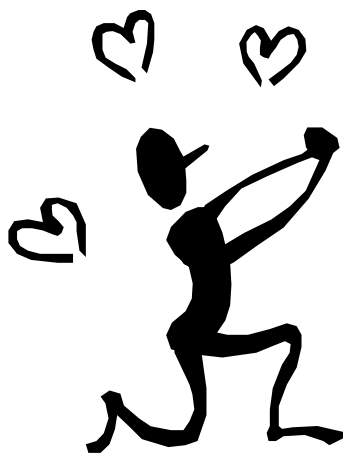
Symposia from the Chemical Information Division include: 3D Searching, Pharma Informatics, Electronic Chemistry Publishing, and Web-based Information Sources. Web site: <http://www.lib.uchicago.cinf>

Symposia from the Computers in Chemistry Division include: Artificial Intelligence, Library Design, Protein Folding, Structure-Based data mining, and Enzyme Modes of Action. Web site: <http://membership.acs.org/C/COMP/>

- Computational Methods in Toxicology and Pharmacology Integrating Internet Resources, Bordeaux, France, July 11-13, 2001. Contacts: Alain Carpy ([acarpy@u-bordeaux.fr](mailto:acarpy@u-bordeaux.fr)) and James Devillers.
- Fall Meeting of the American Chemical Society, Chicago, Aug 26-30, 2001 ([www.acs.org](http://www.acs.org))
- Perspectives in High-Throughput and in silico ADME, London, December 4<sup>th</sup>, 2001. Contact: Han van de Waterbeemd ([han\\_waterbeemd@sandwich.pfizer.com](mailto:han_waterbeemd@sandwich.pfizer.com)).

## 2002

- 5<sup>th</sup> Swiss School on Medicinal Chemistry, October 2002, Leysin, Switzerland. Contact: Gerd Folkers, Bernard Testa, Han van de Waterbeemd.



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Or to Han van de Waterbeemd in the UK (Eurocheques should be drafted in £).



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