



Chemical Structure Association Trust

NEWSLETTER

Autumn 2005 Issue 11

In this issue, friends and colleagues of the late Jaques-Émile Dubois pay tribute to one of the great pioneers in chemoinformatics (pages 4 to 7).

The death of Jaques-Émile was reported in an earlier Newsletter, and with the help of his family, we have been able to assemble contributions which show many aspects of this remarkable man.

It is appropriate that the Sponsor's Spotlight for this issue is from Questel.Orbit which is one of the co-sponsors of the new CSA Trust Jacques-Émile Dubois Grant.



Left to right: Trustees Steve Heller, Wendy Warr and Pierre Buffet enjoying a reception at the Nîmes conference (report on page 3)

AGM Agenda and Dinner

This year's AGM takes place on 29 November in London, followed by the Dinner

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CINF/CSA Trust Symposium

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Chemical Structure Association Trust Annual General Meeting

Monday 28th November 2005 at 4pm
at SCI, 14/15 Belgrave Square, London

Agenda

1. Attendance and apologies
2. Minutes of 2004 AGM
3. Matters arising from the meeting not on the Agenda
4. Chairman's report – Guenter Grethe
5. Treasurer's report – Geoff Downs
6. Update reports from sub-committees
 - 6 a. Public Relations – Janet Ash
 - 6 b. Meetings/training – Peter Nichols
 - 6 c. Grants – Bonnie Lawlor
 - 6 d. Awards – René Deplanque
 - 6 e. Fundraising
7. Election of Trustees
8. Proposal for extension of the AGM electronically and rule changes
9. Any other business
10. AGM 2006

The AGM will be followed by a dinner at Bumbles Restaurant, 16 Buckingham Palace Road, London. To book for the dinner, please contact David Walsh at david.j.walsh@pfizer.com

People and Places

Professor Ivar Ugi died on 29 September after a long illness. He was 75. There are brief announcements on the websites of the Technical University of Munich (<http://www.ch.tum.de/oc1/Iugi/iugi.html>) and the Estonian Chemical Society (<http://ecs.kbfi.ee/ugi.html>); readers may remember the remarkable recovery he made from his first stroke to give the keynote address at the 1996 Noordwijkerhout conference.

Dr Eugene Garfield, pioneer in the field of bibliometrics, celebrated his 80th birthday on September 16. His groundbreaking research in 1955 led to the first *Science Citation Index* in 1964, and ultimately to the creation of *Web of Science*.

Peter Schuhs has retired as financial managing director of FIZ Chemie Berlin. René Deplanque (a CSA Trust Trustee) remains as the sole managing director.

Bill Hayden is now senior vice president, Sales and Marketing, of Coalesix Inc. Based in Cambridge, Massachusetts, Coalesix focuses on the development and commercialisation of technology to improve the efficiency of drug discovery through the use of its Candidate Design Environment (CDE), Mobius. The chief technical officer is Jim Wikel, who has retired after 34 years at Eli Lilly and Company, most recently as head of computational chemistry.

Philip Judson has founded Lexeus Ltd, which develops and supplies software to support chemical hazard communication. The company offers two main products, LabelADVISOplus and SafeTEXT, which together provide a multi-lingual, multi-territory solution for chemical safety datasheets, classification and labelling.

2006 Herman Skolnik Award for Hugo Kubinyi

Hugo Kubinyi is to receive the 2006 Herman Skolnik Award at the Fall ACS meeting in San Francisco.

Born in Vienna, Austria in 1940, Hugo Kubinyi studied chemistry in Vienna, and at the Max Planck Institute of Biochemistry, Munich, Germany. From 1965–1966 he worked at the German Cancer Research Center (DKFZ), Heidelberg, Germany and in 1966 he moved to Knoll AG (now Abbott GmbH & Co. KG), Ludwigshafen, Germany where he was Research Scientist, Natural Products, Project Manager Chemical Research, and later Department Head of Natural Products Research. In 1985 he moved to BASF AG, Ludwigshafen, where he was Head of Drug Design (Molecular Modelling and Protein Crystallography), and then Head of Combinatorial Chemistry and Molecular Modelling (including Pro-

tein Crystallography and Drug Design). From 1986 he was also Professor of Pharmaceutical Chemistry at the University of Heidelberg.

He has received many awards and has published five books on QSAR, 3D QSAR and drug design. He is one of the editors of the book series *Methods and Principles in Medicinal Chemistry*. He was Vice-Chair (1991) and Chair (1993) of the Gordon Research Conference 'Quantitative Structure-Activity Relationships', Chair of the QSAR and Modelling Society and a member of the Editorial Boards of the journals *Current Drug Discovery*, *Current Opinion in Drug Discovery & Development*, *Journal of Chemical Information and Computer Sciences*, *Medicinal Chemistry Research* and *Quantitative Structure-Activity Relationships*.

17th International Chemical Information Conference and Exhibition (ICIC)

The 17th International Chemical Information Conference and Exhibition, organised by Infonortics, Ltd, took place in Nîmes, France from October 16 to 19 2005. There were a large number of attendees and about 25 papers presented by a variety of authors. Presentations can be viewed at <http://www.infonortics.com/chemical/ch05/05chempro.html>.

Some impressions are that the conference is:

- alive, well and robust;
- attended by many new faces;
- relevant to producers and practitioners in the chemical and patent information communities.

Highlights of this year's programme included the usual round of obligatory talks by industry notables (some of which were a little less than stellar) and some new things.

Martin Hicks made an original presentation in the form of a parable on the very interesting topic of scholarly publishing using the new Beilstein journal as an example.

A preview of Steve Arnold's just-published *The Google Legacy* was followed by John Lewis Needham from Google, who confirmed some of the findings and put them in perspective.

Willem Laagemat had the most unpronounceable word in his presentation. It was Dutch, of course, 'uitgerversmaatschappij' the meaning which was relevant and given but forgotten by this reporter. My spell-checker thinks it should be 'interferes' but it is not.

Harry Collier (CSA Trustee and conference organiser) complimented Rob Scoffin, speaker from CambridgeSoft, for his very informative talk that clearly made the case for electronic lab notebooks without being a product review. It was a quite refreshing approach. Indeed, all of the speakers were of the quality expected in a meeting of this calibre.

As usual, some of the most informative (and some of the most dull) presentations were in the product reviews that remain a valuable part of the programme. The exhibition was full and well-staffed. This year's sponsors were generous providing food, drink and transportation as a part of the conference.

Success begets success and next year's ICIC is planned for October 2006, to be held in Nîmes, France 22–25 October 2006.

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ExemplarChem

Normally at this time of the year, we include in the Newsletter a report on the annual ExemplarChem competition prizewinners' meeting in London. Unfortunately, there was no such meeting this autumn.

Dr Sean McWhinnie of the RSC's Science Policy unit has told us that "Having reviewed ExemplarChem

we (the RSC) decided to stop the activity. We felt that we had given the project a good go and detected that there had been a downturn in the number of entries. Therefore, we felt it was better to call a halt whilst ExemplarChem was still a success rather than wait for it to fade away." Sean thanked the CSA Trust for its support over the years.

CINF–IO Informatics Scholarship for Scientific Excellence

The scholarship program of the Division of Chemical Information (CINF) of the American Chemical Society, funded by IO Informatics, is designed to reward graduate students in chemical information and related sciences for scientific excellence and to foster their involvement in CINF.

Five scholarships valued at \$1,000 will be given out at both the Spring and Fall ACS National Meetings in a given year for a total of \$10,000/year. The winners will receive an annual licence, free of charge, of IO Informatics's software Sentient for their academic institution.

Grants were awarded at the 230th ACS National Meeting in Washington, DC, to:

- Jerome Hert, Krebs Institute for Biomolecular Research and the Department of Information Studies, University of Sheffield, for his poster 'Turbo Similarity Searching'
- Kunal Aggarwal, School of Chemical and Biomolecular Engineering, Cornell University, for 'Framework for integrating transcriptomic and proteomic profiles in *Escherichia coli*'
- Ivan Tubert-Brohman, Department of Chemistry, Yale University, for 'Mok – A Domain Specific Language for Molecular Information Processing'.

Applicants must be enrolled at a certified college or university. They have to present a poster at the respective National Meeting. Abstracts for the poster have to be submitted according to ACS rules by the deadline for electronic submission using OASYS (<http://oasys.acs.org/oasys.htm>). Applications are accepted for the 2006 Spring ACS Meeting in Atlanta (March 26–30, 2006). The deadline for submitting an abstract is November 23, 2005. A 2,000-word long abstract describing the work to be presented has to be sent in electronic form before February 1, 2006, to the chair of the selection committee at ggrethe@comcast.net. Questions related to applying for a scholarship should be directed to the same e-mail address.

Winners will be chosen based on content, presentation and relevance of the poster and will be announced at the meeting. The content shall reflect upon the student's work and describe research in the field of chemoinformatics and related sciences.

Jacques-Émile Dubois, the man who wanted to cancel the frontiers

Professor Jacques-Émile Dubois, Emeritus Professor at the Université de Paris 7, died on April 2, 2005. He had a profound influence on the electronic storing, processing and analysis of chemical information, as is recognised in the following personal tributes. The full text of the tributes is to be found on the CSA Trust website, <http://www.csa-trust.org>.



My recollection of Professor Dubois goes back further than for most people in chemical information. In my PhD work in the late 1960s, I was investigating the mechanism of halogenation of cyclooctatetraene and came across his reports of careful measurements of the rate of bromination of alkenes. Jacques-Émile had made himself a name in physical organic chemistry way before venturing into chemical information. He strongly believed in the importance of high-quality data and understood how much work has to go into their acquisition. It became quite important for him to seek methods for sharing such valuable data efficiently – a trait that runs through his entire life, even after retirement as chairman of CODATA (Committee on Data in Science and Technology).

Sharing data in a world where the amount of information was dramatically increasing asked for new approaches, and he saw that this could only be achieved by electronic means. It was also clear to him that physical and chemical data of compounds are intimately tied to the chemical structure. Ways had to be found to store and retrieve chemical structures. The DARC (Documentation & Automated Research on Correlations) system evolved from this

work. His vision in developing the DARC system cannot be overstated. At a time when most approaches to chemical structure coding were using fragment codes and other highly compressed methods, he insisted that the representation of a chemical structure should give access to each individual atom and bond of a molecule. Nowadays, as everybody represents chemical structures by connection tables, the structure coding of the DARC system seems quite obvious; at the time of its inception it was revolutionary!

Jacques-Émile was not simply a theoretician, however, but also worked hard to implement his ideas into workable systems, and to develop globally available systems. Clearly, this meant a lot of effort convincing funding agencies and politicians to finance ambitious projects. Jacques-Émile was good at this: his intellect was quick, his tongue fast and insisting, his arguments convincing, even to politicians! One of his publications had the title 'The French National Policy in Chemical Information'. What else is there to say? When a scientist succeeds in shaping national policy, the science must be sound, the arguments convincing, and the political connections excellent!

It is sad that the databases and retrieval systems based on the DARC system as put up for commercial use by Télésystème-Questel were eventually put on hold and discontinued. The reasons were clearly not in the performance of the system but have to be due to non-scientific considerations.

It would be a difficult task to give a comprehensive overview of his work. I only want to mention his many contributions to the correlation of chemical structures with spectroscopic data. Again, this emphasises his physicochemical background and his strong belief in the importance of data. Even after retirement from academia Jacques-Émile was still highly active, particularly in making CODATA internationally recognised.

Jacques-Émile was an inspiring lecturer who gave flavour to any scientific conference in which he participated. He had broad interests that went way beyond science and I always enjoyed sitting at his table and discussing a wide range of topics. Often he was accompanied by his wife Bernice and their company was always stimulating. The intellectual curiosity of Jacques-Émile kept him young. You certainly would have taken him for 10 to 15 years younger than he actually was. Thus it was for me – and I guess for all of his colleagues and friends – quite a shock to hear that he has passed away.

Jacques-Émile, we will always miss you!

Johnny Gasteiger

In the 1960s, graph theory was akin to the dark side of the moon for most chemists. Jacques-Émile Dubois, however, recognised that it could be the basis of computer programs for chemical structure searching. In 1966, he published the first of a number of papers on what became the DARC system, truly the first structure search system. The software was solidly grounded in chemical graph theory and was ingenious and clever. In contrast to the American systems, DARC relied upon a circular

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motif. Its pathways, based on FRELS, took a circular but exhaustive route through all the possible permutations as it identified and selected correct solutions to the problem at hand.

Today, DARC survives but has lost its first place to systems from CAS. It is still used by structure searching professionals who like its power, particularly in patent searching, and are fond of the techniques inherent in the system. Its inability to retain its place stems from marketing issues and also because Dubois, patriotic Frenchmen that he was, preferred to publish in French journals. The great majority of papers on DARC appeared in journals such as *Bulletin de la Société Chimique de France* and it was only later that publication in, for example, the *Journal of Chemical Information and Computer Sciences* was embarked upon. This guaranteed limited visibility for DARC but Dubois' goals were top flight science and patriotism.

In 1992 the ACS honoured Professor Dubois with the Skolnik Award for achievements in chemical information research. A Symposium marking the award was followed by a reception at the Willard Hotel in Washington, arranged by the French Embassy which selected this 4-star Hotel and provided excellent French cuisine and wines.

Our friendship goes back to the 1960s but between 1989 and 2004, I was Editor in Chief of the *Journal of Chemical Information and Computer Sciences* and I had a great deal of contact with him. Beginning in 1984, he published in *JCICS* four papers describing applications of the DARC software to contemporary problems such as pattern recognition and simulation of IR spectra. I edited these papers and unsurprisingly, found them to be international class and top-flight, a pleasure to read and publish.

So like everyone else, I feel a great sense of loss on Jacques-Émile's passing. He was one of the very few truly great scientists that I have known. He was a clear leader in my own field of computer searching and, as a human being, was someone that I felt privileged to know and count as a friend.

Bill Milne

I want to pay tribute here to a man whose career exceeds the yoke of the scientific disciplines and the professional world. I will evoke the memory of the man who did not stop building bridges between public and private, university and defence, data processing and chemistry, IST (information science and technology) and politics. I will concentrate particularly on his pioneering work for information science and as a constant defender of IST. He was one of the first in France to understand its political value.

Also, I want to remember the man whom I knew in 1974 at the Ministry of Defence, with whom I shared the adventure of AUDIST (University Agency of Scientific and Technical Information). Then our paths crossed regularly during our professional careers till Spring 2004 when, worn out by his sickness, he had to cancel our weekly meetings in his famous office in rue Guy de la Brosse.

Being among the first chemists to introduce data processing into his discipline, he began to cancel frontiers among disciplines. By inventing the DARC system which was operational in 1965, he also became one of the French pioneers of information science.

In the field of documentary achievements, in addition to the PLURIDATA data banks produced at ITODYS and using DARC, he put together a group of data banks inside IST, which all respected certain originality and quality standards for their contents: PLURIDATA, CRISTAL-LODATA, THERMODATA, ERGODATA, JURISDATA.

All his undertakings were part of national policy implemented by the French government. In the context of the cold war, IST, instrument of the space conquest and race for nuclear weapons, was committed to international competition, in what the newspaper *le Monde Diplomatique* in November 1979 called "the data war". The DARC system was not only innovative but it was also a political weapon. It constituted the backbone of the French cooperation with CAS. To counter the CAS monopoly of chemical information, in 1979 the National Center of Chemical Information (CNIC) was created under the influence of Jacques-Émile Dubois. CNIC had the mission of coordinating the national effort for the development of data banks complementary to CAS and also to

promote the DARC system in order not to be a simple customer. In fact, CNIC became a partner of CAS.

Jacques-Émile Dubois had been the Director of the Research Department at the Ministry of National Defence. Then he had an active part in the installation of the IST infrastructure in France during the 1970s. Jacques-Émile Dubois had a leading role in the majority of the decisions concerning the information politics: creation of BNIST, MIDIST, CNIC and then AUDIST.

His important but not always public role in national IST politics would gain visibility with the creation of AUDIST in 1978. He directed the Agency until 1981.

Jacques-Émile Dubois worked out and implemented an overall policy of IST, integrating for the first time in France all aspects of filing, keeping and transferring information and also using all means offered by the National Library, the University Libraries, the CNRS and the network of university data banks. Several frontiers considered closed were crossed: university and industry but, especially, for the first time in France, university libraries and the IST sector.

After the adventure of AUDIST, Jacques-Émile Dubois was elected vice-president of CODATA, then president. Finally from 2000 to 2005 he was the CODATA France chairman. He was working hard for the development of the CODATA site when disease struck him.

Jacques-Émile Dubois's last creation once again testified to his constant will to abolish borders. To encourage the studies of defence in the academic world, in 1993, he founded with Admiral Lacoste the Center of Scientific Studies of Defence at the University of Marne la Vallée.

From now on, we have to speak of Jacques-Émile Dubois in the past tense, but DARC is always active and the man will remain in our minds which he has contributed so much to form. He dedicated his life for the service of an ideal, that of science. He belongs to those explorers who have contributed to draw the contours of information science and who could translate IST problems into political terms.

Serge Cacaly
President of the Paris-Marne University

He was the founder and Director of this lab and, to all of his ex-students, remained its father. Of the various positions he held, the lab was his pride and passion. Very recently, during one of those numerous friendly conversations I was lucky enough to enjoy with him, (since, until forced to stop, he still came to his office some three days a week), he showed me how attentive he remained to its evolution, to the progress we were making. I felt he was both satisfied and happy that all he had given and dedicated to the ITODYS, including the solidarity he had passed on to us, was in such good working order more than 40 years after he'd begun. The research areas of the lab have evolved, but, interestingly, our core research areas, namely organic surface phenomena, bioorganic chemistry, supramolecularity, theoretical and informatic chemistry, and nanometric composite structures, are all a continuation of research ideas he seeded. Every researcher in this lab is fully conscious of the fact, and our choosing to keep the lab's name as ITODYS, even though some of the letters now stand for a new meaning, reflects the gratitude we all felt. That decision warmed his heart at the time.

To describe his personality in a few words is not my purpose. I would simply say he was an exceptional man, of a calibre one seldom meets in a lifetime. His resume alone is eloquent and forces respect and admiration. From a scientific vantage point, he will remain for us a man of challenge, endowed with extraordinary intuition and analytical capability, someone who dismissed ready made wisdom and took an impish pleasure in demonstrating that it was possible to resolve things deemed impossible. An example is the TitraVIT, an automated electronic apparatus devised to analyse solutions. He conceived and patented the machine in the 1950s in the Saar. It enjoyed a great and long-lived commercial success in France. This titrimeter, which functioned smoothly and fully satisfied the needs of the analysts, had a very rare feature for the times, in that it used a pair of metallic electrodes as captors. Analytical electrochemistry specialists, relying on the then prevailing theories for the acids and bases properties, had predicted the failure of such a set-up. Jacques-Émile Dubois seized the challenge, followed his intuition and proved he was right. Explanations came later: the key was that the objective had been reached in the teeth of all predictions to the contrary.

His scientific culture was incredible. With an astonishing and almost boundless intellectual curiosity, as a young researcher in the 1940s, he had assimilated the history of chemistry, conducting a critical analysis of all the publications by French chemists in all disciplines. This thirst for knowledge

and understanding never waned. He kept surprising us by remaining at the cutting edge of information despite a very busy schedule. He would regularly forward us scientific clippings, annotated by him, with on top: "urgent; interesting for us; come back to me quickly on this; try it". That was one of his typical ways of keeping us on our toes and of making sure his ideas progressed. The recipient wasn't always thrilled, but would act on it and our research progressed all the faster.

His broad knowledge of chemistry in its increasing diversity and complexity also made him insist on a multidisciplinary approach, indispensable in studying and resolving the great challenges of chemistry, particularly of physical organic chemistry. Very much in the mode of an orchestra conductor, he would swiftly assemble and coordinate highly varied teams and instrumental means, tailored to the projects underway, such as a group dedicated to electronics and informatics, which contributed to developing, within the lab, the expertise in techniques for data storage and processing. Such groups, made up of informatics-electronics experts, of chemists specialising in rapid kinetics, in photochemistry, in spectroscopy, in electrochemistry and automated solution analysis, soon gave the ITODYS a reputation for excellence, particularly in rapid kinetics and more generally in the area of reactivity of transitory species with an ultra-short lifetime.

In parallel to spectacular advances in instrumentation, Jacques-Émile Dubois set himself another challenge, that of marrying chemistry and informatics. It was due to our studies of reactivity, which featured specific electrochemistry apparatus adapted to the study of olefin reactivity, and in the course of which we noticed some very erratic electrode behaviours, that he conceived the idea of launching the study of surface phenomena in the lab and urged me to undertake research in that field. As usual, we were practically alone in our interest at the time. Electrochemistry colleagues showed little interest in this type of research, which seemed quite esoteric to them, very much in the off-the-wall tradition of the ITODYS researchers on Professor Dubois' team. We continued to swim upstream for a time. Being a young researcher concerned with his career, I was beginning to doubt the validity of that research area and the wisdom of venturing forth in a complete desert. Once more, his persuasiveness carried the day, and I still remember his encouraging words: "Don't worry, Lacaze: surface phenomena, organic films, those are the future". Again, his visionary sense of the evolution of chemistry's centres of interest proved well-founded. As time went by, this research

area was widely taken up in the USA, before, with some lag, taking root in France. It now represents one of the major research poles of the ITODYS, and shows the premonitory and visionary nature of Jacques-Émile Dubois' perception. I hope these few memories have shown his decisive influence on the development of the ITODYS, a laboratory which, some 40 years after its birth, retains an excellent position in the CNRS rankings. With the disappearance of Jacques-Émile Dubois, we lose an emblematic figure of organic physical chemistry, an exceptional scientist, a man of great heart and a friend to us all.

Pierre Lacaze

From Notes at Jacques-Émile Dubois' funeral in April 2005

I first met Jacques-Émile Dubois at, what turned out to be a seminal conference, in 1972 in Noorwijkerhout at the NATO/CNA ASI on Computer Representation and Manipulation of Chemical Information. The DARC system which he described at that conference was years ahead of most anything else available at the time. The work Richard Feldmann and I were involved in at NIH overlapped heavily but he was delighted to discuss his work and was very encouraging.

For more than 30 years, we met often at meetings, and whenever I was in Paris I would go to dinner with Jacques and Bernice, who, being a New Yorker like myself, made these meetings and dinners even more pleasant. He was always working on something new and with an enthusiasm that it is hard to describe. What attracted me so much was his dedication to his projects and to moving the field of computers in chemistry forward. His efforts with CODATA were another example of his international view. He was always there to talk to and bounce ideas off. As a young and junior player in the field he helped encourage me to try new things and not worry about breaking rules. He always was looking to the future and to new things, and this philosophy has helped shape my thoughts and activities throughout my career. I will very much miss him and the stimulation I have received from him over the years.

Steve Heller

I knew Jacques-Émile only from meeting him at conferences, first at the memorable NATO conference in the Netherlands in 1972. This was a highly significant event for those working in the field now called chemoinformatics. It brought together for the first time many scientists working in otherwise disparate fields: some from chemistry laboratories, other from computer science laboratories, information systems, etc. A significant feature of this conference was a transatlantic telecommunications link for demonstrations – the first that most of us had seen, and an early sign of the future that we all enjoy. We owe much to those who conceived the need for such a conference and acted accordingly.

Jacques-Émile and I happened to sit together on the cruise boat during the canal tour. We became so absorbed in our exchanges that the scenes of Amsterdam passed quite unnoticed. That was typical of Jacques-Émile – total absorption in the science to which he contributed so much.

It was interesting and revealing that he found diagrams, like structures, very evocative, and that he used them extensively to suggest, support and develop novel approaches in his work. This related equally to the conceptual level and to the graph theoretical chemical structure level. Which came first, I do not know.

The DARC system evolved directly from the scientific directions he was pursuing in physical organic chemistry, in terms of identifying structure-activity correlations. EURECAS, an early subset of the CAS Registry System, which was inaugurated on the DARC system in 1978 and which anticipated the advent of CAS Online by several years, had a huge impact, besides being an outright imaginative tour de force in computational terms. Its appeal to industry was immediate and widespread. Once again, when the Markush DARC system was introduced at a later date, it was equally valued.

Jacques-Émile and I met at several other conferences, including the International Conference on Computers in Chemical Research and Education (ICCCRE) held in Paris in the mid-90s, which he led. As host to ICCCRE he was magical, with time and attention for everyone, a generous host to an admirable scientific event, an imaginative conference leader with a well-balanced program, and all this in so beautiful a city.

We met most recently at a conference organised by the Chemical Heritage Foundation of Philadelphia in 2002, where he was accompanied by his delightful wife, Bernice. The topic of the conference was the early days of research on computers in chemical information. Jacques-Émile gave not the least indication that he was already in his early 80s; he delivered a sparkling paper which demonstrated how well models had served him in his thinking, and how the development of the chemical and the machine representation ideas stemmed from the same thinking.

His modesty was remarkable; he was not one to boast about his manifold contributions to science outside his mainstream activities, nor about the many awards which he had been given. To learn something more about the huge range of his activities, of which I for one was completely ignorant, has been most instructive, but all of a piece with the man.

Mike Lynch

It is with great emotion that I recall the activities of Jaques-Emile Dubois, the inventor of the DARC system. It was a thrilling adventure, in which he expressed the full range of his talent and personality: creativity, imagination, vision, but also sense of humour, self-deprecation and charisma.

At the outset in 1954, there was curiosity and intuition; the object of curiosity: given a population of ketones and IR spectroscopic data, how could one link the evolutions in the relative location of atoms to the evolutions of experimental data; the intuition: the relative position of the atoms is topology and one needs to quantify the evolution of this topology on a population. From that point on, all was said, and all remained to be done. He set about it with originality, persistence and conviction.

A multi-generational adventure

He conducted his adventure with several waves of researchers. From 1954 on, I've counted 7 to 8 such waves. Our purpose was fundamental research, without any concern yet as to concrete applications, other than satisfying the initial curiosity and validating and fleshing out his early intuition. In the second wave, to which I belonged with H. Viellard, M. Chastrette, F. Hennequin., our endeavours thus concerned the definition and coherence of the concepts, the rigour of processes and the elegance of the logic. The research conducted under his guidance for almost 50 years led to methods of apprehending molecules, chemical reactions, ever broader and fuzzier sets, using concepts such as hyperstructure, correlation and identification methods etc. This fundamental research led to the birth of real chemical informatics systems, among which the DARC is a reference. His action was twofold:

At national level: faced with gaps in our chemical industry, he created or orchestrated the creation of transfer structures which enabled him to demonstrate the operational viability of the system

Internationally: it was key to gain access to the databases of leading US institutions such as CAS in order to enrich them and heighten their value and performance for users. Hardly an easy negotiation! His assets? His conviction, people skills, findings and mastery of English.

A human adventure

For those in my 'wave', as for those who followed us, there was a very human dimension, for he was a man of great heart. Those of us who suffered traumatic events in their personal lives can testify to how intensely present he was for them in such circumstances! Those years are among the best memories of our professional lives. To speak of 'professional life' is almost a misnomer: we did not then have the impression of belonging to a 'profession', of managing a 'career'. We were not in quest of status, but motivated by the sense of belonging to a team engaged in a thrilling race. He was 45 at the time. He already had an international reputation. The average age in the lab was 25 and, under his leadership, we felt like so many fearless conquerors. It is with great emotion that I recall those vivid Saturday or even Sunday meetings in the lab: the atmosphere was stimulating, free, outspoken, sometimes electric, for he knew how to stage an outburst now and then. Jacques Émile was young and always remained it. Open minded, curious of all things and people, he loved life and made us share his passion. Jacques Émile thought big, his vision was far reaching and he took great pleasure in what he was doing. Let me thank him for having drawn us into sharing this pleasure.

Daniel Laurent

Connect 2005

Connect 2005, the 12th National Convention of the Royal Australian Chemical Institute (RACI), took place in Sydney from July 3 to 7. Held once every five years, the convention provides a showcase for Australian chemistry, establishing a platform for the exchange of ideas among Australian chemists, and between Australian chemists and international leaders. The convention was held at the Darling Harbour Convention Centre in Sydney (see right), and attracted almost 1200 participants.

Six outstanding convention plenary speakers gave interesting and unique perspectives on the challenges facing chemistry as a discipline, and on the exciting advances taking place at the boundaries between chemistry and other disciplines. They were:

- Mr Koichi Tanaka (General Manager, Mass Spectrometry Research Laboratory, Shimadzu Corporation, Japan) who is a Nobel Laureate for the development of soft desorption ionisation methods in mass spectrometric analyses of biological macromolecules;
- Professor Richard Zare (Marguerite Blake Wilbur Professor in Natural Science at Stanford University, USA), who is renowned for his research in the area of laser chemistry, resulting in a greater understanding of chemical reactions at the molecular level;
- Professor R. Mark Wightman (W.R. Kenan, Jr Professor of Chemistry, Department of Chemistry, University of North Carolina, USA) whose research interests centre around microelectrodes and their use to probe complex chemical and biochemical phenomena. More recently, Professor Wightman has also extended the applications of these devices to other areas including the generation of excited state, light emitting species from reagents produced electrochemically;
- Professor Bert Meijer (Eindhoven University of Technology, The Netherlands) whose research interests include dendrimers and novel architectures, supramolecular chemistry, organics with unconventional electro-optical properties;
- Peter G. Schultz (Professor of Chemistry, The Scripps Research Institute and Director of the Genomics Institute of the Novartis Research Foundation) who spoke on the development of methods for incorporating unnatural amino acids and base pairs selectively into proteins and nucleic acids, respectively;
- Professor Andrew B. Holmes (FRS, Bio21 Institute, University of Melbourne, Federation Research Fellow) who spoke on electroluminescence of poly(para-phenylene vinylene).



The conference was chaired by Professor Tony Baker from the University of Technology Sydney, with the support of a very able committee. The RACI Division involvement was excellent with 12 of the 13 represented at the Convention, and a relatively large number of cross-disciplinary sessions.

The Biomolecular Chemistry Divisional Program at Connect 2005 covered all aspects of medicinal chemistry from discovery and design to development. The Division ran a four-day meeting. Sessions highlighted current important topics in drug design and development, including bioactive drug discovery; synthesis and biological evaluation of drugs targeting ion channels, G-protein coupled receptors, enzymes, RNA and DNA; structure-activity relationship studies; molecular modelling; biological structural analysis; and the impact of cereals in health. The divisional plenary lecturers were:

- Professor Nobutaka Hirokawa, (University of Tokyo) who spoke on his work on the kinesin superfamily of proteins;
- Professor Peter G. Schultz (Scripps Research Institute and Director of the Genomics Institute of the Novartis Research Foundation) who discussed encoding unnatural amino acids into organisms;
- Dr David Wustrow (Director of CNS Drug Design, Pfizer R&D) who provided an excellent case for the $\alpha_2\delta$ calcium receptor as the mode of action of Pregabalin and Gabapentin in neuropathic pain.

The 13th National Convention takes place in 2010.

Dave Winkler

SPONSOR'S SPOTLIGHT

Questel.Orbit

Questel.Orbit is the result of the merger in 1995 of two online vendors: Orbit, which was founded in the early 1970s, and Questel, which was founded in the late 1970s. Both companies were recognised for their inventiveness. Together with Derwent, Orbit created the first DWPI file, the "must have" patent file used all over the world, and Questel was involved in chemical structure searching with the DARC system from the very beginning. It is worth remembering that, thanks to cooperation between the Paris University and Questel under the sponsorship of the Ministry of Research, the full CAS Registry file became publicly searchable as early as 1980. Consequently, with this expertise, Questel was chosen by both Derwent and INPI for the development of the next generation of DARC, namely Markush DARC aimed at handling generic formulae found in patents.

Another big development in Questel.Orbit has been its strong involvement in the development of EPOQUE, which is used today by thousands of EPO examiners and by SIPO, the Chinese Patent Office in Beijing.

In 1999 Questel.Orbit decided to focus its activities fully on intellectual property; that is, patent and trademark information and related services. All services are based on a vast collection of databases covering well-known files like *Thomson Scientific DWPI* or *EPO INPADOC*, full text patent files as well as proprietary databases like *PlusPat* or *FamPat* covering patents from over 70 patent issuing authorities. Similarly, the trademark collection includes 24 databases covering Europe and North America.

Recent developments include the latest versions of web services for both the expert and professional end user:

- *Qweb* giving access to the whole Questel.Orbit database collection for expert searchers
- *Qpat* designed for professional end users working around patents

- *TrademarkExplorer* for initial screening of trademark name availability
- *TrademarkExpert* for thorough analysis of similar trademark names

as well as a brand new version of *MMS* under Unix monitored by INPI, the French Patent and Trademark Office, which has been greatly enhanced, in particular with much better response times and expanded limits.

Last year, Questel.Orbit decided to expand its offering vertically, covering more needs in the field of intellectual property. In this respect, it acquired several companies:

- *Artegy Telematique*, expert in trademark search engines
- *Digipat*, able to deliver file wrappers on both patent and trademarks, especially in the US where there is great demand for such services
- *Editat*, offering both screening and advances searches on trademarks, and patent and trademark patent portfolio management software.

The company also took shares in Lingway, a leading company in language engineering. This company developed a series of tools such as *PatReader* aimed at facilitating reading of long text documents such as patents.

In order to cover information from the Far East better, Questel.Orbit has signed cooperative agreements with PATOLIS Corp., the largest Japanese company in the field of intellectual property information.

There is further information on these websites:

www.questel.orbit.com
www.digipat.com
www.edital.com
www.lingway.com
or e-mail at pbuffet@questel.fr

Company News

Digital Chemistry

John Barnard, Tony Cook, Geoff Downs, Julian Hayward and Matthew Wright have announced the formation of Digital Chemistry Ltd and its acquisition of Barnard Chemical Information Ltd (BCI). Digital Chemistry was incorporated in September 2005 and has offices in Leeds, UK. The company's goals are to deliver sophisticated software tools and services which address the cheminformatics needs of researchers within the pharmaceutical and related industries. Initial products will be based on the well-known BCI Toolkit and will include new web services. The website is at <http://www.digitalchemistry.co.uk/>

40 years of the CCDC

Founded in 1965, this year the Cambridge Crystallographic Data Centre celebrates 40 years of service to the scientific community. The 40th anniversary of the RSC's *Chemical Communications* also occurs in 2005. The CCDC has contributed a 40th Anniversary article: 'Librarians, Crystal Structures and Drug Design', which has been published in Issue 41 (2005) as *Chem. Commun.*, 5135–5140, 2005, and can be accessed by subscribers to the journal at <http://www.rsc.org/Publishing/Journals/CC/article.asp?doi=b511106b>.

There is more information about the anniversary on the CCDC website at http://www.ccdc.cam.ac.uk/ccdc_40th_anniversary/

EVENTS 2005–2006

November

28	CSA Trust AGM, SCI, 14/15 Belgrave Square, London, followed by the Annual Dinner, Bumbles Restaurant, 16 Buckingham Palace Road, London (see page 2)	To book for the dinner, please contact David Walsh at david.j.walsh@pfizer.com
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29 November – December 1	Online Information, Olympia, London, UK	http://www.online-information.co.uk
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December

15–20	Pacifichem 2005 (International Chemical Congress of Pacific Basin Societies) Honolulu, Hawaii, US	E-mail: Pacifichem@comcast.net http://www.pacifichem.org
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2006

March

5–8	IPI-ConfEx 2006, International Patent Information Conference and Exposition, Athens, Greece	Trudi@IPI-Institute.com www.IPI-ConfEx.com
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13–16	Drug Discovery Technology Europe 2006, Novotel London West, London, UK	http://www.ibc-lifesci.com/novotel/2006/ddt2006/main/ddt2006.asp?Page=overview
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13–16	InfoTechPharma 2006, Novotel London West, London, UK	http://www.ibc-lifesci.com/novotel/2006/it2006/premailer/it2006pre.asp?Mainpage=brochure
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26–30	ACS Spring Meeting, Atlanta, Georgia, US Includes Joint CSAT/CINF symposium, 'De Novo Design and Synthetic Accessibility' (see page 12)	http://www.chemistry.org/portal/a/c/s/1/acsdisplay.html?DOC=meetings%5cfuture.html
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April

24–26	Advances in Drug Discovery and Development, Tokyo, Japan	http://www.drugdisc.com/japan
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May

8–11	MipTec – The 9th International Conference and Exhibition on Drug Discovery, Basel, Switzerland	http://www.miptec.com
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28–31	International Conference on Computational Science (ICCS) 2006: Advancing Science through Computation, University of Reading, Reading, UK	http://www.iccs-meeting.org/iccs2006/ Email: iccs2006@reading.ac.uk
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29 May – 1 June	Workshop on Chemoinformatics in Europe: Research and Teaching, Obernai, France	http://infochim.u-strasbg.fr/recherche/europeen_chemistry/index.php
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August

7–10	IBC's Drug Discovery Technology World Congress Boston Convention & Exhibition Center, Boston, MA	http://www.drugdisc.com/section.asp
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September

10–14	232nd ACS National Meeting & Exposition, San Francisco, CA
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Product News

Marvin 4 and MarvinSpace

ChemAxon has released version 4.0 of its platform independent chemical editing and visualisation suite Marvin. The release includes the launch of MarvinSpace, a new tool for 3D molecular structure visualisation. The release sees many new features and improvements such as template based structure cleaning, 3D editing, lone pair support and an attached data function to annotate atoms with user defined data. 3D conformer generation is improved further giving increased coordinate accuracy. Although at an early development stage, MarvinSpace already provides unique functionalities and high performance within a fast evolving public development. To try out MarvinSpace please visit www.chemaxon.hu/shared/MarvinSpace/index.html. ChemAxon provides free licences for all of its toolkits to teachers and academic researchers. There is more information at www.chemaxon.hu/forum/ftopic193.html

Science of Synthesis Version 3.0

This new release has a completely redesigned interface and brand new functionality. The key topics covered are organometallics; heteroarenes and related ring systems; nitriles, isocyanides, and derivatives; ketones; and heteroatom analogues of aldehydes and ketones. This information together with the Houben-Weyl legacy archive means that the user has access to synthetic chemistry information from the early 1900s up to the present day. New search functionality means that structure and reaction searching is enabled via ISIS/Draw, ChemDraw 7.0, an inbuilt Java applet and the possibility of uploading Molfiles. It is possible to refine a structure/reaction search via CAS Registry Number. Also, the new Name Reactions search option gives the chance to browse through well-known reactions illustrated in the series. The product can be found at the Thieme Chemistry website under <http://www.science-of-synthesis.com/>.

DiscoveryGate for Mac OS X Tiger

Elsevier MDL has released a new Mac OS X version of its DiscoveryGate content platform. The release is fully Tiger compatible and offers the scientific community broader access to a structure-searchable online platform for integrated researching of scientific content from databases, journal articles, patent publications and reference works.

DiscoveryGate incorporates recent upgrades to provide faster responses to complex queries, improved usability and easy installation and maintenance. New data sources recently available through the platform include the xPharm database, the world's largest pharmacological reference work, and MDL Patent Chemistry Database, an extensive collection of reaction and substance data for scientists. For more information, visit discoverygate.com.

IUPAC International Chemical Identifier

InChI is a protocol for converting a chemical structure (connection table) to a unique, predictable ASCII character string. It is not a registry system. Version 1.0 expresses chemical structures in a standard machine-readable format, in terms of

atomic connectivity, tautomeric state, isotopes, stereochemistry, and electronic charge. It deals with neutral and ionic well-defined, covalently-bonded organic molecules, and also with inorganic, organometallic and coordination compounds. The software, documentation, source code and licensing conditions are available from the IUPAC website at <http://www.iupac.org/inchi>. To enable development of InChI facilities and applications in an Open Source context, a project to encompass this work has been registered with SourceForge.net (see <http://sourceforge.net/projects/inchi>); people wishing to participate should contact the project administrator (mcnaughta@rsc.org) or the IUPAC Secretariat (secretariat@iupac.org). To receive and discuss proposals for InChI enhancements, an internet listserver has also been established; people wishing to participate in these discussions should contact Alan McNaught (mcnaughta@rsc.org).

Wiley Registry 7th Ed/NIST 2005 Mass Spectral Library

This comprehensive library of more than 461,000 mass spectra combines the Wiley Registry of Mass Spectral Data, 7th edition and the NIST/NIH/EPA Mass Spectral Library 2005. The coverage is extensive and includes: pharmaceuticals, illegal drugs, chemical weapons, environmental pollutants, metabolites, flavours and fragrances, and various compounds of interest. It features 820,528 unique chemical names and 222,553 unique CAS numbers. Formats include NIST MSSearch/Thermo Xcalibur and Agilent Chemstation. For more information please visit <http://www.wiley.com/go/databases>.

MMS, Merged Markush Service

The Merged Markush Service is the product of a collaboration between Derwent and INPI (the French Patent Office), providing a joint file which combines the existing MPHARM and World Patents Index Markush (WPIM) files on Markush DARC. It provides the largest Markush structure coverage available online with over 1,600,000 structures records representing 450,000,000 specific real and prophetic structures. It also includes the Thomson Derwent Chemical Registry. All chemicals are covered from 1983 to the present; the coverage goes back to 1978 for pharmaceutical patents. Searching is possible via a new Unix version of Markush DARC developed to offer faster and more flexible searches. Results can then be cross-searched with either DWPI or Pharmsearch. There is more information at <http://scientific.thomson.com/products/markush/>

Sentient Suite Version 2.7

IO Informatics has released Sentient Suite, Version 2.7, which allows a user to assemble, view, analyse and search very disparate information in a common environment. The disparate data can be numeric values, images, spreadsheets, web content, public or private databases, or information from applications. Enhancements include new knowledge-building functionality based on all accessible information sources and workflow management of projects across experiments and methods. There is more information at <http://io-informatics.com>

Joint CINF–CSA Trust Symposium

De Novo Design and Synthetic Accessibility

at the ACS Meeting in Atlanta, GA, USA

March 26–30, 2006

Several inroads have been made into the design of novel molecules as potential leads for new drugs. These methods may be either based on a knowledge of the 3D structure of the target protein and its binding pocket or may rest on an analysis of a series of ligands of the protein. The molecules thus designed have quite different complexity and thus an estimate on how easy – or difficult – their synthesis might be is of paramount importance for the medicinal chemist.

This symposium intends to show the present state of affairs both in the de novo design of lead structures and in methods for estimating the synthetic accessibility of organic structures.

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Chair – Fund Raising

Vacant

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