Mass Spectrometry PittCon® 2004

Reviewed by O. David Sparkman
Mass Spectrometry Consultant
5354 Thunderbird Court
Antioch, California, USA
ods@compuserve.com

A lot of things were different between this and last year's Pittsburgh Conference on Analytical Chemistry and Applied Spectroscopy other than the 40 degrees in the evening temperatures. PittCon 2004 was held in Chicago, Illinois, March 7–12. The organizers reported a registration of 25,025 distributed between 12,586 conferees, 12,221 exhibitors, and a press core/business consultant group of 218. This year's registration was slightly higher from last year's, which was 24,057. The actual number of attendees is always somewhat less than the number of registrants. Students (including those from local high schools) are counted with the conferees. The organizers made a special point of the fact that over 1,000 conferees were registered on Thursday. This was more than four times what has taken place in previous years. This year, there were 1,195 companies exhibiting in 2,714 booths compared to last year's 1,260 companies in 2,856 booths. The Exhibition was open from 9:00 a.m. to 5:00 p.m. Monday through Wednesday and from 9:00 a.m. to 3:00 p.m. on Thursday. The small size was evident in your ability to transverse diagonal to diagonal. The appearance was as large as ever, but the ability to cover the area was much greater due to the reduced size.

There have been a number of changes at the Chicago Convention Center since PittCon 96 when the conference was last there. All the interminable construction has been completed, and the shining new facility that greeted the 2001 Fall American Chemical Society (ACS) Meeting availed itself to the PittCon attendees. But what was not gone were the long lines for busses at the end of the day and the bus rides that could take up to one hour in the Chicago rush-hour traffic. The ACS offered two of its traditional mass spectrometry courses, whereas PittCon offered eight. Most of the PittCon courses have been offered in years past with the exception of one new one-day course entitled *Interpretation of LC/MS Spectra of Small Molecules* taught by E. Michael Thurman and Imma Ferrer (Department of Analytical Chemistry, Almeria, Spain). Drs. Thurman and Ferrer are the editors of the ACS Symposium Series 850 entitled *Liquid Chromatography/Mass Spectrometry MS/MS and Time-of-Flight MS: Analysis of Emerging Contaminants* (copyright 2003 American Chemical Society, Washington, DC, and distributed by Oxford University Press, ISBN: 0-8412-3825-1). I attended this course and found that it provided some useful and interesting information. For a one-day course, too much time was spent on discussion of the ionization techniques and the different types of *m/z* analyzers. Some very good examples were provided, but they often lacked clear explanation of fragmentation mechanisms. Attendance at this course, like that of all the mass spectrometry courses offered by the PittCon organizers and the ACS, was well into the double digits.

The technical program has improved over the years. One mass spectrometry exhibitor, in an effort to explain what he perceived to be fewer potential contacts, said that he believed that the technical program had improved to the extent that people were not spending as much time on the exhibition floor and were spending more time in the technical sessions. In the PittCon 2004 Technical Program Focus Areas At-A-Glance section of *The Final Program*, there was listed a total of 26 oral sessions, symposia, or poster sessions under the headings of *Mass Spectrometry, GC and GC/MS, and LC and LC/MS* that would have been of interest to those who are practitioners of mass spectrometry. This included *The Origin and Future of Macromolecule Ionization by Laser Irradiation* presented by Mr. Koichi Tanaka (Shimadzu Corporation, Kyoto, Japan), one of the three recipients of the 2002 Nobel Prize for Chemistry. Following Mr. Tanaka's noon-time presentation was another Special Nobel Prize Lecture held in the afternoon by Dr. Kurt Wüthrich (Institute of Molecular Biology and Biophysics, ETH Hönggerberg CH-8093, Zürich, Switzerland), one of the other 2002 Nobel Prize for Chemistry winners, entitled *The NMR View of Proteins*.

Just as ENC (*Experimental Nuclear Magnetic Resonance Conference*) has replaced PittCon as the venue for the introduction of new products in NMR, it appears that the annual *ASMS Conference on Mass Spectrometry and Allied Topics* is becoming the forum for new mass spectrometry products. Now that the ASMS conference includes an exhibition as well as extensive displays of iron in the users' meetings held by manufacturers in their hospitality suites, the stage has been set for new things in mass spectrometry to be introduced at this venue. A good example is the introduction of the new T-Wave technology for the Micromass tandem-in-space mass spectrometers made by Waters Corporation (Milford, Massachusetts) at the 2003 ASMS Conference, whereas PittCon 2004 was used to place emphasis on their new *Acquity Ultra Performance LC* system, which tied for the Gold for the annual *PittCon Editors' Award* with the TPI terahertz spectrometer from Bruker Optics (Billerica, Massachusetts).

This was the first year in some time since its inception that mass spectrometry did not take any of the prizes presented by the *PittCon Editors' Award* (established in 1995 by Dr. Gordon Wilkinson, the former Managing Editor of *Analytical Instrument Industry Report*, now sponsored by the PittCon Show Daily, which

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is owned and operated by Centcom, the organization that manages advertising for the ACS). However, a number of mass spectrometry products were nominated. They included the *Orthogonal NanoSpray Interface* for the *LC/MSD Trap* (Agilent Technologies, Inc., Santa Clara, California); the *Minotaur 300* cylinder ion trap mass spectrometer (actually introduced last year by Griffin Analytical Technologies, Inc., West Lafayette, Indiana); the *Finnigan LTQ LC-MS* (a linear quadrupole ion trap introduced at the ASMS Conference in 2003 and shown at PittCon for the first time in 2004 by Thermo Electron, San Jose, California); the *CP-4900 Differential Mobility Detector* for its portable GC and the *4000 Ion Trap GC/MS* (Varian, Inc., Palo Alto, California); and the *Micromass Quattro Premier* (introduced at the ASMS Conference in 2003 and shown at PittCon for the first time in 2004 by Waters Corporation).

Two significant business issues that came out of this year's PittCon were Waters Corporation's announcement of the conclusion of its litigation with Applied Biosystems Group (Foster City, California) and MDS/Sciex (Toronto, ON, Canada); and Thermo Electron's post-PittCon announcement that it had shipped its 100th LTQ. According to an article that appeared in *Instrumenta Analytical Instrument Industry Report* (18 March 2004, Vol. 20, 23/24), Richmond, Surrey, U.K., an agreement has been reached on pending litigation in the U.K., Canada, and Japan relating to Waters' loss of a U.S. suit that involved triple-quadrupole mass spectrometry technology; a separate suit brought about by Applied Biosystems relating to MALDI; and a suit initiated by Waters against Applied Biosystems involving electrospray technology. After making a final payment of $18.1 million, the two companies have reached an agreement on cross-licensing resulting in royalties to both parties. This brings to just over $70 million paid by Waters. According to the *Instrumenta* article, "The loss of the triple quadrupole case also led to loss of sales of $30–35 million in 2002/2003 as the affected products were reengineered, according to Waters' own estimates." This $100+ million (not including attorney costs) may be the largest settlement involving mass spectrometry technology to date.

In addition to the Ferrer and Thurman book already mentioned, there were three other books that appeared at PittCon for the first time this year: (1) the Elsevier *Encyclopedia of Mass Spectrometry Vol. 1, Theory and Ion Chemistry*, Peter B. Armentrout, Ed. (ISBN: 0-08-043802-4), which first appeared at the International Mass Spectrometry Conference in Edinburgh, Scotland, in the Fall of 2003, and was reviewed in *JASMS*, May 2004; (2) *Advances in Forensic Applications of Mass Spectrometry*, Jehuda Ynion, Ed.; CRC: Boca Raton, FL, 12/29/03, ISBN: 0849315220; (3) *Mass Spectrometry: A Textbook* by Jürgen H. Gross (Springer-Verlag: Berlin, Germany, ISBN: 3-540-40739-1, © 2004).

The following is an alphabetical listing of companies that presented new products of importance to the field of mass spectrometry. This year, companies that introduced software upgrades, model changes that did not involve new enhancements, or new sample handling devices will not be included.

Academy Savant (Fullerton, CA)

Academy Savant (formerly SAVANT–Sloane Audio Visuals for Analysis and Training) is a producer of computer-based training programs. At Pittcon 2004, Academy Savant introduced a new program entitled *Introduction to Protein and Peptide Analysis with Mass Spectrometry*. The content of this program is authored by Frederick E. Klink (STM, San Ramon, California), who teaches the ACS course *Peptide and Protein Characterization with Mass Spectrometry* with J. Throck Watson (Michigan State University, Departments of Biochemistry and Chemistry, E. Lansing, Michigan). This program is very detailed with comprehensive text, good illustrations, many of which are animated, and narration that can be turned on or off. The programming of the seven chapters was done by Dennis Saunders, who has authored a number of programs on chromatography and mass spectrometry for Savant. The program is well referenced, and there are a number of useful tools found in the Appendix.

Additional information on this and other Academy Savant interactive programs in mass spectrometry and chromatography can be found at http://www.academysavant.com.

Agilent Technologies, Inc. (Santa Clara, CA)

Agilent's Life Sciences and Chemical Analysis (LSCA) group had $1.2 billion dollars in FY'03 revenue with 3,700+ employees. The company continues to have product development in the U.S. in the Bay Area of California and Little Falls, New Jersey; in Europe in Waldbronn, Germany; and in the Far East in Tokyo, Japan, and Shanghai, China, with manufacturing in Little Falls, Waldbronn, and Shanghai. Agilent's LSCA group no longer has manufacturing in the Bay Area. Chris van Ingen, Senior Vice President and General Manager of the LSCA Group said that Agilent has successfully moved all of its gas chromatography manufacturing to Shanghai, where the quality is improved over previous manufacturing. He further stated that Agilent is beginning the manufacture of a 6820 GC, which contains a reduced feature set for sales specifically in China, India, and Eastern Europe. As also reported last year, the Chemical Analysis portion of the business continues to account for approximately 60% with the remaining 40% being attributed to the Life Sciences group. Q1'04 has shown a significant growth over FY'03 in the areas of orders, revenue, and operating profit, indicating a turnaround in the economy. One interesting slide shown in the Agilent Press Conference was a comparison of their operating profits with those of their competitors: Applied Biosystems, Amersham, Thermo Electron, and Waters. Agilent and Waters were

in the 28% region, Amersham and Applied Biosystems were around 13.5%, and Varian and Thermo Electron were both below 10%. In another slide comparing revenue growth, Agilent was somewhat between Waters with the low of 7.3% and Varian with the high of 8.6%. The other three companies were significantly lower with Applied Biosystems having a revenue growth of 3.1%, Amersham having 2.1%, and Thermo Electron having 2.6%.

Agilent's main mass spectrometry new product introductions at PittCon were the *7500ce* inductively coupled plasma mass spectrometer (ICP-MS) system for trace-metals analysis in environmental applications; the *LC/MSD Trap HCT Plus*; 21 CFR Part 11 compliant *GC/MS MSD ChemStation*; the *Orthogonal NanoSpray* interface for the LC/MSD Trap, and *Deconvolution Reporting Software* (DRS), which uses Agilent's *Retention Lock Library* systems with the National Institutes of Standards and Technology's (NIST) *AMDIS* (Automated Mass spectral Deconvolution and Identification System). Other products that were of significance that had been introduced earlier were the *LC/MSD TOF*, the *5973 GC/MSD Inert*, and the G1701DA D.01.00 version of the *GC/MS ChemStation*.

This was the second year in a row that Agilent and Bruker DALTONICS made new introductions regarding their jointly manufactured quadrupole ion trap LC/MS/MS instrument. Little information was provided last year as to the specifics of improved performance other than to say the HIGH CAPACITY TRAP had better sensitivity. This year, Agilent was ready with additional information. The HCT and HCT Plus use superimposed multipoles (hexapole or octupole) to add increased trap capacity that is proportional to the area inside a pseudopotential well. This modification to the traditional 3D QIT is described in "Non Linear Ion Traps" (Johen Franzen, R. H. Gabling, Michel Schubert, and Minga Yang, Chapter 3, *Practical Aspects of Ion Trap Mass Spectrometry,* Volume 1, *Fundamentals of Ion Trap Mass Spectrometry*; Raymond E. March and John F. J. Todd, Eds.; CRC: Boca Raton, FL, 1995). Agilent also reported some nonspecific modifications to the ion detection system. The *HCT Plus* is the new instrument. It is unclear if this instrument is a replacement for the HCT. The HCT was reported to have a sensitivity specification of 50:1 S/N (actually signal-to-background) for 1 pg of reserpine. The HCT Plus has a sensitivity of 50:1 S/N for 250 fg of reserpine. One data example shown in the booth presentation was of a triple-charge ion at *m/z* 461.9. The data obtained on the LC/MSD Trap SL was not capable of having the isotope peak *m/z* values assigned. The data obtained on the LC/MSD Trap HCT (not the HCT Plus) clearly allowed for the assignment of the isotope peaks every 0.3 *m/z* units, and these multiple-charge isotope peaks were clearly resolved. Another addition to the LC/MSD HCT and HCT Plus was the *Orthogonal Nanoelectrospray* source. The performance was reported in an oral presentation by Paul Goodley (WOCam 11:35, LC/MS: Future of Liquid Separations "A Novel Microfluidics Orthogonal Electrospray–APCI Ion Source") at the 2003 ASMS meeting. Although the Bruker DALTONICS Esquire and the Agilent LC/MSD Traps are assembled in the same factory, there are several significant differences, one being the design of the NanoSpray sources and another the software used for protein analysis. The two instruments also have different maximum achievable *m/z* values. These traps appear to be very powerful instruments.

Another mass spectrometer first exhibited at ASMS 2003 from Agilent and shown the first time at PittCon this year is the *LC/MSD TOF*. At PittCon, this LC/MSD TOF prompted a marketing manager from a competitive company to report that Agilent was introducing a Q-q-TOF. That, of course, is not the case. This orthogonal ion-injection reflectron time-of-flight mass spectrometer has an electrospray, nanospray, APCI, and atmospheric MALDI interface available. The brochure, which is downloadable from http://www.chem.agilent.com/temp/rad1E3E4/00042009.pdf, is well worth the read. The instrument has an *m/z* range of 70–7,000 with a resolving power of 10,000 (FWHM measured at *m/z* 2722). It has a reported *m/z* accuracy to 3 ppm achievable with an internal standard. The scan speed [*sic*] (hmm, I wonder what you scan in a TOF mass spectrometer) is 5 spectra sec^{-1} from *m/z* 100 to 3,000. The instrument is capable of positive- and negative-ion detection but not in alternating spectra. Like the JEOL AccuTOF, this instrument uses an analog-to-digital converter to assure a wide dynamic range, the lack of which has been reported with the TOF instruments using a time-to-digital converter. The flight tube is constructed of a special alloy to assure that the variations in ambient temperature do not affect the instrument's performance. The electrospray source used a dual orthogonal spray needle for sample on *m/z* internal standard. Another important aspect of the LC/MSD TOF is the fact that it is using the *Analyst QS* software from Applied Biosystems/MDS Sciex for data analysis. This has been enhanced with application-specific additions from Agilent.

Another instrument featured by Agilent at PittCon 2004 was the *5973 GC/MSD Inert* introduced at the International Mass Spectrometry Conference in Edinburgh in the Fall of 2003. This instrument features a specially constructed ion source to assure that analyte degradation of specially susceptible compounds does not occur. Agilent states that it is the material from which the source is constructed rather than a coating; therefore, the inertness will be permanent. When this GC-MS was introduced, a new revision of the GC/MS MSD ChemStation was released (G1701DA D.01.00). This software was far more than just a revision. Agilent included a number of button bars, one of which has three buttons that can be associated with custom mac-

ros called Custom Tools button. A review of this software can be read on the ChemUserWorld Web site at http://www.chemuserworld.com. Another interesting aspect of Agilent's 5973 and 5973 Inert is the fact that there is now an application note telling you how to tune the CI ion source in such a way as to get good EI spectra in the absence of a reagent gas.

The newly introduced *7500ce* ICP-MS is reported to have 5× the sensitivity of the previous models. This is accomplished through use of new reaction cell technology, new digital-drive RF generator that supplies the ICP RF power, and newly designed ion optics. More information on the Agilent 7500ce ICP-MS can be found at http:// www.agilent.com/chem/icpms.

More information is available on these and all Agilent products and services from the Life Sciences and Chemical Analysis group at http//www.agilent.com/chem.

Applied Biosystems, Inc./MDS Sciex (Foster City, CA/Toronto, Canada)

Applied Biosystems introduced a triple-quadrupole mass spectrometer where the second *m/z* analyzer was a linear quadrupole ion trap with axial ion ejection on their ABI 2000 LC/MS/MS platform (Q Trap™ LC/MS/MS System) at the ASMS Conference in 2002. This instrument first appeared at a PittCon in 2003. At PittCon 2002, Applied Biosystems/MSD Sciex introduced a new generation triple-quadrupole instrument with a dual sprayer (DuoSpray™ Ion Source) orthogonal interface, the API 4000 LC/MS/MS System. The DuoSpray is a combination APCI and TurboIonSpray® (pneumatically assisted electrospray) that allows for software switching between the two modes. According to one of the applications specialists in the Agilent booth, this orthogonal geometry is under license from Agilent to Applied Biosystems/MDS Sciex.

At the 2003 ASMS Conference, in one of the largest attended users' meeting ever held at an ASMS conference, Applied Biosystems/MSD Sciex introduced the *4000 Q Trap™ LC/MS/MS System*. This added the powerful linear quadrupole ion trap as the second *m/z* analyzer that allows for an additional iteration of MS/MS in the third stage of the instrument. The linear QIT can be used to increase sensitivity as well as providing increased specificity. The *4000 Q Trap LC/MS/MS System* made its PittCon debut this year. The 4000 Q Trap probably has the same general performance as the ABI 4000 LC/MS/MS System: *m/z* range of 5–3,000; and an *m/z* accuracy of 0.01% over the entire *m/z* range.

More information is available about the Applied Biosystems line of mass spectrometry products at http://www.appliedbiosystems.com or from the MDS/Sciex Web site at http://www.mdssciex.com.

Bruker DALTONICS (Billerica, MA; Bremen, Germany)

Bruker DALTONICS by far had more new instrument introductions in mass spectrometry than any other manufacturer. This is often the case. Bruker announced six new mass spectrometry models, an upgrade to an existing instrument (*Focus* optics for the ESI-microTOF™ introduced in 2003), and two new software platforms. The six new instruments were the *esquire4000*™, the *esquire6000*™, the *HCTplus* (all three are new models of the ESQUIRE™ quadrupole ion trap LC/MS/MS instrument introduced in 1994 at the 13th International Mass Spectrometry Conference held in Budapest, Hungry), the *microflex*™ MALDI-TOF (a benchtop instrument for proteomics application), the *autoflex II MALDI-TOF and TOF/TOF* (the first vertical TOF/TOF instrument), and the *APEX®-QE 7 Tesla Q-q-FTMS* (an FT-MS with integrated Top↓Pro™, a.k.a. top-down proteomics, software). The two software products were the *Metabolic Profiler*™ (a joint introduction from Bruker DALTONICS and Bruker BioSpin – the NMR group), a way of managing the NMR/TOF mass spectrometry data that are important to toxicity and efficacy studies, and *Proteomics RIMS*™, an integrated database LIMS system for managing all the data of proteomics, mass spectrometry, x-ray crystallography, and NMR in such a way to allow for the extraction of information.

One of the stated strengths of Bruker for biopolymers analyses is their combination of products both in NMR and in mass spectrometry. Bruker and Varian, Inc. are the only companies that combination products are supported from both an applications and hardware standpoint. A good example of Bruker's commitment to this area is *Proteomics RIMS* bioinformatics software development.

Without specifics, Dr. Frank Laukien, President and CEO of Bruker DALTONICS, stated yes to the question as whether the resolution, sensitivity, ion-storage capacity, or increased *m/z* range accounted for the improvements in the *Esquire* line of LC/MS/MS QIT instruments. He stated that all of these were the reason that there is an *esquire4000* replacing the esquire2000, and an *esquire6000* replacing the esquire3000plus; these two new instruments have *m/z* ranges to 4,000 and 6,000, respectively. Bruker claims that these two new Esquire instruments are twice as sensitive as the instruments they replace. The existing HCT continues to be provided with the *HCTplus* being a new member of the family. The main reason for the improved specifications was attributed to improvements in manufacturing. The Bruker Esquire line of LC/MS/MS QIT instruments is a jointly developed product with Agilent Technologies. Both companies sell the instruments but have different performance specifications, software, and, in the case of the nanospray interfaces, different source geometries. The Bruker and Agilent instruments share a common trap and a common APCI ES interface. One of the ways

Bruker differentiates its QIT instrumentation from that sold by Agilent is by providing application-specific solutions with custom software tailored for the application. Another differentiating feature of the Bruker Esquire instruments is the use of a single mass spectrometry software platform, *Compass*™. All of the Bruker mass spectrometers are under the Compass software umbrella.

The *Focus* optics for the ESI-microTOF increases the resolving power of this benchtop instrument from 10K to 15K. This 15K resolving power specification is the same as quoted for the newly introduced *microflex* benchtop MALDI-TOF.

The *autoflex II* is a replacement for the autoflex introduced in 2000. The autoflex is available as a single MALDI-TOF instrument or as a TOF/TOF instrument. A single TOF instrument can be field-upgraded to a TOF/TOF instrument, just as the ultraflex™ (the original TOF/TOF instrument from Bruker introduced at PittCon 2001).

Bruker has had a long history in FTMS. The *APEX-QE 7 Tesla Q-q-FTMS* is another instrument in that lineage. This hybrid allows for MS/MS in the FTMS as well as in the collision cell separating the transmission quadrupole *m/z* analyzer and the FTMS. Because of the integration with the Compass software, the APEX-QE is as easy to operate as the Esquire QIT instruments. The system can be set up for automated overnight analyses.

More information on all of the Bruker DALTONICS line of mass spectrometers and software can be found at http://www.bruker.com.

GV Instruments (Manchester, U.K.)

GV Instruments is barely one year old, being formed as the result of an employee buyout of the inorganic mass spectrometry products of Micromass, Ltd. from Waters Corporation and the acquisition of Analytical Precision Products, Ltd. (a supplier of stable isotope mass spectrometers) and HtX, Ltd. (a developer of mass spectrometers used for the analysis of noble gases); both of these latter two companies were much smaller than the inorganics group of Micromass, Ltd. GV Instruments offers transmission quadrupole and magnetic-sector ICP mass spectrometers for elemental analysis and speciation and stable isotope, thermal ionization, and noble gas mass spectrometers as well as accessories for these instruments.

GV Instruments has posted a rather interesting genealogy of all the companies that had their origins as VG Micromass (which had its beginning in 1962), the mass spectrometry company of vacuum generators. This genealogy can be found on the Web at http://www.gvinstruments.co.uk/history.htm.

At PittCon 2004, GVI announced plans to replace its 5400 NGMS (noble gas mass spectrometer) with a new series of instruments, which include the *HELIX* and the *HELIX SFT*. The *HELIX* has a multicollector array that allows the simultaneous collection of all isotopes of any noble gases. The instrument boasts a resolving power of 1,800 with no loss in ion transmission. This allows research-limiting isotope interferences to be resolved. The company claims this has not been possible with any instrument. The *HELIX SFT*, while not limited to helium, has been designed with particular emphasis on the ^{3}He and ^{4}He isotopes by utilizing a deep-bucket Faraday cup and an ion-counting electron multiplier on two separate spurs to simultaneously carry out this analysis.

More information about GV Instruments can be found at http://www.gvinstruments.co.uk. As of this writing, there was no information on this site about the new instruments announced at PittCon.

In Process Instruments (Bremen, Germany)

In Process was started with the transfer of the transmission quadrupole analyzer technology from the former Balzer AG (now Inficon AG), Liechtenstein, Germany, in 1997. The company specializes in process instrumentation that can also be used in research applications. The company first appeared at PittCon in 2003, somewhat in stealth mode with no press packets, no advertising, and no listing under mass spectrometry in the vendors list. This year, the company made a more effective introduction of its products. In the U.S., the company is represented by Robert Adams of ARLS, Inc. in Atlanta, Georgia (raadams59@comcast.net). The new instrument introduced at this year's PittCon was the *GAM 400* with an *m/z* range of 1–512, a crossbeam ion source, and a Faraday and SEM detector. The instrument can be configured with up to three gas inlets for simultaneous measuring of samples. The instrument is considered to be competitive in the area of automated analysis of ^{13}C- and ^{15}N-enriched samples. The instrument is also targeted for catalysis research. The instrument can be configured with a high-precision quadrupole suitable for the separation of helium/deuterium (4.002603u/4.028204u). The company's Web site (http://www.in-process.com) shows nine different instruments, including one specifically designed for the analysis of gases in lamps. This is a quantitative system. The GAM 600 SI uses a soft ionization technique in addition to electron ionization. The soft ionization technique appears to chemical ionization with the ability to use different reagent gases. One of the instrument's claims is the ability to easily switch between SI and EI modes.

John Wiley & Sons (New York, NY)

Several years ago, John Wiley and Sons acquired the German publisher VCH. VCH owned a company that was involved in database software and databases specific to various types of spectrometries. Now Wiley appears to have combined Chemical Concepts databases and its Wiley Registry of Mass Spectral Data into a unified effort called *Wiley Databases, Chemistry that*

Matters. These databases are being sold through the traditional distribution channels of Wiley, including sales direct to end-users and OEMs. About a year ago, Wiley took over the distribution of the Wiley Registry from Palisade Corporation who had previously been the supplier to OEMs, distributors, and end-users. Shown for the first time at this year's PittCon, in addition to the *Wiley Registry of Mass Spectral Data* (*Wiley 7* ISBN: 0-471-44097-3 and combined with the *NIST02 Database–Wiley 7N* ISBN: 0-471-44098-1) and the 4th edition of Professor Henneburg's *Mass Spectra Chemical Concepts* (40K spectra ISBN: 0-471-44036-1), were a series of boutique databases: A. J. Zeist's TNO *Mass Spectra of Volatile Compounds in Food*, 2nd ed. (ISBN: 0-471-44056-6), number of spectra not specified; J. W. de Leeuw's (Netherlands Institute of Sea Research) *Mass Spectral Collection: Geochemicals, Petrochemicals and Biomarkers*, 2nd ed. (ISBN: 0-471-64798-5), 1,100 spectra; Dr. Peter Roesner's (Regional Department of Criminal Investigation, Kiel, Germany) *Mass Spectra of Designer Drugs* (ISBN: 0-471-47356-1), 1,700 spectra of 1,400 compounds; Dr. Alexander Yarkov's (Chemical Block, Moscow) *Mass Spectra of Organic Compounds* (ISBN: 0-471-66773-0), 37,055 spectra; and Professor H. L. J. Markin's (St. Bartholomew and the Royal London School of Medicine and Dentistry) *Mass Spectra of Androstanes, Oestrogens and Other Steroids* (ISBN: 0-471-44034-5), 2,500 spectra. In addition, the same brochure that promoted all of these collections also promoted the multiple-spectrometries databases and software *SpecInfo* (ISBN: 0-471-21895-2). The SpecInfo Database Server can be accessed through Webclient SuperSurf, which is platform-independent and can be used through the Internet. All of these databases are available in a variety of different instrument manufacturers' formats. Not listed in the Wiley brochure but shown on their Web site was the NIST02 Database with the NIST MS Search Program v.2.0 (ISBN: 0-471-44625-4).

More information on the new Wiley mass spectral databases can be obtained by e-mailing sales@chemicalconcepts.com.

Palisade Corporation (Newfield, NY)

Palisade has introduced a new EI mass spectral database and a new concept in mass spectral database distribution. The *Palisade CompleteMSLibrary 660K* is a combination of the Wiley 7 (Wiley Registry of Mass Spectral Data version 7 ~338K spectra) and the NIST02 (the NIST/EPA/NIH Mass Spectral Database 2002 Release ~170K spectra) databases plus over 150K spectra that have not been previously included in any commercially distributed EI mass spectral database. The *Palisade Complete* has spectra of 495K unique compounds, 327K CAS registry numbers, and 985K chemical names. The new concept in distribution is a subscription program of three or five years that assures the user of ~25K new spectra per year (some of the promotional material said 25K to 50K new spectra per year) at an annual fixed cost. After the subscription period, the purchaser can renew or not with the spectra now in the subscriber's possession belonging to the subscriber. A 30-day demo version was provided at PittCon that allowed various non-spectral-comparison searches of the database through the Palisade Mass Spectral Browser. In addition to the database, it appears that the Palisade Probability Based Matching program will be provided with the database. This program has the ability to extract and search spectra from most commercially available formats. The Palisade Complete will also be provided in a variety of different instrument-specific formats including that used by the NIST MS Search Program. In a brief examination of the Palisade Complete, it was found that some of the spectra were associated with Markush structures with the R and R′ values having multiple definition. Palisade was the sole distributor of the Wiley Registry (to OEMs, distributors, and end-users) until about a year ago.

More information can be found regarding the Palisade Complete at the Palisade mass spectrometry Web site (http://www.palisade-ms.com).

Thermo Electron (San Jose, CA)

In addition to exhibiting the Finnigan LTQ linear quadrupole ion trap mass spectrometer introduced at the 2003 ASMS Conference, Thermo Electron had more than 20 new product introductions, 9 of which were of interest to the mass spectrometrist. One of these was the *vMALDI* interface for the Finnigan LTQ and the Finnigan LTQ FT MS. The Finnigan LTQ is a linear QIT mass spectrometer capable of MS^{10} with an *m/z* range of 50–2,000. This instrument has several unique features, the least of which is not the dual detector design to give maximum sensitivity from the radial ion-ejection device. The *vMALDI* device is a traditional vacuum MALDI system that will automatically handle 96- and 384-well plates. Analyses can be automated using the Crystal Positioning System (CPS™) to determine an optimized sampling pattern. Automatic Spectral Filtering (ASF™) is used to assess real-time data quality, and the system's Automatic Gain Control (AGC™) determines the optimum number of laser shots to fill the trap. The vMALDI adds to the utility of the Finnigan LTQ, and the Finnigan LTQ FT MS has a tool for the analysis of biopolymers. Several self-running movies on the Finnigan LTQ can be found at: http://www.thermo.com/com/cda/resources/resources_detail/1,,22534-111299,00.html.

Another very interesting product from Thermo Electron is the *Finnigan LC IsoLink*, which is an LC isotope ratioing mass spectrometer system. Thermo claims that this is the first such system to be made commercially available. It will not take long for some enterprising analyst to figure out how to hook up a CRIMS interface to this instrument. This instrument is also going to find utility in both the pharmaceutical and the food industry. Information as to the history and origin of a sample can be

gained from IRMS. Until the Finnigan LC IsoLink, this technique was limited to GC ICRMS analyses.

The capability of the Finnigan LTQ FT MS was expanded by adding two new modes of MS/MS: Electron Capture Dissociation – ECD (use of slow electrons from a gated electron gun) and InfraRed MultiPhoton Dissociation – IRMPD (uses IR laser radiation from a 20W CO_2 laser to excite and fragment ions). These capabilities added to the collisionally activated dissociation that can be carried out in the linear QIT enhances the flexibility of the Finnigan LTQ FT MS.

Among the other new product introductions to the mass spectrometrist were two software packages; a new version of *Mass Frontier*™ (fragmentation prediction software) and *EnviroLabs*™ *Forms* (a forms package for U.S. EPA Environmental Method reporting of data acquired, using Xcalibur v.1.3 and the Finnigan DSQ transmission quadrupole GC-MS).

Thermo Electron also introduced a new version of the high-resolution triple quadrupole. This instrument is called the *Finnigan TSQ Quantum Ultra EMR* (extended mass range). This instrument has an *m/z* range to 3,000 while still allowing for the resolution specifications of the Finnigan TSQ Quantum. Another product that could be called a new instrument was the *Finnigan ProteomeX*™ *LTQ* proteomics workstation. This system is based on the Finnigan LTQ. The *ProteomeX LTQ* includes a new proteomics autosampler, the *Finnigan Micro AS*™, and optimized column-method combinations for specific proteomics applications. The ProteomeX LTQ software makes possible high-throughput protein identification, maximum sequence coverage, phosphorylation site mapping, and Multidimensional Protein Identification Technology (MudPIT) with an automated system.

There are two GC/MS specific products: (1) the *Finnigan TriPlus* autosampler that appears to have all the features and capabilities of the CTC autosampler; (2) a new ion source (the *Bright Ion Source*) for the Finnigan Focus DSQ™ and the Finnigan Trace DSQ™.

More information on Thermo Electron's products can be found at http://www.thermoelectron.com.

Varian, Inc. (Palo Alto, CA)

Varian introduced two new products of potential interest to users of mass spectrometry—the *CP-4900 Micro-GC with Differential Mobility Detector* (CP-4900 DMD) and the *Varian 4000 GC/MS* based on an internal/external ionization quadrupole ion trap. The *CP-4900 DMD* is a joint development with Sionex Corporation (Waltham, Massachusetts) using Sionex's patented DMX technology. Sionex calls this *microDMx*™ technology (Differential Mobility). The origin of this technology is in research from the former Soviet Union. Erkinjon Nazarov et al. illustrate the foundation of the technology in what was referred to as FAIMS (Field Asymmetric Ion Mobility Spectrometry). Raanan Miller and co-workers at the Charles Stark Draper Laboratory (Cambridge, Massachusetts) applied MEMS (microelectromechanical systems) and microfabrication technology to the FAIMS concept to produce the microDMx chip. At the same time the MEMS work progressed at Draper, additional work on the chemistry behind the detection mechanisms was being conducted at New Mexico State University by Gary Eiceman. The resulting detection device, which is tuned to specific analyte types such as sulfur species in hydrocarbon streams, sulfur-containing and other odorants in natural gas, ferrons in ambient air, anesthetic gasses (for monitoring gasses in operating and recovery rooms), and so forth, is being interfaced to Varian's micromachined GC. Varian will deliver instruments for specific applications using this mobility detector.

The *Varian 4000 GC/MS* is an instrument that is completely separate from the existing Saturn line of GC/MS instrumentation, which was based on Varian's MS/MS and CI patents but Thermo Electron's licensed scan function. The Varian 4000 GC/MS is based on 18 different Varian patented technologies. The instrument uses unidirectional ion ejection. The ionization time is using a new algorithm that adjusts the prescan time based on the number of ions formed during the previous cycle. In the internal ionization mode, the instrument is capable of EI and CI. In external ionization, the instrument can be operated in EI or CI with detection of positive ions, or resonance electron capture ionization with detection of negative ions. The Varian 4000 GC/MS introduced something Varian calls *Hybrid CI*. This is a process where reagent ions are produced by an external source and injected into the trap where they are allowed to undergo ion/molecule reactions with analyte molecules that are flowing from the GC column into the trap through the normal internal ionization route. The example shown in the Varian booth was that of the hybrid chemical ionization of anthracene and phenanthrene (both polynuclear hydrocarbon with the same molecular mass and number of rings, but different geometries) using the *m/z* 131 positive ion of PFTBA as the reagent ion. The EI and CI spectra of these two compounds were identical with the hybrid CI spectra being very different. These reagent ions can be produced in either the external CI configuration for the source (high pressure) or under EI conditions. The ions injected into the trap for reaction with analyte molecules can be *m/z* selected in the trap. These reagent ions can be either positive or negative. This allows the domain of ion/molecule reactions to be used as a highly specific analytical tool.

Another unique feature of this instrument is that the electron beam in external ionization is deflected rather than interrupted when ions are not being injected into the trap. The instrument is reported to produce a mass spectrum of perfluorotributylamine using external EI that has a base peak at *m/z* 69. The external ionization uses a unique source design that allows for switching between EI and CI without breaking vacuum. This is not quite as convenient as switching between EI and CI

with internal ionization, but it is better than that which is available on many instruments.

The instrument has an *m/z* range of 10–1,000, which is greater than that of the Saturn instruments. Ions can be scanned out of the trap at variable rates between 5,000 and 10,000 *m/z* units per second. Varian, like many other manufacturers, still has difficulty in differentiating between the mass-to-charge ratio and the mass of ions. A lot of their promotional material uses units of mass rather than the unit-less *m/z* value. Another point worth mentioning about the Varian 4000 GC/MS is that it uses a 230 L sec^{-1} turbomolecular pump manufactured by Varian's vacuum division. Varian manufactures more of the components of this instrument than any other manufacturer.

Although not stated as the final specifications, a mass chromatogram of *m/z* 272 was shown for a spectral acquisition range of *m/z* 50–300 in internal ionization EI of octafluoronaphthlene with a signal-to-background of 128:1 for 250 fg injected. The mass spectrum at the apex of the mass chromatographic peak was very acceptable and produced a spectrum of OFN as the first hit when searched against the NIST/EPA/NIH (NIST02) Mass Spectral Database. Data was shown, showing that the instrument could meet the U.S. EPA tune criteria for Method 525.2 using decafluorotriphenylphosphine (DFTPP); however, it was not stated as to whether this was accomplished with internal or external ionization or both. It was stated that performance in the resonance electron capture negative ionization was compound dependent and did not provide for the broad range of halogenated analytes that could be detected with beam-type instruments such as the Varian 1200 GC/MS.

The Varian 4000 GC/MS offers all the capabilities of the Saturn instruments in terms of MS/MS and Selected Ion Storage. As Hybrid CI gets into the hands of more investigators, it is sure to find some important application niches. The extended *m/z* of the Varian 4000 GC/MS is definitely a plus and will increase the capability for the QIT GC/MS user. Varian has elected to stay with its powerful Chromatoprobe device for the introduction of batch solid and liquid samples rather than introducing a direct insertion probe. Direct insertion probes usually mean lots of source-cleaning downtime.

In speaking to the company's overall position to scientific instruments, Gary W. Rodgerson, President and Chief Operating Officer, stated that not only was Varian the company that manufactures more of the components in its mass spectrometers than any other company; but with the production of NMR, LC, and the 1200 ES/APCI triple quadrupole, Varian manufactured more of its LC/NMR/MS product than any other company.

More information on Varian's products can be found at http://www.varianinc.com.

Waters Corporation (Milford, MA)

Waters Corporation, like Thermo Electron and Applied Biosystems/MSD Sciex, had major product introductions at the 2003 ASMS meeting. This product, the *Quattro Premier*, introduces a new concept in ion optics for the triple-quadrupole *m/z* analyzer. As a matter of fact, this instrument can no longer be called a "triple quadrupole." Like the traditional triple-quadrupole instruments, the *Quattro Premier* has two *m/z* analyzers. Rather than the two being separated by a collision cell that uses quadrupole fields applied to a quadrupole, hexapole, or octupole, Quattro Premier uses a traveling wave (T-Wave technology) as the collision cell. This T-Wave technology provides for improved ion transmission and control through the collision cell. The same T-Wave technology has been applied to the ion optics used to bring ions from the atmospheric region of the ion interface into the first *m/z* analyzer. The Quattro Premier is the Quattro Ultima Platinum, which was withdrawn from the U.S. market last year after the Applied Biosystems/MDS Sciex litigation. Waters also introduced a new concept in liquid chromatography that will be of interest to many users of mass spectrometry. This is the *Acquity Ultra Performance LC* system. Another re-introduction was that of the *Quattro Micro GC*, a GC/MS/MS. This is now one of the two commercially available GC/MS/MS products on the market, the other being the Varian 1200.

More information about these and all of Waters products can be found on their Web site at http://www.waters.com.

In conclusion. . .

There were many companies with some new items for their product lines. Shimadzu has new software for their GC/MS and LC/MS instrumentation; Advanced Chemistry Development (http://www.acdlabs.com) announced the release of version 8 of its software; Konik-Tech (http://www.konik-group.com), the Barcelona, Spain, company that introduced GC/MS and LC/MS products last year, was back, talking about their pending shipments; Perkin Elmer Instruments (www.perkinelmer.com) showed their benchtop GC/MS and MDS/Sciex ICP-MS products along with the MDS/Sciex orthogonal MALDI TOF instrument at last year's PittCon; Inficon, developer and manufacturer of the Hapsite portable GC-MS, introduced a *SituProbe* purge and trap GC/MS system for laboratory-quality water analysis in the field and the *Scentograph* series of portable and continuous on-line GC monitoring systems for air and water; JEOL exhibited their *GCmate* (a double-focusing GC-MS) and *AccuTOF* (an ES-TOF) mass spectrometers; and Scientific Instrument Services showed their product line as usual, just to mention a few. As is the case with every year's PittCon, there is still too much to see and do when it comes to mass spectrometry. It is now harder because a number of new products are appearing at the annual ASMS conference before they make their PittCon debut.