Mass Spectrometry PittCon® 2005

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The year 2005 was the most exciting for new mass spectrometry introductions at PittCon in the 11 years that this column has been appearing in JASMS. Although the Silver award from the PittCon Editors’ Award [this award had its origin with Analytical Instrument Industry Report, Dr. Gordon Wilkinson, Founding Editor, in 1995. Since that time, many mass spectrometry products have received the Gold, Silver, and Bronze awards. Last year was the first year that no award was received by a mass spectrometry product] was shared by three products; one was for a mass spectrometry product (the Shimadzu LCMS-IT-TOF). The Gold award went to the JEOL DART and was an overwhelming winner at an almost three-to-one majority. The Bronze award also went to a mass spectrometry product (the Agilent ESI LC Chip).

JEOL introduced DART, a new ionization technique that may well be worthy of the next mass spectrometry Nobel Prize. JEOL also showed at PittCon for the first time the AccuTof-GC, a GC-MS based on their AccuTOF technology introduced as an LC-MS in 2002. Shimadzu introduced an electrospray version of the tandem quadrupole ion trap TOF mass spectrometer introduced in 2001 as the MALDI AXIMA QIT.

Applied Biosystems/SCIEX introduced the API 5000 triple quadrupole mass spectrometer that boasts a ten-fold increase in sensitivity over previous models. Agilent showed at PittCon for the first time the LC Chip with an electrospray interface and introduced a unique simultaneous APCI-ESI source for its 1100 Series of LC/MS single quadrupole instruments.

Thermo Electron introduced an exciting new glow discharge version of its Element II high-resolution double-focusing mass spectrometer, which is the culmination of a joint effort of its Bremen, Germany, mass spectrometry factory and technology from VG Elemental, which was part of the VG acquisition made several years back.

Bruker Daltonics introduced four new mass spectrometers and two novel mass spectrometry components that included a simultaneous MALDI-ESI source.

Waters showed the Micromass Q-Tof Premier, introduced at ASMS in 2004, for the first time at PittCon. This instrument is now MALDI-enabled. Waters also showed new low-flow LC technology that will greatly enhance the performance of its mass spectrometers.

Another product introduction that may be as revolutionary as JEOL’s DART is the cryogen-free 7-tesla FT-MS from IonSpec.

Two non-U.S. companies, exhibiting at PittCon for the first time, introduced products that were very interesting. These companies are Syft (New Zealand), manufacturer of a transmission quadrupole mass spectrometer using SIFT technology for volatile organic analyses (VOA), and Pyrolab (Sweden), manufacturer of a new dimension in pyrolysis.

In addition, two companies that had introduced instrument concepts in previous years were back with products ready to ship. They were Konik (Barcelona, Spain) with its benchtop transmission quadrupole mass spectrometer for GC and LC, and Griffin Analytical Technologies (West Lafayette, IN) with its GC-MS based on the Purdue cylindrical quadrupole ion trap. There was also some interesting news from some of the older standby companies in mass spectrometry.

PittCon 2005 was held in Orlando, FL, beginning Friday, February 25, with short courses offered by the American Chemical Society and ending with the close of the technical program on Friday, March 4. The exposition of instruments, services, and supplies was from March 1 through March 4. The registration was around 20,000 (just under 8000 conferees and just over 10,000 exhibitors, with the remainder being press and students). In recent years, PittCon appears to have become more of a business-to-business conference (companies that make vacuum pumps and detectors dealing with instrument manufacturers), an opportunity for companies publicly traded on the stock market to impress Wall Street, and for venture capitalists and new technologies to get together. There are still instrument users who come to see what is available in new instrumentation. A good sign for the economy was a comment by a representative of one of the major mass spectrometry manufacturers who said, “Unlike previous years when customers would come to the booth to see what was new, and what they might try to get funding for, this year they came already funded and looking to see what they should buy.” Overall, there were a lot of complaints about the Orlando venue, but all the mass spectrometry manufacturers commented that “they were getting plenty of leads” and that the quality of the leads was quite good. There was a rumor that this year’s PittCon had 250 fewer exhibitors than last year. Another indicator of a decline in this year’s attendance was the 7 a.m. United Airlines nonstop flight from Orlando to San Francisco on Friday, March 4. This flight, which has always been full in the past, had most of the center seats open.

The conference and exposition was held in the new addition to the Orange County Convention Center. The south entrance, the entrance closest to the convention...
center hotels, was on the opposite end to the main entrance where the registration was held. Because the exhibition floor occupied the entire center area, this meant that you had to walk around the outside of the building unless you had an exhibitor badge. This was especially inconvenient on Sunday during a day-long hard rainstorm and on Thursday during a less-dramatic rain that conveniently began as the exhibition closed at 3:00 p.m.

As stated in this article every year, there was just too much to attend—press conferences, visiting booths, and the technical presentations. The symposia, oral sessions, and posters at PittCon have undergone a drastic improvement over the last 10 years. This makes the choices as to what to do even more difficult. It is also sometimes difficult to find all the presentations of interest to the mass spectrometrist because they are often hidden in sections such as Food Science and Homeland Security. It was nice when *Analytical Chemistry* would sort this out from the program and publish it in an issue before the meeting. However, with the Preliminary Program reaching conferees quite late these past few years, it would have been difficult for *Analytical Chemistry* to publish such a list.

This year also marked another significant event, and a change, for PittCon. The technical abstracts are now available only on CD-ROM—no more hardcopy abstracts—like ASMS, which changed to electronic version in 1999.

The American Chemical Society offered a three-day course entitled Interpretation of Mass Spectra taught by O. David Sparkman of the University of the Pacific (Stockton, CA), and a two-day course entitled LC/MS taught by Jack Henion of Cornell University and Advion (Ithaca, NY). Among the 100+ courses offered by PittCon between Saturday and Thursday were 14 courses on mass spectrometry: (1) Sample Preparation Strategies in ICP–AES and MS, Isaac (Joe) Brenner, Environmental Analytical Services (1 day); (2) Practical Aspects of Nanoelectrospray and Nano LC–MS/MS with Applications to Mass Spectrometry Based Proteomics (new course), David Muddiman, Mayo Clinic College of Medicine; Ben Madden, Mayo Clinic College of Medicine (1/2 day); (3) Advanced Interpretation of CID Mass Spectra from LC/MS/MS—Developing a Systematic Methodology for Spectral Interpretation (new course), Robert Voyksner, LCMS Limited; Jennifer Townsend, LCMS Limited (2 days); (4) Introduction to Mass Spectrometry, Kenneth Busch, Wyvern Associates (1 day); (5) GC/Mass Spectroscopy [sic]: Fundamentals, Applications, and Troubleshooting, William Coleman, R. J. Reynolds Tobacco Company; Bert Gordon, R. J. Reynolds Tobacco Company (1 day); (6) Interpretation of Electrospray Mass Spectra of Small Molecules, Earl Michael Thurman, University of Almeria; Imma Ferrer, University of Almeria (1 day); (7) Fundamentals of Ion Mobility (IMS) and Ion Mobility Mass Spectrometry (IMMS), Herbert Hill, Washington State University (1/2 day); (8) How to Select an ICP-Mass Spectrometer: The Most Important Analytical Considerations, Robert Thomas, Scientific Solutions (1/2 day); (9) ICP Mass Spectrometry: Principles and Instrumentation, R. S. Houk, Ames Laboratory USDOE (1/2 day); (10) LC–MS–MS, LC–MS and GC–MS Analysis of Endocrine Disruptors [sic] in the Environment (new course), Damia Barcelo, IIQAB-CSIC (1/2 day); (11) Analytical Organic Mass Spectrometry, William Budde, U.S. Environmental Protection Agency (1 day); (12) HPLC Method Development for LC/MS, Shane Needham, Alturas Analytics (1 day); (13) LC/MS Strategies for the Identification of Impurities, Degradants, and Metabolites, Mike Lee, Milestone Development Services; Mark Bayliss, Advanced Chemistry Development (1 day); (14) MALDI Time-of-Flight Mass Spectrometry: Fundamentals and Applications. What you need to know to get started, Pierre Chaurand, Vanderbilt University (1 day). The American Chemical Society and PittCon also offered courses on GC and LC, which would be of interest to many mass spectrometrists.

The big legal news at PittCon 2005 was the final decision in the lawsuit between John B. Fenn (one of the 2002 Nobel Prize in Chemistry recipients) and Yale University over the ownership of one of the primary patents on electrospray ionization. Yale claimed that, without their knowledge, Dr. Fenn applied for a patent that was approved in 1992. When Yale found out about the patent, it claimed rights and asked Fenn to reassign the patent to Yale. Dr. Fenn originally assigned the patent to Analytica of Branford (Branford, CT), which he co-founded with Craig Whitehouse. The U.S. District Court in Hartford, CT, originally found in favor of Yale in 2003. In an article that appeared in the February 21, 2005 issue of *C&EN*, the court is quoted to have found that Dr. Fenn “misrepresented the importance and commercial viability of the invention, . . . actively discouraged Yale from preparing and filing a patent application, and wrongfully filed one himself without notifying Yale and the National Institutes of Health, which helped fund the work.” In the same *C&EN* article, Dr. Fenn is reported to have said, “I filed for a patent because Yale didn’t, after there was insufficient commercial interest.” Dr. Fenn says that two other patents on electrospray worth even more money have been assigned to Yale, and he denies the theft charge. He says that he plans to appeal this decision. The final decision, handed down in February, ordered Dr. Fenn to pay $545K in misdirected royalties and about $500K in attorney fees.

The following is a company-by-company description of new instrumentation. There might be some companies that belong in this category and were overlooked; however, with an exhibition the size of the Pittsburgh Conference on Analytical Chemistry, it is easy to overlook those that do not make a specific effort to be known, or those that may be on the periphery of the field.
**Agilent Technologies, Inc. (Santa Clara, CA)**

Chris van Ingen, Agilent’s President, reported that the company experienced a 13% growth in orders in 2004, and that Q1 2005 had seen a 16% order growth over Q1 2004. Revenue growth was up 12% in 2004 and 13% for Q1 2005, and both 2004 and Q1 2005 showed an operating profit increase of 14% over the previous periods. The 2004 revenue was $1.33 billion.

The major product announcements of interest to mass spectrometry were the HPLC-Chip/MS System for Proteomics, the Simultaneous Multimode Ion Source for Mass Spectrometry, and Lab Resource Management Service for Large Laboratories.

Last year, Agilent introduced the microfluidics-based chip as an LC column. The micro-machine chip places all the LC components on a single surface about the size of a credit card. The chip has a 43-mm × 75-μm column packed with 5-μm Zorbax Bond 300A C-18 for reversed-phase liquid chromatography and a spray tip used in electrospray mass spectrometry. The HPLC-Chip is positioned in an HPLC-Chip Cube that is mounted on the Agilent Nanoflow Proteomics Solution XCT+ quadrupole ion trap mass spectrometer. When the chip is placed in the cube, the chip is automatically loaded and locked into place providing a high-pressure, leak-tight seal with the mass spectrometer. Information on the chip such as ID and type, documentation, diagnostic, and operational data along with comments that are entered by the user are read into the data file header. Necessary information that has been updated is recorded on the chip’s RF tag before it is removed. Switching chips is simple and is accomplished in a few seconds. The HPLC-Chip Cube is a standard molecule for the Agilent 1100 Series LC System for mass spectrometry. The initial offering is with a single-column packing and only for use with the QIT mass spectrometer; however, plans are underway for making the Chip Cube available for the 1100 Series MSD and the TOF mass spectrometer. Agilent claims that the system eliminates more than 50% of the fittings and connections normally used in LC/MS systems. They also claim that reduced sample sizes can yield as much or more information as is available from current nanoflow LC/MS systems. It is still unclear as to whether Agilent plans to make the Chip LC available on other manufacturers’ mass spectrometers. This Chip LC/MS System was introduced at the 2004 ASMS meeting in Nashville, TN, held May 23–27. It was shown for the first time at this year’s PittCon; therefore, it was eligible for the PittCon Editors’ Award and won third place.

Agilent’s Simultaneous Electrospray/APCI Source was a nominated contender for the PittCon Editors’ Award. This is a revolutionary ion source. There have been several combination ion sources in the past, but this is the first one that allows for simultaneous operation of two modes recording data into a single data file. Many of the analyses performed using LC/MS instrumentation are to determine the molecular mass of a compound. As thousands of compounds are synthesized by pharmaceutical manufacturers, the chemist is continuing to look for confirmation of molecular mass. It has been estimated that electrospray will provide information on 80% of these samples. The other 20% can be analyzed by APCI. Agilent’s Simultaneous Ion Source allows for single analysis no matter what the better ionization method is. The following description of the operation of this device appeared in an American Laboratory article by Wayne P. Duncan and Patrick D. Perkins (both of Agilent) in March 2005. LC-MS with Simultaneous Electrospray and Atmospheric Pressure Chemical Ionization: “Under pressure of the nebulizing gas, HPLC eluent is forced through the nebulizer, converting the liquid stream into an aerosol. Upon exiting the nebulizer, the aerosol enters the ESI zone where it is charged by the charging electrode and then separated from the uncharged component by the reversing electrode. The aerosol then enters the thermal container where it is completely vaporized by powerful infrared lamps. ESI ions and neutral analyte molecules then pass into the APCI zone. Ions previously formed by ESI are deflected around the corona, while remaining neutral molecules pass through and are ionized. ESI and APCI ions are then merged into a single stream and directed to the capillary entrance of the MS detector.” Data shown for the simultaneous operation of the ion source show the same signal strength observed when the source is operated in the ESI or APCI mode only. This combination ion source is currently only available on the LC/MSD 1100 but will become available on all of Agilent’s mass spectrometry platforms.

The third introduction of interest to the mass spectrometrist is called Lab Resources Management (LRM) Services for Large Laboratories. This is a new service program by which Agilent will provide maintenance for all instrumentation in a laboratory regardless of the manufacturer. This program will service any manufacturer’s equipment as long as parts are available from the manufacturer or through a third party. When asked about no longer providing service for their own older-model instruments, May Van, vice president and general manager of Agilent’s Consumables and Service Solutions business, said there was a policy change, and under this program, these instruments would be supported. Agilent says that the service program has been demonstrated to reduce instrument downtime by a factor of 4 compared with standard support agreements from individual vendors and reduces labor time from 8.5 employee hours per failure to 75 minutes. In response to a question regarding who will provide the service, Chris van Ingen said that it would be done both by Agilent employees and by third-party contractors.

Another interesting revelation at Agilent’s Monday-morning press conference was that a new GC/MSD is to be introduced in the third quarter of 2005; a new LC/MS platform will be introduced also in the third quarter. The new GC/MSD is reported to have a new
data system that will be backwardly compatible with the current GC/MS ChemStation. When questioned as to the specifics of the LC/MS platform, it was implied that a possibility existed for both a triple quadrupole analyzer and a quadrupole/time-of-flight MS/MS instrument. The desire on Agilent’s part is to be able to provide more specifics at this year’s ASMS conference in San Antonio, TX, in June.

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)

ABI/MDS Sciex introduced the API 5000™ LC/MS/MS System, which uses the QJet™ ion guide technology and the Analyst® 1.4.1 software. This is not just another upgrade to an existing instrument. This is a new instrument using new technology throughout the ion path from atmospheric inlet to detector. The QJet ion guide is an RF-only quadrupole that is positioned so that ions are captured and focused into the high-vacuum chamber rather than the process of skimming off a portion of the gas ion beam emanating from the API 4000 or electro spray source. This instrument uses the Turbo V™ source that has been one of the hallmarks of the API 4000. The m/z range of the API 5000 is 5 to 1250. The instrument uses a higher RF frequency over its ion path than is used in the API 4000; 1.228 MHz compared with 816 KHz used in the API 4000. The orifice diameter on the entrance of Q0 on the API 5000 is 0.62 mm compared with 0.32 mm on the API 4000. The QJet provides for a greater flow of ions from the source into the mass spectrometer than is obtained with conventional optic systems. The QJet also provides for better separation of ions and noncharged particles. This results in a better signal-to-background. Both the improved signal-to-background and the better flow of ions result in the demonstrated improved limits of quantitation. The QJet is reported to be easier to remove and clean than the skimmer used in the API 4000 and to handle larger gas loads. Operation of the QJet involves two additional parameters that must be set for data acquisition; however, ABI says that method transfer from the API 4000 to API 5000 is very easy.

The data shown for the API 5000 was in comparison to the data from the API 4000. In one test using three test compounds for negative-ion electrospray and three for positive-ion electrospray with Q1 and Q3 set for unit resolution, a range of 3.5 to 26.6 was shown for signal improvement with the API 5000 compared to the API 4000 (low: cyanazine in negative-ion detection; high: 5-fluorouracil in negative-ion detection). The other four compounds showed signal strength improvements in the range of 4x to 9x. These same tests showed improvements in signal-to-background of 2.1 to 6.2. The linearity of the API 5000 was from 10⁻³ to 1 pg µL⁻¹ of buspirone (MM 385 Da) acquired using selected reaction monitoring (SRM) with a transition of m/z 386 to 122. These data indicated a lower limit of detection of 1 fg on-column. The linear dynamic range based on these data appeared to be 3 to 4 orders of magnitude. Other SRM data were shown where as many as 20 different transitions were simultaneously monitored with significant improvement in sensitivity over the results obtained on the API 4000.

Applied Biosystems/MDS Sciex has been known for innovations in the area of transmission quadrupole mass spectrometers and especially in the area of MS/MS instrumentation. The API 5000 and the QJet Ion Guide appear to be another one of those innovations that will continue to push the limits of where mass spectrometry can go. 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 Inc. (Billerica, MA; Bremen, Germany)

Bruker Daltonics introduced a new benchtop transmission quadrupole-TOF MS/MS instrument, the microOTOF™-Q: a benchtop MALDI, the microflexLT MALDI-TOF: a new laser system (smartbeam™) incorporated into the ultrasflex™ II MALDI TOF/TOF instrument; and a yet-improved quadrupole ion trap called the HCTultra Ion Trap. In addition, they introduced the Apollo™ II Ion Funnel ESI source for its apex®-Qe line of hybrid Q-q-FTMS instruments; and a computer switchable ESI/MALDI source on the UltrOTOF™-Q quadrupole time-of-flight mass spectrometer.

The microOTOF-Q takes advantage of technology that Bruker Daltonics developed for its floor-standing Q-TOF instruments. This instrument has a reported mass resolving power of 15,000 (FWHM) at full sensitivity using a standard reflectron (not W-reflection). It has a specification of 3-ppm mass accuracy in MS and MS/MS over a wide dynamic range. This instrument claims good suitability for quantitation based on the “use of modern electronics and detector technology...” The instrument’s data system provides precise isotope profile analysis technology (SigmaFit™), which is combined with the 3-ppm mass accuracy to give better elemental compositions than can be obtained by mass accuracy alone. The instrument is capable of 20 full spectra per second. According to the information found on Bruker Daltonics’ Web site, the instrument’s m/z range is 20 to 40,000. This instrument also uses the Apollo II Ion Funnel.

The microflex LT MALDI TOF instrument is a linearly scanned time-of-flight system that uses Bruker Daltonics’ gridless ion source. The instrument is capable of operating in both the positive- and the negative-ion detection modes. The system is compatible with the patented
AnchorChip™ technology and is operated using the integrated Compass™ software. This instrument is designed as a low-cost MALDI system to meet the needs of many clinical proteomics applications.

The introduction of the smartbeam laser technology for the Bruker Daltonics MALDI-TOF/TOF instrument could be considered the third generation for this instrument. This is why it is considered a new instrument. Conventional Nd:YAG lasers used in TOF/TOF instruments have been found to be less suitable for intact protein analysis, MALDI imaging, and protocols such as thin-layer or DHB matrix preparations. These lasers are also not very suitable for the analysis of synthetic polymers. The smartbeam technology (patent applied for) employs a variable repetition rate (1–200 Hz) on all solid-state laser system. Bruker Daltonics is also offering a new software package for this instrument called flexImaging for use in MALDI imaging.

The HCTultra quadrupole ion trap mass spectrometer is the third higher-capacity QIT instrument from Bruker in as many years. This instrument is reported to give better sensitivity in MSn data-dependent analyses. It is said to have “greatly increased acquisition speed and sensitivity, in combination with new Compass software capabilities for data-dependent scans.” There are no specifics in the Bruker press release nor on their Web site describing these improvements.

The Apollo II Ion Funnel ESI source provided on the apex-Qe Q-q-FTMS mass spectrometer gives increased sensitivity by increasing the number of ions that pass from the source to the m/z analyzer. This source is available on all of Bruker Daltonics’ FTMS instruments. The apex-Qe is reported to reduce the limit-of-detection by an order of magnitude.

The other innovation in the ion source introduced by Bruker at PittCon 2005 was the computer-switchable ESI/MALDI source. This is an option for the floor-standing ultrOTOF-Q Q-q-TOF. The ESI portion of this combination source is based on the Apollo II Ion Funnel ESI source and allows for the use of MALDI while acquiring ESI data. This can be very convenient for peak matching to assign accurate mass to ESI data. It also allows for convenient switching between modes of operation without having to replace one source with another, which is often the inertial limiting factor in making switches in operational modes.

More information on all of the Bruker Daltonics line of mass spectrometers and software can be found at http://www.bdal.com. Please note that this is a different Web site from that reported in previous years.

**Elsevier**

**(Amsterdam, The Netherlands)**


**Griffin Analytical Technologies**

**(West Lafayette, IN)**

This company first appeared at PittCon 2003 (J. Am. Soc. Mass Spectrom. 2003, 14, 542–551) shortly after Graham Cooks’ paper on the miniature cylindrical ion trap appeared (Patterson, G. E.; Guymon, A. J.; Riter, L. S.; Everly, M; Griep-Raming, J; Laughlin, B. C.; Ouyang, Z.; Cooks, R. G. Miniature Cylindrical Ion Trap Mass Spectrometer. Anal. Chem. 2002, 74, 6145–6153). All the company had to show at that time was an empty box and a concept of what their quadrupole ion trap product would be. This year, those 2003 dreams became reality in the MINOTAUR 300™, a desktop GC-MS and the MINOTAUR 400™, a “field-ready GC-MS.”

This MINOTAUR 300 is intended more for the educational market but will find its way into a number of different applications. There are still some unrealized specifications such as the ability to do internal chemical ionization, but the company has begun to deliver instruments that are operating with internal (in trap) electron ionization. This instrument claims a limit-of-detection 17–ppb toluene for a continuous real-time monitoring of a gas sample. The instrument’s operating pressure is 10⁻⁴ torr using ambient air as the buffer gas to cool the ions in the trap. The m/z range to 400 and unit resolution are well suited for GC/MS. There is a Griffin data system for use with the MINOTAUR systems. They can provide a wide range of acquisition parameter controls including multiple temperature ramps of the GC. The data output portion is still in development, but data files can be exported as netCDF for use with other data systems. The company is also producing the AROS™, a quadrupole controller that provides both waveform-generating functions and timing controls. This product is intended for use with developmental transmission quadrupole and quadrupole ion trap systems.

Look for this company to have a continued presence in mass spectrometry and to fill the current gaps in its product lines. You can learn more about the company and their products at http://www.griffinanalytical.com.

**IonSpec**

**(Lake Forest, CA)**

This small southern California company founded in 1983 by Robert T. McIver, a pioneer in Fourier trans-
form mass spectrometry, showed at PittCon for the first time a 7-tesla cryogen-free FT-MS. IonSpec is the first of three commercial manufacturers of FTMS to deliver a cryogen-free instrument. These instruments use magnets that are based on cryocoolers capable of operation at about 4°K. This technology was first employed with MRI instruments in hospitals that did not want to deal with the maintenance issues involved with traditional superconducting. These systems operate on 2.5 kW. Although a power outage lasting more than 10 minutes will result in a magnetic quench, the cryogen-free magnets from Cryomagnetics (Oak Ridge, TN) are designed and guaranteed to withstand quenching without damage. The use of cryogen-free magnets adds to the initial cost, but this will quickly be offset by savings experienced from not having to buy liquid helium and nitrogen.

IonSpec is also now shipping its QFT-12 instrument. This is a hybrid triple quadrupole mass spectrometer with a 12-tesla magnet. The use of 12-tesla magnets has been somewhat problematic, but Dr. McIver says that the instruments manufactured and installed by IonSpec have proven to be routine.

In the past year, IonSpec has doubled its manufacturing capability by purchasing a new 9400 sq. ft. building that will be dedicated to manufacturing, final testing, and an applications and demonstration laboratory. The existing building will be used for R and E, software development, and administration. The company has also dramatically increased the number of employees to 24 with dedicated sales people in Canada, the U.K., and the northeastern U.S. They have also added a Western regional account manager based in the Lake Forest facility.

You can view IonSpec’s array of products that include four different system solutions and three different data stations for their instruments at http://www.ionspec.com.

JEOL
(Peabody, MA)

In this reviewer’s opinion, the introduction of a new ionization technique by JEOL is the most significant event since the introduction of electrospray and MALDI. If this were not enough for JEOL, they became the third company to introduce a TOF GC/MS instrument based on their popular LC/MS AccuTOF instrument introduced at PittCon 2002, and for which they won the Bronze Pittcon Editors’ Award that year (J. Am. Soc. Mass Spectrom. 2002, 13, 749–758).

In the past, technology such as MALDI, electrospray, and the triple quadrupole mass spectrometer was developed by research groups, appeared in the literature, and then appeared as implementation by various manufacturers. JEOL’s DART™ (Direct Analysis in Real Time) was invented internally, patented, tested, and introduced before any publications appeared. DART exploded onto the scene with its first mention of the technology and the finished product at the ASMS 2005 Sanibel Conference in Clearwater, FL (Jan 28–Feb 1); again, at a press conference held at JEOL in Peabody, MA, on February 9; and now, at PittCon. DART was invented by James Laramée and Robert B. Cody. A patent was issued to Drs. Cody and Laramée, who assigned the rights to JEOL USA, Inc. JEOL USA, Inc. then granted an exclusive license to IonSense, Inc., who has the rights to sub-license the technology. IonSense manufactures DART, which is sold as an accessory to the JEOL ESI AccuTOF instrument. The idea for DART grew out of the work involved with JEOL’s TEEM electron monochromator, which was introduced on the GCmate at PittCon 2003 (J. Am. Soc. Mass Spectrom., 2003, 14, 542–551).

DART is a technique used to ionize components in air or on the surfaces of material. The process works at zero potential and atmospheric pressure in an open space just in front of the ion inlet for the mass spectrometer. There are several mechanisms involved in ion formation. A gas is introduced into DART where it is subjected to a corona discharge. The resulting ions, unaffected gas atoms or molecules, and metastable species, pass through a series of electrodes designed to strip out any ionic species leaving only metastables. In the case of helium as the input gas, analyte molecular ions can be formed by Penning ionization by the He metastables, which have 19.8-eV energy. The He metastables can also ionize water molecules, affording ultimately protonated water clusters, which in turn will ionize substances on the surface. Negative ions can be formed through ion/molecule reactions with negative ions formed in the area past the ion removal electrodes or through electron capture attributable to the presence of neutralized electrons produced during other ionization mechanisms. For some analytes, a dopant mixed with the analyte or present in the air will enhance the ionization process. An as-soon-as-possible peer-reviewed paper has been posted on the Analytical Chemistry Web site that gives more detail on these mechanisms.

What DART does is more important than how it works. DART forms ions on the surfaces of material without the need for extraction or sample prep. Unlike the recently described desorption electrospray technique, DART does not need a solvent. DART forms ions and can cause ions of salts to be desorbed into the gas phase. Although the sample types that have been analyzed using DART are far too great to include in this report, some examples are explosives in muddy water by placing a drop of water on a glass rod; the anion of sodium γ-hydroxybutyrate (date-rape drug) on the surface of a cocktail glass; trace amount of sarin on a cinder block; uric acid from a drop of urine placed on a glass rod; multiple compounds such as cocaine, DEET, methyl palmitate, and ritalin on a dollar bill; and the difference between dihydroartemisinin (an antimalarial drug) and methyl stearate (used in counterfeit antimalarial pharmaceutical preparations), both having the...
same nominal mass and both detected in their pill form without sample prep of any kind, to name a few. In each of these cases, samples are held in the open space between the exit of the DART generator and the ion inlet to the atmospheric pressure mass spectrometer. The ionizing agent passes over the surface; ions are formed and/or desorbed from the surface and pass into the mass spectrometer. Gunpowder residue was detected from fingerprints on ABS. Sodium perchlorate was found on the surface of paper or cloth. Dr. Cody said that IonSense hopes to develop DART for instruments other than the high-resolution TOF mass spectrometer. The company believes that DART also has potential with MS/MS instrumentation and ion mobility spectrometers. This Gold winner of the 2005 PittCon Editors’ Award is definitely the most significant event in mass spectrometry since the development of MALDI and electrospray and may be worthy of mass spectrometry’s next Nobel Prize. Who knows to the extent to which DART, in combination with a high-resolving-power TOF mass spectrometer, will be utilized. Someday, you may find yourself in the produce department of the supermarket checking the surface of your produce for pesticides on a DART instrument.

JEOL’s other product introduction, the AccuTOF-GC, is a very impressive product. This GC-MS using a high-resolving-power TOF mass spectrometer boasts a mass accuracy capability of 5 ppm, a resolving power of >5000 (FWHM), an acceleration voltage of 7 kV, an m/z range of 4–2000, and a data acquisition rate of up to 16,000 spectra per second (recording speed up to 25 averaged spectra per second). The sensitivity specification ≥100:1 signal-to-background for 1 pg of octafluoronaphthalene injected onto a 0.25-mm × 30-m DB-5ms column with a 0.25-μm film thickness. The instrument is provided standard with electron ionization. There are options for chemical ionization (including electron capture negative ionization) and field ionization/field desorption ion sources. The FI/FD source has a probe onto which the FD emitters can be mounted. There is a direct exposure probe that allows for desorption CI. There are equally impressive specifications for electron capture negative ionization (S/B ≥ 20:1 for 1 pg hexachlorobenzene) and chemical ionization (S/B ≥150:1 for 100 pg benzophenon) modes. The AccuTOF-GC has a linear dynamic range for quantitation, which was established by the ADC ion-detection technique introduced in the original LC/MS AccuTOF. The instrument has an Agilent 6890 GC that can be configured with multiple injectors and fast temperature programming to take advantage of the fast acquisition rate.

Additional information about all of JEOL’s mass spectrometry products can be found on their Web site at http://www.jeol.com. This Web site has a link to Essays and Tutorials that are available in pdf format and offer very good explanations of techniques such as MS/MS, different types of m/z analyzers, ionization techniques used in organic mass spectrometry, and so forth.

John Wiley & Sons (Hoboken, NJ)

There were several announcements of interest to the mass spectrometrist by Wiley. The second edition of Understanding Mass Spectra (ISBN: 0-471-42,949-X) by R. Martin Smith was shown at PittCon for the first time (copyright 2004). This is a book on the interpretation of electron ionization spectra using a number of examples from the author’s experience in analysis of drugs of abuse. This book is expanded and improved from the first edition. This book can be purchased from the usual book outlets on the Web or from the LCMS Bookstore at http://www.LCMS.com.

Wiley also announced the availability of the Analytical Sciences Backfile, which is a collection of about 25K articles from 16 different journals. This collection includes all the volumes of the discontinued journals of Organic Mass Spectrometry and the various names of Biological Mass Spectrometry as well as the volumes of the continuing journals of Rapid Communications in Mass Spectrometry, Mass Spectrometry Reviews, and Journal of Mass Spectrometry that are not already available in electronic format. This collection is available for a one-time price and is fully indexed and searchable. More information on this back file is available at http://www.interscience.wiley.com/backfiles/analyticalscience.

Wiley also announced a new electronic edition of its Designer Drugs mass spectral library, which will have a 74% increase in the number of compounds. There is an upgrade path for those who have the current edition of this library. Also, a new database of steroids was announced. Both of these databases will be available in May of this year. Wiley is also now offering SpecInfo—a spectral identification system which includes IR, NMR, and mass spectral data—as a Web-based product. There is very aggressive academic pricing for this product. More information about these and other mass spectral databases and Wiley’s print books on mass spectrometry can be found on Wiley’s Web site at http://www.wiley.com/WileyCDA/Section/id-3047.html. There is a specific site for the electronic databases at http://www.wiley.com/go/databases.

Konik Instruments, Inc. (Miami, FL; Barcelona, Spain)

A French-Swiss colleague, Pierre Tecon, with whom I worked for many years once said, “It may be a different circus, but it is always the same clowns.” I was reminded of these words two summers ago when I visited old friends from the original Riber mass spectrometry company. Gerard Devant, the scientific/engineering genius behind the R1010 and Automass, and Alain Perot, the programmer who was responsible for a number of
Pyrolab AB
(Lund, Sweden)

This Swedish company manufactures a unique pyrolysis unit that can be used with a GC or a GC-MS. The company was founded in 1983 by Dr. Inger Ericsson, who has worked in the field of pyrolysis and has offered courses on the subject around the world. The company has two products—the PyroLab® 2000 and the PyroLab® 2000 MultiMatic, which is a multiple-sample version that can be automatically operated. The PyroLab 2000 MultiMatic is available in a 6- and 14-position version and offers the advantage of having different pyrolysis methods for each sample without the need for operator intervention. The Pyrola 2000 differs from other pyrolysis units in that it can be programmed for isothermal, fractionated, or sequential pyrolysis and pyrolytomy. The temperature range is 50–1400 °C. Thermal desorption can precede all the programs. Samples can be heated to 1400 °C in 8 milliseconds. Fractional pyrolysis can be done by programming the system to operate at as many as three preset temperatures. Currently, the company has no distributor in the U.S., but there are distributors in Spain, the U.K., Germany, Taiwan, and The Netherlands. This is a new concept in pyrolysis, and for those interested in this field, a closer look at the company’s Web site (http://www.pyrolab.se) is worth the time. The company will be holding a course on pyrolysis in Lund, Sweden, April 18, 19 and April 21, 22, 2005.

Shimadzu
(Columbia, MD)

The LCMS-IT-TOF, a tandem quadrupole ion trap and TOF mass spectrometer, was introduced at PittCon by Shimadzu along with a low-cost GC/MS product, the QP-2010s that has the same performance characteristics as the GCMS-QP2010, which has been a popular instrument for several years. The LCMS-IT-TOF tied for the Silver PittCon Editors’ Award with two non-mass-spectrometry products.

There are several unique features about this first-ever commercial electrospray QIT-TOF mass spectrometer. The trap uses argon rather than helium as the bath gas to cool the ions before transfer to the TOF. The difference illustrated by Shimadzu between the effects of the two gases on resolving power, when multiple-charge ions are involved, is rather remarkable (He at 4.5 × 10⁻² Pa versus Ar at 7.5 × 10⁻³ Pa). The use of argon also facilitates the collisionally activated dissociation (CAD) process. The instrument has a resolving power specification 10,000 (FWHM) at m/z 1000. The instrument can perform MS⁵. The resolving power for a precursor-ion selection is 1000.

The ion optics of the LCMS-IT-TOF are reported to be significantly improved over previous LC/MS instruments. After the heated desolvation capillary, ions enter a set of three hyperbolic quadrupole plates plus an additional set of electrodes. In this area, the first set of quadrupole plates is spaced wider apart than the third set. The combination of RF and DC voltages cause ions to focus to the center of the array as they move through it and move rapidly toward the first skimmer with very little DC voltage needed. After the skimmer, ions enter a set of gold-plated ceramic octupoles. Different portions of the octupole are either conductive or resistive. There is an RF voltage applied at 2.4 MHz and different DC voltages at each end. Towards the end of the octupole is a resistive portion that allows ions to accumulate before the trap. Ions are bunched together and released from the octupole to the trap while an accelerating voltage (~4 V) is applied to the entrance end cap. A retarding voltage is applied to the exit of the trap. Argon is pulsed into the trap along with the ions for ion cooling, over an approximate 10-ms period. For a typical MS⁵ cycle, ions are cooled for 10 milliseconds, isolated for about 30 milliseconds, collisionally activated for approximately 30 milliseconds, and submitted to additional cooling for 25 milliseconds. For ion ejection from the trap, short-duration high voltages are applied to both end caps to squeeze ions to the center of the ring electrode system and then released into the TOF a few milliseconds later by changing the voltage on the outlet end-cap electrode. This results in less energy variability for ions of the same mass, and a smaller angular dispersion getting into the time-of-flight analyzer.

The dual-stage reflectron technology used in the TOF...
portion of the instrument is perceived to be an improvement over the ion mirrors used in previous Shimadzu instruments. A detailed technical description is listed in U.S. patent no. 6803564 by Eizo Kawato (patent issued October 12, 2004). The QIT is used primarily for precursor-ion selection and fragmentation. Operation of the trap is through ballistic ion ejection. Ions are not scanned out of the trap by m/z values as they would be in a typical ion trap mass analyzer.

The LCMS-IT-TOF is reported to give good, stable mass accuracy without need for internal calibration. Initial results with existing customer installations of the LCMS-IT-TOF indicate the mass accuracy is very stable over long periods of time. Shimadzu chemists have been able to use the same autotune file over a month with a simple external calibration. Part of the reason for this stability is due to the thermal control of the flight tube. Compressed ion introduction, improvements to the reflectron, and the ballistic ion ejection from the trap also play a role in this stability of the m/z scale. For more accurate mass determination, up to three internal standards can be used for internal calibration for each mass spectrum.

Additional information about Shimadzu and their products can be found on their Web site at http://www.shimadzu.com.

**Syft™ Technologies Ltd.**
(Christchurch, New Zealand)

Syft Technology was started in 2002 to commercialize development work that had begun in the chemistry department of Canterbury University. The company considers Canterbury to be the leader in selected ion flow tube (SIFT) mass spectrometry with work pioneered by Dr. Murray J. McEwan. At PittCon 2005, Syft introduced their Voice100 for the analysis of volatile organic compounds (VOCs) based on a SIFT mass spectrometer. The company is being represented in the U.S. and Canada by Ardara Technologies (Monroeville, PA), Dr. Randy Pedder, President (randy.pedder@ArdaraTech.com).

The SIFT mass spectrometer uses three precursor ions (H$_3$O$^+$, O$_2^-$, and NO$^-$) to react in the gas phase with organic molecules in air samples. These ion/molecule reactions form product ions that represent the VOCs present in a sample. The product ions are detected over an m/z range of 10 to 300 using a transmission quadrupole m/z analyzer.

A SIFT acquisition can be divided into five fundamental steps: (1) water vapor or air passes through a microwave discharge, generating a mixture of ions; (2) the ions are drawn through an upstream chamber where a quadrupole mass spectrometer filters the ion stream, selecting precursor ions (H$_3$O$^+$, O$_2^-$, and NO$^-$); (3) the precursor ions are injected into the flow tube where they flow in a helium and argon stream and react with VOCs from the sample; (4) the VOC-ions stream into the downstream chamber and pass through a second quadrupole, which filters the ions according to their m/z values; (5) the ions, separated by individual m/z values, sequentially pass to the electron multiplier (detector).

The instrument is fully contained; it was running on the PittCon Exhibit Floor where breath samples from conferees were being analyzed as you watched. This accomplishment was even after a harrowing airplane trip from New Zealand. This new instrument was worthy of a nomination for the PittCon Editors’ Award and missed the Bronze award by only one vote. More information can be found at the company’s Web site at http://www.syft.com or at the Ardara Web site at http://www.ArdaraTech.com.

**Thermo Electron GmbH**
(Bremen, Germany); **Thermo Electron, Inc.**
(San Jose, CA)

Over the past several years, Thermo Electron, Inc. has introduced several new instruments in its line of organic mass spectrometers. This year, it was the other application of mass spectrometry that had the new product spotlight. The Finnigan Element GD is based on the same high-performance double-focusing mass spectrometer used in the Finnigan Element II ICP mass spectrometer. The Finnigan Element GD uses a newly designed glow discharge ion source. This source is the product technology acquired with Thermo Electron’s acquisition of VG elemental and engineering at the Bremen, Germany, research and manufacturing facility. This new glow discharge ion source uses optical imaging that was behind the success of the Grimm source developed at VG Elemental in 1967. The problem with glow discharge sources in the past had to do with sealing the sample holder. The Finnigan Element GD incorporates the sample holder into the ion source and seals the ion source. A sample can be analyzed for 50 elements in 10 minutes (5 minutes for sample and 5 minutes for cleanup). Older systems took anywhere from 20 minutes to all day, depending on the number of elements to be detected. The mass analyzer is capable of three fixed resolving powers (300, 4000, 10,000) with less than 1-second switching time. The mass stability is better than 25 ppm for over 8 hours. Thermo Electron claims that no mass calibration is required for months. The scan speed is less than 150 milliseconds from m/z 7 to 238 to 7. This instrument, which uses 3 different methods of ion detection (Faraday, analog, and counting), has a linear dynamic range over more than 12 orders of magnitude. The majority of elements are detectable in the ppt range.

In other news from Thermo Electron, it was reported that the latest version of SEQUEST was now “accurate mass enabled.” Additional information about the Finnigan Element GD and the other mass spectrometry and chromatography products available from Thermo Electron can be found on the company’s Web site at http://www.thermoelectron.com.
Waters (Milford, MA)

Waters had two important announcements for the mass spectrometrist: (1) the introduction of the Acquity Ultra Performance LC (Acquity UPLC™) Bridged Ethylsioxane/Silica Hybrid (BEH) Columns; and (2) the fact that the Q-Tof Premier, introduced at the 2004 ASMS in Nashville, TN, is now “MALDI-enabled.” This was the first showing for the Q-Tof Premier at a PittCon.

When electrospray burst onto the scene in the early 1990s, mass spectrometry manufacturers scrambled to produce instruments that would handle the high flow rates from the conventional 4.6-mm i.d. LC columns. As electrospray began to mature and to be more understood, its sensitive dependence on concentration became more obvious. All of a sudden, it was the LC system manufacturers who were scrambling to produce micro-LCs to support smaller diameter columns that produce eluate that have higher concentration of analytes. As the development of the micro-LC progressed, Waters realized that it was not just a bunch of micro components connected with a small diameter column, but a whole system was necessary down to the particle size of the column packing material. This realization has resulted in last year’s introduction of the Acquity UPLC and this year’s introduction of the 1.7-μm particle-size Acquity UPLC BEH Column in both C18 and C8. These columns complete the micro-LC package that results in higher analytic concentration in LC peaks, which are required for electrospray.


In Conclusion . . .

There were a number of exciting discussions in the other press conferences. Bio-Rad Informatics Division talked about the current status of its Know-It-All product. This product, used to determine the identity of primarily organic compounds based on various kinds of spectra, continues to evolve like its competitor ACD Labs. Other companies that were there in addition to column, pump, and detector manufacturers were Varian with all three of its mass spectrometers; Palisade with the Palisade Complete Mass Spectral database; and Inficon, developer and manufacturer of the Hapsite portable GC-MS.

Ever year I conclude this column with, “As is the case with every year’s PittCon, there is still too much to see and do when it comes to mass spectrometry.” But, this year was different. As you walked onto the stand of each company, even those that did not have new products, there was a crackling excitement created by all the new technology and innovations introduced here and a few months before at the ASMS meeting in Nashville. With the PittCon 2005 introductions and what I’m sure will be a very exciting year at ASMS, 2005 will be known forever more as the year of mass spectrometry.