Mass Spectrometry PittCon[®] '96

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The 1996 Pittsburgh Conference & Exposition on Analytical Chemistry and Applied Spectroscopy (PittCon[®] '96) was another big event in respect to mass spectrometry. This year's meeting, held in Chicago, IL, March 3–8, had an attendance of 32,000 + . The prestigious Pittsburgh Spectroscopy Award went to David M. Hercules for his many scientific accomplishments including those in mass spectrometry.

Among the 39 short courses offered by the American Chemical Society, three titles were of particular interest to the field of mass spectrometry: GC/MS, Practical LC/MS and CE/MS, and Analytical Inductively Coupled Plasma: Emission and Mass Spectrometry. During the meeting, the PittCon'96 organizers offered half-day courses in LC/MS and Inductively Coupled Plasma/Mass Spectrometry and one-day courses entitled Quadrupole Ion Trap Mass Spectrometry: Fundamentals and Practice, Introduction to Mass Spectrometry, and Environmental Mass Spectrometry.

In addition to the many posters that were presented throughout the week on gas chromatography/mass spectrometry (GC/MS), liquid chromatography (LC/MS), desorption ionization mass spectrometry, and inorganic analyses using mass spectrometry, there were two symposia in addition to the one honoring David Hercules and six half-day sessions pertaining just to mass spectrometry. Other sessions contained talks that were of interest to many different areas of mass spectrometry.

Bruker-HP (Mountain Lakes, NJ–Palo Alto, CA)

The most talked-about event among the mass spectrometry community at this year's PittCon was the joint marketing agreement between Hewlett-Packard (HP) and Bruker for the Bruker Esquire electrospray ionization (ESI) quadrupole ion trap mass spectrometer (first shown at the 1994 International MS conference in Budapest) with the HP 1100 Series high-performance liquid chromatograph (HPLC) (introduced late last year), the HP 3D capillary electrophoresis (CE) system, and HP's ChemStation software. Although both companies will market and distribute these products worldwide, Bruker will continue to provide the quotations, installation, and service for the Esquire. Dr. Frank H. Larkin, executive vice president, Bruker USA, said, "The agreement combines HP's leadership in

HPLC, CE, and in-depth applications experience in LC/MS with Bruker's complementary patented ion trap technology." In addition to the ESI interface, the Esquire also has available options of an atmospheric pressure chemical ionization (APCI) interface and a NanoSPRAY[™] interface for use with microcapillary LC columns. The Esquire has a mass-to-charge ratio (m/z) range of 6000 with a normal resolution of 0.4 m/z and a high resolution of 0.2 m/z . The PC data system accommodates both the MS software and the HP ChemStation, simultaneously. The system also allows for the HP detectors such as the photo diode array. The instrument is reported to be capable of MS¹⁰. The agreement with Bruker for the joint marketing of the Esquire marks HP's long anticipated entrance into MS/MS and quadrupole ion traps.

HP also introduced a new version of its ChemStation software for the HP 5972 series mass selective detector (MSD), which is used with the earlier introduced 6890 GC.

In addition to the Esquire, Bruker showed the Proflex two-stage gridless reflectron TOF-MS for use with MALDI. This instrument has a new option for delayed ion extraction. It offers high-sensitivity post-source decay (PSD), which is of particular use in peptide and protein structural analysis, as a high-resolution sample observation optics. A 1 mm diameter target produces a full-screen display. This instrument is designed for automated use with Bruker's AutoXecute[™] software and the novel MaldiAutoPrep (MAP[™]) for unattended automated MALDI sample preparation, and is reported to have a resolution of > 20,000.

Bruker also emphasized that all their FT-MS instruments are provided with shielded magnets, regardless of size. These instruments are offered with all the various interfaces used by the biomedical mass spectrometerist. A unique feature of the Bruker FT-MS is that the cell rolls out of the magnet.

Bruker also introduced XBIO[™], a versatile molecular weight calculator and mass spectral interpretation tool. It reports true average and monoisotopic masses for chemicals. This is a powerful package for analyzing mass spectrometry data from large molecules.

Varian (Palo Alto, CA)

Varian CSB introduced the Saturn 2000. Although this instrument has the same performance specifications as the earlier Saturn 3, it is a completely redesigned, smaller, and easier to maintain unit. The use of clamps and vacuum-held flanges make disassembly and reassembly quick and easy. The position of the turbo

pump with flow-through cooling assures proper pump performance and may even increase its life. The Saturn 2000 is about 50% smaller than its predecessors. A new trap-heater design eliminates the need to heat the vacuum manifold during normal operation; however, to assist in quick returns to operations after breaking vacuum in humid climates, a manifold heater is provided. An ion gauge is built into the instrument. Varian is offering a SilChrom™ trap as an option for the Saturn 2000. The SilChrom trap is produced by applying the Restek Corporation (Bellefonte, PA) proprietary deactivation process to the three electrodes of the ion trap. The SilChrom trap enhances the performance of the Saturn 2000 with polar compounds and allows for lower trap operating temperatures, which reduces the disassociation of molecular ions. The SilChrom trap also is available as an upgrade to existing Saturn users.

New software, based on the Windows 95 operating system for viewing GC/MS data, also was introduced along with the Saturn 2000. This is the beginning of Windows software for Saturn. The current DOS-based software is still provided and is fully supported as an application in a DOS Window. Links between the two packages are included. As the Saturn Windows software evolves, current purchasers will be upgraded at no charge until the DOS software is no longer in use.

Other options for the Saturn 2000 are positive ion chemical ionization, selected ion storage, and MS/MS. The Varian 3400 GC, supplied with the Saturn 2000, has the 1078 injector as standard. This injector is designed for split and splitless cold on-column injections as well as hot injections. This new feature has allowed for detection of as little as 5 femtograms/ μL with a 100 μL injection.

According to Terry Sheehan, GC/MS product manager, the Saturn 2000 will ship in June, 1996.

Varian OSI introduced an automated "Cool Plasma" technique for use with the Ultra Mass inductively coupled plasma mass spectrometer (ICP-MS). This technique was developed in conjunction with leading chip manufacturers to detect the presence of minerals in process acids and bases at the part-per-quadrillion level. The cool plasma refers to the plasma's temperature during the analysis (2000 °C to 2500 °C as compared to normal ICP temperatures of 7000 °C to 10,000 °C). Varian has installed a specially designed portable clean room to demonstrate the efficacy of ICP-MS for microchip wafer quality control in an environment like that found at semiconductor fabrication plants.

Finnigan (San Jose, CA)

Finnigan continues to add to its reputation as a "Mass Spec. Company." Finnigan showed the GCQ (introduced at Pittcon '95), the LCQ (introduced at ASMS 1995 in Atlanta, GA), quadrupole ion trap mass spectrometers for GC and LC, respectively, its family of SSQ and TSQ (for MS/MS) transmission quadrupole

instruments with LC/MS interfaces, the high-resolution ICP-MS (double-sector instrument), isotope rationing mass spectrometers, its line of gas chromatographs that came as a result of the acquisition of Tremetrics (Austin, TX), and the two latest jewels in its crown: the Finnigan FT-MS, which resulted from the approximately \$1.7 million acquisition of Extral FTMS (Madison, WI) from Waters Technology Corporation (Milford, MA), January 31, 1994, and the Automass™ GC-MS, which resulted from the acquisition of the analytical instrument division of Analytical Technology, Inc. (ATI) for approximately \$34.9 million in cash and \$7 million in assumed debt, December 1, 1995. Both of these acquisitions were made by Thermo Instrument Systems, Inc. (Santa Fe, NM). Finnigan is owned by ThermoQuest Corporation, a subsidiary of Thermo Instrument Systems, Inc.

The Finnigan Automass uses the same GC that is designed for use with the GCQ. The Automass transmission quadrupole mass spectrometer, which is manufactured in France, has its origin in the instrument designed by Nermag. It has an m/z range to 1000 and can be extended to 1500. In addition to a single-pumped EI version, a differentially pumped EI/CI with both positive and negative ion detection is available.

According to Everett Sizemore, marketing manager, the Finnigan FT-MS with a 3-tesla magnet has the same performance as the competition's instrument with a 4.7-tesla magnet. To support this claim, Mr. Sizemore pointed to the MALDI mass spectrum of a single-laser shot on bovine insulin b-chain, shown on the back cover of a new Finnigan FT-MS brochure that showed a resolving power of $>210,000$. It also was pointed out that the Finnigan FT-MS can have a MALDI source mounted on one end and an ESI interface on the other. Spectra can be acquired using either ionization method without having to make any changes to the hardware.

Fisons (Beverly, MA)

The delayed acquisition of Fisons Instruments by Thermo Instrument Systems, Inc. appears to be reaching a climax. The sale to Thermo should be completed by mid to late March. At the same time, Fisons expects to complete the disposal of the parts of the instrument business that were of concern to the US and UK antitrust regulatory authorities to a financially supported group led by Schroder Ventures, including the senior management of VG Analytical and VG Biotech. This business will operate under the name of Micromass. Thermo will receive the MD 800 and newly introduced MD 1000 benchtop GC/MS products in this sale. Micromass will retain all the high-resolution and hybrid instrumentation, the Platform, the Quattro, the isotope rationing instruments, and the Plasma Trace II magnetic-sector ICP-MS. Thermo also will receive the quadrupole-analyzer-based ICP-MS and GC product line.

In addition to the MD 1000, which is a benchtop quadrupole GC-MS with an m/z range to 1000 and reportedly higher sensitivity than the MD 800 (which already has some of the best sensitivity specifications in the benchtop GC/MS industry), Fisons introduced: the new NanoflowTM ESI interface that allows for flow rates between 30 and 100 nL/min.; VG OpenLynx-LC, 32-bit, multitasking Windows-NT LC-MS software that uses two computers to enhance open access performance; enhanced versions of the ToFSpec-E and ToFSpec-SE MALDI-TOF mass spectrometry instruments with MassLynx-NT data handling technology; VG OpenLynx-Diversity software (developed by VG Organic of Altrincham, Cheshire) that is used with fully automated, high-sample throughput API quadrupole mass spectrometry and combinatorial chemistry; and newly enhanced ion source technology with X-Flow Electrospray for a higher tolerance to involatile buffers and samples entrained in complex biological matrices.

Fisons continues to commercialize the Open Access concept in API mass spectrometry so that the technique can be put easily into the hands of the nonmass spectrometerists, i.e., liquid chromatographers, biochemists, and synthetic or medicinal chemists. This is the impetus behind most of the software introductions.

LECO Corporation (St. Joseph, MI)

LECO introduced the Pegasus GC/TOFMS. LECO acquired the rapid detection TOF GC/MS product line from Meridian Instruments. Since the acquisition, LECO has put a great deal of effort into the completion and enhancement of what Meridian started. The Pegasus provides several spectral acquisition rates (not to be confused with scan rates) up to 500 spectra/sec over an m/z range to 650. The TOF-MS has a 1.5 meter mirrored flight tube and left and right side GC access ports. It can perform an analysis of all the components in US-EPA Method TO-14 in less than 4 min without the sacrifice of qualitative or quantitative data integrity.

Shimadzu Scientific Instruments (Columbia, MD)

With the introduction of the Kompact MALDI IV, Shimadzu expanded its already extensive line of MALDI-TOF mass spectrometers. This benchtop instrument is designed to dramatically reduce the time required to obtain peptide sequence information. The MALDI IV uses novel curved field reflectron technology, developed and patented by R. J. Cotter and T. Cornish. Shimadzu has an exclusive license on this patent from The John Hopkins University. Instead of the ability to focus only 10% of the ions produced by post-source decay, the curved field reflectron allows all the ion current to be focused, which results in less sample required and fewer laser shots to obtain sequencing information. The instrument allows a sequence spectrum to be acquired in less than 3 min.

"Seamless data acquisition" (SAD) allows for peptide sequencing without the need for time-consuming enzymatic/chemical digestion followed by database searching. The SAD technique allows sequence data to be obtained at the full sensitivity setting of the instrument. This allows for preservation of valuable samples. The MALDI IV includes the use of a high-performance Sun SPARCstation data system, disposable multiple-sample holders, and automatic tuning and method operating parameters.

Shimadzu also exhibited the QP5000 benchtop mass spectrometer with the GC-17. This benchtop transmission quadrupole GC-MS continues to offer good performance. It now has automated reporting for environmental and drugs of abuse analyses.

Waters (Milford, MA)

Waters did not introduce a new mass spectrometer at PittCon'96; however, they did introduce a new concept in liquid chromatography, which is of interest to those doing LC/MS. The Alliance HPLC Systems are the first to incorporate integrated solvent and sample management technology. This produces more accurate and consistent results. Waters makes the point that this is not a new LC pump but rather "a solvent and sample management system." The 2690 Separation Module comes with a new solvent delivery technology that features independent, digitally controlled piston drives for accurate and pulse-free (very important in LC/MS) isocratic or gradient-solvent delivery. It compensates for changes in eluent viscosity and automatically purges any gaseous mobile phase. Waters showed results of multiple injections with no deviation in retention times. The 2690 Separation Module is standard on the Integrity particle beam LC-MS.

JEOL (Peabody, MA)

The MStation JMS-700, which has never been shown in the US but has been on the market for about a year, was exhibited by JEOL. This is a fully automated version of the successful JMS-SX102, 10 KV source, reverse geometry instrument that has been on the market for many years. This instrument has an extremely well-designed automated data system and will eventually replace the SX102. Like the SX102, the MStation allows for alternate negative-positive ion detection at the full 10 KV accelerating voltage.

JEOL also introduced the CCD (charged coupled device) array detection accessory for a number of its instruments. This scanning CCD array detector is designed to improve sensitivity for recording mass spectra by a factor of 50 or more.

JEOL also showed the GCmate benchtop high-resolution mass spectrometer designed for GC/MS. This instrument was introduced last year. It has an m/z range of 1-1000, a maximum resolution of 5000, and is capable of scanning one decade in 0.07 sec. It uses an

acquisition processor and a PC-based data analysis computer.

NIST (Gaithersburg, MD)

NIST introduced Version 1.5 of its Mass Spectral Search Program for Windows, which includes the NIST/EPA/NIH Mass Spectral Library, and is shipping now. It added two major features to search software: substructure identification and automated batch searching of spectra. In addition, the program now has an interpretation aid utility called ISOFORM. A full-functioning version of ISOFORM is included with the Version 1.5 demo diskette set.

Substructure identification is a routine used in the interpretation of spectra that come from compounds whose spectra are not in the NIST/EPA/NIH Library. After a search of the unknown spectrum has been completed, the search results are examined to determine the probability of the presence of certain substructures in the molecule that produced the spectrum. The probability of the presence and/or absence of substructures is reported. This also reports a possible molecular weight for the unknown along with an accurate estimation of the number of atoms of chlorine and/or bromine that are present. The reported substructures include rings-plus-double-bonds estimation, phenyl groups, a phenolic group, hydroxyls, organic acids, etc.

ISOFORM calculates relative intensities of isotope peaks based on the input of a formula. It also is used to determine formulas that can be produced for a specified peak based on elemental constraints. It can be used to calculate the possible formulas of ions produced by neutral losses. One of the unique features of this program is its calculation of rings and double bonds. Unlike most routines used for this purpose, the RDB formula accounts for sulfur, nitrogen, and phosphorus in their higher valence states.

HD Science (Wilmington, DE and Nottingham, UK)

HD Science exhibited at PittCon for the first time this year. HD Science is a publishing company in the United Kingdom that produces abstracts in various fields of mass spectrometry, which include: *GC/MS Update, Part A, Environmental*; *GC/MS Update, Part B, Biomedical*; and *LC/MS Update and Other Soft Ionization Techniques*. These abstracts are distributed in either a printed or electronic format six times a year. HD Science introduced their *Mass Spectrometry Analyte* series, which are collections of abstracts selected for specific areas of interest: *Pesticides*, *PCDDs/PCDFs/PCBs*, *Water and Sediment Pollutants*, and *Drugs and Metabolites*. HD Science also introduced a *Techniques* series with two offerings: *Electrospray 1991-94* and *MALDI 1991-94*. One significant value of the HD Science abstracts is the detail of the analytical technique that is included.

HD Science also publishes an annual catalog that includes a variety of books, software, and training aids for MS, GC/MS, LC/MS, GC, and LC. In addition to their own products, HD Science used their booth to promote the nascent *European Journal of Mass Spectrometry*.

THRU-PUT Systems, Inc. (Orlando, FL)

THRU-PUT software introduced a Windows 95 version of their Target software, which is due to ship in May, 1996. Target, Version 3.2, introduced in December of 1995, provides for reporting of environmental (CLP and non-CLP formats), drugs of abuse, pharmaceutical, general GC/MS, GC, and LC analyses. A new feature in Version 3.2 is the reporting of pharmaceutical analyses along with system suitability studies. The Target software now can be used in a client/server environment where the server can either be UNIX or Windows NT; and the client can be a UNIX workstation, Windows NT client, or Windows 95. The pharmaceutical module of the Target software has been certified with data files from both the PE SCIEX and Finnigan triple quadrupole mass spectrometer, both of which are of particular interest to the pharmaceutical industry. In addition to the already large number of instrument data system formats supported, Version 3.2 also supports the Analytical Instrument Association (AIA) data format (netCDF) for gas chromatography and mass spectrometry.

Bear Instruments, Inc. (Santa Clara, CA)

The Bear CUB 800 Quadrupole GC-MS-MS, introduced at PittCon'95 with a spectrum of air and water, was exhibited with full-scan data, data acquisition, and a complete data system. The company is taking orders for this rounded hyperbolic quadrupole QQQ instrument for shipment in September. The instrument includes an HP-GC, a computer, and a printer. An optional GC auto sampler also is available. This small footprint mass spectrometer (18w × 21d × 14.5h, not including the GC) has an m/z range to 800 with a 0.1 m/z resolution. The data system comes with a macro-programming language for user-customizable reporting and data analysis. This instrument has many features such as true-triple-quad MS/MS in small footprint.

Palisade Corporation (Newfield, NY)

Palisade exhibited their new Wiley AccessPak, BenchTop/PBM, and MASSTransit. The Wiley AccessPak, introduced late last year, is available with the 6th edition of the Wiley Mass Spectral Library (230,000 spectra), the 6th edition of the Wiley Mass Spectral Library with the spectra from the NIST Database (275,000), or as the Wiley Select Mass Spectral Library (93,000 spectra). This is a CD-ROM that contains data

in a format that can be used by most PC-based commercial data systems' library search routines.

Perkin-Elmer SCIEX® (Foster City, CA)

PE SCIEX added the API-100 LC to its line of IonSpray™ transmission-quadrupole mass spectrometers. This instrument has an m/z range to 1200 Da. Also new this year is LC control from the MacIntosh-based data system. Control of the PE, ABI, HP, and Shimadzu LC is now available from the data system. In addition to the API-300 triple quad, two other 3000 Da instruments are in the API line: the API 100 and the API 100B. The API 100B has the BioToolBox™ software, which enables protein and peptide characterization. The BioToolBox is available as an option for any of the four API instruments offered.

PerSeptive Biosystems (Framingham, MA)

PerSeptive Biosystems introduced the Voyager-DE™, a benchtop linear MALDI-TOF instrument that employs patent-pending delayed extraction (DE) technology. Delayed extraction, or post-ionization extraction, improves the quality of the mass spectrum by reducing the chemical noise due to fragmentation in the ion acceleration region. Sample analyses were performed on request for interested customers. The Voyager-DE is attached to the Integral™ LC system, which has a fraction collector that is modified to use MALDI sample plates. The Voyager-DE uses the same ion optics used in the research-grade Voyager-Elite™.

Infocon (East Syracuse, NY)

Infocon, the US subsidiary of German-based Leybold AG, exhibited Hapsite™, "a portable GC-MS for site seeing." This transmission-quadrupole instrument, introduced in November, 1995, is available in June, 1996.

It has a portable unit and a separate Service Module, which allows the unit to be used as a conventional benchtop GC-MS. The portable unit has a weight of about 35 pounds, including batteries, and has a built-in gas chromatograph and a sampling device. The Hapsite is designed for the onsite analysis of volatile organic compounds (VOCs). The vacuum system of the portable unit is a nonevaporative getter (NEG) pump. The m/z range is 1-300. The acquisition rate is 1000 m/z units/sec@10 points per m/z unit. The gas chromatograph uses nitrogen as the carrier gas. The unit is supplied with a GC column designed for the analysis of VOCs. The Service Module has a 60 L/sec molecular drag/turbo pump with an oil-free backing pump and requires 110 V, 200 watts of power at normal operating conditions. The power consumption of the portable unit is 24 V, 25 watts of power at normal operating conditions.

Too many others to include all

In addition to the above-cited companies, there were a number of other companies who exhibited and are of interest to those working in mass spectrometry. These companies include: GC and LC column manufacturers and distributors, electron multiplier manufacturers, software publishers and distributors, third-party service and training companies, and vacuum equipment manufacturers just to name a few. There are two good sources for mass spectrometry information on the World-Wide-Web:

- (1) The Scientific Instrument Services, Inc. Web Page at <http://www.sisweb.com>
- (2) The Web Page operated by Kermit K. Murray, Emory University, at <http://tswww.cc.emory.edu/~kmurraymslist.html>