

The Newsletter On Analytical Data Interchange

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Andi/Mass Spectrometry Enhances Data Interchange at Eastman Chemical Locations

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The use of Andi/Mass Spectrometry to support transfer of mass spectral data and databases is key to accomplishing our corporate mass spectral goal. Our goal is to share mass spectral data, software and electron impact databases among all mass spectrometers within Eastman Chemical Company (35 instruments, 60 users). Instruments in Tennessee, Texas and Arkansas are connected via Ethernet. Our instruments employ data systems from a variety of manufacturers including Finnigan (PDP-11, UNIX), Hewlett-Packard (DOS, UNIX) and VG (VAX workstations).

Corporate and various commercial databases are used extensively in our research, development and environmental work. Our corporate database is composed of 29,500 electron impact mass spectra and 16,000 structures. The Andi/Mass Spectrometry format is used with other commercial software packages to distribute the database and corresponding structures to our users.

Use of Andi/Mass Spectrometry allows us to transfer files between users with different data systems or to a host computer. The host computer

employs VG's OPUS software to process the files while results of the processing are displayed on the user's local computer. The host computer displays structures for library search results and can search commercial and corporate databases by structure. Use of the host computer is the preferred approach and is employed by users whose primary responsibility is mass spectrometry. Other users, who employ mass spectrometry as an ancillary technique, use the HP DOS software package. This approach only displays structures with library results but does not allow searches of the databases by structure.

The conversion and transfer of data files between users requires extensive knowledge of the UNIX, VAX, DOS and RSX operating systems. This severely limited our initial attempts to share data, software and databases. This was overcome by writing a user-friendly, menu-driven interface for our VAX host computer. The interface employs custom menus for each user, requires no knowledge of the VAX operating system and requires very little user training, generally less than 15 minutes.

Infrared Group Tests Raw Data Information

The Andi/Infrared working group met on October 4 to discuss results of initial round-trip testing. Participants included ATI/Mattson, Bio-Rad/Digilab, Galactic Industries, JCAMP, Nicolet, Perkin-Elmer and Sadtler.

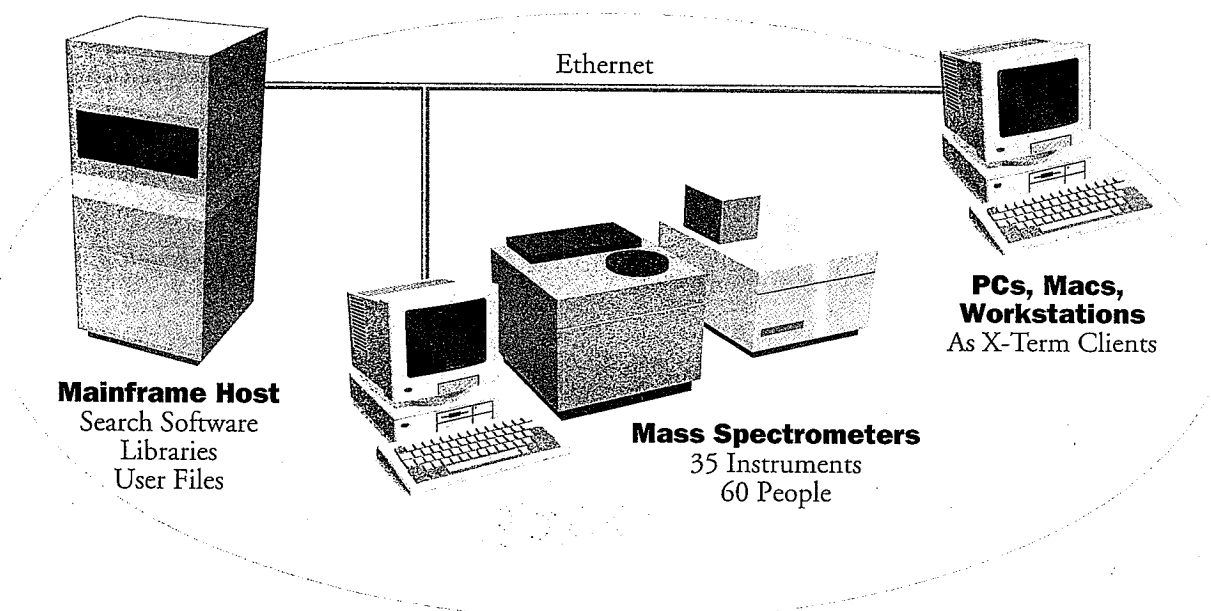
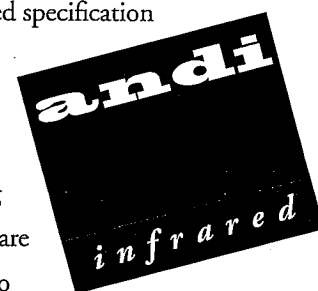
Initial testing took place last summer and marked the beginning of the implementation phase of Andi/Infrared. Participants created data files using the Andi/Infrared specification and information from its Raw Data section. These data files were successfully read using the participants' software and then distributed to other participants for use in round-trip testing.

As a result of the initial tests, questions were raised concerning the scope of the specification, the use of default values and the handling of units. Each of these questions was discussed at the October 4 meeting and resolved. The Andi/Infrared specification was then revised to incorporate changes agreed to at the meeting.

Testing of the revised Raw Data section of Andi/Infrared is currently under way and is scheduled to continue through February.

The working group plans to meet in New Orleans on March 7 to review results of the latest testing. If all goes well, the group plans to begin testing the second and third implementation phases (which cover Final Results and Full Data Processing Method) later this spring. Release of the final version of Andi/Infrared is planned for later this year.

For more information, contact Mike Duff of AIA at 703-836-1360.



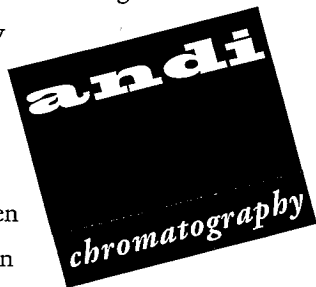
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Working Group Prepares To Update Andi/Chromatography

An AIA working group currently is reviewing suggestions for a number of changes to Andi/Chromatography based on vendor experiences and feedback from users. No modifications have been made since its release in June 1992.

The principal change is an extension of Andi/Chromatography to cover diode array data. This was suggested by several respondents to a recent AIA survey of Andi users.



Other suggestions include upgrading the version of netCDF. A major upgrade of netCDF (Version 2.3.2) occurred after release of Andi/Chromatography (which is based on netCDF Version 2.0.1). Both Andi/Mass Spectrometry, released last summer, and Andi/Infrared, currently under development, use the newer version of netCDF.

Also under consideration are proposals to make the Andi/Chromatography specification more user-friendly, such as by adding an information description information class and a sample description information class. Also being evaluated are proposals to make Andi/Chromatography more consistent with Andi/Mass Spectrometry and Andi/Infrared. Several users, especially from the pharmaceutical industry, would like to see support for GLP regulatory requirements.

The working group is developing a list of priority items for changes and a timetable for implementation. This will allow AIA release of a revised specification later this year. In the meantime, the group welcomes readers' comments and suggestions for changes.

For more information, please contact Mike Duff of AIA at 703-836-1360.

Comments Solicited for Atomic Spectroscopy

The Laboratory Automation Standards Foundation (LASF) of Groton, Massachusetts, is soliciting comments from instrument vendors and users on a draft specification for atomic spectroscopy data interchange. The comment period extends through early March.

Although not sponsored by AIA, the LASF coordinated effort intends to develop a data interchange specification for atomic spectroscopy data that is compatible with AIA's Andi specifications. According to LASF, the purpose of the work, which is funded by the U.S. Army Corps of Engineers, is to provide a means for interchange and archiving of data for techniques including ICP, DCP, AA methods and Spark Emission.

LASF also reports that the atomic spectroscopy specification will be structured so that all data for a sequence of samples and standards is contained in one file. The length of a sequence may range from a tray of material to a long run using robotics equipment. Besides making it easier to work with, having all data in a single file will make it easier to move information while maintaining data integrity. In addition, the specification will address regulatory compliance aspects of data management.

After reviewing comments received on its latest draft specification, LASF plans to develop software to support the specification and to have it available in late spring.

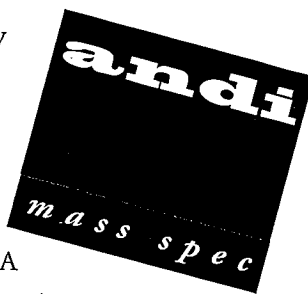
For more information or to receive a copy of LASF's atomic spectroscopy specification, contact Joe Liscouski of LASF at 508-448-6130.

Andi/Mass Spectrometry Use Begins

Since its release last summer, Andi/Mass Spectrometry has been incorporated into at least 17 MS products. See the Andi/Mass Spectrometry scoreboard for a current listing of suppliers and products incorporating the standard.

By early January, AIA had distributed approximately 20 copies of Andi/Mass Spectrometry. On the front page of this issue, an article describes the use of Andi/Mass Spectrometry at Eastman Chemical Company facilities in Tennessee, Texas and Arkansas.

Because its release was less than a year ago, it is premature to consider future extensions of Andi/Mass Spectrometry. Over the next few months, however, the Andi/Mass Spectrometry working group will solicit feedback from suppliers and users on their applications and experiences as well as their priorities and timing for revisions. A poll on this subject will be taken at the upcoming American Society of Mass Spectrometry annual meeting.



Industrial Research Managers Briefed on Andi Progress

Dave Nelson, Chairman of AIA's Andi communication program, presented the Andi program to more than 40 Directors of Industrial Research, Analytical Group (DIR-AG), on October 6, 1994, at their annual meeting held in Piscataway, NJ.

Companies represented included Eastman-Kodak, Colgate-Palmolive, Dow Chemical, DuPont and Occidental Chemical. All members are large companies with major investments in analytical instrumentation and related equipment.

AIA is particularly anxious to communicate with DIR-AG because the larger companies tend to have systems architectural schemes that include networking and information transfer and are mature, well worked out and supported by internal MIS organizations.

Nelson discussed the nature and genesis of the Andi program, the status of each Andi committee (Chromatography, Mass Spectrometry, Infrared), results in terms of published standards and applications and future plans.

This is the second time AIA has presented to this organization. Whereas the first presentation, in the fall of 1993, was greeted with little understanding or familiarity, this second one was different in two important ways:

- Many more of the companies were familiar with the Andi program.
- Much more encouragement and appreciation of the AIA program was evident.

Many DIR-AG members asked how they could help encourage continued development work in support of AIA efforts. In answer, Nelson emphasized the need for broader use of Andi standards within the larger chemical and pharmaceutical companies and continued pressure on instrument vendors to include Andi software as part of their products.

AIA Considers Windows™ Utility

In response to user requests, the Andi/Chromatography working group is considering development of a Windows-based utility that would facilitate use of Andi specifications. Although evaluation would be based on Andi/Chromatography, the Windows utility could easily be adapted to Andi/Mass Spectrometry and Andi/Infrared. A number of vendors and users have already developed such Windows-based data interchange utilities. Kits supplied by AIA, however, do not support Windows.

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AIA is pleased to acknowledge the creative talents generously contributed by Lena Chow Advertising of Palo Alto, California, in the design of this newsletter.

Andi/Chromatography and Andi/Mass Spectrometry: The List Is Growing

The list of AIA member products that support Andi/Chromatography and Andi/Mass Spectrometry is growing as members incorporate Andi specifications into their products. The list does not, however, reflect the full extent of Andi implementation, because only AIA member products are included. Other manufacturers who are not members of AIA and many third party software vendors also currently supply products

that support Andi specifications. Contact your supplier if you have questions as to whether a particular product supports either Andi/Chromatography or Andi/Mass Spectrometry.

The scoreboards were prepared on January 10, 1995, based on information reported by respective vendors, and have not been independently verified. Newer releases of existing products, as well as additional products, continue to

become available. Some products on the current list may already have more functionality than shown.

A similar scoreboard for products supporting Andi/Infrared will be developed after that specification is released. Contact Mike Duff at AIA if your company has released products that support Andi specifications.

a n d i / c h r o m a t o g r a p h y s c o r e b o a r d

Company	Model/Version	Status of Implementation				User Access Via			Level of Implementation				
		Tested, But Not Shipped	Available As Separate Utility	Standard Product	Availability	Standard User Interface	Direct Command	Programming Required	Level 1, Raw Data Read	Level 1, Raw Data Write	Level 2, Results Data Read	Level 2, Results Data Write	
Beckman	System Gold/8.1		√		Now		√			√	√		
Dionex	AI-450/3.32			√	Now	√				√	√	√	√
	PeakNet/4.11			√	Now	√				√	√	√	√
Fisons Instruments	XChrom/1.5			√	Now	√	√			√	√	√	√
	XChrom/2.02			√	Now	√	√			√	√	√	√
	Multichrom/2.1	√		√	Now	√	√			√	√	√	√
Hitachi Instruments	HPLC Manager D6000/14			√	Now	√				√	√		√
	DAD System Manager D6500/4			√	Now	√				√	√		√
	HPLC Manager D7000				June 30, 1995	√				√	√		√
Hewlett-Packard	HP ChemServer 4920 and 4930/A.01.00			√	Now					√	√		
	HP ChemStation for Chromatography/A.03.01			√	Now	√	√			√	√		√
Lachat Instruments	Omnicon/1.0			√	Now	√				√	√		
Perkin-Elmer, PE Nelson Division	Model 1022/8.0			√	Now	√				√	√	√	√
	Turbochrom/4.0			√	Now	√				√	√	√	√
	AccessChrom/1.9			√	Now		√			√	√	√	√
Shimadzu Scientific	Chromatopac Data Archive/3.2		√		Now	√				√	√	√	√
	Shimadzu E-Z Chrom/3.3	√		√	September 1994	√				√	√	√	√
	E-Z Chrom/6.5	√		√	July 1994	√				√	√	√	√
Thermo Separation Products	PC 1000 Chromatography Workstation/2.0			√	Now	√				√	√	√	√
	PC 1000 Chromatography Workstation/2.5			√	Now	√				√	√	√	√
Thru-Put Systems, Inc.	Target 3 30330/3.1			√	Now	√				√			
Varian	Star Chromatography Workstation/4.0/3.0			√	Now		√	√		√	√	√	√
	StarLims			√	Spring 1995	√						√	
Waters Chromatography	Millennium 2010/V2.0			√	Now	√				√		√	
	Millennium 2010/V2.1	√			1Q 1995	√				√	√	√	√
	Millennium 2020 VMS/V2.01			√	Now	√				√			
	Millennium 2020 Novell/V2.02			√	Now	√				√			
	Millennium 2020 VMS/V2.10.1	√			1Q 1995	√				√	√		√
	Millennium 2020 Novell/V2.10.1	√			2Q 1995	√				√	√		√
	Millennium-LIMS Interface/V1.0	√			2Q 1995	√							√

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Finnigan	ICIS/8.1			√	Now	√	√			√	√	√	√
Fisons Instruments	MassLynx/2.0			√	Now	√				√	√		
	MassLab/1.2			√	Now	√				√	√		
	OPUS/4.0			√	Now		√			√	√		
	SpecBase/4.0			√	Now	√				√	√		
Hewlett-Packard	G1034C MS ChemStation/C.03.00			√	Now		√			√	√		
	G1032C Enviroquant/C.00.02			via G1034C	Now		√			√	√		
	G1046A Dry Analysis/A.00.01			via G1034C	Now		√			√	√		
	G1047A LC/MS/A.01.00			via G1034C	Now		√			√	√		
	G1045A GC Enviroquant/A.00.01			via G1034C	Now		√			√	√		
PE Sciex	API 3			√	Now	√				√	√		
	API 1			√	Now	√				√	√		
	API 100			√	Now	√				√	√		
	API 300			√	Now	√				√	√		
Teknivent	Vector Two/2.02			√	Now		√			√	√		
	Envirolink/2.02			√	Now		√			√	√		
Thru-Put Systems, Inc.	Target/3.2			√	May 1995	√				√			

Andi Specifications Available from AIA

Many chromatography and MS instrument and software suppliers incorporate Andi specifications into their products. Contact your favorite supplier if you have questions regarding their implementation of Andi specifications in their products. Copies of Andi specifications also may be obtained directly from AIA for a nominal fee.

AIA packages Andi specifications for chromatography and mass spectrometry in separate kits. Kits contain appropriate specification and implementation guides, software disks and a software development kit, plus the appropriate version of netCDF from Unidata. While no programming expertise is needed to use products that incorporate Andi specifications, some

programming experience is necessary to use the kits supplied by AIA.

The cost of each kit is \$175 to AIA members and \$300 to non-members. Non-members wishing to purchase both kits at the same time can do so for a special fee of \$500.

For more information or to obtain an order form, contact Mike Duff of AIA at 703-836-1360.

Andi Protocols for Analytical Data Interchange



Andi/Chromatography

- Tested and released in 1992
- Incorporated in more than 30 instrument and software products
- Work under way to include diode array data and improve user-friendliness

Andi/Mass Spectrometry

- Tested and released in summer 1994
- Incorporated in 17 instrument and software products

Andi/Infrared

- Testing of specification covering Raw Data and Final Results under way
- Release expected later in 1995

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Andi News is intended to keep you informed on application experiences of users and vendors with Andi protocols. We also intend to keep you informed on AIA's activities and new products related to analytical data interchange.

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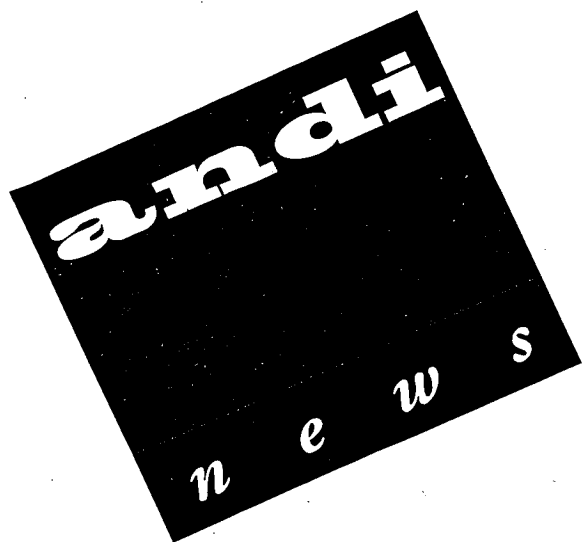
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