# PA13/31 HPLC'99 Granada, 31 May 1999 Creating an HPLC/SPE Databasco Roscourco to Sorvo

Database Resource to Serve Applications Documents as Well as Reference Citations via the Internet

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# **Abstract**

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When faced with developing a new separation or devising a sample preparation protocol, chemists and chromatographers are trained to turn first to the literature to see what might have been done in the past. Even an older reference to a similar separation problem might establish the feasibility of the desired separation goal and/or a starting point for method development. Or, one might discover that the problem has already been solved and that the necessary elements of the separation system are near at hand. In any case, valuable time and resources are saved by the knowledge gained.

For twenty years, we have been collecting references to the applications of HPLC columns, chemistries, instruments and SPE devices. About 15 years ago we began to enter these references into an internal database for electronic searching and retrieval. Recently, we migrated the data to an architecture based on Lotus Notes/Domino servers. Now our database, containing more than 14,000 citations, can be accessed and searched via a web-browser on the Internet.

Because we first painstakingly review the literature ourselves, we select references for inclusion in our database based on experimental details which may not be in abstracts or keyword lists. Such references would therefore not turn up in searches of various on-line databases (e.g., Chemical or Analytical Abstracts). Also, we may include references to documents from sources not available to most libraries or commercial databases.

Recently, we have begun to use the portable document format (PDF) to create actual electronic versions of printed documents and developed an innovative way to access them anytime, day or night, from anywhere in the world. Rather than simply creating an HTML archive of links to these PDF files on a web page, we have linked them directly to records in our database. Thus, when an appropriate record turns up in a list of search results, by clicking on an icon, the actual document cited in that record may be viewed immediately, as may one or more related documents. This saves even more valuable time and effort -- no trips to the library or reprint requests are needed! If copyright permission has been secured, but a PDF file is not available, we have created an e-mail form, immediately available on-line, to request a paper copy of a document.

Examples of the content and utility of this innovative database will be reviewed.

# Importance of Our Database

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- Accelerate Method Development
  - Generate Ideas
  - Establish Feasibility
  - Locate Adaptable/Adoptable Procedure
- Get Product/Applications Information
- Conserve Resources, Save Time
- Access References Not Available Elsewhere
- Download/Order Documents [copyright permitting]
- 24/7 Worldwide No-Fee Access

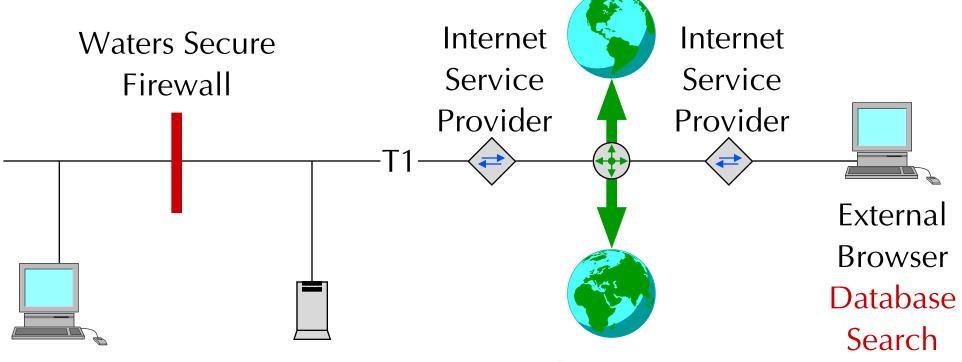
# Database Milestones

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# Network Architecture

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Internal
Network
Client
Database
Entry

Internet [web] Server
http://www.waters.com
Lotus Domino
Waters Applications
Library Database

Internet [Worldwide Web]

# Tools & Search Mechanism

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Web Server

[multiprocessor PC]

- 1. Type Request into Browser form; Click on SEARCH
- 2. Web Server routes request to Lotus Domino database server software.
- 3. Domino translates request & queries Lotus Notes database.



Client with

browser

[& Acrobat Reader v. 3 + toread PDF files.]

- 5. Domino translates results to **hypert**ext **m**arkup language; HTML page is returned via web server to
  - client's Browser.
- 4. Notes performs search & returns results to Domino.

# http://www.waters.com

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To access *Waters* Applications Library database, Select **Applications Library** from HPLC Columns & Supplies picklist.

[Alternate route: select first item from Applications picklist (hidden here, just below HPLC Columns ... list)

# Search Form

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Search Ideas: More effective searching may be done with some simple, standard Boolean operators [Search Tips & Hints]. Words in a typical entry might include, but are not limited to:

### Link to Search Tips Page

- Name of a chemical compound: e.g., acetaminophen.
- Waters product brand name or model number: e.g., Symmetry or 2690.
- Last name of author
- File number of reference: e.g., 981040 or SP95002

– Instant Access: Click on this icon 🔈 to view & print the actual PDF document. File size indicates relative download

**NOTE:** You will need v3.x of Acrobat Reader to access these files. Val'Get Acrobat



**Database Features** Description

SPE References: More than 3,300 SPE references, including all those from the "Solid Phase Extraction Applications Guide and Bibliography: A Resource for Sample Preparation Methods Development, Sixth Edition ", PD McDonald & ESP Bouvier, Eds, Waters, Milford, 1995 [Waters P/N 52853], are now in this database. These references have file numbers with the prefix: SP

Hot Links: On the Search Results page or on each individual Record Detail page, there may be one or more "Hot Links". For example, if they are present, move your cursor over the red star icon, the SPE device icon, the SPE Sorbent name, or the name of the Analytical Technique, and then click to obtain detailed background or reference information

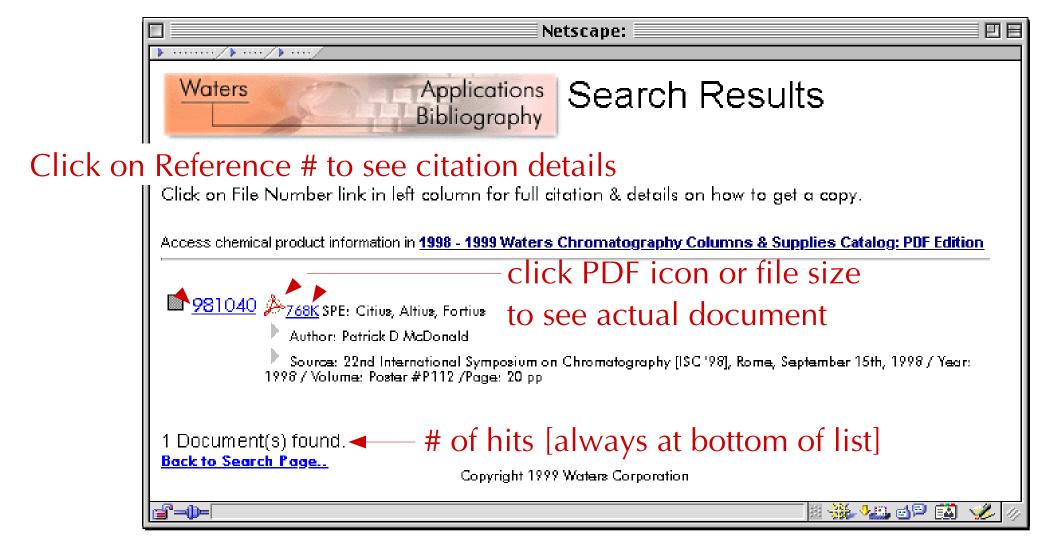
We always welcome your comments and/or suggestions - <a href="InfoCenter@waters.com">InfoCenter@waters.com</a>

# Search Results

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# Search Results lists Title, Author, and Bibliographic citation for all records that match search criteria

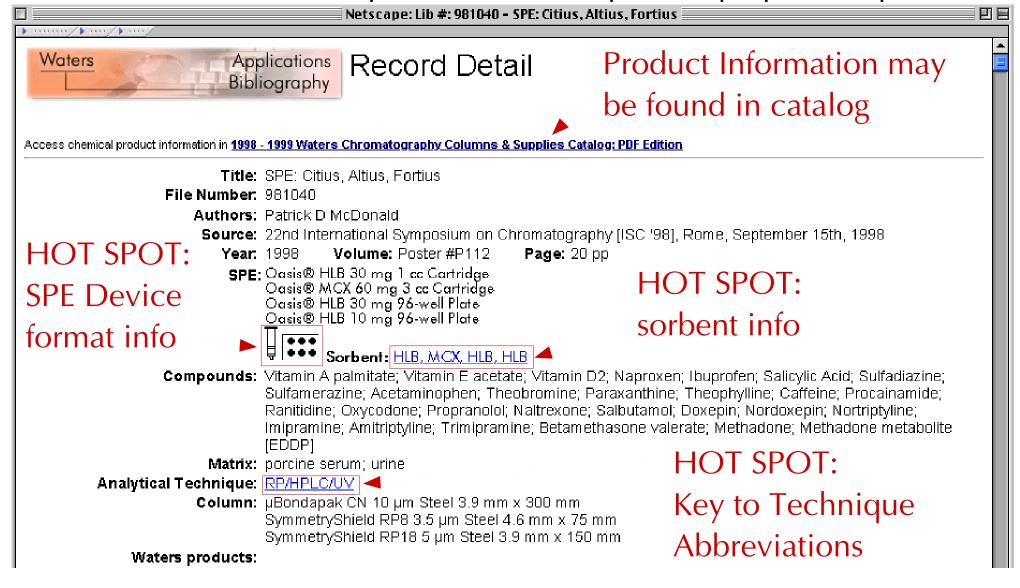


# Record Detail

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Details of SPE device & HPLC column formats & sorbent chemistries are listed as well as sample matrix & compounds prepared/separated.



# More Record Detail

### Details of SPE device & HPLC column formats & sorbent chemistries are listed as well as sample matrix/compounds prepared

(if available)

**Notes:** ABSTRACT: This year marks the twentieth anniversary of the commercialization of the first miniature cartridge columns containing silica-based adsorbents designed for SPE (1). The ideas that led to this Abstract invention, the history of column liquid-solid phase extraction [CLSE - modern SPE], and the rapid development of SPE in the last two decades as a preferred sample preparation technique will be traced. SPE is hundreds of years old: fragrance manufacturers in Grasse to this day still extract labile oils from jasmine petals via the ancient process of embedding them in paraffin wax. Pioneering work by Schwartz in the 1950's and 1960's in which CLSE was performed on both the mini- and micro-scale (in glass) melting-point capillary tubing), with on-column derivatization and/or complexation, specific for certain compound classes, is virtually unrecognized today. So, too, are some of the first laboratorty-scale applications of hydrophobic polymers for reversed-phase CLSE by Bradlow in the late 1960's. There were three characteristics of the first commercial product for CSLE/SPE that led to the rapid adoption of the technique: a convenient, efficient, disposable, miniature column format; a family of Click on link reproducible, reliable sorbents chosen and quality-controlled specially for SPE; and a package that maintained the integrity of the sorbent until it was used.

A new generation of formats and stationary phase chemistries which enable the practice of SPE to be to see PDF of faster, with higher sample throughput, and stronger performance will be emphasized. The unique properties of new sorbents which have spurred a renaissance in the use of polymer packings and actual document dramatically improved SPE performance will be reviewed.
(1) PD McDonald, RV Vivilecchia, DR Lorenz, "Triaxially Compressed Beds", US Patent #4,211,658

(1980).

🥍 Click Here for Document 768k

Related PDFs: Dearn more about Waters Symmetry family of columns and cartridges 1.1 MB

Learn about the family of Oasis® HLB Sample Extraction Products 1 MB

🎤 Learn More about Oasis⊚ MCX Sample Extraction Products 192K

Links to related PDF documents

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# Instant Document Access

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### Actual Document: 24 pages; 744K

# SPE: CITIUS, ALTIUS, ISC '98 ROMA Poster 112 15 Sept 1998 Patrick D. McDonald, Ph.D. Waters Corporation 34 Maple Street Milford, MA 01757 USA mcdonald\_pat@waters.com

This poster, which reviews the history of the development of modern SPE, from the perspective of one of its pioneering inventors, is **not** available anywhere else.

### Related Document: 8 pages; 512K



Columns for Every Step in the Drug Discovery and Development Process

- Superior Peak Shape
- Unmatched Reproducibility
- Extended Column Lifetime
- Fast Analysis Without Sacrificing Resolution
- Direct Scale Up From Analytical to Prep
- Design for LC/MS

### Meeting the Constantly Changing Demands of Pharmaceutical R&D

Phormoceutical scientists are under pressure to brige new drug candidate to market faster. In order to achieve this, you may have to deal with shortened limelines and parallel devel opment projects. If that that reaugh, the new International Conference on Harmonisation (IC-II) regulatory guidelines are placing more stimgent demands on assay sensitivity, making fast and accurate validation more difficult. Because of these pressures, there is one area where you simply cannot afford to compromite: your choice of HPC columns. That's why pharmoceutical scientists around the world put their trust in the Symmetry's manufactures.

family of columns. Symmetry\* columns provide the highest standard of reproducibility for total confidence in the long-term compliance of your HPLC methods, with unmatched peak symmetry for maximum sensitivity and accurate qua titation. No other column delivers as much. Waters offers 3.5.5 ond 7 um particle sizes in the complete range of column lengths and internal diameters to take you all the way from lead generation and optimization to development of volidated assays for stability testing and impurity profiles.

And now, with the introduction of

And now, with the introduction of the innovative SymmetryShield 'RP1a and RP2 columns, based on our patents between the state of the columns of the state of the

Unique among suppliers of HPIC columns, Waters controls the entire column manufacturing process from silica synthesis to column hardware manufacture. Control of the process from start to finish is the investment we've made so that you can meet the constantly changing demands of pharmaceutical R&D.

Waters

In depth information is available *when you need it*.

# **Boolean Operators**

and HPLC.

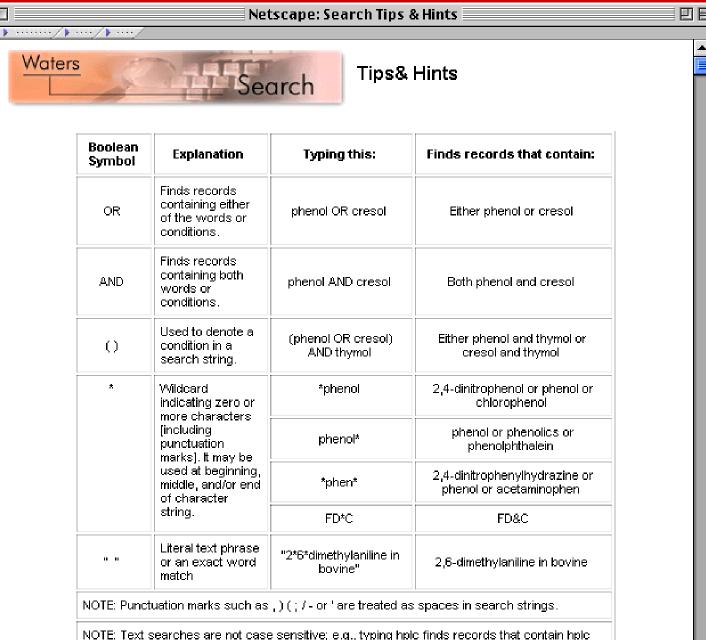
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Boolean Operators can be used to increase the specificity of any search.

The wildcard operator [\*] is especially important:

e.g., *symmetry\** finds
Symmetry,
Symmetry®,
SymmetryShield, &
Symmetry300; while *symmetry* only finds
Symmetry.



# More Search Tips

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When looking for a chemical name, try using the wildcard operator in conjunction with the root or search for the common name or a compound class name: e.g., \*cholesten\* or cholesterol.

### Other Hints for successful searches:

- Don't enter too much information, but try to use enough characters and combinations of words to achieve specificity in your search.
- Try to use search strings that return only those records of interest; e.g., searching for the brand name Symmetry will return several hundred records, but searching for Symmetry AND barbital will only return a few records.
- To search for a word or fragment that contains one or more punctuation marks [but no spaces] that are important
  to its meaning, use an asterisk in place of each punctuation mark in the search string; see the example in the table
  above for FD&C.
- If you need to search for an exact phrase containing punctuation, use the literal text operator; see example in table above for 2,6-dimethylaniline.
- Keep in mind that different authors may express similar things with different forms of the same word; e.g., a
  search for chromatography will not return chromatographic, but a search for chromatogra\* will return both, as
  well as chromatogram and chromatographer. But neither search will return HPLC or LC.
- When searching for a compound name containing an alphanumeric string of numbers, symbols, and punctuation marks, try using the wildcard operator before and/or after the longest root word in the name; e.g., to find 3β-hydroxy-Δ<sup>5</sup>-cholestenol, search for \*cholestenol.
- If you know the common name for a compound, try that before searching for the root of the IUPAC-type name;
   e.g., to find 3β-hydroxy-Δ<sup>5</sup>-cholestenol, search instead for "cholesterol".
- If you are familiar with other Boolean symbols, you may construct more complicated search strings.
- If the first search doesn't work, go back to the form and try another approach.

Go BACK to the Waters Applications Bibliography Search Page

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# Hot Spot Link

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# Clicking on SPE Device Icon in Record Detail accesses detailed information on various formats.



# Hot Spot Link – 2

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Clicking on **SPE Sorbent** name in Record Detail links to more information on sorbent chemistry & properties.



### SPE Sorbents\*

Access Chemical Product Information in <u>Waters 1998-1998 Chromatography Columns & Supplies Catalog:</u>
<u>PDF Edition</u>

- Introduction: Sorbent Chemistries
- Sorbent Properties & Typical Applications: select a Separation Mode or Sorbent below:

### Reversed-Phase Sorbents

- Oasis<sup>®</sup> HLB
- <u>C</u><sub>18</sub>
- <u>tC<sub>18</sub></u>
- <u>C</u>,
- <u>tC</u>₂
- Porapak™ Rox

### Normal- or Reversed-Phase Sorbents

- <u>Aminopropyl</u> [NH<sub>2</sub>]
- Cyano [CN]
- <u>Diol</u>

### Normal-Phase Sorbents

- Silica
- Alumina A, N, B
- FlorisiI™

### Mixed-Mode and Ion Exchange Sorbents

- Oasis<sup>®</sup> MCX
- Accell™ Plus QMA
- Accell™ Plus CM

### Specialty Sorbents

- DNPH-Silica
- XPoSure™

### Introduction: Oasis® and Sep-Pak® Brand SPE Sorbent chemistries

The wide variety of sorbent chemistries available from Waters lets you tailor a sample preparation step to the specific needs of your application. There are hydrophilic phases that

# Hot Spot Link – 3

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### Oasis® HLB

An exceptionally clean, highly reproducible, patented (pending) copolymer synthesized with a unique composition that is hydrophilic-lipophilic-balanced for **both** strong reversed-phase retention **and** water-wettability. Compatible with sample or eluents from pH 1 to 14.

Used to adsorb both polar and non-polar compounds simultaneously from aqueous media; typical applications include drugs and their metabolites from biological fluids, environmental pollutants from water.

HLB can be substituted for, has a wider spectrum of retention, and is more reproducible than  $\mathrm{C}_{18}$  and all other silica- or polymer-based reversed-phase media. Oasis® HLB is the ideal starting point for new reversed-phase SPE method development.

Pore Size (nominal): 80 Å

Particle Size: 30 µm [or 60 µm for LP grade] A

**Surface Functionality:** m-Divinylbenzene & N-vinylpyrrolidone copolymer

Sorbent information includes physical & chemical characteristics.

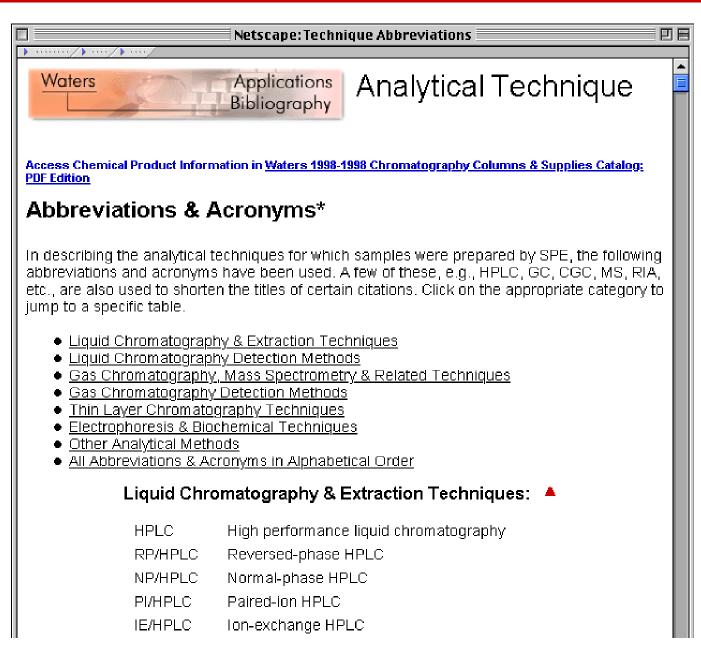
Product information can also be found in brochures linked as **PDF** files to DB records, as well as in linked catalog **PDF** files.

# Hot Spot Link – 4

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An extensive list of abbreviations & acronyms used in database record fields is reached by clicking on the Analytical Technique abbreviation hot spot on the **Record Detail** page.



# What's Included in Database

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- Most Citations are for articles in journals
- Lectures, Posters, Seminars presented by Waters scientists
- Applications Notes, Newsletters, e.g.:
  - Waters Column articles
  - Waters Performance Perspectives
  - Waters AMD & Integrity Mass Spec Notes
  - Waters Symmetry & Oasis Application Notes
- Product Brochures
- Product Manuals [book length]

# How to Obtain Documents

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# Record Detail will specify the appropriate procedure at bottom of page:

- Where available, download the Portable Document Format [PDF] file immediately.
- When copyright permission is available, an email photocopy request form link appears on Record Detail page. Fill it out & send.
- For most articles cited, Waters does not own the copyright. You must take the reference to your local *librarian*.

# Summary

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- We have been compiling HPLC & SPE references for more than 20 years into a succession of database formats.
- Using a fast server & web link, we have now made this collection accessible to everyone on the worldwide web.
- Start your search for ways to prepare or separate a compound *here*, using information not always found in fee-based, private databases of abstracts.

# Suggestions?

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We are pleased to offer you the *benefits of* many thousands of hours we have spent scanning one of the world's highest quality collections of chromatographic information.

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- We *welcome* your *feedback* on our ongoing & evolving project.
- Please email/send us your ideas, suggestions, & stories of how our database may have helped you in some small or significant way! Thank you!

# Gracias Amigos

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### Database Creation & Maintenance



Grace Lavallee

Assistant Librarian
Reference Procurement
& Request Fulfillment

Carla Clayton
Senior Librarian
DB Pioneer, Architect &
Data Entry since 1978!

### IT Architecture



Ken McGovern
Notes /Domino
Programmer & Directory
Architect

Jeff O'Halloran Lotus Notes Consultant FileMaker Pro Migration

Kevin Landry
Notes Programmer &
Web Server Architect

### Maureen Allegrezza

Database Administrator
Design & Ongoing Data Entry

Randy Sheehan: automated rollup of files to web server; Marcos Cerda: set up our intranet server directories; Brian McDonald: [my son] showed us how to return # of records found in Results [Lotus said it was impossible!]

# Want More Information?

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### Please leave your name, address, & email address

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### Please *indicate* which option [A, B or C] you prefer:

- **A**. a *paper* copy of this poster by mail
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- C. an email notification of how & when to view or download a PDF copy of this poster through the Waters Applications Library at http://www.waters.com