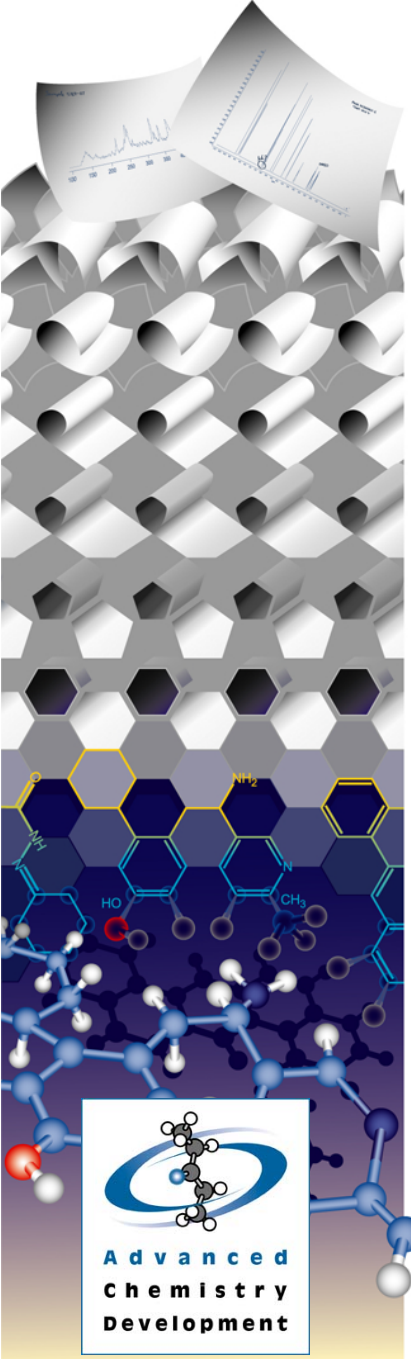


Structured Solutions

Mobile Chemistry: Structure Databases in Your Palm and Your Pocket

Vince Dillman

NJ NMR Users Seminar
10/1/2003

Spectroscopy • Chromatography • PhysChem • Naming • Drawing and Databasing • Enterprise Solutions

Mobile Chemistry

- Mobile computing – Laptops, Tablet PCs, PDAs – Palm and Pocket PC
- Cost-accessibility issue – PDAs are cheap and very accessible
- Current applications are mainly text based.
  - Schedules/appointments
  - Personal/Business contacts
  - Email
  - Notes
  - Recipes/books/music/movies, etc.

Mobile Chemistry

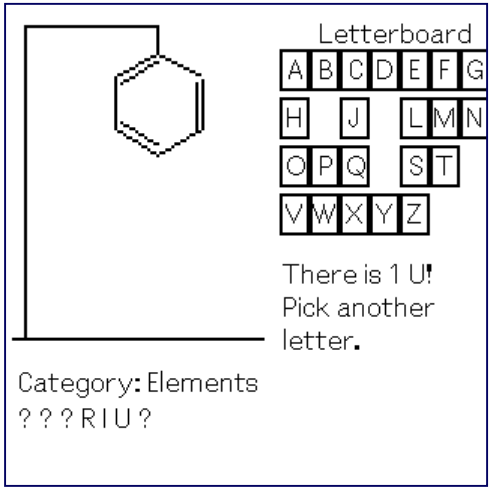
- PDA-based chemistry to date
  - HyperChem – modeling and ab initio calculations on a Pocket PC
  - ChemiCalc – balancing stoichiometry – Text based
  - Periodic Table of Elements, Solution Calculator (ACD/Labs)
  - Others?

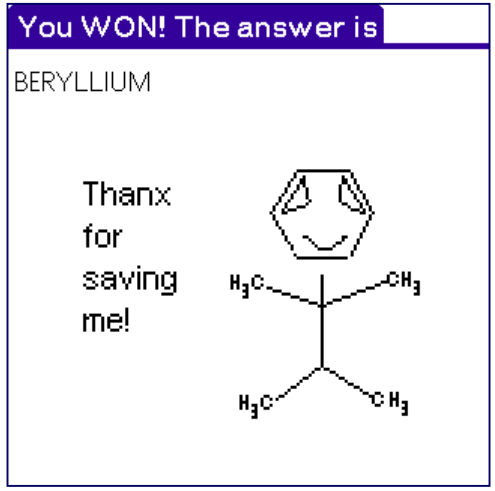
Other ACD/Labs Text-Based Chemistry Applications

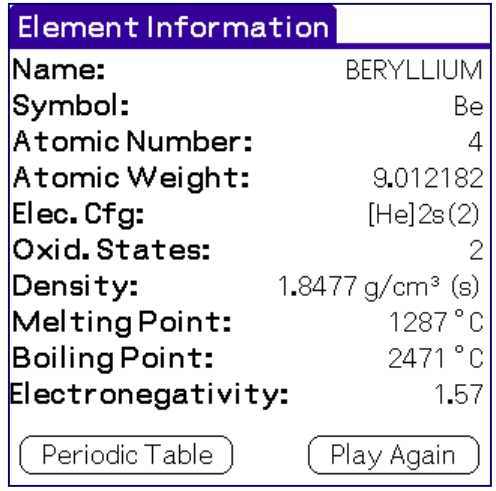
- All are presently available for the Palm
  - ChemHang
  - NMR Solvent Reference Table
  - Column Selector

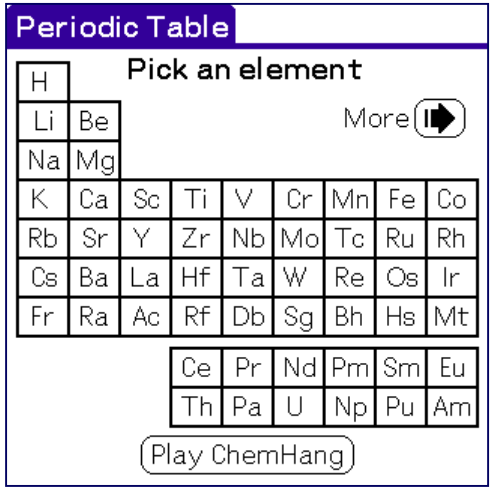
Free downloads available at www.acdlabs.com/download/

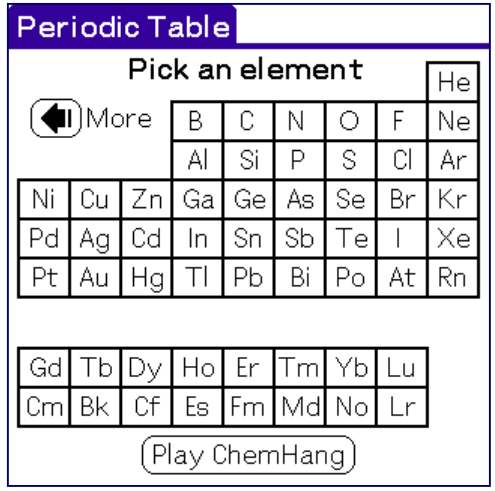
ChemHang









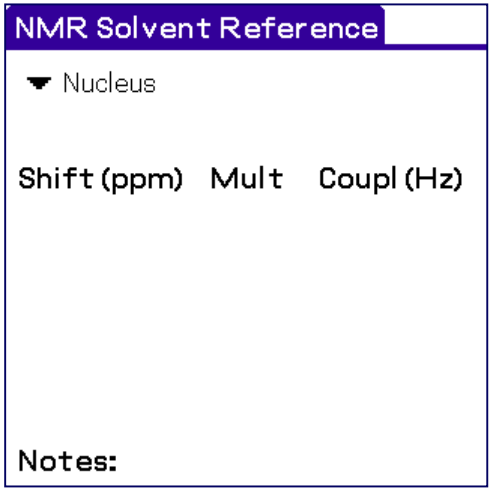


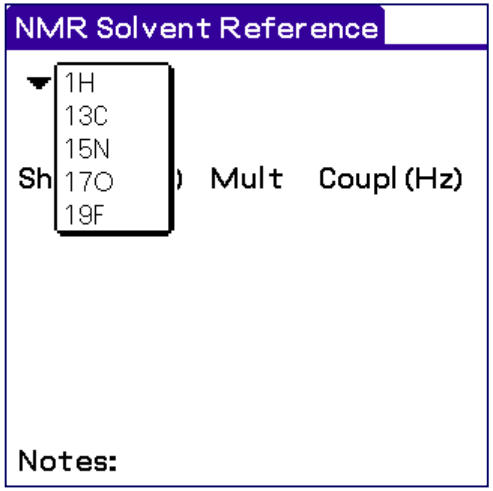
Spectroscopy • Chromatography • PhysChem • Naming • Drawing and Databasing • Enterprise Solutions

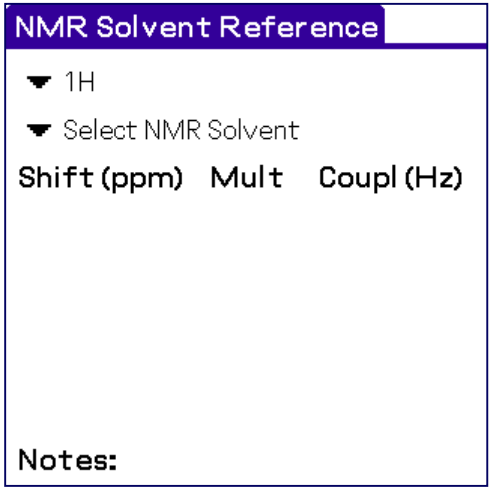
Spectroscopists Like PDAs Too

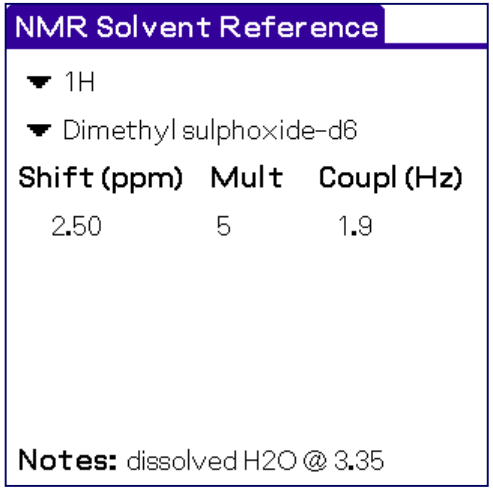
- Useful lookup tables are ideal for the PDA
- Already available online – MS calculator, Units conversion tools
- NMR solvents?

NMR Solvent Reference Table





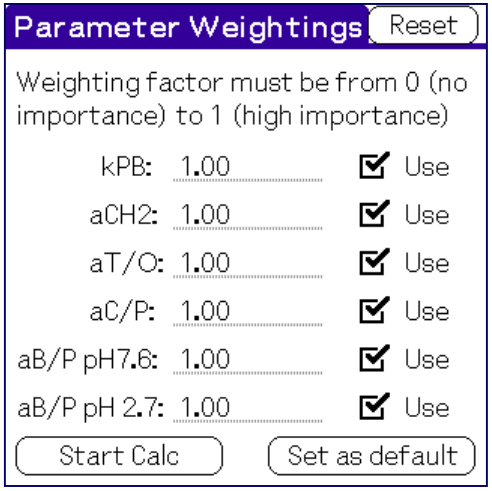


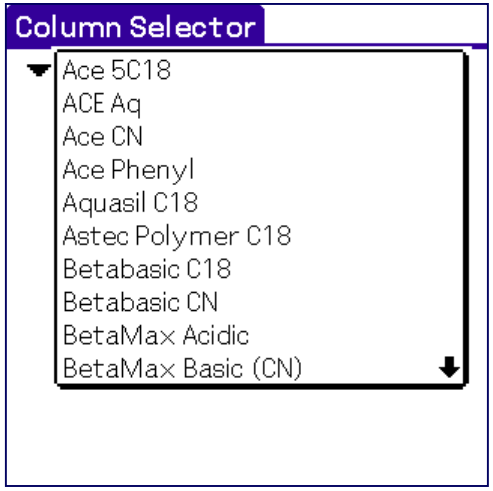


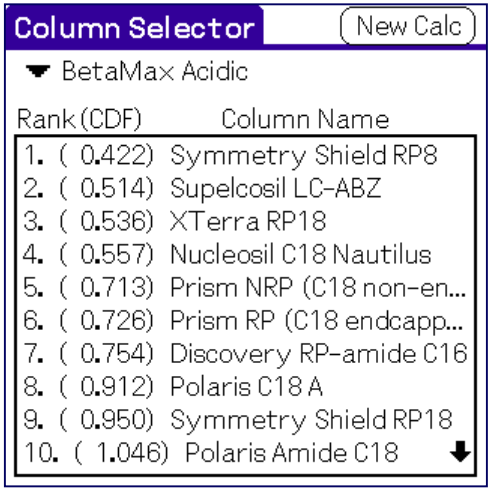
...and Chromatographers?

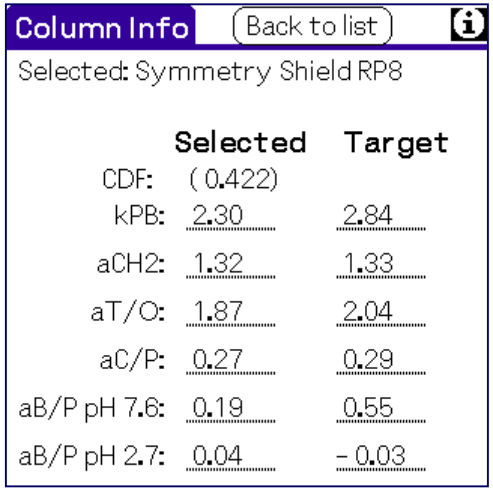
- You do a search in the ACD/AppDB and the column that you need is not at hand:
  - Find the most equivalent, available column.
- The column that you initially tried is not giving you resolution, despite optimization:
  - Find an orthogonal column to try next.
- You have two compounds that differ in a readily discernable fashion, and want to exploit the difference:
  - Find a column with a higher specific coefficient.

Column Selector





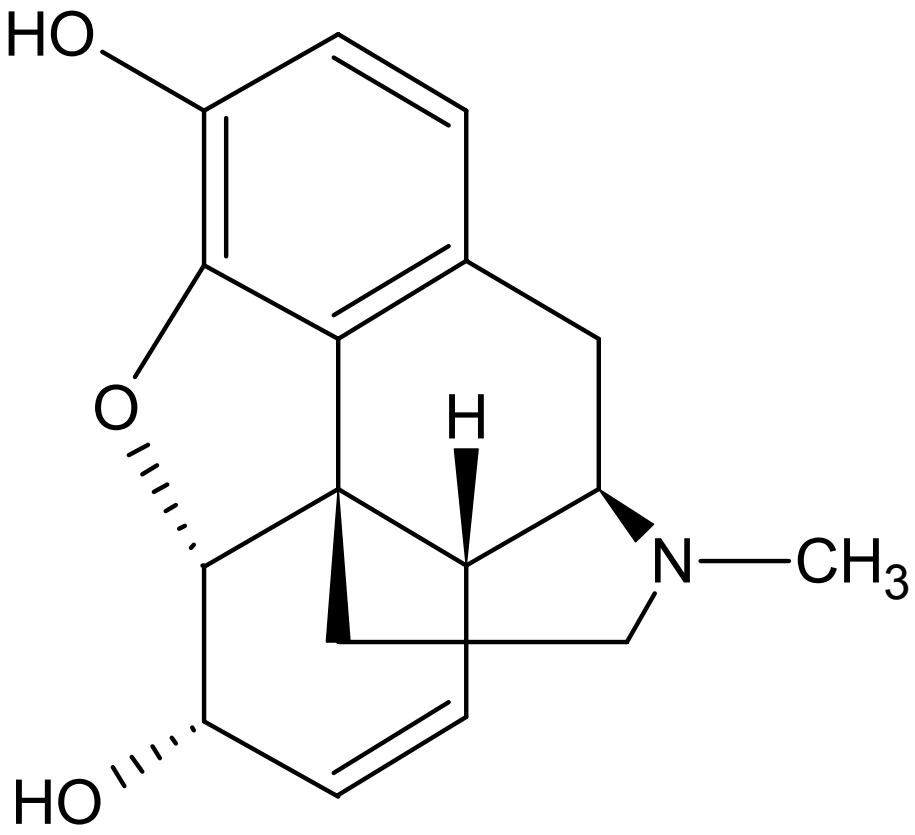




Euerby, MR; Petersson, P. *J. Chromatogr. A*, **2003**, **994**, 13-36.

Chemical Communication

- Structure is the language of chemists

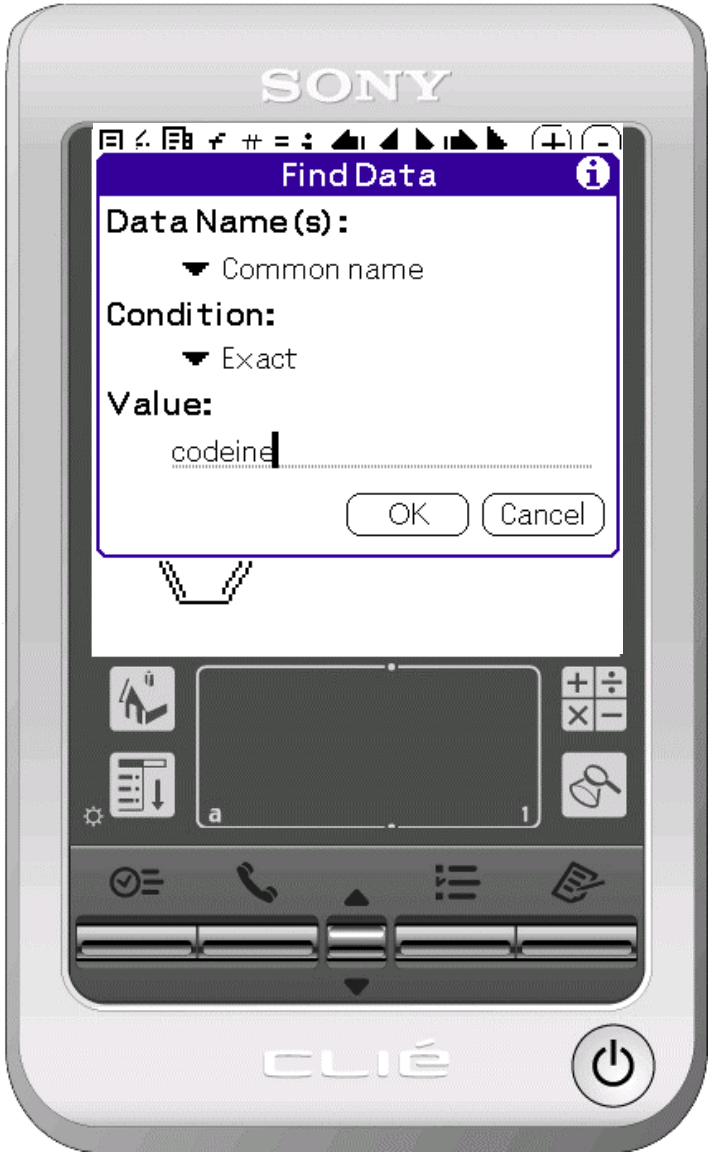


Mobile Chemistry

- What would be the value of structure database viewing on a PDA?
- Chemists communicate via structures. Less chance of misunderstandings.
- Project related structure databases
- A company dictionary
- Vendor databases on a PDA for browsing – The Aldrich catalog?

Advanced Chemistry Development

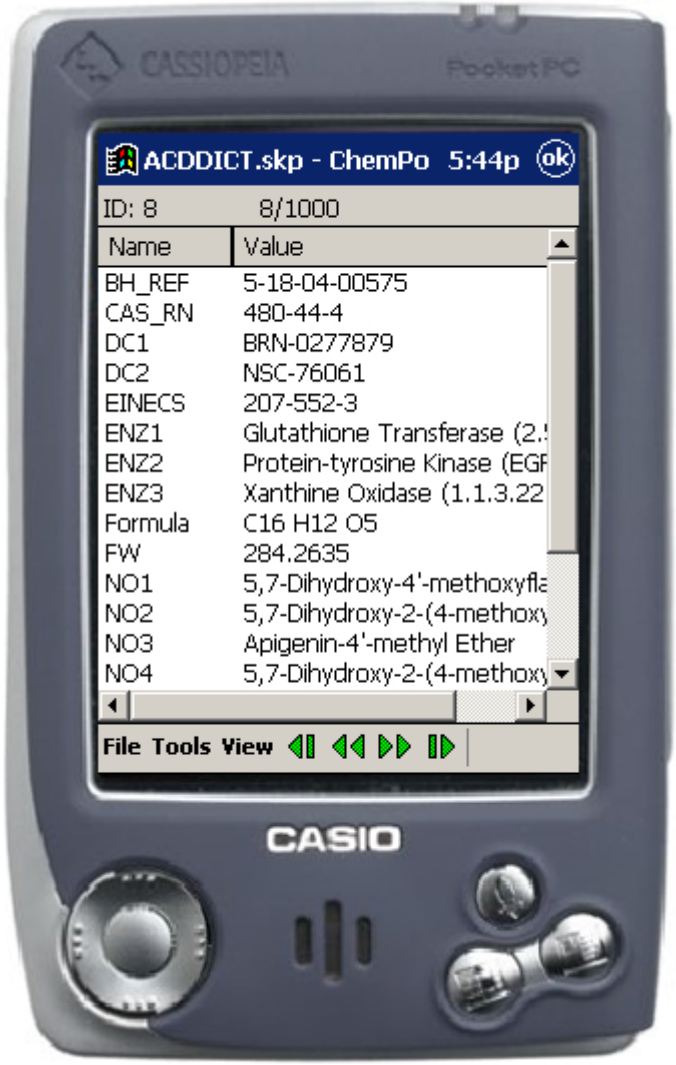
ACD/ChemPalm



Structured Solutions

Advanced Chemistry Development

ACD/ChemPocket



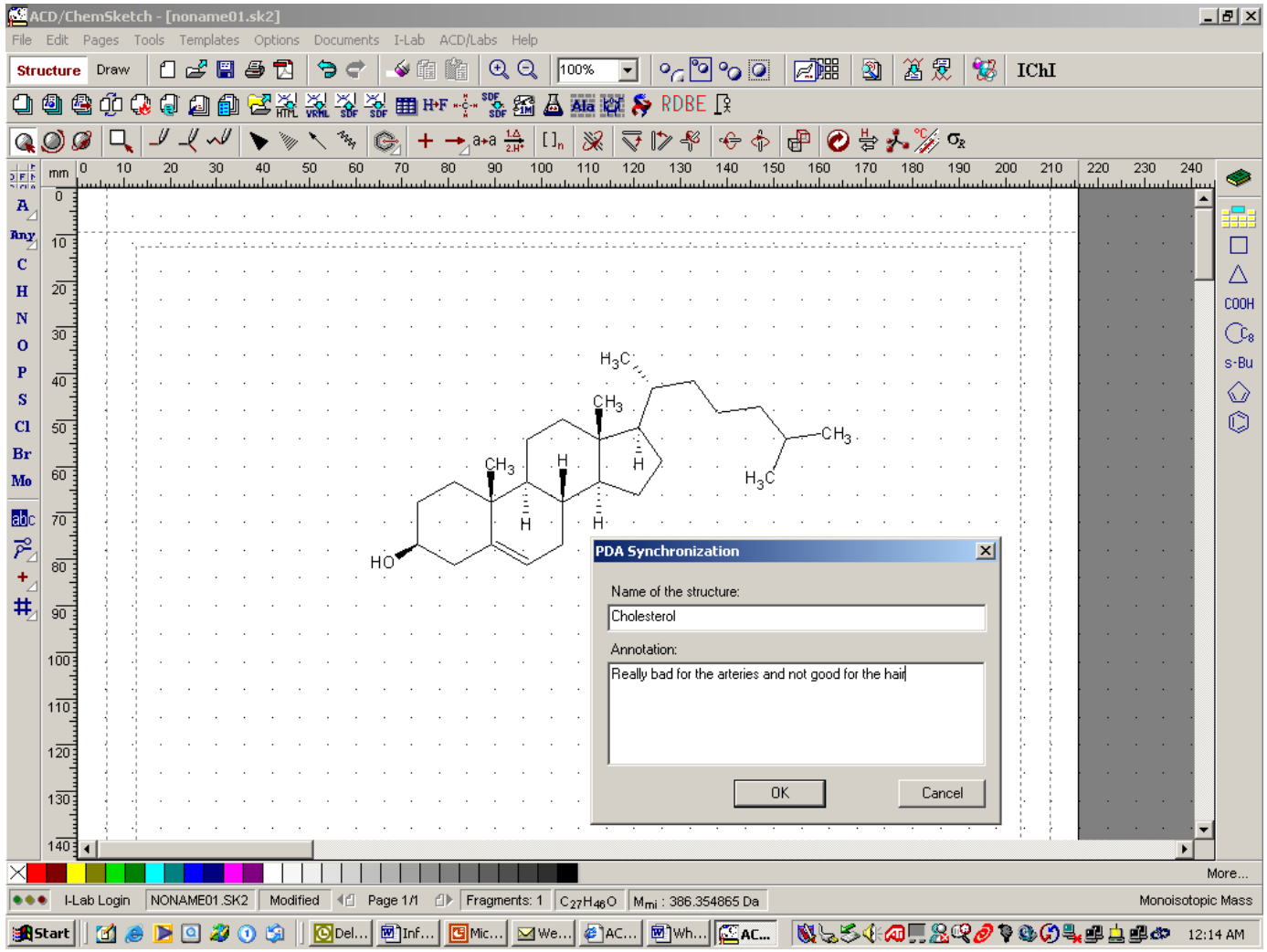
Structured Solutions

Spectroscopy • Chromatography • PhysChem • Naming • Drawing and Databasing • Enterprise Solutions

Integrating Mobile Chemistry

- Structure or structure databases need to be sync'ed to the PDA
- Multiple drawing packages and multiple structure databases
  - ACD/ChemSketch
  - Cambridgesoft ChemDraw
  - MDL/ISIS Draw
- Databases can be exported as SDF

Integration with Drawing Packages



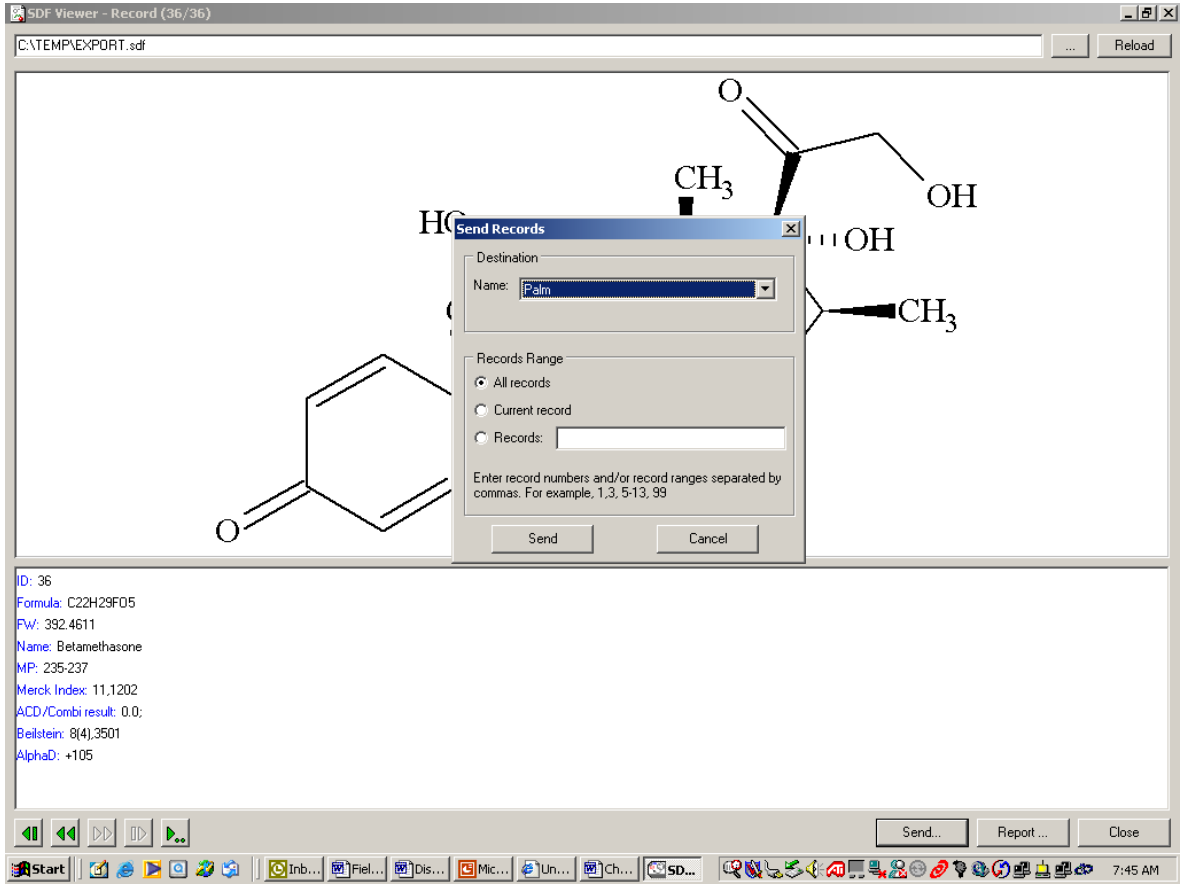
Spectroscopy • Chromatography • PhysChem • Naming • Drawing and Databasing • Enterprise Solutions

ACD/Labs Tools for Multiple Drawing Packages

- ChemPalm and ChemPocket are already integrated to
  - ACD/ChemSketch
  - ChemDraw
  - ISIS Draw

Moving DATABASES to PDA

- ACD/SDFViewer sends all SDF based databases to the PDA. Same tool moves Cambridgesoft and ISIS exported SDF files

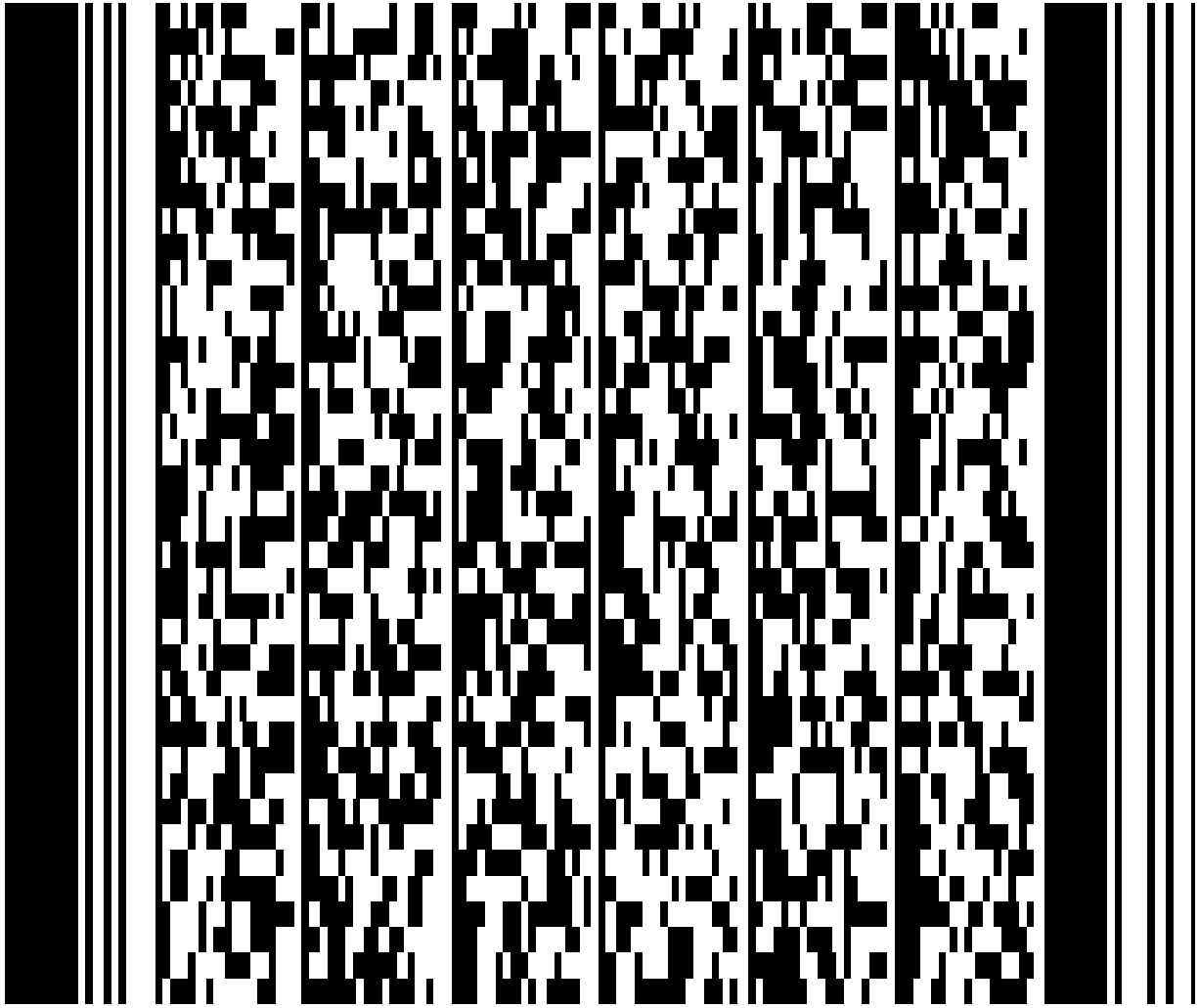


Structure Databases on PDAs

- A small molecule DB containing 20,000 structures occupies 8MB
- Can be searched by text strings and substrings
  - Names
  - ID numbers
  - Organizational dictionary fields
- Does not support structure/substructure searching
  - Who would like to draw complex structures on a PDA?

Advanced Chemistry Development

What's This?

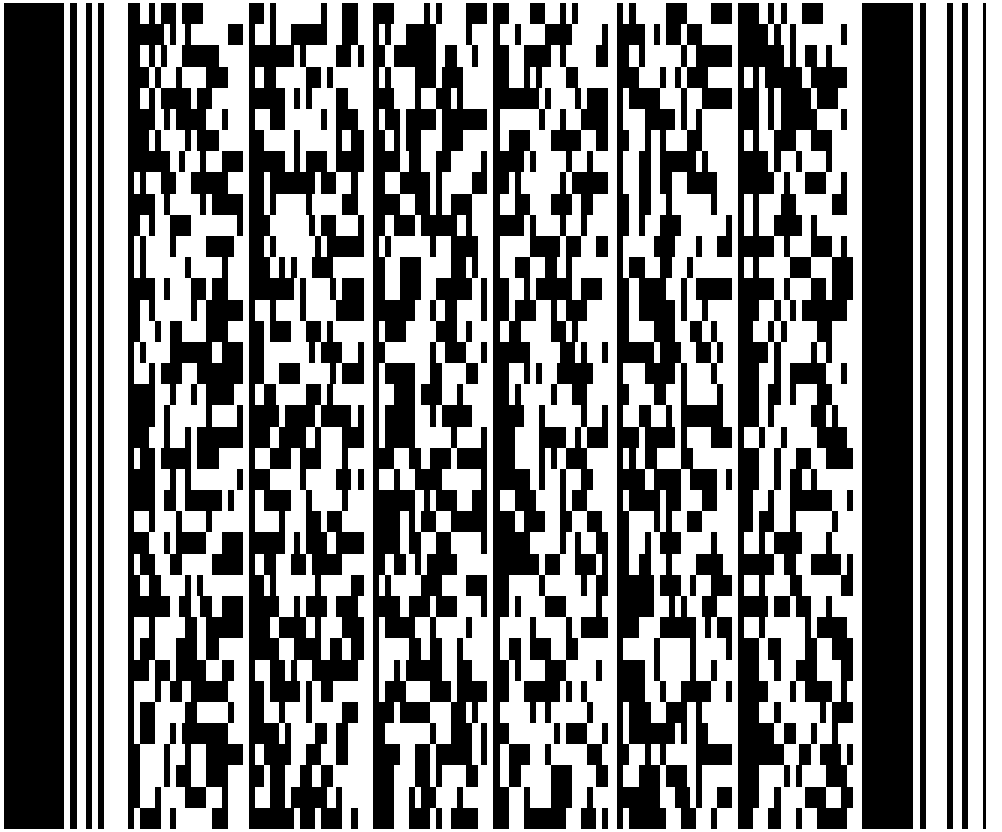


Structured Solutions

Spectroscopy • Chromatography • PhysChem • Naming • Drawing and Databasing • Enterprise Solutions

Structures and Barcodes

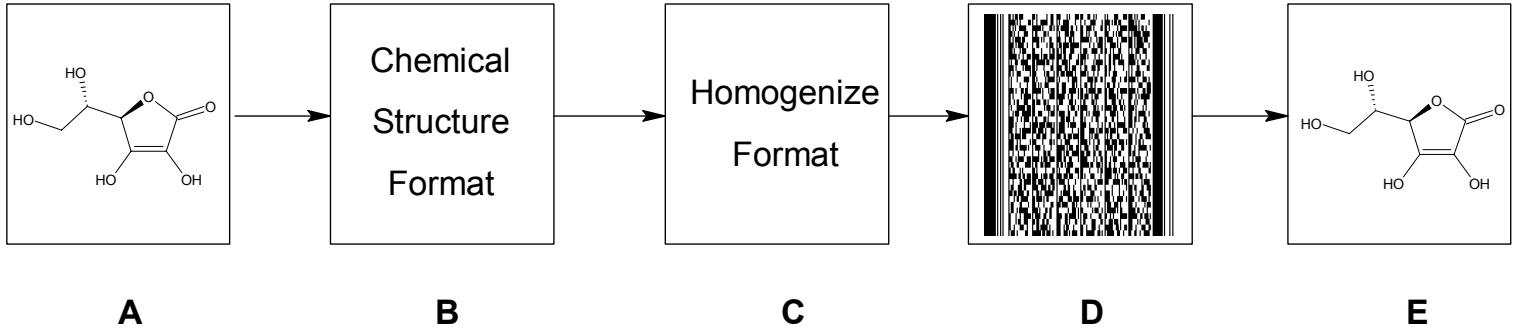
- PDF 417 2D barcode technology – holds 1.1K of information – structures and "user data"



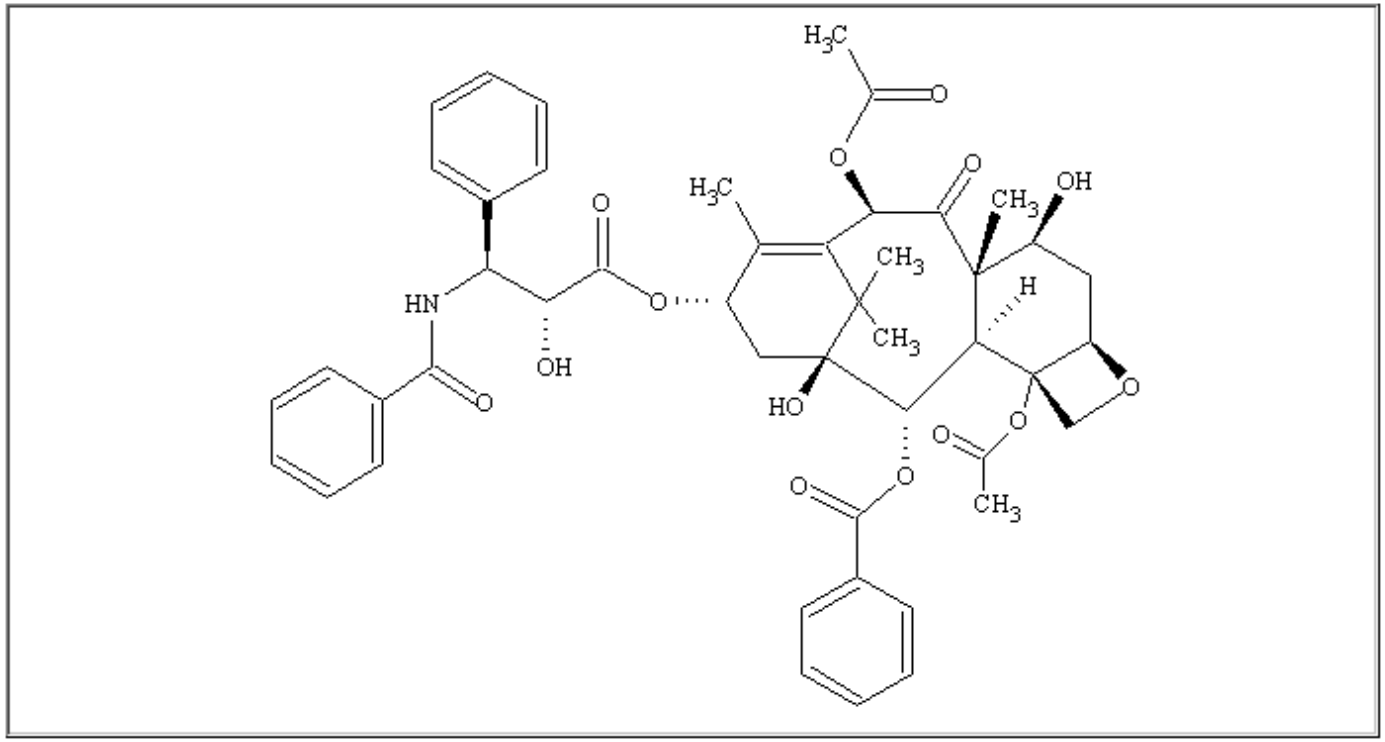
"Scanning Structures on PDAs"

- A vision:
  - Scan a barcode and display the barcode-encoded structure on the PDA
  - Chemical libraries and vendor chemical bottles. Chemists can view structures easier than convert names to structures!
  - Barcode scanners already support Palm and Pocket PC OS
  - Integration with robotic systems – analytical instruments scan the structure – MS fragmentation, NMR prediction

Structures and Barcodes

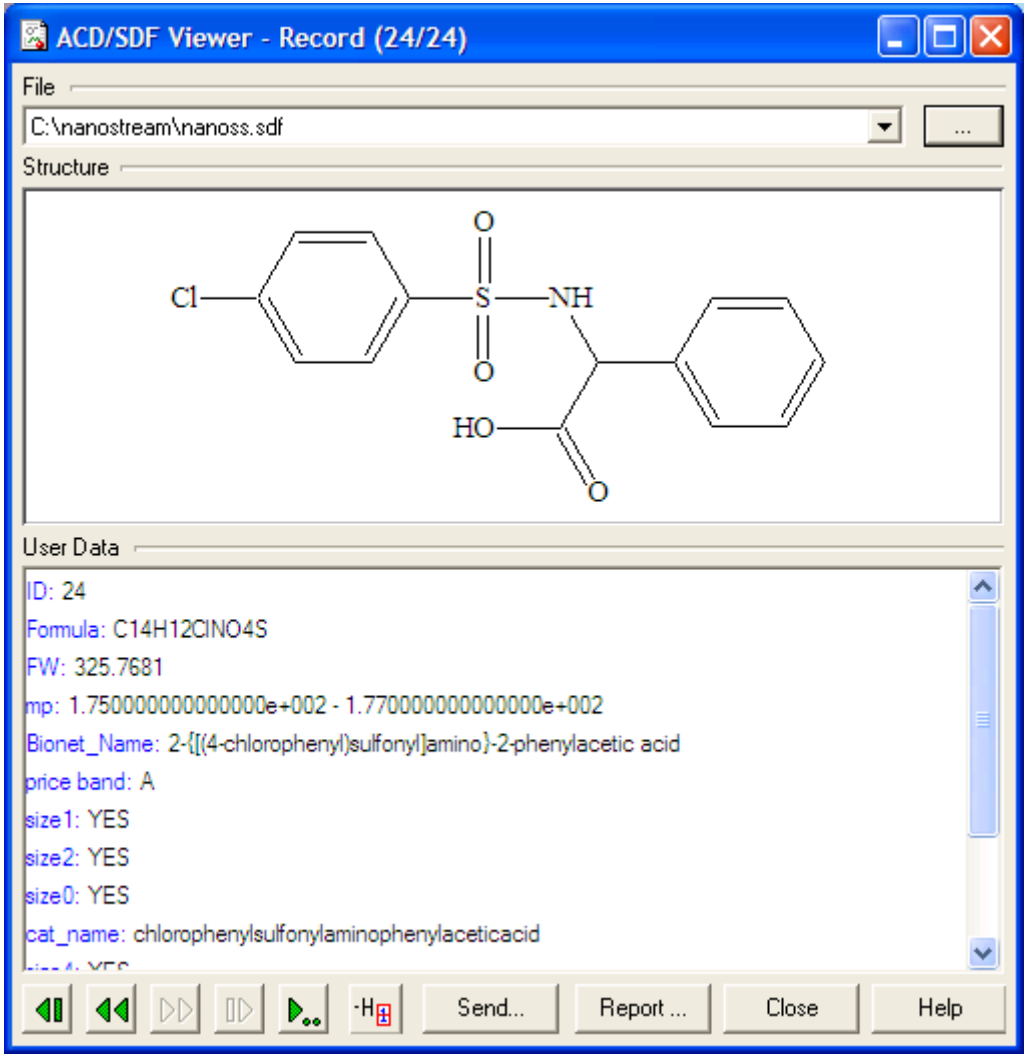


Taxol 2D barcode



Advanced Chemistry Development

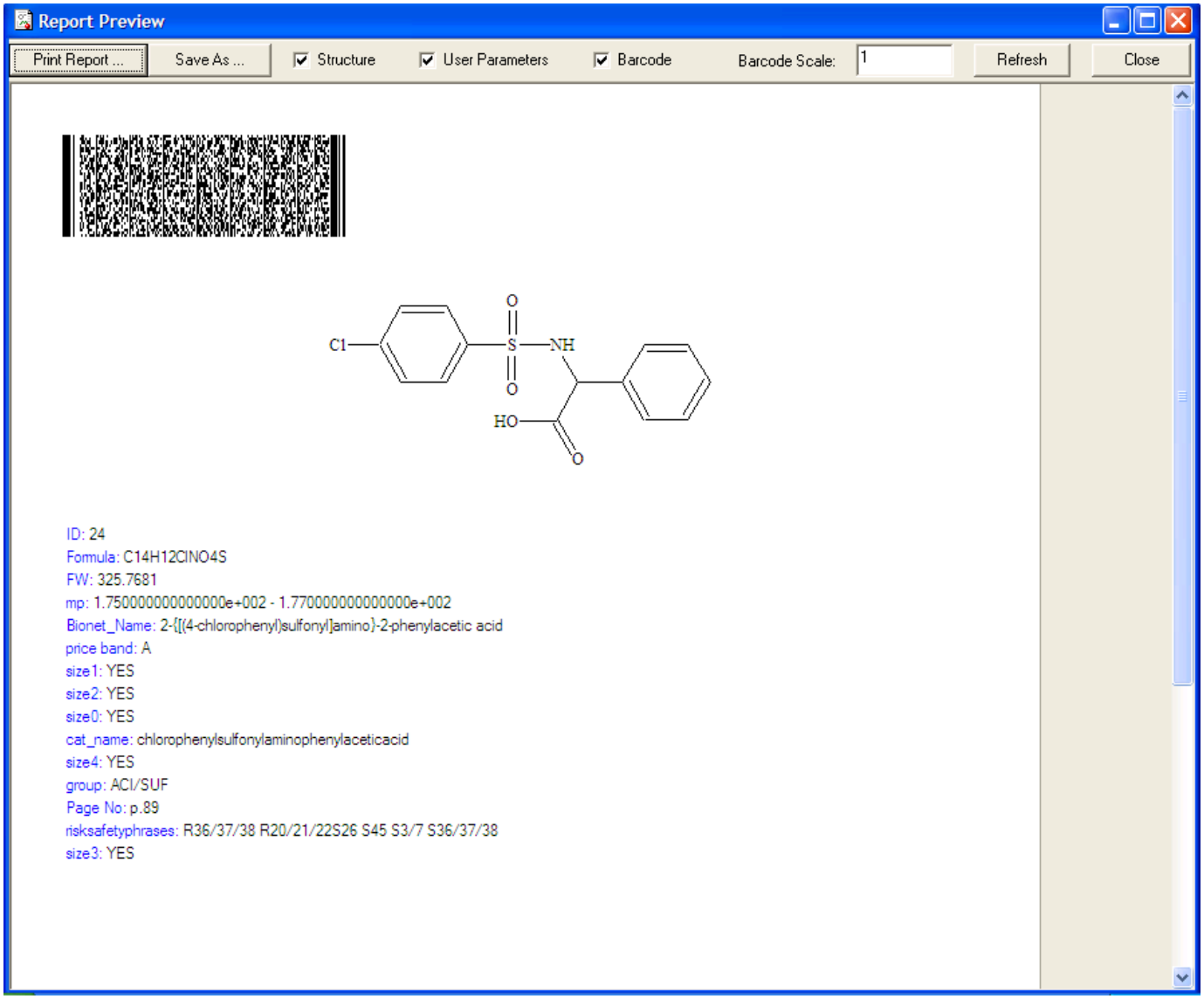
SDF Viewer



Structured Solutions

Advanced Chemistry Development

SDF Viewer



Structured Solutions

Spectroscopy • Chromatography • PhysChem • Naming • Drawing and Databasing • Enterprise Solutions

Future Development

POSSIBILITIES

- Wireless access to databases?
- Wireless access to online predictions (ACD/I-Lab)?

FUTURE DEVELOPMENT

- Barcoding will look up structures in a thick client or web database directly
- ChemiCalc will be integrated into ACD/ChemPalm by Spring 2004

Further Information

- www.acdlabs.com/products
- Mobile Chemistry Article available at http://www.acdlabs.com/download/publ/2003/chemdbpalm.pdf
- This talk online next week at http://www.acdlabs.com/publish/