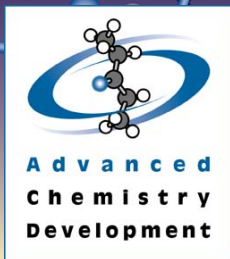


Mobile Chemistry: Structure Databases in Your Palm and Your Pocket

Vince Dillman
NJ NMR Users Seminar
10/1/2003

Structured Solutions



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

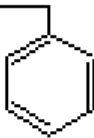
- ♦ PDA-based chemistry to date
 - HyperChem – modeling and ab initio calculations on a Pocket PC
 - ChemiCalc – balancing stoichiometry – Text based
 - Periodic Table of Elements, Solution Calculator (ACD/Labs)
 - Others?

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



Letterboard

A	B	C	D	E	F	G
H	J	L	M	N		
O	P	Q	S	T		
V	W	X	Y	Z		

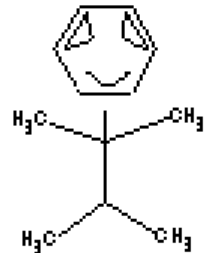
There is 1 U!
Pick another letter.

Category: Elements
???RIU?

You WON! The answer is

BERYLLIUM

Thanx
for
saving
me!



Element Information

Name: BERYLLIUM

Symbol: Be

Atomic Number: 4

Atomic Weight: 9.012182

Elec. Cfg: [He]2s(2)

Oxid. States: 2

Density: 1.8477 g/cm³ (s)

Melting Point: 1287 °C

Boiling Point: 2471 °C


Electronegativity: 1.57

[Periodic Table](#)
[Play Again](#)

Periodic Table

Pick an element

H																
Li	Be															
Na	Mg															
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co								
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh								
Cs	Ba	La	Hf	Ta	W	Re	Os	Ir								
Fr	Ra	Ac	Rf	Db	Sg	Bh	Hs	Mt								
		Ce	Pr	Nd	Pm	Sm	Eu									
		Th	Pa	U	Np	Pu	Am									


More 

[Play ChemHang](#)

Periodic Table

Pick an element

										He
										Ne
										Ar
Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr		
Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe		
Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn		
Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu			
Cm	Bk	Cf	Es	Fm	Md	No	Lr			

 More

[Play ChemHang](#)

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

NMR Solvent Reference

▼ Nucleus

Shift (ppm)	Mult	Coupl (Hz)
-------------	------	------------

Notes:

NMR Solvent Reference

▼ 1H

13C

15N

17O

19F

Shift (ppm)	Mult	Coupl (Hz)
-------------	------	------------

Notes:

NMR Solvent Reference

▼ 1H

▼ Select NMR Solvent

Shift (ppm)	Mult	Coupl (Hz)
-------------	------	------------

Notes:

NMR Solvent Reference

▼ 1H

▼ Dimethyl sulphoxide-d6

Shift (ppm)	Mult	Coupl (Hz)
-------------	------	------------

2.50	5	1.9
------	---	-----

Notes: dissolved H2O @ 3.35

...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

Parameter Weightings Reset

Weighting factor must be from 0 (no importance) to 1 (high importance)

kPB: ☒ Use

aCH2: ☒ Use

aT/O: ☒ Use

aC/P: ☒ Use

aB/P pH7.6: ☒ Use

aB/P pH 2.7: ☒ Use

Start Calc Set as default

Column Selector

- ▼ Ace 5C18
- ACE Aq
- Ace CN
- Ace Phenyl
- Aquasil C18
- Astec Polymer C18
- Betabasic C18
- Betabasic CN
- BetaMax Acidic
- BetaMax Basic (CN)

Column Selector New Calc

▼ BetaMax Acidic

Rank (CDF)	Column Name
1. (0.422)	Symmetry Shield RP8
2. (0.514)	Supelcosil LC-ABZ
3. (0.536)	XTerra RP18
4. (0.557)	Nucleosil C18 Nautilus
5. (0.713)	Prism NRP (C18 non-en...
6. (0.726)	Prism RP (C18 endcapp...
7. (0.754)	Discovery RP-amide C16
8. (0.912)	Polaris C18 A
9. (0.950)	Symmetry Shield RP18
10. (1.046)	Polaris Amide C18

Column Info Back to list i

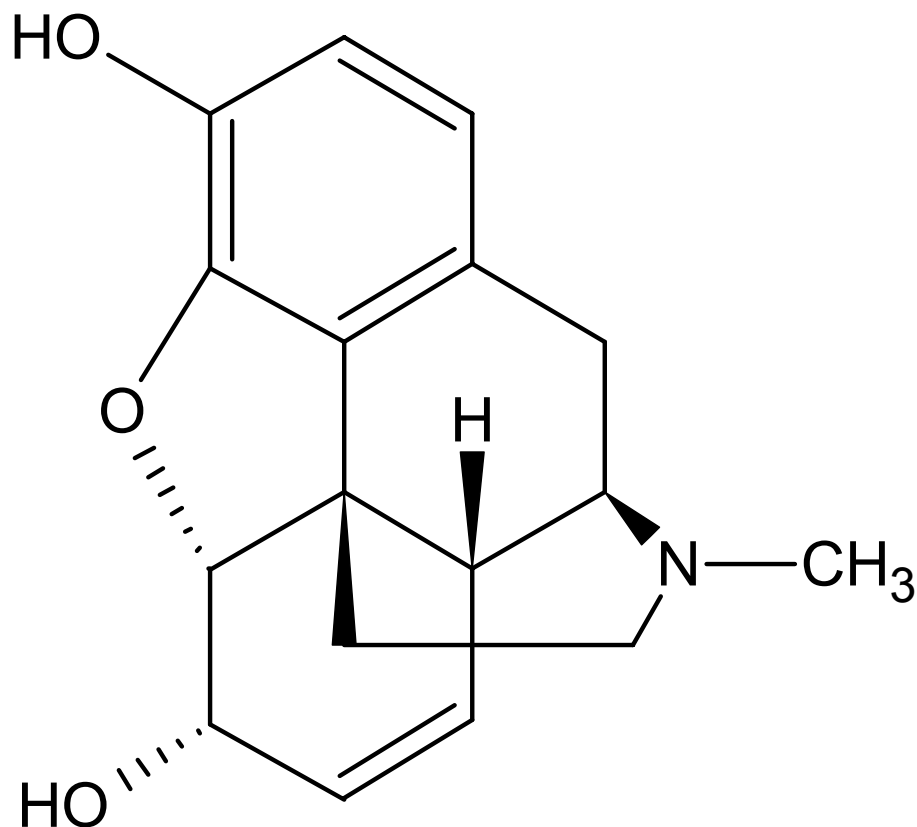
Selected: Symmetry Shield RP8

	Selected	Target
CDF:	(0.422)	
kPB:	<input type="text" value="2.30"/>	<input type="text" value="2.84"/>
aCH2:	<input type="text" value="1.32"/>	<input type="text" value="1.33"/>
aT/O:	<input type="text" value="1.87"/>	<input type="text" value="2.04"/>
aC/P:	<input type="text" value="0.27"/>	<input type="text" value="0.29"/>
aB/P pH 7.6:	<input type="text" value="0.19"/>	<input type="text" value="0.55"/>
aB/P pH 2.7:	<input type="text" value="0.04"/>	<input type="text" value="- 0.03"/>

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

Chemical Communication

- ◆ Structure is the language of chemists

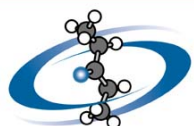


Mobile Chemistry

- ♦ 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?

ACD/ChemPalm





Advanced
Chemistry
Development

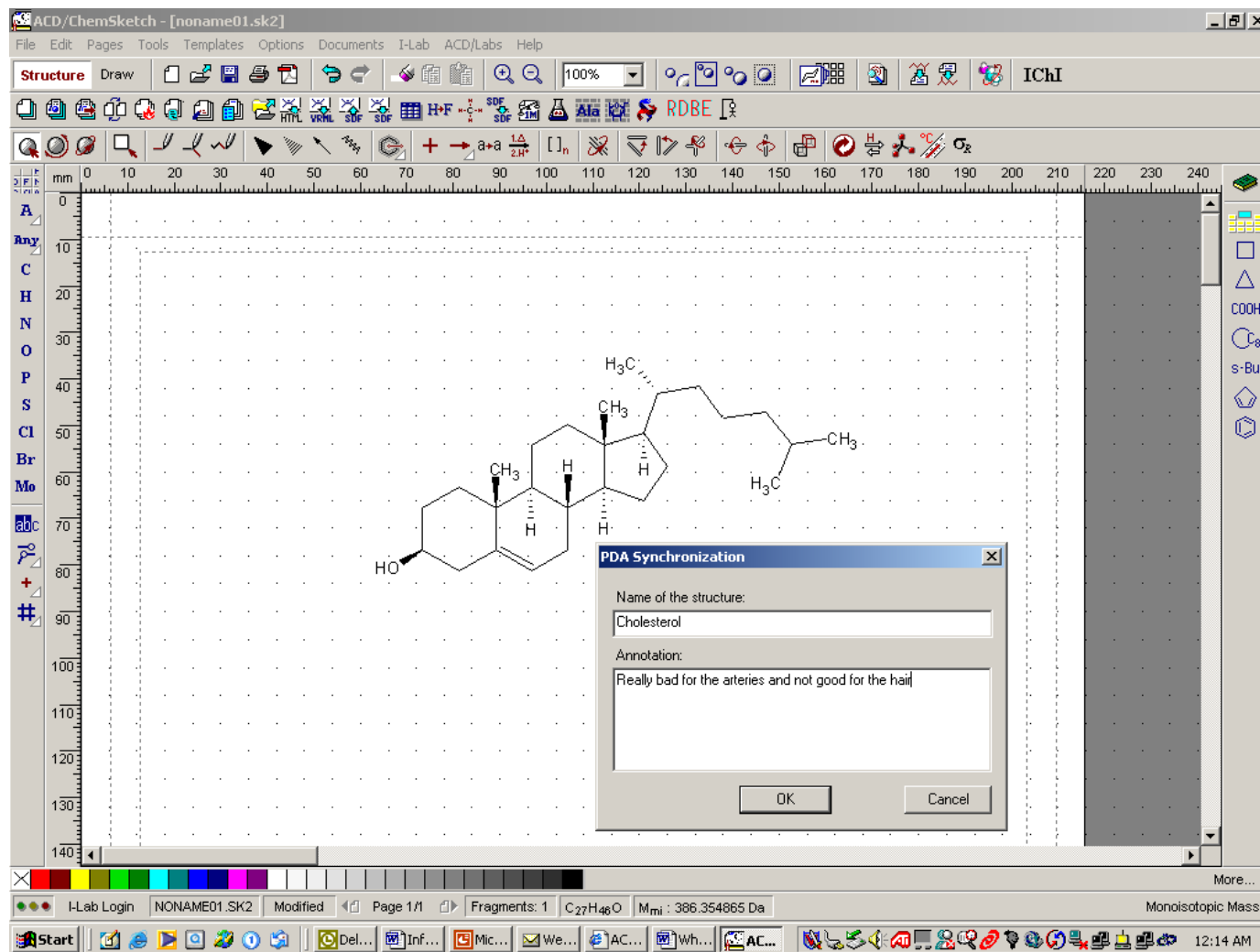
ACD/ChemPocket



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

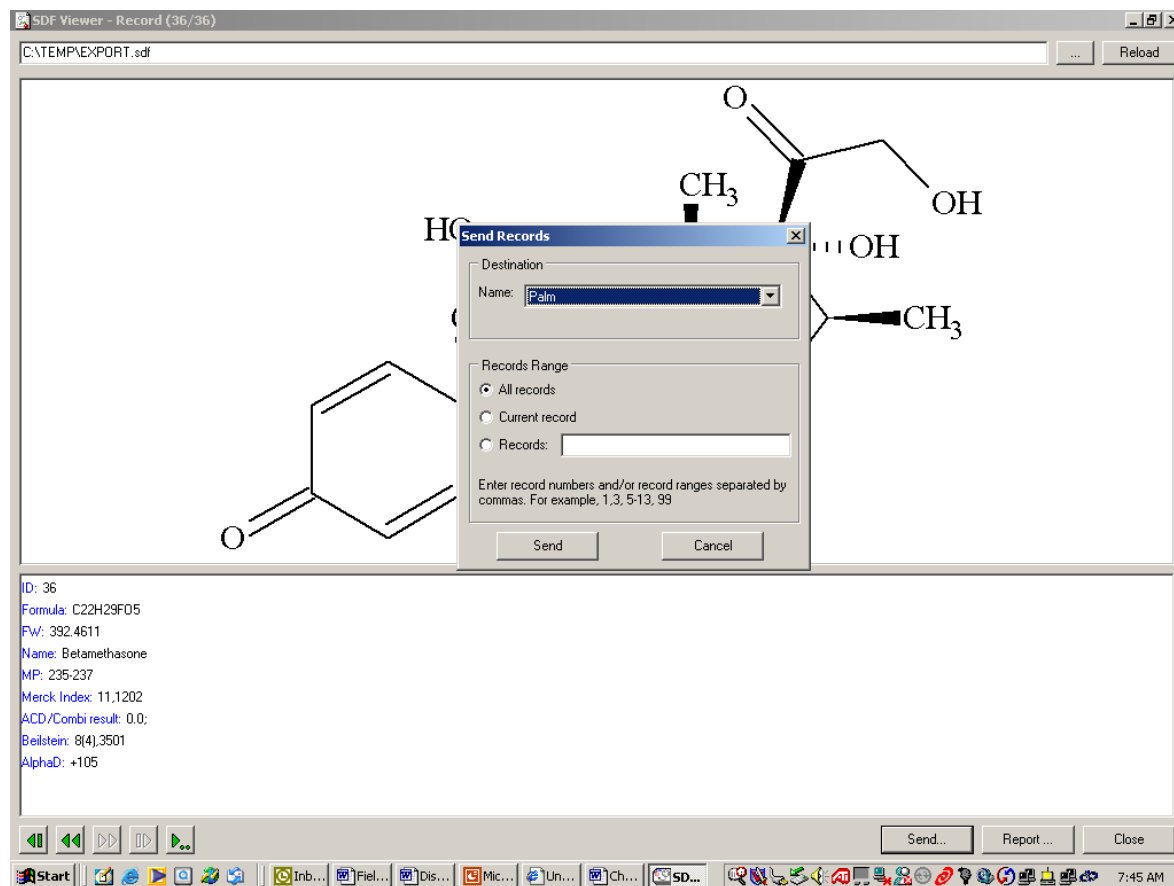


ACD/Labs Tools for Multiple Drawing Packages

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

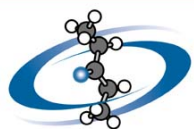
Moving DATABASES to PDA

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



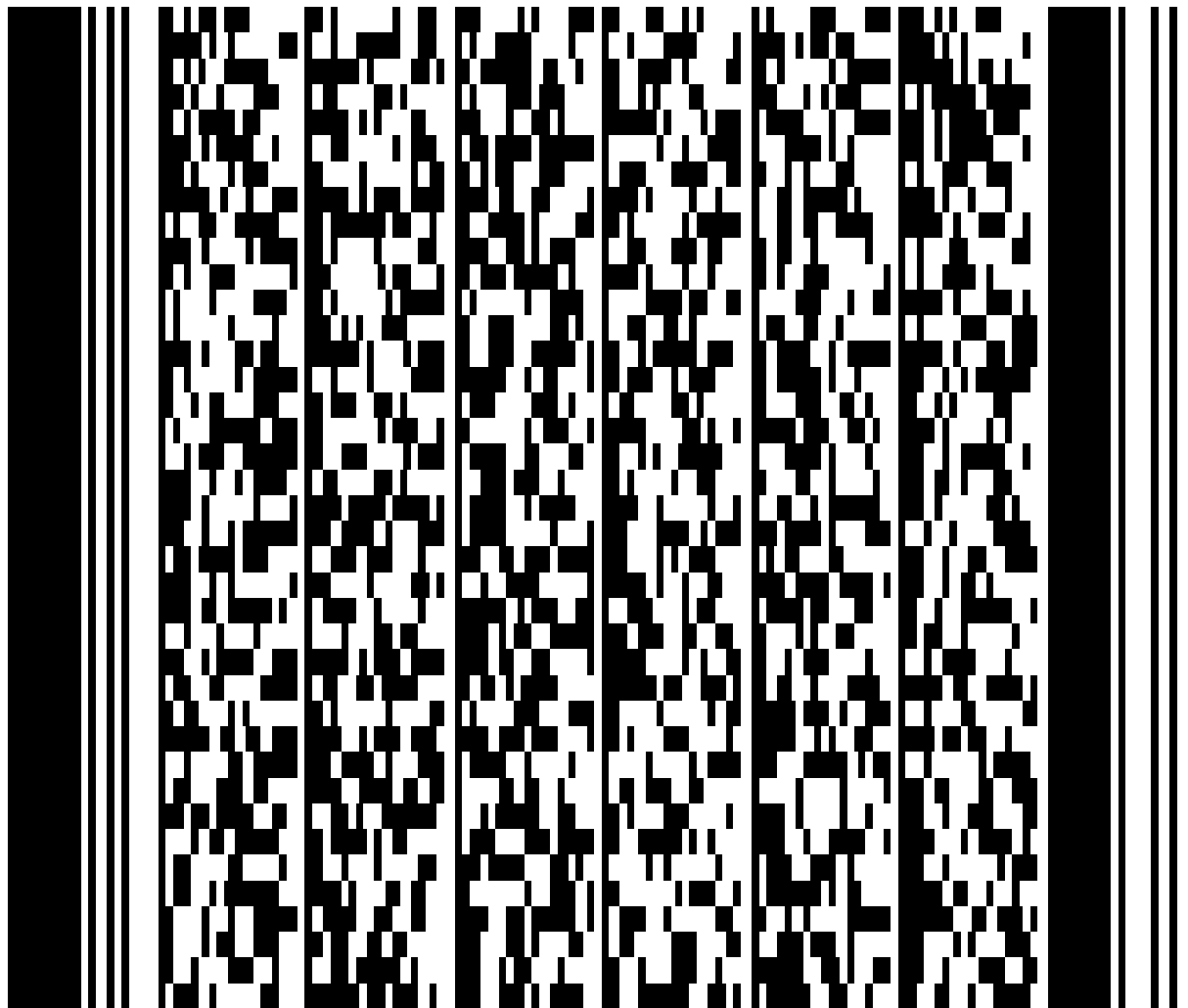
Structure Databases on PDAs

- ◆ 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?



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Development

What's This?

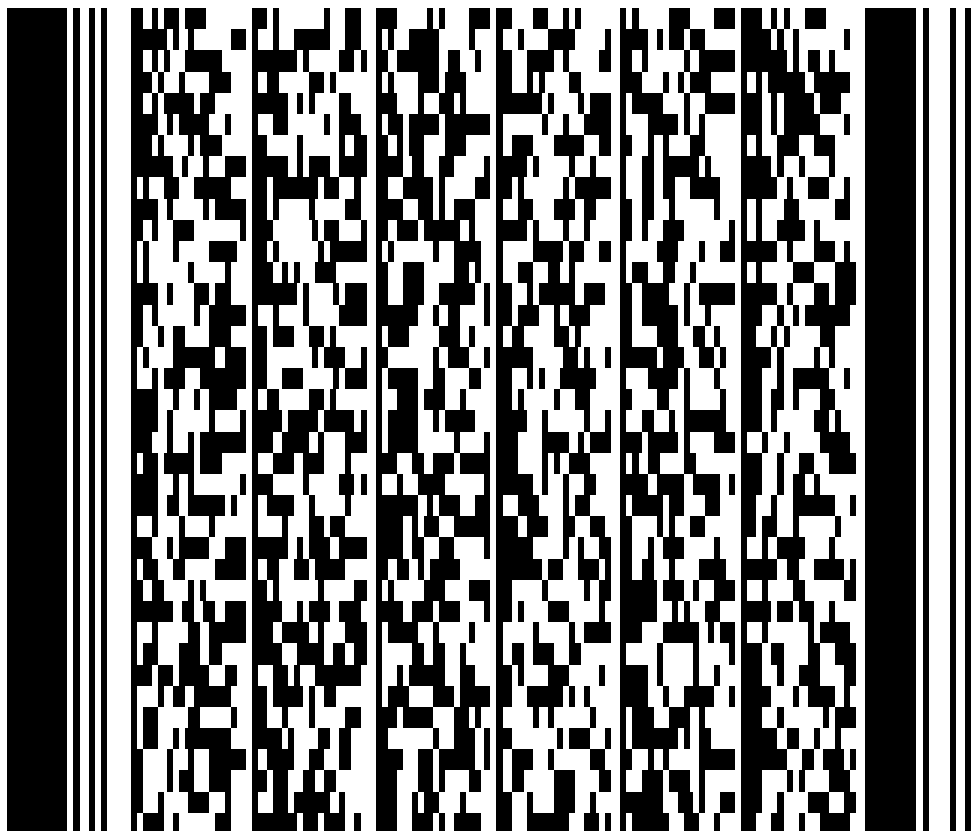


Structured
Solutions

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”

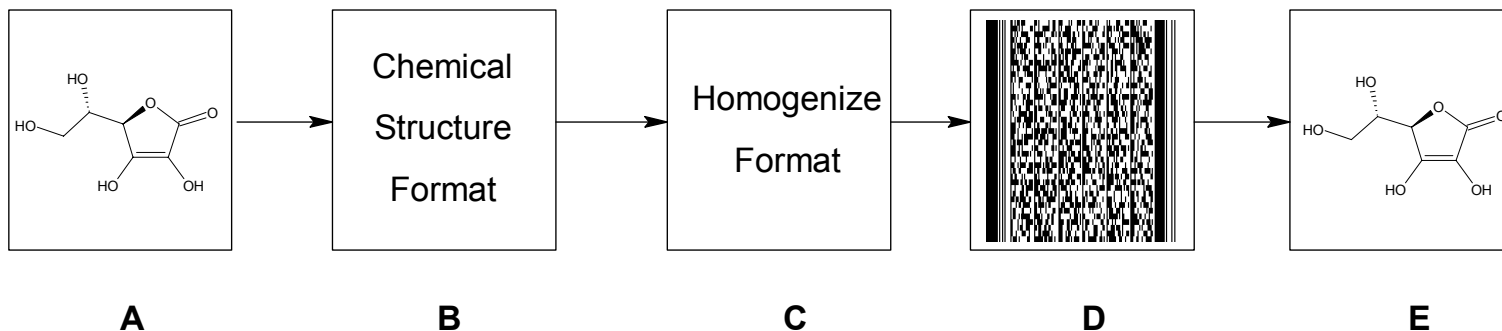


"Scanning Structures on PDAs"

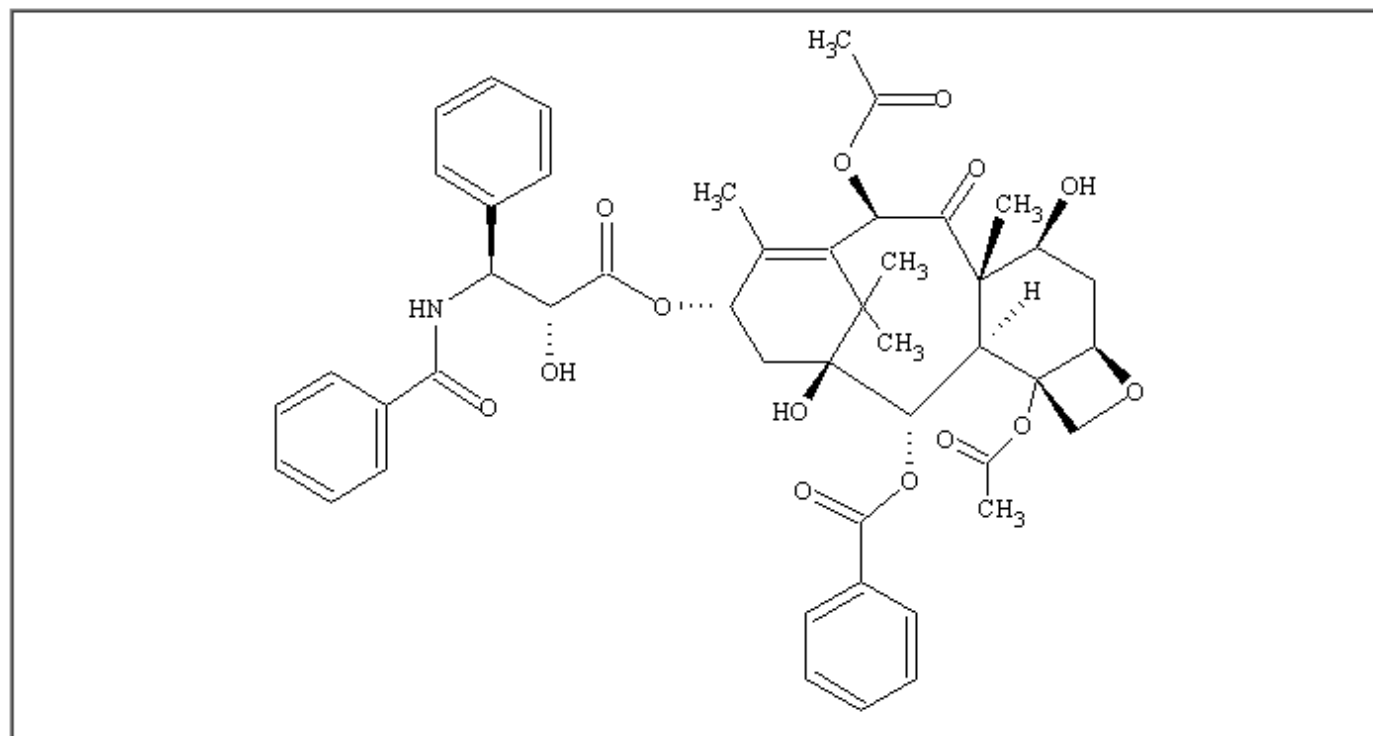
♦ A vision:

- 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

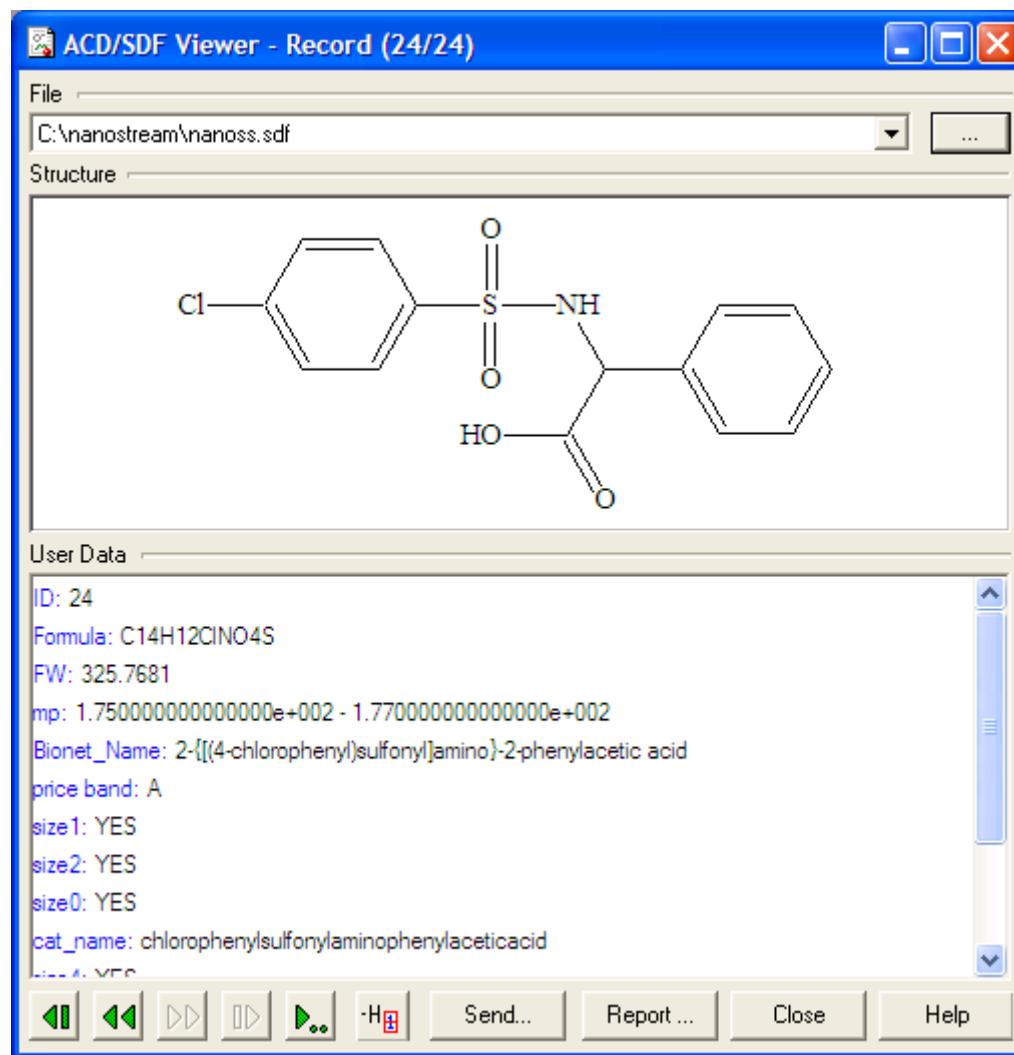
Structures and Barcodes



Taxol 2D barcode




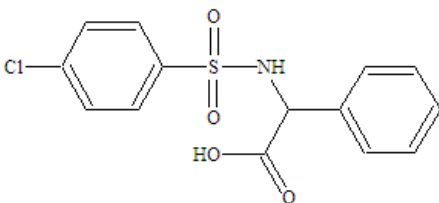
SDF Viewer



SDF Viewer

Report Preview

Print Report ... Save As ... ☒ Structure ☒ User Parameters ☒ Barcode Barcode Scale: 1 Refresh Close

ID: 24
 Formula: C₁₄H₁₂ClNO₄S
 FW: 325.7681
 mp: 1.7500000000000000e+002 - 1.7700000000000000e+002
 Bionet_Name: 2-[(4-chlorophenyl)sulfonylamino]-2-phenylacetic acid
 price band: A
 size1: YES
 size2: YES
 size0: YES
 cat_name: chlorophenylsulfonylaminophenylaceticacid
 size4: YES
 group: ACI/SUF
 Page No: p.89
 risksafetyphrases: R36/37/38 R20/21/22S26 S45 S3/7 S36/37/38
 size3: YES

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/>