

Structured Solutions



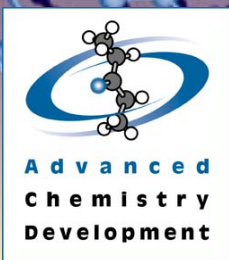
# **What's Available Online? Live Update, Tech Support, I-Lab, and Web Librarian**

***Extending the Technology  
to Enterprise Deployment***

Kevin Turnbull

Account Manager

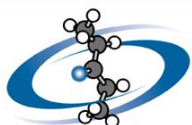
NMR Seminar – October 2, 2003.



# What's Available Online?

## Overview

- ◆ Internet
  - I-Lab on the Internet
  - Live update
  - Tech support Live help
- ◆ Intranet
  - I-Lab
  - Structure-spectrum verification using I-Lab
  - Web Librarian



Advanced  
Chemistry  
Development

# www.acdlabs.com

Advanced Chemistry Development Homepage - Microsoft Internet Explorer

Fichier Edition Affichage Favoris Outils ?

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**Latest News**

September 10, 2003 -  
[ACD/Labs Helps Develop Memory and Nomenclature Skills](#)

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**ACD/Labs, the inventor of ChemAnalytics, develops software that enables the process of discovery for chemists**

Applications

Product Groups

**ACD/Labs Structure Elucidation Challenge:**  
[Can your spectra stump our expert systems?](#)

ACD/Labs Web Site: an incredible source of regularly updated information

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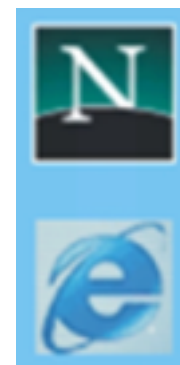
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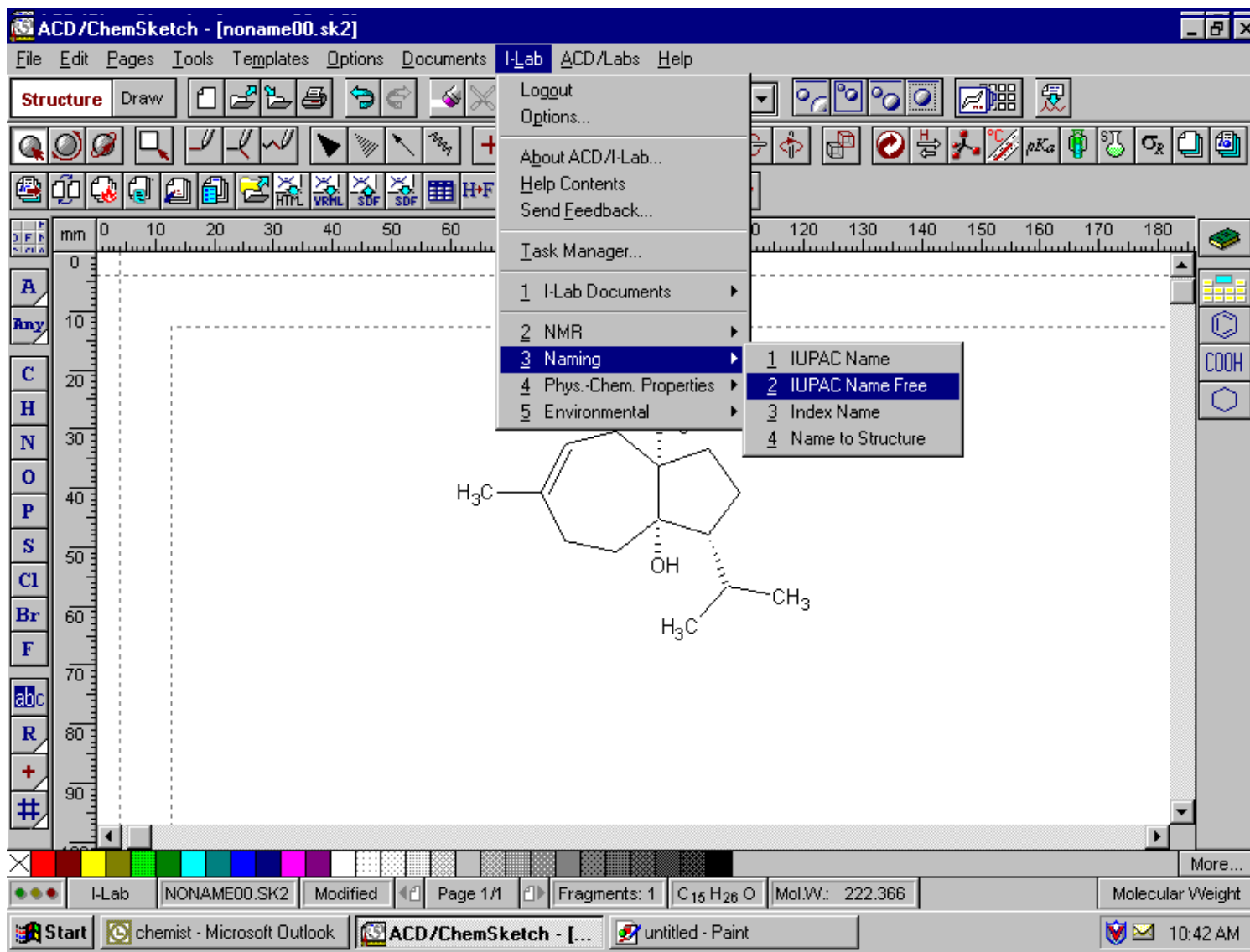
# What Is I-Lab?

- ◆ The Interactive Laboratory
  - Delivering ACD/Labs predictions
    - CNMR, HNMR, FNMR, PNMR, NNMR
    - IUPAC Name, CAS/Index Name, NTS
    - BP, LogP, pKa, LogD Aq Solubility
  - Providing access to non spectral databases
    - NMR DB
    - PhysChem DB

**Via a Web Architecture**

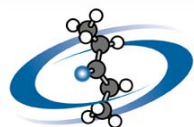


# I-Lab via ChemSketch



The screenshot shows the ACD/ChemSketch software interface. The title bar reads "ACD/ChemSketch - [noname00.sk2]". The menu bar includes File, Edit, Pages, Tools, Templates, Options, Documents, I-Lab, ACD/Labs, and Help. The I-Lab menu is open, showing options: Logout, Options..., About ACD/I-Lab..., Help Contents, Send Feedback..., Task Manager..., and a list of I-Lab Documents. The "Naming" document is selected, and its sub-menu is open, showing: 1 IUPAC Name, 2 IUPAC Name Free (highlighted), 3 Index Name, and 4 Name to Structure.

The main workspace displays a chemical structure of a bicyclic compound with a methyl group (H<sub>3</sub>C) and a hydroxyl group (OH). The structure is drawn on a grid with a ruler at the top and left. The left sidebar contains a vertical list of chemical elements: A, Any, C, H, N, O, P, S, Cl, Br, F, abc, R, +, #. The bottom status bar shows the current document is "NONAME00.SK2", modified, page 1/1, with 1 fragment, molecular formula C<sub>15</sub>H<sub>26</sub>O, and molecular weight 222.366. The taskbar at the bottom shows the Start button, a Microsoft Outlook window, the ACD/ChemSketch window, and an untitled Paint window. The system clock shows 10:42 AM.



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# I-Lab Online

ACD/I-Lab - Microsoft Internet Explorer

File Edit View Favorites Tools Help

Back Forward Stop Home Search Favorites Media Print

Address <http://ilab.acdlabs.com/ilab/perl/work.pl> Go Links

i-Lab Structure Web Librarian NMR Naming LogD New Calc History

CC

Put structure to the Editor/Viewer

LogD:

pH = 0.0 ; logD = -0.6 ± 1.0
pH = 1.0 ; logD = -0.6 ± 1.0
pH = 2.0 ; logD = -0.4 ± 1.0
pH = 3.0 ; logD = 0.3 ± 1.0
pH = 4.0 ; logD = 1.2 ± 1.0
pH = 5.0 ; logD = 1.7 ± 1.0
pH = 6.0 ; logD = 1.9 ± 1.0
pH = 7.0 ; logD = 1.9 ± 1.0
pH = 8.0 ; logD = 1.9 ± 1.0
pH = 9.0 ; logD = 1.8 ± 1.0
pH = 10.0 ; logD = 1.4 ± 1.0
pH = 11.0 ; logD = 0.6 ± 1.0
pH = 12.0 ; logD = -0.3 ± 1.0
pH = 13.0 ; logD = -1.0 ± 1.0
pH = 14.0 ; logD = -1.4 ± 1.0

Balance: \$0.00 Pay Bills Update Account Subscriptions Balance Summary Invoice History

ACD/I-Lab TM Internet



# What's Available Online?

## Overview

### ◆ Internet

- I-Lab on the Internet
- **Live product updates**
- Tech support Live help

### ◆ Intranet

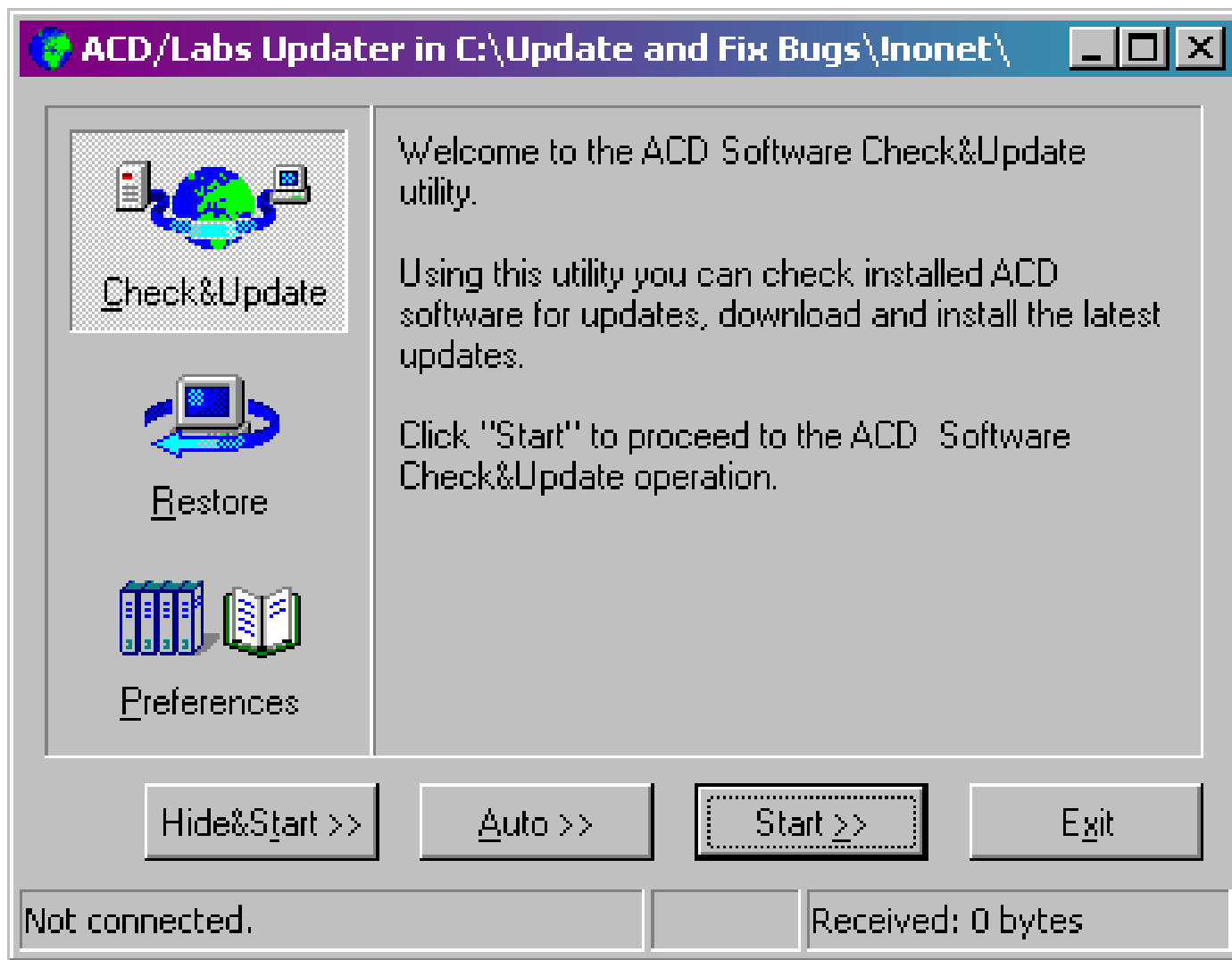
- I-Lab
- Structure-spectrum verification using I-Lab
- Web Librarian



# Online Updates

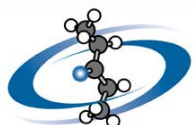
- ◆ New Application for online Updates available since April 2002
- ◆ WUK delivered to those under maintenance
- ◆ Automatic Download and Install
  - All new bug fixes and improvements
  - File format enhancements
  - Ability to restore original
- ◆ Password and Security Protection
- ◆ Verification and Logging of Updates
- ◆ Automated version control

# Online Update Utility



# What's Available Online? Overview

- ◆ Internet
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# Live Help

Advanced Chemistry Development Homepage - Microsoft Internet Explorer

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[Can your spectra stump our expert systems?](#)

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Discussions Abonnement... Discussions non disponibles sur <http://www.acdlabs.com/>

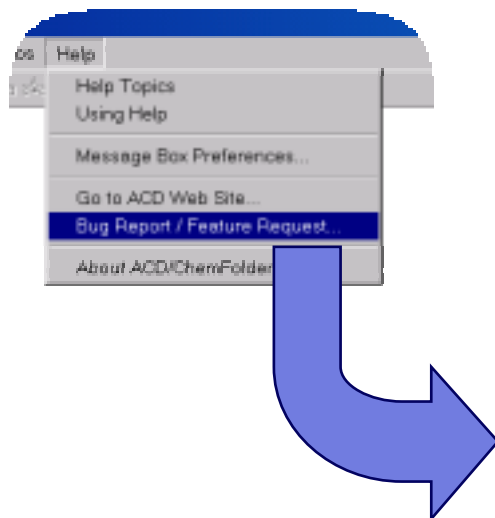
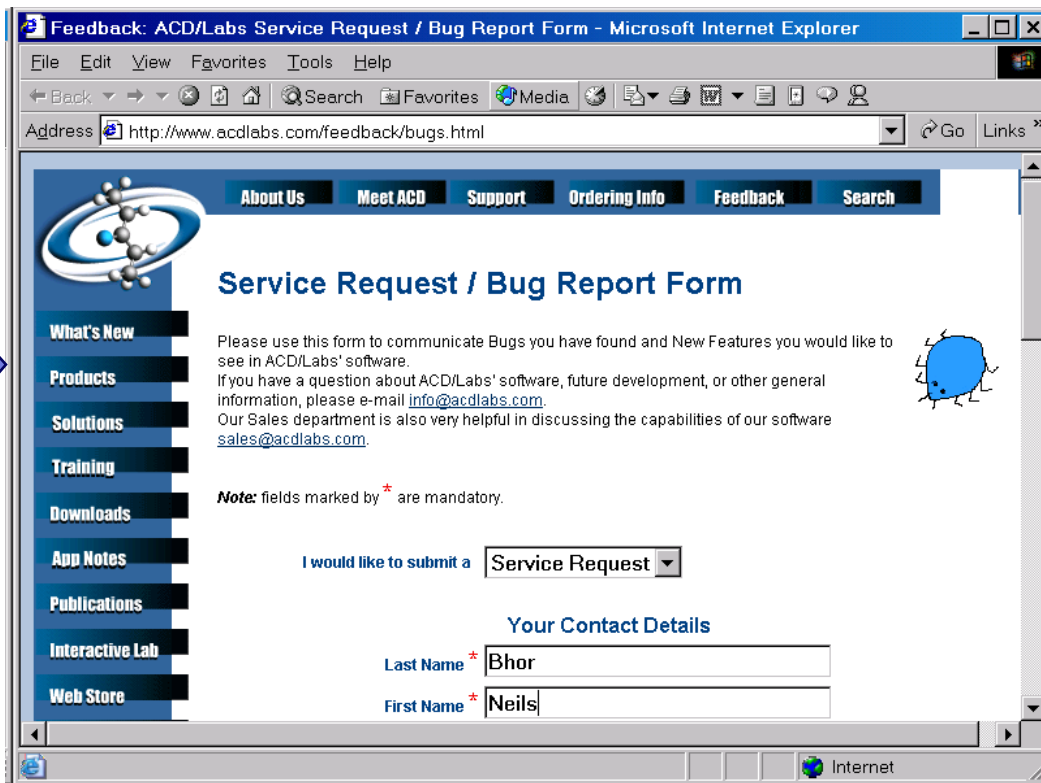
Terminé Internet

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# Contacting Support

Service Request / Bug Report Form :

- Fastest Resolution Time
- Automated

Feedback: ACD/Labs Service Request / Bug Report Form - Microsoft Internet Explorer

File Edit View Favorites Tools Help

Address <http://www.acdlabs.com/feedback/bugs.html>

About Us Meet ACD Support Ordering Info Feedback Search

## Service Request / Bug Report Form

Please use this form to communicate Bugs you have found and New Features you would like to see in ACD/Labs' software.  
If you have a question about ACD/Labs' software, future development, or other general information, please e-mail [info@acdlabs.com](mailto:info@acdlabs.com).  
Our Sales department is also very helpful in discussing the capabilities of our software [sales@acdlabs.com](mailto:sales@acdlabs.com).

**Note:** fields marked by \* are mandatory.

I would like to submit a

### Your Contact Details

Last Name \*

First Name \*

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# I-Lab for Intranets

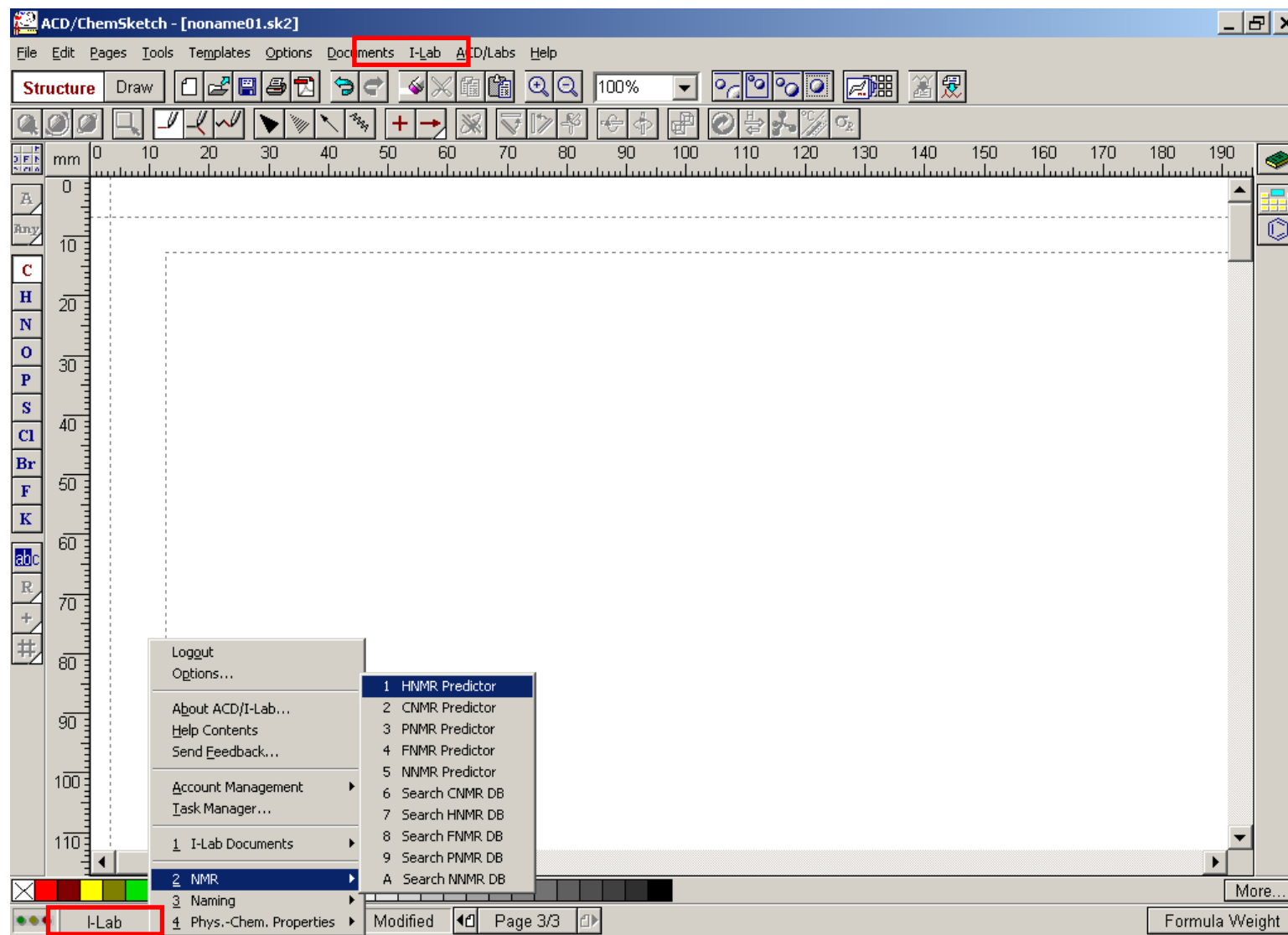
- ◆ “It’s a nightmare to deploy all that software on everyone’s desktop who needs it”
  - o Inventory the hardware;
  - o Inventory the computer resources for each machine;
  - o Install the software on each computer;
  - o Make sure network installations don't cause too much network traffic; and
  - o Re-install for every update.
- ◆ The cost of deployment and maintenance can be a significant financial burden itself.
- ◆ **I-Lab on Intranet offers an equivalent accuracy for less money than the standard Windows interface**



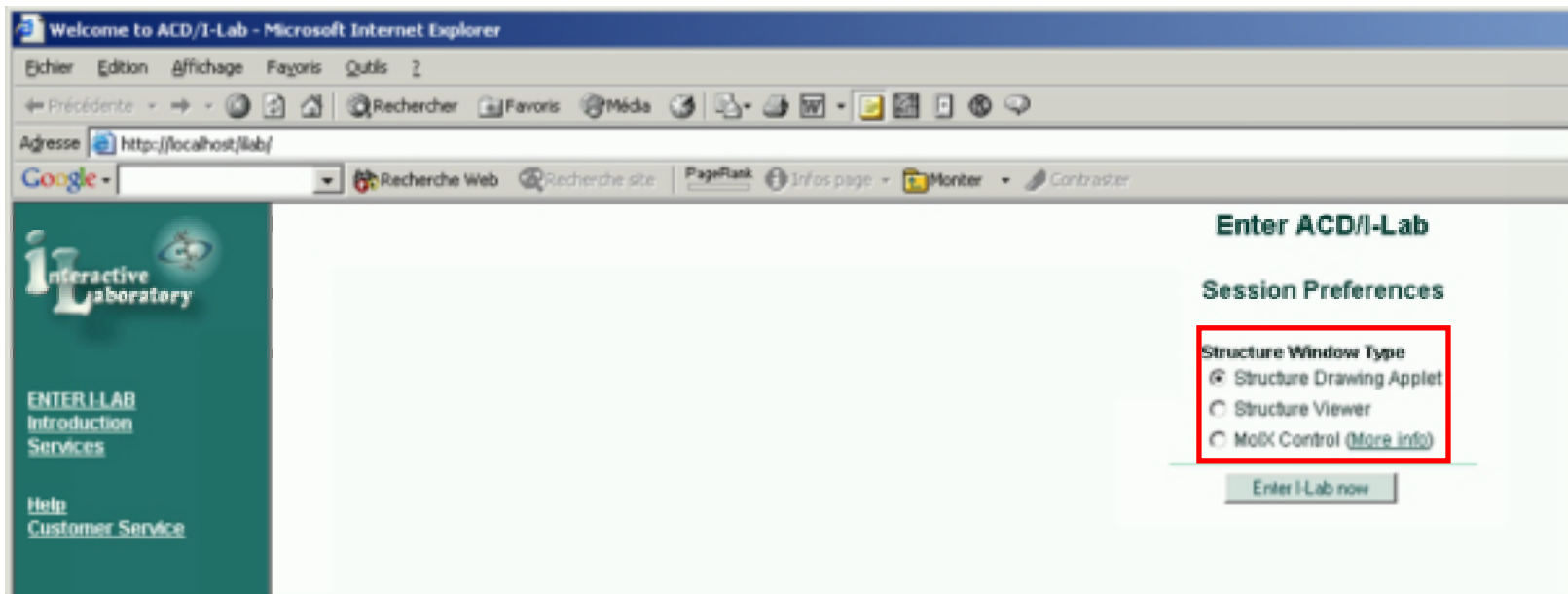
# I-Lab Architecture

- ◆ The I-Lab Prediction Platform is server technology serving up the predictions and providing the transaction handling and integration technology
- ◆ ACD/Labs prediction engines sit on the platform technology
- ◆ The user interface can be
  - ACD/Chemsketch
  - ACD plug-ins on IE or Netscape
  - ACD/ Active-X module used in some customized user interface

# Starting I-Lab from ChemSketch

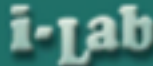






# Starting I-Lab from your Internet Browser



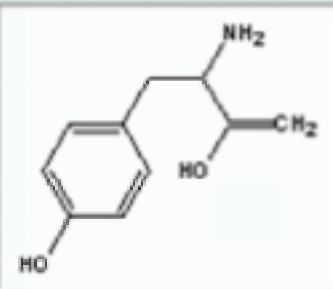




# MolX Control

## Structure

To enter a new structure or edit the entered one double-click on the box below



If the MolX control does not work properly proceed to [troubleshooting](#)

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Your browser window is divided into three parts.

- Top part contains file operations menu and a list of I-Lab services
- Middle part is used to input additional parameters for calculations
- Bottom part is called Account Frame. It contains your account information. If values are shown in red, that means they are incorrect.

The Structure Drawing Applet occupies a separate window. Click on the Structure Drawing icon in the top menu.

Before you request an I-Lab service, the Structure Drawing Applet must be initialized. Click on the Structure Drawing Menu Frame to input existing MOL or ChemDraw file into the applet.

---



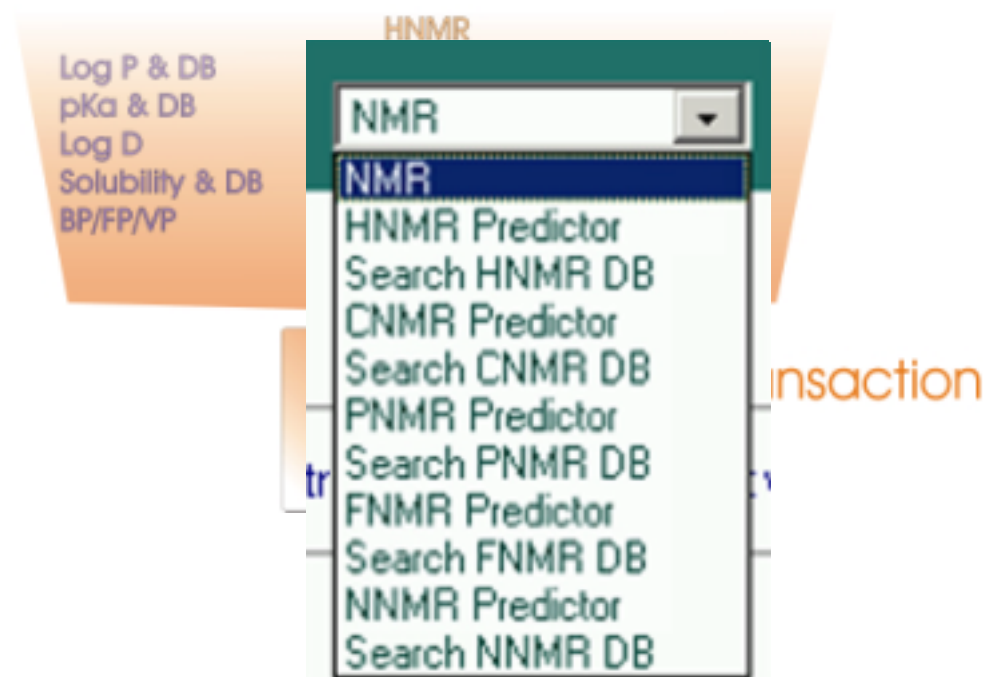
## I-Lab ENGINES



I-Lab Transaction  
Server



## I-Lab ENGINES





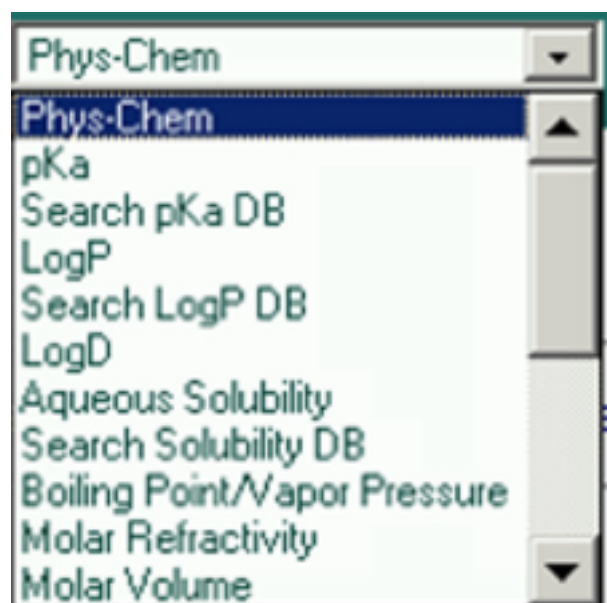


## I-Lab ENGINES

Log P & DB  
pKa & DB  
Log D  
Solubility & DB  
BP/FP/VP



I-Lab Transaction  
Server





## I-Lab ENGINES



action

# I-Lab Request - NMR

**CALCULATE**

**HNMR Options**

Frequency, MHz

**System training**

☒ Not Use [User DB descriptions](#)

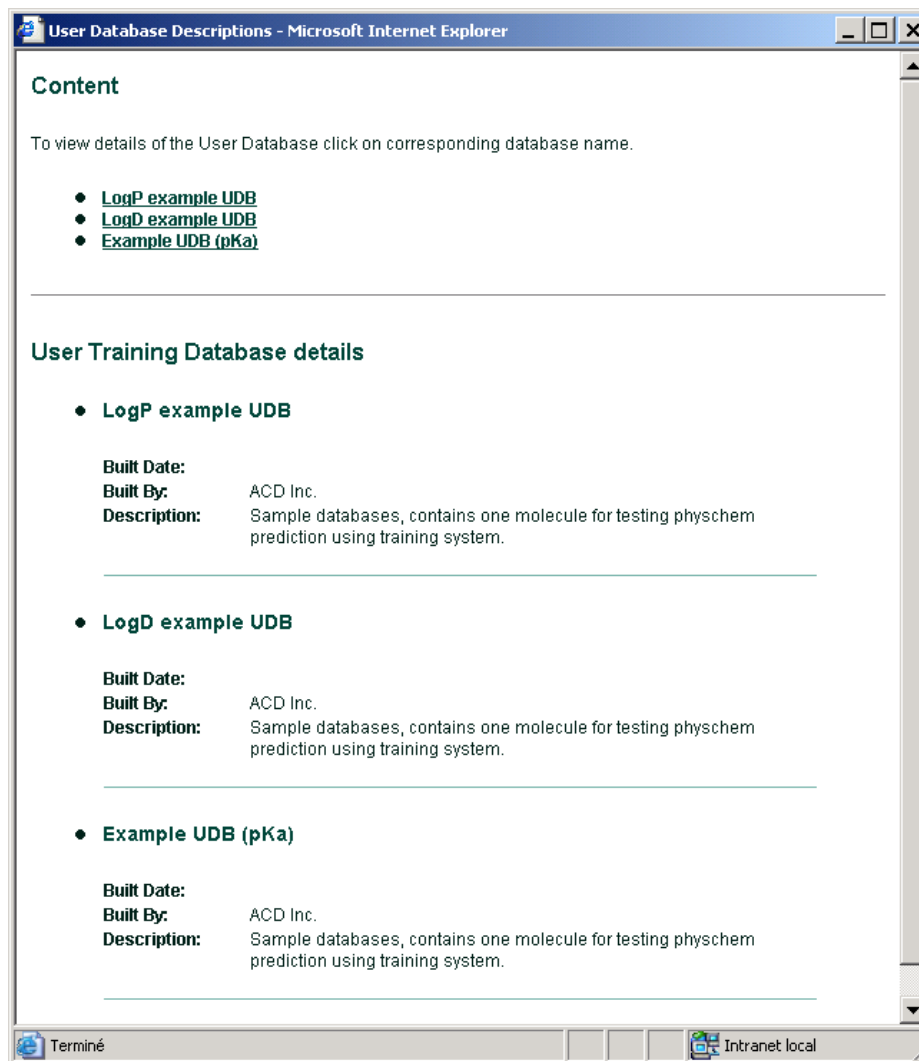
☐ Use System Training [descriptions](#)

**HNMR User Database(s)**

☐ ACD Demo UDB

☐ Example UDB

# User DB Description



**Content**

To view details of the User Database click on corresponding database name.

- [LogP example UDB](#)
- [LogD example UDB](#)
- [Example UDB \(pKa\)](#)

---

**User Training Database details**

- **LogP example UDB**

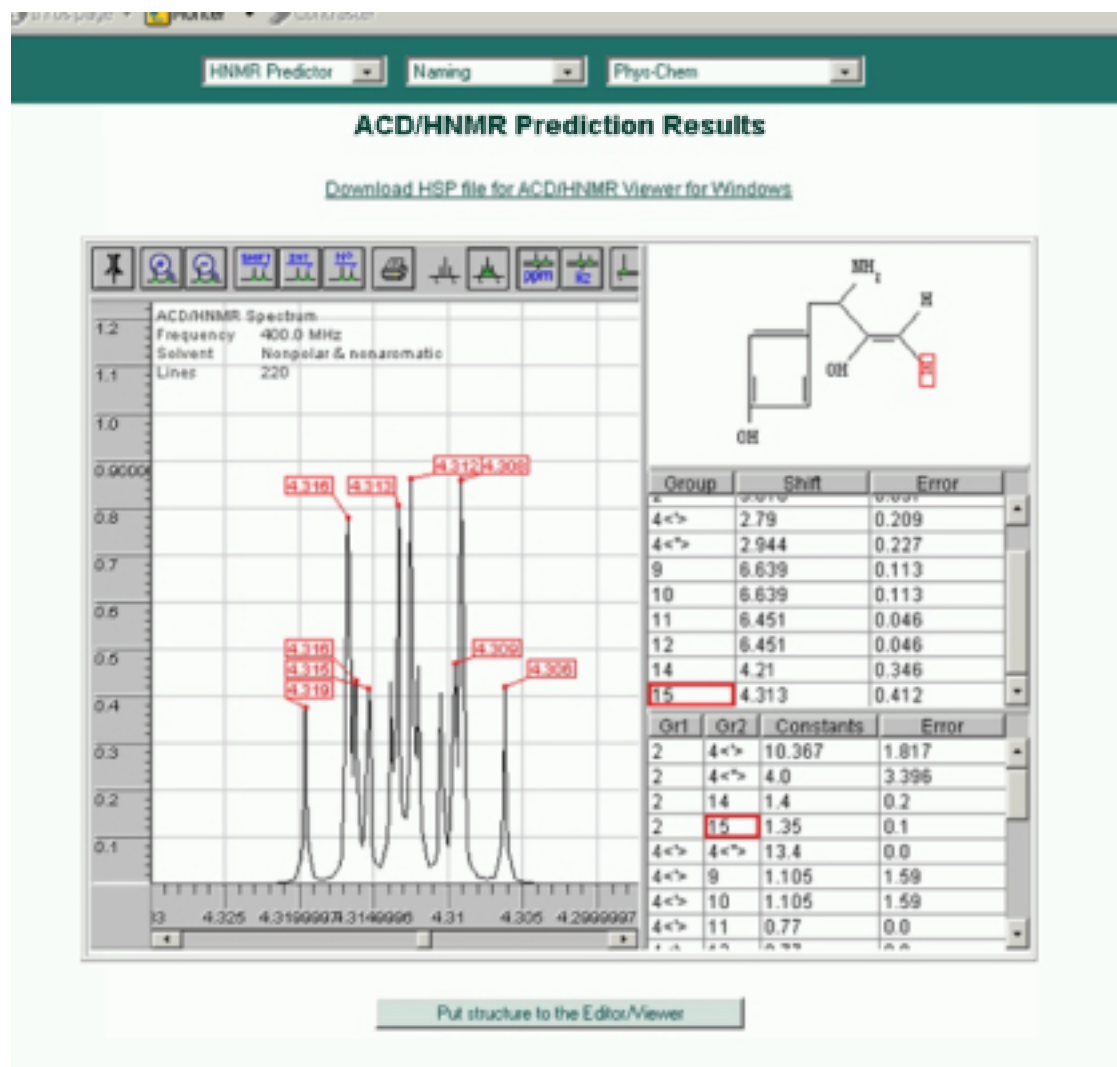
**Built Date:**  
**Built By:** ACD Inc.  
**Description:** Sample databases, contains one molecule for testing physchem prediction using training system.
- **LogD example UDB**

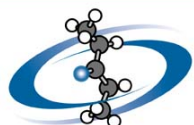
**Built Date:**  
**Built By:** ACD Inc.  
**Description:** Sample databases, contains one molecule for testing physchem prediction using training system.
- **Example UDB (pKa)**

**Built Date:**  
**Built By:** ACD Inc.  
**Description:** Sample databases, contains one molecule for testing physchem prediction using training system.

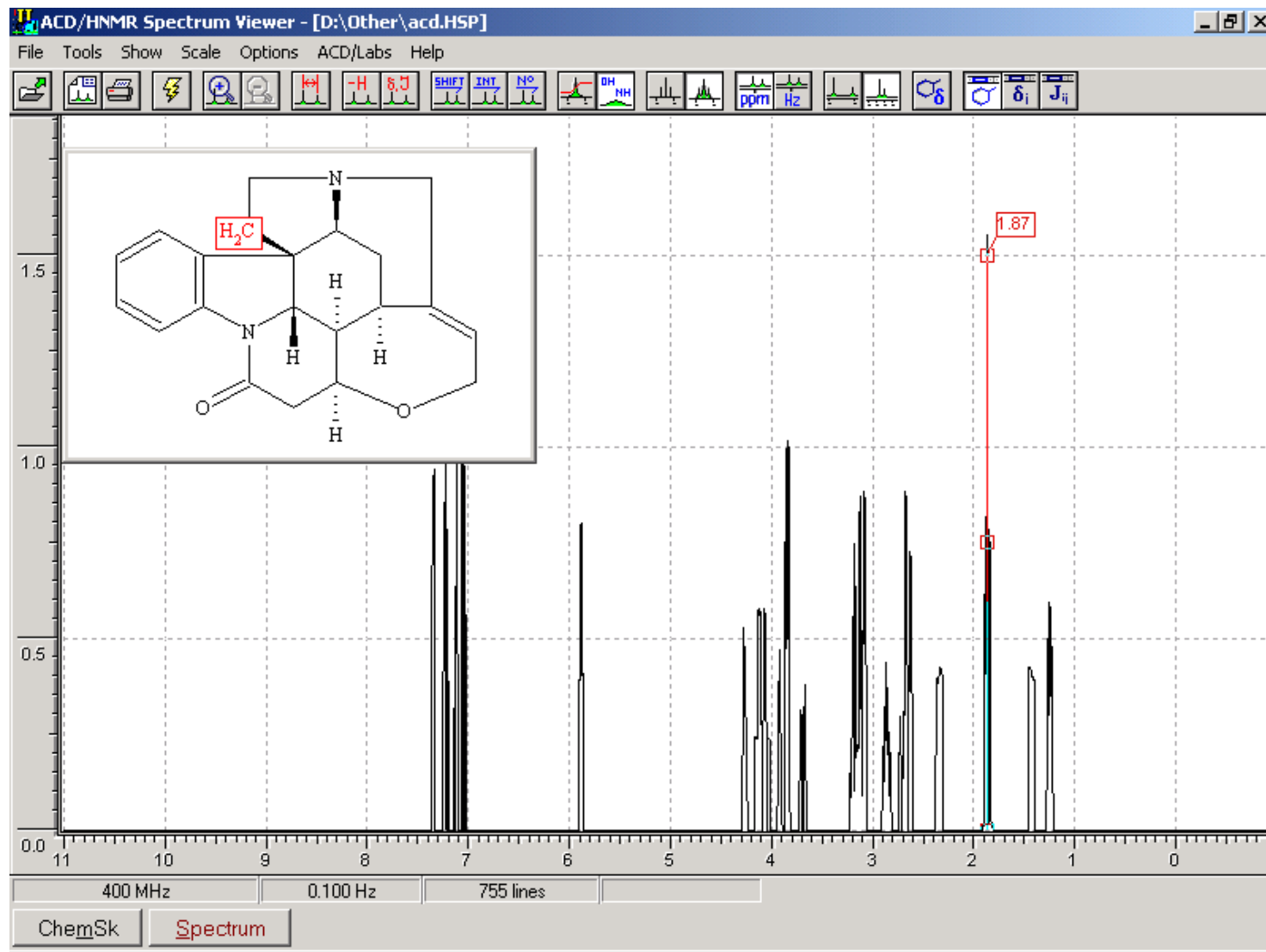
Terminé Intranet local

# I-Lab Result – H1 NMR Prediction





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You can view the NMR spectrum predicted using  
I-Lab with a Windows-based spectrum viewer

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

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# Workflow Scenario Using ACD/Labs Software

- ◆ 10 Spectroscopists are using some modules of SpecManager to make assignments, and/or enriching training databases
- ◆ 20 Chemists are making compounds, running NMRs, and creating NMR Predictor training databases
- ◆ The rest of the organization periodically needs access to NMR information, in addition to other unmeasured structures or access to a simple verification
- ◆ **For those, a deployment of I-Lab Intranet is the best choice**



# I-Lab vs Standard Windows

- ◆ Easy Deployment:
  - → *I-Lab*
- ◆ 100% of the functionality
  - → *Standard Windows*
- ◆ More intuitive interface
  - → *I-Lab*
- ◆ Pricing for large deployment
  - → *I-Lab*
- ◆ Easy upgrade
  - → *I-Lab*
- ◆ Concurrent network
  - → *Standard Windows*
- ◆ No capability to build a user database and train the program but only using Corporate User training DB
  - → *I-Lab*

# What's Available Online?

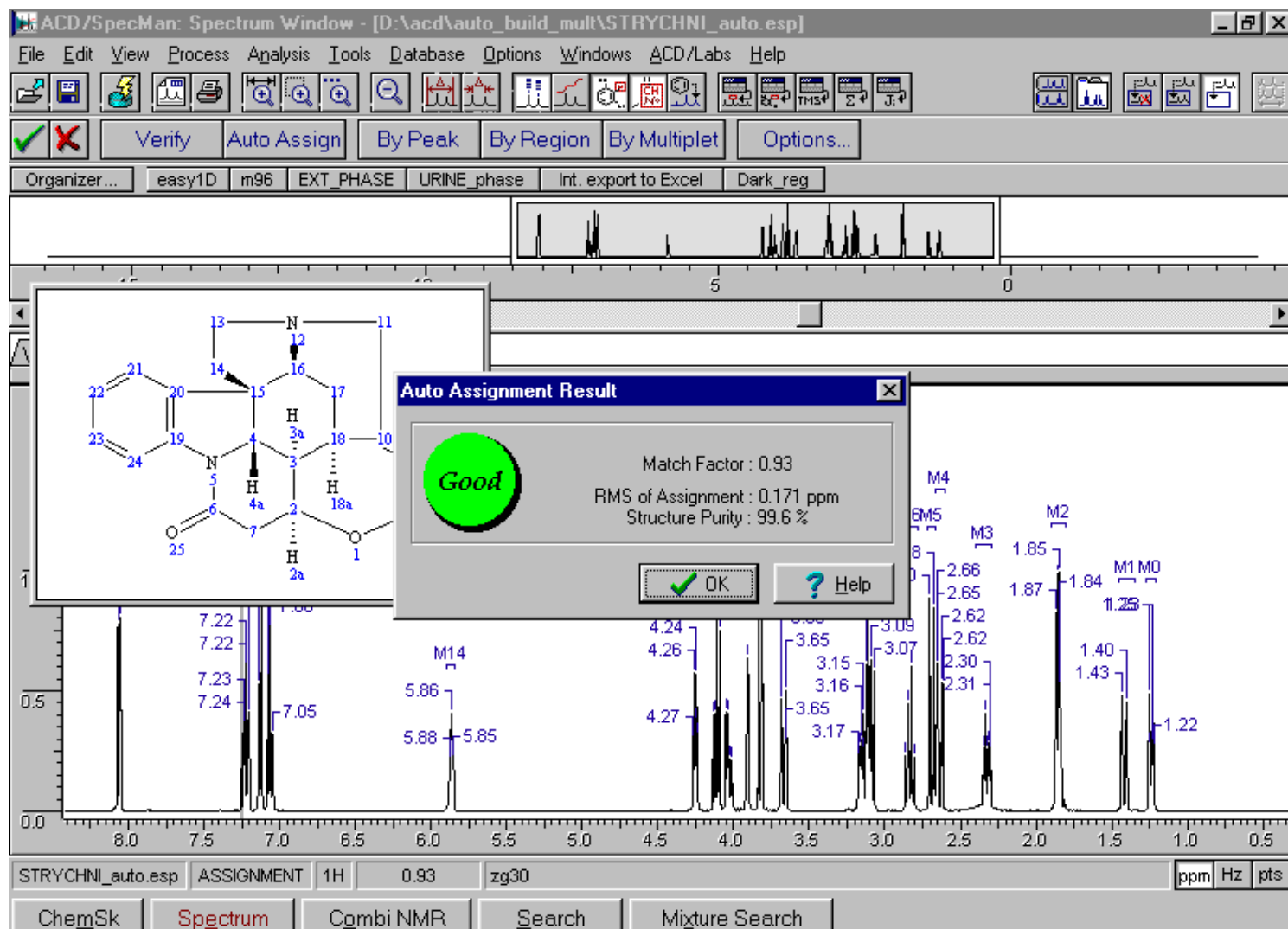
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# NEW: NMR Verification through I-Lab

- ◆ Manual, spectrum-by-spectrum interpretation is the traditional way
- ◆ Use prediction software to predict compound-by-compound, and compare against experimental is faster using ACD/NMR Processor or Manager and H or C NMR Predictor
- ◆ Now easy to deploy using H or CNMR Prediction under I-Lab

# Auto-Assignment



# What's Available Online?

## Overview

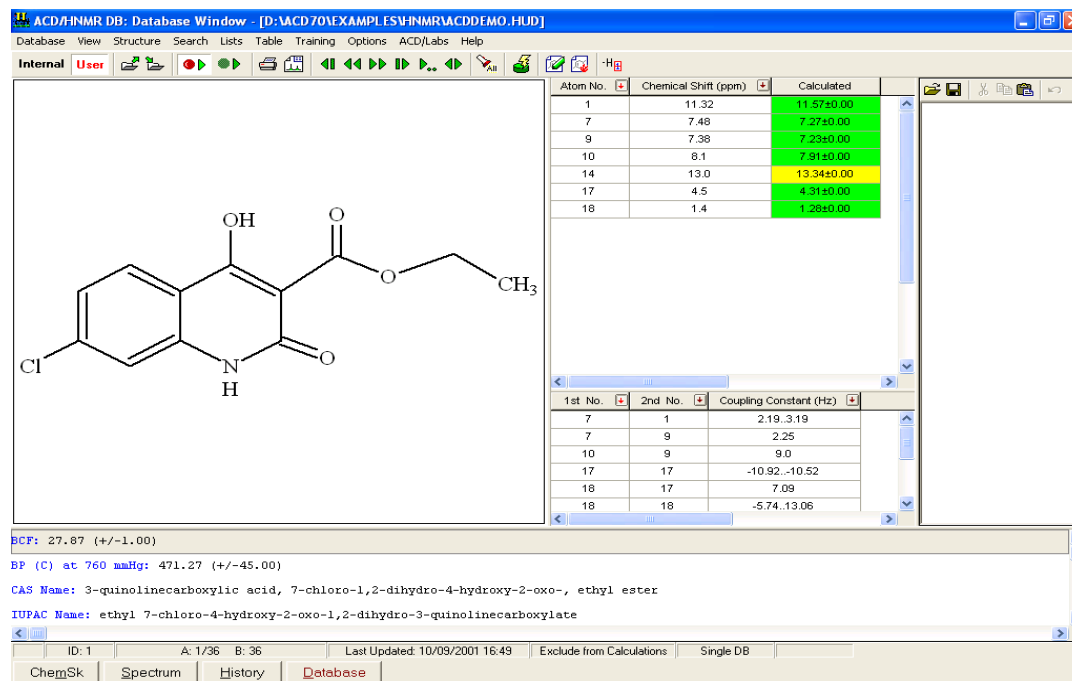
### ◆ Internet

- I-Lab on the Internet
- Live update
- Chromatographic application database on the Web
- Tech support Live help

### ◆ Intranet

- I-Lab
- Structure-spectrum verification using I-Lab
- **Web Librarian**

# Review of Workflow Using ACD/Labs NMR Software



ACD/HNMR DB: Database Window - [D:\ACD70\EXAMPLES\HNMR\ACDDEMO.HUD]

Database View Structure Search Lists Table Training Options ACD/Labs Help

Internal User

Chemical structure: CCOC(=O)C1=C(O)C(=O)NC2=CC=CC=C1Cl

Atom No.	Chemical Shift (ppm)	Calculated
1	11.32	11.57±0.00
7	7.48	7.27±0.00
9	7.38	7.23±0.00
10	8.1	7.91±0.00
14	13.0	13.34±0.00
17	4.5	4.31±0.00
18	1.4	1.28±0.00

1st No.	2nd No.	Coupling Constant (Hz)
7	1	2.19..3.19
7	9	2.25
10	9	9.0
17	17	-10.92..-10.52
18	17	7.09
18	18	-5.74..13.06

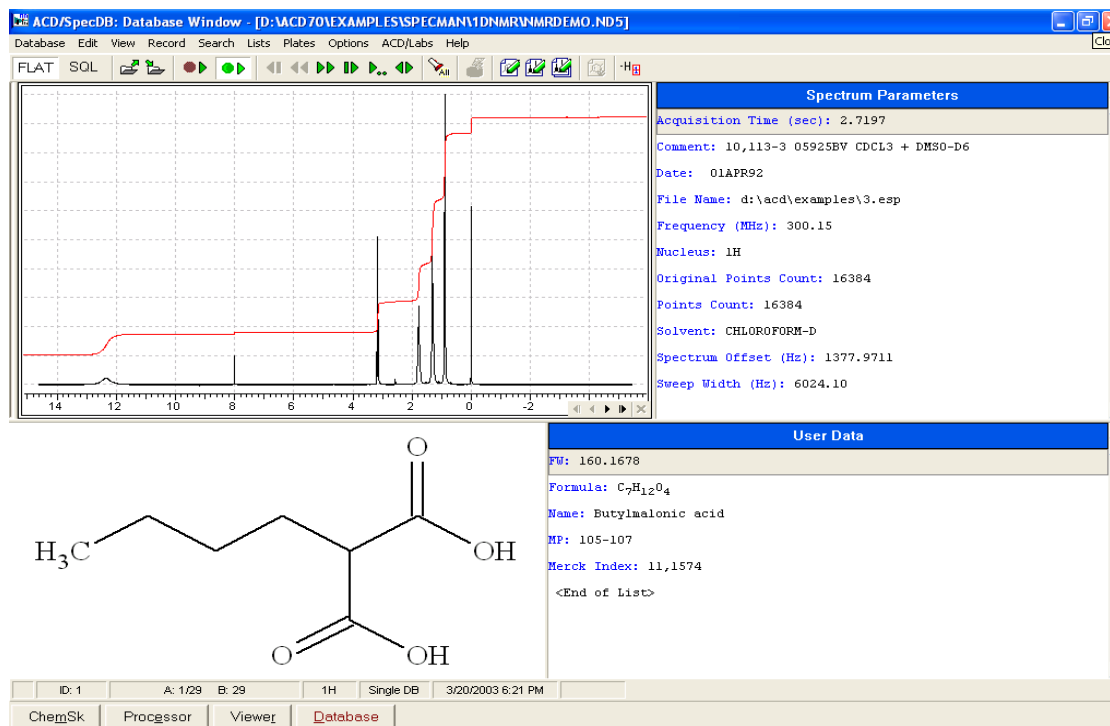
BCF: 27.87 (+/-1.00)  
BP (C) at 760 mmHg: 471.27 (+/-45.00)  
CAS Name: 3-quinolinecarboxylic acid, 7-chloro-1,2-dihydro-4-hydroxy-2-oxo-, ethyl ester  
IUPAC Name: ethyl 7-chloro-4-hydroxy-2-oxo-1,2-dihydro-3-quinolinecarboxylate

ID: 1 A: 1/36 B: 36 Last Updated: 10/03/2001 16:49 Exclude from Calculations Single DB

ChemSk Spectrum History Database

- ◆ Databases of chemical shift information are being created to train the CNMR, HNMR predictions

# Review of Workflow Using ACD/Labs NMR Software



- ◆ Databases of SPECTRA are created and shared with ACD/NMR Manager (1D and 2D)

# Other Types of ACD/Labs Databases Your Company Might Be Creating

- ◆ MS Manager
- ◆ UV-IR Manager
- ◆ ChromManager
- ◆ CurveManager
- ◆ ChemFolder
- ◆ LogP user database
- ◆ pKa user database

***Islands of isolated information that can be leveraged by other groups in your organization?***

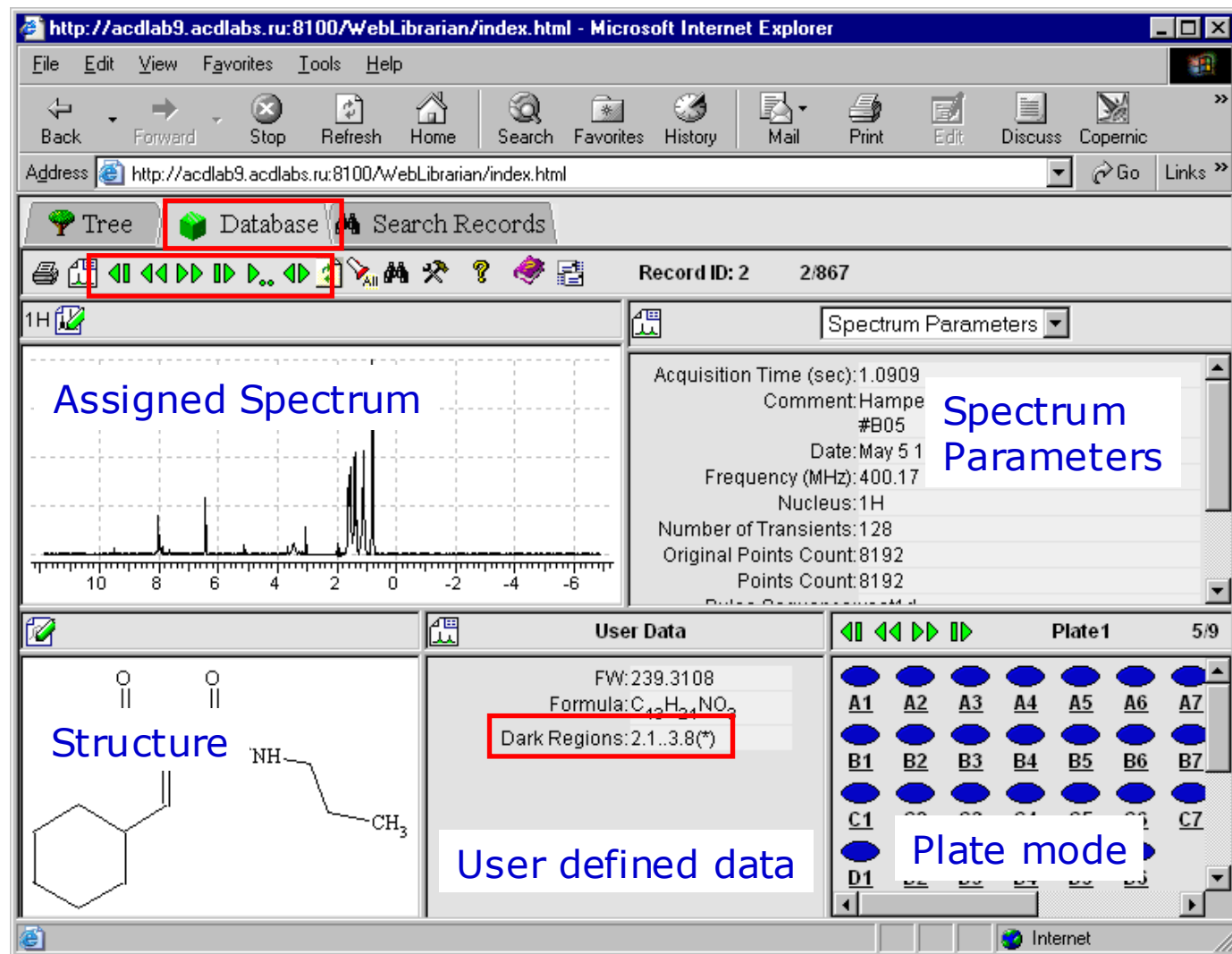


# ACD/Web Librarian

## ◆ Design Objectives

- To provide web-based access to analytical databases built inside SpecManager SQL on ORACLE, and CNMR/HNMR 'training' databases
- To ease deployment across an organization
- To reduce significantly the cost of deployment for spectral DB viewing and searching
- To provide DOWNLOAD access of spectra and structures to ACD/Labs desktop tools for "power users"
- To provide a tool which can be integrated to already existing enterprise solutions

# Visualization of *all* Associated Information



# Viewing Various Tables

http://acdlab9.acdlabs.ru:8100/WebLibrarian/index.html - Microsoft Internet Explorer

File Edit View Favorites Tools Help

Address http://acdlab9.acdlabs.ru:8100/WebLibrarian/index.html Go Links

Tree Database Search Records

Record ID: 1 1/36

1H

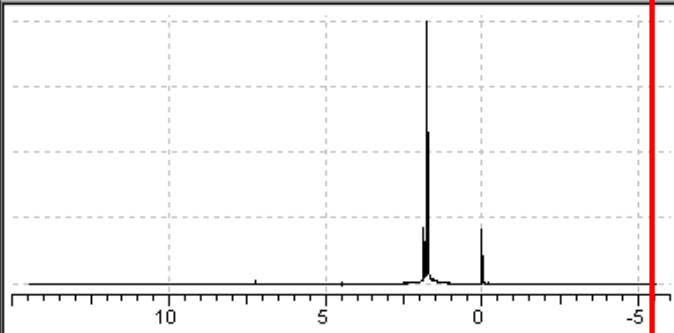
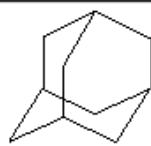


Table of Peaks

No.	(ppm)	(Hz)	*	(ppm)	Area	LF	Function
1	0.00	0.0	-				
2	1.54	463.3	-				
3	1.62	487.6	-				
4	1.63	490.5	-	0.0201	-	-	-
5	1.67	501.2	-	0.0300	-	-	-
6	1.75	526.2	-	1.0000	-	-	-
7	1.76	529.5	-	0.7319	-	-	-
8	1.87	561.5	-	0.2117	-	-	-

Record Note

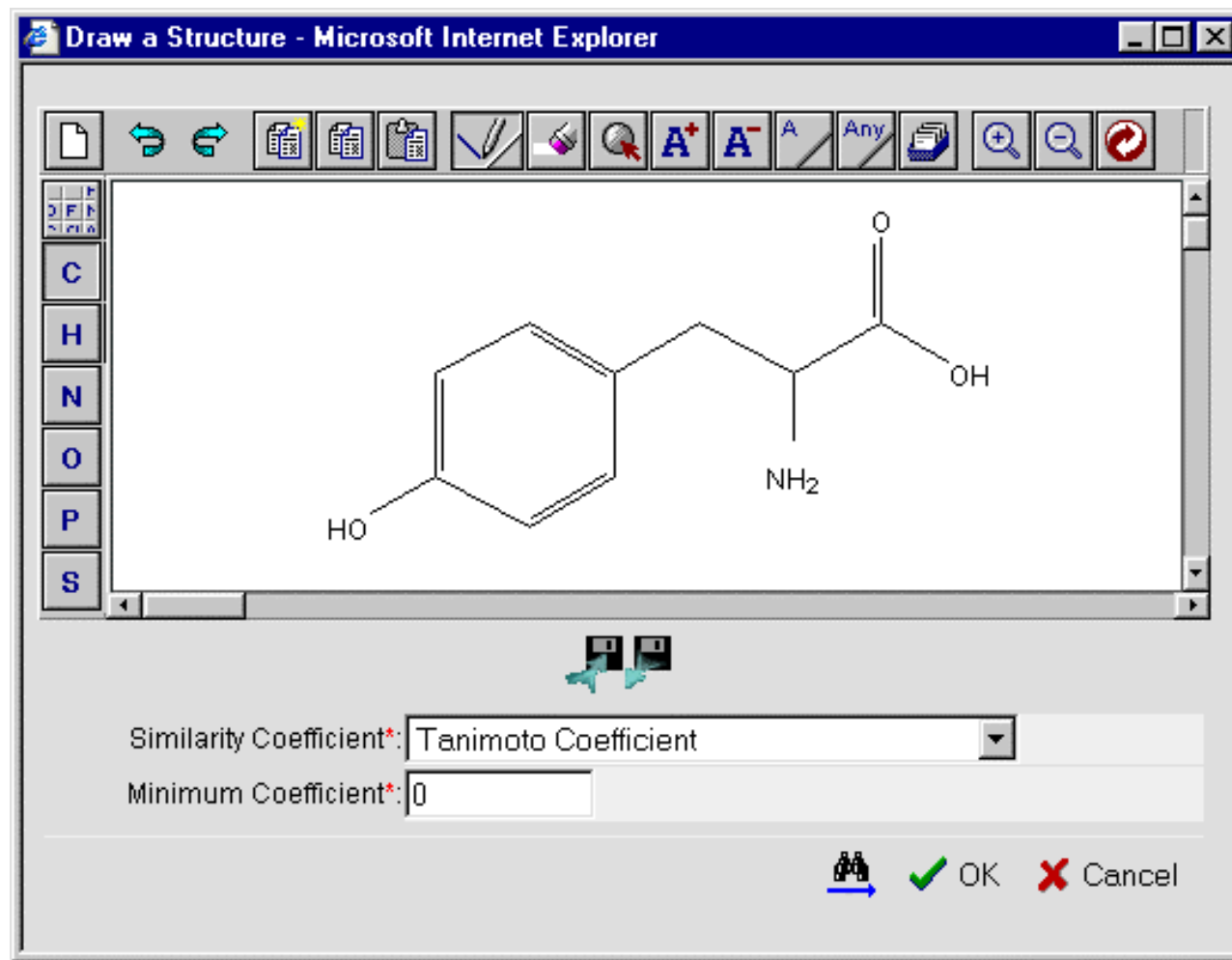


User Data

Name: Adamantane  
MP: 209-212 (sublimes), 268 (sealed tube)  
Merck Index: 11,140  
ACD/Combi result: 0.58636

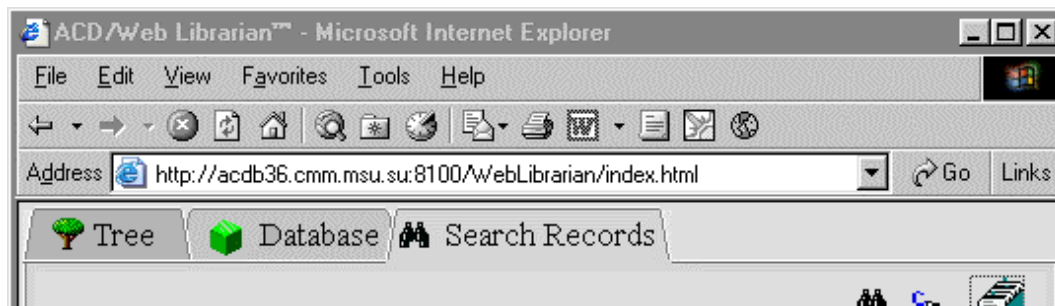
Internet

# Structure Searching





# Multiple DB Searching



**Multiple Search Results - Microsoft Internet Explorer**

Database	Total Records	Number of Hits
<a href="#">f:\webdb\data\Digital.cfd</a>	1340	2
<a href="#">f:\webdb\data\nmrdemo1.nd5</a>	867	0
<a href="#">f:\webdb\data\Poppy.cfd</a>	35	4
<a href="#">f:\webdb\data\Example.ndb</a>	28	0

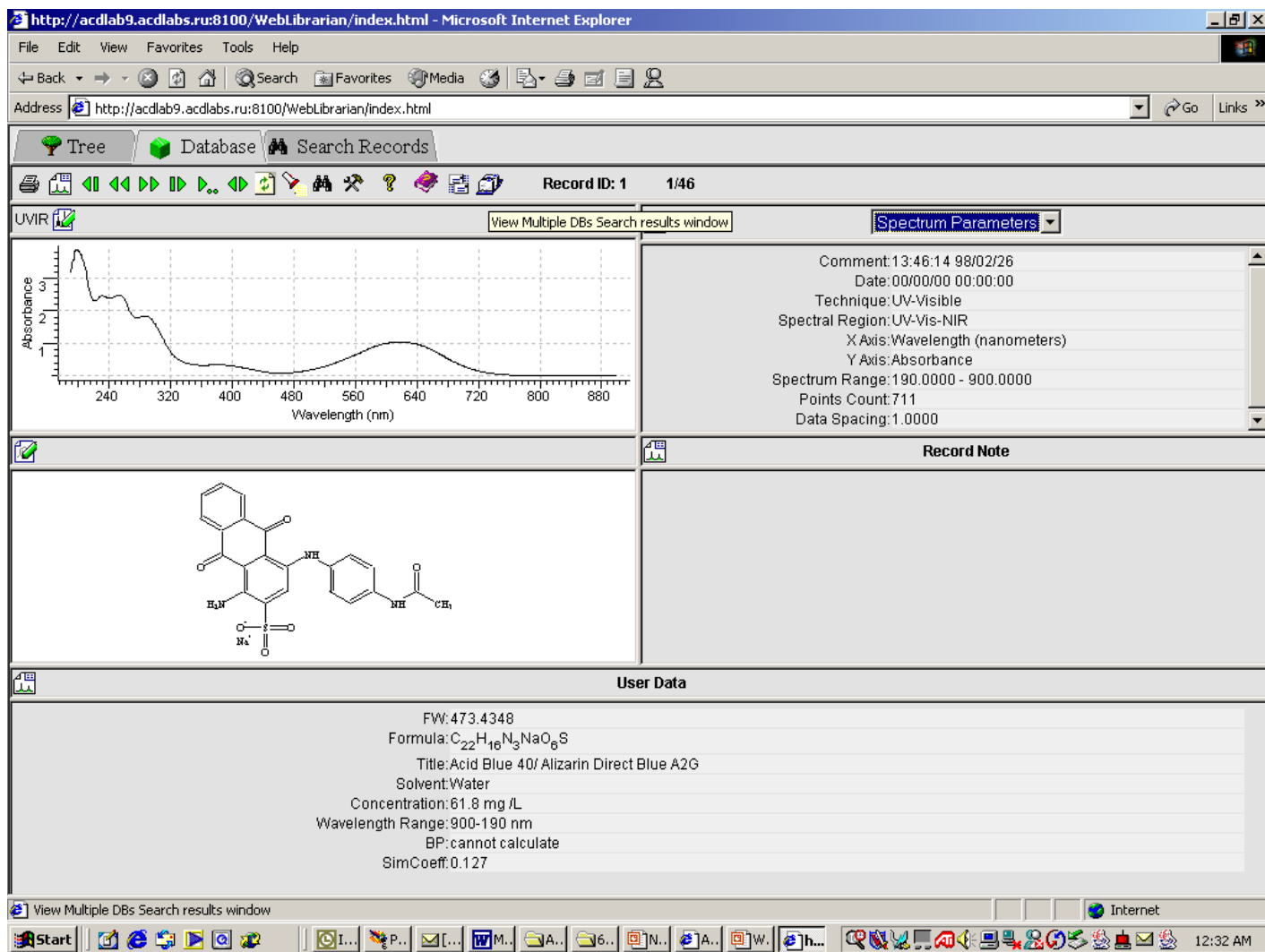
  

3	<input type="checkbox"/>	E:\Projects\WebDB\Data\dict.cfd	X
4	<input type="checkbox"/>	E:\Projects\WebDB\Data\uwis.nd5	X

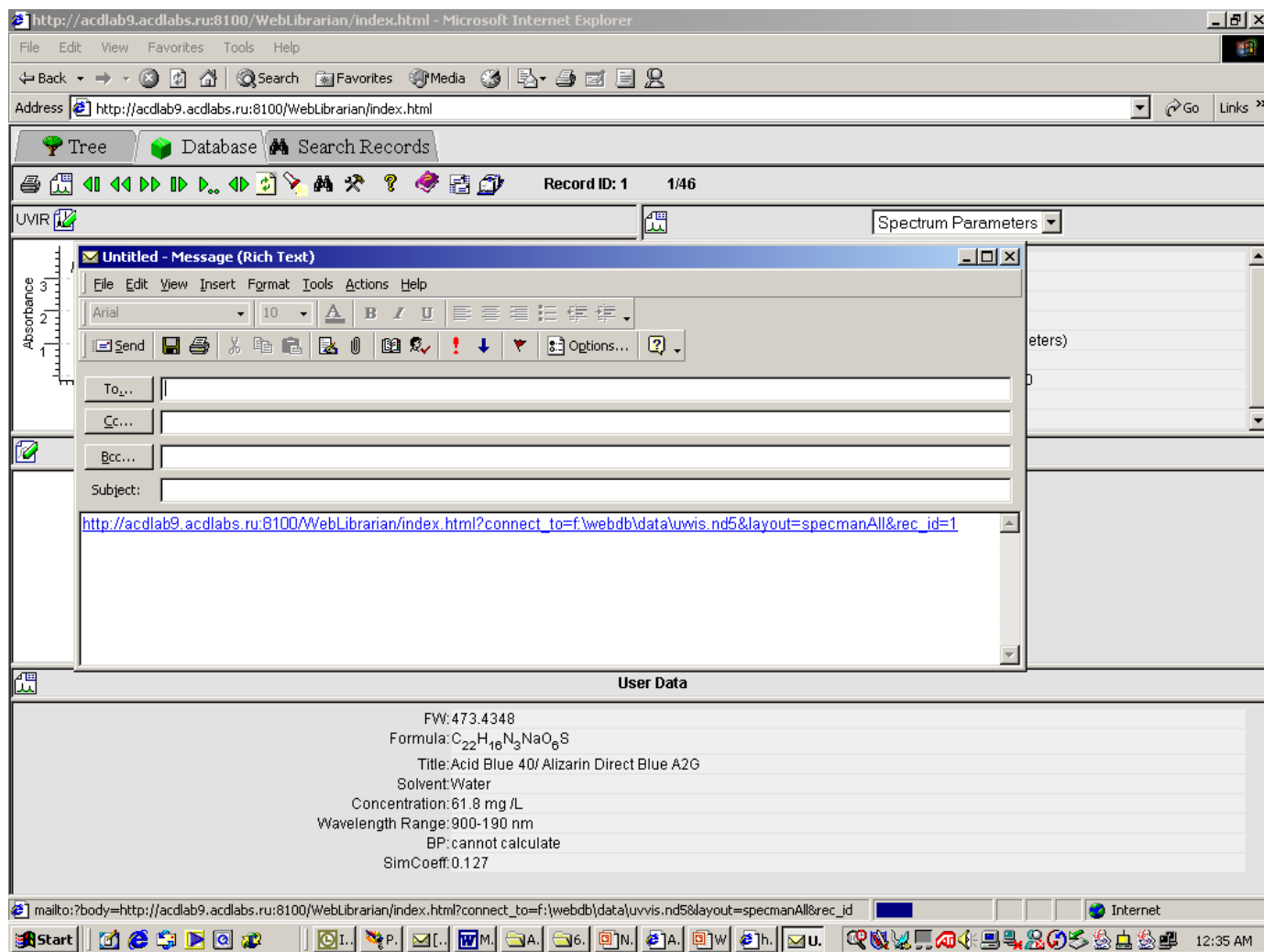
Execute Multiple Databases Search ☐

OK Cancel

# After Searching Multiple DBs



# Email Record Link



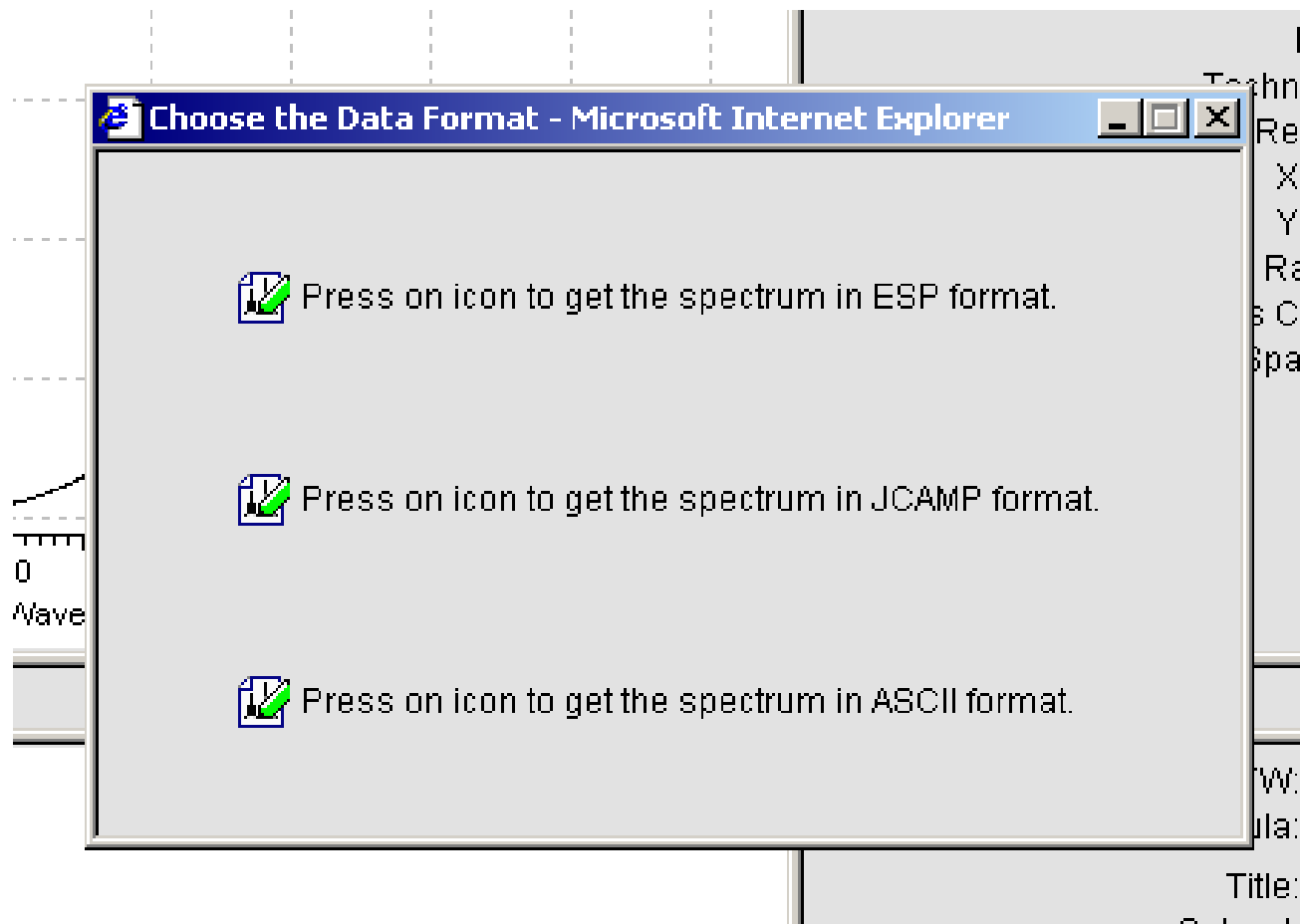
The screenshot shows a Microsoft Internet Explorer window displaying a web application interface. The address bar shows the URL: <http://acdlab9.acdlabs.ru:8100/WebLibrarian/index.html>. The application has tabs for 'Tree', 'Database', and 'Search Records'. Below these are navigation icons and a 'Record ID: 1 1/46' indicator. A 'UVIR' section is visible with a 'Spectrum Parameters' dropdown. A large 'Untitled - Message (Rich Text)' window is open, showing an email composition interface with fields for 'To...', 'Cc...', 'Bcc...', and 'Subject:'. The 'Subject' field contains a long URL: [http://acdlab9.acdlabs.ru:8100/WebLibrarian/index.html?connect\\_to=f:\webdb\data\uwis.nd5&layout=specmanAll&rec\\_id=1](http://acdlab9.acdlabs.ru:8100/WebLibrarian/index.html?connect_to=f:\webdb\data\uwis.nd5&layout=specmanAll&rec_id=1). Below the email composition area, a 'User Data' section displays the following information:

- FW: 473.4348
- Formula:  $C_{22}H_{16}N_3NaO_8S$
- Title: Acid Blue 40/ Alizarin Direct Blue A2G
- Solvent: Water
- Concentration: 61.8 mg /L
- Wavelength Range: 900-190 nm
- BP: cannot calculate
- SimCoeff: 0.127

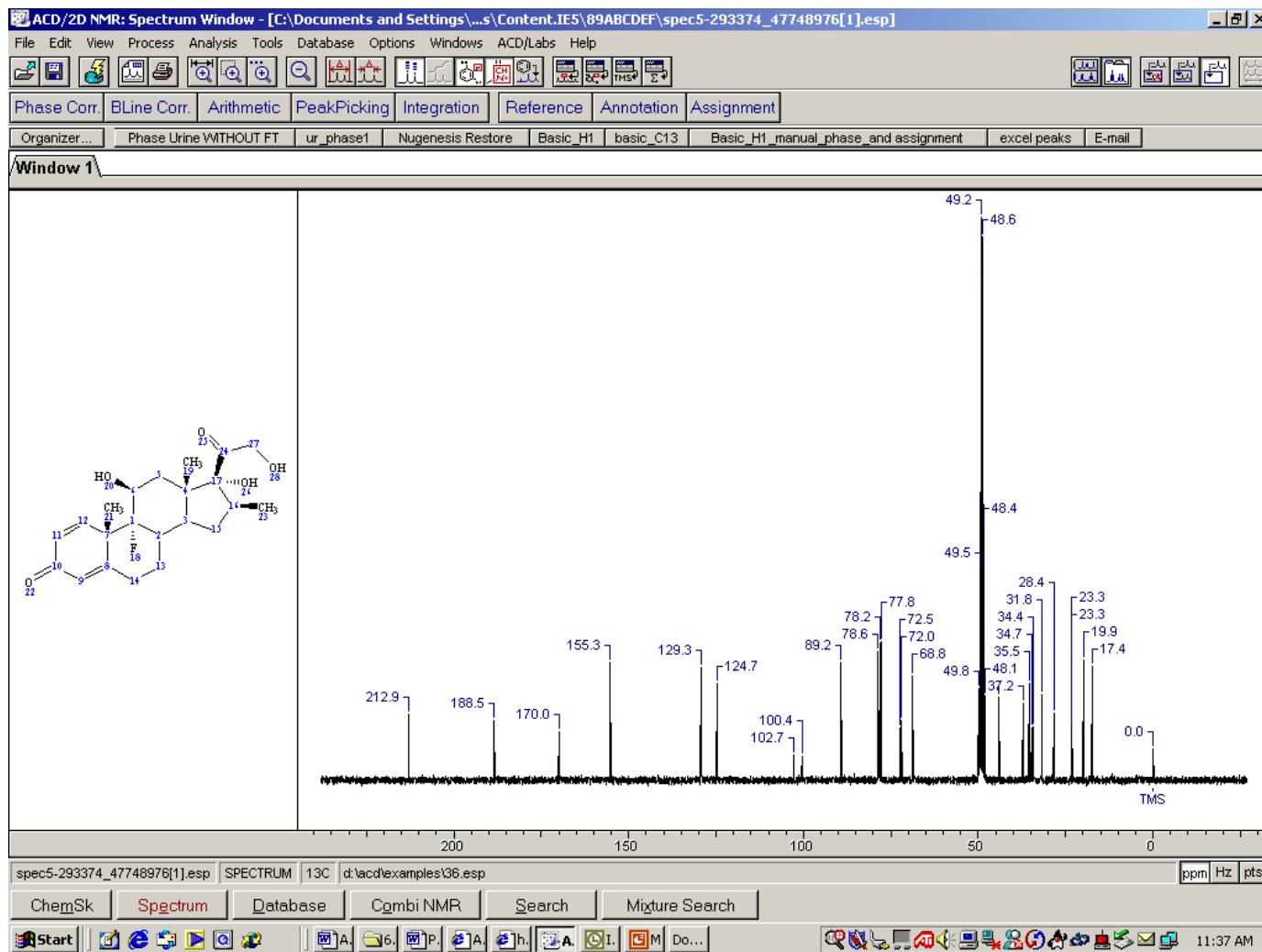
The bottom of the browser window shows the taskbar with various application icons and the system clock displaying 12:35 AM.



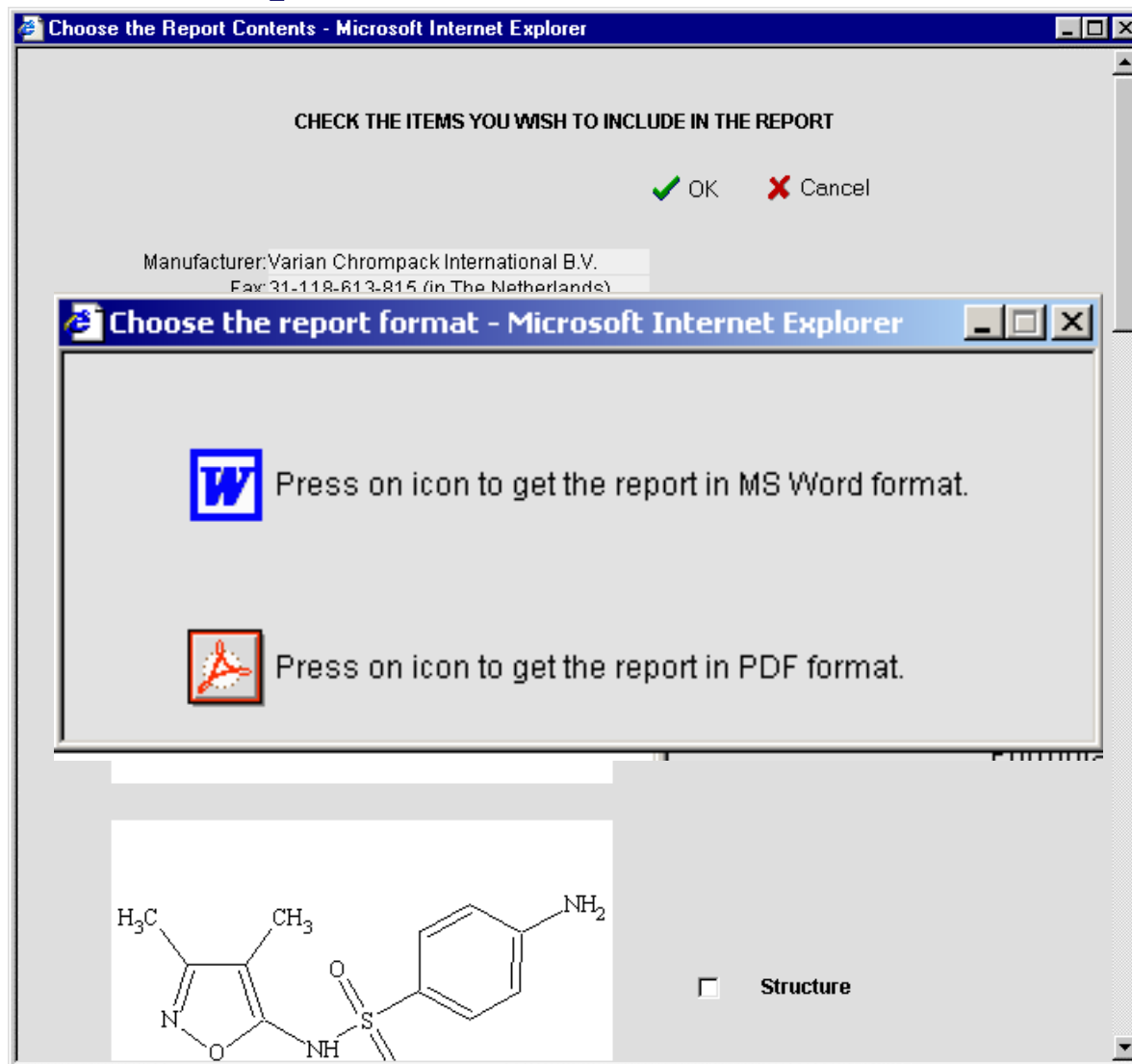
# Download Data



# Download Spectrum



# Report Generation



# Report Generation

RecReport9-575626\_1015937698[1].doc - Microsoft Word

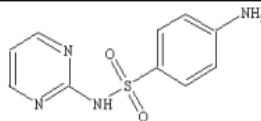
File Edit View Insert Format Tools Table Window Help

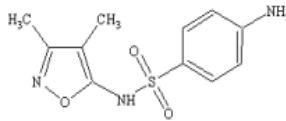
Normal Times New Roman 14 B I U

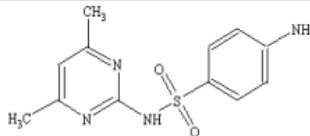
f:\webdb\data\Appl\_DB.nd5 Record ID: 1


**User Data**

Manufacturer	Varian Chrompack International B.V.
Fax	31-118-613-815 (in The Netherlands)
Technology	LC
Web site of vendor	<a href="http://www.varianinc.com/chrompack">http://www.varianinc.com/chrompack</a>
Column pH min	2.5
Column pH max	7.5









Page 1 Sec 1 1/2 At 0,7" Ln 1 Col 1 REC TRK EXT OVR English (U.S)

# ACD/Web Librarian

- ◆ A Thin-Client view of SpecManager (SQL)
- ◆ Fully searchable by usual ACD/Labs methods
- ◆ Ideal method by which to make enterprise reference databases accessible across the company
- ◆ Distribute ORACLE-based data via the web to analysts for downloading (comparison, reporting etc.)
- ◆ Full reporting capabilities

***Flexible, easy to maintain, easy to deploy!***

# What's Available Online? Overview

- ◆ Internet
  - I-Lab on the Internet
  - Live update
  - Tech support Live help
- ◆ Intranet
  - I-Lab
  - Structure-spectrum verification using I-Lab
  - Web Librarian
- ◆ **Extending the Technology to Enterprise Deployment (some examples)**

# Enterprise-Wide Integration

- ◆ Out-of-the-box ACD/Labs Tools
  - I-Lab (Intranet)
  - Web Librarian
  - MS-Windows® Platform
- ◆ ACD/Labs tools for integration
  - ActiveX Components
  - API
  - Batch programs for integration to registration systems or webifying
  - ACD/DLLs
- ◆ Integration directly managed and commercially proposed by ACD/Labs:  
MDL/ISIS Draw, Base and Host integration

# Conclusion

- ◆ Our Web Site is an incredible source of regularly updated informations
- ◆ We developped a lot of capabilities to be used on line
  - I-Lab
  - Updater
  - Access to support
- ◆ Most of this tools are usable on your Intranet for larger deployment