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Spectral Database Libraries: Creation, Management and Access in th

Larry Taylor, Ph
Bio-Rad Laboratories, Inc
Informatics Division
June 11th, 2002

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Sadtler Software & Databases

Bio-Rad Laboratories, Inc.
Informatics Division

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- Founded over 125 years ago (Sadtler Consulting Research Chemists).
- Dedicated to the development of software solutions for spectroscopy and chemical information.
- Developed the first fully integrated solution for spectroscopy information management.
- Part of Bio-Rad Laboratories, Inc. since 1979.
  - A multinational manufacturer and distributor of life science research products, clinical diagnostics and analytical instrumentation, based in Hercules, California.
  - Serves more than 70,000 research and industry customers worldwide through a network of more than 30 wholly owned subsidiary offices.
  - Sales for 2001 were $817.5 million, a 12.6% increase over 2000.

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Outline

- What is a spectral library?
- Benefits of spectral libraries
- Creation and architecture
- Managing change
- Build, purchase or subscribe?
- User interface and searching
- Adding value with database tools
- Wrap up

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What is a Spectral Library?

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- Spectral libraries used to be hard copy collections of spectra, structures and meta data.

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Spectral Library = Spectral Database

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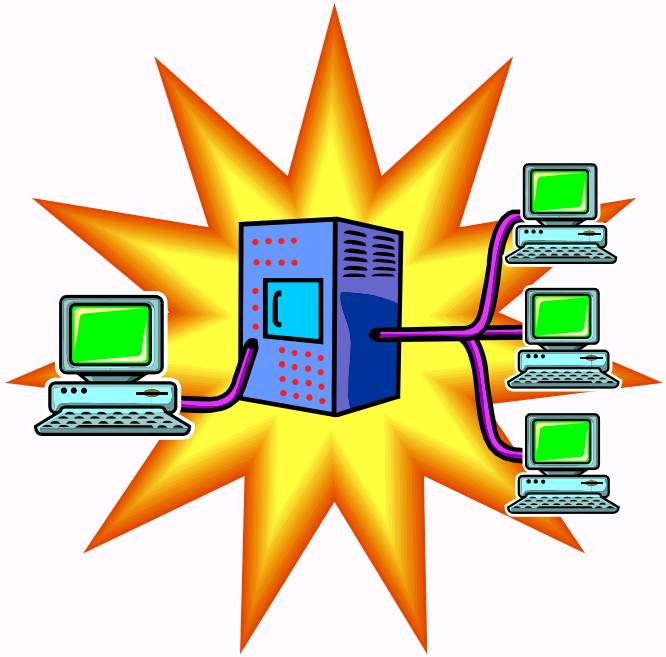
- Today a spectral library is a database made of:
  - Digitized spectra
  - Instrument parameters and conditions
  - Structures
  - Physical and chemical properties
  - Hyperlinks to other data sources



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Benefits of Digital Spectral Libraries

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- Secure and archive intellectual property
- Reduce physical storage space
- Improve searching speed
- Easier to update digital media
- Achieve goal to convert data to knowledge

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Path to Knowledge

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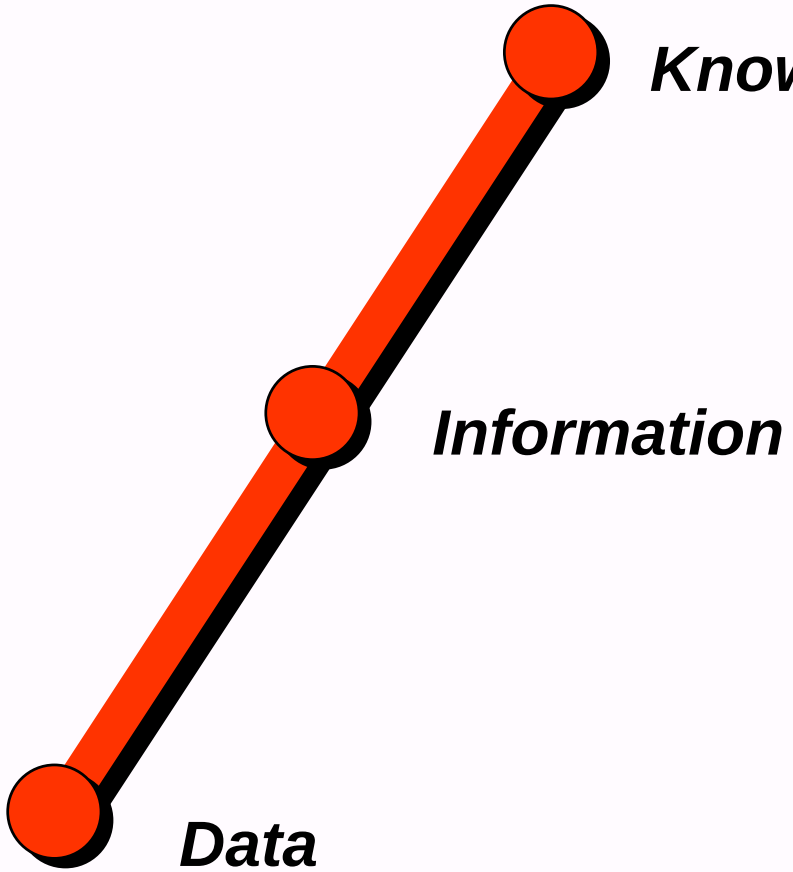

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Role of Digital Libraries

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Publishing Tools

Prediction Tools

Analysis Tools

Analytical Databases

Database Management System

Informatics Environment

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Creation of Spectral Databases

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- Can build, purchase or subscribe.
- To build a database:
  - Synthesize or buy chemicals
  - Prepare samples
  - Run spectra
  - Check quality
  - Refine (clean up) spectra
  - Publish and index
- In-house databases include reference & competitor materials, adulterants, novel or proprietary samples, contaminants, breakdown products, etc.

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Creation of Spectral Databases

- Can build from literature sources:
  - Digitize hard copies of spectra
  - Copy and paste from other sources
  - Create from published peak tables
  - Download spectra from Internet
- Issues for building databases
  - Variable quality of spectra collection
  - Variable ranges of spectra
  - Insufficient property information
  - Non-standard formats

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Creation of Spectral Databases

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- Comparison of built, purchased and subscribed databases
  - Subscribing and purchasing advantages:
    - leverages building cost among many consumers
    - frees internal resources for other tasks
    - in general quality is higher and less variable
  - Building your own database has a higher cost but more content critical to your organization
  - Subscribing is most cost-effective source
  - Best solution is a mix of subscribed data and your own data

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Creation of Spectral Databases

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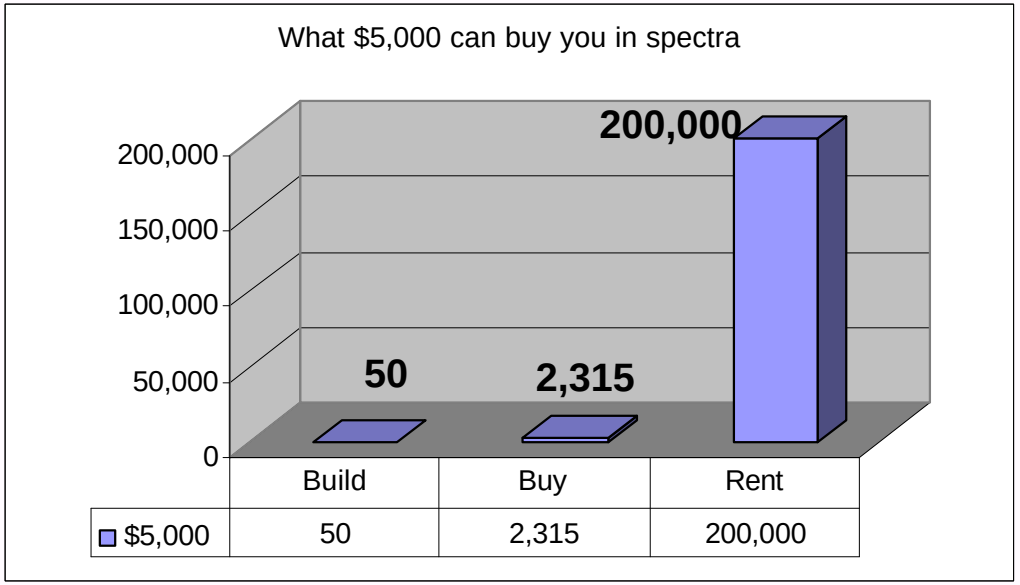
- Cost factors to consider when building
  - Obtaining samples or standards
  - Running and reviewing the spectra.
  - Sample tracking, storage and/or disposal.
  - Data entry (properties, structures, etc.).
  - Uniqueness of the material.
  - Uniqueness of the technique.



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Spectral Database Architecture

- Technology
  - Server, network, database and client
  - Use industry standards (MS, Oracle, etc.)
- Security and archival
  - Protect intellectual property
  - Choose data format carefully
- Design issues
  - Standard data formats
  - User interface
  - Search and cross-reference
  - Customization vs. Configurability

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Architecture and Design

- User interface:
  - Easy to use
  - Familiar to the most users possible
  - Short learning curve to reduce training
  - Common interface for all searches
- Database design:
  - Design database for spectral searching
  - Search by structure and sub-structure
  - Search meta data and indexes
  - Fast search engine speed
  - Build in cross-referencing

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User Interface Design

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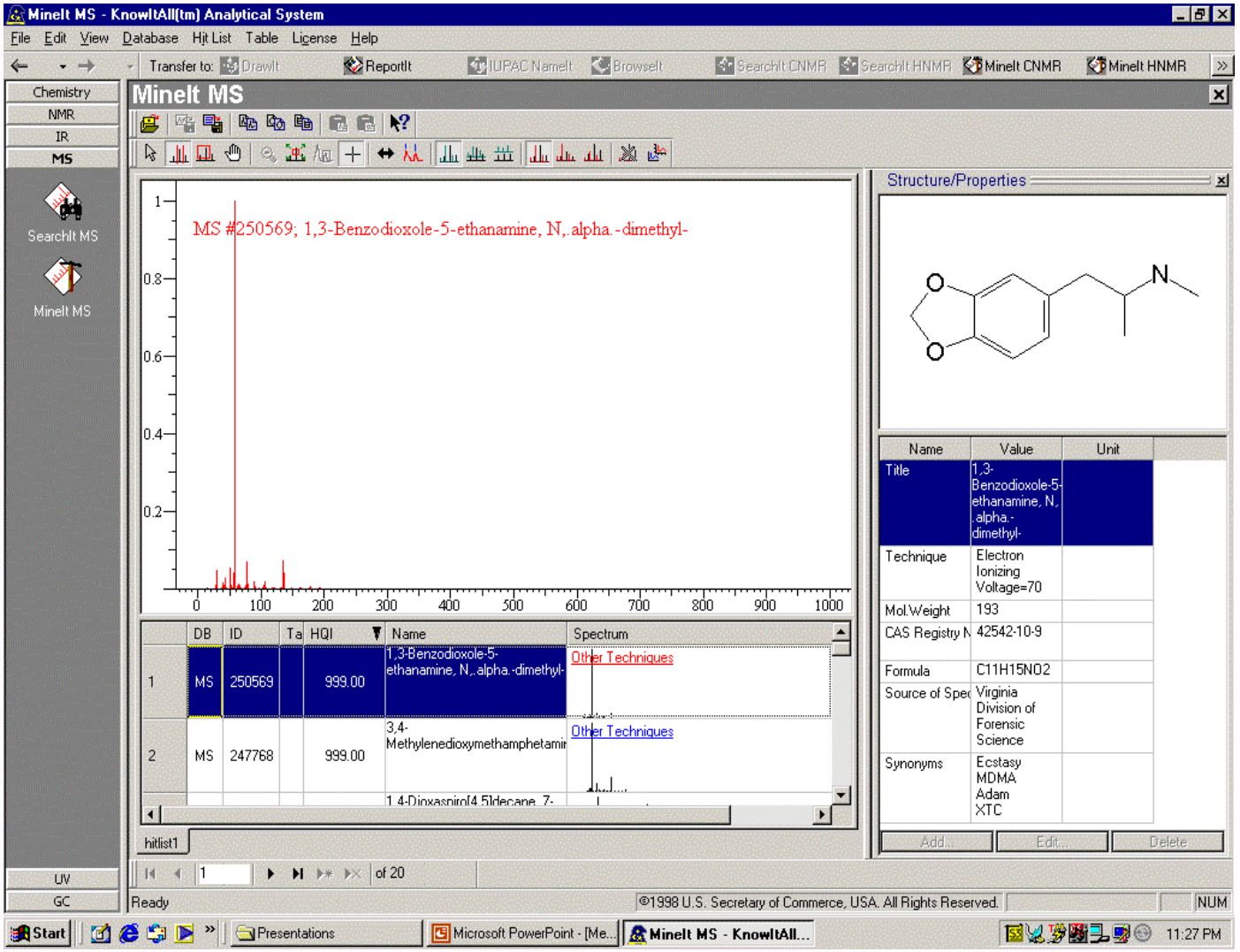

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System

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  - *Search meta data and indexes*
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  - Build in cross-referencing

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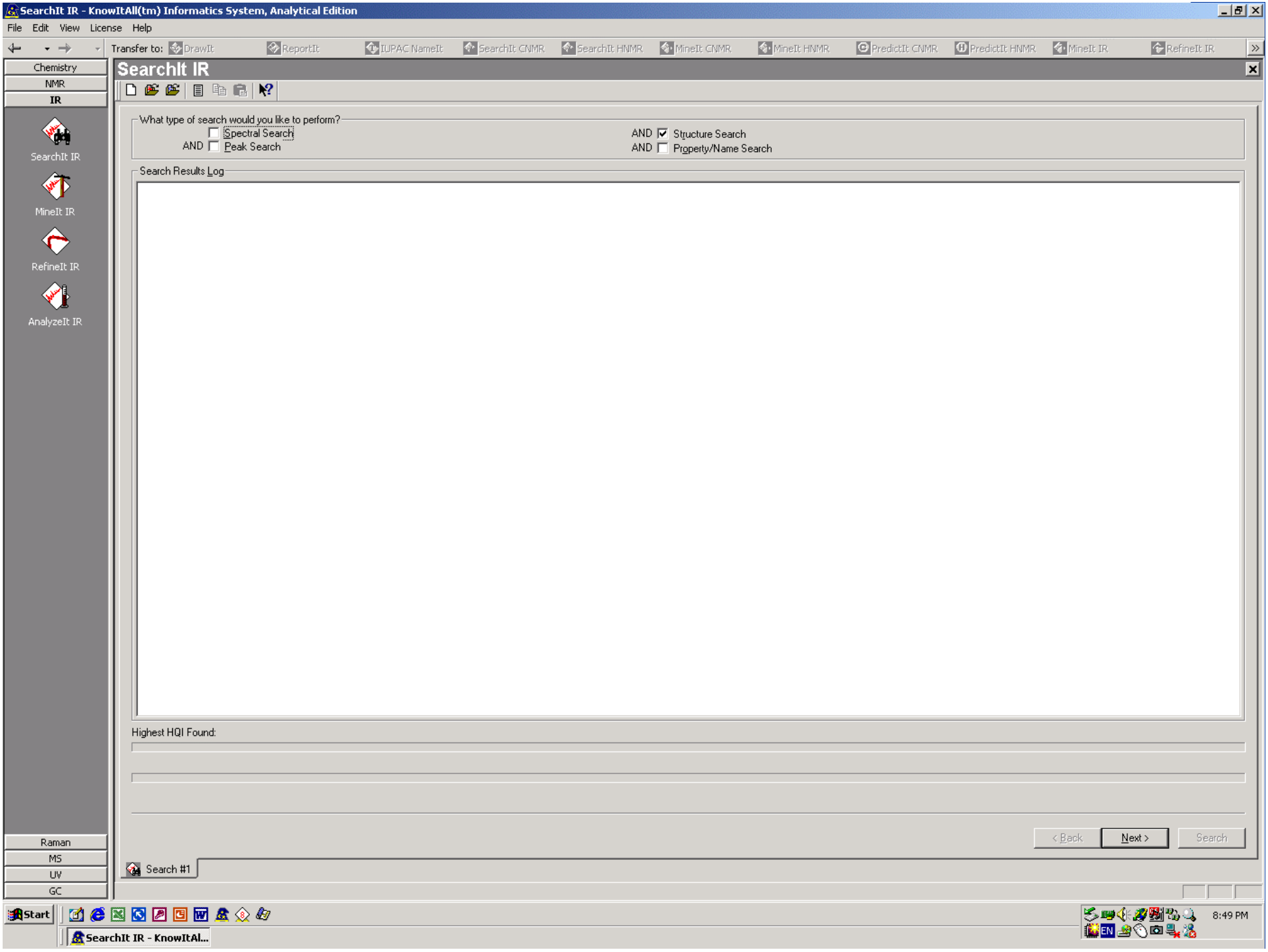
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Chemistry
NMR
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SearchIt IR
What type of search would you like to perform?
Spectral Search
AND Peak Search
AND Structure Search
AND Property/Name Search
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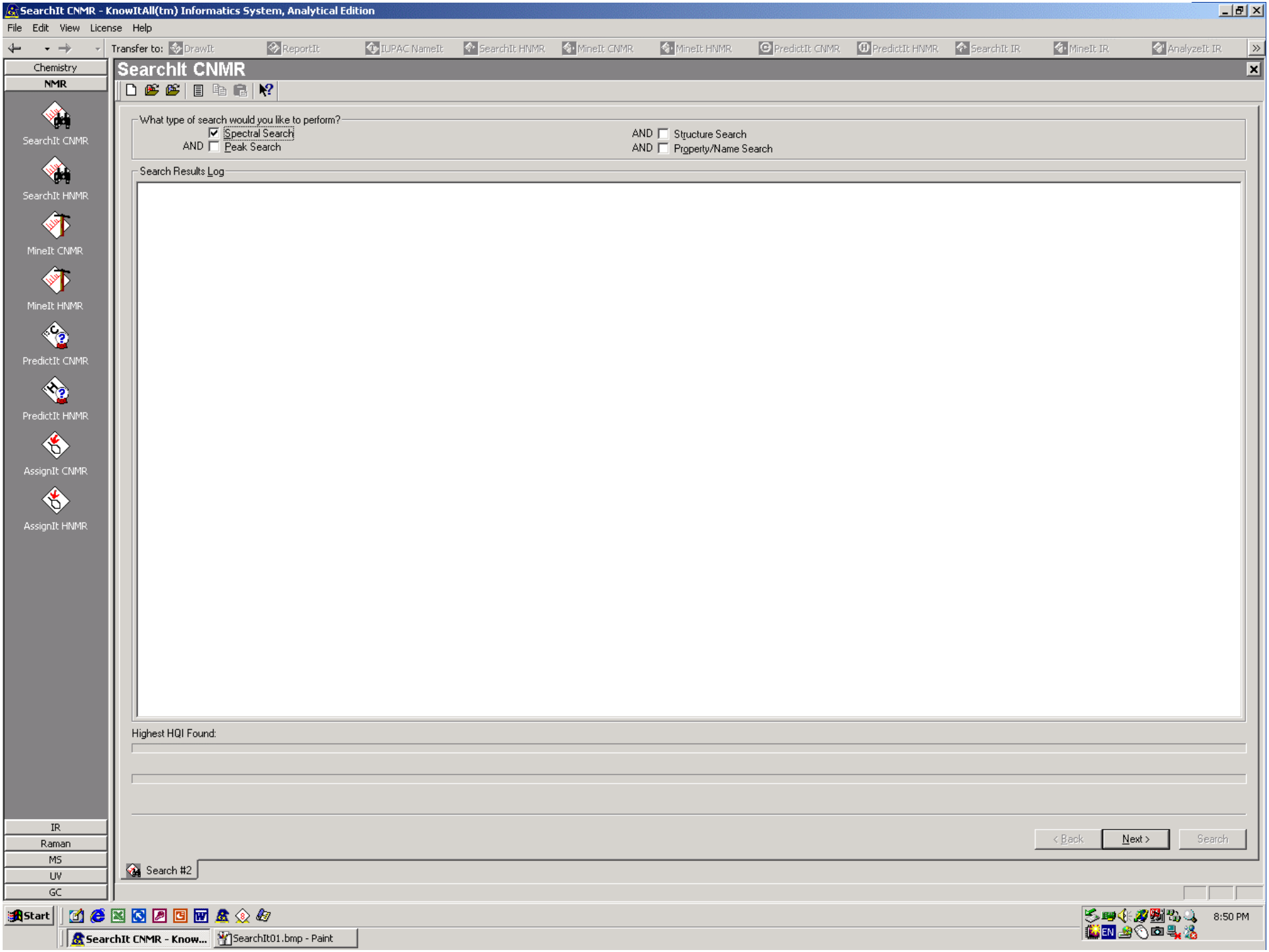
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AND Peak Search
AND Structure Search
AND Property/Name Search
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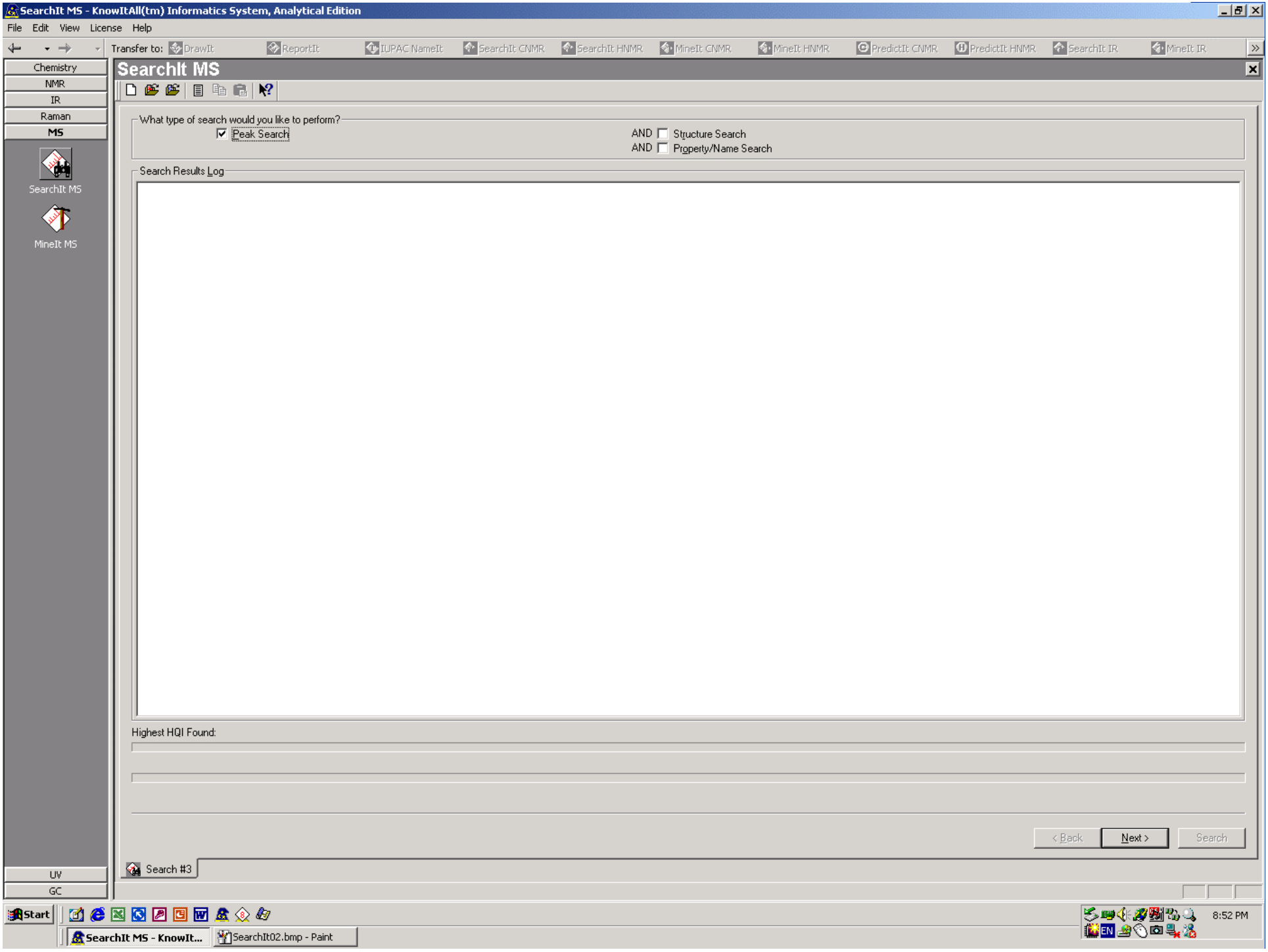
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AND Structure Search
AND Property/Name Search
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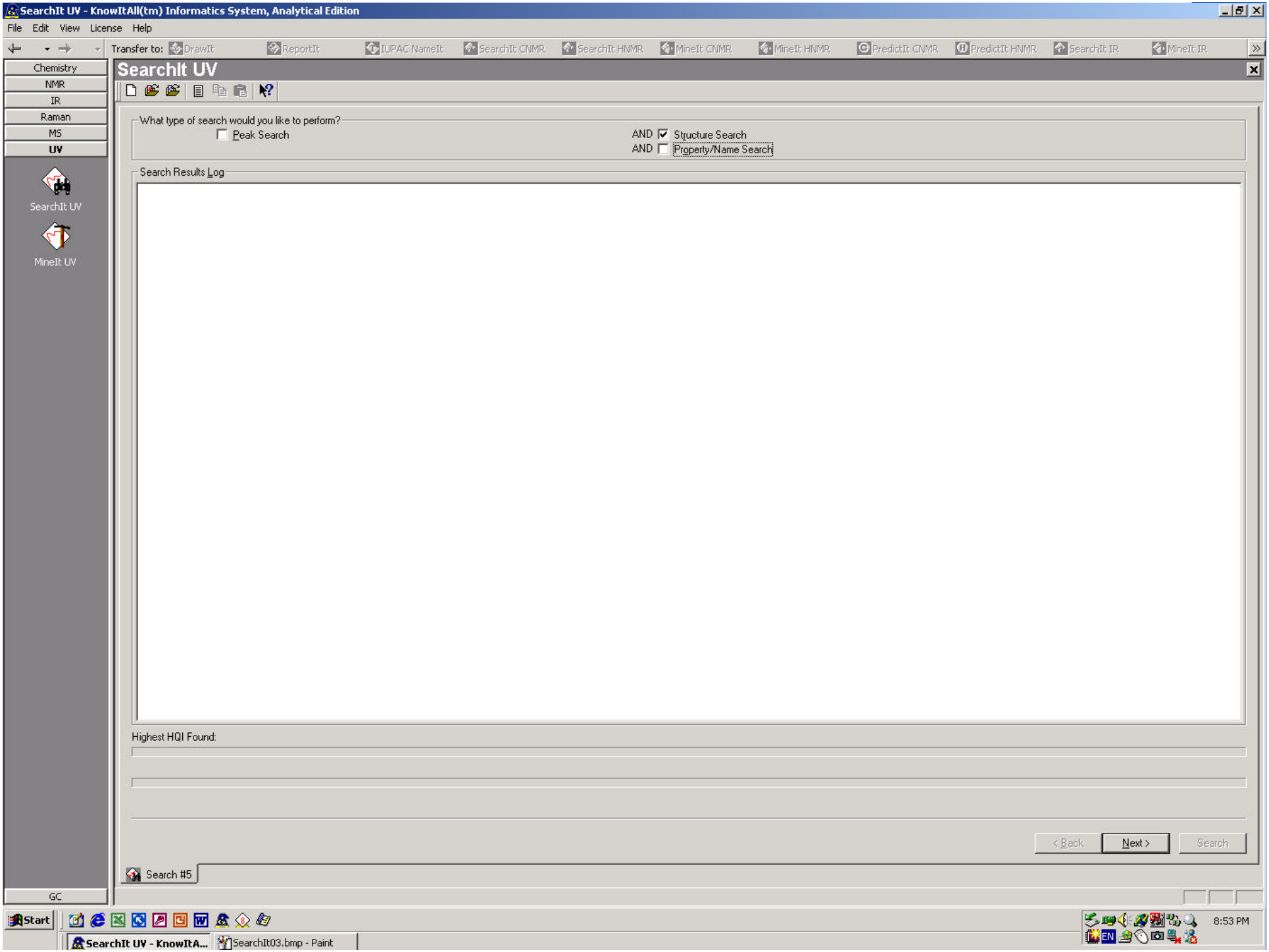
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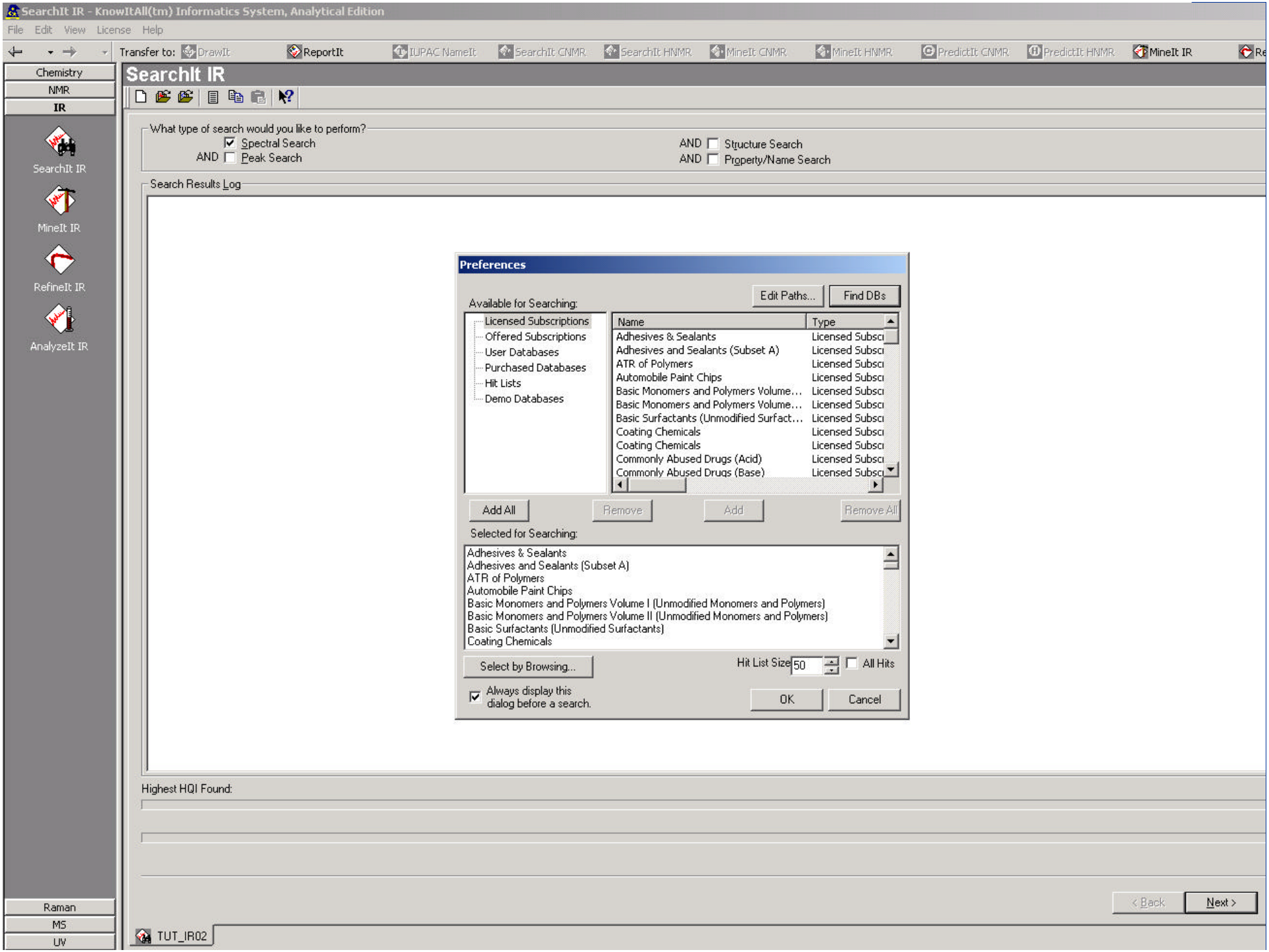
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What type of search would you like to perform?
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AND Peak Search
AND Structure Search
AND Property/Name Search
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Find DBs
Available for Searching:
Licensed Subscriptions
Offered Subscriptions
User Databases
Purchased Databases
Hit Lists
Demo Databases
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Adhesives and Sealants (Subset A)
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Automobile Paint Chips
Basic Monomers and Polymers Volume...
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Basic Monomers and Polymers Volume II (Unmodified Monomers and Polymers)
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Build in Cross-Referencing

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- Maximize your investment in multiple types of analytical instruments by organizing data together easily
- Provide links to data from different sources or labs with different expertise (QC, incoming materials, testing)
- Provide access to additional property information in each data type whether or not a particular lab or user created it
- *Examples of cross-referencing spectra*

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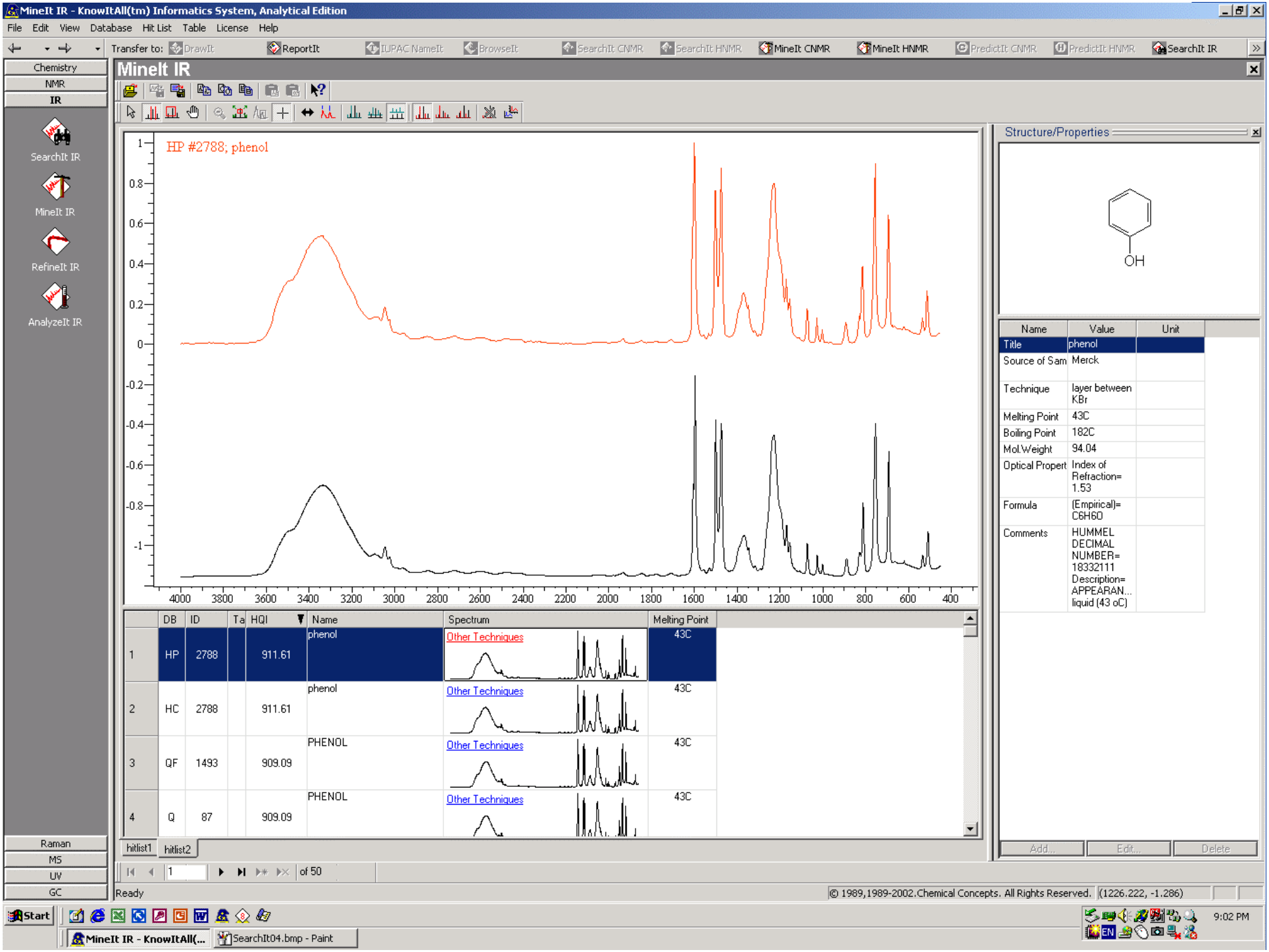
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-0.6
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-1
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DB ID Ta HQI Name Spectrum Melting Point
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2 HC 2788 911.61 phenol Other Techniques 43C
3 QF 1493 909.09 PHENOL Other Techniques 43C
4 Q 87 909.09 PHENOL Other Techniques 43C
hitlist1 hitlist2
1 of 50
Structure/Properties
OH
Name Value Unit
Title phenol
Source of Sam Merck
Technique layer between KBr
Melting Point 43C
Boiling Point 182C
Mol.Weight 94.04
Optical Propert Index of Refraction= 1.53
Formula (Empirical)= C6H6O
Comments HUMMEL DECIMAL NUMBER= 18332111 Description= APPEARAN... liquid (43 oC)
Add... Edit... Delete
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© 1989,1989-2002.Chemical Concepts. All Rights Reserved.
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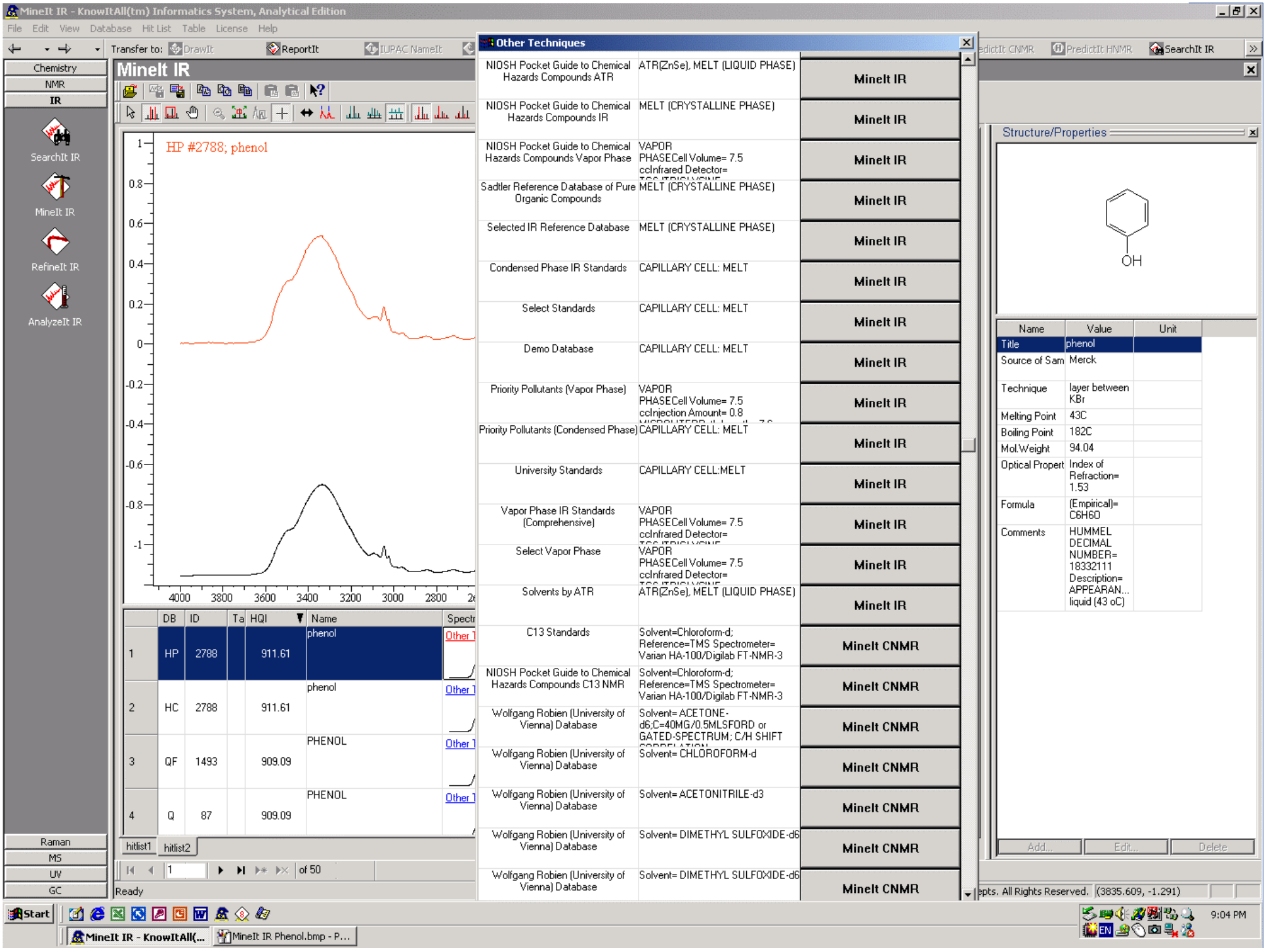
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2 HC 2788 911.61 phenol Other T
3 QF 1493 909.09 PHENOL Other T
4 Q 87 909.09 PHENOL Other T
hitlist1 hitlist2
1 of 50
Ready
Other Techniques
NIOSH Pocket Guide to Chemical Hazards Compounds ATR
ATR(ZnSe), MELT (LIQUID PHASE)
MineIt IR
NIOSH Pocket Guide to Chemical Hazards Compounds IR
MELT (CRYSTALLINE PHASE)
MineIt IR
NIOSH Pocket Guide to Chemical Hazards Compounds Vapor Phase
VAPOR PHASECell Volume= 7.5 ccInfrared Detector=
MineIt IR
Sadtler Reference Database of Pure Organic Compounds
MELT (CRYSTALLINE PHASE)
MineIt IR
Selected IR Reference Database
MELT (CRYSTALLINE PHASE)
MineIt IR
Condensed Phase IR Standards
CAPILLARY CELL: MELT
MineIt IR
Select Standards
CAPILLARY CELL: MELT
MineIt IR
Demo Database
CAPILLARY CELL: MELT
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Priority Pollutants (Vapor Phase)
VAPOR PHASECell Volume= 7.5 ccInjection Amount= 0.8
MineIt IR
Priority Pollutants (Condensed Phase)
CAPILLARY CELL: MELT
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University Standards
CAPILLARY CELL:MELT
MineIt IR
Vapor Phase IR Standards (Comprehensive)
VAPOR PHASECell Volume= 7.5 ccInfrared Detector=
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Select Vapor Phase
VAPOR PHASECell Volume= 7.5 ccInfrared Detector=
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Solvents by ATR
ATR(ZnSe), MELT (LIQUID PHASE)
MineIt IR
C13 Standards
Solvent=Chloroform-d; Reference=TMS Spectrometer= Varian HA-100/Digilab FT-NMR-3
MineIt CNMR
NIOSH Pocket Guide to Chemical Hazards Compounds C13 NMR
Solvent=Chloroform-d; Reference=TMS Spectrometer= Varian HA-100/Digilab FT-NMR-3
MineIt CNMR
Wolfgang Robien (University of Vienna) Database
Solvent= ACETONE-d6;C=40MG/0.5MLSFORD or GATED-SPECTRUM; C/H SHIFT
MineIt CNMR
Wolfgang Robien (University of Vienna) Database
Solvent= CHLOROFORM-d
MineIt CNMR
Wolfgang Robien (University of Vienna) Database
Solvent= ACETONITRILE-d3
MineIt CNMR
Wolfgang Robien (University of Vienna) Database
Solvent= DIMETHYL SULFOXIDE-d6
MineIt CNMR
Wolfgang Robien (University of Vienna) Database
Solvent= DIMETHYL SULFOXIDE-d6
MineIt CNMR
Structure/Properties
OH
Name Value Unit
Title phenol
Source of Sam Merck
Technique layer between KBr
Melting Point 43C
Boiling Point 182C
Mol.Weight 94.04
Optical Propert Index of Refraction= 1.53
Formula (Empirical)= C6H6O
Comments HUMMEL DECIMAL NUMBER= 18332111 Description= APPEARAN... liquid (43 oC)
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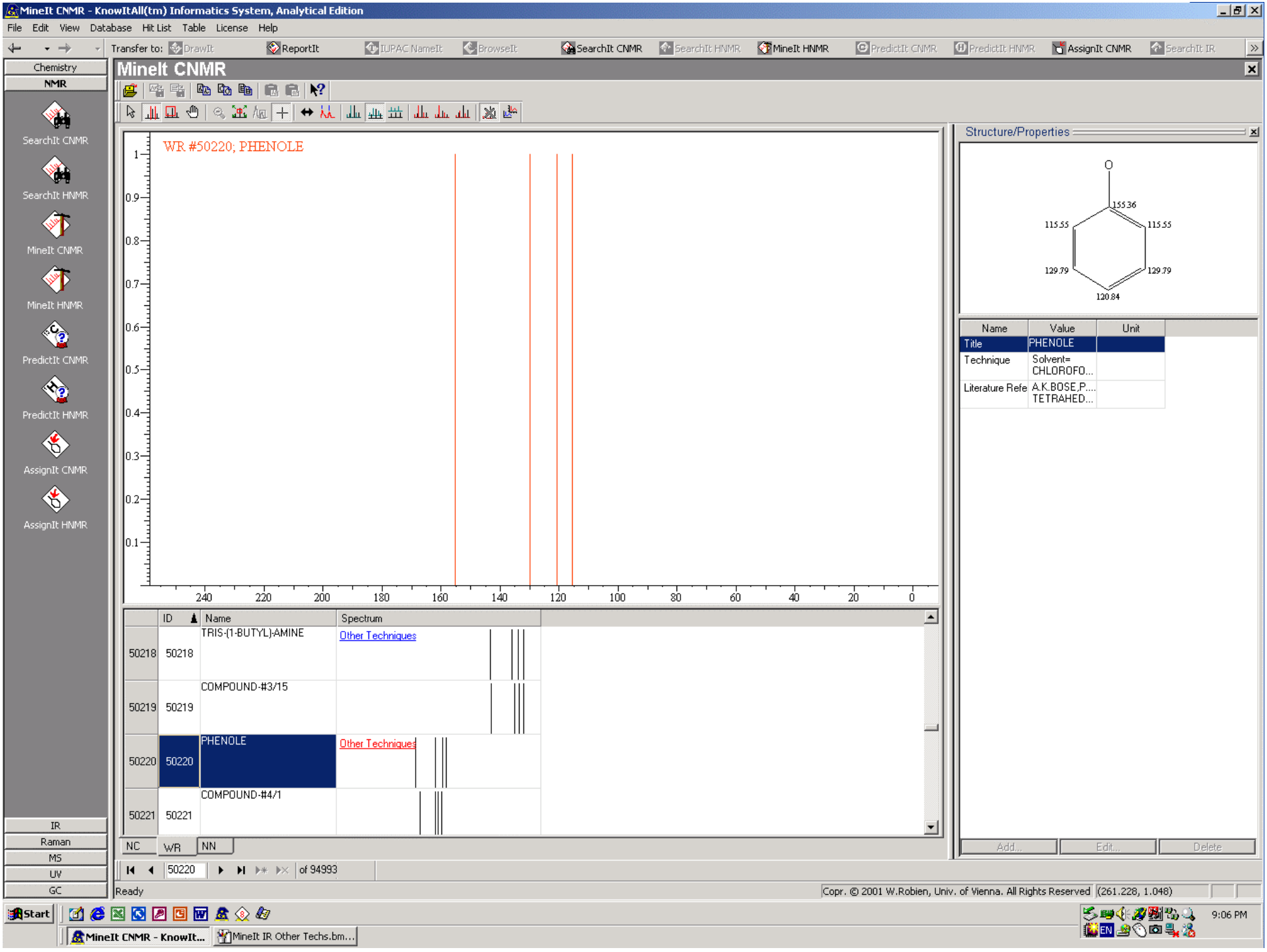
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240 220 200 180 160 140 120 100 80 60 40 20 0
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50218 50218 TRIS-(1-BUTYL)-AMINE Other Techniques
50219 50219 COMPOUND-#3/15
50220 50220 PHENOLE Other Techniques
50221 50221 COMPOUND-#4/1
NC WR NN
50220 of 94993
Structure/Properties
O
155.36
115.55
115.55
129.79
129.79
120.84
Name Value Unit
Title PHENOLE
Technique Solvent= CHLOROFO...
Literature Refe A.K.BOSE,P.... TETRAHED...
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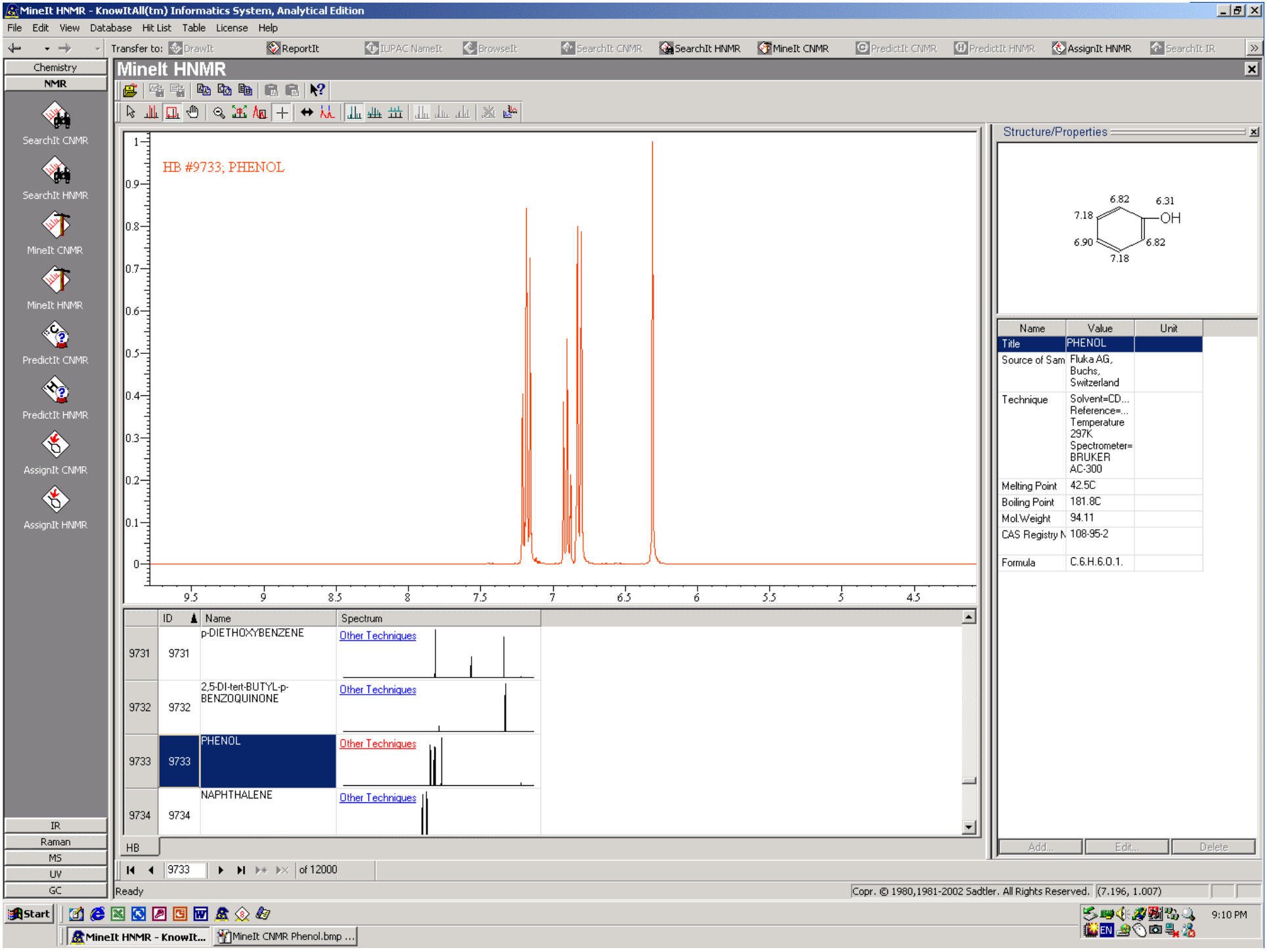
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Other Techniques
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Structure/Properties
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Name
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Unit
Title
PHENOL
Source of Sam
Fluka AG, Buchs, Switzerland
Technique
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Melting Point
42.5C
Boiling Point
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Mol.Weight
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CAS Registry N
108-95-2
Formula
C.6.H.6.O.1.
Add...
Edit...
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Ready
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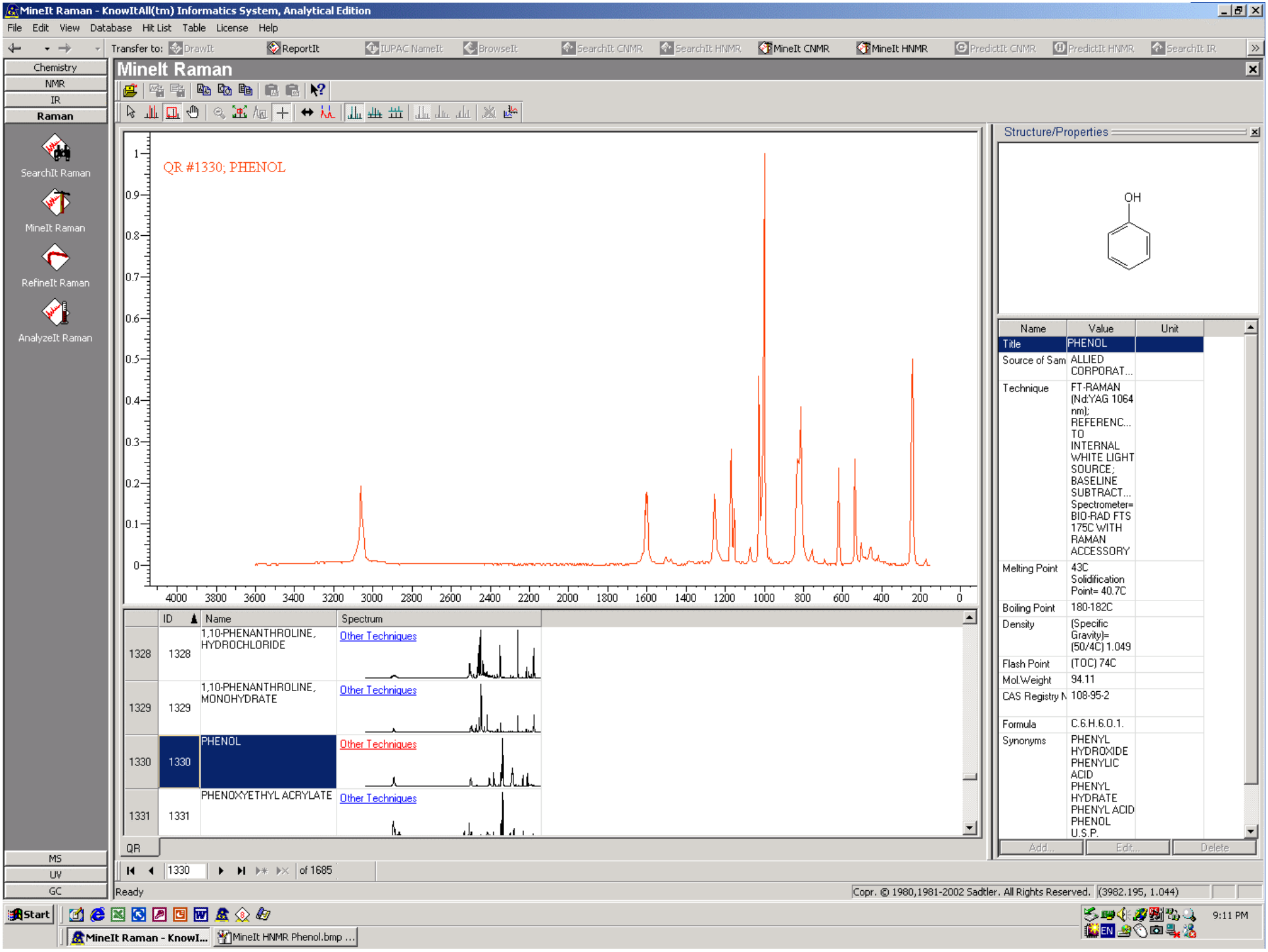
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1328 1328 1,10-PHENANTHROLINE, HYDROCHLORIDE Other Techniques
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1331 1331 PHENOXYETHYL ACRYLATE Other Techniques
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Structure/Properties
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Melting Point 43C Solidification Point= 40.7C
Boiling Point 180-182C
Density (Specific Gravity)= (50/4C) 1.049
Flash Point (TOC) 74C
Mol.Weight 94.11
CAS Registry N 108-95-2
Formula C.6.H.6.O.1.
Synonyms PHENYL HYDROXIDE PHENYLIC ACID PHENYL HYDRATE PHENYL ACID PHENOL U.S.P.
Add... Edit... Delete
Ready
Copr. © 1980,1981-2002 Sadtler. All Rights Reserved. (3982.195, 1.044)
Start
MineIt Raman - KnowI...
MineIt HNMR Phenol.bmp ...
9:11 PM

KnowItAll™
Informatics
System

Spectral Database Management

- Change management process will:
  - Manage adding, changing and deleting data
  - Control who has access
  - Manage updating of database and user interface technology
  - Manage user training
- Database lifecycle

BIO-RAD

Informatics Division
Sadtler Software & Databases

Database lifecycle

KnowItAll™
Informatics
System

BIO-RAD

Informatics Division
Sadtler Software & Databases

Database tools

KnowItAll™
Informatics
System

- Refine spectra baselines, remove noise, pick peaks, smooth spectra
- Analyze spectra to identify peaks and determine structure
- Predict spectra and properties from structures
- Assign shift, functional group and masses to spectral peaks

BIO-RAD

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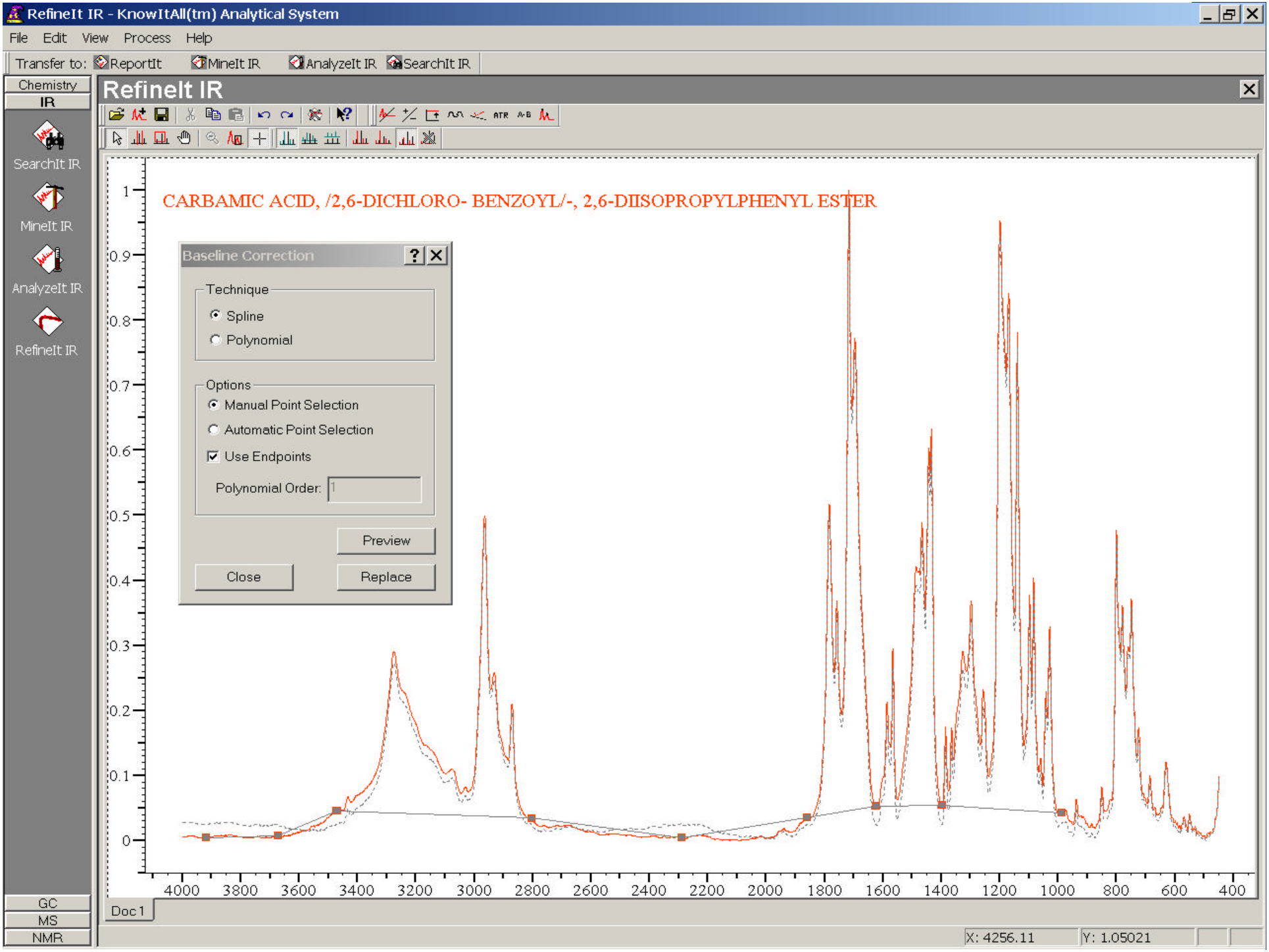
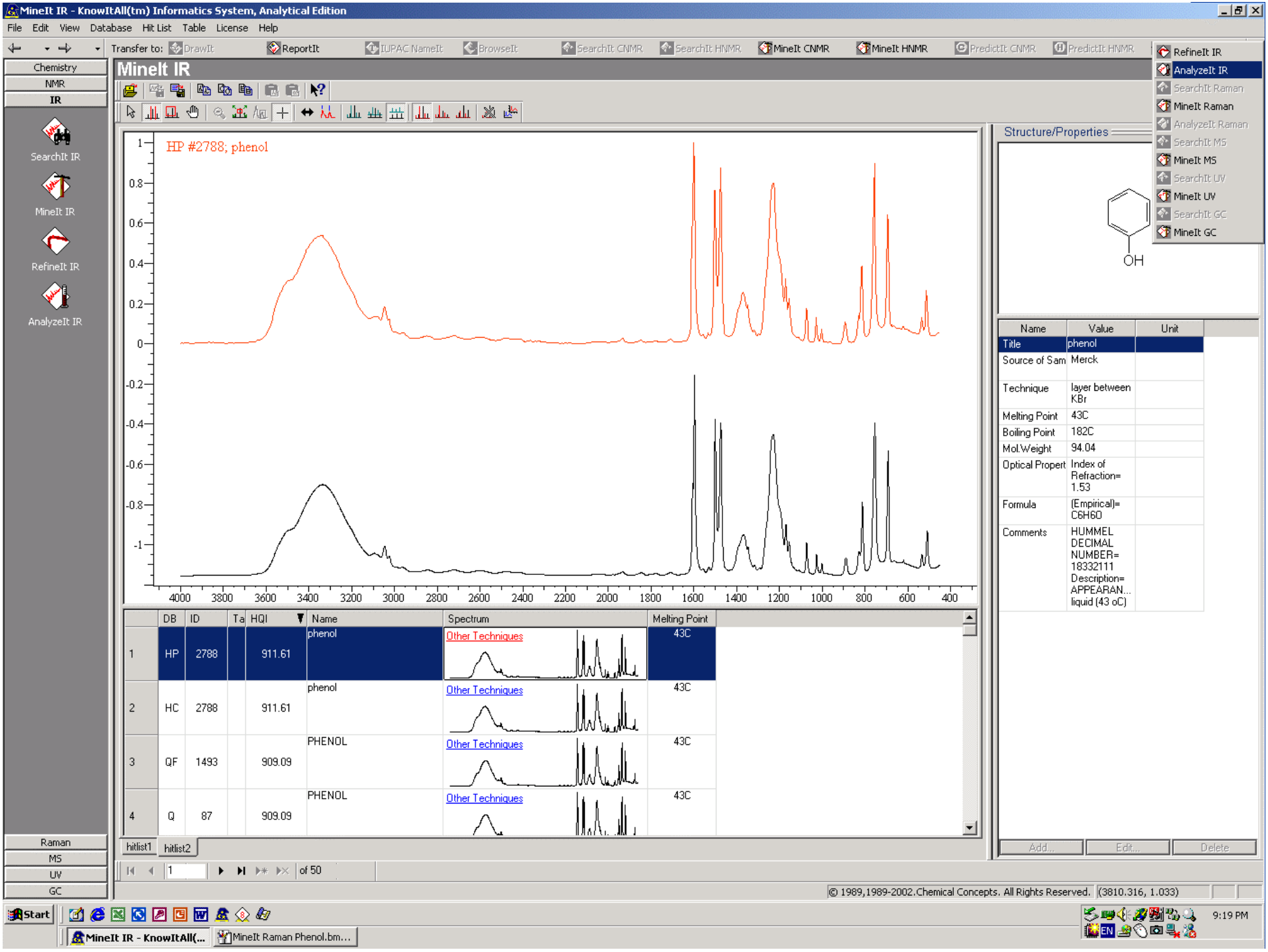
Sadtler Software & Databases


RefineIt IR - KnowItAll(tm) Analytical System
File Edit View Process Help
Transfer to: ReportIt MineIt IR AnalyzeIt IR SearchIt IR
Chemistry
IR
SearchIt IR
MineIt IR
AnalyzeIt IR
RefineIt IR
GC
MS
NMR
RefineIt IR
CARBAMIC ACID, /2,6-DICHLORO- BENZOYL/-, 2,6-DIISOPROPYLPHENYL ESTER
Baseline Correction
Technique
Spline
Polynomial
Options
Manual Point Selection
Automatic Point Selection
Use Endpoints
Polynomial Order: 1
Preview
Close
Replace
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
4000 3800 3600 3400 3200 3000 2800 2600 2400 2200 2000 1800 1600 1400 1200 1000 800 600 400
Doc 1
X: 4256.11
Y: 1.05021


MineIt IR - KnowItAll(tm) Informatics System, Analytical Edition
File Edit View Database Hit List Table License Help
Transfer to: DrawIt ReportIt IUPAC NameIt BrowseIt SearchIt CNMR SearchIt HNMR MineIt CNMR MineIt HNMR PredictIt CNMR PredictIt HNMR
RefineIt IR
AnalyzeIt IR
SearchIt Raman
MineIt Raman
AnalyzeIt Raman
SearchIt MS
MineIt MS
SearchIt UV
MineIt UV
SearchIt GC
MineIt GC
Chemistry
NMR
IR
SearchIt IR
MineIt IR
RefineIt IR
AnalyzeIt IR
Raman
MS
UV
GC
MineIt IR
HP #2788; phenol
Structure/Properties
OH
Name Value Unit
Title phenol
Source of Sam Merck
Technique layer between KBr
Melting Point 43C
Boiling Point 182C
Mol.Weight 94.04
Optical Propert Index of Refraction= 1.53
Formula (Empirical)= C6H6O
Comments HUMMEL DECIMAL NUMBER= 18332111 Description= APPEARAN... liquid (43 oC)
Add... Edit... Delete
DB ID Ta HQI Name Spectrum Melting Point
1 HP 2788 911.61 phenol Other Techniques 43C
2 HC 2788 911.61 phenol Other Techniques 43C
3 QF 1493 909.09 PHENOL Other Techniques 43C
4 Q 87 909.09 PHENOL Other Techniques 43C
hitlist1 hitlist2
of 50
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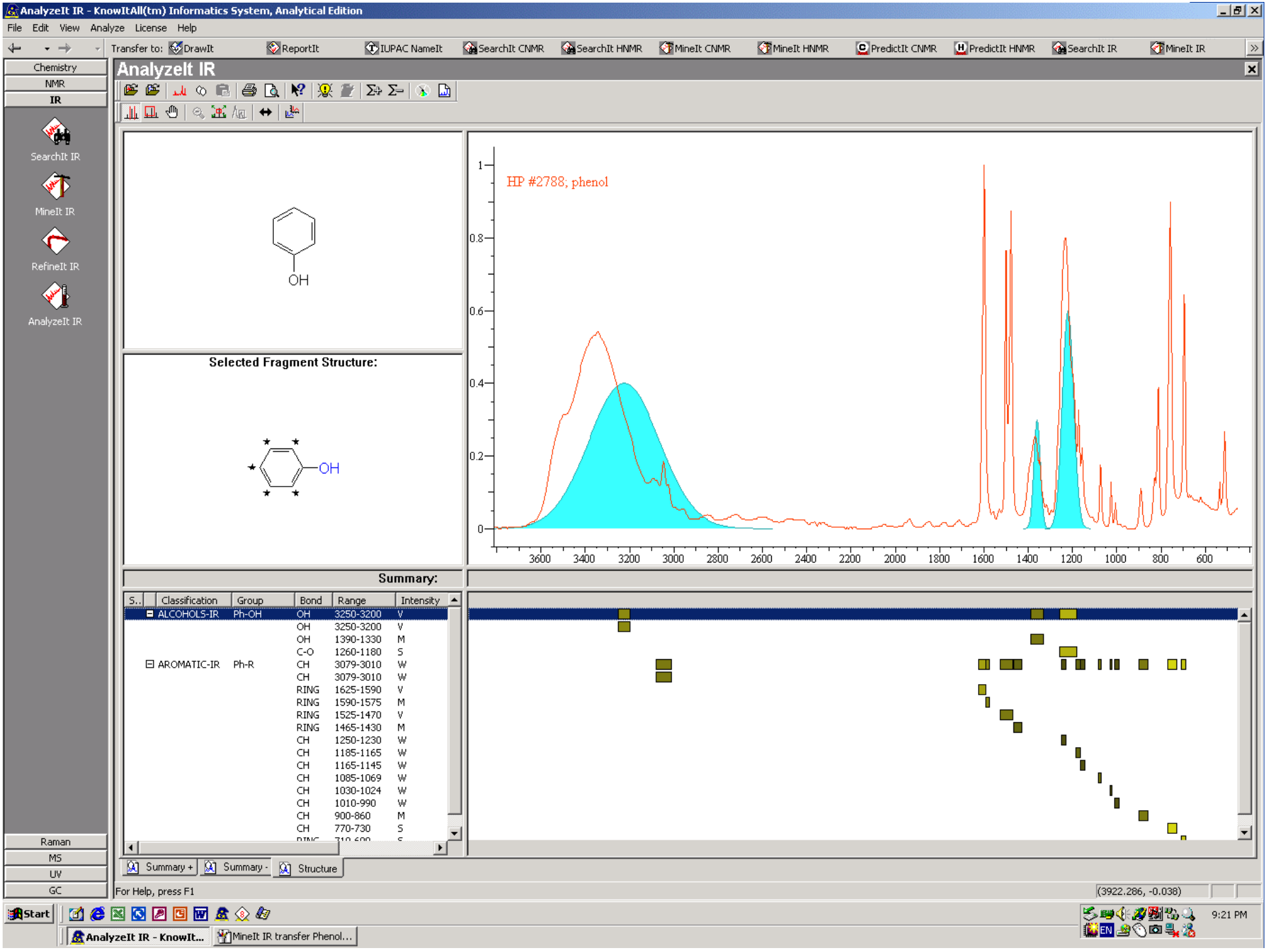
(3810.316, 1.033)
Start
MineIt IR - KnowItAll(...
MineIt Raman Phenol.bm...
9:19 PM


AnalyzeIt IR - KnowItAll(tm) Informatics System, Analytical Edition
File Edit View Analyze License Help
Transfer to: DrawIt ReportIt IUPAC NameIt SearchIt CNMR SearchIt HNMR MineIt CNMR MineIt HNMR PredictIt CNMR PredictIt HNMR SearchIt IR MineIt IR
Chemistry
NMR
IR
SearchIt IR
MineIt IR
RefineIt IR
AnalyzeIt IR
Raman
MS
UV
GC
AnalyzeIt IR
OH
Selected Fragment Structure:
OH
HP #2788; phenol
1
0.8
0.6
0.4
0.2
0
3600 3400 3200 3000 2800 2600 2400 2200 2000 1800 1600 1400 1200 1000 800 600
Summary:
S.. Classification Group Bond Range Intensity
ALCOHOLS-IR Ph-OH OH 3250-3200 V
OH 3250-3200 V
OH 1390-1330 M
C-O 1260-1180 S
AROMATIC-IR Ph-R CH 3079-3010 W
CH 3079-3010 W
RING 1625-1590 V
RING 1590-1575 M
RING 1525-1470 V
RING 1465-1430 M
CH 1250-1230 W
CH 1185-1165 W
CH 1165-1145 W
CH 1085-1069 W
CH 1030-1024 W
CH 1010-990 W
CH 900-860 M
CH 770-730 S
Summary + Summary - Structure
For Help, press F1
(3922.286, -0.038)
Start
AnalyzeIt IR - KnowIt...
MineIt IR transfer Phenol...
9:21 PM

PredictIt CNMR - KnowItAll(tm) Informatics System, Analytical Edition

File Edit View License Help

Transfer to: DrawIt ReportIt IUPAC NameIt SearchIt CNMR SearchIt HNMR MineIt CNMR MineIt HNMR PredictIt HNMR SearchIt IR MineIt IR AnalyzeIt IR

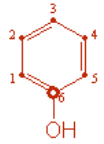
Chemistry
NMR
SearchIt CNMR
SearchIt HNMR
MineIt CNMR
MineIt HNMR
PredictIt CNMR
PredictIt HNMR
AssignIt CNMR
AssignIt HNMR
IR
Raman
MS
UV
GC

PredictIt CNMR

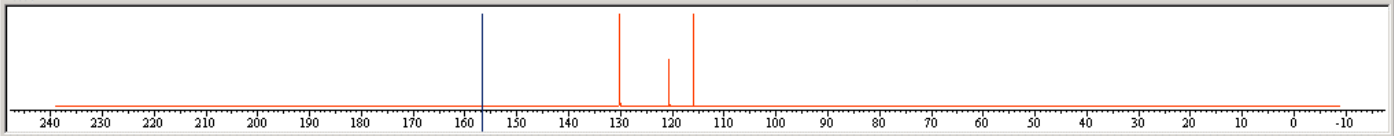
All Solvents

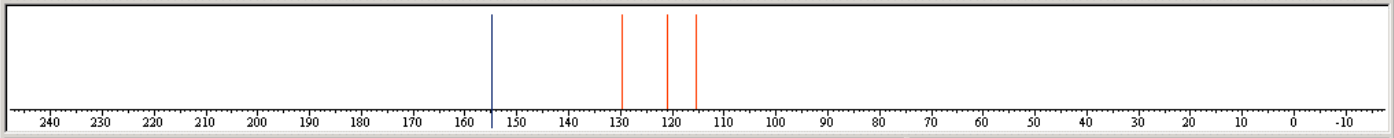
- 130.15±0.58(17)
- 120.62±1.27(17)
- 130.15±0.58(17)
- 115.93±0.55(17)
- 115.93±0.55(17)
- 156.73±1.90(17)
  - * 156.73±1.90(17)
    - 151.80
    - 154.80
    - 154.90
    - 155.00
    - 155.36
    - 155.50
    - 156.40
    - 157.19
    - 157.34
    - 157.90
    - 158.00
    - 158.10
    - 158.24
    - 158.30
    - 158.50
    - 158.58
    - 158.58
  - 4 Double Click to Load
  - 3 Double Click to Load
  - 2 Double Click to Load
  - 1 Double Click to Load

Predicted Shift Information

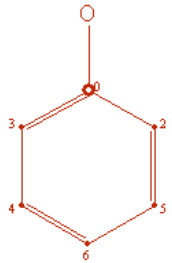


ID	Shift	Multiplicity
1	115.93	s
2	130.15	s
3	120.62	s
4	130.15	s
5	115.93	s
6	156.73	s





Source: WR36092
Solvent: UNKNOWN



ID	Shift
0	154.90
2	115.40
3	115.40
4	129.70
5	129.70
6	121.00

Selected Database Record

Search Record 1

Ready

Start PredictIt CNMR - Know... AnalyzeIt IR Phenol.bmp ... 9:24 PM

PredictIt HNMR - KnowItAll(tm) Informatics System, Analytical Edition

File Edit View License Help

Transfer to: DrawIt ReportIt IUPAC NameIt SearchIt CNMR SearchIt HNMR MineIt CNMR MineIt HNMR PredictIt CNMR SearchIt IR MineIt IR AnalyzeIt IR

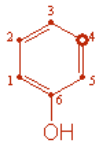
Chemistry
NMR
SearchIt CNMR
SearchIt HNMR
MineIt CNMR
MineIt HNMR
PredictIt CNMR
PredictIt HNMR
AssignIt CNMR
AssignIt HNMR
IR
Raman
MS
UV
GC

PredictIt HNMR

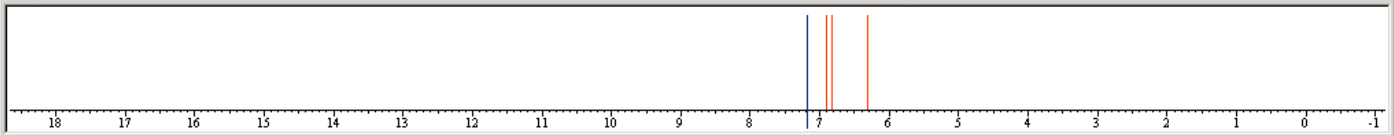
All Solvents

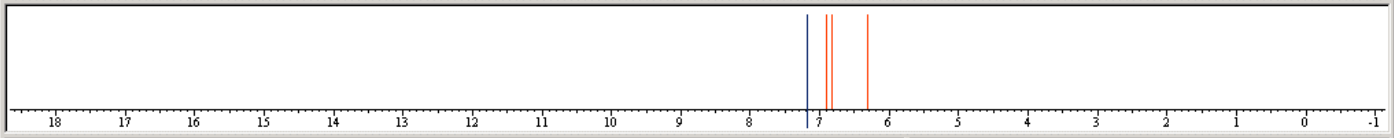
- 6.82±0.00(1)
- 7.18±0.00(1)
- 6.90±0.00(1)
- 7.18±0.00(1)
  - * 7.18±0.00(1)
    - 7.18
    - 4 Double Click to Load
    - 3 Double Click to Load
    - 2 Double Click to Load
    - 1 Double Click to Load
- 6.82±0.00(1)
- 6.31±0.00(1)

Predicted Shift Information

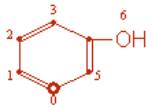


ID	Shift
1	6.82
2	7.18
3	6.90
4	7.18
5	6.82
6	6.31





Source: HB9733
Solvent: CDCl3



ID	Shift
0	7.18
1	6.90
2	7.18
3	6.82
5	6.82
6	6.31

Selected Database Record

Search Record 1 Search Record 2

Ready

Start

PredictIt HNMR - Know... PredictIt CNMR Phenol.b...

9:26 PM

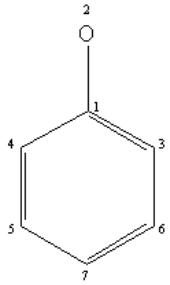
AssignIt CNMR - KnowItAll(tm) Informatics System, Analytical Edition

File Edit View License Help

Return to: MineIt CNMR and Save | MineIt CNMR and Discard

Chemistry
NMR
SearchIt CNMR
SearchIt HNMR
MineIt CNMR
MineIt HNMR
PredictIt CNMR
PredictIt HNMR
AssignIt CNMR
AssignIt HNMR
IR
Raman
MS
UV
GC

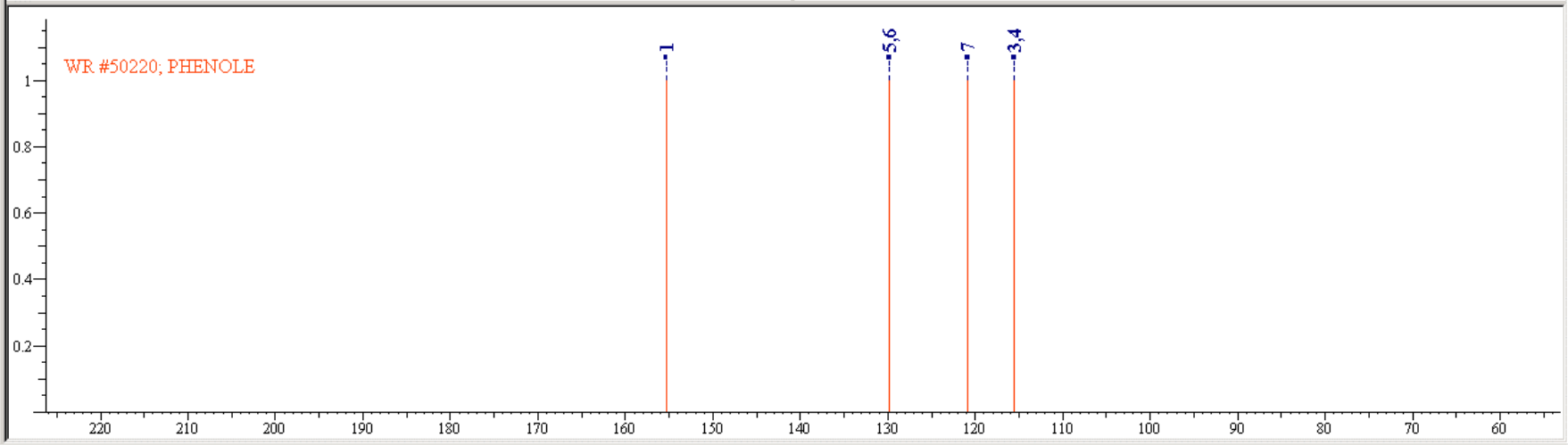
AssignIt CNMR



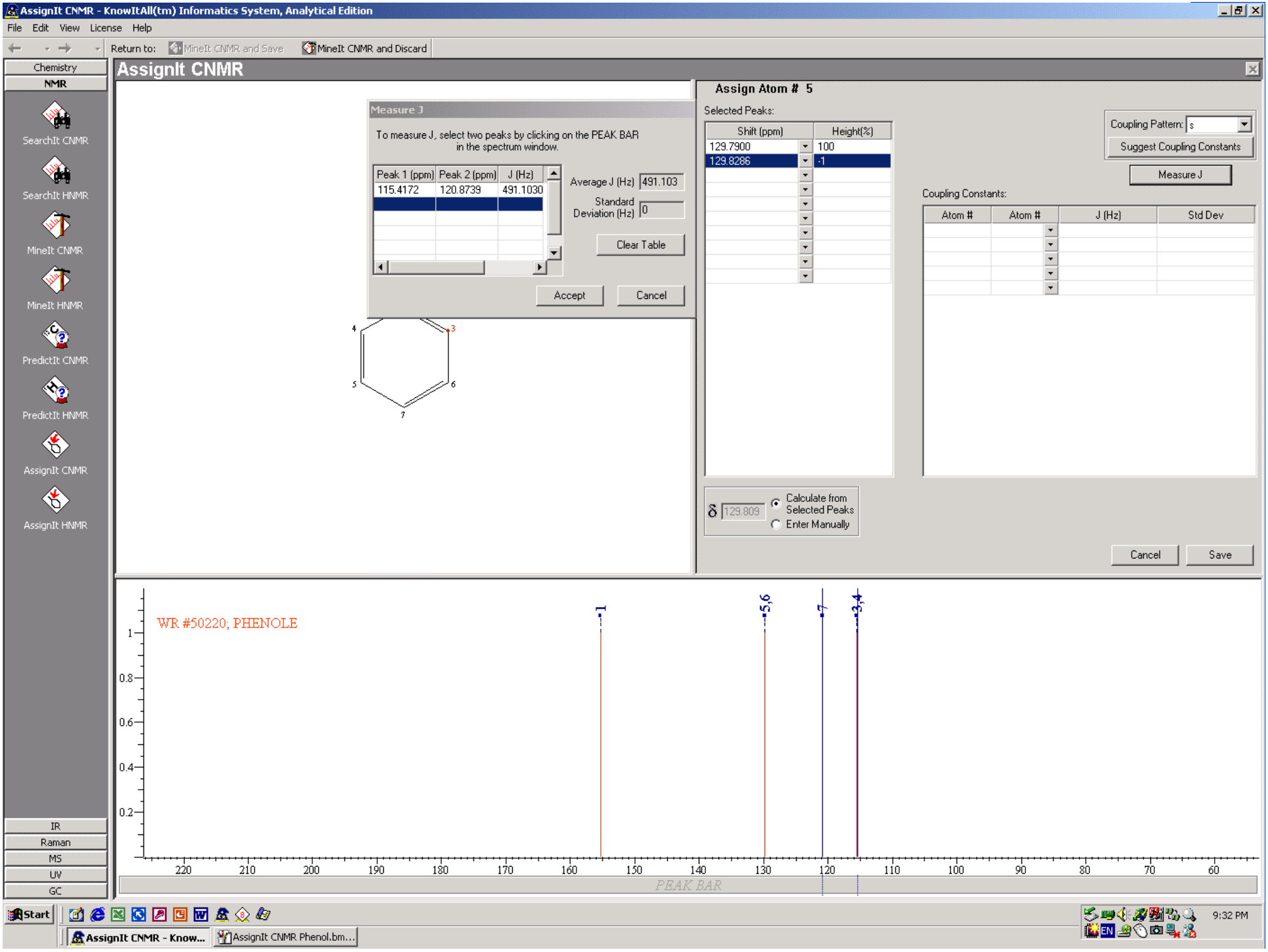
Atom #	δ (ppm)	peaks (ppm)	Pattern	J (Hz)
1		155.3600	s	
3		115.5500	s	
4		115.5500	s	
5		129.7900	s	
6		129.7900	s	
7		120.8400	s	

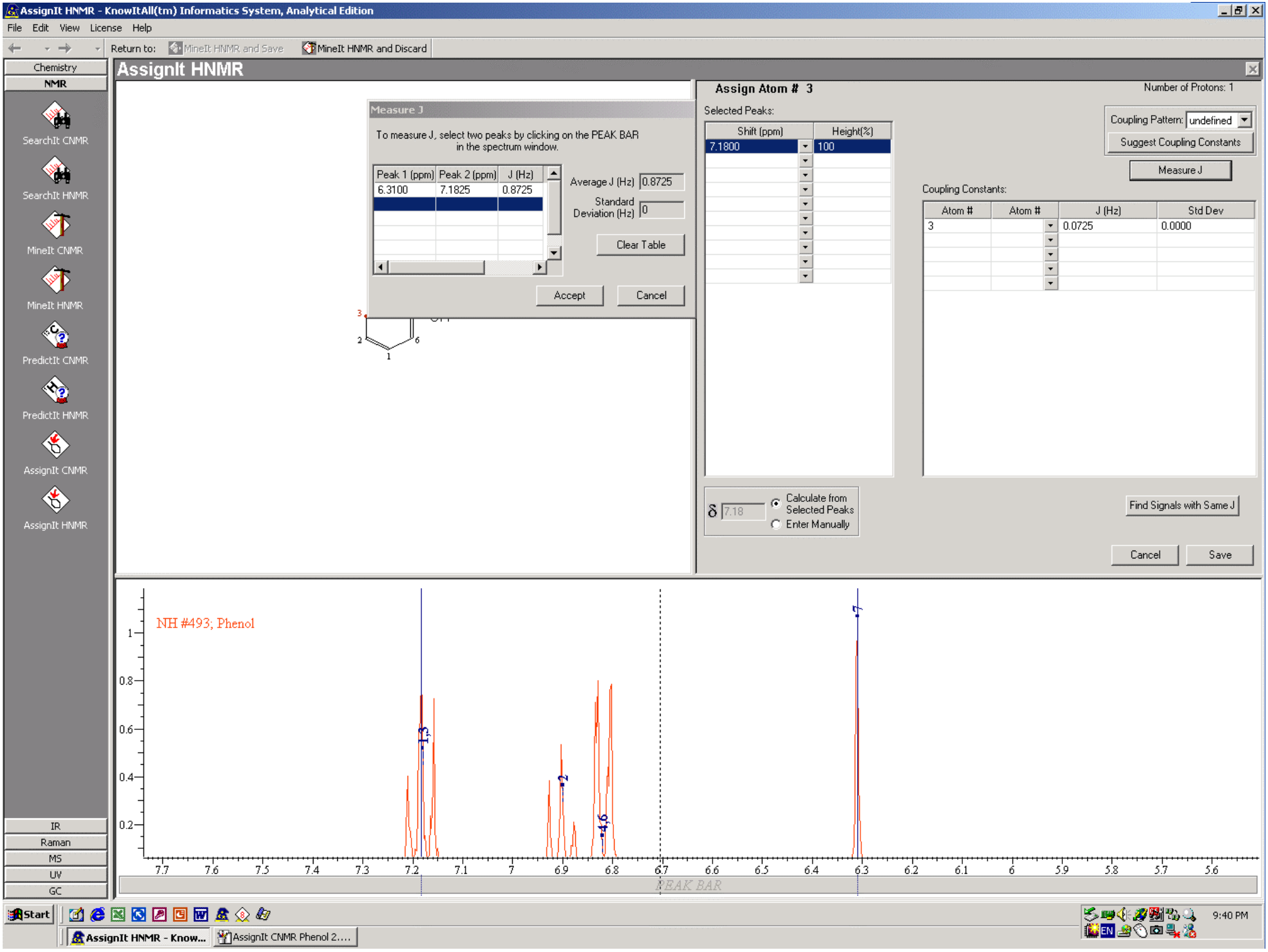
Atom #	Atom #	J (Hz)

New entry | Edit entry | Delete



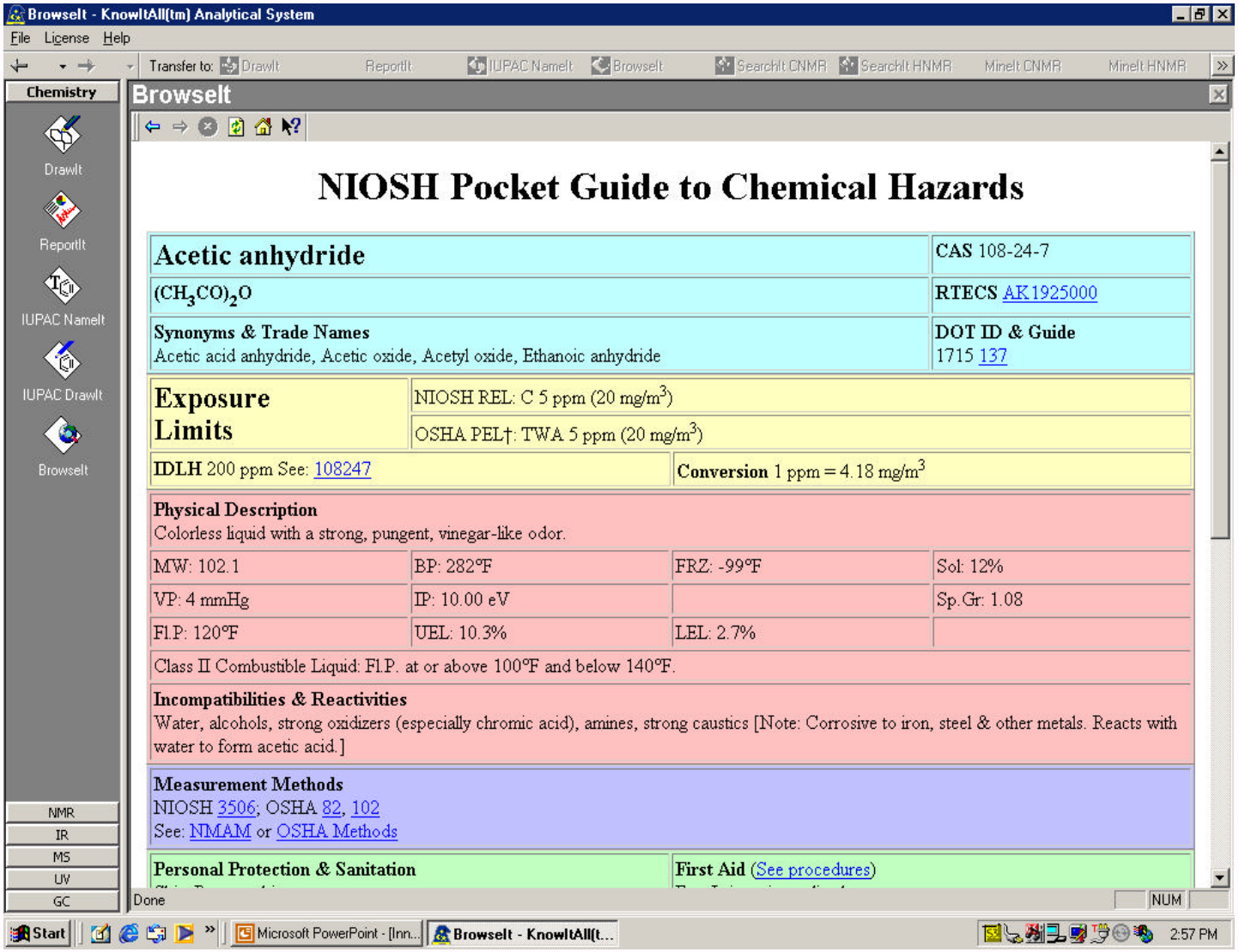
Start | AssignIt CNMR - Know... | PredictIt HNMR Phenol.b... | 9:28 PM


AssignIt CNMR - KnowItAll(tm) Informatics System, Analytical Edition
File Edit View License Help
Return to: MineIt CNMR and Save MineIt CNMR and Discard
Chemistry
NMR
SearchIt CNMR
SearchIt HNMR
MineIt CNMR
MineIt HNMR
PredictIt CNMR
PredictIt HNMR
AssignIt CNMR
AssignIt HNMR
IR
Raman
MS
UV
GC
AssignIt CNMR
Measure J
To measure J, select two peaks by clicking on the PEAK BAR in the spectrum window.
Peak 1 (ppm) Peak 2 (ppm) J (Hz)
115.4172 120.8739 491.1030
Average J (Hz) 491.103
Standard Deviation (Hz) 0
Clear Table
Accept
Cancel
Assign Atom # 5
Selected Peaks:
Shift (ppm) Height(%)
129.7900 100
129.8286 -1
Coupling Pattern: s
Suggest Coupling Constants
Measure J
Coupling Constants:
Atom # Atom # J (Hz) Std Dev
δ 129.809
Calculate from Selected Peaks
Enter Manually
Cancel
Save
WR #50220; PHENOLE
1
5,6
7
3,4
1
0.8
0.6
0.4
0.2
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60
PEAK BAR
Start
AssignIt CNMR - Know...
AssignIt CNMR Phenol.bm...
9:32 PM


AssignIt HNMR - KnowItAll(tm) Informatics System, Analytical Edition
File Edit View License Help
Return to: MineIt HNMR and Save MineIt HNMR and Discard
Chemistry
NMR
SearchIt CNMR
SearchIt HNMR
MineIt CNMR
MineIt HNMR
PredictIt CNMR
PredictIt HNMR
AssignIt CNMR
AssignIt HNMR
IR
Raman
MS
UV
GC
AssignIt HNMR
Measure J
To measure J, select two peaks by clicking on the PEAK BAR in the spectrum window.
Peak 1 (ppm) Peak 2 (ppm) J (Hz)
6.3100 7.1825 0.8725
Average J (Hz) 0.8725
Standard Deviation (Hz) 0
Clear Table
Accept
Cancel
Assign Atom # 3
Number of Protons: 1
Selected Peaks:
Shift (ppm) Height(%)
7.1800 100
Coupling Pattern: undefined
Suggest Coupling Constants
Measure J
Coupling Constants:
Atom # Atom # J (Hz) Std Dev
3 0.0725 0.0000
δ 7.18
Calculate from Selected Peaks
Enter Manually
Find Signals with Same J
Cancel
Save
NH #493; Phenol
PEAK BAR
Start
AssignIt HNMR - Know...
AssignIt CNMR Phenol 2....
9:40 PM

Web-link to other Databases

KnowItAll™
Informatics System



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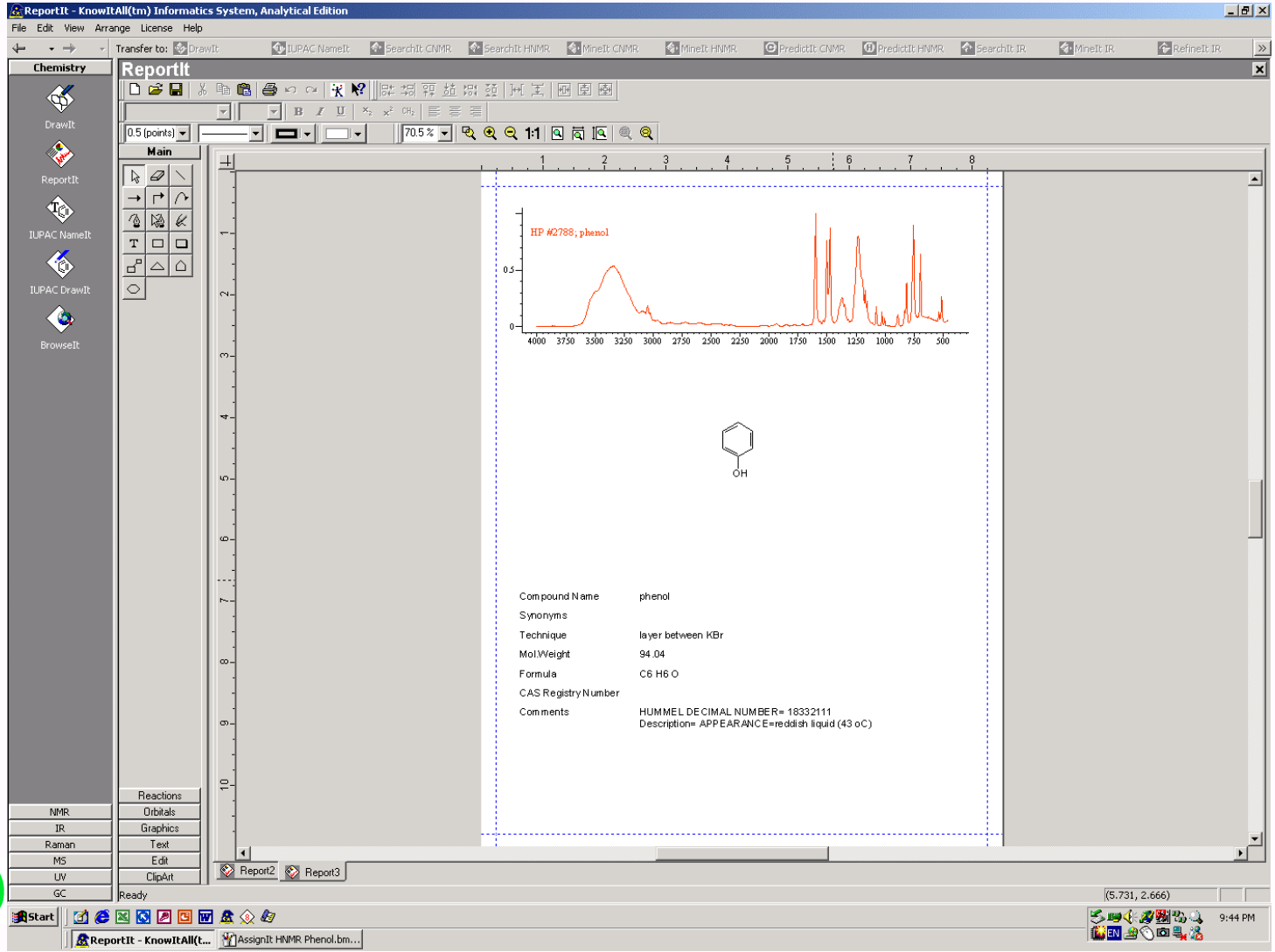
Report Results

KnowItAll™
Informatics
System



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KnowItAll™
Informatics
System

Spectral Database User Needs

- High quality, controlled and verifiable databases in the lab
- Create, import and manage spectral data and physical property information, and save it for the future.
- An easy-to-use interface that links different instrument techniques and all data.
- Capability to draw structures and create department, analyst or lab-specific reports.
- Continue to develop better platforms for shared information, knowledge management and improved productivity.

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System

Thank you!

Larry_Taylor@Bio-Rad.com

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