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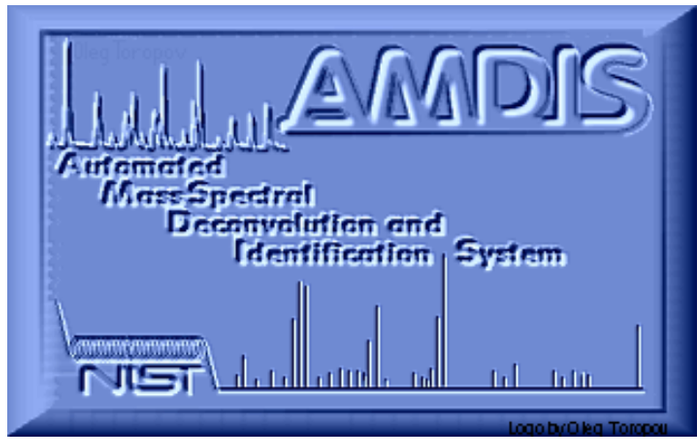
Welcome to
www.amdis.net



AMDIS is a new (easy to use) sophisticated software for GC-MS data interpretation from NIST.

www.amdis.net deals with modern aspects of GC-MS data interpretation - including chemometrics, liquid/gas chromatography and mass spectrometry.

www.amdis.net is open for every contribution from chromatography, chemometrics and mass spectrometry fields.

www.amdis.net is a private owned site - supervised by Tobias Kind

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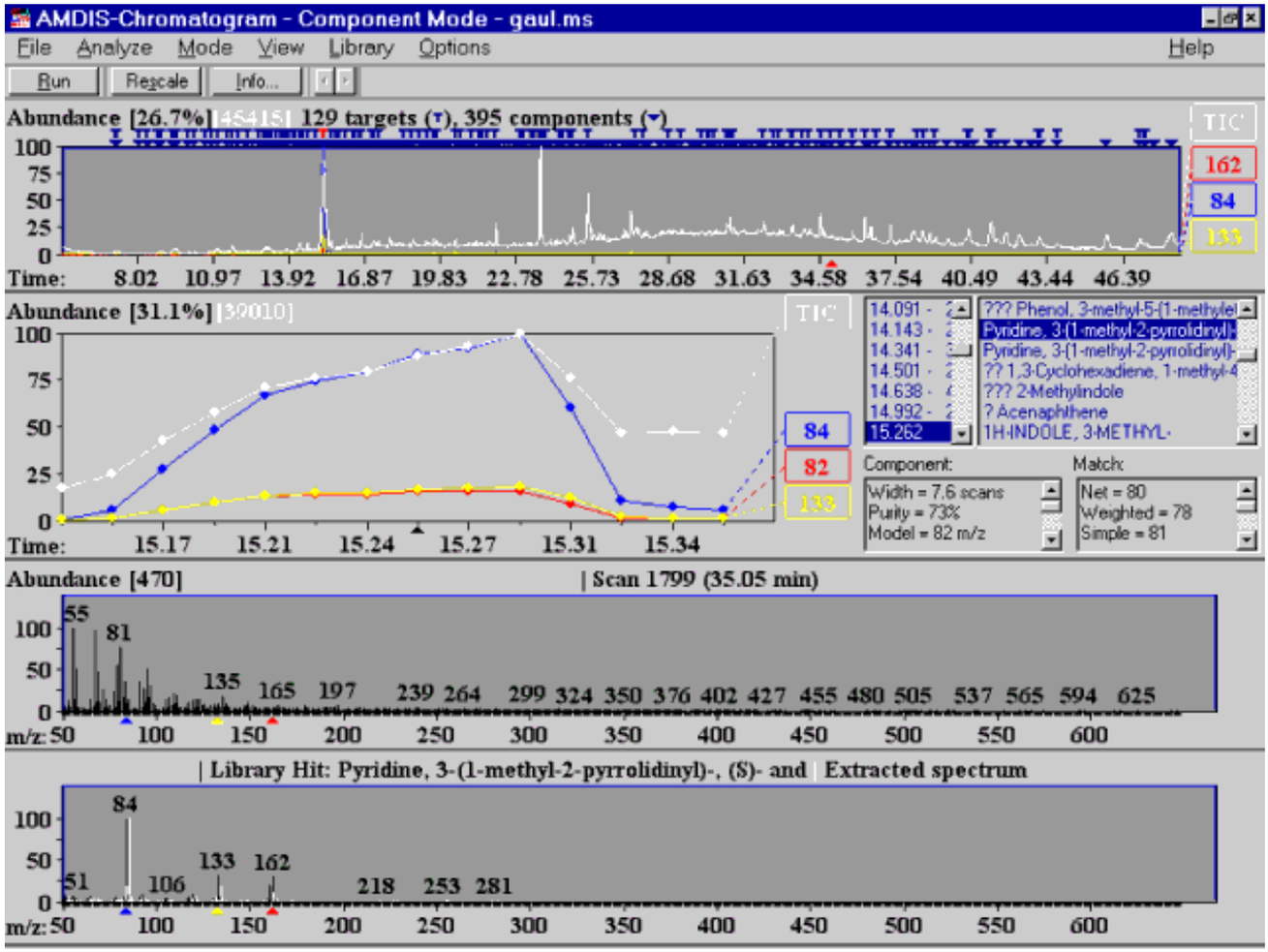
Introduction

AMDIS **(Automated Mass Spectral Deconvolution and Identification System)** is a new (easy to use) sophisticated software for GC-MS data interpretation from NIST.



Just imagine, you are a *non-scientist* working with GC-MS.

You get the task to analyze some complex organic extracts. You are working together with one of the wonderfull technicans who prepare the samples and fill the autosampler for you - but you are responsible for the task - therefore you push the "START" button.

After more or less leisure you go home - free in mind - because on the next day AMDIS will also do the work for you. On the next day you start your PC and AMDIS - you load the files from the different systems to your desktop and press "Analyze". After some seconds you get a list with your target analytes (from some of them you never heard the name). You save the list and send it to your boss or customer. A day later you get your cheque.

Any problems (apart from the GC-MS and the cheque)?

Yes - because you are a *scientist* and have to verify your data. But AMDIS can help you **to save time** and to avoid the "mouse click syndrome" (from subtracting all your spectra manually).

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Detailed Information about AMDIS

AMDIS can help you to analyze GC-MS data of complex mixtures, even with strong background and coeluting peaks. If you are working in SIM mode and you have external standards and want to quantify your compounds, you don´t need AMDIS. But if you have a noisy TIC spectra file and you want to find and identify known or unknown substances - AMDIS is the first choise.

AMDIS automatically extracts pure (background free) component mass spectra from highly complex GC-MS data files and uses these purified spectra for a search in a mass spectral library.

AMDIS can easy build library files from your own components and AMDIS will find these target compounds. You can scan data files only for these specific compounds. (You don´t need to set "time windows" or such things - just click the analyze button) AMDIS can find substances under a straight baseline (of course if there are some). You don´t need to extract all the ions traces manually and in the time consuming way.

AMDIS is free of charge with the omnipresent NIST Mass Spectral Library package.
Never checked your CD? Never detected this nugget in your task list? Fly out and download the latest release for free.

What is this AMDIS not:

After reading the text you may notify that this AMDIS is not that AMDIS (Association of Medical Directors of Information Systems) nor that AMDIS Atomic and Molecular Data Information System). (Read all the text and hate the joke? EMail me!)

AMDIS is not a tool for quantification of GC-MS data.

How AMDIS works:

AMDIS analyses steps: 1. noise analysis, 2. component perception, 3. spectrum deconvolution, 4. compound identification.

First AMDIS analyzes the background and calculates a noise level for later processing. After that, it analyzes the data for an increase of a special ion trace. If there is maxima also for other traces at the same time, is assumes there is a peak and shapes a model peak. In the next step it calculates a "clean" spectra for each peak. And at last it identifies the compound via a library search.

Indeed its more complicated. You can read it in the AMDIS Method Paper:
"An Integrated Method for Spectrum Extraction and Compound Identification from GC/MS Data" by Steven E. Stein

---

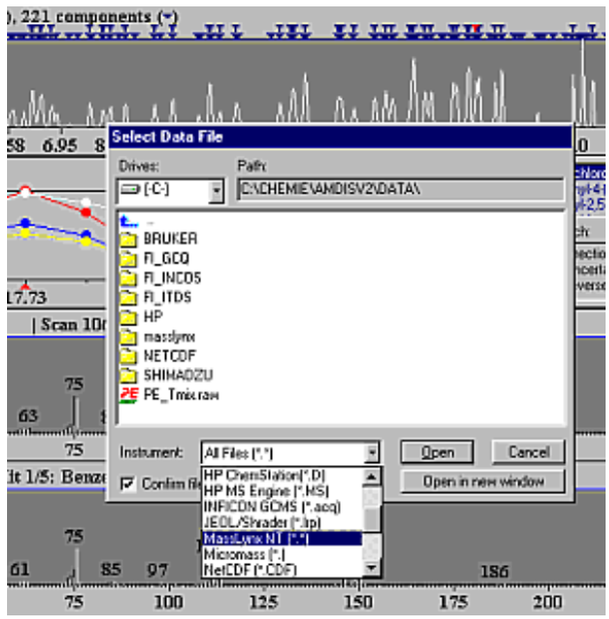
AMDIS needs:

- For large date files with more than 100 substances: A Pentium-200 or better with Windows (for small data a Pentium 90 is ok).
- Windows NT based system (Windows NT/2000) is recommended - because large arrays are handled and memory system and file system are up to 20% faster.
- A user who knows a little bit about GC techniques and MS data evaluation, to avoid false positive and false negative identifications.

AMDIS32 V2.1 can handle files from:

Bruker (*.msf)
Finnigan (GCQ, INCOS, and ITDS formats) (*.ms;*.mi;*.dat)

HP Benchtop and MS Engines (*.ms)
HP Chemstation (*.d)
Inficon GCMS (*.acq)
MassLynx NT Formats (*.*)
MicroMass (*.)
NetCDF (*.netCDF)
Perkin-Elmer Turbo Mass (*.raw)
Saturn SMS (*.sms)
Shimadzu MS Files (*.R##)
Shrader/GCMate (*.lrp)
Varian Saturn Files (*.ms)
Xcalibur (*.raw)



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Advanced

AMDIS (Automated Mass Spectral Deconvolution and Identification System) from NIST has some important features.

Coupling of mass spectra with retention indices:

This is the only wise topic which will survive in the future (apart from a very fast MS^n-Detector) for the identification of organic substances with GC-MS. Identification of substances **only** via mass spectra or retention indices (RI) may lead to false identifiactions. Mass spectra may be very similiar and RI values may be ”false” or overlapping. Its obvious that the more descriptors (vectors) exist for a certain compound, the more trustworthy the information will be.

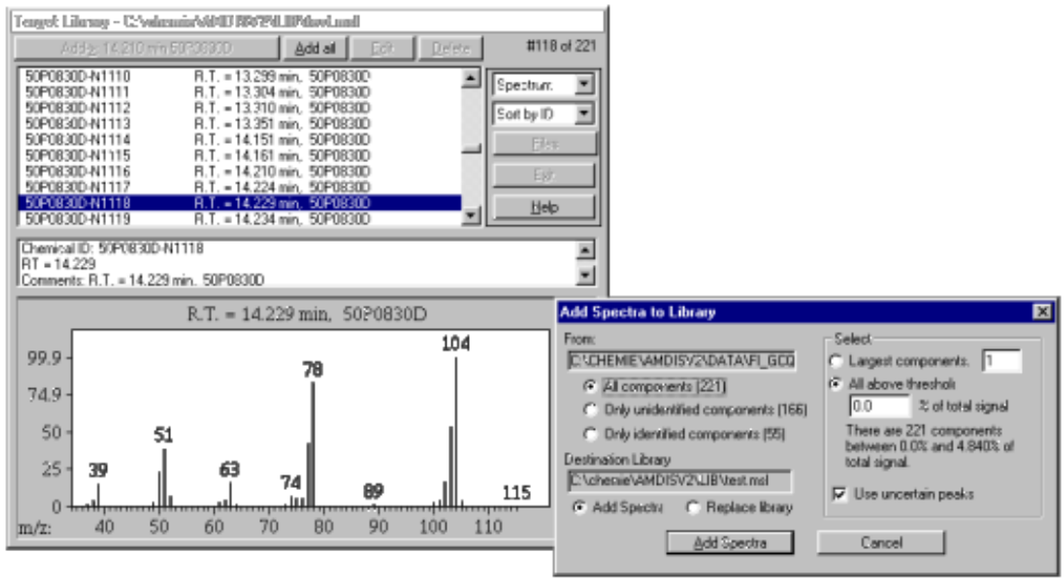
The concept of the AMDIS target libraries

This ingenious topic is a milestone for scientiest working with GC-MS/LC-MS. A stupid search for all substances existing in a certain chromatogram may be interesting but not truly clever.
Always remember - CAS currently knows about 30 million substances (2002) - a **systematization** is indispensable.

Searching for a special group of substances (alkanes, chloro-compounds, nitro-compounds) or a group of substances with a specific principle of action (toxic, endocrine, carcinogenic substances) will lead to a comprehensive identification of substances.

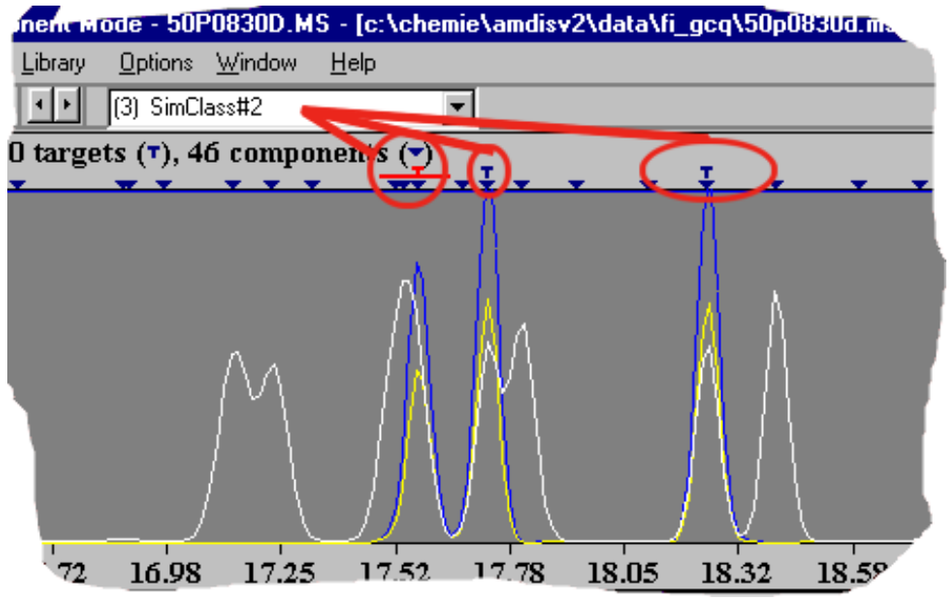
Library handling in AMDIS

Many programs for GC-MS or LC-MS data processing can produce user (mass spectral) libraries from chromatograms. But AMDIS has a unique concept of handling these libraries. Peaks can be added not only peak by peak, but they can be processed in one step.



AMDIS postprocessing - spectral similarity

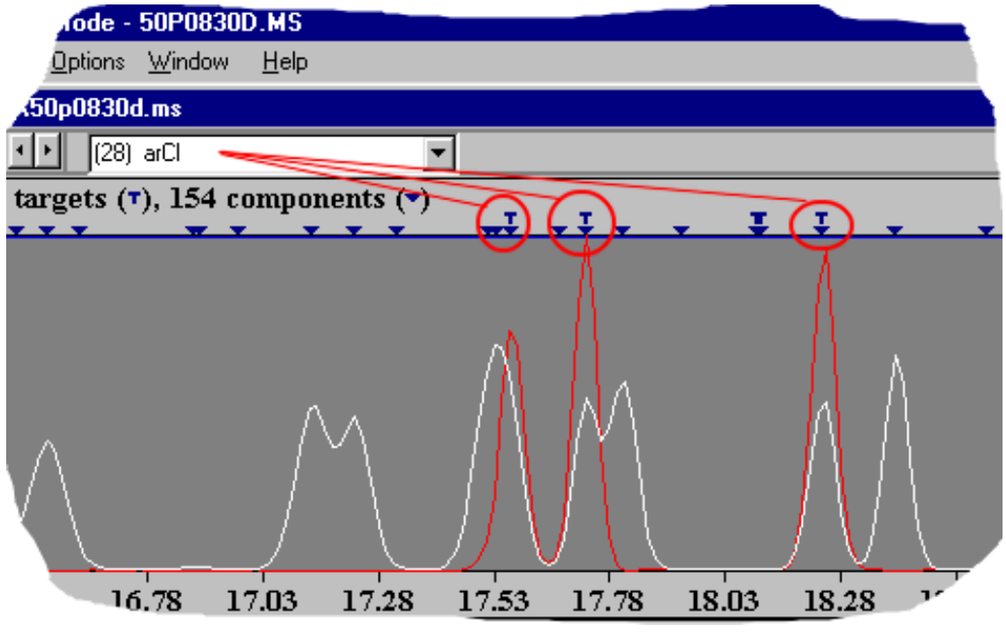
This AMDIS topic classifies (if possible) all compounds in a data file. Even if database search fails you will get an information about certain substances. In most cases these compounds will be related structurally. In the picture you see a SIM-Class with all three Dichlorobenzenes (marked with a **T**). In a former target library search they were not identified. But in the next step one can evaluate them “en bloc”.



This important step of **systematization** will fail in some cases (if the resolution is to low). But with the powerful library editor you can export all pure compounds and can classify the compounds with external programs. You will find some ideas in the amdis.net chemometrics section.

AMDIS postprocessing - VARMUZA classifiers

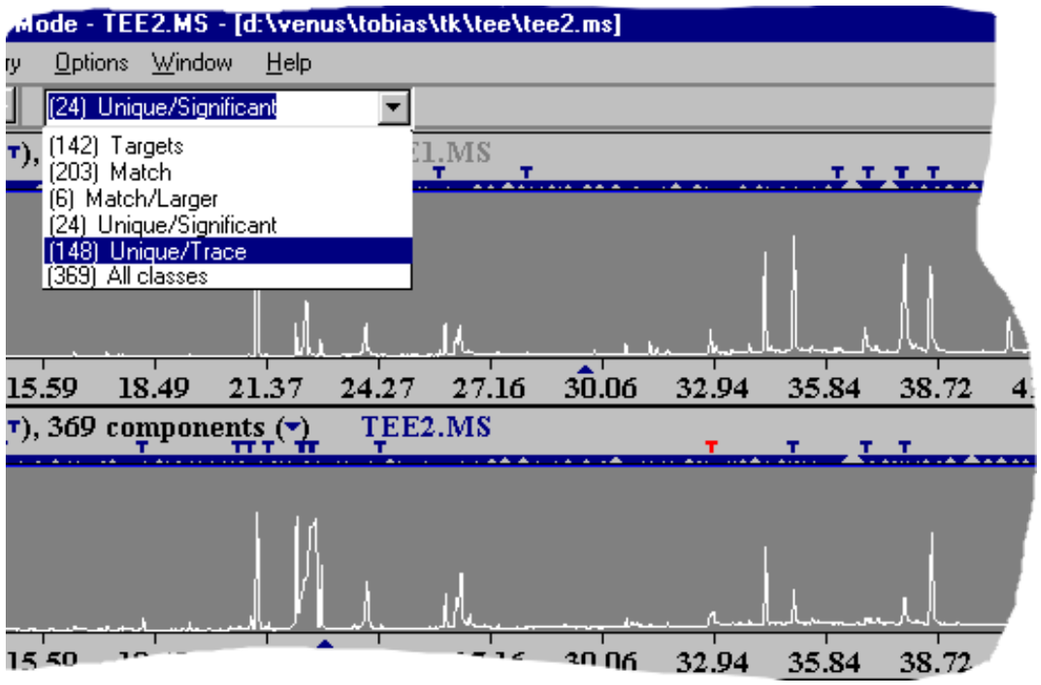
If you have no other information about a certain substance - you can choose this procedure. This is an expert algorithm which will detect special functional groups or substructures. You will find the substructures in the AMDIS handbook (amdis.net literature section).
Only some of these classifiers have a high discriminating power. As an example you will find many targets pointing to elemental sulfur. But there is absolutly no sulfur. In the current version of MSclass exist 160 classifiers for 85 substructures. This modul is also the (vulnerable) backbone of the outstanding MOLGEN-MS program.



As you can see in the graphics - all 3 Dichlorobenzenes are correctly identified as an aromatic system with chlorine.
Another powerful expert algorithm for substructure determination from mass spectra can be found in the NIST-MS-Search program (S.E. Stein, J. Am. Soc. Mass Spectrom., 1995, 6, 644-655). You can use both approaches if you have absolutely no information about a substance.

AMDIS postprocessing - compare datafiles

Every chromatographer knows this nice practice to overlay chromatograms and to compare them via the graphical peak pattern. This may be helpful in some cases but is only a very simple method.
Within AMDIS you can compare them via mass spectra and retention values.
This topic allows to find substances wich are existing or absent in a certain chromatogram. You have to open both runs in one active window.



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Downloads

AMDIS **(Automated Mass Spectral Deconvolution and Identification System)** is a new (easy to use) sophisticated software for GC-MS data interpretation from NIST.

Original sites from NIST:

- AMDIS Home
- AMDIS Download Page - with the AMDIS Handbook and the AMDIS method paper
- NIST/EPA/NIH Mass Spectral Library

Publications with AMDIS: - you can also read the larger page with abstracts [LINK]

- Deconvolution gas chromatography/mass spectrometry of urinary organic acids - potential for pattern recognition and automated identification of metabolic disorders; John M. Halket*, Anna Przyborowska, Stephen E. Stein, W. Gary Mallard,Stephen Down, Ronald A. Chalmers [LINK
- Comparison of gas chromatography pulsed flame photometric detection mass spectrometry, automated mass spectral deconvolution and identification system and gas chromatography tandem mass spectrometry as tools for trace level detection and identification; Shai Dagan, J.Chrom. A., 868, 2000, 229-247 [LINK] [LINK2]
- 1999 IFT Annual Meeting Abstract 48-6 - Effect of salt concentration on the volatile composition of cucumbers fermented with a Lactobacillus plantarum culture that does not produce carbon dioxide from malic acid: R. F. MCFEETERS, C. S. Palma, H. P. Fleming, and F. Breidt [LINK]
- The new Automated Mass Spectrometry Deconvolution and Identification System (AMDIS) May/June 1998; Antony N. Davies (ISAS Dortmund) [PDF]
- 1998 Version of the NIST/EPA/NIHMass Spectral Library—NIST98; By O. David Sparkman [LINK]
- Help files compiled by James L. Little [LINK]
- A step towards Multi-targeted Profiling of Phytohormone levels in Plant samples; C. Wiesner, L.Willmitzer, J,Kopka [PDF]
- A systematic approach to biochemical profiling; Norm Glassbrook and John Ryals; Cur Opin Plant Biol. 4 :186- 190. 13. [LINK]
- An Integrated Method for Spectrum Extraction and Compound Identification from GC/MS Data; S. E. Stein; NIST; Journal of the American Society of Mass Spectrometry in Volume 10, 1999, pages 770-781. [PDF]
- New software solutions for analytical spectroscopists; Antony N. Davies; ISAS Dortmund; [LINK]
- Integrated studies on plant biology using multiparallel techniques; Oliver Fiehn, Sebastian Kloska and Thomas Altmann; Curr.Opp.Biotech, 12,2001,82 [PDF]
- Combining genomics, metabolome analysis, and biochemical modelling to understand metabolic networks, Oliver Fiehn; Comp Funct Genom 2001; 2: 155-168. [PDF]
- Screening of Brazilian fruit aromas using solid-phase microextraction-gas chromatography-mass spectrometry; Fabio Augusto , Antonio Luiz Pires Valente, Eduardo dos Santos Tada, Sandra Regina Rivellino; Journal of Chromatography A, 873 (2000) 117-127; [LINK]
- Molecular and morphologic approaches to discrimination of variability patterns in chub mackerel, Scomber japonicus; Maria Ines Roldan , Ricardo G. Perrotta , Marti Cortey , Carles Pla; Journal of Experimental Marine Biology and Ecology 253 (2000) 63-74 [LINK]
- Resistively Heated Gas Chromatography Coupled to Quadrupole Mass Spectrometry; Jens Dallüge, René Vreuls, Dick van Iperen, Martijn van Rijn, and Udo A.Th. Brinkman [PDF]
- The Rapid Characterisation of Complex Mixtures using a Wide Dynamic Range Benchtop GC/TOF-MS; Jonathan Hughes, Lu Lin, Nick Bukowski [PDF]

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Benchmarks
AMDIS performance

AMDIS Benchmarks

AMDIS is a very CPU and memory intensive program. The following procedures compare the times for deconvolution and library search under different conditions.

- AMDIS test file: 50p0830d; pure standards: low noise; peak shape OK
- EPA method 524.2 purge and trap GC-MS analysis of volatile organic compounds in water (60 volatile compounds).
- target library: NISTEPA.MSL (1112 compounds)
- component width: 20
- VL=very low; L=LOW; M=midlle; H=high; VH=very high
- WIN98; Athlon 1700Mhz; 512 MB RAM; IBM ICSL HD

Results:
Adjecent (neighbouring) peak subtraction (low to high) has no impact in low res mode (see end of this table) - but in high res mode the number of target analytes will increase.

Resolution (low to high) increases number of target analytes and components.

Sensitivity (low to high) increases number of target analytes and components.

Shape requirements (low to high) has no impact in low res mode, but will decrease the number of targets and components in high res mode.

Recommendation:
1. Start with a peak subtraction of 2, shape req. high, low resolution and very low sensitivity
2. Change sensitivity to medium
3. Change resolution to medium
After all steps do a target library search or NIST search and compare your results.
All these factors strongly depend on the kind of your data file (noise, peak overlapp etc.)

Benchmark Table

Peak subtract.	Resolution	Sensitivity	Shape Req.	Targets	Components	Time[s]
2	**L**	**VL**	**L**	**77**	**95**	**2.8**
2	L	L	L	91	117	3
2	L	M	L	100	153	4
2	L	H	L	102	196	4
2	L	VH	L	126	280	6,5
2	L	VL	L	77	95	2,8
2	L	VL	M	78	97	2,5
2	L	VL	H	79	95	2,5
2	L	VH	L	126	280	7
2	L	VH	M	129	277	6
2	L	VH	H	110	213	5
2	M	VL	L	159	167	6
2	M	L	L	194	233	9
2	M	M	L	233	326	10
2	M	H	L	252	361	10
2	M	VH	L	307	559	15
2	M	VH	M	276	550	15
2	M	VH	H	229	476	13
2	H	VL	L	249	259	9
2	H	L	L	302	373	12
2	H	M	L	370	519	17

2	H	H	L	377	586	19
2	**H**	**VH**	**L**	**432**	**878**	**25**
2	H	VH	M	392	868	24
2	H	VH	H	306	775	20
2	H	VL	M	208	259	9
2	H	M	M	320	522	16
2	H	VH	M	392	868	24
2	H	VL	H	173	252	14
2	H	M	H	267	496	14
2	H	VH	H	306	775	20
Impact of peak subtraction **Low res mode**: Trend of increasing peak subtraction has no effect **High res mode**: Increasing targets but constant components and increasing analysis time						
N	L	VL	L	74	95	2,5
1	L	VL	L	76	95	2,5
2	L	VL	L	77	95	2,8
N	H	VH	H	178	748	7
1	H	VH	H	219	777	12
2	H	VH	H	306	775	20

Comparing the impact of different target libraries

- Conditions: see above
- Init variables: Peak subtract:2; Resolution: High; Sensitivity: Very high; Shape Req: Low

Results: Detected targets may me different (due to the selected target library) but detected components (even if false) vary. Why?

Analysis time may not increase with increasing number of target analytes (see nistepa/nisttox). Why?

On a “fast system” (Athlon 1700Mhz; 512 MB RAM) even the search for all 878 components in the NIST98 library may be acceptable.

Target Library	number of targets in library	targets	components	time [s]
0.msl	0	0	858	8
1.msl	1	7	859	9
grobx.msl	57	15	861	9
nistfda.msl	419	179	862	14
nistff.msl	993	148	870	23
nistepa.msl	1112	432	878	25
nisttox.msl	1251	53	862	19
Full NIST98 search (match factor in %) for all 878 components in Normal mode				
NIST98 (70%)	129136	344	878	60
NIST98 (80%)	129136	231	878	60
NIST98 (90%)	129136	83	878	60
NIST98 (95%)	129136	18	878	60
NIST98 (99%)	129136	11	878	60

There can be a speed increase of nearly 10% if the full NIST98 (or any other library) is in the hard disk cache. (f.e., with 512 MB RAM installed)

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Steve Stein

People

This section contains information about people who work in the field of chemometrics,
liquid/gas chromatography, mass spectrometry and programming.
Feel free to include your name here. Send me your “personal” page.

- Stephen E. Stein - NIST - AMDIS, NIST-MS-Search, NIST Webbook
- James Little - on mass-spec-groups has a lot of information about proper using of NIST-MS-Search programm (link contains literature)
- O. D. Sparkman - Sparkman and Associates, Antioch, CA
  some recouces on google and mass-spec-group and literature.
- Don R. Scott - wrote some important algorithms about mass-spectra interpretation - (link contains literature)
- Kurt Varmuza - important chemometrics group - wrote the classifier implementations for AMDIS and MOLGEN-MS
  google1 and google2 and literature
- Antony N. Davies - JCAMP, internet and chemistry and a lot more stuff
- Christoph Steinbeck - cheminformatics group in Jena with some CASE (Computer-Assisted Structure Elucidation) programs and JAVA
- Jörg Hau - (try dejanews) - wrote a fine mass-spec-program (MSGraph) and has netCDF resources and many other interesting stuff.
- Antony Williams - please note the extensive literature section
- Aviv Amirav - fast GC (supersonic molecular beams), pulsed flame photometric detector - google
- Hans Lohninger - chemometrics software and a lot of programming
- Wolf-D. Ihlenfeldt - wrote the CACTVS system and
  Enhanced NCI Database Browser - read the interesting lectures
- Steve Hellers - computers, mass-spectra, chemistry, data handling in chemistry - read the Steven.R. Hellers resume
- Desire Luc Massart - calibration and fundamentals in chemometrics
- Feng Gan - works in several fields of chemometrics (library search of mass specra)
- Barry K. Lavine - data mining and chemometrics
- Plamen Nikolov Penchev - application of chemometric methods for identification of organic compounds
- Frank Antolasic - wrote WSEARCH one of the first free programs for GC-MS data evaluation
- Richard Brereton - chemomtrics group in Bristol - visit about 75 free chemometric articles in The Alchimist and a lot of other useful resources

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Stephen E. Stein (NIST)

Steve works at the National Institute of Standards and Technology as a NIST Fellow, where he has been in charge of the NIST Mass Spectrometry Data Center since 1988. He was born on the lower east side of Manhattan, New York City on December 13, 1948 and grew up in mostly in the Bronx. He graduated from the University of Rochester in 1969 with a degree in Chemistry and earned a Ph.D. in Physical Chemistry from the University of Washington, Seattle in 1974, in the area of Gas Phase Kinetics.

He spent two years in the Thermochemisty and Chemical Kinetics Division of SRI International in Menlo Park, California as a Research Associate/Staff Scientist and five years in the Chemistry Department of West Virginia University as an Assistant/Associate Professor, working mostly in the area of high temperature kinetics, especially in its application to coal chemistry.

He came to NIST (then NBS) in 1980 where he continued work in kinetics for several years before becoming involved in computer applications of chemical reference data, assuming responsibility for the NIST/EPA/NIH Mass Spectral Library in 1988. Since then he has led the comprehensive evaluation of the library and been involved in the development of algorithms and software for evaluating data and extracting chemical information from this resource.

He has also been involved in a number of other reference data projects, including the NIST Chemistry WebBook and several chemical thermodynamics data programs.

He has received the Department of Commerce Gold Medal, the ACS Storch Award in Fuel Science, the ACS Patterson-Crane Award and NIST Applied Research and Schlichter Awards. He has published over 75 research papers and been a principal developer of several data products including the NIST Mass Spectral Search Program, the AMDIS GC/MS Deconvolution Program, the NIST Structures and Properties Program and the NIST/EPA Gas Phase Infrared Library.

(From FACCS information)

- Literature: Scirus (only some citations)
- Address: NIST
- Projects: AMDIS, NIST-MS-Search, NIST Webbook,

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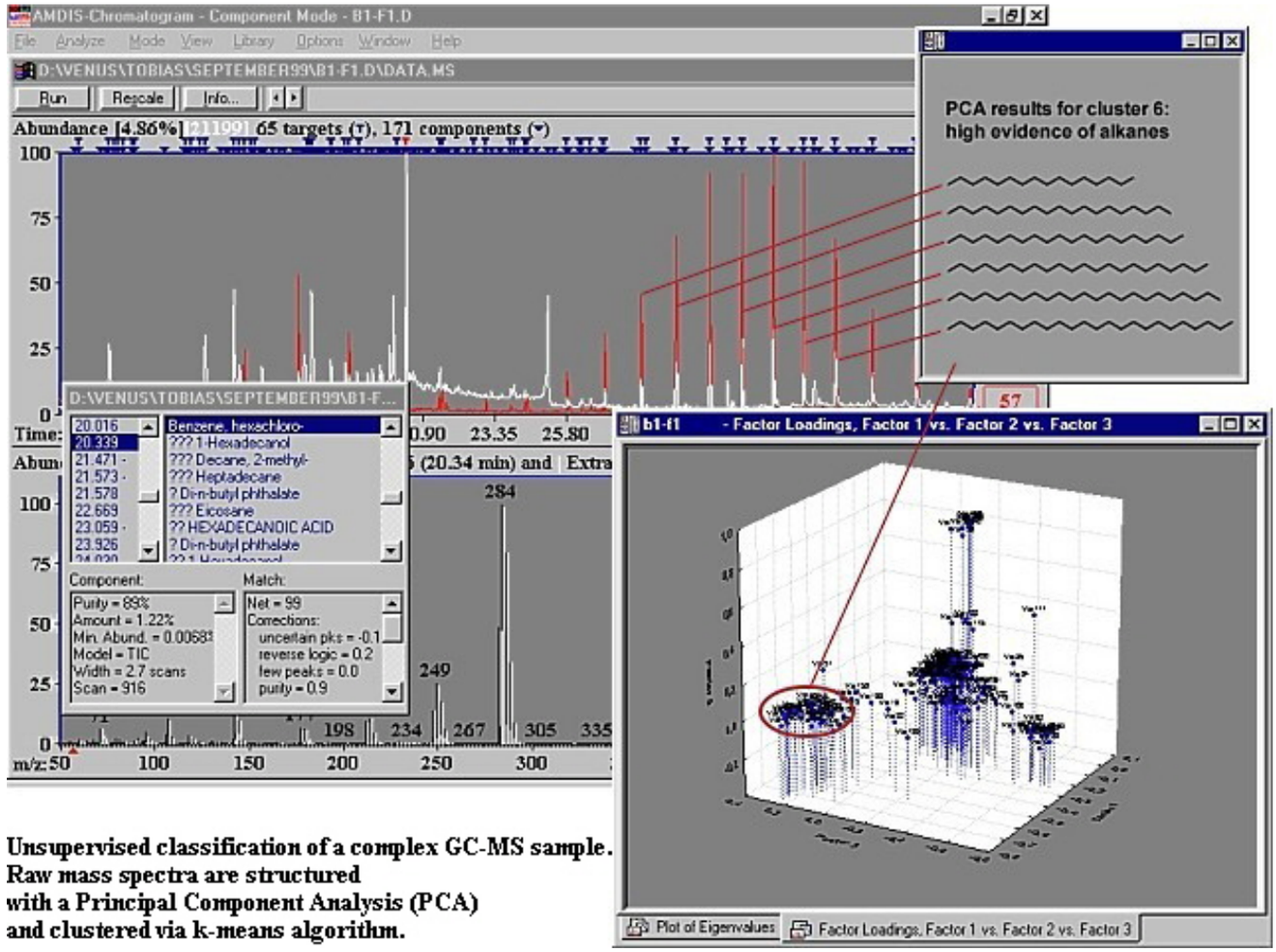
Chemometrics for comprehensive GC/LC-MS data evaluation

The development of new GC-MS or LC-MS devices and techniques made a significant progress in the last years. But the “sticking point” is that these devices produce too much data which can not evaluated in a proper way.

“Comprehensive data evaluation” means that we try to “squeeze out” all information from our raw data - with every possible approach.



Unsupervised classification of a complex GC-MS sample. Raw mass spectra are structured with a Principal Component Analysis (PCA) and clustered via k-means algorithm.

In the following sections you will find some programs which can help you in this way.

- Programs - for multivariate statistics, expert algorithms and databases
- Literature - selected literature for comprehensive data evaluation
- Patents - including most features of modern GC/LC-MS data evaluation

Chemometrics for comprehensive GC-MS data evaluation

Deconvolution and data handling

- **AMDIS32** V2.1 (free download) use with NIST98 [LINK]
- **Mass Frontier** from HighChem and Thermo/Finnigan (no demo) [LINK]
- **MassLIB** (demo available) [LINK]
- **ACD/MS Manager** (demo available) [LINK]
- **RIZA GC/MS Database** (free download) [LINK]
  The free RIZA GC/MS Database allows a coupled search of mass spectra **and** retention indices from AMDIS processed GC-MS files. Thus it keeps formerly processed data in the actual work process.

Mass Spectral Databases

There exist **two** large mass spectral databases which where assembled from different sources. The Wiley 5th edition and NIST98 had an overlap of 36,847 spectra. For a fast and secure identification of unknown spectra you need both libraries.

- **Wiley 7th edition** (338,000 spectra) (demo available) [LINK]
- **NIST98** (129,136 spectra) (demo available) [LINK]
- **NIST02** (175,214 spectra) [LINK]

GC Retention Indices

Up to now there exist no useful (that means large) retention index database. You can use AMDIS for building a user RI database and store the results in the RIZA GC-MS database. As a quick remedy you can look at the RESTEK catalog. Or you can make a rough estimate with the help of boiling points from EPISUITE. If you want to play a little bit with retention times you can use

- **Pro ezGC** (demo available) [LINK] or the
- **ACD/GC Simulator**.(demo available) [LINK]

For common congener analytes (PCBs, PCNs, dioxines) published RI tables exist. You may also use small retention time libraries like the

- **Agilent PCB Congener GC/MS RTL Database** [LINK] or the
- **Agilent/NMSLAB Forensic Toxicology GC/MS RTL Database** [LINK]
- **Tobacco/Smoke Mass Spectral Library** and Retention Time Database [LINK] [PDF]

Programs- Chemicals and Properties

- **EPA EPI Suite** (free download) [LINK] [LINK2]
  The free EPI-Suite contains some 103.000 structures + CAS numbers (SMILECAS database) and (PHYSPROP database) with around 25,000 compounds with some experimental data (logP, bp, henry..) and you can also calculate a lot of physico-chemical properties (bp,logp,simple toxicity)

- **Molgen-MS** (demo available) [LINK]
  Evaluation of Low Resolution Electron Impact Mass Spectra without Database Search; Modules: MSclass (mass spectra classification)
  ElCoCo (elemental composition computation)
  MOLGEN (molecular structure generator)
  ReNeGe (reaction network generator)

Metabolites

As we are working in a â€œliving worldâ€• there are always metabolites or breakdown products of chemicals. For a clever identification you need metabolite databases like:

- **Metabolite database** from MDL (8,590 parent compounds) [LINK]
- **Metabolism Database** from Accelrys [LINK]
- **Environmental Fate Database** (EPA und Syracuse Research) (free) [LINK]
- **University of Minnesota Biocatalysis/ Biodegradation Database** (free) [LINK]

If you want to identify metabolites of new or â€œunknownâ€• chemicals you can use expert algorithms like:

- **MetabolExpert** from CompuDrug (demo) [LINK]
- **Meteor** from Uni Leeds [LINK]
- **CATABOL** from (University Burgas) [LINK]

Programs- Statistics

- **Kyplot** - statistic program [LINK]
  Multivariate analysis, t-tests, ANOVAs, regression, PCA, cluster analysis, factor analysis, discriminant anaylsis, canonical correlation, survival analysis

- **Datalab** (Lohninger) [LINK]
  Univariate linear and parabolic regression, rank correlation, multiple linear regression, principal component analysis, neural networks, KNN-modelling, hierarchical clustering (dendrograms), etc.

- **ADE-4** (Uni Lyon) [LINK]
  PCA (Principal Components Analysis and extensions), COA (COrrespondence Analysis and extensions), HTA (Homogeneous Tables Analysis), MCA (Multiple Correspondance Analysis and extensions), DDUtil (Complements to basic analyses) and MatAlg (Matrix computations).
  UniVarReg, OrthoVar, LinearReg (Linear rgressions),Discrimin (Discriminant analyses, between and within class analyses), Projectors (Principal Component Analysis with respect to Instrumental Variables) and CCA (Canonical Correspondance Analysis).
  DMAUse (multiple distance matrices analysis and biodiversity measures), Clusters (cluster analysis) et Dendrograms (cluster analysis graphics).

Compound Databases

Remember the CAS service knows today around 30 million organic compounds - we know around 0.5 million mass spectra. This is a very large gap. Therefore a smart chromatographer needs to know â€œallâ€• possible compounds.

Q: Why not use CAS? A: Database politics, f.e. in germany is a very delicate subject. Most of the german universities have no money for a full CAS service (without major restrictions). The annual shilly shallying about a new subscription will fail in most cases because there is no money. Database politics in science in general is a difficult thing. Apart from some exceptions it is not reasonable to pay an inadequate amount of money for the â€œownâ€• reengineered results. Policy-makers do not pay attention to this important topic.
Wouldnâ€™t it be better if all OECD countries share the annual costs of CAS (~$30 Mio.) and gain free access?

- **ChemIDPlus** - [LINK]
  Toxline contains also literature for analytical chemistry (coverage 1945...today). You need the MDLI chime-plugin for copy/paste from ISIS Draw and other applications [LINK]

- **Enhanced NCI (CACTVS) database browser** - [LINK]
  Very flexible open database concept with multiple input and output options.

- **SMILECAS database** - [LINK]
  Contains about 103.000 structures with name and CAS numbers as backbone of the EPI-Suite.

- **Available Chemicals Directory** (ACD) - [LINK]
  Contains around 400000 unique compounds from 700 different suppliers. Trail within chemweb.com

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AMDIS

- AMDIS user guide; W. Gary Mallard and Janiel Reed; [PDF]
- An Integrated Method for Spectrum Extraction and Compound Identification from GC/MS Data; S. E. Stein; [PDF]

MS-Database-Search

- Most of useful information are from James D. Little - there are 8 papers [Link]
- The Critical Evaluation of a Comprehensive Mass Spectral Library ;P. Ausloos, C. L. Clifton, S. G. Lias, A. I. Mikaya, S. E. Stein, and D. V. Tchekhovskoi; O. D. Sparkman,V. Zaikin,Damo Zhu; [PDF]
- A Novel Approach of Retrieval of Mass Spectrum of Mixture; Feng Gan and Yizeng Liang [PDF]
- Library Search of Mass Spectra with a New Matching Algorithm Based on Substructure Similarity; Feng Gan, Jia-hong Yang and Yi-zeng Liang [PDF]
- Neural Network as a Pattern Recognition Tool in Spectroscopy; Cheng Kok Choi; Hong Kong Baptist University [LINK]
  Gives a nice overview about the most MS-SEARCH algorithms like (Probability Based Matching (PBM) method from McLafferty and D.B. Stauffer, similarity search, "dot product" search algorithm from S.E. Stein and D.R. Scott) and others.

GC Retention Indices

- Making sense of nontarget compound data from GC-MS library searches; William P.Eckel [PDF] (Lee retention index)
- New Design of the Algorithm for GC Retention Indices of Any Organic Compounds Precalculation from Their Physico-Chemical Constants; Igor G. Zenkevich; [PDF]
- Building a Comprehensive, Evaluated Collection of GC Retention Indices from Literature Data; J.K.Klassen,S.E.Stein,I.G. Zenkevich [PDF]

Chemometrics

- From MS Data via Chemometrics to Chemical Structure Information; K.Varmuza; [PDF]
- Clustering and Classification of Analytical Data; Barry K. Lavine; [PDF]
- Applied Chemometrics: From Chemical Data to Relevant Information; K.Varmuza; [PDF]
- The feasibility of latent variables applied to GC-MS data; F. Brakstad [Scirus]
- Anwendung multivariater Methoden und künstlicher neuronaler Netze zur Klassifizierung von Spirituosen mittels Headspace-GC-MS-Kopplung; P. Kursawe [PDF]

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Patents for GC/LC-MS data evaluation

Patents are nice sources for a special view â€œinsideâ€•. I will list some interesting patents from mass spectrometry, data evaluation, device development. As many services are outdated very fast, you can also search for yourself at the US Patent Office or Delphion.

Mass spectrometry

US5218529: **Neural network system and methods for analysis of organic materials and structures using spectral data**; Meyer; Bernd J. , Athens, GA; Sellers; Jeffrey P. , Suwanee, GA; Thomsen; Jan U. , Fredricksberg, Denmark; University of Georgia Research Foundation, Inc. (Athens, GA)

Apparatus and processes for recognizing and identifying materials. Characteristic spectra are obtained for the materials via spectroscopy techniques including nuclear magnetic resonance spectroscopy, infrared absorption analysis, x-ray analysis, mass spectroscopy and gas chromatography. Desired portions of the spectra may be selected and then placed in proper form and format for presentation to a number of input layer neurons in an offline neural network. The network is first trained according to a predetermined training process; it may then be employed to identify particular materials. Such apparatus and processes are particularly useful for recognizing and identifying organic compounds such as complex carbohydrates, whose spectra conventionally require a high level of training and many hours of hard work to identify, and are frequently indistinguishable from one another by human interpretation. [PDF][PDF2]

Time-of-Flight mass spectrometry

US5175430: **Time-compressed chromatography in mass spectrometry**; Enke; Christie G. , East Lansing, MI; Holland; John F. , Lansing, MI; McLane; Richard D. , Lansing, MI; Yefchak; George E. , Lansing, MI; Meridian Instruments, Inc., Okemos, MI

A process and apparatus employing the time compression of chromatography in mass spectrometry with array detection in which the time compressed informatioin is deconvoluted by mathematical analysis for recovery of analytical information made inaccessible in the time compression and thereby resulting in a decrease in analysis time and improved component identification without loss of sensitivity.[PDF][PDF2]

Deconvolution in Mass spectrometry

EP0708475: **Mass spectra deconvolution method;** Gray, Zachary A.; Abel, Roger H. Hewlett-Packard Company; 1995
Mass spectral analyzer providing automated discovery, deconvolution and identification of mass spectrum. Conventionally acquired mass data file (180) is re-sorted from chronological (181) to primarily ion-mass order (182) and secondarily to chronological order (183) within each ion-mass grouping. For each ion-mass measured, local peaks or maximums are identified through an integrator means. All local maximums are then sorted and partitioned (184) such that a set of deconvoluted spectra is obtained such that each element of the set constitutes an identifiable compound. Compounds are then matched to reference spectra in library datafiles (185) by conventional probabilistic matching routines. [PDF] [LINK]

US4807148: **Deconvolving chromatographic peaks**; Lacey; Richard F. , Palo Alto, CA; Hewlett-Packard Company, Palo Alto, CA; 1989
: Deconvolution of up to three overlapping chromatographic peaks is provided in which pure spectral components are extrapolated from a Euclidean-normalized expression of chromatographic data in the space of the three principal factors. A coordinate transformation to planar coordinates after expansion in factor space and before extrapolation yields the simplicity of linear extrapolation in combination with the inherent accuracy of Euclidean, as opposed to standard, normalization. The estimation of the pure component spectra permits the constructions of a concentration matrix. Improved estimates and an error bound are provided by applying assumptions of non-negativity and limited deviation from the means to the concentration matrix. [PDF]

US4752888: **Method of determining major and minor peaks in a chromatogram using a data processor**; Yoshihara; Touhachi , Katsuta, Japan;Hitachi, Ltd., Tokyo, Japan; 1985
A data processor for chromatography operates to separately recognize the peaks of a composite peak of a chromatogram. At first, in order to separate the peaks, the maximum point of the peak of the chromatogram is determined, and extrapolation lines are drawn from said maximum point to the individual points of the chromatogram, and then the gradients of the lines changing from the minimum to the maximum are determined. By determining the changes of the gradients of the extrapolation lines and intersection points of the extrapolation lines and the chromatogram, the major and minor peak are separated so that the shoulder peak can be judged remarkably accurately. [PDF] [PDF2]

US5453613: **Mass spectra interpretation system including spectra extraction**; Gray; Zachary A. , Palo Alto, CA; Abel; Roger H. , Cupertino, CA; 1994
A mass spectral analyzer system providing automated discovery, deconvolution and identification of mass spectrum is taught. Conventionally acquired mass data files are re-sorted from chronological to primarily ion-mass order and secondarily to chronological order within each ion-mass grouping. For each ion-mass measured, local peaks or maximums are identified through an integrator means. All local maximums are then sorted and partitioned such that a set of deconvoluted spectra is obtained such that each element of the set constitutes an identifiable compound. Compounds are then matched to reference spectra in library datafiles by conventional probabilistic matching routines. [PDF]

US4837434: **Mass spectrometry system and method employing measurement/survey scan strategy**; James; Craig A. , Palo Alto, CA; Hewlett-Packard Company, 1989

A gas chromatography plus mass spectrometry system implements a scan strategy in which each full range scan alternates between a normal measurement mode and a survey mode based on a block/gap map made during the previous scan. Survey mode is used within regions that were determined in the previous scan to lack signal above a predetermined threshold. Spectral data is generated during measurement mode operation. Each scan serves both measurement and mapping functions in a way that avoids mass filter jumps, since each scan is monotonic over the entire scanning range.[PDF] [PDF2]

US6147344: **Method for identifying compounds in a chemical mixture**; Annis; D. Allen , Cambridge, MA; Birnbaum; Mark , New York, NY; Birnbaum; Seth N. , Boston, MA; Tyler; Andrew N. , Reading, MA; Neogenesis, Inc, Cambridge, MA; 2000

A technique for automatically analyzing mass spectrographic data from mixtures of chemical compounds is described consisting a series of screens designed to eliminate or reduce incorrect peak identifications due to background noise, system resolution, system contamination, multiply charged ions and isotope substitutions. The technique performs a mass spectrum operation on a control sample, producing a first group of output values. Next, perform a mass spectrographic operation on a sample to be analyzed, producing a second group of output values. Select a first m/z ratio for a material expected to be present in the mixture from a predetermined library of calculated mass spectrometer output spectrums and subtract the value of the control sample at the expected output value from the value of the analyzed sample, and compare the difference to a predetermined value. If the value is greater than the predetermined value thus indicating that the signal is above the background noise level, generating a record at that m/z value for an expected material. Performing the same mass spectrum operation several times to eliminate random noise and background contamination. Next, identify peak values that donâ€™t have the expected peak width or proper retention time for the separation method. Identify multiply charged ions by examining peak separation. Examine the m/z location of the expected material and compare intensity at the expected m/z location with the intensity at the next lower m/z recorded peak to identify peaks related to atomic isotope substitution. With such a technique, mass spectrograph data analysis may be greatly simplified by the identification of probable spurious signals, and analysis will become simpler and more accurate.[PDF] [PDF2]

Examples for comprehensive GC/LC-MS data evaluation

Classification of GC-MS data

In complex samples up to 200..500 compounds can be detected. Therefore a classification is essential. In some cases a classification via retention time or peak height may be adequate. There are lot of examples with classification of GC data with different multivariate methods. An online example is the Chemometric Analysis of Gas Chromatographic Data of Oils from Eucalyptus species. You will find other examples and reviews in the literature section.

But for a finer analysis you can do a classification of the raw mass spectra (also including retention times). These raw samples can be classified using supervised and unsupervised methods like:

- partial least squares - PLS
- artificial neural networks - ANN
- self-organizing maps - SOM (an ANN method)
- linear discriminant analysis - LDA
- k-nearest neighbours - k-NN
- soft independent modeling of class analogy - SIMCA
- principle component analysis - PCA
- canonical analysis
- cluster analysis

As a first step you can use the *spectral similarity* information from AMDIS postprocessing. This is based on a normalized dot product of the spectra being compared (S.E. Stein, D.R.Scott).
If you want to classify your own spectra you need:

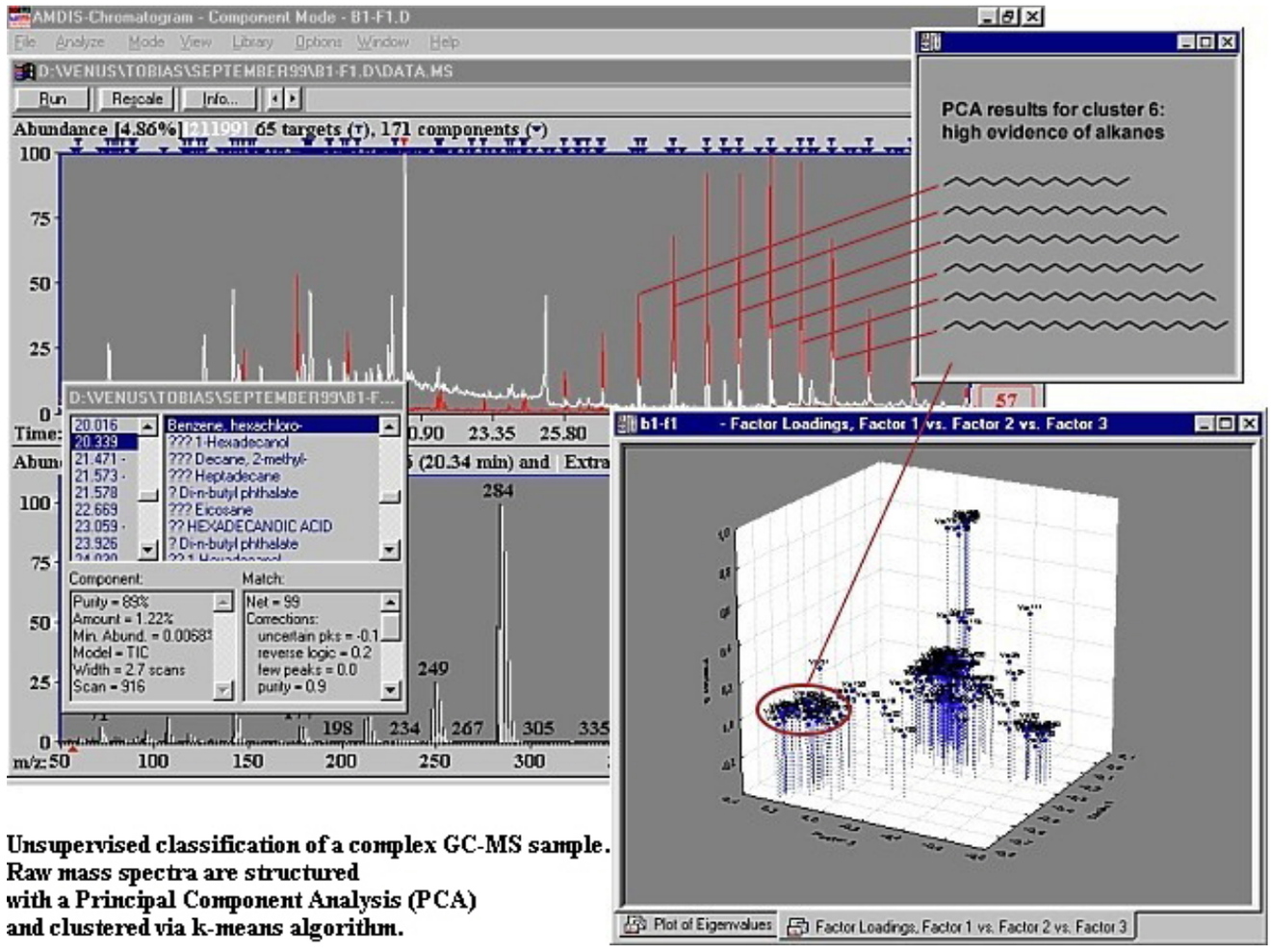
1. **AMDIS and the included AMDIS LIBRARY EDITOR** - [LINK]
   Choose the example file 50p0830d start in low/low/low mode. Export the the peaks via the menu Library/Build one Library/Files/Create New Library/**New target library**/50P0830D.msl
   Now you can add “All components” or selected targets. It is important that you select “save as target library” as this selection allows the creation of a new file with all peaks. In the second step you have to save the *.msl file as *.msp file (simple MS file *.MSP) via the “**Save Library as”** button. You now have a file with raw mass spectra.

2. **LIB2NIST** - [LINK]
   Load the MSP file and convert it to a HP JCAMP file. (External link from NIST)

3. **JCAMP4PCA** - as text [LINK] and the newest version V0.92 as zip file [ZIP]
   Run EXCEL and start the Visual Basic Editor via Extras/Macros/Visual Basic Editor.
   Now import the jcamp4pca.bas via File/Import File *.bas After loading you should start the module via run module after choosing the file in the project window. In the following file dialog box choose 50P0830D.HPJ and convert it. After 5 seconds you now have a nice export version of all peaks. Each column is one cleaned AMDIS peak.

4. **Programs for classification** - [LINK]
   Now you can import all cleaned peaks to your prefered classification program. For confirming the peaks sort the peaks in the AMDIS library editor via “Source: **Sort by ID**”

In the following graphic you can see a simple unsupervised classification of raw mass spectra from a complex GC-MS sample using Principal Component Analysis (PCA) and clustering via k-means algorithm. Please note that the clusters may have similiar mass spectra and most of these compounds will be related structurally, but this is no “must”. You should confirm or verify your results.



Unsupervised classification of a complex GC-MS sample. Raw mass spectra are structured with a Principal Component Analysis (PCA) and clustered via k-means algorithm.

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Nitro PAHs

You will find a collective index about nitrated polycyclic aromatic hydrocarbons on NITRO PAHs.

If you are planning a HPLC analysis I recommend the following critical review: “High-performance liquid chromatography of nitrated polycyclic aromatic hydrocarbons” by Josef Cvacka , Jirí Barek , Arnold G. Fogg , Josino C. Moreira and Jirí Zima from Analyst, February 1998, Vol. 123 (9R18R) [DOI]

HP-Chemstation

The following section gives an overview about the powerful HP Chemstation macro language. Its popularity is based on the “open concept” and simplicity (like BASIC). You can read almost of the code and learn from it. If you want to write your own code you should download the ChemStation Macro Editor (Macropad) from Niels Waleson and the macro debugger.

If you are running the LC(UV-VIS) Chemstation read the “Agilent ChemStation for UV-visible Spectroscopy - Macro Programming Guide” [PDF].
For other revisions you should checkout the 450 page monster “Macro Programming Guide” [PDF].

If you want to program the Agilent ChemStation for GC-MSD (G1034C ,G1032C, G1701AA, G1710,G1701BA) you should do a quick search for all help files in your \hpchem\msexe\ directory (macros.hlp or hpenvda.hlp) they cover most of the implemented commands.
You will find a short summary of macro commands here:

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About the Author of amdis.net

Tobias Kind was born in Dresden and grow up in Taucha near Leipzig.

He studied in Merseburg, Bayreuth and Leipzig. Later he worked for 3 years at the UFZ (Centre for Environmental Research) Leipzig-Halle and is currently finishing his PhD studies.

He is interested in environmental research (lecture) including chromatography (HPLC, GC-MS) and chemometrics for GC-MS data evaluation. Collaboration research: [PDF1] [PDF2] [PDF3].

Other fields of interest are environmental remediation strategies (in general), clean water technologies (polymer adsorption, membrane technologies), medicinal/pharmaceutical chemistry (acetylcysteine) and programming and data management in chemistry.

You can read some of my collected usenet comments.

About this website

www.amdis.net is a contribution to AMDIS and the scientific community.

www.amdis.net would not be possible without the authors of AMDIS:

Steve Stein, **Oleg Toropov**, **Jane Klassen**, **W. Gary Mallard**, **Janiel Reed** and contributors Boyu Yang, W.Werther, H. Lohninger, F. Tancl, H. Scsibrany, Kurt Varmuza, D. Henneberg and B.Weimann, Don R. Scott and the generous free release of AMDIS with the support of DSWA/DTRA, OPCW and NIST.

www.amdis.net deals with modern aspects of GC-MS data interpretation - including chemometrics, liquid/gas chromatography and mass spectrometry.

www.amdis.net is open for every contribution from chromatography, chemometrics and mass spectrometry fields.

www.amdis.net is not responsible for the content of external links.

If you have remarks, questions, critical comments or want to contribute a chapter or link please do not hesitate to contact me:
tk2003deja@amdis.net

About NOF

This website was made with one of the buggiest programs ever - **Netobjects Fusion 5.1**

Nothing is perfect - and NOF 5.1 really has great possibilities, but crashing every 20 minute and restarting the whole system can increase your suffering to **mental confusion.**
Thatswhy I call this proggy **Netobjects Confusion.**

As you can see - they sold a number of copies and counted the produced websites with an Integer-Overflow. Its like 8-bit EXCEL 2000 ;-).

If you don't believe me - try Netobject Fusion crashes. If you compare to MS Frontpage it is even a raw factor of 10 better. But who cares ? Writing HTML like assembler may be fun but is not really advantageous.

Environmental Pollution
Volume 121, Issue 1, January 2003, Pages 81-85

DOI: 10.1016/S0269-7491(02)00200-2
PII: S0269-7491(02)00200-2

This Document
- **Abstract**
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Actions
- E-mail Article

Polychlorinated naphthalenes in sediments from the industrial region of Bitterfeld

Werner Brack[a], Tobias Kind[a], Steffi Schrader[b], Monika Möder[b] and Gerrit Schüürmann[a]

[a] Department of Chemical Ecotoxicology, UFZ Center for Environmental Research Leipzig-Halle, Permoserstraße 15, 04318, Leipzig, Germany
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Received 19 December 2001; accepted 15 March 2002. Available online 15 April 2002.

Abstract

Bitterfeld (Germany) was a major site of chemical production in the former German Democratic Republic with chloralkali electrolysis as the basic process. Effluents were dumped via the creek Spittelwasser into the rivers Mulde and Elbe. Despite the fact that the chloralkali industry is known as a possible source of polychlorinated naphthalenes (PCNs), to date no data about PCN pollution in the region of Bitterfeld and downstream regions are available. Therefore, sediments of the creek Spittelwasser were isomer-specifically analysed for penta-, hexa- and heptachlorinated naphthalenes using GC/MS. Concentrations of 880, 543 and 1120 ng/g dry weight were found, respectively. The isomer pattern suggests chloralkali industry as the major source of PCN contamination. Because of their toxicological relevance we suggest to include PCNs into monitoring and risk assessment programs of the rivers Mulde and Elbe downstream of Bitterfeld.

Abstract

Polychlorinated napthalenes are a major contaminant of sediments in regions of the former German Democratic Republic.

Author Keywords: PCNs; Sediments; Isomer-specific analysis; River Elbe

Corresponding author; email: wb@uoe.ufz.de

Environmental Pollution
Volume 121, Issue 1, January 2003, Pages 81-85

This Document
- **Abstract**
- Full Text + Links
- PDF (145 K)

Actions
- E-mail Article

Environmental Toxicology and Chemistry: **Vol. 21, No. 12, pp. 2654–2662.**

EFFECT-DIRECTED FRACTIONATION AND IDENTIFICATION OF CYTOCHROME P4501A-INDUCING HALOGENATED AROMATIC HYDROCARBONS IN A CONTAMINATED SEDIMENT

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(*Received* 9 *January* 2002; *Accepted* 7 *June* 2002)

Abstract—On the basis of a new fractionation method combined with in vitro ethoxyresorufin-*O*-deethylase (EROD) induction in a rainbow trout liver cell line (RTL-W1) and chemical analysis, halogenated aromatic hydrocarbons with dioxin-like activity were identified in a sediment extract from Bitterfeld, Germany. The fractionation method allowed a separation of different nonplanar and coplanar polychlorinated biphenyls (PCBs), polychlorinated naphthalenes (PCNs), dibenzo-*p*-dioxins (PCDDs), and dibenzofurans (PCDFs) with different degrees of chlorination. The dioxin-like activity at the investigated site could be quantitatively assigned to PCDD/Fs. Both PCBs and PCNs could be excluded as the cause of the measured effects on the basis of the fractionation procedure and bioanalytical results. Thus, the method allowed the chemical analysis to focus on PCDD/Fs, with significant reduction of the analytical expense. The EROD-induction potency of sediment-extract fractions was quantified, and toxicants were confirmed by the application of induction equivalent quantities on the basis of fixed-effect-level concentrations that exhibit 15% of the maximum induction by 2,3,7,8-tetrachlorodibenzo-*p*-dioxin. This approach was designed to minimize methodological limitations due to superimposing inhibitory effects.

Keywords—Effect-directed fractionation Ethoxyresorufin-*O*-deethylase Toxicant identification Sediment extract

Journal of Chromatography A
Volume 986, Issue 1, 31 January 2003, Pages 55-66

DOI: 10.1016/S0021-9673(02)01909-X
PII: S0021-9673(02)01909-X

Sequential fractionation procedure for the identification of potentially cytochrome P4501A-inducing compounds

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Received 6 June 2002; revised 15 October 2002; accepted 19 November 2002. ; Available online 19 December 2002.

Abstract

A multistep fractionation procedure for the separation of nonpolar aromatic compounds with respect to cytochrome P4501A induction is presented. Normal-phase HPLC on nitrophenylpropyl silica and cyanopropyl silica was tested for group-specific separation as a first fractionation step. Subsequent individual compound-specific PAH fractionation was done by means of reversed-phase HPLC. Electron-donor–acceptor HPLC and size-exclusion chromatography were applied to separate PAHs, PCBs, PCNs and PCDD/Fs according to their number of aromatic carbon atoms, their hydrophobicity, their degree of chlorination, their planarity and their molecular size. The method was validated for complex environmental mixtures on the basis of two sediment extracts.

Author Keywords: Cytochrome P4501A-inducing compounds

Subject-index terms: Multistep fractionation; Preparative chromatography

Journal of Chromatography A
Volume 986, Issue 1, 31 January 2003, Pages 55-66

This Document
- **Abstract**
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Tobias Kind

Here are some of my postings from the Dejanews archive.

I know I will never beat Uncle Al [2] - but I know he had a problem with cockroaches :-)

- Septumless injectors
- Chemical Nomenclature Software (dilemma)
- Macro use for Agilents Chemstation
- Fast GC
- SPME and Phosphines (in blood)
- EPI Suite with 103.000 structures and CAS Nos
- Literature on peak detection and peak integration
- Reminder: EPI Suite with 103.000 structures and CAS Nos
- Convert HP ChemStation 3D MSD data to ASCII?-1
- Convert HP ChemStation 3D MSD data to ASCII?-2
- HP Chemstation-to-ASCII--YES
- Chemstation_custom_report
- Water as a solvent for GC --> You can - if you want :-)
- Need info from CAS ---> (YES)
- Chloramphenicol
- chrom software?
- Utility of LC/MS/MS system
- Mass Spectrum Prediction (Simulation) software, algorithm
- ultrafiltration-membran
- Agilent Msd Chemstation Macros
- data file conversion [Finnigan-->HP=GCQ2HP]
- Backup 0n QTof
- Antimony removal from power plant waste streams
- New Web Site: SGS-Polymers
- Heat_capacity_of_methylsiloxane
- Nitro-PAH_determination_1
- Nitro-PAH_determination_2
- PAH analysis with fixed fluo emission
- Identifying Unknowns Using TSCA ---> its a nugget !
- Finding unknown substances
- Authentic TXIB
- Finnigan ITDS software
- silanizing glass injector inlets (+++ bargain)
- Advice_on_HPLC_software

.

Von:**Tobias Kind** (tk2002deja@amdis.net) Search Result 7
Betrifft:Re: Septumless injectors
Newsgroups:sci.chem.analytical
Datum:2002-03-21 14:30:09 PST View: Complete Thread (2 articles) | Original Format

"smithski" <smithski@btinternet.com> wrote in message news:<a77b7q$m9u$1@knossos.btinternet.com>...
> Hi,
> Does anyone have any experience of septumless injectors for GC work?

Dear "smithski",

they work fine but you need a special (cylindrical) syringe.

*Check out the JADE injector for most of the available GCs
http://www.alltechweb.com/literature/brochure/B463.pdf

* checkout the needle system
http://www.sisweb.com/sptd/needles.htm

*checkout the GERSTEL septumless head
http://www.gerstelus.com/appnotes/new/Gerstel%202001/an-2001-07.pdf

*try US4954149 and search for 4954149
http://patft.uspto.gov/netahtml/srchnum.htm

*checkout Merlin microseal system
http://www.alltechweb.com/literature/catalog500/205.pdf

Keywords:
septumless GC injection device,
JADE Inlet,
JADE Valve Injector,
Merlin Microseal,
septumless injector,
GERSTEL Septumless Head,
Solid Phase Microextraction,
SPME,
jade valves,
Septumless Inlets,
Split/Splitless injection

With **kind** regards
Tobias Kind

www.amdis.net

Von:Tobias Kind (tk@theo.uoe.ufz.de) Message 1 in thread
Betrifft:Re: Chemical Nomenclature Software (dilemma)
Newsgroups:sci.techniques.mass-spec
Datum:2001-06-08 14:25:07 PST View this article only

A.N. (Tony) Davies wrote:
}Dear Colleagues
}I would be grateful for any feedback you have on the chemical
}nomenclature programs now available on the internet.

Dear Dr. Davies,
if all applets are installed (chime, ISIS, others) - it should
be no problem.

A) The molecule
http://dtpsearch.ncifcrf.gov/data/chemxdb/molfiles/667542.mol

Autonom (http://chemweb.com/autonom) can solve some lager structures like this
one.

The free version of ACD/IUPAC (http://www.acdlabs.com/ilab/)
has some limitations (only 50 atoms) and will not solve this example
in the free version.

(BTW - they had/have really stunning JAVA applets at the beginning/now.)

B) trimethylaluminium (CAS:75-24-1)

Taken as an example from
http://www.acdlabs.com/products/name_lab/iupac/competit.html

<a href="http://chemweb.com/autonom">Autonom cracks up with
error code "ERR-210 = Atom(s) out of range in organic component".

<a href="http://www2.acdlabs.com/ilab/">I-lab cracks up with
{{{DB.SERV_PACK.s_info.s_short_name}}} Request Error internal error.

But it was not an I-Lab internal error -> It was an error of mine. Al(5+)
I redraw it.
Again an error -- ok -- I remember no Al allowed in the free version.

OK.

I go to <a href="http://www.chemfinder.camsoft.com/">Chemfinder
he tells me : Aluminum trimethyl

mmh it sounds better - I remember everything should be in alphabetic
order, or oxidation state ?

Ok - I start to read the IUPAC recommendations
http://www.chem.qmw.ac.uk/iupac/
but I am confused and understand nothing.

I kick-start <a href="http://chem.sis.nlm.nih.gov/chemidplus/">ChemIDPlus:
and he tells me:Aluminum, trimethyl-

I am tired and decide to attand again to an undergraduate chemical naming
class.

What did we learn from this lesson ?
a) Nothing is perfect.
b) Nur der Tod ist umsonst - und der kostet das Leben.
 (Babelfish)

With kind regards
Tobias Kind

PS:
http://www.spectroscopyeurope.com/td_col.html
I am still confused - left or right ?
PPS: not really :-)

Von:Antony Williams (tony@acdlabs.com) Message 2 in thread
Betrifft:Re: Chemical Nomenclature Software (dilemma)
Newsgroups:sci.techniques.mass-spec

Datum:2001-06-10 11:15:05 PST View this article only

Tobias Kind mentioned the Ilab...THe ACD Ilab is web-based as a commercial
service as well as a free version. It does not have the 50 atom limit...

http://www.acdlabs.com/ilab/services.html

****
            Dr. Antony Williams, B.Sc. Ph.D,
Vice President: Scientific Development and Marketing
            Advanced Chemistry Development,
              US Office, The Settlement,
          225 Jamestown Road, Pittsboro,
                           NC-27312

                  Office 919-928-9035
                Cellular 919-201-1516
                  Efax   425-790-3749
              Email   antony.williams@acdlabs.com

    Head office 416-368-3435
      Support   416-368-3435
      Support   support@acdlabs.com
****

Tobias Kind wrote:
A.N. (Tony) Davies wrote:
}}Dear Colleagues
}}I would be grateful for any feedback you have on the chemical
}}nomenclature programs now available on the internet.
}
}Dear Dr. Davies,
}if all applets are installed (chime, ISIS, others) - it should
}be no problem.
}
}*A*) The molecule
}http://dtpsearch.ncifcrf.gov/data/chemxdb/molfiles/667542.mol
}
}Autonom (http://chemweb.com/autonom) can solve some lager structures like
}this one.
}
}The free version of ACD/IUPAC (http://www.acdlabs.com/ilab/)
}has some limitations (only 50 atoms) and will not solve this example
}in the free version.
}
}(BTW - they had/have really stunning JAVA applets at the beginning/now.)
}
}*B*) trimethylaluminium (CAS:75-24-1)
}
}Taken as an example from

}http://www.acdlabs.com/products/name_lab/iupac/competit.html
}
}<a href="http://chemweb.com/autonom">Autonom cracks up with
}error code "ERR-210 = Atom(s) out of range in organic component".
}
}<a href="http://www2.acdlabs.com/ilab/">I-lab cracks up with
}{{{DB.SERV_PACK.s_info.s_short_name}}} Request Error internal error.
}
}But it was not an I-Lab internal error -> It was an error of mine. Al(5+)
}I redraw it.
}Again an error -- ok -- I remember no Al allowed in the free version.
}
}OK.
}
}I go to <a href="http://www.chemfinder.camsoft.com/">Chemfinder
}he tells me : Aluminum trimethyl
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}mmh it sounds better - I remember everything should be in alphabetic
}order, or oxidation state ?
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} (Babelfish)
}
}With kind regards
}Tobias Kind
}
}PS:
}http://www.spectroscopyeurope.com/td_col.html
}I am still confused - left or right ?
}PPS: not really :-)

Alle Beiträge des Diskussionsthemas "**Macro use for Agilents Chemstation**"

Von:Harry Loris (hloris@MailAndNews.com) Message 1 in thread
Betrifft:Macro use for Agilents Chemstation
Newsgroups:sci.techniques.mass-spec
Datum:2001-03-13 17:26:06 PST View this article only

```
Hi there,

can anybody tell me if the new version (C) of Chemstation supplies some
commands to use the printer in landscape mode for graphics?

thank you


Harald Loris
ESR
Porirua

-------------------------------------------------------------
 Get your FREE web-based e-mail and newsgroup access at:
                http://MailAndNews.com

 Create a new mailbox, or access your existing IMAP4 or
 POP3 mailbox from anywhere with just a web browser.
-------------------------------------------------------------
```

Von:Tobias Kind (kind@rziris.rz.uni-leipzig.de) Message 2 in thread
Betrifft:Re: Macro use for Agilents Chemstation
Newsgroups:sci.techniques.mass-spec
Datum:2001-03-14 10:22:15 PST View this article only

```
Good Morning  Mr. Loris


} can anybody tell me if the new version (C) of Chemstation supplies some
} commands to use the printer in landscape mode for graphics?

I know, you asked for the (C) version.

Believing in the continuation of HPs software, this would be
a inexcusable and unforgivable and unpardonable mistake, or
lets say an fundamental error if AGILENT in an
monitored approach of megalomania has changed some
variables. (I don't believe :-)

In the (B) version of HP Chemstations fabulous macro language
the variable is :

ORIENTPR = 1 for portrait mode printing and
ORIENTPR = 2 for landscape mode.

This variable is defined in cpres.dll

You can find (or have still found) some example macros in the
file macros.mac or msda.mac.

------

If I am wrong - you can use (for yourself) the good old method
```

of printing the graphic in a postscript file - using the landscape
function in the printer settings (f.e., Schlumberger printer, or
Laserjet 5 MP/PS). Later you can load it via PowerPoint or
CorelDraw. This works with any software (I guess :-)

If I am double wrong - use the software FinePrint 2000.

With kind regards
Tobias Kind

PS: triple wrong... Quadrupol wrong ?

Von:Peter Frank (peter@acdlabs.com) Message 3 in thread
Betrifft:Re: Macro use for Agilents Chemstation
Newsgroups:sci.techniques.mass-spec

Datum:2001-03-19 12:42:03 PST View this article only

Advanced Chemistry Development's MS/Manager provides flexible reporting
functions that you may be interested in.

Reports can be printed directly in from the module, or copied to our
ChemSketch software. When using ChemSketch, all of your report elements
(including fragmentsassignments) become drawing objects, chemical
structures, or tables. Providing maximum flexibility in formating since
these objects can be resized, and positioned as required.

Since ChemSketch is free, this will allow distrubution of reports can be
done electronically. As well ChemSketch can save in a variety of formats,
and all objects are OLE compliant and will therefore Cut and Paste to any
Windows Application.

ACD MS/Manager supports marco processing, and will read most ChemStation
formats. I would welcome the opportunity to show you the features MS
Manager has to offer your laboratory. In the meantime, more information
about ACD/MS manager can be found at:
http://www.acdlabs.com/products/spec_lab/exp_spectra/ms/

Regards,
Peter Frank
Customer Support Specialist
Advanced Chemistry Development, Inc.
90 Adelaide St. West, Suite 702
Toronto, ON
Canada M5H 3V9
Phone: 416-368-3435 x243
Fax: 416-368-5596
URL: http://www.acdlabs.com

Tobias Kind <kind@rziris.rz.uni-leipzig.de> wrote in message
news:98ocgb$i8s$1@news-int.gatech.edu...
} Good Morning Mr. Loris
}
}
} } can anybody tell me if the new version (C) of Chemstation supplies some
} } commands to use the printer in landscape mode for graphics?
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```
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} CorelDraw. This works with any software (I guess :-)
}
} -----
}
} If I am double wrong - use the software FinePrint 2000.
}
} With kind regards
} Tobias Kind
}
} PS: triple wrong... Quadrupol wrong ?
}
}
}
```

Alle Beiträge des Diskussionsthemas "**Fast GC**"

Von:c.z42@gmx.net (c.z42@gmx.net) Message 1 in thread
Betrifft:Fast GC
Newsgroups:sci.techniques.mass-spec
Datum:2001-09-19 06:35:07 PST View this article only

I have to present some applications of Fast-GC to our MS hardware
developers. Does anyone have good referneces where Peaks with widths of
less than 1 second are shown ?

Von:Tobias Kind (kind@rziris.rz.uni-leipzig.de) Message 2 in thread
Betrifft:Re: Fast GC
Newsgroups:sci.techniques.mass-spec
Datum:2001-09-20 05:30:03 PST View this article only

"c.z42@gmx.net" wrote:

} I have to present some applications of Fast-GC to our MS hardware
} developers. Does anyone have good referneces where Peaks with widths of
} less than 1 second are shown ?

Dear Carsten,

* ten compounds within 500 ms
Evaluation of time-of-flight mass spectrometric detection for fast gas
chromatography,
Journal of Chromatography A, Volume 878, Issue 2, 12 May 2000, Pages
205-213
M. M. van Deursen, J. Beens, H. -G. Janssen, P. A. Leclercq and C. A.
Cramers

* Fast, Very Fast, and Ultra-Fast Gas Chromatography-Mass Spectrometry of
Thermally Labile Steroids,
Carbamates, and Drugs in Supersonic Molecular Beams
S. Dagan and A. Amirav. J. Am. Soc. Mass Spectrom. 7 (1996), p. 737.

Prof. Amirav also has a page with a fine book showing a lot of gc-runs with
times
under 250 msecs. http://www.tau.ac.il/chemistry/amirav/smbms.shtml

*High-speed gas chromatography: an overview of various concepts,
Journal of Chromatography A, Volume 856, Issues 1-2, 24 September 1999,
 Pages 315-329 Carel A. Cramers, Hans-Gerd Janssen, Marieke M. van Deursen
and Piet A. Leclercq

* also JChromA : Vol 842 and Vol 856 have some articles and
High-speed gas chromatography: an overview of various concepts, Pages
315-329
Carel A. Cramers, Hans-Gerd Janssen, Marieke M. van Deursen and Piet A.
Leclercq
Volume 856, Issues 1-2,

shows this often copied sample (separation of alkanes within 600 ms
from van Es, 2xCramers,Rijks - HRC 11 (1988) very nice ...

*Flash GC
Instrumentation and applications of fast high-resolution capillary gas
chromatography,

Journal of Chromatography A, Volume 842, Issues 1-2, 21 May 1999, Pages
309-319
F. David, D. R. Gere, F. Scanlan and P. Sandra

You will also find alot of other examples (peak width < 1sec) if you search
for applications from
* LECO PEGASUS II
* Restek Flash-GC (EZ-Flash)
* keywords GCxGC comprehensive GC from Analytical Chemistry

With kind regards
Tobias Kind

PS: What means low-cost for the SensiTOF ?
Under 50.000 Euro ?

Von:Don Drinkwater (drinkwd@basf-corp.com) Message 3 in thread
Betrifft:Re: Fast GC
Newsgroups:sci.techniques.mass-spec
Datum:2001-09-20 06:20:04 PST View this article only

I used to do a lot of "fast" GC/MS when I worked for Texaco. There is
a chapter in the recent book "Current Practice of Gas
Chromatography-Mass Spectrometry" edited by W.M.A. Niessen (publisher
Marcel-Dekker) authored by myself and Sam Hsu which shows on pg. 70 a
30-second blow-up of overlaid mass chromatograms of gasoline (we
implemented a 90-min ASTM D5769 method as a 9 min. method on a 0.10mm
ID column). The peaks are about 1 second at the base and 0.4 seconds
at half-height. The quad was scanning at 20 scans/second to get good
profiles.

Hope this helps.
Sincerely,

Don Drinkwater

Von:Phil (gothics@free.fr) Message 4 in thread
Betrifft:Re: Fast GC
Newsgroups:sci.techniques.mass-spec
Datum:2001-09-20 07:30:04 PST View this article only

You can also check the applications published by ThermoFinnigan on their
Website

Von:Karen (karencee@yahoo.com) Message 5 in thread
Betrifft:Re: Fast GC
Newsgroups:sci.techniques.mass-spec
Datum:2001-09-20 17:45:04 PST View this article only

I do the comprehensive two-dimensional gas chromatography (GCxGC) mentioned
by the post below. In complex samples, I have observed up to 20 peaks in a
10 second chromatogram with peak widths ranging between 100 and 200 msec.
The big difference between my work and the references listed below is that
those chromatograms go from start to finish in a second or two and have 10
peaks, while in GCxGC there will be several hundred sequential fast
chromatograms, each containing numerous 100 msec wide peaks. Since the
total analysis can run to several hours, the 100-200 Hz mass spectrum rate
will produce massive data files.

Glenn Frysinger

"Tobias Kind" <kind@rziris.rz.uni-leipzig.de> wrote in message
news:9ocnd4$1b4$1@news-int.gatech.edu...
}
}
} "c.z42@gmx.net" wrote:
}
} } I have to present some applications of Fast-GC to our MS hardware

} } developers. Does anyone have good referneces where Peaks with widths of
} } less than 1 second are shown ?
}
} Dear Carsten,
}
} * ten compounds within 500 ms
} Evaluation of time-of-flight mass spectrometric detection for fast gas
} chromatography,
} Journal of Chromatography A, Volume 878, Issue 2, 12 May 2000, Pages
} 205-213
} M. M. van Deursen, J. Beens, H. -G. Janssen, P. A. Leclercq and C. A.
} Cramers
}
} * Fast, Very Fast, and Ultra-Fast Gas Chromatography-Mass Spectrometry of
} Thermally Labile Steroids,
} Carbamates, and Drugs in Supersonic Molecular Beams
} S. Dagan and A. Amirav. J. Am. Soc. Mass Spectrom. 7 (1996), p. 737.
}
} Prof. Amirav also has a page with a fine book showing a lot of gc-runs with
} times
} under 250 msecs. http://www.tau.ac.il/chemistry/amirav/smbms.shtml
}
} *High-speed gas chromatography: an overview of various concepts,
} Journal of Chromatography A, Volume 856, Issues 1-2, 24 September 1999,
} Pages 315-329 Carel A. Cramers, Hans-Gerd Janssen, Marieke M. van Deursen
} and Piet A. Leclercq
}

Lesen Sie den Rest der Nachricht... *(38 zusätzliche Zeilen)*

Alle Beiträge des Diskussionsthemas "**SPME and Phosphines (in blood)**"

Von:Harry Loris (hloris@MailAndNews.com) Message 1 in thread
Betrifft:SPME and Phosphines (in blood)
Newsgroups:sci.techniques.mass-spec
Datum:2001-04-30 06:40:02 PST View this article only

Looking for this akward combination. Has naybody done or heard something
about
it before? Thank you in advance

Harry

Von:Tobias Kind (kind@rziris.rz.uni-leipzig.de) Message 2 in thread
Betrifft:Re: SPME and Phosphines (in blood)
Newsgroups:sci.techniques.mass-spec
Datum:2001-04-30 09:30:08 PST View this article only

Dear Harry,

Harry Loris wrote:
SPME and Phosphines (in blood)

} Looking for this akward combination. Has naybody done or heard something
} about
} it before? Thank you in advance

I don't want to "pester" you , but

* Which phosphine_s_ ? There are thousands (possible)

there is a difference if you want to measure trimethyl- or
triphenyl-phosphines or GeH5P or
(1,1-dimethylethyl)[5-methyl-2-(1-methylethyl)cyclohexyl](phenylmethyl)-
phosphine
...
  (Kow,Bp,volatility)

* Which analysis method ? GC, HPLC ,CE ?
  ..maybe not so important.

* SPME ?? want to do HEADSPACE or DIRECT ?
   ...maybe not so important.

Maybe there is no direct method from a color prospect,
but you can take for volatiles (trimethyl) (bad peaks):

The measurement of volatile constituents in Foray 48B, an insecticide
prepared from Bacillus thuringiensis var. kurstaki, C. van Netten et al.

The Science of the Total Environment 263 2000 155-160

or for triphenylphoshine (Henry constant = 2.26E-008 atm-m3/mole,
logP=5.69) you have to put the fiber in to the solution (a lot of problems
will occour)

or you are doing first a liquid-liquid extraction or any other
sample preparation...or:

I think - first choose the molecule, second can take any other SPME-BLOOD
method for a molecule with similiar properties.

Or maybe you can tell us the problems which occoured during analysis...

With kind regards
Tobias Kind

Von:**Tobias Kind** (kind@rziris.rz.uni-leipzig.de)
Search Result 4
Betrifft:EPI Suite with 103.000 structures and CAS Nos
Newsgroups:sci.chem.analytical
Datum:2001-09-10 14:34:56 PST
View: (This is the only article in this thread) | Original Format

Hi,
I recommend to use the freely available (copyrighted) EPA EPI suite:

It contains some 103.000 structures + CAS numbers (SMILECAS database)
and (PHYSPROP database) with around 25,000 compounds with
experimental data (logP, bp, henry..) and you can also calculate
a lot of physico-chemical properties.

Instead of repeating all the important things from
http://www.epa.gov/opptintr/exposure/docs/episuite.htm
I will pick out some things:

   AOPWIN - estimates atmospheric oxidation rates
   BCFWIN - estimates bioconcentration factor (BCF)
   BIOWIN - estimates biodegradation probability
   ECOSAR - estimates aquatic toxicity (LD50, LC50)
   HENRYWIN - estimates Henry's law constant
   HYDROWIN - estimates aqueous hydrolysis rates (acid-, base-catalyzed)

   KOWWIN - estimates octanol-water partition coefficient
   MPBPWIN - estimates melting point, boiling point, and vapor pressure
   PCKOCWIN - estimates soil sorption coefficient (Koc)
   WSKOWWIN - estimates water solubility
   DERMWIN - Dermal Permeability Program
   STPWIN - (Sewage Treatment Plant Fugacity Model)
   WVOLWIN - (Volatilization Rate from Water)
   LEVEL3NT - (Level III Fugacity Model)

* EPIWIN allows batch file input for a large number of compounds

* MPBWIN has an experimental database of
11347 compounds (8948 melting points, 6381 boiling points,
and 2857 vapor pressures) - this may be useful for retention time
fitting (assuming same class of compounds).

* KowWIN - contains a database of 13200 experimental log P values.
and also a algorithm for calculating unknowns via smiles structure
input.
(Please take care: blind usage of calculated logP values is like walking
in a mine field:-)
further reading: http://www.lnh.unil.ch/Appl/cchem2.html
and http://esc.syrres.com/interkow/kowdemo.htm

* I also recommend to read:
Identifying Unknowns with "Spectraless" Databases from James Little
http://users.chartertn.net/slittle/files\TSCA_Poster%20Session.pdf
from http://users.chartertn.net/slittle/tsca.html
because it gives some important hints how mass spectra and mol masses
and databases can be linked together.

* Some rare EPIWIN examples for testing
Consul : (CAS 86479-06-3)
Fc1cccc(F)c1C(=O)NC(=O)Nc2cc(Cl)c(OC(F)(F)C(F)F)c(Cl)c2
Transfluthrin: (CAS 118712-89-3)

Fc1c(F)cc(F)c(F)c1COC(=O)C2C(C)(C)C2C=C(Cl)Cl

With kind regards
Tobias Kind

PS: Thanks to U.S.EPA Office of Pollution Prevention Toxics
and Syracuse Research Corporation (SRC) and ...

PPS: Try the incredible CACTVS system at
http://www2.ccc.uni-erlangen.de/ncidb2
It has enhanced features now - this is truly a state-of-the-art "open
database concept"
it has dozen of (multiple) input and output options. Try molsurf and
orbvis!

PPPS: Most molecular editors and some java applets import and export
smiles.
If you have a CAS number you can now use SMILECAS or CHEMIDplus - later
Merlin or ISIS/Base or whatyouwant for a structural
similarity/substructure search.
After data retrieval you can search with the obtained structures
for similiar mass spectra or substructures using NIST MS search V2.0
http://www.nist.gov/srd/nist1a.htm

PPPPS: if you want more information about PPPS you should change
to news:sci.techniques.mass-spec (without any additional cost:-)

Von:**Tobias Kind** (kind@rziris.rz.uni-leipzig.de) Search Result 17
Betrifft:Re: Literature on peak detection and peak integration
Newsgroups:sci.techniques.mass-spec
Datum:2001-02-01 05:35:09 PST View: Complete Thread (2 articles) | Original Format

Dear Mr. Tang,

as good introductions you can read

wilfred_tang@yahoo.com wrote:

} I am interested in peak detection and peak integration. Given a

as good introductions you can read

"An Integrated Method for Spectrum Extraction and Compound Identification
from GC/MS Data"
by Steven E.Stein from NIST "AMDIS Method Paper"
http://chemdata.nist.gov/mass-spc/amdis/

and also

"Peak distortion, data sampling errors and the integrator in the
measurement of
very narrow chromatographic peaks " by Norman Dyson.
Journal of Chromatography A, Volume 842, Issues 1-2, 21 May 1999, Pages
321-340
(From every chemistry library and from http://ww.sciencedirect.com)

With kind regards
Tobias Kind

Von:**Tobias Kind** (kind@rziris.rz.uni-leipzig.de)

Search Result 5

Betrifft:Reminder: EPI Suite with 103.000 structures and CAS Nos

Newsgroups:sci.techniques.mass-spec

Datum:2001-09-10 13:50:03 PST

Dear Colleagues,

an "integrated approach" for GC-MS and LC-MS analysis
(small molecules) may improve our lab work - therefore
I recommend to use the freely available (copyrighted) EPA EPI suite:

It contains some 103.000 structures + CAS numbers (SMILECAS database)
and (PHYSPROP database) with around 25,000 compounds with
some experimental data (logP, bp, henry..) and you can also calculate
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   MPBPWIN - estimates melting point, boiling point, and vapor pressure
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   LEVEL3NT - (Level III Fugacity Model)

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(Please take care: blind usage of calculated logP values is like walking
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Transfluthrin: (CAS 118712-89-3)
Fc1c(F)cc(F)c(F)c1COC(=O)C2C(C)(C)C2C=C(Cl)Cl
Viridicatin (CAS 129-24-8) remember ?
c(ccc1C(c(ccc2)c(c2)N3)=C(O)C3=O)cc1

With kind regards
Tobias Kind

P.S.: Thanks to U.S.EPA Office of Pollution Prevention Toxics
and Syracuse Research Corporation (SRC) and ...

P.P.S.: Try the incredible CACTVS system at
http://www2.ccc.uni-erlangen.de/ncidb2
It has enhanced features now - this is truly a state-of-the-art "open
database concept"
it has dozen of (multiple) input and output options. Try molsurf and
orbvis!

P.P.P.S.: Most molecular editors and some java applets import and export
smiles.
If you have a CAS number you can now use SMILECAS or CHEMIDplus - later
Merlin or ISIS/Base or whatyouwant for a structural
similarity/substructure search.
After data retrieval you can search with the obtained structures
for similiar mass spectra or substructures using NIST MS search V2.0
http://www.nist.gov/srd/nist1a.htm

Beiträge 1-10 des Diskussionsthemas "**Convert HP ChemStation 3D MSD data to ASCII?**"

Nächste 4

Springen zu [Ende des Diskussionsthemas]

Von:Pham Tuan Hai (PhamTuanHai@rocketmail.com) Message 1 in thread
Betrifft:Convert HP ChemStation 3D MSD data to ASCII?
Newsgroups:sci.techniques.mass-spec
Datum:2001-08-14 05:25:38 PST View this article only

Dear all,

I am new to the list and do not know if the problem has been voiced an answered
before. If yes, pls point me to the right direction.

I am looking for a way to convert the entire HP Chemstation MSD data file into
ASCII format. It can be a macro or an independent program. I have found in the
ChemStation itself only a feature to convert either selected chromatogram or
spectrum to an ASCII file. Does anyone have experience with the same problem?

Thanks a lot for your help,
Dr. Pham Tuan Hai
Unilever Research Vlaardingen
Central Analytical Sciences / A4471
Postbox 114
3130 AC Vlaardingen
The Netherlands
Tel: 0031-10-460 55 46
Fax: 0031-10-460 56 71

Von:Pham Tuan Hai (PhamTuanHai@rocketmail.com) Message 2 in thread
Betrifft:Re: Convert HP ChemStation 3D MSD data to ASCII?
Newsgroups:sci.techniques.mass-spec
Datum:2001-08-14 10:07:17 PST View this article only

Oh, I have but did not find the right answer. Maybe somebody else has done it.
Thanks anyway.
Hai

--- stms <cminvms@acme.gatech.edu> wrote:
} Try the archived questions/answers at the sci.techniques.mass-spec website
} at <http://www.chemistry.gatech.edu/stms> under archives-by-topic in the
} computer section.
} Thanks,
} Sarah Shealy
} backup moderator for sci.techniques.mass-spec
}
} At 05:02 AM 8/14/01 -0700, you wrote:
} }Dear all,
} }
} }I am new to the list and do not know if the problem has been voiced an
} }answered
} }before. If yes, pls point me to the right direction.
} }
} }I am looking for a way to convert the entire HP Chemstation MSD data file into
} }ASCII format. It can be a macro or an independent program. I have found in the

} }ChemStation itself only a feature to convert either selected chromatogram or
} }spectrum to an ASCII file. Does anyone have experience with the same problem?
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} }Thanks a lot for your help,
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} }Unilever Research Vlaardingen
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} }Postbox 114
} }3130 AC Vlaardingen
} }The Netherlands
} }Tel: 0031-10-460 55 46
} }Fax: 0031-10-460 56 71
} }
} }_____
} }Do You Yahoo!?
} }Make international calls for as low as $.04/minute with Yahoo! Messenger
} }http://phonecard.yahoo.com/
}

_____
Do You Yahoo!?
Make international calls for as low as $.04/minute with Yahoo! Messenger
http://phonecard.yahoo.com/

Von:David Sparkman (ods@compuserve.com) Message 3 in thread
Betrifft:Re: Convert HP ChemStation 3D MSD data to ASCII?
Newsgroups:sci.techniques.mass-spec
Datum:2001-08-17 06:20:08 PST View this article only

There is a program from ChemSW that will do this. http://www.chemsw.com. The program is called GC GCMS File Translator. There are two versions. You probably can get by with the cheaper one. There is also a program available from Palisade software, http://www.palisade.com, for a lot more money. This is called Mass Transit.

The subject line of your message makes me think that you believe that both MS and chromatographic data are stored in a GC/MS or LC/MS data file. This is incorrect. The data stored are mass spectral data of m/z value and intensity pairs for each spectrum acquired. Chromatograms are reconstructed from these mass spectral data either by summing all the intensities with in each mass spectrum and plotting this summed intensity as a function of the spectrum number, which is also a function of time (the reconstructed total ion current chromatogram -- RTICC) or by plotting the intensities of one are more ions with in each mass spectrum as a function of time (the mass chromatogram -- or RIC on the ChemStation).

Regards;

David

--
O. David Sparkman
Consultant-At-Large
ods@compuserve.com
"Pham Tuan Hai" <PhamTuanHai@rocketmail.com> wrote in message
news:9lbljltp1@news-int.gatech.edu...
} Oh, I have but did not find the right answer. Maybe somebody else has done it.
} Thanks anyway.
} Hai
}
} --- stms <cminvms@acme.gatech.edu> wrote:
} } Try the archived questions/answers at the sci.techniques.mass-spec website
} } at <http://www.chemistry.gatech.edu/stms> under archives-by-topic in the
} } computer section.
} } Thanks,
} } Sarah Shealy
} } backup moderator for sci.techniques.mass-spec
} }

} } At 05:02 AM 8/14/01 -0700, you wrote:
} } }Dear all,
} } }
} } }I am new to the list and do not know if the problem has been voiced an
} } }answered
} } }before. If yes, pls point me to the right direction.
} } }

Lesen Sie den Rest der Nachricht... *(38 zusätzliche Zeilen)*

Von:Joerg Hau (joerg.hau@swissonline.ch) Message 4 in thread
Betrifft:Re: Convert HP ChemStation 3D MSD data to ASCII?
Newsgroups:sci.techniques.mass-spec
Datum:2001-08-17 14:25:04 PST View this article only

On Tue, 14 Aug 2001 05:02:03 -0700 (PDT), Pham Tuan Hai wrote:

} I am looking for a way to convert the entire HP Chemstation MSD data file into
} ASCII format. It can be a macro or an independent program.

I don't know what you want to do with these ASCII data, and I don't
know in which form you need them, so I have to guess ... but three
possibilities come to mind:

(1) Export dataset as netCDF file, then use 'MSGraph' (available at
http://www.mysunrise.ch/users/joerg.hau/sci/msgraph/). This program can
export mass spectra, chromatograms or a complete run (!) as ASCII
data. However, it's limited to integer mass processing.

(2) Export dataset as netCDF file (as above), then use a home-made
program to access the netCDF data directly. 'cdf2msg' is available at
the same URL as above (with source code) and will require only a few
modifications to do what you need.

(3) ... and of course you could [have someone] write a macro that writes
them out spectrum-by-spectrum, but that's programming-at-large again.

HTH,

-- Joerg

---
joerg.hau(at)swissonline.ch * Lausanne, Switzerland
http://www.diax.ch/users/joerg.hau/
"All standard disclaimers apply".

Von:Tobias Kind (kind@rziris.rz.uni-leipzig.de) Message 5 in thread
Betrifft:Re: Convert HP ChemStation 3D MSD data to ASCII?
Newsgroups:sci.techniques.mass-spec
Datum:2001-08-18 09:40:03 PST View this article only

Pham Tuan Hai wrote:

} I am looking for a way to convert the entire HP Chemstation MSD data file into
} ASCII format. It can be a macro...

Nazdar,

!HP2ASCII.MAC starts here

```
name HP2ASCII
!***
!*** this macro fully converts a HP Chemstation file to ASCII or JCAMP-DX
!*** (c)TK4ICBINB
!*** if an error occours during macro execution:false line break in macro
!***
```

```
!***(1) load a GC-MS file in HP Chemstation
!***(2) Choose Options Dialog Box --> Command line
!***(3) enter "macro" at command line and load HP2ASCII
!***(4) enter HP2ASCII at the command line to start
!***(5) Choose an option TIC+MS, TIC, JCAMP-DX
!***(6) Read in with XCL with ";" separator
!***    (from the actual HP data path)
!***
!*** possible files are : xMSspec.txt, xspecrow.txt,
!***                              xTIConly.txt , JCMPGCMS.jdx
!*** BEWARE: XCL can read only a 256x65536 matrix!!! Yes 3x!



  LOCAL label, button, choice
  SDim label, 4
  SDim button, 3
  label[1] = "TIC+spectra nice output"
  label[2] = "TIC+spectra ín one line"
  label[3] = "Only TIC"
  label[4] = "JCAMP 4 Lib2NIST"
  button[1] = ""
  button[2] = "OK"
  button[3] = ""
  choice = 1
  INPUT6 3, 4,"HP2ASCII", label, button, choice
  mychoice = choice

  POINTS R0  ! Get scan range in NPOINTS
  lowscan = 1
  highscan = NPOINTS

  if (mychoice = 1) then
      NiceOutput
  endif
  if (mychoice = 2) then
      LineOutput
  endif
  if (mychoice = 3)  then
      TICOutput
  endIF
  if (mychoice = 4)  then
      JCAMP4Lib2NIST
  endIF

CLOSE #1
Alert "Beware: EXCEL is only 8-bit!",2
return



name NiceOutput
  fileName$ = _DATAPATH$+_DATAFILE$ + "\xMSspec.txt"
  OPEN fileName$ FOR OUTPUT AS #1
 !change for header line output
  PRINT USING #1,"%;%;%;%;%;%/","Scan","Time","TIC","MSPeaks","Mass","Abund"
  i = 1
  while i <= highscan
    scan i
    points x !get the number of spectra points

    !***array starts from 0 , scans start from 1 aarrgghh
    PRINT USING #1, "#;#.###;#;#/",i,r0[i-1,0],r0[i-1,1],NPOINTS

    !**************************************
    !*** write out the mass pairs
    masscount = 0 !array starts from zero
    while masscount < NPOINTS

    !*** take care !
    !*** if you want true mass values use #.###
```

```
    !*** and remove the round() function
    !*** give out mass, abundance
    print using #1 ,";;;;#.##;#/",round(x[masscount,0]),x[masscount,1]

    masscount = masscount+1
    endwhile
    !**************************************
    i = i+1
    print i
  endwhile
return


name LineOutput

  fileName$ = _DATAPATH$+_DATAFILE$ + "\xspecrow.txt"
  OPEN fileName$ FOR OUTPUT AS #1
  !header line output
  PRINT USING #1,"%;%;%;%;%;%/","Scan","Time","TIC","MSPeaks","Mass","Abund"

  i = 1
  while i <= highscan
    scan i
    points x !get the number of spectra points

    !***array starts from 0 , scans start from 1 aarrgghh
    PRINT USING #1, "#;#.###;#;#",i,r0[i-1,0],r0[i-1,1],NPOINTS

    !**************************************
    !*** write out the mass pairs
    masscount = 0 !array starts from zero
    while masscount < NPOINTS
      ! All spectra in one line
      print using #1 ,";#.##;#",round(x[masscount,0]),x[masscount,1]
    masscount = masscount+1
    endwhile
    !**************************************
    print using #1, "/"
    i = i+1
    print i
  endwhile
return

name TICOutput
  fileName$ = _DATAPATH$+_DATAFILE$ + "\xTIConly.txt"
  OPEN fileName$ FOR OUTPUT AS #1
  PRINT USING #1, "%;%;%;%;/","Scan","Time","TIC","MSPeaks"
  i = 1
  while i <= highscan
    scan i
    points x !get the number of spectra points
    !***array starts from 0 , scans start from 1 aarrgghh
    PRINT USING #1, "#;#.###;#;#/",i,r0[i-1,0],r0[i-1,1],NPOINTS
    i = i+1
    print i
  endwhile
return

name JCAMP4Lib2NIST
! HP Chemstation GC-MS file to JCAMP-DX (HP2JCAMP)
! my contribution to the IUPAC year :-)
! but anyway, it would be better to use AMDIS32  and Lib2NIST
! and use only pure extracted peaks...
! for JCAMP look at
! http://wwwchem.uwimona.edu.jm:1104/software/jcampdx.html
! http://www.isas-dortmund.de/projects/jcamp/
! no compressed format -> ever built a hashtable in Chemstation ?

fileName$ = _DATAPATH$+_DATAFILE$ + "\JCMPGCMS.jdx"
OPEN fileName$ FOR OUTPUT AS #1
```

```
  i = 1
  while i <= highscan
    scan i
    points x !get the number of spectra points

    !***array starts from 0 , scans start from 1 aarrgghh
    PRINT USING #1, "% % %#/","##TITLE=",_DATAFILE$,"Scan ",i
    PRINT #1, "##JCAMPDX= Revision 5.0"
    PRINT #1, "##DATA TYPE= MASS SPECTRUM"
    PRINT #1, "##DATA CLASS= PEAK TABLE"
    PRINT #1, "##XUNITS= m/z"
    PRINT #1, "##YUNITS= RELATIVE ABUNDANCE"
    PRINT USING #1, "% #/", "##NPOINTS=", NPOINTS
    PRINT #1, "##PEAK TABLE= (XY..XY)"

    !**************************************
    !*** write out the mass pairs
    masscount = 0 !array starts from zero
    while masscount < NPOINTS

    !*** take care !
    !*** if you want true mass values use #.###
    !*** and remove the round() function
    !*** give out mass, abundance
    print using #1 ,"# #/",round(x[masscount,0]),x[masscount,1]

    masscount = masscount+1
    endwhile
    !**************************************
    i = i+1
    print i
  endwhile

return

!*** HP2ASCII.MAC ends here

With kind regards
Tobias Kind


PS:
I still can´t decide wether to take ICBINB
http://www.tasteyoulove.com/product/index.html
or My Three Suns
http://home.nikocity.de/stoesser/Tierrechte/txt/futurama.html
:-)
```

Von:Dave White (dave_white@spectrachrom.com) Message 6 in thread
Betrifft:Re: Convert HP ChemStation 3D MSD data to ASCII?
Newsgroups:sci.techniques.mass-spec
Datum:2001-08-18 09:40:03 PST View this article only

Just to be pedantic :-) ChemStation files actually store the RTICC
information in the data file. Each scan has a header record which specifies
the number of peaks in the scan, the base peak, retention time, etc, and
also the TIC for that scan.

--
Dave White
SpectraChrom Software
www.spectrachrom.com
dave(underscore)white@spectrachrom.com   replace the (underscore) with _ to
e-mail directly

"David Sparkman" <ods@compuserve.com> wrote in message
news:9lj5lsauj1@news-int.gatech.edu...

snip

} is incorrect. The data stored are mass spectral data of m/z value and
} intensity pairs for each spectrum acquired. Chromatograms are reconstructed
} from these mass spectral data either by summing all the intensities with in
} each mass spectrum and plotting this summed intensity as a function of the
} spectrum number, which is also a function of time (the reconstructed total
} ion current chromatogram -- RTICC) or by plotting the intensities of one
are

Von:Phil (gothics@free.fr) Message 7 in thread
Betrifft:Re: Convert HP ChemStation 3D MSD data to ASCII?
Newsgroups:sci.techniques.mass-spec
Datum:2001-08-18 11:10:04 PST View this article only

Tobias,

Good stuff, however Pham requires a macro for the LC/MS CHEMSTATION and it
ain't the same
macro language or at least a lot different !!

Phil

"Tobias Kind" <kind@rziris.rz.uni-leipzig.de> a écrit dans le message news:
9lm5im$7h1$1@news-int.gatech.edu...
}
}
} Pham Tuan Hai wrote:
}
} } I am looking for a way to convert the entire HP Chemstation MSD data file into
} } ASCII format. It can be a macro...
}
}
}
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} !*** (c)TK4ICBINB
} !*** if an error occours during macro execution:false line break in macro
} !***
} !***(1) load a GC-MS file in HP Chemstation
} !***(2) Choose Options Dialog Box --> Command line
} !***(3) enter "macro" at command line and load HP2ASCII
} !***(4) enter HP2ASCII at the command line to start
} !***(5) Choose an option TIC+MS, TIC, JCAMP-DX
} !***(6) Read in with XCL with ";" separator
} !***   (from the actual HP data path)
} !***
} !*** possible files are : xMSspec.txt, xspecrow.txt,
} !***   xTIConly.txt , JCMPGCMS.jdx
} !*** BEWARE: XCL can read only a 256x65536 matrix!!! Yes 3x!
}
}
}
}   LOCAL label, button, choice
}   SDim label, 4
}   SDim button, 3
}   label[1] = "TIC+spectra nice output"

Lesen Sie den Rest der Nachricht... *(183 zusätzliche Zeilen)*

Von:Volker Haeupl (vh@quasium.de) Message 8 in thread
Betrifft:Re: Convert HP ChemStation 3D MSD data to ASCII?
Newsgroups:sci.techniques.mass-spec
Datum:2001-08-19 18:45:03 PST View this article only

Ehmmm ... to be even more pedantic ;-) the ChemStation data
file also has so called "directory records" behind all the spectral
records which consist of
 1 - a pointer to the spectral record,
 2 - retention time, and
 3 - total ion abundance at this retention time.
Neglecting the pointer, this basically is the Total Ion Chromatogram!

This and more details were documented in the HP-UX ChemStation
manual, for instance.

Volker Haeupl - vh@quasium.com

"Dave White" <dave_white@spectrachrom.com> wrote in message
} news:9lm5k0$7h4$1@news-int.gatech.edu...
} Just to be pedantic :-) ChemStation files actually store the RTICC
} information in the data file. Each scan has a header record which specifies
} the number of peaks in the scan, the base peak, retention time, etc, and
} also the TIC for that scan.
}
} --
} Dave White
} SpectraChrom Software
} www.spectrachrom.com
} dave(underscore)white@spectrachrom.com   replace the (underscore) with _ to
} e-mail directly

Von:Pham Tuan Hai (PhamTuanHai@rocketmail.com) Message 9 in thread
Betrifft:Re: Convert HP ChemStation 3D MSD data to ASCII?
Newsgroups:sci.techniques.mass-spec
Datum:2001-08-20 04:35:06 PST View this article only

Hi Tobias, Phil, Joerg et all.

Yes, sorry that I did not make it clear in the first message (call for help). I
was talking about the LC/MS data and it seems that the macro you've sent me is
not compatible. I tried to load it into the ChemStation and got the syntax
error message.

The HP ChemStation does not have to ability to export data set into net CDF
file, so the option to use MSgraph is also not OK.

I should explain a bit more about the purpose of having data in the ASCII
format. We want to play around with retention time shifting problem, then do
the PCA analysis for a set of data. This will be done by an data science guy in
our group. I am responsible for providing the data, but he will need them in
ASCII format to play around. Data taken on the MassLynx system has no such
problem due to the built in option for conversion. HP does not provide an
explicite function. That why I am asking for help.

Hai

Von:Tobias Kind (kind@rziris.rz.uni-leipzig.de)
Message 10 in thread
Betrifft:Re: Convert HP ChemStation 3D MSD data to ASCII?
Newsgroups:sci.techniques.mass-spec
Datum:2001-08-20 06:28:29 PST
View this article only

Phil wrote:

} Tobias,
}
} Good stuff, however Pham requires a macro for the LC/MS CHEMSTATION and it
} ain't the same
} macro language or at least a lot different !!

Dear Phil,

yes! But my data system also has a RP18 column in the Agilent picture book. :-)
or :-(

[Maybe Pham Tuan Hai can answer if he has HP G1047A LC/MS Software or G2710AA
system ?
he already answered]

And I know Lin DeNoyer claims to know how to read HP LC/MS ChemStation data.

And maybe he can send the header format and I will write a converter for a
piece of ICBINB...

PS:

Mmmhh... Philippe I found you in 167 out of my 1400 macros - so I guess
you also know the HP 3D LC/MS Chemstation format ?? :-)

Nächste 4
Springen zu [Ende des Diskussionsthemas]

Beiträge 11-14 des Diskussionsthemas "**Convert HP ChemStation 3D MSD data to ASCII?**"

Vorherige 10

Springen zu [Anfang des Diskussionsthemas]

Von:oblada oblado (obladi63@yahoo.com) Message 11 in thread
Betrifft:Re:Convert HP ChemStation 3D MSD data to ASCII?
Newsgroups:sci.techniques.mass-spec
Datum:2001-08-20 13:50:04 PST View this article only

[Moderator's note: The Excel file mentioned below has been saved to the STMS FTP site at ftp.gatech.edu/pub/mass-spec/trans8.xls. It is available using a Web browser or by anonymous FTP. DB]

Dear Pham,
For my Chemstation G1047A LC/MS, there is a "tabulate" menu bar command that allows the clipboard to be written with a 4-column output of the spectrum in ASCII. This is awkward to reformat when the clipboard is pasted to Excel, so I wrote a visual basic excel macro to do the reformat. To use it (trans8.xls), just clear the sample data from the spreadsheets, and paste in your own tabulate output. Then select run macro from the menu bar. The text file will be written out to the directory specified in the macro. Hope this helps,
Larry

Larry Gross obladi63@yahoo.com
HHMI - University of California, San Diego

}Dear all,
}I am new to the list and do not know if the problem
}has been voiced an answered before. If yes, pls point
}me to the right direction.
}I am looking for a way to convert the entire HP
}Chemstation MSD data file into
}ASCII format. It can be a macro or an independent
}program. I have found in the
}ChemStation itself only a feature to convert either
}selected chromatogram or
}spectrum to an ASCII file. Does anyone have
}experience with the same problem?
}Thanks a lot for your help,
}Dr. Pham Tuan Hai

Von:Pham Tuan Hai (PhamTuanHai@rocketmail.com) Message 12 in thread
Betrifft:Re: Convert HP ChemStation 3D MSD data to ASCII?
Newsgroups:sci.techniques.mass-spec
Datum:2001-08-24 11:05:05 PST View this article only

Hi Tobias,

} And I know Lin DeNoyer claims to know how to read HP LC/MS ChemStation data.

Is he also on the list or do you know how I can reach him?

} And maybe he can send the header format and I will write a converter for a
} piece of ICBINB...

How can I get the header format out of the HP LC/MS data file? I don't exactly
understand what you mean.

Hi Larry,

} Dear Pham,
} For my Chemstation G1047A LC/MS, there is a "tabulate"
} menu bar command that allows the clipboard to be
} written with a 4-column output of the spectrum in
} ASCII. This is awkward to reformat when the
} clipboard is pasted to Excel, so I wrote a visual
} basic excel macro to do the reformat. To use it
} (trans8.xls), just clear the sample data from the
} spreadsheets, and paste in your own tabulate output.
} Then select run macro from the menu bar. The text file
} will be written out to the directory specified in the
} macro. Hope this helps,
} Larry

No, it is not the average spectra over a time range that I want to get. I would
like to have the every scan from the MS file. I know the tabulate command and
can "export" scan by scan but it will take years before I can convert one
complete MS data file into the ASCII :-) Thanks anyway.

Cheers
Hai

Von:Lin DeNoyer (lkd1@cornell.edu) Message 13 in thread
Betrifft:Re: Convert HP ChemStation 3D MSD data to ASCII?
Newsgroups:sci.techniques.mass-spec
Datum:2001-08-24 13:58:11 PST View this article only

Just found this...

}} And I know Lin DeNoyer claims to know how to read HP LC/MS ChemStation data.

I checked my harddrive. I have a fortran source file
with a little program that reads ChemStation files.
Program was developed in Oct 97, so that is the version it reads.
As far as I know, it works for current Chemstation LCMS files also.

Send me an email. I'll ship you the source file.
If you want to know whether this source file will read your particular
data file, send me the file, I will put it into our MOP program, and
see if the data appears on the screen.

Lin

Von:Lin DeNoyer (lkd1@cornell.edu) Message 14 in thread
Betrifft:Re: Convert HP ChemStation 3D MSD data to ASCII?
Newsgroups:sci.techniques.mass-spec
Datum:2001-08-24 13:58:11 PST View this article only

Just found this...

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If you want to know whether this source file will read your particular
data file, send me the file, I will put it into our MOP program, and
see if the data appears on the screen.

Lin

Vorherige 10
Springen zu [Anfang des Diskussionsthemas]

Von:**Tobias Kind** (tk2002deja@amdis.net)
Search Result 8
Betrifft:Re: HP Chemstation -> ASCII --> YES
Newsgroups:sci.chem.analytical
Datum:2002-03-21 12:51:56 PST

Franz Borrmann <franz.borrmann@tu-berlin.de> wrote
> Dear Colleagues,
>
> we're looking for a possibility to get ASCII-files (TIC or
> SIM-chromatogram data) out of a HP-Chemstation (ver.G1034C) ..snip
> Thanks a lot

Dear Franz,

sometimes ago I wrote a nice :-) macro:

```
--------------------------------------------------------------------------------
!HP2ASCII.MAC starts here

name HP2ASCII
!***
!*** this macro fully converts a HP Chemstation file to ASCII or JCAMP-DX
!*** (c)TK4ICBINB
!*** if an error occours during macro execution:false line break in macro
!***
!***(1) load a GC-MS file in HP Chemstation
!***(2) Choose Options Dialog Box --> Command line
!***(3) enter "macro" at command line and load HP2ASCII
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!***(5) Choose an option TIC+MS, TIC, JCAMP-DX
!***(6) Read in with XCL with ";" separator
!***    (from the actual HP data path)
!***
!*** possible files are : xMSspec.txt, xspecrow.txt,
!***                           xTIConly.txt , JCMPGCMS.jdx
!*** BEWARE: XCL can read only a 256x65536 matrix!!! Yes 3x!



  LOCAL label, button, choice
  SDim label, 4
  SDim button, 3
  label[1] = "TIC+spectra nice output"
  label[2] = "TIC+spectra ín one line"
  label[3] = "Only TIC"
  label[4] = "JCAMP 4 Lib2NIST"
  button[1] = ""
  button[2] = "OK"
  button[3] = ""
  choice = 1
  INPUT6 3, 4,"HP2ASCII", label, button, choice
  mychoice = choice

  POINTS R0  ! Get scan range in NPOINTS
  lowscan = 1
  highscan = NPOINTS

  if (mychoice = 1) then
      NiceOutput
  endif
```

```
  if (mychoice = 2) then
      LineOutput
  endif
  if (mychoice = 3)  then
      TICOutput
  endIF
  if (mychoice = 4)  then
      JCAMP4Lib2NIST
  endIF

CLOSE #1
Alert "Beware: EXCEL is only 8-bit!",2
return



name NiceOutput
  fileName$ = _DATAPATH$+_DATAFILE$ + "\xMSspec.txt"
  OPEN fileName$ FOR OUTPUT AS #1
 !change for header line output
  PRINT USING #1,"%;%;%;%;%;%/","Scan","Time","TIC","MSPeaks","Mass","Abund"
  i = 1
  while i <= highscan
    scan i
    points x !get the number of spectra points

    !***array starts from 0 , scans start from 1 aarrgghh
    PRINT USING #1, "#;#.###;#;#/",i,r0[i-1,0],r0[i-1,1],NPOINTS

    !**************************************
    !*** write out the mass pairs
    masscount = 0 !array starts from zero
    while masscount < NPOINTS

    !*** take care !
    !*** if you want true mass values use #.###
    !*** and remove the round() function
    !*** give out mass, abundance
    print using #1 ,";;;;#.##;#/",round(x[masscount,0]),x[masscount,1]

    masscount = masscount+1
    endwhile
    !**************************************
    i = i+1
    print i
  endwhile
return


name LineOutput

  fileName$ = _DATAPATH$+_DATAFILE$ + "\xspecrow.txt"
  OPEN fileName$ FOR OUTPUT AS #1
  !header line output
  PRINT USING #1,"%;%;%;%;%;%/","Scan","Time","TIC","MSPeaks","Mass","Abund"

  i = 1
  while i <= highscan
    scan i
    points x !get the number of spectra points

    !***array starts from 0 , scans start from 1 aarrgghh
    PRINT USING #1, "#;#.###;#;#",i,r0[i-1,0],r0[i-1,1],NPOINTS

    !**************************************
    !*** write out the mass pairs
    masscount = 0 !array starts from zero
    while masscount < NPOINTS
      ! All spectra in one line
      print using #1 ,";#.##;#",round(x[masscount,0]),x[masscount,1]
    masscount = masscount+1
```

```
    endwhile
    !***************************************
    print using #1, "/"
    i = i+1
    print i
  endwhile
return

name TICOutput
  fileName$ = _DATAPATH$+_DATAFILE$ + "\xTIConly.txt"
  OPEN fileName$ FOR OUTPUT AS #1
  PRINT USING #1, "%;%;%;%;/","Scan","Time","TIC","MSPeaks"
  i = 1
  while i <= highscan
    scan i
    points x !get the number of spectra points
    !***array starts from 0 , scans start from 1 aarrgghh
    PRINT USING #1, "#;#.###;#;#/",i,r0[i-1,0],r0[i-1,1],NPOINTS
    i = i+1
    print i
  endwhile
return

name JCAMP4Lib2NIST
! HP Chemstation GC-MS file to JCAMP-DX (HP2JCAMP)
! my contribution to the IUPAC year :-)
! but anyway, it would be better to use AMDIS32  and Lib2NIST
! and use only pure extracted peaks...
! for JCAMP look at
! http://wwwchem.uwimona.edu.jm:1104/software/jcampdx.html
! http://www.isas-dortmund.de/projects/jcamp/
! no compressed format -> ever built a hashtable in Chemstation ?

fileName$ = _DATAPATH$+_DATAFILE$ + "\JCMPGCMS.jdx"
OPEN fileName$ FOR OUTPUT AS #1

  i = 1
  while i <= highscan
    scan i
    points x !get the number of spectra points

    !***array starts from 0 , scans start from 1 aarrgghh
    PRINT USING #1, "% % %#/","##TITLE=",_DATAFILE$,"Scan ",i
    PRINT #1, "##JCAMPDX= Revision 5.0"
    PRINT #1, "##DATA TYPE= MASS SPECTRUM"
    PRINT #1, "##DATA CLASS= PEAK TABLE"
    PRINT #1, "##XUNITS= m/z"
    PRINT #1, "##YUNITS= RELATIVE ABUNDANCE"
    PRINT USING #1, "% #/", "##NPOINTS=", NPOINTS
    PRINT #1, "##PEAK TABLE= (XY..XY)"

    !***************************************
    !*** write out the mass pairs
    masscount = 0 !array starts from zero
    while masscount < NPOINTS

    !*** take care !
    !*** if you want true mass values use #.###
    !*** and remove the round() function
    !*** give out mass, abundance
    print using #1 ,"# #/",round(x[masscount,0]),x[masscount,1]

    masscount = masscount+1
    endwhile
    !***************************************
    i = i+1
    print i
  endwhile

return
```

```
!*** HP2ASCII.MAC ends here
-------------------------------------------------------------------------------
```

A good starting point are the google-groups:
http://groups.google.de/groups?hl=en&q=tic+chemstation+macro
and also the sci.techniques.mass-spec group (moderated).

The HP Chemstation has a really powerful and open concept.
If you want to have a nice programming environment please
download the macropad from
http://www.chem.agilent.com/cag/servsup/usersoft/main.html

There are a also a lot of examples in //hpchem/msexe/macros.hlp

With **kind** regards
Tobias Kind
www.amdis.net

PS:
Ever noticed SGS-Polymers ?
http://wwwstud.uni-leipzig.de/~che94beq/pradiobr.htm

Von:**Tobias Kind** (tk2002deja@amdis.net)

Search Result 6

Betrifft:Re: Chemstation
Newsgroups:sci.chem.analytical

Datum:2002-03-21 15:54:34 PST

luszniak@yahoo.com (Mark Luszniak) wrote in message news:<bd613128.0203211024.66faf068@posting.google.com>...

> I have a client who is running EnviroQuant Chemstation (Version
> G1701AA Version A.03.00), and they'd like to be able to use methods
> with more than 250 items in the quantitation database.
>
> After taking a (admittedly quick) look though the macros, and the help
> files, I have a feeling that the 250 limit is imposed by the
> application. However, I'm by no means an expert with Chemstation, can
> anybody give the definitive answer as to if it's possible to exceed
> 250 items, and if so how?

Dear Mark,

the custrpt.exe (custom report) from HP Chemstation has hardcoded AI x
16000 values (256). (The maximum capacity of a Custom Reports database
is 250 columns by 16,000 says the handbook).
Guess we are still in 8-bit age :-) similiar to 8-bit EXCEL2002. :-(

But there are only around 220 predefined items from the wizard, and
only if you define some additional items you will have no place.

I think there are a lot of "useless" predefined items.
So, a practical way would be to kill some items.

Another way is to transpose all the values. But you have to rewrite
some macros. :-(

Or use another software :-)

Keywords:
chemstation ,250 columns ,NPEAKS ,maxpeaks ,Database Wizard ,custom
reports ,
Database Capacity Considerations

With **kind** regards
Tobias Kind

www.amdis.net

Von:**Tobias Kind** (kind@rziris.rz.uni-leipzig.de) Search Result 8
Betrifft:Re: Water as a solvent for GC --> You can - if you want :-)
Newsgroups:sci.chem.analytical
Datum:2001-07-02 15:33:45 PST View: (This is the only article in this thread) | Original Format

Kevin wrote:

> Hi all,
>
> I have read in several places that water shouldn't be used as a
> solvent for GC especially when using capillary columns. However other
> references seem to dispute this. Is there a definitive answer to
> this.

..snip, snip

Hi,

you can do a direct injection of water in a GC if you use a special
injector -
a programmed temperature vaporizer (PTV) injector
and a technique called: Large Volume Injection (LVI).

But indeed its a trick, because you
1) inject water in the GC injector
2) enrich the components on an adsorbent
3) dry the adsorbent
4) heat the adsorbent
5) and let this gas stream flow through the gc column.

There is a nice review giving a lot of references and also showing some
chromatograms obtained by direct water injection in GC from:

W. Engewald , J. Teske and J. Efer
Programmed temperature vaporisers-based large volume injection in
capillary gas chromatography
Journal of Chromatography A ; Volume 842, Issues 1-2 ; Pages 143-161

http://www.sciencedirect.com/science?_ob=GatewayURL&_origin=ScienceSearch&_method=citationSearch&_piikey=S0021967399000801&_returnURL=http://www.scirus.com&_version=1&md5=9e9a6e04098843a97110947a198d5059

or you can find a lot of other literature if you go to
http://www.scirus.com

and enter the words: large volume injection ptv
http://www.scirus.com/index.php?viewresults=yes&wordtype=all&query=large+volume+injection+++ptv+&docsource=dsall&saall=on#results

(I don't know if the robots will break these long links)

Some other good keywords are (all mixed together or alone)
* PTV - programmed temperature vaporisation
* PTV- programmed temperature vaporization (yes some search engines have
no phonetic search :-(
* thermo desorption
* gas-phase adsorption
* SPE (Solid Phase Extraction), Tenax, cold-trap, cryo-trap
* ATAS , Gerstel , Varian , Agilent
* LVI - Large Volume Injection
* Programmable Temperature Vaporizing Injector
* PTV-GC-MS
* injection of aqueous samples

With kind regards from LE
Tobias Kind

--

Von:**Tobias Kind** (kind@rziris.rz.uni-leipzig.de)
Search Result 10
Betrifft:Re: Need info from CAS ---> (YES)
Newsgroups:sci.chem.organic.synthesis, sci.chem, sci.chem.analytical
Datum:2001-04-18 09:58:41 PST

Dear Fred,

>
> secoisolariciresinol (CAS # 29388-59-8) is obtained from the stinging

...maybe its too late

I think you can not buy this chemical but you can ask the group in Finland if they
kindly
donate or sell you something.

Or you can ask for the original synthesis.

http://www.helsinki.fi/~orgkm_ww/Hase.html

or other experts (Prof. Herman Adlercreutz).

You can also find a synthesis of Secoisolariciresinol at
http://www.sciencedirect.com/

Oxidative cyclisation of 3,4-dibenzyltetrahydrofurans using ruthenium
tetra(trifluoroacetate)
R. S. Ward, D. D. Hughes / Tetrahedron 57 (2001) 2057±2064
Department of Chemistry, University of Wales Swansea, Singleton Park, Swansea SA2
8PP, UK

(compound (13) 3.1.5) --> please ask for reprint :-)

Maybe you already know ChemIDPlus form NIH - for toxicity you can have a look
(with CAS or name) at
http://chem.sis.nlm.nih.gov/chemidplus/

and you can also search for Secoisolariciresinol in Delphion (world patents and US
patents)
http://www.delphion.com/

With kind regards
Tobias Kind

PS: hope you avoided hoarding flax seeds... :-)
PPS: sorry for the search engines...

--
Paul J. Franklin(moderator - sci.chem.organic.synthesis)
http://users.pandora.be/synthesis/newsgroup/wnewshp.html
Georgia State University <chepjf@panther.gsu.edu>
Atlanta, GA

Von:**Tobias Kind** (tk2002deja@amdis.net)
Search Result 1
Betrifft:Re: Chloramphenicol
Newsgroups:de.sci.chemie
Datum:2002-04-26 07:10:23 PST
View: Complete Thread (6 articles) | Original Format

Sven wrote in message news:<9m8rnf$1p8$06$1@news.t-online.com>...
>Weiß einer von Euch wie man Chloramphenicol am besten GC gängig machen
>kann???

Hallo Sven,

CHLORAMPHENICOL hat die CAS: 56-75-7
falls du keinen Scifinder (CAS) hast, dann schau doch mal nch bei:

* http://www.scirus.com (elsevier+Beilstein)
* http://chem.sis.nlm.nih.gov/chemidplus/ (ChemIDPlus)
* http://toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen?TOXLINE (Toxline)

Bei Toxline suchst Du nach: 56-75-7 and gas chromatography
Das gibt ca. 19 Titel - viele davon mit GC.
Toxline sammelt auch analytische Literatur (ab 1945).

Das beantwortet zwar vielleicht nicht direkt Deine Frage,
aber vielleicht hilfts ja :-)

Viele Gruesse nach Norderstedt
Tobias Kind

www.amdis.net

PS:
Chloramphenicol auf einer 25m CP-Sil 5 CB
google: 56-75-7 gc-ms filetype:pdf
http://www.google.de/search?hl=de&q=56-75-7+gc-ms++filetype%3Apdf&meta=

Post a follow-up to this message

Alle Beiträge des Diskussionsthemas "**chrom software?**"

Von:ckf (craig@fulton52.freeserve.co.uk) Message 1 in thread
Betrifft:chrom software?
Newsgroups:sci.chem.analytical
Datum:2001-04-03 10:45:15 PST View this article only

```
Hi all

Does anyone know of any freeware or shareware that can be used for viewing
chromatographs from agilent equipment. It's not important enough to buy
another copy of chemstation (or license) I'm just too lazy to walk to the
lab and use the computer there.

Cheers

Craig
```

Von:Tobias Kind (kind@rziris.rz.uni-leipzig.de) Message 2 in thread
Betrifft:Re: chrom software?
Newsgroups:sci.chem.analytical
Datum:2001-04-04 04:38:08 PST View this article only

```
Dear Craig,

> Does anyone know of any freeware or shareware that can be used for viewing
> chromatographs from agilent equipment. It's not important enough to buy
> another copy of chemstation (or license) I'm just too lazy to walk to the
> lab and use the computer there.

for LC or GC ?

For GC you can take AMDIS from NIST (link is a little review):

http://wwwstud.rz.uni-leipzig.de/~che94beq/amdis.htm

or WSEARCH by Frank Antolasic

http://minyos.its.rmit.edu.au/~rcmfa/index.html


With kind regards
Tobias Kind

--
```

Von:Rico (Rico@nospam.nl) Message 3 in thread
Betrifft:Re: chrom software?
Newsgroups:sci.chem.analytical
Datum:2001-04-04 06:46:06 PST View this article only

```
On Wed, 04 Apr 2001 12:46:23 +0200, Tobias Kind
<kind@rziris.rz.uni-leipzig.de> wrote:

>
>--------------4E3AA4FFF8E98CAF53C48161
>Content-Type: text/plain; charset=us-ascii
>Content-Transfer-Encoding: 7bit
>
>
>Dear Craig,
>
>> Does anyone know of any freeware or shareware that can be used for viewing
>> chromatographs from agilent equipment. It's not important enough to buy
>> another copy of chemstation (or license) I'm just too lazy to walk to the
>> lab and use the computer there.
```

>
>for LC or GC ?
>
>For GC you can take AMDIS from NIST (link is a little review):
>
>http://wwwstud.rz.uni-leipzig.de/~che94beq/amdis.htm
>
>or WSEARCH by Frank Antolasic
>
>http://minyos.its.rmit.edu.au/~rcmfa/index.html
>
>
>With kind regards
>Tobias Kind
>
>--------------4E3AA4FFF8E98CAF53C48161
>Content-Type: text/html; charset=us-ascii
>Content-Transfer-Encoding: 7bit
>
><!doctype html public "-//w3c//dtd html 4.0 transitional//en">
><html>
>
>
Dear Craig,
><blockquote TYPE=CITE>Does anyone know of any freeware or shareware that
>can be used for viewing
>
chromatographs from agilent equipment. It's not important enough to
>buy
>
another copy of chemstation (or license) I'm just too lazy to walk
>to the
>
lab and use the computer there.</blockquote>
>for LC or GC ?
><p>For GC you can take AMDIS from NIST (link is a little review):
><p><a
href="http://wwwstud.rz.uni-leipzig.de/~che94beq/amdis.htm">http://wwwstud.rz.uni-leipzig.de/~che94beq/amdis.htm
><p>or WSEARCH by Frank Antolasic
><p>http://minyos.its.rmit.edu.au/~rcmfa/index.html
>

><p>With kind regards
>
Tobias Kind</html>
>
>--------------4E3AA4FFF8E98CAF53C48161--
>
http://www.dataset.fr
They have remote control, may be of some use for U, I use it to
control my PC with LC-MS(MS) attached to it.

Good luck,
Rico

Alle Beiträge des Diskussionsthemas "**Utility of LC/MS/MS system**"

Von:Hubert (chhubert@hotmail.com) Message 1 in thread
Betrifft:Utility of LC/MS/MS system
Newsgroups:sci.techniques.mass-spec
Datum:2001-03-19 17:26:36 PST View this article only

```
Dear all,

I am wondering if anyone knows any web sites or sources for measuring the
utility rate of different LC/MS/MS systems, in partcular to PE/Sciex API3000
and Micromass Quattro Ultima in research paper.

Thanks in advance.

Regards,
Hubert Tang


_________________________________________________________________
Get Your Private, Free E-mail from MSN Hotmail at http://www.hotmail.com.
```

Von:Justin Withers (justin_withers@hotmail.com) Message 2 in thread
Betrifft:Re: Utility of LC/MS/MS system
Newsgroups:sci.techniques.mass-spec
Datum:2001-03-20 05:57:14 PST View this article only

```
My instinctive reaction to that would be to go to my colleague's cube, grab
her ASMS CD-ROMs from the last two years and use Acrobat to search them.
Strikes me as one easy approach, but I AM biased,

Justin Withers
AB|MDS Sciex
"Hubert" <chhubert@hotmail.com> wrote in message
news:996bb7$g2o$1@news-int.gatech.edu...
} Dear all,
}
} I am wondering if anyone knows any web sites or sources for measuring the
} utility rate of different LC/MS/MS systems, in partcular to PE/Sciex API3000
} and Micromass Quattro Ultima in research paper.
}
} Thanks in advance.
}
} Regards,
} Hubert Tang
}
} _________________________________________________________________
} Get Your Private, Free E-mail from MSN Hotmail at http://www.hotmail.com.
}
}
}
```

Von:Tobias Kind (kind@rziris.rz.uni-leipzig.de) Message 3 in thread
Betrifft:Re: Utility of LC/MS/MS system
Newsgroups:sci.techniques.mass-spec
Datum:2001-03-20 14:12:02 PST View this article only

```
Dear Mr. Tang,

the best way if you do not have time and money and the magic cube
```

and if you are only interested in the mathematical or lets say statistical
point of view is to contact
a) Micromass: mailto:nicola.wright@micromass.co.uk
b) Appliedbiosystems and PE: mailto:prodinfo@appliedbiosystems.com
c) ask for a bibliography of the system (100% existing)
c1) in most cases they are pleased as punch because you ask for their child's
if not
c2) tell them you want to buy a system (ooops:-)
d) calculate
e) realize that even this number is only a vulgar fraction

With kind regards
Tobias Kind

PS: chopping between 0.08 and 0.53 - maybe fuzzy logic helps...

} My instinctive reaction to that would be to go to my colleague's cube, grab
} her ASMS CD-ROMs from the last two years and use Acrobat to search them.
} Strikes me as one easy approach, but I AM biased,
}
} Justin Withers
} AB|MDS Sciex
} "Hubert" <chhubert@hotmail.com> wrote in message
} news:996bb7$g2o$1@news-int.gatech.edu...
} } Dear all,
} }
} } I am wondering if anyone knows any web sites or sources for measuring the
} } utility rate of different LC/MS/MS systems, in partcular to PE/Sciex API3000
} } and Micromass Quattro Ultima in research paper.
} }
} } Thanks in advance.
} }
} } Regards,
} } Hubert Tang

Alle Beiträge des Diskussionsthemas "**Mass Spectrum Prediction (Simulation) software, al...**"

Von:Chemist (pgong@cambridgesoft.com) Message 1 in thread
Betrifft:Mass Spectrum Prediction (Simulation) software, algorithm
Newsgroups:sci.techniques.mass-spec
Datum:2001-12-14 12:06:05 PST View this article only

```
Hi,
   Anybody has information about where can I find Mass Spectrum
Prediction or Simulation software or algorithm?

   Searching CA does not turn out much information( Maybe the way I
search is not proper ).

   Could you please email pgong@cambridgesoft.com for your info?  I
will summerize and post.

   Thanks!

Paul
```

Von:Tobias Kind (kind@rziris.rz.uni-leipzig.de) Message 2 in thread
Betrifft:Re: Mass Spectrum Prediction (Simulation) software, algorithm
Newsgroups:sci.techniques.mass-spec
Datum:2001-12-19 09:20:02 PST View this article only

```
Dear Paul,

} Hi,
}    Anybody has information about where can I find Mass Spectrum
} Prediction or Simulation software or algorithm?
}    Searching CA does not turn out much information( Maybe the way I
} search is not proper ).
}    Could you please email pgong@cambridgesoft.com for your info?  I
} will summerize and post.
}    Thanks!
} Paul

I can only speak for small molecules and this is NO full reference,
therefore --> please don't hit me if you see
that an important work is not mentioned here.

Two ways are possible :
(A) from mass spectra to structure
(B) from structure to mass spectra

****** (A)
One of the most sophisticated (A) programs  I've ever seen (handful)
MOLGEN-MS. http://www.molgen.de follow the link to
MOLGEN-MS. Please read the full homepage. Really nice !

It features a fully independent machine. You give a mass spectrum -->
MOLGEN-MS gives you a structure. (Keywords: MSclass, ElCoCo, MOLGEN, MS
reaction network)

C. Benecke , T. Gruner , A. Kerber ,R. Laue ,T. Wieland
Fresenius J Anal Chem (1997) 359: 23-32
MOLecular structure GENeration with MOLGEN, new features and
future developments
```

****** (B)
MASP - from The Richert Research Group at Tufts University

http://microvirus.chem.tufts.edu/MASP/masp.html

[1] C. Steinbeck, K. Berlin, and C. Richert, MASP - a program predicting

mass spectra of combinatorial libraries, submitted for publication.

[2] K. Berlin, R. K. Jain, C. Tetzlaff, C. Steinbeck and C. Richert, Spectrometrically monitored selection experiments: quantitative laser desorption mass spectrometry of small chemical libraries, submitted for publication.

Prof. Steinbeck also has a page at:
http://vanilla.ice.mpg.de/~stein/

******

There are a lot of expert algorithms built in in spectra prediction software:
you will find (rare) some algorithms in the references.
* NIST-MS Search http://www.nist.gov/srd/nist1a.htm
with
Empirical Pattern Recognition/Expert System for Molecular Weight Estimation of Low Resolution Mass Spectra; D.R. Scott; Analytica Chemica Acta 285 (1994)
or
Chemical Substructure Identification by Mass Spectral Library Searching; Stein, S.E.; J. Am. Soc. Mass Spectrom., 1995, 6, 644-655

* MASSLIB www.masslib.com
* Mass-Frontier www.highchem.com
* MS interpreter from ACDlabs
  http://www.acdlabs.com/products/spec_lab/exp_spectra/ms/

****
Varmuza group :
http://www.lcm.tuwien.ac.at/vk/

with VARMUZA classifiers:
Feature selection by genetic algorithms for mass spectral classifiers
H. Yoshida , R. Leardi , K. Funatsu , K. Varmuza
Analytica Chimica Acta 446 (2001) 485–494
or
Systematic structure elucidation of organic compounds by mass spectra classification
Journal of Molecular Structures 408/409 (1997) 91-96
K. Varmuza, P. Penchev, F. Stancl and W. Werther

These classifiers are used in MOLGEN-MS and AMDIS

****

Don't forget AMDIS (NIST/ S.E.Stein) with the VARMUZA post processing
http://wwwstud.rz.uni-leipzig.de/~che94beq/amdis.htm
(my small review :-)

****

Please also check additional literature
* from Steven E. Stein (NIST)
* Stephen R. Heller www.hellers.com
* Don R. Scott http://www.flash.net/~donrscot/index.htm
* DENDRAL project (Search the Joshua Lederberg Papers)
  http://www.profiles.nlm.nih.gov/BB/search/
  enter DENDRAL (its fun, fun, fun :-)

and and and...

With kind regards
Tobias Kind

PS: Peaceful holidays !
PPS: For all...

Alle Beiträge des Diskussionsthemas "**ultrafiltration-membran**"

Von:andreas (aheerwag@gmx.de) Message 1 in thread
Betrifft:ultrafiltration-membran
Newsgroups:sci.chem.analytical
Datum:2001-02-16 05:21:01 PST View this article only

```
Greetings,
Does anyone know if any manufacture exists for generated cellulose
ultrafiltration-membran with cut-off of about 1000kD.
Thanks for every help.

Andreas Heerwagen
```

Von:Tobias Kind (kind@rziris.rz.uni-leipzig.de) Message 2 in thread
Betrifft:Re: ultrafiltration-membran
Newsgroups:sci.chem.analytical
Datum:2001-02-19 01:39:05 PST View this article only

```
> Greetings,
> Does anyone know if any manufacture exists for generated cellulose
> ultrafiltration-membran with cut-off of about 1000kD.
> Thanks for every help.

Dear Mr. Heerwagen,

you can call Millipore Germany (Herr Meier/Mayer/Meyer - product
specialist for UF membranes)
06196 4940 (Eschborn).

http://www.millipore.com:80/analytical\pubdbase.nsf/docs/TN1000ENUS.html

With kind regards
Tobias Kind

PS:
Give them my name - they will send me a coffee machine as a gift :-)
```

Alle Beiträge des Diskussionsthemas "**Agilent Msd Chemstation Macros**"

Von:Paul Overaa (pauloveraa@cleanaway.com) Message 1 in thread
Betrifft:Agilent Msd Chemstation Macros
Newsgroups:sci.chem.analytical
Datum:2001-02-12 11:38:39 PST View this article only

I'm writing a Visual Basic Data-Vet (data-verification) program that, having
been
launched from a Msd Chemstation macro, sets up a DDE channel in order to
send collected
gc/ms quantitation results to the Data-Vet for verification.

In the main I've encountered very few difficulties and all the Agilent
DDE-based macro
functions work as documented... except for one, namely DDEExecute, which
generates a DDE
error 26 error message. Unfortunately, the DDE error codes are not
documented in the
system on-line manuals and I'm not at all sure that the DDEExecute command
is documented
as fully as it should be.

Needless to say I'm more than happy to provide full details of what I am
doing but,
before wasting newsgroup space, I thought I'd better check to see if anyone
else is
working with these Agilent Macro language DDE functions.

I ought to mention that I have already done the obvious: I've read the
Agilent docs,
studied a number of the system macros, checked and re-checked my code, and
have
been in regular contact with Agilent's technical support team.

Thanks in advance for any possible help &/or interest - Paul Overaa

Von:Tobias Kind (kind@rziris.rz.uni-leipzig.de) Message 2 in thread
Betrifft:Re: Agilent Msd Chemstation Macros
Newsgroups:sci.chem.analytical
Datum:2001-02-13 07:34:23 PST View this article only

Paul Overaa wrote:

> I'm writing a Visual Basic Data-Vet (data-verification) program that, having
> been
> launched from a Msd Chemstation macro, sets up a DDE channel in order to
> send collected
> gc/ms quantitation results to the Data-Vet for verification.
>
> In the main I've encountered very few difficulties and all the Agilent
> DDE-based macro
> functions work as documented... except for one, namely DDEExecute, which
> generates a DDE
> error 26 error message. Unfortunately, the DDE error codes are not
> documented in the
> system on-line manuals and I'm not at all sure that the DDEExecute command
> is documented
> as fully as it should be.

>
> Needless to say I'm more than happy to provide full details of what I am
> doing but,
> before wasting newsgroup space, I thought I'd better check to see if anyone
> else is
> working with these Agilent Macro language DDE functions.
>
> I ought to mention that I have already done the obvious: I've read the
> Agilent docs,
> studied a number of the system macros, checked and re-checked my code, and
> have
> been in regular contact with Agilent's technical support team.
>
> Thanks in advance for any possible help &/or interest - Paul Overaa

Dear Paul,

DDE is truly "crap" ... sometimes it works .. sometimes not...
I have only some tips, maybe it helps.

* Did you use the DDESPY.EXE ? (use correct version for operating system)

* DDExecute works fine on my computer within HPChemstation as long the command
is registered correctly... (search with regedit in registry)

(from www.distributive.com/CustomerSupport/documents/ScriptDevelopmentGuide.pdf)

f.e., type on the command line

```
ChanNum = DDEInitiate("PROGMAN","PROGMAN")
DDEExecute ChanNum,"[CreateGroup(XXX)]"
DDETerminate ChanNum
```

...explorer popups and has group xxx

* DDE errors are external problems - go to
http://support.microsoft.com/ - and search there for DDEEXECUTE

* DDE errors are only documented in win32 API reference guides
   not in HPCHEMSTATTION

* at least you can contact Niels Waleson from HP.
 or somebody from www.msconsult.dk

With kind regards
Tobias Kind

Von:Jean-Marc Szalies (dontdisturb.szalies@yahoo.com) Message 3 in thread
Betrifft:Re: Agilent Msd Chemstation Macros
Newsgroups:sci.chem.analytical
Datum:2001-02-13 09:35:34 PST View this article only

DDE worked great until I switched from Win 3.11 to NT
So I used a text file as output for Chemstation that I could acces by
Excel.
Since NT, DDE wasn't that great anymore (or was it since Office 95 or
97 ? Is this "progress" ? ;)))))

>
>Dear Paul,
>
>DDE is truly "crap" ... sometimes it works .. sometimes not...
>I have only some tips, maybe it helps.
>

Email without the dontdisturb
http://web.wanadoo.be/szalies/

Von:Paul Overaa (pauloveraa@cleanaway.com)

Betrifft:Re: Agilent Msd Chemstation Macros
Newsgroups:sci.chem.analytical
Datum:2001-02-15 00:45:15 PST
View this article only

Tobias,

Thanks for your help. Things have, however, taken an unexpected twist in the last day. I got a DDE example from Kenneth Weiner, an Agilent software guy. He sent the VB source, a VB executable and a small Msd Chemstation script (attached).

Here's the crunch - his code works fine on my system and the DDEExecute command gave no DDE error 26 messages, yet I looked at his code and his DDE function use was exactly the same as mine. I recompiled his example and guess what - the DDE error 26 messages then appeared with his code as well.

So... looks like we've got a VB version specific problem here. I'm using Visual Basic Professional 4.0, Ken's original executable was done in VB5. Needless to say I'm going to order an upgrade ASAP.

Just shows you doesn't it - Over the last few weeks I thought I'd been systematically working through all possible 'error-cause' scenarios but I didn't once think we'd be dealing with a version specific VB function snag.

Funny old life isn't it (:

Regards and thanks again - Paul

p.s. If anyone else wants a copy of the example code just mail me!
pauloveraa@cleanaway.com

Paul Overaa wrote in message ...

>I'm writing a Visual Basic Data-Vet (data-verification) program that, having
>been aunched from a Msd Chemstation macro, sets up a DDE channel in order to
>send collected gc/ms quantitation results to the Data-Vet for verification.
>
>In the main I've encountered very few difficulties and all the Agilent
>DDE-based macro functions work as documented... except for one, namely
>DDEExecute, which generates a DDE error 26 error message. Unfortunately,
>the DDE error codes are not documented in the system on-line manuals and
> I'm not at all sure that the DDEExecute command is documented as fully as it
>should be.
>
>Needless to say I'm more than happy to provide full details of what I am
>doing but, before wasting newsgroup space, I thought I'd better check to see if
>anyone else is working with these Agilent Macro language DDE functions.
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>I ought to mention that I have already done the obvious: I've read the
>Agilent docs, studied a number of the system macros, checked and
>re-checked my code, and have been in regular contact with Agilent's
> technical support team.
>
>Thanks in advance for any possible help &/or interest - Paul Overaa
>
>

Von:**Tobias Kind** (kind@wwwserv.rz.uni-leipzig.de) Search Result 19
Betrifft:Re: data file conversion [Finnigan-->HP=GCQ2HP]
Newsgroups:sci.techniques.mass-spec
Datum:2000-09-22 11:20:14 PST View: (This is the only article in this thread) | Original Format

Rich Yelton wrote:

} Does anyone know of any software available capable of
} converting Finnigan format data (.ms files) into HP format (.d files)?

Dear Mr. Yelton,

yes - if the files are in ITS40 format (from Finnigan GCQ) you can use
GCQ2HP GCQ2HP converts Finnigan GCQ Ion-Trap files (ITS40) to HP
Chemstation files. http://wwwstud.rz.uni-leipzig.de/~che94beq/gcq2hp.htm

And the best: it is zero quid (marks/bucks) - if you have a GCQ. Yes its
free.

GCQ2HP is for those people who used the IonTrap and got (some) trouble
with the support (not the software) and where hangig between an old
program and the unfinished MassFrontier (cool tool). Sorry for my 10
cents.

If you have only Incos 50/500, TSQ 70/700 go for the other programs
suggested on the bottom of the GCQ2HP page.

Or again, use AMDIS (can also read *.ms).
http://wwwstud.rz.uni-leipzig.de/~che94beq/amdis.htm

With kind regards
Tobias Kind

PS: Why do YOU wanna convert Finnigan files today ?
Think you are heretical :-)

Alle Beiträge des Diskussionsthemas "**Backup 0n QTof**"

Von:Kenneth Chan (Kenneth.Chan@nrc.ca) Message 1 in thread
Betrifft:Backup 0n QTof
Newsgroups:sci.techniques.mass-spec
Datum:2000/07/24 View this article only

```
Hello NG,

We recently got a QTof (and soon there would be two) and we are
generating 2 GB of data a night.  Do anybody have any thoughts on
backups the data we are generating??

CD-R vs. Tapes vs. DVD-RAM? vs. ??
Any Good archive programs?
How are you dealing with the flood of data??

We were thinking of CD-R (Cause it is so inexpensive) but at the end of
the year we could end up with 1000 CD!  Please share your experience
with the NG.

Swimming in CDs

Ken
```

Von:Pat Thompson (patrick.thompson@kodak.com) Message 2 in thread
Betrifft:Re: Backup 0n QTof
Newsgroups:sci.techniques.mass-spec
Datum:2000/07/24 View this article only

```
You ask a good question.  We have a ToF-SIMS that can generate what are
called "*.raw" files that can be up to 2 Gb in size.  We've decided to
upload the date onto a server where 3 - 6 months of data can be made
availabe for more or less instant access and the post 3 - 6 month data
gets stored on tape in case it's ever needed.

Even with these large files we certainly don't normally generate 2
Gb/day.  We looked at the idea of CR-R, tapes, optical drives, Jazz
drives plus a few others and as far as we could see there isn't a good
solution to the problem.  Tapes are big on storage but too slow, most
everything else is fairly fast but too small.



Kenneth Chan wrote:
}
} Hello NG,
}
} We recently got a QTof (and soon there would be two) and we are
} generating 2 GB of data a night.  Do anybody have any thoughts on
} backups the data we are generating??
}
} CD-R vs. Tapes vs. DVD-RAM? vs. ??
} Any Good archive programs?
} How are you dealing with the flood of data??
}
} We were thinking of CD-R (Cause it is so inexpensive) but at the end of
} the year we could end up with 1000 CD!  Please share your experience
} with the NG.
}
```

} Swimming in CDs
}
} Ken

Von:Tobias Kind (kind@wwwserv.rz.uni-leipzig.de) Message 3 in thread
Betrifft:Re: Backup 0n QTof
Newsgroups:sci.techniques.mass-spec
Datum:2000/07/25 View this article only

}We recently got a QTof (and soon there would be two) and we are
}generating 2 GB of data a night.
}
}We were thinking of CD-R (Cause it is so inexpensive) but at the end of
}the year we could end up with 1000 CD! Please share your experience
}with the NG.

Hi,
this is a very interesting discussion.

(1000 CDs are 650 MB * 1000 = 650 GByte) at a rough guess

If you need your data only in the next 5 years - take CDs 1000 * $1 =
$1000
(I have old CDs and can not read them) - but use some good quality CDs.

If you need your data in the next 5 years and want to get rid of 1000 CDs
take the new ADR streamers they are fast and have 50GB space
take the OnStream Tape-Drive SC50 50GB SCSI-2
its $600 in germany and tapes (1x =$50) will cost you again $600
http://www.onstream.com/server/pricelist.html

If you _really_ need your data only use MOs
http://fujitsu.dynamit.net/web/mo_disk/htm/index.htm
but you will get poor. Because the GIGAMO-drive costs you
around $600 but the media (1,3Gbyte 1x=$40) will cost you $20.000 (oooops)

ok buy the HP-MO solution
http://www.hp-optical.com/products/fs_products.htm
its the HP 5200ex $2500 and Media (5Gbyte = $80) = $10.000 (ooops)

If you want DVD use toshiba or panasonic DVD-RAM
but Medium 5 GByte will cost (1x=$40) you $5200 (oops)
http://www.toshiba.com/taecdpd/products/features/SDW1111-Over.shtml

Prices may differ, but best thing:
A) life time --> go for MO
B) Optimum --> go for 50 GByte ADR-Streamer

(GC files are in most cases compressed, but you can crunch them down
to 60% of the original size)

For compression UNIX go for a ZIP derivate
For WINDOWS go for ARJ
at the and use an automatic batch converter for compressing all the files
and save them.

Kind regards
Tobias Kind

...mmhh print it out ???

Von:Kenneth Chan (Kenneth.Chan@nrc.ca) Message 4 in thread
Betrifft:Re: Backup 0n QTof
Newsgroups:sci.techniques.mass-spec
Datum:2000/07/25 View this article only

Here is something we been playing around / thinking about here:

We are going to try to setup a file server with the biggest hard disk we could find (in
Canada Maxtor Diamond Max 60 = $440 cdn.) When the hard drive gets full we will pull
the full hard drive out and replace it with a fresh HD.

Cost per Gb (in Canadian dollars)
HD = $7.33
DVD = $12.50 ($65 / disk 5.2Gb)
Tape = $3.00 depending on formats
CD = $2.00

It sounds crazy, but it has the fastest transfer rate of the medium and it does not
require an interface.

Got any better ideas??? Cause this sounds too crazy to work (or could it?)

Ken

Tobias Kind wrote:

} Hi,
} this is a very interesting discussion.
}
} ---> sorry for the snip!
}
} If you want DVD use toshiba or panasonic DVD-RAM
} but Medium 5 GByte will cost (1x=$40) you $5200 (oops)
} http://www.toshiba.com/taecdpd/products/features/SDW1111-Over.shtml
}
} Prices may differ, but best thing:
} A) life time --> go for MO
} B) Optimum --> go for 50 GByte ADR-Streamer
}
} Kind regards
} Tobias Kind
}
} ...mmhh print it out ???

Von:Ken Weir (ken.weir@netcom.ca) Message 5 in thread
Betrifft:Re: Backup 0n QTof
Newsgroups:sci.techniques.mass-spec
Datum:2000/08/04 View this article only

All,

In regards to data acquired on Q-TOF type instruments. Although
expensive, the data capacity of a RAID type 3 or type 5 would be much more
benificial. for $5,000 (US) you can now purchase units up to 250Gb (5x50Gb
drives) They all sit in a single case, and then the processed data can be
backed up onto another media (i.e. CD-R) this would provide fast access
to the raw data, and then allow for selection of the archival data.

This is the method now being used for DVD development of Video.

Regards,

Ken Weir
Media Development Coordinator
MDS Sciex Instruments
Kenneth Chan <Kenneth.Chan@nrc.ca> wrote in message
news:8lkheq$9ks$1@news-int.gatech.edu...
} Here is something we been playing around / thinking about here:
}
} We are going to try to setup a file server with the biggest hard disk we could find (in
} Canada Maxtor Diamond Max 60 = $440 cdn.) When the hard drive gets full we will pull
} the full hard drive out and replace it with a fresh HD.
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} Cost per Gb (in Canadian dollars)
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} CD = $2.00
}
} It sounds crazy, but it has the fastest transfer rate of the medium and it does not
} require an interface.
}
} Got any better ideas??? Cause this sounds too crazy to work (or could it?)
}
} Ken
}
} Tobias Kind wrote:
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} }
} } Prices may differ, but best thing:
} } A) life time --> go for MO
} } B) Optimum --> go for 50 GByte ADR-Streamer
} }
} } Kind regards
} } Tobias Kind
} }
} } ...mmhh print it out ???
}
}
}

Von:Jens Höhndorf (Jens.Hoehndorf@t-online.de)
Message 6 in thread
Betrifft:Re: Backup 0n QTof
Newsgroups:sci.techniques.mass-spec
Datum:2000/08/13
View this article only

Hi Ken,

Do you have an idea what and especially WHEN you will do something (e.g.
process) with this data? This will maybe lead you to your appropriate
solution. If you don't get the time and capacity to process you can as
well record 2 GB of noise a night.

IMHO the solution is to process the data online, i.e. as fast as you
generate them. Archive only the REAL RESULTS.
If you just store the masses (and maybe a width and a reliability
score), you will have only one CD instead of 1000.

Jens

Kenneth Chan wrote:
}
} Hello NG,
}
} We recently got a QTof (and soon there would be two) and we are
} generating 2 GB of data a night. Do anybody have any thoughts on
} backups the data we are generating??
}
} CD-R vs. Tapes vs. DVD-RAM? vs. ??
} Any Good archive programs?
} How are you dealing with the flood of data??
}
} We were thinking of CD-R (Cause it is so inexpensive) but at the end of
} the year we could end up with 1000 CD! Please share your experience
} with the NG.
}
} Swimming in CDs

}
} Ken

Von:Kenneth Chan (Kenneth.Chan@nrc.ca) Message 7 in thread
Betrifft:Re: Backup 0n QTof
Newsgroups:sci.techniques.mass-spec
Datum:2000-08-14 06:36:06 PST View this article only

Hello Jens

We do "Real Time" processing (i.e.. When the MS/MS spectrums are ran, we do
an automated peptide search). And yes most of the time we only look at the
processed data. However, deleting the original data file is not possible
because of chain of causticity.(sp?) issues, i.e.. where the data comes form,
how it was processed, can we get anything else out of the data?

The scary part is that we have rarely had 2 GB of junk... Only twice did an
over night run gone bad. And in was an HPLC problem, not the mass spec....

Ken

Jens Höhndorf wrote:

} Hi Ken,
}
} Do you have an idea what and especially WHEN you will do something (e.g.
} process) with this data? This will maybe lead you to your appropriate
} solution. If you don't get the time and capacity to process you can as
} well record 2 GB of noise a night.
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} generate them. Archive only the REAL RESULTS.
} If you just store the masses (and maybe a width and a reliability
} score), you will have only one CD instead of 1000.
}
} Jens

Alle Beiträge des Diskussionsthemas "**Antimony removal from power plant waste streams**"

Von:ejh4286@dukepower.com (ejh4286@dukepower.com) Message 1 in thread
Betrifft:Antimony removal from power plant waste streams
Newsgroups:sci.engr.chem
Datum:1996/01/15 View this article only

```
Does anyone have any relevant expereince on the best way to remove antimony (Sb-125) from nuclear power plant liquid
waste?  Ion exchange has not been very effective.

Ed Haack, PE
```

Von:Marc Andelman (drgonfly@biosource.ultranet.com) Message 2 in thread
Betrifft:Re: Antimony removal from power plant waste streams
Newsgroups:sci.engr.chem
Datum:1996/01/15 View this article only

```
ejh4286@dukepower.com wrote:
>
> Does anyone have any relevant expereince on the best way to remove antimony (Sb-125) from nuclear power plant liquid
> waste?  Ion exchange has not been very effective.
>
> Ed Haack, PE
> Can you tell me what the electrochemical breakdown voltage
of your particular antimony species is?  If you can measure
current in a conductivity bridge, while applying
increasing voltages, that would be the best answer.
Depending on the number you get, I may have a solution.
Marc Andelman
```

Von:Tobias Kind Sekt. Chemie/Mineralogie SS96 (kind) Message 3 in thread
Betrifft:Re: Antimony removal from power plant waste streams
Newsgroups:sci.engr.chem
Datum:1996/01/23 View this article only

```
Dear Ed,
have a look at http://rzaix340.rz.uni-leipzig.de/~kind/rgseng.htm

This problem was solved using SGS-polymers.

Industrial application:
SGS-filters removes about 94% of antimony from a complex acid solution with
1 g/l of antimony.
Achieved concentration in eluate is 45-50 g/l and flow rate 1200 specific
volumes. Eluate is 15% solution of HCl.

These values are from literature. In most cases a better cleaning (up to
microgram per liter oer better) is possible.

Please feel free to Email me.
With regards
Tobias Kind
```

Von:**Tobias Kind** (kind@rzaix340.rz.uni-leipzig.de)

Search Result 22

Betrifft:New Web Site: SGS-Polymers
Newsgroups:sci.polymers

Datum:1995/11/18

Polymers of Spatial Globular Structure are highly porous materials,
wich are used as ion exchangers, sorbents, filters and demulsifiers.

Informations about SGS-Polymers are now available at

http://rzaix340.rz.uni-leipzig.de/~kind/rgseng.htm

Tobias Kind

Von:Daniel Koch (danielkoch@gmx.net)
Search Result 2
Betrifft:Re: Heat capacity of methylsiloxane
Newsgroups:sci.chem.analytical
Datum:2002-04-25 15:02:10 PST
View: Complete Thread (4 articles) | Original Format

Thanks **Tobias** for your **kind** answer. This really helps a lot !

Daniel

Tobias Kind wrote:

> Bernd Koch <b.j.koch@T-Online.de> wrote in message news:<3CC07091.4080602@T-Online.de>...
>
>>Does anyone know where to find the specific heat capacity (cp) of
>>methylsiloxane (Silikonkautschuk, silicon resin) ? I `d appreciate any help.
>>
>>Daniel
>>
>
>
> Dear Daniel,
> you can also try the CHEOPS software with the Andrey A. Askadskii approach
> http://www.millionzillion.com.pl/cheops/home02.htm
>
> It calculates among others the:
> Specific heat capacity at 298 for glassy state
> Specific heat capacity at 298 K for liquid state
> http://www.millionzillion.com.pl/cheops/products03.htm
> They also have a large polymer database.
>
> Or go to http://www.dtwassociates.com/ the have some
> Polymer design Tools. They also use other methods
> (Askadskii,van Krevelen, Bicerano).
>
> ----
> Without warranty:
> Heat capacity of solid polymer at 298 K
> Poly(methylsiloxane) [-OSiH(CH3)-] 100,9 J/(mole*K) (calc)
> Poly(dimethy siloxane) [-OSi(CH3)2-] 124 J/(mole*K)(calc)
> ----
>
> With **kind** regards
> **Tobias Kind**
>
> www.amdis.net
>

Post a follow-up to this message

Von:**Tobias Kind** (tk2002deja@amdis.net)
Search Result 5
Betrifft:Re: Nitro-PAH determination
Newsgroups:sci.chem.analytical
Datum:2002-04-04 06:01:51 PST

Dear Jose ,

>1) which method/s are the best for the determination of nitro-PAH?
>2) Can somebody explain in deept these methods?

*1)
Depends on your available devices
with HPLC or CE : fluorescence, electrochemical, chemiluminescence
with GC-MS: chemical ionization or EI in positive or negative mode
with LC-MS: ESI, APCI in positive or negative mode

If you only have some known targets go for HPLC or LC-MS. The reduction
step to amines in HPLC may be problematic or time consuming.

If you have complex samples go for GC-MS in SIM or MS/MS mode. But also
during this analysis you need a cleanup step.
I got best results with low signal/noise ratio in MS/MS mode.

*2) I made a page with some literature with abstracts for you:
http://www.amdis.net/external/nitro-pahs.html

or try:
google and search for: "nitro PAHs" filetype:PDF
http://www.google.de/search?hl=de&q=%22nitro+PAHs%22+filetype%3APDF

*3) If you search additional publications about
3-nitro-7H-benz[d,e]anthracen-7-one (3-nitrobenzanthrone)
you can also search the Elsevier database
http://scirus.com

With **kind** regards
Tobias Kind

www.amdis.net

Keywords:
Nitro-PAH, Nitro-PAHs
776-34-1 1-Amino-4-nitronaphthalene 602-60-8 9-Nitroanthracene
20268-51-3 7-Nitrobenz[a]anthracene 63041-90-7 6-Nitrobenz[a]pyrene
86-00-0 2-Nitrobiphenyl 2113-58-8 3-Nitrobiphenyl
92-93-3 4-Nitrobiphenyl 7496-02-8 6-Nitrochrysene
5410-97-9 3-Nitrodibenzofuran 6639-36-7 2-Nitrodibenzothiophene
892-21-7 3-Nitrofluoranthene 86-57-7 1-Nitronaphthalene
581-89-5 2-Nitronaphthalene 17024-19-0 3-Nitrophenanthrene
82064-15-1 4-Nitrophenanthrene 954-46-1 9-Nitrophenanthrene
5522-43-0 1-Nitropyrene 33685-60-8 9,10-Dinitroanthracene
2436-96-6 2,2'-Dinitrobiphenyl N/A 2,8-Dinitrodibenzothiophene
5405-53-8 2,7-Dinitrofluorene 31551-45-8 2,7-Dinitro-9-fluorenone
606-37-1 1,3-Dinitronaphthalene 605-71-0 1,5-Dinitronaphthalene
602-38-0 1,8-Dinitronaphthalene 75321-20-9 1,3-Dinitropyrene

42397-64-8 1,6-Dinitropyrene 42397-65-9 1,8-Dinitropyrene
129-79-3 2,4,7-Trinitro-9-fluorenone 98-95-3 Nitrobenzene
88-72-2 2-Nitrotoluene 121-14-2 2,4-Dinitrotoluene
606-20-2 2,6-Dinitrotoluene 51-28-5 2-Nitrophenol
100-02-7 4-Nitrophenol 51-28-5 2,4-Dinitrophenol
88-74-4 2-Nitroaniline 99-09-2 3-Nitroaniline
100-01-6 4-Nitroaniline 534-52-1 4,6-Dinitro- o-cresol
607-57-8 2-Nitrofluorene

Post a follow-up to this message

Von:**Tobias Kind** (tk2002deja@amdis.net)
Search Result 4
Betrifft:Re: Toxicity of nitro PAH
Newsgroups:sci.chem.analytical
Datum:2002-04-06 17:24:31 PST

picallo_de@yahoo.com (Jose M. Santos Picallo) wrote in some messages
and news:<4e262f3b.0204050555.154f2366@posting.google.com>...

Jose M. Santos Picallo wrote:

>which method/s are the best for the determination of nitro-PAH?
>Can somebody explain in deept these methods? ...
>Hi, im searching some information about 3-nitrobenzathron and how is
>generated for a diesel engine. ...
>im researching about nitroPAH and oder combustion gases from diesel
>engines. Im interesting in their toxicity (from example in the Ames
>Test). Also im interesting in some information about particle
>measurement devices (SMPS) and particle generator (CAST).

Dear Manolo,

again I have to peddle with the literature section I made (esp.)
for you: http://www.amdis.net/external/nitro-pahs.html

If you can afford some bucks you should buy or read two
very compact books. They contain all (most) information
you want and cover most of the fields of modern PAH research.
            -----   -------------------
(A)
The Handbook of Environmental Chemistry Vol3/Part J
Neilson, A.N., (Ed.)
PAHs and Related Compounds
Chemistry
http://www.springer.de/cgi-bin/search_book.pl?isbn=3-540-62394-9

(B)
The Handbook of Environmental Chemistry Vol3/Part J
Neilson, A.H., Stockholm, Sweden (Ed.)
PAHs and Related Compounds
Biology (With contributions by numerous experts)
http://www.springer.de/cgi-bin/search_book.pl?isbn=3-540-63422-3

With **kind** regards
Tobias Kind

www.amdis.net

PS:
Por qué no das una vuelta a la biblioteca?
Te he buscado tantos libros. Cómo te puede
ayudar alguien si no te ayudas a ti mismo?
!Que te diviertas investigando!
Saludos,
Tobias

PPS: Yes they are green and expensive :-)

Keywords:
(A)
Contents: R.G. Harvey: Environmental Chemistry of PAHs.-
A. Colmsjö: Concentration and Extraction of PAHs from Environmental
Samples.
- D.L. Poster, L.C. Sander and S.A. Wise: Chromatographic Methods of
Analysis
for the Determination of PAHs in Environmental Samples.-
M. Howsam and K. Jones: Sources of PAHs in the Environment.- B.R.T.
Simoneit: Biomarker PAHs in the Environment.- A.H. Neilson and P.-A.
Hynning: PAHs: Products of Chemical and Biochemical Transformation of
Alicyclic Precursors.- A.A. Herod: Azaarenes and Thiaarenes.- D.
Mackay and D. Callcott: Partitioning and Physical Chemical Properties
of PAHs.- J. Arey: Atmospheric Reactions of PAHs Including Formation
of Nitroarenes.
(B)
Contents: A.H. Neilson and A.-S. Allard: Microbial Metabolism of PAHs
and Heteroarenes.- E. Cavalieri and E. Rogan: Mechanisms of Tumor
Initiation by Polycyclic Aromatic Hydrocarbons in Mammals.- R.
Jankowiak and G.J. Small: Analysis of PAH-DNA Aduccts - Fluorescence
Line-Narrowing Spectroscopy.- R. Ramanathan and M.L. Gross: Mass
Specrometry Techniques: DNA Adducts of PAHs and Related Carcinogens.-
T.C. van Brummelen, B. van Hattum, T. Crommentuijn and D.F. Kalf:
Bioavailability and Ecotoxicity of PAHs.- G.-J. de Maagd and A.D.
Vethaak: Biotransformation of PAHs and Their Carcinogenic Effects in
Fish.- D. Delistraty: A Critical Review of the Application of Toxic
Equivalency Factors to Carcinogenic Effects of Polycyclic Aromatic
Hydrocarbons in Mammals.

Bargain section:
http://www.google.de/search?hl=de&q=Nitroarenes+ames+filetype%3Apdf&meta=

Post a follow-up to this message

Alle Beiträge des Diskussionsthemas "**PAH analysis with fixed fluo emission**"

Von:Tobias Kind (tk@theo.uoe.ufz.de)

Message 1 in thread

Betrifft:Re: PAH analysis with fixed fluo emission
Newsgroups:sci.chem.analytical

Datum:2001-08-09 12:34:18 PST

Dear Gerd,

> I'm trying to set up an HPLC method for analysis
> of pah in soil. Everything is working fine, now I
> want to change from UV to fl detection. I have
> a Kratos 980, which allows programming of the excitation
> wavelength, but not the emission wavelength. All publications

you want to to find only the 16 priority PAHs ? or extended list ?

(1)
try to set the excitation wavelength according to their lambda max.
(similar to their maximum in the UV-spectra) - if you have a strong
"baseline jumping" during wavelength switching - group your
molecules - like:
280 nm - Naphthalene, Acenaphtylene, Acenaphthene,Fluorene
250 nm - Phenanthrene,Anthracene
260 nm - Fluoranthene,Pyrene
265 nm - Benzo[a]anthracene,Chrysene
305 nm - Benzo[b]fluoranthene,Benzo[k]fluoranthene,
Benzo[a]pyrene,Dibenz[a,h]anthracene,Benzo[g,h,i]perylene,

Indeno[1,2,3-cd]pyrene
(2)
set your (fixed) emission wavelength to 335 nm for the first run
for the first 5-6 PAHs
set your (fixed) emission wavelength to 420 nm for the second run
for the rest

(2.1) Why 2 runs ? This is the price for a high sensitivity.

(A) from a monetary point of view I would say if you have to
do a lot of runs - try to get a exc./em. switchable device :-)

(B) from a chemometrical point of view I nevertheless suggest
to do 8 runs with settings from (1) and try emission wavelength
from 320 nm to 480 nm (20 nm steps).
This will take one day or night and will solve your problem in the best
way
(solvent, sensitivity,column, number of PAHs).

(C) Beware - this is not trivial - you will even lose some molecules
with 2 runs because PAHs also have different emission intensities.

For further reading:
(These publications have all pictures from fluorescence spectra and
listed
excitation and emission wavelengths and will also list some "uncommon"
PAHs - I write this because there are millions of PAH publications...)

*Investigation on simultaneous analysis of multicomponent polycyclic

aromatic hydrocarbon mixtures in water samples: a simple synchronous
fluorimetric method, Talanta, Volume 55, Issue 1, 3 August 2001, Pages
143-153
Digambara Patra and A. K. Mishra

*Fluorescence spectroscopy of aromatic species produced in rich
premixed ethylene flames, Chemosphere, Volume 42, Issues 5-7,
February 2001, Pages 835-841 A. Ciajolo, R. Ragucci, B. Apicella,
R. Barbella, M. de Joannon and A. Tregrossi

*Fish Biliary Polycyclic Aromatic Hydrocarbon Metabolites Estimated
 by Fixed-Wavelength Fluorescence: Comparison
with HPLC-Fluorescent Detection
EDITH L. C. LIN,SUSAN M. CORMIER, AND JONI A. TORSELLA
ECOTOXICOLOGY AND ENVIRONMENTAL SAFETY 35, 16–23 (1996)

*Invited Review
Photochemistry and Photobiology, Vol. 70, Iss. 1, July 1999
A Compilation of Physical, Spectroscopic and Photophysical Properties of

Polycyclic Aromatic Hydrocarbons
Reza Dabestani* and Ilia N. Ivanov
 http://www.pol-us.net/PAPHome/Vol70/pdfs/vol70iss1pp10-34.pdf

*Investigation on simultaneous analysis of multicomponent
polycyclic aromatic hydrocarbon mixtures in water samples:
a simple synchronous fluorimetric method
Talanta 55 (2001) 143–153
Digambara Patra, A.K. Mishra

With kind regards
Tobias Kind

PS:
Try also the NIST (Sander/Wise)
"Polycyclic Aromatic Hydrocarbon Structure Index"
http://ois.nist.gov/pah/

and
the Jinno Lab Polycyclic Aromatic Hydrocarbons (PAHs) Data Base
http://chrom.tutms.tut.ac.jp/JINNO/DATABASE/00database.html

and if you want to see their nice Kirschbaumbluetenfest (o-hanami) take
http://chrom.tutms.tut.ac.jp/JINNO/Memory/memory_frame.html

...ooops they cutted their last pictures - hope they had no
"sake excess" - just kidding :-)

Von:Gerd Klaassen (klaassen@coastweb.de) Message 2 in thread
Betrifft:Re: PAH analysis with fixed fluo emission
Newsgroups:sci.chem.analytical

Datum:2001-08-09 23:22:45 PST View this article only

Tobias Kind wrote:
>
> Dear Gerd,
>
> > I'm trying to set up an HPLC method for analysis
> > of pah in soil. Everything is working fine, now I
> > want to change from UV to fl detection. I have
> > a Kratos 980, which allows programming of the excitation
> > wavelength, but not the emission wavelength. All publications
>
> you want to to find only the 16 priority PAHs ? or extended list ?
>
> (1)
> try to set the excitation wavelength according to their lambda max.
> (similar to their maximum in the UV-spectra) - if you have a strong

> "baseline jumping" during wavelength switching - group your
> molecules - like:
> 280 nm - Naphthalene, Acenaphtylene, Acenaphthene,Fluorene
> 250 nm - Phenanthrene,Anthracene
> 260 nm - Fluoranthene,Pyrene
> 265 nm - Benzo[a]anthracene,Chrysene
> 305 nm - Benzo[b]fluoranthene,Benzo[k]fluoranthene,
>   Benzo[a]pyrene,Dibenz[a,h]anthracene,Benzo[g,h,i]perylene,
>
>   Indeno[1,2,3-cd]pyrene
> (2)
> set your (fixed) emission wavelength to 335 nm for the first run
> for the first 5-6 PAHs
> set your (fixed) emission wavelength to 420 nm for the second run
> for the rest
>
> (2.1) Why 2 runs ? This is the price for a high sensitivity.
>
> (A) from a monetary point of view I would say if you have to
> do a lot of runs - try to get a exc./em. switchable device :-)
>
> (B) from a chemometrical point of view I nevertheless suggest
> to do 8 runs with settings from (1) and try emission wavelength
> from 320 nm to 480 nm (20 nm steps).
> This will take one day or night and will solve your problem in the best
> way
> (solvent, sensitivity,column, number of PAHs).
>
> (C) Beware - this is not trivial - you will even lose some molecules
> with 2 runs because PAHs also have different emission intensities.
>
> For further reading:
> (These publications have all pictures from fluorescence spectra and
> listed
> excitation and emission wavelengths and will also list some "uncommon"
> PAHs - I write this because there are millions of PAH publications...)
>
> *Investigation on simultaneous analysis of multicomponent polycyclic
> aromatic hydrocarbon mixtures in water samples: a simple synchronous
> fluorimetric method, Talanta, Volume 55, Issue 1, 3 August 2001, Pages
> 143-153
> Digambara Patra and A. K. Mishra
>
> *Fluorescence spectroscopy of aromatic species produced in rich
> premixed ethylene flames, Chemosphere, Volume 42, Issues 5-7,
> February 2001, Pages 835-841 A. Ciajolo, R. Ragucci, B. Apicella,
> R. Barbella, M. de Joannon and A. Tregrossi
>
> *Fish Biliary Polycyclic Aromatic Hydrocarbon Metabolites Estimated
> by Fixed-Wavelength Fluorescence: Comparison
> with HPLC-Fluorescent Detection
> EDITH L. C. LIN,SUSAN M. CORMIER, AND JONI A. TORSELLA
> ECOTOXICOLOGY AND ENVIRONMENTAL SAFETY 35, 16–23 (1996)
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> *Invited Review
> Photochemistry and Photobiology, Vol. 70, Iss. 1, July 1999
> A Compilation of Physical, Spectroscopic and Photophysical Properties of
>
> Polycyclic Aromatic Hydrocarbons
> Reza Dabestani* and Ilia N. Ivanov
> http://www.pol-us.net/PAPHome/Vol70/pdfs/vol70iss1pp10-34.pdf
>
> *Investigation on simultaneous analysis of multicomponent
> polycyclic aromatic hydrocarbon mixtures in water samples:
> a simple synchronous fluorimetric method
> Talanta 55 (2001) 143–153
> Digambara Patra, A.K. Mishra
>
> With kind regards
> Tobias Kind
>

> PS:
> Try also the NIST (Sander/Wise)
> "Polycyclic Aromatic Hydrocarbon Structure Index"
> http://ois.nist.gov/pah/
>
> and
> the Jinno Lab Polycyclic Aromatic Hydrocarbons (PAHs) Data Base
> http://chrom.tutms.tut.ac.jp/JINNO/DATABASE/00database.html
>
> and if you want to see their nice Kirschbaumbluetenfest (o-hanami) take
> http://chrom.tutms.tut.ac.jp/JINNO/Memory/memory_frame.html
>
> ...ooops they cutted their last pictures - hope they had no
> "sake excess" - just kidding :-)

Thanks a lot!

I try to find "only" the 16 PAH's. I used UV detection before,
which runs pretty good, but I recently got a used FL detector
and so I thought I can use it to increase sensitivity. A new
one is not possible.

The students can't do two runs of each sample, so I have
to find out a way with switching only the ex wavelength.

The german DIN method suggests 365/470 nm, but I found the results
were really bad. (Maybe I have to use a xenon lamp instead of
the D2 one, but I don't have the power supply for it).

Best results up to now are something like 270/340 nm using
a cut-off filter (which allows detection of all emissions
above about 340 nm.)

Thanks also for the links. BTW - Agilent has a nice PAH handbook
in pdf available with all spectra on their hompepage.

Kind regards,
Gerd Klaassen

Von:**Tobias Kind** (tk@theo.uoe.ufz.de)

Betrifft:Re: Identifying Unknowns Using TSCA ---> its a nugget !
Newsgroups:sci.techniques.mass-spec
Datum:2001-06-08 14:05:14 PST

"Little, James" wrote:

} We have had good success using the TSCA Inventory (list of chemical
} substances in use in the United States). We employ either the MW or MF
} obtained by LC-MS data. For more information, go to the section on NIST
} Search: Standard PC Approach, and look for TSCA link.

...snip ...snip :-)
and now the important thing:

}
} "A Little Mass Spectrometry and Sailing":
} http://users.chartertn.net/slittle

Dear James,

Again - thank you very much.

Detailed instructions - its really fun (=work) to read all the new things.
I know TSCA is not CAS, but I found on-the-fly some interesting
compounds.

A good example for a former "unknown" CAS is:

Benzene, 1,1'-(2,2,2-trichloroethylidene)bis-
Formula: C14H11Cl3
MW: 284 CAS#: 2971-22-4 NIST#: NA

It was not found before. But now its here in "my house".
Really good together with the isotopic calculator and/or HRGCMS.

Another good example:
C16H35O2PS2: 0 hits before - 5 hits now.

But there's still a "large" gap.

If you look at some very "problematic" PAH-structures
like C21H14 you will only find a few substances in
NIST and Wiley but around 32 in ChemIDPlus with
detailed records and toxicological research since 30 or 40 years.

OK, they have all a molecular weight of 266 and spectra are
not very different. But to "know" about it is important.

Again I can go to the
Polycyclic Aromatic Hydrocarbon Structure Index from NIST
http://ois.nist.gov/pah/
and search for all the 252-PAHs and can now calulate
and think about all possible isomers (252-1+15)....

But it takes time...

But its good to have some more substances now :-)

With kind regards
Tobias Kind

PS: 17831-67-3 was not found :-(

PPS: Ahhh it was found in ISPRA at the
Existing Chemicals Bureau (former EINECS)

http://ecb.ei.jrc.it/existing-chemicals/

Von:**Tobias Kind** (tk@theo.uoe.ufz.de)
Search Result 26
Betrifft:Finding unknown substances
Newsgroups:sci.techniques.mass-spec
Datum:2001-01-03 16:00:05 PST

Dear Colleagues,

finding unknown "known" substances (identified by GC-MS) is sometimes horrible. In most cases customers of
GC-MS services want a little background knowledge about the identified substance.

Costs for 24h-online databases (CA,WOS,STN) can exceed the cost of a GC-MS device by a factor of 10.
Again, all the following links may be well known, therefore --> to whom it may concern.

I suppose you identified a substance manually or you have a proposal by NISTor Wiley databases.
As an arbitrary example I take CAS: [205-43-6] - Benzo(b)naphtho(1,2-d)thiophene.
You have to find retention data (boiling point), toxicity, and source and standards. (and you have no money)

(1) ***** 49 hits (by toxline//SIS//NLM)
http://chem.sis.nlm.nih.gov/chemidplus/

The people at toxline should win a prize for cleverness - they have dozens of CAS numbers. Especially many
old chromatography abstracts (its an eldorado). Don't forget to check medline.
And in the near future other clever people will link the whole databases to NIST an Wiley... :-)

(2) ***** 0 usefull links (by chemfinder)
http://www.chemfinder.camsoft.com/

Don't wonder - in this case Chemfinder found nothing - but this is the NUMBER ONE if you want to find
anything about a substance. Ever wondered what "grass hopper ketone" is? Try it! Or find out all the
features of chemfinder - using a substance like lindane. (people at chemfinder also should win a prize)
They link to NIST Chemistry WebBook and ECR Physprop (and many many other databases).

(3) ***** 3 hits (CAS), 19 hits name (by google)
http://www.google.com

Forget all other search engines, google is double sized (1,4E9 pages) and truly at time the biggest internet-engine.
Use the cache function - even if the other side is offline, you can read the page, because google has a carbon copy!
Remember, stemming (using wildcards *) is not allowed, and no phonetic search...

(4) *** 10-14 hits (by Beilstein)
http://www.chemweb.com/databases/beilstein

This is the free Beilstein abstract service by chemweb (you can join for free).

... and if you are a lucky subscriber (sorry)
(5) *** 4 hits (by sciencedirect)
www.sciencedirect.com together with the (german based) document delivery service SUBITO

I know that there are a lot more of services, databases, meta engines, full-text libraries, but I think that these
are the most useful free services one can use without professional help.

With kind regards
Tobias Kind

PS: If someone finds more (useful) hits with 4 other free services he/she will also win a price :-)

Alle Beiträge des Diskussionsthemas "**Authentic TXIB**"

Von:Jens Glastrup (jens.glastrup@natmus.dk) Message 1 in thread
Betrifft:Authentic TXIB
Newsgroups:sci.techniques.mass-spec
Datum:2000-12-15 05:50:06 PST View this article only

Dear colleaques
Could anyone provide me with a few mg's of a component named TXIB, CAS
#: 74381-40-1
Thank you very much in advance

Jens Glastrup
The National Museum of Denmark
Dept. of Conservation
Brede, Post Box 260
DK 2800 Lyngby
Denmark

Von:Tobias Kind (tk@theo.uoe.ufz.de) Message 2 in thread
Betrifft:Re: Authentic TXIB
Newsgroups:sci.techniques.mass-spec
Datum:2000-12-15 11:45:18 PST View this article only

Jens Glastrup wrote:

} Dear colleaques
} Could anyone provide me with a few mg's of a component named TXIB, CAS
} #: 74381-40-1
} Thank you very much in advance

Dear Dr. Glastrup,

I wonder where you got this number. TXIB (Kodaflex) is a brand from
Eastman.
And TXIB is 2,2,4-Trimethyl-1,3-pentanediol diisobutyrate (CAS#:
6846-50-0)

http://www.eastman.com/Brands/TXIB/OnlinePub.asp

http://www.eastman.com/Productfiles/Prod0197.htm

If you took this from NIST - maybe you can contact the group of Prof.
Hites (contributor).

http://www.indiana.edu/~hiteslab/

I think - as a multi (million) ton product TXIB could be contaminated
with
Propanoic acid, 2-methyl-, 1-(1,1-dimethylethyl)-2-methyl-1,3-propanediyl
ester (CAS#: 74381-40-1).
(And even 2,4,4-trimethyl-1, 3-pentanediol is very rare)
But this is my opinion (not veryfied) and there are many other ways. But
maybe you can contact Eastman.
(6846-50-0 and the corresponding diols are also produced by other
companies.)

Witgh kind regards
Tobias Kind

Alle Beiträge des Diskussionsthemas "**Finnigan ITDS software**"

Von:Dr. Dickie (dr_dickie@my-deja.com) Message 1 in thread
Betrifft:Finnigan ITDS software
Newsgroups:sci.techniques.mass-spec
Datum:2000-08-29 08:45:40 PST View this article only

I have a Perkin-Elmer ITD (really a Finnigan ITD with a Perkin-Elmer
8420 GC) and I am running the Finnigan ITDS version 4.10 software. Since
this software is no longer supported (the Finnigan web page lists this
software a obsolete) I was wondering if anyone had up-dated versions of
this software and or libraries for this software that I might be able to
get a copy of. We use this instrument for instrumental analytical
chemistry lab and better software and library searching capabilities
would allow for better (more real world) labs.
I would assume that this is not considered illegal since the software is
obsolete and no longer supported.
Yes I know that several companies make special software that can be used
to convert the ITDS into chemstation-type chromatagrams, but our budget
for this instrument is whatever I happen to have in my pocket at the
moment.
Thanks in advance.

--
Dr. Dickie

"The important thing is not to stop questioning.
Curiosity has its own reason for existing."
A. Einstein

Von:Tobias Kind (kind@wwwserv.rz.uni-leipzig.de) Message 2 in thread
Betrifft:Re: Finnigan ITDS software
Newsgroups:sci.techniques.mass-spec
Datum:2000-08-29 12:51:23 PST View this article only

"Dr. Dickie" wrote:

} I have a Perkin-Elmer ITD (really a Finnigan ITD with a Perkin-Elmer
} 8420 GC) and I am running the Finnigan ITDS version 4.10 software. Since
} .....snip....
} I would assume that this is not considered illegal since the software is
} obsolete and no longer supported.
} Yes I know that several companies make special software that can be used
} to convert the ITDS into chemstation-type chromatagrams, but our budget
} for this instrument is whatever I happen to have in my pocket at the
} moment.
}

...snip

Hi,
you can use AMDIS from NIST - it works with IDTS and ITS40 files
(remember to choose Finnigan IDTS form the Analyze Settings)
Its really powerfull and you can download a 32-bit version from NIST
and a handbook and library conversion... (following a review :-)

http://wwwstud.rz.uni-leipzig.de/~che94beq/amdis.htm

Or you can use WSearch from Frank Antolasic (but maybe only ITS40)
http://minyos.its.rmit.edu.au/~rcmfa/search.htm

Assuming you have a chemstation - you can export spectra from AMDIS to your
NIST-library.

Kind regards
Tobias

PS:
Assuming you have a quarter in your pocket :-)

Von:MC Guy (ktreier@fuse.net) Message 3 in thread
Betrifft:Re: Finnigan ITDS software
Newsgroups:sci.techniques.mass-spec

Datum:2000-08-31 13:02:43 PST View this article only

We provide an upgraded version of ITDS 4.1 software which provides the
following enhancements:

1) Ability to run on Pentium and Pentium II class machines
2) Ability to support Hard Drive partitions <32MB to <2GB
3) 10-20% sensitivity improvement under identical operating conditions
NEW
4) HP Laserjet Support
5) Ability to adjust Scan Segment break points ***NEW***

available for $249

Karl Treier
ktreier@fuse.net

We also provide ITDS data format converters:

DAT2XML (ITDS DAT format to XML)
DAT2TXT (ITDS DAT format to delimited ASCII for import to Excel)
DAT2MS (ITDS DAT format to Magnum MS format)

$49/ea (written in 100% Java, will run on Windows, Solaris, Linux, etc)

Dr. Dickie <dr_dickie@my-deja.com> wrote in message
news:8ogli1mkp1@news-int.gatech.edu...
} I have a Perkin-Elmer ITD (really a Finnigan ITD with a Perkin-Elmer
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} this software is no longer supported (the Finnigan web page lists this
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} I would assume that this is not considered illegal since the software is
} obsolete and no longer supported.
} Yes I know that several companies make special software that can be used
} to convert the ITDS into chemstation-type chromatagrams, but our budget
} for this instrument is whatever I happen to have in my pocket at the
} moment.
} Thanks in advance.
}
} --
} Dr. Dickie
} -----------------
} "The important thing is not to stop questioning.
} Curiosity has its own reason for existing."
} A. Einstein
} -----------

```
}
}
} Sent via Deja.com http://www.deja.com/
} Before you buy.
}
}
```

Von:**Tobias Kind** (kind@rziris.rz.uni-leipzig.de)
Search Result 18
Betrifft:Re: silanizing glass injector inlets (+++ bargain)
Newsgroups:sci.techniques.mass-spec
Datum:2001-01-11 09:31:04 PST

Dear Mr. Kitchen,

} What is the process for silanization of injector inlet glassware inside
} of injector sleeves. We currently use split inlets and buy new ones
} although we would like to start cleaning our own. Thanks.

Answer: (c)Alltech

All untreated glass surfaces contain –OH or silanol groups. These groups interact with most compounds that are injected into your GC. The interaction usually takes the form of tailing peaks (reversible adsorption) or irreversible adsorption of the compound, both of which make quantitation difficult. However, you have several options to counteract this problem. You can either buy deactivated liners or deactivate the liners yourself.

To deactivate the liner, you must first prepare it for silylation. Rinse the new liner with your sample solvent to remove any manufacturing residues that might interfere with this process.

The liner must then be dehydrated. Silylation reagents preferentially react with small polar compounds such as water, alcohols, and amines, so these compounds must be removed before beginning the silylation process. To dehydrate the liner place it in an oven and heat it at 180°C for 1 hour.

Cool the oven to approximately 50°C and immediately place the liner in a 5% solution of dimethyldichlorosilane (DMDCS) preferably in toluene, but methylene chloride and pentane will also work. Place a piece of laboratory stretch film such as Saran Wrap™ or Dura Seal™ over the reaction vessel. Soak the liner in the 5% DMDCS solution for 10 minutes. Use caution when removing the liner from the reaction vessel because anhydrous hydrochloric acid is formed during this reaction as demonstrated by Figure 1. Due to their volatile and flammable nature, silylating reagents (and their solvents in some cases) should be kept away from open flames and sources of heat and should be handled only in a hood.

The liner should be rinsed with the same solvent used in the DMDCS solution and then soaked in methanol for 10 minutes. Once again cover the reaction vessel with laboratory stretch film. This step takes the reaction to completion and Residual reagent, if left on the liner, will often mimic column bleed which could require several hours to stabilize. The liner should then be removed from the methanol and allowed to air dry. Once dry, the liner is thoroughly deactivated and ready for use. Do not store opened solutions or leave covered for long periods of time.

Alltech has created a new deactivation kit specifically designed for deactivating
injection port liners. The kit comes with 4 x10mL ampules of 5% dimethyl-dichlorosilane (DMDCS) solution, a pair of tweezers for easy liner

handling, four test
tubes which act as the reaction vessel, and detailed instructions. This kit
includes
enough DMDCS to deactivate four injection port liners.

This is was taken from Alltech catalog: “Specialists in Chromatography”
Deactivation Kit 18107 $33.00
http://www.alltechweb.com/literature/brochure/363p7.pdf
or
http://www.alltechweb.com/searchmain.asp
(search for DMDCS - use Adobe Acrobat reader for reading PDF files)

With kind regards
Tobias Kind

PS: OK - here comes the bargain basement:

Additionally to my previous post: Finding unknown substances
(stuff,junk,everything)
I add another useful service: The "Search Adobe PDF Online"
In most cases you can instantly read "PDF-files" and you will
find exclusive documents which are not covered by other
search services!

http://searchpdf.adobe.com/

Enter: silylation liner dmdcs
If the links contain no usefull information - try "more like this document"

(...theres a gap - I walked manually to alltechweb...)

PPS: Sorry - J. Throck Watson :-)

Von:**Tobias Kind** (tk2002deja@amdis.net)
Search Result 3
Betrifft:Re: Advice on HPLC software
Newsgroups:sci.chem.analytical
Datum:2002-04-17 04:23:46 PST

"F.M.S." <fmstr@netcom.ca> wrote in message news:<NB0v8.8433$a04.39894@tor-nn1.netcom.ca>...
> Hi there I need some advice on HPLC software. I do not need the names of the
> software. I am looking more for features.

...snip snip

Dear Fred,

depends on your detectors and your tasks.

If you work with MS or DAD (Diode-Array-Detector) or
full scan fluorescence (multi-wavelength detection) where
you can get additional *spectral* information, you
need some more features.

If you work only with a raw peak (retention, height)
like UV or ELSD (Evaporative light scattering detector)
you need some basic features.

I assume basic functions (manual peak integration)
are implemented...
Some points from my developer database:

* software should *easily* integrate other devices.
  Important because if you do a "tricky research" you need
  different devices, no producer has all excellent
  detectors, pumps, autosamplers etc.pp..

* software should have an internal macro language.
  if you work with standard GLP you do not need it.

* software should have a "peak marker" or "post-it".
  most important function, often forgotten, people
  fight with printouts

* software should have export functions for *all* data.
  - maybe I have another software for interpretation
  - will save data in other formats (netCDF)
  - want a nice *vector* graphic

* software should have tools for batch processing.
  don't like to write 1000 rows manually

* software should have overlay/compare functions.
  not only a graphic version - but if you have a
  spectroscopic information also based on locking
  the same peaks on different chromatograms

* software should export all data to excel :-(.
  after integrating, batching etc. this is a must

* software should use spectroscopic functions.
  if you have UV-DAD, scanning fluo or MS - please look
  at a software which handles only this data.

Remember all the features and come back to your
HPLC software.

Nice 3-D graphics are funny but don't help us.
But a
* nice peak purity function or a
* peak deconvolution for UV/fluo/MS data or a
* spectra interpretation for UV-VIS data or fluo data (!)
* library manager for UV, fluorescence data
* funny enough those device vendors acquired millions of chromatograms
  but never saved the UV-VIS or fluorescence spectra
  for huge solvent corrected libraries... hahaahaa
  poor user souls...

* software should automatic correct drifts from
  multi-detector systems.

* software should have an inbuilt HPLC troubleshooter.
  peak has tailing, peak has fronting, no signal?
  which solvent to use?
  Easy example of a simple decision tree software

* software should have a integrated pKa, pH, logP unit.
  most separation problems with basic/acidic substances
  are problem of false solvent/pH conditions

* may help you in "automated method method development".
  multiple runs for best peak separation

* list goes on...

With **kind** regards
Tobias Kind

www.amdis.net

keywords:
waters, agilent, shimadzu, beckman, pharmacia,
kontron, hitachi, dionex, gynkotek, knauer, kratos,
linaer, perkin elmer, signal, varian

PS: Normally software producers don't read newsgroups
They are "in business". Therefore I've never seen such
a software. But one should say that the users
accept to suffer from (all) silly software and
in most cases "drain the cup of sorrow to the dregs"
until they (never) wake up...

PPS: counting replies ... tending to sifr(0) :-)

Post a follow-up to this message
