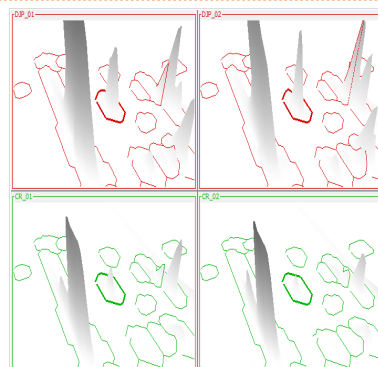
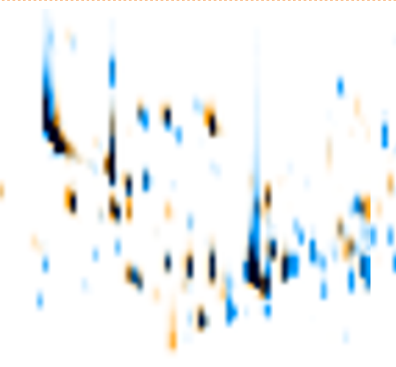


GasPedal

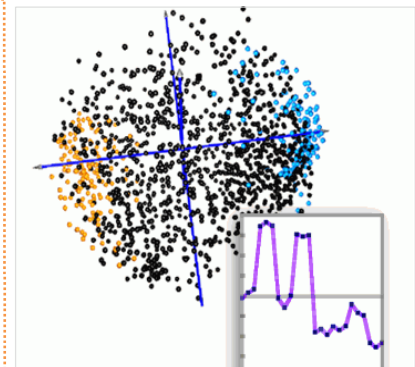
Boost Your GCxGC Analysis



Spots selected on image 'DJP_01'

Total number of selected spots shown in this report: 10.

| Profile | Label(s) ↓ | Spot ↑ | DJP (direct juice pasteurized) | | CR (concentrate + recovery aroma) | |
|---------|------------|--------|--------------------------------|--------|-----------------------------------|-------|
| | | | DJP_01 | DJP_02 | CR_01 | CR_02 |
| | ID17432 | 17432 | | | | |
| | ID17448 | 17448 | | | | |
| | ID17455 | 17455 | | | | |
| | ID17499 | 17499 | | | | |
| | ID34482 | 34482 | | | | |
| | ID35967 | 35967 | | | | |



GasPedal – explore a new era of analysis

You spend a lot of time optimizing your sample preparation and GCxGC protocols. You analyze single runs and want to compare them, to get the most information out of them.

As GasPedal is based on modern technologies you get reliable and statistically significant results. Furthermore with GasPedal you reduce the analysis time to a minimum – your time matters to us.

More reliable results, better statistical analysis

GasPedal includes an approach that generates complete spot profiles, i.e. without missing values, to make statistical analysis much more reliable.

The approach as implemented in GasPedal is unique, transparent, time-saving, and under your full control.

Why GasPedal?

- Comparison of different runs
- Workflow support for beginners
- Complete spot profiles
- Automatic image alignment to remove distortions between runs
- Spot detection and editing only on one image necessary
- Spectra export compatible to e.g. NIST MS Search
- Advanced statistical methods, based on absence of missing values
- Various visualization, reporting and exporting features
- Flexible pricing/licensing models
- Available for current Windows, Mac, and Linux operating systems

Image warping (alignment of spot positions) was introduced in 2000 and improved by SmartVectors™, GasPedal's leading technology for automatic alignment of chromatograms.

The idea to create complete spot profiles resulting in 100% spot matching has been invented by DECODON to increase statistical confidence significantly.

Deciding for GasPedal means deciding for innovation.

DECODON – committed to customer satisfaction and innovation

Established in 2000, we are committed to developing and delivering innovative software tools for modern life sciences and dedicated to customer satisfaction. Our team of mathematicians, computer scientists, and biologists carefully listens to you, analyses your needs, and transforms innovative ideas into outstanding software solutions that really make a difference.

Analyze ALL your GCxGC experiments with ONE software

Comprehensive two-dimensional gas chromatography (GCxGC) has seen many innovations in the past.

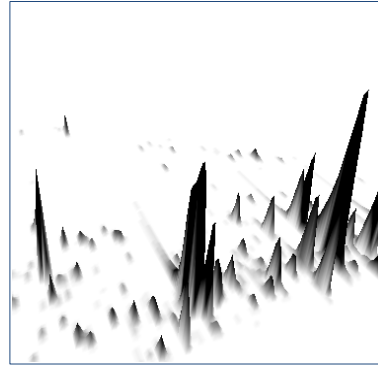
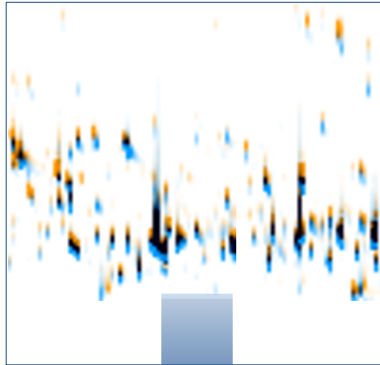
With GasPedal you can experience one more: Different chromatograms can be analyzed and compared easily.

Whatever you want to explore, GasPedal will help you to get the most information out of your runs.

Various visualization and exporting features

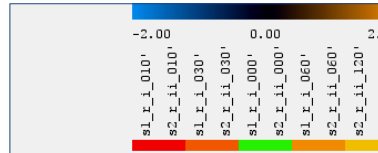
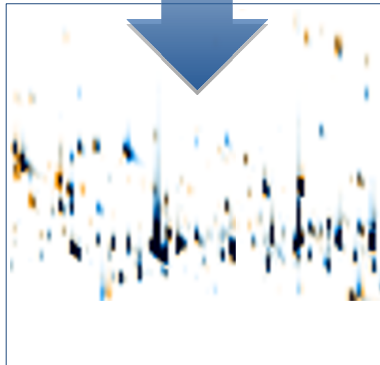
It is good to achieve reliable results. Being able to easily prepare them for publication and presentation is even better. GasPedal helps you with that: Use a broad range of modern data visualization and various exporting features.

Dual color channel overlay of two images (blue represents image A; orange image B) before initialization of automatic warping.

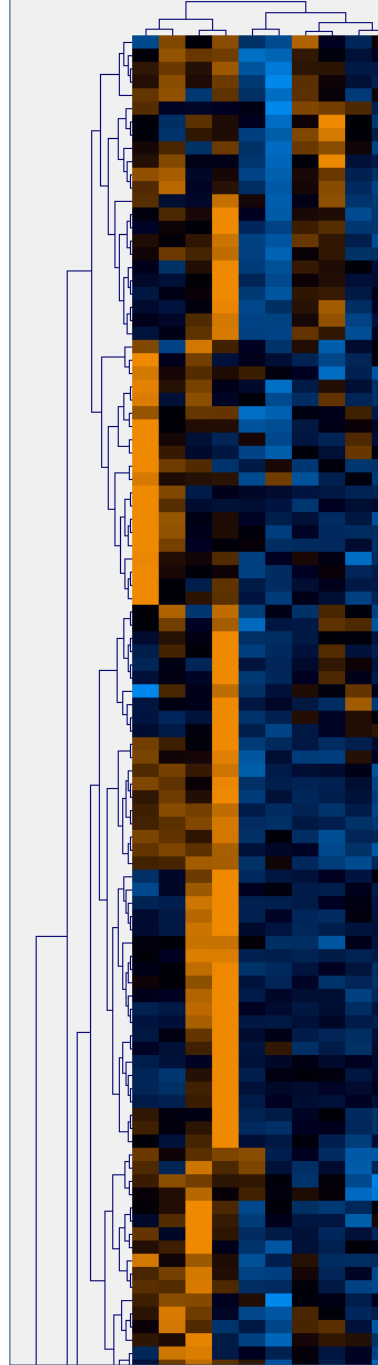


3D spot views help to determine spot boundaries during spot editing, supportable by a NIST database search

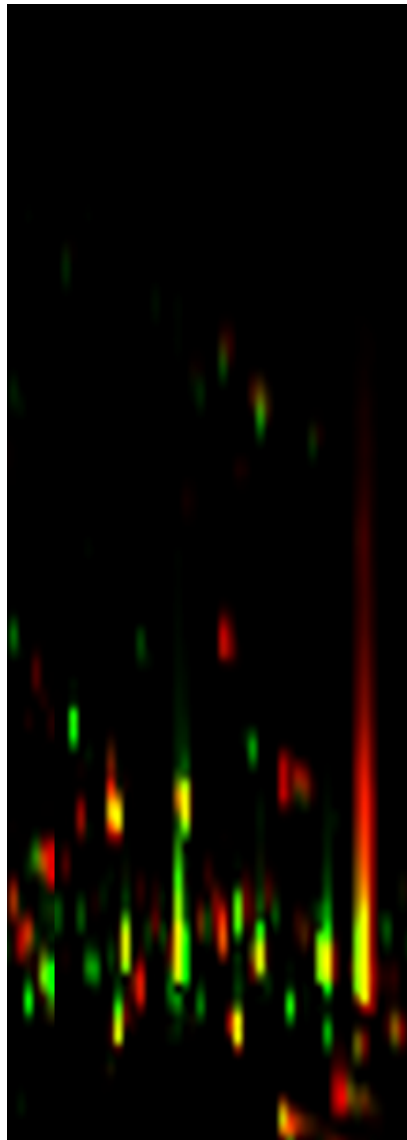
Result of the automatic warping process: black and gray spots are present in both images with similar signal intensity.



Complete spot profiles allow for the application of a variety of clustering methods and statistical test.



Dual color channel image of two image in a dark design after compensating run differences



2D chromatogram of a pineapple extract (section).

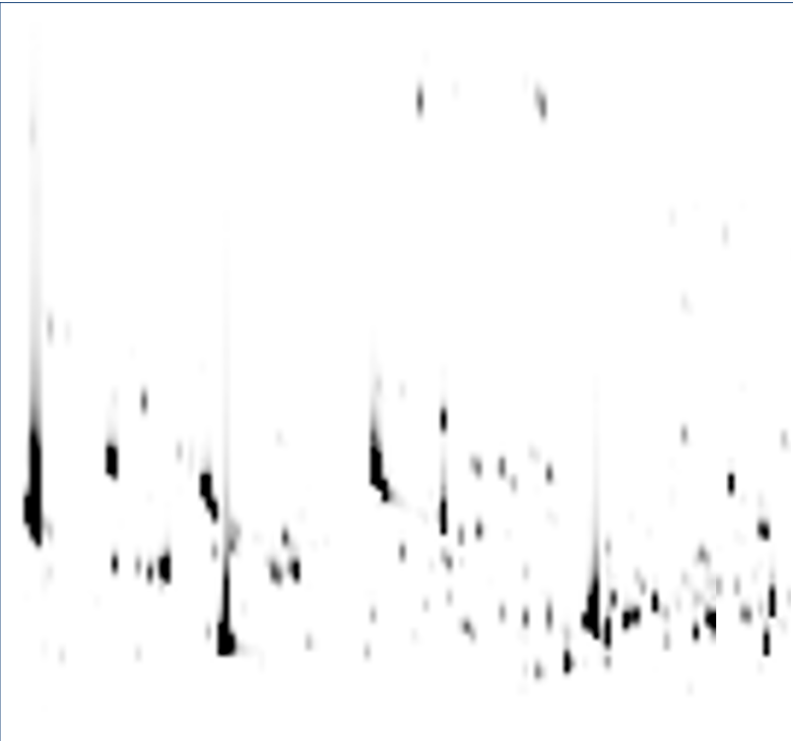
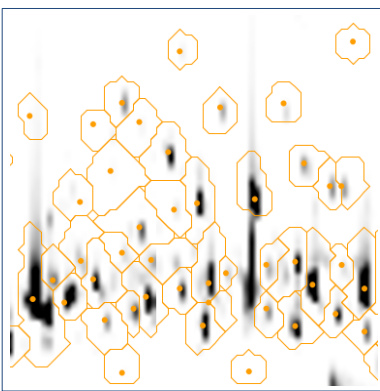


Image with detected and modelled spot boundaries



Unique analysis workflow for 100% matching spots

The recommended analysis workflow for GasPedal is a unique approach that leads to complete and correct spot matching for reliable data. Users are free to use the Workflow component as a guideline for the complete analysis process or enjoy the flexibility of the sophisticated capabilities of GasPedal.

Image warping – making virtually perfect GCxGC runs

GasPedal's SmartVectors™ technology uses the whole image information to automatically eliminate running differences between chromatograms to align them.

You are not forced to decide for a reference image to be aligned with all other images in your project. Use predefined warping strategies or freely connect images according to your individual experiment along the similarity of the chromatograms. As a result all spots have the same position on each image – as if you had perfect runs without any distortions.

Simplified and flexible project setup

With GasPedal's Light Table, organizing images into groups is done in the blink of an eye: You can freely setup your project so that it fits to your experimental setup.

The missing values problem ... no problem for GasPedal

All images of a project can be fused into one synthetic image using the Union Fusion algorithm (introduced in 2003 in Delta2D). The resulting image looks like a real chromatogram and is actually the substance map for your project – containing all spots from all images of the project.

One image with all spots – a perfect basis for spot detection and editing. Let GasPedal transfer the complete pattern of spot boundaries from your substance map to all the images in your project and spot matching is finished – completely and correctly.



GasPedal introduces innovations, e.g.:

Image warping (alignment of spot positions) was introduced with Delta2D 1.0 in year 2000. The concept of creating complete spot profiles resulting in 100% spot matching was made a reality in 2003. In 2006 SmartVectors™ were introduced to provide a transparent and hybrid method to integrate automatic and manual image warping. Web reports have been developed in 2007, along with advanced multivariate statistical methods. Since 2008, Delta2D offers a guided workflow and a modern, more effective window management. Many further improvements and innovations followed – among them 3D view across all images in 2014 and export of images as presentation slides.

GasPedal, developed as a sibling product of Delta2D, now lets you benefit from all of these innovations also in comprehensive two-dimensional gas chromatography (GCxGC).

GasPedal – decide for leading technology.

Workflow component of GasPedal guides you step by step through the whole image analysis process.

Project: Pineapple Juices

- 1 Setup Project
- 2 Warp Images
- 3 Detect and Quantify Spots
- 4 Analyze Spot Profiles
- 5 Present Results

Connect images

Setup *direct warpings* such that all images in the project are connected, directly or indirectly.

All images are connected.

Automatic warping

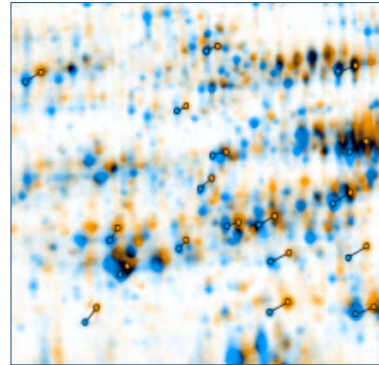
Use the *Job Manager* to let GasPedal find warpings for multiple image pairs. Each pair that has warp mode set to *automatic* will be included in the job manager's list. You can review and change completed warpings while the job manager is still working.

Review direct warpings

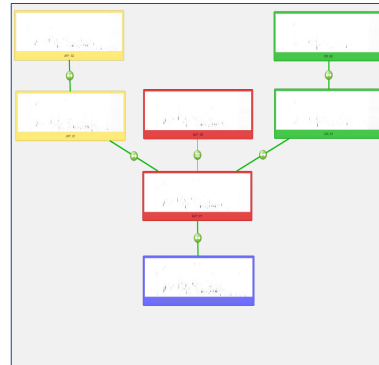
Double click on any pair in the list to open it in the Dual View.

| 1st Image | 2nd Image | Status | Approve |
|-----------|-----------|--------|---------|
| DJP_01 | DJP_02 | OK | |
| DJP_01 | CR_01 | OK | |
| CR_01 | CR_02 | OK | |
| DJP_01 | JRP_01 | OK | |
| JRP_01 | JRP_02 | OK | |

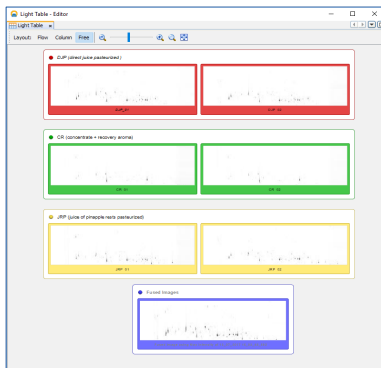
You can change the match vectors there or even let GasPedal find additional vectors using the Find Match Vectors button. When you are satisfied with the warping click on *Approve* in the table above to approve all match vectors.



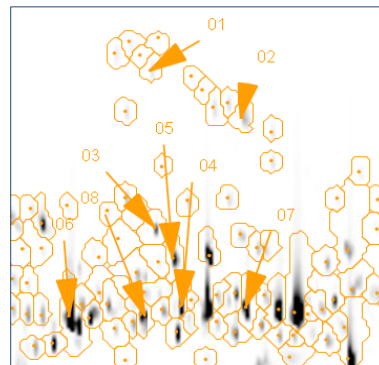
Warp vectors represent correspondences between two images.



The Warping Setup shows how pairwise warpings connect all images in your project.

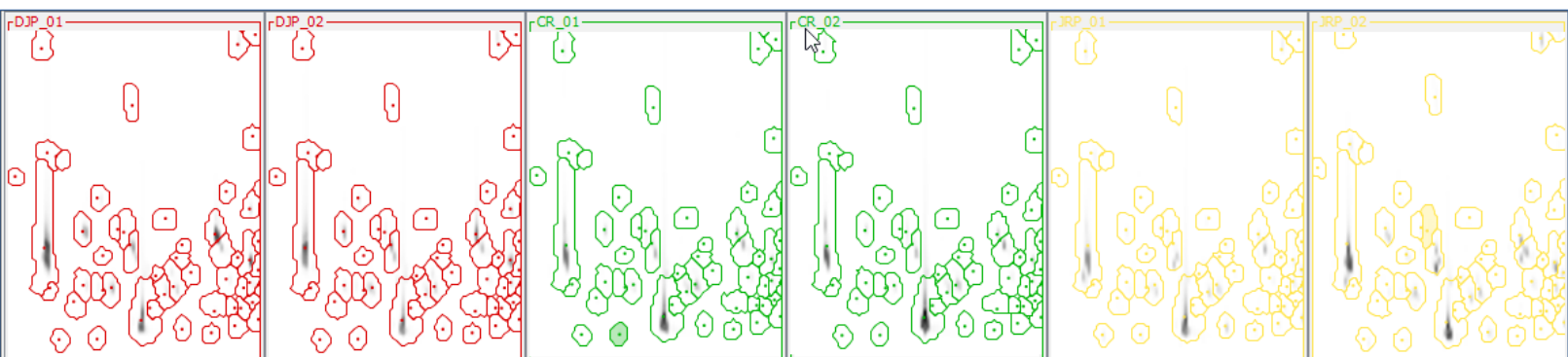


The Light Table supports project organization, e.g. naming of groups and images and grouping of replicates.

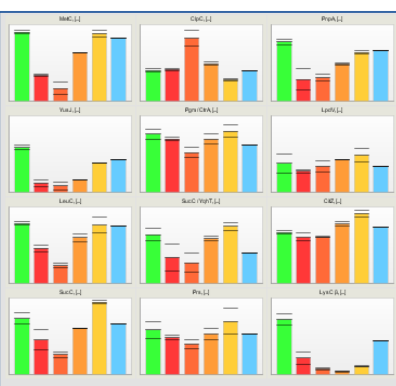


After positional correction, images are fused into a fusion image condensing the spot pattern of the whole experiment in one image. Spot identifications can be managed on the fusion image. Spot detection and editing is performed here only once per experiment ...

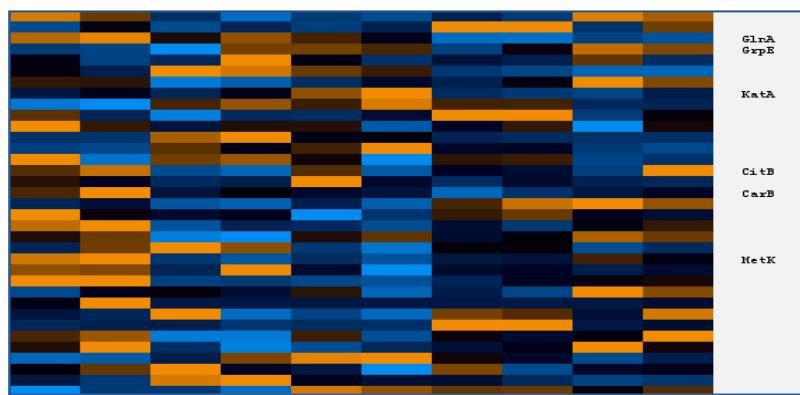
... while transfer of this spot pattern results in 100% matching spots for all images of your experiment.



detection data of 100% matching spots result in complete bar charts ...



... or in heat maps (orange means high, black average, and blue low quantity).



Advanced statistical methods

With GasPedal's 100 Percent Spot Matching, matching problems are eliminated. It also results in highest statistical confidence as there are no missing values.

GasPedal incorporates advanced algorithms provided and tightly integrates them into the 2D chromatogram analysis workflow.

Identify structures in your data and detect outliers

A very powerful method to detect outliers is **Principal Component Analysis (PCA)** or clustering methods.

Both can also be used to identify structures in the experiment. Ideally, the cluster composition will reflect the real structure of the experiment, i.e. replicates and images from the same sample should have similar expression levels and thus end up in the same cluster.

Clustering also help to group spot profiles. This can be very useful for getting an overview of all spot profiles before proceeding to more detailed analysis.

These methods are currently available:

- **Hierarchical Clustering (HCL)**,
- **k-means / k-medians Clustering (KMC)**.

Furthermore, **Paulidis Template Matching (PTM)** allows for selecting substances that follow a given spot pattern.

Nonparametric tests – the gold standard for spot quantities

Nonparametric tests do not require a normal distribution assumption. They are therefore especially suitable for small projects.

In GasPedal, these nonparametric tests can be applied:

- **Wilcoxon Rank Sum Test** for testing one factor in two experimental groups
- **Kruskal-Wallis Test** for testing one factor in multiple experimental groups
- **Mack-Skillings Test** for testing two factors in multiple experimental groups
- **Fisher Exact Test** for testing non-random associations between two categorical variables.

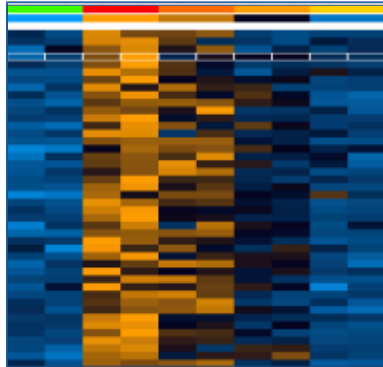
Find significantly changed spots

In the simplest case, the experiment is a comparison of two samples, e.g. diseased vs. control, mutant vs. wild type etc. The challenge is finding those substances that show significant differences in expression levels. Certainly the most popular test in this area is **Student's t-Test**. In GasPedal, different variations of the t-Test are available.

Spots that have significant differences in means across three or more groups of samples can be found with the **Analysis of Variance (ANOVA)**. In GasPedal, **one-way** analysis of variance and **two-factor** analysis of variance are implemented.

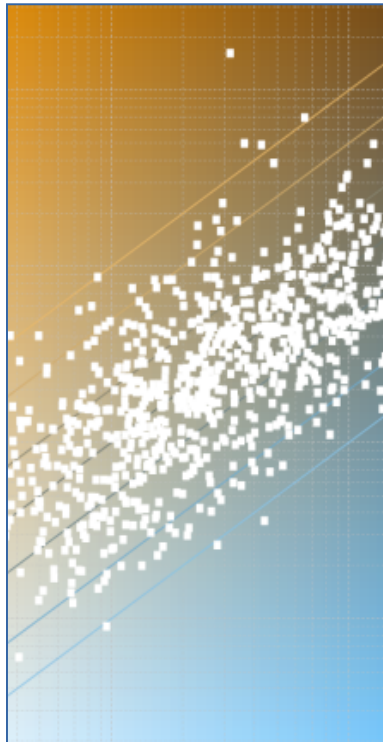
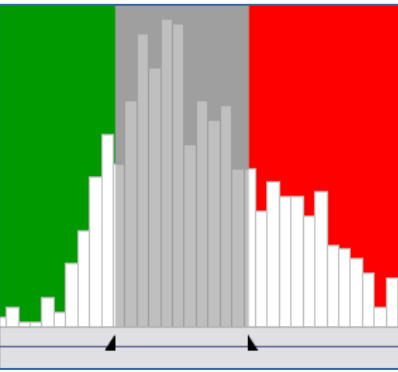
All tests can be supplemented with controlling the **False Discovery Rate (FDR)**, since multiple testing can be a real pitfall.

You can use filters to find volatile spots within a specified induction range, within a specific intensity class or with other properties of interest. Filters can be combined to find spots that match a combination of different criteria.

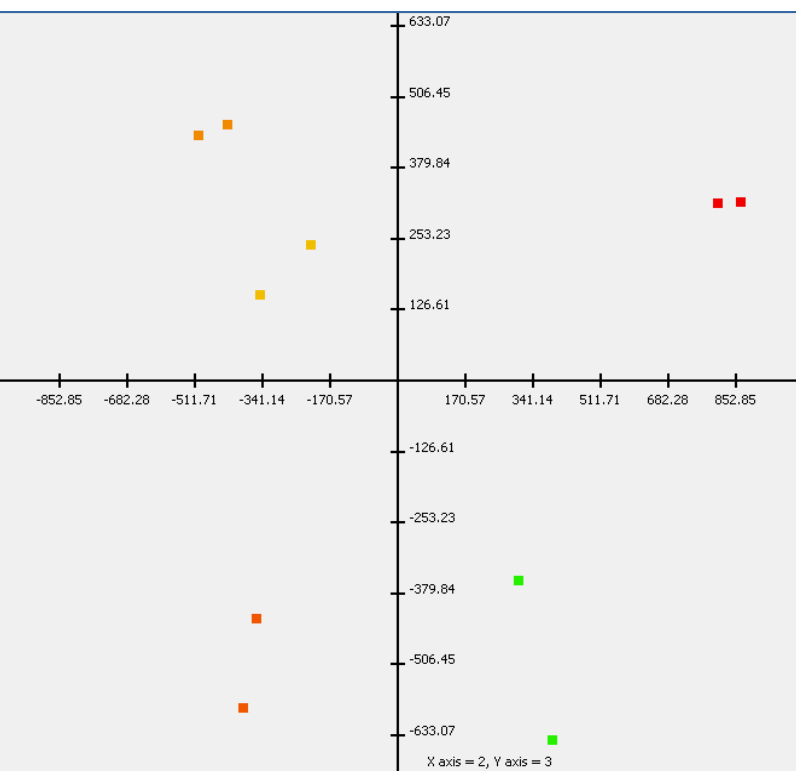


If you are looking for certain kind of spot profiles, you can predefine a template (shown in the second row of the heat map header). All spots behaving similar to the profile template will be found.

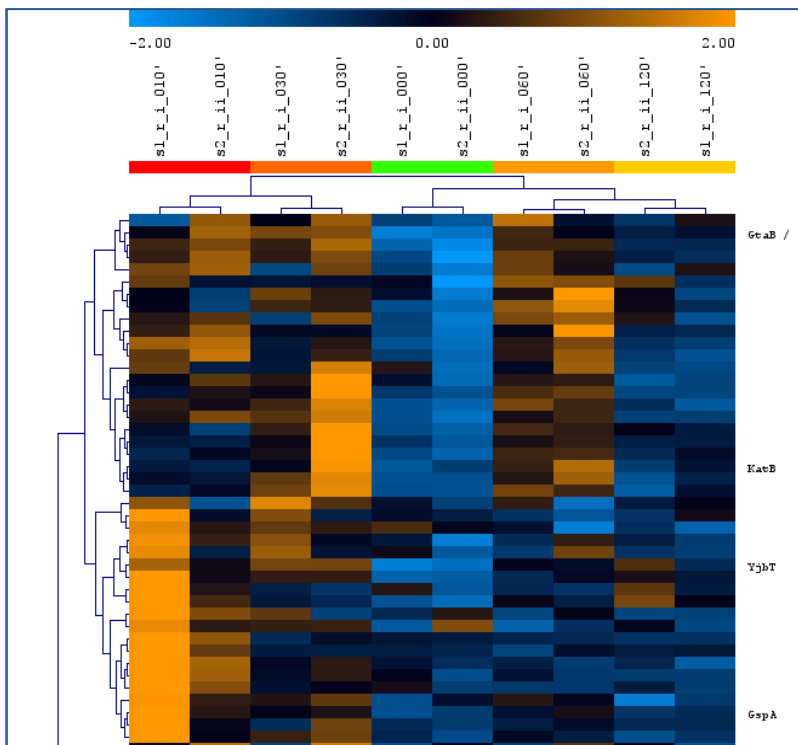
The Quantitation Table gives an overview of the expression data of your chromatograms.



Principal Component Analysis is a tool to reduce data complexity in multidimensional data sets. A set of data points were projected onto a two dimensional data space. This shows that samples clearly differ from each other while replicates are closely related.



| s1 %V | s2 %V | s1 %V | s2 %V | s1 %V | s2 %V | s1 %V | s2 %V | s1 %V | s2 %V | s1 %V | s2 %V | s1 %V | s2 %V | Label |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| 0.039 | 0.029 | 0.010 | 0.001 | 0.009 | 0.006 | 0.012 | 0.009 | 0.040 | 0.035 | | | | | |
| 0.010 | 0.017 | 0.010 | 0.013 | 0.011 | 0.013 | 0.031 | 0.029 | 0.012 | 0.023 | | | | | |
| 0.261 | 0.278 | 0.206 | 0.247 | 0.220 | 0.187 | 0.121 | 0.119 | 0.146 | 0.135 | GlnA | | | | |
| 0.115 | 0.112 | 0.078 | 0.159 | 0.160 | 0.152 | 0.114 | 0.140 | 0.174 | 0.162 | GrpE | | | | |
| 0.016 | 0.006 | 0.009 | 0.054 | 0.016 | 0.008 | 0.012 | 0.011 | 0.026 | 0.009 | | | | | |
| 0.144 | 0.095 | 0.286 | 0.252 | 0.197 | 0.171 | 0.073 | 0.060 | 0.033 | 0.032 | | | | | |
| 0.143 | 0.141 | 0.047 | 0.063 | 0.091 | 0.111 | 0.098 | 0.121 | 0.241 | 0.170 | | | | | |
| 0.054 | 0.063 | 0.048 | 0.064 | 0.101 | 0.161 | 0.046 | 0.041 | 0.037 | 0.052 | KatA | | | | |
| 0.067 | 0.030 | 0.199 | 0.233 | 0.193 | 0.264 | 0.198 | 0.197 | 0.125 | 0.127 | | | | | |
| 0.015 | 0.007 | 0.000 | 0.007 | 0.006 | 0.009 | 0.024 | 0.022 | 0.005 | 0.011 | | | | | |
| 0.043 | 0.028 | 0.021 | 0.027 | 0.027 | 0.015 | 0.023 | 0.028 | 0.006 | 0.026 | | | | | |
| 0.008 | 0.005 | 0.154 | 0.269 | 0.054 | 0.065 | 0.019 | 0.012 | 0.008 | 0.009 | | | | | |
| 0.008 | 0.004 | 0.072 | 0.041 | 0.065 | 0.160 | 0.034 | 0.035 | 0.010 | 0.003 | | | | | |
| 0.075 | 0.019 | 0.059 | 0.064 | 0.047 | 0.014 | 0.051 | 0.052 | 0.028 | 0.032 | | | | | |
| 0.289 | 0.325 | 0.212 | 0.197 | 0.288 | 0.204 | 0.251 | 0.245 | 0.219 | 0.352 | CitB | | | | |



Hierarchical Clustering sorts samples (columns) according to similar global expression of substances, or spots (rows) according to similar expression on all chromatograms.



TIGR MeV, an analysis suite for expression data analysis, is used inside GasPedal to perform advanced expression studies.

Do more with your data

Since its beginning GasPedal supports open data formats which allow you to easily transfer your analysis data to, for example, your in-house database. The powerful exporting and visualization features can be used to prepare results for publication and presentation.

Export tables and images

We want you to get the most out of your data and save it in the format you prefer. Currently, you can export data from GasPedal

- as MS Excel worksheets – flexibly configure visibility of table columns since what you see is what is exported,
- as MS PowerPoint slides – works for single, dual channel, and color coding images (spot boundaries and labels appear as MS PowerPoint objects),
- as CSV-files – to be imported to 3rd party software,
- as snapshots – single or dual channel images and Color Coding images can be exported in standard image file formats (like TIFF, JPEG, PNG, PNM, BMP).

Standard MS Office files can also be opened by other packages like LibreOffice or OpenOffice.

Color Coding – Summarize your results on a single image

Spot Color Coding lets GasPedal display a component map (or a single chromatogram) with spots colored according to their spot profiles. Independent of the experiment all results can be shown at a glance.

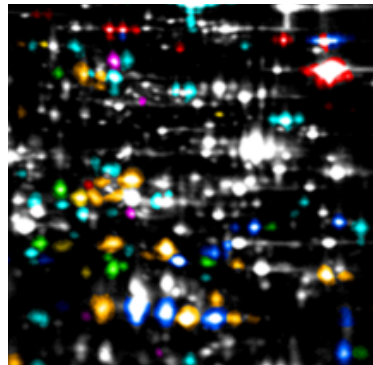
Search and identify volatiles by their spectra

You can easily copy individual spectra to your clipboard and paste them into your NIST MS Search database. If you want to search for multiple spectra at once, you can export subsets or even all spectra of a chromatogram to a MGF file and use it to identify your volatiles.

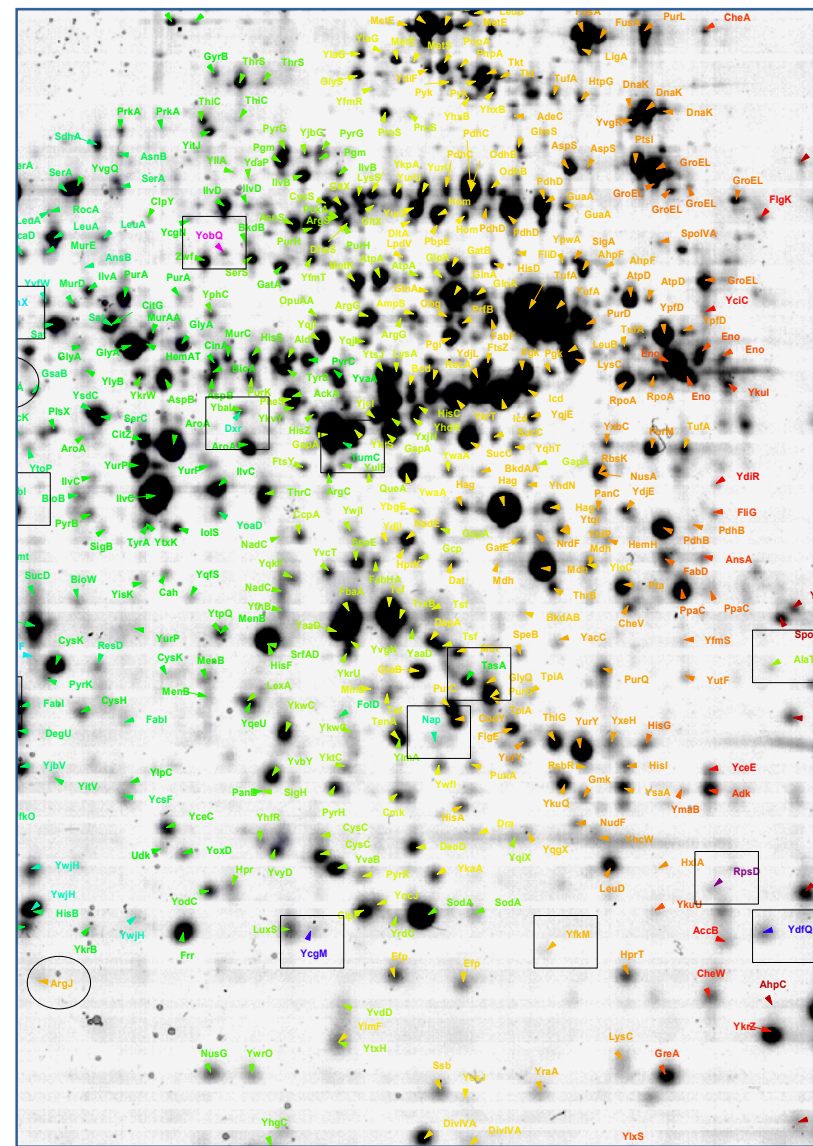
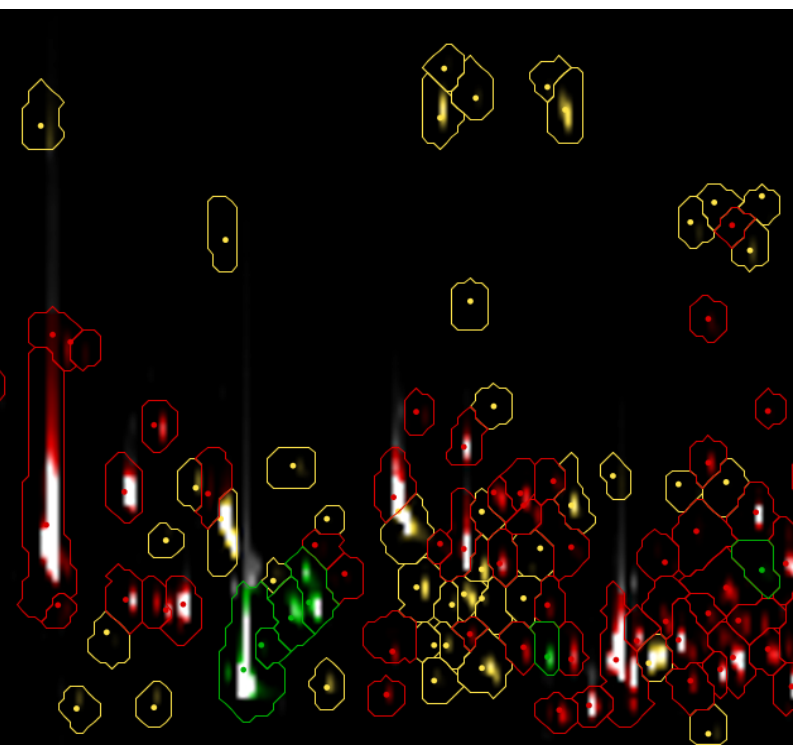
Min/Max Color Coding colors spots according to their maximum (or minimum) intensity within a series of samples.



Subset Color Coding produces a component map that shows which volatiles get increased or reduced by certain combinations of experimental conditions, treatments, or stimuli.



Color Coding according to arbitrary properties highlights outliers.



"Delta2D has greatly enhanced our ability to quickly and more reliably align our gel images, which greatly reduces errors in protein spot reproduction and alignment. The alignment feature in Delta2D is superior to the warping feature we were using with our previous software, and as a result our processing times have decreased significantly. This allows us to get to the actual spot analysis more quickly, make decisions, and move on to the next experiment."

*Joseph MacFarland
Framingham, USA*

DECODON Scouts – Retrieve data from databases in the web

DECODON Scouts are small software applications that go out to web resources or local files (like CSV) and come back with useful information about a label on a image.

Scout data can be properties, annotations such as identifications, functional categories, and much more.

GasPedal offers an API to easily create customized Scouts to retrieve data from arbitrary web resources when offered as XML.

The information being retrieved by scouts is attached to labels. The data is organized in groups of related data about a spot.

The data is saved along with the pool so it does not need to be retrieved from the web again.

Labels and the retrieved Scout data can easily be exported using GasPedal's Label report (see below).

Interactive web reports – The modern way of exporting data

GasPedal's web reports make it easy to present and summarize your experimental setup, relevant spots, and quantitative data. They are based on HTML so you can put them on the web easily.

The reports are shown in your web browser. You can copy all or part of a report into your favorite word processor or presentation program.

Project report includes global information that is available for samples, groups, chromatograms (including the images) and the warping strategy (including the respective dual channel images).

Spot Album report includes information about spot profiles in the form of the respective areas on the chromatograms.

Spot Quantities report includes detailed quantitative information about spot profiles.

Labels report includes information about all labels on a certain image or those belonging to a certain set of spots on a an image, including Scout data if available.

All reports are interactive: They include controls to change the reports' content.

Furthermore the reports are connected with GasPedal: For example, clicking on a dual channel image in the Project Report will open the corresponding chromatogram in GasPedal, or clicked spots will automatically be highlighted in GasPedal. All reports can be accessed via the Reports menu in the Project Manager.

The report design is based on a HTML stylesheet, so they can be adapted to any corporate design.

Show spot profiles in the form of the respective chromatogram thumbnails.

Spots selected on image 'DJP_01'

Total number of selected spots shown in this report: 10.

| Profile | Label(s) | Spot | DJP (direct juice pasteurized) | | CR (concentrate + recovery aroma) | |
|---------|----------|-------|--------------------------------|--------|-----------------------------------|-------|
| | | | DJP_01 | DJP_02 | CR_01 | CR_02 |
| | ID17432 | 17432 | | | | |
| | ID17448 | 17448 | | | | |
| | ID17455 | 17455 | | | | |
| | ID17499 | 17499 | | | | |
| | ID34482 | 34482 | | | | |
| | ID35967 | 35967 | | | | |

Automate your queries with DECODON's scout technology.

Scout Data Editor

Physicochemical properties

Label: 4680

Data Table Physicochemical properties

MW [Da] Isolelectric Point

Notes

Name: Heptanoic acid, 2-ethyl-
 Formula: C9H18O2
 MW: 158 CAS#: 3274-29-1 NIST#: 5503 ID#: 490 DB: mainlib
 Other DBs: TSCA, HODOC, EINECS
 Contributor: F.M.TRENT RES. DIV., U.S. IND. CHEM. CO., CINCINNATI, USA

10 largest peaks:

| | | | | | | | |
|----|-----|----|-----|-----|-----|----|-----|
| 88 | 999 | 73 | 861 | 101 | 353 | 41 | 247 |
| 55 | 193 | 87 | 168 | 57 | 163 | 29 | 121 |

Synonyms:
 1,2-Ethylheptanoic acid
 2,3-Octanecarboxylic acid

Estimated non-polar retention index (n-alkane scale):
 Value: 1208 iu
 Confidence interval (Carboxylic acids): 51(50%) 220(95%) iu

The Spot Quantities report shows either a condensed or a detailed set of table columns for selected or marked expression profiles.

The Labels Report lists all available label data, including the data retrieved by a DECODON Scout.

Quantities for spots marked on image 'DJP_01'

Table shows normalized volumes (i.u.) of spots marked on image 'DJP_01'. Ratios and p-values (using t-Tests) are computed relative to group 'DJP' (direct juice pasteurized). Total number of marked spots shown in this report: 32.

| DJP_01 | | DJP (direct juice pasteurized) | | | | CR (concentrate + recovery aroma) | | | | JRP (juice of pineapple rests pasteurized) | | | |
|------------|-------|--------------------------------|----|--------|--------|-----------------------------------|--------|-------|-------|--|--------|-------|---------|
| Label | Spot | X | Y | DJP_01 | DJP_02 | Mean | RSD | CR_01 | CR_02 | Mean | RSD | Ratio | p-value |
| (no label) | 17349 | 109 | 40 | 0.11 | 0.10 | 0.014 | 18.083 | 0.037 | 0.047 | 0.042 | 12.990 | 3.000 | 0.043 |
| (no label) | 17351 | 257 | 41 | 0.056 | 0.097 | 0.077 | 26.501 | 0.025 | 0.015 | 0.020 | 23.866 | 0.264 | 0.114 |
| (no label) | 17360 | 282 | 55 | 0.256 | 0.387 | 0.321 | 20.604 | 0.130 | 0.074 | 0.102 | 27.456 | 0.319 | 0.093 |
| ID17364 | 17364 | 290 | 59 | 0.055 | 0.080 | 0.070 | 21.769 | 0.035 | 0.021 | 0.028 | 24.648 | 0.390 | 0.127 |
| ID17379 | 17379 | 250 | 78 | 0.111 | 0.162 | 0.137 | 18.781 | 0.011 | 0.012 | 0.012 | 3.739 | 0.087 | 0.040 |
| (no label) | 17385 | 180 | 78 | 0.048 | 0.059 | 0.053 | 10.988 | 0.070 | 0.071 | 0.071 | 0.479 | 1.323 | 0.099 |
| (no label) | 17399 | 258 | 86 | 0.417 | 0.481 | 0.454 | 8.072 | 0.125 | 0.093 | 0.109 | 14.593 | 0.240 | 0.013 |
| ID17400 | 17400 | 407 | 88 | 0.113 | 0.134 | 0.124 | 8.626 | 0.546 | 0.423 | 0.485 | 12.696 | 3.920 | 0.029 |
| (no label) | 17413 | 158 | 91 | 0.024 | 0.039 | 0.032 | 24.403 | 0.039 | 0.027 | 0.033 | 19.900 | 1.049 | 0.890 |

Labels

| Labels for marked spots on gel image 'control_01' | | All Labels on gel image 'control_01' | | | | | | | | | | | | | | | |
|---|------|--------------------------------------|-------|-----------|-------------|-----------|---------------|--------------------|---|------------------|---|----------|---------------------|--|------|------|---|
| Label | Spot | PI/MW Estimation | | Uniprot | | | | | | | | | | | | | |
| Name | X | Y | ID | Accession | Amino Acids | Gene name | Gene Ontology | Isolelectric Point | Keywords | Molecular Weight | NCBI Taxonomy | Organism | Original label name | Query text | Ref | | |
| AtpC | 876 | 689 | 13405 | N.A. | N.A. | M1UDY3 | 187 | atpC | <ul style="list-style-type: none"> F: cytochrome-c peroxidase activity [GO:0004130] F: peroxidase activity [GO:0008055] F: response to oxidative stress [GO:0009779] | 4.2224 | <ul style="list-style-type: none"> Complete proteome Chloroplast Peridont | 20627.12 | 1147161 | Bacillus subtilis subsp. spizizenii DSM 9851:HDW | AtpC | AtpC | 1 |
| AtpF | 711 | 271 | 13694 | N.A. | N.A. | M1UZW0 | 509 | atpF | <ul style="list-style-type: none"> F: alkyl hydroperoxide reductase activity [GO:0008763] F: electron carrier activity [GO:0008055] F: flavin adenine dinucleotide binding [GO:0006600] F: FAD binding [GO:0030137] F: protein disulfide | 4.8273 | <ul style="list-style-type: none"> Complete proteome Disulfide bond FAD Flavoprotein NADP Oxidoreductase Nucleic-acid center | 54874.4 | 1147161 | Bacillus subtilis subsp. spizizenii DSM 9851:HDW | AtpF | AtpF | 1 |

„My students and I have tested several programs and Delta2D has turned out to be by far the best 2D gel image analysis program. Most importantly, the service is superb. It does not matter which time zone you are in, they call you and walk you through any problem you may encounter.“

*Lars Tomanek
California, USA*

Premium service is our standard

When you decide for GasPedal you do not only get a great application. Providing accessible and quick support is one of our highest goals. We know that each customer's problem is important and you will receive prompt attention from our support team. By prioritizing the request, our support team ensures that the most urgent ones are solved first.

Our experienced support team is dedicated to providing effective support that helps our customers to use GasPedal. The team continuously ensures customer satisfaction by one-to-one communication via email, phone, and web sessions.

The DECODON Support Team
Phone: +49 (0)3834 515 235
Email: support@decodon.com

Enjoy working with GasPedal!

Remote Assistance – Just sit back and see how to solve your problem

The DECODON support team often uses a very time-efficient way to support GasPedal users: Interactive web sessions.

You only need a computer with internet connection and a phone. A support member will call you at an agreed time to have a look on your screen and to present a solution.

We provide support

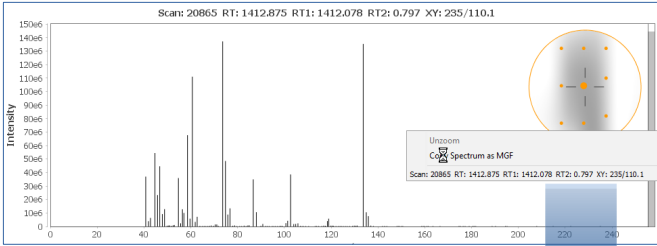
- to introduce GasPedal to new users,
- to discuss experimental design,
- to help with individual problems,
- to guide through statistical analysis.

We offer

software training on site or online.

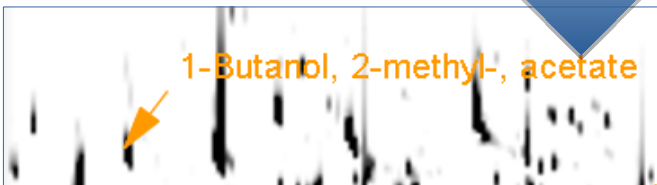
“The support I've experienced from DECODON has been nothing short of perfect.“

*Daniel Kay
Porirua, New Zealand*



Targeted search for a spectrum:
copy spectrum via clipboard,
e.g. to NIST MS Search,
copy name and create a label.

Name: 1-Butanol, 2-methyl-, acetate
Formula: C₇H₁₄O₂
MW: 130 **CAS#:** 624-41-9 **NIST#:** 236871 **ID#:** 353 **DB:** mainlib
Other DBs: Fine, TSCA, RTECS, HODOC, EINECS
Contributor: Japan AIST/NIMC Database- Spectrum MS-NW-9411
10 largest peaks:
 43 999 | 70 342 | 55 163 | 73 156 | 41 101 |
 29 81 | 42 79 | 57 61 | 74 53 | 72 52 |
Synonyms:
 1. 2-Methyl-1-butyl acetate
 2. 2-Methylbutyl acetate
 3. Acetic acid 2-methylbutyl ester

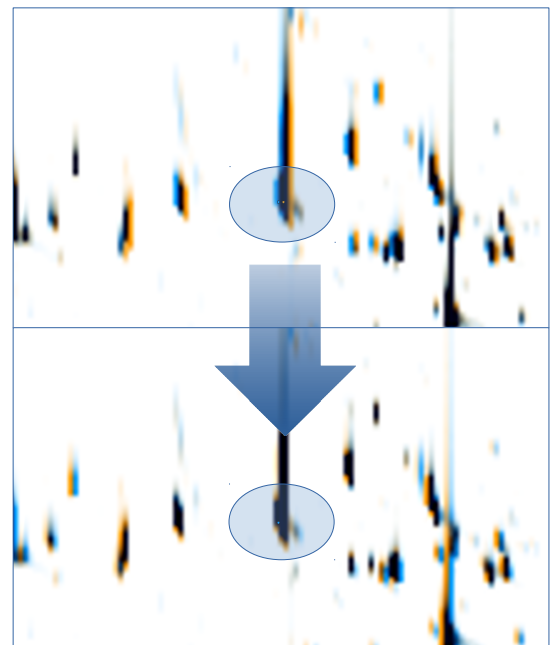


Identify your volatiles for all, spotted, selected
or labeled spectra of a chromatogram
e.g. using NIST MS Search

| # | Lib | Match | R Match | Prob. (%) | Name |
|---|-----|-------|---------|-----------|----------------------------|
| 1 | M | 737 | 845 | 59.6 | 3-Methyl-3-oxetanemethanol |
| 2 | M | 708 | 754 | 16.9 | 1-Penten-3-ol |
| 3 | M | 692 | 691 | 5.05 | 2-Hexen-1-ol (E) |
| 4 | M | 664 | 671 | 2.60 | Cyclohexanol |

Simplify fine tuning of alignment
by comparing spectra

GasPedal's Warping is supported
by spectra comparison



GasPedal: Features and functions at a glance

Image Processing

| | |
|---|--|
| Dual Channel Images (overlay of two images colored in false colors) | See differences in spot patterns at a glance, e.g. enables qualitative analysis of chromatograms |
| SmartVectors™ HQ Technology for automatic alignment, i.e. image warping | Minimizes hands-on time No need for initial landmarks Eliminates running differences between chromatograms that prevent for a fast and reliable analysis Allows verification and adjusting of automatically found vectors |
| Image Fusion and Spot Maps | Combine several chromatograms to one synthetic (but realistically looking) image See all spots of all conditions on just one image – the map of volatiles Minimizes time needed for spot detection and editing |
| Color Coding for Spots and Labels | Condense your analysis results in just one image, e.g. in your map of volatiles See at a glance the distribution and also outliers in a selected property over a complete image |
| Background Subtraction | Compensates for strong and inhomogeneous background Complete visual and quantitative control |

Export and Reporting

| | |
|---|---|
| Interactive Web Reports (Project Report, Spot Album, Spot Quantities, and Labels) | Present and summarize your experimental setup, relevant spots, quantitative data, and annotations (incl. database details) at a glance. Can be put on the web easily as they are in HTML file format Copy all or part of a report into your favorite word processor or presentation program Allows to check in GasPedal as all reports are interactive Data ready for sharing and documentation |
| Export of Quantitative Data as Excel file or as CSV file | Complete control about what will be exported by making columns and/or rows of the Quantitation Table visible or invisible Provide information to colleagues, collaborators, etc. |
| Export of images (single or dual view, warped / unwarped, Fusion images or Color Coding Images) as Powerpoint file or as snapshot (TIFF, JPEG, PNG, PNM, BMP) | Use images for publication and presentation Edit spot boundaries and spot labels as objects Open slides with other packages like LibreOffice or Openoffice |
| Export of single or multiple spectra as MGF files or transfer spectra directly via clipboard | Use MGF files for database search and identification, e.g. in NIST MS Search or paste spectra from the clipboard |

Quantitation

| | |
|-------------------------------------|--|
| Support of various file formats | Import .cdf, .mzml, .tif, .tiff, .ti4, .jpg, .jpeg, .png, .pnm, .gif, or .bmp files Correct quantitation, incl. calibration information |
| Various Data Normalization methods | Select the normalization method that is suitable for your data Enables correct quantitative analysis of all kinds of GCxGC experiments |
| Quantitation on the original images | Reliable Data: Changes of spot shapes due to warping do not affect spot quantities |

Statistical Analysis

| | |
|---|---|
| Heat map display of expression profiles | Get a colorful visualization of all quantitative data of your project in just image See differences and similarities between expression profiles and images at a glance |
| Hierarchical Clustering (HCL) | Cluster expression profiles of spots or images, optional bootstrapping and jackknifing support |
| k-Means/Medians Clustering (KMC) | Cluster expression profiles of spots or images |
| t-Test (various methods) | Find significantly differentially expressed spots between two replicate groups, including control of False Discovery Rate (FDR) |
| Pavlidis Template Matching (PTM) | Find spots that follow a given expression pattern |
| Analysis of Variance (ANOVA) | Find significantly differentially expressed spots between n replicate groups |
| Principal Component Analysis (PCA) | Detect structures in your experiment and find outliers |
| Nonparametric Tests | No normal distribution assumption is needed to apply these tests on your data No assumptions about the parameters of the distribution (e.g. mean, standard deviation, etc.) are needed. Includes Wilcoxon Rank Sum Test, Mann-Whitney Kruskal-Wallis Test, Mack-Skillings Test, and Fisher Exact Test. |

Data Handling

| | |
|---|---|
| Use of Open Data Formats (open XML) | Easily read data and import it into your databases |
| Store Data in Projects within Pools | All data related to your chromatograms, including the images themselves, in one folder only – the 'Pool' Transfer data to e.g. another computer easily Store several subprojects in just one folder |
| Spot Annotations kept independently from spots | Allows for re-detection, spot editing, and/or cancelling without losing annotations which can also contain information like MW, etc. Export as you prefer: Images with or without spot annotations, or spot annotations only |
| Automated Web Data Retrieval with DECODON Scouts | No manual retrieval of information from local files or web resources necessary Fully automatic: Scout data will be attached to the label of a certain spot Data is saved along with the pool so it does not need to be retrieved from the web again |
| Statistical Analysis can be opened independently from the rest of the project | Send the statistical analysis to a statistician to continue your analysis – an additional installation of GasPedal is not needed, the free statistics tool TIGR MeV can be used |

Data Visualization

| | |
|---------------------------------------|---|
| Color Coding for Spots and Labels | Condense your analysis results in just one image, e.g. in your map of volatiles See at a glance the distribution and also outliers in a selected property (MW, etc.) over a complete image |
| Scatter Plot | Find interesting spots, check normalization method |
| Bar charts of Spot profiles | Get a summary of a spots expression over a complete experiment Find interesting spots by just rolling over an image |
| Image Regions | See all images of your project in one window to compare them and / or find corresponding spots, use 2D or 3D view |
| Show / hide particular image overlays | See only those overlays that you are currently interested in, i.e. spot labels, spot boundaries, and/or match vectors |
| Color Schemes | Choose any predefined or customized color scheme for the overlay shown in the Dual Window, find spots that are only present on one image, or on both images (i.e. find intersection, union, or complement sets) |
| 3D Spots | See spots in a 3D view Check spot detection, i.e. find artifacts or spots that have to be deleted, splitted, or merged, compare spots from two images |



GasPedal 1.0



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