Manual for the use of deco

This manual describes the basic use of the Deco program. Commands to be entered or buttons to be pressed are indicated in the text by the button name within array hooks ([ ]) in the format [button pressed] .

The first step in using the Deco deconvolution program is collecting appropriate data. With this we mean collecting data in the NetCDF format (http://en.wikipedia.org/wiki/NetCDF). Most manufactures of MS equipment provide software to export data in that format, other files can be translated using for instance ACD-software. When data is collected Matlab can be started, after moving to the deco directory, deco started by entering the command deco.

The deco command will activate the deco program and show the main window

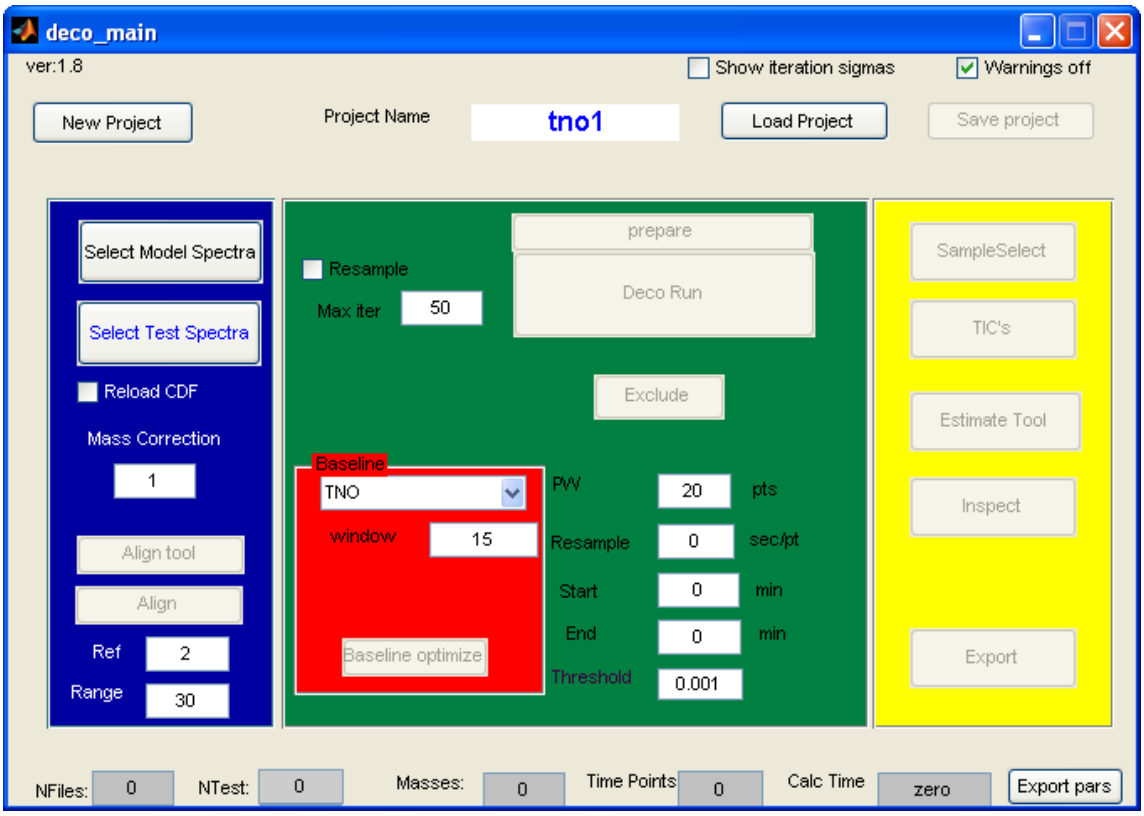


Figure 1: main deco window

This window has been subdivided into a general part (grey area) and four main processing area's addressing different aspects of the program. The blue part deals with entering and aligning the data. The green part is dedicated to the deconvolution of the data. The red part is used for baseline correction while the yellow part deals with displaying the results. Options that are not yet available to the operator are disabled.

The first step in the analysis is to assign a project name for the current processing. Setting the project name is done by pressing the [new project] button in the gray top area. This will activate a popup window (Figure 2) where a project name can be entered. If the name already exists then a warning will be shown and the user is then requested to either enter a new name or accept the name and overwrite the previous project.

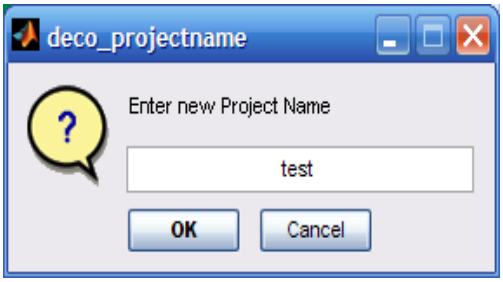


Figure 2: project window

Some background
Deco data generally consists of a number of model spectra and maybe some test files. The model spectra are used to build the deconvolution model and generate sets of compounds that are present in the data. The general process of the deconvolution process is to enter data, align the data, apply some baseline processing and then use a combination of Multiple curve resolution (MCR), Alternating Least Squares and unimodal restriction algorithms to build a set of pure compound spectra which are then used to generate concentration profiles for each compound in each file. Main difference between Deco and most other deconvolution programs is that deco processes the full set of spectra simultaneously while most other programs process each file separately. The Deco approach has the advantage that small differences in retention time for a compound between spectra are eliminated during the processing instead of by post-processing. However, because of the size of the data, the algorithm is not capable to process complete spectra. Spectra must first be cut into blocks (regions) which are then processed individually and later combined back into a single overall result. The size of the blocks is determined by the number of files (block-height) and an estimation of the peakwidth (block-width) of the peaks in the data. For optimal processing the width of the blocks is set to 4 times the estimated peakwidth (pw). The default value for pw in Deco is 20 points . Because it is possible that some peaks are located at the end of the blocks and therefore can (partially) be shared by different blocks. The processing is most reliable in the central part of the block. For this reason in Deco an approach was adopted where the blocks are shifted through the data with a window of 2 times the estimated peakwidth. This implies that each block overlaps both with the previous and the next block. (Block 1 = [1..4pw]; Block2 = [2pw .. 6pw]; Block3 [4pw…8pw] etc…). Using this approach each peak will pass through the central most reliable area of a block (between pw and 3*pw) at least once during the processing. After processing the results from the blocks are combined and overlap issues are solved to produce a full set of pure compounds with no double entries. Pure compounds spectra are calculated solely from the model spectra which are then used to predict the concentration in the test samples.

Step 2 in the processing is to enter some data into the program. This can be achieved by pressing the [Select model spectra] in the blue area. After pressing this button a familiar windows file window will appear where the directory can be changed and were the appropriate files can be selected. All the usual multiple file selection options cab be used in this program including CTRL to select individual files and SHIFT to select ranges of files.

After selecting the relevant CDF files these are then read and converted into smaller DBC files that are then used to import data into the main deco routines. When a DBC file is already available in the selected directory this will be read instead of the original CDF file. Re-

reading the original CDF file can be forced by ticking the reload box in the blue area of the main window. During the processing the high resolution masses in the CDF files are converted to modal masses using the formula

```
mas = round(multifactor*V_mass_values(massas_in_scan))';    [1]
```

Where multifactor is the mass correction factor in the blue part of the main window. This factor can be used to correct for the mass deficiency of large compounds with many protons. Default this value is set to 1 (no action). For mass deficiency correction this value is generally set to 1.001 (a 1 percent mass correction)

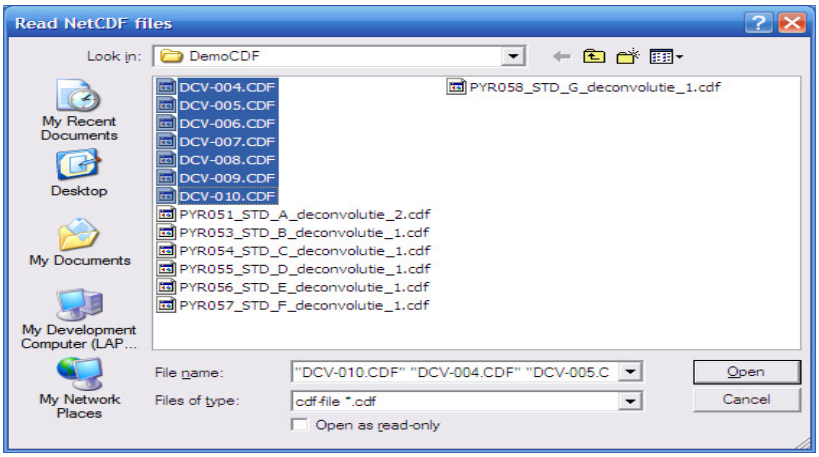


Figure 3 : Data entry window

After entry the next (optional) step is to select some test samples by pressing the [Select Test Spectra] button. An identical window to selecting the model spectra will appear. Selection test samples is an option not a requirement. This step can be skipped if no test samples are available.

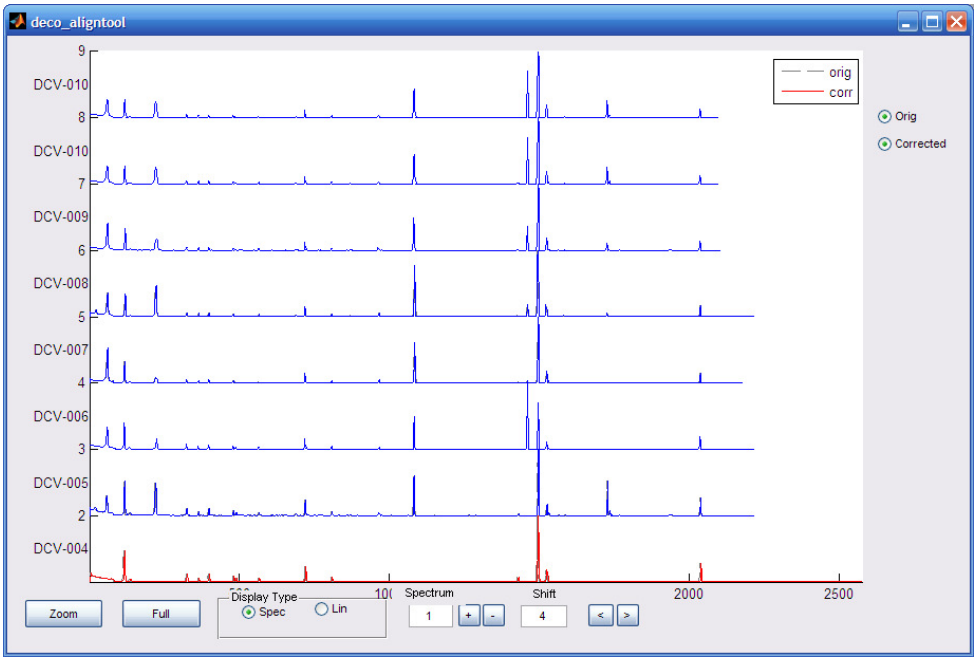


Figure 4: Alignment tool

Sometimes the spectra are shifted in position due to small changes in the start time of the equipment. To correct for this an alignment option has been build into the program where each file is compared to a reference spectrum using an autocorrelation algorithm (Matlab xcorr command). To use this option both the reference (Ref) spectrum and the maximum range (Range) of the autocorrelation must be entered into the blue area of the main window. The effect of this step can be evaluated using the [Align tool] button (Figure 4). This tool shows the original and corrected spectra and the factor used to shift each individual spectrum. If necessary, new permutations of reference spectrum and shift can be tried. However for application these values must be re-entered into the [ref] and [Range] boxes of the main window before they are finally applied to the spectra. (This option will be added to the program at a later date).

The next step is to correct the baselines of the spectra. To do this interactively the [Baseline optimize] button in the Red area of the main window can be pressed.

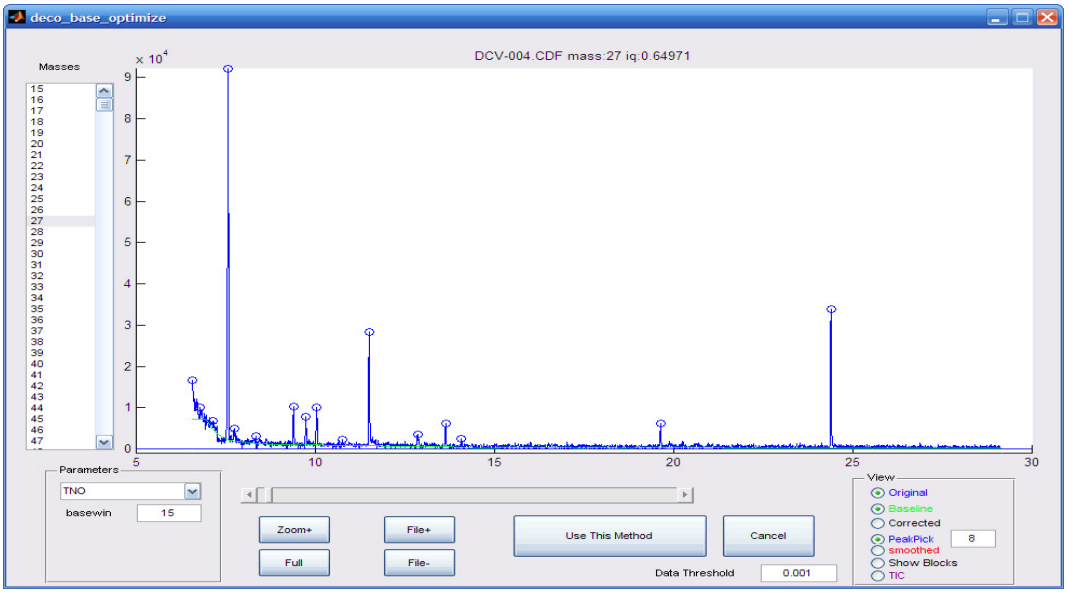


Figure 5: Baseline optimize window

In this tool for each of the spectra the individual mass traces of each spectrum can be selected and the effect of the selected baseline correction method evaluated. Four baseline methods are preprogrammed these are the Groningen method, the TNO method, the convex hull method and the Eilers method. The Groningen option is mainly used for processing LCMS files and the convex hull method is still experimental. Most commonly used are the Eilers method [4] and the TNO method which is based on the median value of a range (basewin) of points to calculate the baseline value this is the default option. When selecting one of the other choices the appropriate options for these methods will appear in the parameters window. See figure 6. For evaluation during the selection of the most appropriate method the [original], [baseline], [Corrected], [smoothed] and [tic] spectra can be shown simultaneously in the window. Also for evaluation the spectrum can be peaks picked and the future separation into blocks of the spectra can be shown. The Data threshold and Peakpick (minimum signal to noise ratio) parameter are used to limit the number of peaks picked. When the appropriate method has been determined then it can be selected using the [Use This Method] button. The [Cancel] button can be used to leave the tool with no action taken.

Remark : This tool is a modal window that means that it must be closed before further processing is possible.

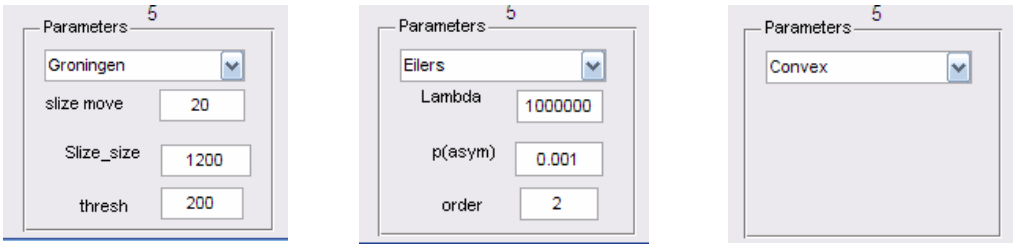


Figure 6: Baseline method correction windows for Groningen / Eilers of convex (hull) method.

The baseline method can be skipped by entering the method and parameters directly into the baseline boxes in the red part of the main window.

Processing

The data is now ready to be processed. In the green part of the main window several options for the processing an be entered. Of these options the ones most frequently changed are the [start] and [end] time and the peak width [pw]. Often the first few minutes of the files contain mainly solvent peaks these can be skipped by setting the start value. Similarly the final part of the spectra can be eliminated using the end time option. The peak width option is an important but difficult parameter to enter. The default value is 20 points, this is generally a sensible choice for GCMS spectra but it should be increased for LCMS files. For heavily overlapped spectra or spectra with small peaks widths this value should be lowered. Selecting small pw-values increases the number of blocks and therefore the calculation time, while selecting large values for pw generally increases the number of estimated peaks per block this will also increase the calculation time. The other options in the green field are estimated from the data while is was being read such as resample which is the minimum time found in the data between two sample points. In many GCMS applications this time is constant but like in LCMS methods it can change. If the ms sample frequency is not constant then the spectra are resampled using a spline based algorithm. Even if the frequency is constant the data can be forced to be resampled by ticking the [Resample box]. Another option is to set the threshold option this option regulates the minimum height of the individual masses in the pure component mass spectra. If the height of a calculated mass is below this threshold it is eliminated. The last option in the green field is the [Max Iter] field. In this field the maximum number of iterations that the deconvolution process can run to process a single block of data can be entered. Default value is 50. For blocks containing well defined peaks the value that the deconvolution will take is generally much lower than 50. Typical values are between 5 and 10. For more complex blocks containing many peaks the value is generally much higher. Higher values will take more time. From daily experience a value of 15 to 25 points should generally be sufficient to process most files without sacrificing essential information.

The processing can be started using either the [prepare] button or [Deco run] button, if prepare has not been selected before then the deco run button will automatically include the action normally performed in the prepare step.

Prepare step

After pressing the [prepare] button the model set spectra are aligned, resampled and baseline corrected using the supplied parameters. The information of the different spectra in the set is then combined to create a global data set which contains the common information from all spectra. Traces that do not occur in all the spectra are eliminated. The next, and crucial, step is to estimate the number of pure compounds per block. For this estimation the data from a single block is analyzed using a svd-based rank estimation algorithm where the eigenvalues of the mean centered spectrum data are compared to the eigenvalues of a block of random data. The point where the level of the data eigenvalues drop below the random eigenvalues is marked as being equal to the number of potential pure compounds in the block. Other methods to estimate this "rank" such as the Imbedded error, the Indicator function or a scree-plot [2] are available but generally not used. The result of this rank-estimation step can be evaluated and modified by the estimate tool available through the [estimate tool] button in the yellow part of the main window.

Deco Run

After the prepare step the data is deconvoluted [Deco run] per block using a combination of Multiple curve resolution, Alternating least squares under a number of non-negative and unimodal restriction. The time spend in this step is governed by the number of files, the estimated number of compounds per block, the noise level of the data and the maximum number of iterations per block. At the moment the number of spectra is not limited, the estimated number of compounds is determined by the eigenvalues and the maximum number of iterations is set default to 50. The current 1.8 version of the program is already a big improvement over the earlier version however the estimation of the number of pure compounds should still be further optimized. Also the used algorithm of ALS with the non-negative and unimodal restriction should receive some extra attention, trying some new approaches. The latest modification to the algorithm is the addition of the restriction that if the spectra of two components after ALS and after application of a threshold 90.05) are completely equal then the number of compounds is reduced and the calculation repeated.

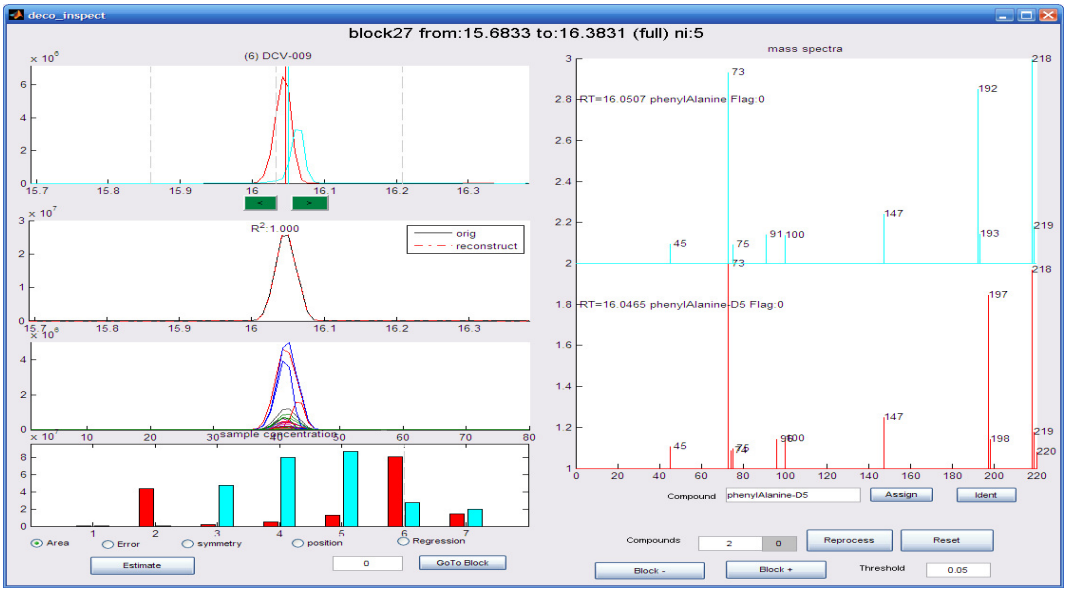


Figure 7: Inspect window

During the processing the progress in blocks and per iteration within a given block is indicated by progress windows. More detail can be obtained by ticking the [Show iteration

sigmas] in the gray part of the main window. During the processing all warnings such as “divisions by zero” and “singular matrix” are switched off by the default ticking of the [Warnings off] tic box in the gray part of the main window.

After the processing the Deco run the program automatically switches to the Inspect window. In this window (see Figure 7) an overview of the calculated spectra and chromatograms per block is generated. The tool contains several windows. Top Left is a view of the peaks calculated for a single spectrum. Default the spectrum which has the lowest regression with is reconstructed spectrum (calculated spectrum * chromatogram) is shown. By pressing the [<] and [>] keys the user can switch between all model spectra. The vertical colored lines in the display are indicators of the average value of the corresponding compounds in all files. If the position of the line does not match with the chromatogram then this is generally an indication that the corresponding compound does not exists in the file. The algorithm tries to fit all lines in all spectra. When a compound is not present then it is predicted at a random position with a low area. The dotted gray lines in the display indicate the “hot”-zone of the block. Peaks within these blocks are generally reliable while peaks outside this area become less reliable when close to the edges of the block.
The second window on the left of the tool shows the relation between the original and the reconstructed tic for the selected file in the selected block. From this window together with the individual mass spectra in the third window missing peaks can be detected. Fixing a missing peak is not straightforward. Often when increasing the number of compounds in a spectrum that contains a large peak and a smaller non-modeled peak the program generally favors the split of a larger peak into 2 smaller peaks over the addition of a small extra peak. Ideally the MCR and/or ALS algorithms should be extended by an extra restriction that some peaks are not allowed to shift more than an indicated amount. However, such an algorithm is at the moment not available.

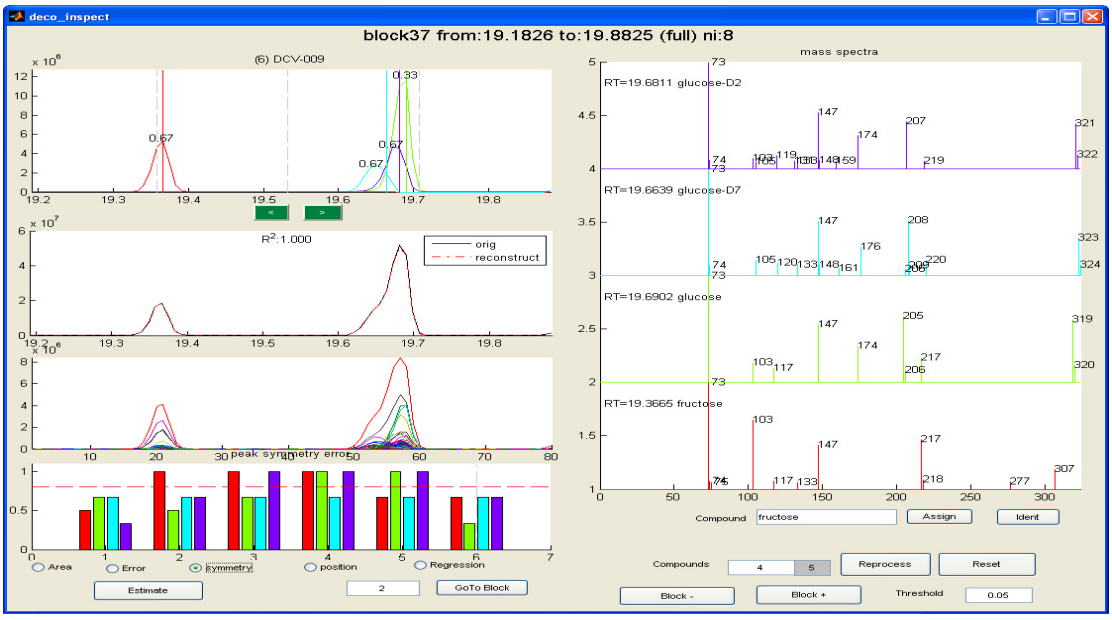


Figure 8: Symmetric option window

The bottom window on the left side of the tool is a quality control window with several options such as a choice to display per file either the area’s, the error between the fitted and a Gaussian modeled peak, the Symmetry (peak-width left/right ratio), the position versus the median position, and a regression between the original and the fitted chromatogram. If either

the error, the symmetry or position options are chosen then, if peaks deviate form the “normal” value, in the top window the corresponding peaks are marked with the deviating value. For instance in figure 8 where for a given set of spectra the symmetry option is selected. From the bottom left window it can be seen that in file DCV-009 (number 6) all the peaks have a symmetry value below 1.0 i.e. all peaks are wider on the left than on the right this is especially true for the green component which has a symmetry value of 0.33. The left side is twice as wide as the right side. Similar observations can be made for the position and error visualizations. In general these values help the researcher into deciding whether a peak is real or false (a random fit).

The right side of the tool is fully dedicated to the display and evaluation of the generated pure component spectra. The colors of the spectra correspond to the same colored chromatograms in the top and bottom left windows. Inside the window the masses of the components above the threshold are plotted. The titles show the average retention time and the peak name. The peak name can be edited by clicking the chromatogram and then entering a new name in the compound window followed by a click on the [assign] button. Clicking on the [ident] button exports the currently selected chromatogram into a NIST [3] database and compares it to the stored compounds (see figure 9)

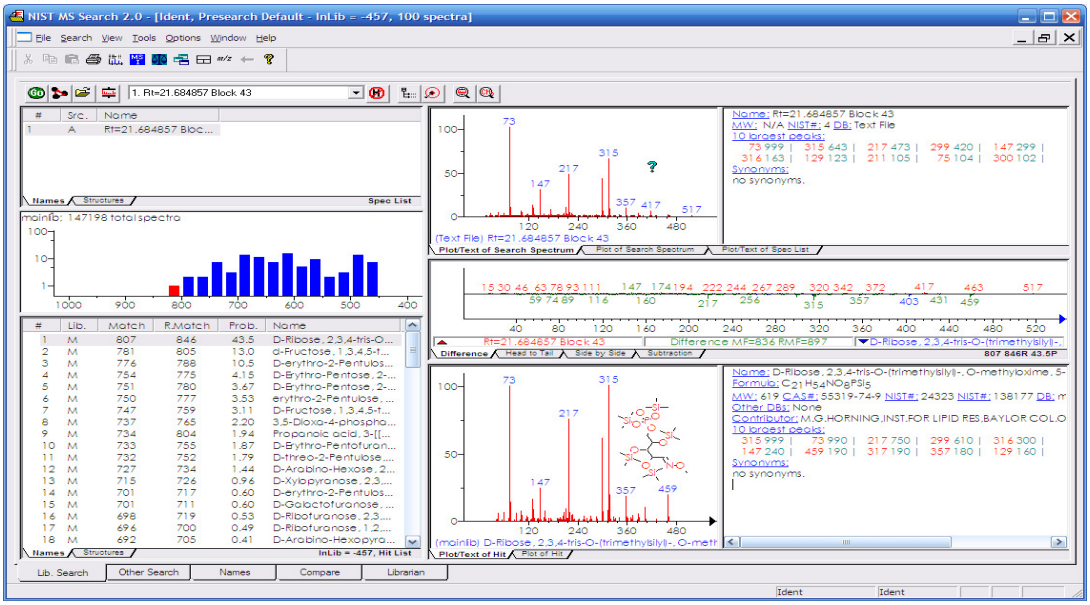


Figure 9: NIST database

Here the compound under scrutiny is identified as D-ribose which corresponds to the known identity of this compound.

Further buttons in this tool are used to switch between blocks (empty blocks are skipped) or to jump to specific block. The last button is the [Estimate] button which allows the user to start up the estimate tool as in figure 10. This tool is the same tool as accessed from the [Estimate Tool] button in the yellow area of the main window.

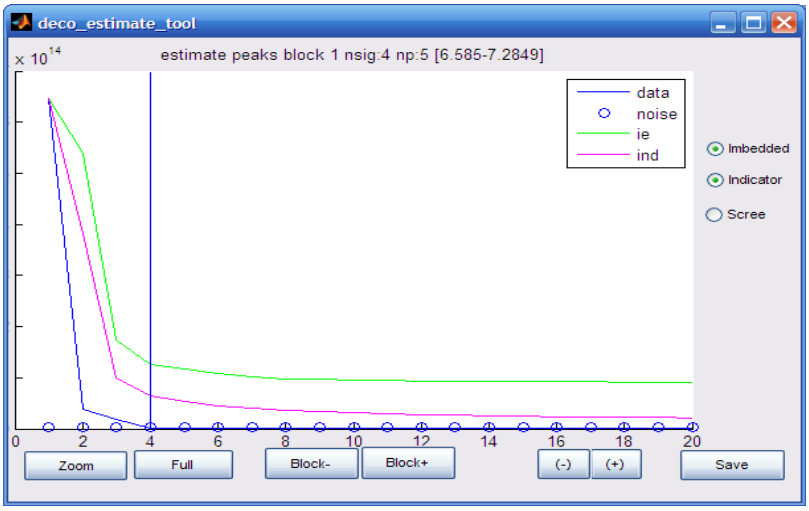


Figure 10: Estimate tool

Exporting

The final step in the Analysis is to export the results this can be achieved through pressing the Export button in the main Deco window. This action produces several files (depending on the settings in [export pars].

Project_name_Area.xls (combination of all cleaned areas in the project)

Microsoft Excel - tno_AREA.xls

	A	B	C	D	E	F	G	H	I	J	K
1	nr	rt(min)	ident	DCV-004	DCV-005	DCV-006	DCV-007	DCV-008	DCV-009	DCV-010	
2	1	7.07	pk(1)3	0.00E+00	1.04E+07	5.05E+06	1.09E+07	3.55E+07	3.82E+07	4.78E+07	
3	2	7.08	pk(1)1	0.00E+00	3.50E+07	0.00E+00	0.00E+00	5.10E+07	5.38E+06	2.33E+07	
4	3	7.09	pk(1)4	0.00E+00	9.03E+05	6.60E+07	1.42E+08	3.58E+07	9.29E+07	4.39E+07	
5	4	7.59	pk(3)1	4.13E+07	4.80E+07	5.14E+07	5.28E+07	5.37E+07	5.82E+07	5.59E+07	
6	5	7.75	pk(3)2	1.43E+07	1.60E+07	1.65E+07	1.45E+07	1.51E+07	1.67E+07	1.68E+07	
7	6	7.85	pk(4)2	4.89E+05	7.91E+05	8.20E+05	9.81E+05	0.00E+00	1.13E+06	1.35E+06	
8	7	8.05	pk(4)5	0.00E+00	1.80E+07	0.00E+00	0.00E+00	1.84E+07	1.88E+07	1.95E+07	
9	8	8.49	alanine-D4	2.01E+06	7.23E+07	1.81E+06	1.85E+07	1.17E+08	3.75E+07	7.68E+07	
10	9	8.53	pk(6)3	1.81E+07	1.61E+07	0.00E+00	1.68E+07	1.39E+07	0.00E+00	0.00E+00	
11	10	8.53	pk(6)1	1.30E+05	2.13E+05	3.17E+07	1.50E+07	7.95E+06	5.11E+07	3.35E+07	
12	11	9.02	pk(7)3	0.00E+00	2.52E+06	3.39E+06	2.16E+06	2.06E+06	2.70E+06	2.42E+06	
13	12	9.35	pk(8)3	1.32E+07	1.36E+07	1.42E+07	1.35E+07	1.48E+07	1.46E+07	1.49E+07	
14	13	9.4	pk(8)2	1.06E+07	9.58E+06	1.01E+07	9.92E+06	9.71E+06	9.72E+06	1.01E+07	
15	14	9.69	pk(8)1	3.37E+06	4.70E+06	5.15E+06	5.54E+06	2.43E+05	6.55E+06	6.19E+06	
16	15	9.81	pk(9)2	1.19E+07	1.18E+07	1.33E+07	1.16E+07	1.23E+07	1.32E+07	1.30E+07	
17	16	10.04	pk(10)2	1.88E+06	1.55E+06	1.40E+06	1.40E+06	1.44E+06	1.43E+06	1.48E+06	
18	17	10.04	pk(10)3	1.13E+07	9.06E+06	8.41E+06	7.32E+06	7.57E+06	7.50E+06	7.55E+06	
19	18	10.59	pk(11)3	1.09E+07	8.97E+06	1.22E+07	8.91E+06	1.08E+07	9.96E+06	1.30E+07	

tno_AREA

Figure 11: example project_Area.xls file

Cleaned in this context means that all overlapping areas are analyzed, cleaned and combined into a single integral for each peak. A peak is selected if it is located in the ‘hot zone’ of an area between pw and 3*pw. If for one or more spectra in the project the peak of the

corresponding compound is located outside this zone then this peak is, depending on its position, located in the next or the previous block and added to the final result. The criterion for a matching peak is that between the different blocks the calculated mass spectrum must have a regression coefficient of more than 0.95.

Project_name.msp : this file contains the mass spectra as calculated in the deco deconvolution procedure. The content of this file is in ascii and can be used to import spectra directly into the NIST database. General shape is

- retention time and identity of the peak
- number of masses
- (list of) mass intensity …. (combinations describing the compound)

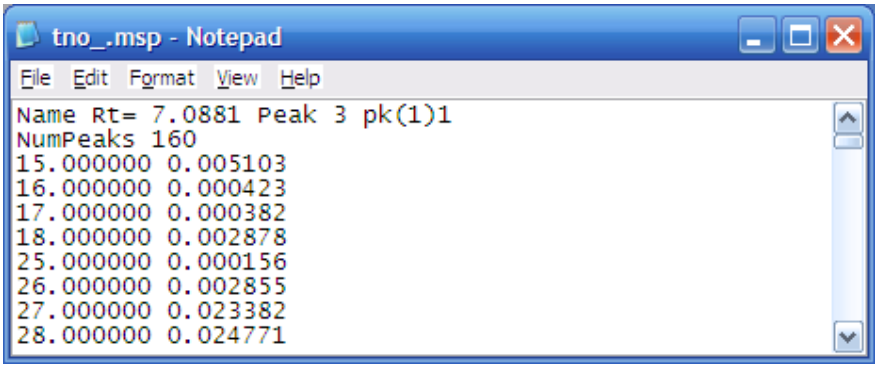


Figure 12: content of example projectname.msp file

For analysis purposes at the moment a second spectrum file called project_name_full.msp is exported containing the raw calculated spectrum information from each peak in each block. The export of this file will be terminated in the next deco version.

Filename_area.are.txt (collection of text files containing the area information for a single file)

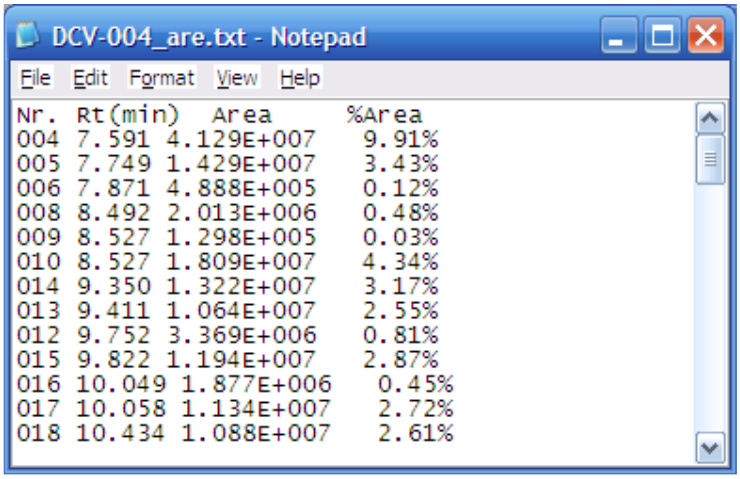
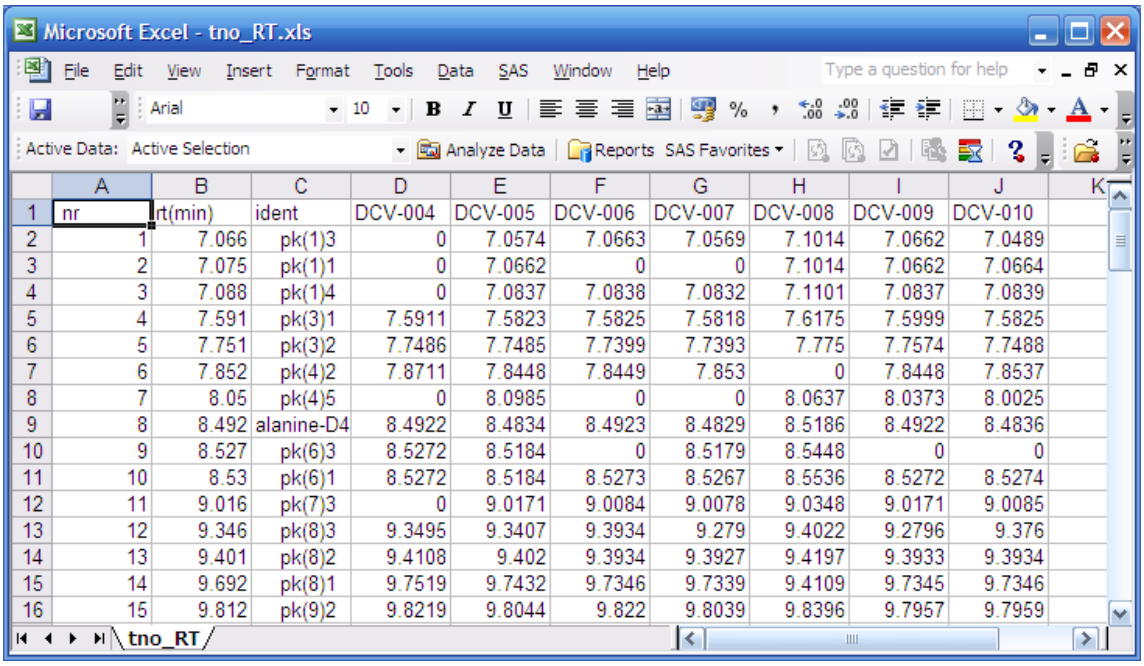


Figure 13: Content of an example filename_are.txt file.

Project_name_rt.xls : This file contains the retention time of each found peak in each spectrum. The content of this file makes it easier to locate the peaks from the project_name_area.xls files in the original mass spectra.



Microsoft Excel - tno_RT.xls

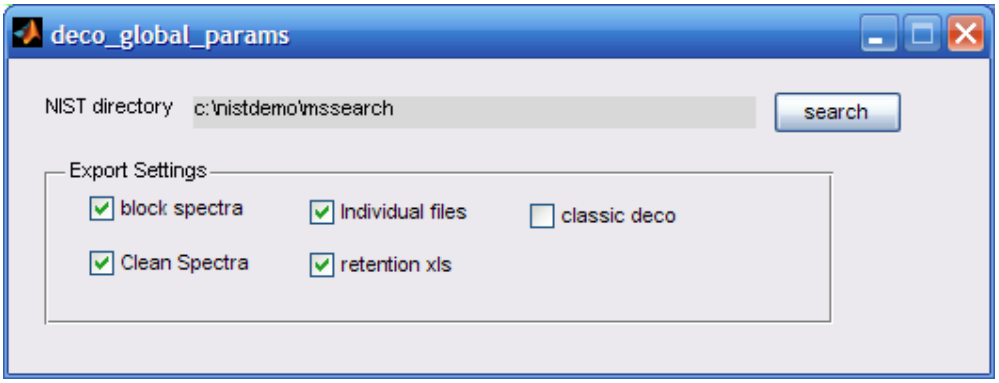
File Edit View Insert Format Tools Data SAS Window Help

Active Data: Active Selection | Analyze Data | Reports | SAS Favorites

	A	B	C	D	E	F	G	H	I	J
1	nr	rt(min)	ident	DCV-004	DCV-005	DCV-006	DCV-007	DCV-008	DCV-009	DCV-010
2	1	7.066	pk(1)3	0	7.0574	7.0663	7.0569	7.1014	7.0662	7.0489
3	2	7.075	pk(1)1	0	7.0662	0	0	7.1014	7.0662	7.0664
4	3	7.088	pk(1)4	0	7.0837	7.0838	7.0832	7.1101	7.0837	7.0839
5	4	7.591	pk(3)1	7.5911	7.5823	7.5825	7.5818	7.6175	7.5999	7.5825
6	5	7.751	pk(3)2	7.7486	7.7485	7.7399	7.7393	7.775	7.7574	7.7488
7	6	7.852	pk(4)2	7.8711	7.8448	7.8449	7.853	0	7.8448	7.8537
8	7	8.05	pk(4)5	0	8.0985	0	0	8.0637	8.0373	8.0025
9	8	8.492	alanine-D4	8.4922	8.4834	8.4923	8.4829	8.5186	8.4922	8.4836
10	9	8.527	pk(6)3	8.5272	8.5184	0	8.5179	8.5448	0	0
11	10	8.53	pk(6)1	8.5272	8.5184	8.5273	8.5267	8.5536	8.5272	8.5274
12	11	9.016	pk(7)3	0	9.0171	9.0084	9.0078	9.0348	9.0171	9.0085
13	12	9.346	pk(8)3	9.3495	9.3407	9.3934	9.279	9.4022	9.2796	9.376
14	13	9.401	pk(8)2	9.4108	9.402	9.3934	9.3927	9.4197	9.3933	9.3934
15	14	9.692	pk(8)1	9.7519	9.7432	9.7346	9.7339	9.4109	9.7345	9.7346
16	15	9.812	pk(9)2	9.8219	9.8044	9.822	9.8039	9.8396	9.7957	9.7959

tno_RT

Export Pars



The export pars window offers the ability to change the export options of the deco program. The [classic deco] option is only used for backward compatibility issues that may arise from using this program in projects that were processed with earlier versions of the program. This option will be fased out in new versions of the program. Changes in these export settings are local (just for this project) but will be stored with the project file. In future versions of deco an option will be added to safe these settings as new default option for new projects.

Literature and Software

Conversion Software:
Conversion program for sms files: ACD Labs MS manager (version 11)
http://www.acdlabs.com/products/spec_lab/exp_spectra/ms/

Literature:

[1] Paul Eilers, A Perfect Smoother, Anal chem. 2003, 75,3631-3636
[2] Data handling in science and technology, Multivariate pattern recognition in chemometrics, edited by R.G. Brereton, Elsevier Amsterdam 1992. chapter 5.
[3] NIST Database, free download from http://www.nist.gov/srd/nist1a.htm
[4] Tauler http://www.ub.edu/mcr/welcome.html

Known Bugs

- **xcorr present only in signal toolbox**
  - Status : fixed by including deco_corr function) 27-10-2008 JV.
- **Division by zero error in ALS**
  - Status: open
- **Error on export of empty blocks**
  - Status: Fixed in deco_export code 27-10-2008 JV

Comparison of results of deco analysis on TNO sugar mix data

Step1 : areas are collected
Step2 : areas are scaled against file DCV-10 * 20 (or * 180 for phenylalanine)
Step3 : areas are divided by reference values (from manual mixing)

Table 1

Reference	acetoin	Butane diol	alanine-D4	alanine	phenylA-D5	phenylA	fructose	glucose-D7	glucose-D2	glucose	ribose-5P	Dicyclo hexylIP
DCV-010	20	20	20	20	180	180	20	20	20	20	20	20
DCV-009	10	30	10	30	270	90	10	10	10	30	10	20
DCV-008	30	5	30	5	45	270	5	30	10	5	5	20
DCV-007	2	40	5	10	15	270	1	5	30	2	1	20
DCV-006	0	20	0	20	0	180	20	0	0	20	0	20
DCV-005	20	0	20	0	180	0	0	0	20	0	20	20
DCV-004	0	0	0	0	0	0	0	20	0	0	0	20

Deco	1	2	7	8	48	49	63	65	66	67	73	79
rt(min)	7.07	7.12	8.49	8.53	16	16.01	19.26	19.63	19.65	19.66	21.66	24.38
ident	acetoin	Butane diol	alanine-D4	alanine	Phenyl A-D5	phenylA	fructose	glucose-D7	glucose-D2	glucose	ribose-5P	Dicyclo hexylIP
DCV-010	20.0	20.0	20.0	20.0	180.0	180.0	20.0	20.0	20.0	20.0	20.0	20.0
DCV-009	10.5	31.7	9.8	29.8	268.6	82.3	10.0	10.4	12.6	32.3	9.3	19.4
DCV-008	27.7	7.9	31.5	5.2	43.7	269.6	4.5	29.8	7.3	3.9	4.1	19.4
DCV-007	2.1	40.6	4.8	9.6	18.0	246.9	1.0	6.8	25.4	0.5	1.2	19.5
DCV-006	0.8	18.8	0.5	18.9	7.2	149.1	19.8	1.6	3.0	18.9	0.8	19.8
DCV-005	15.9	1.4	18.8	0.9	147.7	1.6	0.4	2.4	14.1	0.2	18.7	18.6
DCV-004	0.0	0.1	0.5	1.2	3.4	2.1	0.8	15.8	0.4	1.6	0.9	19.2

From these tables it can be seen that the Deco calculations are very reliable and indicative of the experimental design.

To get an insight into the performance of Deco compared to other methods the above results are compared to a manual analysis using the machine software and an alternative deconvolution program called AMDIS. The results of these comparisons are displayed in table 2.

Table 2

Deco Error	1	2	7	8	48	49	63	65	66	67	73	79
rt(min)	7.07	7.12	8.49	8.53	16	16.01	19.26	19.63	19.65	19.66	21.66	24.38
Ident	Ace toin	butaned iol	alanine-D4	Ala nine	phenylA-D5	phenylA	Fruc tose	glucose-D7	glucose-D2	Glu cose	ribose-5P	Dicyclo hexylIP
DCV-010	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
DCV-009	1.05	1.06	0.98	0.99	0.99	0.91	1.00	1.04	1.26	1.08	0.93	0.97
DCV-008	0.92	1.57	1.05	1.05	0.97	1.00	0.90	0.99	0.73	0.79	0.82	0.97
DCV-007	1.06	1.02	0.96	0.96	1.20	0.91	1.01	1.36	0.85	0.26	1.21	0.98

Manual Error	acetoin	butaned iol	alanine-D4	alanine	phenylA-D5	phenylA	fructos e	glucose-D7	glucose-D2	glucose	ribose-5P	Dicyclo hexylIP
DCV-010	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
DCV-009	0.56	1.76	0.50	1.60	1.57	0.47	0.41	0.46	0.61	1.52	0.40	1.00
DCV-008	1.51	0.23	1.65	0.28	0.22	1.56	0.15	1.44	0.40	0.21	0.13	1.00
DCV-007	0.11	2.26	0.23	0.46	0.06	1.42	0.03	0.40	1.22	0.10	0.02	1.00

Amdis error	acetoin	butaned iol	alanine-D4	alanine	phenylA-D5	phenylA	fructos e	glucose-D7	glucose-D2	glucose	ribose-5P	Dicyclo hexylIP
DCV-010	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
DCV-009	0.00	2.02	0.40	1.46	1.86	0.31	0.92	0.81	0.00	0.92	0.51	1.00
DCV-008	1.71	0.58	1.69	0.27	0.00	1.37	0.00	1.47	0.53	0.00	0.18	1.00
DCV-007	0.00	2.67	0.24	0.44	0.00	1.22	0.00	0.17	1.21	0.00	0.02	1.00

From these tables it can be seen that the Deco results are far more reliable than those obtained from either a manual processing or a processing by the Amdis software.

Achieved

1. Better / faster Baseline correction
2. Faster ALS algorithm
3. Inclusion of test spectra
4. Export of Retention times and data in xls format
5. Integration with NIST database
6. Updated GUI's
7. Inspect window with editing capabilities
8. Interactive baseline window
9. Methods for estimating number of compounds per block
10. Cleanup of algorithm
11. Cleanup of m-files and content of files
12. Help texts added to buttons in guis
13. Automatic rejection of partial spectra
14. Transfer of technology
15. Manual for the use of the software

To do

1. Baseline correction per block (better estimation of compounds per block)
2. Interactive ALS with positional fix (set and fix peak positions)
3. Detection of noise masses per block (better estimation and better speed)
4.