

hyperSpec Plotting functions

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Reproducing the Examples in this Vignette

All spectra used in this manual are installed automatically with *hyperSpec*.
Note that some definitions are executed in `vignette.defs`.

Contents

1	Predefined functions	1
2	Arguments for plot	3
3	Spectra	5
3.1	Stacked spectra	7
4	Levelplot	9
5	Spectra Matrix	9
6	Calibration Plots, (Depth) Profiles, and Time Series Plots	11
7	False-Colour Maps	11
8	3 D	13
9	Troubleshooting	13
9.1	No output is produced	13
10	Interactive Graphics	13
10.1	<code>spc.identify</code> : finding out wavelength, intensity and spectrum	13
10.2	<code>map.identify</code> : finding a spectrum in a map plot	13
10.3	Related functions provided by base graphics and lattice	14
10.4	Interactively changing graphics	14

1 Predefined functions

hyperSpec comes with 5 major predefined plotting functions.

plot main switchyard for most plotting tasks

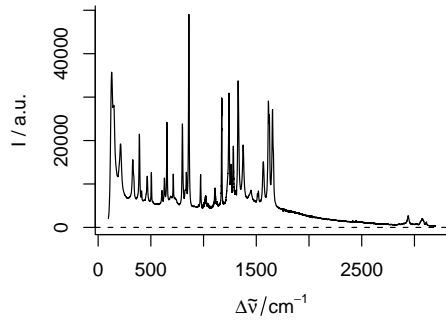
levelplot *hyperSpec* has a levelplot method

plotspc plots spectra

plotc calibration plot,time series, depth profile

plotmap version of levelplot allowing some more preprocessing of the data.

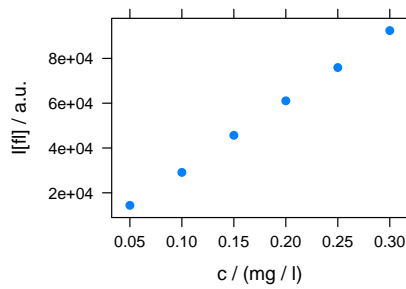
plotspc



plots the spectra, i.e. the intensities `$spc` over the wavelengths `@wavelength`.

```
> plotspc (paracetamol)
```

plotc

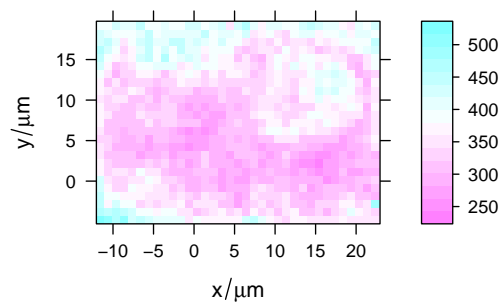


plots an intensity over a single other data column. e. g.

- time series
- calibration
- depth profile

```
> plotc (flu)
```

levelplot

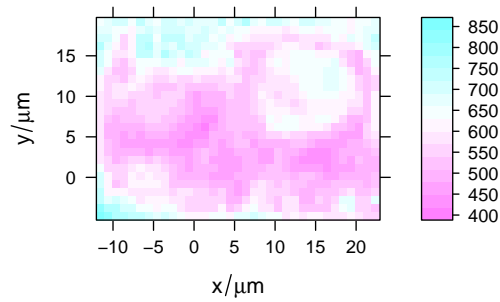


plots a false colour map, defined by a formula.

```
> levelplot ( spc ~ x * y, chondro, aspect = "iso")
```

Warning: only the first wavelength is used.

plotmap



plotmap is a specialized version of levelplot. It uses a single value (e.g. average intensity or cluster membership) over two data columns (default x and y)

```
> plotmap (chondro)
```

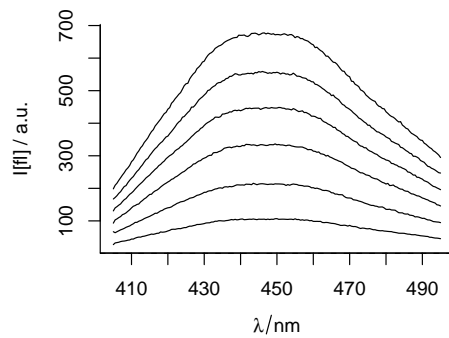
2 Arguments for plot

The three specialized functions are also accessible via *plot*:

hyperSpec's *plot* method uses the second argument to determine which of the three specialized plot functions to call. All further arguments are handed over to this function.

This allows a few more handy abbreviations.

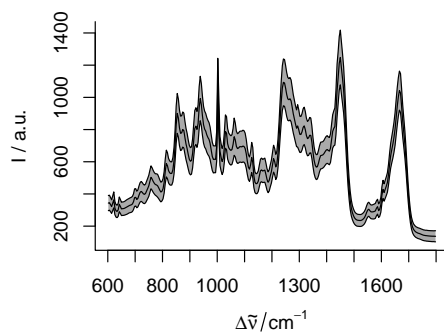
plot (x, "spc")



is equivalent to `plotspc (flu)`

```
> plot (flu, "spc")
```

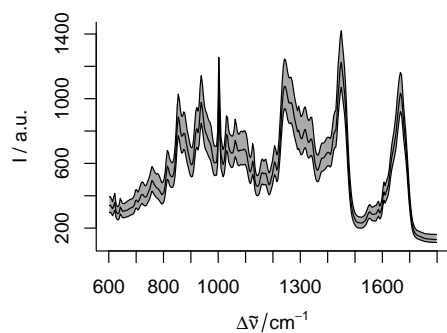
plot (x, "spcmeansd")



plots mean spectrum ± 1 standard deviation

```
> plot (chondro, "spcmeansd")
```

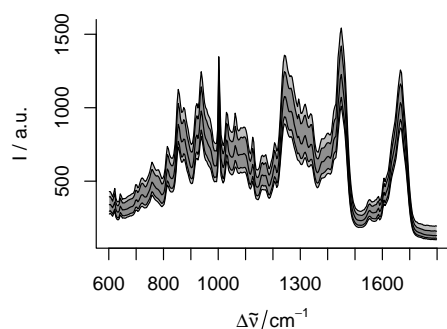
`plot (x, "spcprctile")`



plots median, 16th and 84th percentile for each wavelength. For Gaussian distributed data, 16th, 50th and 84th percentile are equal to mean \pm standard deviation. Spectroscopic data frequently are not Gaussian distributed. The percentiles give a better idea of the true distribution. They are also less sensitive to outliers.

`> plot (chondro, "spcprctile")`

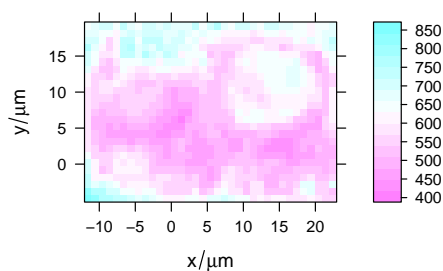
`plot (x, "spcprctl5")`



like "spcprctl" plus 5th and 95th percentile.

`> plot (chondro, "spcprctl5")`

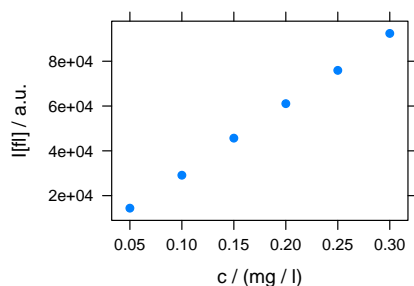
`plot (x, "map")`



is equivalent to `plotmap (chondro)`

`> plot (chondro, "map")`

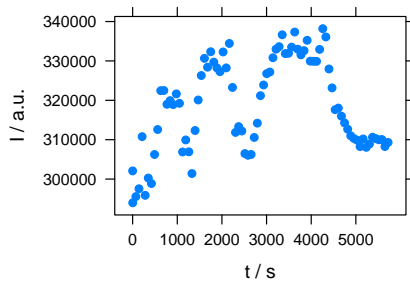
`plot (x, "c")`



is equivalent to `plotc (flu)`

`> plot (flu, "c")`

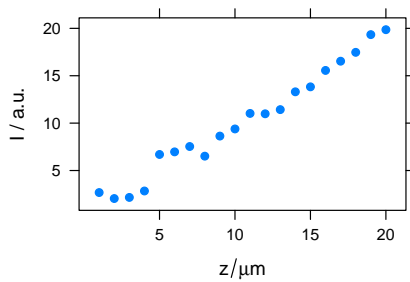
`plot (x, "ts")`



plots a time series plot, equivalent to `plotc (laser, spc ~ t)`

```
> plot (laser, "ts")
```

`plot (x, "depth")`

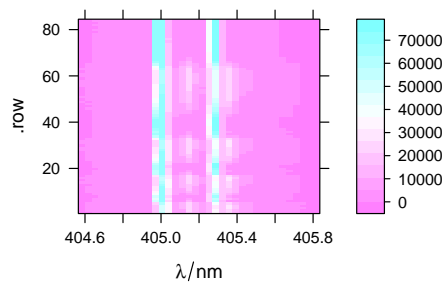


plots a depth profile plot, equivalent to `plotc (laser, spc ~ z)`

```
> depth.profile <- new ("hyperSpec",
+   spc = as.matrix (rnorm (20) + 1:20),
+   data = data.frame (z = 1 : 20),
+   label = list (spc = "I / a.u.",
+     z = expression (z, mu*m)),
+   .wavelength = expression (lambda))
```

```
> plot (depth.profile, "depth")
```

`plot (x, "mat")`



plots the spectra matrix.

```
> plot (laser, "mat")
```

Equivalent to

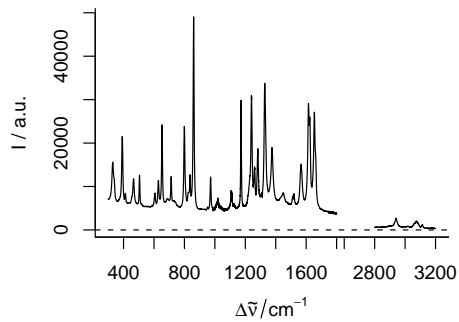
```
> levelplot (spc ~ .wavelength * .row, laser)
```

3 Spectra

`plotspc`

`plotspc` offers a variety of parameters for customized plots. To plot ...

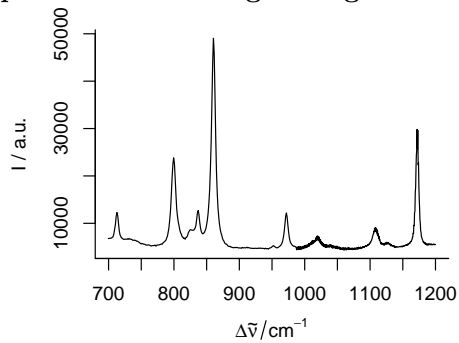
particular wavelength ranges



use `wl.range = list (600 ~ 1800, 2800 ~ 3100)`.
If `wl.range` already contains indices: use `wl.index = TRUE`. Cut the wavelength axis appropriately with `xoffset = 750`

```
> plotspc (paracetamol,
+          wl.range = c (300 ~ 1800, 2800 ~ max),
+          xoffset = 750)
```

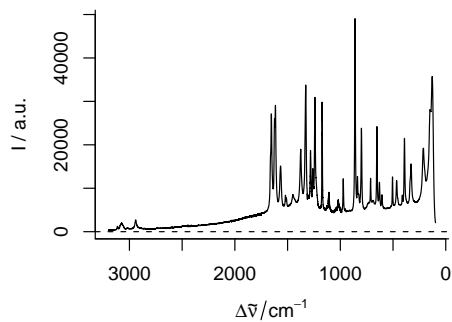
particular wavelength ranges II



if only one wavelength range is needed, the `extract` command is handier:

```
> plotspc (paracetamol[, 700 ~ 1200])
```

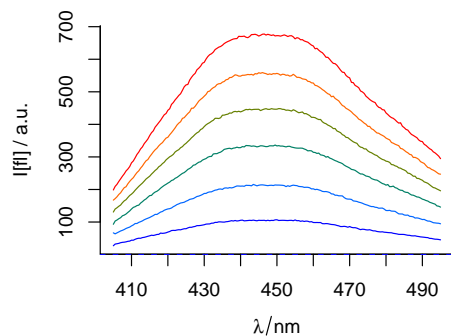
with reversed abscissa



use `wl.reverse = TRUE`

```
> plotspc (paracetamol, wl.reverse = TRUE )
```

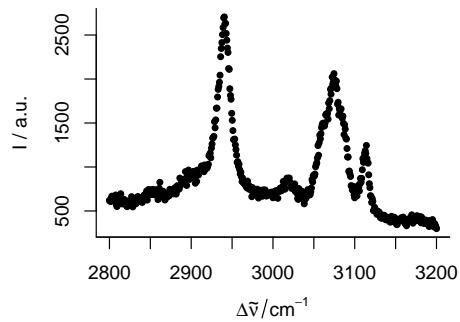
in different colours



use `col = vector.of.colours`

```
> plotspc (flu, col = matlab.dark.palette(6) )
```

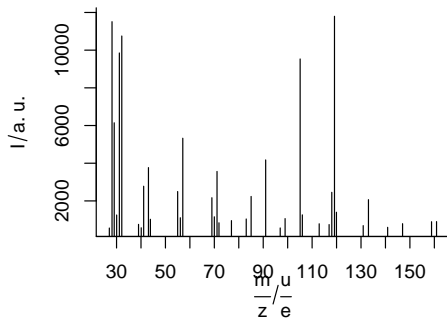
dots instead of lines



```
use lines.args = list (pch = 20, type = "p")

> plotspc (paracetamol [, 2800 ~ 3200],
+         lines.args = list (pch = 20, type = "p"))
```

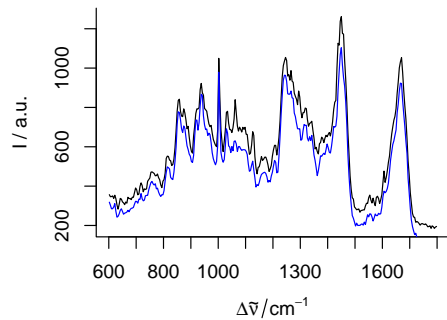
mass spectra



```
use lines.args = list (type = "h")

> plot (barbituates [[1]], lines.args = list (type = "h"))
```

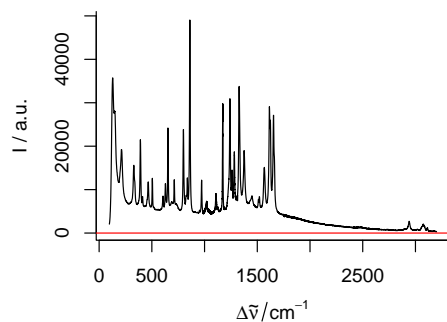
more spectra into an existing plot



```
use add = TRUE

> plotspc (chondro[30,,])
> plotspc (chondro[300,,], add = TRUE, col = "blue")
```

with different line at $I = 0$

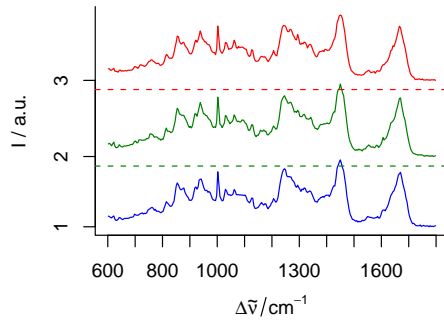


```
use zeroline = list.of.arguments.to.abline.
NULL suppresses the line.

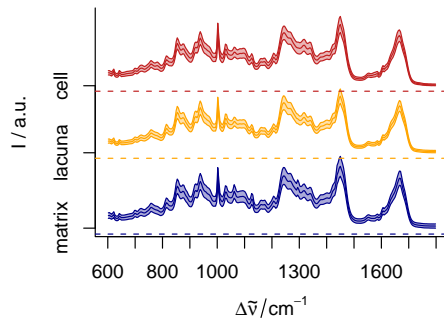
> plotspc (paracetamol,
+         zeroline = list (col = "red"))
```

3.1 Stacked spectra

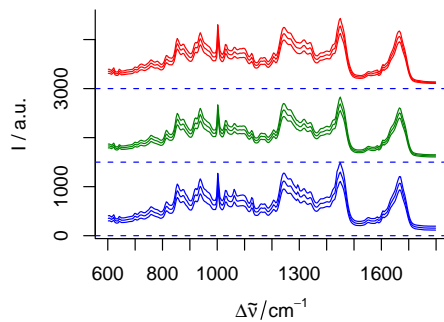
stacked = TRUE



Stacking groups of spectra



yoffset



use *stacked = TRUE*

```
> plotspc (chondro[1:3,,],
+         col = matlab.dark.palette (3),
+         stacked = TRUE)
```

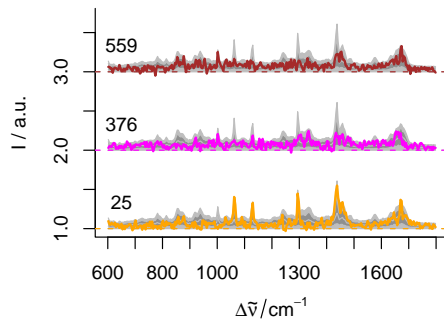
if you want to plot mean spectrum \pm 1 standard deviation of each of the clusters, use *stacked = grouping.column ".name"*

```
> cols <- c ("dark blue", "orange", "#C02020")
> cluster.means <- aggregate (chondro,
+                             chondro$clusters,
+                             mean_pm_sd)
> plot (cluster.means,
+       stacked = ".aggregate",
+       fill = ".aggregate",
+       col = cols)
```

or use *yoffset =*

```
> cluster.means <- aggregate (chondro,
+                             chondro$clusters,
+                             mean_pm_sd)
> plotspc (cluster.means,
+         yoffset = rep (c (0,1500,3000), each = 3),
+         col = rep (matlab.dark.palette (3), each = 3))
```


Manually with normalized spectra



it's also possible to normalize and stack the spectra like this:

```
> out <- c (25, 376, 559)
> outcols <- c ("orange", "magenta", "brown")
```

Preprocessing of the spectra:

```
> bl <- spc.fit.poly.below (chondro)
Fitting with npts.min = 15
> chondro <- chondro - bl
> chondro <- sweep (chondro, 1, mean, "/")
> chondro <- sweep (chondro,
+                   2,
+                   apply (chondro,
+                           2,
+                           quantile,
+                           0.05),
+                   "-")
```

The figure:

```
> ## coordinate system:
> plot(chondro[1],
+      plot.args = list (ylim = c (1, length (out) + .7)),
+      lines.args = list( type = "n")
+      )
> ## stacked spectra:
> for (i in seq (along = out)){
+   plot(chondro,
+        "spcprctl5",
+        yoffset = i,
+        col = "gray",
+        add = TRUE)
+   plot (chondro [out[i]],
+         yoffset = i,
+         col = outcols[i],
+         add = TRUE,
+         lines.args = list (lwd = 2))
+   text (650, i + .33, out [i]) }
```

4 Levelplot

Levelplot can use two special column names:

.wavelength for the wavelengths

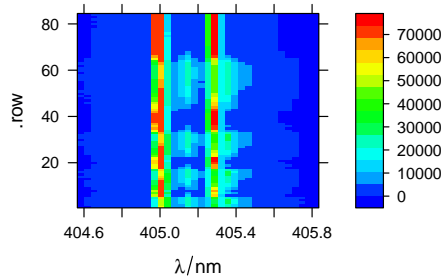
.row for the row index (i.e. spectrum number) in the data

5 Spectra Matrix

It is often useful to plot the spectra against an additional coordinate, e.g. the time for time series, the depth for depth profiles, etc.

This can be done by `plot (object, "mat")` or `levelplot (model = spc ~ .wavelength * other.data.column, object)`. The actual plotting is done by `levelplot`, so the plots can be grouped or conditioned.

different palette

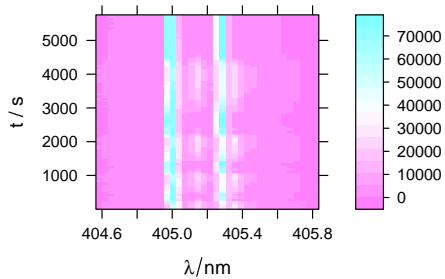


```
> plot (laser, "mat",
+       col.regions = matlab.palette (20) )
```

is the same as

```
> levelplot (spc ~ .wavelength * .row,
+            laser,
+            col.regions = matlab.palette (20))
```

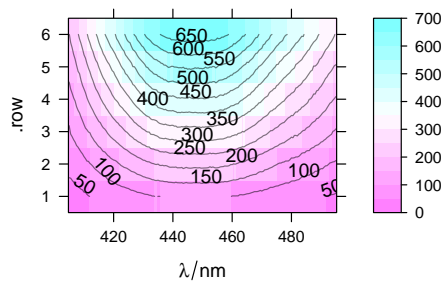
different y axis



Changing the y axis is only possible with `levelplot`:

```
> levelplot (spc ~ .wavelength * t,
+            laser)
```

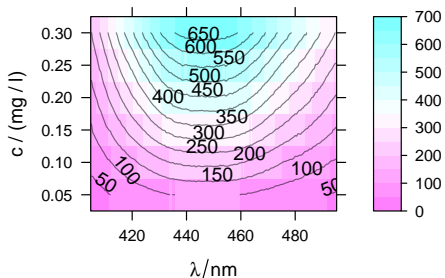
contour lines with plot



Contourplots are possible with `plot` and `levelplot`:

```
> plot (flu,
+       "mat",
+       contour = TRUE,
+       labels = TRUE,
+       col = "#00000080",
+       at = seq (0, 700, by = 50))
```

contour lines with levelplot



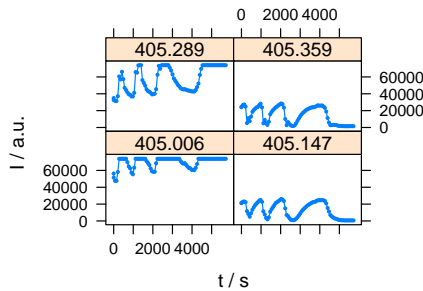
Contourplot with a different y axis:

```
> levelplot (spc ~ .wavelength * c,
+            flu,
+            contour = TRUE,
+            labels = TRUE,
+            col = "#00000080",
+            at = seq (0, 700, by = 50))
```

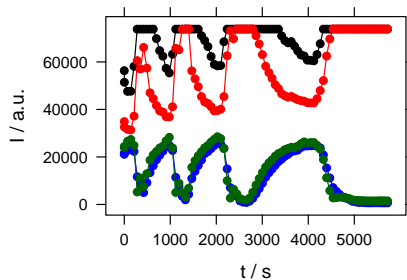
6 Calibration Plots, (Depth) Profiles, and Time Series Plots

plotc

`plotc` plots an intensity over one of the extra data columns. The abscissa uses column `$c` by default, another column can be specified using a proper formula. The ordinate can be calculated as a sum characteristic (with parameter `func= function`, defaulting to `sum`).



```
> plotc (laser [, c (13, 17, 21, 23),
+         wl.index = TRUE],
+        spc ~ t | .wavelength,
+        type = "b",
+        cex = .3)
```



```
> plotc (laser [, c (13, 17, 21, 23),
+         wl.index = TRUE],
+        spc ~ t,
+        groups = .wavelength,
+        type = "b",
+        col = c ("black", "blue", "red", "darkgreen"))
```

7 False-Colour Maps

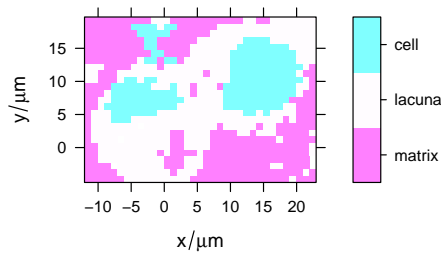
plotmap

`plotmap` uses `levelplot`, a *lattice* function. Therefore, in loops, functions, Sweave chunks, etc. the lattice object needs to be printed explicitly by `print (plotmap (object))` ([R FAQ: Why do lattice/trellis graphics not work?](#)).

`plotmap` produces a 3d plot, with the *z* axis colour-coded. `plotmap`'s arguments *x* and *y* take the name of extra data columns.

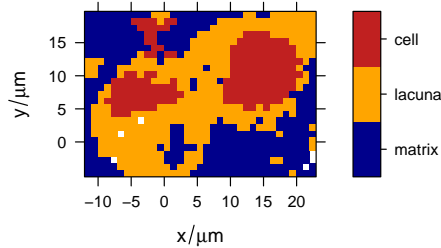
The colour-coded axis. Also *z* can be used to select one column of the extra data by name. Alternatively, it may be a numeric or factor directly giving the values to be used. Each level of a factor will have one colour. It is also possible to plot a sum characteristic of the spectra: supply the function in argument `func`. The default setting is to plot the average intensity (no *z* and `func=mean`).

plotting clusters



```
> plotmap (chondro, clusters ~ x * y)
```

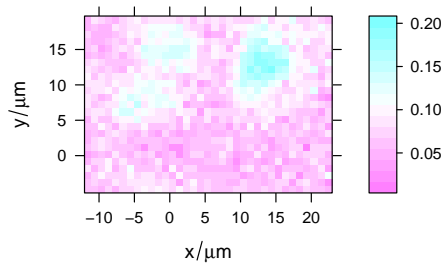
different palette



To plot with a different palette, use *trellis.args= list* (*col.regions = palette*).

```
> cols <- c ("dark blue", "orange", "#C02020")
> print (plotmap (chondro,
+               clusters ~ x * y,
+               col.regions = cols))
```

defined wavelengths



To plot a map with particular wavelengths use this:

```
> plotmap (chondro[, , c( 728, 782, 1098, 1240,
+                          1482, 1577)])
```

Examples

Conditioning. Lattice graphics have a concept of conditioning a plot. Instead of plotting all data in one diagram, a diagram is produced for each of the groups specified by the condition. *plotmap*'s argument *cond* takes the name of the extra data column used for conditioning. This could e.g. be a column containing the sample number of a *hyperSpec* object that contains several samples.

Beispiele: voronoi

8 3 D

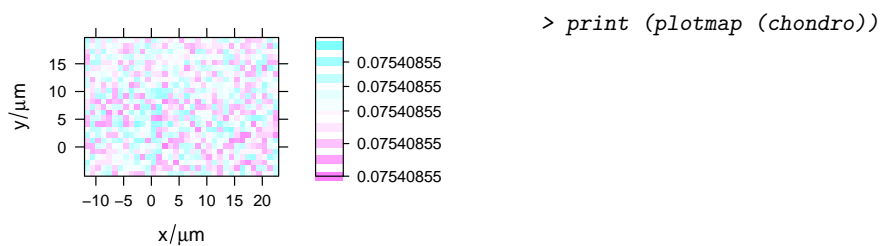
9 Troubleshooting

9.1 No output is produced

`plotmap` and `plotc` use `levelplot`, a *lattice* function. Therefore, in loops, functions, Sweave chunks, etc. the lattice object needs to be printed explicitly by `print (plotmap (object))` ([R FAQ: Why do lattice/trellis graphics not work?](#)).

In `vignettes.defs` is shown how the lattice functions can be redefined so that the result is printed without external print command.

in functions



10 Interactive Graphics

hyperSpec offers two basic interaction functions, `spc.identify`, and `map.identify`. They identify points in spectra plots and map plots, respectively.

10.1 `spc.identify`: finding out wavelength, intensity and spectrum

`spc.identify` allows to measure points in graphics produced by `plotspc`. It works correctly with reversed and cut wavelength axes.

```
> spc.identify (plotspc (paracetamol, wl.range = c (600 ~ 1800, 2800 ~ 3200), xoffset = 800))
```

The result is a data.frame with the indices of the spectra, the wavelength, and its intensity.

10.2 `map.identify`: finding a spectrum in a map plot

`map.identify` returns the spectra indices of the clicked points.

```
> map.identify (chondro)
```

10.3 Related functions provided by base graphics and lattice

For base graphics (as produced by `plotspc`), `locator` may be useful as well. It returns the clicked coordinates. Note that these are *not* transformed according to `xoffset` & Co.

For lattice graphics, `grid.locator` may be used instead. If it is not called in the panel function, a preceding call to `trellis.focus` is needed:

```
> plot (laser, "mat")
> trellis.focus ()
> grid.locator ()
```

`identify` (or `panel.identify` for lattice graphics) allows to identify points of the plot directly. Note that the returned indices correspond to the plotted object.

10.4 Interactively changing graphics

hyperSpec's lattice functions work with *playwith* and *lattice*. These packages allow easy customization of the plots and also identification of points.