Barcode Pre-Processing

C. Beleites, IPHT Jena

March 30, 2012

Definition im Artikel [1]: 2. Ableitung > 0.1 max (2. Ableitung)
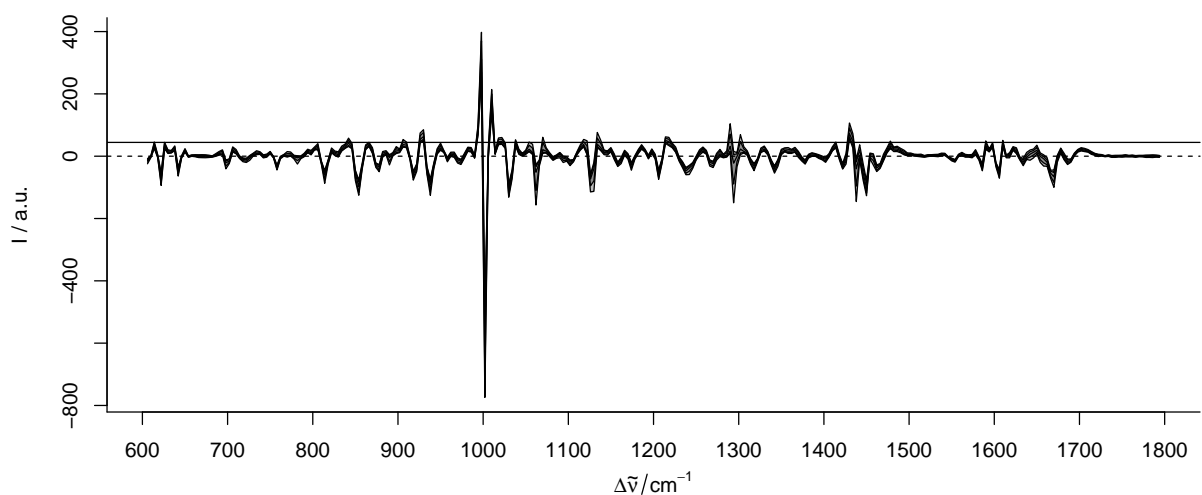
```
library(hyperSpec)
```

ungeglättete 2. Ableitung:

```
d2 <- apply(chondro, 1, diff, differences = 2, new.wavelength =
wl(chondro)[2:(nwl(chondro) -
    1)])
```

Grenzwert:

```
(threshold <- 0.1 * max(d2))

## [1] 44.29

barcode <- d2
barcode[[]] <- barcode[[]] > threshold
```
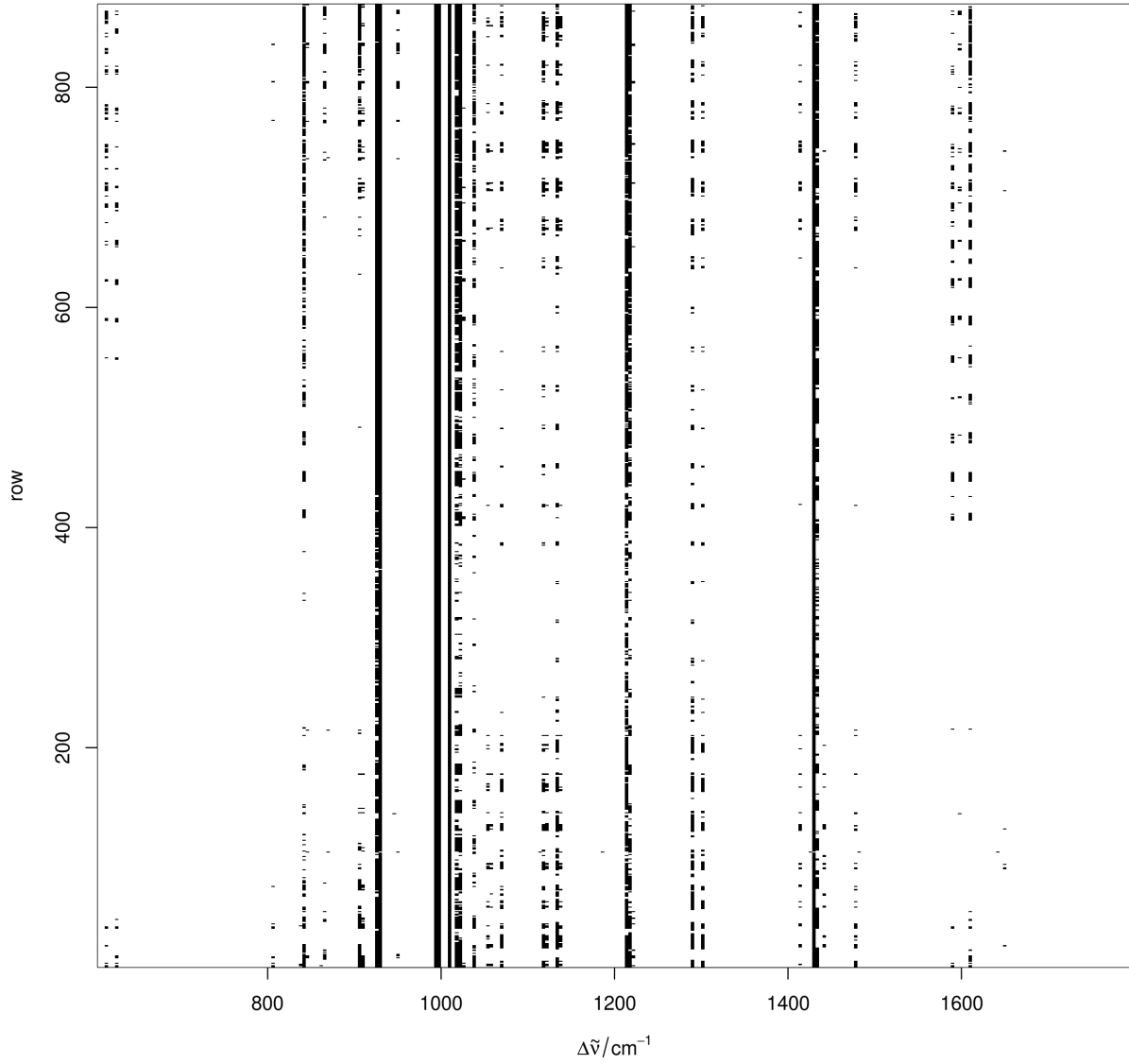
```
plot(d2, "spcprctl5")
abline(h = threshold)
```
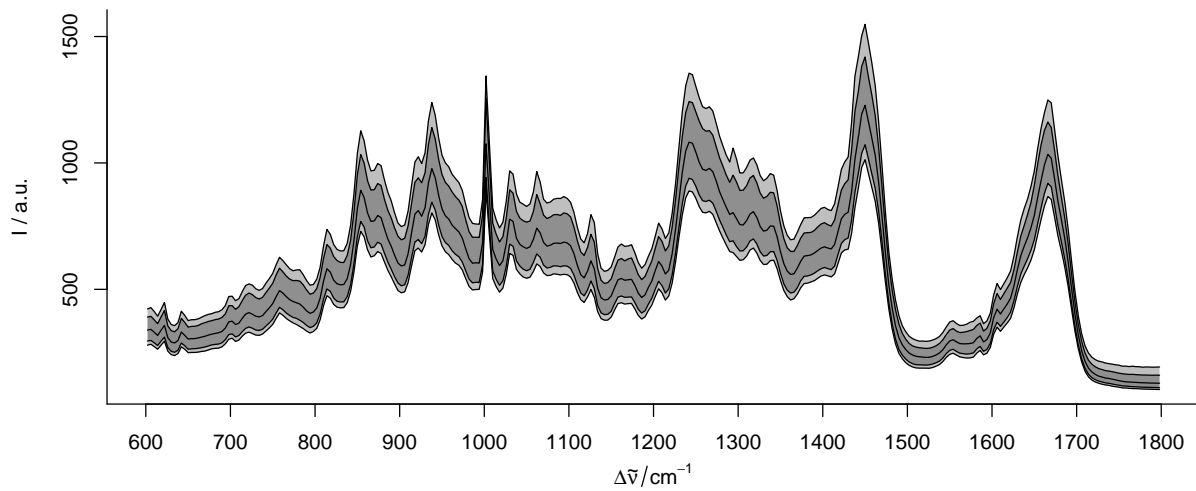
Barcode-Spektrenmatrix:

```
plotmat(barcode, col = c("white", "black"))
```
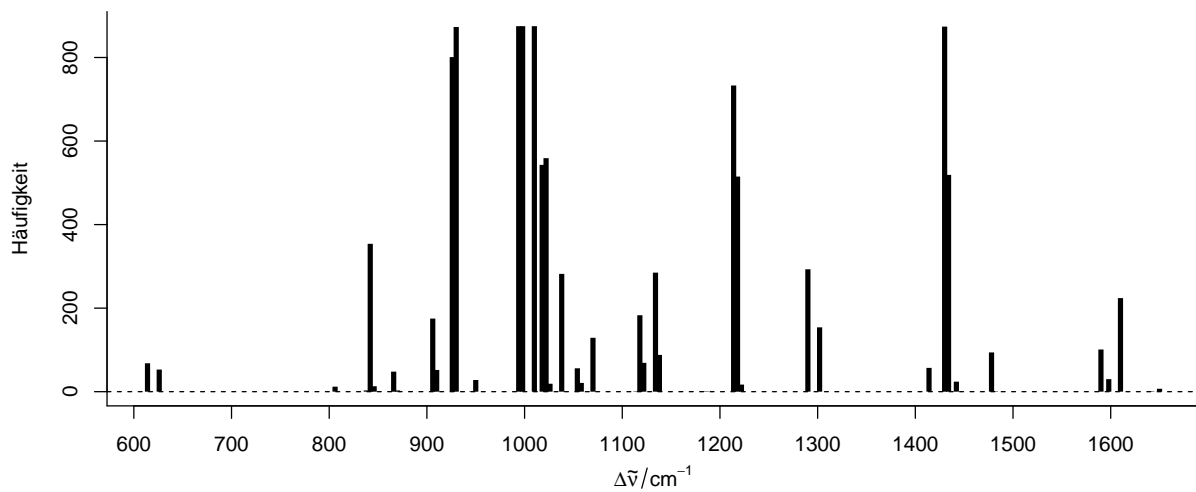
Rohspektren:

```
plot(chondro, "spcprctl5")
```


Häufigkeit, dass Datenpunkt mit 1 codiert ist:

```
f.barcode <- colSums(barcode)
f.barcode <- f.barcode[, , f.barcode > 0, wl.index = TRUE]
labels(f.barcode, "spc") <- "Häufigkeit"
plot(f.barcode, lines.args = list(type = "h", lwd = 4, lend = "butt"))
```

Alternative zu `diff`: geglättete Ableitung mit Savitzky-Golay-Filter:

```
library(signal)
d2 <- apply(chondro, 1, sgolayfilt, p = 3, m = 2)
```

References

[1] I. S. Patel, W. R. Premasiri, D. T. Moir, and L. D. Ziegler. Barcoding bacterial cells: A sers based methodology for pathogen identification. *J Raman Spectrosc*, 39(11):1660–1672, Nov 2008. doi: 10.1002/jrs.2064. URL http://dx.doi.org/10.1002/jrs.2064.