

**Global Parametric Time Warping in R**  
**The PTW package**

*Tom Bloemberg*

*Institute for Molecules  
and Materials*

*Dept. Chemometrics /  
Analytical Chemistry*

[www.ru.nl/imm](http://www.ru.nl/imm)

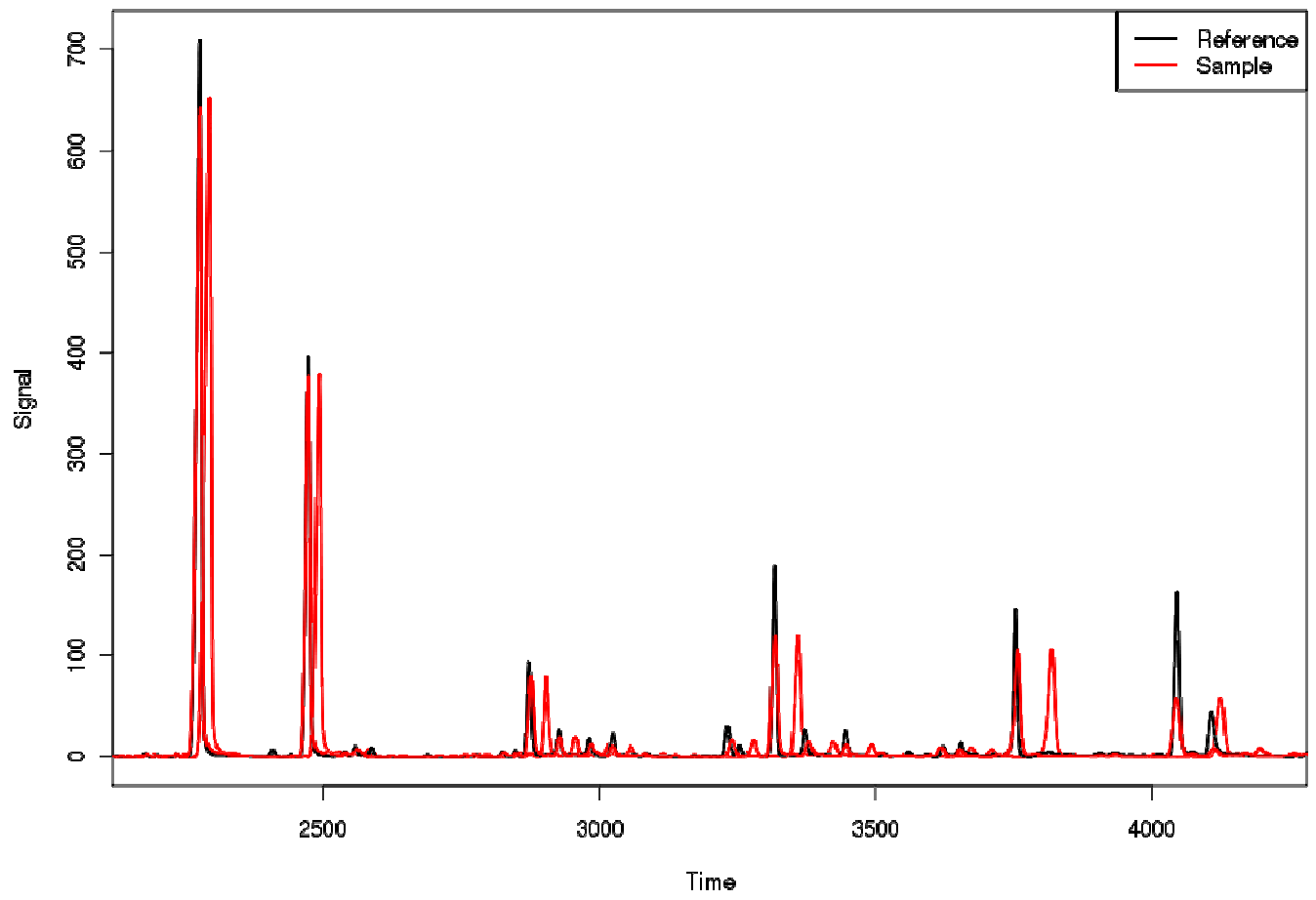
**Radboud University Nijmegen**





# Chromatographic example

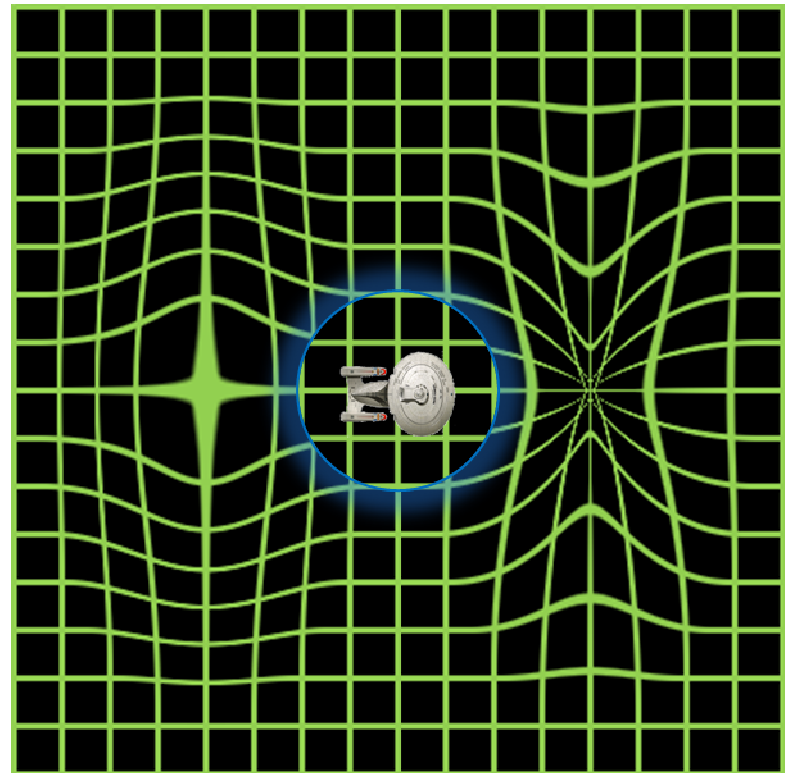
Figure





## Alignment

- Also:
  - ‘Synchronization’
  - ‘(Time) Warping’
- Shift, stretch, compress
- Applications in:
  - Speech analysis
  - Chromatography
  - NMR
  - ...





## Parametric Time Warping<sup>1</sup>

- Before warping:  $\text{Reference}(t) \leftrightarrow \text{Sample}(t)$
- After warping:  $\text{Reference}(t) \leftrightarrow \text{Sample}(w(t))$
- Polynomial model of warping function:

$$w(t) = \sum_{q=0}^Q a_q t^q$$

$$w(t) = a_0 + a_1 t + a_2 t^2 + \dots$$

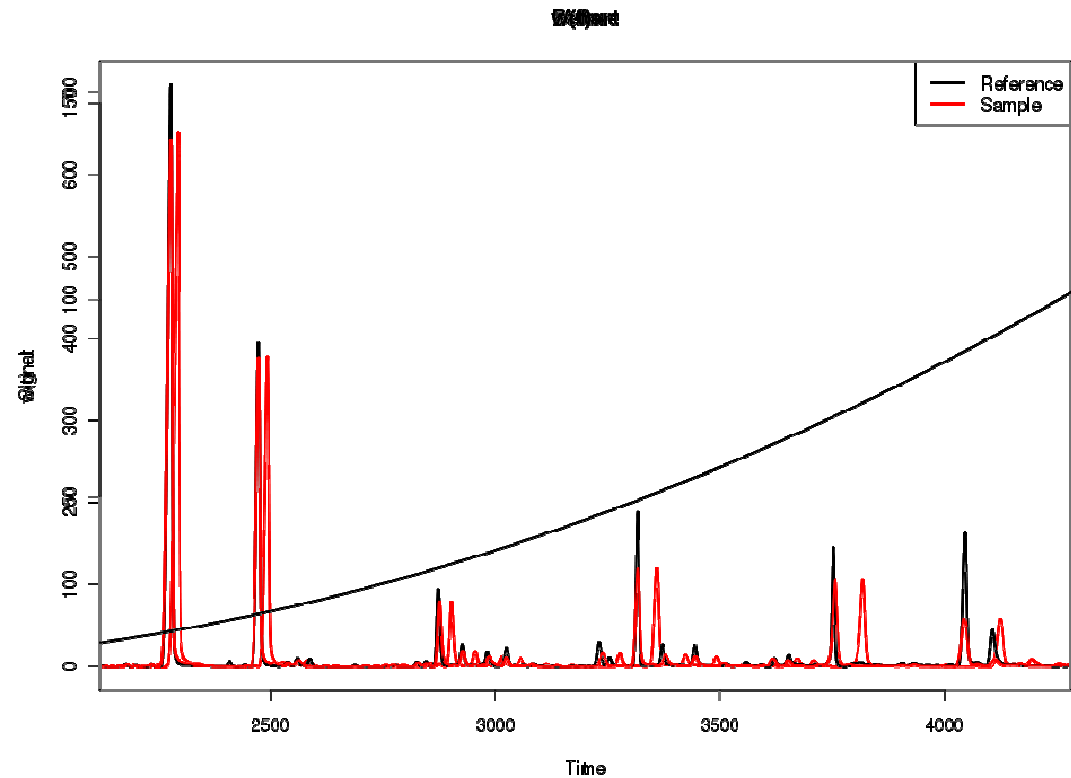
- Minimize:

$$\sum_i (\text{Reference}(t_i) - \text{Sample}(w(t_i)))^2$$

<sup>1</sup>Eilers, P.H.C. *Analytical Chemistry* 76 (2) 404-411 2004



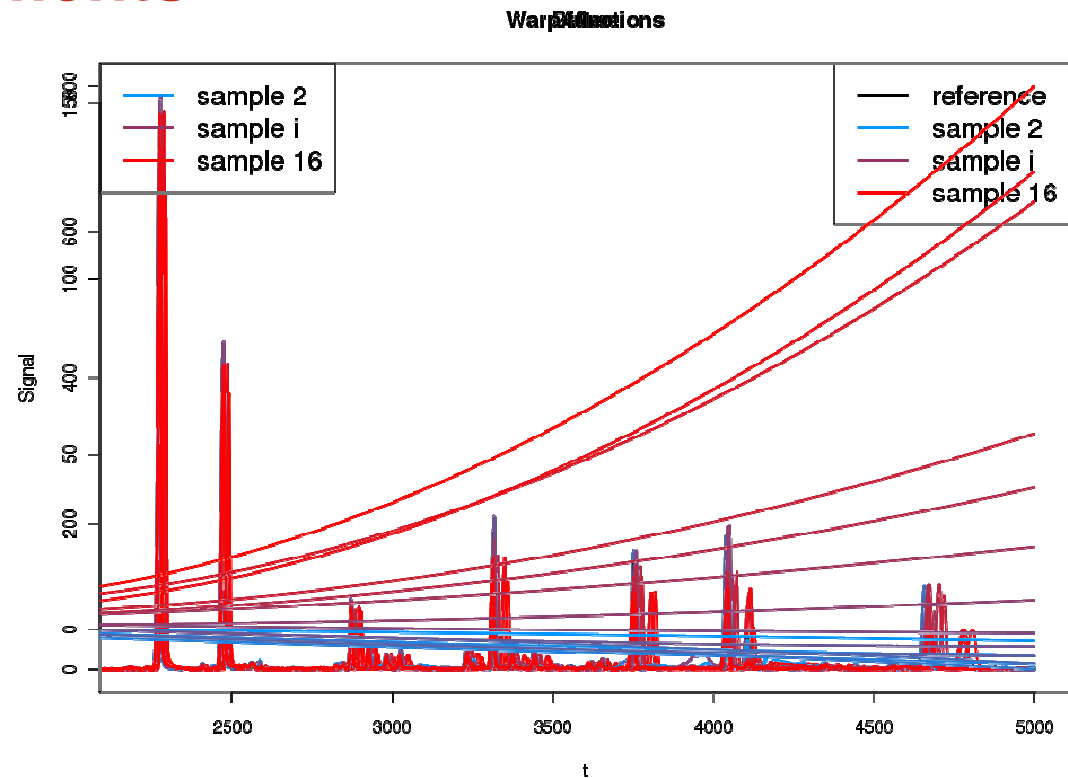
## A single alignment



```
> library(ptw)
> data(chromatograms)
> chromatograms <- basel.off(chromatograms)
> C.warped <- ptw(chromatograms[1, ], chromatograms[16, ])
> plot(C.warped, plot.orig=TRUE, plot.wf=TRUE)
```



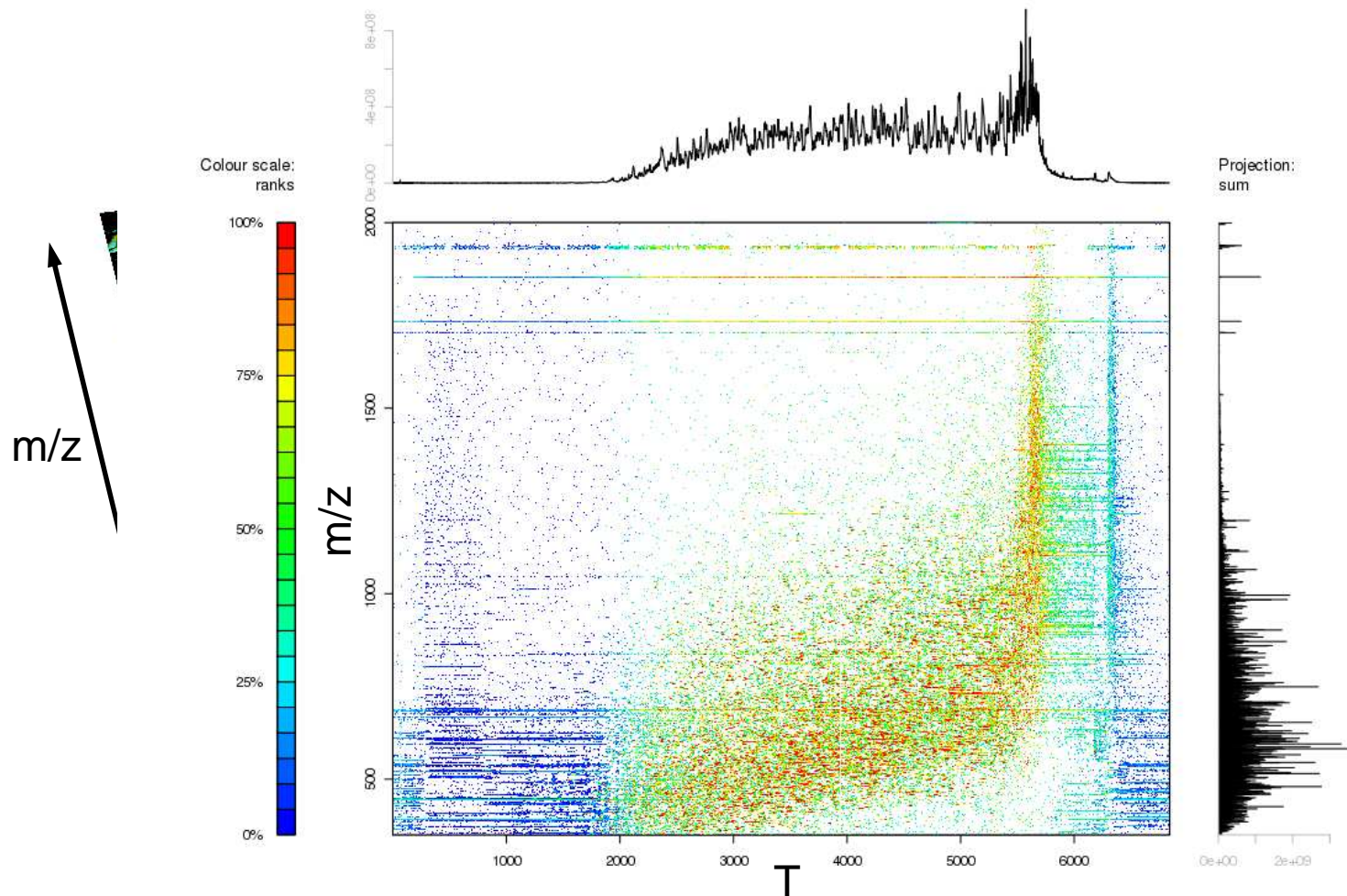
## Multiple alignments



```
> library(ptw)
> data(chromatograms)
> chromatograms <- basel.off(chromatograms)
> C.warped <- ptw(chromatograms[1;8], chromatograms[16;16])
> plot(C.warped, plot.orig=TRUE, plot.wf=TRUE)
```

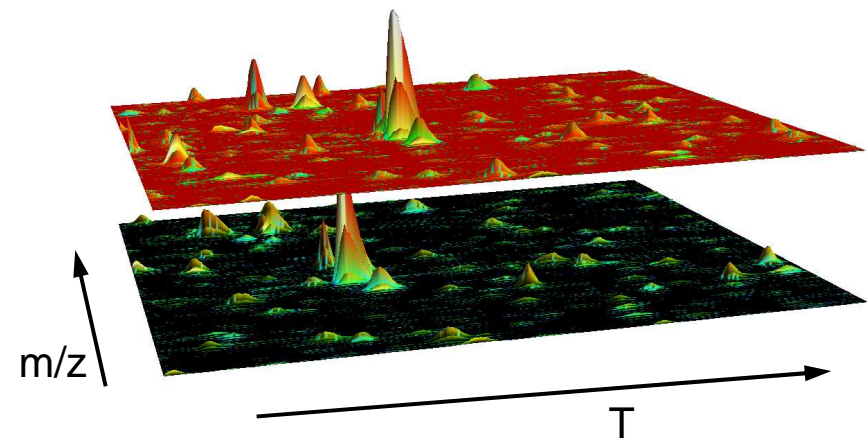
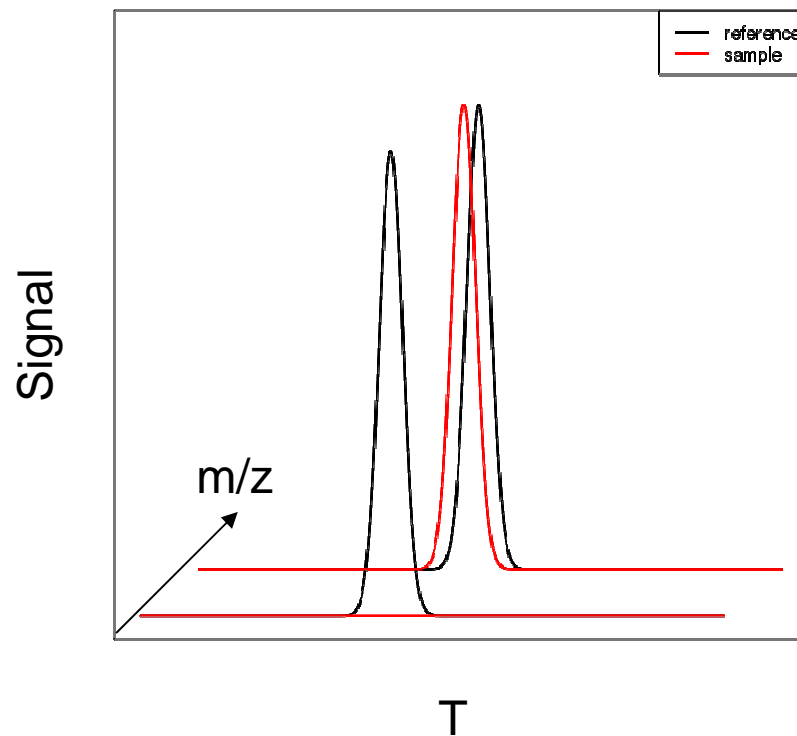


## LC-MS data





## LC-MS data

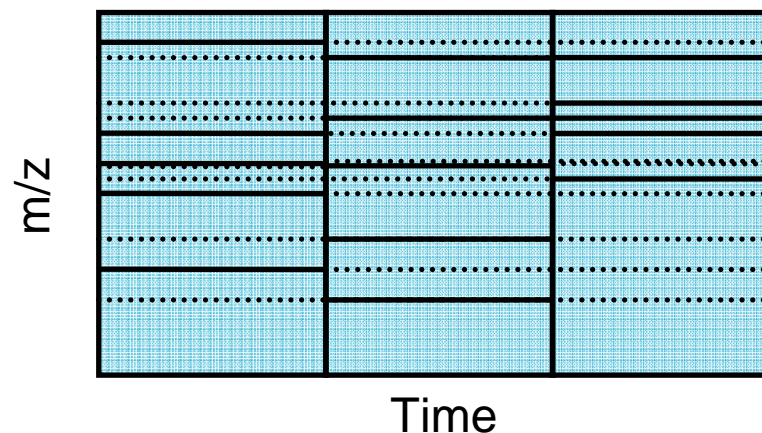






## Global Alignment

- Choose 'High Quality' traces using CODA<sup>2,3</sup>



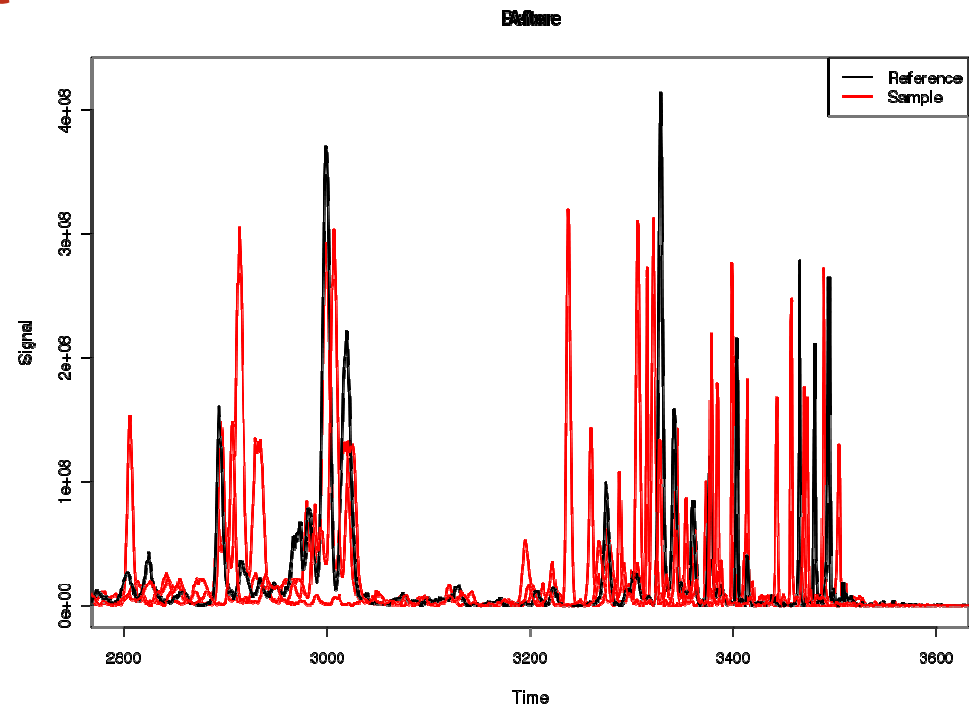
```
> library(ptw)
> data(LCMS)
> HQ <- coda(LCMS, combine=c(1,2), windows=c(3,1), nChroms=5)
> LCMS.Warped <- ptw(LCMS[1, , ], LCMS[2, , ], HQ=HQ,
  align.method="global")
```

<sup>2</sup>Windig, W. *Analytical Chemistry* 68 (20) 3602-3606 1996

<sup>3</sup>Christin, C. *Analytical Chemistry* 80 (18) 7012-7021 2008



## Global Alignment



```
> library(ptw)
> data(LCMS)
> HQ <- coda(LCMS, combine=c(1,2), windows=c(3,1), nChroms=5)
> LCMS.Warped <- ptw(LCMS[1,], LCMS[2, HQ]) HQ=HQ,
align.method = "individual")
```



## Discussion

- Second alignment package for R (next to **dtw**)
- Individual, multiple and global warpings
- Trace selection (CODA)
- Baseline removal (asymmetric LS)
- Smoothing (Whittaker)

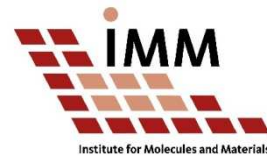


## Planning

- Implement semi-PTW
- Implement other distance measures
- Connect with **dtw**-package
- Release on 1 September 2009



## Acknowledgements



Jan Gerretzen  
Hans Wouters  
Ron Wehrens  
Lutgarde Buydens



Paul Eilers



Jolein Gloerich  
Hans Wessels  
Bert van der Heuvel