WEB337 - HPLC analysis

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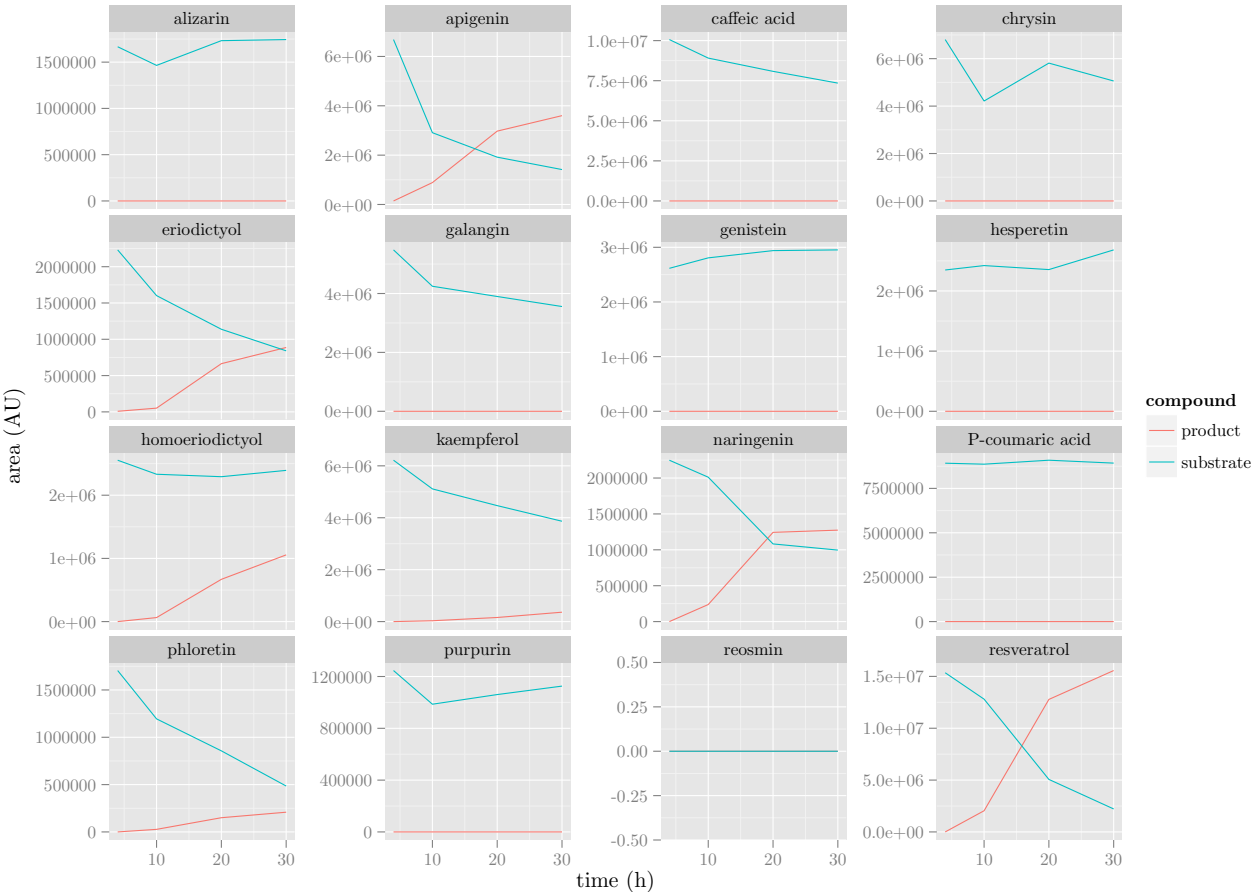
The area data, which was automatically aquired by the HPLC software and stored in ASCII files was transferred manually into a table and stored as a `csv` file. Were no area value was present the `NA` value was set to *0*.

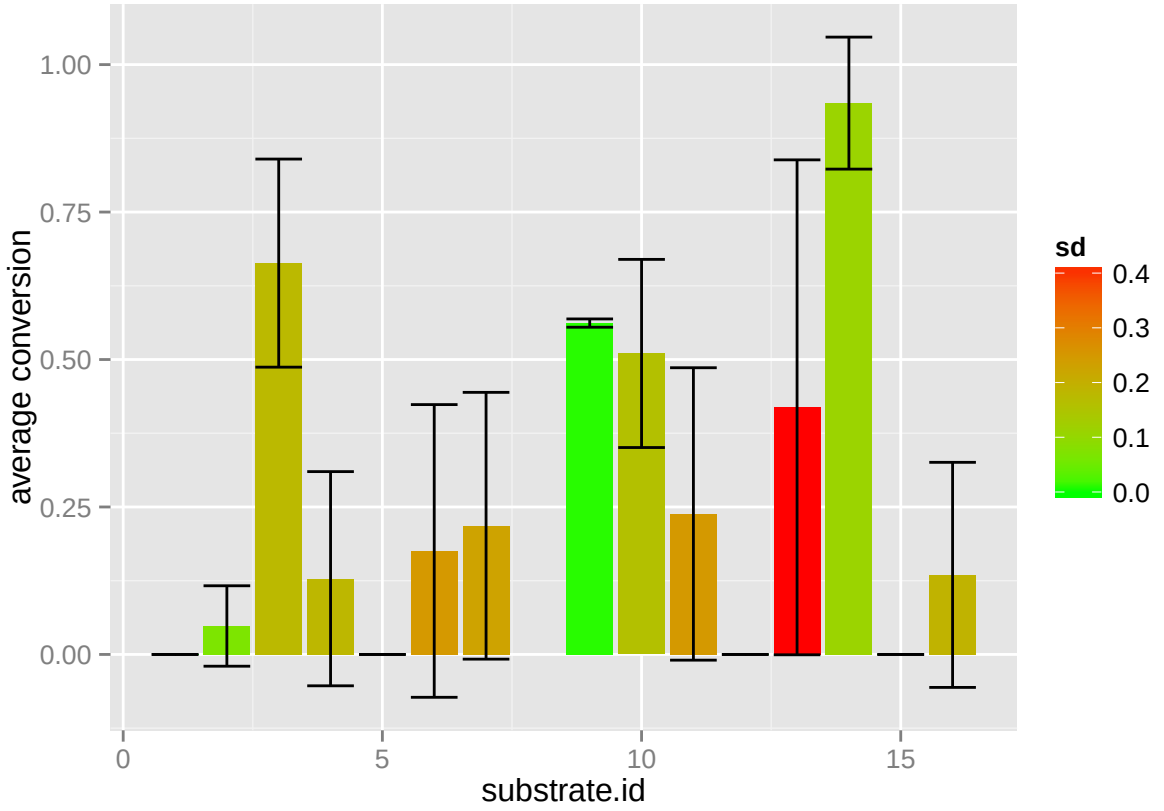
```
knitr::opts_chunk$set(size='tiny')
```

```
library(ggplot2)
library(dplyr)
library(magrittr)
df <- read.csv("~/IPB//Experimente//WEB337 - in vivo SOMT//RAW//results_area.csv")

df %<>% filter(substrate.id != 17)
df$area[is.na(df$area)] <- 0

ggplot(data=df, aes(x=time, y=area, color=compound)) +
  geom_line() +
  facet_wrap(~substrate.name, ncol = 4, scales = "free_y") +
  labs(x="time (h)", y="area (AU)")
```



Conversion can be observed with multiple substrates. Coumaric acid derivatives (coumaric acid, caffeic acid and reosim), anthraquinones (alizarin, purpurin) are not converted. Only flavonoids with a free 4' hydroxyl are converted, as is evident by the non-conversion of hesperetin.

```
tmp <- df %>% filter((time == 4 & compound=="substrate") | (time == 30 & compound=="product"))

tmp.a <- reshape2::melt(tmp, id.vars=c("compound", "substrate.id"), measure.vars="area") %>%
  reshape2::dcast(formula = substrate.id ~ compound) %>%
  mutate(conversion.p = product/substrate)  %>% select(c(1,4))

tmp <- df %>% filter((time == 4 & compound=="substrate") | (time == 30 & compound=="substrate"))
tmp$time <- paste("t", tmp$time, sep=".")
tmp.b <- reshape2::melt(tmp, id.vars=c("compound", "substrate.id", "time"), measure.vars="area") %>%
  reshape2::dcast(formula = substrate.id ~ time) %>%
  mutate(conversion.s = 1-t.30/t.4) %>% select(c(1,4))

tmp.b$conversion.s[which(tmp.b$conversion.s < 0)] <- as.numeric(!(tmp.b$conversion.s < 0))[which(tmp.b$

tmp <- merge(x = tmp.a, y=tmp.b, by = "substrate.id") %>%
  tidyr::gather(key = type, value = conversion, -substrate.id) %>%
  group_by(substrate.id) %>% summarize(mean = mean(conversion), sd = sd(conversion))

ggplot(data=tmp, aes(x=substrate.id, y=mean)) +
  geom_bar(stat = "identity", aes(fill=sd)) +
  labs(y="average conversion") +
  geom_errorbar(aes(ymin = mean - sd, ymax=mean+sd)) +
  scale_fill_gradient(low = "green", high = "red")
```



The conversions obtained by using the product area at 30 hours (a) or the substrate areas at 30 houzrs (b) and setting the substrate area at 4h as 100%. % latex table generated in R 3.1.2 by xtable 1.7-4 package % Tue Jul 21 22:00:55 2015

	substrate.id	conversion.p	conversion.s	mean	sd
1	1	0.00	0.00	0.00	0.00
2	2	0.00	0.10	0.05	0.07
3	3	0.54	0.79	0.66	0.18
4	4	0.00	0.26	0.13	0.18
5	5	0.00	0.00	0.00	0.00
6	6	0.00	0.35	0.18	0.25
7	7	0.06	0.38	0.22	0.23
8	8				
9	9	0.57	0.56	0.56	0.01
10	10	0.40	0.62	0.51	0.16
11	11	0.41	0.06	0.24	0.25
12	12	0.00	0.00	0.00	0.00
13	13	0.12	0.72	0.42	0.42
14	14	1.01	0.86	0.93	0.11
15	15	0.00	0.00	0.00	0.00
16	16	0.00	0.27	0.13	0.19

Table 1: Crude calculated conversions of substrates by product or substrate.