

# WEB272 – SOMT Refolding

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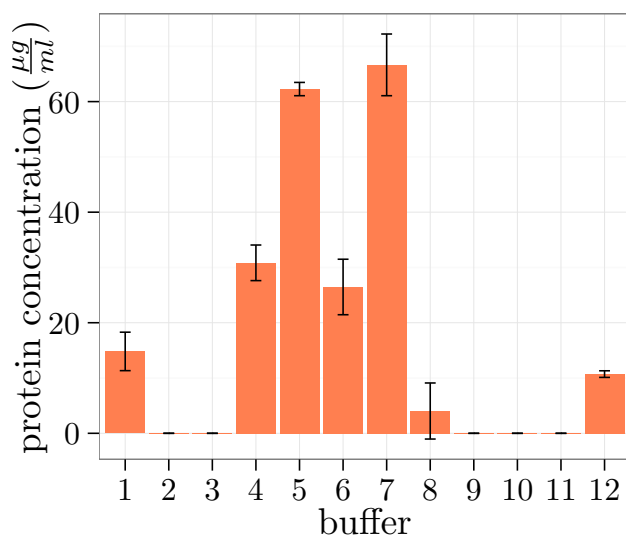
*07/23/2015*

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After rebuffering protein concentrations were measured by Bradford:

## 1 Protein concetration



### 1.1 Regression tree

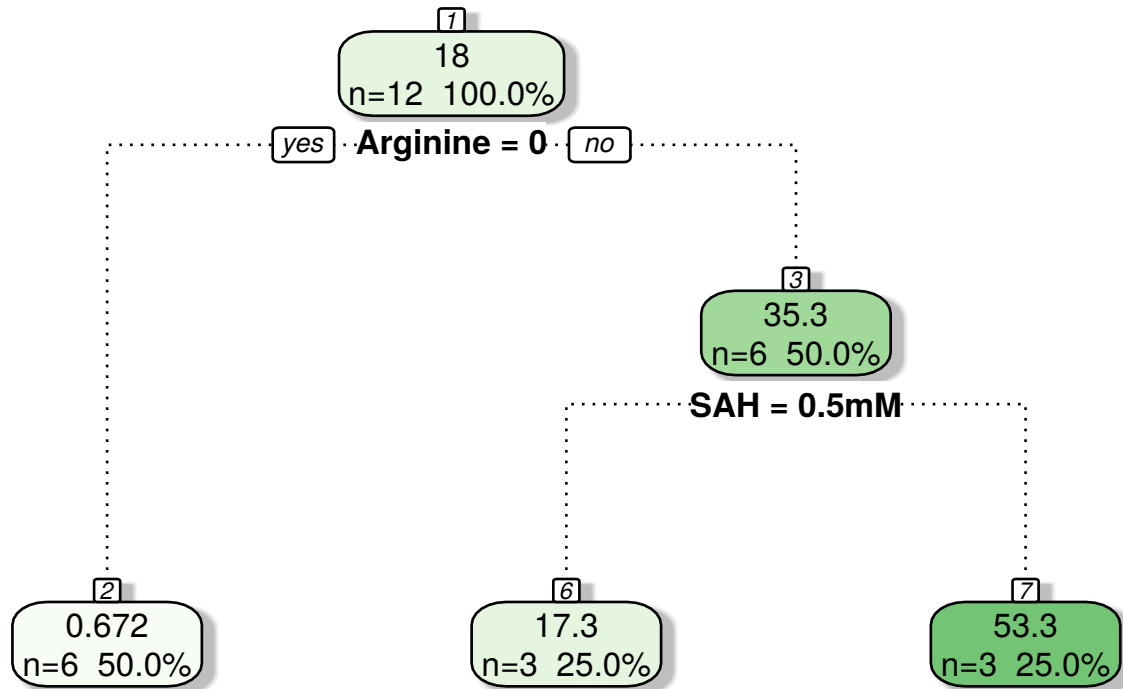
Next we build a regression tree. To see, which factors have the most influence on the protein concentration.

```
somttree2 <- rpart(BFmean ~ .,  
  data=df[,c(1:11,21)],  
  control = c(minsplit = 3,
```

```

minbucket = 2,
complexity = 0.001))
fancyRpartPlot(somttree2, digits=3)

```

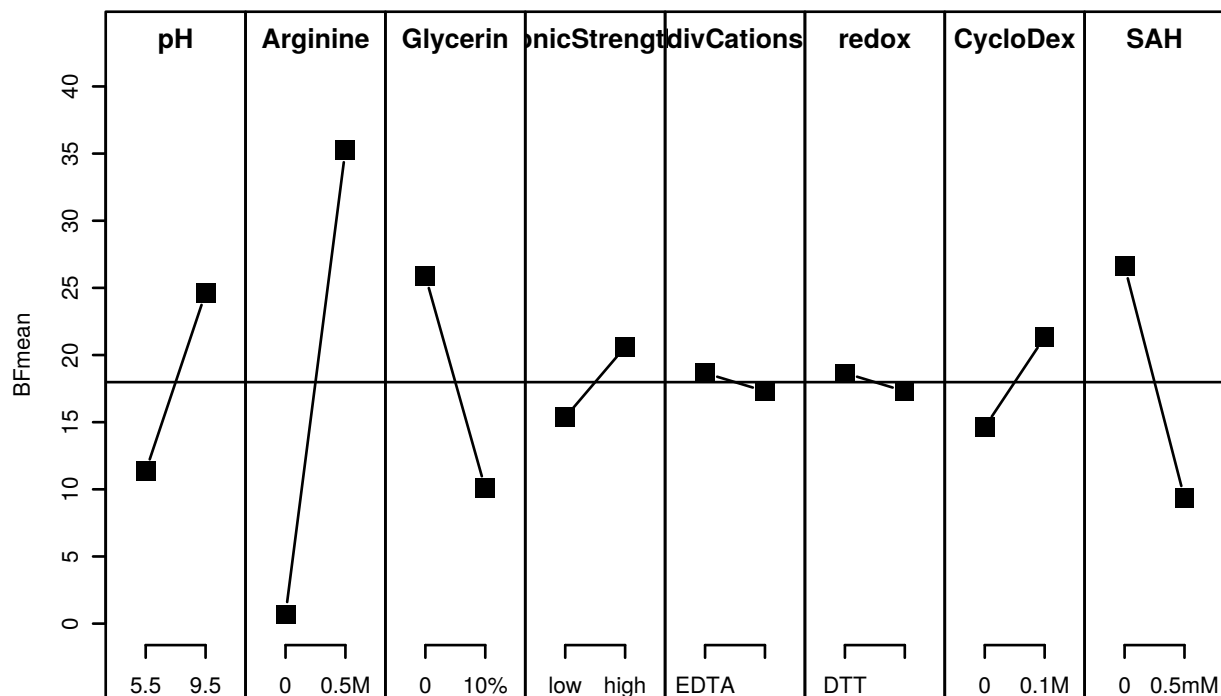


Rattle 2015-Okt-22 11:41:40 mori

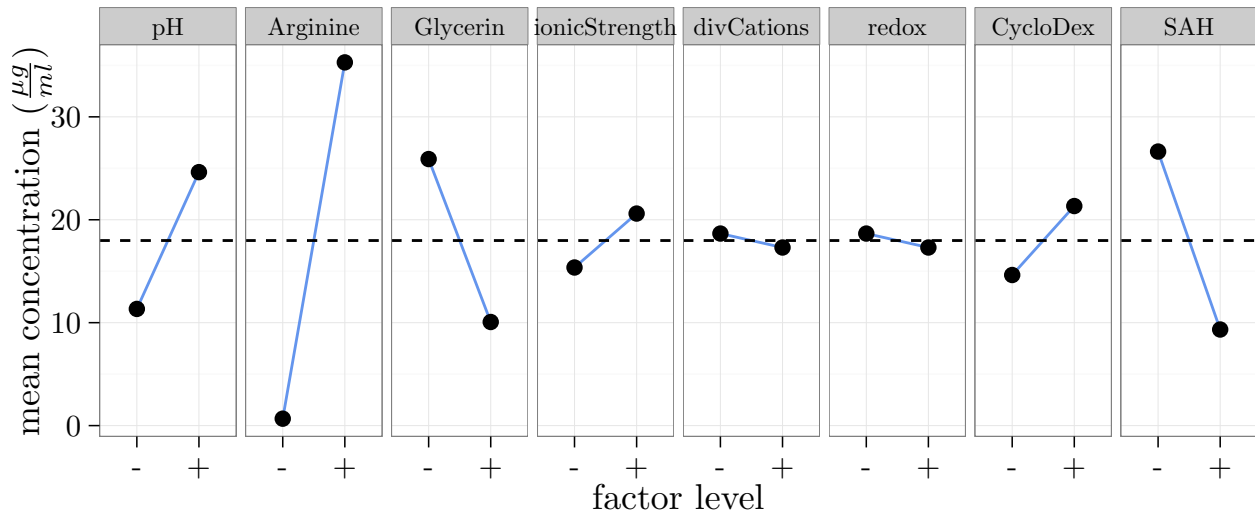
Arginine seems to have the biggest impact on refolding efficiency (Arginine addition is better). Then comes SAH (no SAH is better).

## 1.2 Main effects plot

**Main effects plot for BFmean**



```
## % latex table generated in R 3.1.2 by xtable 1.7-4 package
## % Thu Oct 22 11:41:42 2015
## \begin{table}[ht]
## \centering
## \begin{tabular}{rlllr}
## \hline
## & state & ME & value & \\
## \hline
## 1 & - & pH & 11.34 & \\
## 2 & + & pH & 24.63 & \\
## 3 & - & Arginine & 0.67 & \\
## 4 & + & Arginine & 35.29 & \\
## 5 & - & Glycerin & 25.90 & \\
## 6 & + & Glycerin & 10.07 & \\
## 7 & - & ionicStrength & 15.36 & \\
## 8 & + & ionicStrength & 20.60 & \\
## 9 & - & divCations & 18.66 & \\
## 10 & + & divCations & 17.30 & \\
## 11 & - & redox & 18.66 & \\
## 12 & + & redox & 17.30 & \\
## 13 & - & CycloDex & 14.63 & \\
## 14 & + & CycloDex & 21.33 & \\
## 15 & - & SAH & 26.63 & \\
## 16 & + & SAH & 9.34 & \\
## \hline
## \end{tabular}
## \end{table}
```



### 1.3 Statistical test

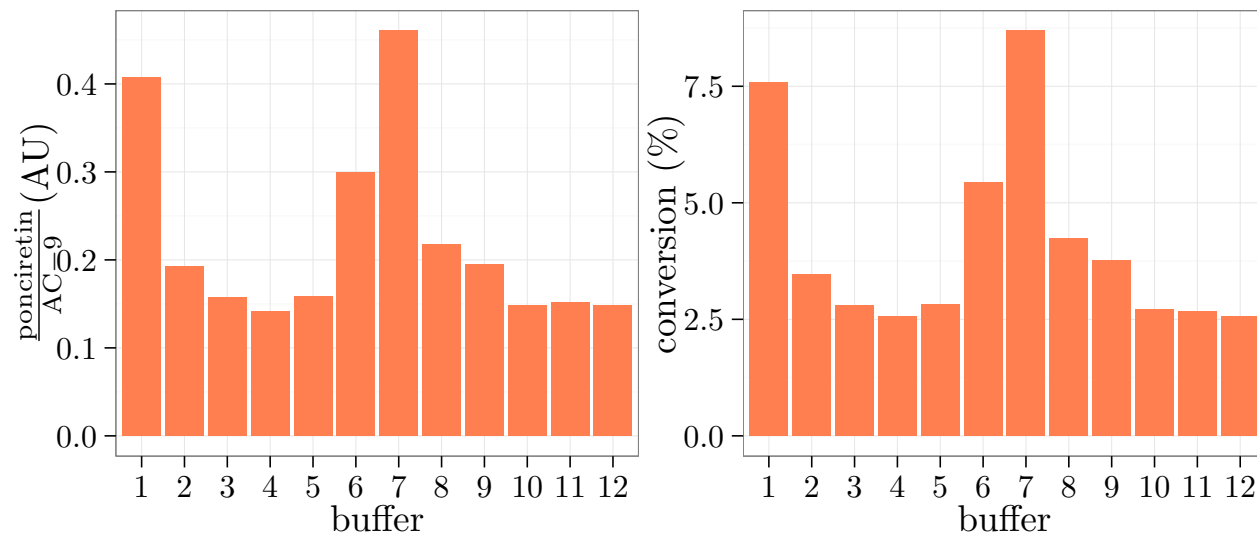
Test the statistical significance of main effects. Only Arginine is statistically significant to a p-value of 0.05. SAH to a p-value of 0.1.

% latex table generated in R 3.1.2 by xtable 1.7-4 package % Thu Oct 22 11:41:44 2015

	Df	Sum Sq	Mean Sq	F value	Pr(>F)
Arginine	1	3595.63	3595.63	24.56	0.0158
pH	1	529.87	529.87	3.62	0.1533
Glycerin	1	752.08	752.08	5.14	0.1083
ionicStrength	1	82.37	82.37	0.56	0.5077
divCations	1	5.49	5.49	0.04	0.8588
redox	1	5.52	5.52	0.04	0.8584
CycloDex	1	134.67	134.67	0.92	0.4083
SAH	1	896.83	896.83	6.13	0.0897
Residuals	3	439.26	146.42		

```
## Error in eval(expr, envir, enclos): could not find function "LenthPlot"
```

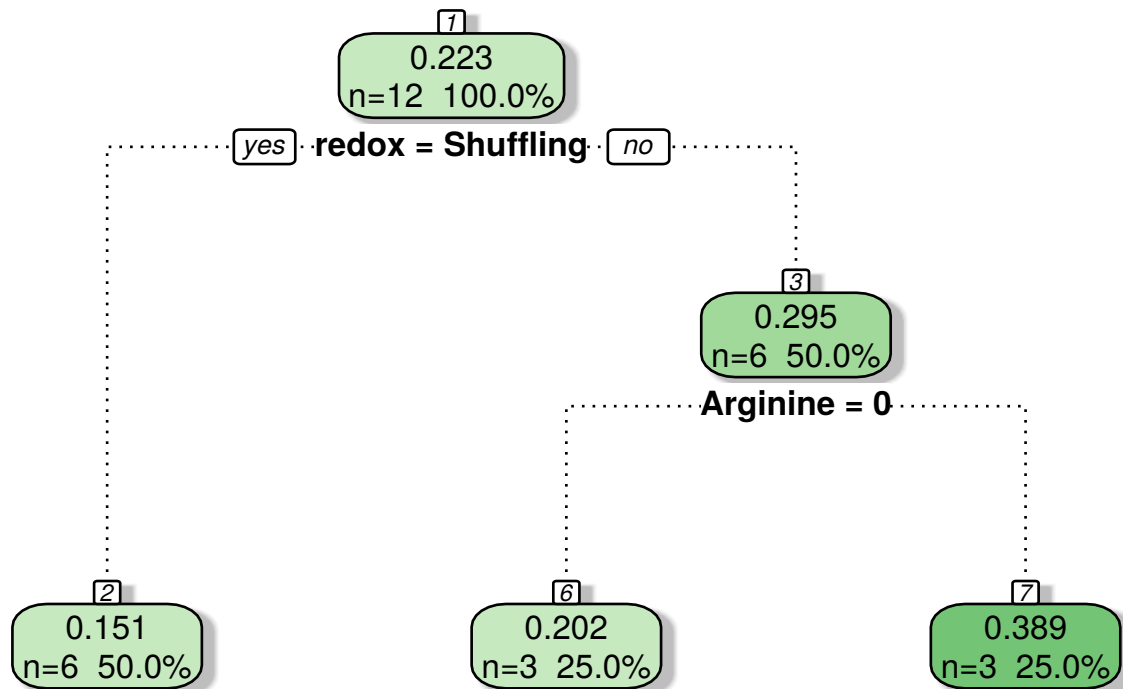
## 2 Protein volume activity



### 2.1 Regression tree

Next we build a regression tree. To see, which factors have the most influence the SOMT activity.

```
somttree2 <- rpart(P1_AC ~ .,  
  data=df[,c(1:8,12)],  
  control = c(minsplit = 3,  
    minbucket = 2,  
    complexity = 0.001))  
fancyRpartPlot(somttree2, digits=3)
```

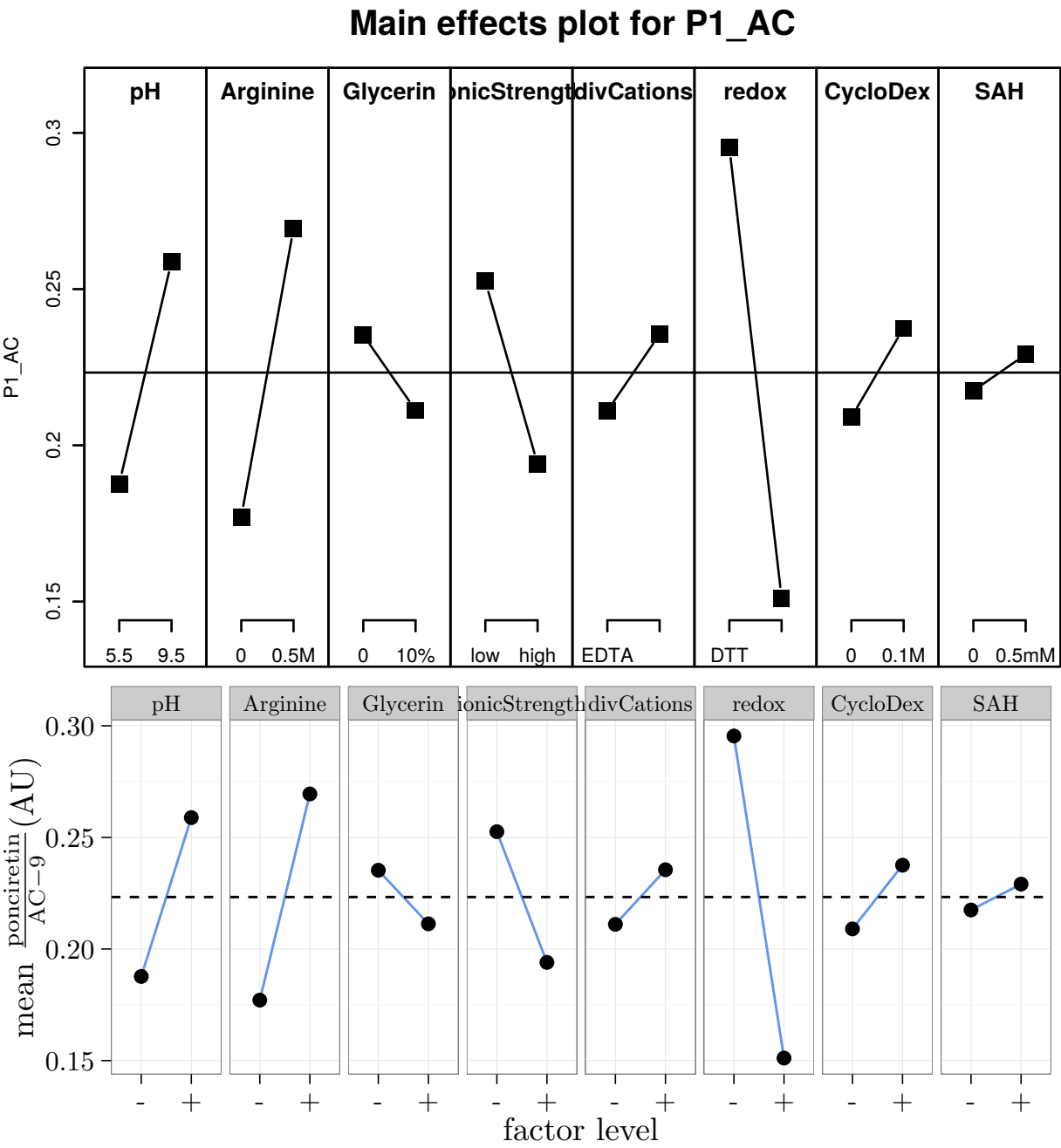


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The redox status seems to have the biggest impact on refolding efficiency measured by activity (reducing is better, DTT). Then comes arginine (arginine is better).

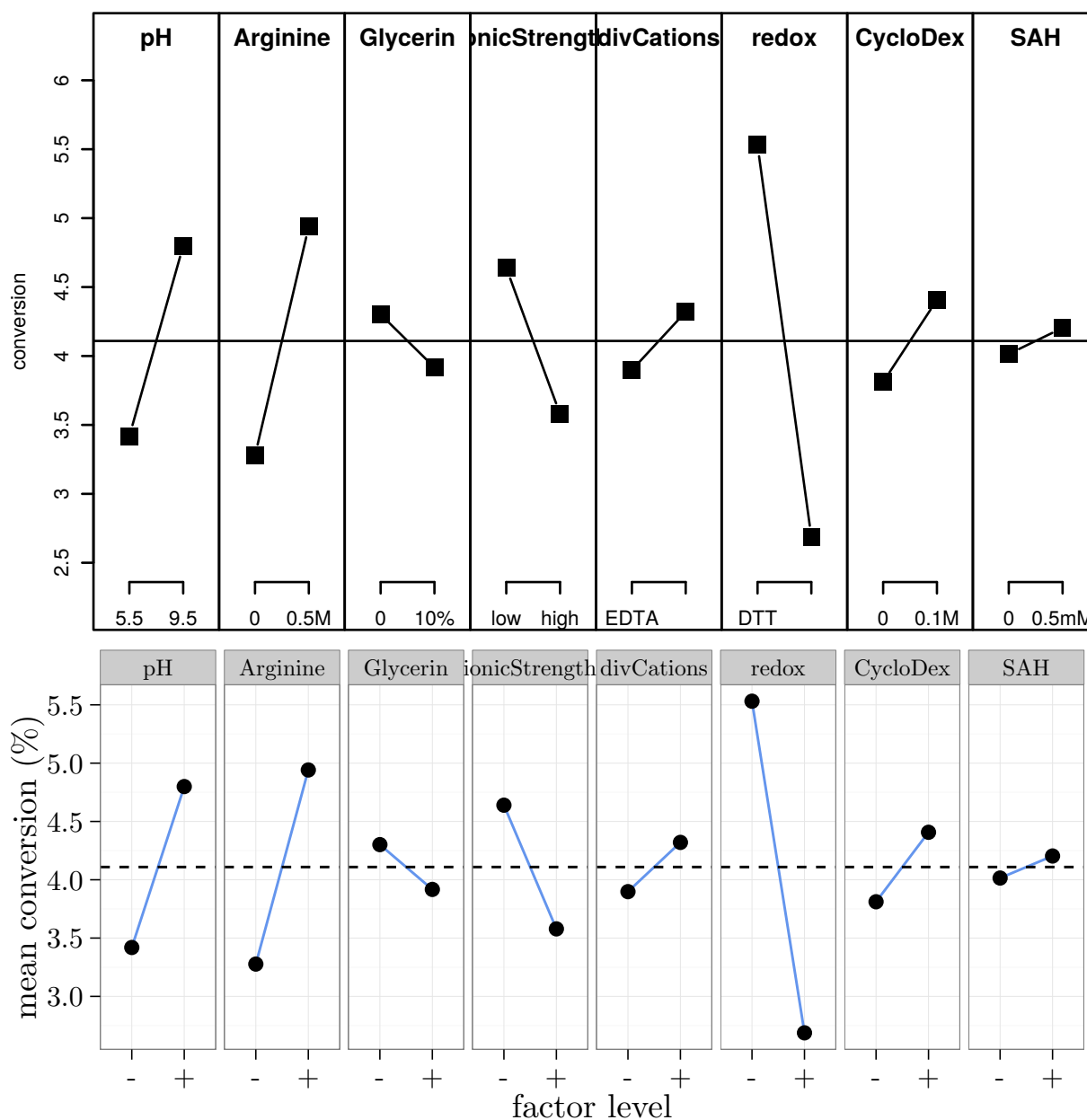
2.2 Main effects plot

2.2.1 ÁUC



## 2.2.2 conversion

**Main effects plot for conversion**



## 2.3 Statistical test

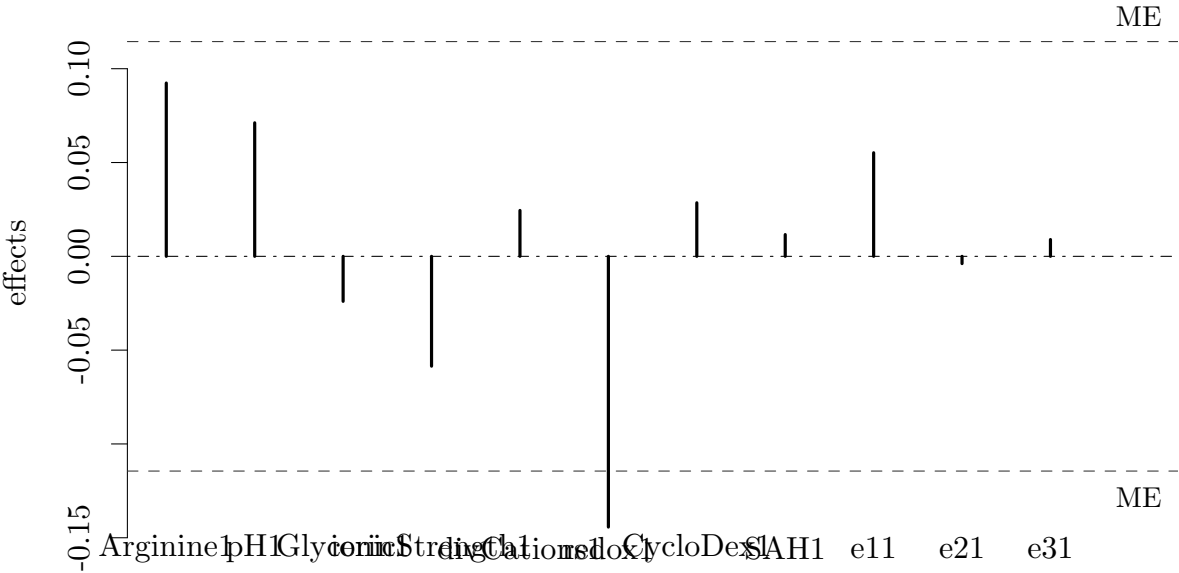
Test the statistical significance of main effects. Only Arginine is statistically significant to a p-value of 0.05. SAH to a p-value of 0.1.

### 2.3.1 AUC

% latex table generated in R 3.1.2 by xtable 1.7-4 package % Thu Oct 22 11:41:50 2015



	Df	Sum Sq	Mean Sq	F value	Pr(>F)
pH	1	0.02	0.02	4.83	0.1153
Arginine	1	0.03	0.03	8.14	0.0649
Glycerin	1	0.00	0.00	0.55	0.5122
ionicStrength	1	0.01	0.01	3.27	0.1682
divCations	1	0.00	0.00	0.57	0.5047
redox	1	0.06	0.06	19.88	0.0210
CycloDex	1	0.00	0.00	0.78	0.4428
SAH	1	0.00	0.00	0.13	0.7439
Residuals	3	0.01	0.00		

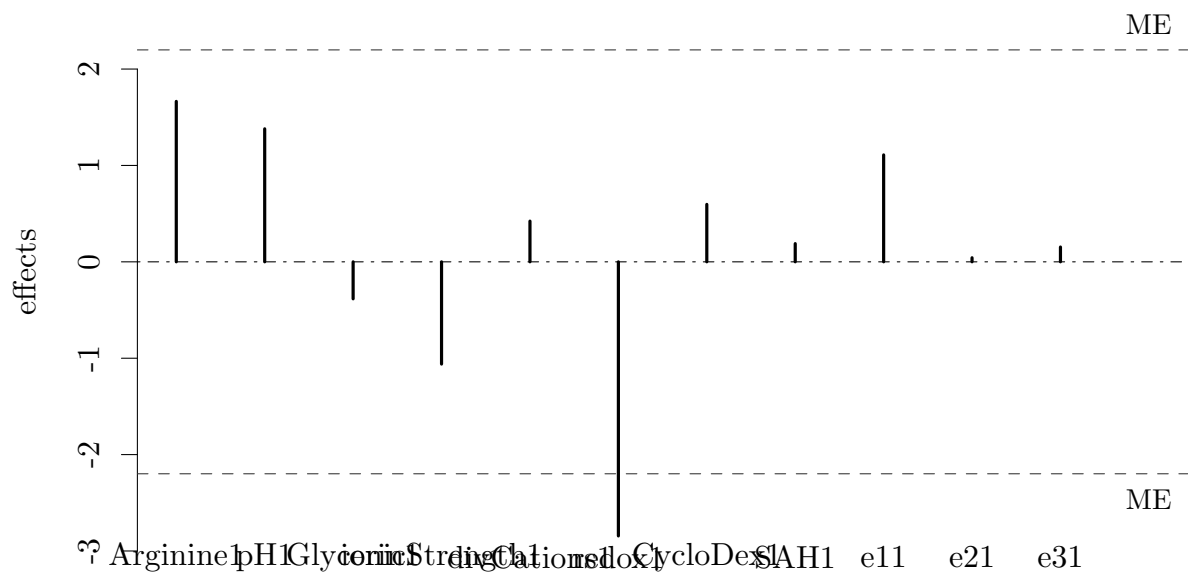


factors  
 PSE ME SME 0.05000000 0.03975856 0.11446004 0.24518392

### 2.3.2 conversion

% latex table generated in R 3.1.2 by xtable 1.7-4 package % Thu Oct 22 11:41:50 2015

	Df	Sum Sq	Mean Sq	F value	Pr(>F)
pH	1	5.71	5.71	4.55	0.1227
Arginine	1	8.31	8.31	6.62	0.0824
Glycerin	1	0.44	0.44	0.35	0.5945
ionicStrength	1	3.38	3.38	2.69	0.1997
divCations	1	0.54	0.54	0.43	0.5605
redox	1	24.26	24.26	19.31	0.0218
CycloDex	1	1.07	1.07	0.85	0.4250
SAH	1	0.11	0.11	0.09	0.7893
Residuals	3	3.77	1.26		



PSE ME SME 0.0500000 0.7637776 2.1988227 4.7100805

alpha