Calmodulin model plots

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Load necessary libraries

```
library(ggplot2)
library(reshape2)
```

Figure 3

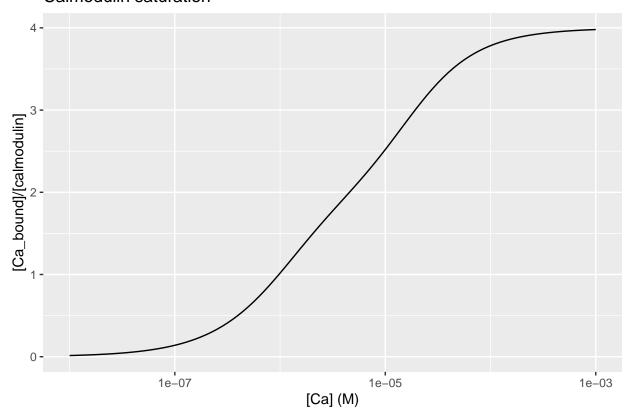
Import data (this assumes the working directory is set correctly)

```
figure3 <- read.table("Figure3.txt",sep="\t",header=FALSE)
names(figure3) <- c("Ca","saturation")</pre>
```

Plot the data

```
p3 <- ggplot(figure3, aes(x=Ca,y=saturation))
p3 <- p3 + geom_line() + scale_x_log10()
p3 <- p3 + ylab("[Ca_bound]/[calmodulin]") + xlab("[Ca] (M)")
p3 <- p3 + ggtitle("Calmodulin saturation")
p3</pre>
```

Calmodulin saturation



```
png("calmodulin_saturation.png", width = 4, height = 4, units = 'in', res = 300)
p3
dev.off()
## pdf
## 2
```

Figure 4

The data is stored in four different data files (one for each curve). Import them and a column specifying their condition.

```
figure4a <- read.table("Figure4a.txt",sep="\t",header=FALSE)
names(figure4a) <- c("Ca","ybar")
figure4a$condition <- "no target"

figure4b <- read.table("Figure4b.txt",sep="\t",header=FALSE)
names(figure4b) <- c("Ca","ybar")
figure4b$condition <- "R state"

figure4c <- read.table("Figure4c.txt",sep="\t",header=FALSE)
names(figure4c) <- c("Ca","ybar")
figure4c$condition <- "T state"

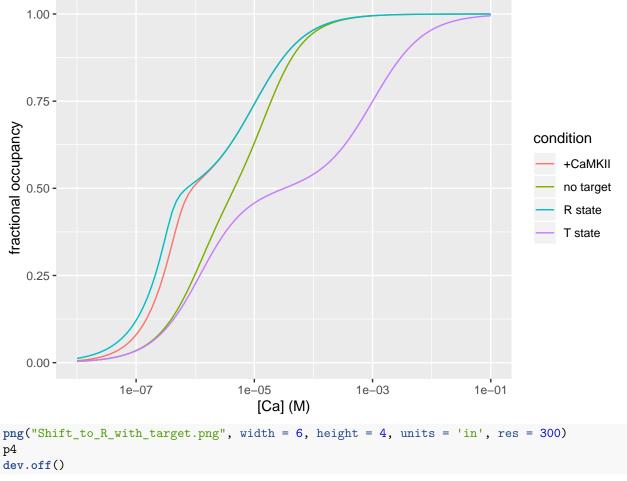
figure4d <- read.table("Figure4d.txt",sep="\t",header=FALSE)
names(figure4d) <- c("Ca","ybar")
figure4d$condition <- "+CaMKII"</pre>
```

Concatenate all the data for figure 4 into one big data frame

```
figure4 <- rbind(figure4a,figure4b,figure4c,figure4d)</pre>
```

Plot the data:

```
p4 <- ggplot(figure4, aes(x=Ca,y=ybar,col=condition))
p4 <- p4+geom_line()+ scale_x_log10()
p4 <- p4 + ylab("fractional occupancy") + xlab("[Ca] (M)")
p4</pre>
```



```
p4
dev.off()
```

pdf

Figure 5

Import the data; get rid of extra column

```
figure5 <- read.table("Figure5.txt",sep="\t",header=FALSE)</pre>
figure5 <- figure5[,1:3]</pre>
```

In order to name the columns, we need to know in which order they were defined in the model: First CaMKII, then PP2B

```
names(figure5) <- c("Ca", "CaMKII", "PP2B")</pre>
```

Normalise CaMKII and PP2B to their respective max, then melt the dataset

```
figure5$CaMKII <- figure5$CaMKII/(max(figure5$CaMKII))</pre>
figure5$PP2B <- figure5$PP2B/(max(figure5$PP2B))</pre>
figure5 <- melt(figure5,id="Ca")</pre>
```

Plot the data

```
p5 <- ggplot(figure5, aes(x = Ca,y=value, color=variable))</pre>
p5 <- p5 + geom_line()
p5 <- p5 + scale_x_log10()
p5 <- p5 + ylab("activity (normalised)") + xlab("[Ca] (M)")
р5
    1.00 -
   0.75 -
activity (normalised)
                                                                                       variable
                                                                                          - CaMKII
    0.50 -
                                                                                            PP2B
   0.25 -
   0.00 -
         1e-07
                          1e-06
                                           1e-05
                                                            1e-04
                                                                             1e-03
                                         [Ca] (M)
png("CaMKII_PP2B.png", width = 6, height = 4, units = 'in', res = 300)
p5
```

```
dev.off()
```

pdf ## 2