Data preparation for modeling

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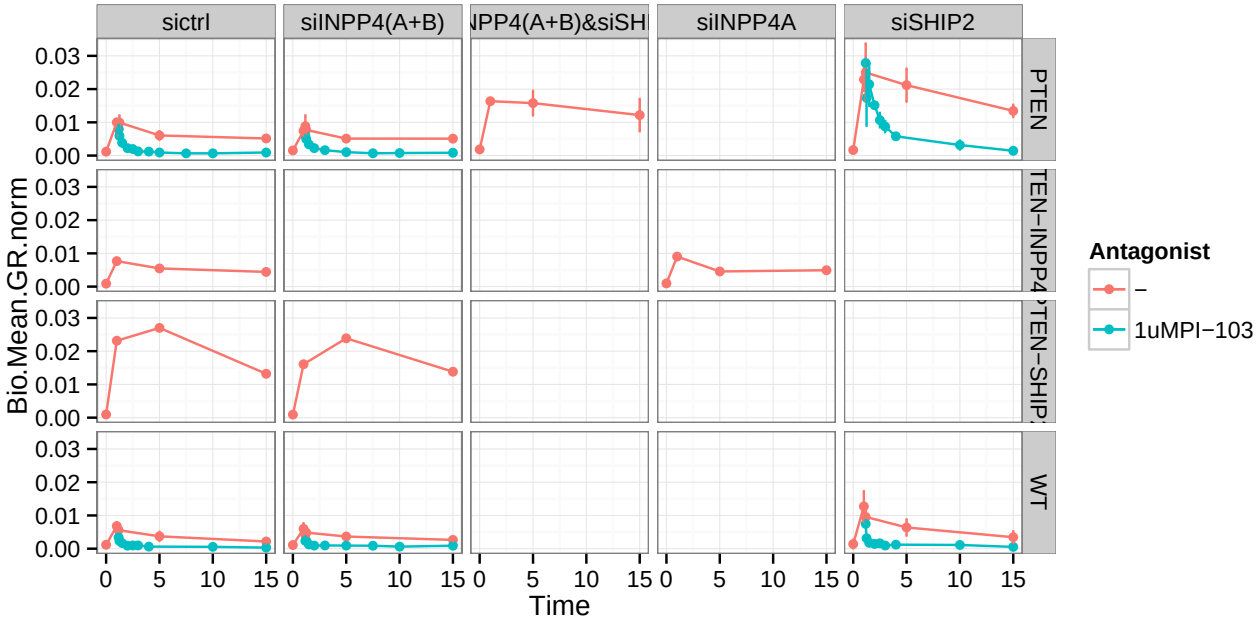
Contents

In this report I will show how I convert Golden Ratio units into uM (umol/l) and how I do regression analysis to get smooth curves for the modeling part.

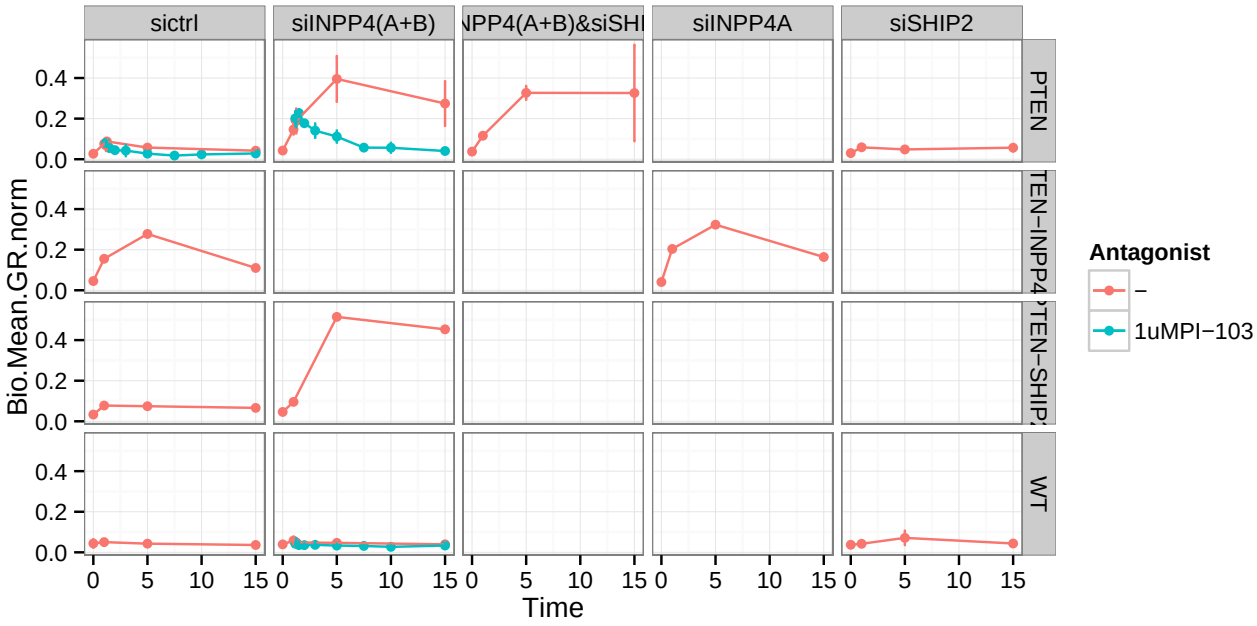
1 Golden Ratio –> uM units

First of all, the final data for both PIP3 and PI(3,4)P2:

PIP3



PI(3,4)P2



Let's now convert Golden Ratio units in M units. First, define all parameters:

```
cell.radius <- 10e-6 # [m]; Malek: average diameter of MCF10a cells: 18.7 um
cell.volume <- 4/3*3.14*cell.radius^3*1e3 # [l]
nucleus.volume <- 0.1*cell.volume # [l]; 10% of cell volume - from Wikipedia
cytoplasm.volume <- cell.volume - nucleus.volume # [l]
ms.cell.number <- 250000 # number of cells involved in each mass spec experiment
# for the following factors - see golden-ratio-mol-conversion.txt
# 1 point in the Golden Ratio PIP3  is equal to  0.036718508 nmol
p3.conversion.factor <- 0.036718508
# 1 point in the Golden Ratio PI(3,4)p2 ( C18 column )  is equal to  0.033106953 nmol
p2.conversion.factor <- 0.033106953
```

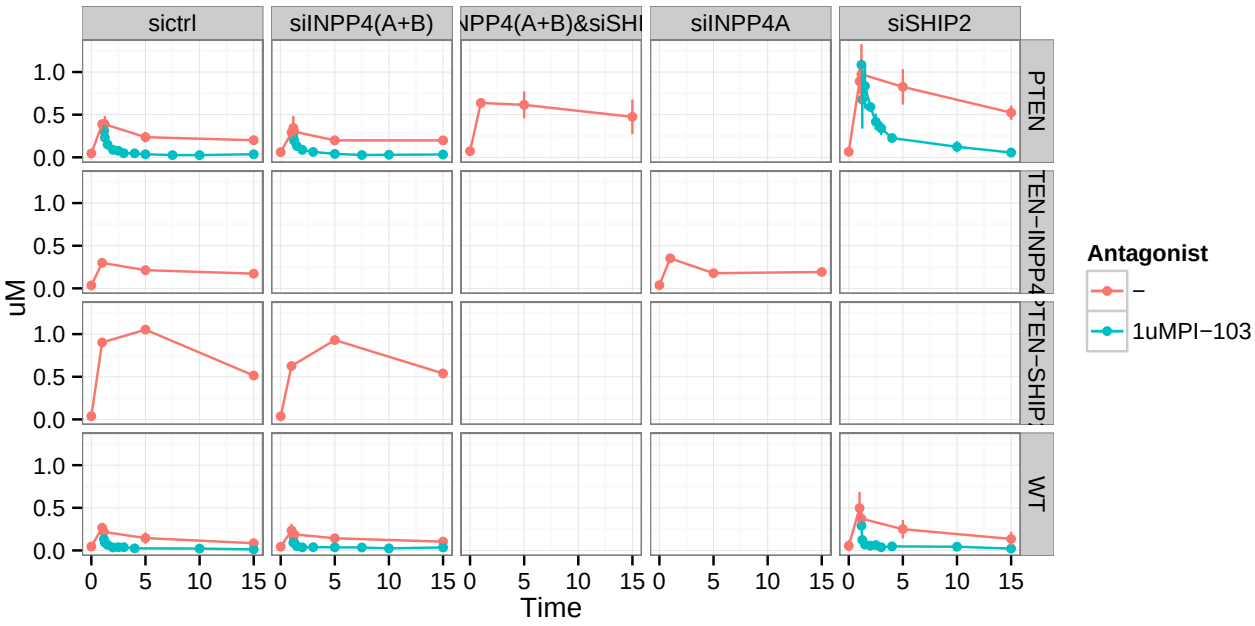
Now make the conversion:

```
# convert to nmols
p2$nm <- p2$Bio.Mean.GR.norm*p2.conversion.factor
p2$nm.sd <- p2$Bio.SD.GR.norm*p2.conversion.factor
p3$nm <- p3$Bio.Mean.GR.norm*p3.conversion.factor
p3$nm.sd <- p3$Bio.SD.GR.norm*p3.conversion.factor
# convert to uM concentration
p2$uM <- p2$nm/
        ms.cell.number*    # per 1 cell
        1e-9/              # nmol --> mol
        cytoplasm.volume/ # divide by the cell volume and get
                          # concentration in M
        1e-6               # M --> uM
p2$uM.sd <- p2$nm.sd/
        ms.cell.number*    # per 1 cell
        1e-9/              # nmol --> mol
        cytoplasm.volume/ # divide by the cell volume and get
                          # concentration in M
        1e-6               # M --> uM
p3$uM <- p3$nm/
```

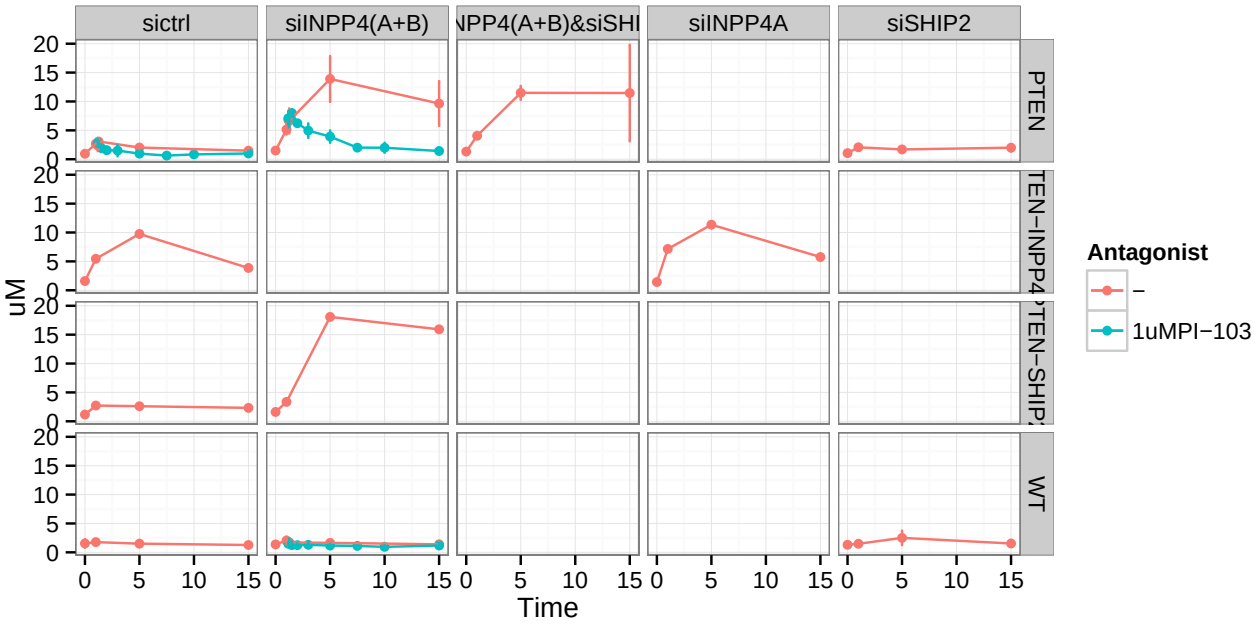
```
        ms.cell.number*    # per 1 cell
        1e-9/              # nmol --> mol
        cytoplasm.volume/ # divide by the cell volume and get
                           # concentration in M
        1e-6               # M --> uM
p3$uM.sd <- p3$nm.sd/
        ms.cell.number*    # per 1 cell
        1e-9/              # nmol --> mol
        cytoplasm.volume/ # divide by the cell volume and get
                           # concentration in M
        1e-6               # M --> uM
write.csv(p2, file = "all-data/bio-rep-av/pi34p2-uM.csv", row.names = F, quote = F)
write.csv(p3, file = "all-data/bio-rep-av/p3_4-uM.csv", row.names = F, quote = F)
```

Now plot data represented in uM:

PIP3



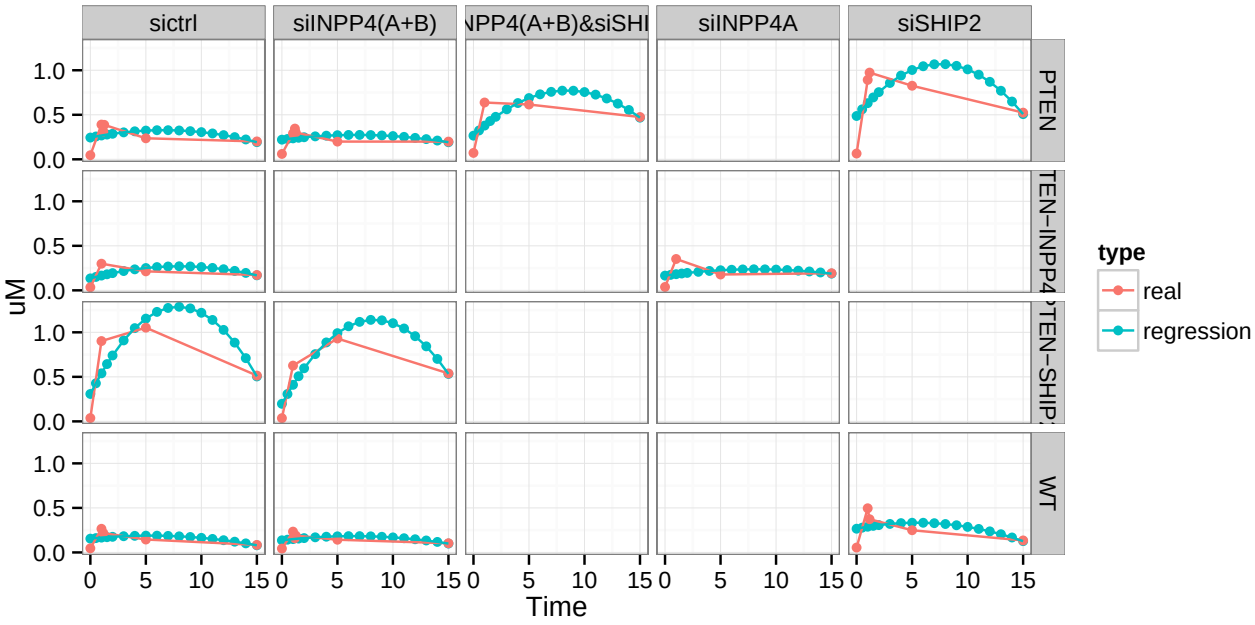
PI(3,4)P2



2 Regressions

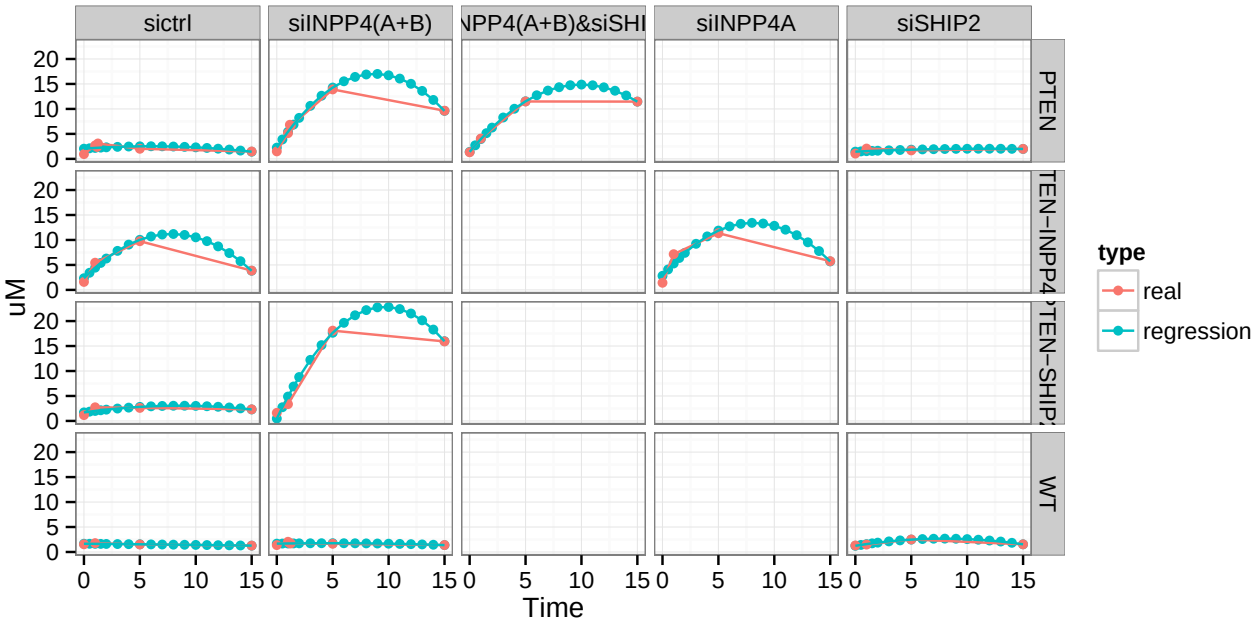
Now let's try to fit smooth curves to the data. I start with data with no PI3K inhibitor. I try to fit it with polynomial function of degree 2.

PIP3



It is not easy to fit polynomial function to PIP3 (I also tried degrees 3 and 4) and it looks like the time course is biphasic with the peak point as a changing point...

PI(3,4)P2



PI(3,4)P2 was easy to fit with the degree of 2.

Data with the inhibitors is fit with an exponentional function but it requires more time to fit, because one has to take into account only few points of the time course - it is not possible to fit the total time course with just one exponent.

In the model I will start with the raw data and see if I need to use regression at all.