

A

## Select parameters for the plot.

☐ Theoretical calculations

Choose values type:

- ☒ relative  
☐ absolute

Comparison plot parameters:

Time point  
CHOSEN

1

Time point IN

0.01

Time point OUT

1440

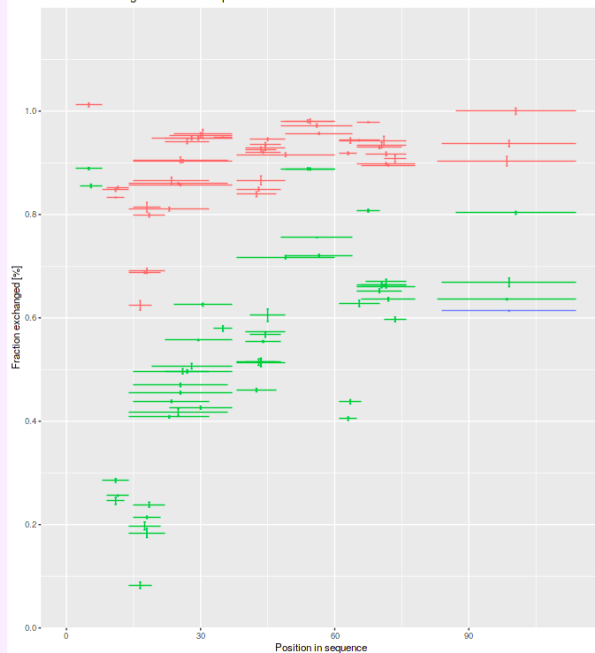
Choose states for comparison:

- ☒ S100A9 (NaCl)  
☐ S100A9 + Ca (z NaCl)  
☐ S100A9 + Ca + Zn 110uM (z NaCl)  
☐ S100A9 + Mn (z NaCl)  
☒ S100A9 + Zn 110uM (z NaCl)  
☐ S100A9 + Zn 500uM (z NaCl)  
☐ S100A9 (NaCl):Oxidation M (I1)  
☐ S100A9 + Ca (z NaCl):Oxidation M (I1)  
☐ S100A9 + Ca + Zn 110uM (z NaCl):Oxidation M (I1)  
☐ S100A9 + Mn (z NaCl):Oxidation M (I1)  
☒ S100A9 + Zn 110uM (z NaCl):Oxidation M (I1)  
☐ S100A9 + Zn 500uM (z NaCl):Oxidation M (I1)

Comparison plot

Data

Fraction exchanged in state comparison in 1 min



— S100A9 (NaCl) — S100A9 + Zn 110uM (z NaCl) — S100A9 + Zn 110uM (z NaCl):Oxidation M (I1)

B

Choose state:

- ☒ S100A9 (NaCl)  
☐ S100A9 + Ca (z NaCl)  
☐ S100A9 + Ca + Zn 110uM (z NaCl)  
☐ S100A9 + Mn (z NaCl)  
☐ S100A9 + Zn 110uM (z NaCl)  
☐ S100A9 + Zn 500uM (z NaCl)  
☐ S100A9 (NaCl):Oxidation M (I1)  
☐ S100A9 + Ca (z NaCl):Oxidation M (I1)  
☐ S100A9 + Ca + Zn 110uM (z NaCl):Oxidation M (I1)  
☐ S100A9 + Mn (z NaCl):Oxidation M (I1)  
☐ S100A9 + Zn 110uM (z NaCl):Oxidation M (I1)  
☐ S100A9 + Zn 500uM (z NaCl):Oxidation M (I1)

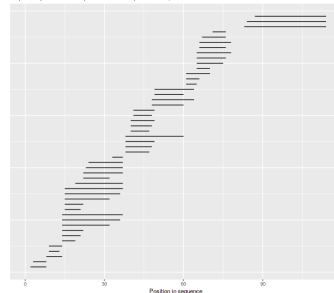
Choose range:



Peptide Coverage

Data

Peptides positions compared to whole protein sequence



C

Woods plot parameters:

State 1

S100A9 (NaCl)

State 2

S100A9 + Zn 110uM (z NaCl)

Choose confidence limit:

98%

Choose second confidence limit:

99%

Adjust plot:

Choose y range for comparison plot:



Choose y range for Woods plot:



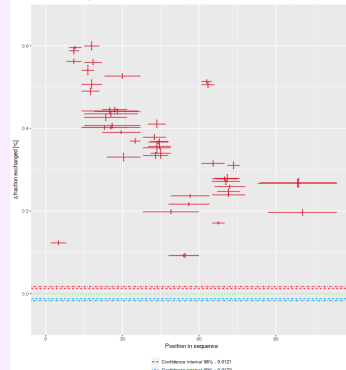
Choose x range for both plots:



Woods plot

Data

Δ Fraction exchanged in 1 min between S100A9 (NaCl) and S100A9 + Zn 110uM (z NaCl)



— Confidence interval 95% - 0.0121  
 — Confidence interval 95% - 0.0172