20211122_spinrelaxation_plotting_R.R

kelse

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```r
# 20211122 plotting of spin relaxation data collected on 500 MHz and 600 MHz
# spectrometers. Plots of R1, R2, NOE, and calculated order parameters by residue.

library(tidyverse)
```

```
## -- Attaching packages ------------------------------------ tidyverse 1.3.0 --

## v ggplot2 3.3.3     v purrr   0.3.4
## v tibble  3.1.0     v dplyr   1.0.5
## v tidyr   1.1.3     v stringr 1.4.0
## v readr   1.4.0     v forcats 0.5.1

## Warning: package 'stringr' was built under R version 4.0.5

## -- Conflicts -------------------------------------------- tidyverse_conflicts() --
## x dplyr::filter() masks stats::filter()
## x dplyr::lag()    masks stats::lag()
```

```r
library(readxl)

#load file - edited in excel
#raw data included in folder

order_param <- read_excel("20211122_spinrelaxation_plotting.xlsx", sheet = 1)

R1 <- read_excel("20211122_spinrelaxation_plotting.xlsx", sheet = 2)

R2 <- read_excel("20211122_spinrelaxation_plotting.xlsx", sheet = 3)

NOE <- read_excel("20211122_spinrelaxation_plotting.xlsx", sheet = 4)


#Combined data - R1, R2, and HetNOE

#R1
R1 %>%
  ggplot(., aes(x = residue, y = R1, color = as.factor(field), shape=as.factor(field))) +
  geom_pointrange(aes(ymin=R1-R1err, ymax=R1+R1err), position=position_dodge(0.9),
                  size=0.3) +
  scale_color_manual(values=c("gray15", "orchid4")) +
```
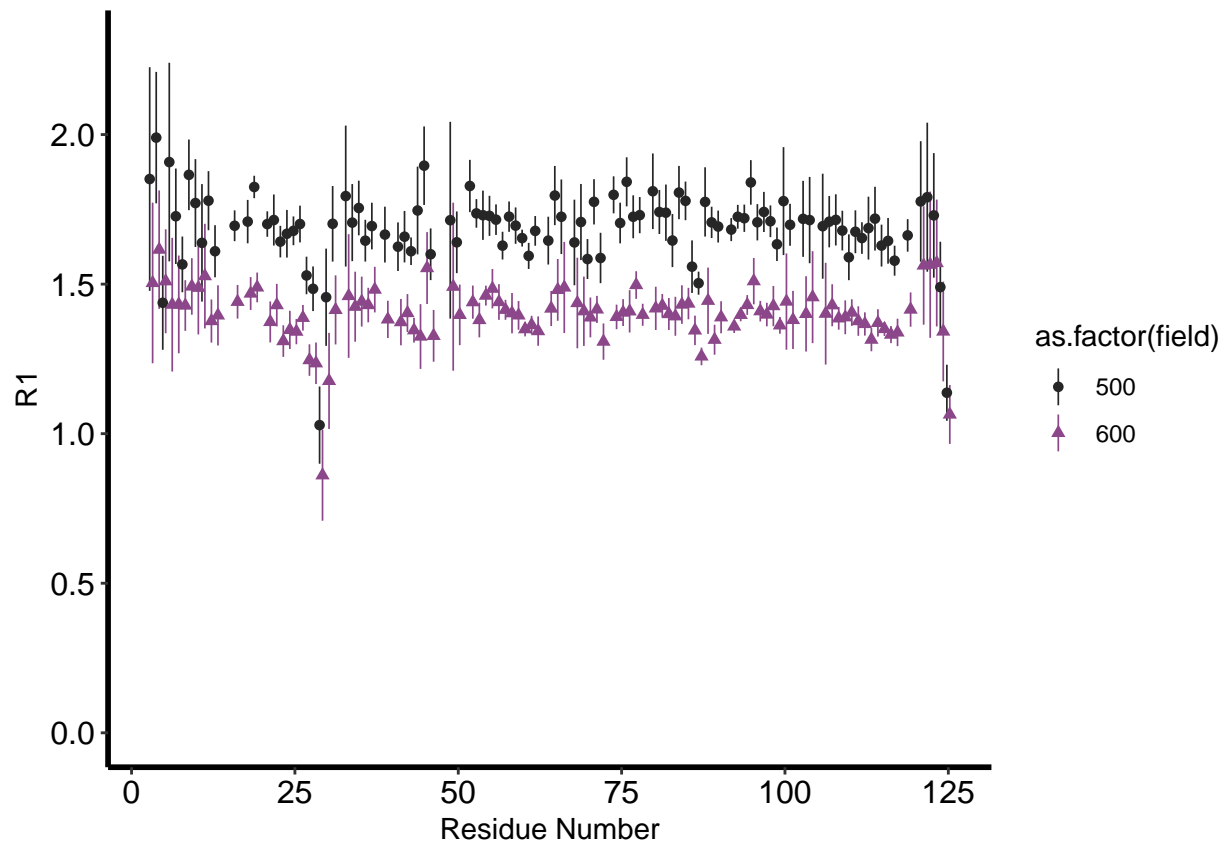
```
    labs(x = "Residue Number", y = "R1") +
    theme_bw() +
    scale_y_continuous(limits = c(0, 2.3), breaks = c(0, 0.5, 1.0, 1.5, 2.0)) +
    theme(axis.text = element_text(color = "black", size = 12),
          panel.grid.major = element_blank(),
          panel.grid.minor = element_blank(),
          panel.border = element_blank(),
          panel.background = element_blank(),
          axis.line.x = element_line(color = "black", size = 1, linetype = 1),
          axis.line.y = element_line(color = "black", size = 1, linetype = 1)
    )
```



```
ggsave("20211122_Fis1_R1.png",
       width = 16, height = 10, units = "cm")

ggsave("20211122_Fis1_R1.pdf",
       width = 16, height = 10, units = "cm")

#R2
R2 %>%
  ggplot(., aes(x = residue, y = R2, color = as.factor(field), shape=as.factor(field))) +
  geom_pointrange(aes(ymin=R2-R2err, ymax=R2+R2err), position=position_dodge(0.9),
                  size=0.3) +
  scale_color_manual(values=c("gray15", "orchid4")) +
  labs(x = "Residue Number", y = "R2") +
```
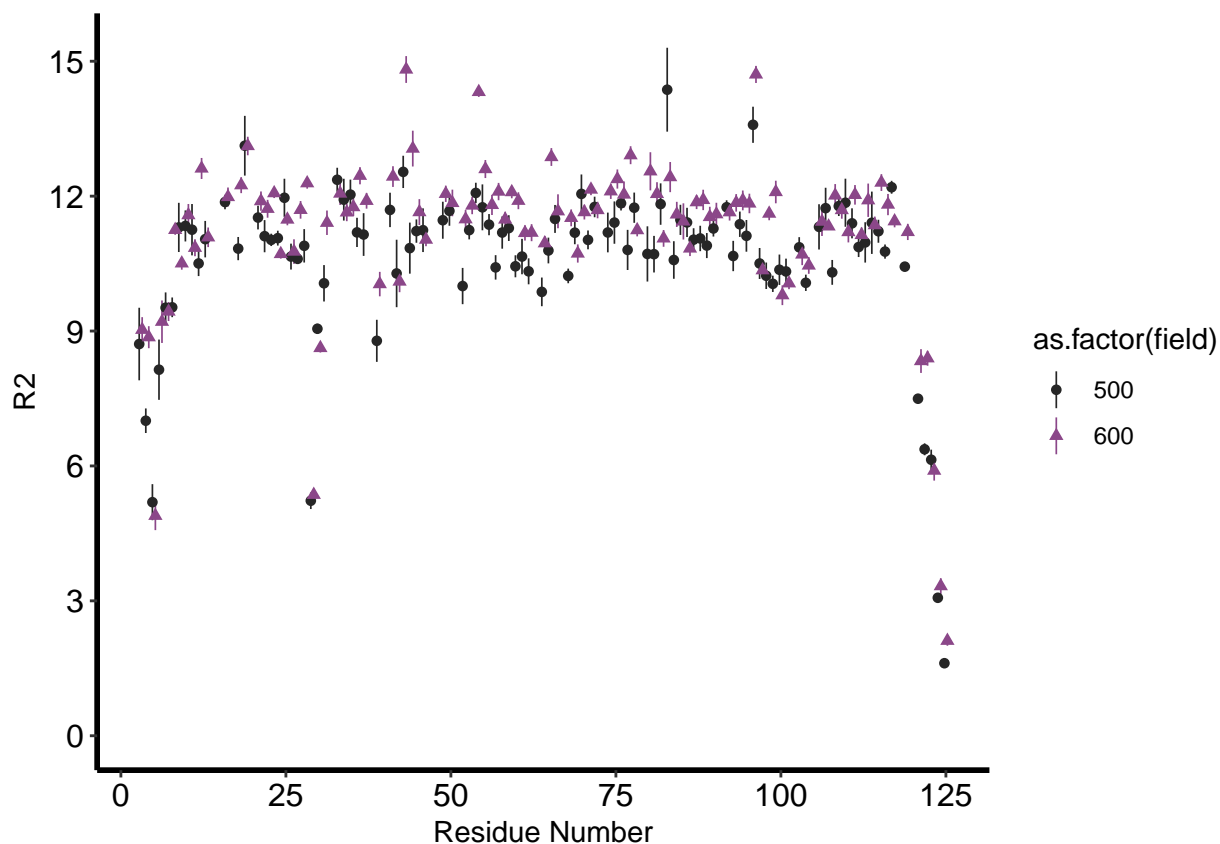
```
theme_bw() +
scale_y_continuous(limits = c(0, 15.3), breaks = c(0, 3, 6, 9, 12, 15)) +
theme(axis.text = element_text(color = "black", size = 12),
      panel.grid.major = element_blank(),
      panel.grid.minor = element_blank(),
      panel.border = element_blank(),
      panel.background = element_blank(),
      axis.line.x = element_line(color = "black", size = 1, linetype = 1),
      axis.line.y = element_line(color = "black", size = 1, linetype = 1)
)
```



```
ggsave("20211122_Fis1_R2.png",
       width = 16, height = 10, units = "cm")

ggsave("20211122_Fis1_R2.pdf",
       width = 16, height = 10, units = "cm")

#NOE
NOE %>%
  ggplot(., aes(x = residue, y = NOE, color = as.factor(field), shape=as.factor(field))) +
  geom_pointrange(aes(ymin=NOE-NOEerr, ymax=NOE+NOEerr), position=position_dodge(0.9),
                  size=0.3) +
  scale_color_manual(values=c("gray15", "orchid4")) +
  labs(x = "Residue Number", y = "NOE") +
  theme_bw() +
```
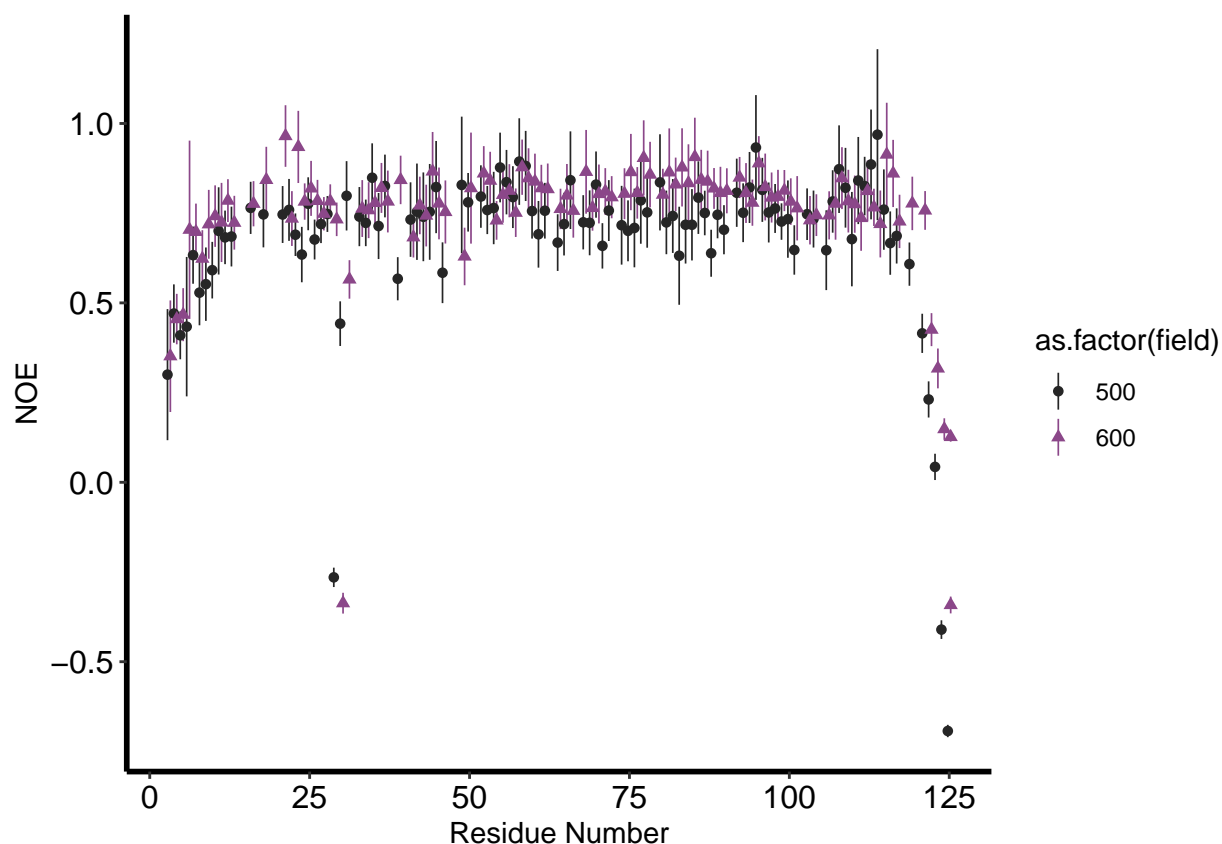
```
theme(axis.text = element_text(color = "black", size = 12),
      panel.grid.major = element_blank(),
      panel.grid.minor = element_blank(),
      panel.border = element_blank(),
      panel.background = element_blank(),
      axis.line.x = element_line(color = "black", size = 1, linetype = 1),
      axis.line.y = element_line(color = "black", size = 1, linetype = 1)
)
```



```
ggsave("20211122_Fis1_NOE.png",
       width = 16, height = 10, units = "cm")

ggsave("20211122_Fis1_NOE.pdf",
       width = 16, height = 10, units = "cm")


#Plot order parameter figure
order_param %>%
  filter(., residue!= 5) %>%
  ggplot(., aes(x = residue, y = S2, color = secondary)) +
#  geom_point(stat = "identity",  color = "gray40", size = 1.0) +
  geom_pointrange(aes(ymin=S2-S2err, ymax=S2+S2err), size = 0.3) +
  scale_y_continuous(limits = c(0, 1.1), breaks = c(0, 0.2, 0.4, 0.6, 0.8, 1.0)) +
  scale_color_manual(breaks = c("arm", "helix", "loop"),
                     labels = c("N-arm", "Helix", "Loop"),
```
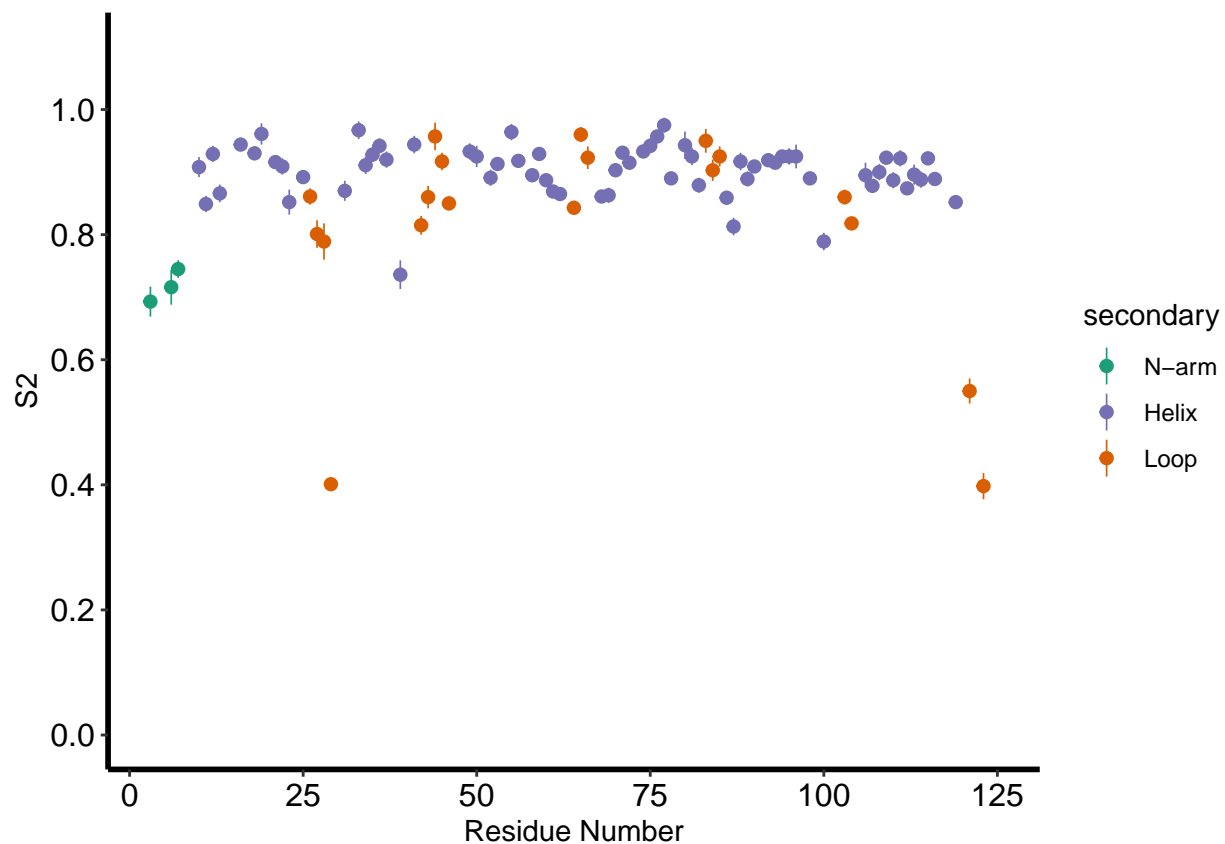
```
                      values = c("#1b9e77", "#7570b3", "#d95f02")) +
  labs(x = "Residue Number", y = "S2") +
  theme_bw() +
  theme(axis.text = element_text(color = "black", size = 12),
        panel.grid.major = element_blank(),
        panel.grid.minor = element_blank(),
        panel.border = element_blank(),
        panel.background = element_blank(),
        axis.line.x = element_line(color = "black", size = 1, linetype = 1),
        axis.line.y = element_line(color = "black", size = 1, linetype = 1)
  )
```

Warning: Removed 14 rows containing missing values (geom_pointrange).


```
ggsave("20211122_Fis1_order_parameters_color.png",
       width = 16, height = 10, units = "cm")
```

Warning: Removed 14 rows containing missing values (geom_pointrange).

```
ggsave("20211122_Fis1_order_parameters_color.pdf",
       width = 16, height = 10, units = "cm")
```

Warning: Removed 14 rows containing missing values (geom_pointrange).