

20211022_Fis1_Fis1dN_CSP_plot.R

kelse

2022-05-31

```
# Reanalyzing Ryan Bonate's CSP data
# and plotting the CSP plot of Fis1dN-Fis1
# so that it matches standard style of lab
# and gradient color scheme of Pymol figure
# to be incorporated into the JBC manuscript

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()

library(broom)
library(minpack.lm)
library(readxl)

raw <- read_csv("20211022_Fis1_Fis1dN_peaklists_edit.csv")

##
## -- Column specification -----
## cols(
##   residue = col_double(),
##   aa = col_character(),
##   H_Fis1 = col_double(),
##   N_Fis1 = col_double(),
##   H_dN = col_double(),
##   N_dN = col_double()
## )
```

```
# Calculate total chemical shift perturbations and plot against residue
```

```
total_shift <- raw %>%
  mutate(., CSP = sqrt(((5*(H_Fis1 - H_dN))^2) + (N_Fis1 - N_dN)^2))
```

```
# Determine mean and SD of chemical shift perturbations
```

```
mean_sd <- total_shift %>%
  filter(., CSP >= 0) %>%
  summarise(., mean = mean(CSP),
            sd = sd(CSP)) %>%
  mutate(twoSD = 2*sd, sigma = mean + sd, twosigma = sigma*2)
```

```
mean_sd
```

```
## # A tibble: 1 x 5
##   mean    sd twoSD sigma twosigma
##   <dbl> <dbl> <dbl> <dbl>   <dbl>
## 1 0.311 0.404 0.807 0.715     1.43
```

```
total_shift <- total_shift %>%
  mutate(., STDEV = 0.402, TwoSTDEV = 0.805, sigma = 0.714693,
         twosigma = 1.429386, mean = 0.3110453)
```

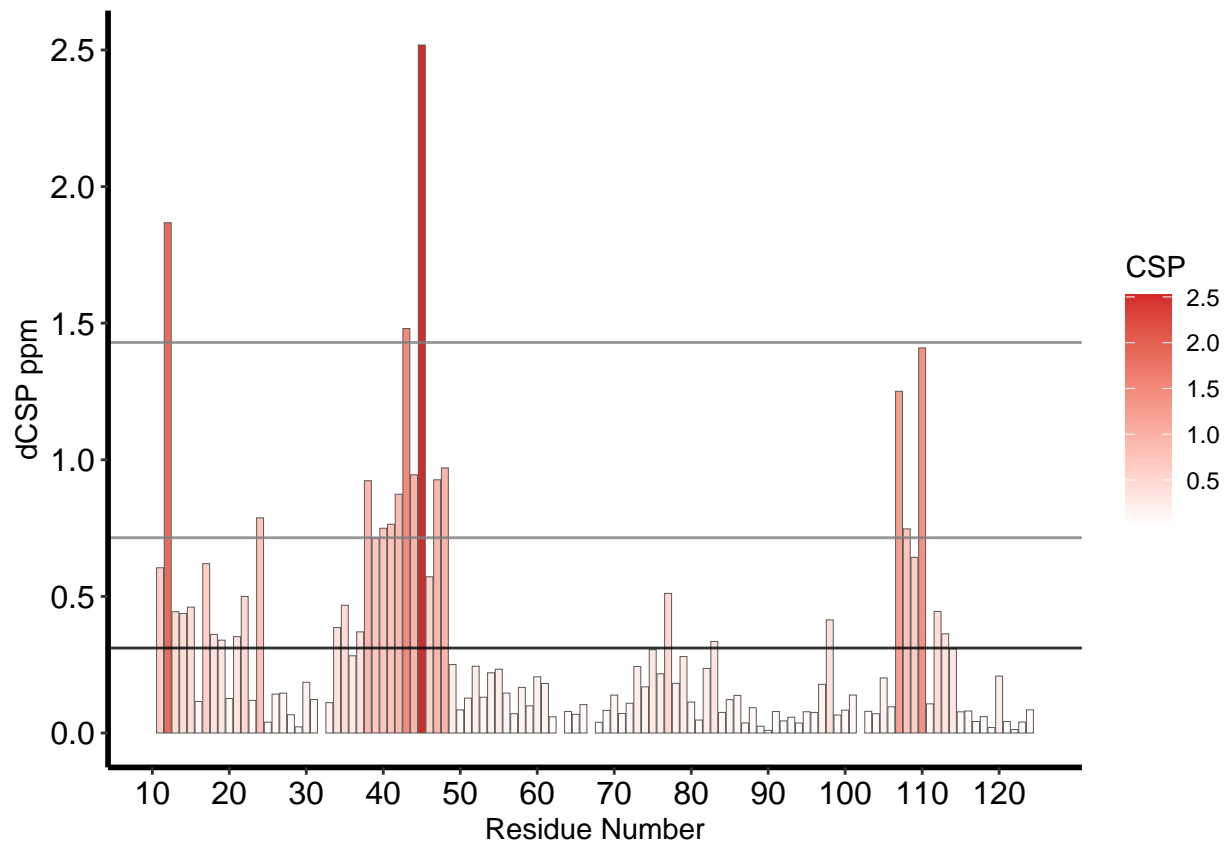
```
write_csv(total_shift, "20220310_dN_hFis1_CSPs_from_nativeN.csv")
```

```
# CSP by Fis1 Residue # for dN and WT Fis1
# in red gradient to match surface representation in Pymol
# Using W40 indole as reporter for residue W40.
```

```
total_shift %>%
  filter(., aa!= "TRP") %>%
  ggplot(., aes(x = residue, y = CSP, fill = CSP)) +
  geom_bar(stat = "identity", color = "gray35", size = 0.05) +
  scale_fill_gradient(low = "white", high = "#D32A2A") +
  geom_hline(yintercept = c(0.714693 , 1.429386, 0.3110453), color = c("grey50", "grey50", "black"),
            alpha = 0.8) +
  scale_x_continuous(limits = c(10, 125),
                    breaks = c(0, 10, 20, 30, 40, 50, 60,
                               70, 80, 90, 100, 110, 120)) +
  labs(x = "Residue Number", y = "dCSP ppm") +
  theme_bw() + # green line = 1 SD and purple line = 2 SD from zero
  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 8 rows containing missing values (position_stack).
```

```
## Warning: Removed 2 rows containing missing values (geom_bar).
```



```
ggsave("20220310_Fis1_Fis1dN_CSP_plot_sigma.png",
       width = 16, height = 10, units = "cm")
```

```
## Warning: Removed 8 rows containing missing values (position_stack).
```

```
## Warning: Removed 2 rows containing missing values (geom_bar).
```

```
ggsave("20220310_Fis1_Fis1dN_CSP_plot_sigma.pdf",
       width = 16, height = 10, units = "cm")
```

```
## Warning: Removed 8 rows containing missing values (position_stack).
```

```
## Warning: Removed 2 rows containing missing values (geom_bar).
```