

# Stokes Radius Analysis by Gel Filtration

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```
require(ggplot2)
```

```
## Loading required package: ggplot2
```

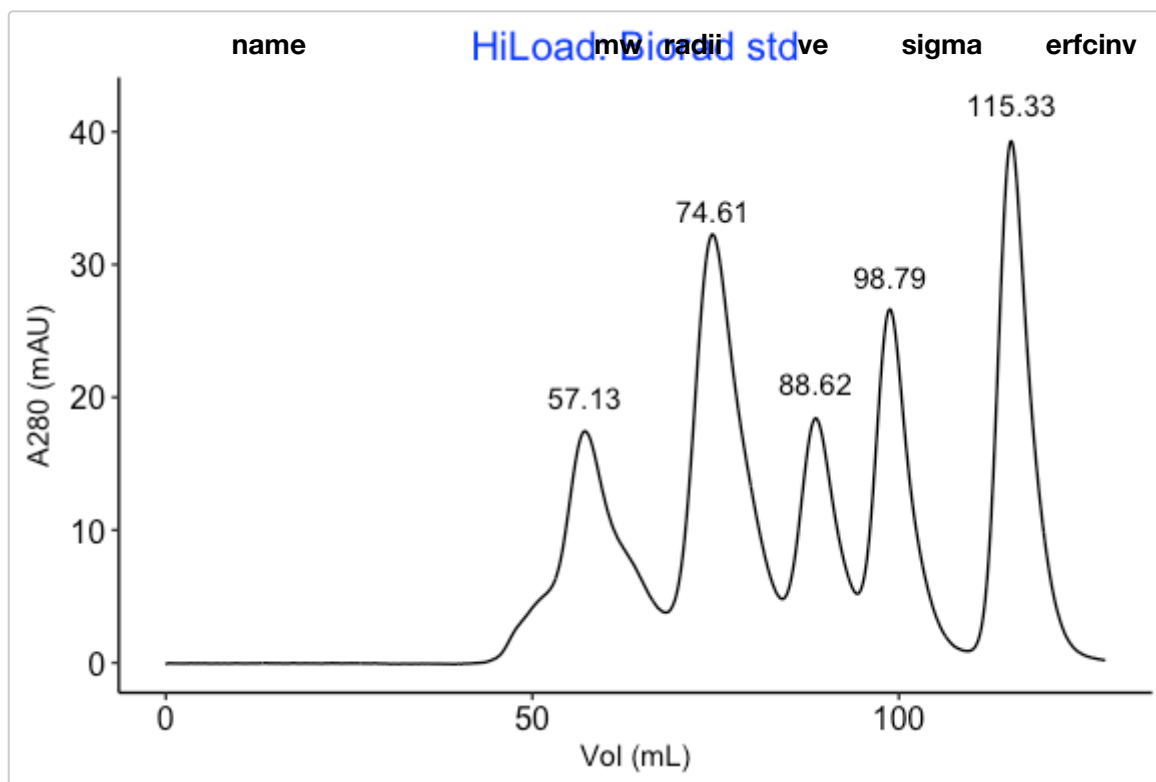
```
##  
## Attaching package: 'ggplot2'
```

```
## The following object is masked from 'package:radii':  
##  
##      ggplot
```

```
require(radii)
```

## Load and plot the gel filtration data

```
# Load the data: the gel filtration elution profile  
file <- system.file("extdata", "160826bioradstdph74EDTA_HiLoad.asc", package="radii")  
HiLoad_std <- read.csv(file, header = TRUE, skip=2, sep = "\t");  
HiLoad_std <- na.omit(HiLoad_std[, 1:2])  
  
# plot the data: gel filtration profile  
# with(HiLoad_std, plot(mAU ~ mL, type = "l", main = "HiLoad: Biorad STD"))  
#  
g <- radii::ggplot()  
g <- g + ggplot2::geom_line(aes(mL, mAU), data=HiLoad_std)  
g <- g + ggtitle("HiLoad: Biorad std") + xlab("Vol (mL)") + ylab("A280 (mAU)")  
label=as.character(radii::protein_std_HiLoad$ve)  
pos <- data.frame(x= as.numeric(label), y = c(42, 29, 21, 34, 20))  
g <- g + annotate("text", label=label, x=pos$x, y=pos$y)  
print(g)
```



## Transform the standard and then fit to the Stokes radius model

```
# superdex 200 HiLoad 16/60
vt = mean(c(122.31,122.93))
vo = mean(c(47.26,46.59))

protein_std_HiLoad$sigma <- radii::partition_coef(protein_std_HiLoad$ve, vo=vo, vt=vt)
protein_std_HiLoad$erfcinv <- radii::erfcinv(protein_std_HiLoad$sigma)
#
knitr::kable(protein_std_HiLoad, format = "markdown")
```

name	mw	radii	ve	siga	erfcinv
vitamin B12	1350	NA	115.33	0.9036924	0.0855587
horse myoglobin	17000	1.89	98.79	0.6851840	0.2866607
chicken ovalbumin	44000	2.75	88.62	0.5508290	0.4218022
bovine gamma-globulin	158000	5.22	74.61	0.3657441	0.6395597
bovine thyroglobulin	670000	8.50	57.13	0.1348174	1.0573877

```
protein_std_HiLoad <- na.omit(protein_std_HiLoad)

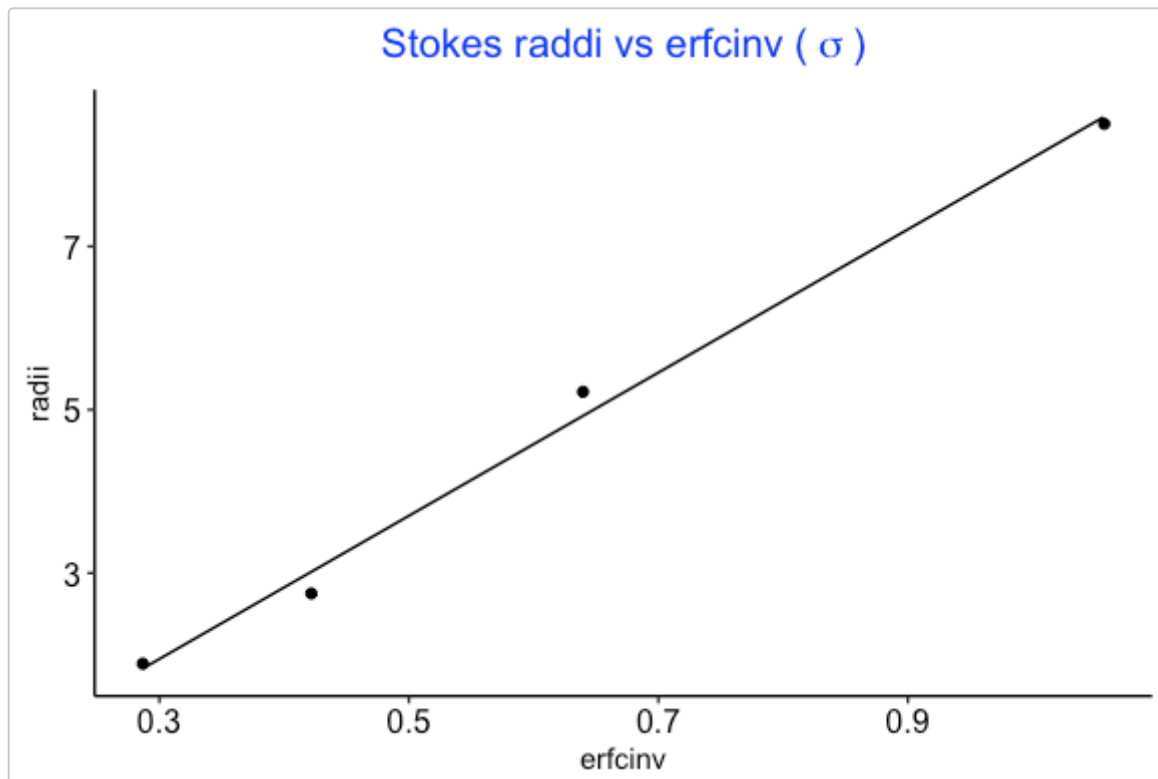
fit <- lm (radii~erfcinv+1, data = protein_std_HiLoad)
summary(fit)
```

```
##
## Call:
## lm(formula = radii ~ erfcinv + 1, data = protein_std_HiLoad)
##
## Residuals:
##      2      3      4      5
## 0.05920 -0.26571  0.29500 -0.08848
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept)  -0.6826     0.3329  -2.051  0.17676
## erfcinv       8.7679     0.4980  17.608  0.00321 **
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.2907 on 2 degrees of freedom
## Multiple R-squared:  0.9936, Adjusted R-squared:  0.9904
## F-statistic: 310 on 1 and 2 DF, p-value: 0.00321
```

```
xdat <- seq(min(protein_std_HiLoad$erfcinv), max(protein_std_HiLoad$erfcinv), by = 0.01 )
pred <- predict(fit, newdata = data.frame(erfcinv=xdat))
```

```
# Plotting
```

```
g = radii::ggplot() + geom_point(data = protein_std_HiLoad, aes(erfcinv, radii))
g <- g + ggtitle(expression("Stokes raddi vs erfcinv (" ~ sigma ~ ")"))
g + geom_line(aes(xdat, pred))
```



## Purified VWF Propeptide

```
# superdex 200 HiLoad 16/60
vt = mean(c(122.31,122.93))
vo = mean(c(47.26,46.59))
# sample data
ve_D1D2_pure = 74.36
sigma_D1D2_pure=radii::partition_coef(ve_D1D2_pure, vo=vo, vt=vt)
erfcinv_D1D2_pure= radii::erfcinv(sigma_D1D2_pure)
r_D1D2_pure = predict(fit, newdata = data.frame(erfcinv=erfcinv_D1D2_pure))
print(paste("Stokes radius of the purified D1D2", r_D1D2_pure, "nm"))
```

```
## [1] "Stokes radius of the purified D1D2 4.9637398754402 nm"
```

## Plasma D1D2

```
# D1D2
ve_D1D2_plasma = 81
sigma_D1D2_plasma=radii::partition_coef(ve_D1D2_plasma, vo=vo, vt=vt)
erfcinv_D1D2_plasma= radii::erfcinv(sigma_D1D2_plasma)
r_D1D2_plasma = predict(fit, newdata = data.frame(erfcinv=erfcinv_D1D2_plasma))
print(paste("Stokes radius of the purified D1D2", r_D1D2_plasma, "nm"))
```

```
## [1] "Stokes radius of the purified D1D2 3.99917971664297 nm"
```

```
summary(fit)
```

```
##
## Call:
## lm(formula = radii ~ erfcinv + 1, data = protein_std_HiLoad)
##
## Residuals:
##      2      3      4      5
## 0.05920 -0.26571 0.29500 -0.08848
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept)  -0.6826     0.3329  -2.051  0.17676
## erfcinv       8.7679     0.4980  17.608  0.00321 **
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.2907 on 2 degrees of freedom
```

```
## Multiple R-squared:  0.9936, Adjusted R-squared:  0.9904  
## F-statistic:    310 on 1 and 2 DF,  p-value: 0.00321
```