

In []:

In []: *## Pharmacokinetic Analysis Using R*

In []:

```
In [5]: install.packages("dplyr")
install.packages("ggplot2")
install.packages("PK")
install.packages("pracma")
```

```
library(dplyr)
library(ggplot2)
library(PK)
library(pracma)
```

Warning message:

"package 'dplyr' is in use and will not be installed"

Warning message:

"package 'ggplot2' is in use and will not be installed"

Warning message:

"package 'PK' is in use and will not be installed"

Installing package into 'C:/Users/dgous/AppData/Local/R/win-library/4.4'
(as 'lib' is unspecified)

package 'pracma' successfully unpacked and MD5 sums checked

The downloaded binary packages are in

C:\Users\dgous\AppData\Local\Temp\Rtmp0IWjhx\downloaded_packages

```
In [6]: # Sample dataset of time (hours) and plasma concentration (mg/L)
time <- c(0, 0.5, 1, 2, 3, 4, 6, 8, 10, 12, 24)
concentration <- c(0, 15, 20, 18, 15, 12, 8, 5, 3, 1.5, 0.5)

pk_data <- data.frame(time, concentration)
```

```
In [7]: # Calculate AUC using the trapezoidal rule
auc <- trapz(pk_data$time, pk_data$concentration)

# Calculate half-life (t1/2) using Linear regression on the Log-transformed data
log_concentration <- log(pk_data$concentration[pk_data$concentration > 0])
log_time <- pk_data$time[pk_data$concentration > 0]
lm_fit <- lm(log_concentration ~ log_time)
half_life <- log(2) / abs(lm_fit$coefficients[2])

# Calculate clearance (CL) assuming a dose of 100 mg
dose <- 100
clearance <- dose / auc

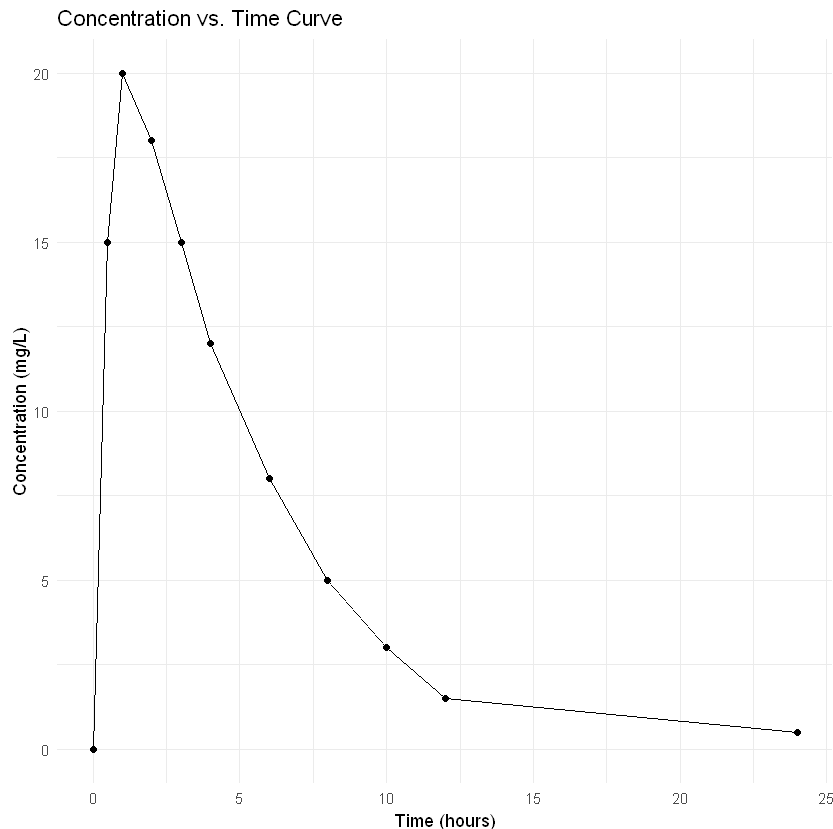
auc
half_life
clearance
```

119

log_time: 4.12487988501384

0.840336134453782

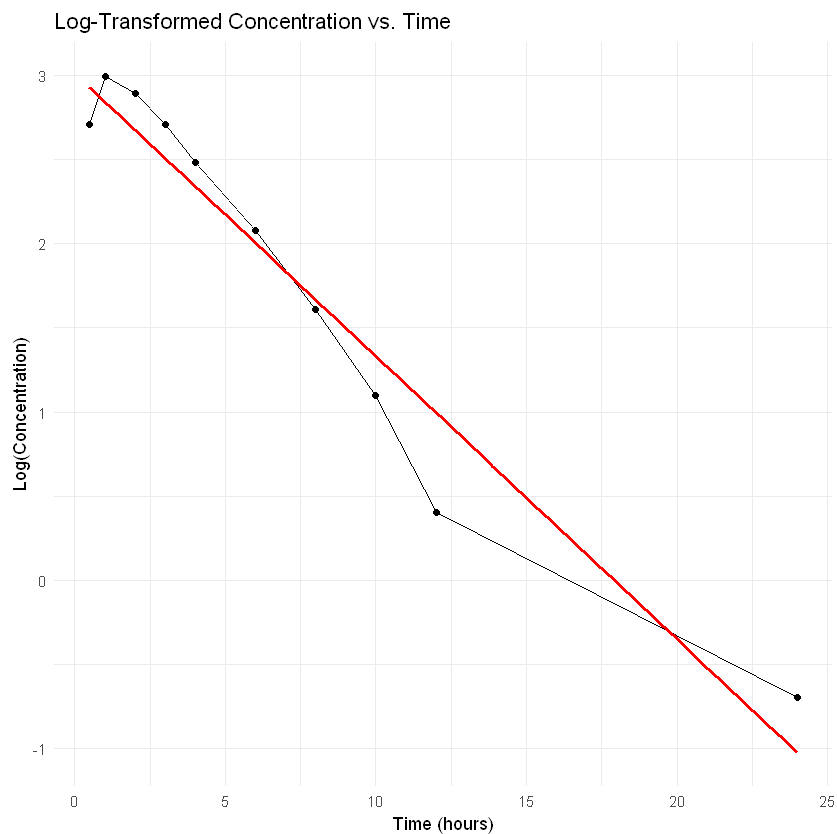
```
In [8]: ggplot(pk_data, aes(x = time, y = concentration)) +
  geom_line() +
  geom_point() +
  labs(title = "Concentration vs. Time Curve",
       x = "Time (hours)",
       y = "Concentration (mg/L)") +
  theme_minimal()
```



```
In [9]: log_pk_data <- data.frame(log_time, log_concentration)

ggplot(log_pk_data, aes(x = log_time, y = log_concentration)) +
  geom_line() +
  geom_point() +
  geom_smooth(method = "lm", se = FALSE, col = "red") +
  labs(title = "Log-Transformed Concentration vs. Time",
       x = "Time (hours)",
       y = "Log(Concentration)") +
  theme_minimal()
```

`geom_smooth()` using formula = 'y ~ x'



```

In [10]: # Load necessary packages
library(dplyr)
library(ggplot2)
library(pracma)

# Sample dataset
time <- c(0, 0.5, 1, 2, 3, 4, 6, 8, 10, 12, 24)
concentration <- c(0, 15, 20, 18, 15, 12, 8, 5, 3, 1.5, 0.5)
pk_data <- data.frame(time, concentration)

# Calculate AUC using the trapezoidal rule
auc <- trapz(pk_data$time, pk_data$concentration)

# Calculate half-life
log_concentration <- log(pk_data$concentration[pk_data$concentration > 0])
log_time <- pk_data$time[pk_data$concentration > 0]
lm_fit <- lm(log_concentration ~ log_time)
half_life <- log(2) / abs(lm_fit$coefficients[2])

# Calculate clearance
dose <- 100
clearance <- dose / auc

# Print calculated parameters
print(paste("AUC:", auc))
print(paste("Half-life (t1/2):", half_life))
print(paste("Clearance (CL):", clearance))

# Plot Concentration vs. Time
ggplot(pk_data, aes(x = time, y = concentration)) +
  geom_line() +
  geom_point() +
  labs(title = "Concentration vs. Time Curve",
       x = "Time (hours)",
       y = "Concentration (mg/L)") +
  theme_minimal()

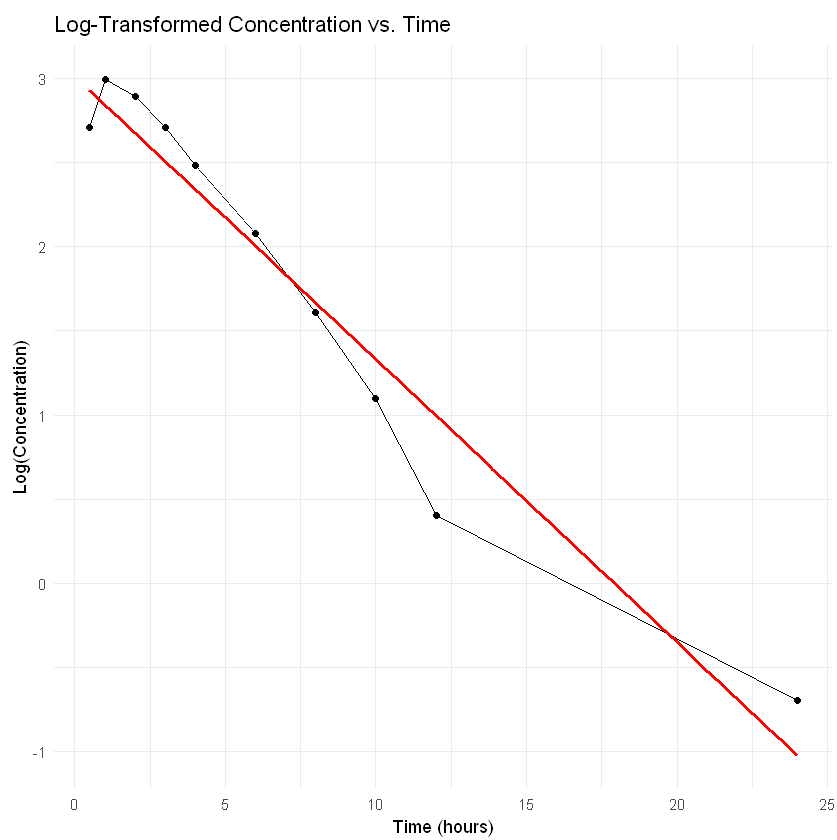
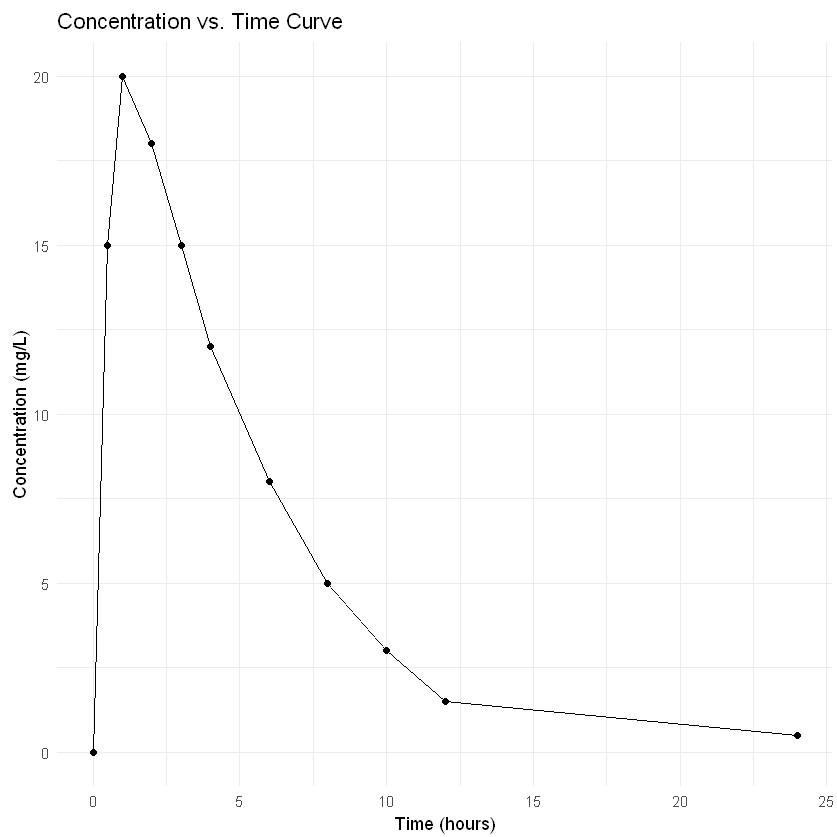
# Plot Log-Transformed Concentration vs. Time
log_pk_data <- data.frame(log_time, log_concentration)

ggplot(log_pk_data, aes(x = log_time, y = log_concentration)) +
  geom_line() +
  geom_point() +
  geom_smooth(method = "lm", se = FALSE, col = "red") +
  labs(title = "Log-Transformed Concentration vs. Time",
       x = "Time (hours)",
       y = "Log(Concentration)") +
  theme_minimal()

[1] "AUC: 119"
[1] "Half-life (t1/2): 4.12487988501384"
[1] "Clearance (CL): 0.840336134453782"

```

```
`geom_smooth()` using formula = 'y ~ x'
```



In []:

