

Plot Interval Graph (Prediction Vs Observed inhibitory activities)

*Saw Simeon, Nuttapat Anuwongcharoen, Watshara Shoombuatong, Aijaz Ahmad Malik,
Virapong Prachayasittikul, Jarl E. S. Wikberg and Chanin Nantasenamat*

June 16, 2016

Create a predicted and IC50 plot

```
file <- function(x) {  
  library(randomForest)  
  library(caret)  
  library(ranger)  
  library(cowplot)  
  set.seed(10)  
  para <- dplyr::sample_n(x, size = 2570, replace = TRUE)  
  set.seed(3)  
  in_train_para <- sample(nrow(para),  
                           size = as.integer(nrow(para) * 0.8),  
                           replace = FALSE)  
  
  set.seed(4)  
  Train <- para[in_train_para, ]  
  Test  <- para[-in_train_para, ]  
  
  model <- ranger::ranger(pIC50~., data = Train, write.forest = TRUE, save.memory = TRUE)  
  #actual <- train$Activity  
  prediction <- predict(model, Train)  
  prediction_Internal <- prediction$predictions  
  value <- data.frame(obs = Train$pIC50, pred = prediction_Internal)  
  labeling <- c("obs", "pred")  
  colnames(value) <- labeling  
  value$Label <- c("Internal")  
  prediction_External <- predict(model, Test)  
  prediction_External <- prediction_External$predictions  
  value_external <- data.frame(obs = Test$pIC50, pred = prediction_External)  
  colnames(value_external) <- labeling  
  value_external$Label <- c("External")  
  results <- rbind(value, value_external)  
  return(results)  
}  
  
get_interval <- function(x) {  
  file <- file(x)  
  x <- file[, 1]  
  y <- file[, 2]  
  label <- file[3]  
  fit <- lm(y~x)  
  pred.int <- predict(fit, interval = "prediction")  
}
```

```

pred.lower = pred.int[,2]
pred.upper = pred.int[,3]
df <- cbind(x, y, label, pred.lower, pred.upper)
return(df)
}

plot_graph_interval <- function(x) {
  library(ggplot2)
  ok <- get_interval(x)
  good <- ggplot(ok, aes(x = x)) +
    geom_point(size = 7, colour = "black", pch = 21, alpha= 0.4,
               aes(y = y, fill = factor(Label))) +
    geom_line(aes(y = pred.lower), size = 1.5, colour = "grey", linetype = 2) +
    geom_line(aes(y = pred.upper), size = 1.5, colour = "grey", linetype = 2) +
    xlab(expression(paste('Predicted ', pIC[50]))) + ylab(expression(paste('Experimental ', pIC[50]))) +
    #geom_abline(intercept = ok$pred.lower[[1]], linetype = 2, size = 1.5, colour = "grey") +
    #geom_abline(intercept = ok$pred.upper[[1]], linetype = 2, size = 1.5, colour = "grey") +
    theme(
      panel.border = element_rect(linetype = "solid", colour = "black",
                                   fill = NA, size = 1),

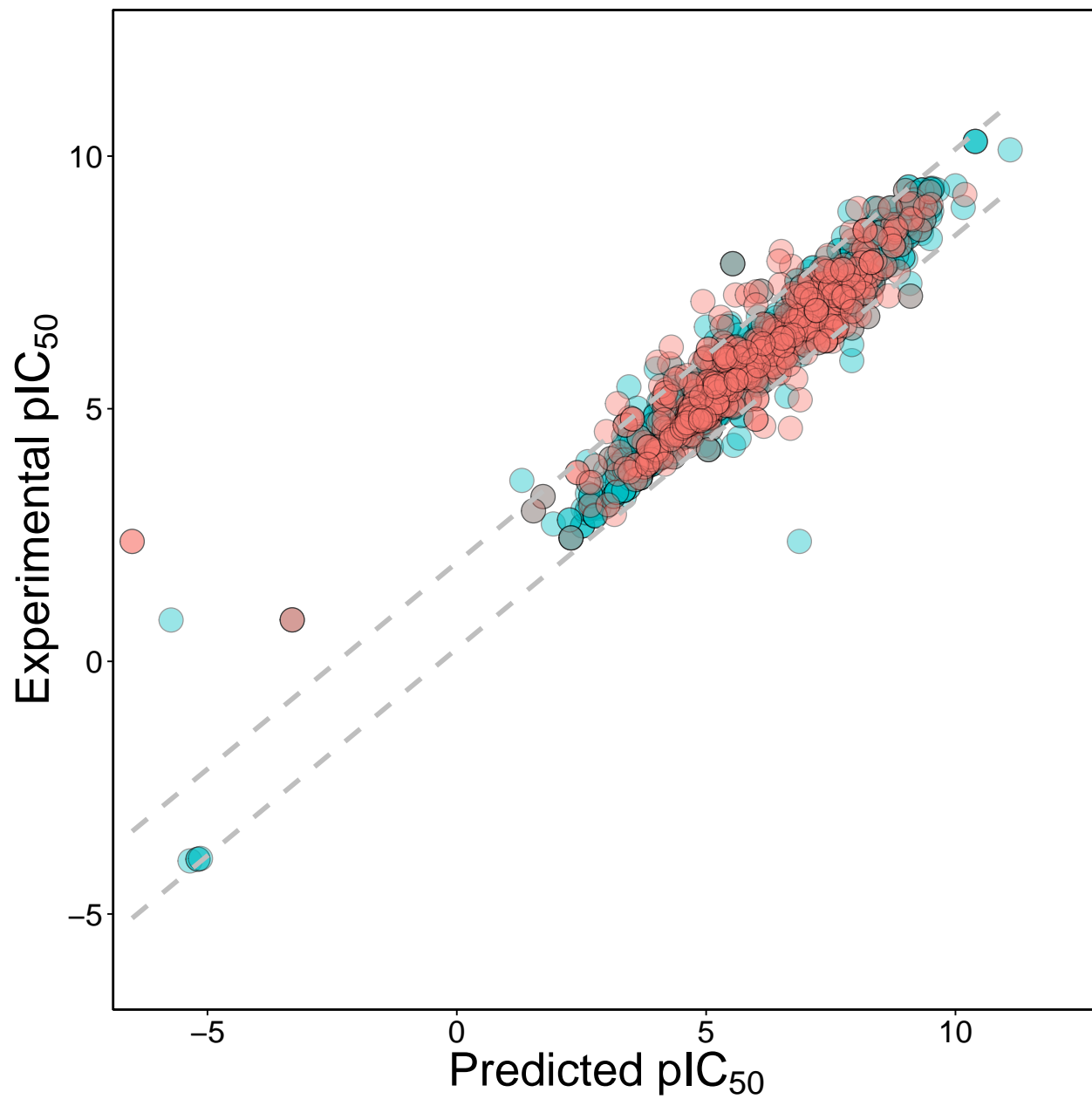
      axis.text.y = element_text(size = 20, colour = "black"),
      axis.text.x = element_text(size = 20, colour = "black"),
      axis.title.x = element_text(size = 30, color = "black", face = "bold"),
      axis.title.y = element_text(size = 30, color = "black", face = "bold"),

      legend.position = ("none")) +
    coord_cartesian(ylim = c(-6, 12), xlim = c(-6, 12))
  return(good)
}

```

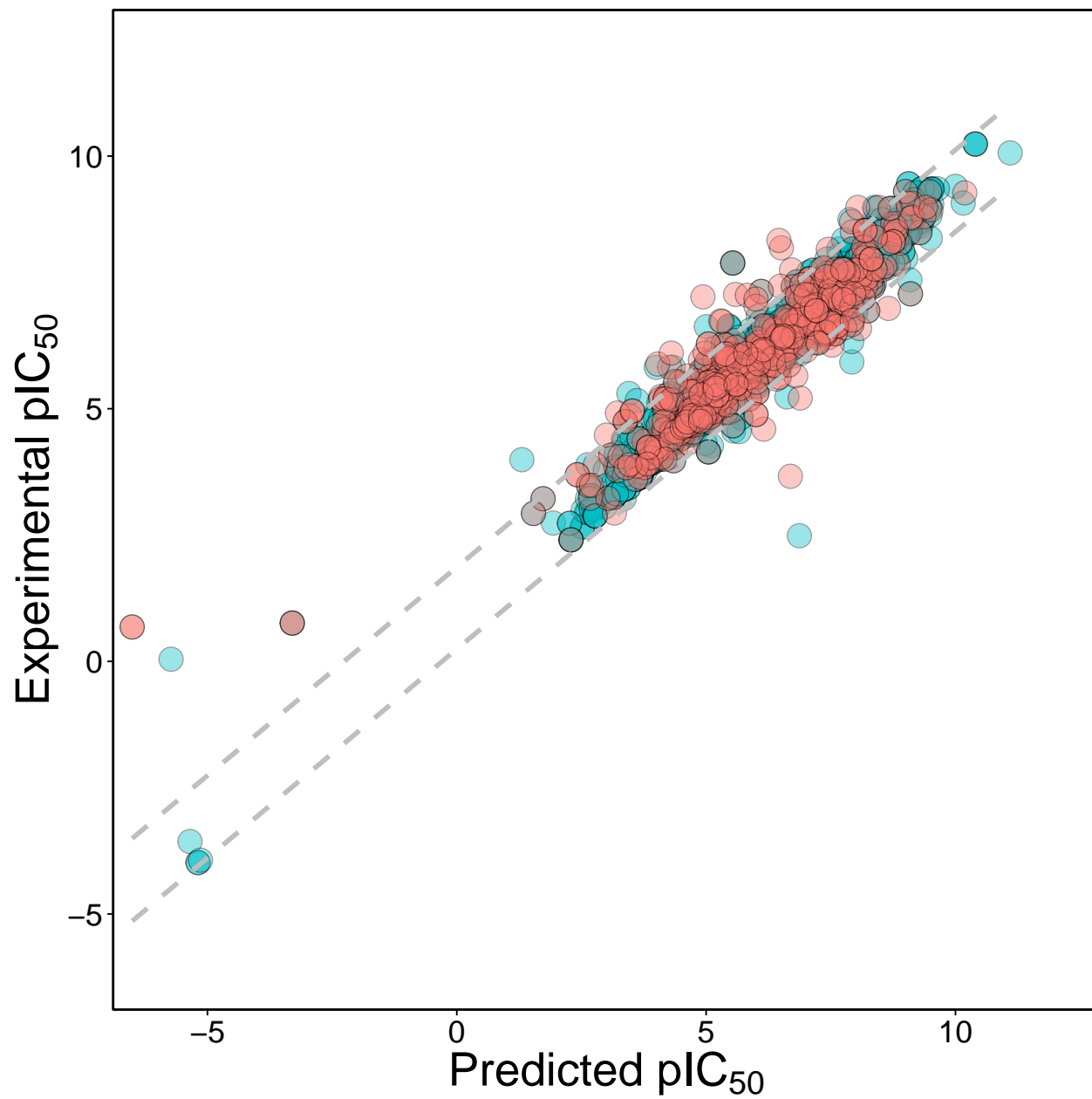
CDK fingerprint

```
input <- readRDS("data.Rds")  
df <- input$FingerPrinter  
plot_graph_interval(df)
```



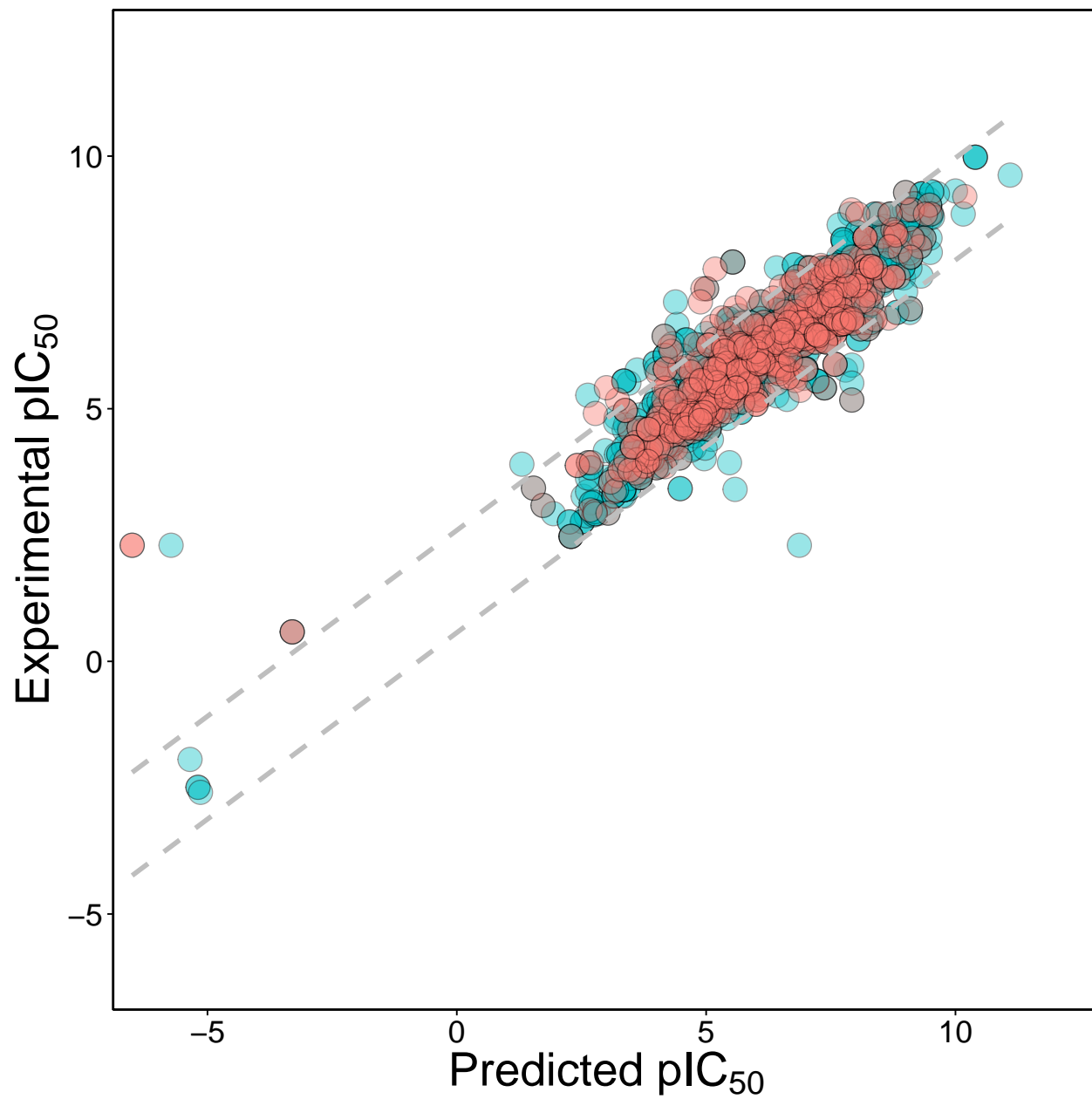
CDK extended fingerprint

```
input <- readRDS("data.Rds")  
df <- input$Extended_finterPrinter  
plot_graph_interval(df)
```



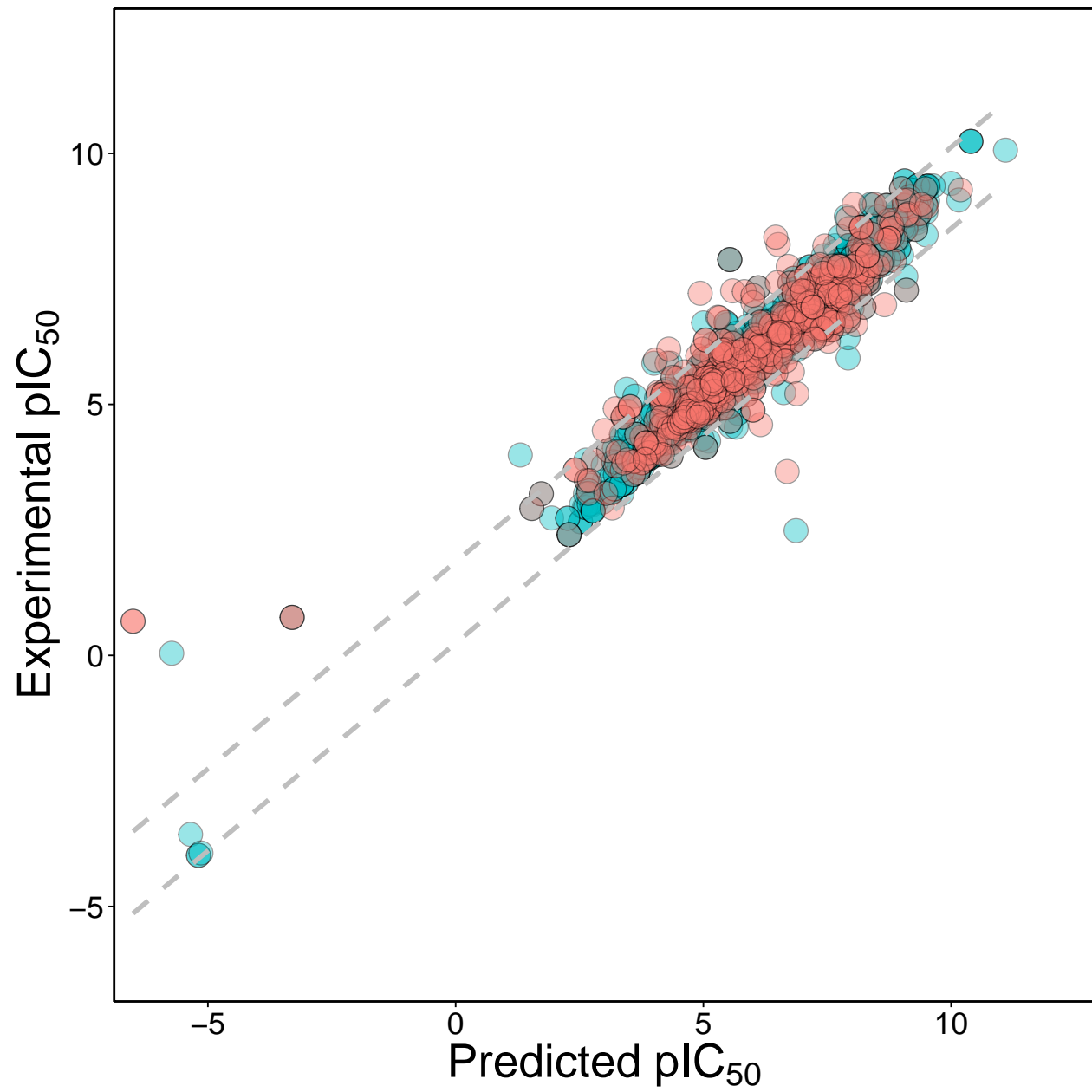
CDK graph only fingerprint

```
input <- readRDS("data.Rds")  
df <- input$GraphOnly_FingerPrinter  
plot_graph_interval(df)
```



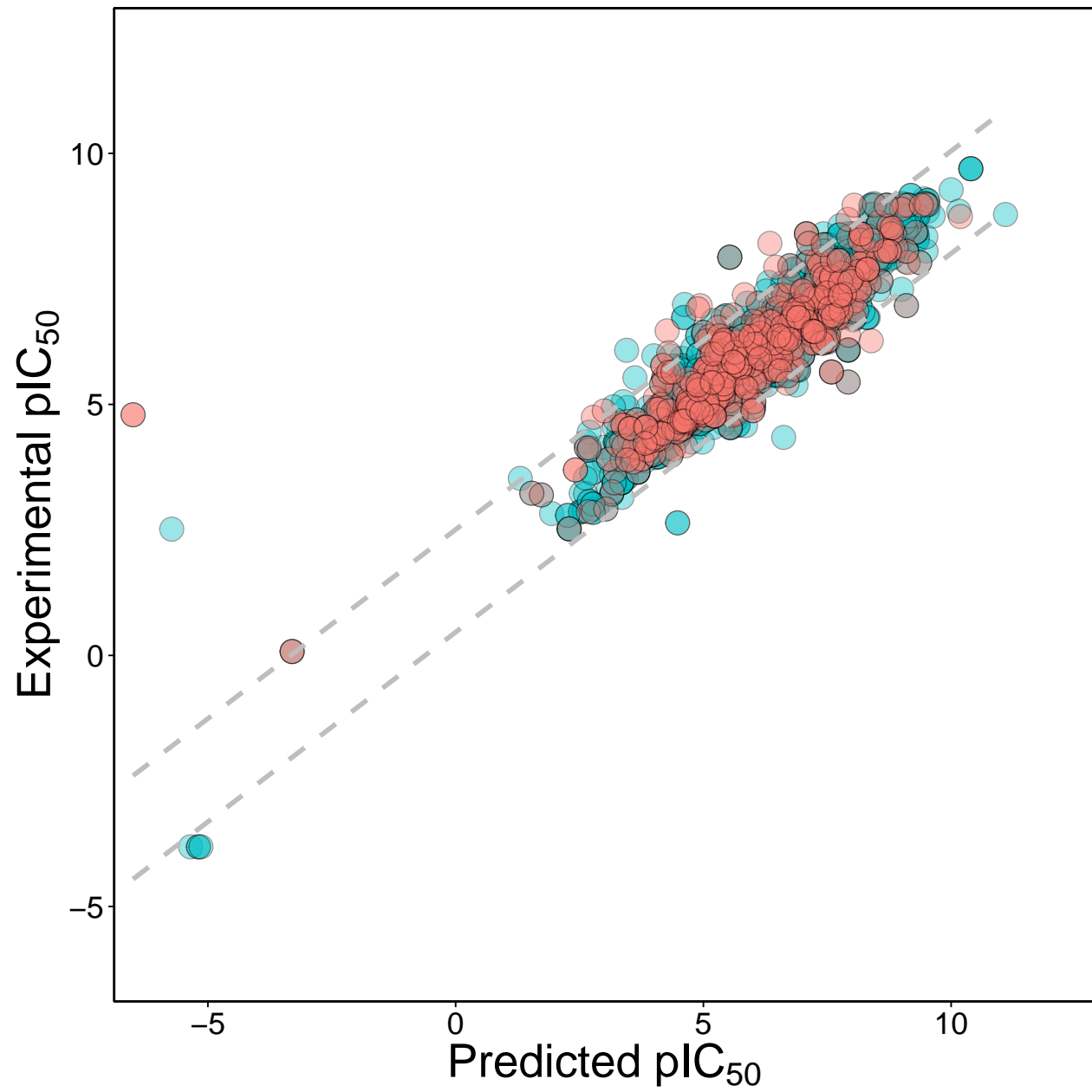
E-state fingerprint

```
input <- readRDS("data.Rds")  
df <- input$Extended_finterPrinter  
plot_graph_interval(df)
```



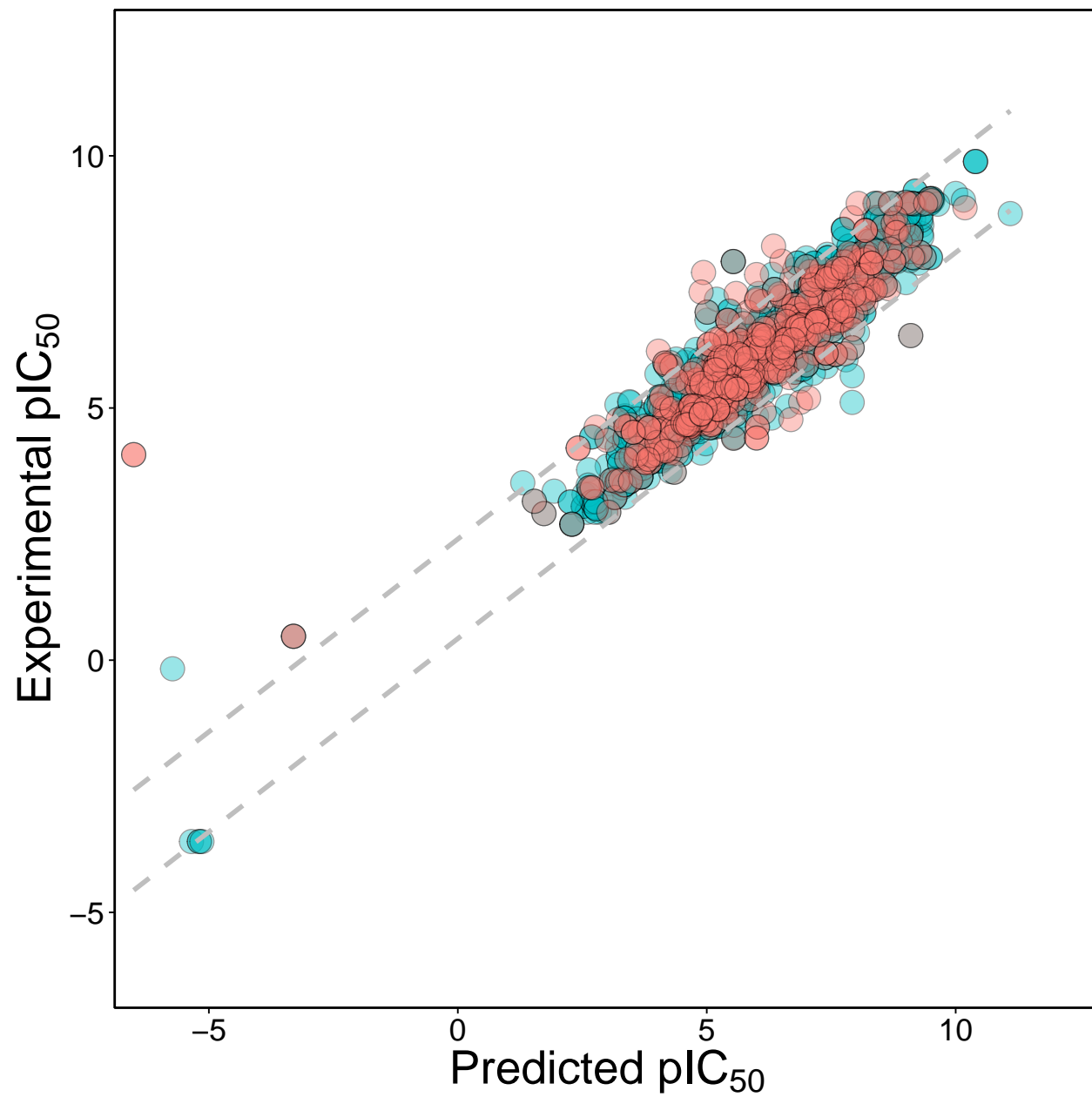
MACCS fingerprint

```
input <- readRDS("data.Rds")  
df <- input$MACCS_FingerPrinter  
plot_graph_interval(df)
```



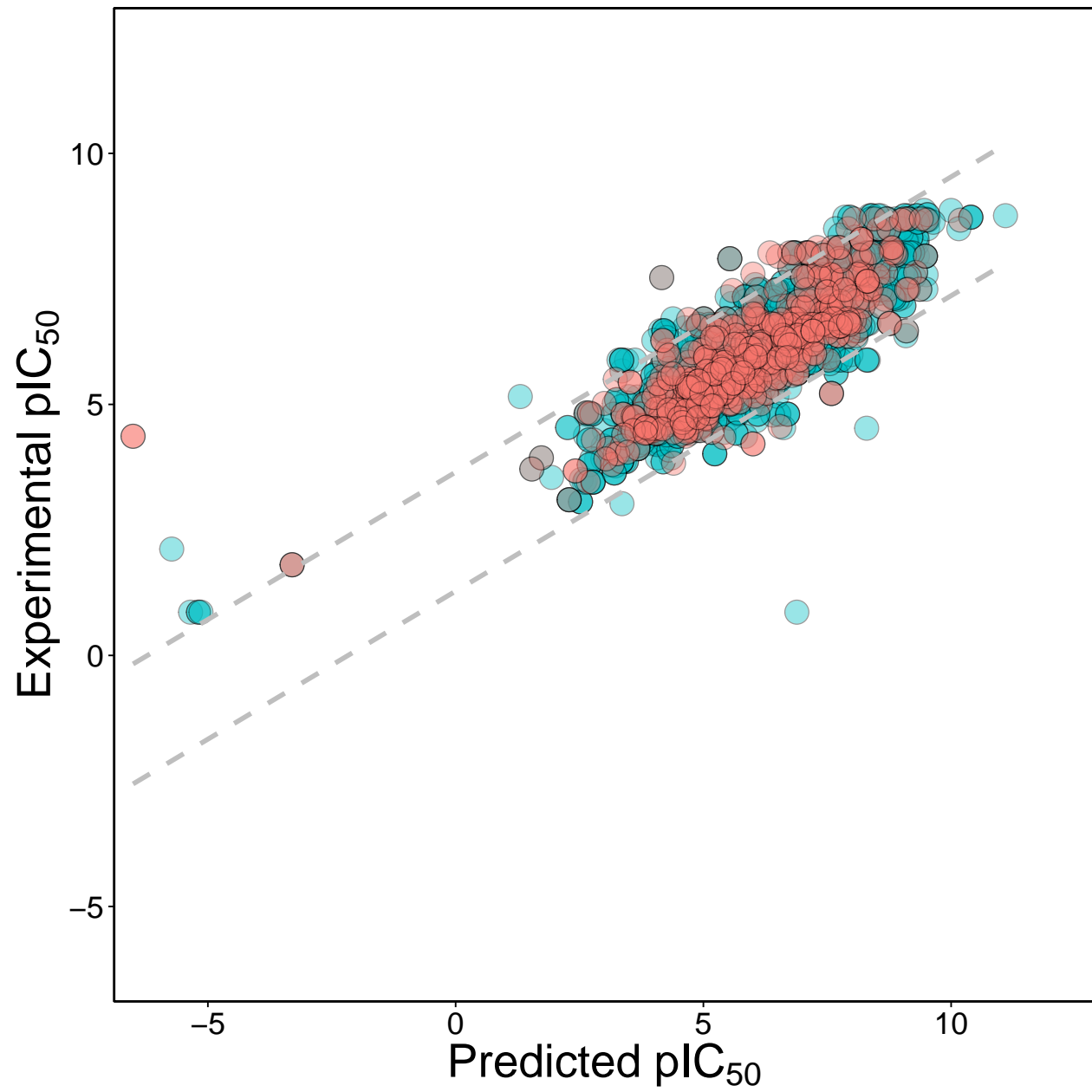
PubChem fingerprint

```
input <- readRDS("data.Rds")  
df <- input$Pubchem_FingerPrinter  
plot_graph_interval(df)
```



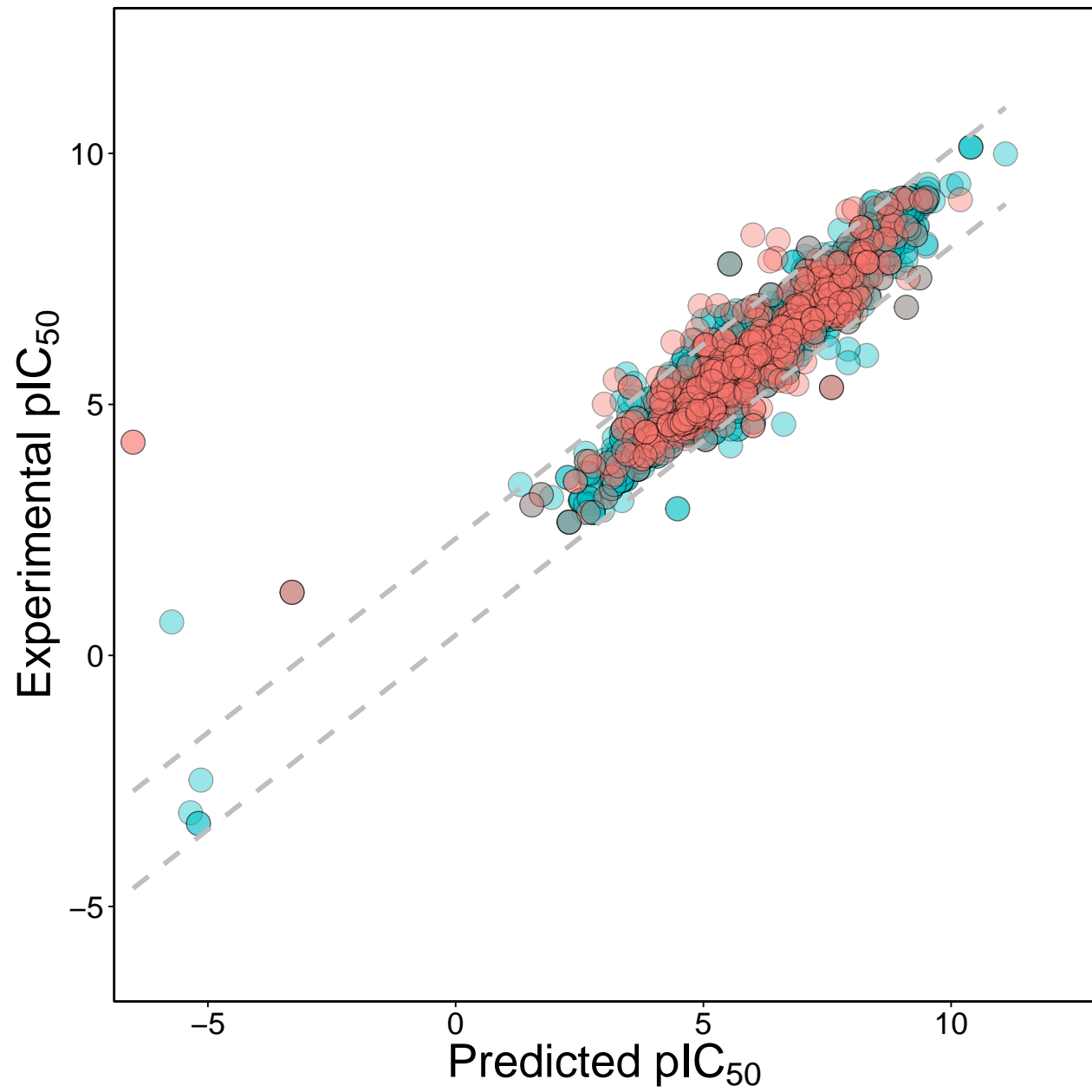
Substructure fingerprint

```
input <- readRDS("data.Rds")  
df <- input$Substructure_fingerPrinter  
plot_graph_interval(df)
```



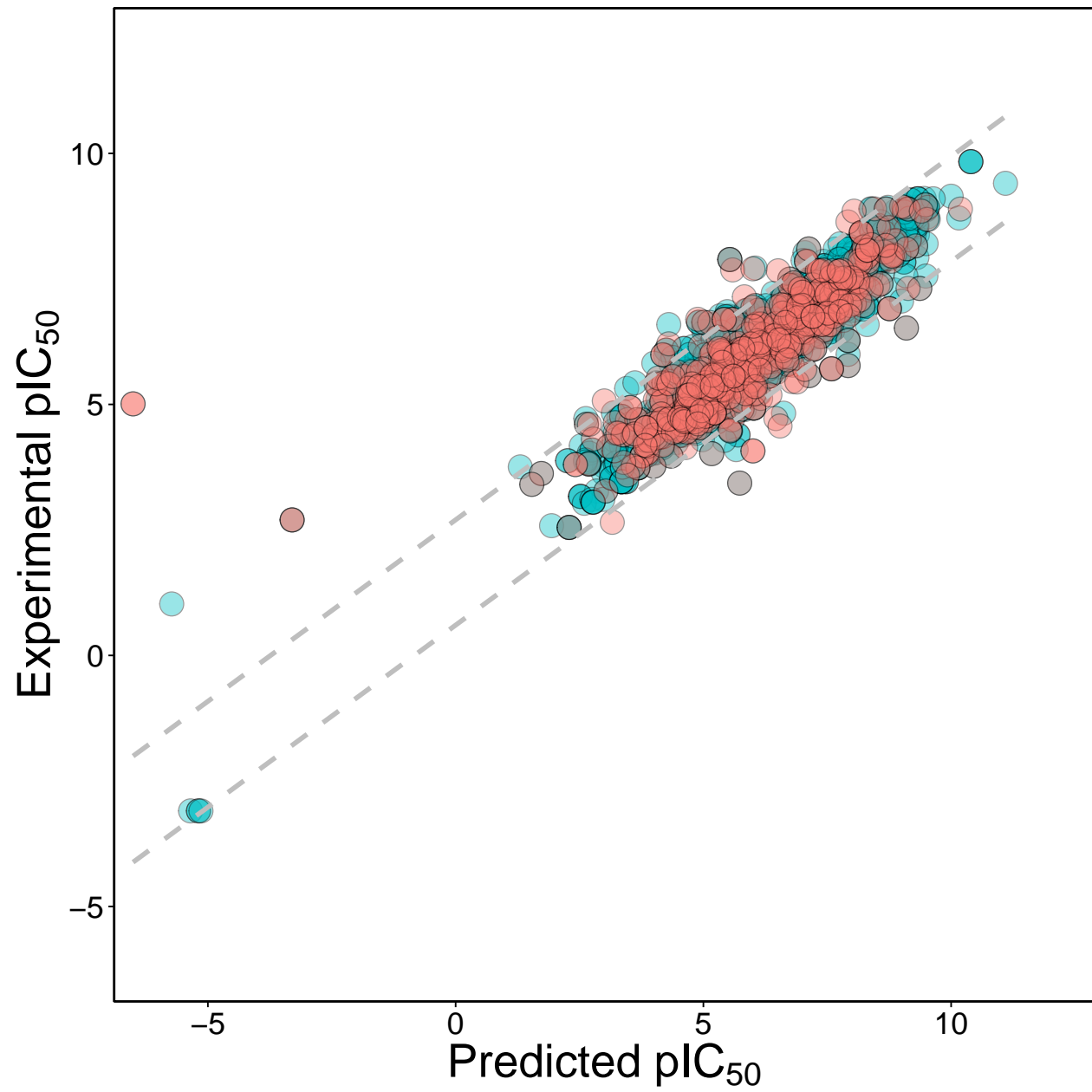
Substructure count

```
input <- readRDS("data.Rds")  
df <- input$Substructure_fingerPrintCount  
plot_graph_interval(df)
```



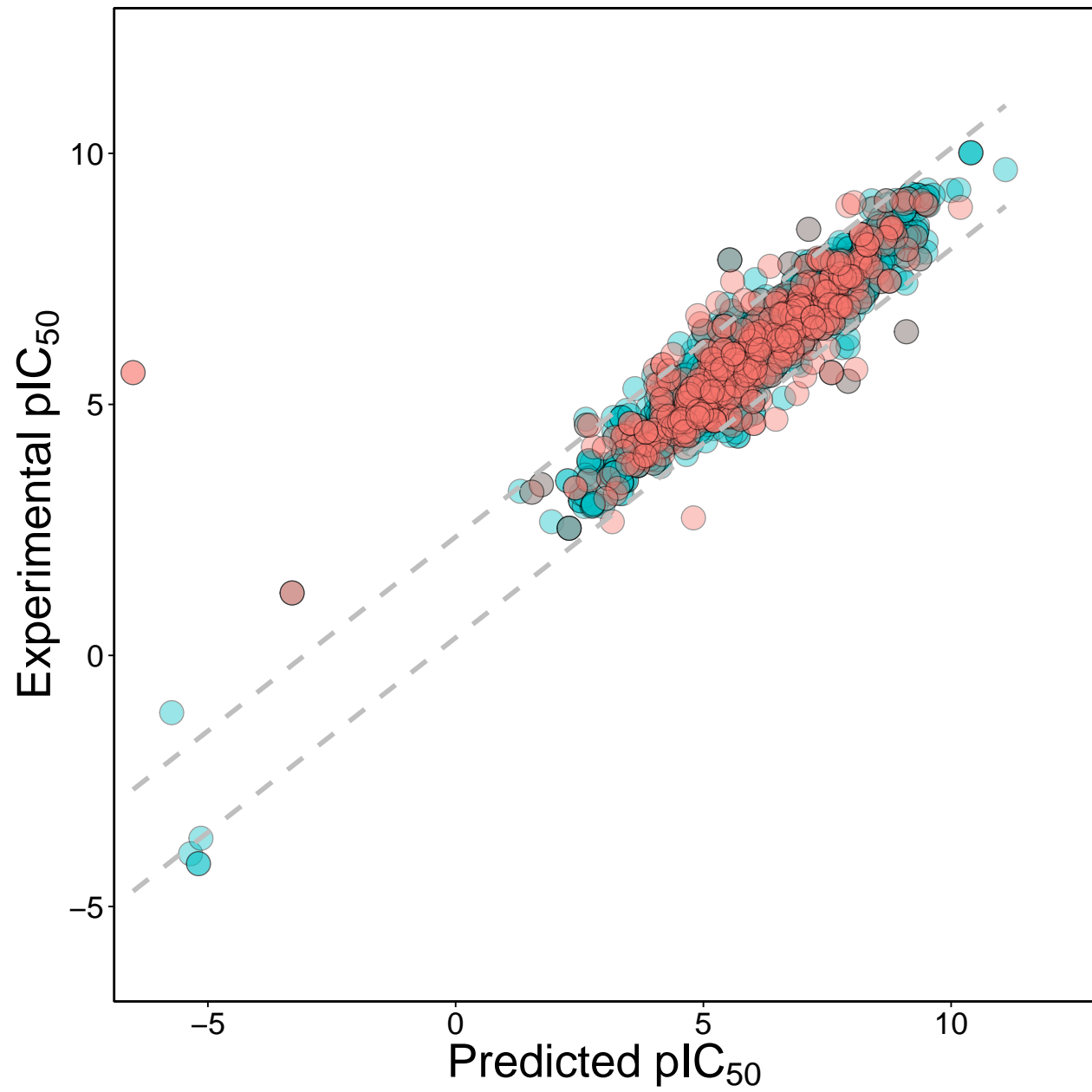
Klekota-Roth fingerprint

```
input <- readRDS("data.Rds")  
df <- input$KlekotaRoth_FingerPrinter  
plot_graph_interval(df)
```



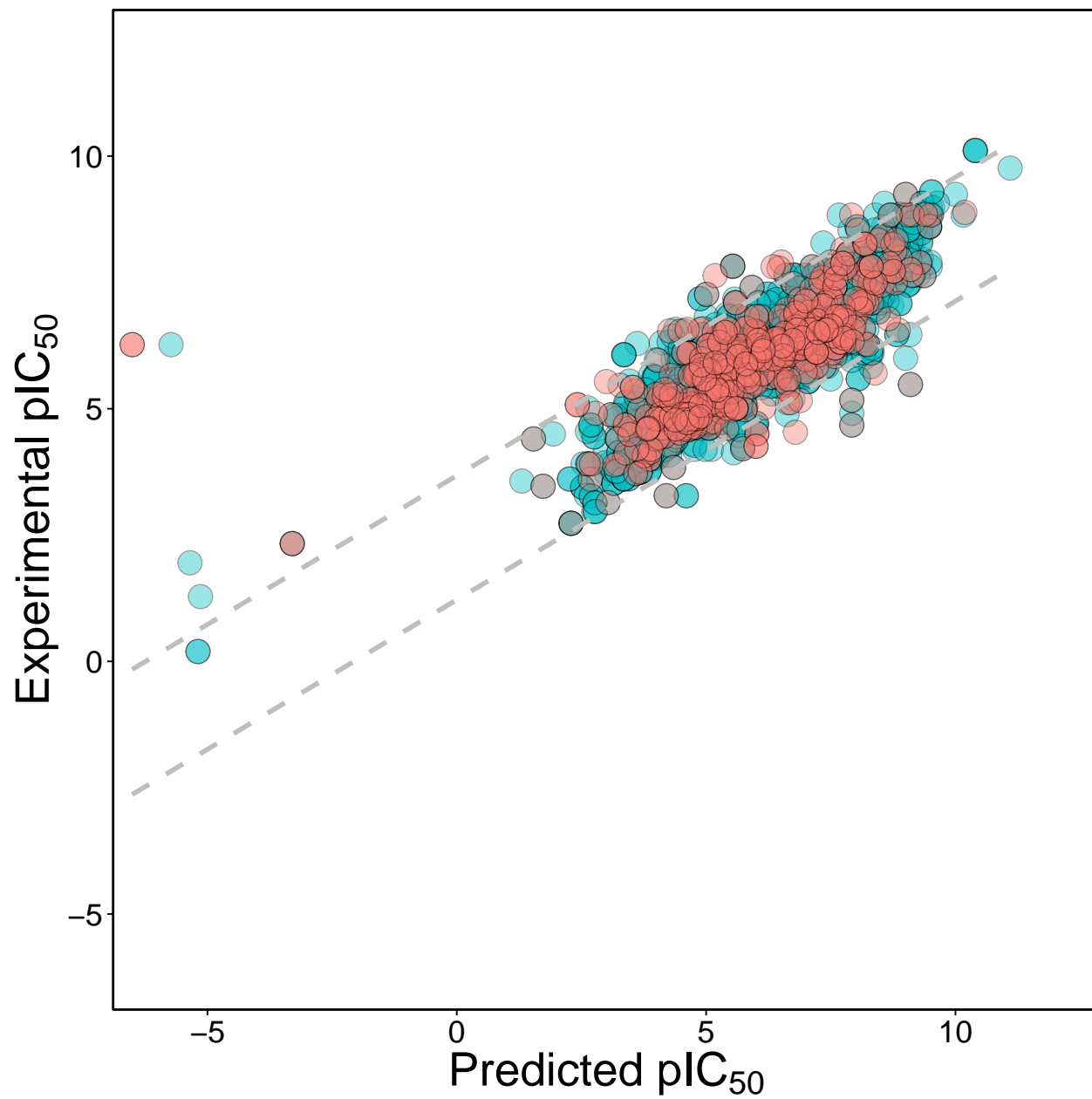
Klekota-Roth count

```
input <- readRDS("data.Rds")  
df <- input$KlekotaRoth_FingerprintCount  
plot_graph_interval(df)
```



2D atom pairs

```
input <- readRDS("data.Rds")  
df <- input$AtomPairs2D_fingerPrinter  
plot_graph_interval(df)
```



2D atom pairs count

```
input <- readRDS("data.Rds")  
df <- input$AtomPairs2D_fingerPrintCount  
plot_graph_interval(df)
```

