







Supplemental File

RStudio/2023.03.1+446 © 2009-2023 Posit Software, PBC.

"Cherry Blossom" Release (6e31ffc3, 2023-05-09) for windows

The following algorithm was used to produce the figures from raw data material of IC50 spectrophotometry analysis.

```

library(gcookbook)
library(viridis)
library(ggpmisc)
#Absorbance_Extracts2.0
ggplot(data=IC50_R_Studio, mapping = aes(x = E, y = Absorbance, color = Absorbance))+
  # geom_point()
  #str(IC50_R_Studio)
  #IC50_R_Studio %>% ggplot(aes(x = E, y = Absorbance, color = Absorbance))+
  geom_point(size = 3, alpha = 0.7)+
  facet_wrap(~ Conc, nrow = 1, scales = "free")+
  #facet_grid()+
  #gradient_color("RdYlBu")+
  #scale_fill_viridis(discrete = FALSE, option = "C")+
  xlab("Extracts") +

```

```

ylab("Absorbance (T = 30 mins,  $\lambda$  = 517nm)") +
#theme_minimal() +
theme(legend.position = "bottom")+
theme(axis.title.x=element_text(size=13))+
theme(axis.title.y=element_text(size=13))+
guides(colour = guide_colorbar(title.position = "top"))+
theme(axis.title.x = element_text(vjust=-1.5))
#theme(legend.title = element_text(size=13))
ggsave("Absorbance_Extracts.tiff", width = 9, height = 5)

```

```

#Absorbance_Ascorbic Acid
ggplot(data=IC50_R_Studio_AA, mapping = aes(x = Concentrations.ppm, y = Absorbance, color
= Absorbance))+
#geom_point()
#str(IC50_R_Studio_AA)
#IC50_R_Studio_AA %>% ggplot(aes(x = Concentrations.ppm, y = Absorbance, color =
Absorbance))+
geom_point(size = 3, alpha = 0.7)+
#facet_wrap(~ Concentrations.ppm, nrow = 1, scales = "free")+
#labs(fill = "Absorbance")+
#theme(legend.title = element_text ("Absorbance")) +
xlab("Concentrations (ppm)") +
ylab("Absorbance (T = 30 mins,  $\lambda$  = 517nm)")
ggsave("Absorbance_AA.tiff", width = 9, height = 3)

```

```

#Linear_regression_KA
ggplot(IC50_R_Studio_IN, aes(ConcEx, RC, linetype = Repetitions, grp.label = Repetitions))+
geom_point(aes(color = RC), size = 3, alpha = 0.7) +
stat_poly_line(fill= "#001128", color = "#FFE45C", alpha = 0.2) +
stat_poly_eq(use_label(c("eq", "r2")), size = 3, label.y = 40) +
#scale_color_viridis(discrete = TRUE, option = "D")+
#scale_fill_viridis(discrete = TRUE, option = "D") +
facet_wrap(~ Repetitions)+
#theme_minimal() +
theme(legend.position = "bottom") +
theme(legend.box = "horizontal")+
guides(colour = guide_colorbar(order = 1))+
guides(colour = guide_colorbar(title.position = "top"))+
labs(x=expression(paste(italic("Log")["e"], italic("x"), " of Concentrations")))+
ylab("Inhibitions (%)")
ggsave("Inhibitions_KA.tiff", width = 9, height = 3)

```

```

#Linear_regression_MA
ggplot(IC50_R_Studio_IN, aes(ConcEx, RM, linetype = Repetitions, grp.label = Repetitions))+

```

```

geom_point(aes(color = RM), size = 3, alpha = 0.7) +
stat_poly_line(fill= "#001128", color = "#FFE45C", alpha = 0.2) +
stat_poly_eq(use_label(c("eq", "r2")), size = 3, label.y = 40) +
#scale_color_viridis(discrete = TRUE, option = "D")+
#scale_fill_viridis(discrete = TRUE, option = "D") +
facet_wrap(~ Repetitions)+
#theme_minimal() +
theme(legend.position = "bottom") +
theme(legend.box = "horizontal")+
guides(colour = guide_colorbar(order = 1))+
guides(colour = guide_colorbar(title.position = "top"))+
labs(x=expression(paste(italic("Log")["e"], italic("x"), " of Concentrations")))) +
ylab("Inhibitions (%)")
ggsave("Inhibitions_MA.tiff", width = 9, height = 3)

```

```

#Linear_regression_KD

```

```

ggplot(IC50_R_Studio_IN, aes(ConcEx, LC, linetype = Repetitions, grp.label = Repetitions))+
geom_point(aes(color = LC), size = 3, alpha = 0.7) +
stat_poly_line(fill= "#001128", color = "#FFE45C", alpha = 0.2) +
stat_poly_eq(use_label(c("eq", "r2")), size = 3, label.y = 40) +
#scale_color_viridis(discrete = TRUE, option = "D")+
#scale_fill_viridis(discrete = TRUE, option = "D") +
facet_wrap(~ Repetitions)+
#theme_minimal() +
theme(legend.position = "bottom") +
theme(legend.box = "horizontal")+
guides(colour = guide_colorbar(order = 1))+
guides(colour = guide_colorbar(title.position = "top"))+
labs(x=expression(paste(italic("Log")["e"], italic("x"), " of Concentrations")))) +
ylab("Inhibitions (%)")
ggsave("Inhibitions_KD.tiff", width = 9, height = 3)

```

```

#Linear_regression_MD

```

```

ggplot(IC50_R_Studio_IN, aes(ConcEx, LM, linetype = Repetitions, grp.label = Repetitions))+
geom_point(aes(color = LM), size = 3, alpha = 0.7) +
stat_poly_line(fill= "#001128", color = "#FFE45C", alpha = 0.2) +
stat_poly_eq(use_label(c("eq", "r2")), size = 3, label.y = 40) +
#scale_color_viridis(discrete = TRUE, option = "D")+
#scale_fill_viridis(discrete = TRUE, option = "D") +
facet_wrap(~ Repetitions)+
#theme_minimal() +
theme(legend.position = "bottom") +
theme(legend.box = "horizontal")+
guides(colour = guide_colorbar(order = 1))+

```

```
guides(colour = guide_colorbar(title.position = "top"))+
labs(x=expression(paste(italic("Log")["e"], italic("x"), " of Concentrations")))+
ylab("Inhibitions (%)")
ggsave("Inhibitions_MD.tiff", width = 9, height = 3)
```

```
#Linear_regression_ED
ggplot(IC50_R_Studio_IN, aes(ConcEx, LE, linetype = Repetitions, grp.label = Repetitions))+
geom_point(aes(color = LE), size = 3, alpha = 0.7) +
stat_poly_line(fill= "#001128", color = "#FFE45C", alpha = 0.2) +
stat_poly_eq(use_label(c("eq", "r2")), size = 3, label.y = 40) +
#scale_color_viridis(discrete = TRUE, option = "D")+
#scale_fill_viridis(discrete = TRUE, option = "D") +
facet_wrap(~ Repetitions)+
#theme_minimal() +
theme(legend.position = "bottom") +
theme(legend.box = "horizontal")+
guides(colour = guide_colorbar(order = 1))+
guides(colour = guide_colorbar(title.position = "top"))+
labs(x=expression(paste(italic("Log")["e"], italic("x"), " of Concentrations")))+
ylab("Inhibitions (%)")
ggsave("Inhibitions_ED.tiff", width = 9, height = 3)
```

```
#Linear_regression_AA
ggplot(IC50_R_Studio_INA, aes(ConcExAA, AA, linetype = Repetitions, grp.label = Repetitions))+
geom_point(aes(color = AA), size = 3, alpha = 0.7) +
stat_poly_line(fill= "#001128", color = "#FFE45C", alpha = 0.2) +
stat_poly_eq(use_label(c("eq", "r2")), size = 3, label.y = 40) +
#scale_color_viridis(discrete = TRUE, option = "D")+
#scale_fill_viridis(discrete = TRUE, option = "D") +
facet_wrap(~ Repetitions)+
#theme_minimal() +
theme(legend.position = "bottom") +
theme(legend.box = "horizontal")+
guides(colour = guide_colorbar(order = 1))+
guides(colour = guide_colorbar(title.position = "top"))+
labs(x=expression(paste(italic("Log")["e"], italic("x"), " of Concentrations")))+
ylab("Inhibitions (%)")
ggsave("Inhibitions_AA.tiff", width = 9, height = 3)
```