Supplementary Data

This supplementary data is a part of paper entitled "Employing an R Software Package rsm for Optimizing of Genistein, Daidzein, and Glycitein Separation and Its Application for Soy Milk Analysis by HPLC Method".

S1. R formula for analyzing genistein data

```
library(rsm)
gen = read.csv("gen2.csv")
gen

##setting up coded levels for genistein model
gen.rsm <- coded.data(gen, x1 ~ (methanol - 65)/5,
                      x2 ~ (flowrate - 0.8)/0.2,
                      x3 ~ (temp - 40)/10)
gen.rsm

##RSM for analyzing retention time for genistein
gen.ret.rsm <- rsm(retention ~ SO(x1, x2, x3), data = gen.rsm)
gen.ret.rsm
summary(gen.ret.rsm)

par(mfrow = c(1,3))
persp(gen.ret.rsm, ~ x1 + x2 + x3, at = summary(gen.ret.rsm)$canonical$xs,
      contours = "col", col = rainbow(40),
      zlab = "Retention Time",
      xlabs = c("Methanol Concentration (%)", "Flowrate (mL/min)", "Temperature
(oC)"))

##RSM for analyzing resolution for genistein
gen.res.rsm <- rsm(resolution ~ SO(x1, x2, x3), data = gen.rsm)
gen.res.rsm
summary(gen.res.rsm)

par(mfrow = c(1,3))

persp(gen.res.rsm, ~ x1 + x2 + x3, at = summary(gen.res.rsm)$canonical$xs,
      contours = "col", col = rainbow(40),
      zlab = "Resolution",
      xlabs = c("Methanol Concentration (%)", "Flowrate (mL/min)", "Temperature
(oC)"))

##RSM for analyzing tailing factor for genistein
gen.tai.rsm <- rsm(tailing ~ SO(x1, x2, x3), data = gen.rsm)
gen.tai.rsm
summary(gen.tai.rsm)

par(mfrow = c(1,3))
persp(gen.tai.rsm, ~ x1 + x2 + x3, at = summary(gen.tai.rsm)$canonical$xs,
      contours = "col", col = rainbow(40),
      zlab = "Tailing Factor",
```

```
      xlabs = c("Methanol Concentration (%)", "Flowrate (mL/min)", "Temperature
(oC)"))

##RSM for analyzing N for genistein
gen.n.rsm <- rsm(n ~ SO(x1, x2, x3), data = gen.rsm)
gen.n.rsm
summary(gen.n.rsm)

par(mfrow = c(1,3))
persp(gen.n.rsm, ~ x1 + x2 + x3, at = summary(gen.n.rsm)$canonical$xs,
      contours = "col", col = rainbow(40),
      zlab = "Theoretical Plates Number",
      xlabs = c("Methanol Concentration (%)", "Flowrate (mL/min)", "Temperature
(oC)"))
```

S2. R formula for analyzing daidzein data

```
library(rsm)
dai = read.csv("dai2.csv")
dai

##setting up coded levels for daidzein model
dai.rsm <- coded.data(dai, x1 ~ (methanol - 65)/5,
                      x2 ~ (flowrate - 0.8)/0.2,
                      x3 ~ (temp - 40)/10)
dai.rsm

##RSM for analyzing retention time for daidzein
dai.ret.rsm <- rsm(retention ~ SO(x1, x2, x3), data = dai.rsm)
dai.ret.rsm
summary(dai.ret.rsm)

par(mfrow = c(1,3))
persp(dai.ret.rsm, ~ x1 + x2 + x3, at = summary(dai.ret.rsm)$canonical$xs,
      contours = "col", col = rainbow(40),
      zlab = "Retention Time",
      xlabs = c("Methanol Concentration (%)", "Flowrate (mL/min)", "Temperature
(oC)"))

##RSM for analyzing resolution for daidzein
dai.res.rsm <- rsm(resolution ~ SO(x1, x2, x3), data = dai.rsm)
dai.res.rsm
summary(dai.res.rsm)

par(mfrow = c(1,3))
persp(dai.res.rsm, ~ x1 + x2 + x3, at = summary(dai.res.rsm)$canonical$xs,
      contours = "col", col = rainbow(40),
      zlab = "Resolution",
      xlabs = c("Methanol Concentration (%)", "Flowrate (mL/min)", "Temperature
(oC)"))
##RSM for analyzing tailing factor for daidzein
dai.tai.rsm <- rsm(tailing ~ SO(x1, x2, x3), data = dai.rsm)
```

```
dai.tai.rsm
summary(dai.tai.rsm)

par(mfrow = c(1,3))
persp(dai.tai.rsm, ~ x1 + x2 + x3, at = summary(dai.tai.rsm)$canonical$xs,
      contours = "col", col = rainbow(40),
      zlab = "Tailing Factor",
      xlabs = c("Methanol Concentration (%)", "Flowrate (mL/min)", "Temperature
(oC)"))

##RSM for analyzing N for daidzein
dai.n.rsm <- rsm(n ~ SO(x1, x2, x3), data = dai.rsm)
dai.n.rsm
summary(dai.n.rsm)

par(mfrow = c(1,3))
persp(dai.n.rsm, ~ x1 + x2 + x3, at = summary(dai.n.rsm)$canonical$xs,
      contours = "col", col = rainbow(40),
      zlab = "Theoretical Plates Number",
      xlabs = c("Methanol Concentration (%)", "Flowrate (mL/min)", "Temperature
(oC)"))
```

S3. R formula for analyzing glycitein data

```
library(rsm)
gly = read.csv("gly2.csv")
gly

##setting up coded levels for glycitein model
gly.rsm <- coded.data(gly, x1 ~ (methanol - 65)/5,
                      x2 ~ (flowrate - 0.8)/0.2,
                      x3 ~ (temp - 40)/10)
gly.rsm

##RSM for analyzing retention time for glycitein
gly.ret.rsm <- rsm(retention ~ SO(x1, x2, x3), data = gly.rsm)
gly.ret.rsm
summary(gly.ret.rsm)

par(mfrow = c(1,3))
persp(gly.ret.rsm, ~ x1 + x2 + x3, at = summary(gly.ret.rsm)$canonical$xs,
      contours = "col", col = rainbow(40),
      zlab = "Retention Time",
      xlabs = c("Methanol Concentration (%)", "Flowrate (mL/min)", "Temperature
(oC)"))

##RSM for analyzing resolution for glycitein
gly.res.rsm <- rsm(resolution ~ SO(x1, x2, x3), data = gly.rsm)
gly.res.rsm
summary(gly.res.rsm)
par(mfrow = c(1,3))
persp(gly.res.rsm, ~ x1 + x2 + x3, at = summary(gly.res.rsm)$canonical$xs,
```

```
      contours = "col", col = rainbow(40),
      zlab = "Resolution",
      xlabs = c("Methanol Concentration (%)", "Flowrate (mL/min)", "Temperature
(oC)"))

##RSM for analyzing tailing factor for glycitein
gly.tai.rsm <- rsm(tailing ~ SO(x1, x2, x3), data = gly.rsm)
gly.tai.rsm
summary(gly.tai.rsm)

par(mfrow = c(1,3))
persp(gly.tai.rsm, ~ x1 + x2 + x3, at = summary(gly.tai.rsm)$canonical$xs,
      contours = "col", col = rainbow(40),
      zlab = "Tailing Factor",
      xlabs = c("Methanol Concentration (%)", "Flowrate (mL/min)", "Temperature
(oC)"))

##RSM for analyzing N for glycitein
gly.n.rsm <- rsm(n ~ SO(x1, x2, x3), data = gly.rsm)
gly.n.rsm
summary(gly.n.rsm)

par(mfrow = c(1,3))
persp(gly.n.rsm, ~ x1 + x2 + x3, at = summary(gly.n.rsm)$canonical$xs,
      contours = "col", col = rainbow(40),
      zlab = "Theoretical Plates Number",
      xlabs = c("Methanol Concentration (%)", "Flowrate (mL/min)", "Temperature
(oC)"))
```