#1 A Partial Least Squares-Based Consensus Regression Method for the Analysis of Near-Infrared Complex Spectral Data of Plant Samples

##60-20 10

###1~mp6 0.159

```
## 0.1224099 0.1466523 0.02424241 0.1708948
```

```
##    user  system elapsed
##   0.014   0.003  10.036
```

#1 A Partial Least Squares-Based Consensus Regression Method for the Analysis of Near-Infrared Complex Spectral Data of Plant Samples

##60-20 10

###2~mp6 0.107

```
## 0.08169381 0.09496089 0.01326708 0.108228
```

```
##    user  system elapsed
##   0.012   0.002  10.459
```

#1 A Partial Least Squares-Based Consensus Regression Method for the Analysis of Near-Infrared Complex Spectral Data of Plant Samples

##60-20 10

###3~mp6 0.150

```
## 0.1210491 0.1431659 0.0221168 0.1652827
```

```
##    user  system elapsed
##   0.011   0.003  10.475
```

#1 A Partial Least Squares-Based Consensus Regression Method for the Analysis of Near-Infrared Complex Spectral Data of Plant Samples

##60-20 10

###4~mp6 0.370

```
## 0.3182161 0.3661988 0.04798274 0.4141816
```

```
##    user  system elapsed
##   0.013   0.001  10.506
```

#2 A strategy that iteratively retains informative variables for selecting optimal variable subset in multivariate calibration

##64-16 9 CV=5

###1~m5 RMSEC = 0.0149; RMSEP = 0.0201

```
## 0.01433805 0.01513965 0.0008016005 0.01594125
## 0.01682591 0.02026211 0.003436204 0.02369832
```

```
##    user  system elapsed
##   0.015   0.000   4.131
```

#3 Cross-validation for the selection of spectral variables using the successive projections algorithm

##60-20 SavitzkyGolay filler (in) 3-fold but Loo better

###1~m5 0.040(5)

```
## Error in library("MALDIquant"): there is no package called 'MALDIquant'
```

```
## Error in library(prospectr): there is no package called 'prospectr'
```

```
## Error in checkForRemoteErrors(val): 36 nodes produced errors; first error: there is no pa
```

#3 Cross-validation for the selection of spectral variables using the successive projections algorithm

##60-20 SavitzkyGolay filler (in) 3-fold

###2~m5 0.029(12)

```
## Error in library("MALDIquant"): there is no package called 'MALDIquant'
```

```
## Error in library(prospectr): there is no package called 'prospectr'
```

```
## Error in checkForRemoteErrors(val): 36 nodes produced errors; first error: there is no pa
```

#3 Cross-validation for the selection of spectral variables using the successive projections algorithm

##60-20 SavitzkyGolay filler (in) 3-fold

###3~m5 0.119(6)

```
## Error in library("MALDIquant"): there is no package called 'MALDIquant'
```

```
## Error in library(prospectr): there is no package called 'prospectr'
```

```
## Error in checkForRemoteErrors(val): 36 nodes produced errors; first error: there is no pa
```

#3 Cross-validation for the selection of spectral variables using the successive projections algorithm

##60-20 SavitzkyGolay filler (in) 3-fold but Loo better

###4~m5 0.196(6)

```
## Error in library("MALDIquant"): there is no package called 'MALDIquant'
```

```
## Error in library(prospectr): there is no package called 'prospectr'
```

```
## Error in checkForRemoteErrors(val): 36 nodes produced errors; first error: there is no pa
```

#4 Reduced PCR/PLSR models by subspace projections

##40-40 Scale 12

###1~m5 0.3506

```
## 0.01971152 0.02375771 0.004046195 0.02780391
```

```
##    user  system elapsed
##   0.012   0.002   7.989
```

#4 Reduced PCR/PLSR models by subspace projections

##40-40 Scale 14

###2~m5 0.6912

```
## 0.3338348 0.3932385 0.05940365 0.4526421
```

```
##    user  system elapsed
##   0.013   0.001   8.762
```

#4 Reduced PCR/PLSR models by subspace projections

##40-40 Scale 8

###3~m5 0.4466

```
## 0.3003264 0.3528507 0.05252433 0.405375
```

```
##    user  system elapsed
##   0.011   0.002   6.644
```

#4 Reduced PCR/PLSR models by subspace projections

##40-40 Scale 9

###4~m5 0.5010

```
## 0.3136586 0.3605722 0.04691361 0.4074858
```

```
##    user  system elapsed
##   0.012   0.003   7.144
```

#5 Stability competitive adaptive reweighted sampling (SCARS) and its applications to multivariate calibration of NIR spectra

##40-40 Scale 10

###1~mp5 0.357

```
## 0.3598559 0.4064021 0.04654622 0.4529483
```

```
##    user  system elapsed
##   0.014   0.001   6.924
```

#6 Pretreating near infrared spectra with fractional order Savitzky–Golay differentiation (FOSGD)

##64-16 savitzkyGolay filler=(0,2,13) 7 5-fold

###2~m5 RMSECV=0.0729; RMSECP=0.0855

```
## Error in library("MALDIquant"): there is no package called 'MALDIquant'
```

```
## Error in library(prospectr): there is no package called 'prospectr'
```

```
## Error in checkForRemoteErrors(val): 36 nodes produced errors; first error: there is no pa
```

#6 Pretreating near infrared spectra with fractional order Savitzky–Golay differentiation (FOSGD)

##64-16 savitzkyGolay filler=(1,2,13) 7 5-fold

###2~m5 RMSECV=0.0577; RMSECP=0.0682

```
## Error in library("MALDIquant"): there is no package called 'MALDIquant'
```

```
## Error in library(prospectr): there is no package called 'prospectr'
```

```
## Error in checkForRemoteErrors(val): 36 nodes produced errors; first error: there is no pa
```

#6 Pretreating near infrared spectra with fractional order Savitzky–Golay differentiation (FOSGD)

##64-16 savitzkyGolay filler=(2,2,13) 7 5-fold

###2~m5 RMSECV=0.0370; RMSECP=0.0397

```
## Error in library("MALDIquant"): there is no package called 'MALDIquant'
```

```
## Error in library(prospectr): there is no package called 'prospectr'
```

```
## Error in checkForRemoteErrors(val): 36 nodes produced errors; first error: there is no pa
```

#6 Pretreating near infrared spectra with fractional order Savitzky–Golay differentiation (FOSGD)

##64-16 savitzkyGolay filler=(0,2,7) 8 5-fold

###4~m5 RMSECV=0.312; RMSECP=0.214

```
## Error in library("MALDIquant"): there is no package called 'MALDIquant'
```

```
## Error in library(prospectr): there is no package called 'prospectr'
```

```
## Error in checkForRemoteErrors(val): 36 nodes produced errors; first error: there is no pa
```

#6 Pretreating near infrared spectra with fractional order Savitzky–Golay differentiation (FOSGD)

##64-16 savitzkyGolay filler=(1,2,7) 8 5-fold

###4~m5 RMSECV=0.248; RMSECP=0.221

```
## Error in library("MALDIquant"): there is no package called 'MALDIquant'
```

```
## Error in library(prospectr): there is no package called 'prospectr'
```

```
## Error in checkForRemoteErrors(val): 36 nodes produced errors; first error: there is no pa
```

#6 Pretreating near infrared spectra with fractional order Savitzky–Golay differentiation (FOSGD)

##64-16 savitzkyGolay filler=(2,2,7) 8 5-fold

###4~m5 RMSECV=0.347; RMSECP=0.228

```
## Error in library("MALDIquant"): there is no package called 'MALDIquant'
```

```
## Error in library(prospectr): there is no package called 'prospectr'
```

```
## Error in checkForRemoteErrors(val): 36 nodes produced errors; first error: there is no pa
```

#7 A variable elimination method to improve the parsimony of MLR models using the successive projections algorithm

##60-20 savitzkyGolay filler=(1,2,21) (in)

###1~m5 0.045(06)

```
## Error in library("MALDIquant"): there is no package called 'MALDIquant'
```

```
## Error in library(prospectr): there is no package called 'prospectr'
```

```
## Error in checkForRemoteErrors(val): 36 nodes produced errors; first error: there is no pa
```

#7 A variable elimination method to improve the parsimony of MLR models using the successive projections algorithm

##60-20 savitzkyGolay=(1,2,21) (in)

###2~m5 0.028(10)

```
## Error in library("MALDIquant"): there is no package called 'MALDIquant'
```

```
## Error in library(prospectr): there is no package called 'prospectr'
```

```
## Error in checkForRemoteErrors(val): 36 nodes produced errors; first error: there is no pa
```

#7 A variable elimination method to improve the parsimony of MLR models using the successive projections algorithm

##60-20 savitzkyGolay=(1,2,21) (in)

###3~m5 0.110(07)

```
## Error in library("MALDIquant"): there is no package called 'MALDIquant'
```

```
## Error in library(prospectr): there is no package called 'prospectr'
```

```
## Error in checkForRemoteErrors(val): 36 nodes produced errors; first error: there is no pa
```

#7 A variable elimination method to improve the parsimony of MLR models using the successive projections algorithm

##60-20 savitzkyGolay=(1,2,21) (in)

###4~m5 0.228(05)

```
## Error in library("MALDIquant"): there is no package called 'MALDIquant'
```

```
## Error in library(prospectr): there is no package called 'prospectr'
```

```
## Error in checkForRemoteErrors(val): 36 nodes produced errors; first error: there is no pa
```

#8 Using consensus interval partial least square in near infrared spectra analysis

##52-26 Delete 75 , 77; 10

###1~m5 RMSECV=0.0124; RMSEP=0.0157

```
## 0.0203417 0.02197847 0.001636774 0.02361525
## 0.0161657 0.01882367 0.002657967 0.02148163
```

```
##    user  system elapsed
##   0.013   0.002   2.442
```

#8 Using consensus interval partial least square in near infrared spectra analysis

##52-26 Delete 75 , 77; 13

###2~m5 RMSECV=0.0613; RMSEP=0.0673

```
## 0.05669571 0.06393391 0.007238201 0.07117211
## 0.05285865 0.06176522 0.008906579 0.0706718
```

```
##    user  system elapsed
##   0.014   0.001   2.031
```

#8 Using consensus interval partial least square in near infrared spectra analysis

##52-26 Delete 75 , 77 13

###3~m5 RMSECV=0.1080; RMSEP=0.1353

```
## 0.1027958 0.1176843 0.01488856 0.1325729
## 0.09463264 0.1114396 0.01680692 0.1282465
```

```
##    user  system elapsed
##   0.011   0.004   2.693
```

#8 Using consensus interval partial least square in near infrared spectra analysis

##52-26 Delete 75 , 77 10

###4~m5 RMSECV=0.2579; RMSEP=0.2356

```
## 0.2561056 0.2896935 0.03358789 0.3232814
## 0.2419548 0.2847371 0.04278225 0.3275193
```

```
##    user  system elapsed
##   0.013   0.001   2.353
```