The „AUCS*“ mode of Aquagram: Fix Scale & Confidence Intervals

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*Area Under Curve Stabilized
AUCS Aquagrams with Fix Scale & Confidence Intervals: Main Advantages

Fix Scale
• time resolved experiments - compare across time
• same shape as the classical mode, but
  • now we have the added benefit of a meaningful scale, which is
  • an independent temperature scale (the differences in the aquagram can be translated to the effect of temperature);
  • additional benefit: the modification of the dataset does not effect the shape of the lines

Confidence Intervals
• well… 😊😊😊
20-74°C, average
The areas under the specific WAMACS are calculated and expressed in relation to the area change occurred by different temperature.

The areas under the specific WAMACS are calculated and expressed in relation to the area change occurred by different temperature. The area change at C12 by 1°C is compared to the change of perturbation.
MVA package with additional focus on Aquaphotomics

```
## universal peak picker
xPeaks <- function(ObjectToPickPeaks, bandwidth=25, comps=1:4, disc=FALSE) {
  if (class(ObjectToPickPeaks) == "mvr") {
    allColNames <- colnames(ObjectToPickPeaks$coefficients[,1:length(allColNames)]
    lastName <- allColNames[length(allColNames)]
    if (!is.character(lastName)) {
      lastName <- "1 comps"
    }
    mat <- ObjectToPickPeaks$coefficients[, ObjectToPickPeaks$ncomp]
    dfToPickPeaks <- data.frame(X=mat)
    colnames(dfToPickPeaks) <- lastName
  }
  if (class(ObjectToPickPeaks) == "PCA") {
    pickPeaks <- data.frame(ObjectToPickPeak$loading[,comps])
  }
  if (class(ObjectToPickPeaks) == "data.frame") {
    pickPeaks <- ObjectToPickPeaks
  }
  pickResultsList <- pickPeaks$pickers(dftPickPeaks, bandwidth, disc)
  EOF
}
```

```
## pick results object created by pickPeaks as input; contains the vector that was used for picking!
pickResults <- function(pickResults, onSub="onSub", persVarName=NULL, customColor=NULL) {
  if (length(pickResults$rawVector) < 1) {stop("An Error at plotPickResults: Call: NULL")}
  a <- colnames(pickResults$rawVector)
  b <- substr(a, stings$charPrevWVL+1, stings$charWVL) # to get rid of the "W" in front of the numbers
  wavelengths <- as.numeric(b) # so we have the wavelength in the column, and the vectors to be picked for
  res <- pickResults$picks$pickResult
  colPos <- stings$colPosPeaks
  colNeg <- stings$colNegPeaks
  positionTable <- res[1: (nrow(res)/2) ,]
  heightTable <- res)[(nrow(res)/2)+1):nrow(res) ,]
  yrange <- range(pickResults$rawVector)[2] - range(pickResults$rawVector)[1]
  onSub <- paste(onSub, ", bw=", pickResults$picks$pickWindow, sep="")
```
Quick Update — How to Install / Update the package „aquap2“

For those who were at the workshop on Saturday:

library(aquap2)
updateAquap2()
updateAquap2(TRUE)

For new (or re-)installing:

• http://aquaphotomics.com
• download and follow the instructions in the file (~ 3 min until up and running!)
Fix Scale - Time Resolved Experiments

DZ_Timesequence_Ob, T0 @1300–to–1600

grouping by C_Group (each N=20)

Cont
GDum
GPos
MQ

Mode: auc.sdc--diff
Minus: MQ
Calib: 26.6–30.6 deg. C.
T Exp.: 28.6 deg. C
Fix Scale - Time Resolved Experiments

DZ_Timesequence_Ob, T1−30min @1300−to−1600

grouping by C_Group (each N=20)

Mode: aucs.dce−diff
Minus: MQ
Calib: 26.6−30.6 deg. C.
T Exp.: 28.6 deg. C
Fix Scale - Time Resolved Experiments

DZ_Timesequence_Ob, T2–6h @1300–to–1600

Mode: auc.s.dce--diff
Minus: MQ
Calib: 26.6–30.6 deg. C.
T Exp.: 28.6 deg. C.

grouping by C_Group (each N=20)
Fix Scale - Time Resolved Experiments

DZ_Timesequence_Ob , T3–24h @1300–to–1600

Mode: aucs.dce--diff
Minus: MQ
Calib: 26.6–30.6 deg. C.
T Exp.: 28.6 deg. C.

grouping by C_Group (each N=20)
Fix Scale - Time Resolved Experiments

DZ_Timesequence_Ob , T4–48h @1300–to–1600

Mode: aucs.dce–diff
Minus: MQ
Calib: 26.6–30.6 deg. C.
T Exp.: 28.6 deg. C

grouping by C_Group (each N=20)
Confidence Intervals: Visualizing Significant Differences
KCl & NaCl Solutions — Displaying Averages

Strong Separation between Groups

Mode: aucs.dce
Calib: 26–30 deg. C.
T Exp.: 28 deg. C

N= 120, 108, 110, 60

grouping by C_Range (not N corr.)
KCl & NaCl Solutions — Displaying Conf. Int.

Strong Separation between Groups

chemicals, T1 @1300–to–1600

C01
C12
C11
C10
C09
C08
C07
C06
C05
C04
C03
C02
C01

KCI
NaCl

Mode: aucv.dce
Calib: 26–30 deg. C.
T Exp.: 28 deg. C
N= 120, 108, 110, 60

grouping by C_Range (not N corr.) 95% CI based on 1194 bootstrap replicates (bca)
KCl & NaCl Solutions — Displaying Conf. Int.

Strong Separation between Groups

N= 120, 108, 110, 60

Mode: auc.g.dce
Calib: 26 - 30 deg. C.
T Exp.: 28 deg. C

KCl
NaCl
KCl & NaCl Solutions — Displaying Conf. Int.

Strong Separation between Groups

Mode: aucs.dce
Calib: 26–30 deg. C.
T Exp.: 28 deg. C
N = 120, 108, 110, 60

KCl
NaCl
KCl & NaCl Solutions — (Conf. Int.)

Mode: auc.s.dce
Calib: 26–30 deg. C.
T Exp.: 28 deg. C

N= 218, 180

grouping by C_Names (not N corr.) 95% CI based on 1194 bootstrap replicates (bca)
KCl Solutions — Group by Consec. Scan

**Significant difference between Cons. Scans in C04 and C05 only!**
KCl Solutions — Group by Consec. Scan

Mode: aucs.dce  
Calib: 26−30 deg. C. 
T Exp.: 28 deg. C.
Low Concentration KCl Solutions — Mode: aucs.dce-diff

Subtract MilliQ from every other group

chemicals KCl, only MQ and R2, T1 @1300–to–1600

Mode: aucs.dce-diff
Minus: MQ
Calib: 26–30 deg. C.
T Exp.: 28 deg. C

N= 120, 120, 168

N= 120, 120, 168

grouping by C_Range (not N corr.)  95% CI based on 1224 bootstrap replicates (bca)
Low Concentration KCl Solutions — Mode: aucs.dce-diff

Subtract MilliQ from every other group
Just two lines away:

in R-Studio, you type one line at a time:

```r
> install.packages(c("devtools", "iterators"))
> library(devtools)
> install_github(repo="bpollner/aquap2", ref="latestPublic", build_vignettes=FALSE, force=TRUE)
```

or, go to http://aquaphotomics.com, there download the file with the installer-instructions.

or, write an email to bernhard.pollner@mac.com, and we will send you the installation-instruction file.
Thank You