

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

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*Area Under Curve Stabilized

Aquaphotomics: Understanding Water in Biology
at the 2nd International Aquaphotomics Symposium
26.-29. November 2016, Kobe, Japan

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

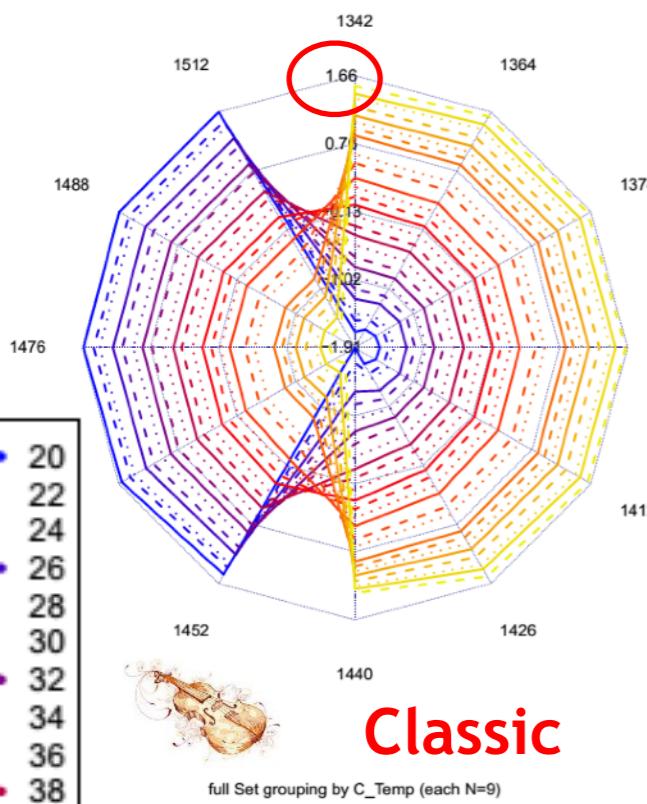
Confidence Intervals

- well...

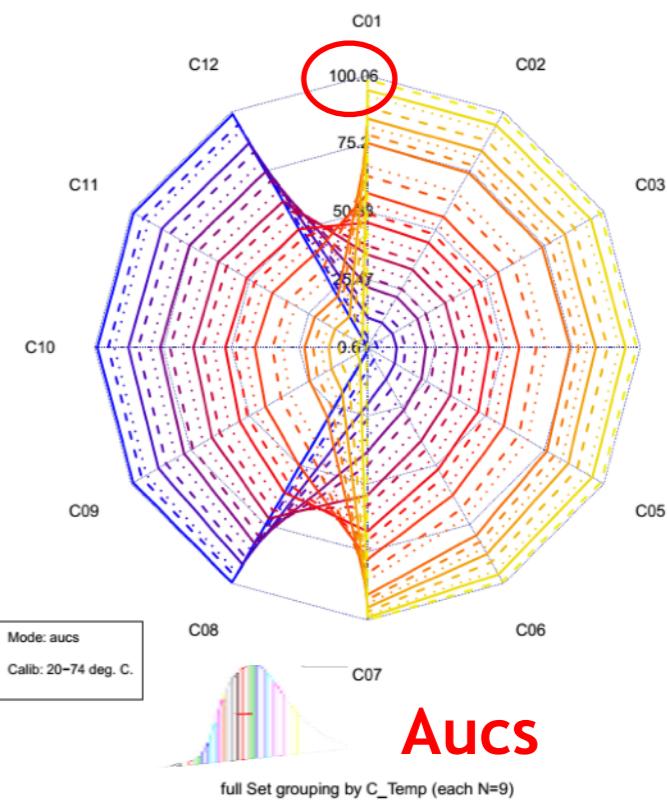


20-74 °C, average

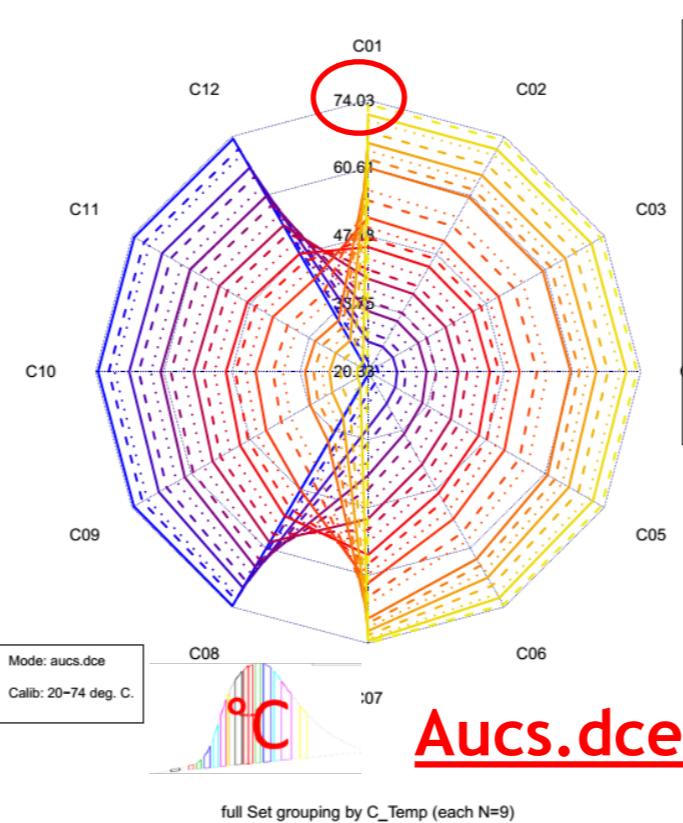
Temperature Calibration Full Set, all@1300-to-1600



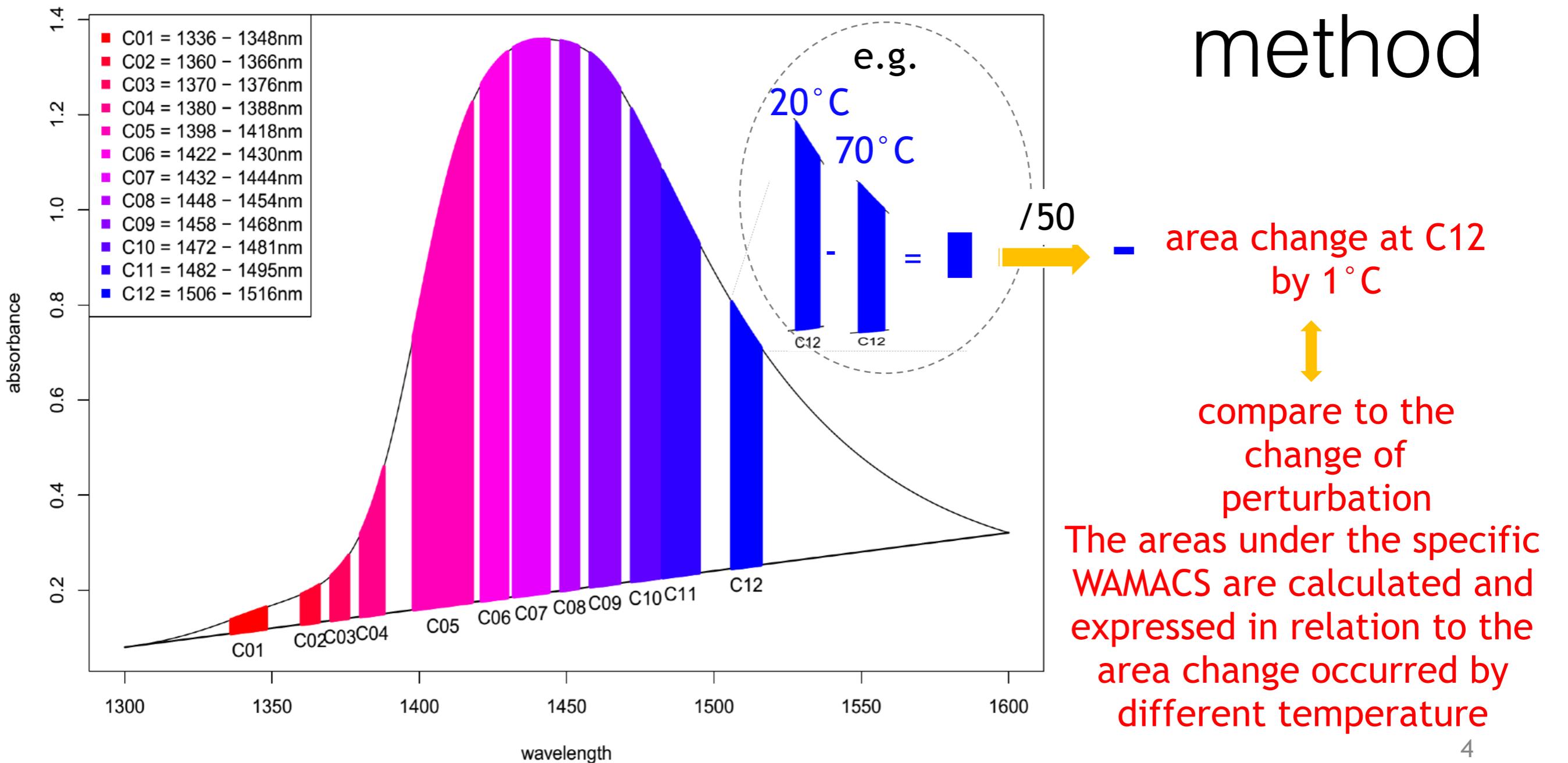
Temperature Calibration Full Set, all@1300-to-1600



Temperature Calibration Full Set, all@1300-to-1600



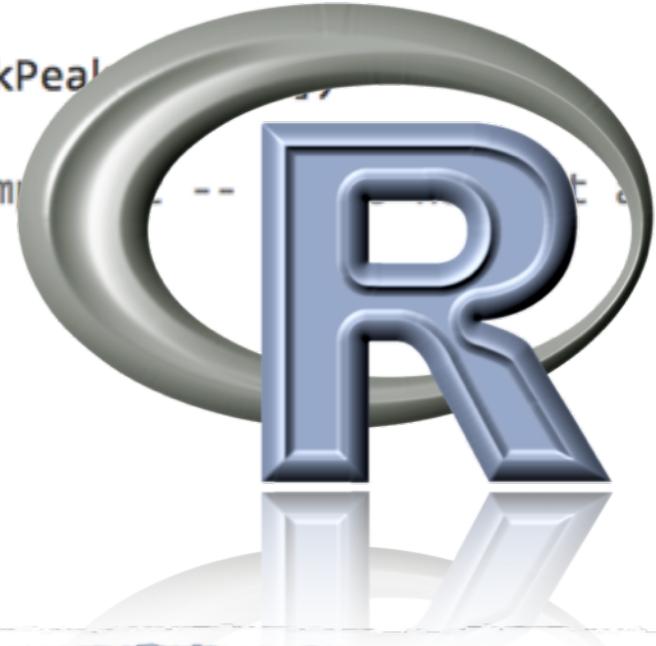
Scheme of the calculation for Area under the curve (AUC) aquagram method



```
the universal input, checking for the class of the input-object
pickPeaks <- function(ObjectToPickPeaks, bandwidth=25, comps=1:4, discrim=FALSE) {      ##### universal peak picker
if (class(ObjectToPickPeaks) == "mvr") {
  allColNames <- colnames(ObjectToPickPeaks$coefficients[, , 1:ObjectToPickPeaks$ncomp])
  lastName <- allColNames[length(allColNames)]
  if (!is.character(lastName)) {      ## problem if there is only one component
    lastName <- "1 comps"
  }
  mat <- ObjectToPickPeaks$coefficients[, , ObjectToPickPeaks$ncomp]
  dfToPickPeaks <- data.frame(X=mat)
  colnames(dfToPickPeaks) <- lastName
}
if (class(ObjectToPickPeaks) == "PCA") {
  dfToPickPeaks <- data.frame(ObjectToPickPeaks$loadings[, comps])
}
if (class(ObjectToPickPeaks) == "data.frame") {
  dfToPickPeaks <- ObjectToPickPeaks
}
pickResultsList <- pickPeaksInner(dfToPickPeaks, bandwidth, discrim)
EOF
```

MVA package with additional focus on Aquaphotomics

```
needs the pick results object created by pickPeaks as input; contains the vector that was used for picking !
plotPickResults <- function (pickResults, onMain="", onSub="", pcaVariables=NULL, customColor=NULL) {
  if (length(pickResults$rawVector) < 1) {
    stop("An Error at plotPickResults: did you call it?")
  }
  a <- colnames(pickResults$rawVector)
  b <- substr(a, strings::strcharprevL1, nchar(a))           # remove 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
  res <- pickResults$picks$pickResult
  colPos <- stngs$colPosPeaks
  colNeg <- stngs$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“

```
lastName <- allColNames[length(allColNames)]
```

```
if (!is.character(lastName)) { ## problem if there is only one component -- we do not get a name back
```

```
lastName <- "1 comps"
```

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
and running!)

AQUAPHOTOMICS: UNDERSTANDING WATER in BIOLOGY

2nd INTERNATIONAL SYMPOSIUM

@ Kobe University, Kobe, Japan

Latest Worldwide Research

Collaboration

26th-29th November 2016

1-1 Rokkodai, Nada, Kobe 657-8501,
Japan

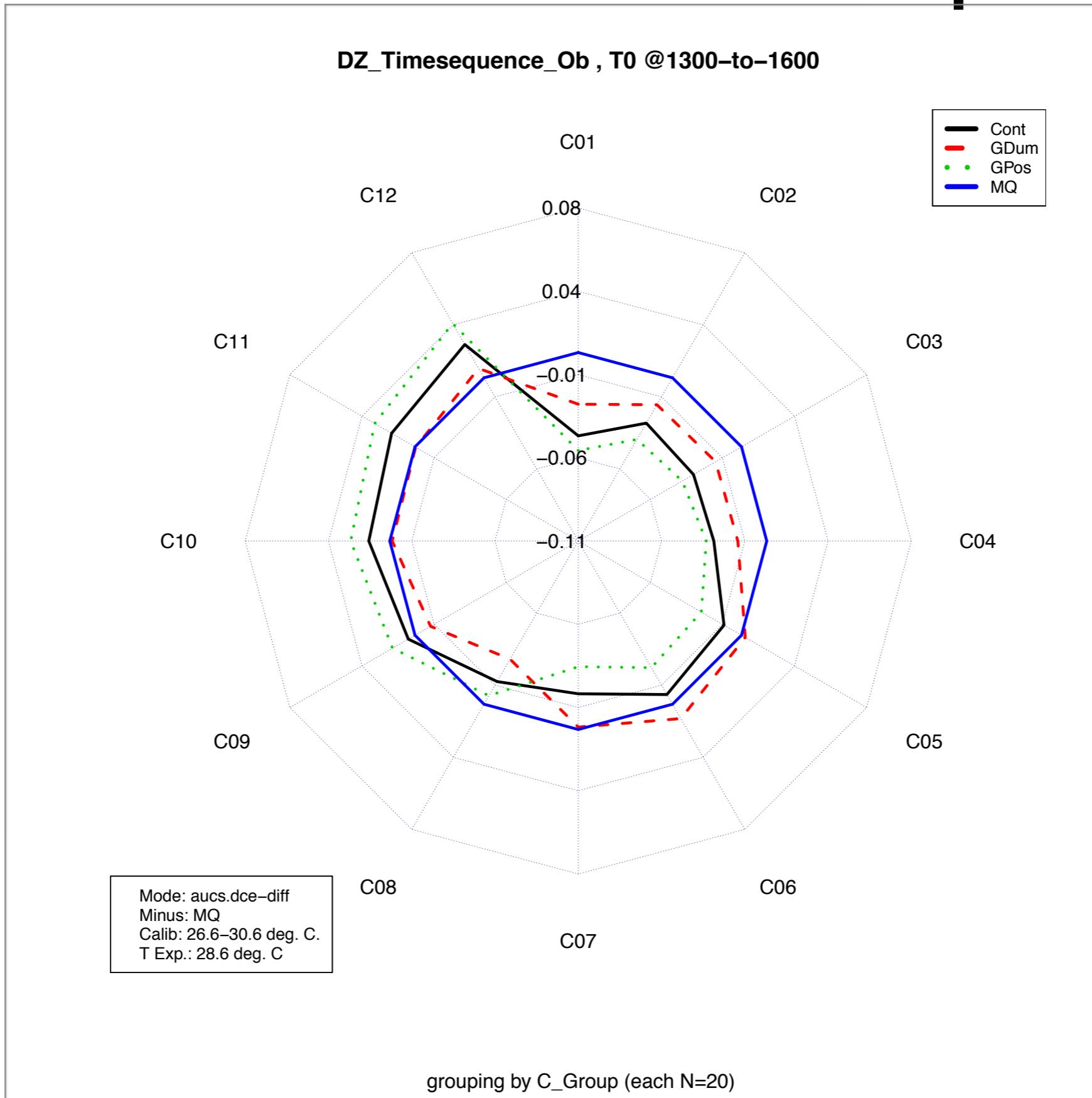


New! [aquap2_installation package \(28th November\)!](#)

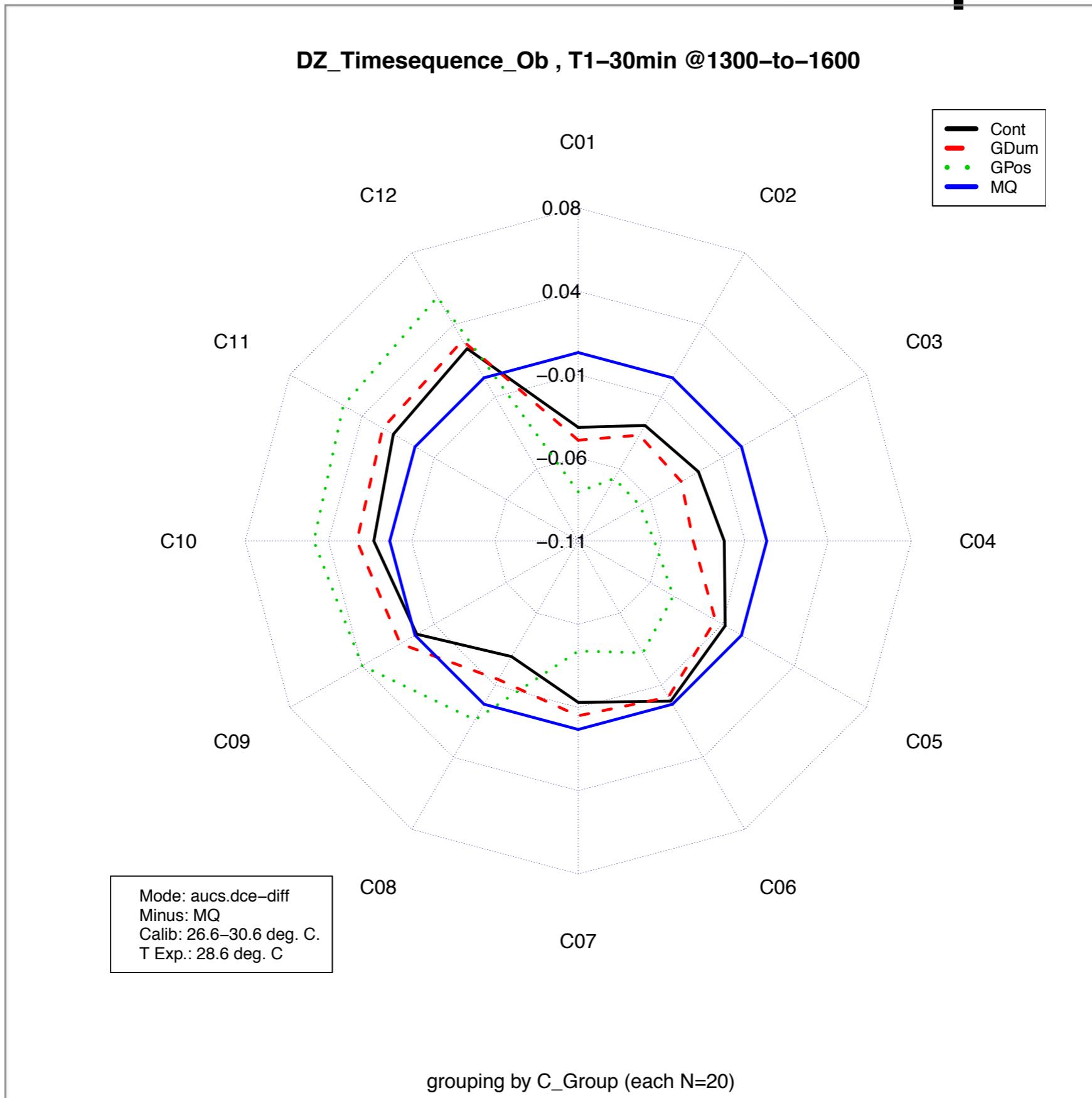
New! [List of Speakers is updated\(22nd November\)!](#)

New! [Conference Program is updated\(22nd November\)!](#)

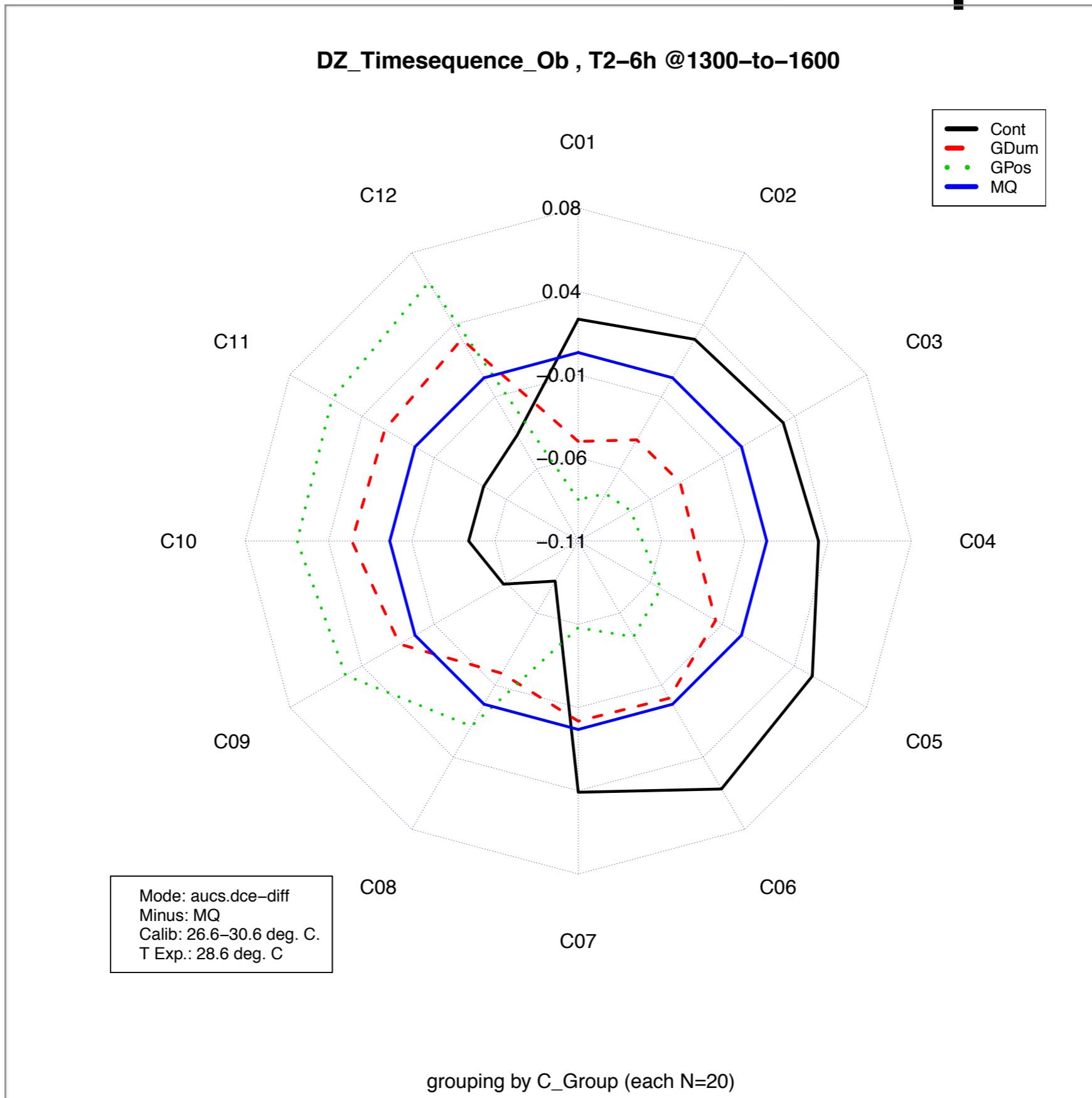
Fix Scale - Time Resolved Experiments



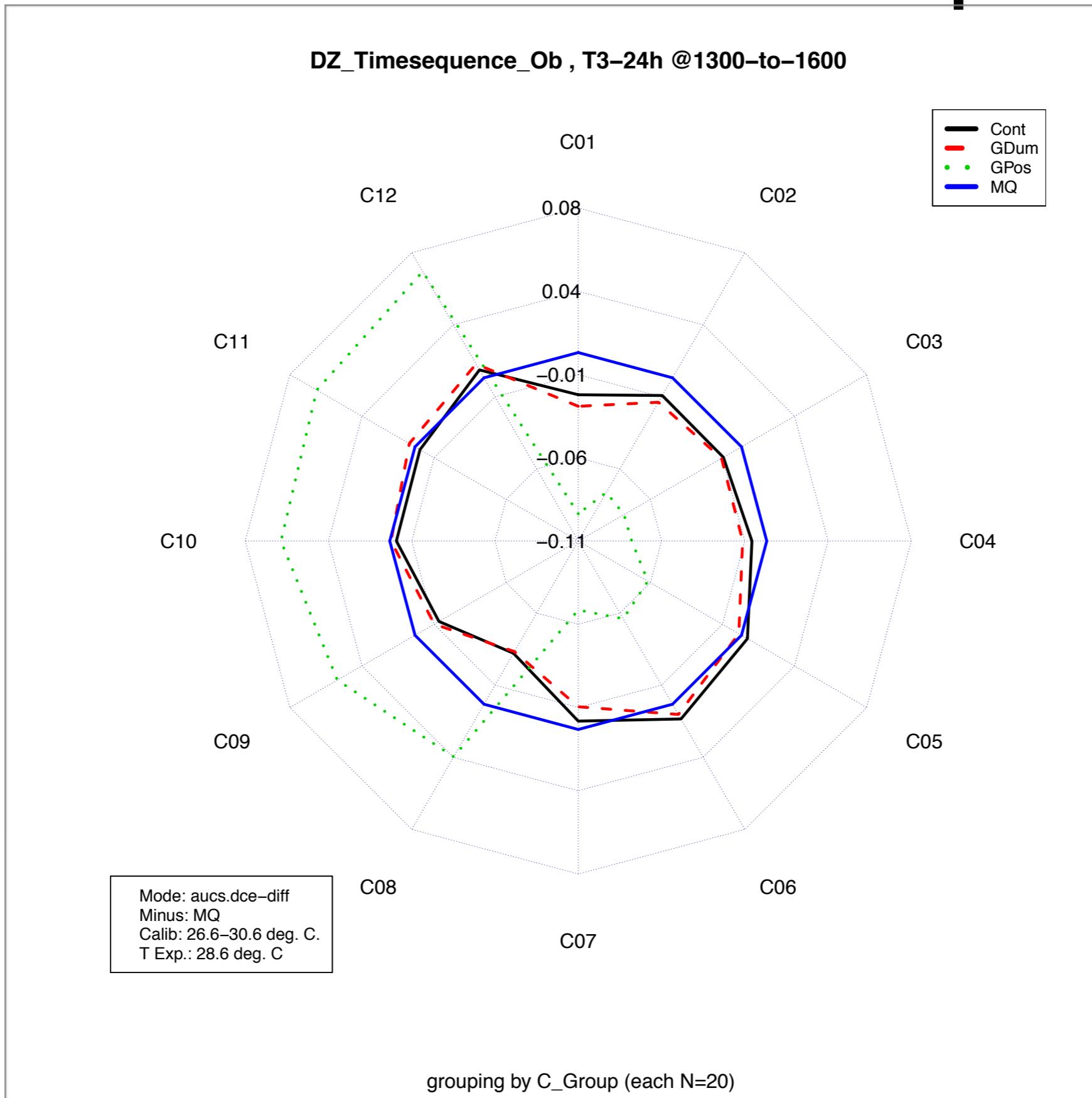
Fix Scale - Time Resolved Experiments



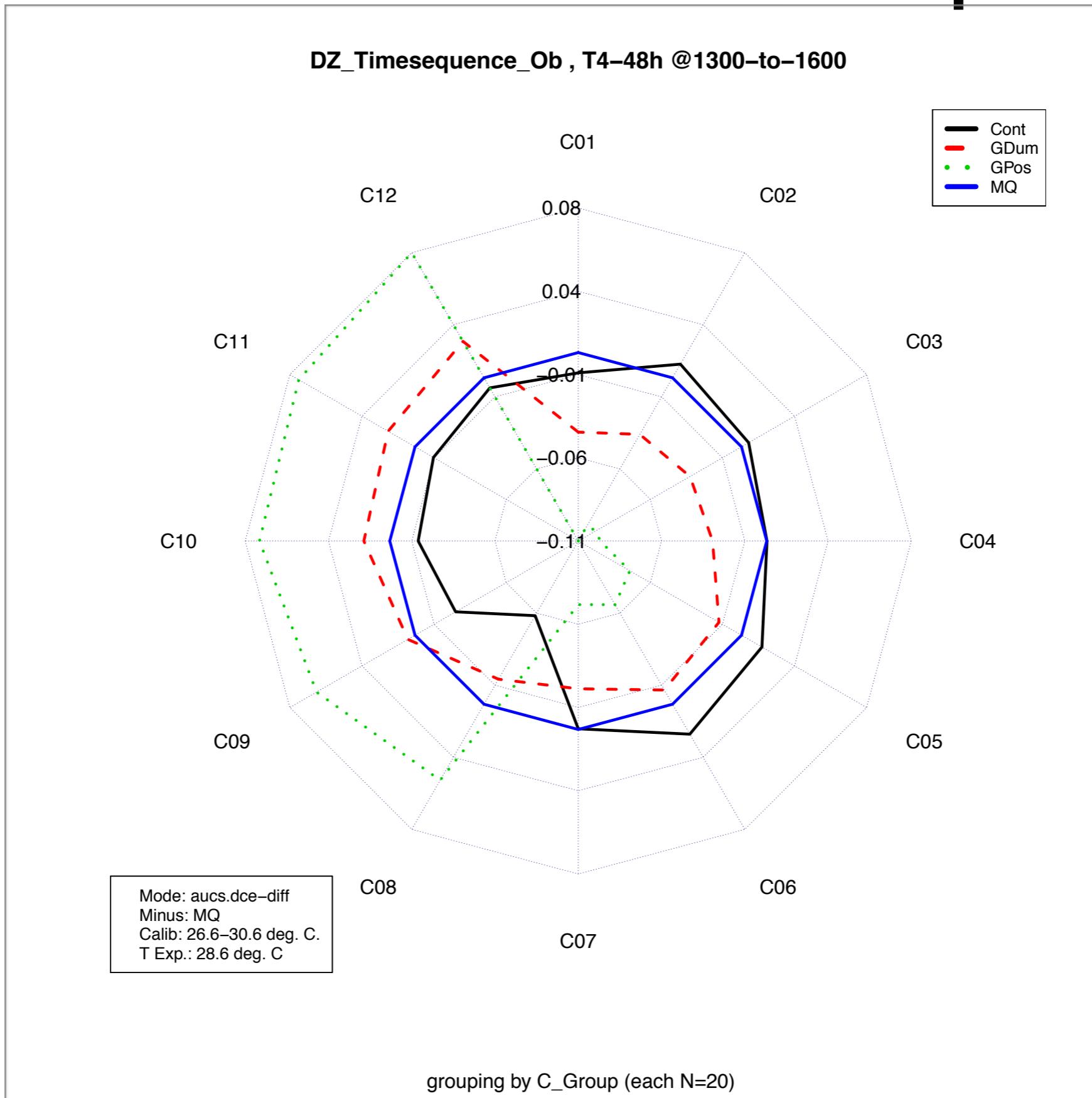
Fix Scale - Time Resolved Experiments



Fix Scale - Time Resolved Experiments



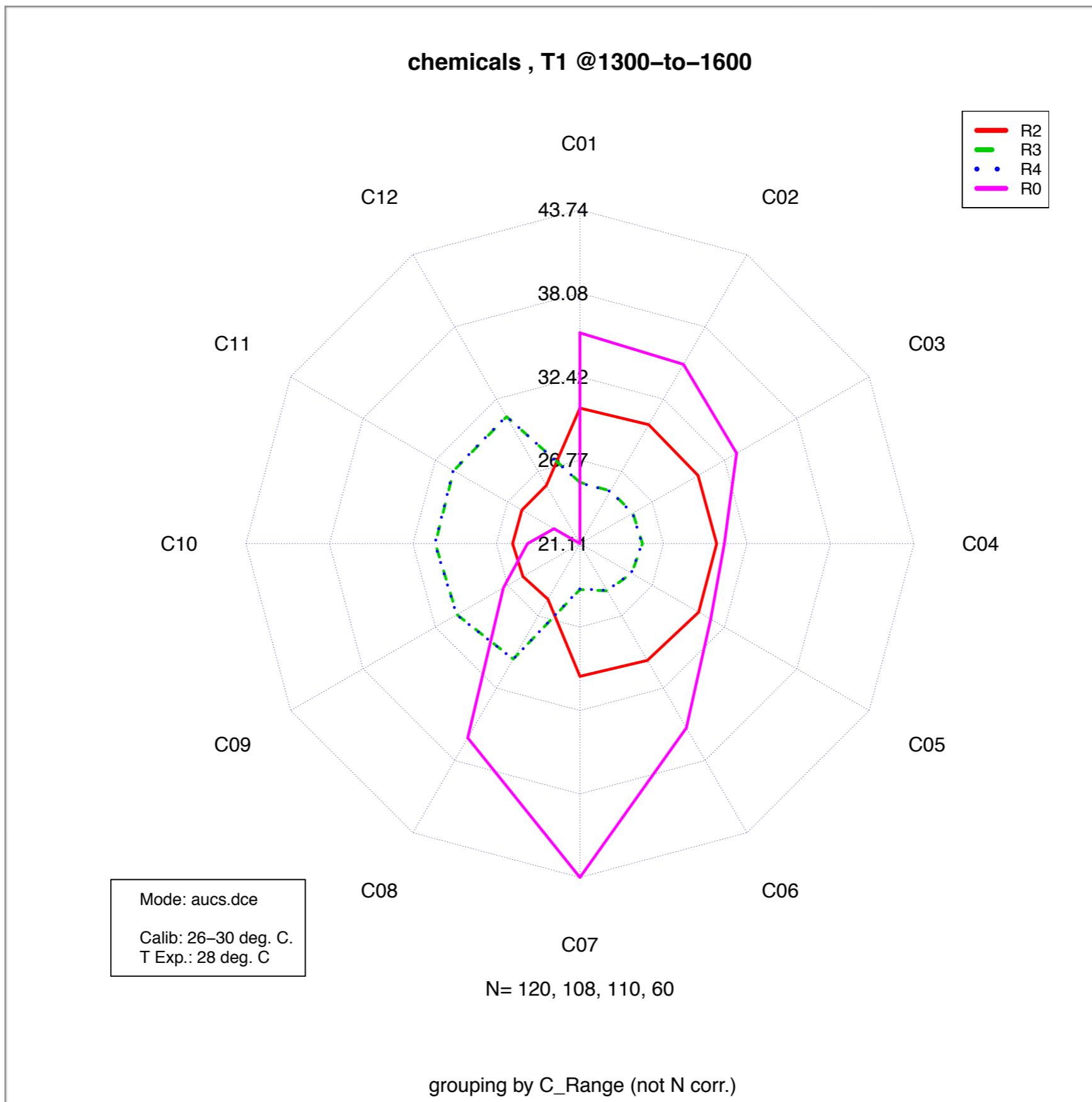
Fix Scale - Time Resolved Experiments



Confidence Intervals: Visualizing Significant Differences

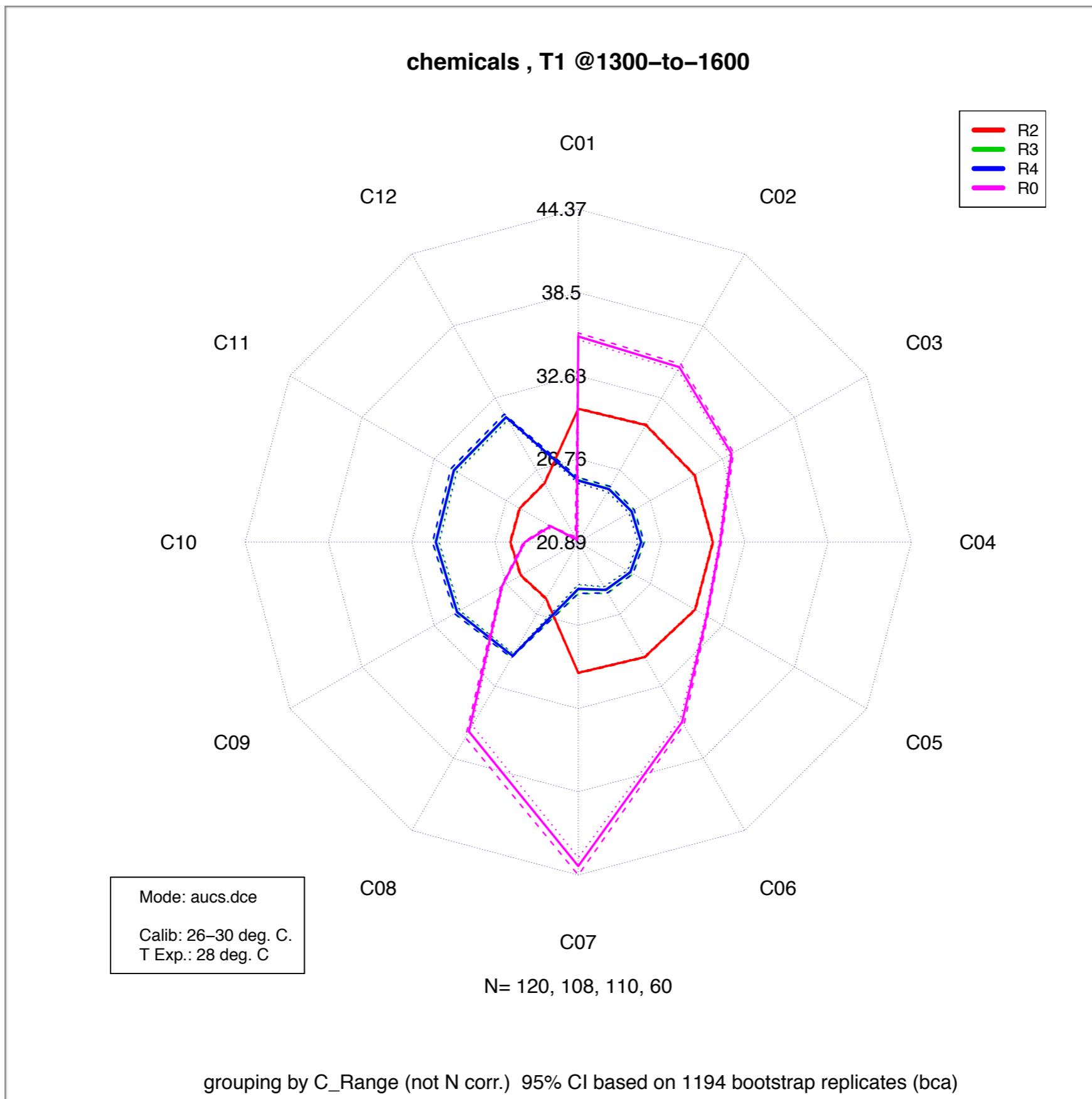
KCl & NaCl Solutions — Displaying Averages

Strong Separation between Groups



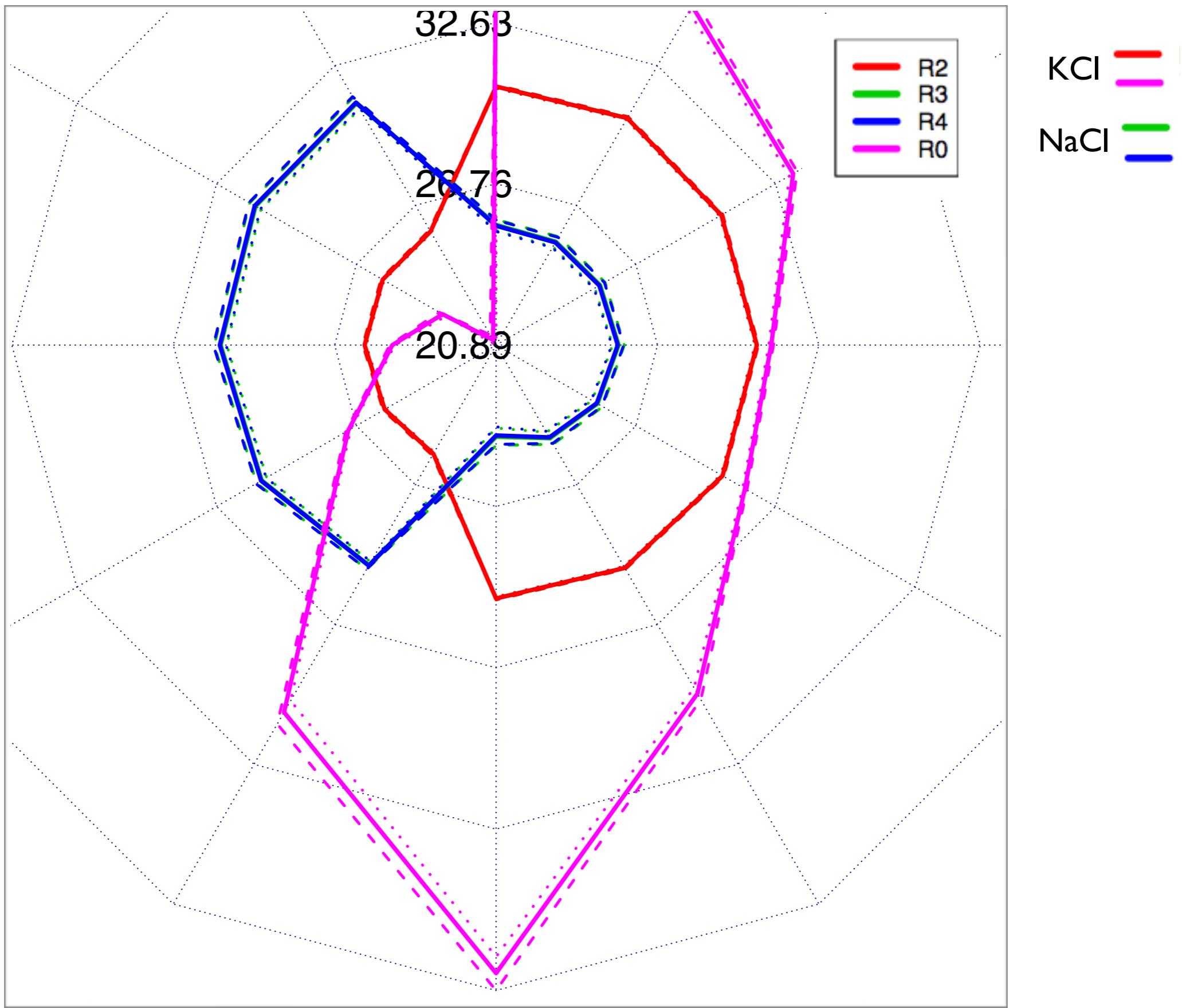
KCl & NaCl Solutions — Displaying Conf. Int.

Strong Separation between Groups



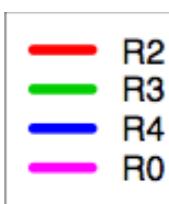
KCl & NaCl Solutions — Displaying Conf. Int.

Strong Separation between Groups



KCl & NaCl Solutions — Displaying Conf. Int.

Strong Separation between Groups

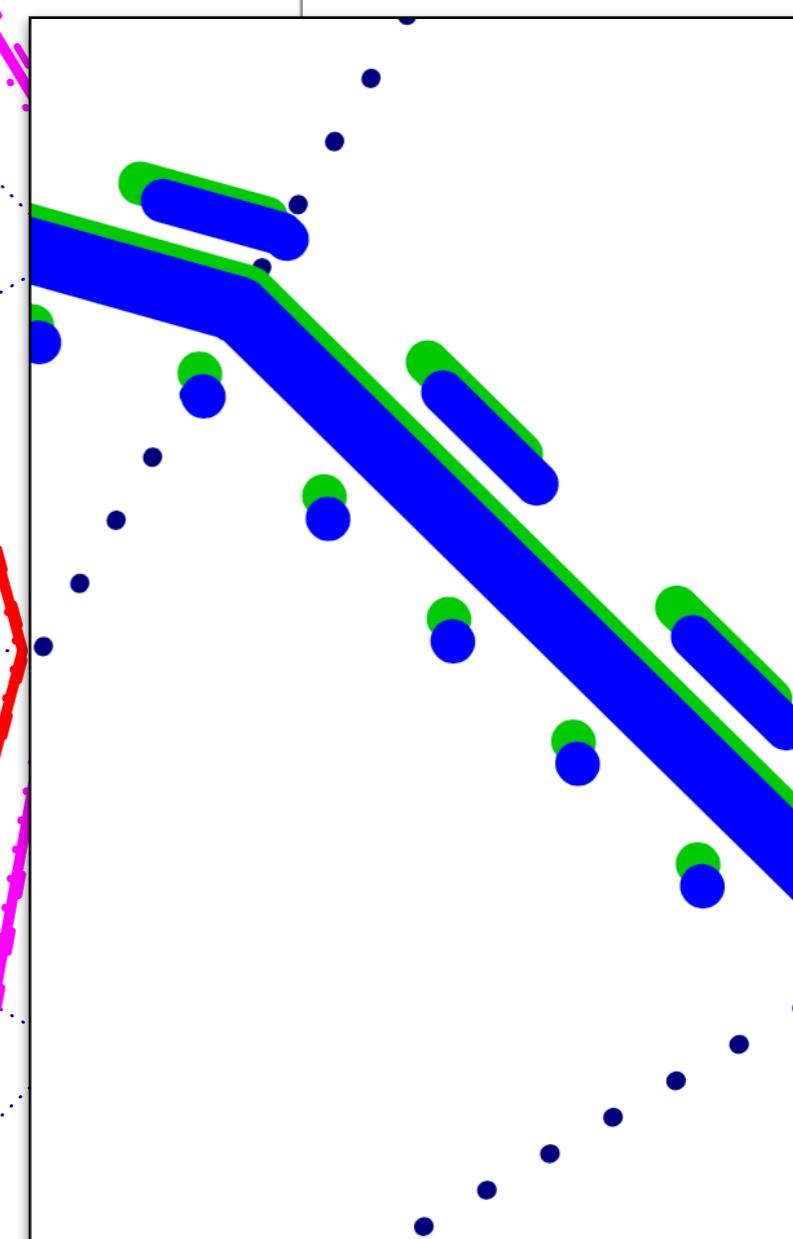


KCl

NaCl

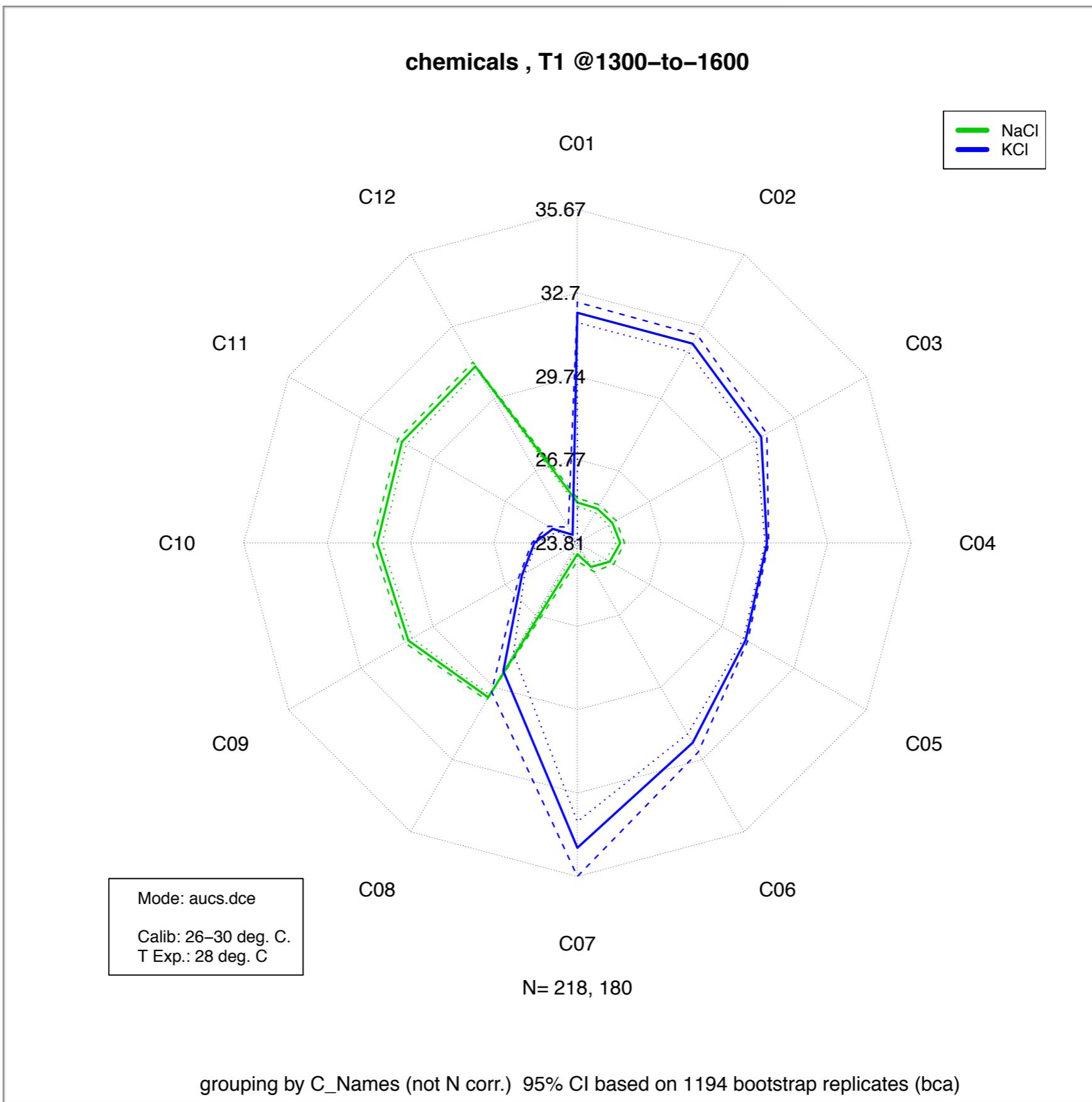
26.76

20.89



KCl & NaCl Solutions — (Conf. Int.)

Strong Separation between Groups

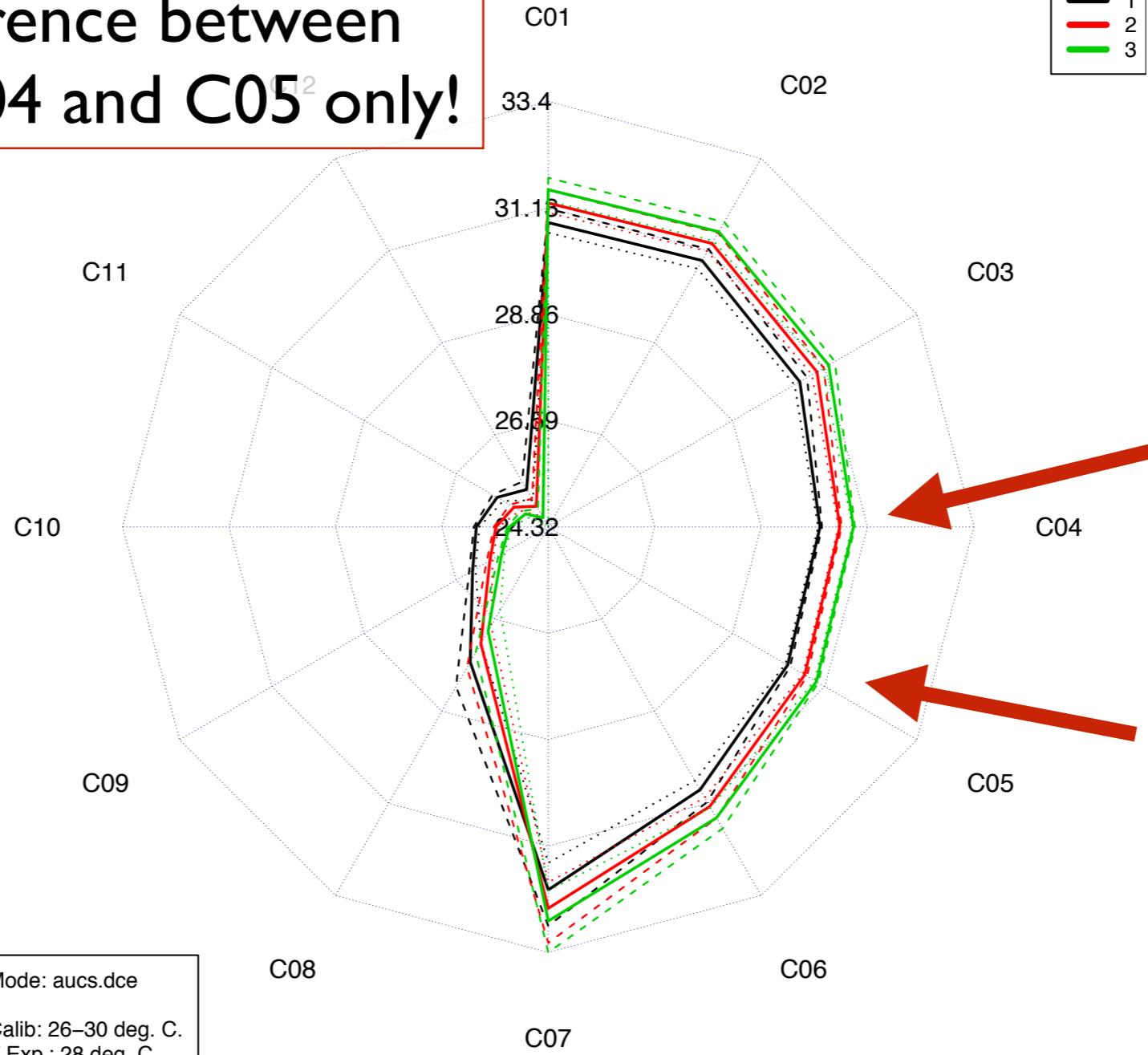


KCl Solutions — Group by Consec. Scan

Significant difference between
Cons. Scans in C04 and C05 only!

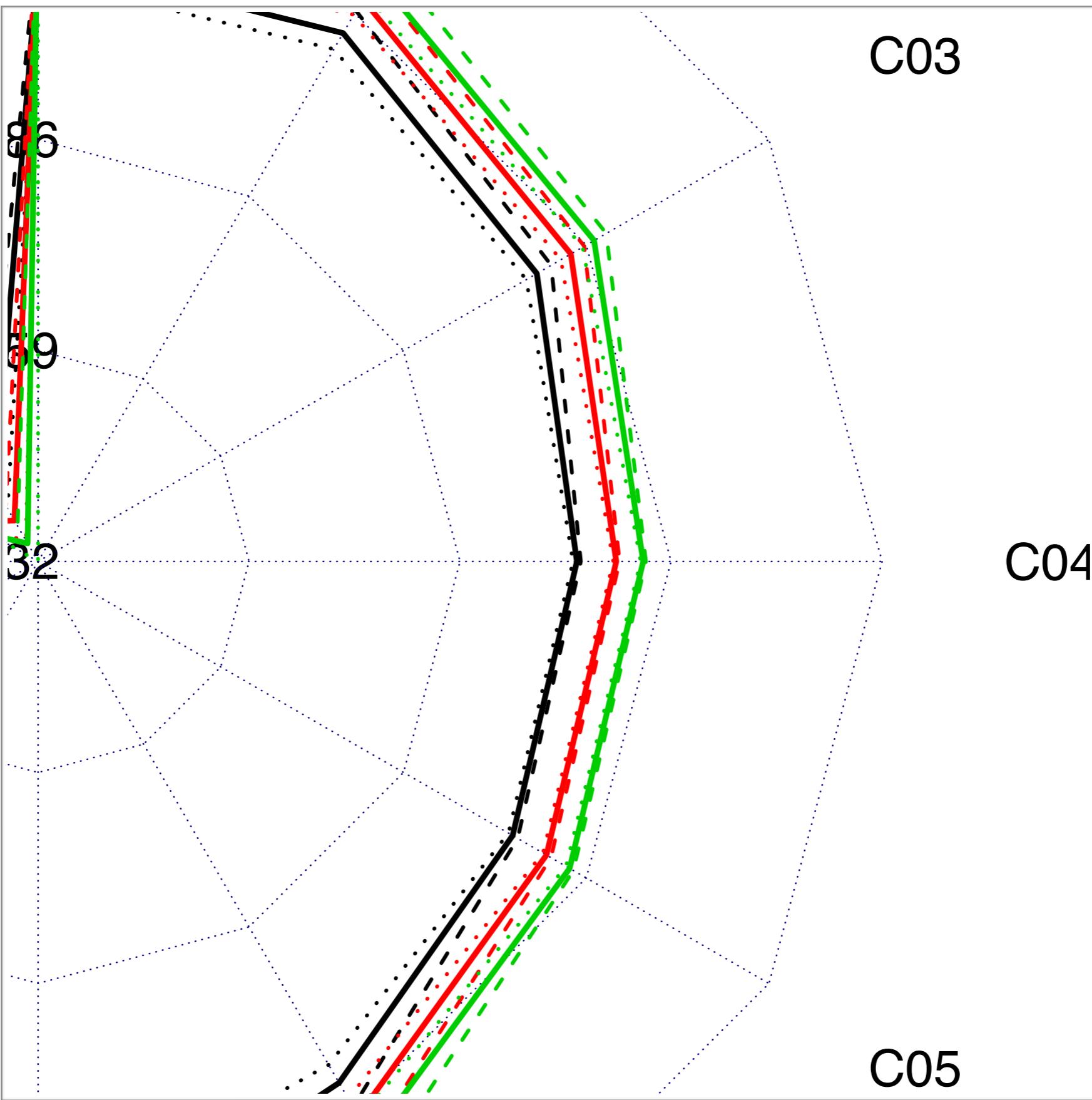
chemicals only KCl, T1 @1300-to-1600

— 1
— 2
— 3



grouping by C_conSNr (each N=176) 95% CI based on 1584 bootstrap replicates (bca)

KCI Solutions — Group by Consec. Scan

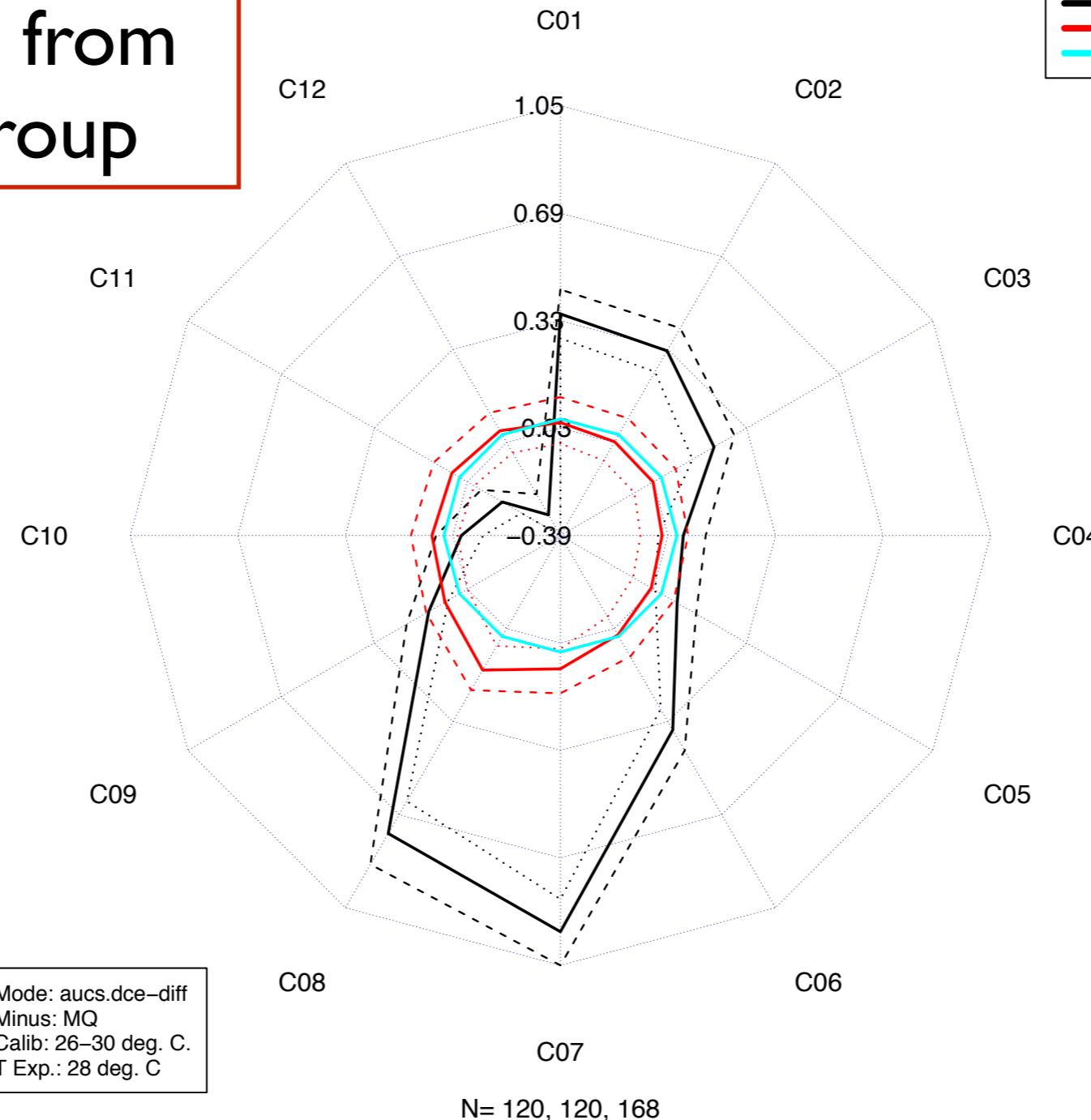


Low Concentration KCl Solutions — Mode: auc_S.dce-diff

Subtract MilliQ from
every other group

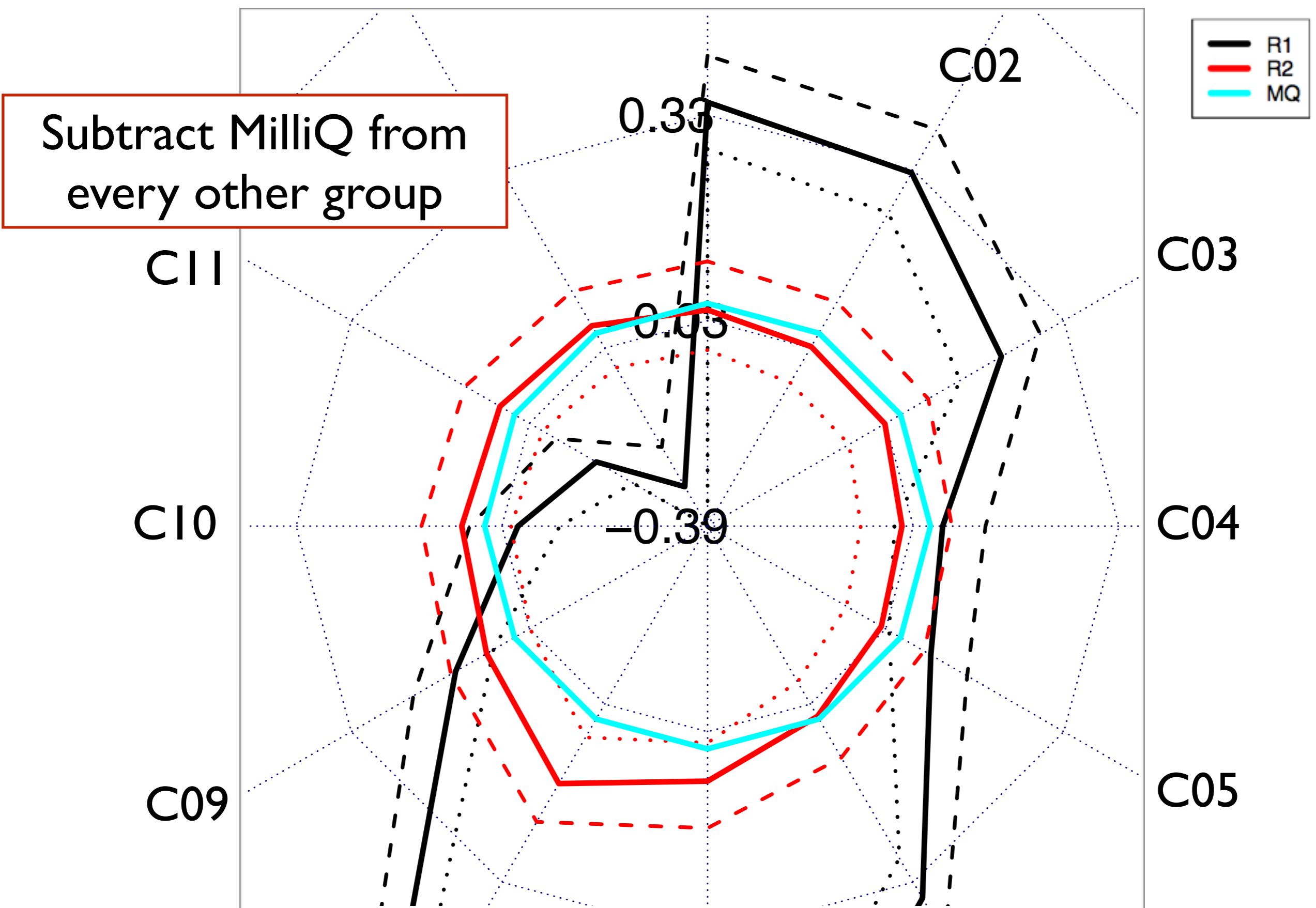
chemicals KCl, only MQ and R2, T1 @1300-to-1600

R1
R2
MQ



grouping by C_Range (not N corr.) 95% CI based on 1224 bootstrap replicates (bca)

Low Concentration KCl Solutions — Mode: auc*s*.dce-diff



!!! All this is at YOUR Fingertips !!!

With our R-Package
aquap2

Just two lines away:

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

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

or, go to <http://aquaphotonics.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

