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

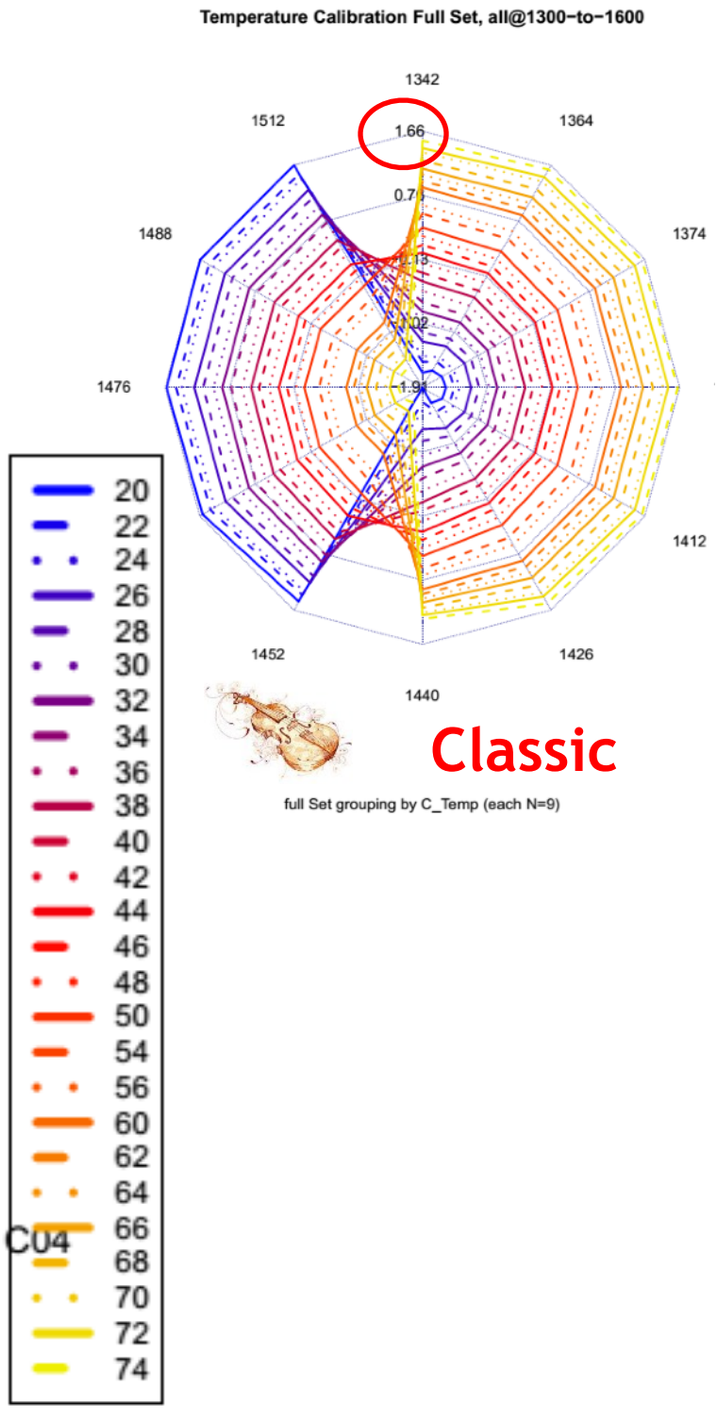
Fix Scale

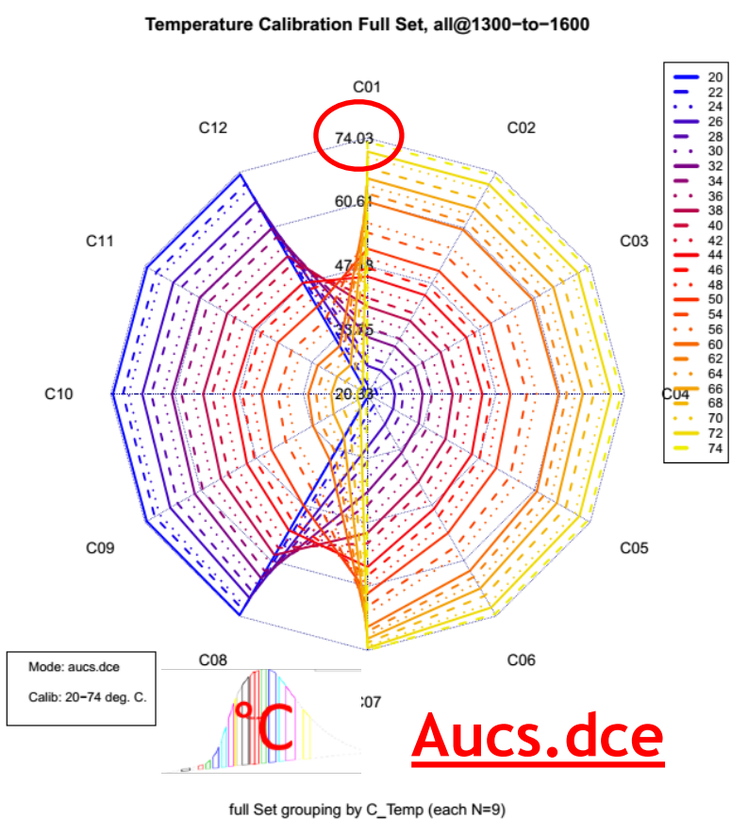
- time resolved experiments - compare across time
- same shape as the classical mode, but
  - now we have the added benefit of a meaningful scale, which is
  - an independent temperature scale (the differences in the aquagram can be translated to the effect of temperature);
- additional benefit: the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

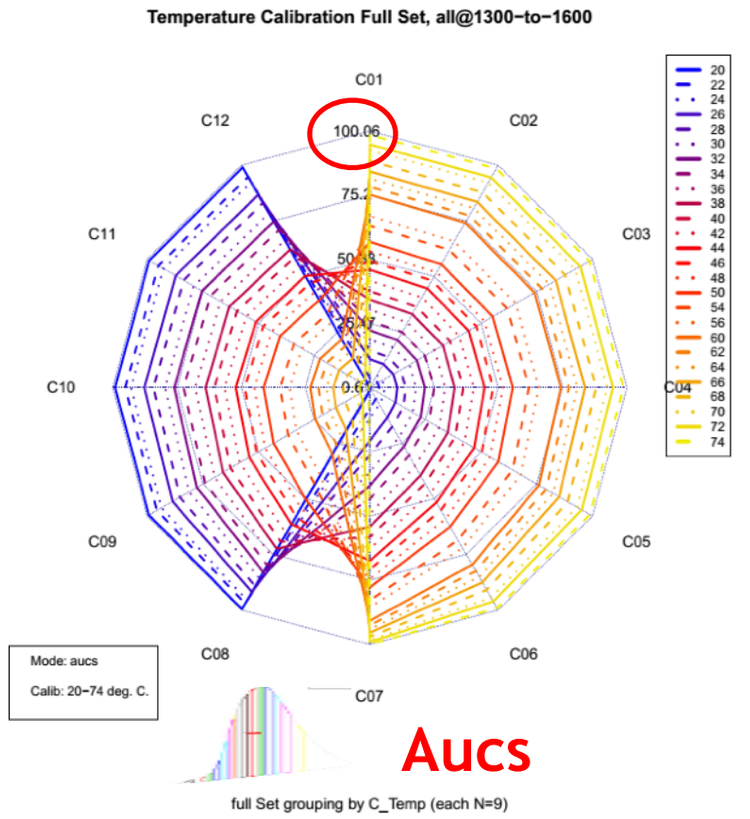
Confidence Intervals

- well… 

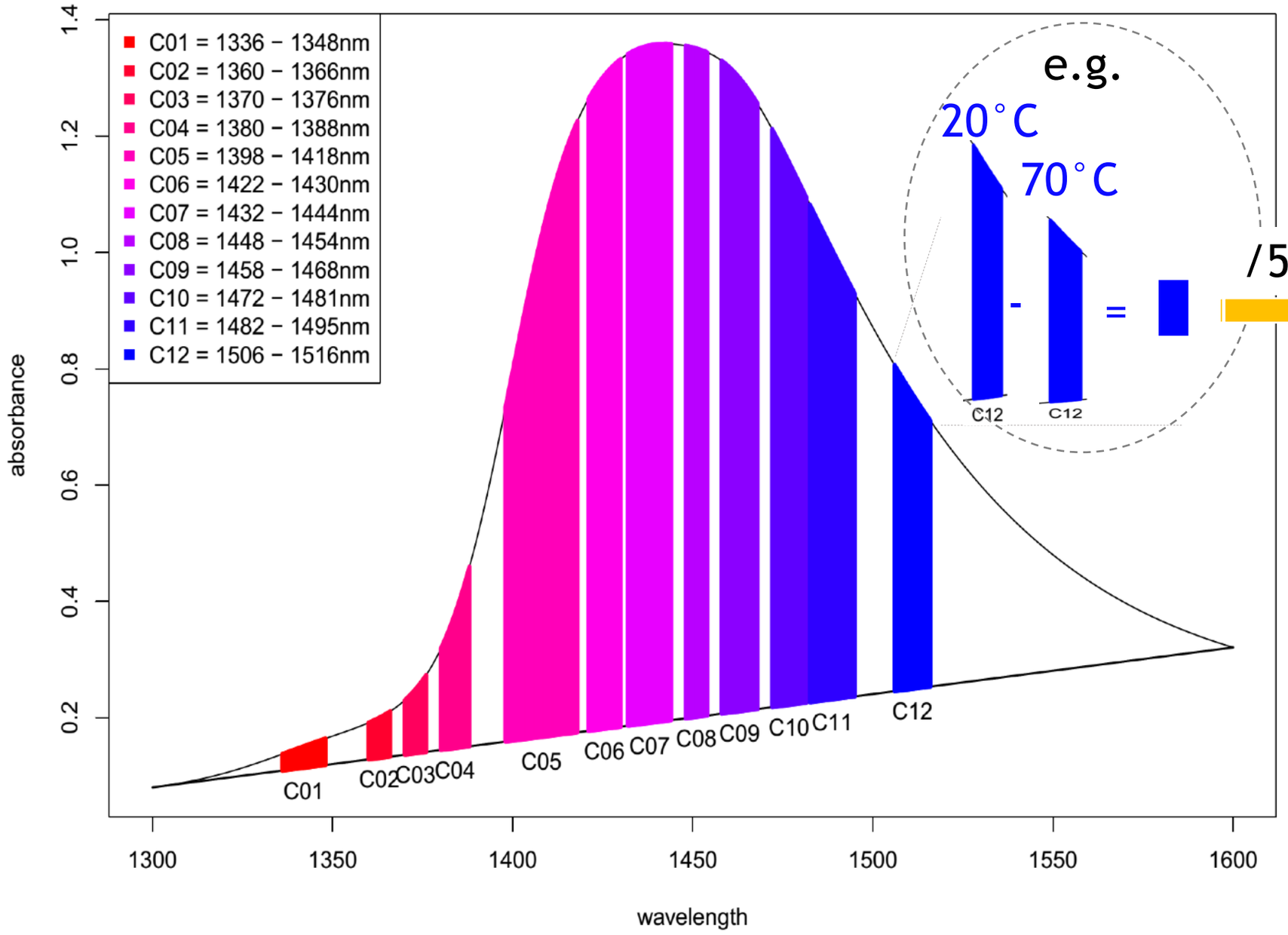
20-74°C, average







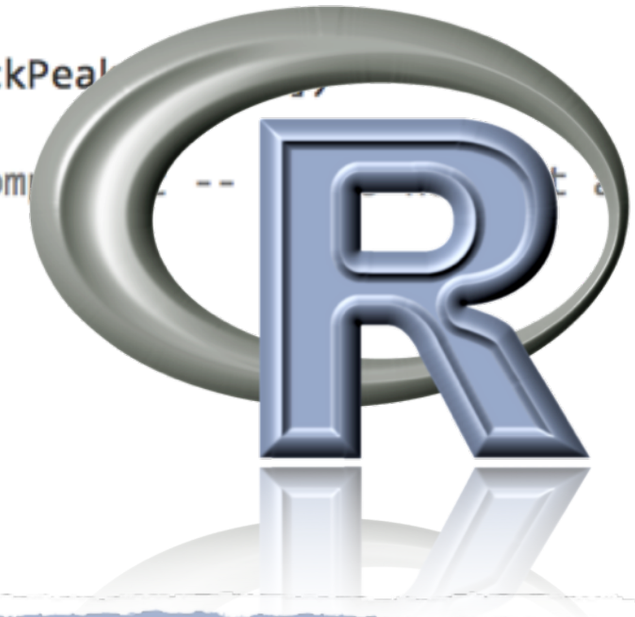
Scheme of the calculation for Area under the curve (AUC) aquagram method



area change at C12 by 1°C

compare to the change of perturbation

The areas under the specific WAMACS are calculated and expressed in relation to the area change occurred by different temperature



MVA package with additional focus on Aquaphotomics

„aquap2“

Quick Update — How to Install / Update the package „aquap2“

<u>For those who were at the workshop on Saturday:</u>

library(aquap2)

updateAquap2()

updateAquap2(TRUE)

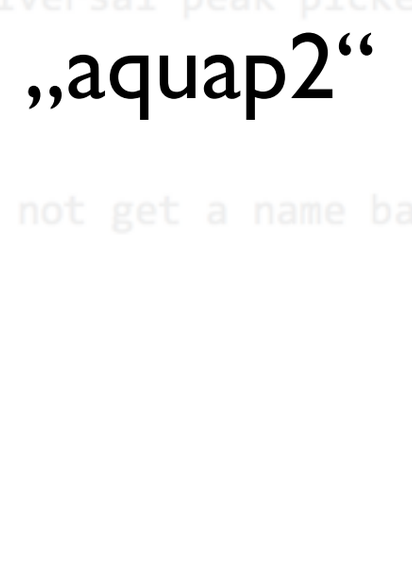
<u>For new (or re-)installing:</u>

- http://aquaphotomics.com
- download and follow the instructions in the file
  (~ 3 min until up and and running!)

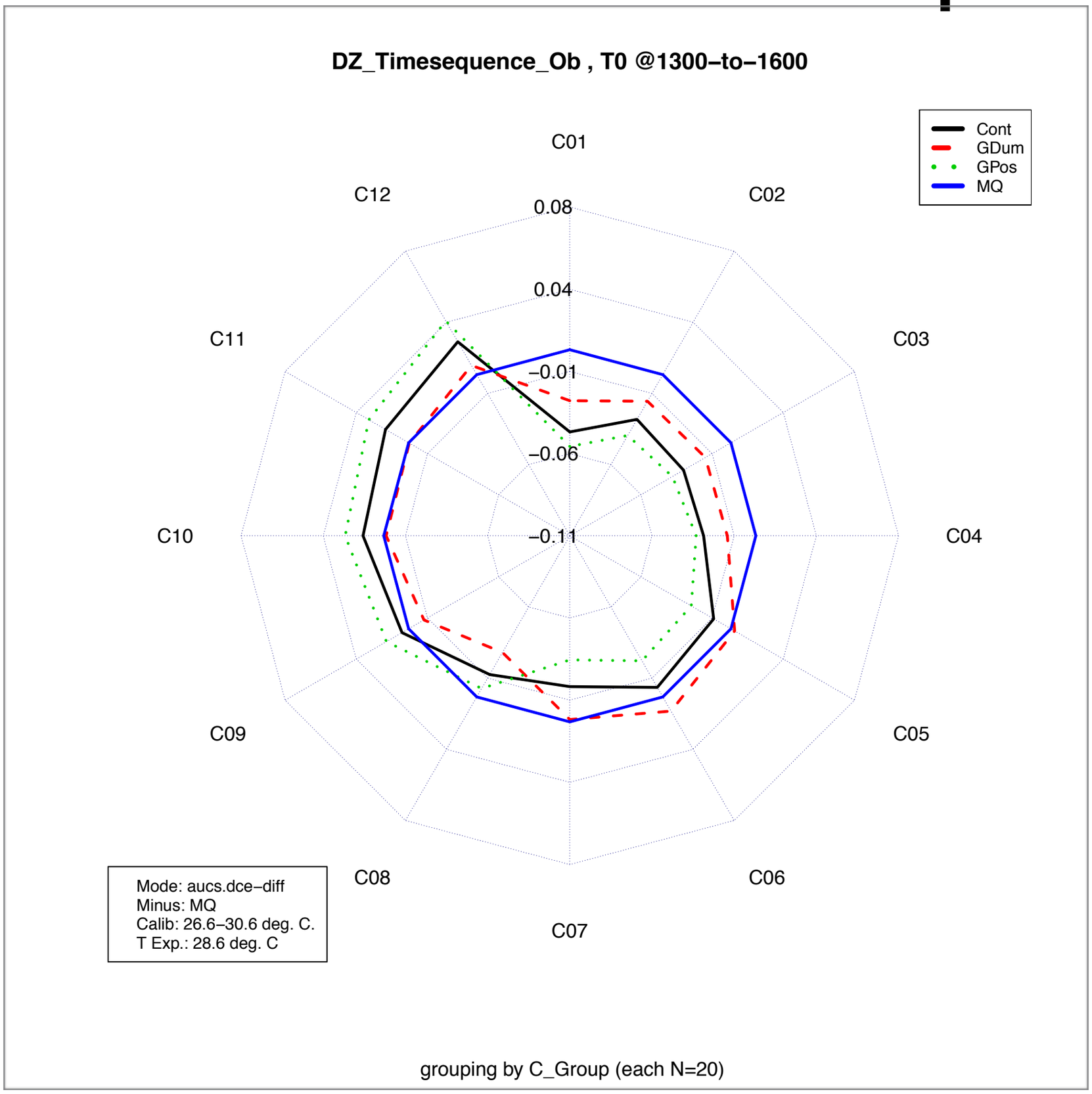
AQUAPHOTOMICS: UNDERSTANDING WATER in BIOLOGY
2nd INTERNATIONAL SYMPOSIUM
@ Kobe University, Kobe, Japan

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



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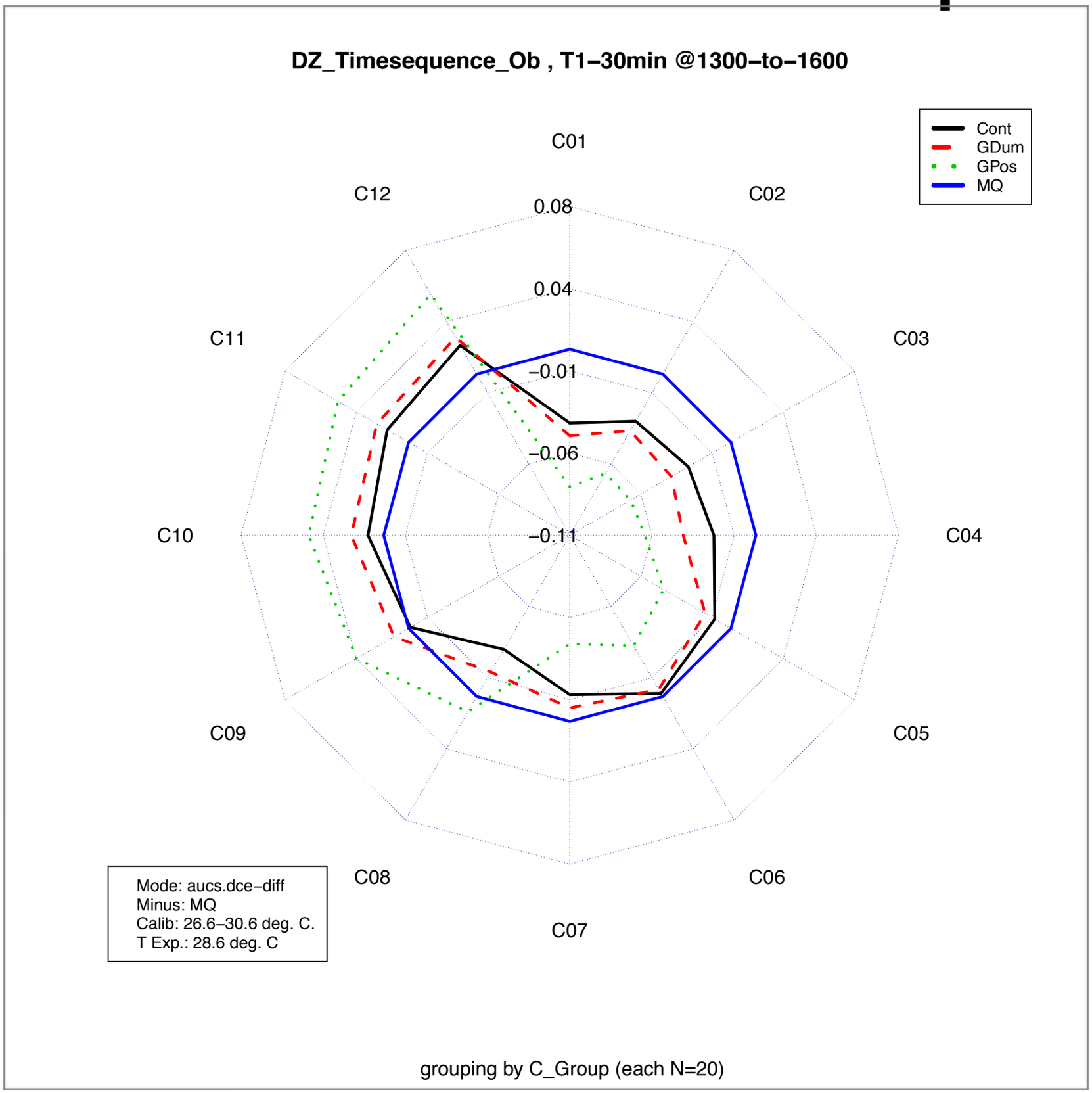

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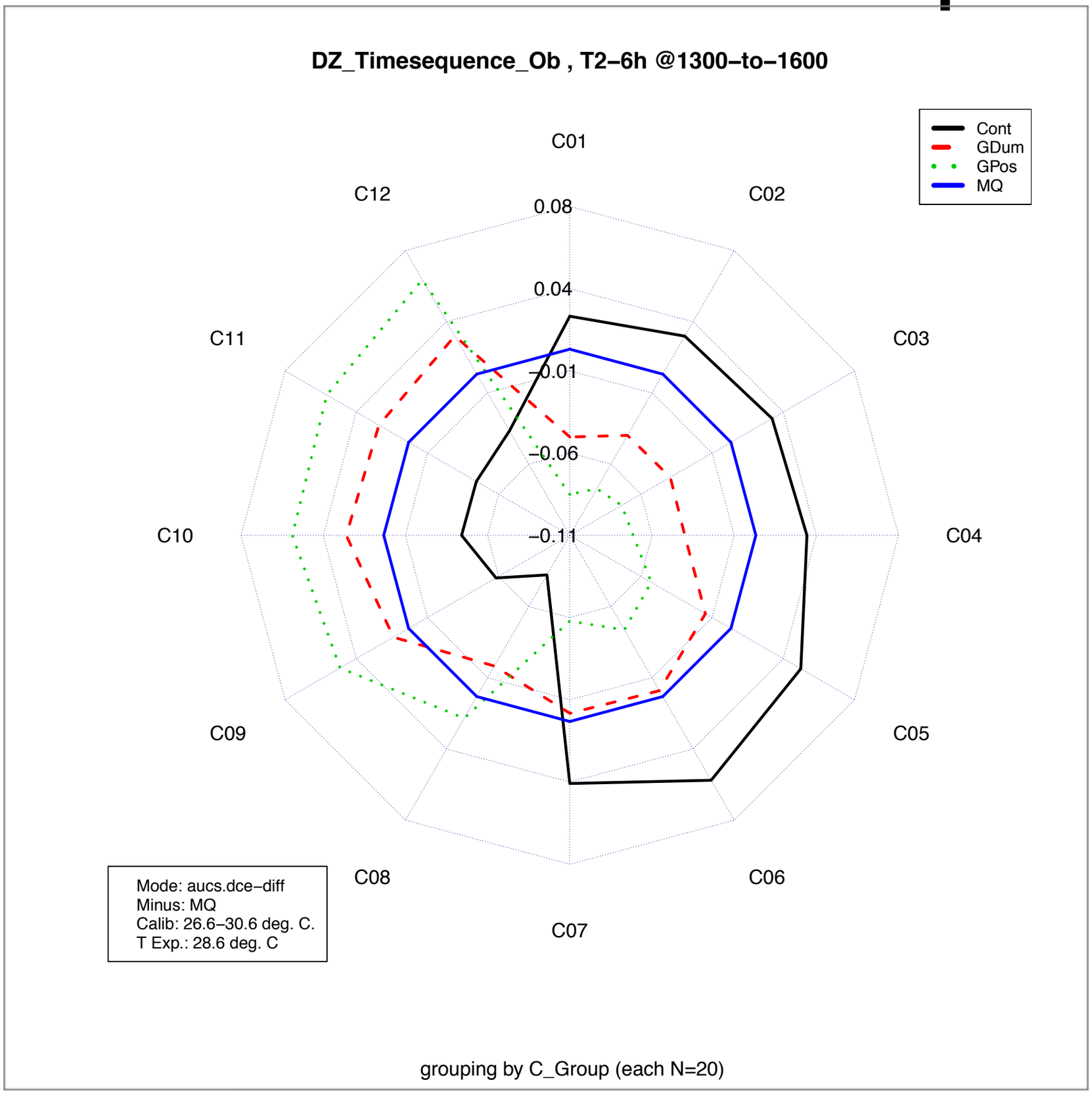

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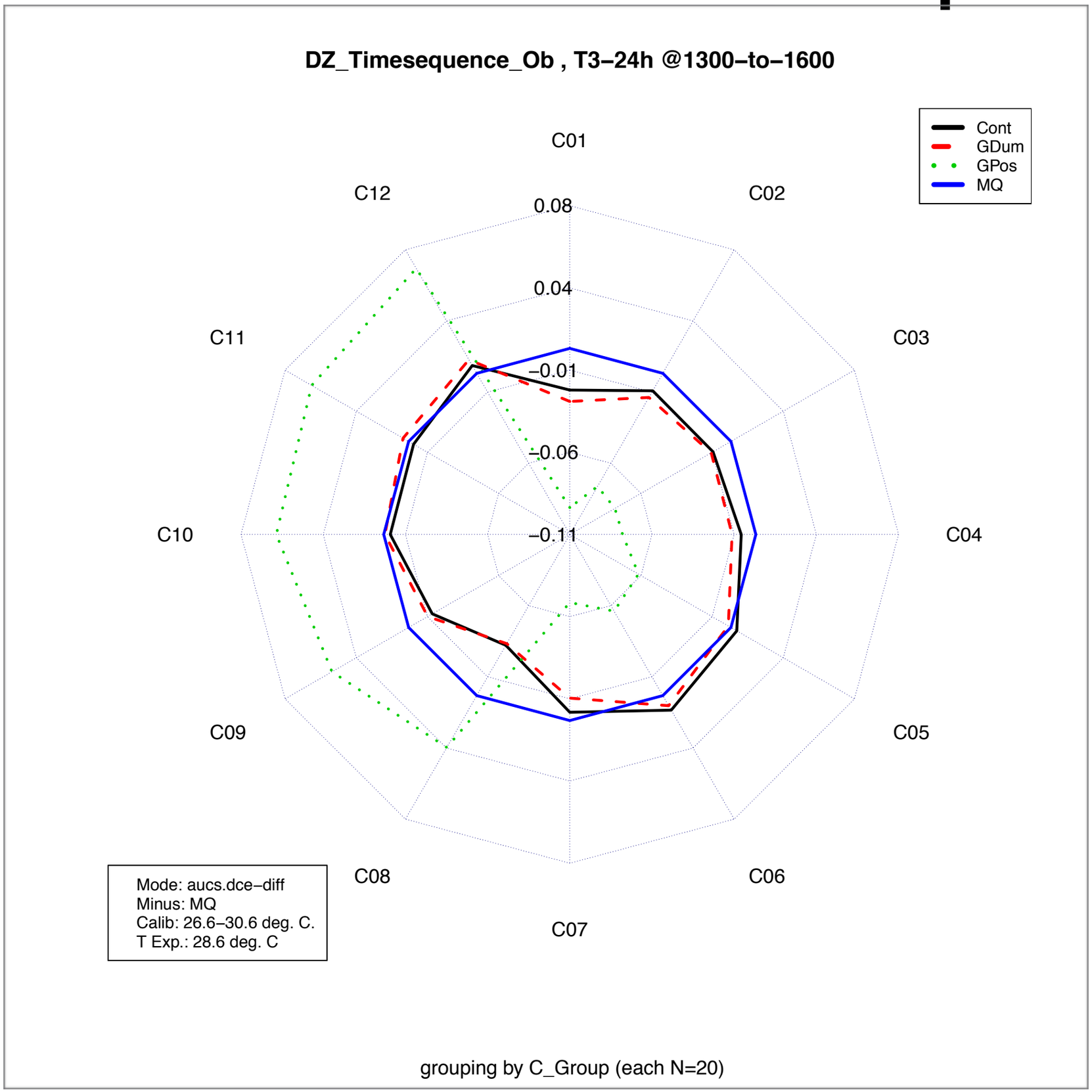

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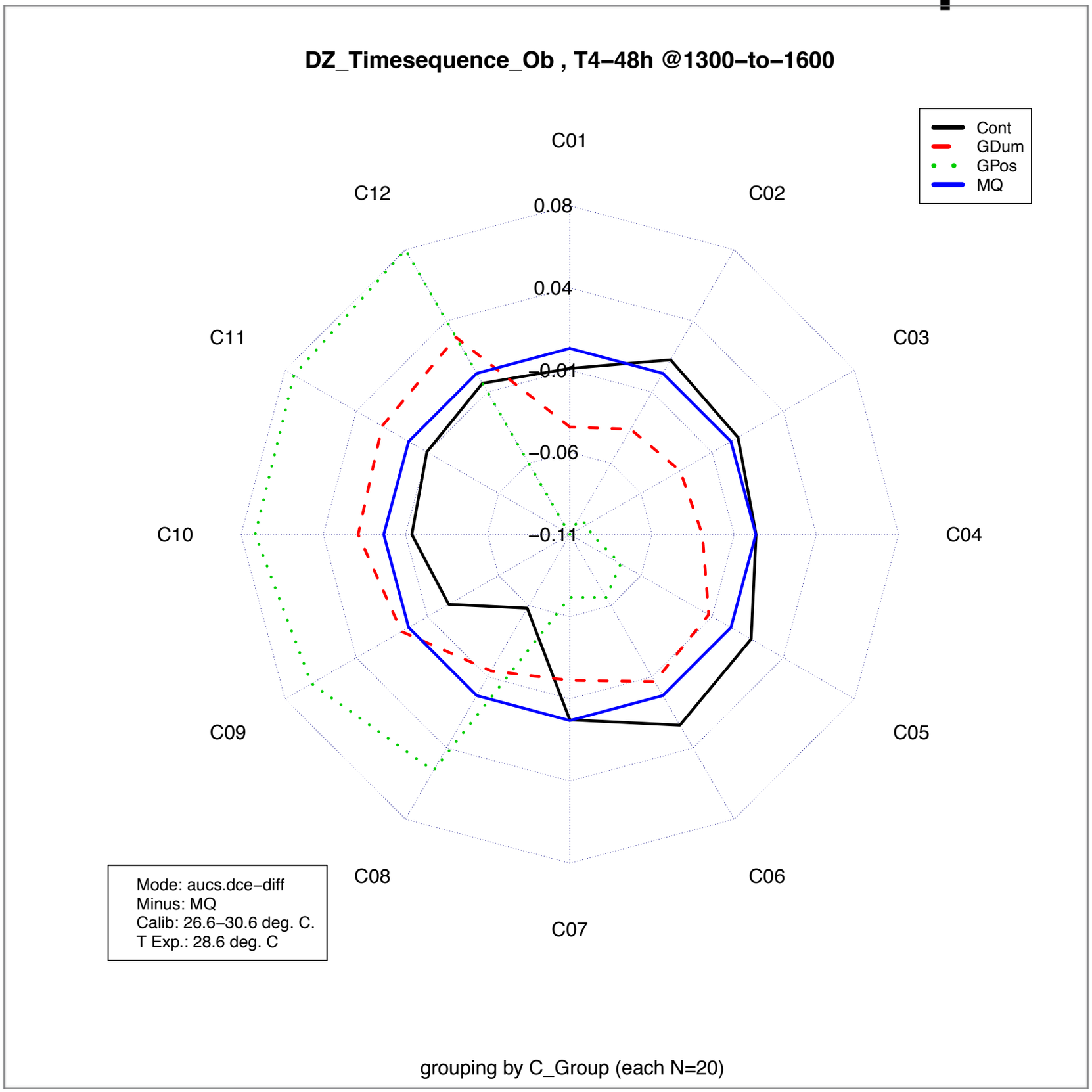
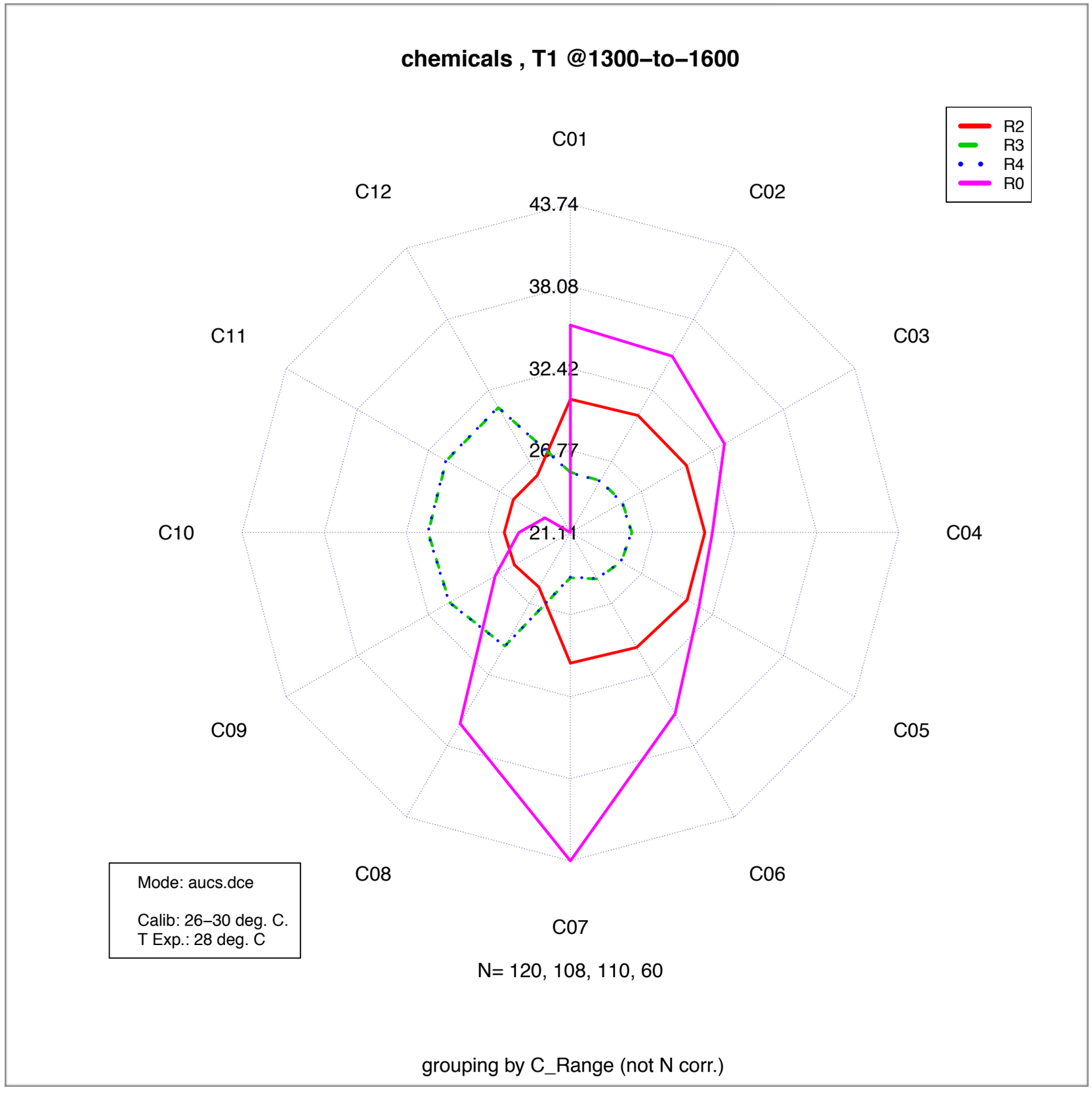


Confidence Intervals:
Visualizing Significant Differences

KCl & NaCl Solutions — Displaying Averages

Strong Separation between Groups

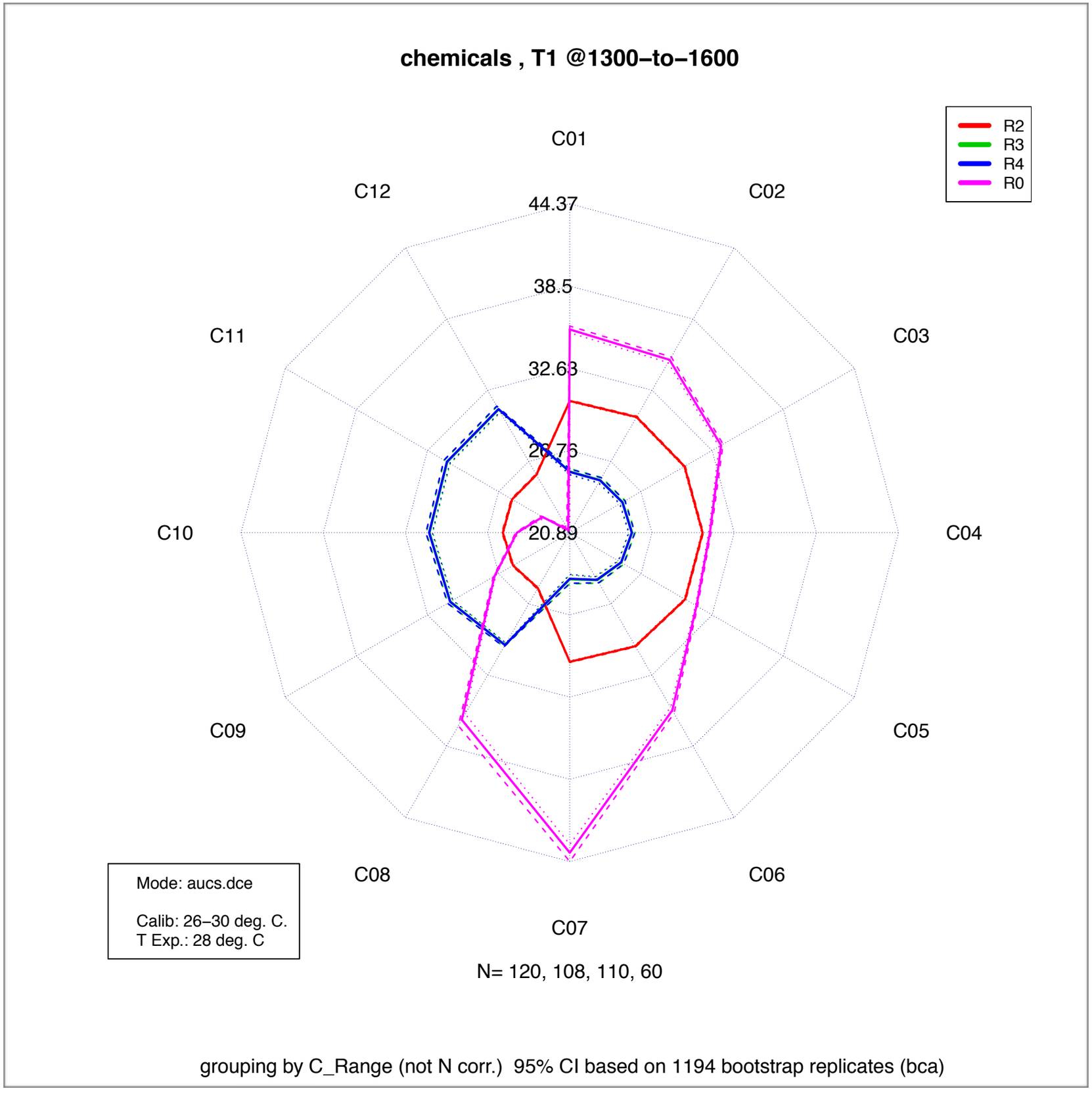


KCl

NaCl

KCl & NaCl Solutions — Displaying Conf. Int.

Strong Separation between Groups



KCl

NaCl

KCl & NaCl Solutions — Displaying Conf. Int.

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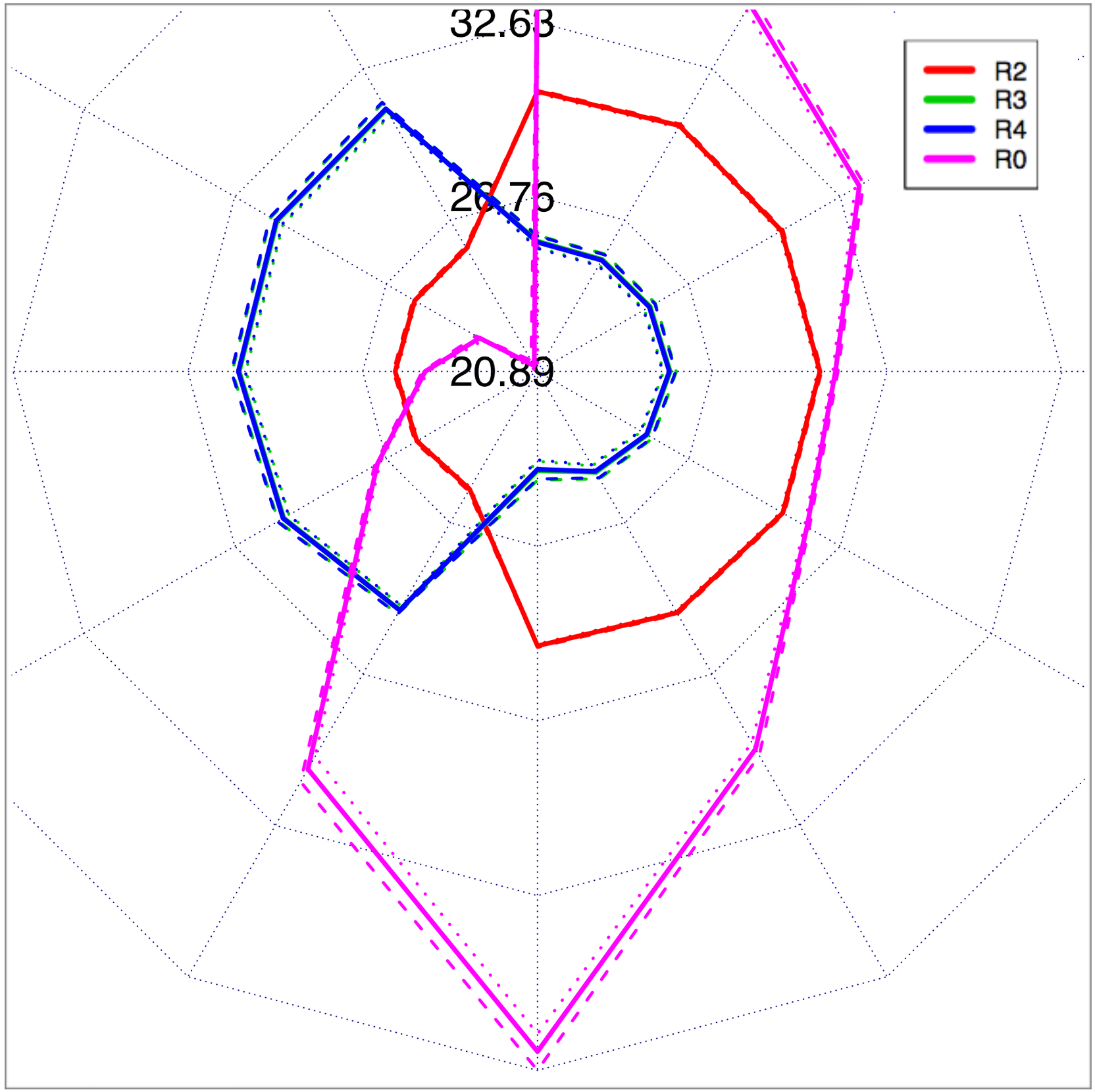
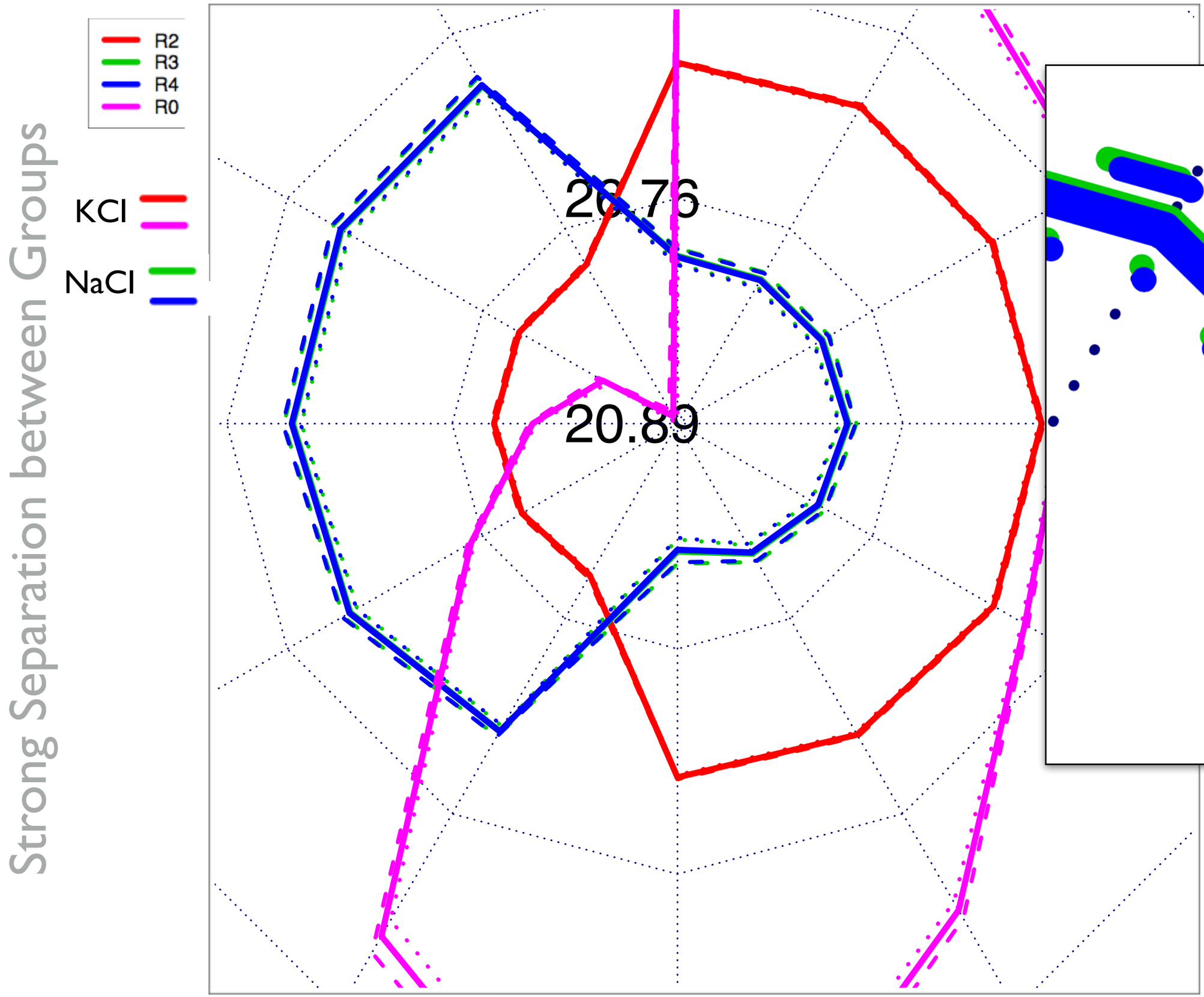
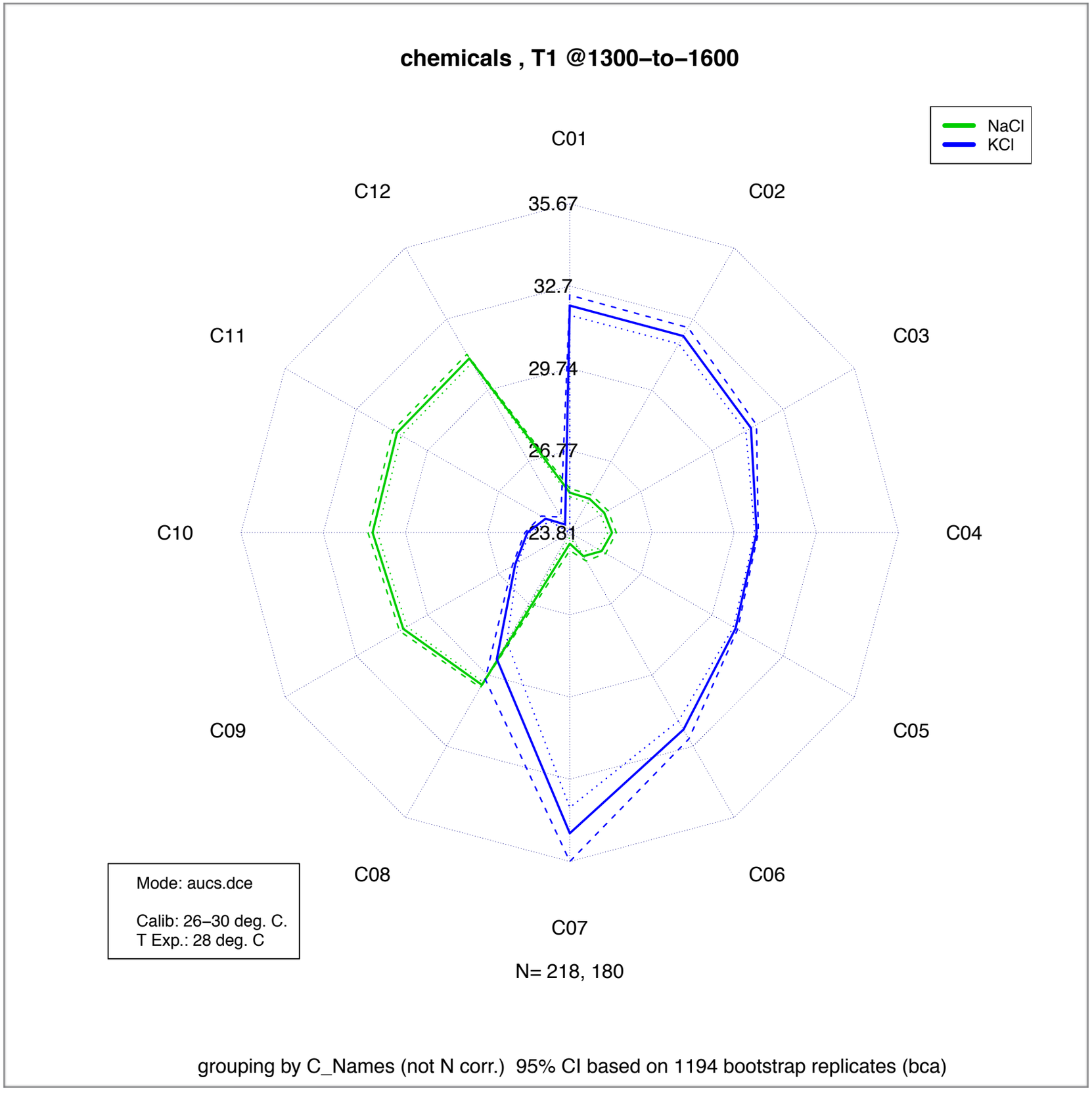


KCl & NaCl Solutions — Displaying Conf. Int.



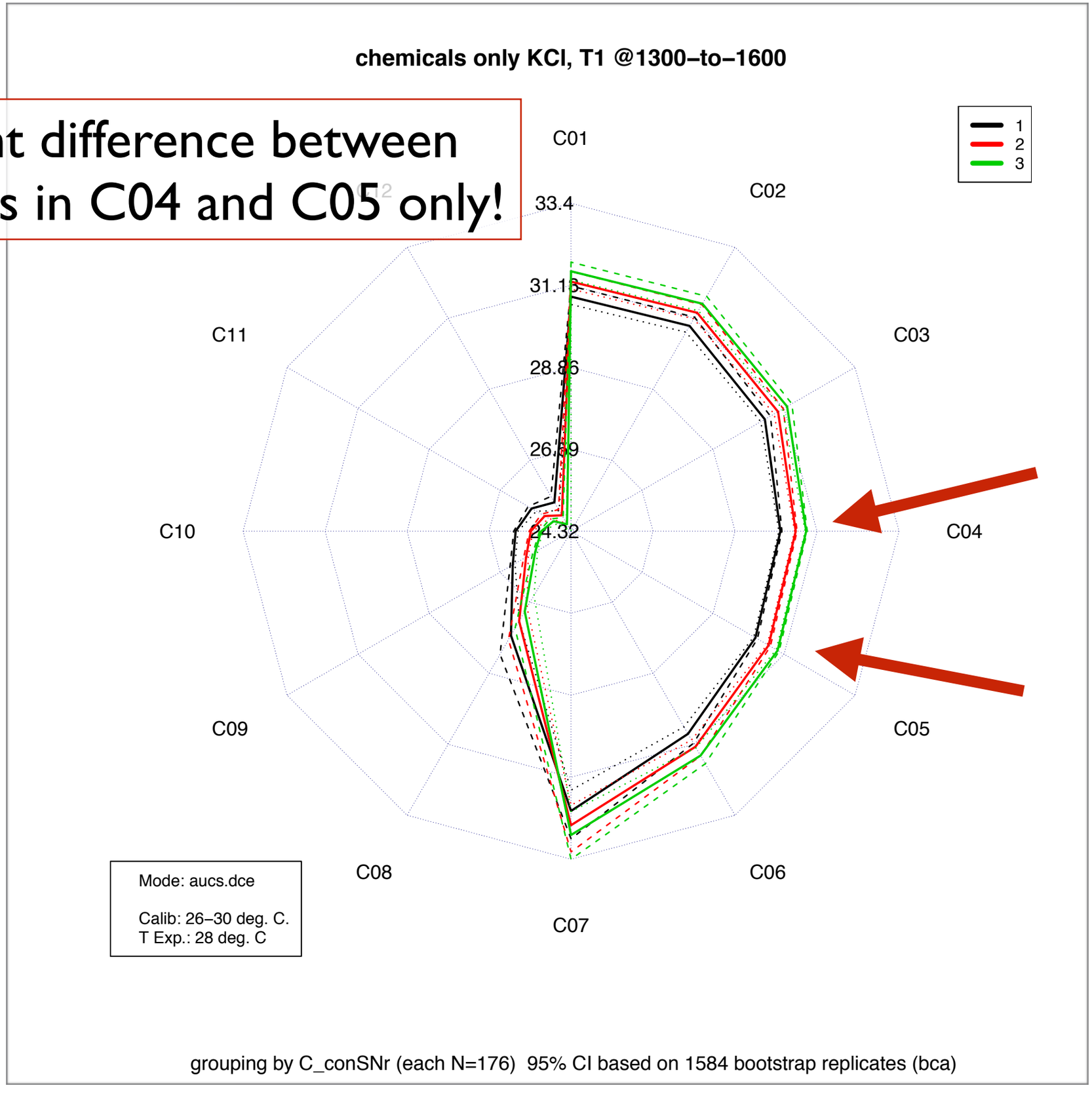
KCl & NaCl Solutions — (Conf. Int.)

Strong Separation between Groups



KCl Solutions — Group by Consec. Scan

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



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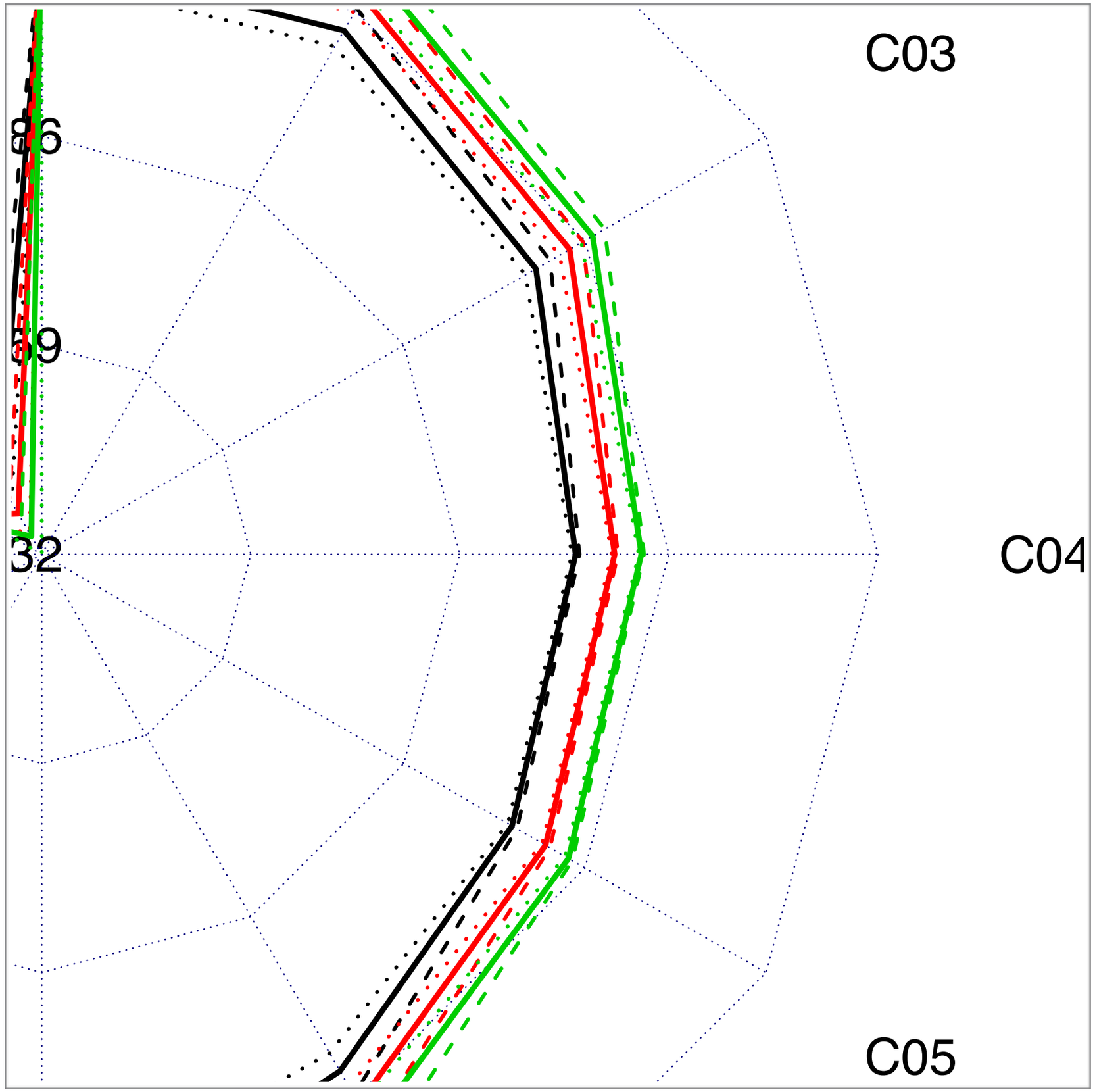
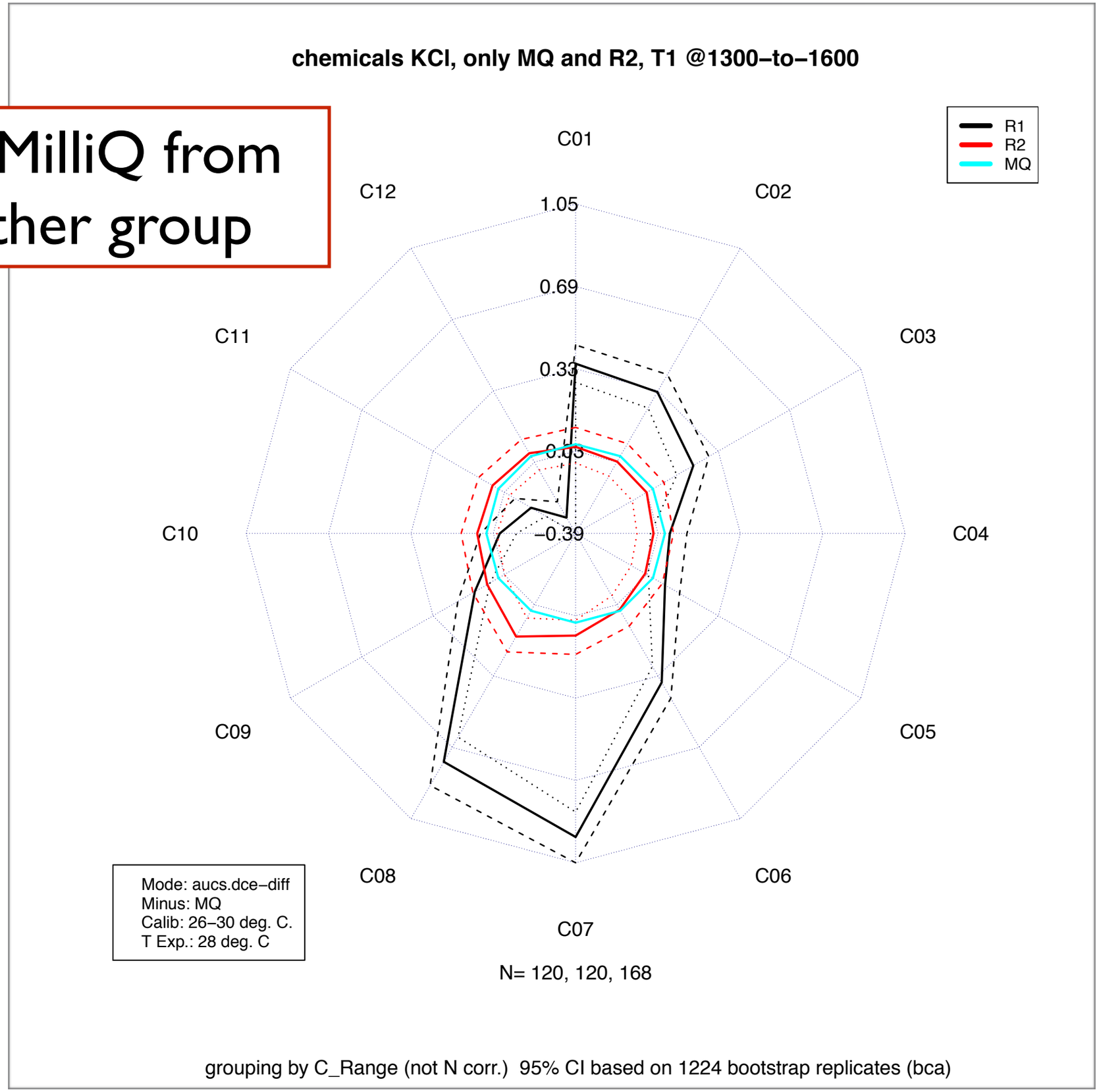


Low Concentration KCl Solutions — Mode: aucs.dce-diff

Subtract MilliQ from every other group



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

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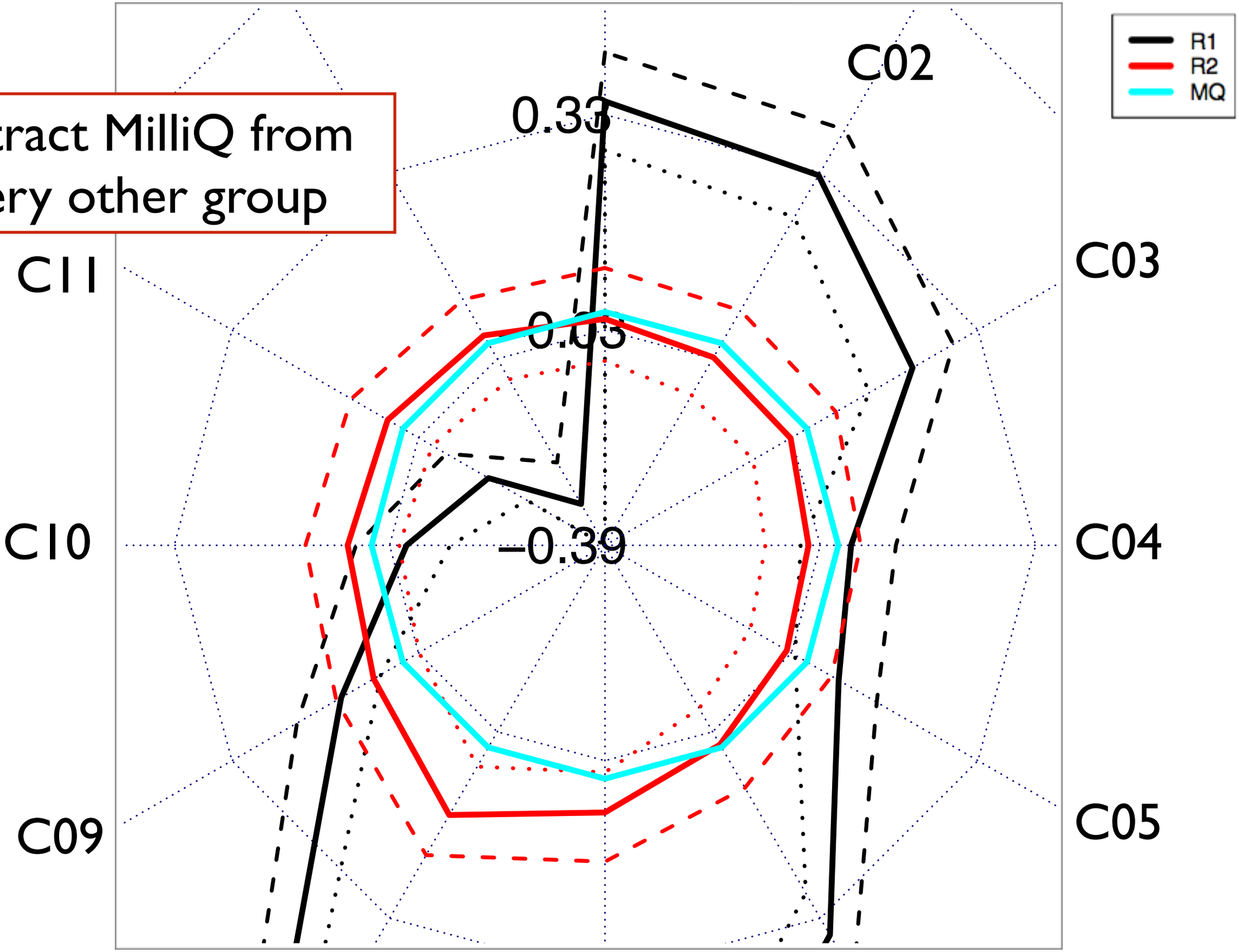

!!! All this is at YOUR Fingertips !!!

With our R-Package

aquap2

<u>Just two lines away:</u>

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://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