

AMS Blanks

Brett Longworth

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Summary of AMS blanks (JME and C1) for both machines from Sep 2014 to present. Raw ratio data are from `snics_raw`, normalized and blank corrected values are from `snics_results`. I'm still working on pulling out acetanilides that were used as test samples, so for now I'm rejecting data $F_m > 0.02$. Only targets larger than 40 μmol and from the SPL used (disregarding JME).

Data getting and munging

```
library(RODBC)
library(dplyr)
library(ggplot2)
library(knitr)
#library(ggthemr)

#ggthemr("fresh")

source("~/R/dbconfig.R") #DB connection info
#Open DB connection
db <- odbcConnect(database, uid = uid, pwd = pwd)

#Get raw blank data
c1r = sqlQuery(db, paste("
  SELECT runtime, target.tp_date_pressed, sample_name, target.tp_num, gf_co2_qty,
         he12c, he13c, d13c, he14_12, he13_12, wheel, ok_calc
  FROM snics_raw, target, graphite
  WHERE target.tp_num = snics_raw.tp_num
  AND target.osg_num = graphite.osg_num
  AND tp_date_pressed > '2014-09-01'
  AND target.rec_num = 83028
  AND graphite.gf_co2_qty > 40
  AND graphite_lab = 1
"))

acetr = sqlQuery(db, paste("
  SELECT runtime, target.tp_date_pressed, sample_name, target.tp_num, gf_co2_qty,
         he12c, he13c, d13c, he14_12, he13_12, wheel, ok_calc
  FROM snics_raw, target, graphite
  WHERE target.tp_num = snics_raw.tp_num
  AND target.osg_num = graphite.osg_num
  AND sample_name LIKE 'Acet%'
  AND tp_date_pressed > '2014-09-01'
  AND graphite.gf_co2_qty > 40
  AND graphite_lab = 1
"))

jmer = sqlQuery(db, paste("
  SELECT runtime, target.tp_date_pressed, sample_name, target.tp_num, gf_co2_qty,
         he12c, he13c, d13c, he14_12, he13_12, wheel, ok_calc
  FROM snics_raw, target, graphite
  WHERE target.tp_num = snics_raw.tp_num
  AND target.osg_num = graphite.osg_num
  AND sample_name LIKE 'JME%'
  AND tp_date_pressed > '2014-09-01'
  AND graphite.gf_co2_qty > 40
  AND graphite_lab = 1
"))
```

```

SELECT runtime, target.tp_date_pressed, sample_name, target.tp_num,
       he12c, he13c, d13c, he14_12, he13_12, wheel, ok_calc
FROM snics_raw, target
WHERE target.tp_num = snics_raw.tp_num
AND target.rec_num = 32491
AND tp_date_pressed > '2014-09-01'))

#add type columns, combine data frames
clr$type <- "C1"
acetr$type <- "Acet"
jmer$type <- "JME"
jmer$gf_co2_qty <- NA
blanks.r <- rbind(clr, acetr, jmer)
blanks.r$type <- ordered(blanks.r$type, levels = c("Acet", "C1", "JME"))

#average by target and filter
blanks.a <- blanks.r %>%
  mutate(system = ifelse(grepl("CFAMS", wheel), "CFAMS", "USAMS")) %>%
  #filter(ok_calc == 1) %>%
  group_by(tp_num, tp_date_pressed, system, type) %>%
  summarize(
    he12c = mean(ifelse(ok_calc == 1, he12c, NA), na.rm = TRUE),
    he1412 = mean(ifelse(ok_calc == 1, he14_12, NA), na.rm = TRUE),
    flagged = ( (n() - sum(ok_calc == 1)) / n()) # fraction of runs flagged
  ) %>%
  filter(he1412 < 1e-13) %>%
  mutate(c1412x = he1412 * 1e16)

###
#Get normalized blank data
###

c1 = sqlQuery(db, paste("
SELECT runtime, wheel, target.tp_date_pressed, sample_name, target.rec_num, target.tp_num, gf_co2,
       norm_ratio, int_err, ext_err, blk_corr_method, fm_corr, sig_fm_corr, ss
FROM snics_results, target, graphite
WHERE target.tp_num = snics_results.tp_num
AND target.osg_num = graphite.osg_num
AND tp_date_pressed > '2014-09-01'
AND target.rec_num = 83028
AND graphite.gf_co2_qty > 40
AND graphite_lab = 1
"))

acet = sqlQuery(db, paste("
SELECT runtime, wheel, target.tp_date_pressed, sample_name, target.rec_num, target.tp_num, gf_co2,
       norm_ratio, int_err, ext_err, blk_corr_method, fm_corr, sig_fm_corr, ss
FROM snics_results, target, graphite
WHERE target.tp_num = snics_results.tp_num
AND target.osg_num = graphite.osg_num
AND sample_name LIKE 'Acet%'
AND tp_date_pressed > '2014-09-01'
AND graphite.gf_co2_qty > 40

```

```

        AND graphite_lab = 1
    "))

#Commented out because no JME data in snics_results?
# jme = sqlQuery(db, paste("
#     SELECT runtime, wheel, target.tp_date_pressed, sample_name, target.rec_num, target.tp_num, gf_c
#         norm_ratio, int_err, ext_err, blk_corr_method, fm_corr, sig_fm_corr, ss
#     FROM snics_results, target, graphite
#     WHERE target.tp_num = snics_results.tp_num
#     AND target.osg_num = graphite.osg_num
#     AND target.rec_num = 32491
#     AND tp_date_pressed > '2014-09-01'"))

#Close DB
odbcClose(db)

c1$type <- "C1"
acet$type <- "Acet"
#jme$type <- "JME"
#jme$gf_co2_qty <- NA
blanks.n <- rbind(c1, acet)
blanks.n$type <- ordered(blanks.n$type, levels = c("Acet", "C1"))
blanks.n <- mutate(blanks.n, system = ifelse(grepl("CFAMS", wheel), "CFAMS", "USAMS"))

#combine data

blanks.as <- select(as.data.frame(blanks.a), -tp_date_pressed, -system, -type)
blanks <- left_join(blanks.n, blanks.as, by="tp_num")

blanks <- blanks %>%
  filter(norm_ratio < .05, fm_corr < .05) %>%
  mutate(merr = pmax(int_err, ext_err))
#Export data as CSV
write.csv(blanks, "blanks.csv")

```

Summary

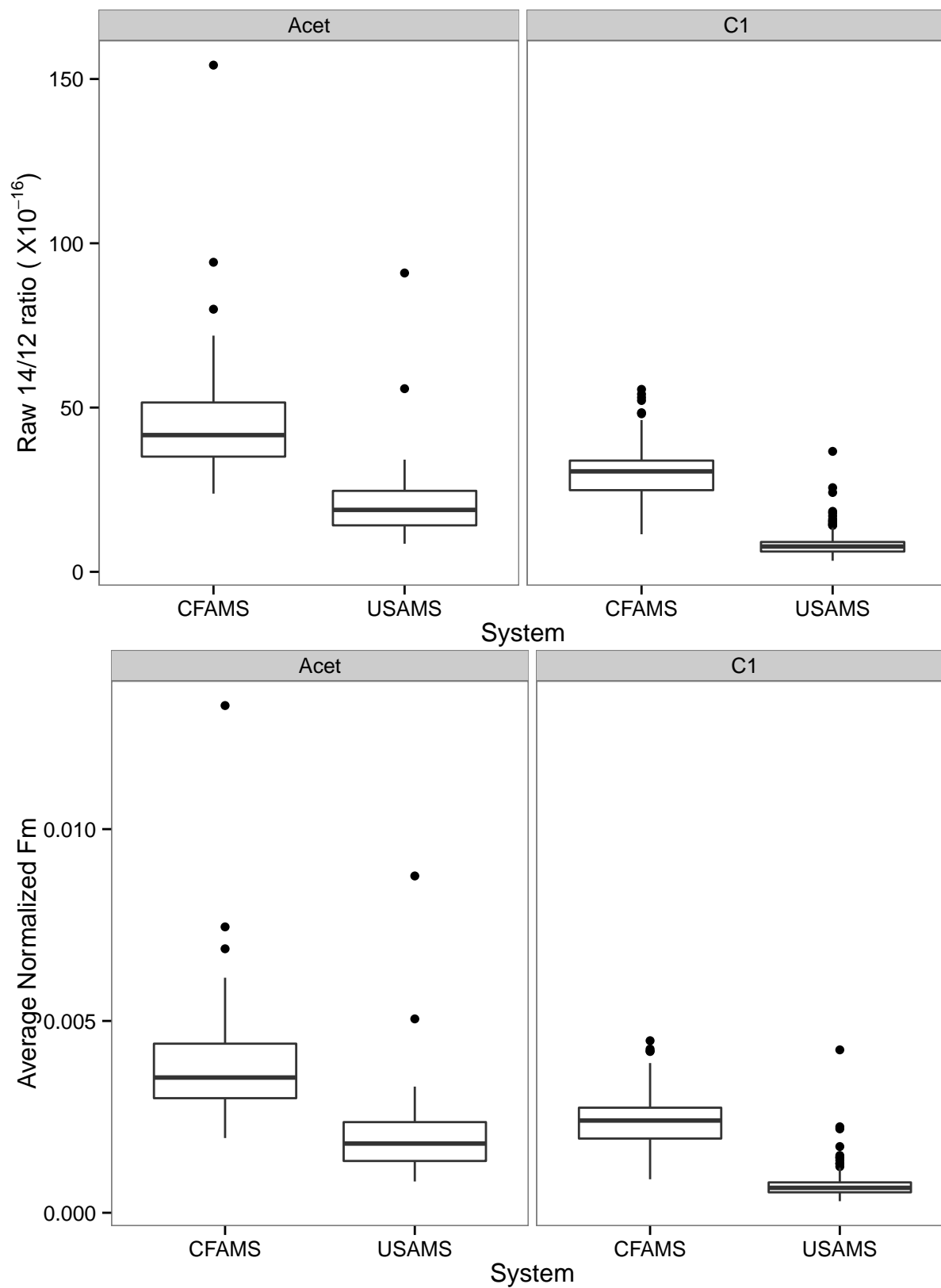
Raw data (Raw1412, Raw1412.sd) are means by target of accepted (unflagged) points. Points above 1e-14 removed. normFm, normFm.sd, and normFm.err are the mean normalized Fm, standard deviation of norm Fm, and mean reported error of normalized blanks. BlkCorrFm is the mean blank Fm after normalization and blank correction. This should distribute around 0.

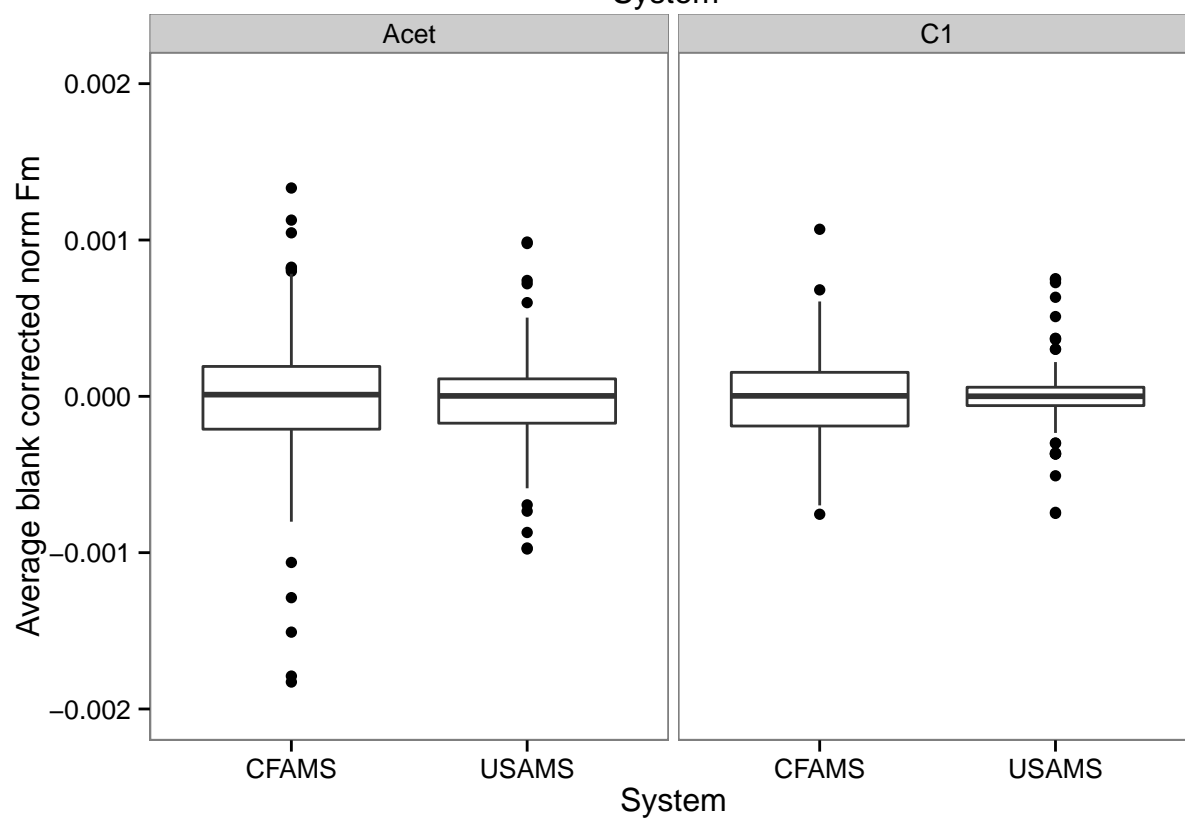
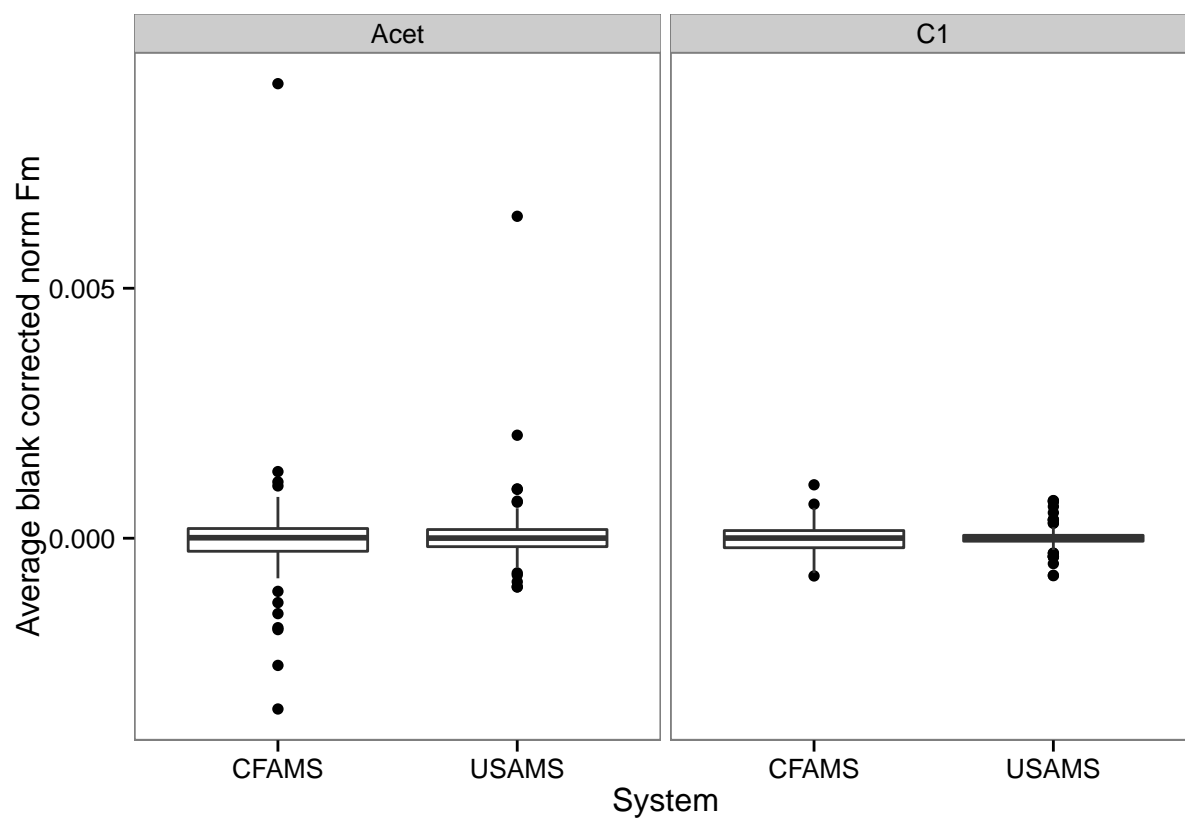
Summary table

system	type	Raw1412	Raw1412.sd	normFm	normFm.sd	normFm.err	BlkCorrFm	N
CFAMS	Acet	46.82	19.463	0.0040	0.00165	0.00021	0.000001	66
CFAMS	C1	30.36	9.292	0.0024	0.00074	0.00016	-0.000014	101
USAMS	Acet	20.88	11.661	0.0020	0.00111	0.00010	0.000109	68

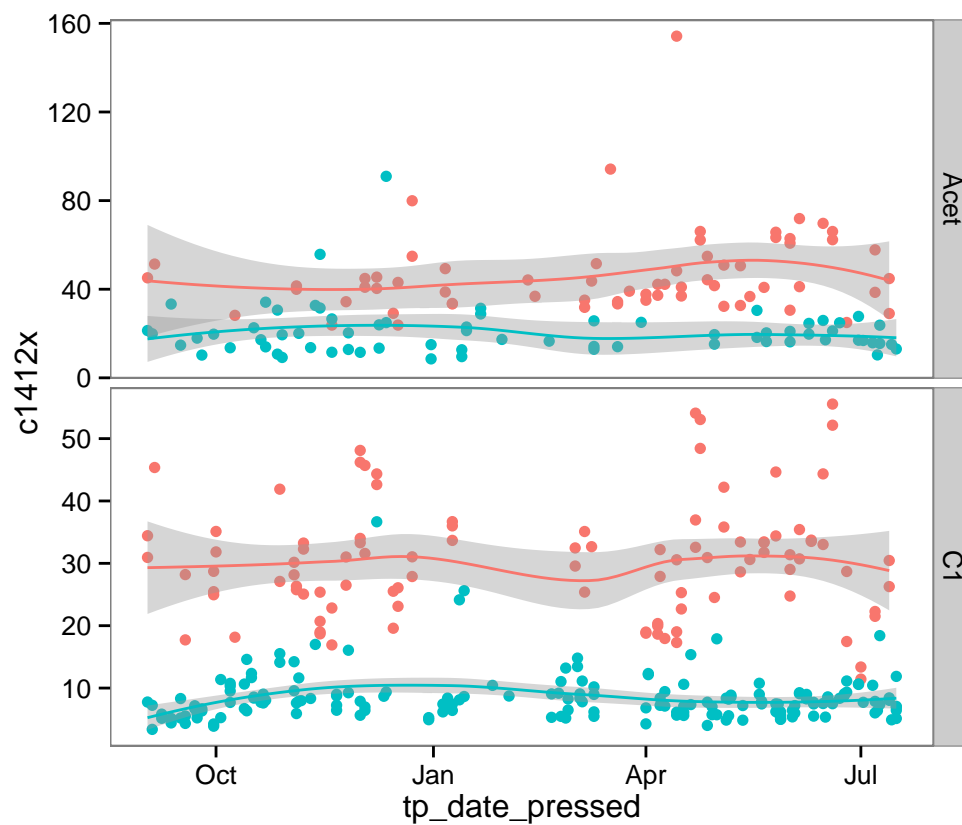
system	type	Raw1412	Raw1412.sd	normFm	normFm.sd	normFm.err	BlkCorrFm	N
USAMS	C1	8.45	3.923	0.0007	0.00039	0.00008	0.000004	175

Boxplots by system and sample type for all data.





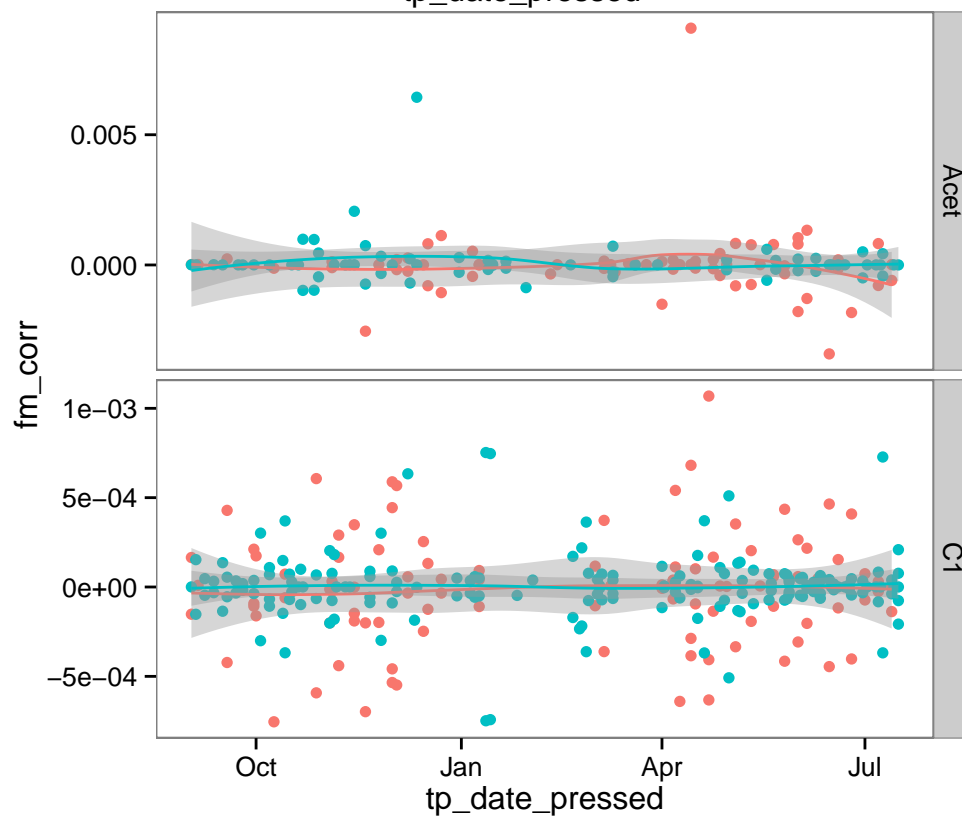
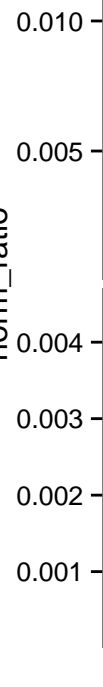
Variability of blanks over time.



system

- CFAMS
- USAMS

$norm_ratio$



system

- CFAMS
- USAMS

Flagging

