PCB Peak Processing V3 - no diagnostics or tcpl

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October 23, 2017

## Load R functions

source("ChiuPeakProcessingAlgorithm.R")  
source("ChiuPeakProcessingUtilities.R")  
source("tcpl\_fit\_functions.R")  
library(tcpl)

## Warning: package 'tcpl' was built under R version 3.3.3

## Loading required package: data.table

## tcpl (v1.2.2) loaded with the following settings:  
## TCPL\_DB: C:/Users/wchiu/Documents/R/win-library/3.3/tcpl/sql/tcpldb.sqlite  
## TCPL\_USER: NA  
## TCPL\_HOST: NA  
## TCPL\_DRVR: SQLite  
## Default settings stored in TCPL.conf. See ?tcplConf for more information.

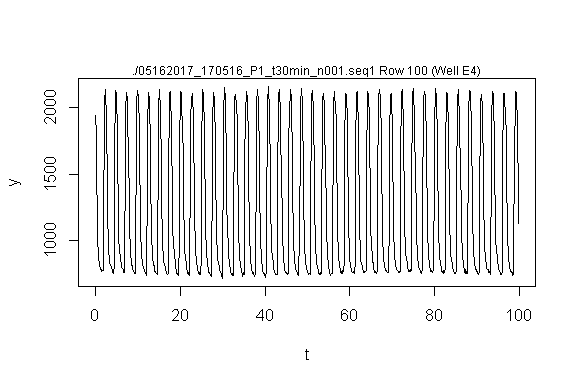
## Load and process multiple plates

### Read files

seq1.file.list<- get.seq1.file.list(".")  
n.files<-length(seq1.file.list)  
dat.list<-list()  
for (n in 1:n.files) {  
 fname<-seq1.file.list[n]  
 dat.list[[n]]<-get.seq1.dat(fname)  
}

### Plot an example

## While file?  
filenum<-2  
dat<-dat.list[[filenum]]  
t<-as.numeric(sub("X","",colnames(dat)[-1]))  
  
## "dat" is a data frame with Well (e.g., E3) in the first column, and the data in the other columns  
  
## Which row?  
rownum<-100  
y<-dat[rownum,-1]  
well<-dat[rownum,1]  
plot(t,y,cex=0.5,type="l");  
mtext(paste(seq1.file.list[filenum]," Row ",rownum," (Well ",well,")",sep=""),side=3,cex=0.75)

 ### Derive peak parameters

peak.parms.vec.list<-list()  
peak.parms.sum.list<-list()  
for (n in 1:n.files) {  
 peak.parms.vec.list[[n]]<-get.peak.parms(dat.list[[n]],trimsec=10)  
 peak.parms.sum.list[[n]]<-summarize.peak.parms(peak.parms.vec.list[[n]])  
}  
print(t(head(peak.parms.sum.list[[n]],3)))

## 1 2 3   
## Well "A1" "A2" "A3"   
## baseline "113.0920" "117.5753" "114.5949"  
## height "113.0920" "117.5753" "114.5949"  
## amplitude "0" "0" "0"   
## notch.amp "0" "0" "0"   
## notch.frac "0" "0" "0"   
## n.peaks "0" "0" "0"   
## n.peaks.expected "0" "0" "0"   
## BPM "0" "0" "0"   
## peak.max.avg "113.0920" "117.5753" "114.5949"  
## peak.max.sd NA NA NA   
## peak.max.cv NA NA NA   
## peak.amp.avg "0" "0" "0"   
## peak.amp.sd NA NA NA   
## peak.amp.cv NA NA NA   
## peak.spacing.avg "0" "0" "0"   
## peak.spacing.sd NA NA NA   
## peak.spacing.cv NA NA NA   
## peak.freq.avg "0" "0" "0"   
## peak.freq.sd NA NA NA   
## peak.freq.cv NA NA NA   
## peak.width.avg "0" "0" "0"   
## peak.width.sd NA NA NA   
## peak.width.cv NA NA NA   
## rise.times.avg "0" "0" "0"   
## rise.times.sd NA NA NA   
## rise.times.cv NA NA NA   
## decay.times.avg "0" "0" "0"   
## decay.times.sd NA NA NA   
## decay.times.cv NA NA NA   
## decay.rise.ratio.avg NA NA NA   
## decay.rise.ratio.sd NA NA NA   
## decay.rise.ratio.cv NA NA NA

### Merging with plate map and chemical lists

nplates<-1  
plate.map.frame<-get.plate.design(nplates=nplates)  
chem.map<-get.chem.map(fname="chemicals.dat.txt")  
plate.map.frame$Chemical.name<-chem.map[paste(plate.map.frame$Chemical.Number),]  
plate.peak.parms.sum.list<-list()  
timepoint<-c("15min","30min","60min","90min","24hr")  
for (n in 1:n.files) {  
 plate.peak.parms.sum.list[[n]]<-merge(plate.map.frame,  
 peak.parms.sum.list[[n]],  
 by.x="rowcol",by.y="Well",sort=FALSE)  
 plate.peak.parms.sum.list[[n]]<-plate.peak.parms.sum.list[[n]][  
 order(plate.peak.parms.sum.list[[n]]$Chemical.Number,  
 plate.peak.parms.sum.list[[n]]$Solvent,  
 plate.peak.parms.sum.list[[n]]$Chemical.Concentration),]  
 ## Add timepoint to data frame  
 plate.peak.parms.sum.list[[n]]$TimePoint<-timepoint[n]  
 ncol<-dim(plate.peak.parms.sum.list[[n]])[2]  
 plate.peak.parms.sum.list[[n]]<-plate.peak.parms.sum.list[[n]][,c(ncol,1:(ncol-1))]  
}  
print(t(head(plate.peak.parms.sum.list[[n]],3)))

## 17 18 19   
## TimePoint "24hr" "24hr" "24hr"   
## rowcol "B2" "C2" "D2"   
## Plate "1" "1" "1"   
## Chemical.Number "1" "1" "1"   
## Chemical.Concentration "0.01" "0.01" "0.10"   
## Solvent "DMSO" "DMSO" "DMSO"   
## Chemical.name "PCB3" "PCB3" "PCB3"   
## baseline "469.6908" "405.0372" "471.1429"   
## height "605.6712" "645.7417" "471.1429"   
## amplitude "135.9804" "240.7045" " 0.0000"   
## notch.amp "0" "0" "0"   
## notch.frac "0" "0" "0"   
## n.peaks "58" "50" " 0"   
## n.peaks.expected "64.36729" "56.69314" " 0.00000"   
## BPM "34.84181" "30.03604" " 0.00000"   
## peak.max.avg "620.7759" "660.4400" "471.1429"   
## peak.max.sd "9.053531" "6.969789" NA   
## peak.max.cv "0.01458422" "0.01055325" NA   
## peak.amp.avg "151.0851" "255.4028" " 0.0000"   
## peak.amp.sd "9.053531" "6.969789" NA   
## peak.amp.cv "0.0599234" "0.0272894" NA   
## peak.spacing.avg "1.557018" "1.765306" "0.000000"   
## peak.spacing.sd "0.09176766" "0.07958491" NA   
## peak.spacing.cv "0.05893810" "0.04508278" NA   
## peak.freq.avg "0.6444462" "0.5676126" "0.0000000"  
## peak.freq.sd "0.03798141" "0.02582137" NA   
## peak.freq.cv "0.05893651" "0.04549119" NA   
## peak.width.avg "0.5977586" "0.7776000" "0.0000000"  
## peak.width.sd "0.06263352" "0.06355329" NA   
## peak.width.cv "0.10478063" "0.08173005" NA   
## rise.times.avg "0.1644828" "0.1946000" "0.0000000"  
## rise.times.sd "0.05801308" "0.06322006" NA   
## rise.times.cv "0.3527001" "0.3248718" NA   
## decay.times.avg "0.4332759" "0.5830000" "0.0000000"  
## decay.times.sd "0.06292262" "0.07008013" NA   
## decay.times.cv "0.1452253" "0.1202061" NA   
## decay.rise.ratio.avg "2.967144" "3.454533" NA   
## decay.rise.ratio.sd "1.050942" "1.486215" NA   
## decay.rise.ratio.cv "0.3541930" "0.4302216" NA

### Merge into one data frame and write as CSV

peak.parms.sum.all<-plate.peak.parms.sum.list[[1]]  
if (n.files>1) {  
 for (n in 2:n.files) {  
 peak.parms.sum.all<-rbind(peak.parms.sum.all,plate.peak.parms.sum.list[[n]])  
 }  
}  
write.csv(peak.parms.sum.all,file="Peak.Parms.Summary.csv",row.names=FALSE)