NIST Spectral Upload

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```r
source('src/compliance.R')
```

```
##
## Attaching package: 'tools'

## The following object is masked from 'package:XML':
##
##      toHTML

## Loading required package: rcdklibs

## Loading required package: rJava
```

```r
compoundtable <- read.csv('src/gather/pfas_cmpds.csv', header = TRUE, row.names = NULL)
```

Exporting all files generated by NIST

Set up the directory

```r
file_dir <- "input"
all_jsonfile <- list.files(file_dir, ".JSON", full.names = TRUE)
all_methodjson <- lapply(all_jsonfile, parse_methodjson)
all_mzml <- sapply(1:length(all_jsonfile), function(x) paste(dirname(all_jsonfile[x]), "/", all_methodj
```

Extract data and copy into JSON

```r
for (i in 1:length(all_jsonfile)) {
  methodjson <- all_methodjson[[i]]
  mzml <- mzMLtoR(all_mzml[[i]])
  dat <- peak_gather_json(methodjson, mzml, compoundtable)
  for (j in 1:length(dat)) {
    qc <- gather_qc(dat[[j]], exactmasses)
    output <- dat[[j]]
    output$qc <- qc
    write_json(output, paste("output/NIST_MS/", gsub("\\.", "_", dat[[j]]$sample$filename), "_cmpd", da
  }
}
print("DONE")
```

```
## [1] "DONE"
```