

# NIST Spectral Upload

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```
source("src/compliance.R")
compoundtable <- read.csv("src/gather/pfas_cmpds.csv", header = TRUE, row.names = NULL)
```

## Exporting all files generated by NIST

Set up the directory

```
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_methodjson[[x]]$sample$filename, sep = ""))
```

## Extract data and copy into JSON

```
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$filename),
      "_cmpd", dat[[j]]$compounddata$ID, ".JSON", sep = ""), auto_unbox = TRUE)
  }
}
print("DONE")
```

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