

# Field Spectral Upload

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

**Note:** JSON has been updated with new format.

## Exporting all files generated by Barzen-Hanson et al.

Set up the directory

```
file_dir <- "input/FIELDupload"
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]]$sample$name, 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, ms1range = c(0.5, 3), ms1isomatchlimit = 0.5,
      minerror = 0.01) #minerror is larger for the QTOF data
    output <- dat[[j]]
    output$qc <- qc
    write_json(output, paste("output/FIELD_MS/", gsub("\\\\.", "_", dat[[j]]$sample$name),
      "_cmpd", dat[[j]]$compounddata$ID, ".JSON", sep = ""), auto_unbox = TRUE,
      pretty = TRUE)
  }
}
print("DONE")
```

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