Database model

compounds.xlsx

```
compounds              3329 obs. of 5 variables
    $ compound_id      : int [1:3329] 4305 11151 10519 10708
    $ compound_name    : chr [1:3329] "(+-)-Fluazifop-d4" "(+
    $ molecular_formula: chr [1:3329] "C15H8[2]H4N1O4F3" "C19
    $ type             : chr [1:3329] NA "internal standard"
    $ computed_mass    : num [1:3329] 331 375 347 353 309 ...
```

Primary Key

measured-compounds.xlsx

```
measured_compounds    605 obs. of 6 variables
    $ measured_compound_id: int  1 2 3 4 5 6 7 8 9 10
    $ compound_id         : int  4 7 8 15 15 16 21 24
    $ retention_time_id   : int  1 2 3 4 4 5 6 7 8 8 .
    $ adduct_id           : int  1 3 3 1 3 3 3 3 1 3 .
    $ measured_mass       : num  188 205 202 224 222 .
    $ molecular_formula   : chr  "C10H10N3O1" "C9H2[2]
```

Primary Key

Foreign Key

Foreign Key

Foreign Key

```
rt                    500 obs. of 3 variables
    $ retention_time_id: int  1 2 3 4 5 6 7 8 9 10 ...
    $ retention_time   : num  5.31 9.7 18.8 9.24 9.4 7
    $ comment          : chr  "nan" "nan" "nan" "nan"
```

Primary Key

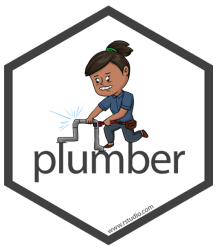
Adducts.json

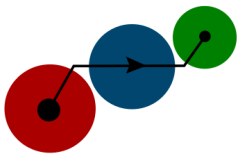
```
adducts               3 obs. of 4 variables
    $ adduct_id      : int  1 2 3
    $ adduct_name    : chr  "M+H" "M+Na" "M-H"
    $ mass_adjustment: num  1.01 22.99 -1.01
    $ ion_mode       : chr  "positive" "positive" "negative"
```

Primary Key

Implementation

- MongoDB as noSQL database option
- API designed with plumber in R
- Calculation with enviPat





Further steps, not implemented:

- Docker container with dependencies 

- More consistency checks, especially after adding a new entry into the database
- Duplicate information on molecular formula, check if calculated masses fit as consistency check
- Mongoid schema configuration
- Error handling in API started, not yet fully established