DynaStI – Command line parameters for the DynMetID core

DynMetID can be run as a command line command line tool with the following parameters

```
>dynmetid <database host>...
     <database user> <password>...
     <database name> <compound property table>...
     <feature list file> <adduct list file>...
     <mass tolerance ppm>...
     <exp. ret. time tol. %> <QSRR ret. time tol. %>...
     <gradient start %> <gradient end %>...
     <gradient time min> <flow rate mL/min>...
     <dead time min> <dwell volume mL> [calibration list file]
```

The database must be an SQL database, with a table of compounds with the fields `name`, `logkw` and `s`, corresponding to each of the relevant parameters of the compound. The concrete database measured and curated in the context of the accompanying article is hosted at `dynasti.vital-it.ch`, as part of the Vital-IT infrastructure. The feature list must be a path to a plain-text file containing single line entries of the form

`<retention time min>_<m/z of ion>m/z`

or

`<retention time min>_<exact neutral mass>n`

in the case of features for which the neutral mass is already known. The adduct list must equally point to a plain-text file with entries providing

`<adduct name>;<adduct mass excess>;<adduct charge>`

Finally, the optional calibration list file should contain entries with

`<compound name>;<experimental retention time min>`

The name of the compound must, of course, match one of those in the database.