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# **DO-MS-Processing**

***Release 1.0***

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## PROCESSING

Command line tool for feature detection in shotgun MS experiments. Can be used together with DIA-NN to provide additional information on the peptide like features identified in the MS1 spectra.

```
usage: FeatureDetection [-h] --raw-parser-location RAW_PARSER_LOCATION
                        [--dinosaur-location DINOSAUR_LOCATION] [-m] [-d] [-v]
                        [-t TEMPORARY_FOLDER] [--no-feature-detection]
                        [--no-fill-times] [--no-tic] [--no-sn]
                        [--no-mzml-generation] [--mz-bin-size MZ_BIN_SIZE]
                        [--tic-dense] [--resolution RESOLUTION] [-p PROCESSES]
                        [--isotopes-sn]
                        report
```

## 1.1 Positional Arguments

**report** Path pointing to report.tsv output from DIA-NN.  
Default: /home/runner/work/ActionsPlayground/ActionsPlayground/docs

## 1.2 options

**--raw-parser-location** Path pointing to the ThermoRawFileParser executable.

**--dinosaur-location** Path pointing to the dinosaur jar executable.

**-m, --mono** Use mono for ThermoRawFileParser under Linux and OSX.  
Default: False

**-d, --delete** Delete generated mzML and copied raw files after successfull feature generation.  
Default: False

**-v, --verbose** Show verbose output.  
Default: False

**-t, --temporary-folder** Input Raw files will be temporarilly copied to this folder. Required for use with Google drive.

- no-feature-detection** All steps are performed as usual but Dinosaur feature detection is skipped. No features.tsv file will be generated.  
Default: False
- no-fill-times** All steps are performed as usual but fill times are not extracted. No fill\_times.tsv file will be generated.  
Default: False
- no-tic** All steps are performed as usual but binned TIC is not extracted. No tic.tsv file will be generated.  
Default: False
- no-sn** Signal to Noise ratio is not estimated for precursors  
Default: False
- no-mzml-generation** Raw files are not converted to .mzML. Nevertheless, mzML files are expected in their theoretical output location and loaded. Should be only be carefully used for repeated calculations or debugging  
Default: False
- mz-bin-size** Bin size over the mz dimension for TIC binning.  
Default: 10
- tic-dense** Return dense TIC matrices. If this option is selected dense TIC matrices are exported for every dataset separately. The default behavior is a single sparse output file.  
Default: False
- resolution** Set the resolution used for estimating counts from S/N data  
Default: 70000
- p, --processes** Number of Processes  
Default: 10
- isotopes-sn** Use all isotopes from the same scan as the highest intensity datapoint for estimating the SN and copy number.  
Default: False

## INDICES AND TABLES

- `genindex`
- `modindex`
- `search`