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| **Category** | **Minimum information** | **Definition** |  |
| General Features | Contact information/responsible person or role | The (stable) primary contact person for this data set. | The (stable) primary contact person for this data set; In all cases give affiliation including e-mail address and stable contact information. |
|  | Experiment identifier or name | Descriptive name and/or an identifier assigned to the experiment (may be assigned later by a public repository). | Include keywords indicating which disease, model... was studied. |
|  | Quality control generating software customization | Quality control tool's name, version and any customizations to the default setup of the software. |  |
|  | Availability of the software | The references of the vendor or public URL if a publicly available version has been used. |  |
| Experimental design and sample description | Experiment strategy |  | Experimental strategy (workflow). e.g. Total protein extraction -> Digestion -> SCX -> RPLC -> MALDI -> MS, Total protein extraction -> Digestion -> SEC -> SCX -> RPLC -> ESI -> MS |
| Experimental protocol | Quality control strategies. Including bioinformatics processing and analytical analysis. | Downstream elements of analytical pipeline, which represents critical steps to generate the final comparative results. |
| Groups | A group is a sample set that corresponds to a certain experimental condition with its value . | Description of the experimental sample grouping including group names (if appropriate). |
| Biological and/or technical replicates | Technical replicates: Replicates that share the same sample; i.e. the measurements are repeated. The technical variability is tested. Biological replicates: Replicate where different samples are used for testing the biological variability between the selected samples. | Description of the biological and/or technical replicate structure (if appropriate). This is also a group structure like above, but hierarchically ordered. |
| Number of QC runs | How many QC runs are included in the experiment. |  |
| Sample description (sample name, type, count ..) | Short description samples. | Including sample name, sample type, sample count.. In the case of label-based quantification methods, provide the sample labelling with assay definition, i.e. MS run / data set together with reporting ion mass, reagent or isotope labelled amino acid. |
| Input data description | Description and reference of dataset used. | Including type, format and availability of the input data. |
| MS acquisition parameters | Chromatogram count |  |  |
|  | Retention time (ranges) | A time interval from the start of chromatography when an analyte exits a chromatographic column. |  |
|  | Ionization mode (if applicable) | The ionization mode of ESI. | Positive/Negative |
|  | Instrument settings | The optimized parameters for ESI ion source. | e.g. Block temp, CDL temp. |
|  | MZ ranges |  |  |
|  | Ion injection time | Full MS scan ion injection time which contains the accumulation time in the ion trap device used in machine settings during MS acquisition. |  |
|  | MS1 scan time | Average scan time for Full MS scan used in machine settings. |  |
|  | MS1 scan spectra count | Number of full MS scan spectra. |  |
|  | MS1 intensity variation for peptides |  |  |
|  | MS1 scans | Number of full MS scans taken over time period over which 50% of peptides were identified. |  |
|  | MS2 scans | Number of tandem MS scans taken over time period over which 50% of peptides were identified. |  |
|  | MS2 scan spectra count | Number of tandem MS scan spectra. |  |
|  | MS2 scan time | Average scan time for tandem MS scan used in machine settings. |  |
| MS identification parameters | Mass spectrometry customization | Free text description of a single customization made to the instrument; for several modifications, use several entries. |  |
| Estimated spectra FDR | The false discovery rate of the estimated spectra. |  |
| Identification rate in terms of spectra | The number of identified spectra vs. The number of total spectra. |  |
| Precursor error | The maximum and median number of precursor error. |  |
| Estimated peptide FDR | Provide the false discovery rate of the estimated peptide. |  |
| Identification rate in terms of peptides | The number of identified peptides vs. The number of recorded Tandem MS spectrum. |  |
| Peptide count | This number indicates the number peptides that were identified. |  |
| Identification rate in terms of PSMs |  |  |
| Protein count | Total number of identified proteins. |  |
|  | Modified peptides count | This number indicates the number modified peptide sequences that were identified (after FDR). |  |
|  | Protein coverage |  |  |
|  | Estimated protein FDR | The false discovery rate of the estimated protein. |  |
|  | Protein count for parsimony protein group | The average and median protein count for parsimony protein group. |  |
|  | Protein group ratio | Ratio of unique protein group to parsimony protein group. |  |
| MS quantitation parameters | Quantitation software comment or customization | Quantitation software comment or any customizations to the default setup of the software. |  |
| Protocol of label-based quantification methods (if applicable) |  | In the case of label-based quantification methods, describe the labelling protocol, including the labelling level: if labelling occurs at the element, amino acid, peptide (terminus) or protein (terminus) level. |

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|  | general features |  |  |  |  |  |  |  |  |
|  | experimental design |  | sample description |  |  |  |  |  |  |
|  | chromatography |  | ion source |  | MS1 signal |  | dynamic sampling |  | MS2 signal |
|  | spectrum identification |  | peptide identification |  | protein identification |  | protein group and inference |  |  |
|  | quantitation |  |  |  |  |  |  |  |  |