**Requirements for studies that include mass spectrometry data**

All manuscripts submitted to JMCC that contain mass spectrometry data (*e.g.* proteomics, metabolomics, glycomics) must be in compliance with established [guidelines](http://www.mcponline.org/page/content/mass-spec-guidelines) [for acquiring and reporting these types of data.](http://www.mcponline.org/page/content/mass-spec-guidelines) These include those described for *Molecular and Cellular Proteomics* and the *Journal of Proteome Research* found at these links:

<https://www.mcponline.org/content/4/9/1223>

[http://pubsapp.acs.org/paragonplus/submission/jprobs/jprobs\_proteomics\_guidelines.pdf?](http://pubsapp.acs.org/paragonplus/submission/jprobs/jprobs_proteomics_guidelines.pdf)

[http://pubsapp.acs.org/paragonplus/submission/jprobs/jprobs\_mass\_spectrometry\_guidelines.pdf?](http://pubsapp.acs.org/paragonplus/submission/jprobs/jprobs_mass_spectrometry_guidelines.pdf)

Importantly, data provided in the supporting information should enable the reviewer and reader to reproduce the analysis and readily assess the quality of the underlying data supporting the conclusions. For proteomics data, this includes describing peptide-level data to support the protein-level inferences.

Raw data files must be available in a public repository (*e.g.* MASSive, PRIDE).

<https://massive.ucsd.edu/ProteoSAFe/static/massive.jsp>

<https://www.ebi.ac.uk/pride/>

**Check list for Publication of Mass Spectrometry Data in JMCC**

The following checklist is used by the editorial team when screening submitted manuscripts that contain mass spectrometry data. Manuscripts not meeting these requirements will be returned to the author without peer review.

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| General Requirements | Y | N/A | Page |
| 1 | Peak list-generating software (name and release version number or date) |  |  |  |
| 2 | Search engine (name and release version number or date) |  |  |  |
| 3 | Sequence database or spectral library searched (name, number of entries, and release version number or date)🡪If the database was generated in-house, include the source of protein sequences and software used to compile it |  |  |  |
| 4 | Protease specificity of all enzymes used to generate peptides |  |  |  |
| 5 | Allowed number of missed and/or non-specific cleavages  |  |  |  |
| 6 | List of all variable and fixed modification(s) (including residue specificity) allowed |  |  |  |
| 8 | Mass tolerance for precursor and fragment ions |  |  |  |
| 9 | Known contaminants that were excluded post-searching |  |  |  |
| 10 | Threshold score or expectation value for accepting individual spectra |  |  |  |
| 11 | Estimation of false discovery rate (FDR) and how it is calculated |  |  |  |

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| Peptide and Protein Data | Y | N/A | Page |
| 1 | Accession number (and database from which it is derived) for all protein identifications |  |  |  |
| 2 | List (in tabular form) of all peptide sequences, including any deviations from expected cleavage specificity |  |  |  |
| 3 | Precursor charge state and mass/charge (*m/z*) for each peptide assignment |  |  |  |
| 4 | All modifications observed, including showing modified and unmodified forms of the same peptide, if applicable |  |  |  |
| 5 | Peptide identification Score(s) |  |  |  |
| 6 | Number of unique peptides assigned to each protein |  |  |  |
| 7 | Sequence coverage (%) of each protein assigned  |  |  |  |
| 8 | For single peptide identifications, annotated spectra are provided for each protein |  |  |  |

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| Post-Translational Modifications | Y | N/A | Page |
| 1 | Site(s) of modification within each peptide are clearly located |  |  |  |
| 2 | Justification of any localization score threshold |  |  |  |
| 3 | Separate table for all peptides with ambiguous modification site assignments |  |  |  |
| 4 | Annotated, mass labeled spectra for all modified peptides are provided either in public repository or as supplemental material with the manuscript |  |  |  |

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| Quantification | Y | N/A | Page |
| 1 | Quantification measurements for each peptide and protein |  |  |  |
| 2 | Description of how raw MS data were processed to yield quantification data |  |  |  |
| 3 | Description of technical replicates and statistical treatments |  |  |  |
| 4 | Label free quantification should include use of blocking and randomization. If not, suitable justification is required. |  |  |  |
| 5 | Description of biological replicates, independent experiments, statistical analyses |  |  |  |
| 6 | Description of any adjustments for systematic errors |  |  |  |
| 7 | How random error issues were addressed (outliers, exclusion limits etc.) |  |  |  |
| 8 | Estimates of uncertainty for individual proteins |  |  |  |
| 9 | How the identity of the analyte was verified (in non-database identifications) |  |  |  |
| 10 | How quantification of multiple isoforms in the same sample was handled |  |  |  |
| 11 | Number of peptides or number of spectra used for the quantification |  |  |  |
| 12 | Inclusion of modified, semi-tryptic or shared peptides (from different isoforms) |  |  |  |

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| Raw Data Submission | Y | N/A | Page |
| 1 | The raw mass spectrometry data has been deposited into a public repository. The location and identifying information (URL of repository, deposit ID, username, hash code/identifier, password) are provided in the results or methods section. The reviewers’ login information (username, password) to access the raw data is included in the cover letter. |  |  |  |