

Code and Software Submission Checklist

Prior to submitting your work to Nature Research, we strongly recommend that you ask at least one colleague who is unfamiliar with your software to install the tool(s), follow the instructions, and provide feedback. This process will help ensure that reviewers will also be able to run your software.

You must submit all required content as a single zip file prior to peer review or provide a link where editors and reviewers can access all required content.

► Required content

- ☒ Compiled standalone software and/or source code
- ☐ A small (simulated or real) dataset to demo the software/code

A README file that includes:

1. System requirements

- ☒ All software dependencies and operating systems (including version numbers)
- ☒ Versions the software has been tested on
- ☒ Any required non-standard hardware

2. Installation guide

- ☒ Instructions
- ☒ Typical install time on a "normal" desktop computer

3. Demo

- ☒ Instructions to run on data
- ☒ Expected output
- ☒ Expected run time for demo on a "normal" desktop computer

4. Instructions for use

- ☒ How to run the software on your data
- ☐ (OPTIONAL) Reproduction instructions

We encourage you to include instructions for reproducing all the quantitative results in the manuscript.

► Additional information

Describe your software's license for use. We strongly recommend using a [license](#) approved by the [Open Source Initiative](#).

UniDec is distributed under a completely open source license.

UniDec License:

Copyright (c) 2016, University of Oxford 2017-2023, University of Arizona All rights reserved.

Redistribution and use in source and binary forms, with or without modification, are permitted provided that the following conditions are met:

Redistributions of source code must retain the above copyright notice, this list of conditions, and the following disclaimer.

Redistributions in binary form must reproduce the above copyright notice, this list of conditions, and the following disclaimer in the documentation and/or other materials provided with the distribution.

Neither the name of the copyright holders nor the names of its contributors may be used to endorse or promote products derived from this software without specific prior written permission.

Any publications that result from use of the software should cite Marty et al. Anal. Chem. 2015. DOI: 10.1021/acs.analchem.5b00140. If UniDec is redistributed or incorporated into other software, it must be clearly indicated to the end user that UniDec is being used, and the request to cite Marty et al. Anal. Chem. 2015. DOI: 10.1021/acs.analchem.5b00140 must be passed on to the end user.

Provide a link to the code in an open source repository (when available).

<https://github.com/michaelmarty/UniDec/tree/master/PublicScripts/DIA-PTCR>

Your manuscript should include a complete, detailed description of the code's functionality (i.e. pseudocode).

Please indicate where this is found:

- ☐ Main text
- ☒ Methods section

☐ Elsewhere (specify):

► Examples of well-structured software packages

1. <https://github.com/neurodata-papers/MGC>
2. <https://github.com/neurodata-papers/LOL>
3. <https://www.nature.com/nbt/journal/v34/n6/abs/nbt.3569.html#supplementary-information>
4. <https://www.nature.com/nature/journal/v548/n7669/full/nature23463.html#extended-data>
<https://github.com/yasharhezaveh/Ensa>
5. <https://www.nature.com/nbt/journal/v34/n11/full/nbt.3685.html#supplementary-information>
<https://github.com/IFIProteomics/LFQbench>