2023 special issue on software tools and resources: accelerating research with new and evolving open source software

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Editorial

2023 Special Issue on Software Tools and Resources: Accelerating Research with New and Evolving Open Source Software

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The third biennial *Journal of Proteome Research* Special Issue on Software Tools and Resources contains novel and significantly updated tools and resources for computational proteomics. The purpose of the Special Issue is to promote with high visibility a collection of peer-reviewed analytical tools that demonstrate applicability, availability, and ease-of-use to the proteomics community. For the developers of these tools, the Special Issue focuses their work on the target audience that would benefit the most from these tools, ensuring dissemination and further development of these valuable resources. The diversity of topics within the proteomics and computational mass spectrometry field captured in this Special Issue reflects the vivid and active bioinformatics community continuously moving the field forward.

One of the tenets of this Special Issue is to accommodate significantly updated software tools. Although it is generally understood that the life cycle of a successful software application begins with publication, the work performed to keep the software functional and relevant in an ever-evolving proteomics field often goes unnoticed. Just as the evolution of proteomics technology is often incremental rather than paradigm-shifting, the software tools that make proteomics research possible evolve incrementally as well. It is often more efficient to adapt existing software tools with a strong foundation to satisfy the needs of new research techniques than to continuously rebuild the tools from scratch. Unfortunately, the incremental improvements that are made throughout the life cycle of a software tool are rarely recorded through scientific publications beyond the initial manuscript. However, the accumulation of these incremental improvements does have a significant impact on proteomics research, whether they broaden the scope of the software, incorporate newly developed technology, or enable integration of the software into new pipelines. This Special Issue is part of a series that was created explicitly to provide an outlet for publication of this necessary and beneficial aspect of proteomics software development. For many tools, this is only the second time they are described in a dedicated paper, including compareMS2 2.0, pmartR 2.0, and Cytoscape stringApp 2.0. Still, others are presenting versions well beyond the second, such as the Trans-Proteomic Pipeline and the Crux Toolkit. We hope this Special Issue continues to serve as a platform for proteomics software developers to achieve new goals and reach a broader audience as their tools adapt and expand to meet the demands of tomorrow's research.

Like past Special Issues on Software Tools and Resources, the content of the papers also reflects the state-of-the-art in proteomics. Topics with multiple contributions include structural and top-down proteomics, machine/deep learning applications, spectral libraries, and quality control and statistical methods. Applications for bottom-up proteomics are still among the majority. Development languages and platforms are diversely represented, with particular emphasis on Python and R. However, perhaps an interesting component to this Special Issue's contributions is the inclusion of software libraries and application programming interfaces (APIs) such as pyAscore and psm_utils. Software publications often present the development of applications for users, but it is equally important to also present software tools that enable the developers of tomorrow's applications. In many ways this helps promote the axioms of FAIR software (Findable, Accessible, Interoperable, and Reusable), in which the software should be both sustainable and open, keeping up with new types of experiments and be interoperable with new databases or formats. Ideally, this also allows access to, and reuse of, the code itself, as generally provided by software libraries and APIs. By highlighting such software in this Special Issue, we hope to add to the visibility these projects deserve and encourage supporting their continued development. Proteomics runs on software, as much as on mass spectrometers.

We were highly impressed by the quality and abundance of the contributions to this Special Issue as well as the passionate and constructive engagement of the reviewers. These are all evidence of the vitality of proteomics as a scientific enterprise, and of the increasing emphasis placed on computational tools for robust and reproducible analysis of proteomics data.

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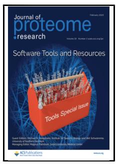

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Notes

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