



OPEN ACCESS

EDITED AND REVIEWED BY

Zhi-Ping Liu,
Shandong University, China

*CORRESPONDENCE

Diego Mariano,
✉ diegomariano@ufmg.br
Raquel Cardoso de Melo-Minardi,
✉ raquelcm@dcc.ufmg.br

RECEIVED 24 June 2023

ACCEPTED 28 June 2023

PUBLISHED 04 July 2023

CITATION

Mariano D, Da Fonseca Júnior NJ,
Santos LH and de Melo-Minardi RC
(2023), Editorial: Bioinformatics in the age
of data science: algorithms, methods, and
tools applied from Omics to
structural data.
Front. Bioinform. 3:1246859.
doi: 10.3389/fbinf.2023.1246859

COPYRIGHT

© 2023 Mariano, Da Fonseca Júnior,
Santos and de Melo-Minardi. This is an
open-access article distributed under the
terms of the [Creative Commons
Attribution License \(CC BY\)](#). The use,
distribution or reproduction in other
forums is permitted, provided the original
author(s) and the copyright owner(s) are
credited and that the original publication
in this journal is cited, in accordance with
accepted academic practice. No use,
distribution or reproduction is permitted
which does not comply with these terms.

Editorial: Bioinformatics in the age of data science: algorithms, methods, and tools applied from Omics to structural data

Diego Mariano^{1*}, Neli José Da Fonseca Júnior²,
Lucianna Helene Santos³ and Raquel Cardoso de Melo-Minardi^{1*}

¹Laboratory of Bioinformatics and Systems, Universidade Federal de Minas Gerais, Belo Horizonte, Brazil, ²European Molecular Biology Laboratory, European Bioinformatics Institute (EMBL-EBI), Wellcome Genome Campus, Hinxton, Cambridgeshire, United Kingdom, ³Biomolecular Simulations Group, Institut Pasteur de Montevideo, Montevideo, Uruguay

KEYWORDS

bioinformatics, web tools, algorithms, methods, structural bioinformatics, omics sciences, software

Editorial on the Research Topic

Bioinformatics in the age of data science: algorithms, methods, and tools applied from Omics to structural data

In recent years, researchers have been confronted with an overwhelming influx of data, resulting from novel technologies utilized for sequencing data and acquiring three-dimensional structures of macromolecules. The increasing demand for computing power has allowed an evolution of data processing technologies, ranging from using CPUs with increasingly miniaturized lithography to the adaptation of graphics cards for efficient data analysis. As a result, we live in a new era: the age of data science.

We extended an open invitation to researchers and general software developers to disclose and share their methods, algorithms, and tools with the community of bioinformatics and computational biology in a Research Topic entitled “Bioinformatics in the age of data science: algorithms, methods, and tools applied from Omics to structural data”.

We received four submissions: two data reports (Rodrigues et al.; Martins et al.), one technology and code (Mohsen et al.), and one brief research report (Oliveira et al.). Thus, this Research Topic contains a combination of articles describing new algorithms, methods, and tools that are applicable to the domains of bioinformatics and computational biology. Below, we summarize the contributions that comprise this Research Topic.

In the data report section, we received two remarkable contributions that yielded significant works in terms of source code and user-friendly tools. Rodrigues et al. presented an application for the analysis of multi-omic bacterial genomes entitled “PanViTa: Pan Virulence and resisTance analysis”. PanViTa (Pan Virulence and resisTance Analysis) was developed in Python, accessible at <https://github.com/dlnrodrigues/panvita>.

Martins et al. presented an update for the public database entitled “Propedia v2.3: A novel representation approach for the peptide-protein interaction database using graph-based structural signatures (Martins et al.)”. Propedia is a public database of three-dimensional protein-peptide complexes, and it is available at <http://bioinfo.dcc.ufmg.br/propedia2>. In this new version,

Propedia received an increment of approximately 150% in the number of protein–peptide complexes available (from ~19,800 to ~49,300). Additionally, the authors provided graph-based structural signature data for subsets of sequence-based and complex-type data. These signature vectors can be used in several machine-learning tasks, such as protein–peptide docking prediction.

In the technology and code section, [Mohsen et al.](#) presented a Snakemake pipeline for QIIME2 16S data analysis, called Snaq, in the paper “Snaq: A Dynamic Snakemake Pipeline for Microbiome Data Analysis With QIIME2.”. Snaq is available at <https://github.com/attayeb/snaq>.

In the brief research report section, [Oliveira et al.](#) presented a tool called SPLACE in their article “SPLACE: A tool to automatically SPLit, Align, and Concatenate genes for phylogenomic inference of several organisms.” The authors described SPLACE as a tool to split, align, and concatenate the genes automatically and then generate a supermatrix file and phylogenetic tree. SPLACE is available at <https://github.com/reinator/splace>.

These recently developed software programs are accessible to the public or offered as open source, thereby enabling the scientific community to benefit from them. All the software programs presented here display easy-to-access graphical interfaces, sometimes considered essential for most users, and comprehensive documentation and availability of tutorials.

In summary, this Research Topic highlights important contributions to the field of bioinformatics and computational biology. We hope the works presented here can give insights into and inspiration for developing new tools and lead to new scientific discoveries.

Author contributions

All authors listed have made a substantial, direct, and intellectual contribution to the work and approved it for publication.

Acknowledgments

We thank the Brazilian Funding Agencies CAPES, CNPq, and Fapemig. The authors also thank Dr. Arne Seitz for contributing to this Research Topic.

Conflict of interest

The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

Publisher's note

All claims expressed in this article are solely those of the authors and do not necessarily represent those of their affiliated organizations, or those of the publisher, the editors and the reviewers. Any product that may be evaluated in this article, or claim that may be made by its manufacturer, is not guaranteed or endorsed by the publisher.