
biobb Documentation

Release 3.6.0

Bioexcel Project

Oct 01, 2021

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CONTENTS**1.1 biobb****1.1.1 Summary**

The **BioExcel Building Blocks (BioBB)** library is a collection of portable wrappers on top of common biomolecular simulation tools Andrio, P., *et al.* **BioExcel Building Blocks, a software library for interoperable biomolecular simulation workflows.** *Sci Data* **6**, 169 (2019). Created and implemented within the **BioExcel CoE**, the library is designed to i) increase the interoperability between the tools wrapped; ii) ease the implementation of biomolecular simulation workflows; and iii) increase the reusability and reproducibility of the generated workflows. The library is being developed following the FAIR principles for research software development best practices. The result is a collection of building block modules, classified according to the tool being wrapped (e.g. `biobb_amber` for AMBER MD package) or the functionalities offered by the tools being wrapped (e.g. `biobb_vs` for Virtual Screening, `biobb_chemistry` for chemoinformatics). Each of the module is built from a combination of software packaging (Pip, BioConda, BioContainers), documentation (ReadTheDocs, OpenAPI, Swagger), registry and findability (bio.tools, BioSchemas, OpenEBench, WorkflowHub), source code (GitHub) and WfMS integration -adapters- (CWL, Galaxy, PyCOMPSs, Jupyter Notebook).

A collection of **demonstration workflows** have been developed to showcase the library possibilities. Built using the Jupyter Notebook GUI, the demonstration workflows offer a graphical and interactive interface, including documentation (integrated markdown) related to the workflow and the building blocks used, and also information about the pipeline and the biomolecular simulation methods used. The set of demonstration workflows are available from the **BioExcel GitHub** repository, with step-by-step instructions on how to reproduce them in a local machine using the Conda packaging software.

All the information regarding the BioExcel Building Blocks library can be found in the central **BioBB web page**. Links to source code, documentation, packages, containers, tutorials, and information from training events (e.g. BioExcel Summer/Winter School) can be found in the different web sections.

Feedback and contact: <http://mmb.irbbarcelona.org/biobb/contact>

1.1.2 Documentation

The latest documentation of our biobb collections can be found in our readthedocs sites:

- [biobb_io \[GitHub\]](#): Biobb_io is the Biobb module collection to fetch data to be consumed by the rest of the Biobb building blocks.
- [biobb_model \[GitHub\]](#): Biobb_model is the Biobb module collection to check and model 3d structures, create mutations or reconstruct missing atoms.
- [biobb_md \[GitHub\]](#): Biobb_md is the Biobb module collection to perform molecular dynamics simulations.
- [biobb_analysis \[GitHub\]](#): Biobb_analysis is the Biobb module collection to perform analysis of molecular dynamics simulations.
- [biobb_adapters \[GitHub\]](#): Biobb_adapters is the Biobb module collection to use the building blocks with several workflow managers.
- [biobb_common \[GitHub\]](#): Biobb_common is the base package required to use the biobb packages
- [biobb_template \[GitHub\]](#): Boilerplate code and template examples to create your own Biobbs.
- [biobb_chemistry \[GitHub\]](#): Biobb_chemistry is the Biobb module collection to perform chemistry over molecular dynamics simulations.
- [biobb_pmx \[GitHub\]](#): Biobb_pmx is the Biobb module collection to perform [PMX](#) executions.
- [biobb_structure_utils \[GitHub\]](#): Biobb_structure_utils is the Biobb module collection to modify or extract information from a PDB structure file.
- [biobb_ml \[GitHub\]](#): Biobb_ml is the Biobb module collection to perform machine learning predictions.
- [biobb_amber \[GitHub\]](#): Biobb_amber is a BioBB category for AMBER MD package, allowing setup and simulation of atomistic MD simulations using AMBER MD package and its associated AMBER tools.
- [biobb_vs \[GitHub\]](#): Biobb_vs is the Biobb module collection to perform virtual screening studies.
- [biobb_dna \[GitHub\]](#): Biobb_dna is the Biobb module collection to perform analyses and transformations on nucleic acid trajectories and helical parameter data.

1.1.3 Videos

- Introduction to BioExcel Building Blocks: <https://www.youtube.com/watch?v=I7ZxRBhYO3E>
- Introduction to workflows with BioExcel Building Blocks: <https://www.youtube.com/watch?v=ou1DOGNs0xM>

1.1.4 Version

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1.1.5 Copyright & Licensing

This software has been developed in the MMB group at the BSC & IRB for the European BioExcel, funded by the European Commission (EU H2020 823830, EU H2020 675728).

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