

## Structural Bioinformatics

# BioExcel Building Blocks REST API (BioBB REST API), programmatic access to interoperable biomolecular simulation tools – Supplementary Material

Genís Bayarri<sup>1</sup>, Pau Andrio<sup>2</sup>, Adam Hospital<sup>1,\*</sup>, Modesto Orozco<sup>1,3,\*</sup>, Josep Lluís Gelpí<sup>2,3,\*</sup>

<sup>1</sup> Institute for Research in Biomedicine (IRB Barcelona), Barcelona Institute of Science and Technology, Barcelona 08028, Spain, <sup>2</sup> Barcelona Supercomputing Center (BSC), <sup>3</sup> Department of Biochemistry and Molecular Biomedicine, University of Barcelona, Barcelona 08028, Spain

\*To whom correspondence should be addressed.

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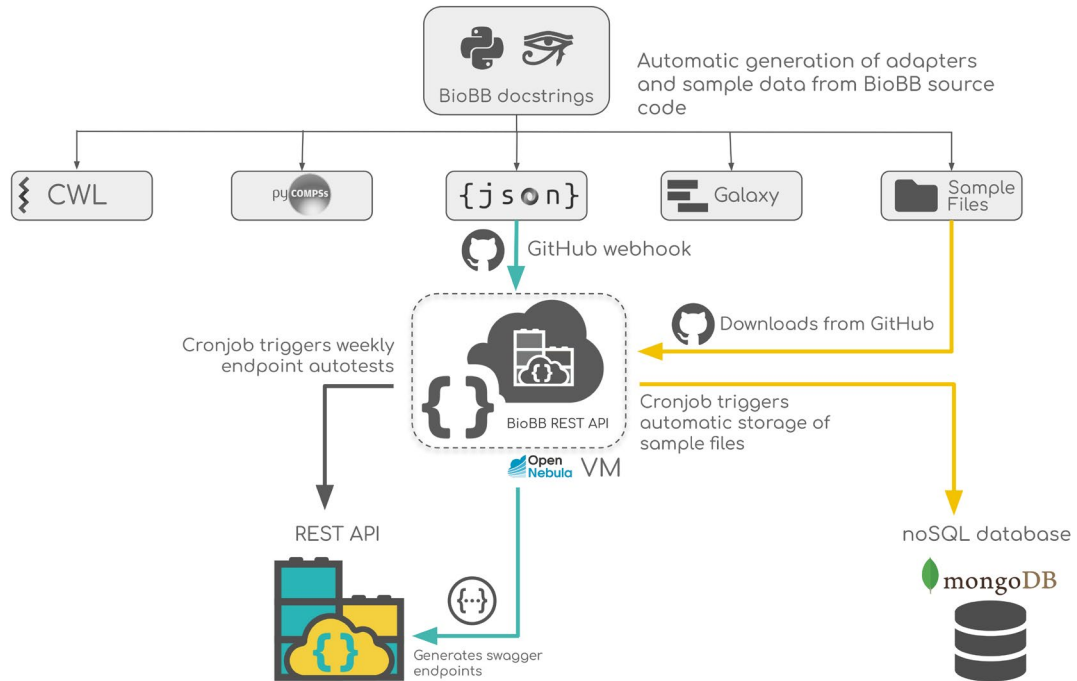
**Contact:** [adam.hospital@irbbarcelona.org](mailto:adam.hospital@irbbarcelona.org), [gelpi@ub.edu](mailto:gelpi@ub.edu) or [modesto.orozco@irbbarcelona.org](mailto:modesto.orozco@irbbarcelona.org)

**Supplementary information:** Supplementary data are available at *Bioinformatics* online.

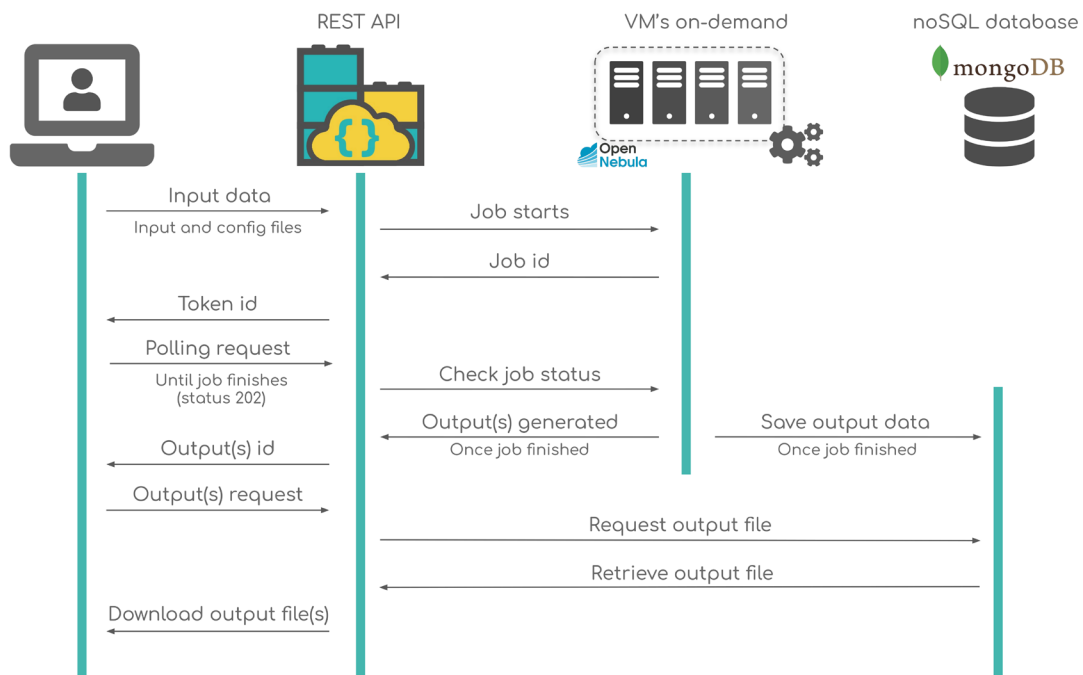
**Suppl. Table 1:** Documentation available from the **BioBB REST API** web site. Description of the information included in the web section and links to the respective section are shown in the table.

Description	Link
Landing Web Page	<a href="https://mmb.irbbarcelona.org/biobb-api/">https://mmb.irbbarcelona.org/biobb-api/</a>
OpenAPI Documentation	<a href="https://mmb.irbbarcelona.org/biobb-api/rest">https://mmb.irbbarcelona.org/biobb-api/rest</a>
Endpoints List	<a href="https://mmb.irbbarcelona.org/biobb-api/tools-documentation">https://mmb.irbbarcelona.org/biobb-api/tools-documentation</a>
Endpoints Examples	<a href="https://mmb.irbbarcelona.org/biobb-api/tools-execution">https://mmb.irbbarcelona.org/biobb-api/tools-execution</a>
Endpoints Tutorial	<a href="https://mmb.irbbarcelona.org/biobb-api/tutorials/restapi">https://mmb.irbbarcelona.org/biobb-api/tutorials/restapi</a>
Protein MD Setup Workflow Tutorial	<a href="https://mmb.irbbarcelona.org/biobb-api/tutorials/mdsetup">https://mmb.irbbarcelona.org/biobb-api/tutorials/mdsetup</a>
Read-The-Docs Documentation	<a href="https://biobb-rest-api-documentation.readthedocs.io/">https://biobb-rest-api-documentation.readthedocs.io/</a>
bio.tools entry	<a href="https://bio.tools/bioexcel_building_blocks_rest_api_biobb-api">https://bio.tools/bioexcel_building_blocks_rest_api_biobb-api</a>

**Suppl. Figure 1:** BioBB REST API automatic endpoints generation schema. Information contained in the Python docstring documentation for each of the BioBB building blocks is automatically parsed and used to generate the API endpoints. GitHub webhooks ensure consistency between the available BioBB building blocks and the REST API endpoints, triggering automatic updates with every push in the repositories. Sample files are also automatically downloaded from the corresponding repositories, stored in the API database, and used for the weekly auto tests.



**Suppl. Figure 2:** BioBB REST API user's interaction diagram. API endpoints executions comprise three different steps: launch, poll, and data retrieval. The launch process involves sending the input data files, with the endpoint returning a token id (asynchronous execution). The token is then used to query for the job status (Polling request). Once the execution is finished, a set of output id(s) (unique identifiers) for the generated data are sent, and can be used to retrieve the final results (Output request).



**Suppl. Figure 3:** BioBB REST API internal schema, including a private on-demand cloud infrastructure and a noSQL mongoDB.

