pdbmine: A Node.js API for the RCSB Protein Data Bank (PDB)

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Abstract

Summary: The advent of Web-based tools that assist in the analysis and visualization of macromolecules require application programming interfaces (APIs) designed for modern web frameworks. To this end, we have developed a Node.js module pdbmine that allows any user to generate faster data-request queries to the RCSB Protein Data Bank (PDB). This JavaScript API acts as a layer over the XML-based RCSB PDB RESTful API. The relatively simple nature of the function calls within this module allows the user to easily implement and integrate pdbmine into larger Node.js web applications.

Availability: This module can be installed via the Node Package Manager (NPM) at https://www.npmjs.com/package/pdbmine/ and is hosted on GitHub under the open-source MIT license at https://github.com/nnj1/pdbmine/. Relevant documentation is detailed at https://nnj1.github.io/pdbmine/

Introduction

The RCSB Protein Data Bank (PDB) contains a plethora of structural biology information, including X-ray diffraction structures, CryoEM models and NMR ensembles [1]. These structures are widely accessed and used for structural analysis and computational work. The PDB website provides various in-browser features that enable researchers to visualize, manipulate, and inspect structures, as well as obtain meta-data pertaining to a structure [2].

The PDB database can be envisioned as a representative of the expanding initiative to move scientific tools and resources into web environments, where the prerequisite of stringent hardware and softwares can be easily bypassed through a mere web connection [3].

Web applications that offer scientific tools and analytical functionalities usually require access to the PDB. While the PDB database does provide a RESTful API for making data requests, an additional layer of abstraction in the form of a language-specific API will assist researchers and developers in incorporating PDB data into their applications. This article introduces a Node.js API for querying and requesting data from the PDB.

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Modern web applications are increasingly being developed using Node.js, a server-side JavaScript run-time environment that leverages Google’s V8 JavaScript engine [6]. Advantages of using this framework include easy scalability, seamless integration of client-side and server-side code, and modular development practices that utilize of the node package manager registry. pdbmine aims to address the lack of Node.js specific PDB querying APIs. This API essentially acts as a layer of abstraction over the XML query requests that the PDB RESTful API generally accepts.

Usage

This module can be easily acquired using the npm command line tool and invoking npm install pdbmine. Once the module is added as a dependency to a project, it can be referenced in scripts and used to make various PDB queries. The core functions of this library are described in Table 1.

**Table 1. List of the functions provided by this API.** Further details are available in the full documentation which is available on the GitHub repository.

| Function            | Details                                                                 |
|---------------------|-------------------------------------------------------------------------|
| get_all_ids(cb)     | Returns a list of strings containing every PDB ID in the database as an argument to the callback. |
| query(query_string, cb) | Accepts a query string argument and returns a list of PDB IDs pertinent to the search query as an argument to the callback. |
| describe_pdb(ids, params, cb) | Accepts a list of PDB IDs, along with a list of parameters to return for each ID. Returns a list of JSON documents relevant to the provided PDB IDs as an argument to the callback. |
| download(id, format, cb) | Accepts PDB ID along with a string specifying the format (.pdb or .cif), and returns a a string representation of the file as an argument to the callback. |

Common to all methods is the callback parameter, which is a function that is invoked after the asynchronous HTTP request returns the relevant data. However, after the ECMAScript 6 Standard introduced the concept of JavaScript Promises, support for Promises was added to the above functions [7]. Usage details are described in the module documentation.

The `query` function returns a array of JSON documents, given that JSON is the most natural JavaScript data structure for document-style data. Arrays in JavaScript can be filtered using custom functions. Hence, the JSON documents returned by `query` be further filtered based on conditions on the comprising element values. An example of such usage is depicted in the code block below:

```javascript
miner.query("ribozyme")
  .then(results => miner.describe_pdb(results, ["macromoleculeType"])
  .then(descriptions => descriptions.filter(obj => obj.macromoleculeType == "RNA")
  .then(rnas => console.log(rnas));
```

The output is a list of structures pertaining to the “ribozyme” query that consist of RNAs. Additional methods are in the process of development and any contributions to the Git repository for the project are welcomed.
Example Case

![Figure 1](image.png)

Figure 1. Example of usage. A plotly graph displaying the frequency of various DSSP assignments for structures corresponding to the query “transmembrane protein.”

The PDB was queried for the terms “transmembrane protein,” and the kabschSander parameter was requested. One of eight characters, corresponding to a secondary structural element, is assigned to each residue in the primary structure[4]. The resulting 1,857,175 total assignments corresponding to the matching PDB entries were plotted using the external plotly Node.js module[5]. This serves as one simple example for the kind of data wrangling that this module aims to simplify.

Conclusion

We have introduced an API for Node.js that serves as a wrapper around the RESTful RSCB PDB API, for the purpose of simplifying the task of PDB querying in modern web applications. This tool can fit well into larger web-based bioinformatics pipelines that may make use of PDB/mmCIF parsers and/or external visualization modules.

The latest release of the code is available on the npm registry and issues, along with development progress, can be tracked on the GitHub repository.

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