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Applications Note

Systems biology

NMRPro: an integrated web component for interactive processing and visualization of NMR spectra

Ahmed Mohamed*, Canh Hao Nguyen and Hiroshi Mamitsuka

Bioinformatics Center, Institute for Chemical Research, Kyoto University, Kyoto, Japan

*To whom correspondence should be addressed.

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Abstract

Summary: The popularity of using NMR spectroscopy in metabolomics and natural products has driven the development of an array of NMR spectral analysis tools and databases. Particularly, web applications are well used recently because they are platform-independent and easy to extend through reusable web components. Currently available web applications provide the analysis of NMR spectra. However, they still lack the necessary processing and interactive visualization functionalities. To overcome these limitations, we present NMRPro, a web component that can be easily incorporated into current web applications, enabling easy-to-use online interactive processing and visualization. NMRPro integrates server-side processing with client-side interactive visualization through three parts: a python package to efficiently process large NMR datasets on the server-side, a Django App managing server-client interaction, and SpecdrawJS for client-side interactive visualization.

Availability and implementation: Demo and installation instructions are available at http://mamitsukalab.org/tools/nmrpro/

Contact: mohamed@kuicr.kyoto-u.ac.jp

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

1 Introduction

Nuclear magnetic resonance (NMR) spectroscopy is indispensible for structure identification of chemical compounds, becoming a crucial part of metabolomics and natural products studies. Web applications are attractive environments for analysis and storage of NMR spectra because (i) web is a platform-independent highly interactive environment and (ii) existing web applications can be easily extended through integrating 'web components', such as JavaScript libraries and web services, to provide additional functionalities.

Online processing and interactive visualization of spectra are necessary functionalities for all NMR web applications (Mohamed *et al.*, 2015). However, web applications for NMR analysis such as MetaboAnalyst (Xia *et al.*, 2012), MetaboHunter (Tulpan *et al.*, 2011) and COLMAR (Zhang and Brüschweiler, 2007) require NMR spectra to be processed offline beforehand. Also, interactive investigation of NMR spectra in databases such as HMDB (Wishart *et al.*, 2013) requires raw spectra to be downloaded and visualized offline.

Although processing and interactive visualization of NMR spectra are needed for web applications, web components providing these functionalities are still lacking. In fact, previously used Java applet components, such as JSpecView (Lancashire, 2007) and Nemo, suffer from security concerns and require installation of additional software. Also, although the recently developed jsNMR (Vosegaard, 2015) and SpeckTackle (Beisken *et al.*, 2015) offer JavaScript-based visualization, they have very limited processing functionalities.

The development of web components for processing NMR spectra is hampered by three challenges caused by the large size of NMR spectra: (i) processing of large datasets is computationally intensive, requiring server-side integration. (ii) A compressed spectral format, required for efficient transfer across the Web, is lacking. (iii) Visualization of large number of spectral data points presents a

computational load on users' computers. Automatic reduction of data points is needed.

We present NMRPro, an open-source easy-to-integrate web component for processing and visualization of NMR data, which is highly extensible to include new functionalities according to the needs of each application. NMRPro consists of three integrated parts, (i) Python package with extensible functionality plugins for server-side spectral processing, (ii) Django App for spectral compression and managing communication between server- and client-sides and (iii) SpecdrawJS, a JavaScript library for visualization of 1D and 2D NMR datasets. Advantages over existing tools are summarized in the supplement (Tables S1 and S2).

2 Component architecture

The general application architecture (Fig. 1) consists of three main subcomponents, NMRPro python package, Django-NMRPro App and SpecdrawJS. Below, we discuss the role of each subcomponent.

2.1 Python package

NMRPro python package consists of two main parts: (i) core part, providing four classes for programmatic representation of NMR spectra, which keep necessary information about the spectra and processing history and (ii) plugins, which provide functions necessary for automatic spectral processing (Fig. 1). Each plugin also contains a GUI information entry, which is displayed in the web browser on the client-side, allowing the user to customize processing parameters. The plugin architecture allows extensibility of the subcomponent by installing new plugins on the server-side, and the GUI is updated automatically to match installed plugins.

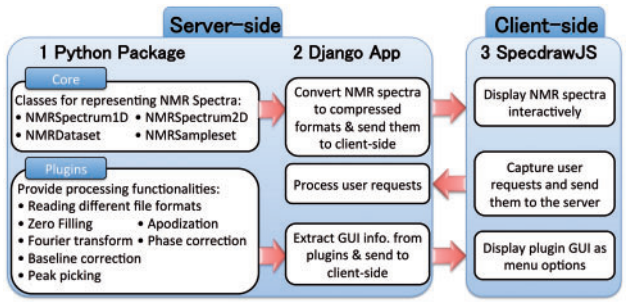

Fig. 1. Component architecture of NMRPro

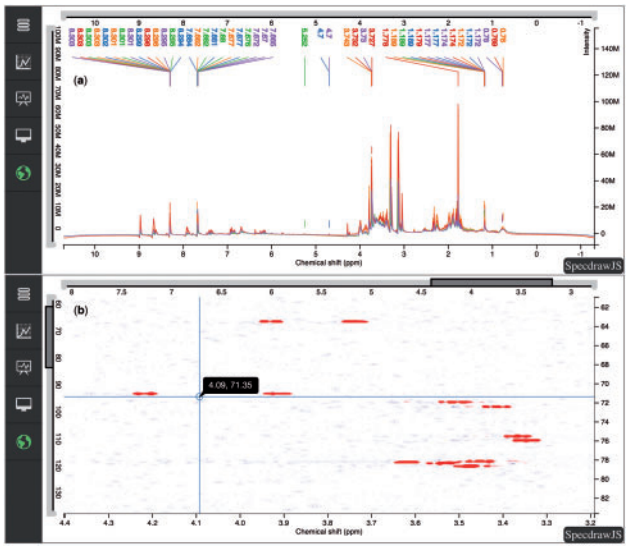

Fig. 2. SpecdrawJS visualization. (**a**) 1D NMR dataset. (**b**) 2D NMR spectrum

2.2 Django App

Django framework enables the development software packages, 'Apps', that can be directly integrated into existing web applications, interfacing between python processing functionalities and client-side visualization. Django App controls the interaction between the server and client-side by managing three roles: (i) efficient transfer of spectral to client-side, using a scaled down and compressed format that can be read in the web browser, utilizing PNG image compression (see supplement, Fig. S1). (ii) Storage and retrieval of user spectra for processing on the server-side. (iii) Aggregation of server-side plugins and sending their GUI information to the client-side.

2.3 SpecdrawJS

SpecDrawJS is a platform-independent JavaScript library for visualization of 1D and 2D NMR spectra (Fig. 2). SpecdrawJS can be used in four different configurations, static view, interactive view, full client-side and connected modes, with functionalities ranging from static visualization to full interactive processing (see supplement, Table S1 for details).

To enable visualization of NMR datasets, SpecdrawJS improves visualization performance by implementing two approaches: (i) Reducing the number of points in an NMR spectra using topology-preserving line simplification algorithm. NMR spectra are reduced to the number of rendered pixels in the browser without affecting the perceived spectral shape. (ii) Parallel programming using newly introduced web-worker technology.

3 Conclusion

We present NMRPro, an extensible web component that can be easily integrated in current web applications and databases, providing NMR processing and visualization functionalities. Future work is to extend NMRPro by implementing new plugins to add further functionalities such as covariance NMR and multivariate analysis for wider application in metabolomics and natural products.

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