

# Programmatic Access to the Macromolecular Structure Information

*PDBe Workshop for Programmers, 20-21 Nov 2014*

## What?

The Protein Data bank in Europe (PDBe; <http://pdbe.org>) is organising a hands-on, interactive workshop for developers interested in using primary and value-added information about the 3D structures in PDB and EMDB. Programmatic access to macromolecular structure data as well as information about assemblies, structure quality, literature and citations, and up-to-date cross-references to other biomedical resources (UniProt, Pfam, CATH, SCOP, etc.) is a critical requirement for integrative bioinformatics analyses and workflows.

PDBe has developed a set of REST APIs (<http://wwwdev.ebi.ac.uk/pdbe/api/doc>) that provide easy access to high-quality information regarding biomacromolecular structures archived in PDB and EMDB. They provide a simple, reliable, light-weight mechanism to query macromolecular structure data, select entries or molecules of interest, and access targeted information about them, including information about the molecules, experimental details, assemblies, motifs, function, taxonomy, structure quality, etc. The API is used by the PDBe services and is also integrated in Jmol/Jsmol. We will also present Solr/Lucene based query API for macromolecular structure information including PDB, EMDB and value added information on assemblies, structure quality and up-to-date cross-reference information to other biomedical databases based on SIFTS (<http://pdbe.org/sifts>).

## Is it for me?

Do you (plan to) develop software or on-line resources that use or need access to information about structures in PDB or EMDB? Would you rather not maintain your private infrastructure for retrieving, parsing, storing and updating such information? If so, then this workshop is for you!

In the workshop, we will explain what information is available through the API and how you can access it from your own software or resource. There is plenty of time for hands-on work where experienced PDBe developers will try to help you use the API for your specific needs.

## When?

20 & 21 November 2014.

## Where?

EMBL-EBI (<http://www.ebi.ac.uk>), Cambridge.

## How much does it cost?

We expect you to pay for (and arrange) your own travel to and from Cambridge. However, there is no fee for the workshop, and we will provide free accommodation (Holiday Inn Express; <http://www.hiexpresscambridgeduxford.co.uk>), transportation between the hotel and the EMBL-EBI, coffee/tea, lunches and a workshop dinner on the 20th. This is all thanks to generous funding from the Wellcome Trust to PDBe.

## How can I apply?

E-mail Swanand Gore ([swanand@ebi.ac.uk](mailto:swanand@ebi.ac.uk)) or Jose Dana ([dana@ebi.ac.uk](mailto:dana@ebi.ac.uk)) at PDBe no later than 20 October 2014 with the following details:

- a brief description of the software you have developed or are developing - i.e. what it does, in which field, how many users, relevant publications, etc.
- programming language(s) you are specifically interested in (python examples and tutorials will be provided).
- how you would benefit from this workshop.
- any specific topics or questions you would like to see addressed in the workshop.

If the workshop is oversubscribed, we will select participants based on the information provided.

You will be informed by the end of October if you have been selected or not, or whether you are on the stand-by list.

## Prerequisites?

Basic programming experience in use of REST API's. Bring your own laptop with *git* and *iPython notebook* pre-installed if you want to follow the python tutorial and examples. If you need to make plots, make sure that *matplotlib* is also installed.

## Questions?

Swanand Gore ([swanand@ebi.ac.uk](mailto:swanand@ebi.ac.uk)) or Jose Dana ([dana@ebi.ac.uk](mailto:dana@ebi.ac.uk)) at PDBe will be happy to answer your queries.