

# User Document 1. Description of the submission process of a simulation into the P-found system

In the present document, it is described the process of uploading a new simulation into the P-found system. Only registered users can upload data into the system.

This process consists of three major steps:

1. Uploading trajectory and topology files onto an FTP server
2. Submitting the parameters associated with simulation through the P-found webpage, associating the trajectory and topology files with it.
3. Calculating the molecular properties for the new simulation being uploaded, and making it available in the P-found system.

The two first steps are carried out by the user, and the third is performed automatically by the P-found system. Next, it is described in further detail the first two steps.

## **Step 1 – Upload trajectory and topology files onto an FTP server**

- FTP server name: matrix.scic.ulst.ac.uk
- Login name and password as in the P-found system

## **Step 2 – Submit the parameters associated with simulation**

1. Go to P-found webpage and access the **Registered User** area
2. Once the user has logged in to the system, he may Start a New Submission or continue pending submissions.
3. The final step is to associate to these set of parameters with the trajectory and topology file.

## **Step 3 – Calculate and upload into the P-found system the molecular properties for the new simulation submitted**