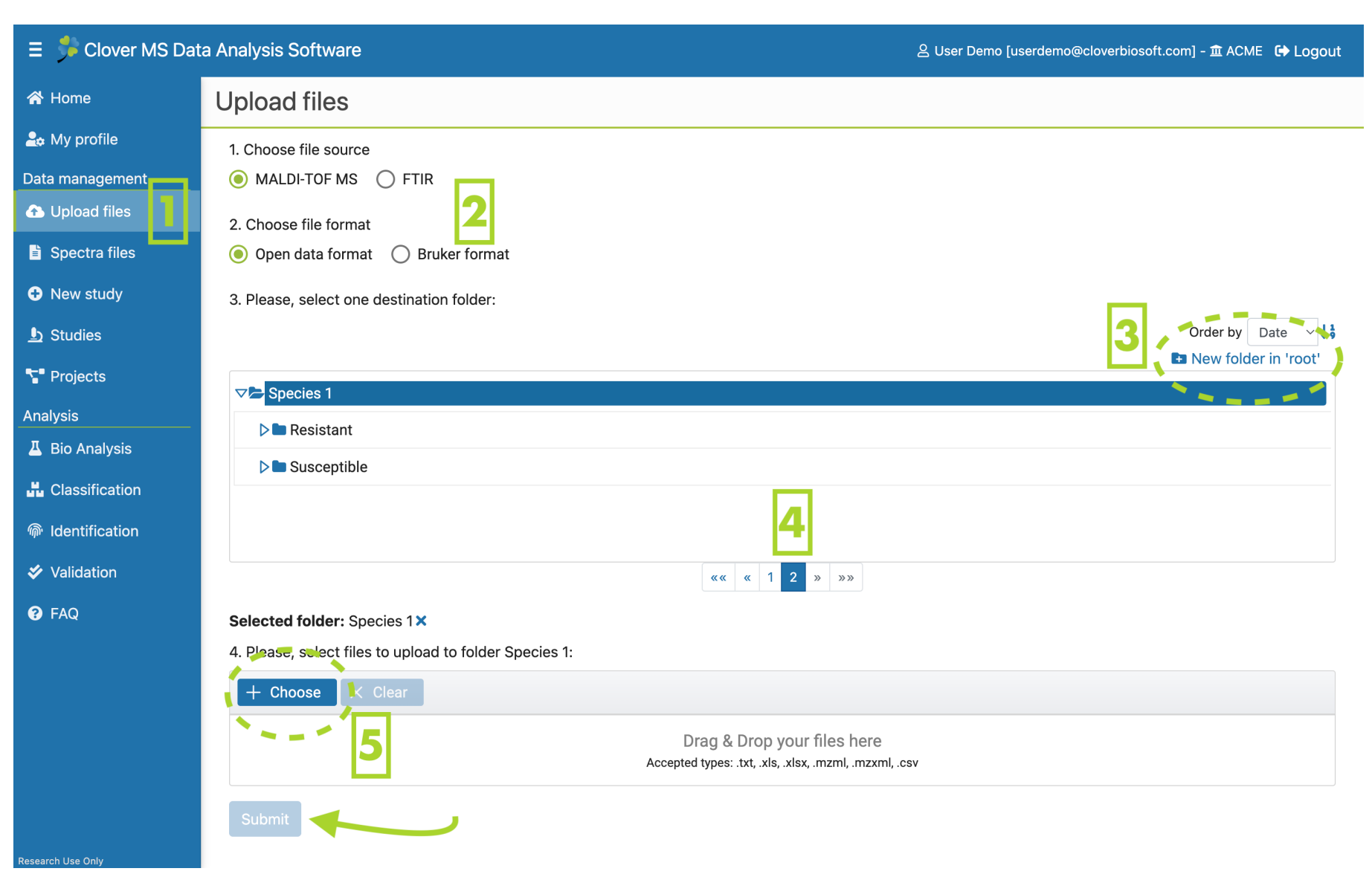


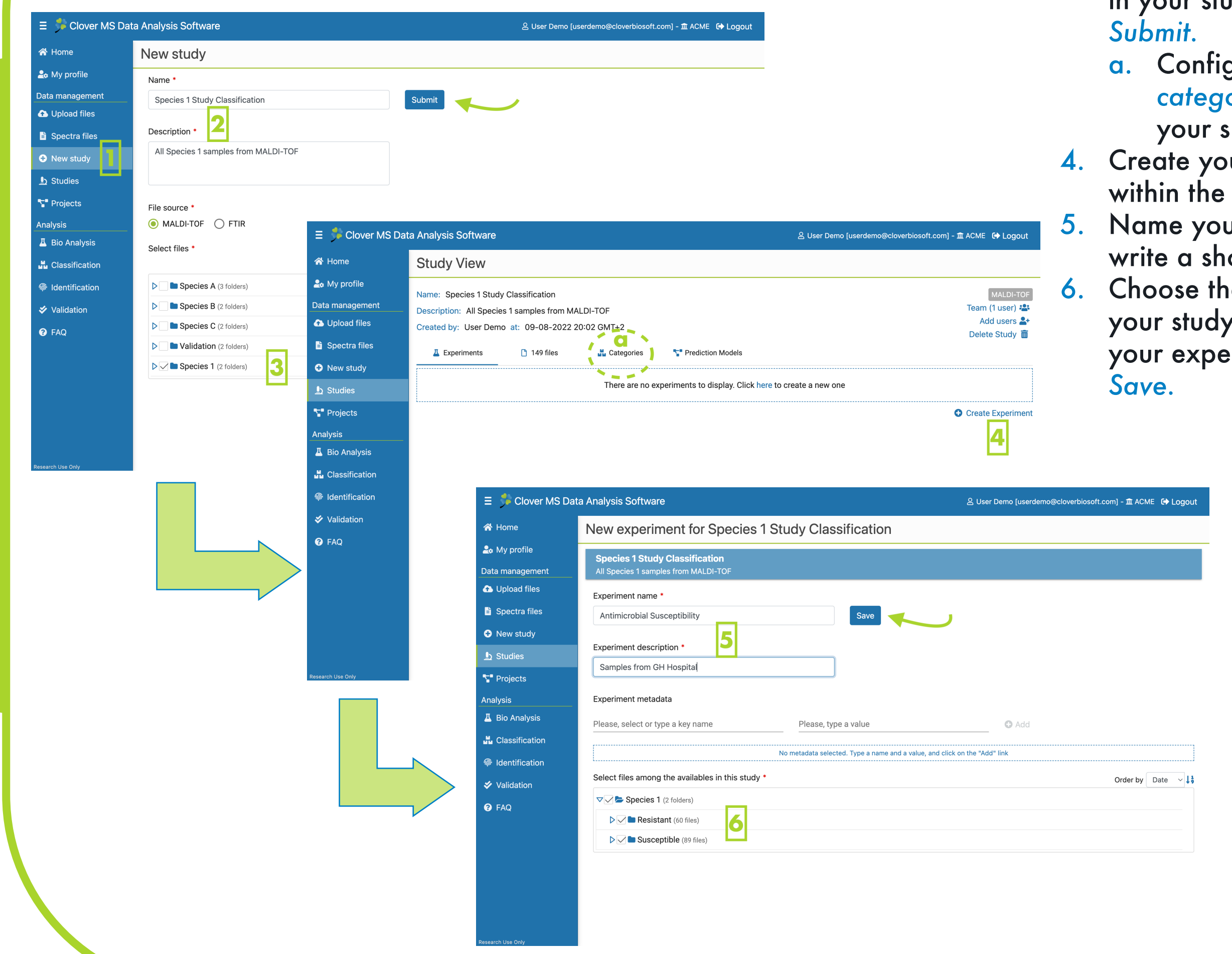
Quick Start Guide CLOVER MS Data Analysis Software

1 Upload Data



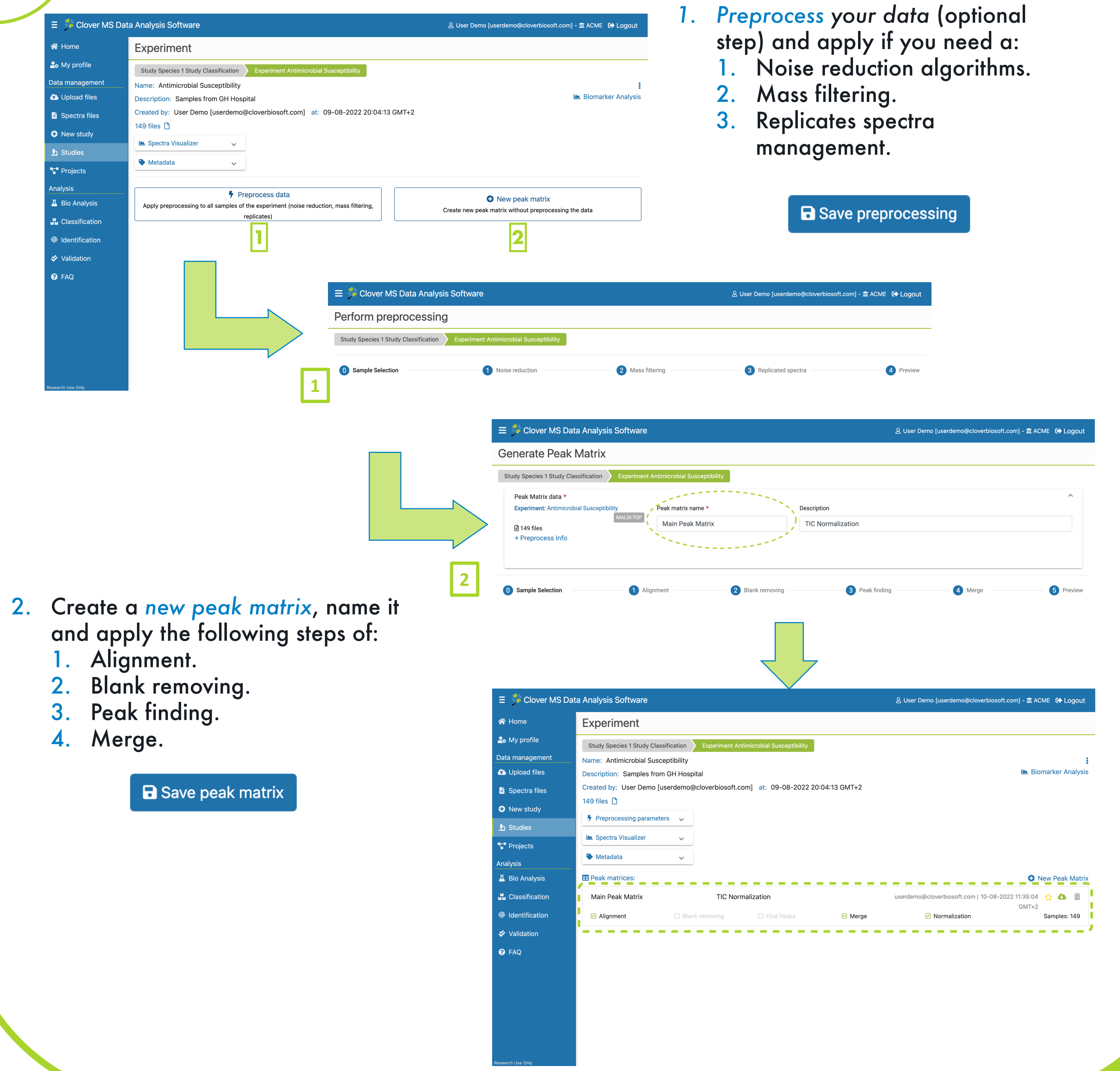
1. Go to **Upload files** section.
2. Choose the file source and format.
3. Create the folder(s) you need.
4. Choose the destination folder.
5. Choose or Drag & Drop your files and press **Submit**.

2 Study and Experiments creation



1. Go to **New Study** Section
2. Name your study.
3. Choose the files to include in your study and press **Submit**.
  - a. Configure the **categories** and label your spectra.
4. Create your experiment within the study.
5. Name your experiment and write a short description.
6. Choose the samples inside your study to include in your experiment and press **Save**.

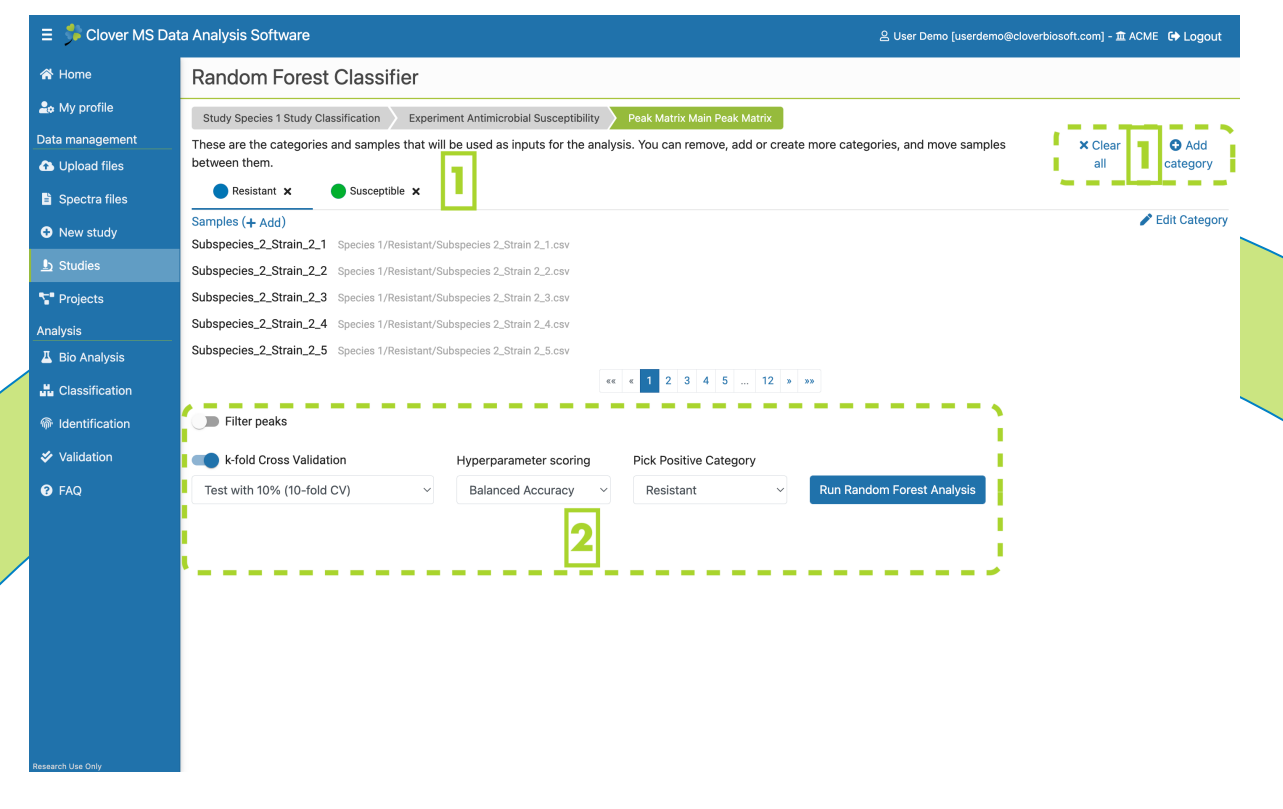
3 Preprocess and Peak Matrix Generation



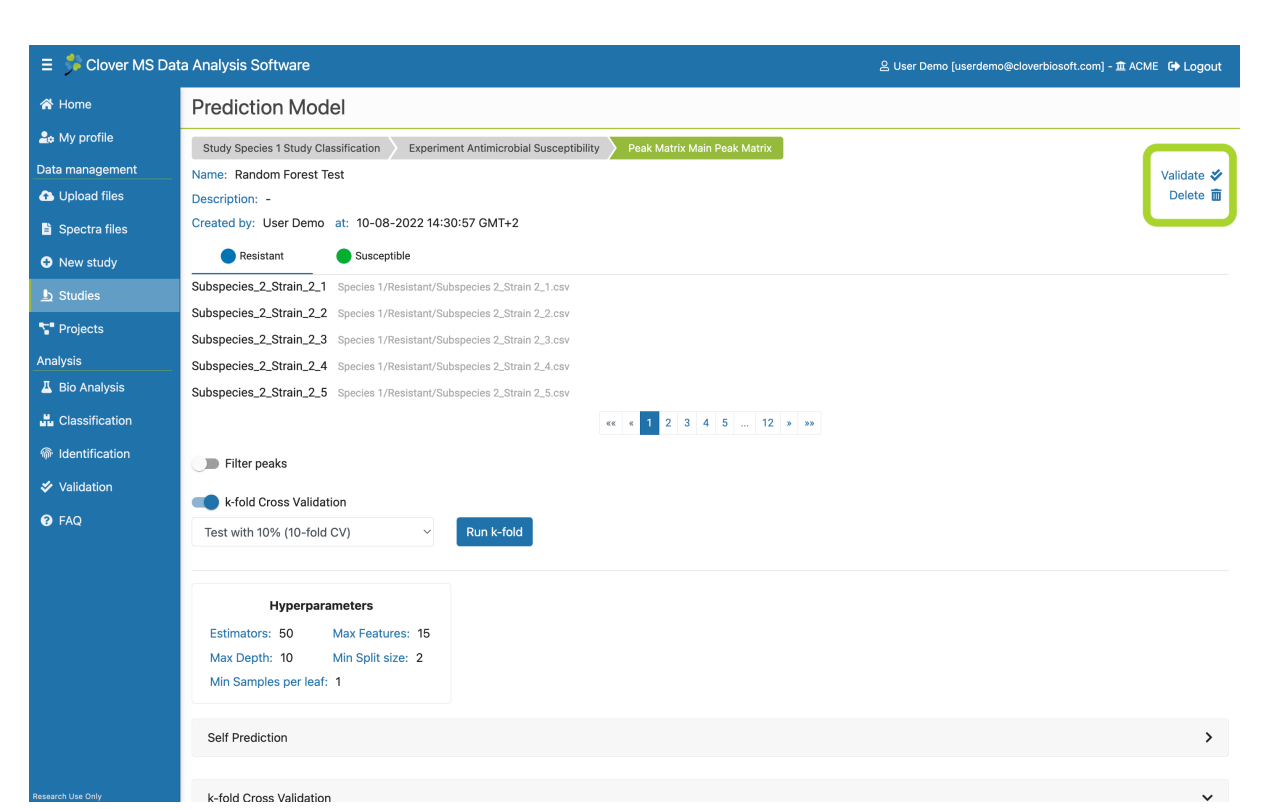
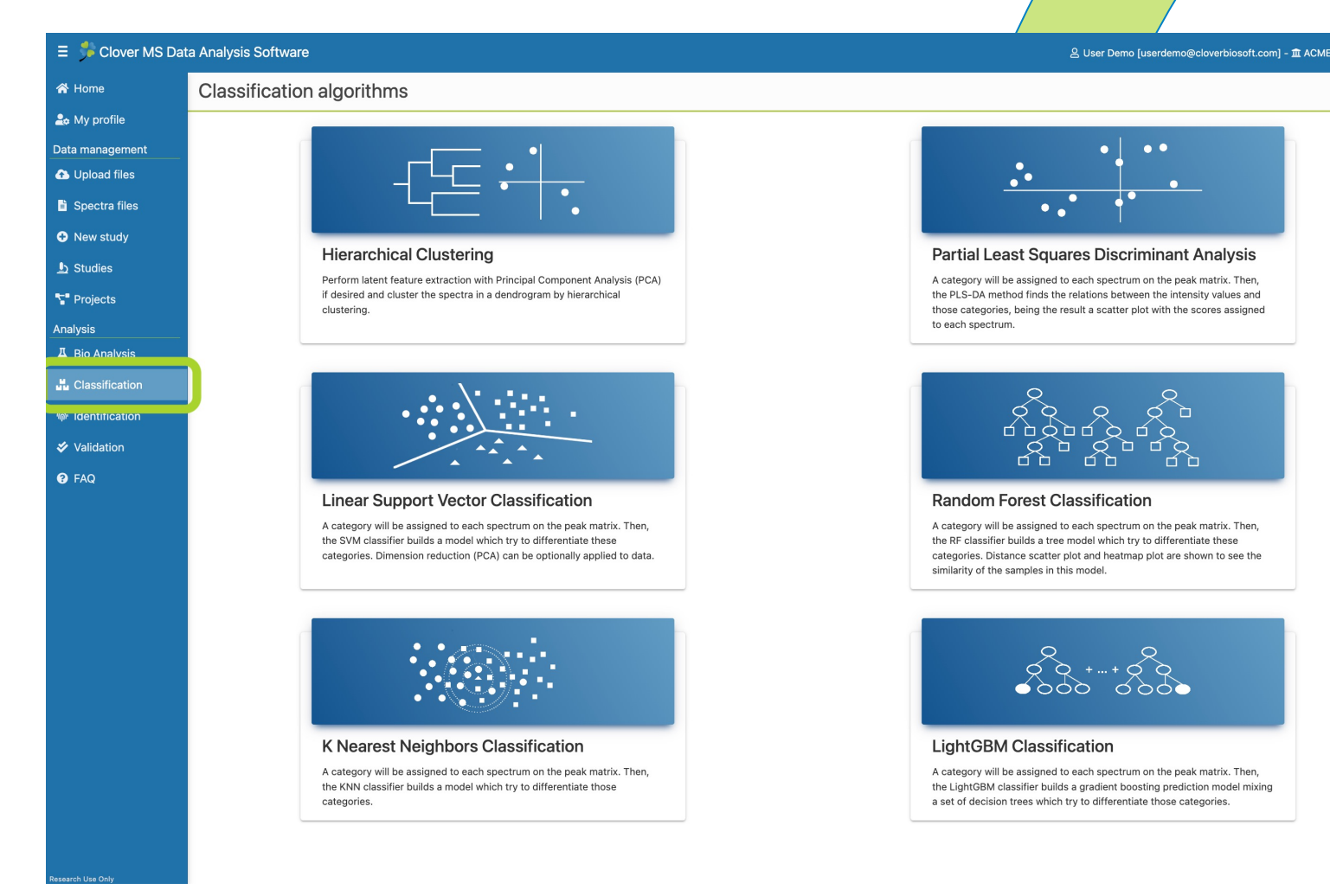
1. **Preprocess** your data (optional step) and apply if you need a:
  1. Noise reduction algorithms.
  2. Mass filtering.
  3. Replicates spectra management.
2. Create a **new peak matrix**, name it and apply the following steps of:
  1. Alignment.
  2. Blank removing.
  3. Peak finding.
  4. Merge.

4 Perform Classification

- In **Classification** section you can chose the algorithm you want to use for test your **peak matrix**.
- In this case, **Random Forest Classification** is chosen to analyze the peak matrix.



- After press in any **Algorithm box** and select your peak matrix from your experiment and study:
1. Configure the **categories** of your samples you want to be classified.
  2. Choose the algorithm parameters like k of k-fold cross validation, the hyperparameter scoring and the positive category if applicable and press **Run Analysis**.



- You can save your optimized analysis as **Prediction Model**, and it will display in that section.
- The prediction model can be consulted any time as well as **validated** with external samples.

Analysis Tools



- K-Fold Cross Validation
- Shapley Values
- Distance Plots
- ROC & PR Curves
- Feature graphs
- Heat Maps



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