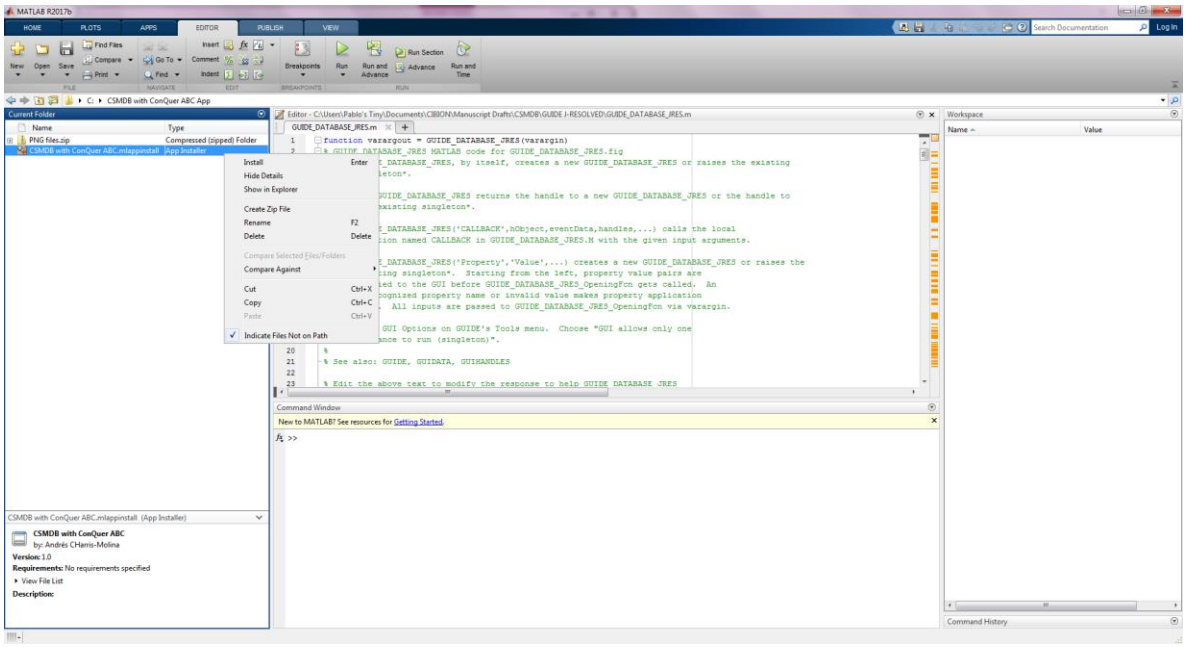
Consecutive Queries to Assess Biological Correlation in NMR Metabolomics: Performance of Comprehensive Search of Multiplets over Typical 1D ^{1}H NMR Database Search

GUIDE

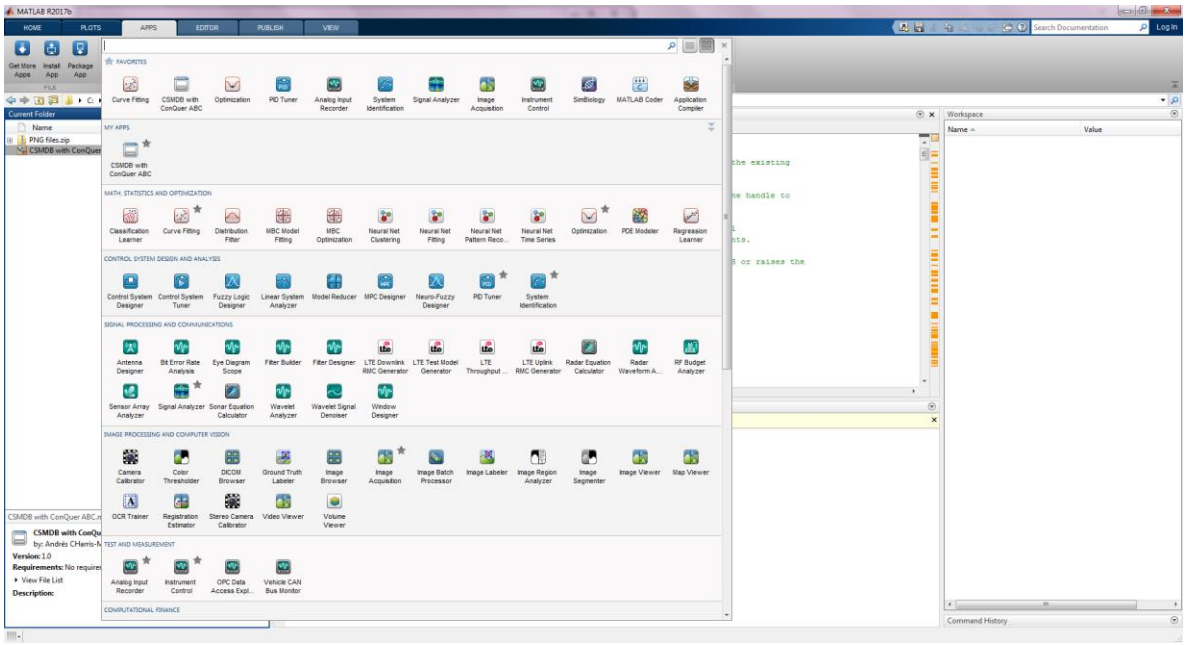
1. Download “CSMDB with ConQuer ABC.mlappinstall” and “PNG files.zip”.

2. Paste files into your Matlab working directory and Install app.

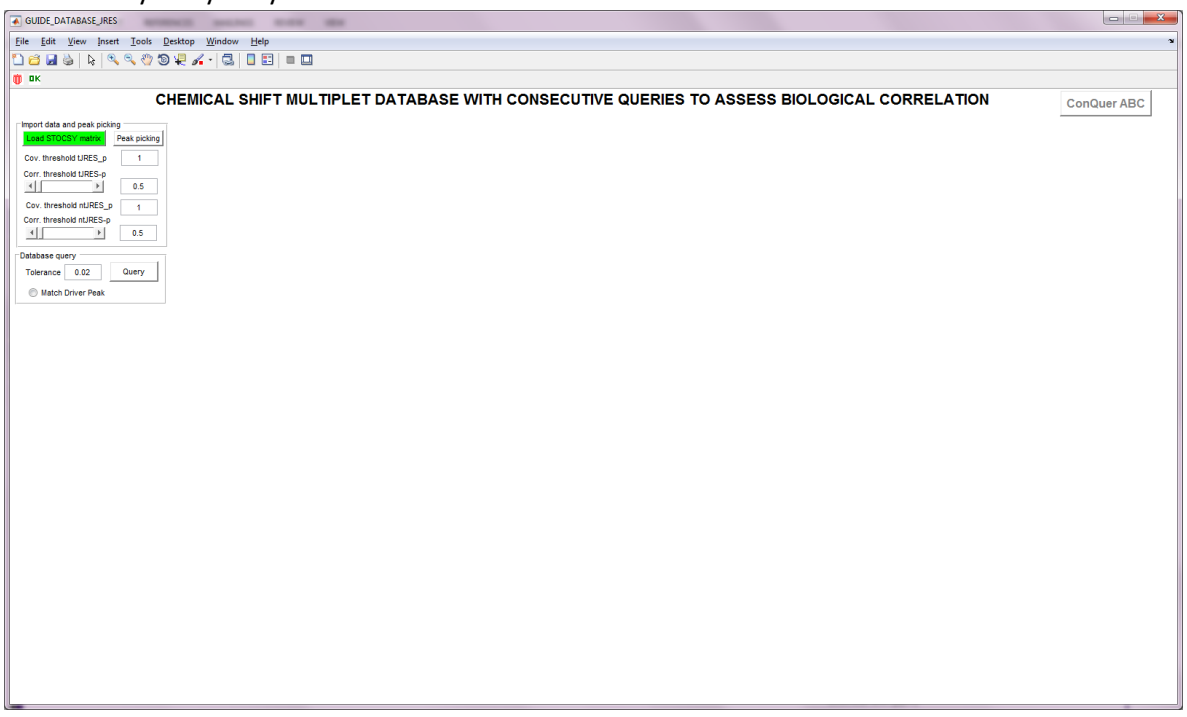


3. Explore the App installation folder (C:\Users\<User Name> \Documents\MATLAB\Add-Ons\Apps\CSMDBWithConQuerABC\code) and unzip the “PNG files.zip” folder there.

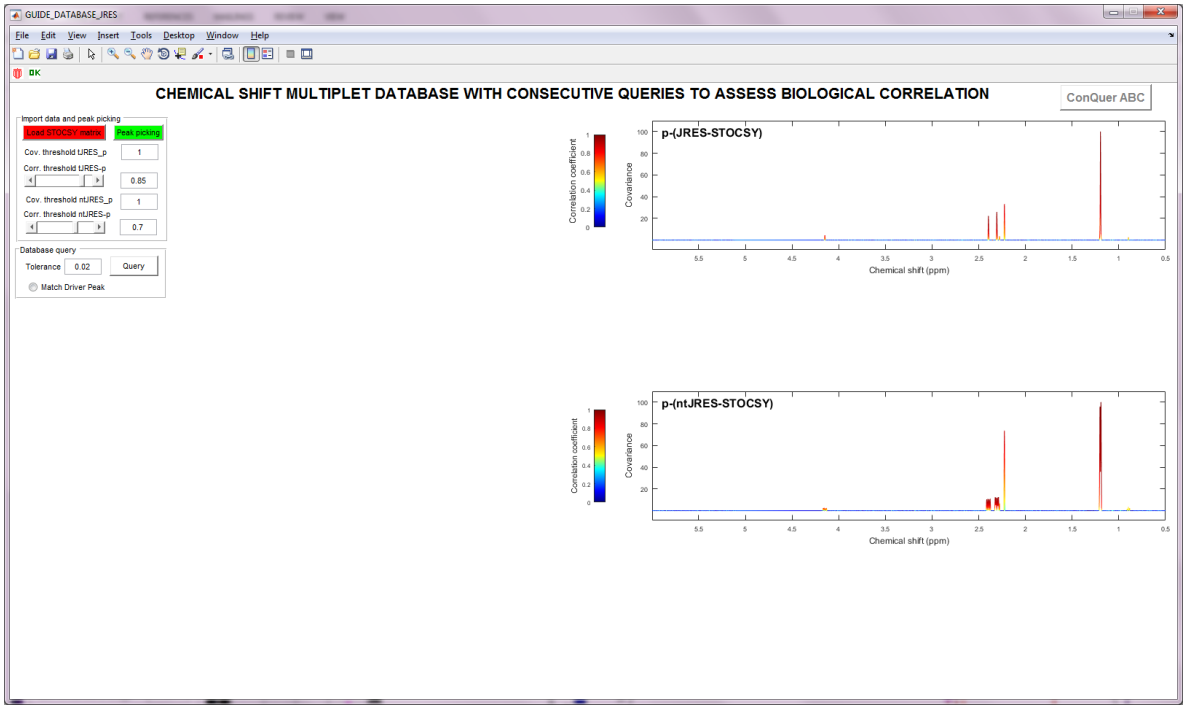
4. Click on Apps in Matlab and select “CSMDB with ConQuer ABC” to start the App.



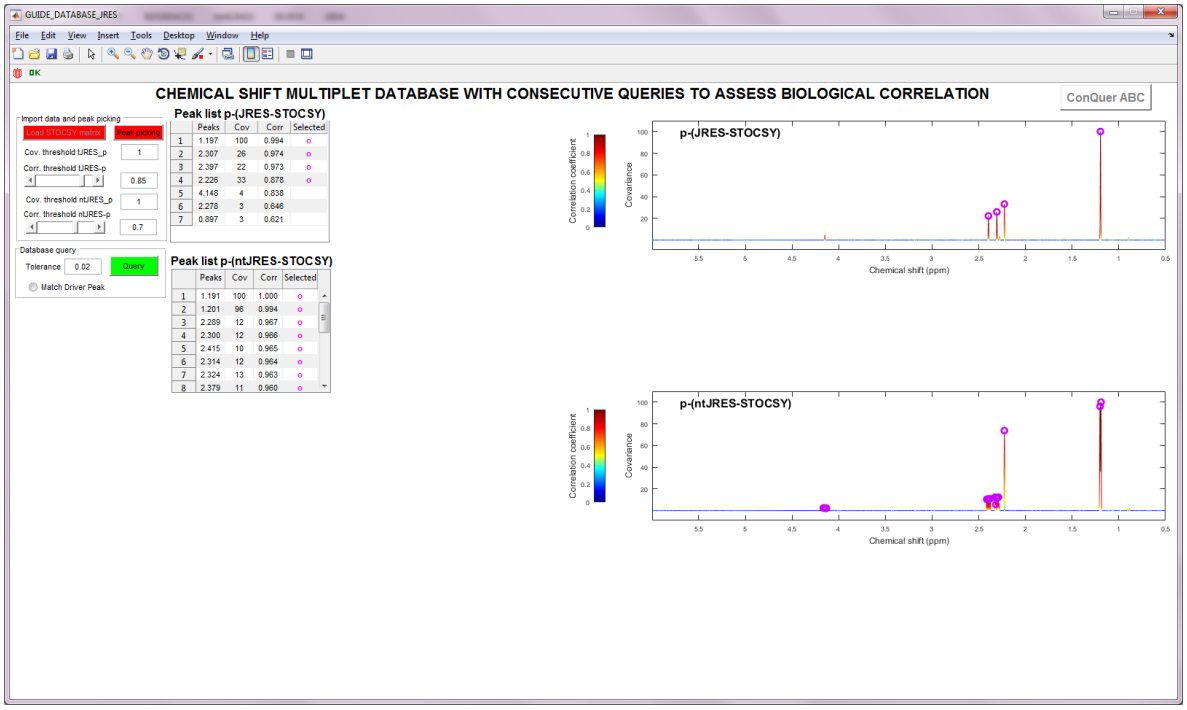
5. Begin by clicking the green “Load STOCSY matrix” button. Green buttons are clickable, red buttons are not clickable. The App contains two examples in the MAT files folder: driver peaks for ethanol and for 3-hydroxy-butyrate. The latter was selected for the rest of this Guide.



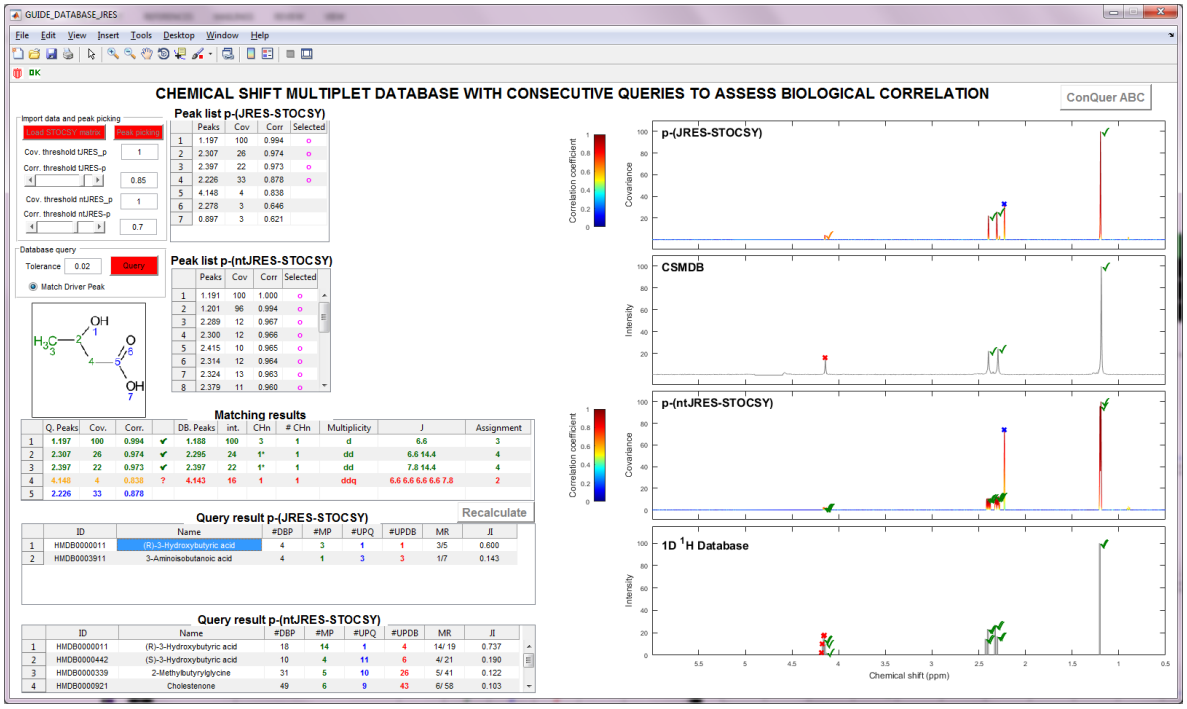
6. Press the button “Peak picking” to select peaks to be searched. In this part, you can set covariance and correlation threshold values for each pseudospectrum STOCSY trace, p-(JRES-STOCSY) and p-(ntJRES-STOCSY). If you want to remove a peak from the selected peak list, select the cell and approve the removal.



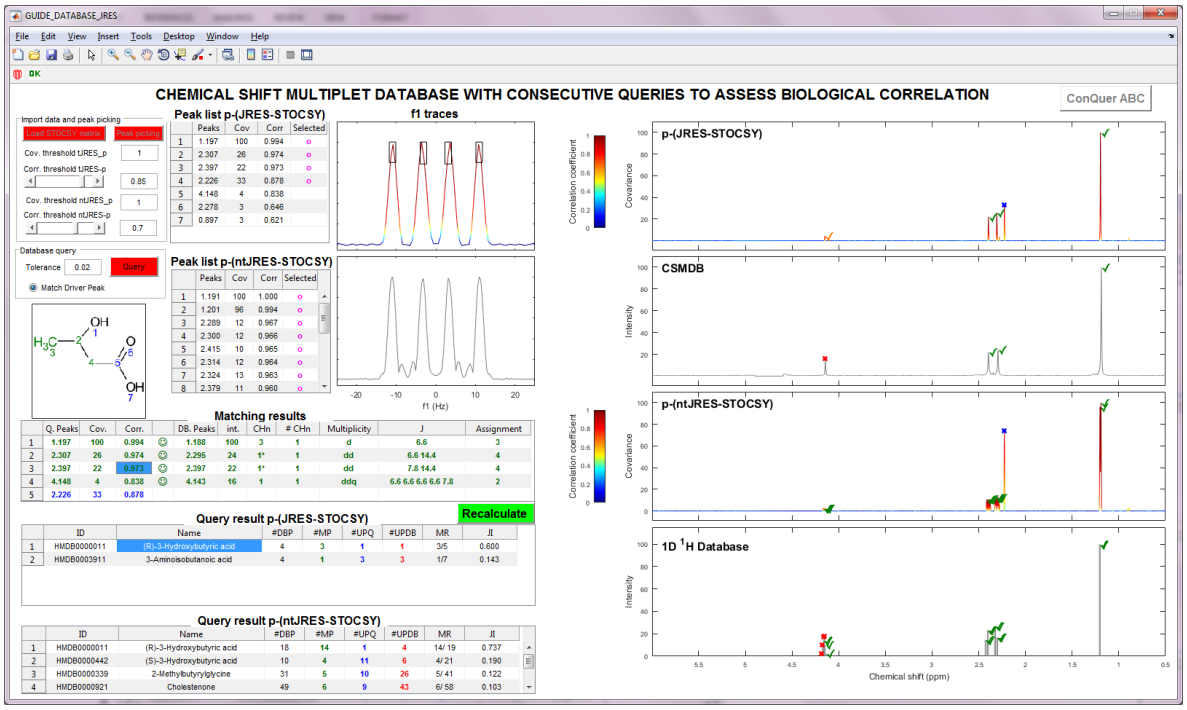
7. Press the “Query” button to find the compounds whose peaks are within the tolerance to the selected ones. The “Match Driver Peak” option could be set before pressing “Query”, if desired. Tables “Query result p-(ntJRES-STOCSY)” and “Query result p-(tJRES-STOCSY)” will now be visible.



8. Select the compound of interest in the table “p-(JRES-STOCSY)”. Table “Matching results” and subplots p-(JRES-STOCSY), CSMDB, p-(ntJRES-STOCSY) and 1D ^{1}H will then be visible.

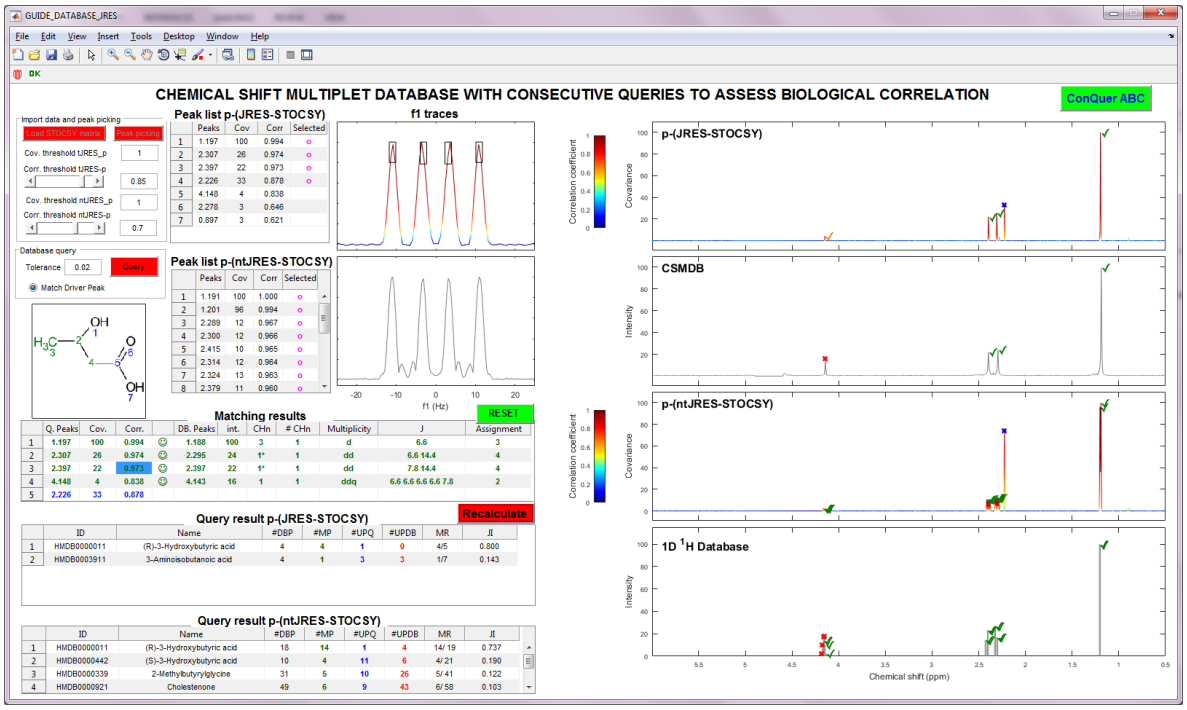


9. Select a desired peak from the table “Query result p-(JRES-STOCSY),” and (in the top left corner) press  or  to disapprove or approve the corresponding f1 trace. Repeat this step until you approve or disapprove all multiplet matches. Once this step is finished press “Recalculate”.

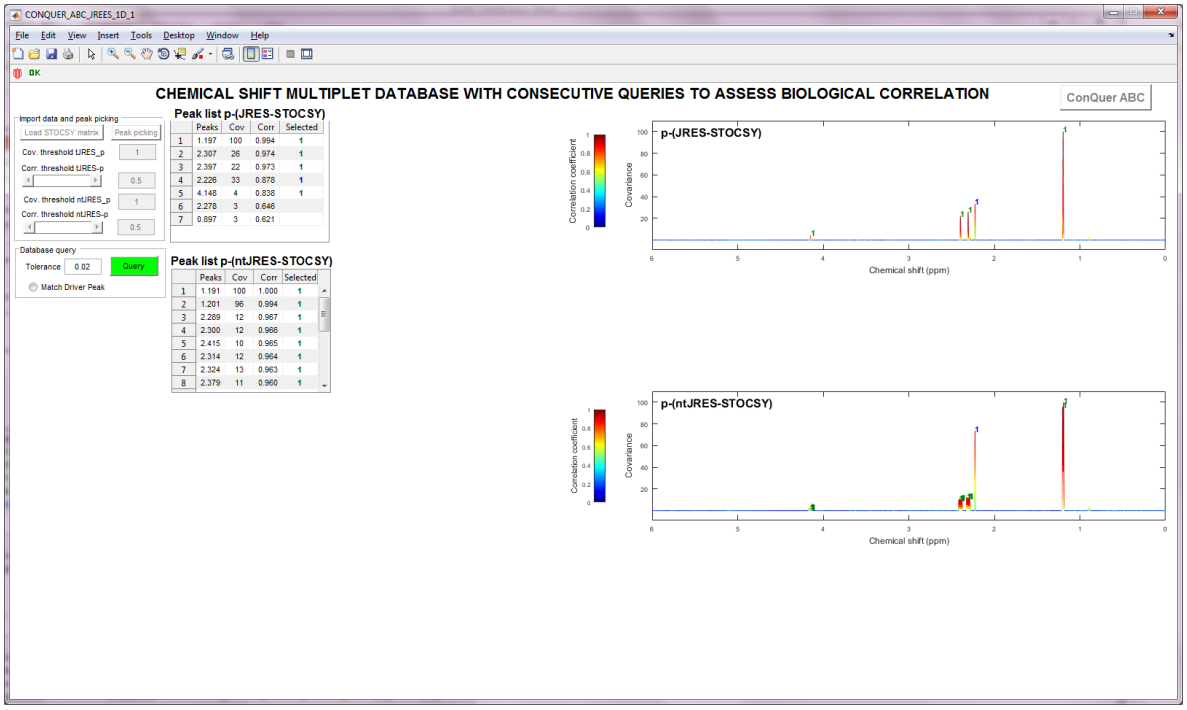


10. If in need to redo trace matching approval and disapproval data for a compound, press RESET and repeat step 9.

If there are unmatched peaks on query list (UPQ) a new query is performed for a selected hit from the original query (table "**Query result p-(JRES-STOCSY)**", to detect the possibility of those peaks pertaining to the spectrum of a biologically correlated compound. Press the "ConQuer" button to open the next query figure window.



11. A new figure is now visible, with information from the previous query. In the peak list tables, subplot p-(JRES-STOCSY) and subplot p-(ntJRES-STOCSY) the blue numbers correspond to unmatched peaks on the query list, the green numbers correspond to matched peaks, and the orange numbers correspond to matched peaks through the "reverse query".



12. Press the “Query” button and repeat steps 8 to 11. Again, the “Match Driver Peak” option can be selected if desired, prior to the query. Repeat this process if peaks remain unmatched in the UPQ list.