N:\figures\Figure_4.tif

Figure 4: Schematic representation of ISPyBB data model. Image has been divided by modules in order to show the tables in a logical layout. Different modules have been labelled in grey and with different background colours for clarity. The date tables correspond to the labelled boxes in blue showing their relations with a line. Table’s fields are not shown for simplicity.

N:\figures\FIGURE_5_A.tif

Figure 5A

N:\figures\FIGURE_5_B.tif

Figure 5 B

N:\figures\FIGURE_5_C.tif

Figure 5 C

N:\figures\FIGURE_5_D.tif

Figure 5 D

N:\figures\Figure_6_A.tif

Figure 6 A Data Acquisition list shows the list of data acquisitions sorted by type: HPLC, sample changer, calibration or all. By clicking on download button will download a zip file with all the files associated to such data acquisition.

N:\figures\Figure_6_B.tif

Figure 6 B

N:\figures\Figure_6_C.tif

Figure 6C

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Figure 6 D

N:\figures\FIGURE_7.tif

Figure 7

N:\figures\Figure_8.tif

Figure 8: A 3D representation shows how models overlap in a customizable way, they can be hidden or their opacity can be modified for a easier visualization. Damaver (in brown), damfilt (in blue) and dammin (in green). Visualization allows to zoom in and zoom out as well as to rotate the model.

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Figure 9 A: Overview shows in customizable view several parameters for all the frames. By selecting a point we can get a plot with the logarithm of the intensity of the sample 9 (in green), the logarithm of the intensity of the average of the buffer (in blue) and the subtraction.

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Figure 9 B. It shows the subtraction of the average of two different peaks.

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Figure 9 C: HPLC’s file manager allows download the frames, averages and subtraction directly from the HDF5 file in a zip format.

N:\figures\FIGURE_10_A.tif

Figure 10 A

N:\figures\FIGURE_10_B.tif

Figure 0 B