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Supplemental information

Advanced analysis of single-molecule spectroscopic data

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This Supplemental Information contains additional screenshot examples as referenced in the main text.

1 Graphical User Interface Examples

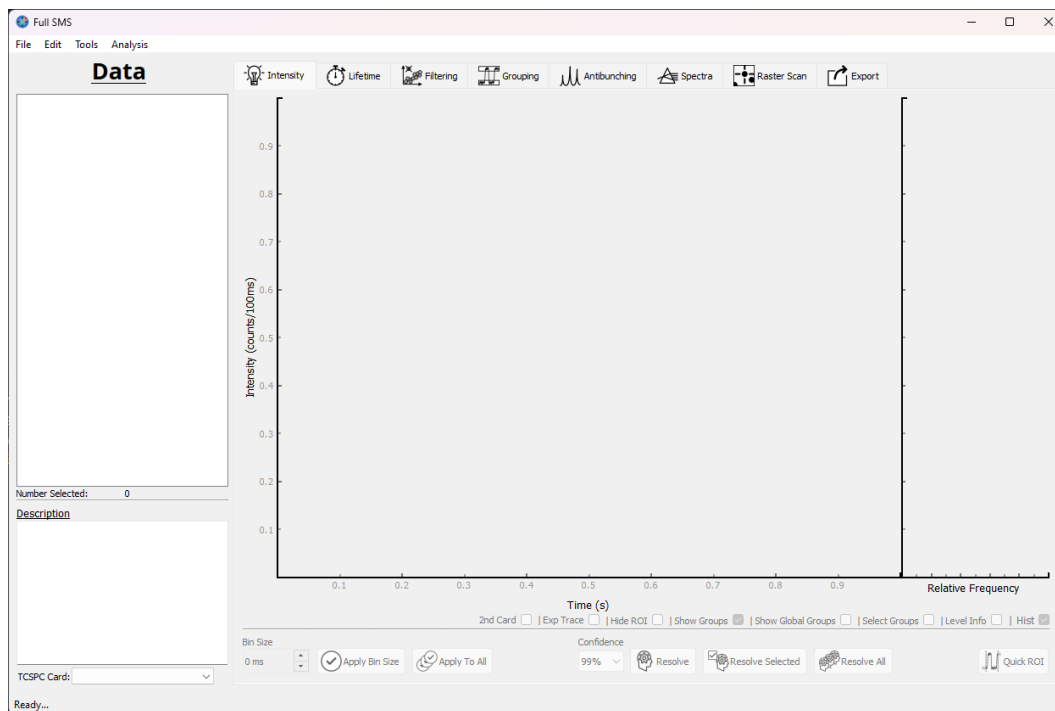


Fig. S 1: Main window of *Full SMS* without any data file loaded. The analysis is separated into separate tabs for each major operation, starting with the *Intensity* tab and ending with the *Export* tab.

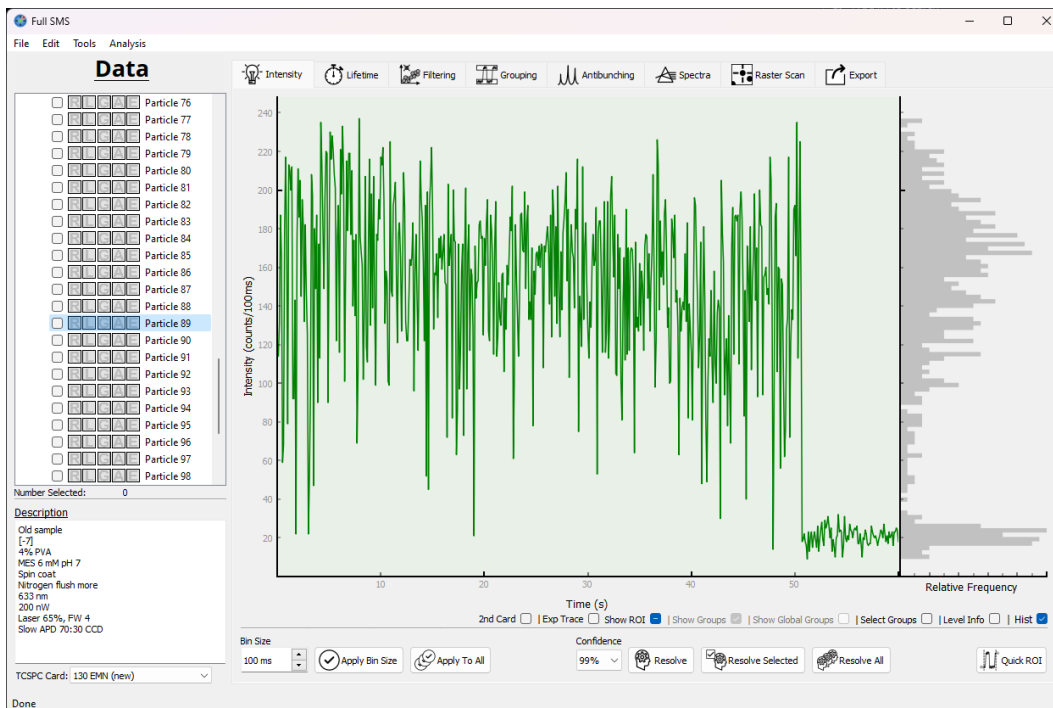


Fig. S 2: Intensity trace example of Alexa as shown in the *Intensity* tab, showing a binned intensity trace before the resolving of the intensity levels is actioned. The same trace is shown in Fig. 1 with the levels resolved.

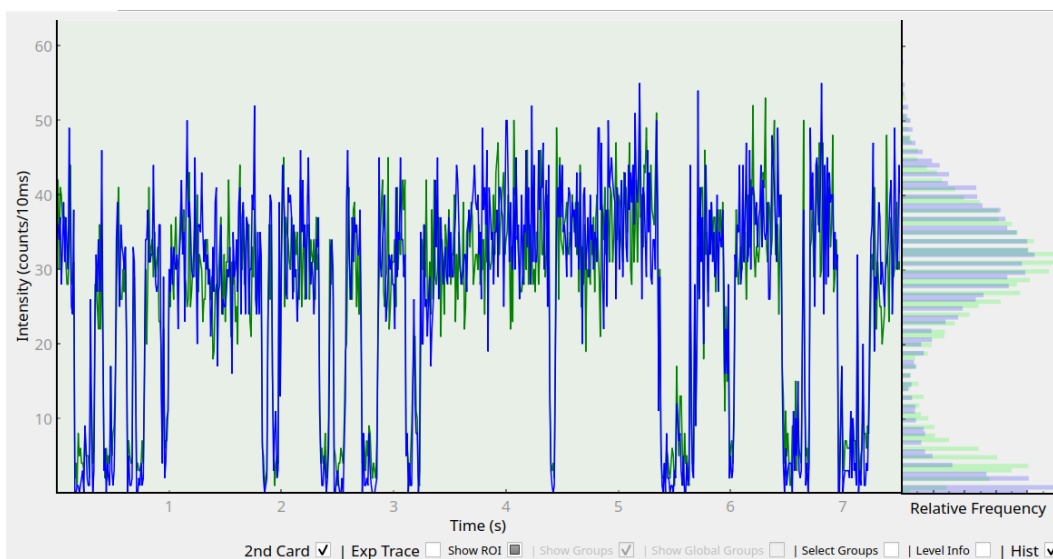


Fig. S 3: Two-channel intensity trace example, showing the binned intensity traces from each channel as a separate colour.



Fig. S 4: Group selection example using the groups shown in Fig. 5. The group's intensity, dwell time, and number of photons are displayed.

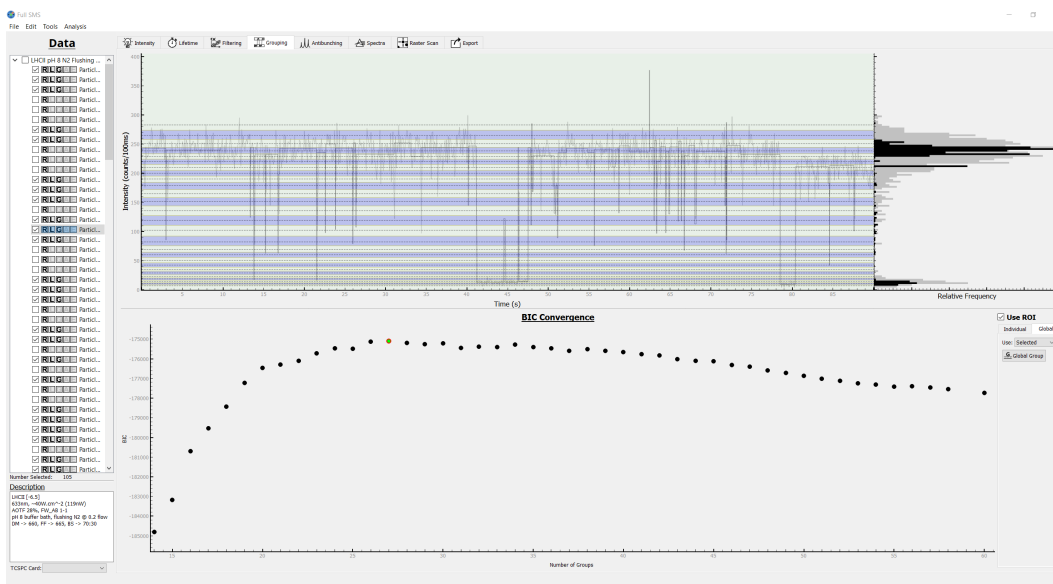


Fig. S 5: Global grouping example of the data of 105 LHCII complexes. The bottom pane shows the progression of the grouping of the appended data, which originally comprised $\sim 10^5$ individual intensity levels. The largest BIC value corresponds to 27 distinct states (down from $\sim 10^5$ states), some of which are not accessed in the intensity trace in the upper pane.

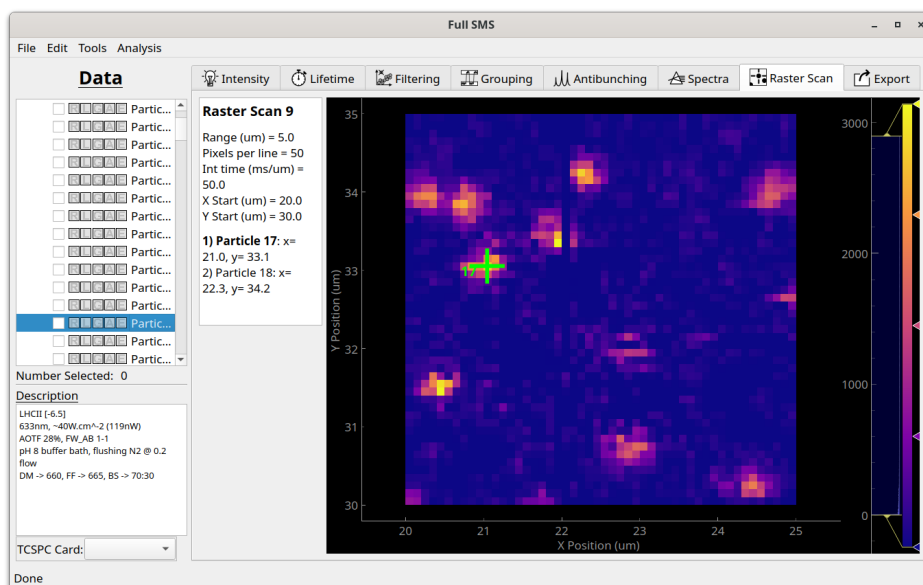


Fig. S 6: Example of a raster-scan image of a few LHCII complexes immobilised on a glass coverslip via poly-L-lysine, indicating the position of the currently selected particle with a green plus. The raster-scan details and coordinates of selected particles are indicated on the left of the image.

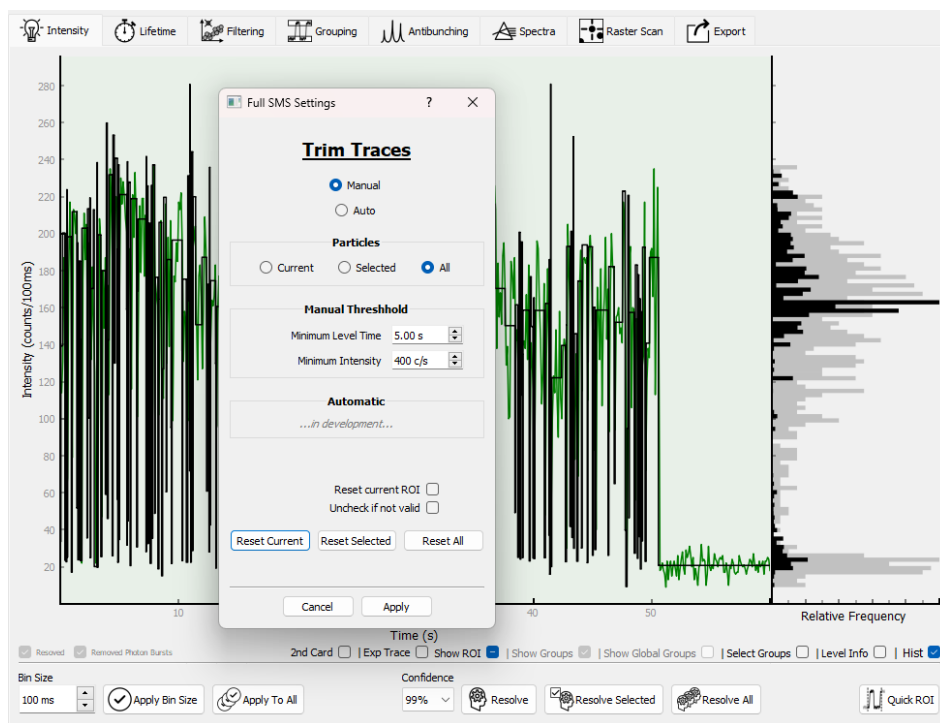


Fig. S 7: Trace trimming tool dialog with the Alexa intensity trace shown in Fig. 1. The end of a trace is trimmed if it is below the given minimum intensity and longer than the given minimum dwell time. An automated choice of these parameters is a future extension that is currently under development.

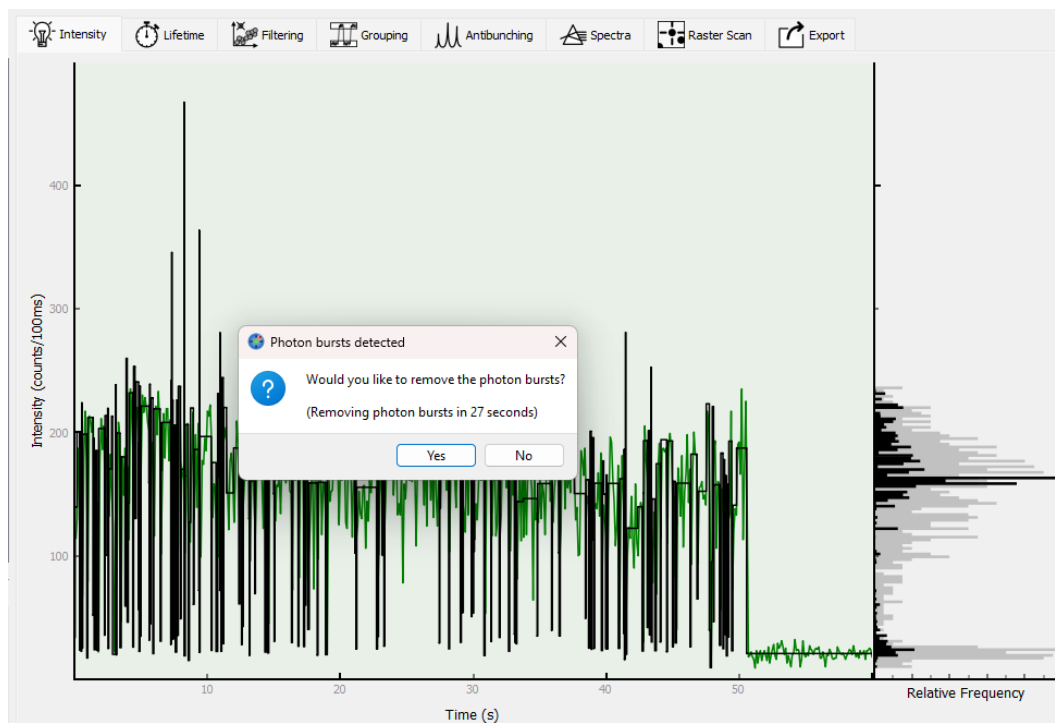


Fig. S 8: Photon burst dialog example with the Alexa intensity trace shown in Fig. 1. This dialog is presented automatically after resolving levels, if photon bursts are detected.