Supporting Information: Quantitative assessment of polymer molecular shape based on changes in the slope of the Mark-Houwink plot derived from size-exclusion chromatography with triple detection

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Supporting Information S-1: Mark-Houwink plots of polyamide-4,6

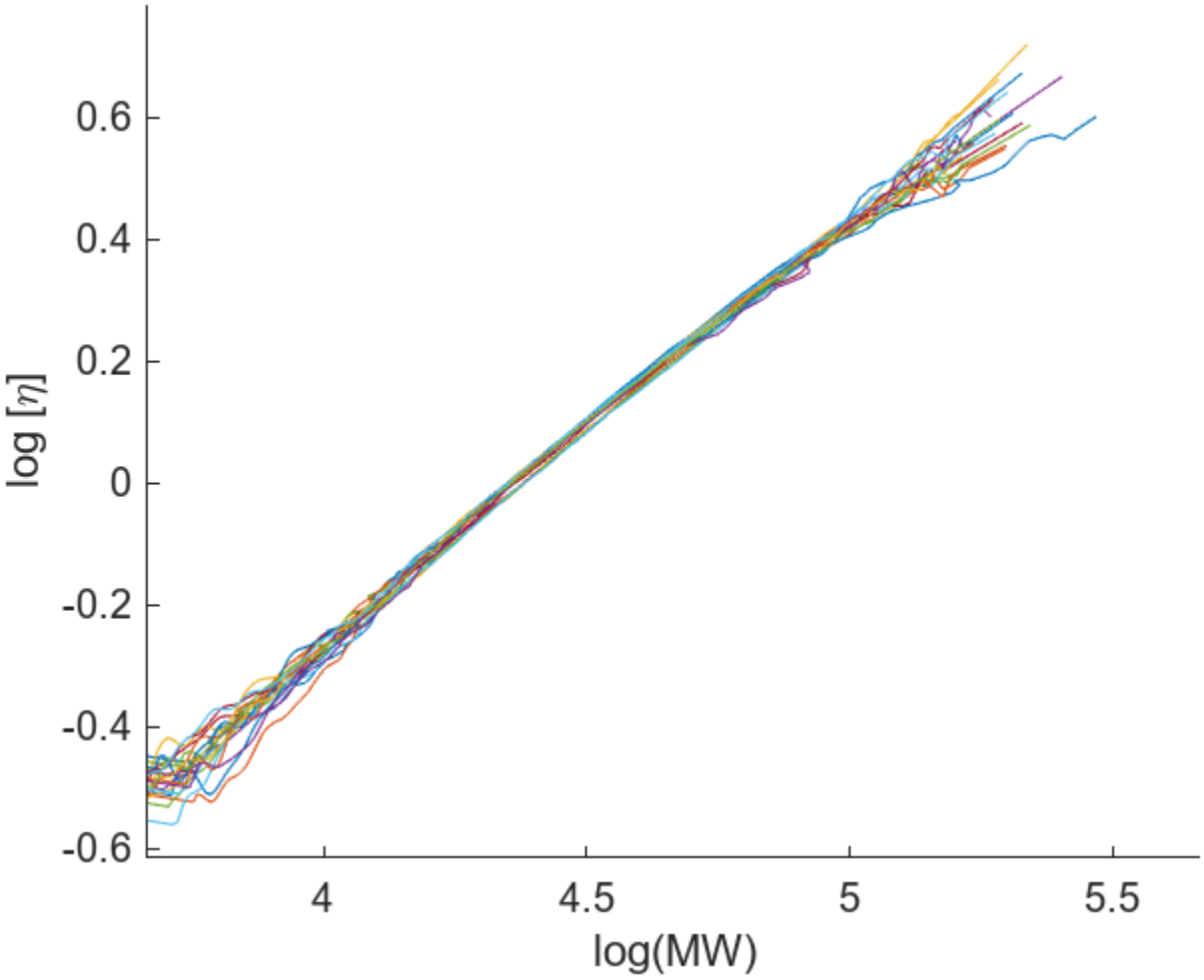

Figure S-1: MH plots derived from twenty SEC-TD analyses of the same polyamide-4,6 sample (1.5 mg/mL) over the course of more than 12 months.

Supporting Information S-2: Mark-Houwink plot of cellulose ethers at

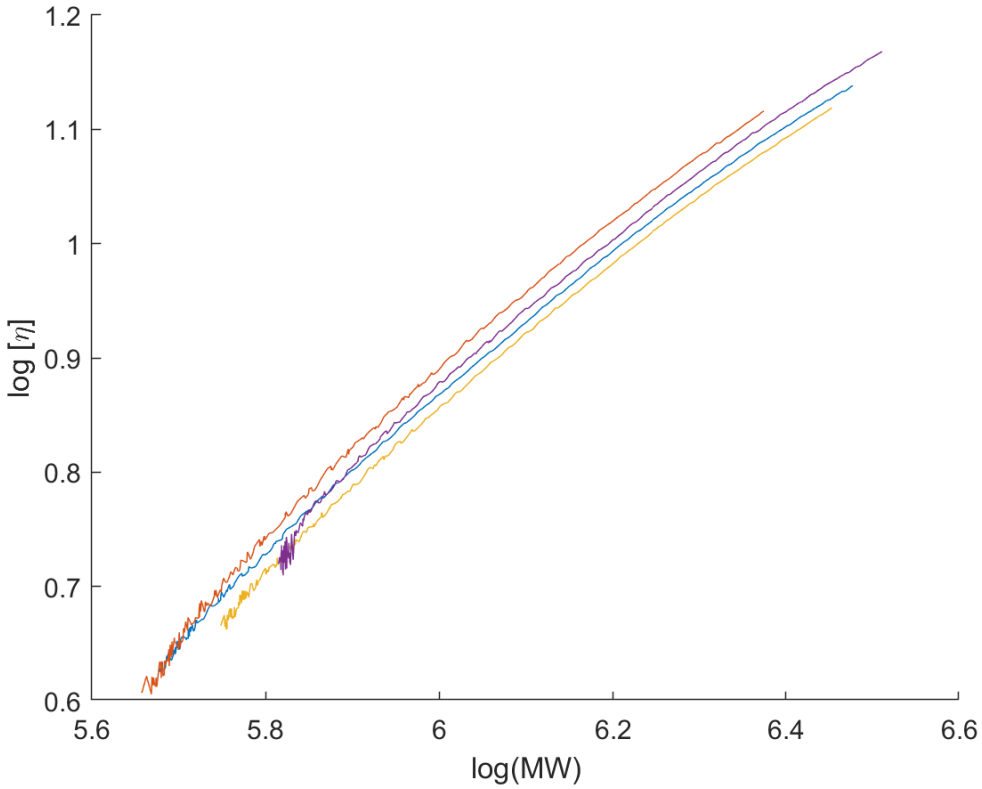

Figure S2: Mark-Houwink plot of the 4 CEs of interest at 25°C. Colors: blue, EHEC (1); orange, EHEC (2); yellow, MEHEC (1); purple, MEHEC (2).

Supporting Information S-3: Manual of the tool to determine the curvature in Mark-Houwink plots

First, the .xlsx file of interest must be loaded by clicking the Load File button. This will open an explorer window in which you can navigate the file of interest. The .xlsx file should have one measurement per sheet of which column A should be the log(MW) and column B should be the log(IV)

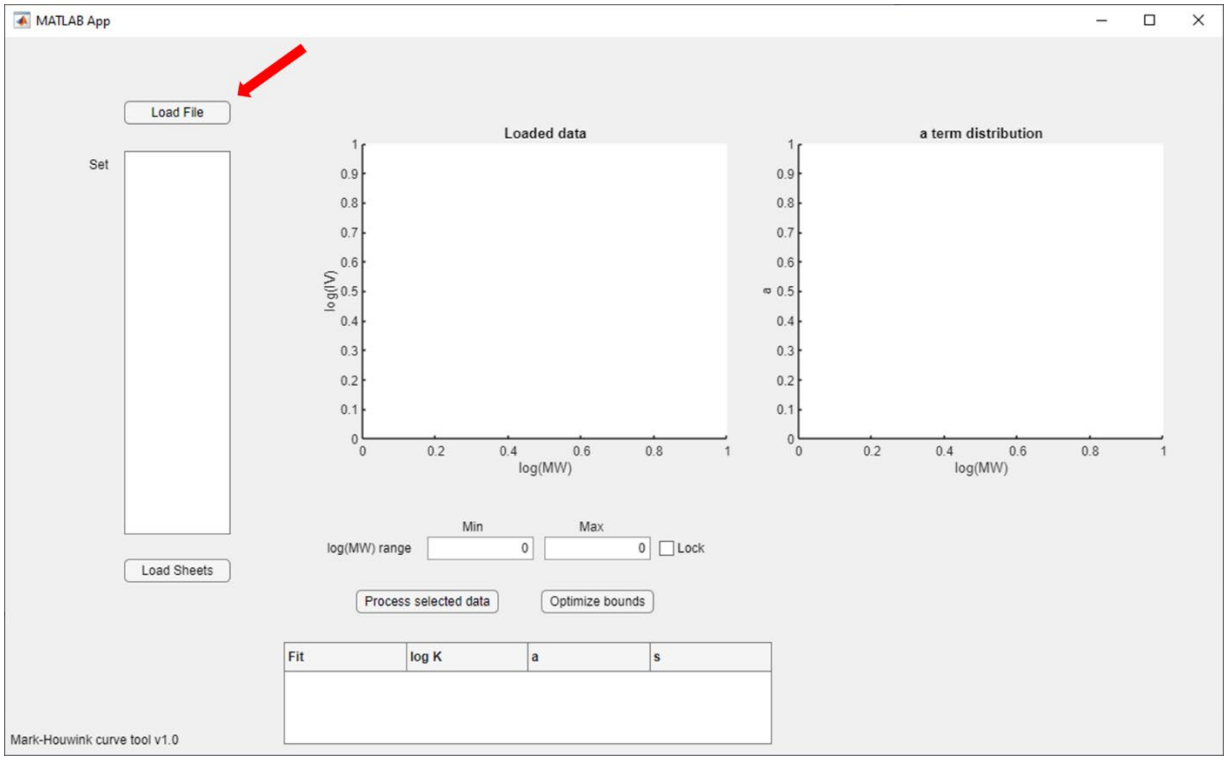

Figure S3: Main screen of the tool.

The list shows the detected sheets. Select individual measurements or multiple replicates of the same sample by using ctrl and/or the shift function.

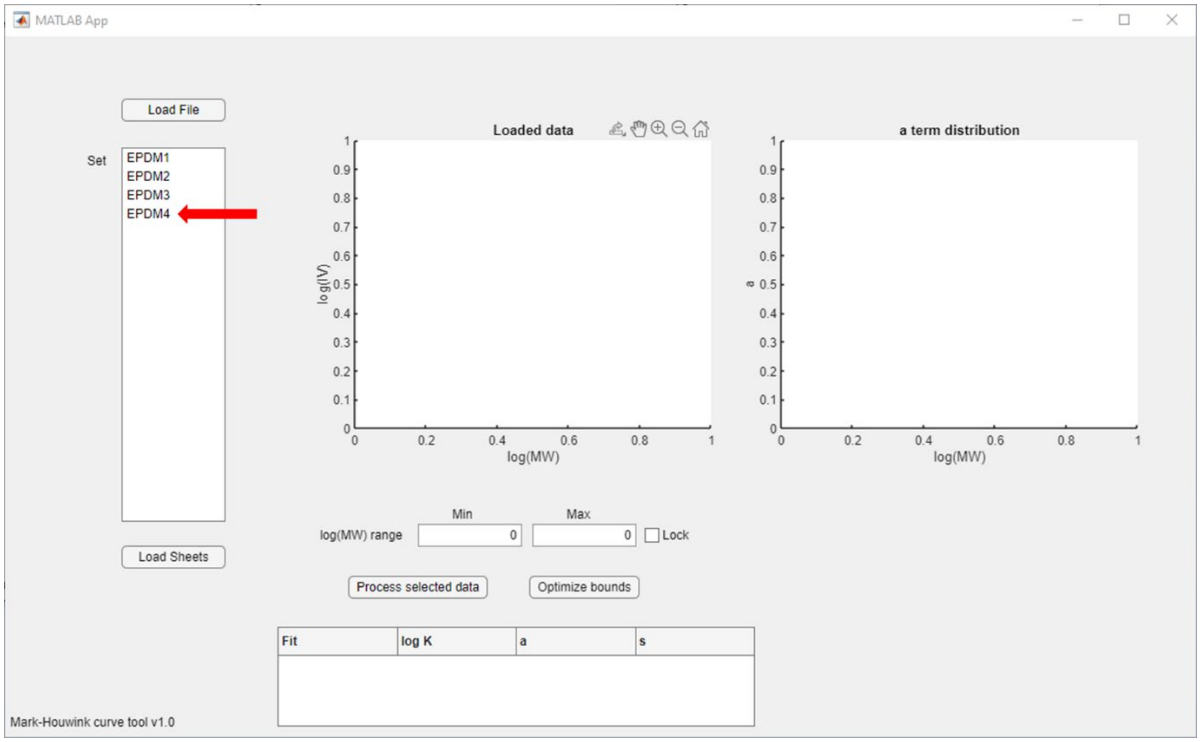

Figure S4: Main screen of the tool when the Excel file of interest has been loaded.

To load the selected measurements into the memory the Load Sheets button needs to be pressed.

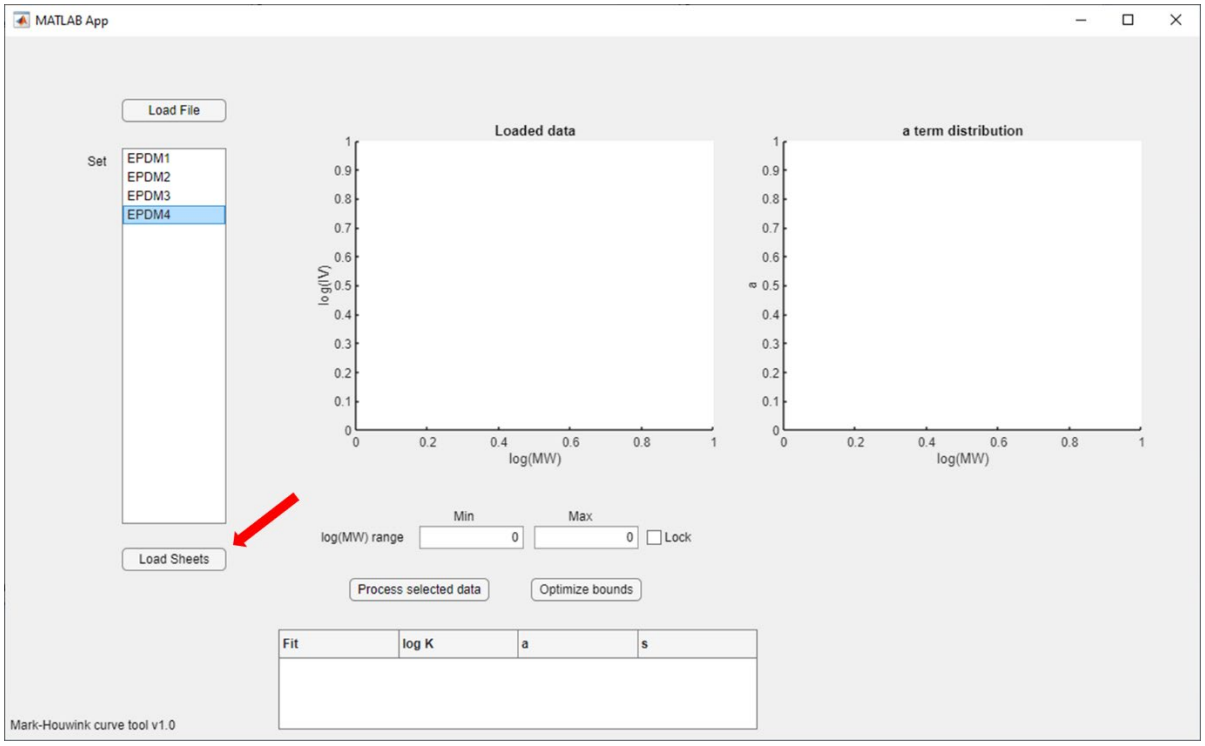

Figure S5: Main screen of the tool when the Excel sheets of interest have been selected.

The loaded Mark-Houwink plots will be shown in the left figure. Now the log(MW) interval can be set manually or optimized automatically with the Optimize bounds button if two or more replicates are loaded. The lock function locks the interval when new data is loaded.

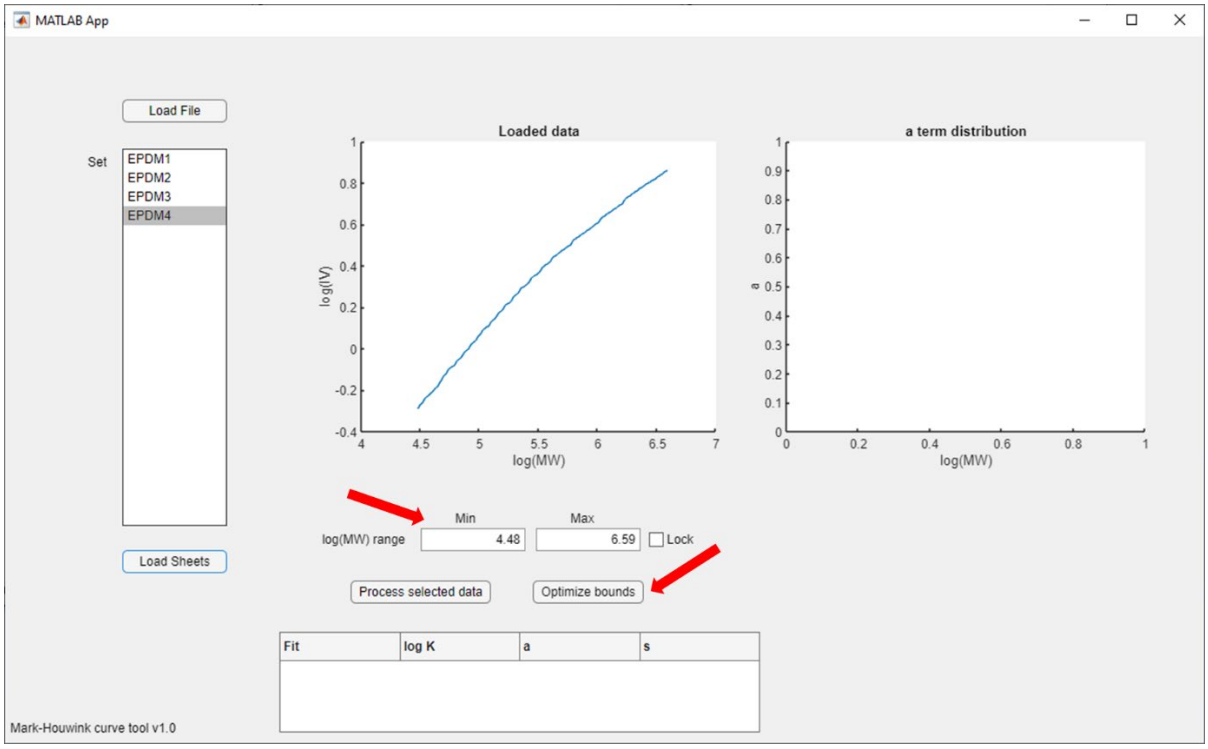

Figure S6: Main screen of the tool when the Excel sheets of interest have been loaded.

The measurements can be processed with the selected interval by pressing the Process selected data button.

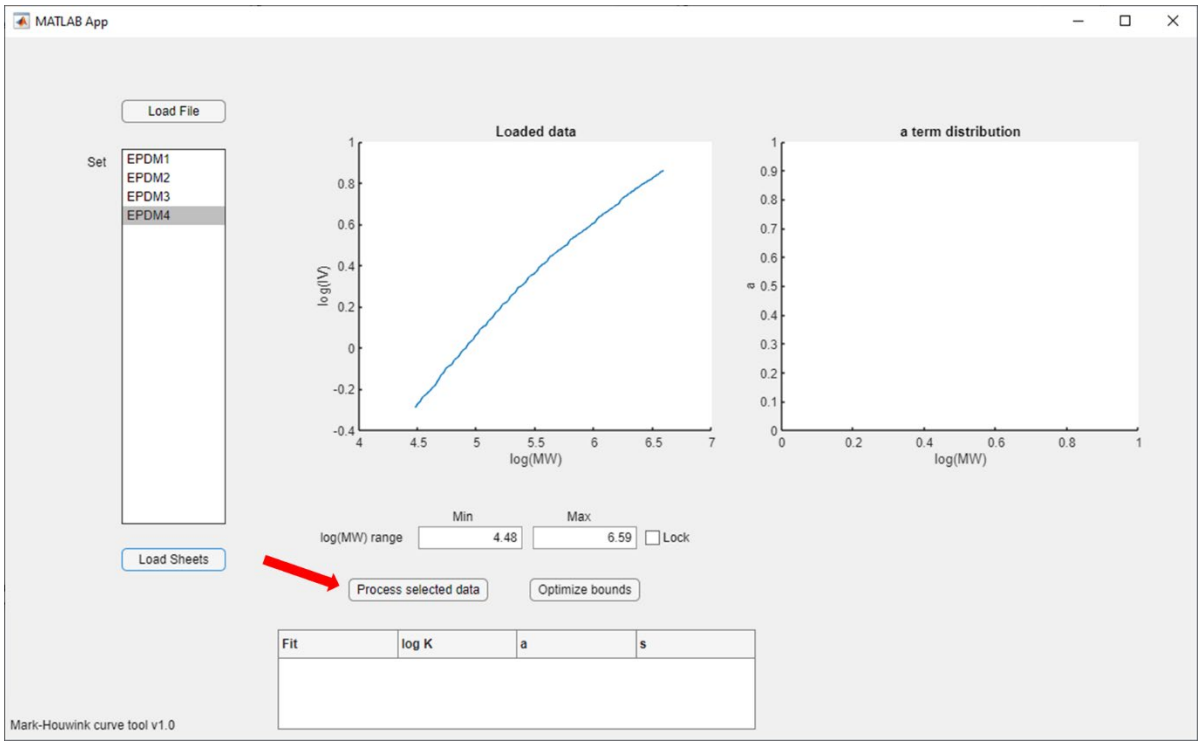

Figure S7: Main screen of the tool when the log(MW) interval of interest has been selected.

The resulting parameters are shown in the table and the fits are plotted in the left figure. The right figure shows the *a* term distribution with the derivative of the fitted MH plot.

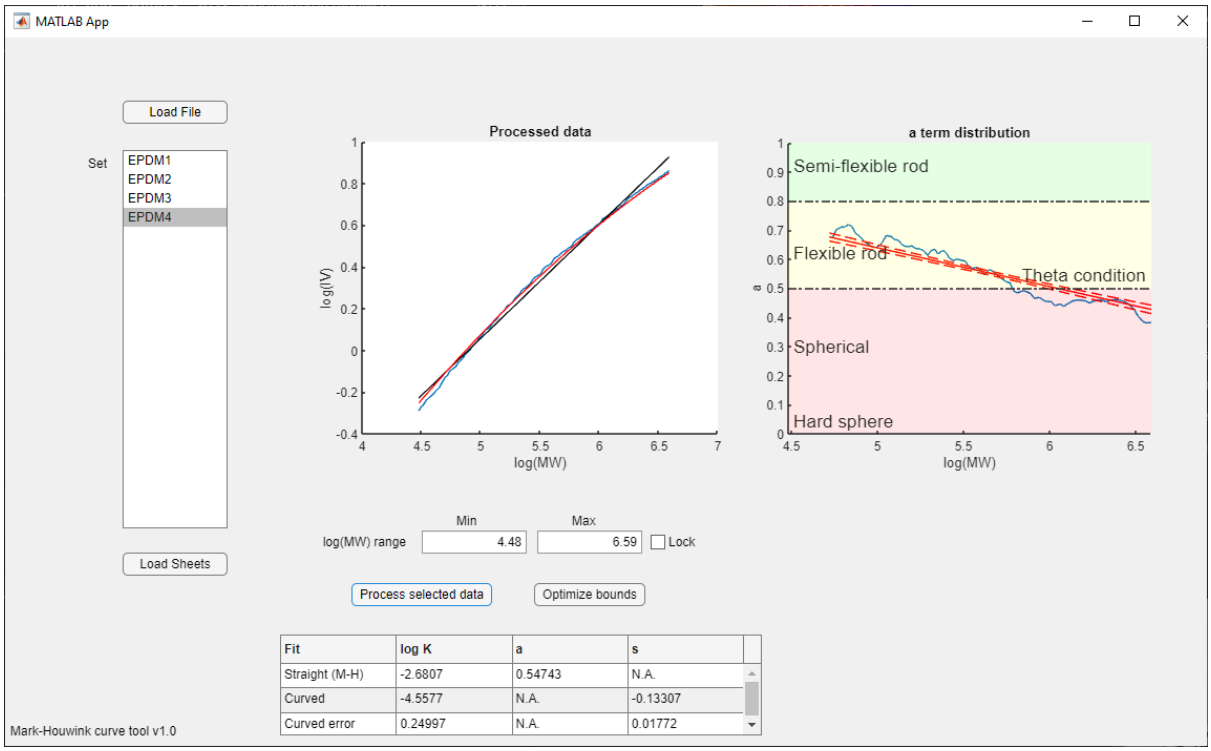

Figure S8: Main screen of the tool when the Excel sheets of interest have been processed.

Supporting Information S-4: sigmoidal description of the a vs log(MW) trend

Sigmoidal *a* exponent equations

$$a = \frac{n}{s_c * e^{\log MW - \mu}} + o_b$$

$$\int \left(\frac{n}{s_c * e^{\log MW - \mu}} + o_b \right) d \log MW =$$

$$o_b * \log MW - \frac{n * e^{\log MW - \mu}}{s_c} + \log k_\circ$$

Where a is the slope in the Mark-Houwink plot, n is the height normalization, s_c is the scale, o_b is the offset of the derivative, $\log MW$ is the logarithm of the molecular-weight, μ is the location parameter, and $\log k_\circ$ is the offset of the Mark-Houwink plot.