Article:

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Supplementary Material

I. DIFFICULTY WITH RESOLUTION OF NARROW MWD PEAKS

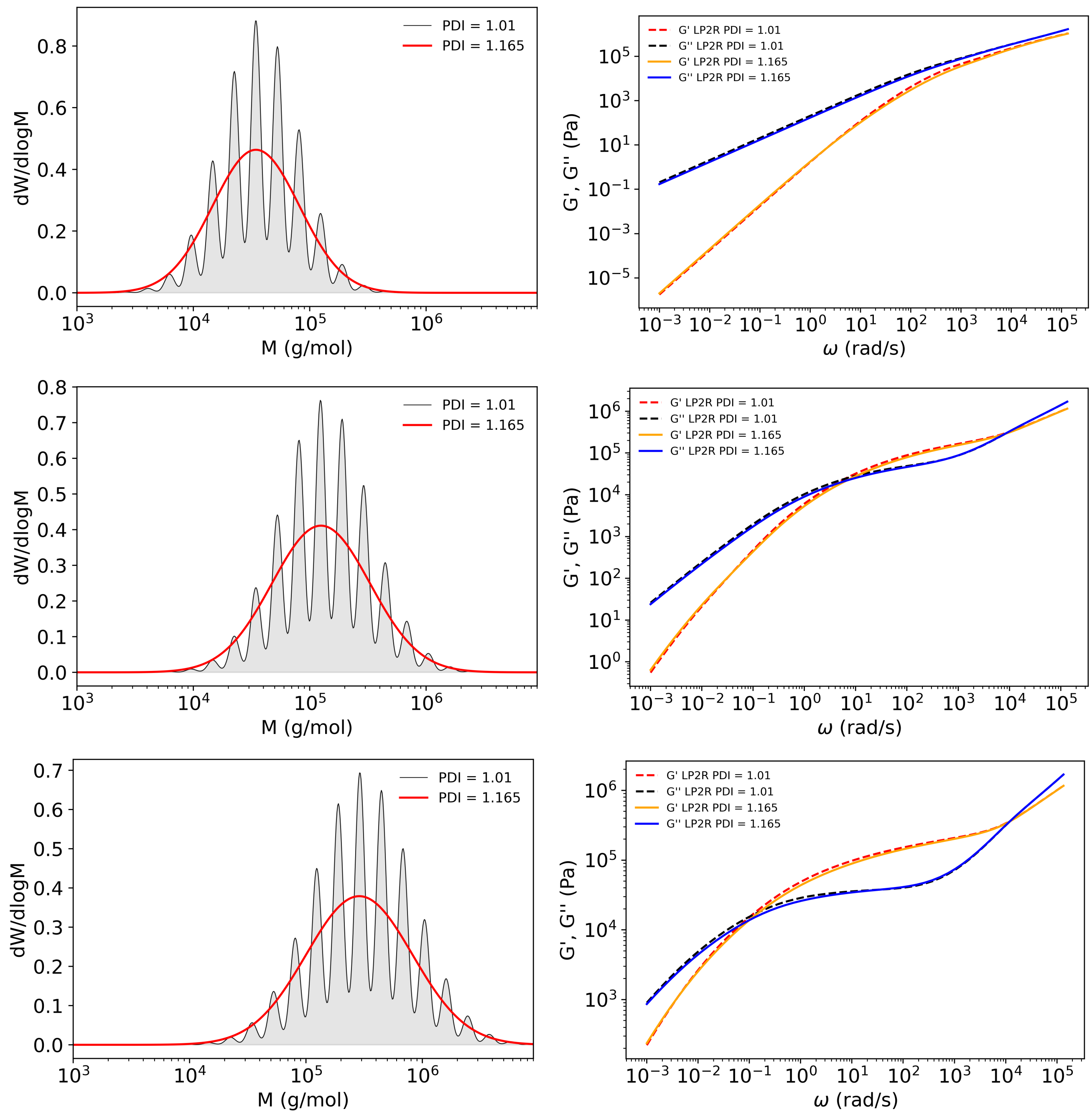

FIG. S1: Artificial rheology predictions using sample log-Gaussian MWDs with different dispersities for each of the sub-distributions. Rheology is not altered significantly, showing there is a clear resolution limit of the rheology with regards to sharp peaks in the MWD. If a lower dispersity was used for the sub-distributions, a greater number of sub-distributions would have to be used to cover the molecular weight range. In this case, many different combinations of the $\{\phi_i\}$ variables could produce the same rheology. The more broad sub-distributions act as a regularisation to mitigate this effect, by reducing the number of $\{\phi_i\}$ solutions for a particular rheology measurement.

II. PREDICTION VARIATION FOR PS SAMPLES

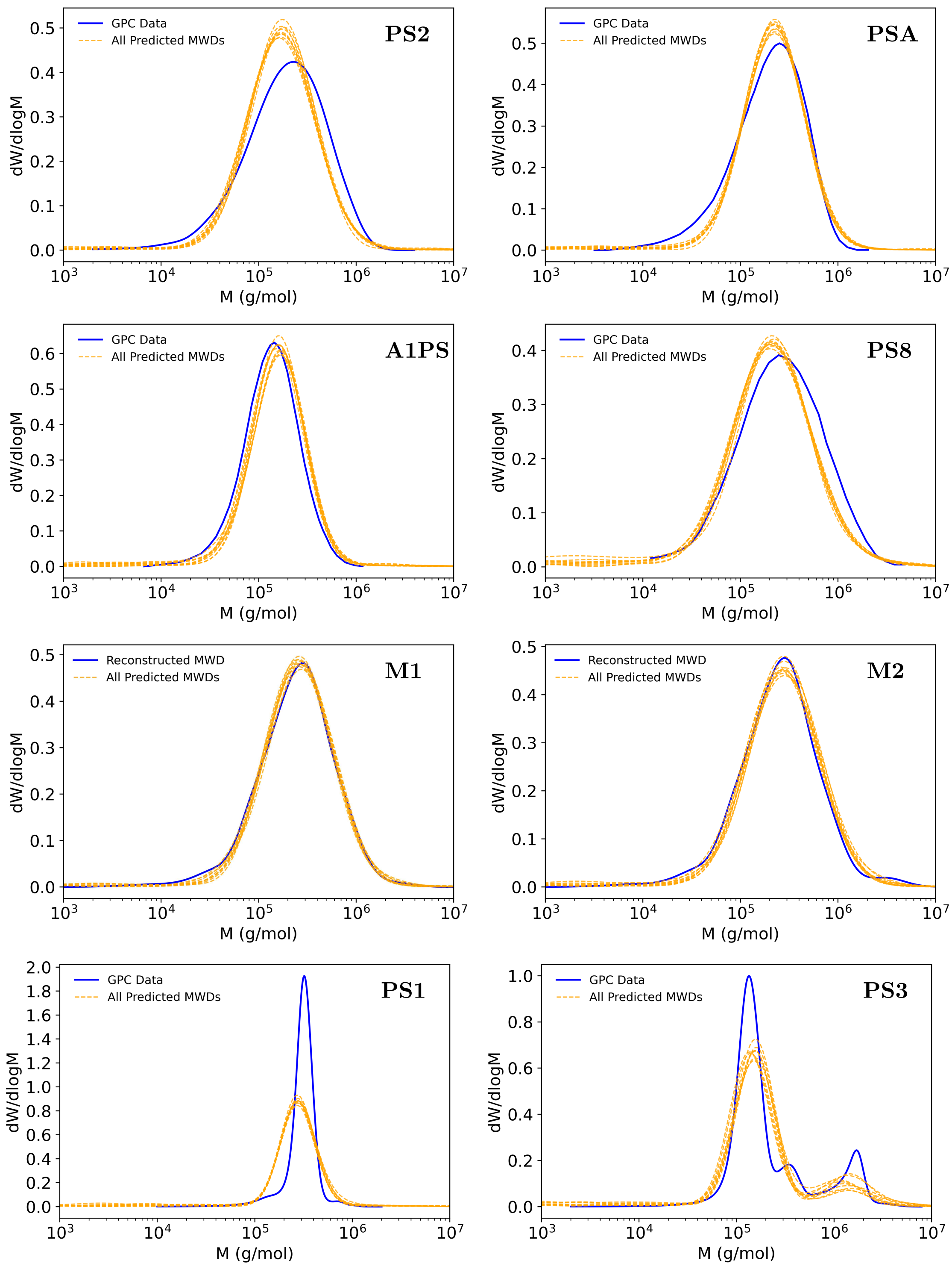

FIG. S2: GPC data overlaid with the MWD prediction from each of the nine NN models. All PS samples included other than PScom, for which the comparative plot is in the main manuscript. Each plot shows qualitatively the variation between the predictions for the NN models, which is quantitatively given as the Std Dev measure in Table III in the main manuscript.

III. M1 AND M2 DISPERSITY CHOICE

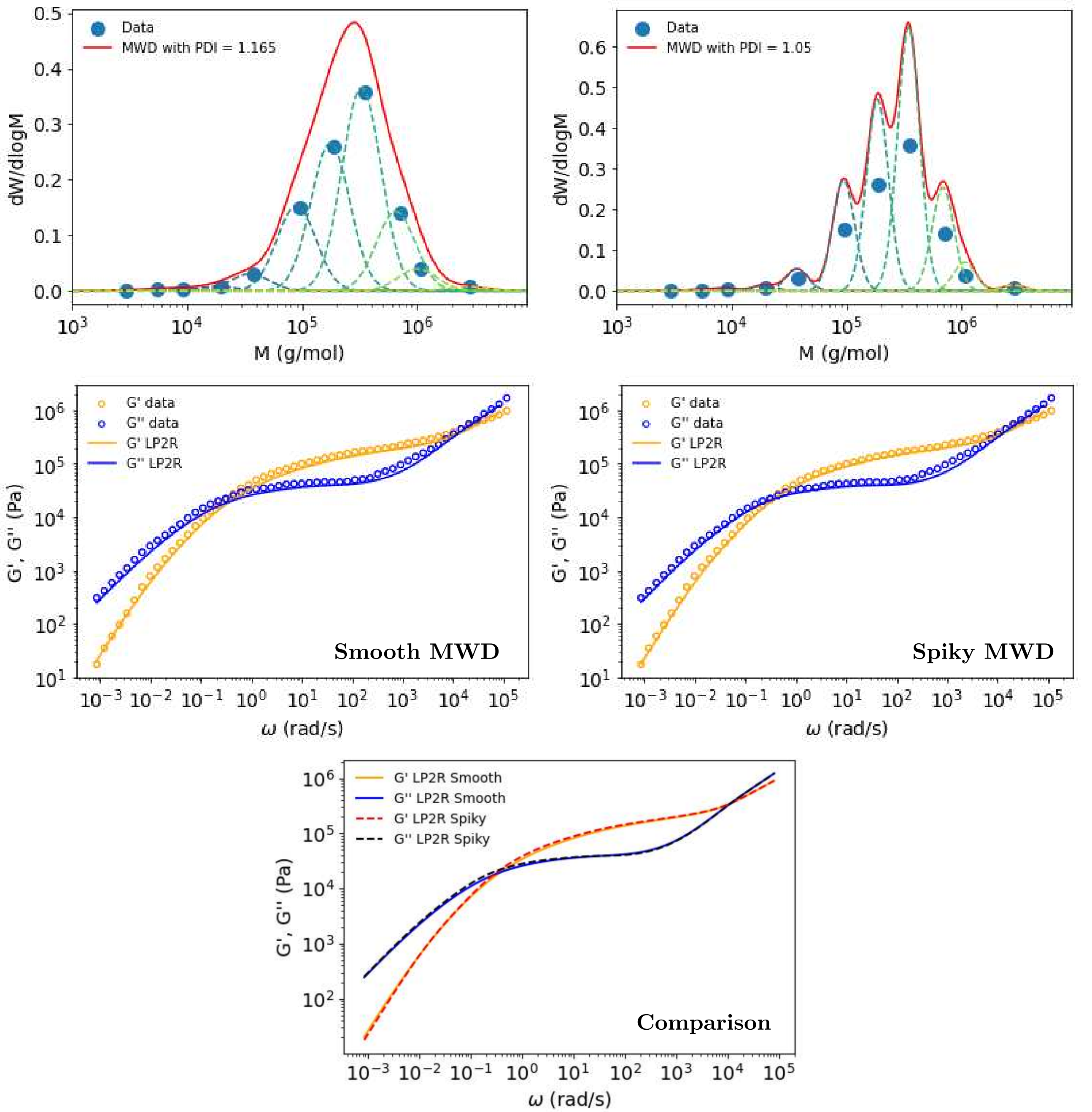

FIG. S3: Comparing LP2R predictions with experimental rheology data when assuming different dispersities for the components in the M1 PS mixture of PS standards. Very little difference is seen in the rheology produced by the 'spiky' and smoothed-out MWDs, and both match the experimental data well. The same is true for the very similar MWD of M2.

IV. MAXWELL MODE FITTING REGULARISATION

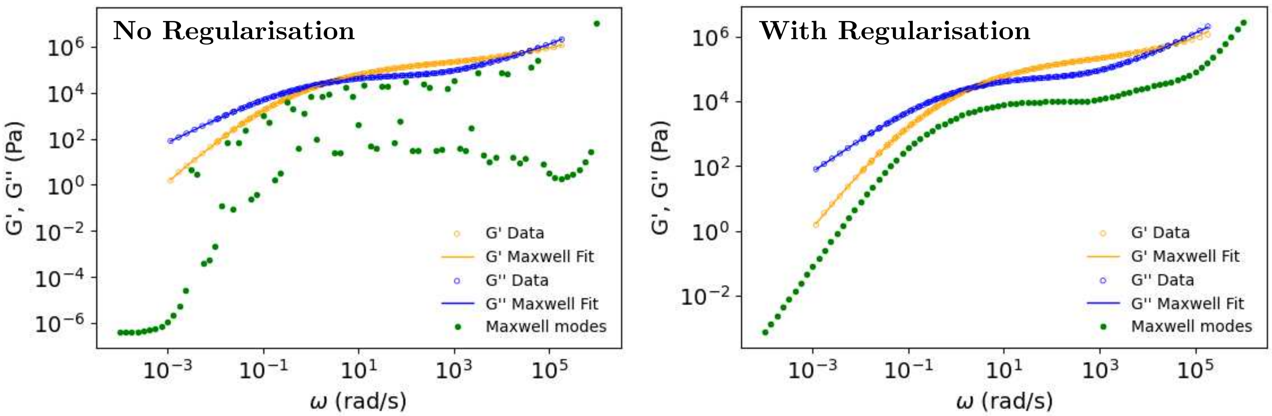

FIG. S4: Comparing Maxwell mode fit to experimental rheology data, first without any regularisation and secondly with the smoothness penalty included as a regularisation. Both sets of Maxwell modes fit the data well, but when no regularisation is used, the modes oscillate as some are not needed to produce an adequate fit. Smoothness is enforced to make the interpolation between training data more simple for the NN. Fitting is also much less computationally costly with the smoothness regularisation.

V. TUBE MODEL RHEOLOGY PREDICTION FROM NN MWD PREDICTION

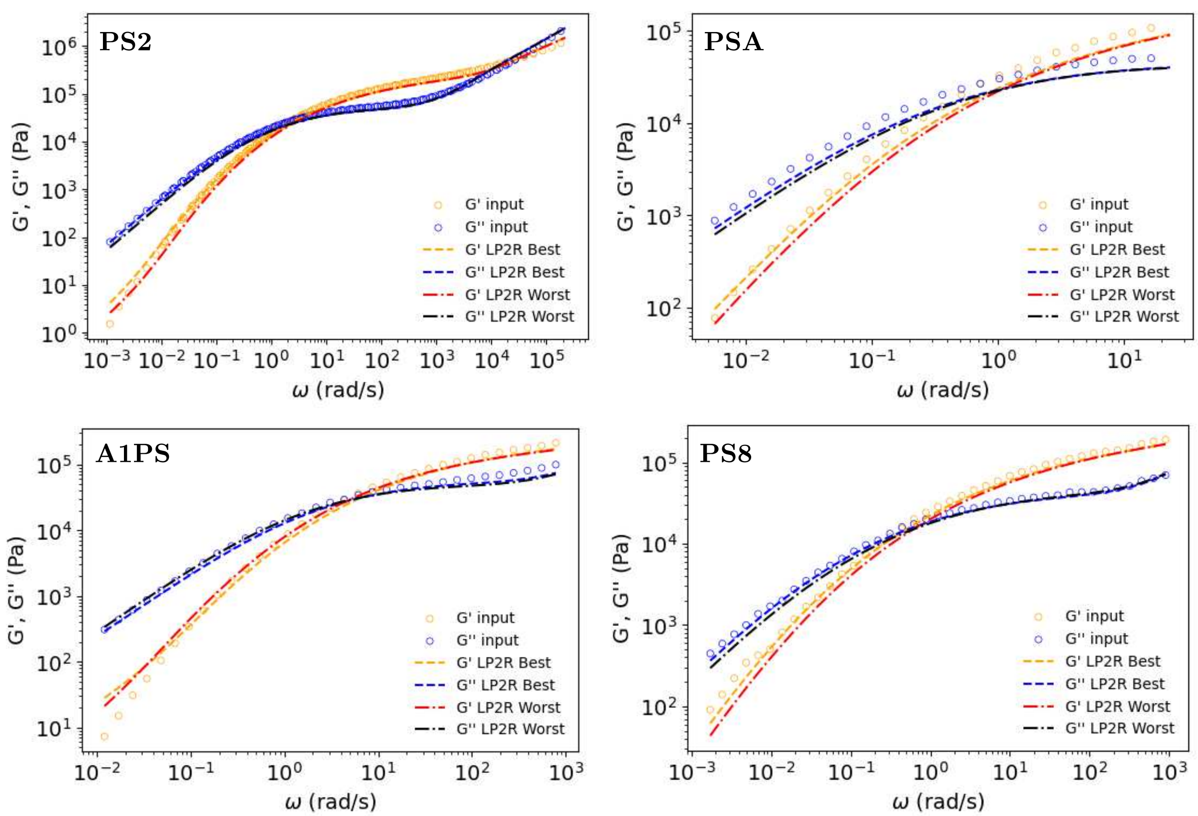

FIG. S5: First set of results of using the NN-predicted MWDs as input for the tube-model tool LP2R to predict the rheology. The highest and lowest RMSE MWD predictions were used, and are shown here compared to each other and to the experimental rheology data for each sample.

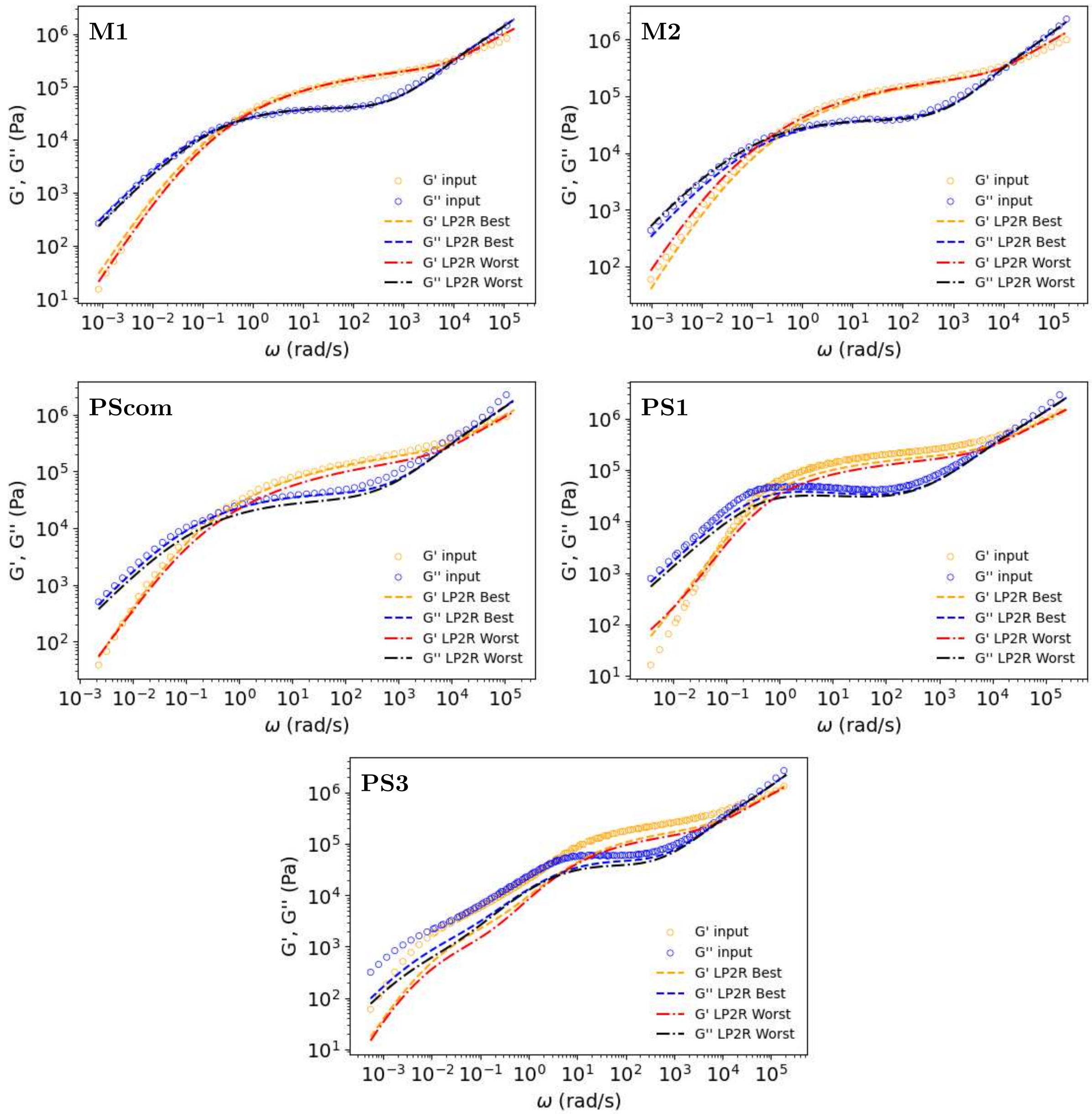

FIG. S6: Remaining results (first set in Fig 5) of using the NN-predicted MWDs as input for the tube-model tool LP2R to predict the rheology. The highest and lowest RMSE MWD predictions were used, and are shown here compared to each other and to the experimental rheology data for each sample. The rheology does not significantly differ for the two NN predictions, showing that the errors in different MWD predictions do not lead to large changes in the rheology. The variation in rheology for the two MWDs used in each case is likely due to the necessary addition of noise to the training dataset. This noise will produce slight inconsistencies between dataset entries in the relationship between the MWD and the rheology. As NN training is not deterministic, each NN "learns" a similar (but not identical) mapping between the MWD parameters and the corresponding rheology parameters. The result is that each model is slightly more or less suitable for each of the inherently noisy sets of experimental rheology data. However, the predictions match the experimental rheology well in most cases, meaning that despite these differences, each of the nine NNs has achieved the goal of this work. The most notable exceptions are PS1 and PS3, and we propose that this is due to the incompatibility of our parameter system (targetting broad MWDs with the dispersity assumed for each sub-distribution) with these samples' narrow MWDs.

VI. COMPARISON WITH PREVIOUS WORK

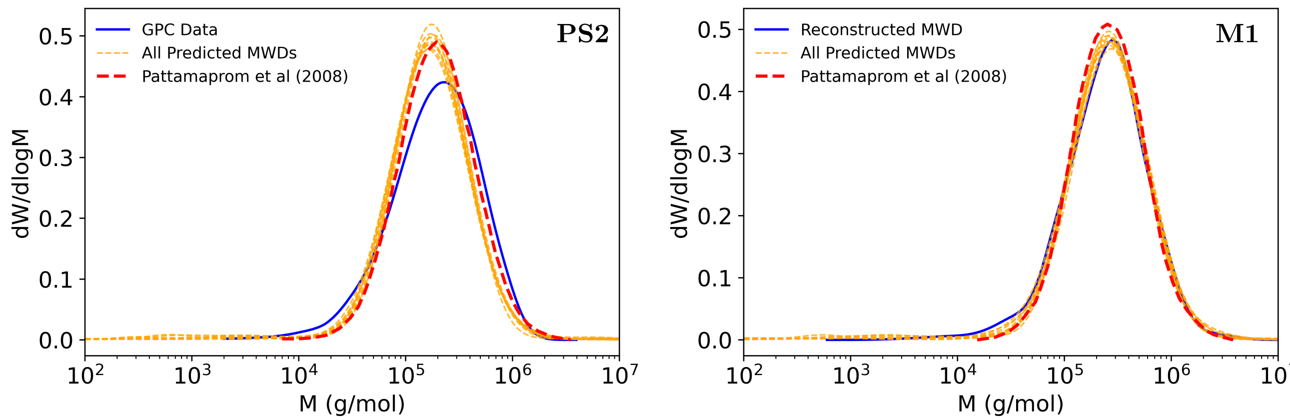

FIG. S7: Comparing predictions made by Pattamaprom et al [1] for PS2 and M1 with those made in this work. Results are comparable in both cases, and the NN predictions match the reconstructed M1 MWD more closely. The shape of the predicted MWD for PS2 is consistent between both works, suggesting that the lack of agreement with the GPC data is not simply an error of this work, but may be due to some unknown factor affecting the rheology or MWD measurements.

REFERENCES

[1] Pattamaprom, C., R. G. Larson, and A. Sirivat, "Determining polymer molecular weight distributions from rheological properties using the dual-constraint model," Rheol Acta **47**, 689–700 (2008).