Supplementary Information (SI) for Polymer Chemistry.

Polymer Chemistry Informed Neural Networks (PCINNs) for data-driven modelling of polymerization processes

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SUPPORTING INFORMATION

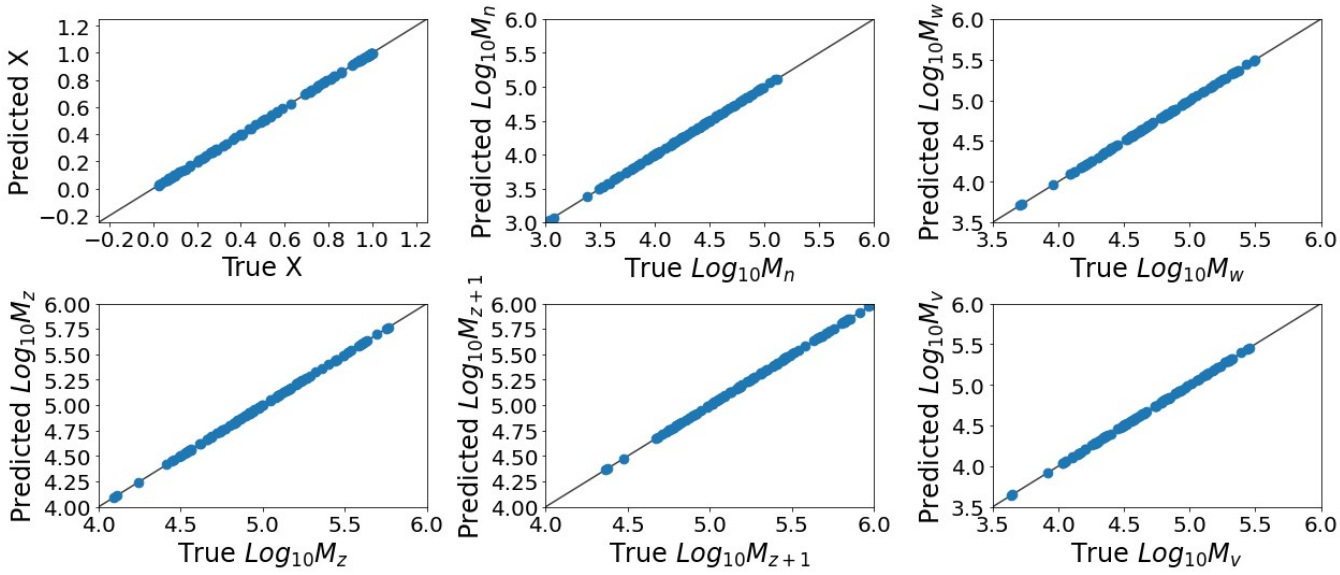

Figure S1. Performance of theory neural network by comparison of predicted values from the "theory" neural network and the values from the kinetic model for 100 different randomly selected sets of ([M], [I], [S], T and time) from the test set.

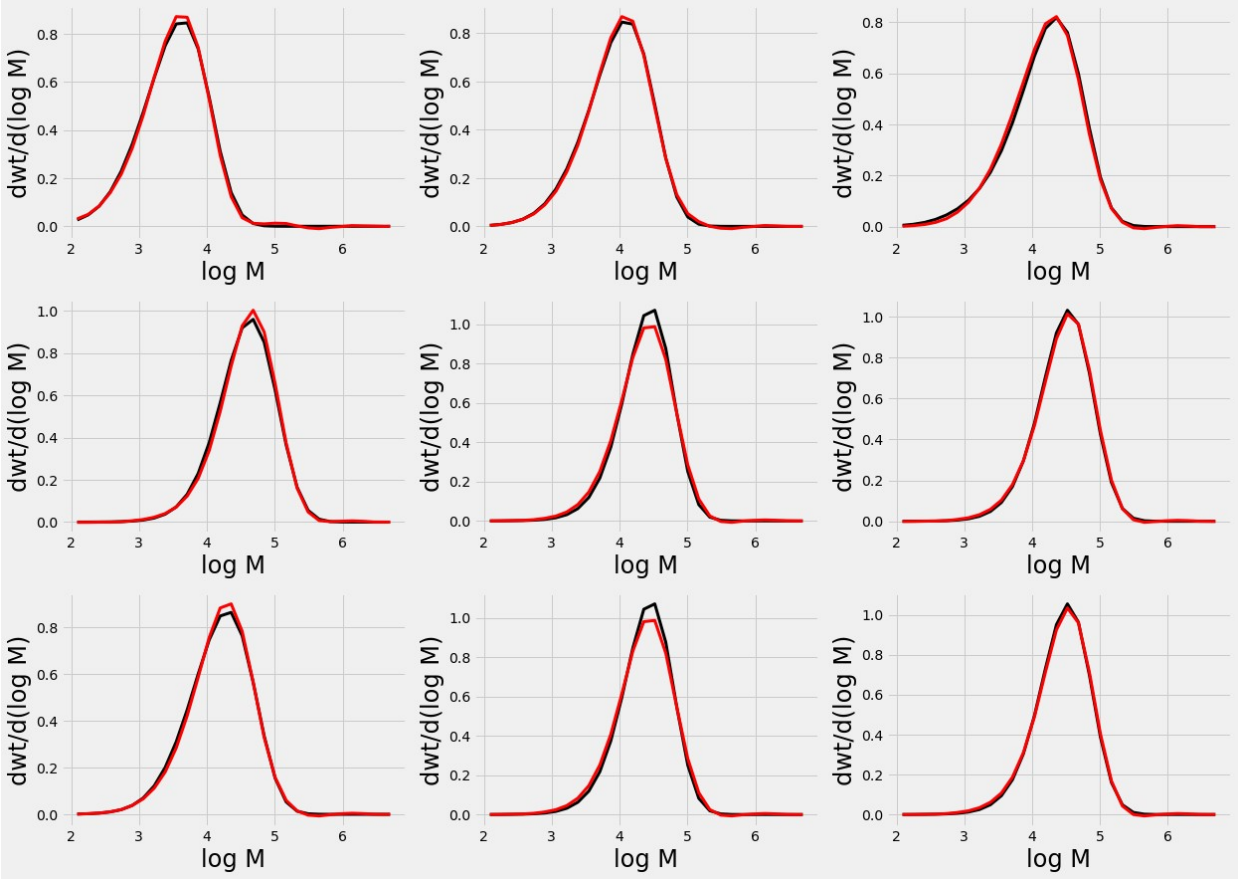

Figure S2. Performance of predictor of molecular weight distribution on 9 different randomly selected samples from the test set.

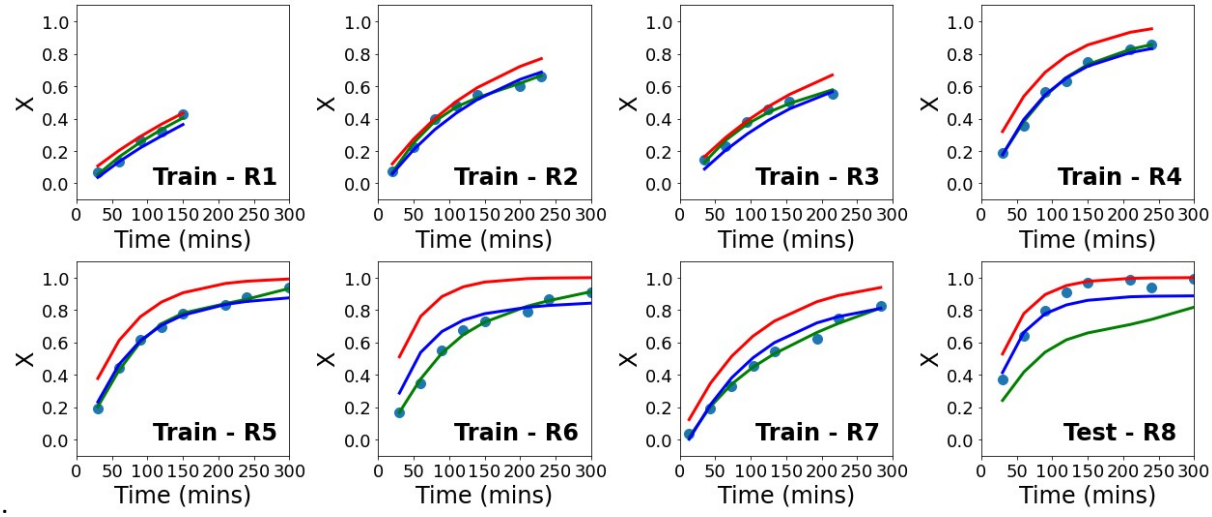

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Figure S3. Evolution of conversion with time for experimental data (circles), in comparison to the theoretical evolution of conversion following equation 6 (red), a purely data-driven neural network (green), and a PCINN (blue). This data corresponds to the model trained using reactions **R1-R7** and tested on reaction **R8**.

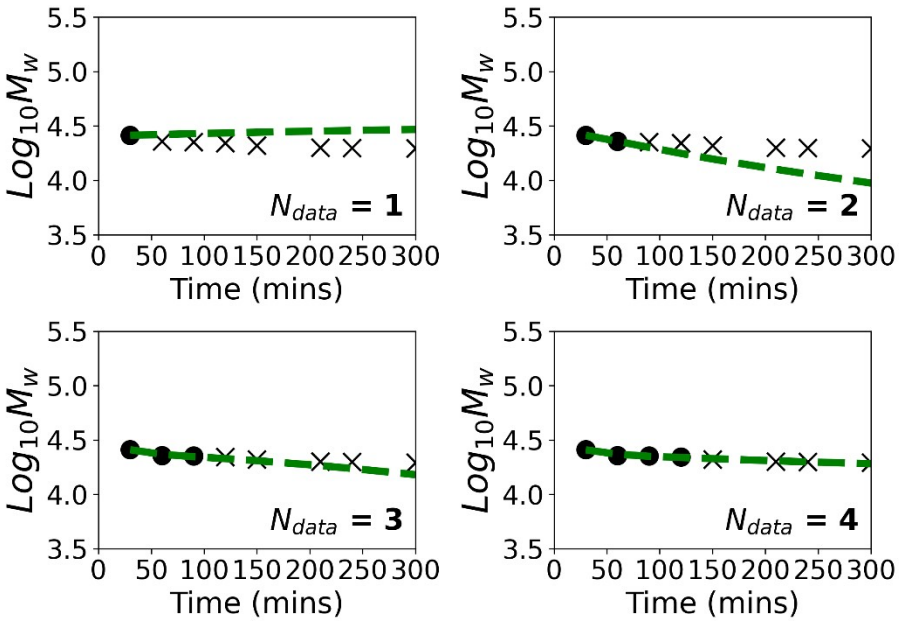

Figure S4. Predicted evolution of molecular weight with time (dashed lines) for purely data-driven neural network based on real-time updates with samples from reaction (Reaction 8). The crosses show future, as-yet unknown values while the circles show the measured values which are used as training data.

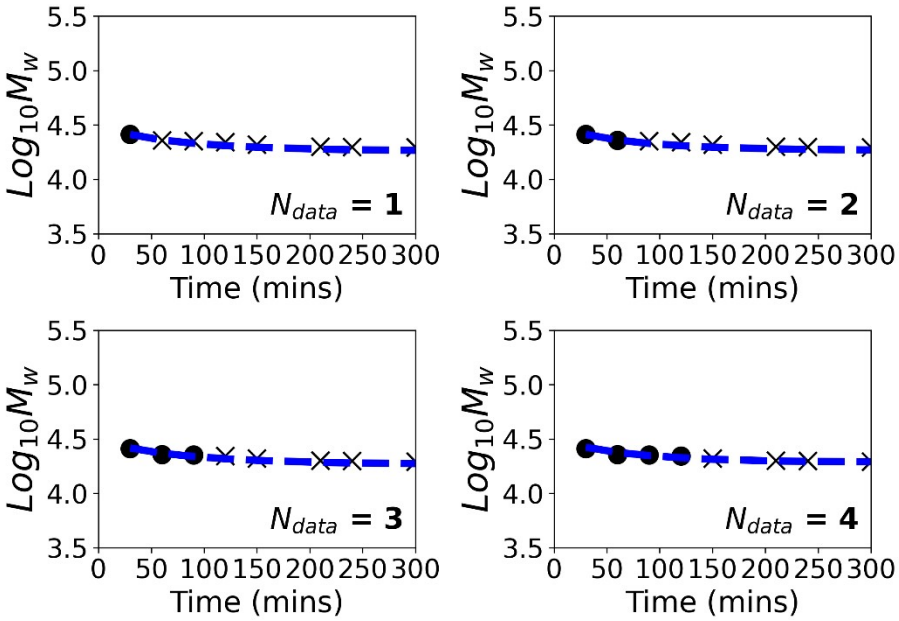

Figure S5. Predicted evolution of molecular weight with time (dashed lines) for PCINN based on real-time updates with samples from reaction (Reaction 8). The crosses show future, as-yet unknown values while the circles show the measured values which are used as training data.