Supplementary Information: Machine Learning-Assisted Profiling of a Kinked Ladder Polymer Structure using Scattering

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Effect of temperature variation We confirm the sample is fully dissolved and without aggregation by comparing the scattering function $I(Q)$ measured under different temperatures: 25 °C, 75 °C and 125 °C. As shown in Fig. S1, the $I(Q)$ spectrum are consistent cross all three temperatures, indicating that the polymer sample we used is fully dissolved.

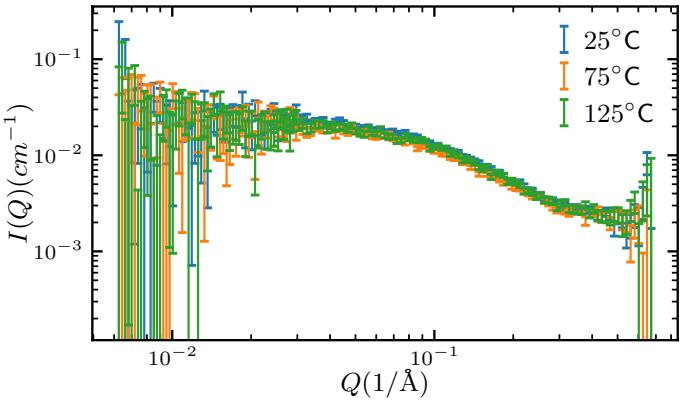

Fig. S1 Scattering intensity of the synthesized CANAL polymer under three different temperature: 25 °C, 75 °C and 125 °C.

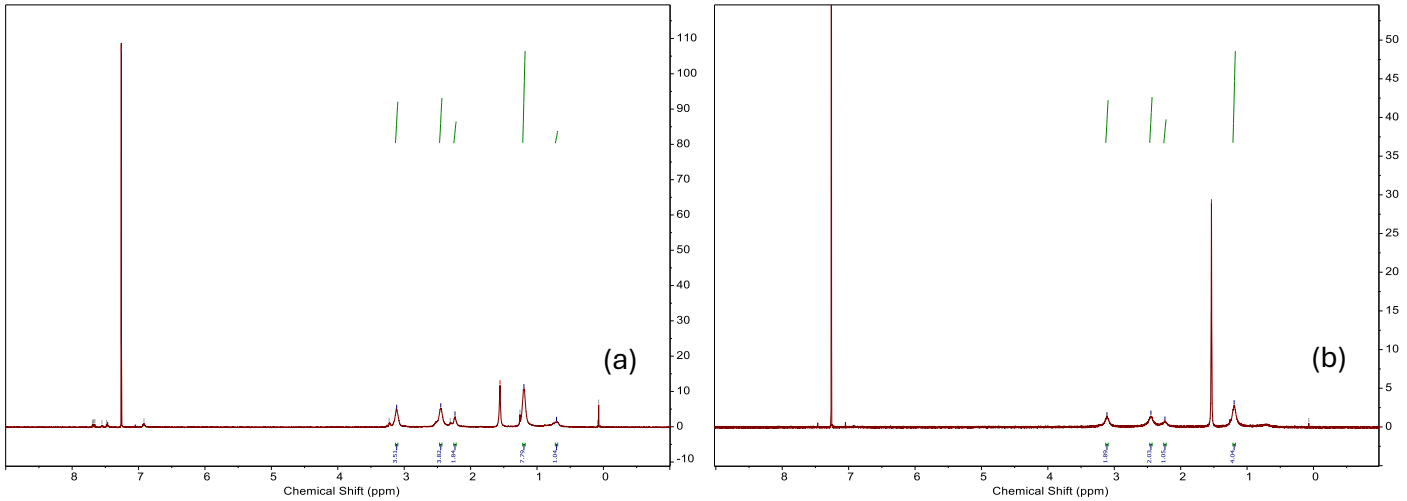

Fig. S2 Nuclear magnetic resonance spectra for the CANAL ladder polymer. (a) Low molecular weight. (b) high molecular weight

Characterization of synthesized ladder polymer All chemicals, including 1,4-diethylbenzene, were purchased from commercial sources and used as received unless otherwise noted. 1,4-dibromo-2,5-diethylbenzene was prepared following known literature procedures (Sugamata et al., 2021). All reactions were performed under nitrogen in oven- or flame-dried glassware unless otherwise noted. Flash column chromatography was carried out with Silica 60 (230–400 mesh; Fisher). Analytical thin-layer chromatography (TLC) was carried out using 0.2 mm silica gel plates (silica gel 60, F254, EMD Chemical).

Proton nuclear magnetic resonance (^{1}H NMR) and carbon nuclear magnetic resonance (^{13}C NMR) spectra were recorded in $CDCl_3$ using 500 MHz Varian NMR spectrometers. Chemical shifts are reported in parts per million (ppm)

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relative to residual protonated solvent for ^{1}H ($CHCl_3 = \delta 7.26$, DCM $= \delta 5.30$, methanol-$d_4 = \delta 3.31$) and relative to carbon resonances of the solvent for ^{13}C ($CDCl_3 = \delta 77.0$). Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, dd = doublet of doublets, t = triplet, q = quartet, m = multiplet, br = broad signal, and associated combinations), coupling constant(s) (Hz), and integration.