Supporting Information for: "Cosolvent Pretreatment in Cellulosic Biofuel Production: Effect of Tetrahydrofuran-Water on Lignin Structure and Dynamics"

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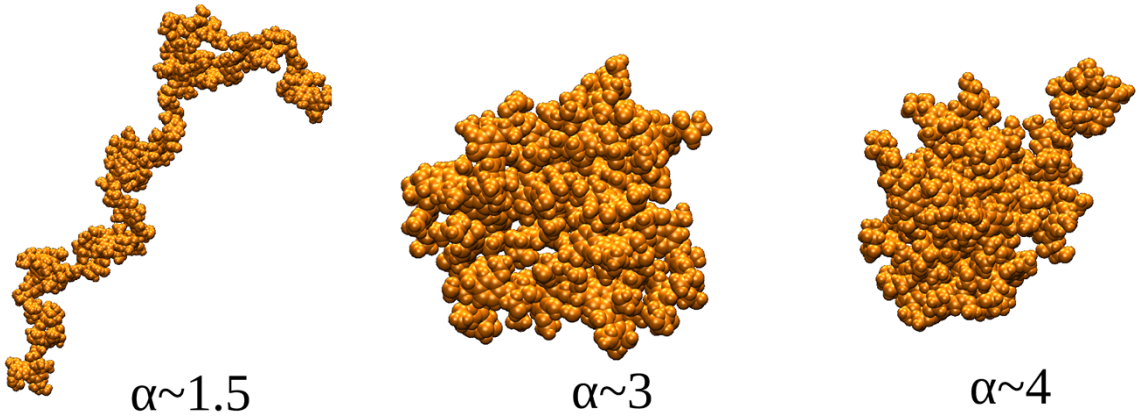
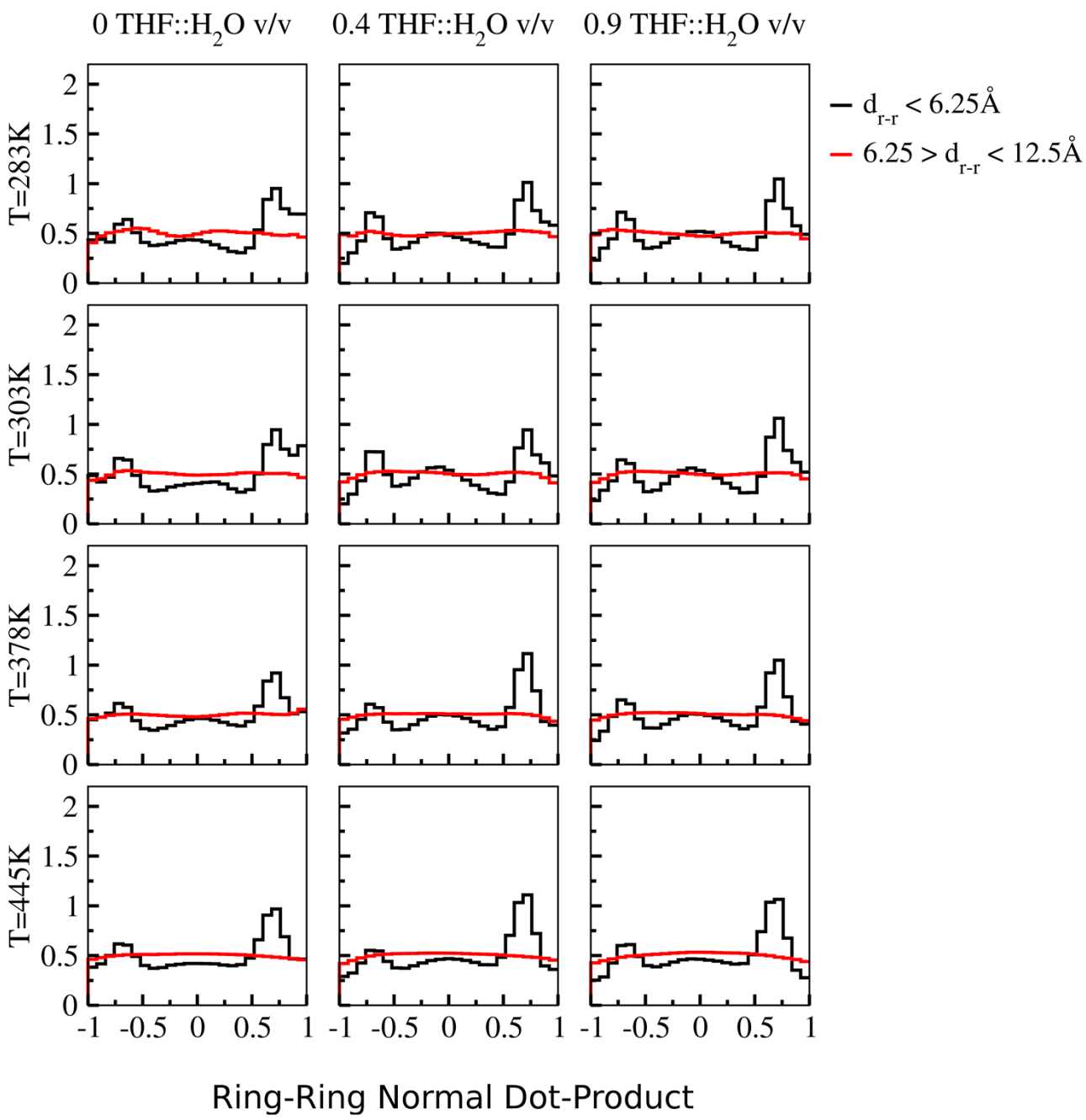
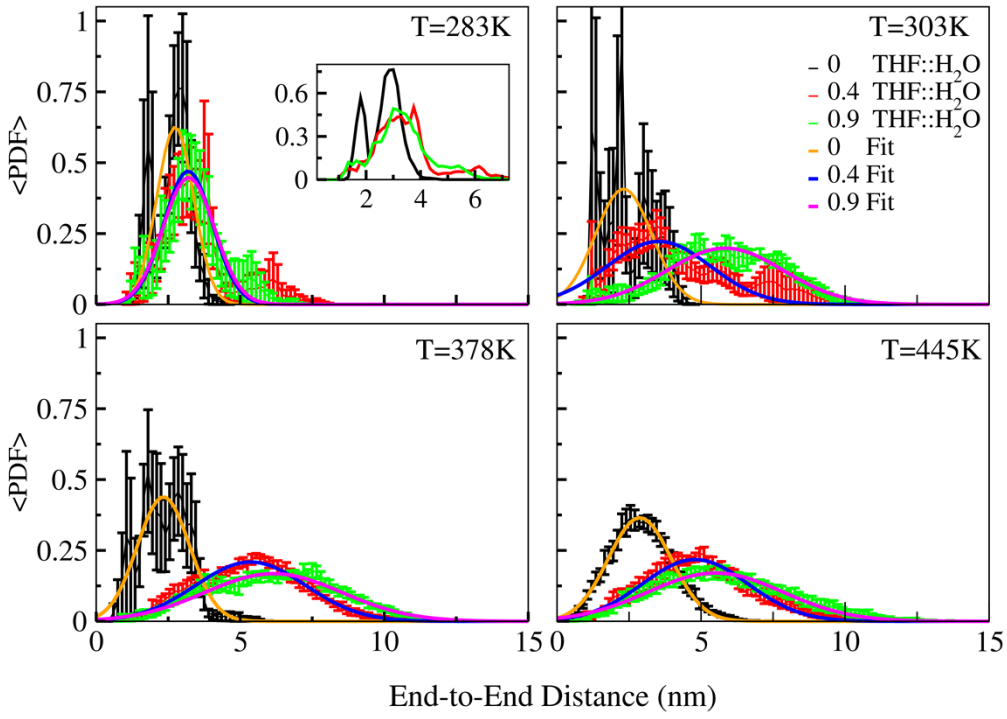
This section contains figures designed to aid the reader in understanding the meaning of the fractal dimension calculations as well as figures and tables that further support the conclusions contained in the main text. These figures are discussed in and are directly referenced from the main text. For this reason, they are presented below with figure captions, but without further discussion.



SI Figure 1) Example fractal structures. Below each structure is the approximate fractal dimension. Note that as the fractal dimension becomes larger, the structures become more compact.



SI Figure 2) A "Zoom-in" of the first distance bins from Figure 4 of the main text. These "zooms" are recalculated 1D histograms of the ring-ring normals for the given distance cutoffs noted in the legend.



SI Figure 3) Average End-to-End distance distributions. Error-bars are standard error of the mean. Inset plot in upper left sub-figure is of the distributions at T=283K without error-bars. Fitted distributions are Gaussian[1] with the form:

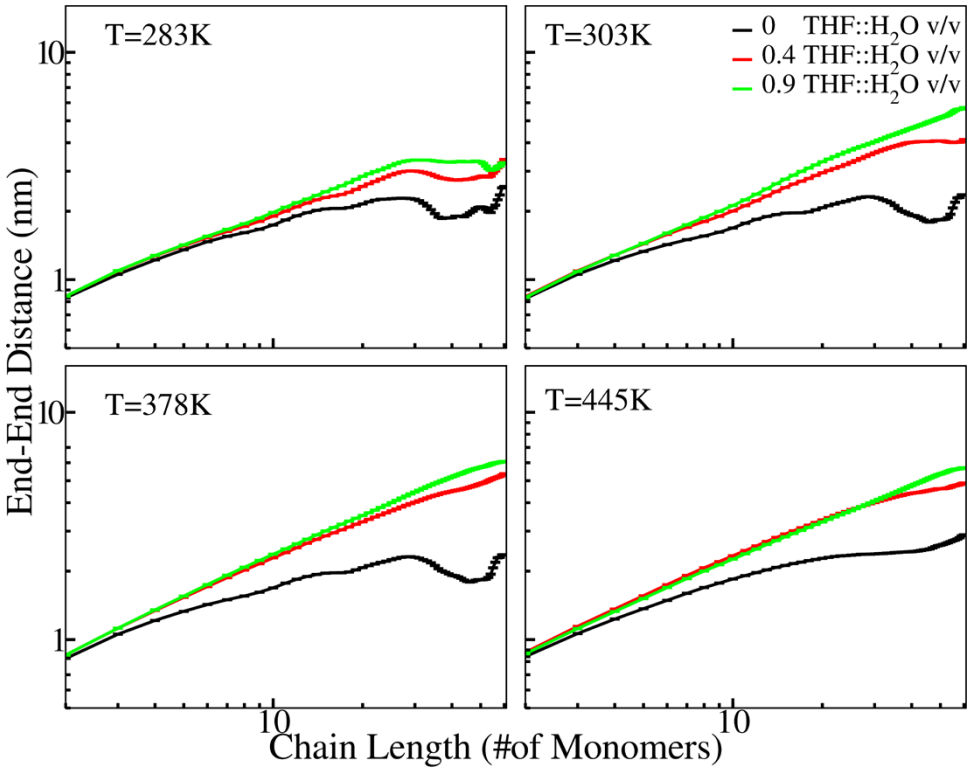
$$\mathrm{P}(R) = \sqrt{\frac{3}{4\pi\, L_c l_p}}\mathrm{e}^{\frac{-3R^2}{4L_c l_p}}$$

where L_c and l_p are the contour and persistence length, respectively.

SI Table 1) Persistence lengths (in nm) obtained from fitting of end-to-end distance distribution from figure SI 3. Contour length is taken to be ~39nm. Value in parenthesis is chi-square value of fit.

	T=283K	T=303K	T=378K	T=445K
0.0 THF::H_2O v/v	0.01556(0.509)	0.0367 (0.894)	0.03164(0.155)	0.0456(0.0069)
0.4 THF::H_2O v/v	0.0276(0.115)	0.1231(0.1013)	0.1394(0.0083)	0.12854(0.00763)
0.9 THF::H_2O v/v	0.0305(0.0706)	0.1546(0.0219)	0.216(0.0134)	0.2102(0.0087)

Note that all persistence lengths are less than of the diameter of one ring unit of the lignin (~0.28nm).



SI Figure 4) Log-log scale rendering of figure 5 from the main-text. Error-bars are approximately the width of the line and are the standard error of the mean.

SI Table 2) Fitted slopes of lines in SI figure 4 (power-law exponents from figure 5 of the main text). Standard-error of the slopes obtained from the fits are given in parenthesis.

	T=283K	T=303K	T=378K	T=445K
0.0 THF::H_2O v/v	0.232 (0.021)	0.18 (0.0212)	0.18 (0.02)	0.28 (0.01)
0.4 THF::H_2O v/v	0.35 (0.016)	0.45 (0.0103)	0.506 (0.0063)	0.472 (0.0097)
0.9 THF::H_2O v/v	0.39 (0.0176)	0.555 (0.0037)	0.568 (0.004)	0.546 (0.0025)

1. M. Rubinstein, R. H. Colby and Knovel (Firm), Oxford University Press,, Oxford ; New York 2003, p. 1 online resource (460 p.).