Supplementary Information

Table S1: Non-bonded LJ parameters of the four force fields for the different interaction sites in N-isopropyl-acrylamide

		OPLS-AA			**AMBER**	
Site	ε (kcal/mol)	R_{min}(Å)	Partial charge *q* (e)	ε (kcal/mol)	R_{min}(Å)	Partial charge *q* (e)
C	–0.105	2.09	0.50	–0.0860	1.9080	0.72
O	–0.21	1.657	–0.50	–0.1520	1.7683	–0.58
N	–0.17	1.82	–0.50	–0.1700	1.8240	–0.79
H-(N)	0.00	0.00	0.30	–0.0150	0.6000	0.32
CH(-N)	–0.066	1.96	0.14	–0.1094	1.9080	0.67
CH	–0.066	1.96	–0.06	–0.1094	1.9080	0.11
CH_2	–0.066	1.96	–0.12	–0.1094	1.9080	–0.34
CH_3	–0.066	1.96	–0.18	–0.1094	1.9080	–0.47
H			0.06	–0.0150	1.3870	0.09/0.11

		CHARMM			**GROMOS53A6**	
Site	ε (kcal/mol)	R_{min}(Å)	Partial charge *q* (e)	ε (kcal/mol)	R_{min}(Å)	Partial charge *q* (e)
C	–0.11	2.00	0.51	–0.066	2.005	0.45
O	–0.12	1.7	–0.51	–0.305	1.545	–0.45
N	–0.20	1.85	–0.47	–0.15	1.76	–0.31
H-(N)	–0.0460	0.2245	0.31			0.31
CH(-N)	–0.0780	2.05	–0.27	–0.022	2.81	0
CH	–0.0560	2.01	–0.18	–0.022	2.81	0
CH_2	–0.0560	2.01	–0.18	–0.098	2.27	0
CH_3	–0.0780	2.05	–0.27	–0.207	2.09	0
H	–0.0240/ –0.0450/ –0.0350	1.34	0.09			0

Table S2: Free energy of hydration, solvation and partition coefficient as predicted by AMBER, CHARMM, GROMOS and OPLS-AA force fields as a function of temperature

T= 275 K	**AMBER**	**CHARMM**	**GROMOS**	**OPLS-AA**
ΔG^{HYD} (kcal/mol)	–5.4±0.4	–5.2±0.3	–3.8±0.35	–6.3±0.4
ΔG^{SOLV} (kcal/mol)	–9.4±0.4	–5.7±0.3	–7.2±0.3	–5.1±0.3
Log K_{ow}	3.2±0.3	0.4±0.2	2.7±0.3	–0.9±0.3
T= 300 K	**AMBER**	**CHARMM**	**GROMOS**	**OPLS-AA**
ΔG^{HYD} (kcal/mol)	–4.9±0.3	–3.8±0.3	–2.2±0.4	–5.6±0.3
ΔG^{SOLV} (kcal/mol)	–10.8±0.4	–4.9±0.3	–6.3±0.4	–4.9±0.3
Log K_{ow}	4.2±0.3	0.8±0.4	2.9±0.3	–0.5±0.3
T= 310 K	**AMBER**	**CHARMM**	**GROMOS**	**OPLS-AA**
ΔG^{HYD} (kcal/mol)	–3.7±0.2	–3.9±0.3	–2.2±0.3	–5.2±0.2
ΔG^{SOLV} (kcal/mol)	–6.6±0.2	–5.9±0.3	–6.2±0.2	–6.5±0.3
Log K_{ow}	2.1±0.2	1.4±0.2	2.8±0.3	0.9±0.2
T= 330 K	**AMBER**	**CHARMM**	**GROMOS**	**OPLS-AA**
ΔG^{HYD} (kcal/mol)	–3.0±0.4	–3.4±0.4	–1.8±0.3	–4.3±0.4
ΔG^{SOLV} (kcal/mol)	–5.0±0.4	–5.8±0.3	–5.8±0.4	–6.7±0.4
Log K_{ow}	1.3±0.3	1.5±0.4	2.7±0.4	1.7±0.3

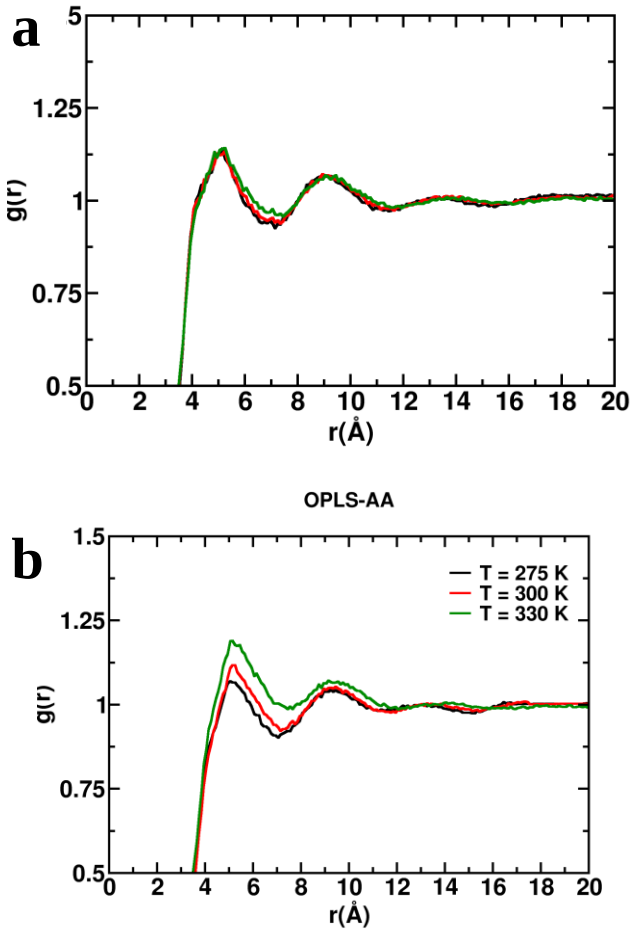

Figure S1 Radial distribution function of the isopropyl carbon chains with the octyl chain of 1-octanol as a function of temperature using (a) CHARMM and (b) OPLS-AA force fields. T=275 K shown as black line, T=300 K shown as red line and T=330 K as green line.

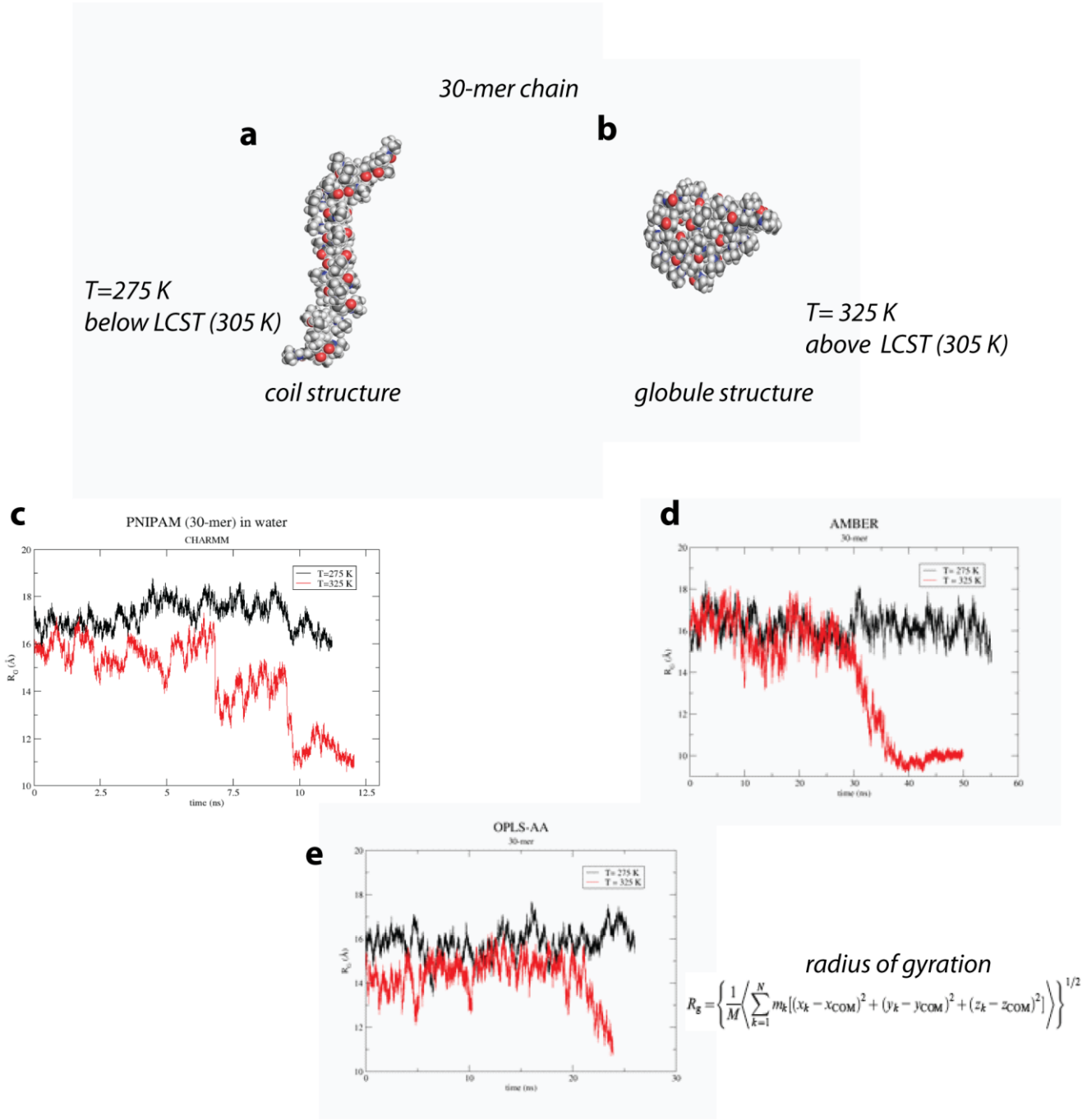

Figure S2 Modeled a 30-mer PNIPAM polymer in NAMD using AMBER, CHARMM and OPLS-AA force fields. Use of SPC/E water for AMBER and OPLS-AA and modified TIP3P water model with CHARMM to look into the relaxation dynamics of the polymer across LCST. The coil structure of the 30mer at 275 K (a) and globule structure at 325 K (b). The radius of gyration of the 30-mer as a function of time scale is shown in c, d and e