Soft Matter

ARTICLE

Supplementary Information for "Universal Localization Transition Accompanying Glass Formation: Insights from Efficient Molecular Dynamics Simulations of Diverse Supercooled Liquids"

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Table S1 provides additional properties of the systems simulated, including fit parameters for the "Cooperative Model" of Schmidtke et al[1] employed to fit the temperature dependence of our relaxation times. Values of T_g and kinetic fragility index m are determined via an extrapolation of this functional form to 100 seconds. T_A is obtained as described in the text. Also reported are fit parameters α employed in the main text. Supplementary figures S1 through S4 illustrate the collapse of reduced Debye-Waller factor vs reduced temperature shown in the main text, albeit with each system shown in a separate plot. Relaxation time data and trajectory files for these simulations are available upon request to the corresponding author.

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Table S 1. Supplementary data for simulated systems: degree of polymerization, T_g and m as determined from an extrapolation to 100 seconds of fits to the cooperative model of Schmidtke et al, ratio of T_A to $3T_{g,coop}$, fit values of α parameter leading to figure 11c collapse in the main text, and parameters and coefficient of determination for fits to the cooperative model of Schmidtke et al.

Material	dop	$T_{g,coop}$	m_{coop}	$T_A/3T_{g,coop}$	α	$\tau_{0,coop}$	E_{inf}	u	b	R^2 of fit
PIB_3	3	103.0	29.9	1.062	3.68	226.79	905	12.39	0.198	0.9997
PIB_5	5	156.9	35.4	0.972	4.07	219.39	1233	14.53	0.209	0.9991
PIB_{10}	10	198.6	33.3	0.933	4.80	252.97	1445	11.89	0.246	0.9994
PIB_{15}	15	209.8	31.7	1.073	3.96	257.81	1558	11.17	0.247	0.9988
PIB_{20}	20	218.7	32.2	1.036	3.93	227.51	1786	12.92	0.211	0.9994
PIB_{30}	30	215.2	29.0	1.108	3.87	270.65	1653	9.88	0.253	0.9995
PIB_{50}	50	215.2	27.6	1.148	4.01	303.11	1576	8.46	0.287	0.9991
PIB_{75}	75	228.2	29.6	1.085	4.14	269.20	1747	10.26	0.249	0.9996
PIB_{100}	100	219.7	27.6	1.064	4.47	293.82	1639	8.63	0.279	0.9989
PS_3	3	206.1	47.8	0.820	4.26	217.05	1261	16.89	0.253	0.9992
PS_5	5	243.7	48.2	0.821	4.55	237.83	1446	16.23	0.263	0.9983
PS_{10}	10	291.4	49.8	0.799	4.97	256.67	1706	17.09	0.262	0.9980
PS_{15}	15	295.9	43.3	0.861	4.90	303.27	1630	13.08	0.306	0.9974
PS_{20}	20	338.2	59.0	0.740	5.43	188.97	2290	25.42	0.202	0.9985
PS_{30}	30	333.6	50.1	0.781	5.29	249.74	2025	17.99	0.249	0.9969
PS_{50}	50	325.4	43.9	0.779	6.04	306.91	1829	13.67	0.295	0.9977
PS_{60}	60	333.4	46.5	0.789	5.62	277.09	1971	15.76	0.267	0.9950
PS_{75}	75	347.3	51.2	0.783	5.54	227.90	2236	19.85	0.228	0.9968
PS_{100}	100	344.9	47.8	0.757	5.87	293.44	1912	15.22	0.287	0.9967
PS_{200}	200	382.8	66.6	0.704	5.66	160.13	2725	31.50	0.183	0.9961
PS_{400}	400	381.5	62.7	0.702	5.94	181.97	2562	27.26	0.200	0.9955
PVC_{10}	10	235.5	49.3	0.795	4.07	223.45	1395	16.97	0.260	0.9997
PVC_{20}	20	263.0	49.1	0.825	3.91	227.37	1542	16.69	0.264	0.9995
PVC_{30}	30	271.6	48.3	0.830	3.91	242.21	1525	15.52	0.282	0.9995
PVC_{50}	50	276.8	46.6	0.809	4.30	244.59	1542	14.60	0.290	0.9991
PVC_{75}	75	274.7	44.5	0.860	4.01	253.25	1522	13.58	0.300	0.9990
PVC_{100}	100	279.0	45.2	0.824	4.25	258.76	1494	13.37	0.311	0.9989
PEI_{10}	10	470.3	63.1	0.651	6.11	224.97	2212	18.06	0.313	0.9982
PB_{10}	10	220.0	46.3	0.736	5.94	254.83	1161	13.60	0.313	0.9974
PB_{30}	30	252.2	41.8	0.767	6.36	268.15	1393	12.37	0.312	0.9978
PB_{50}	50	221.8	47.7	0.811	4.71	238.36	1242	15.19	0.285	0.9975
PB_{100}	100	280.7	45.4	0.791	5.81	272.97	1426	12.67	0.333	0.9967
P(Methyl)A	30	274.5	42.4	0.920	4.26	238.69	1723	14.67	0.260	0.9988
P(Ethyl)A	30	247.2	40.5	0.903	4.32	246.10	1626	14.49	0.250	0.9988
P(Propyl)A	30	223.8	37.5	0.914	4.36	249.12	1569	13.87	0.239	0.9993
P(Butyl)A	30	207.6	34.2	0.986	4.20	272.96	1404	11.39	0.269	0.9984
P(Pentyl)A	30	205.0	35.0	1.005	3.97	248.94	1459	12.60	0.245	0.9993
P(Hexyl)A	30	208.1	36.2	1.014	3.76	242.21	1462	13.13	0.244	0.9986
P(Octyl)A	30	223.6	41.4	0.764	5.22	226.94	1481	15.07	0.244	0.9994

Material	*dop*	$T_{g,coop}$	m_{coop}	$T_A/3T_{g,coop}$	α	$\tau_{0,coop}$	E_{inf}	*u*	*b*	R^2 *of fit*
P(Dexyl)A	30	246.8	52.2	0.725	4.85	193.31	1624	20.82	0.220	0.9982
P(Dodecyl)A	30	268.6	63.4	0.676	4.80	179.48	1667	25.05	0.221	0.9975
UA-PS	30	257.7	49.0	0.673	7.19	128.25	2263	27.01	0.153	0.9985
M-PS	30	276.1	73.0	0.642	6.13	51.6714	3059	61.29	0.104	0.9940
Glycerol	1	172.2	41.7	0.920	3.80	68.6308	1704	24.22	0.139	0.9996
α-D-Glucose	1	256.1	43.8	0.761	4.97	56.43	2629	27.19	0.130	0.9998
Trehalose	1	281.5	38.4	0.993	3.74	140.881	2126	15.37	0.214	0.9996
OTP	1	226.8	101.3	0.509	10.03	18.70	2264	74.96	0.113	0.9976
Cu_4-Ag_6	1	484.8	82.8	0.603	6.99	0.0364	3882	45.09	0.152	0.9967
SiO_2	1	1046	25.4	0.814	7.09	0.0611	3139	2.19	1.415	0.9994
KG	20	0.343	83.56	0.616	6.57	0.0582	2.585	43.04	0.163	0.9987
bLJ	1	0.292	86.24	0.533	8.78	0.029	2.522	51.73	0.138	0.9991

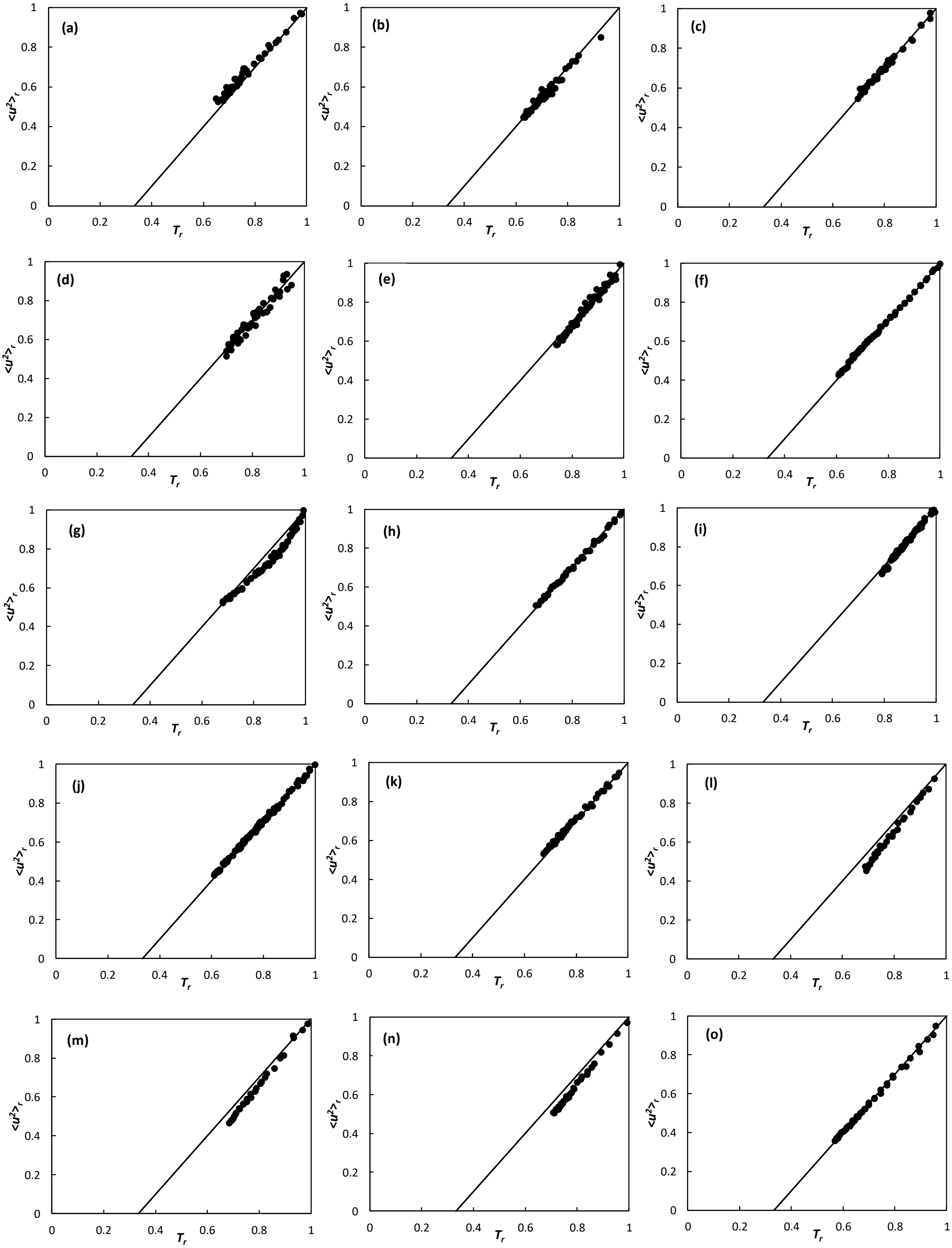

Figure S 1. Reduced Debye-Waller factor vs reduced temperature for (a) PB-100, (b) PB-50, (c), PB-30, (d) PB-10, (e) Binary-LJ, (f) bead-spring polymer, (g) SiO_2, (h)Cu_4Ag_6, (i) OTP, (j) Martini PS, (k) UA-PS, (l) Poly(dodecyl)acrylate, (m) Poly(decyl)acrylate, (n) Poly(octyl) acrylate, (o) Poly(hexyl)acrylate.

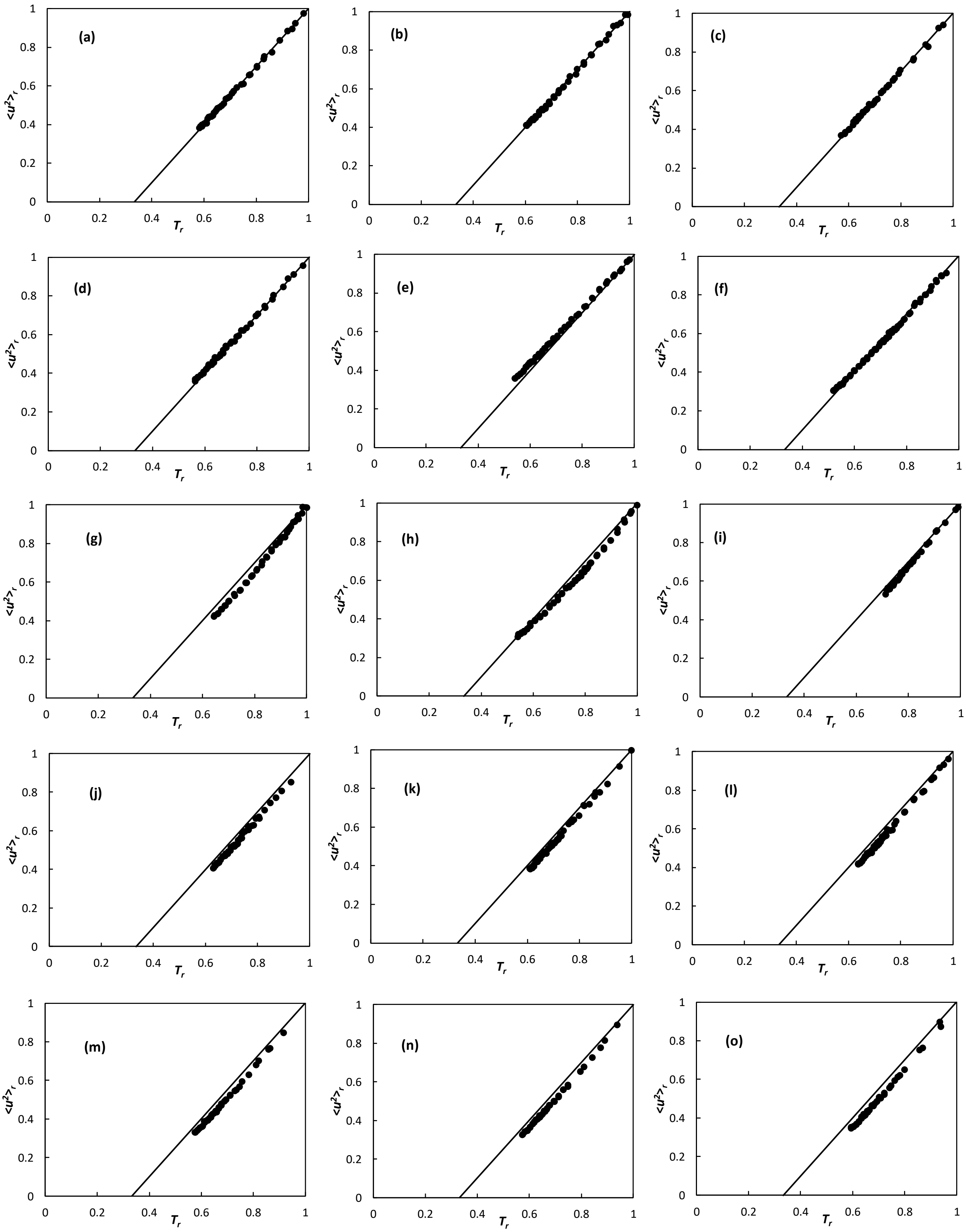

Figure S 2. Reduced Debye-Waller factor vs reduced temperature for (a) Poly(pentyl)acrylate, (b), poly(butly)acrylate, (c) poly(propyl)acrylate, (d) poly(ethyl)acrylate, (e) poly(methyl)acrylate, (f) trehalose, (g) glucose, (h) glycerol, (i) PEI, (j) PVC-100, (k) PVC-75, (l) PVC-50, (m) PVC-30, (n) PVC-20, (o) PVC-10.

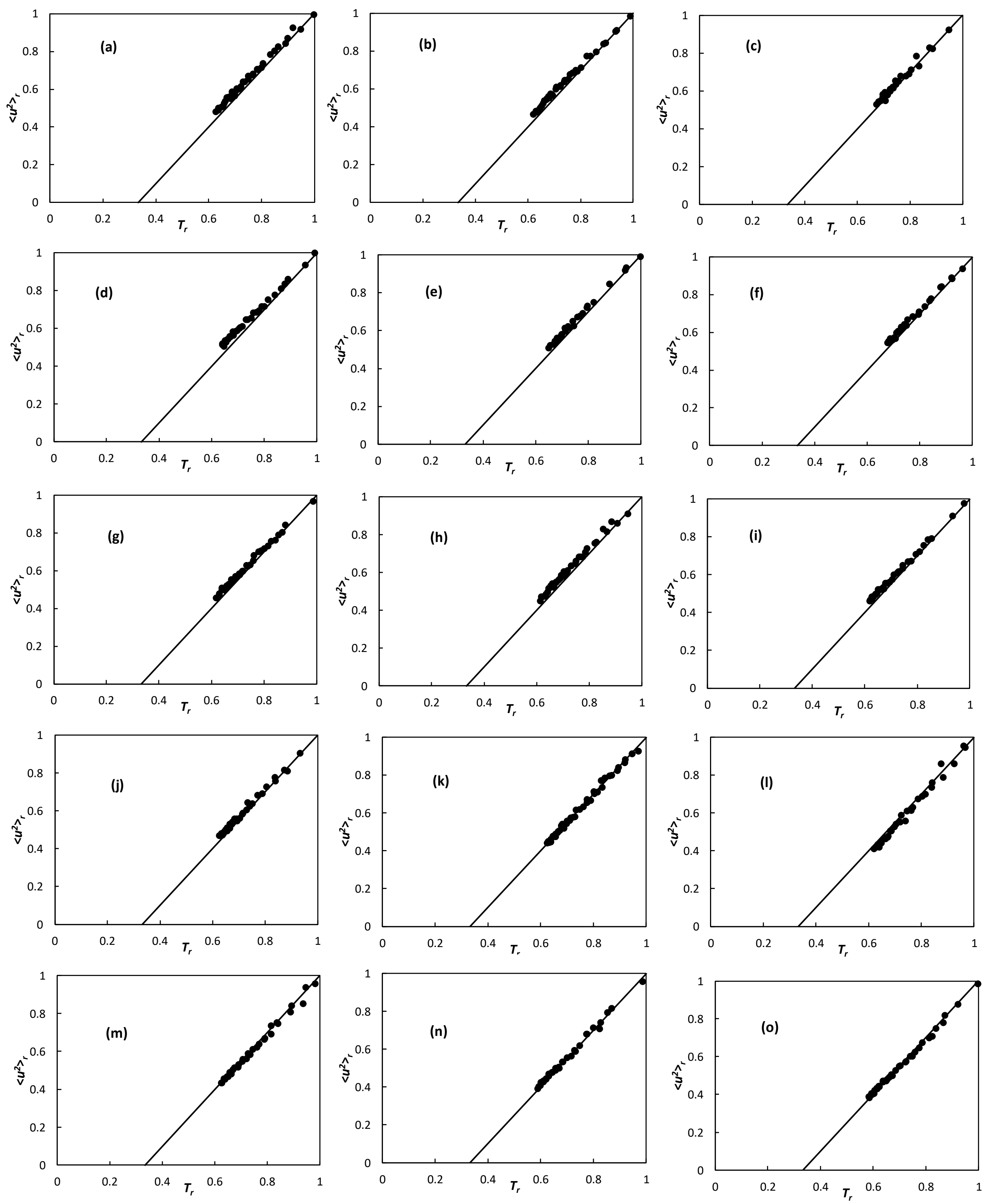

Figure S 3. Reduced Debye-Waller factor vs reduced temperature for (a) PS-400, (b) PS-200, (c) PS-100, (d) PS-75, (e) PS-60, (f) PS-50, (g) PS-30, (h) PS-20, (i) PS-15, (j) PS-10, (k) PS-5, (l) PS-3, (m) PIB-100, (n) PIB-75, (o) PIB-50.

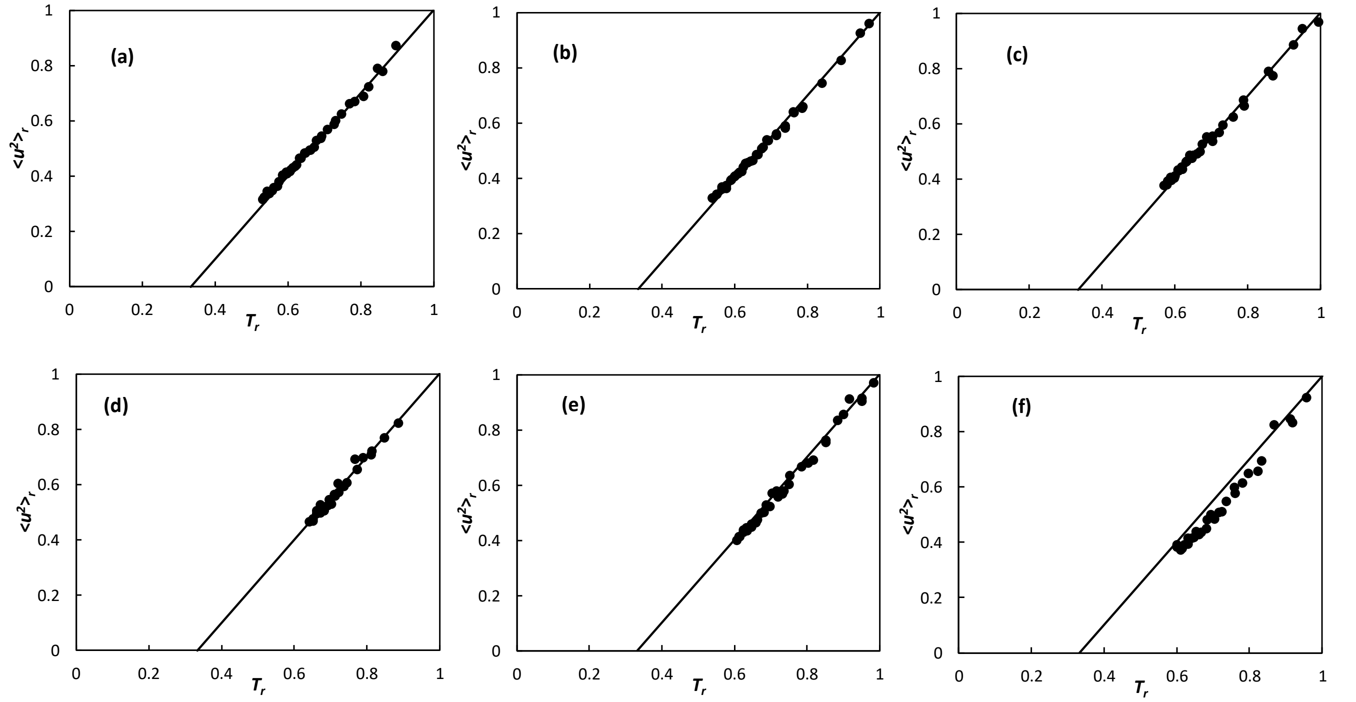

Figure S 4. Reduced Debye-Waller factor vs reduced temperature for (a) PIB-30, (b) PIB-20, (c) PIB-15, (d) PIB-10, (e) PIB-5, (f) PIB-3.

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Notes and references

1. Schmidtke, B., Hofmann, M., Lichtinger, A. & Rössler, E. A. Temperature Dependence of the Segmental Relaxation Time of Polymers Revisited. *Macromolecules* **48**, 3005–3013 (2015).