Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Molecular Dynamics Simulation Studies of Hyperbranched Polyglycerols and Their Encapsulation Behaviors of Small Drug Molecules

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Table S1. Summary of the simulation systems.

Number of solute atoms	DB	DP	Number of water molecules	Number of solute atoms	DB	DP	Number of water molecules
298	0.6_max	26	3115	1046	0.2_min	94	12632
298	0.6_min	26	2773	1046	0.4_max	94	15321
518	0.0	46	30037	1046	0.4_min	94	6702
518	0.2_max	46	12408	1046	0.6_max	94	6723
518	0.2_min	46	8559	1046	0.6_min	94	5518
518	0.4_max	46	5665	1046	0.8_max	94	5527
518	0.4_min	46	3926	1046	0.8_min	94	5520
518	0.6_max	46	5559	1046	1.0	94	4900
518	0.6_min	46	3160	2212	0.6_max	200	13109
518	0.8_max	46	4624	2212	0.6_min	200	9171
518	0.8_min	46	3541	738	0.6_max	66	6881/7524
518	1.0	46	3599	2775	0.6_max_arm	66	62657
1046	0.0	94	205305	738	0.6_min	66	5605/6472
1046	0.2_max	94	25643	2775	0.6_min_arm	66	40558

Table S2. Radius of gyration (R_g) (Å) as functions of *DP* and *DB*.

DP	DB	WI	R_g(Å)	DP	DB	WI	R_g(Å)
26	0.6	2039	8.6±0.1	66	0.6	14642	10.7±0.1
26	0.6	1464	7.5±0.2	94	0.0	138415	18.8±0.6
46	0.0	16215	15.8±0.6	94	0.2	93397	15.2±0.5
46	0.2	12646	11.7±0.5	94	0.2	51209	13.0±0.2
46	0.2	8372	9.9±0.3	94	0.4	68410	13.8±0.3
46	0.4	10762	11.2±0.4	94	0.4	39947	12.7±0.1
46	0.4	6973	9.0±0.1	94	0.6	53802	13.9±0.3
46	0.6	8807	10.9±0.2	94	0.6	35774	12.3±0.1
46	0.6	6082	9.3±0.1	94	0.8	44610	13.8±0.1
46	0.8	8010	9.9±0.1	94	0.8	32472	11.9±0.1
46	0.8	5827	9.5±0.1	94	1.0	31293	11.7±0.1
46	1.0	5661	10.0±0.1	200	0.6	334411	17.0±0.2
66	0.6	22928	12.0±0.3	200	0.6	212832	15.2±0.1

Table S3. Aspect ratios and asphericities for various HPGs molecules.

DP	DB	WI	I_z/I_x	I_z/I_y	δ
26	0.6	2039	2.58±0.26	1.04±0.02	0.063±0.010
26	0.6	1464	2.30±0.18	1.25±0.05	0.059±0.008
46	0.0	16215	12.16±2.23	1.02±0.01	0.192±0.010
46	0.2	12646	2.94±0.36	1.13±0.04	0.075±0.012
46	0.2	8372	1.76±0.18	1.07±0.05	0.026±0.009
46	0.4	10762	2.16±0.09	1.32±0.04	0.044±0.004
46	0.4	6973	1.33±0.06	1.16±0.04	0.007±0.002
46	0.6	8807	2.02±0.33	1.18±0.09	0.037±0.015
46	0.6	6082	1.57±0.10	1.36±0.06	0.019±0.003
46	0.8	8010	1.61±0.08	1.09±0.02	0.019±0.004
46	0.8	5827	1.70±0.11	1.23±0.05	0.022±0.005
46	1.0	5661	1.90±0.14	1.08±0.03	0.033±0.007
66	0.6	22928	2.42±0.45	1.17±0.09	0.054±0.019
66	0.6	14642	1.76±0.07	1.35±0.03	0.027±0.003
94	0.0	138415	3.55±0.35	1.21±0.05	0.094±0.011
94	0.2	93397	2.79±0.22	1.18±0.04	0.069±0.008
94	0.2	51209	2.01±0.07	1.30±0.03	0.037±0.003
94	0.4	68410	2.60±0.12	1.14±0.03	0.062±0.005
94	0.4	39947	1.61±0.06	1.32±0.04	0.020±0.003
94	0.6	53802	2.26±0.21	1.25±0.04	0.047±0.009
94	0.6	35774	1.65±0.07	1.22±0.03	0.020±0.003
94	0.8	44610	2.38±0.11	1.26±0.03	0.053±0.005
94	0.8	32472	1.58±0.04	1.25±0.02	0.017±0.002
94	1.0	31293	1.70±0.04	1.40±0.03	0.025±0.002
200	0.6	334411	1.70±0.04	1.40±0.03	0.025±0.002
200	0.6	212832	1.45±0.02	1.15±0.02	0.011±0.001

Table S4. Solvent accessible surface for various HPGs molecules.

DP	DB	WI	SASA (nm^2)	DP	DB	WI	SASA (nm^2)
26	0.6	2039	17.93±0.60	66	0.6	14642	41.63±1.20
26	0.6	1464	20.26±0.70	94	0.0	138415	60.32±1.57
46	0.0	16215	33.30±1.09	94	0.2	93397	57.58±1.72
46	0.2	12646	32.93±1.03	94	0.2	51209	58.56±2.68
46	0.2	8372	30.97±1.43	94	0.4	68410	56.38±1.29
46	0.4	10762	32.72±0.98	94	0.4	39947	56.55±0.97
46	0.4	6973	30.10±0.88	94	0.6	53802	55.79±1.54
46	0.6	8807	31.95±0.87	94	0.6	35774	56.27±1.77
46	0.6	6082	29.85±0.83	94	0.8	44610	54.67±1.13
46	0.8	8010	31.83±0.83	94	0.8	32472	54.43±1.03
46	0.8	5827	30.49±0.87	94	1.0	31293	54.28±0.98
46	1.0	5661	30.77±0.62	200	0.6	334411	108.22±1.53
66	0.6	22928	39.46±1.07	200	0.6	212832	103.30±2.40

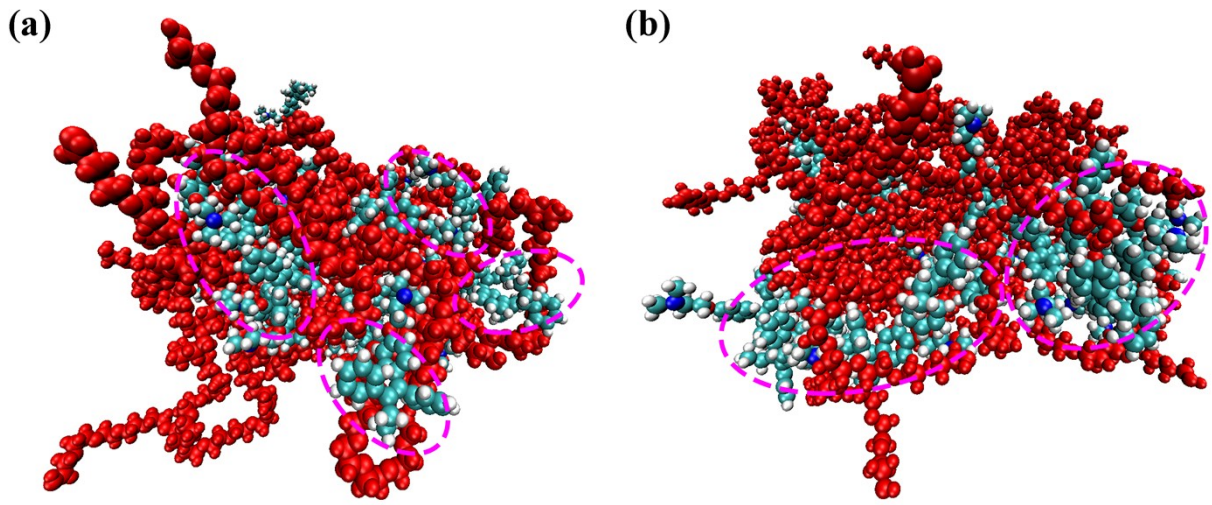

Fig. S1. Snapshot of clusters of tamoxifen molecules associating to the HPG-star-PEG (red). (a) max WI HPG-star-PEG/tamoxifen complex; (b) min WI HPG-star-PEG/tamoxifen complex. The HPG-star-PEG are shown as the red beads; The tamoxifen clusters are marked with carmine circle. Water molecules are not shown for visual clarity.