

SUPPLEMENTARY DATA

Conformational analysis of oligomers of non-ionic thermoresponsive polymers containing amide groups

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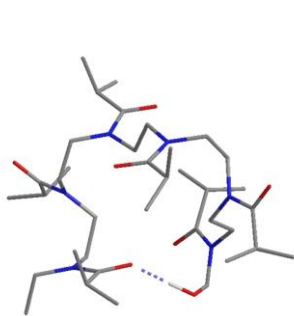
Table S1. Cluster analysis of conformations of oligomers of thermoresponsive polymers.

	IPOZ-6	IPOZ-12	NIPAM-6
Clustering method	Single linkage		
Distance (similarity) index	Torsional distance		
Distance threshold	10.0°		
Distance definitions (number of torsions)	17	34	10
Number of conformers clustered	4552	15378	14947
Number of clusters	621	3233	101
Minimum size of cluster	1		
Maximum size of cluster	181	1199	4764

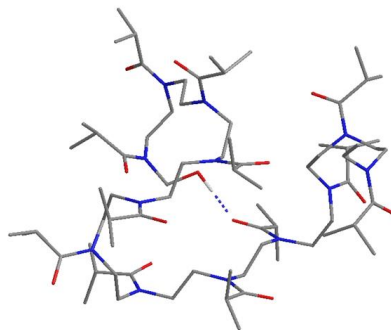
Cluster	Number of members in the cluster	Distribution of the cluster	ID's of the lowest-energy conformers	Relative Steric Energy (kcal mol ⁻¹)	Population (%)
IPOZ-6					
A	55	48.3	03831	0.0	80.3
			03917	1.4	7.4
			03908	1.9	3.3
			03906	2.2	1.8
			03905	2.3	1.5
			03915	2.4	1.4
			03909	2.6	1.0
			03910	2.8	0.7
B	126	10.2	01927	1.2	54.7
			01675	1.7	19.8
			01928	2.5	6.0
			01965	2.5	5.2
			01926	2.6	5.1

			01674	3.1	2.1
C	149	10.1	04109	1.3	43.3
			04177	1.6	24.0
			04110	2.2	9.0
			04196	2.6	4.9
			04176	2.9	2.8
D	39	2.9	01732	1.6	82.0
			01731	3.0	8.8
			01923	3.2	5.8
E	33	2.5	03314	1.8	74.2
			03300	2.6	20.0
			03352	3.9	2.1
F	112	2.8	00883	1.8	62.0
			00916	2.7	15.5
			00884	3.2	5.8
			00906	3.4	4.4
G	114	6.9	04004	2.1	17.4
			04021	2.2	14.1
			04187	2.3	11.5
			03950	2.4	9.5
			04019	2.5	7.8
			04020	2.6	7.6
			04027	2.8	5.3
			04097	2.8	4.6
			03951	3.0	3.8
			04214	3.1	3.3
H	181	2.7	01056	2.1	40.6
			01563	2.7	13.2
			01261	2.8	7.2
			01264	3.1	2.3
			00990	3.8	2.2
			01623	3.8	1.5
			01255	4.1	1.1
I	95	2.4	02413	2.2	40.3
			02555	2.7	17.1
			02304	3.0	10.7
			02436	3.4	4.9
			02556	3.5	4.6
			02407	3.5	4.5
J	25	1.1	01783	2.2	82.6
			01946	3.4	12.2
			01940	4.5	2.0
			01948	4.6	1.5
K	38	0.7	01185	2.6	75.9
			01269	3.8	9.1
			01276	4.0	6.3
IPOZ-12					
A	15	76.6	15235	0.0	94.5
			15236	1.6	4.4
			15077	3.0	0.6

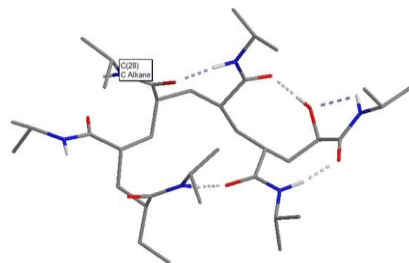
B	278	17.6	14973	1.6	29.0
			14977	1.8	21.0
			14993	2.0	13.5
			15348	2.4	7.2
			15068	2.7	4.3
			14995	2.8	3.6
			14989	2.9	3.2
			14981	2.9	2.9
C	18	2.9	15250	2.0	84.1
			15249	3.3	9.3
			15149	3.9	3.2
			15251	4.3	1.6
			15255	5.0	0.5
			15347	5.1	0.4
			15036	5.3	0.3
D	8	0.8	15272	2.7	90.3
			15292	4.3	6.0
			15367	5.0	2.0
			15271	5.4	1.0
E	210	1.1	14398	3.2	30.2
			14517	3.3	24.1
			14507	3.8	10.8
			14698	3.9	8.4
F	1	0.1	15341	4.0	100.0
NIPAM-6					
A	4764	77.4	05665	39	from
			05918	(0.0 ÷ 1.0)	2.9%
			05677		
			05472	170	to
			05930	(1.0 ÷ 2.0)	0.02%
			05473		
			05922	325	
			05664	(2.0 ÷ 3.0)	
05688					
05963					
B	3137	20.6	06605	36	
			06741	(1.3 ÷ 2.0)	
				
			286	
....	(2.0 ÷ 3.0)				
C	1947	2.0	05240	1.9	4.2
			04787	2.0	3.6
			05247	2.2	2.9
				
			20	from 1.7%
	(2.5 ÷ 3.0)	to 0.7%			
D	419	0.0	13276	4.7	
E	29	0.0	14340	6.3	
F	13	0.0	14847	6.5	



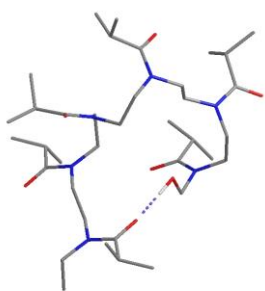
IPOZ-6_A-03831 (0.39)



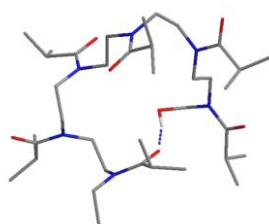
IPOZ-12_A-15235 (0.72)



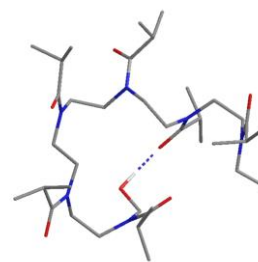
NIPAM-6_A-05665 (0.02)



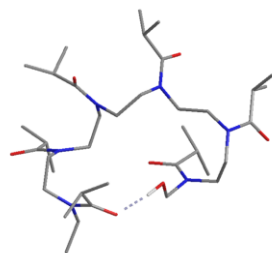
IPOZ-6_B-01927 (0.06)



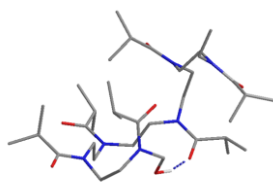
IPOZ-6_C-04109 (0.04)



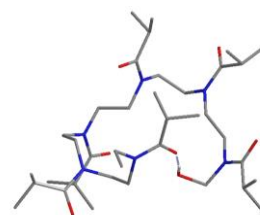
IPOZ-6_D-01731 (0.02)



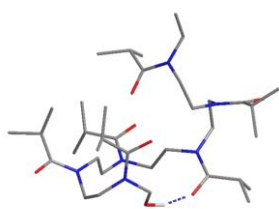
IPOZ-6_E-03314 (0.02)



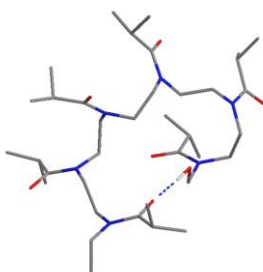
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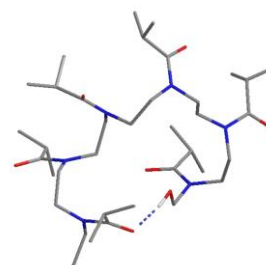
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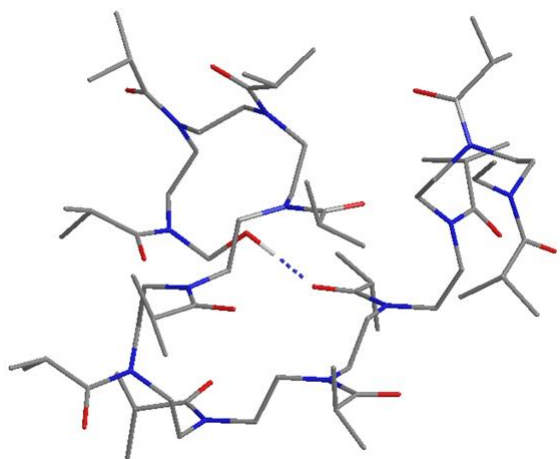
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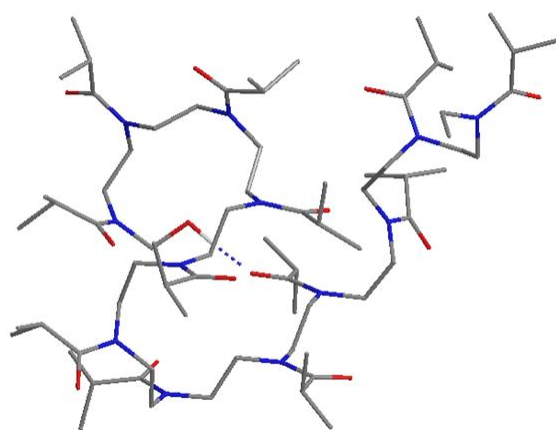
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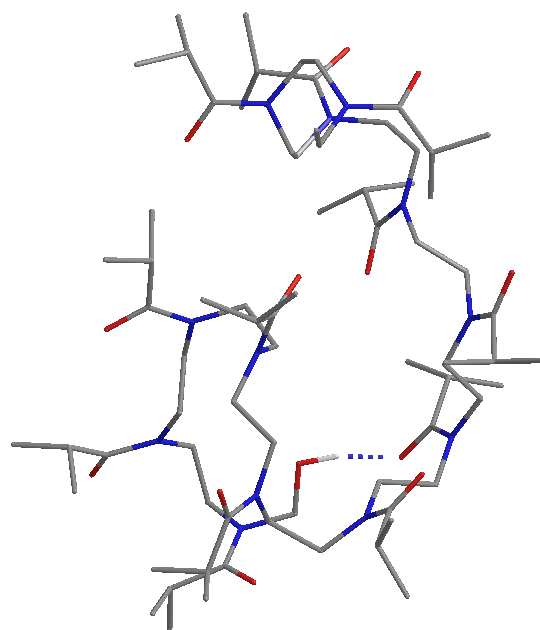
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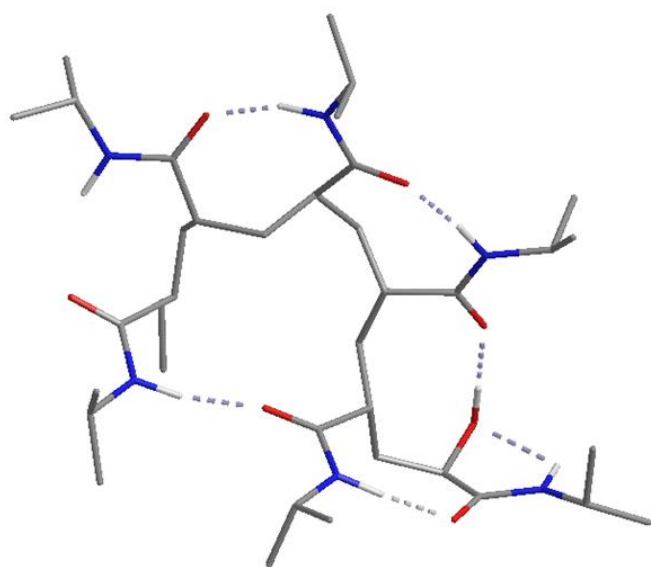
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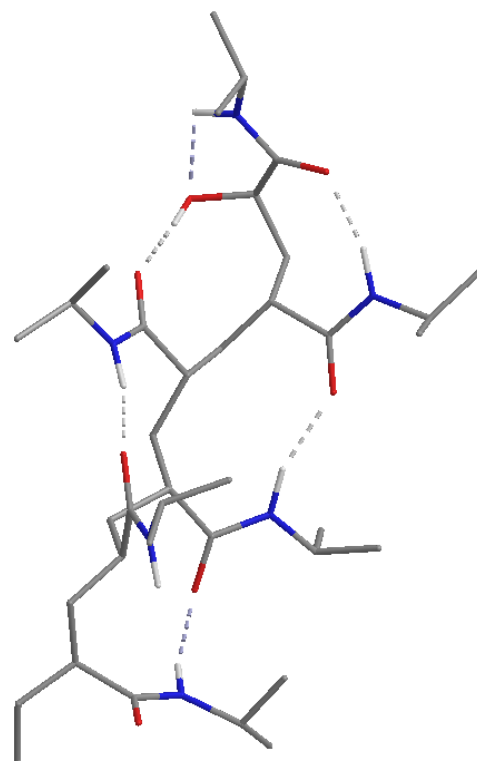
IPOZ-12_C-15250 (0.02)



IPOZ-12_D-15272 (0.03)



NIPAM-6_B-06605 (0.003)



NIPAM-6_C-05240 (0.01)

Fig. S1. Optimized geometries of low-energy conformations of some clusters (populations of conformers are given in parenthesis).