

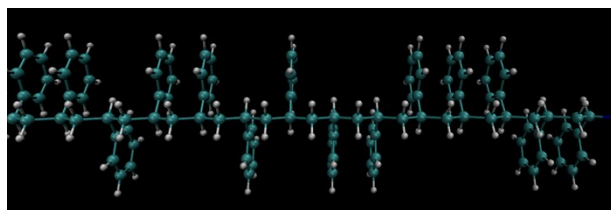
Supporting information for:

Tacticity Dependence of Single Chain Polymer Folding

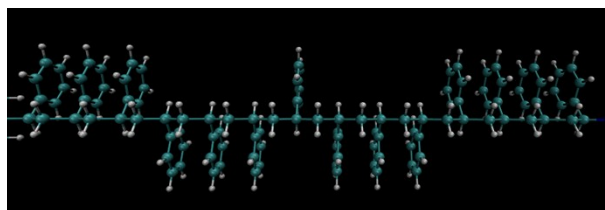
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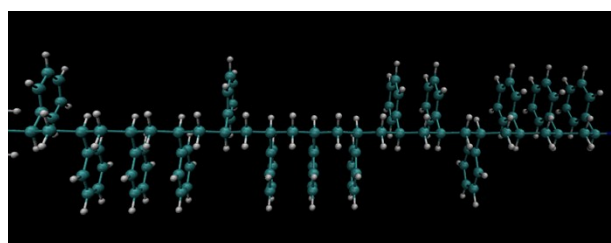
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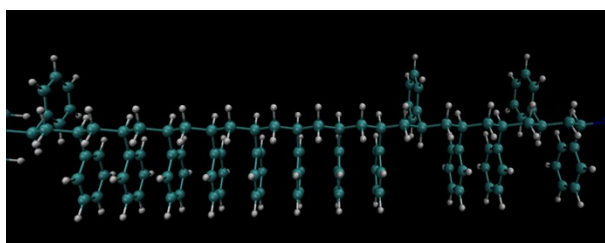
A1



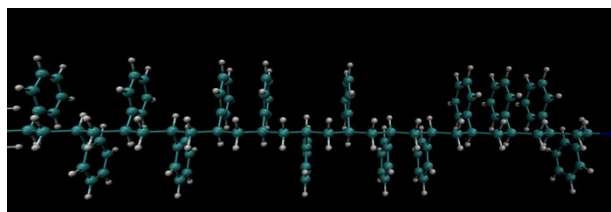
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Figure S1. Different random stereochemistries of atactic polymers of L=14 studied in this work.

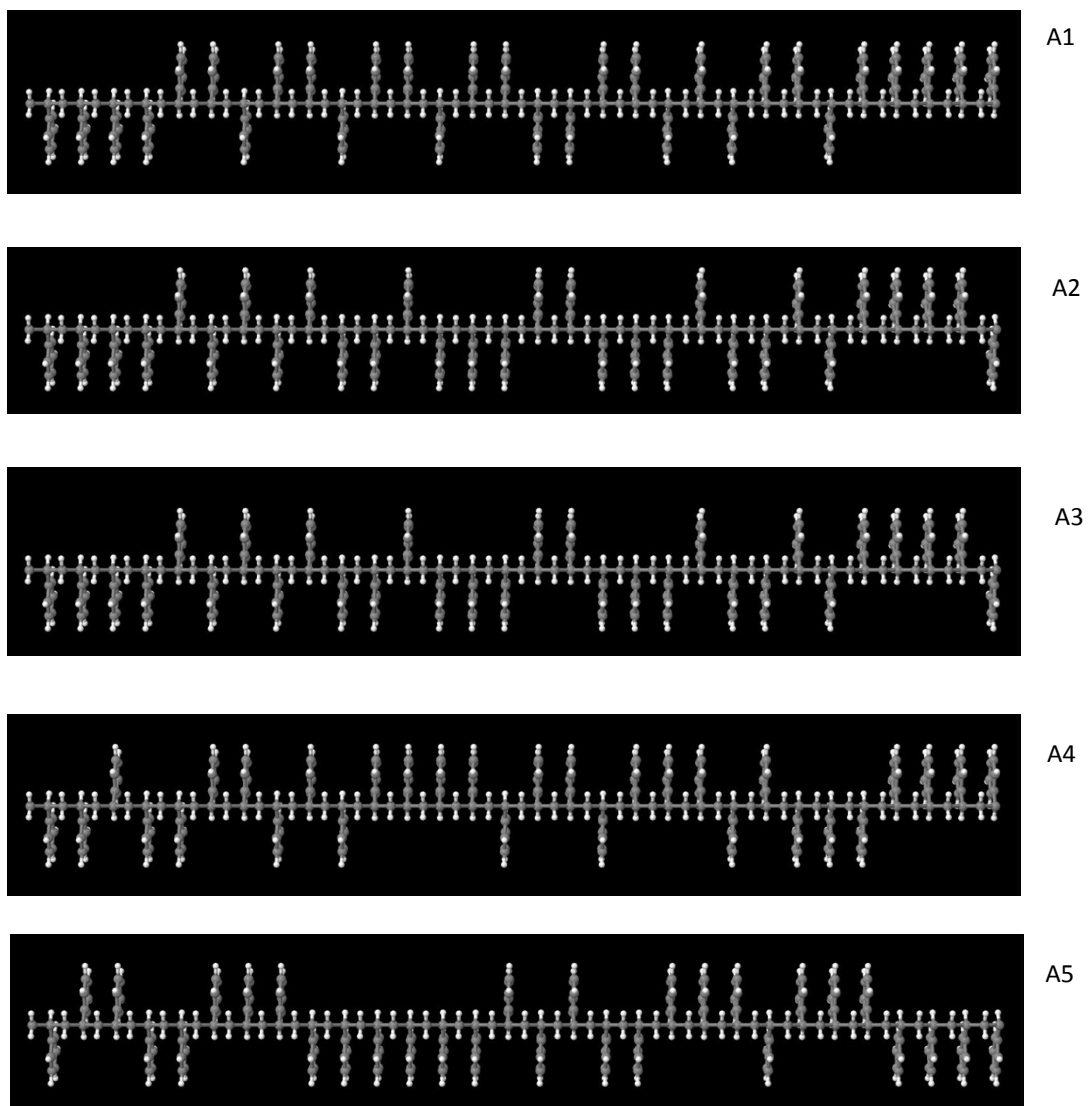


Figure S2. Different random stereochemistries of atactic polymers of L=30 studied in this work.

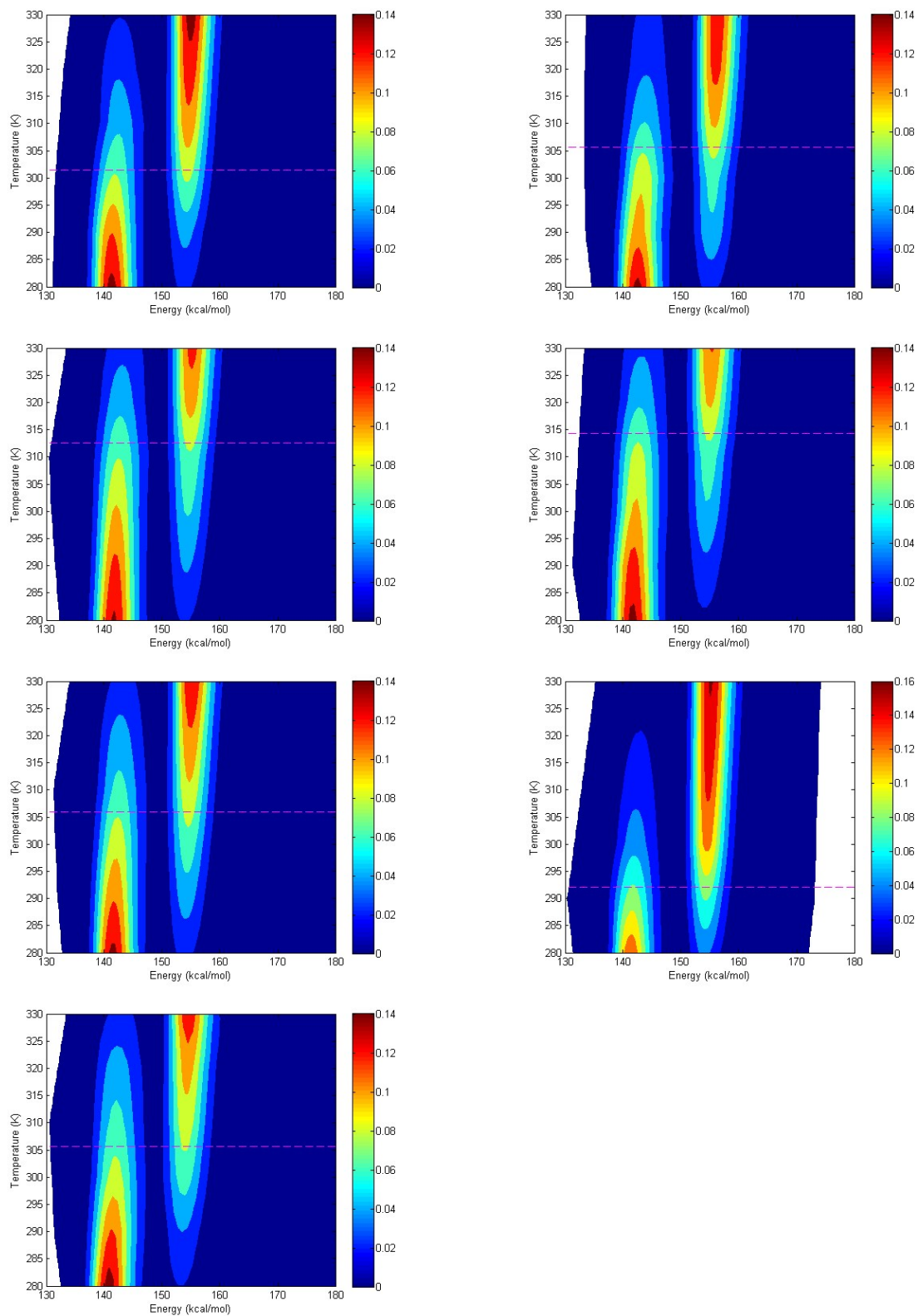


Figure S3. Free energy diagrams for five different atactic polymers and also syndiotactic and isotactic polymers of length $L=18$ derived from the trajectories.

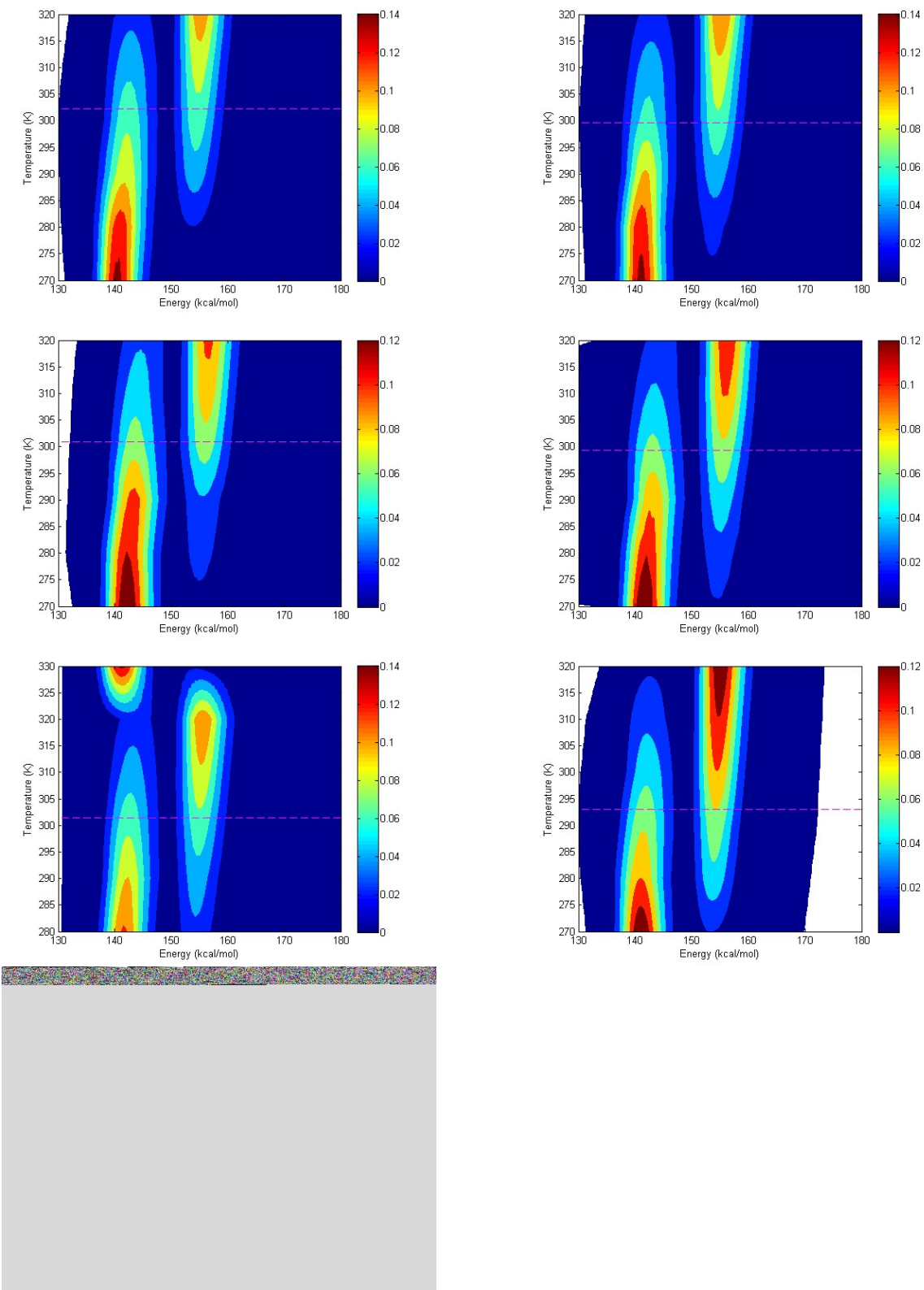


Figure S4. Free energy diagrams for five different atactic polymers and also syndiotactic and isotactic polymers for $L=20$ derived from the trajectories.

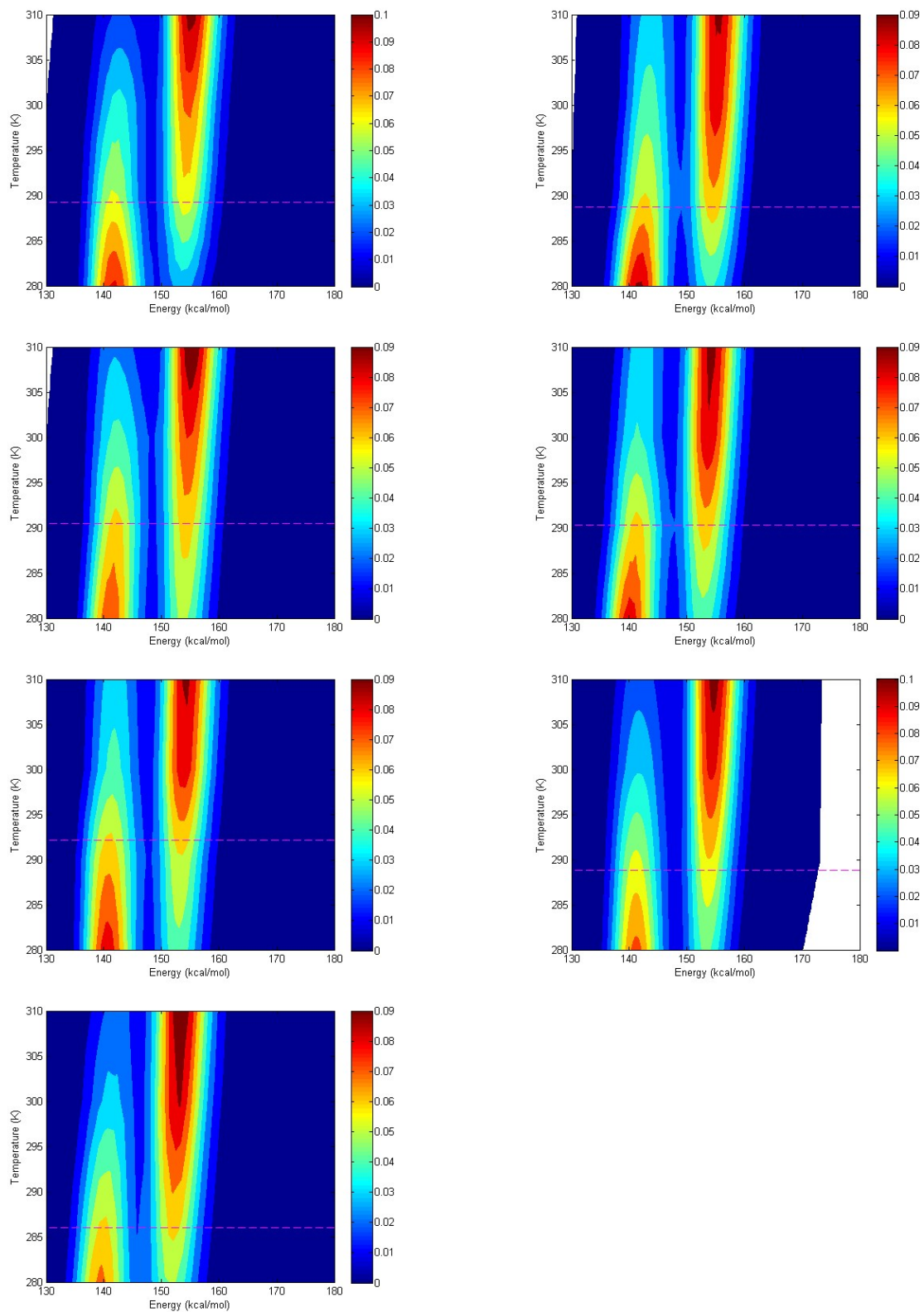


Figure S5. Free energy diagrams for five different atactic polymers and also syndiotactic and isotactic polymers for $L=30$ derived from the trajectories.

Table S1. Folding temperatures and thermodynamic properties for isotactic, syndiotactic and atactic polymers of different chain lengths. The symbols A-1 to A-5 denotes different configurations of atactic polymers with random tacticities.

isotactic			
Length	T_m(K)	ΔH (kcal mol⁻¹)	ΔS(kcal.mol⁻¹K⁻¹)
10	320.6	11.91	0.0371
12	315.5	12.10	0.0383
14	305.7	11.91	0.0390
16	300.6	11.90	0.0396
18	301.8	12.00	0.0398
20	292.1	12.62	0.0432
30	286.0	12.41	0.0434

syndiotactic			
Length	T_m(K)	ΔH (kcal mol⁻¹)	ΔS (kcal.mol⁻¹K⁻¹)
10	298.0	12.47	0.0418
12	295.9	12.36	0.0418
14	292.1	12.63	0.0432
16	290.6	12.48	0.0430
18	293.5	12.50	0.0426
20	293.1	12.39	0.0423
30	288.8	12.59	0.0436

Atactic				
length	polymer	T _m (K)	ΔH (kcal.mol ⁻¹)	ΔS (kcal.mol ⁻¹ K ⁻¹)
10	A-1	316.9	11.92	0.0376
	A-2	320.0	12.13	0.0379
	A-3	317.9	11.98	0.0377
	A-4	307.4	12.14	0.0395
	A-5	320.1	12.08	0.0378
12	A-1	312.9	11.95	0.0382
	A-2	311.9	12.01	0.0385
	A-3	314.6	11.95	0.0380
	A-4	311.0	12.05	0.0387
	A-5	310.7	12.10	0.0390
14	A-1	301.4	12.28	0.0408
	A-2	305.6	12.04	0.0394
	A-3	312.5	12.13	0.0388
	A-4	314.3	12.10	0.0385
	A-5	305.9	12.06	0.0394
16	A-1	304.7	12.18	0.0400
	A-2	303.6	12.29	0.0405
	A-3	311.7	12.08	0.0388
	A-4	301.2	12.35	0.0410
	A-5	303.8	12.19	0.0401
18	A-1	297.6	12.28	0.0413
	A-2	296.2	12.27	0.0414
	A-3	302.9	12.29	0.0406
	A-4	300.7	12.17	0.0405
	A-5	305.3	12.20	0.0399
20	A-1	302.3	12.20	0.0404
	A-2	299.6	12.39	0.0414
	A-3	300.9	12.24	0.0407
	A-4	299.3	12.43	0.0415
	A-5	301.5	12.37	0.0410
30	A-1	289.2	12.56	0.0434
	A-2	288.7	11.94	0.0414
	A-3	290.5	12.30	0.0424
	A-4	290.3	12.12	0.0418
	A-5	292.2	12.44	0.0426