Supplemental Information:

Table S1. Energies with Zero-Point Correction for Conformations of the Monomer.

Conformer	Characteristics	Energy (H)	E(kcal/mol)	ZPE (H)	**E(kcal/mol)**
1	*cis*-Eq(–176.4)	-589.586321	0.00	-589.359271	**0.00**
2	*trans*-Ax(–72.1)	-589.586216	0.07	-589.358875	**0.25**
3	*trans*-Eq(–62.2)	-589.585881	0.28	-589.358881	**0.24**
4	*cis*-Eq(–56.8)	-589.585436	0.56	-589.358466	**0.51**
5	*trans*-Eq(–171.2)	-589.585231	0.68	-589.358199	**0.67**
6	*cis*-Ax(–178.9)	-589.585017	0.82	-589.357720	**0.97**
7	*cis*-Ax(–62.5)	-589.584687	1.03	-589.357389	**1.18**
8	*trans*-Ax(–160.7)	-589.584534	1.12	-589.357206	**1.30**
9	*trans*-Eq(57.9)	-589.584396	1.21	-589.357137	**1.34**
10	*cis*-Eq(54.7)	-589.584322	1.25	-589.357060	**1.39**
11	*trans*-Ax(56.1)	-589.583482	1.78	-589.356082	**2.00**
12	*cis*-Ax(44.5)	-589.582773	2.23	-589.355422	**2.42**

Table S2. Energies with Zero-Point Correction for Conformations of the Dimer.

Conformer	Characteristics	Energy (H)	E(kcal/mol)	ZPE (H)	**E(kcal/mol)**
1	*cis*-Eq(–150)	-912.335283	0.00	-911.978138	**0.00**
2	*trans*-Ax(–85)	-912.335182	0.06	-911.977514	**0.39**
3	*trans*-Eq(–88)	-912.334012	0.80	-911.977067	**0.67**
4	*trans*-Ax(–154)	-912.333253	1.27	-911.975582	**1.60**
5	*cis*-Ax(–82)	-912.332646	1.65	-911.975002	**1.97**
6	*cis*-Ax(–168)	-912.332005	2.06	-911.974523	**2.27**
7	*cis*-Eq(72)	-912.325772	5.97	-911.968350	**6.14**
8	*trans*-Eq(69)	-912.325380	6.21	-911.967902	**6.42**
9	*trans*-Ax(7)	-912.322661	7.92	-911.964797	**8.37**
10	*cis*-Ax(27)	-912.322022	8.32	-911.964228	**8.73**
11	*trans*-Ax(89)	-912.319115	10.15	-911.960852	**10.85**

Table S3. Energies for Conformations of the Dimer with Differing Ester Torsions [C –C –C–O(CH_3)]. These calculations verify that the scans provided the lowest energy minima (in bold). Scans of *cis* conformers were based on an ester torsion of 180°, while the scans of the *trans* conformers were based on ester torsions of –60°.

cis-Eq (,ester torsion) minima:			
cis-Eq (-150,54)	-912.333147 H	*cis*-Eq (71,53)	-912.323823 H
***cis*-Eq (-150,-176)**	**-912.335283 H**	***cis*-Eq (72,-176)**	**-912.325772 H**
cis-Eq (-150,-56)	-912.334355 H	*cis*-Eq (72,-57)	-912.324931 H
trans-Eq (,ester torsion) minima:			
trans-Eq (-88,58)	-912.332396 H	*trans*-Eq (68,59)	-912.324158 H
trans-Eq (-89,-171)	-912.333505 H	*trans*-Eq (67,-173)	-912.324836 H
***trans*-Eq (-88,-63)**	**-912.334012 H**	***trans*-Eq (69,-61)**	**-912.325380 H**
cis-Ax (,ester torsion) minima:			
cis-Ax (-85,36)	-912.328781 H	*cis*-Ax (-165,44)	-912.329347 H
***cis*-Ax (-82,180)**	**-912.332646 H**	***cis*-Ax (-168,-178)**	**-912.332005 H**
cis-Ax (-82,-61)	-912.330437 H	*cis*-Ax (-164,-63)	-912.331252 H
cis-Ax (19,15)	-912.319285 H		
***cis*-Ax (27,-175)**	**-912.322022 H**		
cis-Ax (13,-55)	-912.321775 H		
trans-Ax (,ester torsion) minima:			
trans-Ax (-151,57)	-912.330188 H	*trans*-Ax (-82,56)	-912.332400 H
trans-Ax (-154,-157)	-912.332101 H	*trans*-Ax (-82,-161)	-912.333864 H
***trans*-Ax (-154,-79)**	**-912.333253 H**	***trans*-Ax (-85,-73)**	**-912.335182 H**
trans-Ax (12,52)	-912.320515 H	*trans*-Ax (89,60)	*Unstable, ring flip to Eq*
trans-Ax (9,-164)	-912.321859 H	*trans*-Ax (89,180)	*Unstable, ring flip to Eq*
***trans*-Ax (7,-71)**	**-912.322661 H**	***trans*-Ax (89,-63)**	**-912.319115 H**

Table S4. Energies with Zero-Point Correction for Conformations of the Hexamer.

Conformer	Characteristics	Energy (H)	E(kcal/mol)	ZPE (H)	**E(kcal/mol)**
1	*cis*-Eq(–150)	-2203.332618	0.00	-2202.455194	**0.00**
2	*trans*-Ax(–85)	-2203.331765	0.54	-2202.452887	**1.45**
3	*trans*-Ax(–155)	-2203.327571	3.17	-2202.448299	**4.33**
4	*cis*-Ax(–85)	-2203.326653	3.74	-2202.447646	**4.74**
5	*trans*-Eq(–94)	-2203.325840	4.25	-2202.448667	**4.10**
6	*cis*-Ax(–173)	-2203.322869	6.12	-2202.444525	**6.69**
7	*trans*-Eq(60)	-2203.286521	28.93	-2202.406736	**30.41**
8	*cis*-Eq(75)	-2203.282588	31.39	-2202.403959	**32.15**