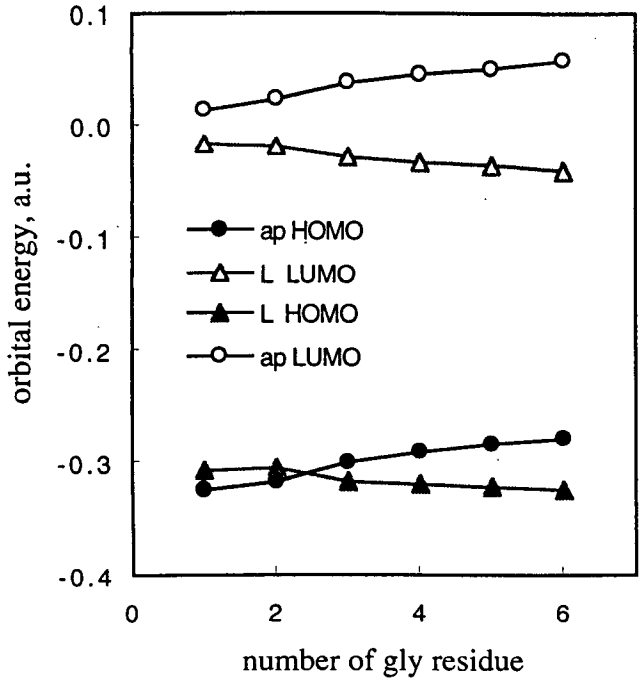
Supplementary Material 1. Total dipole moment vs. the number of glycine units between cbpy and ap.

#gly	α-helix	3_{10}-helix	β-strand	polypro II	polypro I	$(CH_2)_{3n}$
1	5.34	5.85	0.77	2.25	-1.52	-3.09
2	9.63	10.15	0.39	4.09	-4.98	-4.15
3	14.94	14.82	1.64	5.32	-9.40	-3.37
4	20.24	19.26	1.35	7.17	-13.48	-2.27
5	25.29	23.51	1.52	8.60	-17.66	-3.21
6	30.98	28.93		10.24	-21.82	-3.85
7				11.47		
Δμ/#gly	**5.16**	**4.57**	**0.25**	**1.54**	**-4.10**	**0.00**

Supplementary Material 2. Orbital energies (in atomic unit) of ap and L in cbpy-$(gly)_n$-ap where $(gly)_n$ is in the α-helical conformation.

	ap		cbpy	
#gly	HOMO	LUMO	HOMO	LUMO
1	-0.325	0.0153	-0.306	-0.0164
2	-0.316	0.0233	-0.305	-0.0192
3	-0.299	0.0378	-0.316	-0.0290
4	-0.289	0.0456	-0.320	-0.0337
5	-0.284	0.0504	-0.321	-0.0361
6	-0.278	0.0564	-0.325	-0.0395



Supplementary Material 3. Distance dependence of the charge transfer transition energy in peptide secondary structures.

	ap-to-cbpy transition		cbpy-to-ap transition	
# of gly	$\Delta\mu_{DA}$ (D)	ΔE (kK)	$\Delta\mu_{DA}$ (D)	ΔE (kK)
		β-strand		
1	31.4	56.7	21.3	55.3
2	58.1	60.6	26.9	58.7
3	65.0	60.6	73.9	61.3
4	86.3	62.3	89.1	62.3
5	98.7	63.1	98.7	63.2
		polyporoline II		
1	21.1	48.7	29.1	56.7
2	35.2	51.9	32.8	60.2
3	58.3	54.3	60.0	60.1
4	64.1	55.7	76.0	64.7
5	73.8	56.5	87.8	65.9
6	99.8	57.4	104.2	68.8
7	112.4	57.9		
		α-helix		
1	2.8	48.5	2.7	55.6
2	13.7	44.9	3.6	48.8
3	26.2	41.1	11.5	62.7
4	33.9	42.1	14.9	66.8
5	39.8	42.4		
6	46.6	45.1		
		3_{10}-helix		
1	12.1	49.9	12.8	58.1
2	25.5	49.3	27.6	66.4
3	40.2	43.3		
4	48.3	43.0		
5	60.1	43.6		
6	72.8	43.6		
		polyproline I		
1	8.6	48.2	6.8	49.4
2	20.6	60.3	31.0	54.1
3	24.3	62.1	36.8	49.0
4	38.4	66.7	47.1	49.8
5	54.1	68.0	57.2	49.3

Supplementary Material 4. Distance dependence of the charge transfer transition energy in hydrocarbon bridged structures.

	ap-to-cbpy transition		cbpy-to-ap transition	
# of gly	$\Delta\mu_{DA}$ (D)	ΔE (kK)	$\Delta\mu_{DA}$ (D)	ΔE (kK)
bpy-$(CH_2)_{3n}$-ap in the α-helix conformation				
1	19.7	54.5	20.1	49.2
2	19.3	50.3	17.2	44.1
3	19.0	55.3	31.1	48.8
4	39.0	59.0	45.7	52.6
5	50.7	60.0	49.2	53.6
bpy-$(CH_2)_{3n}$-ap in the polyproline II conformation				
1	35.3	59.8	37.7	59.4
2	43.5	58.4	38.7	51.7
3	62.8	61.2	59.2	54.7
4	75.6	62.4	72.9	56.3
5	85.2	63.3	82.5	57.4
6	103.3	64.3	99.2	58.4

Supplementary Material 5. Angle between the ground state peptide dipole and the change in dipole moment upon electronic transition in bpy-$(gly)_n$-ap molecules.

	ap-to-bpy transition			bpy-to-ap transition		
# of gly	$\Delta\mu$ (D)	ΔE (cm^{-1})	$\mu_g \cdot \Delta\mu$	$\Delta\mu$ (D)	ΔE (cm^{-1})	$\mu_g \cdot \Delta\mu$
			α-helix			
1	15.9	48.5	-0.178	22.3	55.6	0.120
2	19.2	44.9	-0.714	9.0	48.8	0.399
3	27.6	41.1	-0.950	14.1	62.7	0.818
4	38.6	42.1	-0.879	24.3	66.8	0.614
5	46.5	42.4	-0.855			
6	48.7	45.1	-0.957			
			3_{10}-helix			
1	22.1	49.9	-0.665	25.4	58.1	0.479
2	35.5	49.3	-0.859	33.3	66.4	0.830
3	43.0	43.3	-0.934			
4	51.2	43.0	-0.943			
5	62.3	43.6	-0.964			
6	74.7	43.6	-0.974			
			polyproline I			
1	13.0	48.2	0.658	12.2	49.4	-0.556
2	21.8	60.3	0.946	33.6	54.1	-0.922
3	26.1	62.1	0.929	40.2	49.0	-0.916
4	40.6	66.7	0.945	50.2	49.8	-0.939
5	54.5	68.0	0.992	58.4	49.3	-0.980

Supplementary Material 6: Structural Information used in Calculating Electrostatic Potentials given in Table 3.

For α-helix

n	d(bpy-ap)	d(bpy-CO)	angle(bpy...CO)	d(ap-CO)	angle(ap...CO)
0	3.8	2.2	110	2.9	97
1	5.4	5.2	126	4.2	77
2	5.0	6.5	147	3.6	46
3	6.1	6.8	166	3.4	8
4	8.5	8.3	154	5.9	39
5	9.9	10.5	159	7.7	38
6	10.5	11.7	172	8.2	14
7	12.1	12.7	167	9.5	17
8	14.0	14.4	162	11.7	32
9	15.3	16.2	172	13.0	26
10	16.1	17.4	176	14.1	12

For polyproline II helix

n	d(bpy-ap)	d(bpy-CO)	angle(bpy...CO)	d(ap-CO)	angle(ap...CO)
0	3.9	2.2	108	2.9	102
1	6.1	4.5	91	3.9	47
2	8.3	7.7	120	6.7	69
3	11.5	10.1	115	9.7	75
4	14.2	12.8	103	12.2	61
5	16.7	15.8	116	15.0	68
6	19.7	18.4	114	17.9	71
7	22.5	21.2	106	20.6	65
8	25.0	24.1	115	23.3	65
9	27.8	26.8	113	26.2	72
10	30.8	29.5	106	29.0	67