



Supporting Information

for

Angew. Chem. Int. Ed. Z53249

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69451 Weinheim, Germany

Mixed Helices - A General Folding Pattern in Homologous Peptides?

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Table S1: Backbone torsion angles^[a] of the mixed helix $\mathbf{H}_{14/16}$ and the 3_{10} -helix (\mathbf{H}_{10}) in hexamers of α -peptides at the HF/6-31G* and DFT/B3LYP/6-31G* level of ab initio MO theory

Type ^[b]	HF/6-31G*		B3LYP/6-31G*	
	φ	ψ	φ	ψ
$\mathbf{H}_{14/16}$	85.5	-75.2	81.4	-72.1
	-73.6	131.1	-73.6	129.9
	81.1	-66.6	78.6	-67.6
	-80.8	84.5	-76.7	80.2
	121.7	-73.2	123.7	-78.1
	-81.4	82.2	-76.6	78.4
\mathbf{H}_{10} ^[c]	-67.1	-25.5	-65.6	-25.2
	-62.9	-19.5	-59.6	-19.9
	-63.0	-20.1	-60.6	-20.0
	-64.4	-18.3	-61.6	-18.7
	-68.6	-12.9	-67.2	-10.7
	-94.5	-4.8	-100.2	11.3

[a] Angles in degrees. [b] $\mathbf{H}_{x/y}$ denotes mixed helices with alternating rings with x and y atoms, respectively, closed by hydrogen bonds. \mathbf{H}_x denotes periodic helices with rings of x atoms. [c] 3_{10} -helix.

Table S2: Backbone torsion angles^[a] of mixed and periodic helices in hexamers of β -peptides at the HF/6-31G* and DFT/B3LYP/6-31G* level of ab initio MO theory

Type ^[b]	HF/6-31G*			B3LYP/6-31G*		
	φ	θ	ψ	φ	θ	ψ
H_{12/10}^I	-97.7	56.6	96.8	-97.6	54.7	96.1
	85.7	65.5	-111.1	87.0	64.7	-109.4
	-101.8	61.4	88.9	-103.0	58.7	88.0
	89.6	66.1	-111.0	92.4	64.8	-107.8
	-101.1	63.0	93.7	-104.2	61.8	93.5
	85.0	61.1	-132.8	85.2	61.8	-124.3
H_{10/12}^{II}	79.7	58.6	-103.1	80.8	58.9	-97.6
	-16.2	-54.6	165.2	-21.3	-52.4	160.4
	87.4	60.8	-96.2	90.8	59.1	-94.1
	-27.2	-49.6	160.0	-30.0	-47.8	155.0
	82.1	67.6	-93.8	84.7	66.6	-94.2
	-73.3	-60.7	-86.7	-73.6	-59.8	-85.8
H_{10/12}^{III}	-85.8	-58.5	-67.2	-94.0	-56.6	-57.7
	-93.0	56.1	80.6	-94.8	54.2	77.4
	178.9	-61.8	-20.8	-178.5	-60.6	-22.1
	-92.7	50.6	87.0	-93.3	49.1	84.5
	177.2	-60.7	-23.4	179.3	-59.2	-26.0
	-90.7	52.0	90.8	-90.5	51.4	87.5
H_{20/18}^I	75.7	57.4	-162.3	75.8	53.1	-158.5
	-81.6	-79.3	137.8	-81.8	-81.8	136.1
	90.7	66.4	171.1	97.6	65.2	166.1
	-78.5	-56.8	148.6	-78.5	-49.3	145.9
	71.0	74.6	173.9	69.1	79.4	164.5
	-86.4	-60.4	165.1	-83.9	-56.4	162.2
H_{20/18}^{II}	76.7	61.3	-168.2	76.1	59.1	-170.5
	-173.4	67.5	4.9	-170.9	67.7	-3.5
	98.8	66.8	172.7	110.5	66.7	163.9
	-150.2	56.6	47.3	-138.1	55.5	49.3
	69.6	69.6	-157.2	68.5	73.6	-155.9
	178.3	57.4	91.1	-179.9	53.8	105.2
H_{20/18}^{III}	80.5	-176.7	143.2	81.5	-172.6	114.3
	62.2	43.6	-106.6	57.7	43.6	-103.1
	152.5	162.4	69.1	141.3	166.1	70.7
	72.9	51.7	-143.9	73.6	51.0	-145.4
	168.9	159.4	76.7	169.7	159.3	74.4
	77.0	54.1	-145.7	80.0	50.9	-144.8
H_{18/20}^{IV}	77.1	159.5	86.9	80.1	159.4	75.7
	101.7	-54.7	-85.3	105.1	-56.6	84.0
	79.3	-170.7	99.7	77.0	-168.1	102.0
	109.6	-47.5	-43.0	105.7	-49.8	-35.0
	84.0	170.8	73.3	83.9	169.3	75.9
	111.6	-56.7	-32.3	107.3	-57.6	-28.8

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Table S2 continued:

Type ^[b]	HF/6-31G*			B3LYP/6-31G*		
	φ	θ	ψ	φ	θ	ψ
H₁₄	-146.6	62.6	-119.4	-136.3	62.7	-119.5
	-156.2	62.3	-127.1	-152.1	63.4	-129.8
	-148.3	60.7	-137.5	-144.9	61.6	-137.4
	-135.3	60.1	-143.2	-133.7	61.3	-143.6
	-130.9	58.3	-138.5	-129.9	58.5	-138.2
	-135.3	64.5	-160.3	-132.9	63.7	-154.3
H₁₂	-97.2	80.2	-106.8	-92.5	81.7	-111.7
	-80.4	93.6	-118.2	-90.0	95.6	-117.5
	-86.9	92.1	-108.5	-90.7	93.9	-99.8
	-87.2	91.0	-107.9	-91.8	89.0	-99.1
	-87.3	92.0	-108.9	-90.0	91.2	-102.3
	-83.8	88.6	-107.9	-84.4	86.5	-103.7

[a] Angles in degrees. [b] **H_{x/y}** denotes mixed helices with alternating rings with x and y atoms, respectively, closed by hydrogen bonds. **H_x** denotes periodic helices with rings of x atoms.

Table S3: Backbone torsion angles^[a] of mixed and periodic helices in hexamers of γ -peptides at the HF/6-31G* and DFT/B3LYP/6-31G* level of ab initio MO theory

Type ^[b]	HF/6-31G*				B3LYP/6-31G*			
	φ	θ	ζ	ψ	φ	θ	ζ	ψ
H_{14/12}^I	-92.8	78.2	-74.4	162.4	-96.9	78.0	-70.7	154.9
	95.8	81.0	-74.5	-29.9	105.1	76.7	-78.4	-24.5
	-91.1	79.4	-79.5	161.5	-94.1	80.3	-76.1	154.0
	94.4	84.4	-72.8	-29.2	101.1	82.4	-75.0	-26.9
	-96.2	81.4	-79.7	164.7	-101.2	82.9	-76.4	158.2
	85.3	76.9	-53.7	-87.5	89.2	73.6	-55.5	-92.1
H_{14/12}^{II}	77.1	58.4	-84.3	-79.2	78.4	61.1	-77.0	-90.9
	-71.2	-36.2	-56.4	142.6	-66.6	-31.1	-56.8	144.5
	65.4	56.2	-125.6	-53.1	59.7	54.8	-130.5	-48.0
	-63.8	-37.0	-60.5	142.5	-60.8	-37.7	-59.6	139.4
	68.4	55.6	-121.9	-58.5	67.3	54.9	-122.8	-55.2
	-65.6	-34.8	-52.5	157.0	-63.8	-37.1	-51.0	152.6
H_{24/22}^I	108.9	-172.5	-169.1	-153.4	104.9	-173.8	-168.2	-154.5
	-101.7	63.5	-94.4	122.2	-98.6	65.1	-93.4	117.7
	74.2	-176.5	-79.7	-167.7	75.2	-174.8	-76.6	-169.8
	-125.1	61.8	-77.2	154.3	-123.6	61.3	-74.7	154.4
	115.5	-176.9	-177.3	-138.0	114.9	-171.7	-177.3	-137.3
	-160.0	66.9	-74.9	152.9	-158.7	66.5	-72.9	155.3
H_{24/22}^{II}	79.3	66.6	-66.3	-80.3	83.4	61.5	-65.6	-79.8
	84.3	69.4	74.8	9.7	85.2	66.3	75.5	7.3
	93.6	79.3	-65.5	-102.1	102.1	74.7	-66.1	-105.4
	122.9	64.4	66.2	16.2	129.3	65.3	66.5	16.0
	74.5	74.4	-73.8	-76.6	71.7	73.9	-72.3	-84.3
	75.2	83.9	65.9	70.5	73.2	84.2	64.5	80.6
H_{24/22}^{III}	128.9	-64.9	-178.8	104.8	120.4	-65.9	179.4	97.8
	-75.1	-63.0	80.5	29.3	-68.0	-62.6	83.0	17.6
	116.7	-68.4	-173.7	127.5	128.9	-69.7	-174.9	128.9
	-89.1	-71.9	82.8	57.7	-93.9	-68.2	85.8	52.3
	103.6	-65.7	-173.2	124.3	104.8	-64.1	-171.8	127.2
	-80.4	-74.0	58.5	87.2	-81.6	-72.4	58.3	97.4
H₁₄	106.1	-62.6	-67.5	165.6	106.1	-62.6	-67.5	165.6
	136.5	-63.2	-68.2	138.3	136.5	-63.2	-68.2	138.3
	138.0	-60.1	-65.1	141.4	138.0	-60.1	-65.1	141.4
	132.9	-61.0	-66.0	144.4	132.9	-61.0	-66.0	144.4
	135.3	-63.4	-66.7	143.0	135.3	-63.4	-66.7	143.0
	138.3	-61.0	-64.1	139.7	138.3	-61.0	-64.1	139.7

[a] Angles in degrees. [b] **H_{x/y}** denotes mixed helices with alternating rings with x and y atoms, respectively, closed by hydrogen bonds. **H_x** denotes periodic helices with rings of x atoms.

Table S4: Backbone torsion angles^[a] of mixed and periodic helices in hexamers of δ -peptides at the HF/6-31G* and DFT/B3LYP/6-31G* level of ab initio MO theory

Type	HF/6-31G*					B3LYP/6-31G*				
	φ	θ	ζ	ρ	ψ	φ	θ	ζ	ρ	ψ
H_{14/16}	-80.2	152.4	-74.0	-69.8	118.0	-80.8	154.6	-70.2	-69.0	112.9
	80.8	73.5	-165.9	70.6	-107.9	81.6	74.9	-162.7	70.6	-107.6
	-171.7	159.1	-77.3	-68.1	130.5	-172.2	158.8	-76.5	-69.3	132.4
	75.9	68.6	-167.5	82.1	-125.8	76.9	67.3	-166.8	81.6	-126.7
	-145.8	89.0	-70.9	-69.6	162.7	-141.8	87.6	-68.8	-70.0	167.9
	70.7	63.1	-165.3	71.9	-121.2	67.5	61.6	-160.1	71.0	-111.3
H_{16/14}	111.7	-46.4	-59.6	152.0	151.4	108.9	-45.3	-58.5	151.3	147.0
	-120.5	83.9	-66.9	-65.0	161.8	-117.3	85.1	-65.2	-65.0	163.0
	113.4	-53.8	-62.3	167.4	158.7	111.8	-53.6	-59.8	169.9	153.5
	-125.9	82.3	-65.9	-67.4	164.4	-122.1	82.9	-64.3	-67.7	164.1
	113.3	-52.6	-63.3	164.6	157.8	112.7	-52.4	-59.9	167.4	150.8
	-12.1	-153.3	101.1	-5.7	-80.9	-6.0	-153.9	101.2	-5.5	-81.2
H₁₀	97.3	-62.8	-68.2	169.2	-86.1	96.9	-61.2	-67.0	166.9	-84.8
	97.9	-62.6	-68.3	168.6	-84.7	97.9	-61.3	-67.0	166.5	-84.1
	98.1	-62.4	-68.4	168.5	-84.5	98.0	-60.9	-67.4	166.2	-83.6
	98.2	-62.4	-68.4	168.4	-84.4	98.3	-61.0	-67.3	166.1	-83.9
	98.3	-62.4	-68.4	168.7	-84.5	98.2	-61.1	-67.7	166.3	-83.0
	99.0	-62.6	-68.8	168.7	-87.1	98.8	-61.2	-67.8	167.1	-85.5
H₈	-178.8	66.5	-143.5	69.1	-171.2	-178.4	64.5	-139.6	68.5	-171.5
	-179.0	66.4	-142.5	69.2	-172.7	-179.1	64.2	-138.6	68.4	-172.5
	-179.5	66.4	-142.2	69.1	-172.5	-179.3	64.2	-138.1	68.3	-172.1
	-179.3	66.4	-142.2	69.2	-172.9	-178.7	64.2	-138.0	69.0	-173.1
	-179.4	66.4	-142.5	69.3	-173.1	-179.2	64.6	-138.8	68.4	-172.9
	-178.7	66.6	-143.9	69.7	-173.8	-178.4	64.7	-140.0	69.0	-173.9

[a] Angles in degrees. [b] **H_{x/y}** denotes mixed helices with alternating rings with x and y atoms, respectively, closed by hydrogen bonds. **H_x** denotes periodic helices with rings of x atoms.

Table S5: Total energies^[a] of periodic helices used as references for the calculations of stabilisation energies at the HF/6-31G*, DFT/B3LYP/6-31G* and PCM//HF/6-31G* level of ab initio MO theory

Type	E _T		
	HF/6-31G*	B3LYP/6-31G*	PCM//HF/6-31G*
		<i>α-Peptides</i>	
H₁₀	-1487.918103	-1496.607967	-1487.945670
		<i>β-Peptides</i>	
H₁₄	-1722.127594	-1732.493651	-1722.147167
H₁₂	-1722.132691	-1732.503571	-1722.138542
		<i>γ-Peptides</i>	
H₁₄	-1956.361656	-1968.407950	-1956.340687
		<i>δ-Peptides</i>	
H₁₀	-2190.562661	-2204.282712	-2190.528328
H₈	-2190.555385	-2204.271987	-2190.543623

[a] In a.u.