Supporting Information

δ-Peptides and δ-Amino Acids as Tools for

Peptide Structure Design – A Theoretical Study

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Table S1. HF/6-31G* backbone torsion angles for the δ-peptide helices with 10-membered pseudocycles of **1** (n=6)^a

Conf.^{b}	φ	θ	ζ	ρ	ψ	Conf.^{b}	φ	θ	ζ	ρ	ψ
H_{10}^{I}	-97.3	62.8	68.2	-169.2	86.1	H_{10}^{VI}	-100.2	67.2	98.3	-67.1	-35.5
	-97.9	62.6	68.3	-168.6	84.7		-100.0	67.1	98.6	-67.9	-33.5
	-98.1	62.4	68.4	-168.5	84.5		-99.8	67.0	98.6	-67.9	-33.4
	-98.2	62.4	68.4	-168.4	84.4		-99.8	66.9	98.7	-67.8	-33.6
	-98.3	62.4	68.4	-168.7	84.5		-99.7	66.8	99.0	-67.1	-34.4
	-99.0	62.6	68.8	-168.7	87.1		-100.2	66.9	98.7	-62.4	-42.3
H_{10}^{II}	-81.7	160.6	-71.4	-69.2	100.4	H_{10}^{VII}	-50.2	-49.0	176.9	-71.7	-3.9
	-83.1	160.8	-71.2	-69.2	98.7		-50.7	-47.6	175.0	-72.6	-1.9
	-83.3	160.8	-71.1	-69.1	98.4		-50.9	-47.4	174.6	-72.5	-2.0
	-83.3	160.8	-71.1	-69.2	98.3		-51.1	-47.3	174.5	-72.7	-1.6
	-83.5	160.8	-71.3	-69.3	98.7		-51.3	-47.3	174.7	-72.7	-1.7
	-84.1	161.8	-71.7	-68.8	101.4		-52.6	-47.1	175.4	-71.4	-6.4
H_{10}^{III}	-121.2	54.0	47.0	56.9	-128.3	H_{10}^{VIII}	-65.4	119.7	-169.1	70.0	15.5
	-121.5	55.1	45.5	57.3	-126.8		-65.9	120.5	-168.2	70.7	13.6
	-121.3	55.0	45.2	57.1	-126.6		-65.9	120.0	-168.0	70.8	13.5
	-121.2	55.0	45.3	57.2	-126.5		-66.0	119.9	-168.0	70.7	13.6
	-121.1	55.4	45.5	57.4	-126.9		-66.1	119.7	-168.2	70.5	14.0
	-121.5	54.5	45.0	52.8	-128.4		-66.7	119.4	-168.7	69.2	16.5
H_{10}^{IV}	-95.7	73.3	-87.6	167.4	-76.9	H_{10}^{IX}	-66.1	-53.4	89.0	71.1	-94.6
	-95.0	74.0	-87.9	166.6	-76.9		-63.3	-54.1	90.0	70.8	-94.4
	-94.7	73.9	-88.0	166.5	-77.1		-63.1	-54.2	89.9	70.7	-94.4
	-94.8	73.7	-88.0	166.6	-76.9		-63.2	-54.2	89.8	70.8	-94.3
	-94.9	73.7	-88.0	166.8	-77.1		-63.3	-54.3	89.7	71.0	-94.0
	-95.6	73.2	-87.7	167.1	-83.4		-65.2	-52.7	92.2	67.2	-105.9
H_{10}^{V}	-81.0	155.8	-76.0	89.8	-113.1						
	-78.7	157.3	-78.5	88.4	-109.2						
	-78.4	157.6	-78.9	88.1	-108.5						
	-78.3	157.5	-78.8	88.2	-108.6						
	-78.3	157.7	-78.4	88.0	-109.6						
	-77.5	162.0	-79.3	82.1	-110.0						

^{a} Angles in degrees. ^{b} H_x denotes a helix with hydrogen-bonded pseudocycles of x atoms. The superscript Roman number arranges helices of the same ring size according to their stability (cf. Table 2 of the paper).

Table S2. HF/6-31G* backbone torsion angles for the δ-peptide helices with 16- and 22-membered pseudocycles of **1** (n=6)^a

Conf.^{b}	φ	θ	ζ	ρ	ψ	Conf.^{b}	φ	θ	ζ	ρ	ψ
H$_{16}^{I}$	-77.8	179.8	-170.6	67.3	-113.1	H$_{22}^{I}$	-94.1	-175.4	177.0	70.7	-135.9
	-75.3	-179.3	-170.6	70.1	-109.9		-91.3	-173.4	179.6	71.3	-136.3
	-76.7	-178.8	-173.4	68.3	-108.0		-88.2	-173.7	178.1	72.8	-134.8
	-75.6	-179.0	-173.6	68.5	-108.9		-88.5	-173.2	176.5	71.4	-128.4
	-77.5	-177.0	-174.4	70.7	-107.1		-96.2	-172.5	175.6	72.2	-120.1
	-78.7	-175.3	178.5	72.6	-105.8		-91.5	-179.8	173.2	64.2	-109.8
H$_{16}^{II}$	-97.2	67.2	178.5	-177.3	-88.2	H$_{22}^{II}$	-108.3	68.3	179.9	-172.9	-127.6
	-95.1	67.1	-175.6	-175.9	-89.5		-106.6	69.4	179.6	-171.8	-116.2
	-96.9	66.3	-175.0	-176.8	-88.7		-106.4	71.3	-177.8	-169.6	-124.7
	-96.0	66.0	-174.9	-176.3	-89.2		-112.5	72.6	-173.9	-169.1	-110.3
	-98.9	68.0	-173.1	-175.0	-85.6		-122.7	71.0	-175.6	-170.5	-114.2
	-106.7	67.6	-172.2	-174.6	-87.3		-116.8	68.5	-178.7	-174.5	-108.9
H$_{16}^{III}$	-77.6	-61.2	-175.4	-60.6	-63.9	H$_{22}^{III}$	175.2	-173.6	-65.6	79.9	-147.1
	-77.4	-59.6	-173.0	-57.2	-66.4		157.0	-174.2	-66.2	77.6	-144.3
	-77.0	-59.6	-173.4	-57.8	-65.7		176.2	-178.0	-69.4	79.1	-140.1
	-77.0	-59.1	-173.0	-57.7	-65.7		149.3	179.4	-62.1	84.1	-145.7
	-78.8	-58.5	-171.8	-57.3	-62.3		158.0	-178.5	-60.9	84.2	-139.1
	-79.5	-62.2	-174.9	-58.4	-68.6		154.6	178.3	-66.0	82.3	-136.4
H$_{16}^{IV}$	-154.2	68.4	96.0	-63.7	-91.0						
	-151.6	66.9	106.1	-59.8	-69.8						
	-169.5	73.3	94.6	-61.6	-71.9						
	-165.0	67.3	98.6	-57.3	-77.8						
	-162.0	69.3	93.4	-57.1	-87.3						
	-155.0	68.3	86.4	-61.3	-78.8						

^{a} Angles in degrees. ^{b} H$_x$ denotes a helix with hydrogen-bonded pseudocycles of x atoms. The superscript Roman number arranges helices of the same ring size according to their stability (cf. Table 2 of the paper).

Table S3. HF/6-31G* backbone torsion angles for the δ-peptide helices with 8-, 14- and 20-membered pseudocycles of **1** (n=6)[a]

Conf.[b]	φ	θ	ζ	ρ	ψ	Conf.[b]	φ	θ	ζ	ρ	ψ
H8^I	-178.8	66.5	-143.5	69.1	-171.2	H14^V	-93.9	-173.3	52.7	41.0	50.0
	-179.0	66.4	-142.5	69.2	-172.7		164.9	-164.6	61.0	42.3	60.0
	-179.5	66.4	-142.2	69.1	-172.5		166.0	-160.0	61.3	40.6	60.5
	-179.3	66.4	-142.2	69.2	-172.9		166.1	-160.6	60.2	40.3	59.2
	-179.4	66.4	-142.5	69.3	-173.1		165.7	-163.2	62.9	43.7	70.1
	-178.7	66.6	-143.9	69.7	-173.8		124.5	-166.1	71.0	60.7	87.4
H8^II	98.8	64.9	-79.9	113.4	128.3	H14^VI	123.2	-45.6	98.6	-144.9	-165.3
	99.8	66.2	-79.3	111.1	128.6		112.1	-43.0	98.5	-149.6	-161.5
	101.4	65.8	-79.7	111.6	126.6		111.4	-42.8	98.0	-147.2	-162.2
	101.6	65.8	-79.8	111.6	126.8		111.0	-43.2	98.8	-148.0	-160.7
	101.4	66.1	-79.6	111.4	126.6		109.9	-43.9	100.3	-150.2	-152.3
	93.7	74.3	-71.0	104.2	100.1		104.7	-53.0	98.6	-164.6	-94.6
H14^I	117.5	-73.5	169.9	-79.9	110.8	H20^I	158.6	-65.2	-176.6	178.0	129.4
	102.6	-71.9	172.1	-75.4	110.8		130.4	-60.5	-177.5	-176.0	109.2
	105.9	-73.1	170.5	-77.1	111.5		145.4	-59.5	-176.8	-174.5	132.7
	106.8	-73.0	170.0	-77.6	111.6		115.7	-55.4	-172.8	-171.0	133.7
	106.0	-71.1	171.1	-75.0	108.8		112.5	-56.8	-175.7	-174.3	140.2
	100.3	-74.1	175.8	-76.1	128.9		111.7	-68.1	178.0	179.4	-151.4
H14^II	172.1	69.1	175.3	68.1	100.1	H20^II	79.7	61.2	174.1	172.7	51.1
	88.4	75.4	-157.9	82.5	98.8		75.7	55.6	171.2	168.7	70.2
	90.4	74.9	-161.4	82.0	99.4		72.4	57.5	177.2	173.3	57.9
	89.1	74.6	-161.5	83.5	101.0		70.6	54.0	176.8	171.1	68.7
	85.8	76.3	-158.9	85.9	98.7		72.2	57.3	177.7	171.5	56.5
	86.4	63.0	-177.1	74.2	-179.8		69.5	53.8	174.7	169.2	122.9
H14^III	86.5	58.2	175.1	164.8	70.6	H20^III	80.1	-176.4	-75.3	-76.8	116.3
	71.1	55.5	-174.3	165.5	83.2		76.2	173.9	-68.0	-59.8	114.9
	75.0	51.5	-108.9	160.9	31.5		77.4	-173.4	-66.4	-68.0	134.2
	79.5	52.1	-100.5	160.4	29.2		75.2	174.7	-79.2	-72.3	110.6
	78.3	51.6	-97.6	159.7	33.4		73.6	174.7	-66.4	-56.9	148.7
	74.8	47.2	-101.8	162.4	55.2		102.6	-175.1	-173.9	-68.1	177.2
H14^IV	84.1	174.0	-63.2	-53.7	122.6						
	75.9	144.7	-66.1	-59.1	158.8						
	78.9	98.2	-52.6	-67.7	-169.9						
	76.1	88.2	-52.2	-67.1	-159.4						
	72.9	84.9	-52.0	-64.3	-150.1						
	79.6	72.4	-73.4	-60.4	-86.2						

[a] Angles in degrees. [b] H_x denotes a helix with hydrogen-bonded pseudocycles of x atoms. The superscript Roman number arranges helices of the same ring size according to their stability (cf. Table 2 of the paper).

Table S4. DFT/B3LYP/6-31G* backbone torsion angles for the δ-peptide helices with 10-membered pseudocycles of **1** (n=6)[a]

Conf.[b]	φ	θ	ζ	ρ	ψ	Conf.[b]	φ	θ	ζ	ρ	ψ
H_{10}^{I}	-96.9	61.2	67.0	-166.9	84.8	H_{10}^{VI}	-97.4	69.5	94.6	-68.8	-32.4
	-97.9	61.3	67.0	-166.5	84.1		-98.3	68.9	95.2	-69.6	-30.5
	-98.0	60.9	67.4	-166.2	83.6		-97.7	68.8	95.4	-70.1	-29.9
	-98.3	61.0	67.3	-166.1	83.9		-97.5	69.6	94.6	-69.9	-30.3
	-98.2	61.1	67.7	-166.3	83.0		-97.7	69.0	95.2	-67.9	-33.3
	-98.8	61.2	67.8	-167.1	85.5		-98.6	67.8	96.8	-65.0	-34.9
H_{10}^{II}	-83.2	160.9	-68.6	-67.5	95.3	H_{10}^{VII}	-47.4	-50.0	174.9	-71.1	-3.4
	-84.1	161.2	-68.7	-67.3	94.7		-49.4	-48.6	172.3	-73.6	2.0
	-83.7	161.7	-68.1	-67.7	92.7		-49.0	-47.8	172.6	-71.0	-3.1
	-84.6	161.1	-68.4	-67.0	95.3		-49.5	-47.7	172.2	-71.7	-1.7
	-82.6	162.4	-68.4	-68.1	91.8		-50.0	-47.5	172.2	-72.0	-1.0
	-85.3	161.9	-69.0	-67.2	96.6		-51.6	-47.3	172.4	-71.5	-3.2
H_{10}^{III}	-117.6	51.2	42.9	54.3	-120.0	H_{10}^{VIII}	-64.4	118.1	-167.1	70.2	12.6
	-117.8	52.9	40.7	55.4	-119.6		-65.0	117.6	-166.0	70.1	12.2
	-117.3	52.1	41.2	55.4	-118.6		-64.5	115.5	-166.0	70.2	13.0
	-117.0	51.9	41.1	55.6	-118.1		-64.5	115.9	-166.1	69.2	14.7
	-116.8	52.3	41.4	55.4	-118.9		-64.4	117.0	-166.6	70.2	12.0
	-117.1	52.8	43.3	51.7	-122.6		-65.4	114.1	-166.6	68.3	16.4
H_{10}^{IV}	-93.8	72.3	-86.6	165.1	-77.4	H_{10}^{IX}	-63.6	-54.0	87.0	70.4	-94.0
	-93.3	72.4	-87.3	164.4	-77.1		-61.2	-55.7	87.2	70.9	-91.7
	-92.7	72.2	-87.7	164.5	-75.8		-60.5	-55.8	87.8	70.2	-94.1
	-93.0	72.2	-87.2	164.3	-78.0		-61.9	-55.5	87.1	70.4	-93.4
	-93.1	71.7	-87.6	164.7	-76.2		-61.9	-55.8	87.3	70.4	-92.7
	-93.4	71.5	-87.1	165.5	-80.2		-63.6	-53.2	90.1	67.8	-102.3
H_{10}^{V}	-83.5	149.6	-71.7	93.7	-112.3						
	-79.8	153.0	-76.4	90.3	-106.8						
	-78.7	155.3	-78.4	87.8	-104.2						
	-78.9	155.6	-79.3	88.6	-102.0						
	-77.9	152.6	-75.9	90.2	-106.6						
	-77.5	158.0	-77.8	84.7	-105.4						

[a] Angles in degrees. [b] H_x denotes a helix with hydrogen-bonded pseudocycles of x atoms. The superscript Roman number arranges helices of the same ring size according to their stability (cf. Table 2 of the paper).

Table S5. DFT/B3LYP/6-31G* backbone torsion angles for the δ-peptide helices with 16- and 22-membered pseudocycles of **1** (n=6)$^{\alpha}$

Conf.^{b}	φ	θ	ζ	ρ	ψ	Conf.^{b}	φ	θ	ζ	ρ	ψ
H_{16}^{I}	-77.1	176.6	-170.1	67.1	-112.6	H_{22}^{I}	-103.8	-174.9	179.0	71.5	-130.0
	-74.7	179.2	-169.3	70.7	-111.2		-94.0	-173.9	-178.9	71.0	-136.2
	-77.8	179.5	-172.5	68.6	-107.8		-89.1	-174.8	179.5	73.3	-133.9
	-75.4	179.6	-173.4	68.2	-109.6		-88.9	-174.3	177.9	71.4	-127.1
	-78.9	-177.6	-172.5	71.5	-108.6		-101.6	-171.2	179.2	73.8	-116.8
	-83.0	-174.1	-179.2	75.2	-105.8		-96.0	179.3	174.5	64.6	-109.4
H_{16}^{II}	-95.1	66.9	-179.6	-179.3	-91.4	H_{22}^{II}	-105.9	67.9	179.3	-172.3	-131.6
	-93.1	67.1	-175.4	-175.6	-92.6		-108.1	69.6	-178.4	-169.1	-121.0
	-95.7	67.0	-174.2	-177.3	-91.8		-103.7	72.1	-177.5	-167.5	-125.7
	-94.7	66.2	-173.7	-176.7	-92.8		-112.2	72.9	-171.6	-167.4	-120.4
	-98.0	69.0	-171.6	-174.5	-88.9		-114.9	70.3	-173.7	-169.1	-114.4
	-109.0	69.2	-170.6	-172.3	-89.4		-116.9	68.3	-177.6	-173.1	-112.4
H_{16}^{III}	-74.4	-61.1	-177.3	-61.5	-63.0	H_{22}^{III}	-171.4	-175.3	-68.3	78.1	-142.4
	-80.0	-59.7	-173.2	-56.2	-66.5		147.8	-173.2	-64.2	76.5	-145.4
	-75.2	-57.9	-174.9	-55.5	-68.5		-174.3	179.6	-73.1	77.2	-131.7
	-76.0	-57.4	-175.1	-55.0	-66.1		130.2	-178.6	-56.7	83.9	-140.5
	-79.8	-58.0	-175.0	-54.8	-62.9		153.0	-177.5	-58.7	84.0	-134.1
	-76.7	-61.6	-178.8	-56.0	-68.8		147.7	178.3	-64.3	81.3	-134.9
H_{16}^{IV}	-154.9	68.1	94.0	-63.8	-86.4						
	-151.5	69.1	96.8	-59.6	-71.3						
	-171.9	74.2	91.6	-62.1	-61.6						
	-170.6	68.3	92.6	-58.0	-74.1						
	-161.1	67.7	89.8	-56.3	-90.0						
	-149.7	68.6	84.2	-59.3	-79.1						

^{a} Angles in degrees. ^{b} H_x denotes a helix with hydrogen-bonded pseudocycles of x atoms. The superscript Roman number arranges helices of the same ring size according to their stability (cf. Table 2 of the paper).

Table S6. DFT/B3LYP/6-31G* backbone torsion angles for the δ-peptide helices with 8-, 14- and 20-membered pseudocycles of **1** (n=6)[a]

Conf.[b]	φ	θ	ζ	ρ	ψ	Conf.[b]	φ	θ	ζ	ρ	ψ
H$_8^{I}$	-178.4	64.5	-139.6	68.5	-171.5	H$_{14}^{V}$	-103.3	-171.6	52.2	38.7	50.9
	-179.1	64.2	-138.6	68.4	-172.5		166.9	-162.7	58.8	40.2	58.9
	-179.3	64.2	-138.1	68.3	-172.1		164.5	-154.9	61.3	41.1	56.6
	-178.7	64.2	-138.0	69.0	-173.1		166.1	-155.1	59.6	39.9	56.3
	-179.2	64.6	-138.8	68.4	-172.9		164.2	-158.2	63.1	43.4	69.1
	-178.4	64.7	-140.0	69.0	-173.9		121.4	-164.5	71.0	59.8	91.2
H$_8^{II}$	111.2	60.7	-80.7	114.7	123.4	H$_{14}^{VI}$	115.1	-42.3	94.9	-144.9	-163.5
	110.9	61.8	-81.0	112.6	123.7		109.8	-42.2	96.5	-148.9	-162.4
	111.0	62.2	-80.2	111.8	122.3		110.0	-42.1	96.6	-145.8	-163.2
	112.5	61.8	-81.5	112.1	123.4		109.1	-42.1	96.3	-146.8	-161.8
	112.1	60.9	-82.1	112.8	126.9		109.1	-44.1	99.8	-148.9	-153.4
	108.0	65.5	-77.7	109.7	113.3		102.4	-51.4	97.3	-164.0	-96.8
H$_{14}^{I}$	115.3	-73.4	167.7	-80.2	113.0	H$_{20}^{I}$	141.7	-62.3	-177.2	178.4	130.4
	101.5	-71.8	170.4	-75.6	109.2		126.5	-59.5	-179.5	-178.6	120.8
	106.3	-72.8	169.4	-76.9	111.2		135.1	-59.3	-178.3	-176.1	131.5
	105.3	-72.0	168.4	-77.0	109.7		118.1	-55.9	-175.1	-173.8	131.8
	105.3	-70.6	170.2	-74.6	107.4		117.1	-56.7	-176.1	-174.8	137.5
	98.7	-72.0	176.2	-74.8	126.4		110.9	-68.9	176.2	-178.9	-143.9
H$_{14}^{II}$	161.6	69.8	178.1	68.0	101.3	H$_{20}^{II}$	79.9	63.1	178.2	174.5	44.6
	89.1	73.7	-156.9	77.7	101.9		75.0	54.9	171.2	167.7	73.9
	91.8	72.7	-159.0	77.9	100.9		69.9	59.1	-179.5	174.8	51.2
	91.1	73.0	-159.1	79.9	101.3		68.5	54.6	-179.2	171.6	65.7
	88.3	74.8	-157.7	81.8	99.8		71.3	59.8	-176.2	174.0	42.2
	87.5	61.2	-174.6	71.6	-172.2		69.8	56.0	177.3	167.7	131.8
H$_{14}^{III}$	91.8	58.4	177.4	163.8	67.2	H$_{20}^{III}$	78.3	-177.4	-77.5	-78.8	124.6
	71.7	53.0	-177.6	165.9	89.5		75.5	169.7	-70.0	-62.8	113.5
	72.0	50.0	-106.8	160.0	25.4		78.6	-171.4	-65.2	-70.6	130.9
	81.5	52.6	-99.2	162.3	24.5		74.1	175.6	-78.2	-72.8	108.2
	77.7	50.3	-95.6	159.3	32.7		72.9	176.3	-65.1	-55.8	146.4
	74.3	46.6	-98.9	162.1	49.4		102.9	-174.8	-176.3	-66.8	174.5
H$_{14}^{IV}$	84.7	173.3	-63.9	-54.8	120.9						
	80.5	136.8	-64.6	-61.0	162.0						
	81.4	92.9	-51.7	-67.4	-166.2						
	74.1	86.1	-51.8	-66.3	-160.0						
	74.2	83.2	-52.9	-62.0	-152.9						
	80.4	71.2	-73.9	-58.6	-83.7						

[a] Angles in degrees. [b] H$_x$ denotes a helix with hydrogen-bonded pseudocycles of x atoms. The superscript Roman number arranges helices of the same ring size according to their stability (cf. Table 2 of the paper).

Table S7. DFT/B3LYP/6-31G* backbone torsion angles for conformers of **1** (n=1) forming 10-membered hydrogen bonded pseudocycles[a]

Conf.[b]	φ	θ	ζ	ρ	ψ
C_{10}^{I}	98.0	-60.9	-67.3	167.7	-88.4
C_{10}^{II}	84.8	-160.7	69.4	67.3	-101.1
C_{10}^{III}	117.5	-51.7	-45.1	-50.7	123.4
C_{10}^{V}	80.9	-156.0	73.6	-86.8	112.1
C_{10}^{IV}	95.0	-71.1	86.2	-166.3	79.6
C_{10}^{VI}	97.3	-68.6	-95.8	63.6	37.0
C_{10}^{IX}	65.6	52.7	-88.9	-68.2	102.8
C_{10}^{VII}	49.3	49.0	-175.9	69.6	7.4
C_{10}^{VIII}	65.8	-115.6	167.1	-67.2	-18.3

[a] Angles in degrees. [b] Nomenclature corresponds to the helix notations (cf. Tables 1 and 2 of the paper).