

## Supplemental file

### Theoretical Prediction of the Basic Helix-Types in $\alpha,\beta$ -Hybrid Peptides

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#### Contents

**TABLE SI.** DFT/B3LYP/6-31G\* Backbone Torsion Angles of all Helix Conformers in Octamers of  $\alpha,\beta$ -Hybrid Peptides

**TABLE SI DFT/B3LYP/6-31G\* Backbone Torsion Angles<sup>a</sup> of All Helix Conformers in Octamers of  $\alpha,\beta$ -Hybrid Peptides**

Conf.	$\phi$	$\theta$	$\psi$	Conf.	$\phi$	$\theta$	$\psi$
H <sub>11</sub>	72.1		18.0	H <sub>16/18</sub> <sup>I</sup>	124.9		-31.4
	90.9	-79.2	91.7		-77.7	-61.4	179.7
	70.8		16.6		82.8		-63.8
	96.4	-75.9	84.2		-68.6	-57.4	158.3
	70.9		16.5		117.8		-109.8
	96.2	-76.5	84.9		-45.3	-50.0	125.0
	74.7		12.7		160.8		-142.9
	102.4	-76.2	84.2		-30.3	-52.0	147.3
H <sub>14/15</sub>	-69.0		-22.0	H <sub>16/18</sub> <sup>II</sup>	82.5		-55.1
	-103.7	81.6	-120.7		-142.7	60.2	117.9
	-79.3		-23.2		92.1		-68.0
	-116.0	74.1	-117.4		-173.1	58.3	78.3
	-70.7		-34.6		112.7		-134.9
	-114.5	82.0	-120.3		-104.1	60.3	33.4
	-95.3		1.8		168.1		-137.8
	-126.4	66.0	-109.1		-101.9	61.4	41.6
H <sub>12</sub>	-137.4		15.5	H <sub>18/16</sub> <sup>I</sup>	131.4		-148.1
	66.4	44.5	63.2		-62.0	-61.7	109.1
	104.8		98.7		132.9		-150.5
	59.7	40.8	62.9		-68.4	-54.7	138.2
	94.9		99.7		96.5		-115.2
	63.3	44.4	44.8		-85.6	-63.7	169.7
	105.0		104.3		76.5		-127.7
	62.8	47.5	96.7		-83.0	-52.3	149.6
H <sub>9/11</sub>	140.1		-40.9	H <sub>18/16</sub> <sup>II</sup>	124.2		-162.6
	-91.6	54.5	89.4		-122.2	57.3	21.4
	133.0		-63.1		112.2		-135.9
	-94.2	58.4	85.5		-134.3	58.6	45.0
	133.2		-60.8		81.1		-77.7
	-95.0	58.5	87.6		177.0	63.4	37.0
	130.1		-61.9		78.8		-82.7
	-90.4	52.7	85.0		-179.7	62.1	26.3
H <sub>11/9</sub>	65.1		-147.9				
	-79.3	-58.1	95.6				
	58.6		-146.7				
	-79.8	-58.4	94.4				
	58.9		-147.8				
	-79.4	-57.6	94.5				
	57.3		-146.6				
	-76.5	-64.0	99.5				

<sup>a</sup> Torsion angles in degrees.