

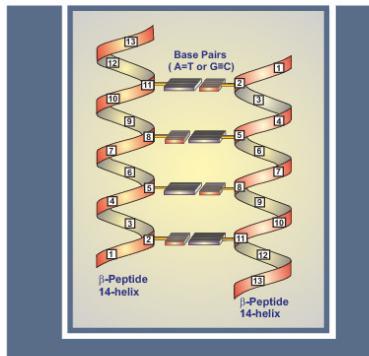


Pradip Chakraborty (Autor)

# Design, Synthesis, and Structural Investigation of Nucleobase Functionalized $\beta$ -Peptides

DESIGN, SYNTHESIS, AND STRUCTURAL INVESTIGATION  
OF NUCLEOBASE FUNCTIONALIZED  $\beta$ -PEPTIDES

Pradip Chakraborty



Cuvillier Verlag Göttingen

<https://cuvillier.de/de/shop/publications/2517>

Copyright:

Cuvillier Verlag, Inhaberin Annette Jentzsch-Cuvillier, Nonnenstieg 8, 37075 Göttingen,  
Germany

Telefon: +49 (0)551 54724-0, E-Mail: [info@cuvillier.de](mailto:info@cuvillier.de), Website: <https://cuvillier.de>

---

## Table of Contents

<b>1</b>	<b>Introduction.....</b>	<b>1</b>
<b>2</b>	<b>Artificial helical secondary structures .....</b>	<b>5</b>
2.1	Foldamers.....	5
2.2	$\beta$ -Peptides.....	6
2.3	Association of $\beta$ -peptide helices .....	13
<b>3</b>	<b><i>De novo</i> design of helical tertiary structures .....</b>	<b>16</b>
3.1	Helical bundles: coiled coils .....	16
3.2	<i>De novo</i> design of helical bundles .....	19
3.3	Metal ion induced $\alpha$ -helical bundles.....	21
3.4	Template-assembled synthetic proteins .....	23
3.5	Self-assembly of nucleobase functionalized oligomers.....	27
<b>4</b>	<b>Synthesis of nucleo-<math>\beta</math>-amino acids.....</b>	<b>30</b>
4.1	Synthesis of nucleo- $\beta^3$ -amino acids.....	32
4.2	Synthesis of ( <i>S</i> )- <i>N</i> -( <i>tert</i> -butoxycarbonyl)- $\gamma$ -(adenine-9-yl)- $\beta$ -homoalanine ...	35
4.3	Synthesis of ( <i>S</i> )- <i>N</i> -( <i>tert</i> -butoxycarbonyl)- $\gamma$ -(7-deazaguanine-9-yl)- $\beta$ -homoalanine .....	36
4.4	Synthesis of other $\beta$ -amino acid building blocks.....	40
<b>5</b>	<b>Nucleobase functionalized <math>\beta</math>-peptides .....</b>	<b>41</b>
5.1	$\beta$ -Homoalanyl PNA .....	43
5.2	Design of nucleobase functionalized $\beta$ -peptide helices.....	45
5.3	Structural characterization by UV and CD spectroscopy .....	46
5.4	Synthesis of nucleobase functionalized $\beta$ -peptides .....	47
5.5	Dimeric association of $\beta$ -peptide helices by nucleobase pairing.....	49

5.5.1	Adenine-thymine pairing in $\beta$ -peptide recognition.....	49
5.5.2	Relative orientation of complementary 14-helices .....	51
5.5.3	Influence of the helix propensity on duplex stability .....	62
5.5.4	Reduced aggregation of 7-deazaguanine functionalized $\beta$ -peptides .....	68
5.5.5	Unexpected self-pairing of the sequence TGAT .....	74
5.5.6	Thermodynamics of base-pairing .....	77
5.6	Tetrameric association of $\beta$ -peptides by G-quadruplex formation.....	81
5.7	Higher aggregation of the nucleobase-modified $\beta$ -peptides.....	86
<b>6</b>	<b>Summary.....</b>	<b>93</b>
<b>7</b>	<b>Zusammenfassung .....</b>	<b>95</b>
<b>8</b>	<b>Experimental part.....</b>	<b>98</b>
8.1	General.....	98
8.2	Characterization .....	100
8.3	General Synthesis .....	103
8.3.1	Determination of enantiomeric excess.....	103
8.3.2	Loading of first amino acid on the resin .....	103
8.3.3	General procedure for the solid phase $\beta$ -peptide synthesis: .....	103
8.4	Synthesis of <i>N</i> -Boc-nucleo- $\beta^3$ -amino acids .....	106
8.5	Synthesis of nucleobase functionalized $\beta$ -peptides .....	122
<b>9</b>	<b>Abbreviations .....</b>	<b>136</b>
<b>10</b>	<b>References.....</b>	<b>140</b>