

Table of Contents

	Preface	<i>IX</i>
	List of Contributors	<i>XI</i>
1	Artificial (Pseudo)peptides for Molecular Recognition and Catalysis	1
	<i>L. J. Prins, P. Scrimin</i>	
1.1	Introduction	1
1.2	Recognition of Biological Targets by Pseudo-peptides	2
1.2.1	Introduction	2
1.2.2	Polyamides as Sequence-specific DNA-minor-groove Binders	2
1.2.3	Peptide Nucleic Acids	12
1.2.4	Protein Recognition by (Pseudo)peptides	17
1.3	Synthetic (Pseudo)peptide-based Supermolecules: From Structure to Function	20
1.3.1	Catalytic (Pseudo)peptides	21
1.3.2	(Pseudo)peptides Altering Membrane Permeability	27
1.3.3	Nanoparticle- and Dendrimer-based Functional (Pseudo)peptides	30
1.4	Combinatorial Selection of Functional (Pseudo)peptides	35
1.5	Conclusions	38
	References	39
2	Carbohydrate Receptors	45
	<i>A. P. Davis, T. D. James</i>	
2.1	Introduction	45
2.2	Carbohydrate Receptors Employing Noncovalent Interactions	47
2.2.1	Recognition in Organic Solvents	48
2.2.2	Recognition in Two-phase Systems	62
2.2.3	Carbohydrate Recognition in Water	69
2.3	Receptors Employing B–O Bond Formation	79
2.3.1	Carbohydrate Recognition in Water	80
2.3.2	Carbohydrate Recognition in Water	84
	References	104

3	Ammonium, Amidinium, Guanidinium, and Pyridinium Cations	111
	<i>T. Schrader, M. Maue</i>	
3.1	Introduction	111
3.2	Ammonium Cations	112
3.2.1	New Receptor Structures	112
3.2.2	Theoretical Investigations	119
3.2.3	New Functions	122
3.2.4	Peptide and Protein Recognition	125
3.2.5	Conclusion and Outlook	131
3.3	Amidinium Cations	132
3.3.1	Introduction	132
3.3.2	Artificial Receptors	133
3.3.3	Conclusion	138
3.4	Guanidinium Cations	138
3.4.1	Introduction	138
3.4.2	Artificial Receptors	139
3.4.3	Conclusion	148
3.5	Pyridinium Cations	149
3.5.1	Introduction	149
3.5.2	Artificial Receptors	149
3.5.3	Conclusion	157
3.6	Conclusions and Outlook	157
	References	159
4	Artificial Pyrrole-based Anion Receptors	165
	<i>W.-S. Cho, J. L. Sessler</i>	
4.1	Introduction	165
4.2	Anions in Biological Systems	166
4.3	Cationic Pyrrole-based Receptors	170
4.3.1	Cyclic Receptors	170
4.3.2	Linear Receptors	180
4.4	Neutral Pyrrole-based Anion Receptors	183
4.4.1	Cyclic Receptors	183
4.4.2	Linear Receptors	200
4.5	Anion Carriers in Transport Applications	203
4.6	Anion Sensing	212
4.7	Guanidinium-based Anion Receptors	228
4.8	Amide-based Anion Receptors	234
4.9	Urea-based Anion Receptors	245
4.10	Conclusions	249
	Acknowledgment	250
	References	250

5	Molecular Containers in Action	257
	<i>D. M. Rudkevich</i>	
5.1	Introduction	257
5.2	Variety of Molecular Containers	258
5.3	Chemistry Inside Capsules	272
5.3.1	Observing Unusual Species Through Encapsulation	272
5.3.2	Changing Reaction Rates by Encapsulation	275
5.3.3	Encapsulated Reagents	277
5.4	Storage of Information Inside Capsules	280
5.5	Materials and Sensors by Encapsulation	283
5.5.1	Molecular Containers as Sensors and Sensing Materials	283
5.5.2	Supramolecular Polymers	286
5.6	Biologically Relevant Encapsulation	290
5.6.1	Entrapment of Biologically Active Guests	290
5.6.2	Encapsulation of Gases	292
5.7	Concluding Remarks	294
	Acknowledgment	295
	References	295
6	Formation and Recognition Properties of Dynamic Combinatorial Libraries	299
	<i>A. D. Hamilton, D. M. Tagore, K. I. Sprinz</i>	
6.1	Introduction	299
6.2	Covalent Interactions Used in DCC Design	302
6.2.1	Acyl Hydrazone and Imine Exchange	302
6.2.2	Transesterification	310
6.2.3	Disulfides	311
6.2.4	Olefin Metathesis	313
6.3	Noncovalent Interactions Used in DCC Design	315
6.3.1	Metal Ligand Coordination	315
6.3.2	Hydrogen Bonding	321
6.4	Conformational/Configurational Isomerization	326
6.5	Receptor-based Screening, Selection, and Amplification	328
6.6	Conclusions	331
	Acknowledgment	331
	References	331
7	Synthetic Molecular Machines	333
	<i>E. R. Kay, D. A. Leigh</i>	
7.1	Introduction	333
7.1.1	Molecular-level Machines and the Language Used to Describe Them	334
7.1.2	Principles of Motion at the Molecular Level – the Effects of Scale	335
7.2	Controlling Conformational Changes	336
7.3	Controlling Configurational Changes	340

7.4	Controlling Motion in Supramolecular Systems	346
7.4.1	Switchable Host–Guest Systems	347
7.4.2	Intramolecular Ion Translocation	348
7.5	Controlling Motion in Interlocked Systems	350
7.5.1	Basic Features	350
7.5.2	Inherent Dynamics: Ring Pirouetting in Rotaxanes	351
7.5.3	Inherent Dynamics: Ring Pirouetting in Catenanes	353
7.5.4	Inherent Dynamics: Shuttling in Rotaxanes	358
7.5.5	Controlling Translational Motion: Molecular Shuttles	361
7.5.6	Controlling the Motion: Ring Pirouetting in Rotaxanes	376
7.5.7	Controlling the Motion: Switchable Catenanes – the Issue of Directionality	377
7.6	From Laboratory to Technology: Toward Useful Molecular Machines	383
7.6.1	Current Challenges	383
7.6.2	Reporting Motion: Switches and Memories	383
7.6.3	The Interface with Real-world Technology	393
7.7	Summary and Outlook	395
	References	397
8	Replicable Nanoscaffolded Multifunctionality – A Chemical Perspective	407
	<i>W.-M. Pankau, S. Antsyovich, L. Eckardt, J. Stankiewicz, S. Mönninghoff, J. Zimmermann, M. Radeva, G. von Kiedrowski</i>	
	Abstract	407
8.1	Introduction	407
8.2	A Manifesto for Nanorobot Implementation	408
8.2.1	Noncovalent Informational Nanoscaffolding	409
8.2.2	Self-assembly From Synthetic Three-arm Junctions	409
8.2.3	Tensegrity and Maximum Instruction as the Keys for Nanoarchitecture Control	411
8.2.4	Chemical Copying of Connectivity Information (CCC) as the Key for Nanomachine Replication	412
8.2.5	Cloning and Copying on Surfaces Using eSPREAD	413
8.2.6	Linear Conjugates as Building Blocks for Junction eSPREADING and Nanoscaffolded Multifunctionality	414
8.2.7	Directed Evolution of Replicable Nanomachines	416
8.2.8	Probing the Existence of Nanoepitopes on the Surface of Biological Cells	417
8.2.9	External Control of the Operation of Such Nanomachines by GHz Radio-frequency Magnetic Field Inductive Heating of Metal Clusters Attached to Such Constructs	417
8.3	Conclusion	419
	Acknowledgment	419
	References	420
Index		421