

## Index

### a

ACE (affinity capillary electrophoresis) 121  
 acetylcholine receptor, nicotinic 120  
 acyl hydrazone exchange 302 ff, 305  
 – acetylcholinesterase 305  
 adding and removing electron 369, 371  
 – cyclic voltammetry 371  
 – redox-switched shuttle 369  
 adding and removing proton 366  
 affinity capillary electrophoresis (ACE) 121  
 affinity chromatography 145, 208  
 AFM 394  
 atomic force microscopy 394  
 air/water interface 81, 116  
 alternating-current (a.c.) electric field 376  
 amide-based anion receptor 234, 237, 240, 243  
 – cyclic hexapeptide 240  
 – dihydrogen phosphate 237  
 – fluorescence chemosensor 237  
 – hydrogen sulfate 237  
 – polyamide cage-type receptor 243  
 – thioamide motif 240  
 amide-based caatenane 354  
 amidinium recognition 132, 135 ff  
 – bis(pentamidine) 135 ff  
 – DAPI 136 ff  
 – solid-phase extraction 137  
 amino acid recognition 140  
 – chiral recognition of arginine 140  
 – chiral recognition of lysine 140  
 amino acid, unnatural 19, 24  
 – amino acid,  $\alpha,\alpha$ -disubstituted 19  
 – ATANP 24  
 ammonium cation recognition 112 ff, 117 f, 150  
 – adrenaline receptor, ditopic 117  
 – alkylammonium, encapsulated 113  
 – bicyclopentane, based on 150  
 – bisphosphonate, based on 114 ff

– cyclophane, based on 114  
 – deep cavitand, resorcinarene-based 118  
 – porphyrin, based on 114  
 amplification 299  
 – DCL 299  
 amplification 326  
 anion recognition 167 ff, 180, 203, 212 ff, 227 ff  
 – cationic pyrrole-based receptor 170 ff  
 – extraction 192 ff  
 – guanidinium based receptor 168  
 – molecular cage, based on 227 ff  
 – natural occurring receptor 167 ff, 180  
 – sensor 212 ff  
 – transport 203  
 anion shuttling 369  
 anthracene fluorescence 390  
 antibody 326  
 – synthetic 45  
 arginine cork 114 ff, 141ff  
 arginine fork 139  
 aromatic wall 260  
 artificial catalyst 229  
 autocatalysis 279  
 azobenzene 341

### b

BAM (Brewster-angle-microscope) 116, 126  
 barbiturate 270  
 $\beta$ -barrel, synthetic 29  
 Bartter's syndrome 168  
 o-benzynes 272  
 biological motor 334  
 biological recognition 291  
 – amino acid ester 291  
 – glucopyranoside 291  
 biologically relevant encapsulation 289  
 – acetyl choline 289  
 – choline 289

- nucleotide 289
  - biomolecular recognition 1 ff
  - biopolymer library 330
    - peptide epitope library 330
    - phage display 330
  - biosensor, semisynthetic 93
  - bis-(catechol) 316
  - bistable molecular shuttle 367
    - pH-responsive 367
  - B-N interaction 96 ff
  - boronic acid 79 ff, 100
  - Brownian motion 333
- c**
- cage, molecular 154
  - calixarene 258 ff
  - capsule 263, 266
    - kinetic stability 263
    - tetraurea capsule 263
  - capsule, reversible 154
    - endo-cavity complexation 155
  - carbohydrate recognition 47 ff, 56, 58 f, 61 f, 64, 66, 68 ff, 84 ff, 94
    - „amino sugar cork“ 114
    - anthracene, based on 78
    - boronic acid, based on 79 ff
    - calixarene 49
    - calorimetric study 47
    - CD-spectroscopy 49, 94
    - cholaphane 50
    - cleft, hydrophobic 71
    - copper(II) complex, based on 77
    - cyclodextrine, based on 72 ff
    - cyclophosphorylated binaphthol, based on 56
    - diastereoselectivity 51 ff
    - extraction 62, 64, 82
    - face-to-face geometry 56
    - fluorescence spectroscopy 70
    - glucosidase activity 58
    - glycopane, based on 78
    - in organic solvent 48 ff
    - in water 69 ff
    - NMR-spectroscopy 70, 72
    - noncovalent interaction 47, 69, 78
    - octahydroxycalixarene, based on 64
    - phase transfer 48, 64
    - polyaza cleft/cavity, based on 53
    - porphyrin, based on 52, 75
    - sensing 62, 84 ff
    - transport 62, 66, 68, 82 ff
    - tricyclic hexalactam, based on 61
    - tricyclic oligoamide, based on 59
    - two phase system, in 62
    - UV/Vis-spectroscopy 70
  - carceplexe 261
    - hemicarceplexe 261
  - carcerand 257 ff
    - hemicarcerand 261
  - casting 301
  - catalysis 1, 21 ff, 149 ff
  - catalyst, biomimetic 22
  - catenane 350
  - $\pi$ -cation interaction 149 ff
  - caviplexe 258 ff
  - cavitand 257 ff, 285 f
    - polymer-bound cavitand 286
    - solid-supported cavitand 285
  - cavity 257 ff
    - inner cavity 258
  - cavity, spheroidal 150
  - CD spectroscopy 49, 94
  - cell proliferation 18
  - cell surface oligosaccharide 69
  - chemical connectivity copying 413
    - CCC 413
  - chemical copying 412
  - chemical fuel 340
  - chiroptical molecular switch 343
  - chromosome 9
  - circular dichroism 344
  - circular helicate 321
  - circumrotation 353
  - circumvolution 353
  - cis-azobenzene 273
  - cis-trans isomerization 340
  - clip, molecular 151 ff
  - co-conformational change 350
  - combinatorial chemistry 299
  - combinatorial library 35, 131, 300
    - parallel synthesis 300
    - split-mix technique 300
  - competitive binding assay 72, 98 ff, 121
  - concave surface 258 ff
  - configurational change 340
  - conformational change 336
  - conformational/configurational isomerization 326
  - connectivity information 412
  - constrictive binding 268
  - continuous 360° rotation 344
  - crown ether 111, 119
  - CV (cyclic voltammetry) 212 ff
  - cyclic hexapeptide 241 f
    - dimeric receptor 242
    - iodide 241
    - molecular oyster 242
    - sulfate 241

- cyclic trimeric silanol 273  
cyclic voltammetry 378  
cyclobisparaquat-*p*-phenylene 356  
– CBPQT<sup>4+</sup> 356  
cyclophane 149 ff  
– catalysis 149 ff
- d**  
DAPI 136 ff  
DCC (dynamic combinatorial library) 117  
DCL 300, 304, 308 f  
– compartmentalization 304  
– covalent interaction 300  
– disulfide bond formation 300  
– hydrogen-bonding 300  
– metal coordination 300  
– noncovalent force 300  
– olefin metathesis 300  
– oxime and hydrazone exchange 300  
– oxime exchange 309  
– peptide-hydrazone DCL 308  
– transesterification 300  
– transimination 300  
– weak binder 304  
deep cavitand 258 ff  
dendrimer 122, 137  
– core polarity 137  
– porosity 137  
Dent's disease 166  
device 334  
dibenzoyl peroxide 275  
dicyclohexylcarbodiimide 275  
5,5-diethylbarbituric acid 322  
dimelamine 323  
dinuclear titanium(IV) architecture 316  
dipolar cycloaddition 328  
directed evolution 416  
directed motion 395  
distal isomer 356  
distamycin 2 ff  
disulfide 311, 313  
– concanavalin A 313  
– tripeptide 311  
DNA 1 ff, 10, 12 ff, 23, 134 ff  
– base pair 4 ff  
– dimer 13  
– double helix 10  
– intercalator 14  
– major groove 10  
– metallointercalator 23  
– minor groove 2 ff, 134 ff  
– mitochondrial 14  
– oligonucleotide (ODN) 15  
– recognition of 12  
DNA-protein complex 120  
double-rosette 270  
DPQ (dipyrrolylquinoxaline) 223 ff  
dynamic combinatorial chemistry 299  
– DCC 299  
dynamic combinatorial library 299 ff  
dynamic combinatorial template-assisted synthesis 300  
dynamic library 271
- e**  
enantioselective recognition 231  
encapsulated reagent 277 f  
encapsulation 257 ff, 291  
– gas 291  
– O<sub>2</sub> 291  
enhancer region 10  
enol 273  
enrichment factor 137  
entrapped 261  
entropy-driven shuttling 374  
– temperature 374  
enzyme, artificial 146 ff  
equilibrium composition 331  
evolutionary process 145 ff  
extraction 64, 62, 82, 192 ff
- f**  
fibrosis, cystic 165  
film-balance 117, 128  
fluorescence energy transfer 90  
fluorescence spectroscopy 70, 74, 125  
fluorescence switching 391  
– 4-aminonaphthalimide 391
- g**  
GAG (glycosylaminoglycan) 126  
GAG-mimic 126  
gas 293  
– Xe 293  
gear 336  
gene activation 11  
gene inhibition 9  
glucose sensing, PET-based 102  
glycocluster 326  
gold cluster 407, 418  
– inductive heating 418  
– RUBiGold 418  
guanidinium recognition 138 ff, 143 ff  
– cyclophane, based on 144  
– photoisomerizable receptor, based on 145 ff  
– sensor, chromogenic 143  
– sensor, electrochemical 145

- torand, based on 141
- trisphosphonate, based on 141
- guanidinium-based anion receptor 228 f, 230
  - bicyclic guanidium 230
  - bis-acylguanidium-based receptor 229
  - polyguanidinium-based receptor 232
- guest 12 ff, 48 ff, 54, 57 ff, 71 ff, 77 ff, 91 f, 94, 98, 100, 113 ff, 119 ff, 125, 133 ff, 140 ff, 144 f, 147, 149 ff, 153 f, 171 ff, 189 ff, 192 ff, 212 ff, 216 ff, 227
  - acetate 192 ff, 227
  - ACh (acetylchoilne) 120, 125, 150
  - adenosine 153
  - adrenaline 115
  - alizarin red S 100
  - allose 94
  - amino alcohol 115 ff
  - amino saccharide 114 ff
  - aminocaproic acid 143
  - AMP 206 ff
  - arabinose 64 ff, 72
  - arginine 114 ff, 140 ff
  - benzoate 192 ff, 212 ff
  - benzylamine 140
  - bis(pentamidine) 133 ff
  - bromine 172, 189 ff, 212 ff
  - butanol 72
  - carboxyfluorescein 98
  - cellobiose 58, 61, 74
  - chloride 171 ff, 189 ff, 212 ff
  - CMP 206 ff
  - creatine 143
  - creatinine 140
  - cyanide 190
  - cyclo(RGDfV) 144
  - cyclodextrine 72
  - D-Ala-D-Ala 121
  - DAPI 136 ff
  - deoxyribose 54, 64 ff
  - dihydrogenphosphate anion 187 ff, 212 ff
  - dimethylguanidine 140
  - disaccharide 61
  - DNA 12 ff
  - erythrose 73
  - fluoride 171 ff, 189 ff, 212 ff
  - fructose 63, 73, 77, 79 ff, 97 ff
  - fucose 64 ff, 71 ff
  - Furanose 65
  - GABA ( $\gamma$ -amino-butyrac acid) 113
  - galactose 48 ff, 60, 73, 77, 79, 97
  - glucarate 91
  - glucofuranose 92
  - glucose 48 ff, 60 ff, 73 ff, 77, 79 ff, 97 ff
  - glucose-6-phosphat 98
  - glucoseamine hydrochloride 58, 91
  - GMP 206 ff
  - guanidinium cation 119 ff, 147
  - heparin 98
  - hexamethylguanidine 145
  - hydrogensulfate 190
  - iodide 189
  - lactose 57 ff, 61, 75, 77
  - lactulose 89
  - Lipid A 78
  - lysine 140 ff
  - lyxose 64 ff
  - maltose 57 ff, 73, 77 ff
  - maltotriose 73
  - mandelic acid 187
  - mannose 48 ff, 60, 72 ff
  - melamine 147
  - melibiose 57
  - methyl glucoside 66, 72, 77
  - methyl picolinium 154
  - methylguanidine 140 ff
  - methylquinoline 145
  - monosaccharide 64, 72
  - NAD<sup>+</sup> 153
  - NADP 153
  - nicotinamide 153
  - nitrate 190
  - p-nitrophenyl glycoside 78
  - N-methyl alkylammonium 117 ff
  - oxalate 227
  - paraquat 151
  - phenyl glycoside 78
  - propylamine 143
  - pyranose 54, 65
  - pyrochatechol violet 98
  - ribofuranoside 66
  - ribose 63 ff
  - RNA 12 ff
  - saccharose 81
  - squaric acid 187
  - succinate 227
  - tartaric acid 187
  - tetrafluoroborate 189
  - TMP 216 ff
  - trifluoroacetate 189
  - UMP 216 ff
  - viologen 149
  - xylose 64 ff, 72 ff
- guest exchange rate 260
- guest exchange 260, 294

**h**

hairpin 9  
 half-live 262  
 halide anion recognition 165  
 – pyrrole-based receptor, based on 165  
 hard nanotechnology 396  
 H-bond acceptor, anionic 56  
 hemisphere 261  
 heterocircuit catenane 356  
 heterodimer 266  
 HIV-1 10  
 HIV-1 protease 17  
 – dimerization domain 17  
 homocircuit catenane 353  
 homodimer 266  
 homoleptic and heteroleptic species 318  
 Hox protein 11 ff  
 hydrazone exchange 309  
 hydrogen bond 260  
 hydrogen bond complementarity 141  
 – intramolecular hydrogen bond 260  
 hydrogen bond, guest-induced 141  
 hydrogen bond, ion-pair-reinforced 114, 135  
 hydrogen bonding 321, 325  
 – tetrameric capsule 325  
 hyperphosphatemia 203

**i**

ICD (induced circular dichroism) 114  
 ICT (internal charge transfer) 84 ff  
 imine exchange 302, 305 f  
 – aldolase 306  
 – carbonic anhydrase II 302  
 – imine reductase 305  
 – influenza A virus neuraminidase 302  
 – *N*-acetylneuraminic acid 306  
 – template-directed synthesis of nucleic acid 306  
 imprinted polymer 77, 136 ff  
 induced circular dichroism 388  
 induced fit 136, 328  
 information storage 282  
 – chirality expression 282  
 – supramolecular isomer 282  
 inhibitor screening 329  
 interaction, electrostatic 165  
 interaction, hydrophobic 149 ff  
 interlocked system 350  
 internal volume 294  
 intramolecular ion translocation 348  
 ion channel, artificial 28  
 ISE (ion selective electrode), anion specific 215 ff

ISE (ion selective electrode), nucleotide specific 216 ff  
 ITC (isothermal calorimetry) 47, 72, 175, 184

**j**

Janus molecule 321  
 Job-plot 136

**k**

kinetic stability 261  
 kinetically associated species 350

**l**

lasalocid 123  
 LB (Langmuir-Blodgett) film 81 ff  
 liquid crystal 341  
 logic circuit 385  
 luciferase gene 15

**m**

machine 334  
 – mechanical movement 334  
 macroscopic effect 393  
 mass spectrometry 154  
 maximum instruction 408, 411 f  
 – instructed mixture paradigm 412  
 mechanical switch 388  
 – chiroptical switch 388  
 melamine 270  
 memory 383  
 memory device 395  
 metal ligand coordination 315, 319  
 – counteraction 319  
 – DNA binding ligand 315  
 – double-level library 319  
 – metallocryptate 319  
 – salicylaldimine 315  
 methyl red 71  
 Michaelis complex 275  
 micro-electromechanical system (MEMS) 396  
 molding 301  
 molecular amplification 309  
 molecular brake 337  
 molecular capsule 124  
 molecular container 257 ff  
 molecular electronic device 383  
 molecular evolution 326  
 molecular muscle 387  
 molecular ratchet 338  
 molecular recognition 1  
 molecular rotor 344  
 – thermal isomerization 344

- molecular shuttle 363
  - stimuli-responsive 363
- molecular switchable tunnel junction 384 ff
- molecular syringe 349
- molecular turnstile 337
- molecular-level motion 333
- molecule-within-molecule complex 294
- multicomponent system 99
- multivalency 30, 120 ff
- mutation 327
  
- n**
- NAD<sup>+</sup> 153
- NADH 149
- NADPH 149
- nanoepitope 417
- nanometer-scale electromechanical system (NEMS) 396
- nanobject 409
- nanorobot 407, 417
  - medical nanomachine 417
- nanoscaffolding 407
- nanoscale container 261
- nitrosating reagent 278
- NMR spectroscopy 70, 72, 75, 140, 185, 199, 212
- NO<sup>+</sup> cation 278
- nucleus 9
  
- o**
- olefin metathesis 313 f
  - [2]catenane 313
  - vancomycin dimer 314
- on/off ratio 385
- osteopetrosis 166
- oxoanion substrate 228
  
- p**
- pairwise selection 281
- Pendred's syndrome 168
- peptide recognition 125 ff, 131, 209
  - aurointricarboxylic acid, based on 131
  - calix[n]arene, based on 126 ff
  - enantioselective recognition 125, 209
  - oligophenoxyacetic acid 131
  - porphyrin, based on 125 ff
- peptide, self-replicating 26
- PET (photoinduced electron transfer) 87 ff
- phase transfer 48, 64
- photochromic system 342
- photoisomerization 341
- pirouetting rate 376
- PNA 12, 14 ff
  - (PNA)<sub>2</sub>/RNA triplex 16
  - antigene 15
  - antisense 15 ff
  - pseudo-complementarity 14
  - regulation of gene expression 14
  - transcription activation 15
- PNA-DNA complex 13
- polyamide, cyclic 6
- polyzopeptide 343
  - load 343
- polycap 286 f, 289
  - CO<sub>2</sub> 289
  - polymeric liquid crystal 287
  - switchable polycap 287
- polyguanidinium-based receptor 233 f
  - 2,3-bisphosphoglycerate 234
  - citrate content 233
  - inorganic phosphate 234
- polymer sensor 101
- porphyrin, expanded 174 ff
- portal 263
- positional integrity 369, 382
- prodiogiosin 180 ff, 203 ff
- promoter region 10
- propeller 336
- protein 15 f, 20, 23, 32, 46, 77, 93, 133, 138 ff, 168
  - BamH1 endonuclease 23
  - catalytic site 32
  - chymotrypsin (ChT) 20
  - ConA (Concanavalin A) 93
  - cytochrome c 20
  - fluorescent protein, enhanced green (EGFP) 16
  - fluorescent protein, green (GFP) 15
  - integrin 133, 139
  - lectin 46, 77
  - RepA 167
  - RNA-binding 138
  - Tat-regulator protein 140
- protein-carbohydrate interaction 73
- protein-protein interaction 17
- protein recognition 125, 128 ff
  - basic domain 128 ff
  - cytochrome c 128 ff
- protein surface 17, 130
  - hot spot 17
- proximal isomer 356
- (pseudo)peptide 1 ff, 6, 11, 17, 19 f, 27 f, 30, 34 ff
  - antibody mimic, artificial 19
  - apo-peptide 6
  - catalysis 1, 21 f, 25, 36
  - combinatorial library 35
  - decarboxylation 1

- dendrimer 34
  - enhancer region 11
  - foldamer 20
  - functional 30
  - functional, combinatorial selection of 35
  - gene activation 11
  - hydrolysis 2
  - ion channel, artificial 28
  - kinase mimic 35
  - membrane permeability 27
  - metallopeptide 36
  - molecular recognition 1
  - promoter region 11
  - protein recognition 17
  - transamination 2
  - transesterification 2
  - transport, transmembrane 28
  - pyranine dye 99
  - pyridinium recognition 149 ff
    - aromatic tweezer, based on 152 ff
    - bicyclophane, based on 150
    - calix[n]arene, based on 154
    - cyclophane, based on 149 ff
    - glycoluril-based clip, based on 151 ff
    - reversible capsule, in 154
    - transport 155
  - pyrrole based anion receptor, cationic 178, 183, 204
    - calix[n]pyrrole 183
    - sapphyrin 178, 204
  - pyrrole based anion receptor, neutral 185, 195, 197 ff
    - calix[4]pyrrole, capped 195
    - calixpyrrole, three-dimensional 198
    - extended-cavity calix[n]pyrrole 185
    - oligopyrrole 197 ff
  - pyrrole based receptor, cationic 172 ff, 177
    - anthraphyrin 177
    - cyclo[n]pyrrole 173 ff
    - isosmaragdyrin 172
    - pentaphyrin 172
    - rosarin 173 ff
    - rubyrin 173 ff
    - turcasarin 175
- q**
- quench 300
- r**
- random connectivity 416
  - rate acceleration 275
  - reaction rate 275
  - real-world technology 393
  - receptor domain, self-aggregated) 116
  - receptor, photoisomerizable 123
  - receptor-assisted combinatorial synthesis 314
    - RACS 314
  - receptor-based screening 328
  - recognition of carboxylic acid, enantioselective 187 ff
  - redox-driven cation translocation 349
  - redox-switched shuttling 370, 372
    - mono- and divalent cation 370
  - resolution, chiral 111
  - resorcinarene 258 ff, 266
  - reversible switching 388
  - Reynolds number 335
  - RGD-sequence 139, 144
  - ring pirouetting 351
  - RNA 1 ff
  - RNA polymerase 9
  - Rossmann fold 149
  - rotaxane 153, 156, 350
- s**
- salmonella typhumurium 168
  - SAM 150
  - sandwich complex 239
  - sandwiching 73
  - sandwich-type structure 240
  - seam 259
  - second law of thermodynamic 336
  - selection 327
  - SELEX 409
  - self-assembling capsule 257 ff, 263, 266, 268
    - metal-induced 266
    - self-assembly 266
    - water solubility 268
  - self-binding 373
  - self-complementary 266
  - self-folding 260
  - self-replicating 407
  - self-sorting 311
  - sensing material 283
    - FRET 283
  - sensor 283, 286
    - mass sensor for alcohol 286
    - NO<sub>x</sub> sensing 283
  - sensor, colorimetric 94 ff, 143, 217 ff
  - sensor, electrochemical 97, 103, 122, 145, 212 ff
  - sensor, fluorometric 218 ff
  - sensor system 122 ff, 212 ff, 101 ff, 122 ff, 93
  - sequential movement 379
  - β-sheet 1, 17
  - shielding 261

- ship-in-a-bottle 275
  - shuttling 358 ff
    - Boltzmann distribution 361
    - degenerate shuttle 358
    - free-energy profile 359
    - physical model 360
    - potential energy surface 360
  - single-station switchable shuttle 362 f
    - kinking 263
    - tedox-active ferrocenyl residue 362
  - SNP (nucleotide polymorphism, single) 14
  - soft ball 263
  - soft nanomaterial 396
  - solvent composition 355
  - SPREAD 407, 413 f
    - cloning and amplification technology (CAT) 414
    - eSPREAD 414
  - static library 300
  - STM 394
  - storage of information 280
  - $\beta$ -strand 29
  - supramolecular isomerism 280
  - supramolecular polymer 286
  - surface property 395
  - switch 383
  - switchable catenane 377 f
    - color change 378
  - switchable host-guest system 347
  - switching 395
  - synthetic molecular machine 333
- t**
- tag, lanthanide-binding 37
  - tail-biting crown ether 347
  - target-directed enrichment 321
  - template method 351
  - temporary barrier 382
    - follow-the-leader 382
  - tennis ball 263
  - tensegrity 408, 411
  - thermolysin 330
  - thodopsin 341
  - three-arm junction 408, 410
    - tris-oligo junction 410
  - thrombin inhibitor, artificial 132
  - through-shell borane reduction 277
  - TICT (twisted internal charge transfer) 85 ff
  - torand 141
  - transesterification 310
    - ester-exchange 310
  - living macrolactonization library 310
  - translation inhibition 15
  - translation, ribosomal 16
  - translational isomer 379
  - translational isomerism 378
  - transport, transmembrane 28, 82 ff, 111, 123, 155, 178, 203 ff, 62, 66, 68 ff
  - Tren (tris(2-aminoethyl)amine) 25 ff
  - syn*-triazole 329
  - tritycene 336
  - tumor suppressor 18
  - tweezer, molecular 151 ff
  - two-station 363 f
    - thermally activated motion 364
    - stimuli-responsive 363
- u**
- unidirectional motion 339, 395
  - unidirectional rotation 382
  - unusual species 272
  - upper rim 260
  - urea-based anion receptor 245 ff
    - glutarate 246
    - metacyclophane-type anion receptor 247
    - TNT 245
    - tricarboxylate anion 248
  - UV/Vis-spectroscopy 70, 78
- v**
- vancomycin 121
  - virtual combinatorial library (VCL) 301
- w**
- wired-logic gate 384
  - wiring 383