

## Index

### a

ABB Lummus/Albemarle AlkyClean process 168  
 ABB Lummus/UOP SMART process 172  
 $\alpha$ -abstraction 86, 87  
 abzyme 213–214  
 acrylamide 18, 217, 218  
 activation energy 41, 45, 64  
 active site 11, 27, 49, 51–52, 68, 79–80, 131, 144, 156, 194, 197–198, 211, 235, 255  
 activity modifier 134  
 adiponitrile 100  
 adsorption isotherm 146, 147–148, 173, 176  
 agostic interaction 93, 238  
 allosteric site 68  
 alloy leaching 137  
 antigen 213  
 apoenzyme 192  
 aqueous biphasic catalysis 159, 160–161  
 Arrhenius equation 41, 42, 45  
 artificial neural network (ANN) 262  
 aspartame 220  
 associative mechanism 81  
 atom economy 4–5, 6, 19, 22, 31, 111–112, 167  
 autoscaling 260, 268

### b

BHC Ibuprofen process 22  
 bifunctional catalysis 197  
 bimolecular reaction 43  
 biocatalysis 12, 16, 17–18, 27, 40, 56, 79, 129, 189, 193, 199–200, 203, 205, 209–210, 214, 235, 256  
 biodiesel 12, 108, 145, 168, 169–171  
 bioprospecting 210  
 bite angle 91, 102, 242, 248, 252

BMS Paclitaxel process 218  
 $\sigma$ -bond metathesis 87  
 bootstrapping 265, 266  
 BP AVADA ethyl acetate process 166  
 BRENDA 192, 221

### c

calcination 140, 141, 142–143, 149, 153  
 calibration set 265  
 Car–Parrinello molecular dynamics 236  
 catalyst descriptors 29, 241, 265  
 catalyst diversity 249, 250, 252, 256, 266  
 catalyst precursor 25, 27, 58, 60, 62, 89, 98, 108, 139, 149, 236  
 catalyst recovery and recycling 108  
 catalyst reservoir 58  
 catalyst stability 135, 145  
 catalytic constant 56  
 catalytic converter 66, 143, 154, 155–156  
 catalytic cycle 4, 12, 13, 15, 19, 21, 27, 43, 44, 45–46, 51–52, 56, 58, 60, 62–64, 69, 78, 81, 83, 98–101, 113, 130, 133–134, 193, 199, 231, 233, 238–239, 262  
 catalytic distillation 171  
 catalytic intermediates 12, 27, 44, 52–53, 57–58, 63, 66, 78, 131, 160, 240  
 catalytic RNA 214  
 catalytic triad 194, 198  
 chemisorption 134–135, 146, 176  
 chemoselectivity 12  
 Ciba–Geigy metolachlor process 102  
 Circe effect 195  
 classification analysis 264  
 classification tree 264  
 click chemistry 111  
 click reaction 111, 112  
 coenzyme 193, 194–195

cofactor 192, 193–195, 200–201  
 common name 192  
 comparative molecular field analysis (CoMFA) 243  
 competitive adsorption 68  
 competitive inhibition 68  
 concentration effects 61, 62  
 cone angle 88, 89, 116, 241, 242, 245  
 conversion 4, 33, 35, 39, 40, 48, 66, 71  
 coupled enzyme approach 200, 201  
 coupled substrate approach 201  
 covalent catalysis 198  
 cross-linking of enzymes 202, 204  
 cross-validation 260, 265  
 cyclometallation 82

**d**

data mining 233, 247, 256, 257, 259, 268  
 deactivation 66, 145, 167–168  
 de-insertion 79, 85  
 density-functional theory (DFT) 28, 235  
 dependent variable 260, 266  
 descriptor space 241, 251, 256  
 detour matrix 246  
 dextrose equivalent 216  
 diastereoselectivity 12, 107  
 directed evolution 17, 210, 211, 212–213  
 dissociative mechanism 81  
 distance matrix 246  
 DNA shuffling 211  
 drying 141, 142, 220  
 Du Pont synthesis of adiponitrile 100  
 dynamic kinetic resolution 208

**e**

Eadie–Hofstee plot 56  
 E-factor 4, 5–6, 21, 189  
 effective prediction domain (EPD) 266  
 electron microscopy 151  
 electronic promoter 134  
 elementary reaction 15, 42, 43–44, 61, 101  
 elementary steps 28, 29, 78, 92, 197, 231, 240  
 Eley–Rideal mechanism 130  
 $\beta$ -elimination 79, 85, 98  
 enantioselectivity 12, 92, 95, 213  
 environmental quotient 6  
 enzyme number 192  
 enzyme screening 212  
 enzyme selection 212  
 epitope 213  
 error-prone PCR 211  
 exploration diversity 252  
 expression host 212

expression vector 212  
 external validation 265  
 extraction mechanism 164  
 extremophile 210  
 extrusion 85, 143  
 Eyring equation 41

**f**

fermentation processes 202  
 figure of merit 241, 244, 249, 252, 255, 257, 265–266  
 first-order kinetics 71  
 Fischer–Tropsch synthesis 127  
 fluororous biphasic catalysis 161  
 forcefield models 233  
 forming 141  
 frequency factor 41

**g**

gene recombination 211  
 general acid catalysis 105  
 glycolic acid 208, 209  
 green chemistry 1, 2, 3–4, 9–10, 14, 19–20, 23, 111, 129, 154, 161, 165, 220  
 – principles 2, 4, 20, 111

**h**

Haber–Bosch ammonia synthesis 127  
 Hapten 214  
 Hartree–Fock approach 235  
 heavy chain 213  
 Heck reaction 12, 60, 161, 264  
 Henry reaction 107  
 heterogeneous catalysis 11, 12, 15, 16, 27, 40, 49, 51, 53, 66, 68, 77, 127, 129, 131, 133, 146–147, 154, 157, 159, 165, 202, 233, 236–237, 255  
 high-fructose corn syrup (HFCS) 216, 223  
 high-temperature fusion 137  
 holoenzyme 192  
 homogeneous catalysis 11, 12, 25, 27, 40, 50, 53, 58, 77, 78, 80, 88, 93, 96, 101, 104, 111, 113, 129, 157, 197, 251, 256  
 hybrid catalyst 110  
 $\alpha$ -hydride elimination 86  
 hydroformylation reaction 77  
 hydrothermal synthesis 136, 139, 140

**i**

ibuprofen 22, 23  
 IFP biodiesel process 170  
 immobilised enzyme 129, 202

- incipient wetness method 139  
independent variable 260, 262  
indigo 202, 206  
induced fit model 194, 195  
infrared (IR) spectroscopy 153  
inhibition 66, 68–69  
insertion 84, 238–239  
interfacial mechanism 165  
ionic liquids 163, 198  
isolated enzyme 200, 205
- j**  
Josiphos ligand 104
- k**  
kinetic resolution 204, 208  
kinetically perfect enzyme 56
- l**  
Langmuir–Hinshelwood kinetics 49  
Langmuir–Hinshelwood mechanism 130  
latent variable 259, 260–261  
L-DOPA 95, 96, 104  
leave-one-out validation 265  
life cycle assessment 9  
ligand 13, 79–89, 91–93, 104, 156, 244–247  
ligand bite angle 91  
ligand bulk radius 89, 116  
ligand exchange 79, 87  
ligand flexibility 91  
light chain 213  
Lineweaver-Burk plot 56  
lock-and-key model 194
- m**  
macroporous 144, 147  
macroscopic level 27, 129  
magic angle spinning 153  
maximum velocity 55  
mean-centring 268  
mercury porosimetry 148  
mesoporous 144  
metalloenzyme 193, 197  
metolachlor 96, 102, 104  
Michaelis–Menten kinetics 54, 195  
microporous 140, 144, 147  
microscopic level 27, 129, 131  
microscopic reversibility  
– principle 15, 83  
migration 66, 68, 79, 84  
migratory insertion 84  
Mitsubishi Rayon acrylamide process 217  
model catalyst systems 132, 133  
model domain 266  
modifier 134  
molecular dynamics 233, 236  
molecular graph 245  
molecular shuttle bus 164  
molecular sieve 140, 147  
molecularity 43  
monolayer capacity 148  
Monte-Carlo 234
- n**  
neoteric solvents 163  
noncompetitive inhibitor 68, 69  
nonelementary reaction 42, 61  
nucleophilic catalysis 197, 198
- o**  
optimisation diversity 252  
organocatalysis 105, 106–107  
orthometallation 87  
oxidative addition 79, 81, 82–84, 86–87, 92  
oxidative coupling 21, 82
- p**  
paclitaxel 218, 219–220  
parallel reactions 57  
partial least-squares (PLS) 260  
pelleting 143  
peptide bond 112, 191  
permutation test 266  
perovskite 266, 267  
phase-transfer catalysis 164  
phase-transfer catalyst 159, 164  
physisorption 146  
poisoning 52, 65, 66, 69, 135, 145  
pore size distribution 146, 148, 149  
pore volume 139, 146, 148, 177  
prediction set 265  
predictive modeling 29, 233, 240, 255, 256, 265  
pre-equilibrium 58, 60, 100  
pre-exponential factor 41  
primary structure 191, 192, 256  
principal component 233, 252, 259, 261  
principal components analysis (PCA) 259  
product life cycle 9  
product selectivity 4, 5, 12, 44, 57, 99, 102, 112, 135, 221  
product yield 4, 5, 6, 91, 117, 255  
promoter 134, 135  
prosthetic group 193  
proximity effect 195, 196  
Pseudo-order conditions 62

**r**

random mutagenesis 211  
 Raney nickel 138  
 rate constant 41, 45–46, 49, 56–57, 61–62, 141  
 rate equation 40, 41, 46, 48, 52, 57–58, 61–62, 80  
 rate-determining step 40, 43, 45, 51–52, 57, 60, 62, 135  
 rational catalyst design 240  
 rational design 210, 211  
 REACH 3  
 reactant conversion 4  
 reaction coordinate 44, 45–46, 238  
 reaction efficiency 4  
 reaction order 40, 42, 43, 45, 60–63  
 reaction pocket 88, 89, 91  
 reaction profile 44  
 reactive distillation 171  
 reductive elimination 79, 82, 83–84, 87, 92–93, 101  
 regioselectivity 12  
 residue  
 ribozyme 214, 215

**s**

Sabatier's principle 65, 194  
 saturation kinetics 55, 80  
 scanning electron microscope 27, 152  
 secondary structure 192  
 second-order kinetics 46, 60  
 selectivity 4–6, 12, 14, 22, 27, 57, 77, 102, 104, 108, 112, 130, 134–135, 159, 173, 255  
 shell higher olefins process (SHOP) 97  
 ship-in-a-bottle catalyst 110  
 sintering 52, 66, 68, 131, 133, 135, 143, 145  
 skeletal catalyst 138  
 small-angle X-ray scattering 151  
 smart polymer 203  
 solid acid 16, 108, 140, 145, 168, 171, 173  
 solid angle 89, 245  
 solid state nuclear magnetic resonance 27, 150, 153  
 Sonogashira reaction 113  
 spectroscopy 25, 27–28, 44, 146, 149, 150–154  
 specific acid catalysis 105  
 specific surface area 144  
 specificity constant 55  
 sphere occupation 89, 242

spray drying 142  
 steady-state approximation 52, 53–54  
 steady-state concentration 52, 193  
 steric crowding 91  
 steric effect 88  
 substrate 10, 12, 15, 17, 25, 33, 50, 54–56, 58, 65, 68, 77, 85, 92, 104, 111, 134–135, 192, 195, 197, 201, 235, 259, 261  
 substrate accessibility 144  
 substrate binding model 194  
 surface organometallic chemistry 110, 156, 157  
 sustainability 1, 2, 10  
 sustainable development 1, 2, 154, 166  
 Suzuki cross-coupling 105

**t**

tableting 143  
 taxol 218, 220  
 technical enzyme 199  
 termolecular reaction 43  
 tertiary structure 192  
 test set 262, 265  
 textural modifier 135  
 thalidomide 94  
 thermal degradation 66  
 thermophilic enzyme 213  
 3D descriptors 242, 243, 245, 248, 255  
 three-way catalyst (TWC) 155  
 Tolman's cone angle 88, 242  
 Tosoh/DSM aspartame process 220  
 training set 262, 265  
 transmission electron microscope 151  
 trial moves 234  
 turnover frequency (TOF) 11, 40, 255  
 turnover number (TON) 11, 40, 255  
 2D descriptors 245, 247–248, 254, 268

**u**

Ullmann reaction 19, 20  
 unimolecular reaction 43

**v**

vacuum pore impregnation 139, 177  
 variable importance parameter (VIP) 261  
 – plot 261, 262  
 virtual library 254

**w**

Wacker oxidation process 99  
 wet impregnation 139

white biotechnology 205

window effect 237

## **x**

xerogel 141

X-ray diffraction 149, 150, 151, 204, 248,  
256

X-ray photoelectron spectroscopy 149, 151

## **y**

yield 4–6, 21–22, 39, 40, 44, 57, 87, 102, 208,  
231, 255

Y-randomising 266

## **z**

zeolites 16, 110, 131–132, 140, 237–238

zero-order kinetics 46

