

Index

a

accelerated membrane assisted clean-up (AMAC) 117
 acetonitrile 331
 7-acetoxy-1-methylquinolinium iodide 325
 acetylcholinesterase 328
 affinity capillary electrophoresis (ACE)
 – dynamic equilibrium 276
 – kinetic 280
 – pre-equilibrium 279
 affinity capillary electrophoresis–mass spectrometry (ACE–MS)
 – application 286, 287
 – specific requirements 284
 affinity ligands 281
 agonists and allosteric modulators 323
 air bubbles 337
 alkaline phosphatase 328
 allosteric modulator 340
 α -lactalbumin 92
 amyloid beta oligomers 368
 amyloidogenic proteins 96
 analogue acetylcholine binding protein (AChBP) 328
 androgen chemical activated luciferase expression (AR-CALUX) 117
 angiotensin-converting enzyme 328
 anti-Alzheimer drug 328
 anti-Alzheimer target protein 328
 antibiotic enrofloxacin 306
 anti-digoxigenin-antibody/digoxigenin + digoxin 327
 antivenomics 370
 ArMet 215
 assay quality parameters 351
 assay signal 344
 association constants 276, 278
 association kinetics 342

atmospheric pressure chemical ionization (APCI) 10, 341
 automated ligand identification system (ALIS) 135

b

background electrolyte (BGE) 271
 base-peak chromatogram (BPC) 2
 benzophenones 66
 β -isoform 355
 Biacore 2000 instrument 305
 binding affinity
 – frontal affinity chromatography 246, 264
 – staircase method 247
 – zonal chromatography 255
 bioactive peptides 348
 bioaffinity 323
 – analysis 131, 133
 – chromatogram 349
 – chromatography 243, 366
 bioassay 336
 – chromatogram 333, 343
 – detector 346
 bioassay guided fractionation (BGF) 124
 biocatalysis 351, 356
 biochemical band broadening 345
 bioengineering 301, 302
 biological assays 323
 biological buffer systems 326
 biosensor immunoassays (BIAs) 300
 bottom-up approach 40
 bulk refractive index 368

c

CALUX assays 138
 capillary electrophoresis (CE) 272, 273, 275, 367

capillary electrophoresis–mass spectrometry (CE–MS) 207

- ACE-MS 284
- general requirements 283
- IA 284

capillary zone electrophoresis (CZE) 275

cell reproduction tests 137

charged residue model (CRM) 8, 86

chemical cross linking proteomics 136

chemical cross-linking MS 64

chemical proteomics approach 136

chip capture and release chromatography 306

chromatographic detector 343

chromatographic dilution 331

cluster analysis 263

collisional cooling 89

collisional heating 89

collision-induced dissociation 20

collision induced unfolding 98

competition assay

- GAT1 176
- SERT 186

competitive binding assay (CBA) 300

competitive binding immunoassays (CBIA)s 305

conformational mobility 264

Coumestrol 325

crude synthesis mixture 330

cyclodextrin 290, 292

cytochrome P450 354

d

data acquisition 5, 30

data analysis 68

data-dependent acquisition (DDA) 143

data interpretation methods 348

deconvolution 144

de novo synthesized compounds 324

desalting 83

desorption electrospray ionization (DESI) 309

desorption electrospray ionization mass spectrometry (DESI-MS) 212

desorption ionization on porous silicon (DIOS) 304

dextromethorphan 265

dialysis 83, 117

3,4-diaminobenzoic acid (DABA) 304

diazirines 66

dilution calculations 346

diode array detector (DAD) 327

direct analysis in real time (DART) 309

direct binding assay (DBA) 300

dissociation constant 280

dopamine receptors 188

dose–response curve 353

double-bond equivalent 7

DriftScope 95

drug metabolites 33

drug–protein interactions 254

dynamic combinatorial chemistry 181

dynamic equilibrium ACE 276

dynamic protein affinity selection 365

e

effect directed analysis (EDA) 111, 342, 368

- automated ligand identification system (ALIS) 135
- bioassay testing 136
- fractionation 126
- identification and confirmation 141
- principles 113
- RapidFire system 134
- sample preparation 113
- size exclusion chromatographic (SEC) approaches 133
- SpeedScreen technology 135
- ultrafiltration 134
- workflow of 127

electron capture dissociation 21, 90

electron ionization 206

electron multiplier 18

electron transfer dissociation 21, 90

electroosmotic flow (EOF) 274, 275

electroosmotic mobility 274

electrophoresis 273

electrophoretic mobility 274

electrospray ionization (ESI) 8, 84, 283, 332

electrospray ionization mass spectrometry (ESI-MS) 305

ELISA blocking reagent 339

Ellman's reagent 324

elution time 255

energy-sudden techniques 7

enhanced product ion analysis 25

Envimass 147

enzymatic catalysis 324

enzyme assisted extraction (EAE) 202

enzyme-linked immunosorbent assays (ELISAs) 282, 300

equilibrium dissociation constant 168

ESI capillaries 335

estrogen receptor (ER) 329, 354, 355

ethoxyresorufin-*O*-deethylase (EROD) assay 116

evanescent wave silicon waveguides 308

evaporative light scattering detection (ELSD) 356
 extracted ion chromatograms (EIC/XIC) 2, 329
 extracted ion currents (EIC) 349

f

filtration based assays 367
 first generation antivenomics 229, 230
 FlashQuant MS system quantitation 179
 flavor and fragrance analysis 123
 flow injection analysis (FIA) 353
 flow splitting 334
 fluorescence 320
 fluorescence detection (FLD) 322
 fluorescence detector 335
 fluorescence enhancement based bioaffinity assay 329
 fluorophore 325, 367
 fluoxetine 184–186
 formic acid (FA) 332
 Fourier transform ion cyclotron resonance mass spectrometry (FT-ICR-MS) 16, 210
 fragmentation 20
 frontal affinity chromatography (FAC) 244, 245, 365
 frontal analysis continuous capillary electrophoresis (FACCE) 279
 fused-silica capillaries 274
 fused-silica reactors 338

g

Galantamine 328
 γ -aminobutyric acid (GABA) 171
 gas chromatography olfactometry (GC-O) 122
 gas chromatography–mass spectrometry (GC–MS) 128, 141
 Gaussian distribution 345
 gel electrophoresis 42
 gel permeation chromatography (GPC) 119
 glass microfluidic chips 338
 Global Snakebite Initiative (GSI) 228
 GLUT1 244
 glycopeptide antibiotics 286
 GPR17 249
 GraphPad Prism 278
 GroEL 84

h

headspace analysis 122
 heat dissipation 273

heterobifunctional cross-linker 70
 high-efficiency free-zone electrophoresis 272
 high-field asymmetric waveform ion mobility spectrometry 29
 high performance liquid chromatography (HPLC) 131, 331
 high-precision nano-FAC system 247
 high-resolution screening (HRS)
 – bioassay 336
 – flow splitting 334
 – fluorescence 320
 – vs. HTS 342
 – MS detection 340
 – on-line post-column assays 321
 – separation 330
 – trends 354
 high-temperature liquid chromatography (HTLC) 334
 high throughput affinity screening 252
 high-throughput screening (HTS) 124, 319
 homobifunctional cross-linker 69
 hydrazone libraries 181
 hydrolysis catalyzing enzymes 328
 7-hydroxy-1-methylquinolinium iodide 325

i

IC₅₀ measurement curves 350
 ideal Gaussian distribution 347
 immobilized artificial membrane (IAM) stationary phase 244
 immobilized proteins 244
 immunoaffinity capillary electrophoresis (IA-CE) 271, 272, 281
 immunoaffinity capillary electrophoresis–mass spectrometry (IA-CE–MS)
 – applications 292
 – specific requirements 284
 immunoaffinity chromatography 233, 235
 incubation times 342
 inductively-coupled plasma (ICP) 284
in silico tools 145
 interactomics 136, 372
 intermediate complexation kinetics, *see* kinetic ACE
 internal energy 7
in vitro bioassays 137
 ion detection 18
 ion dissociation 20
 ion electrophoretic mobility 273
 ion-evaporation model 8
 ionization suppression effects 326

ion mobility 90
 ion-mobility mass spectrometry (IMMS)
 81, 210
 ion mobility spectrometry (IMS) 28, 357
 ion-trap instrument 328
 ion-trap mass analyzer 15
 ion trap mass spectrometers 209
 ion-trap-time-of-flight (IT-TOF) 328
 isocratic solvent 334

j

Joule heating 285

k

kinase inhibitors 98
 kinetic ACE 280
 kinetic assay
 – GAT1 175
 – SERT 186

l

label-free biosensors 299, 367
 label free techniques 366
 laser ablation electrospray ionization
 (LAESI) 213, 309
 laser desorption imaging (LDI)-MS 213
 ligand binding 88
 linear-acceleration high-pressure collision
 cell 22
 linear discriminant analysis (LDA) 215
 linear ion trap quadrupole (LTQ) 209
 linear regression analysis 249
 linear solvent energy relation (LSER) model
 147
 linear two-dimensional ion traps 15
 lipophilic analytes 343
 liquid chromatography (LC) separation
 method 61
 liquid chromatography with diode array
 detector–MS (LC/DAD–MS) 301
 liquid chromatography–mass spectrometry
 (LC–MS) 142, 203, 206
 localized surface plasmon resonance (LSPR)
 368
 logarithm of thermodynamic retention
 factors 262
 low-resolution methods 371

m

mass analyzer 12
 – ion-trap 15
 – Orbitrap 17
 – quadrupole 13
 – time-of-flight 15

mass defect 4
 mass spectrum 2
 matrix effect 11
 matrix-assisted laser desorption ionization
 (MALDI) 10, 211
 matrix-free ion sources 309
 mecamlamine 261
 membrane bound proteins 366
 Merck index 145
 metabolic reactions 348
 Metabolomics Standards Initiative (MSI)
 215
 META-PHOR 216
 methanol 331
 METLIN 145
 Michaelis–Menten kinetics 325, 340
 micro-affinity column 247
 microchannel plate detectors 18
 microfluidic chips 337
 micro/nano-fluidic instrumentation 336
 Microsoft Excel 278
 microwave-assisted extraction (MAE) 201
 middle-down approach 43
 miniaturized bioassay 357
 minimal void volume connectors 338
 mobility-shift ACE 276, 277
 MOLGEN-MS 146
 MS Binding Assays 167
 – analytics 170
 – competitive 176
 – dopamine receptors 188
 – γ -aminobutyric acid (GABA) 171
 – GAT1 179
 – kinetic 175
 – library screening 181, 183
 – vs. radioligand binding assays 167, 168
 – saturation assay 174
 – serotonin transporter (SERT) 183
 MS-coupled biosensor platforms 299
 MS detection 340
 MS structure elucidation 347
 multiple reaction monitoring 22
 multiprotein stationary phase 252

n

nano-electrospray 284
 nanoelectrospray ionization (nano-ESI) 9,
 86
 nanoflow-electrospray ionization source
 60
 nanofractionation 129
 nanoplasmonics 307
 native ion mobility 371
 native MS analysis 58, 60

natural extracts 330
N-hydroxysuccinimide (NHS) esters 64
 nicotinic acetylcholine receptor (nAChR) 328
 nicotinic receptors 261
 nitrogen rule 7
 noise 344
 nominal mass 4
 noncovalent protein–ligand complexes 284
 non-equilibrium CE 276
 non-equilibrium CE of equilibrium mixtures (NECEEM) 280
 non-linear chromatography (NLC) 261
 non-volatile buffers 326
 nonvolatile phosphate BGE 284
 NORMAN network 145
 novel screening method 249
 nucleoproteins 305

o

olfactometric analysis 130
 oligonucleotides 304
 on-chip approaches
 – SPR-LDI-MS 304
 – SPR-MALDI-MS 301
 online affinity analysis 141
 online bioluminescence 139
 on-line post-column assays 353
 on-line post-column bioaffinity screening methodology 368
 on-line pre-column synthesis 354
 opioid peptides 292
 Orbitrap 17, 143, 209
 orphan receptors 366
 orthogonal partial least squares discriminant analysis (OPLS-DA) 215
 orthogonal separation methods 343
 overlaid frontal chromatograms 251

p

paperspray ionization 11
 passive sampler device 113
 pentasaccharide 289
 pentaxin 3 (PTX3) 308
 peptides 347
 P-glycoprotein transporter 259, 260
 phosphate-binding protein 324
 phosphodiesterase (PDE) 328
 photoreactive cross-linkers 65
 plant extracts 330
 plant metabolomics approach 370
 plasma polymerized poly-acrylic acid (ppAA) 308

PLE extraction 120
 p38 mitogen-activated protein kinase 321, 325, 329
 polyethylene glycol (PEG) 338
 porous silver nanoparticles (AgNP) 304
 post-column bioaffinity 368
 – measurement 327
 post-fractionation liquid handling 343
 pre-equilibrium ACE 279
 precursor-ion analysis 356
 pressurized hot water extraction (PHWE) 201
 pressurized liquid extraction (PLE) 117, 201
 principal component analysis (PCA) 214
 projection approximation 96
 protein analysis 58
 protein concentration 352
 protein fishing 372
 protein–ligand interaction 332
 protein molecular-weight determination 37
 protein–protein interactions, *in vivo* strategy 71
 protein target 328
 protein unfolding 333
 proteomics 39, 368
 protonation 38
 pseudostatic libraries 182
 PSP toxins analysis 306, 307
 PubChem 145
 pulse dampeners 336
 pulsed ultrafiltration 135

q

QTAX approach 70
 quadrupole mass analyzer 13
 quadrupole mass spectrometer 208
 quadrupole-time-of-flight (q-TOF) 328
 – mass spectrometer 208
 qual/quant strategy 32
 quantitative analysis 31
 quantitative structure–retention relationships (QSRRs) 257

r

radioflow detector system 245
 radioimmunoassays 300
 radiolabeled thyroxine–transthyretin (T₄*-TTR) binding assay 117
 radioligand binding assays 366
 RapidFire system 134
 reconstitution methods 59

resolving power 2
retention factor 255, 256

s

sandwich type assay design 300, 301
saturation assay
– GAT1 174
– SERT 185
Scatchard analysis 279
second generation antivenomics 232, 234
secondary ion mass spectrometry (SIMS) 212
selected-reaction monitoring 22
semi permeable membrane device 115
semi-quantitative determination 88
separation 330
serine protease assay 331
serotonin transporter (SERT) 183
sheath liquid interface 283
sigmoidal dose–response curve 345
signal-to-noise ratio 350
size exclusion chromatography (SEC) 133, 366
size exclusion methodology 365
SKF86002 325
slow association kinetics 339
slow complexation kinetics, *see* pre-equilibrium ACE
snake venomics approach 231
solid-phase extraction (SPE) 114, 115
solid-phase microextraction (SPME) 115, 123
soluble epoxide hydrolase (sEH) 328
solvent assisted flavor extraction (SAFE) 122
solvent composition 257
solvent viscosity 335
Soxhlet extraction 125
spectrophotometric LC detector 339
SpeedScreen technology 135
split ratio 335
SPR-LDI-MS 304
SPR-MALDI-MS 301
staircase method 247, 248
stir-bar sorptive extraction (SBSE) 115, 122
streptavidin/biotin 327
stromal cell-derived factor-1 290
structure-affinity matching 349
supercritical fluid extraction (SFE) 201
superloop 337
surface-enhanced laser desorption ionization 10
surface-induced dissociation 101
surface plasmon polariton (SPP) 307

surface plasmon resonance imaging (SPRi) 308
switching function 261

t

tag-mass concept 310
tandem mass spectrometry 18
– hybrid instruments 25
– ion dissociation 20
– ion mobility spectrometry 28
– ion-trap instrument 23
– MS–MS configuration 21
– Orbitrap-based hybrid systems 27
– TOF–TOF instruments 23
target antigen 281, 282
target protein immobilization 365
theoretical dose response curve 345
thin layer chromatography (TLC) 124
thiocholine 324
tiagabine 172
time-of-flight (TOF)
– mass analyzer 15
– mass spectrometer 208
time-to-digital converter 18
top-down approach 39
total-ion chromatogram (TIC) 2
toxicity identity evaluation (TIE) 112
transient protein–protein interactions 70
transthyretin 190
travelling-wave IMS 92
tribrid Orbitrap-based system 27
two-enzyme dual-HRS assay 354

u

ultrafiltration 134, 365
ultrahigh performance liquid chromatography system 191
ultrasound assisted extraction (UAE) 201
unmatched HRS chromatogram 349

v

vancomycin 286
vinblastin 260
volatile ammonium acetate BGE 284
volatile BGE 284

y

yeast (anti)androgen assay 116

z

zeta potential 274, 275
Z'-factor 351
zonal affinity chromatography 253
zonal elution 258
zonal elution experiment 255, 256