

Index

a

absorbance gradient 306
 acetaminophen 380ff., 390ff., 412ff.
 – non-invasive Raman spectrum 423
N-acetylglucosamine (NAG) 493
 acetylsalicylic acid (ASA) 335ff., 390
 – PLS model 339
 acousto-optic tunable filter (AOTF) 38,
 259
 active principle ingredient (API) 103
 adenocarcinoma
 – cervical 210
 AFM, *see* atomic force microscopy
 AFMIR 489
 – imaging 490
 age-related macular degeneration (AMD)
 142
 agricultural science
 – near-infrared hyperspectral imaging
 260ff.
 algae 254
 Alzheimer's disease 461
 amorphous calcium phosphate (ACP) 152
 anabolic agent 161
 analyte dissociation 495
 animal feed
 – NIR chemical imaging 269
 anisotropic material
 – imaging 321
 anomalous spectral reading 70
 antiresorptive agent 161
 AOTF, *see* acousto-optic tunable filter
 aperture-SNOM (a-SNOM) 474
Arabidopsis 250
 artificial neural network (ANN) 208f.
 – 3-D image 217
 ascorbic acid (ASC) 335ff.
 – PLS model 339
 aspirin, *see* acetylsalicylic acid (ASA)

atomic force microscopy (AFM) tip 475
 ATR (attenuated total reflection) 458
 ATR FT-IR imaging 347ff.
 – diamond accessory 352
 – expanded field of view 354
 – forensic application 370
 – FPA detector 347ff.
 – high-throughput (HT) 367
 – material sciences 358
 – microfluidics device 369
 – pharmaceutical science 347
 – pressure 310
 – quantitative 356
 – variable angle of incidence 355
 ATR FT-IR spectroscopic imaging
 – penetration depth gradient 306
 ATR imaging 53
 ATR microspectroscopy 21ff.
 ATR prism
 – inverted 351

b

band target entropy minimization (BTEM)
 151, 409
 bandpass filter
 – Raman signal enhancement 412
 basal cell carcinoma (BCC) 140
 baseline correction 69
 Beer–Lambert law 67f.
 Beer–Lambert model
 – Raman emulsion image 74
 Bessel function 21
 bias 79
 biological sample preparation 458
 biology 473, 486ff.
 biomedical application
 – infrared microscopy 451ff.
 – synchrotron radiation 451ff.

- biomedical sample
 – 3-D imaging 203ff.
 biopolymer 311
 – phase separation 318
 – structure 251
 bisphosphonate alendronate (ALN) 155f.
 blinking 495
 bone 149ff.
 – adaptation in response to external stress 156
 – adaptation in response to osteoporosis 159
 – composition 461
 – genetic modification 154ff.
 – infrared and Raman imaging 150
 – infrared and Raman spectroscopy 149
 – probing 414
 – Raman spectrum 418
 – subchondral 165
 brain tissue 128
 – mouse 129
 brain tumor 128
 – primary 131
 – secondary 133
 breast cancer (BC) 416
 – metastase 133
 buccal cell 175ff.
- c**
- caffeine 335ff., 390
 – PLS model 339
 calcification 416
 calcium hydroxyapatite 417
 calcium oxalate 417
 calibration model 78f.
 cancer diagnosis 140
 carbon nanotube (CNT) 480
 – single-walled (SWNT) 480
 – TERS 480
 cardiac muscle cell (cardiomyocyte) 215
 carotenoid 141
 cartilage
 – infrared and Raman imaging 164ff.
 – infrared and Raman spectroscopy 162f.
 – mineralized 165
 – unmineralized tissue 164
 – zone 163
 Cassegrain objective 7
 CCD (charge-coupled device) array detector 25f.
 CCD detector 29ff.
 CCD-Raman spectrometer 26f.
 cell
 – cervical 188
 – cultured 176
 – exfoliated 175
 – human urine-borne 185
 – infrared spectrum 182
 – liposome uptake 196
 – morphology 192
 – oral mucosa (buccal) 184
 – plant 234
 – Raman spectrum 182
 – subcellular organization 192
 cell collection 175
 cell culturing method 175
 cell wall
 – ester 253
 – heterogeneity 253
 – mutation 252
 – *Staphylococcus epidermidis* 493
 cell wall architecture 248
 – FT-IR spectrum 249
 cellulose polymer 391
 – IMS 247
 central nervous system (CNS) 117
 cervical adenocarcinoma, *see*
 adenocarcinoma
 cervical cell
 – human and canine 188
 cervix uteri 135
 chemical imaging analysis 285, 369
 chemical mapping
 – on-line 286
 chemical specificity 263
 chemimage (chemical imaging) 209
 – 3-D 210
 chemometrics 65ff.
 chondroitin sulfate 163
 Christiansen effect 21
 chromosome 196
 cluster analysis 81, 126
 – hierarchical 81, 135f., 181
 clustering process 81
 coastal Bermuda grass (CBG) 244
 collagen 127, 150, 414
 – crosslinking 461
 – type II 163ff.
 colon tissue 124
 colorectal cancer (CC)
 – metastase 133
 compatibilizer 361
 concentration matrix 392
 confocal microscope 27
 confocal Raman microspectroscopy
 – human cell 192
 connective tissue 115f.
 continuous-scanning FT-IR imaging 437

- continuous-scanning FT-IR spectroscopy 437
 corn – NIR imaging 263
 corneocyte biology 139
 correlation coefficient 392
 counterfeit drug – non-invasive detection 421
 counterfeit tablet 372 – imaging 372
 cytology – infrared 184
 CytoSpec software 209
 Czerny-Turner monochromator 25
 Czerny-Turner spectrograph 429
- d**
 data acquisition 178 – Raman spectral mapping 178 – Raman spectroscopy 178
 data analysis 179, 388 – Raman image 393 – spectroscopy 388 – supervised 392 – unsupervised 388ff.
 data collection – mode 458
 data pretreatment/preprocessing 70, 179
 data processing 290
 data reproduction 90
 de-noising 69
 deoxynivalenol (DON) 277
 desiccation study 243
 detection limit 382
 detector – FPA, *see* focal plane array detector – hybrid linear array 50 – infrared 458 – InSb FPA 39, 431 – low-frequency 458 – MCT, *see* MCT detector – mid-infrared microspectroscopy 9 – single element 337ff. – two-dimensional array 45
 deuterated triglycine sulfate (DTGS) detector 9
 DEXA, *see* dual energy X-ray absorptiometry
 diamond ATR accessory 353ff.
 diamond ATR imaging 365
 differential interference contrast (DIC) 457
 diffuse reflection (DR) measurement – FT-NIR spectrometer 337
 diffuse reflection spectroscopy 9
 diffusion 327ff., 357 – coefficient 333 – exponent 332 – Fick's law 327 – FT-IR imaging spectroscopy 328ff.
 – polyamide 327ff.
 digital mirror array (DMA) 290
 dimyristoylphosphatidylcholine (DMPC) 451
 direct classic least square (DCLS) method 389ff.
 DIRLD, *see* dynamic IR linear dichroism
 disease diagnosis 140 – probing of bone 414
 distance 181
 DNA 461 – apertureless s-SNOM IR imaging 488 – BCB-labeled 492 – mitosis 196
 DR, *see* diffuse reflection
 drug delivery system 197
 dual aperturing 17f.
 dual energy X-ray absorptiometry (DEXA) 414
 dynamic IR linear dichroism (DIRLD) 442
 dynamic mechanical analysis (DMA) 442
- e**
 electron multiplying CCD (EMCCD) 30
 emission IR spectroscopy (IRES) 444 – PA-IR spectrograph 444
 emission PA-IR imaging 444
 enamel 465
 energy-dispersive X-ray fluorescence (EDXRF) 377
 – hyperspectral imaging 401
 epithelium 114
 – cancerous oral epithelial cell 461
Erysiphe cichoracearum 250
Escherichia coli 277, 489
 étendue 10
 Euclidean distance 81ff., 181, 392
 evanescent wave 122
 extracellular matrix (ECM) 115
- f**
 fibroblast – infrared a-SNOM 486
 film – ultrathin 434
 finger surface 371
 fish – NIR hyperspectral imaging 286

- fixed-size image window-evolving factor analysis (FSIW-EFA) 87ff.
 - flat field correction 31
 - flax fiber 250
 - focal plane array (FPA) detector 347ff., 429, 452
 - ATR FT-IR imaging 347ff.
 - focal plane array imaging system 17, 52, 227
 - food
 - candling 282
 - chilling injury 281
 - external contamination 275
 - foreign body 275ff.
 - human detectable defect 280
 - internal defect 282
 - internal quality trait 284
 - near-infrared hyperspectral imaging 260ff.
 - potential defect 281
 - potential greening area 281
 - quality control 271ff.
 - surface liquid contamination 277
 - surface and subsurface nonconformity 279
 - forensic application 370
 - attenuated total reflection (ATR) FT-IR imaging 370
 - Fourier transform, *see* FT
 - Fourier transform infrared, *see* FT-IR
 - Fourier transform near infrared, *see* FT-NIR
 - free electron laser (FEL) 12f., 486
 - front-surface reflection 8
 - fruit
 - NIR hyperspectral imaging 285
 - FT-IR/FT-NIR polarization spectroscopy 321ff.
 - FT-IR imaging (FT-IRI) 452ff.
 - instrumentation 299ff.
 - preparation of soft tissue 121
 - reflection 457
 - transmission 457
 - FT-IR imaging microscope 452
 - FT-IR image
 - measurement 305
 - FT-IR microspectroscopy (FT-IRM) 457
 - reflection 457
 - spatial resolution 228, 452
 - synchrotron-based 461
 - transmission 457
 - FT-IR reflection-absorption spectroscopy (FT-IRRAS) 436
 - FT-IR spectroscopic imaging
 - material sciences 297ff.
 - pharmaceutical sciences 297ff.
 - FT-IR spectrometer 6ff.
 - IRES 444
 - FT-NIR spectrometer 41
 - diffuse-reflection measurement 337
 - single-element detector 337
 - FT-Raman spectrometer 26
 - FT-TIRS 445
 - full-width at half height (FWHH) 38
 - Fusarium* 277
 - fuzzy C-means (FCM) 136
- g**
- GBM (glioblastoma multiforme) 131f.
 - genetic modification
 - adaptation of bone 154
 - genetic network 249
 - genetically modified organism (GMO) 261ff.
 - NIR chemical imaging 267
 - geometric control point (GCP) calibration 291
 - germination study 241
 - glandular tissue 212
 - β -glucan 253
 - glycosaminoglycan (GAG) 163
 - GNU image manipulation program (GIMP) 207
- h**
- hard tissue 149ff.
 - hardware development 289
 - heart
 - adult mouse 215
 - hierarchical cluster analysis (HCA) 81, 135, 181
 - unsupervised (UHCA) 205ff.
 - HIV transcriptional activator-derived (TAT) peptide 197ff.
 - modified deuterated liposome (TATp-LIP) 197ff.
 - hollow-fiber bioreactor (HFBR) 164ff.
 - hyaluronic acid (HA) 163
 - hybrid linear array detector 50
 - hydroxylpropylmethylcellulose (HPMC) 356ff.
 - hypercube 379, 391
 - hyperspectral image 66
 - Beer-Lambert law 67f.
 - data set 66
 - hyperspectral imaging 378ff.
 - mid-infrared 45

i

ICA, *see* independent component analysis
 image
 – 3-D 209
 image analysis
 – chemometric 65ff.
 – exploratory 72ff.
 – monolayer 84
 – multilayer 84
 – between-image quantitation 105
 – within-image quantitation 105
 image compression 71
 – resolution 95f.
 image evaluation 313
 image information
 – quantitative 77
 image preprocessing 68
 image quality 380
 image representation 72
 – classical 72
 image resolution 84, 92ff.
 – concept 84
 image segmentation 80
 image total rank 93
 imaging
 – 1-D imaging 427
 – 3-D imaging of biomedical sample 203ff.
 – anisotropic material 321
 – compacted tablet 361
 – introduction 3
 – single plant cells 234
 IMS, *see* infrared microspectroscopy
 independent component analysis (ICA) 76
 index of compactness 81
 indium antimonide (InSb) FPA 431
 – Stirling-engine-cooled detector 39
 infinity correction 20
 infrared a-SNOM 486
 infrared absorption spectroscopy (IRA) 478
 – near-field 478
 infrared beamline 455
 – extraction 456
 infrared data collection 458ff.
 infrared detector 458
 infrared FPA detector 458
 infrared imaging
 – bone 150
 – cartilage 164ff.
 infrared instrumentation 179
 infrared microscope 226, 451ff.
 infrared microspectrum
 – reflection mode 459
 – transmission mode 459

infrared microspectroscopy (IR-MSP, IMS)
 225, 451ff.
 – application 240
 – biomedical application 451ff.
 – cellulose polymer 247ff.
 – flax 250
 – polarized 248
 – sample preparation 177
 – stem 247
 infrared s-SNOM 484
 infrared spectral imaging
 – individual cell 173ff.
 infrared spectroscopy
 – bone 149
 – cartilage 162f.
 – individual cell 173ff.
 infrared spectrum
 – cell 182
 interferometer
 – continuous 9
 – rapid-scan 9
 InSb FPA 431
 internal reflection element (IRE) 21ff.
 IR-PLAN microscope 226ff.
 IRES, *see* emission IR spectroscopy

k

kernel 230ff., 264
 – 3-D NIR chemical imaging 265
 Kohonen algorithm 249
 Kramers–Kronig reflection 8

l

lack of fit 90
 leave 244
 lens 142
 library spectrum 97f.
 lightning rod effect 476
 lignification 247
 linear discriminant analysis (LDA) 131ff.
 liposome 196
 – deuterated 197f.
 liquid crystal (LC) 437
 liquid crystal tunable filter (LCTF) 36f.,
 259, 300
 liquid-based method 173
 liver fibrosis 461
 loading vector 180
 local rank constraint 92f.
 local rank pixel 93
 Lorentzian function 284
 low-density lipoprotein 141
 low-frequency detector 458

- lung cancer (LC)
 - metastase 133
- Lyot filter 37

- m**
- macro ATR-FT-IR imaging
 - counterfeit tablet 372
 - macro FT-IR imaging 304f.
 - magnesium image 399
 - Mahalanobis distance 181
 - mapping 386
 - chemistry of a sample 285
 - DuoScan 387f.
 - introduction 3ff.
 - plant tissue section 231
 - point 387
 - pulsed terahertz radiation 56
 - transition across botanical parts 232
 - material sciences 297ff., 473
 - ATR FT-IR imaging 358
 - FT-IR spectroscopic imaging 297ff.
 - NIR spectroscopic imaging 297ff.
 - MATLAB 205ff.
 - matrix 181
 - MCR-ALS, *see* multivariate curve resolution-alternating least squares
 - MCT (mercury cadmium telluride) array 227, 428
 - MCT detector 9, 431, 458
 - narrow-band 9
 - wide-band 9
 - MCT FPA 431
 - MCT PA-IR spectrograph 433
 - MIA, *see* multivariate image analysis
 - Micrasterias hardyi* 461
 - micro ATR FT-IR imaging 360
 - tablet compaction 363
 - tablet dissolution 364
 - micro ATR imaging 351
 - micro FT-IR imaging 303
 - spatial resolution 312
 - micro-PA-IR system 447
 - microcrack 157f.
 - microelectromechanical system (MEMS) 289
 - microfluidics 369
 - microscope 5ff.
 - microspectroscopy
 - transmission, *see* transmission microspectroscopy
 - mid-infrared hyperspectral imaging 45
 - mid-infrared microspectroscopy 5ff.
 - detector 9
 - source 12
 - Mie scattering 21
 - mineralized tissue 151
 - missing component 93
 - mitochondrial distribution 195
 - mitosis 196
 - morphological analysis 394
 - morphology-dependent resonance 21
 - mosaicing 4
 - multi-image analysis 100ff.
 - multilayer resolution 100
 - multimodal hyperspectral imaging
 - Raman 397
 - multispectral imaging 276
 - multiplicative signal correction (MSC) 336
 - multivariate analysis
 - unsupervised 389
 - multivariate curve resolution-alternating least squares (MCR-ALS) 90
 - multivariate image analysis (MIA) 65, 72
 - multivariate image construction 205
 - multivariate image regression (MIR) 77
 - calibration 78
 - prediction 78
 - muscle tissue 116
 - musculoskeletal tissue 150f.
 - mycotoxin 277
 - myocardial fibrosis 216
 - myoglobin 451

 - n**
 - natural moisturizing factor (NMF) 139
 - Nd : YAG laser 26
 - near-field Raman imaging
 - tip-enhanced coherent anti-Stokes Raman scattering (TE-CARS) 488
 - near-field scanning optical microscopy (NSOM) 34
 - near-field spectroscopic method 479
 - near-infrared, *see* NIR
 - nervous tissue 117
 - neural network 249
 - NeuroDeveloper software 209
 - NIR (near-infrared) chemical imaging method 262ff.
 - genetically modified organism (GMO) 267
 - plant breeding 267
 - NIR diffuse-reflection single-element detector spectroscopy 341
 - NIR diffuse-reflection imaging spectroscopy 341
 - NIR hyperspectral imaging 36, 259ff.
 - agricultural science 260ff.
 - food 260ff.

– pharmaceutical drug formulation 335
 NIR imaging
 – calibration 290
 – characterization 290
 – external contamination 275ff.
 – industrial scale 271
 – instrumentation 299ff.
 – internal defect 282ff.
 – laboratory-based 261ff.
 – on-line 272
 NIR imaging spectroscopy
 – pharmaceutical drug formulation 335
 – quality control 335
 NIR radiation
 – pathlength 301
 NIR spectroscopic imaging
 – material sciences 297ff.
 – pharmaceutical sciences 297ff.
 NIR spectrum 338
 – median imaging 338
 – single pixel imaging 338
 noise equivalent power (NEP) 10
 noise equivalent power temperature (NEPT)
 429
 nucleic acid 451

o

octadecanephosphonic acid (OPA) 14
 octadecyltrichlorosilane (OTS) 434ff.
 ocular tissue 141
 on-line application
 – food quality 272ff.
 – NIR hyperspectral imaging 288
 on-line setting
 – NIR imaging 274
 OPA, *see* octadecanephosphonic acid or
 optical parametric amplifier
 optical parametric amplifier (OPA) 485
 optical parametric oscillator (OPO) 483
 optical path difference (opd) 9
 optical throughput 10
 oral mucosa cell 175ff.
 osteoarthritis 461
 osteogenesis imperfecta (OI) 155, 414
 osteon 152
 osteopetrosis 461
 osteoporosis 159, 416, 461

p

PA (planar array)-DIRLD 443
 PA-IR microscopy 447
 PA-IR spectrophotograph 427
 PA-IR spectroscopy 427ff., 441
 – time-resolved 437ff.

PA-IRES spectral image 446
 PA-TIRS 445
 paracetamol, *see* acetaminophen
 parenchyma bundle sheath (PBS) 244
 Parkinson's disease 461
 pathlength 301, 357
 penetration depth gradient
 – ATR FT-IR spectroscopic imaging 306
 4-n-pentyl-4'-cyanobiphenyl (5CB) 437ff.
 pharmaceutical capsule
 – quality control 421
 pharmaceutical drug formulation 335
 – quality control 419
 – quantitative determination of active
 ingredient 335ff.
 – spatial distribution of active ingredient
 340
 pharmaceutical science
 – attenuated total reflection (ATR) FT-IR
 imaging 361ff.
 – FT-IR spectroscopic imaging 297ff.
 – NIR spectroscopic imaging 297ff.
 pharmaceutical tablet, *see* tablet
 pharmacology 140
 phase separation 318
 phospholipid 451
 photomultiplier tube (PMT) 25
 pixel 66ff.
 – anomalous 70
 planar array, *see* PA
 plant material
 – FT-IR microspectroscopic imaging 225ff.
 – IMS 230
 – kernel 230
 – seed 230
 – tissue section 231
 PLS-discriminant analysis (PLS-DA) 82
 polarizability 478
 polarization spectroscopy 322
 polarized radiation, *see* radiation
 polyamide (PA) 327
 – diffusion 327ff.
 – FT-IR imaging spectroscopy 328
 – PA11 327ff.
 polycarbonate (PC)
 – FT-IR/ATR imaging 314f.
 poly(dimethyl siloxane) (PDMS) 353ff., 368
 poly(ethyl acrylate) (PEA) 486
 polyethylene
 – blend 361
 – FT-IR/ATR imaging 314f.
 poly(ethylene glycol) (PEG) 357
 poly(ethylene naphthalate) (PEN) 431
 poly(ethylene terephthalate) (PET) 313

- aluminium-metallized 316
 - FT-IR/ATR image 316
 - poly(3-hydroxybutyrate) (PHB) 318ff.
 - blend 318ff.
 - FT-IR transmission spectrum 318
 - phase separation 321
 - poly(lactic acid) (PLA) 318ff.
 - blend 318ff.
 - FT-IR transmission spectrum 318
 - phase separation 321
 - polymer
 - attenuated total reflection (ATR) FT-IR imaging 347
 - FT-IR imaging 318
 - interdiffusion 357
 - IR s-SNOM 484
 - quality control 318
 - polymer/carbon fiber interface 358
 - poly(methyl methacrylate) (PMMA) 30, 53, 407, 484
 - polymorphonuclear leukocyte (PMN) 138
 - polypropylene
 - isotactic (iPP) 442
 - polystyrene (PS) 361, 430f., 484
 - poly(vinyl alcohol) (PVA) 437
 - poly(vinylidene fluoride) (PVDF) 324ff.
 - stress-induced phase transformation 324
 - poly(vinyl pyrrolidone) (PVP) 355
 - interdiffusion 357
 - Powell lens 41
 - principal component 73, 180
 - principal component analysis (PCA) 69ff., 87, 180
 - model 74
 - vibrational spectroscopic image 129
 - process analytical technology (PAT)
 - pharmaceutical 419
 - prostate tissue 142
 - protein 451
 - secondary structure 251
 - pulsed terahertz radiation 56

 - q**
 - quality control
 - food 271ff.
 - near-infrared (NIR) imaging spectroscopy 335
 - pharmaceutical capsule 419
 - pharmaceutical tablet 419
 - polymer 318
 - quantitation
 - between-image 105
 - within-image 105
 - quilting 4
- r**
- radiation
 - polarized 321ff., 439
 - Raman a-SNOM 491
 - Raman emulsion image 74
 - Raman hyperspectral imaging 41, 379ff., 396ff.
 - acetaminophen 396
 - aspirin 396
 - caffeine 396
 - pharmaceutical sample 383
 - spectroscopy 383
 - Raman image 381, 396
 - caffeine 395
 - data analysis 393
 - histogram 394
 - Raman imaging
 - bone 150
 - cartilage 164ff.
 - preparation of soft tissue 123
 - Raman imaging microscope 44
 - Raman map 386
 - tablet 397
 - Raman microscope
 - confocal dispersive 383
 - Raman microspectroscopy 24ff.
 - confocal, *see* confocal Raman microspectroscopy
 - sample preparation 177
 - Raman scattering 379f.
 - Raman signal enhancement 412
 - Raman spectral imaging
 - individual cell 173ff.
 - instrumentation 383
 - pharmaceutical product 377
 - Raman spectral mapping
 - data acquisition 178
 - Raman spectroscopy
 - bone 149
 - cartilage 162f.
 - data acquisition 178
 - deep, non-invasive 405ff.
 - diffusely scattering medium 405
 - individual cell 173ff.
 - spatial method 407
 - technique 406
 - temporal method 406
 - ultrafast gating 406
 - Raman spectrum
 - cell 182
 - Raman tomography 424
 - random walk model 301
 - Rayleigh criterion of resolution 16
 - redundant aperturing 17

- region of interest (ROI) 336ff.
 renal cell carcinoma (RCC)
 – metastase 133
 resilient back propagation (Rprop) algorithm 209
 resolution 15f.
 – compressed image 95f.
 – method 85
 – postprocessing identification 98
 – process 89ff.
 – spatial 15ff., 31, 228, 312, 452
 – spectral 382
 – subcellular 453
 retina 142
 – macular degeneration 142
 RGB (red/green/blue) system
 – food quality control 271
 – image 342f.
 Riccati–Bessel function 21
 RNA 461
 root mean square error in prediction (RMSEP) 79, 339f.
- s**
- sample deposition 177f.
 sample preparation 177, 204
 sampling 52
 – techniques 5ff.
 scanning near-field infrared microscopy (SNIM) 483
 scanning near-field optical microscopy (SNOM) 474
 – aperture probe 474
 – illumination mode 486
 scattering medium
 – diffusely 405
 scattering SNOM (s-SNOM) 474ff.
 Schwarzschild objective 7, 452
 SCIRun 207ff.
 scrapie 461
 seed 230ff.
 segmentation method 80
 – fuzzy 83
 – hard 83
 – supervised 80
 – unsupervised 80
 self-assembled monolayer (SAM) 434
 self-interactive modelling class analogy (SIMCA) 82, 133
 self-modeling curve resolution (SMCR) 151
 semiconductor 481
 SERS, *see* surface-enhanced Raman scattering
 Si phonon signal 482
- signal modulation 494
 – surface roughness 494
 – TERS 494
 signal preprocessing 69
 signal-to-noise ratio (SNR) 10ff., 49ff., 380
 – image quality 380
 silk fibroin
 – near-IR spectroscopy 251
 SIMPLISMA 71, 85ff.
 skin 139
 – Raman system 141
 soft tissue 113ff.
 – application 124
 – preparation for FT-IR-imaging 121
 – preparation for Raman imaging 123
 – preparation for vibrational spectroscopic imaging 118
 source
 – mid-infrared microspectroscopy 12
 spatial offset Raman spectroscopy (SORS) 407ff., 423
 – inverse 410
 spatial resolution 15ff., 31, 228, 312, 452
 spectral cytology 175ff.
 – fixation 177
 spectral imager
 – calibration 291
 spectral resolution 382
 spectrograph
 – prism based 447
 spectroscopic imaging 479
 – biological application 491
 – nanometer resolution 473ff.
 – near-field method 473ff.
 spectroscopy
 – biomedical sample 204f.
 spectrum
 – vibrational 119ff.
 specular reflection 8
 squamous cell carcinoma 135
Staphylococcus epidermidis
 – cell wall 493
 statistical analysis 393
 stem
 – IMS 247
 Stingray hyperspectral imaging spectrometer 45ff.
 subsampling problem 411ff.
 subsurface signal
 – discrimination 407
 surface chemistry 473
 surface-enhanced Raman scattering (SERS) 34ff., 475
 synchrotron 12f.

- biological sample preparation 458
- instrumentation 455
- radiation 451ff.
- synchrotron FT-IRM 463ff.
- synchrotron IR microscope 457
- synchrotron IR microscopy
 - kernel 237
 - plant tissue 237
 - seed 237
- synchrotron IR microspectroscopy (IMS) 461ff.
- biological and medical application 461ff.
- synchrotron IR source 454
- beam line extraction 456

- t**
- T-Ray FT-IRM 466
- tablet 397
 - compacted 361ff.
 - counterfeit tablet 372
 - quality control 419
- target factor analysis 97
- targeted chemical composition analysis 285ff.
- TAT, *see* HIV transcriptional activator-derived (TAT) peptide
- terahertz (THz) FT-IRM 466
- terahertz spectrometer 59
- test system 313
- tip
 - contamination 495
 - performance 494
- tip-enhanced coherent anti-Stokes Raman scattering (TE-CARS) 488
- tip-enhanced Raman spectroscopy (TERS) 33, 474ff.
- analyte dissociation 495
- carbon contamination 495
- gap-mode 477
- signal modulation 494
- surface roughness 494
- tip-enhanced Raman (TER) spectrum 493
- tissue
 - engineering 166
 - glandular, *see* glandular tissue
 - hard, *see* hard tissue
 - internal defect in food 283
- mineralized, *see* mineralized tissue
- normal and healthy 151
- plant 231ff.
- soft, *see* soft tissue
- trace detection 370
- ATR FT-IR imaging 370
- training matrix 392
- transflection spectroscopy 8
- transient infrared spectroscopy (TIRS) 445
- transmission microspectroscopy 20
- transmission Raman spectroscopy 411
- two-dimensional array detector 45

- u**
- ultrafast gating 406
- Raman spectroscopy 406
- univariate image construction 205
- unsupervised hierarchical clustering analysis (UHCA) 205ff.
- ANN model 219
- image 210
- stack plot 209
- urine cytology 186

- v**
- vibrational hyperspectral imaging 3
- vibrational spectrometry 36, 56ff.
- vibrational spectroscopic imaging
 - hard tissue 149ff.
 - soft tissue 113ff.
- vibrational spectrum
- reference material 119ff.
- vitreous 142
- voxel 40, 66

- w**
- Ward's algorithm 81, 181
- wheat quality 241
- wood
 - NIR hyperspectral imaging 286

- x**
- X-ray fluorescence (XRF) mapping 399

- z**
- ZnSe ATR accessory 351ff.
- ZnSe ATR imaging 365