
INDEX

Illustrations and figures are in *italics*.

Tables are in **bold**.

- accreditation 338
accuracy 13, 234, 312, 336, 338, 422–3
ACD/ChemSketch 119
ACD/ChromManager 118
ACD/GC Simulator 117–18
ACD/MS Fragmenter 118
ACD/Name Chemist Version 119
ACD/SpecManager Analytical Data Management System 118
acetaldehyde 399–400
acetaldehyde adducts **396**, 399–400
acetaminophen 376, 377
acquisition rate 32–3 *see also* scanning speed
 high-resolution LC/MS instruments 52
 tandem quadrupole instruments 50
 time-of-flight (TOF) analysers 17, 128–9
acrylamide (AA) 402
adenine adducts 402–3
adsorbents 242, **244**
aerial surveillance maps 254
aerodynamic lens systems 363
aerosol analysis 177–80, 353–81, 437
 classes 369
 single-particle analysis 361–76
aerosol mass spectrometers (AMS) 376
aerosol TOF mass spectrometer (ATOFMS) 372–4
Agilent Technologies 99
air analysis *see* atmospheric analysis
aircraft volcanic emission mass spectrometer 209
alachlor (2-chloro-2',6'-diethyl-N-(methoxymethyl)-acetanilide) 156, 213–14, 215
alcohol consumption 399
alcohols 98
aldehydes 34
aliphatic aldehydes 34
aliphatic amines 98
alkanes 247
alkenes 247
alkylguanine DNA adducts 406
alkynaphthalenes 24, 25
Alzheimer's disease 403
ambient conditions 246, 249–52
ambient ionisation 192, 217–18, 434 *see also*
 desorption electrospray ionisation (DESI);
 direct analysis in real time (DART)
ambient mass spectrometry 147–61
AMDIS *see* automated mass spectral deconvolution and identification system (AMDIS)
American Petroleum Institute 93
American Society for Testing and Materials (ASTM) 93
aminomethylphosphonic acid (AMPA) 319–22, 323
AMPA *see* aminomethylphosphonic acid (AMPA)
angular velocity 417
animal feed 181
anion abstraction 7
anthropogenic pollutants 239, 240, 247–9
anti-benzo[a]pyrene diol epoxide (BPDE) 81
antibiotics 288–9
APCI *see* atmospheric pressure chemical ionisation (APCI)
APPI *see* atmospheric pressure photoionisation (APPI)
archaeology 486, 487
aromatic amine adducts 81, 393–8, **394**
aromatic amino acids 81
aromatics 247
arsenic 231 *see also* organoarsenics
arsenobetaine 294, 295
arson accelerants 438
ASAP *see* atmospheric solids analysis probe (ASAP)
ash clouds 353, 354
asphaltenes 422, 423
Atlas of Mass Spectra, The 94
atmospheric analysis
 ambient mass spectrometry 155
 desorption electrospray ionisation (DESI) 155
 Fourier transform ion cyclotron resonance (FT-ICR) analysers 437
 gases 241–2, 358–60
 inductively coupled plasma mass spectrometry (ICP/MS) 229

- particles 229, 360–1
proton-transfer reaction mass spectrometry (PTR/MS) 242, 243
sample collection 243
semi-permeable membranes 187–8
urban 246–9
volatile organic compounds (VOCs) 241–2
- atmospheric gas monitoring 209
atmospheric organic matter 437
atmospheric pressure chemical ionisation (APCI) 10, 45–6, 47 *see also* atmospheric solids analysis probe (ASAP)
fullerenes 298–9
herbicides 78
hydrocarbon compounds 213
natural organic matter (NOM) 451–2
organotins 292, 293
pesticides 317
pharmaceutical contaminants 78
portable devices 193, 194
sensitivity 317
sludge analysis 78
wastewater analysis 78
- atmospheric pressure desorption ionisation 167 *see also* desorption electrospray ionisation (DESI)
- atmospheric pressure ionisation (API) 42, 45–7 *see also* atmospheric pressure chemical ionisation (APCI); atmospheric pressure photoionisation (APPI); electrospray ionisation (ESI)
- desorption electrospray ionisation (DESI) 150
mixed modes 47, 48
pesticides 317
- atmospheric pressure photoionisation (APPI) 10, 46, 48
CDDs/CDFs 344
Fourier transform ion cyclotron resonance (FT-ICR) analysers 433–5
natural organic matter (NOM) 451–2
petroleomics 434, 435
polycyclic aromatic hydrocarbons (PAHs) 434
atmospheric solids analysis probe (ASAP) 149, 151
atomic absorption spectrometry (AAS) 361
atomic masses 423, 424
atrazine (2-chloro-4-(ethylamino)-6-(isopropylamino)-1,3,5-triazine) 156, 213–14
- Australia 249
automated mass spectral deconvolution and identification system (AMDIS) 91, 112–15
automation 65, 347–8
autonomous underwater vehicles (AUVs) 204–5, 206, 207, 212
- AUVs *see* autonomous underwater vehicles (AUVs)
average carbon oxidation state (OS_C) 452, 454
averaging 23
- background subtraction 23, 24, 129
barium salts 225
- benz[a]anthracene 217
benzene 212, 213, 214
benzo[a]pyrene (BP) 400
benzo[e]pyrene 217
benzyl chloride 2
beryllium 225
beverage analysis 484, 488–90
biogenic pollutants 239, 240, 249–52 *see also* emerging contaminants (ECs)
biological tissue imaging 173, 461–2, 469, 470, 471, 472, 473
biomass burning 178–9
biomass-burning organic aerosol 378
biosignatures 453
bird migration 486, 487
bitumen 431, 433
bladder cancer 267
blanks 334
blind samples 338
blood samples 388–9
brain tissue 403
breast tissue 402–3
broad spectrum analysis 23
bromate 265, 276–7
bromine isotopes 3, 275
bulk particle analysis 360–1
bulk stable isotope analysis technique (BSIA) 481–2
Bureau Communautaire de Référence (BCR) 235
1,3-butadiene (BD) 396, 401, 404
- CAD *see* collisionally activated dissociation (CAD)
cadmium 225
caffeine 291
calibration
Fourier transform ion cyclotron resonance (FT-ICR) analysers 422
high-resolution mass spectrometers (HRMS) 335, 336
isotope dilution mass spectrometry (IDMS) 337
matrix effects 336
multi-point 335
proton-transfer reaction mass spectrometry (PTR/MS) 245–6
standards 336
calibration plots 38, 61, 174, 336
cancer 267, 387, 398, 399
capillary columns
film thickness 124, 125, 127
height 124, 125, 127
limitations 123
capillary electrophoresis (CE) 10
capillary HPLC/nanospray ionisation MS (capLC/nanoESI) 402–3
carbon 475, 477, 478, 488
carbon dioxide 208, 209
carbon number 427
carbon number distribution plots 430–3

- carboxylic acids 437
carcinogens 387, 398
carrier gas velocity 124
catalytic convertors 231
CDDs *see* chlorinated dibenzo-*p*-dioxins (CDDs)
CDFMS *see* compact double focusing mass spectrometer (CDFMS)
CDFs *see* chlorinated dibenzofurans (CDFs)
CE *see* capillary electrophoresis (CE)
cellulose 253–4
certified reference material (CRM) 234–5, 335, 337–8 *see also* standard reference material (SRM)
charge exchange 7
Chemical Abstract Services registry number (CASrn) 95, 96
chemical ionisation (CI) 6–8
 CDDs/CDFs 344
 limitations 8
 pesticides 313
 sensitivity 313–14
ChemSite Pro 119
chip/MS 406–7, 408
chlorinated dibenzo-*p*-dioxins (CDDs) 329–49
 delay time 342, 343
 dwell time 342, 343
 fragmentation 340
 ionisation energy (IE) 340
 limits of analysis 349
 regulatory methods 346
 sample preparation 332–5
 selected ion monitoring (SIM) 341–2
 structure 330
 theoretical isotope ratio 342, 343
chlorinated dibenzofurans (CDFs) 329–49
 delay time 342, 343
 dwell time 342, 343
 fragmentation 340
 ionisation energy (IE) 340
 limits of analysis 349
 regulatory methods 346
 sample preparation 332–5
 selected ion monitoring (SIM) 341–2
 structure 330
 theoretical isotope ratio 342, 343
chlorine isotopes 2, 3, 275
chlorite 265
chloroform 265
chondritic organic matter (COM) 447, 448–52
chromium 231
ChromView 120
CID *see* collision-induced dissociation (CID)
cigarette smoke 35, 37, 393, 398
1,8-cineole 240–1
cis-1,2-diol compounds 170–1, 172
CIT *see* cylindrical ion trap (CIT)
classification algorithms 368
climate change 355, 356
cluster ion guns 467
coal samples 430
coelution 36, 114, 129
cold electron ionisation (EI) 132, 134
collision-induced dissociation 68, 136–7, 150, 291, 376, 391 *see also* collisionally activated dissociation (CAD)
collision/reaction cells 51, 69, 227, 228
collisionally activated dissociation (CAD) 68, 74, 76, 78, 109–10 *see also* collision-induced dissociation (CID)
colon cancer 399
columns
 CDDs/CDFs 339
 clean-up 347, 348
 efficiency 124
 film thickness 124, 125, 127
 height 124, 125, 127
 switching methods 401, 403–6, 407–8
 validation 335
compact double focusing mass spectrometer (CDFMS) 200, 201
compositional space 444, 445, 446
compound-specific isotope analysis (CSIA) 481, 482
confirmatory analysis 53–4, 55
containers 242–3
continuous-dynode electron multipliers 203
continuous flow isotope ratio MS (CF-IRMS) 481
corona discharge 47, 178, 193
costs of mass spectrometry 167
Coulomb contribution 421
Coulombic repulsion 168
crude oil 436
 abiotic changes 436
 ambient mass spectrometry 157, 159, 160
 asphaltenes 423
 biotic changes 436
 carbon number distribution plots 433
 consumption 436
 double bond equivalents (DBE) 433, 434
 electrospray ionisation (ESI) 420
 Fourier transform ion cyclotron resonance (FT-ICR) analysers 416, 420
 heteroatom class 432
 Kendrick mass defect (KMD) 429
 Kendrick plots 429
 van Krevelen diagrams 430, 431, 432
cryosections 173
cycloidal focusing mass analyser 201
cyclotron frequency 417–18, 422
cylindrical ion trap (CIT) 16, 197, 202, 213–14
 β -cypermethrin 156–7
DAPI *see* discontinuous atmospheric pressure interface (DAPI)
DART *see* direct analysis in real time (DART)

- data-dependent experiments 61
data interpretation principles 1–3
data systems 347
database search programs 92, 93–4, 96, 98–9
databases *see* mass spectral databases
daughter ion scan *see* product ion scan
DBE *see* double bond equivalents (DBE)
DBPs *see* disinfection by-products (DBPs)
DDT *see* dichlorodiphenyltrichloroethane (DDT)
DEB *see* diepoxybutane (DEB)
deconvolution 129–30
Deconvolution Reporting System 113
Deepwater Horizon oil spill 185, 212, 289, 299–300
DEET (*N,N*-diethyl-*m*-toluamide) 156, 213–14, 215
delay time
 aerosol particles 363
 CDDs/CDFs 342, 343
 volatile organic compounds (VOCs) 246
delta value 475–6, 480
 carbon 478
 nitrogen 478
 water 490
derivatisation 35, 290
DESI *see* desorption electrospray ionisation (DESI)
desorption electrospray ionisation (DESI) 148–50,
 167–81, 196
 advantages 194–5
 aerosol analysis 177–80
 air analysis 155
 atmospheric inlet 168–70
 atmospheric pressure ionisation (API) 150
 calibration plots 174
 cylindrical ion trap (CIT) 213–14
 direct analysis 180–1
 efficiency 175
 electrosonic sprayer 168, 169
 explosives analysis 157, 158
 herbicides 156
 ion formation 168
 ion source 168
 limits of detection (LOD) 150, 181
 liquid samples 174
 molecular imaging 471, 472
 nanospray 180, 193–4
 non-invasive sampling 180–1
 optimal parameters 170
 pesticides 156–7, 213–14, 215
 polycyclic aromatic hydrocarbons (PAHs) 155,
 214–16, 217
 portable devices 155, 181, 194–5
 pre-concentration 175
 pressure changes 192
 quantitative analysis 174
 reactive desorption 170–2
 sample introduction methods 190
 sample stage 168, 169
 sensitivity 175, 177, 180
tandem mass spectrometry 150
vacuum manifold 192
water analysis 175–7
detection limits *see* limits of detection (LOD)
diaphragm pump 202
diazomethane 279, 290
dichlorodiphenyltrichloroethane (DDT) 287
diepoxybutane (DEB) 401
diesel 142, 143
diethylstilbestrol 76
differential ion mobility mass spectrometry 186
diffusion coefficient 124
dimethylarsinic acid 294
dimethylnitrosamine 406
N,N'-dimethylphenethylamine (DMPEA) 291
diode array detection 82
Dioxin International Intercalibration Study (Intercal)
 338
dioxins 53, 329–49
2,6-diphenyl-*p*-phenylene oxide 242
direct analysis in real time (DART) 149, 150–1
 ionisation 151, 246
 oil spill dispersants 300
 petroleomics 434
 plant tissue emissions 242
 thermal desorption 246
 volatile organic compounds (VOCs) 242, 246
direct aqueous sample injection 317
direct inlet system 4
direct introduction probes 65
discontinuous atmospheric pressure interface (DAPI)
 191, 195
discrete-dynode electron multipliers 203
disinfectants 264, 265
disinfection by-products (DBPs) 263–81
 analytical methods 268–80
 classes 267
 derivatisation methods 278–80
 extraction methods 268–72
 formation 264
 Fourier transform ion cyclotron resonance
 (FT-ICR) analysers 273
gas chromatography/mass spectrometry (GC/MS)
 273–6
high-field asymmetric waveform ion mobility
 spectrometry (FAIMS) 277–8
inductively coupled plasma mass spectrometry
 (ICP/MS) 276–7
ion chromatography (IC) 276–7
liquid chromatography/mass spectrometry
 (LC/MS) 276
membrane introduction mass spectrometry
 (MIMS) 277
MS detection methods 272–8
multiple reaction monitoring (MRM) 273, 276
negative ion chemical ionisation (NICI) 279
quadrupole mass filters (QMFs) 273

- quantitative analysis 276
regulatory requirements 266
selected ion monitoring (SIM) 273, 276
selected reaction monitoring (SRM) 273
two-dimensional GC/GC/MS (GC \times GC) 273
- dispersants 299–301, 302
dissolved gases 207
dissolved oxygen concentration 212
DMPEA *see N,N'*-dimethylphenethylamine (DMPEA)
DNA adducts 387–408
 acetaldehyde adducts 399–400
 aromatic amines 393–8
 carcinogenesis role 387–8
 electrospray ionisation (ESI) 390
 ethanol 399–400
 exocyclic 399
 high-performance liquid chromatography (HPLC) 390
 immunoaffinity purification 390
 isotope dilution mass spectrometry (IDMS) 81, 394–7
 limits of detection (LOD) 394–7
 liquid–liquid extraction (LLE) 390
 matrix effects 403–4
 MS instrumentation 390–3
 multiple reaction monitoring (MRM) 81
 nitrosamines 398–9
 polycyclic aromatic hydrocarbons (PAHs) 400–1
 sample preparation 389, 390, 403–6
 selected ion monitoring (SIM) 391
 selected reaction monitoring (SRM) 391
 solid-phase extraction (SPE) 390
 sources for analyses 388–9
 structure 388
 tandem mass spectrometry 81–2
 triple quadrupole mass spectrometry 81
 ultra performance liquid chromatography (UPLC) 81
- dopant 10
doping control 487, 488
dot-product search 99
double bond equivalents (DBE) 426, 427, 428, 430–4, 445, 446
double-focusing high-resolution mass spectrometer (HRMS) 341–2
double sector mass spectrometer 11
doublets 425
Dow Chemicals Company 93
drift 228
drift tube reactor 244
drinking water *see* water analysis
droplet pick-up 168
drug metabolites 407
dwell time 50, 342, 343
dyes 74, 82
dynamic range 52
dynodes 18, 203, 341, 375
- EASI *see* easy ambient sonic-spray ionisation (EASI)
easy ambient sonic-spray ionisation (EASI) 152, 153–4, 157, 160
EBD *see* epoxybutanediol (EBD)
ecosystems 486
ECs *see* emerging contaminants (ECs)
EESI *see* extractive electrospray ionisation (EESI)
efficiency
 desorption electrospray ionisation (DESI) 175
 electrospray ionisation (ESI) 175
EI *see* electron ionisation (EI)
electrochemical sensors 186
electron ionisation (EI) 5–6, 9
 cold 132, 134, 136–7
 fragmentation 313
 gas chromatography/mass spectrometry (GC/MS) 21
 hydrocarbon compounds 213, 214
 limitations 6
 mass spectral databases 92
 miniaturisation 192
 pesticides 313
 sensitivity 313
 tandem mass spectrometry 74
 water analysis 315
electron multipliers 18, 203
electron probe X-ray microanalysis (EPXMA) 361
electron tunnelling effect 8
electrophilic addition 7
electrosonic spray ionisation (ESSI) 168, 169, 194
electrospray ionisation (ESI) 8–10, 45, 46, 48, 67–8, 193–4 *see also* extractive electrospray ionisation (EESI)
chip/MS 406
crude oil 420
DNA adducts 390–1, 402
dyes 82
efficiency 175
Fourier transform ion cyclotron resonance (FT-ICR) analysers 434, 443–4, 448
fullerenes 298
herbicides 78
matrix effects 296–7
molecular imaging 462
natural organic matter (NOM) 443–4, 448, 452
oil spill dispersants 300
with orbitraps 73
organomercury 295
organotins 293
ozone 82–3
pesticides 317
petroleomics 434
pharmaceutical contaminants 78, 296–7
sensitivity 10, 317
sludge analysis 78
solid-phase extraction (SPE) 80
use with ion traps 71–2

- wastewater analysis 78, 82
electrostatic sectors 11, 12
elemental analysers (EA) 481–2
ELISA see enzyme-linked immunosorbent assay (ELISA)
elution times 113, 134, 141, 339, 340
emerging contaminants (ECs) 53, 287–303, 310
 classes 288
 tandem mass spectrometry 74–7
emissions patterns 254
endocrine-disrupting chemicals *see also oestrogenic compounds*
 liquid chromatography/mass spectrometry (LC/MS) 76
 tandem mass spectrometry 76
 wastewater analysis 76
enhanced product ion (EPI) mode 391
Environmental Protection Agency *see US Environmental Protection Agency*
Environmental Semi-VOAS RTL Library 96
enzyme-linked immunosorbent assay (ELISA) 76
epoxides 401–2
epoxybutanediol (EBD) 401
ESI *see electrospray ionisation (ESI)*
ethane 247
ethanol 399–400, 488, 489
ethanol adducts 396, 399–400
etheno DNA adducts 399
ethylbenzene 213
eucalypt plants 249, 252–3, 254–5, 257
eucalyptol *see* 1,8-cineole
European Reference Material (ERM) 235
European Water Policy 315
exact mass 423–6
excitation 418
exocyclic DNA adducts 395, 399
explosives analysis 135, 155, 157, 158, 438
external ionisation 192, 193–5
external standard calibration 336
external standardisation 38
extracted ion chromatogram (XIC) 60, 61
extracted ion chromatogram (XIC) plots 23, 322
extraction methods 268–72, 332–3
extractive electrospray ionisation (EESI) 151–3,
 155–6, 157, 158
Eyjafjallajökull volcano 185, 353, 354

factor analysis 378
FAIMS *see* high-field asymmetric waveform ion mobility spectrometry (FAIMS)
false-negatives 76, 334
false-positives 291, 334
Faraday cup 203, 358, 478, 479, 480
farming 213
FD *see* field desorption (FD)
Federal Drug Administration (FDA) *see* US Federal Drug Administration (FDA)
 wastewater analysis 78, 82
femtosecond lasers 234
FI *see* field ionisation (FI)
fibre introduction mass spectrometry (FIMS) 189–90
field desorption (FD) 8, 416, 434, 436
field instruments *see* portable devices
field ionisation (FI) 8, 9
film thickness 124, 125, 127
FIMS *see* fibre introduction mass spectrometry (FIMS)
fingerprint analysis 142–5
flame ionisation detector (FID) 130, 133
fluorescence detection 42
food adulteration 216–18, 438–9, 488–90
forensic studies 74, 142, 438
forests 245–6, 249–52, 254
Fourier transform ion cyclotron resonance (FT-ICR)
 analysers
 advantages 17
 angular velocity 417
 atmospheric pressure photoionisation (APPI) 434
 basic process 17
 calibration 422
 CDDs/CDFs 344
 characteristics 419
 compositional space 444
 cyclotron frequency 417–18
 disinfection by-products (DBPs) 273
 DNA adducts analysis 391–2
 electrospray ionisation (ESI) 434, 443–4, 448
 with gas chromatography 435–6
 history 17
 ion rotation 417–18
 ionisation methods 433–5
 isobaric compounds 419
 limitations 17
 with liquid chromatography 436
 magnetic field strength 417–18, 419
 mass resolution (R) 17, 420–3
 mass to charge ratio (m/z) 418
 molecular imaging 469–71
 natural organic matter (NOM) 273, 443–56
 petroleumics 416–38
 spectral resolution 420
 ultra-high resolution 443–56
fragmentation
 CDDs/CDFs 340–1
 disadvantages 313
 efficiencies 38
 internal energy 6
 pathways 2, 6, 63, 118
 structural determination 325
fragmentation tree 118, 297
free flow electrophoresis 444
frequency-sweep ('chirp') excitation 418
fruit juice 484, 488–90
FT-ICR *see* Fourier transform ion cyclotron resonance (FT-ICR) analysers

- full-spectrum acquisition techniques 322–4, 326
full width at half maximum (FWHM) 420–1
fullerenes 298–9
fulvic acid 264, 448, 452, 455, 456
fumaroles 209
fused droplet ESI (FD-ESI) 152
FWHM *see* full width at half maximum (FWHM)
- gas chromatograph 21
gas chromatography
 CDDs/CDFs 339–40, 347
 fast mode 124–8
 flame ionisation detector (FID) 130, 133
 validation 335
gas chromatography/mass spectrometry (GC/MS)
 21–40
 acquisition rate 32–3
 atmospheric analysis 241–2
 benefits 242
 CDDs/CDFs 340–1
 disadvantages 242, 435–6
 disinfection by-products (DBPs) 273–6
 electron ionisation (EI) 21
 emerging contaminants (ECs) 290
 environmental pollutants 67
 fast mode 123–30, 141
 isotope dilution mass spectrometry (IDMS) 482–3
 low pressure 127–8
 miniaturisation 186
 oil spill dispersants 300
 organomercury 295
 organotins 292
 pesticides 313–16
 petroleomics 436
 pharmaceutical contaminants 296
 pre-concentration 242, 243
 pressure difference 21
 selectivity 136
 semi-volatiles analysis 35
 sensitivity 136
 separation efficiency 124
 supersonic molecular beams interface (SMB)
 130–8
 target analysis 67
 two-dimensional GC/GC/MS (GC×GC) 138–45,
 273, 347, 415
 volatile organic compounds (VOCs) 241–2
- gas samples
 collection 243
 solid sorbent traps 188–9
- gas sampling bags 243
- GasBench preparation system and interface 483–4
- gasoline 157–9, 161
- GC and GC/MS File Translator Professional 119
- GC/MS *see* gas chromatography/mass spectrometry
- GC×GC *see* two-dimensional GC/GC/MS
- GDEI *see* glow discharge electron ionisation (GDEI)
- gdG *see* glioaldeoxyguanosine (gdG)
- GeoRem database 235
- GFAAS *see* graphite furnace atomic absorption spectrometry (GFAAS)
- glioaldeoxyguanosine (gdG) 398
- Global Atmosphere Watch programme 365
- glow discharge electron ionisation (GDEI) 192, 193
- glufosinate 319, 321–2
- glycidamide (GA) 402
- glyoxal 398
- glyphosate 319–21, 323
- Golay equation 124–5, 126, 127
- GOSAT *see* Greenhouse Observing SATellite (GOSAT)
- gradient elution mode 42
- graph theory 453–5
- graphite furnace atomic absorption spectrometry (GFAAS) 225
- greenhouse gases 208, 355
- Greenhouse Observing SATellite (GOSAT) 239
- groundwater run-off 213
- guaiacols 241
- guanine 398, 399–400, 402
- Guardion-7 gas chromatograph/toroidal mass spectrometer system 202–3
- Gulf of Mexico oil spill 185, 212, 289
- HAAAs *see* haloacetic acids (HAAAs)
- halo ion traps 199
- haloacetic acids (HAAAs) 265, 276–7, 278
- halogenated compounds 247, 329–49
- haloketones 267
- hard ionisation 5 *see also* electron ionisation (EI)
- Hazardous Chemical RTL Library 96
- headspace technique (HS or HSGC) 243, 244, 252 *see also* purge-and-trap (P/T) extraction
- heart-cutting 138, 139
- height equivalent to theoretical plate (*H*) 124
- helium 125, 151, 209–10
- herbicides
 atmospheric pressure chemical ionisation (APCI)
 78
 desorption electrospray ionisation (DESI) 156,
 213
 electrospray ionisation (ESI) 78
 ion traps 78
 limits of quantitation (LOQ) 78, 80
 liquid chromatography/mass spectrometry (LC/MS) 319–21
 matrix effects 78
 tandem mass spectrometry 78–80
 triazines 310
- heroin 488
- heteroatom classes 427–8, 430, 432, 446
- high-field asymmetric waveform ion mobility spectrometry (FAIMS)
- disinfection by-products (DBPs) 277–8

- organometallics 296
high-performance liquid chromatography (HPLC)
atmospheric pressure chemical ionisation (APCI) 170
CDDs/CDFs 333
DNA adducts 81, 389, 390–2
electrospray ionisation (ESI) 81, 82, 295, 389, 390–2
inductively coupled plasma mass spectrometry (ICP/MS) 295
isotope dilution mass spectrometry (IDMS) 483, 484
isotope ratio mass spectrometry (IRMS) 483
mercury 295
natural organic matter (NOM) 444
oestrogenic compounds 290
pesticides 43
sensitivity 43
surfactants 82
high-resolution mass spectrometers (HRMS) 68, 332, 334, 341–2, 343
calibration 335
costs 345
sensitivity 342
validation 335
homocysteine 81
HPLC *see* high-performance liquid chromatography (HPLC)
HRMS *see* double-focusing high-resolution mass spectrometer (HRMS)
HS *see* headspace technique (HS or HSGC)
HSGC *see* headspace technique (HS or HSGC)
humic acid 264
huminomics *see* natural organic matter (NOM)
hydrocarbon compounds 142–5, 211–13, 214
hydrocarbon-like organic aerosol 378
hydrogen 475
carrier gas 125
deficiency 426
hydrology 485, 486
hydrophilic interaction liquid chromatography (HILIC)/ESI-MS 293–4
hydrothermal vents 205
hydroxyethyl radicals 399
hyphenated techniques 231

IC *see* ion chromatography (IC)
Iceland 185, 208
ICP/AES *see* inductively coupled plasma atomic emission spectrometry (ICP/AES)
ICP/MS *see* inductively coupled plasma mass spectrometry (ICP/MS)
IDMS *see* isotope dilution mass spectrometry (IDMS)
IE *see* ionisation energy (IE)
image current 17
imaging methods 461–73
basic procedure 462–4
qualitative analysis 468
quantitative analysis 462
in situ 461, 472
immunoaffinity purification 390
immunochemistry 81
Indoor Air Toxics RTL Library 96
inductively coupled plasma atomic emission spectrometry (ICP/AES) 225
inductively coupled plasma mass spectrometry (ICP/MS) 225–35
air analysis 229
applications 229–35
benefits 227
disinfection by-products (DBPs) 276–7
ion mass separation 227
matrix effects 228–9
sensitivity 227, 277
spectral interferences 227–8
water analysis 229–30
industrial aerosols 177
inert coatings 243
informative order 446
inlet systems 363
Institute of Reference Materials and Measurements (IRMM) 234–5
Intercal 338
interlaboratory studies 335, 338
internal energy 6
internal ionisation 192
internal standard calibration 336, 338
internal standards 39–40, 229, 320, 337, 392
International Organization for Standardization (ISO) 229, 230
International Space Station 209
international standards 28, 229–30
ISO 17025 338
isotopes 475, 476
interscan delay 50
intrinsic order 446
ion chromatography (IC) 276–7, 361
ion cyclotron resonance (ICR) mass analyser 391–2, 417
ion detection 18–19
ion internal energy 6
ion mobility mass spectrometry 64, 186, 444
ion rotation 417–18
ion source temperature 130–1, 132, 133
ion traps 16, 51, 69–71
advantages 374
atmospheric analysis 358
combined with triple quadrupoles 391
cylindrical 197
DNA adducts analysis 391
electrospray ionisation (ESI) 71–2
halo 199
herbicides 78
linear 71–2, 198

- non-resonant excitation 71, 74, 75
particle analysis 374–6
pesticides 314, 322
quadrupole 70–1, 196–7
qualitative analysis 314
radiofrequency 196
rectilinear 198
resonant excitation 71, 74, 75
sensitivity 51, 314, 391
tandem mass spectrometry 374
toroidal 198–9
- ionisation 5–11
ambient 192
atmospheric pressure chemical ionisation (APCI) 10, 47, 193
atmospheric pressure photoionisation (APPI) 434
CDDs/CDFs 344
chemical (CI) 6–8
complex mixtures 434–5
desorption electrospray ionisation (DESI) 167–81, 194–5
direct analysis in real time (DART) 151, 246
electron (EI) 5–6, 9, 192–3
electrospray (ESI) 8–10, 193–4, 434
external 192
field (FI) 8, 9
internal 192
low-temperature plasma (LTP) 153, 195
matrix-assisted laser desorption/ionisation (MALDI) 10–11
Penning 151
portable devices 191–5
sonic-spray (SSI) 153, 154
- ionisation efficiency 38
ionisation energy (IE) 7, 340
ionisation suppression 52
false negatives 76
matrix effects 59, 297, 312
soil analysis 320–2
- IRMS *see* isotope ratio mass spectrometry (IRMS)
ISO 17025 338
- isobaric compounds 242, 244, 249, 341
crude oil 421, 422
exact mass 424–6
Fourier transform ion cyclotron resonance (FT-ICR) analysers 419
- isobaric interferences 227
- isomer analysis 22, 64
- isoprene 239, 250–2
- isoprenoids 252
- isoprostanes 81
- isotope dilution mass spectrometry (IDMS) 38–9
advantages 337, 338
benzo[a]pyrene (BP) 400–1
CDDs/CDFs 331, 335, 336–7
continuous flow 481
corrections 480
- DNA adducts 81, 392, 394–7, 407–8
elemental analysers (EA) 481–2
gas chromatography 482–3
ion collection 480
ionisation 478–9
liquid chromatography 483
mass separation 479–80
multiple loop injection 483–4
sample preparation 480–5
target analysis 39
- isotope ratio mass spectrometry (IRMS) 475–90
- isotopes
atomic masses 424
bromine 3, 275
carbon 475, 477, 488
CDDs/CDFs 342, 343
chlorine 2, 3, 275
delta value 475, 478, 480, 490
equilibrium effects 476
hydrogen 475
international standards 475, 476
kinetic effects 476
lead 2
nitrogen 477–8, 482, 486, 488
oxygen 486
photosynthesis 476–7
stable isotopes 475, 476
temperature effects 476
variations 476–8
- isotopic analysis 233, 471, 472 *see also* isotope dilution mass spectrometry (IDMS)
- Japanese Positive List Pesticide RTL Library 96
- jet separation phenomena 131
- Jungfraujoch, Switzerland 365–6
- Kendrick mass 427–8, 446
Kendrick mass defect (KMD) 427–8
Kendrick mass diagrams 428–30, 430, 446–7, 452, 453
- kerosene 157–9, 161
- KMD *see* Kendrick mass defect (KMD)
- labelling, reactive desorption ionisation 170
- laboratory accreditation 338
- LACE 98 *see* Lindenberg aerosol characterisation experiment (LACE 98)
- LAMPAS *see* laser mass analyser for particles in the airborne state (LAMPAS)
- laser ablation (LA) 233–4
- laser desorption/ionisation (LDI) 372, 373, 376
imaging methods 462, 471
soil analysis 471
- laser mass analyser for particles in the airborne state (LAMPAS) 365–6, 367–71
- laser microprobe mass analysis (LAMMA, LMMS) 361, 462

- LC/MS *see* liquid chromatography/mass spectrometry (LC/MS)
lead 287
lead isotopes 2, 233
lead salts 225
lense contamination 44
libraries 96 *see also* databases
library searches 62, 68, 91, 96 *see also* mass spectral database search
background subtraction 23
GC/MS ChemStation PBM 96
NIST MS Search 96
light-beam oscillographic recorder 90
lignin 253–4, 256–7
limits of detection (LOD) *see also* sensitivity
aircraft volcanic emission mass spectrometer 209
arsenic species 181
column switching 406
desorption electrospray ionisation (DESI) 150, 181
DNA adducts 394–7
extractive electrospray ionisation (EESI) 155, 157
fullerenes 298
matrix-assisted laser desorption ionisation (MALDI) 467
organotins 292
polycyclic aromatic hydrocarbons (PAHs) 216
quadrupole ion traps (QIT) 80
secondary ion mass spectrometry (SIMS) 466–7
selected ion monitoring (SIM) 466
spatial resolution 467
tandem mass spectrometry (MS/MS) 314
time-of-flight (TOF) analysers 391
triple quadrupole mass spectrometry (TQMS or QQQ) 314, 391
limits of quantitation (LOQ) 76, 78, 80
Lindenberg aerosol characterisation experiment (LACE 98) 367–72, 371
linear ion traps 71–3, 198
combined with orbitraps 72–3, 392
combined with quadrupole 51
dyes 82
tandem mass spectrometry 71–2, 82
lipid peroxidation 81
liquid chromatograph/hybrid linear ion trap/Fourier transform-orbitrap mass spectrometry (LC/ LTQ/FT-OT) 297
liquid chromatography/mass spectrometry (LC/MS) 41–65
atmospheric pressure ionisation (API) 45–7
challenges 43–5
detection limits 52
disinfection by-products (DBPs) 276
emerging contaminants (ECs) 290–1
endocrine-disrupting chemicals 76
fullerenes 298–9
gradient elution mode 42
high-resolution instruments 49, 51–2
isotope dilution mass spectrometry (IDMS) 483
low-resolution instruments 47–8, 49–51
low-temperature plasma (LTP) 47
NIST/EPA/NIH Database 109–10
non-volatiles analysis 42
orbitraps 51–2
organotins 292–3
pesticides 316–22
pharmaceutical contaminants 296
polar compounds analysis 42
quadrupole/time of flight (QTOFs) 51–2
sensitivity 42, 43, 317
source design 44–5
tandem quadrupole instruments 49–51, 54–9
target analysis 67
thermo-labile compounds analysis 42
water analysis 52–3
liquid–liquid extraction (LLE)
CDDs/CDFs 333
disinfection by-products (DBPs) 269
DNA adducts 390
pesticides 311
water analysis 175
liquid samples
collection 242–3
desorption electrospray ionisation (DESI) 174
pesticides 311
pressurised liquid extraction (PLE) 311
quantitative analysis 174
solid-phase extraction (SPE) 311
solid-phase microextraction (SPME) 311
LLE *see* liquid–liquid extraction (LLE)
localisation 462
lockmass 342
London, UK 248
loop modulation 139, 140
low pressure gas chromatography (LP-GC) 127–8
low-temperature plasma (LTP) ionisation 152, 153, 195, 197
molecular imaging 471, 472, 473
LTP *see* low-temperature plasma (LTP)
lung cancer 398
magnetic field strength 417–18, 419
magnetic sector mass analysers 11, 273, 341–2, 391
mainlib *see* NIST11
MALDI *see* matrix-assisted laser desorption ionisation (MALDI)
marine ecosystems 211–13
mass accuracy 13, 312, 336, 338
calibration 422
standard reference material (SRM) 234
mass chromatogram 23, 90–1
mass defect 423–6 *see also* Kendrick mass defect (KMD)
mass discrimination 38

- mass fractions aerosol analysis 378, 380
mass fragmentography 26
mass resolution (*R*) 12–13
 CDDs/CDFs 341
 Fourier transform ion cyclotron resonance (FT-ICR) analysers 17, 420–3
 linear ion traps 72
 orbitraps 73
 quadrupole mass filters (QMFs) 15
 time-of-flight (TOF) analysers 322
mass spectrometry concepts 1–3
mass spectrometry/mass spectrometry (MS/MS) *see*
 tandem mass spectrometry
Mass Spectra of Pesticides 2009 96
mass spectral database search 92, 93–4, 96, 98–9 *see also* library searches
mass spectral databases 92–7
 development 91, 93–4
 Mass Spectral Search System (MSSS) 94
 NIST/EPA/NIH Database 92, 94, 95–6
pesticides 96, 313
 Wiley Registry of Mass Spectral Data 94, 95–6,
 109
Mass Spectral Library of Drugs, Poisons, Pesticides, Pollutants and Their Metabolites 2007 96
Mass Spectral Search System (MSSS) 94
Mass Spectrometry Data Centre (MSDC) 93, 95
mass ‘splits’ 425
mass to charge ratio (*m/z*) 1, 2, 9, 55
 CDDs/CDFs 343
 databases 95, 97–8
 Fourier transform ion cyclotron resonance (FT-ICR) analysers 418
 peak deconvolution algorithm 129
 quadrupole mass filters (QMFs) 198, 391
 sector analysers 11
 visualisation 446
MassFragment software 63
MassLynx 99
MassSpec Calculator Professional 119–20
Masstrix metabolic pathway annotation (MassTRIX)
 453
MassWorks 109, 116
matrix-assisted laser desorption ionisation (MALDI)
 10–11, 172–4, 465–7
 atmospheric pressure 472
 matrix application 465–6
 miniaturisation 200
 molecular imaging 462, 471
 sensitivity 465
 soil analysis 471
 spatial resolution 467
matrix effects 52
 calibration 336
 chip/MS 406
 DNA adducts 403–4
 electrospray ionisation (ESI) 296–7
herbicides analysis 78
inductively coupled plasma mass spectrometry (ICP/MS) 228–9
liquid chromatography/mass spectrometry (LC/MS) 317
pesticides analysis 312, 314, 317–19
pharmaceutical contaminants 296–7
selected ion monitoring (SIM) 314
sensitivity 52, 312, 465
spatial resolution 467
supersonic molecular beams interface (SMB)
 GC/MS 136
matrix-enhanced SIMS (ME-SIMS) 467
MDMA 291
melamine detection 216
melittin 171
membrane inlet system 4, 5
membrane introduction 187–8
membrane introduction mass spectrometry (MIMS)
 disinfection by-products (DBPs) 277
 fibre introduction mass spectrometry (FIMS)
 189–90
 portable devices 187–8, 198, 204
 quadrupole mass filters (QMFs) 198
 TETHYS 212–13
 underwater mass spectrometry 204
mercury *see* organomercury
methamphetamine 291
method detection limits (MDLs) 230, 231
methylarsonic acid 294
methylene 445, 446
methylmercury 295
4-(methylnitros-amino)-1-(3-pyridyl)-1-buanol
 (NNAL) 398–9
4-(methylnitrosamino)-1-(3-pyridyl)-1-butaneone
 (NNK) 398–9
1-methylpyrene (1-MP) 401
micro-channel plates (MCPs) 364
micropores 461–2
Milan, Italy 248
MIMS *see* membrane introduction mass spectrometry (MIMS)
miniaturisation 181, 195–201, 199, 380 *see also*
 portable devices
MIPs (molecularly imprinted polymers) 80
modulation 139, 140
molecular imaging 461–73
 basic procedure 462–4
 single compound images 464
molecular imprinting sensors 186
molecularly imprinted polymers (MIPs) 80
Monitoring Certification Scheme (MCERTS) 230
motor boat exhaust 206, 207
MPMS *see* multiple-particle mass spectrometers (MPMS)
MRM *see* multiple reaction monitoring (MRM)
MS/MS *see* mass spectrometry/mass spectrometry

- (MS/MS); tandem mass spectrometry (MS/MS)
- MS Tools 119
- MS^E 325–6
- multi-residue methods 309, 345–9
- multichannel plate detectors 203
- multiple loop injection 483–4
- multiple-particle mass spectrometers (MPMS) 376–9
- multiple reaction monitoring (MRM) 29–30, 31, 49–50
- CDDs/CDFs 342–4, 345
- confirmatory analysis 53–4, 55
- disinfection by-products (DBPs) 273, 276
- DNA adducts 81
- oestrogenic compounds 76
- pesticides 80
- pharmaceutical contaminants 78
- tandem mass spectrometry 76, 343
- target analysis 54–9
- water analysis 273
- m/z* value *see* mass to charge ratio (*m/z*)
- nandrolone 35, 36
- Nanoflow HPLC/nanospray ionisation mass spectrometry (nanoLC/nanESI) 403
- nanomaterials 297–9
- nanometallics 299
- nanoparticles 289
- nanosecond lasers 234
- nanoSIMS 471, 472
- nanospray 402, 403, 408
- nanospray desorption electrospray ionisation (nano-DESI) 180, 193–4
- naphthalene 39, 218
- naphthenic acids 436–7
- narotics 486–7
- National Bureau of Standards (NBS) *see* US National Bureau of Standards (NBS)
- National Heart and Lung Institute (NHLI) 93
- National Institute of Standards and Technology (NIST) 91, 94, 234–5
- National Institutes of Health (NIH) 93
- natural organic matter (NOM)
- atmospheric pressure chemical ionisation (APCI) 451
 - atmospheric pressure photoionisation (APPI) 451–2
 - disinfection by-products (DBPs) 264
 - electrospray ionisation (ESI) 443–4, 448, 452
 - Fourier transform ion cyclotron resonance (FT-ICR) analysers 273, 443–56
 - Kendrick mass diagrams 453
 - molecular compositions 447
 - sulfur chemistry 448, 451
 - van Krevelen diagrams 448–9, 450, 454
- NDELA *see* *N*-nitrosodiethanolamine (NDELA)
- nebulising gas 167–8
- negative ion chemical ionisation (NICI) 8, 279, 344
- negative ion detection 203–4
- NEREUS (novel, efficient, rapid evaluation of underwater spectra) 207, 207
- neuropeptides 469, 470
- neutral desorption EESI (ND-EESI) 152–3
- neutral loss scan 69, 344
- Neutral Loss Search 109–10
- NICI *see* negative ion chemical ionisation (NICI)
- NIST11 *see* NIST/EPA/NIH Database
- NIST/EPA/NIH Database 92, 94, 95–6, 109–10
- NIST MS Interpreter 106–8
- NIST MS Search Program 99, 100–3, 104–6, 109–10
- Any Peaks 116
 - Similarity Search 116
- NIST MS Search routine 99
- NIST retention index (RI) database 111–12
- NIST standard reference materials 234–5
- nitrogen 477–8, 482, 486, 488
- nitrosamine adducts 394–5, 398–9
- N*-nitrosodiethanolamine (NDELA) 398
- N*-nitrosodiethylamine 406
- N*-nitrosodimethylamine 264, 265, 406
- 3-nitrotyrosine 81
- NNAL *see* 4-(methylnitros-amino)-1-(3-pyridyl)-1-buanol (NNAL)
- NNK *see* 4-(methylnitrosamino)-1-(3-pyridyl)-1-butanone (NNK)
- NOM *see* natural organic matter (NOM)
- nominal mass 95
- non-invasive sampling 180–1
- non-resonant excitation 71, 74
- non-volatiles analysis
- electrospray ionisation (ESI) 193–4
 - gas chromatography/mass spectrometry (GC/MS) 35
 - liquid chromatography/mass spectrometry (LC/MS) 42, 67
 - nozzle/skimmer systems 363
 - nuclear binding energy 424, 426
 - nuclear magnetic resonance (NMR) 64
- octafluoronaphthalene (OFN) 132
- oestrogenic compounds 52, 53, 76, 290
- off-line particle analysis 360–1
- OFN *see* octafluoronaphthalene (OFN)
- oil spill dispersants 299–301, 302
- oil spills 144–5, 211–12, 289, 436
- ambient mass spectrometry 157, 159
 - olive oil 489, 490
- open-air ionisation mass spectrometry 242
- open split interface 481
- oral buccal samples 388–9
- orbitraps 18, 51–2
- CDDs/CDFs 344
- combined with linear ion traps 392
- DNA adducts analysis 392

- with electrospray ionisation (ESI) 73
pharmaceutical contaminants 78
resolution 51
use with linear ion traps 72–3
wastewater analysis 78
- organic acids 178–9
organoarsenics 181, 294, 295
organomercury 295–6
organometallics 290, 291–6
organotin 288, 292–4
orthogonal separation 138, 141
oxidative stress markers 81–2
oxygen 486
oxygenated organic aerosol (OOA) 378
ozone 82–3, 247, 265
- palaeoclimatology 485
pancreatic tissue 393
paper spray ionisation (PSI) 149, 150
paraquat 155–6
parent ion scan *see* precursor ion scan
particle exposure effect on health 355–6, 357
Paul trap *see* quadrupole ion traps (QIT)
PBDE *see* polybrominated diphenyl ethers (PBDEs)
PCB *see* polychlorinated biphenyl (PCB)
peak deconvolution algorithm 129–30
Penning ionisation 151
pentafluoroanisole 210
peptides 407, 469, 470
perdeuterated polycyclic aromatic hydrocarbons 40
perfluorinated compounds 53, 210–11
persistent organic pollutants (POPs) 345 *see also*
chlorinated dibenz-p-dioxins (CDDs);
chlorinated dibenzofurans (CDFs)
pesticides 213–15, 309–26
atmospheric pressure chemical ionisation (APCI)
317
atmospheric pressure ionisation (API) 317
confirmatory analysis 58
desorption electrospray ionisation (DESI) 156–7
electrospray ionisation (ESI) 317
fast GC/MS 130
limits of quantitation (LOQ) 78
liquid chromatography/mass spectrometry
(LC/MS) 42
mass spectral databases 96
multiple reaction monitoring (MRM) 80
pressurised liquid extraction 311
quadrupole mass filters 314
residue analysis 53–4, 55, 310–13
selected ion monitoring (SIM) 314
selected reaction monitoring (SRM) 317
solid-phase extraction (SPE) 59, 78, 80, 311
solid-phase microextraction (SPME) 311
tandem mass spectrometry 78–80
toxicity 311
transformation products (TPs) 310, 311–12
- triple quadrupole mass spectrometry (TQMS or
QqQ) 78, 314, 317
ultra performance liquid chromatography
(UPLC) 78
water analysis 52–3, 60, 310, 316, 317–19, 324–6
- Pesticides RTL Library 96
petroleumics 157, 415–16, 433
petroleum 415–16, 421
PFE *see* pressurised fluid extraction (PLF)
PGMs *see* platinum group metals (PGMs)
pharmaceutical contaminants 288–9, 296–7
atmospheric pressure chemical ionisation
(APCI) 78
collisionally activated dissociation (CAD) 78
derivatisation 290
electrospray ionisation (ESI) 78
multiple reaction monitoring (MRM) 78
orbitraps 78
sediment analysis 77–8
selected reaction monitoring (SRM) 78
sludge analysis 77–8
triple quadrupole mass spectrometry (TQMS) 78
water analysis 53, 56, 64, 77–8, 79, 297
- PHB *see* pyridylhydroxybutyl (PHB)
phenanthrene 39
phenylboronic acid 170–1, 172
phosgene 225
phospholipids 468–9
photomultiplier tubes (PMTs) 363
photosynthesis 206, 476–7
planar samples 172–4
plant tissue analysis 181, 213–14, 215, 252, 253–5
plant tissue emissions 242
plasma 6, 226
platinum group metals (PGMs) 231
PLE *see* pressurised liquid extraction (PLE)
POB *see* pyridyloxobutyl (POB)
polar compounds analysis
gas chromatography/mass spectrometry
(GC/MS) 35
liquid chromatography/mass spectrometry
(LC/MS) 42, 67
polyaromatic hydrocarbons 74, 75, 217
polyatomic interferences 227
polybrominated diphenyl ethers (PBDEs) 340, 343
polychlorinated biphenyl (PCB) 330, 343
polycyclic aromatic hydrocarbons (PAHs) 179,
214–16, 217, 218
atmospheric pressure photoionisation (APPI) 434
desorption electrospray ionisation (DESI) 155,
178
DNA adducts 395, 400–1
health impact 372
polyols analysis 35
polysaccharides 253–4, 256–7
population transition 486
portable devices 185–219

- air analysis 155
atmospheric pressure chemical ionisation (APCI) 193
cylindrical ion trap (CIT) 197
desorption electrospray ionisation (DESI) 155, 181, 194–5
discontinuous atmospheric pressure interface (DAPI) 191
electron ionisation 192–3
electron multiplier 203
electrospray ionisation 193–4
Faraday cup 203
fibre introduction mass spectrometry (FIMS) 189–90
halo ion traps 199
ion detection 203–4
ion traps 374, 374
ionisation methods 191–5
linear ion traps 198
low-temperature plasma (LTP) ionisation 195
mass analysers 195–201
membrane introduction 187–8
membrane introduction mass spectrometry (MIMS) 204
pumps 202–3
quadrupole ion traps (QIT) 196–7
quadrupole mass filters (QMFs) 198
radiofrequency ion traps 196
rectilinear ion trap (RIT) 198
sample introduction methods 187–91
sector analysers 200
solid sorbent traps 188–9
speed of analysis 185
time-of-flight (TOF) analysers 199–200
toroidal ion traps 198–9
vacuum systems 187, 200–2
volatile organic compounds (VOCs) 188
poultry feed 181
pre-concentration
 automation 347
 desorption electrospray ionisation (DESI) 175
 detection limits 57
 gas chromatography/mass spectrometry (GC/MS) 242, 243
 oestrogenic compounds 76
 tandem mass spectrometry (MS/MS) 55–7, 58
 transformation products (TPs) 312
 volatile organic compounds (VOCs) 242, 243, 244
 water analysis 175, 317
precursor ion scans 69, 71, 276, 344
pressurised fluid extraction (PFE) 333
pressurised liquid extraction (PLE) 311, 333, 347–8
primary organic aerosols (POAs) 378, 454
probability based matching (PBM) system 98, 99–105, 106
product ion scan 69, 71
prostaglandin metabolites 81
proteins 194
proteomics 392, 403
proton-induced X-ray emission (PIXE) 361
proton transfer 7
proton-transfer reaction mass spectrometry (PTR/MS) 242–6, 249, 252, 358
proton-transfer reactions 245–6
protonation 7
protozoae 468–9
PSI *see* paper spray ionisation (PSI)
P/T *see* purge-and-trap (P/T) extraction
PTR/MS *see* proton-transfer reaction mass spectrometry (PTR/MS)
pumps, portable devices 202–3
purge-and-trap (P/T) extraction 98, 243, 244, 269–71
 see also headspace technique (HS or HSGC)
pyrene 75, 217
pyridylhydroxybutyl (PHB) 399
pyridyloxobutyl (POB) 398–9
pyrolysis 252
pyrolytic pollutants 241, 253–4
QIT *see* quadrupole ion traps (QIT)
QTrap 51
quadrupole ion traps (QIT) 70–1, 196–7, 199, 244
quadrupole mass filters (QMFs) 14–16, 198 *see also*
 tandem mass spectrometry
 atmospheric analysis 358
 development 89
 disinfection by-products (DBPs) 273
 DNA adducts analysis 391
 fast GC/MS 128
 MassWorks use 116
 pesticides 314
 profile mode 116–17
 proton-transfer reaction mass spectrometry (PTR/MS) 243
underwater mass spectrometry 204
volcanology 209
quadrupole/time of flight instruments (QTOFs) 51–2, 53, 59–63
qualitative analysis 314, 468
quantitative analysis 26, 35–9
 desorption ionisation (DI) 174
 equations 40
 imaging methods 462
 liquid chromatography/mass spectrometry (LC/MS) 47
 tandem quadrupole instruments 49–50
 time-of-flight (TOF) analysers 33
 triple quadrupole mass spectrometry (TQMS or QqQ) 314
QUASIMEME (Quality Assurance of Information for Marine Environmental Monitoring in Europe) 338
radio frequency (RF) coil 226

- radiofrequency ion traps 196
radioisotopes 475
radionuclide analysis 233
Raman spectrometers 186
rastering 463
RE *see* recombination energy (RE)
REACH programme 41
reaction rate constants proton-transfer reactions 245
reactive desorption 170–2
reactive desorption ionisation 170–2
reactive oxygen species (ROS) 399–400
reagent gas 6
reagent ions 6
recombination energy (RE) 7
reconstructed ion chromatogram (RIC) 23
reconstructed total ion current (RTIC) chromatogram 23, 91–2, 100, 112–13
rectilinear ion trap (RIT) 198, 202
reference materials 337–8 *see also* certified reference material (CRM)
reflectron lens systems 347
refractive index (RI) detection 42
regulatory requirements 41, 266, 346
remotely operated vehicles (ROVs) 204–5
replics *see* NIST11
replicate sample analysis 335
residual gas analyser (RGA) 358
resolution 12–13, 16, 17, 51
resonance enhanced multiphoton ionisation (REMPI) 372–4
resonant excitation 71, 74
respiration 206
response factors (RFs) 40
Retention Time Locking databases 113
retention times 22, 26, 36
 acceptance window 53
 deconvolution 130
 liquid chromatography/mass spectrometry (LC/MS) 68
 use with database searches 98, 111–12, 113
reverse geometry 68
reverse osmosis (RO) membranes 264–5, 272
RFs *see* response factors (RFs)
RIC *see* reconstructed total ion current (RTIC) chromatogram
RIT *see* rectilinear ion trap (RIT)
RO *see* reverse osmosis (RO) membranes
rotary vane pumps 202
ROVs *see* remotely operated vehicles (ROVs)
RTIC *see* reconstructed total ion current (RTIC) chromatogram
sample collection 242–3, 311
sample introduction methods 3–5
 direct inlet system 4
 discontinuous atmospheric pressure interface (DAPI) 191
fibre introduction mass spectrometry (FIMS) 189–90
membrane introduction 187–8
portable devices 187–91
semi-permeable membranes 4, 5
solid sorbent trap 188–9
sample preparation *see also* pre-concentration
 CDDs/CDFs 332–5
 digestion 226
 gases 243
 inductively coupled plasma mass spectrometry (ICP/MS) 226
 isotope dilution mass spectrometry (IDMS) 480–5
 liquids 226, 242–3
 minimisation 147
 solids 226, 242–3
 urine 389
 volatile organic compounds (VOCs) 242–3
sample purification online 403–6
sampling lines 246, 249
SANCO 53, 55, 312, 313, 319
scanning electron microscopes (SEMs) 361
scanning microprobe matrix-assisted laser desorption/ionisation (SMALDI) 466, 469, 470, 473
scanning speed 32 *see also* acquisition rate
screening 23, 73–4
secondary ion mass spectrometry (SIMS)
 limits of detection (LOD) 466–7
 matrix-enhanced 467
 molecular imaging 462, 463, 466–7, 471
 nanoSIMS 471, 472
 spatial resolution 468
secondary organic aerosols (SOAs) 358, 378, 447, 448, 454
sector analysers 11–14, 68, 128, 200
sediment analysis 77–8, 230–1
selected ion chromatogram (SIC) 23
selected ion monitoring (SIM) 26, 28–30
 CDDs/CDFs 340, 341–2, 345
 disinfection by-products (DBPs) 273, 276
 DNA adducts 391
 fast GC/MS 128
 matrix effects 314
 pesticides 314
 sensitivity 26, 276, 314, 341, 462
 soil analysis 471
 target analysis 26, 28
 water analysis 273
selected reaction monitoring (SRM) 29, 31
 disinfection by-products (DBPs) 273
 DNA adducts 391, 402
 homocysteine 81
 nitrosamine adducts *see* glioxaldehydeguanosine (gdG)
 oestrogenic compounds 76
 organotins 292
 pesticides 314, 317

- pharmaceutical contaminants 78
sensitivity 315, 317
tandem mass spectrometry 76
thiols 81
triple quadrupole mass spectrometry (TQMS or QQQ) 314, 317
urine analysis 401
water analysis 273, 315
semi-permeable membranes 4, 5, 187–8
semi-volatiles analysis
 direct analysis in real time (DART) 246
 fibre introduction mass spectrometry (FIMS) 190
 gas chromatography/mass spectrometry (GC/MS) 34, 35
sensitivity *see also* limits of detection (LOD)
atmospheric pressure chemical ionisation (APCI) 317
chemical ionisation (CI) 313–14
chip/MS 408
column switching 406
desorption electrospray ionisation (DESI) 175, 177, 180
electron ionisation (EI) 313
electrospray ionisation (ESI) 10, 317
fast GC/MS 126
high-performance liquid chromatography (HPLC) 43
high-resolution mass spectrometers (HRMS) 342
inductively coupled plasma mass spectrometry (ICP/MS) 227, 277
internal standards 337
ion traps 51, 314, 391
liquid chromatography/mass spectrometry (LC/MS) 42, 43, 317
matrix-assisted laser desorption ionisation (MALDI) 465
matrix effects 52, 312, 465
nanospray 402, 403, 408
negative ion chemical ionisation (NICI) 8
QTrap 51
quadrupole ion traps (QIT) 244
selected ion monitoring (SIM) 26, 276, 314, 341, 462
selected reaction monitoring (SRM) 315, 317
solid-phase extraction (SPE) 57, 59, 317
solid-phase microextraction (SPME) 177
supersonic molecular beams interface (SMB) GC/MS 136
tandem mass spectrometry (MS/MS) 49, 51, 65, 72, 312, 317
time-of-flight (TOF) analysers 17, 322–24
triple quadrupole mass spectrometry (TQMS or QQQ) 314, 317, 391
ultra performance liquid chromatography (UPLC) 43, 319
separation efficiency 124
sewage influent 198, 205 *see also* wastewater analysis
sewage leachate 316
SIC *see* selected ion chromatogram (SIC)
signal enhancement 18
signal suppression 227–8, 392, 403
SIM *see* selected ion monitoring (SIM)
SIMS *see* secondary ion mass spectrometry (SIMS)
single-particle analysis 361–72
single-particle mass spectrometers (SPMS) 364–72
sludge analysis 77–8, 230–1
SMALDI *see* scanning microprobe matrix-assisted laser desorption/ionisation (SMALDI)
sodium tetrtaethylborate (STEBA) 292
soft ionisation 5, 6, 8, 15, 313
 atmospheric pressure ionisation (API) 45–7
 electrospray ionisation (ESI) 193 4
 pesticides 325
 petroleomics 434–5
soil analysis 230–1
 ambient mass spectrometry 160
herbicides 319–22
imaging methods 471
isotopes 477
laser desorption/ionisation (LDI) 471
matrix-assisted laser desorption ionisation (MALDI) 471
nitrogen cycle 477
polycyclic aromatic hydrocarbons (PAHs) 214–16
scanning microprobe matrix-assisted laser desorption/ionisation (SMALDI) 473
selected ion monitoring (SIM) 28, 471
solid-phase microextraction (SPME) 471, 473
solid-phase extraction (SPE) 57, 59
CDDs/CDFs 332–3
desorption electrospray ionisation (DESI) 175–6
disinfection by-products (DBPs) 268, 269
disposable cartridges 243
DNA adducts 390
electrospray ionisation (ESI) 80
fullerenes 298–9
isoprostanes 81
liquid samples 311
oestrogenic compounds 76
off-line 317
on-line 317
organotins 292, 293
pesticides 78, 80, 311, 319
pharmaceutical contaminants 296
sensitivity 57, 59, 317
tandem mass spectrometry 76
volatile organic compounds (VOCs) 243
water analysis 175–6, 317
solid-phase microextraction (SPME)
 blood samples 270
desorption electrospray ionisation (DESI) 177
disinfection by-products (DBPs) 268–9, 270
disposable cartridges 243

- fibre introduction mass spectrometry (FIMS) 189–90
liquid samples 311
oestrogenic compounds 76, 77
organomercury 295
organotins 292
pesticides 311
pharmaceutical contaminants 296
sensitivity 177
soil analysis 471, 473
tandem mass spectrometry 76, 77
volatile organic compounds (VOCs) 243
water analysis 177
solid samples
 collection 242–3
 preparation 333
solid sorbent traps 188–9
solid waste analysis 230–1
sonic-spray ionisation (SSI) 153, 194
Soxhlet extraction
 CDDs/CDFs 333
 disinfection by-products (DBPs) 271
spatial resolution
 limits of detection (LOD) 467
matrix-assisted laser desorption ionisation
 (MALDI) 465–6, 467, 472
scanning microprobe matrix-assisted laser
 desorption/ionisation 466
 secondary ion mass spectrometry (SIMS) 468
SPE *see* solid-phase extraction (SPE)
speciation 231–2
spectral editing 450–1
spectral quality 23, 32
spectral resolution 420
spectral skewing 32, 113, 130
speed of analysis 185
split ratios 126, 127
SPME *see* solid-phase microextraction (SPME)
SPMS *see* single-particle mass spectrometers (SPMS)
SRM *see* selected reaction monitoring (SRM);
 standard reference material (SRM)
SSI *see* sonic-spray ionisation (SSI)
stable isotope thermometry 485
stable isotopes 40, 475, 476
Stan Pesticides MS Library 96
standard addition 38
standard matrix 465–6
standard reference material (SRM) 234–5
steroid metabolism 488
sulfonamides 297
sulfur 448, 451, 486, 487
sulfur dioxide 208, 209
sulfuric acid 208
supersonic molecular beams interface (SMB) GC/MS 130–8, 133–4, 136
surface guided vehicles 205, 206
surfactants 82, 299
surrogates 39
synthetic oestrogens 76
tandem mass spectrometry (MS/MS) 15, 16, 17, 30, 67–83
 CDDs/CDFs 342–4
 collision cell 343
 collisionally activated dissociation (CAD) 74
 desorption electrospray ionisation (DESI) 150
 DNA adducts 81–2
 dyes 82
 with electron ionisation (EI) 74
 emerging contaminants (ECs) 74–7
 endocrine-disrupting chemicals 76
 herbicides 78–80
 high-resolution instruments 68
 homocysteine 81
 ion traps 374
 isobaric compounds 244
 isoprostanes 81
 miniaturisation 186
 multiple reaction monitoring (MRM) 76, 343
 organomercury 295
 ozone 82–3
 perfluorinated compounds 210–11
 pesticides 78–80, 312, 314, 322
 pre-concentration 55–7, 58
 radio frequency (RF) mode 343
 selected reaction monitoring (SRM) 76
 sensitivity 49, 51, 65, 72, 312, 317
 single-particle analysis 376
 solid-phase extraction (SPE) 76
 solid-phase microextraction (SPME) 76, 77
 surfactants 82
 thermospray ionisation 74
 thiols 81
 tandem quadrupole instruments 49–51, 53, 54–9, 60
target analysis
 external standardisation 38
 gas chromatography/mass spectrometry (GC/MS) 67
 isotope dilution mass spectrometry (IDMS) 39
 liquid chromatography/mass spectrometry
 (LC/MS) 67
 multiple reaction monitoring (MRM) 54–9
 screening 55
 selected ion monitoring (SIM) 26, 28
targeted screening 55
TCDD *see* 2,3,7,8-tetrachlorodibenzo-*p*-dioxin
 (TCDD)
tea tree oil 240–1
TEF *see* toxic equivalent factor (TEF)
TEM *see* transmission electron microscopy (TEM)
temperature-dependent classification 252–3
temperature ramps 125
Tenax 242
TEQ *see* toxic equivalent quantity (TEQ)

- terpenes 239, 240–1, 252
testosterone 137–8
TETHYS (tethered yearlong spectrometer) 212–13
tetrachlorobiphenyl 3, 4
2,3,7,8-tetrachlorodibenzo-*p*-dioxin (TCDD) 329
tetracyclines 83, 297
tetraethyl lead 2–3
THBG *see* N7-trihydroxybutyl-guanine (THBG)
theoretical plates 124
thermal desorption 246
thermal modulator 139
thermo-labile compounds analysis 42
thermospray ionisation 67–8, 74, 82, 293
thiols 81
THMs *see* trihalomethanes (THMs)
TIC *see* total ion current (TIC) chromatogram
time-of-flight (TOF) analysers 16–17, 199–200 *see also* laser microprobe mass analysis (LAMMA, LMMS)
aerosol analysis 361–4, 372–6, 376–7, 379
CDDs/CDFs 347
combined with triple quadrupoles 391
compared to QTOF analysers 60–1
decoupling 71
direct analysis in real time (DART) 246
DNA adducts analysis 391
fast GC/MS 128, 130
flight path 364
flight time 364
investigative analysis 62–3
ion mass calculation 364
mass resolution (R) 322
multi-purpose 372–4
oil spill dispersants 300
on-line 361–4
orthogonal geometry 71
particle analysis 372–4, 376–7, 379
pesticides 324
plant tissue analysis 252
proton-transfer reaction mass spectrometry (PTR/MS) 243–5
quantitative analysis 33
reflectron lens systems 347
screening speed 61
sensitivity 324
speed of analysis 347
structural determination 71
tandem mass spectrometry 71
two-dimensional GC/GC/MS 138
use with quadrupole ion traps 71
use with quadrupole mass filters (QMFs) 71
water analysis 53
tin *see* organotins
tin salts 225
tissue sections 172–4
tobacco smoke 35, 37, 393, 398
TOF *see* time-of-flight (TOF) analysers
toluene 205, 213, 214
topology 462, 465–6
toroidal ion traps 198–9
total ion current (TIC) chromatogram 23, 34
total mass concentration 378, 380
total organic carbon 52
toxic equivalent factor (TEF) 330
toxic equivalent quantity (TEQ) 330, 338
toxic industrial compounds (TICs) 188–9
TQMS *see* triple quadrupole mass spectrometry (TQMS)
transfer optics 44
transformation products (TPs) 52, 64, 310, 311–12, 319
translational kinetic energy 71
transmission electron microscopy (TEM) 361, 472
tree architecture 254
triazine herbicides 310
triazines 319
tribromophosphine 3, 4
tributyltin (TBT) chloride 293–4
trichlosan 53
triethyleneglycol 35, 37
triethyltin (TET) 292
trihalomethanes (THMs) 265, 267, 268–9
N7-trihydroxybutyl-guanine (THBG) 401
trimethylarsine oxide 294
trimethylsilyl (TMS) 290
trimethyltin (TMT) 292
triphenyltin (TPT) chloride 293–4
triple quadrupole mass spectrometry (TQMS or QqQ) 68–9
combined with ion traps 391
combined with time-of-flight analysers 391
DNA adducts 81, 391, 401, 402
enhanced product ion (EPI) mode 391
oil spill dispersants 300
pesticides 78, 314, 317, 322
pharmaceutical contaminants 78, 296–7
selected reaction monitoring (SRM) 314, 317, 391
sensitivity 314, 317, 391
urine analysis 401
water analysis 82, 314–16
tropolone 293
turbo pumps 202
turbomolecular pumps 202
two-dimensional GC/GC/MS (GC×GC) 138–45, 273, 347, 415
tyrosine 81

UK Environment Agency 230
ULISSES (utilisation of in-situ instrumentation and remote sensing for the study of gaseous emissions at active volcanoes) 209–10, 358–60

ultra-fast gas chromatography 125
ultra performance liquid chromatography (UPLC) 42,
 43, 50
 DNA adducts 81
 pesticides 78, 317–19
 pharmaceutical contaminants 296–7
 sensitivity 43, 319
 wastewater analysis 317–19
ultrafiltration 390
ultrafiltration membranes 276
ultraviolet (UV) detection 42
underwater mass spectrometry 197, 198, 202, 204–8
 autonomous underwater vehicles (AUVs) 204–5,
 206, 207
 dissolved gases 207
 Faraday cup 203
 membrane introduction mass spectrometry
 (MIMS) 204
 quadrupole mass filters (QMFs) 204
 surface guided vehicles 205, 206
 volatile organic compounds (VOCs) 197, 204–8
unit resolution 12
unmanned aerial vehicles 210
UPLC *see* ultra performance liquid chromatography
 (UPLC)
urban air analysis 178, 246–9
urethane 399
urine 389, 400–1, 404–5, 487
US Environmental Protection Agency 41, 89, 93,
 229–30
US Federal Drug Administration (FDA) 94
US Geological Survey (USGS) 41
US National Bureau of Standards (NBS) 94

V-EASI *see* Venturi easy ambient sonic-spray ionisation (V-EASI)
vacuum distillation GC/MS 300
vacuum systems 192, 200–2
valley method 421
van Krevelen diagrams 430, 446
 crude oil 430, 431, 432
 fulvic acid 452
 natural organic matter (NOM) 448–9, 450, 454
 primary organic aerosols (POAs) 454
 secondary organic aerosols (SOAs) 454
vegetable oils 438–9
vehicular emissions 214, 355, 373
Venturi easy ambient sonic-spray ionisation (V-EASI)
 152, 154, 155, 157–9, 161
veterinary drug residues 53
vials 242–3
vineyards 241
vinyl carbamate epoxide 399
VOCs *see* volatile organic compounds (VOCs)
volatile organic compounds (VOCs) 239–58, 353–4
 anthropogenic 239, 240, 247–9
 biogenic 239, 240, 249–53

direct analysis in real time (DART) 242
economic impact 241
fibre introduction mass spectrometry 190
forests 245–6, 249–52
health impact 240–1
hydrocarbon compounds 211–13
isobaric compounds 242
MS analysis methods 241–6
portable devices 188
pre-concentration 242, 243, 244
proton-transfer reaction mass spectrometry
 (PTR/MS) 242
sample preparation 242–3, 244
temperature-dependent classification 252–3
underwater mass spectrometry 197, 204–8
urban areas 246–9
 wastewater analysis 205
volcanic emissions 202, 207–10, 358–60

wastewater analysis
 electrospray ionisation (ESI) 78
 endocrine-disrupting chemicals 76
 orbitraps 78
 ozone 83
 pesticides 316, 317–19, 324–6
 pharmaceutical contaminants 77–8, 79, 297
 portable devices 205
 surfactants 82
 tetracycline 83
 thermospray ionisation 82
 triple quadrupole mass spectrometry (TQMS) 82
 ultra performance liquid chromatography (UPLC)
 317–19
 volatile organic compounds (VOCs) 205
water analysis *see also* underwater mass spectrometry
 ambient mass spectrometry 160
 desorption electrospray ionisation (DESI) 175–7
 disinfection by-products 263–81
 dissolved oxygen concentration 212
 drinking water 59, 60, 263–81
 electron ionisation (EI) 315
 electrospray ionisation (ESI) 78
 endocrine-disrupting chemicals 76
 extractive electrospray ionisation (EESI) 155–6
 gas chromatography/mass spectrometry (GC/MS)
 273–6
 groundwater run-off 213
 herbicides 319–21
 high-field asymmetric waveform ion mobility
 spectrometry (FAIMS) 277–8
 hydrocarbon compounds 211–13
 hydrology 485, 486
 inductively coupled plasma mass spectrometry
 (ICP/MS) 229–30, 276–7
 ion chromatography (IC) 276–7
 liquid chromatography/mass spectrometry
 (LC/MS) 52–3, 276

- liquid–liquid extraction (LLE) 269, 332
membrane introduction mass spectrometry (MIMS) 277
methods for DBP detection 268–80
multiple reaction monitoring (MRM) 273
naphthalene 218
natural organic matter (NOM) 444
negative ion chemical ionisation (NICI) 279
oestrogenic compounds 52, 53
orbitraps 78
ozone 83
pesticides 52–3, 60, 310, 316
pharmaceutical contaminants 53, **56**, 64, 77–8, 79, 297
polycyclic aromatic hydrocarbons (PAHs) 214–16
pre-concentration 317
purge-and-trap (P/T) extraction 269–71
reverse osmosis (RO) membrane extraction 272
selected ion monitoring (SIM) 273
selected reaction monitoring (SRM) 273, 315
semi-permeable membranes 187–8
solid-phase extraction (SPE) 268, 269, 317
solid-phase microextraction (SPME) 268–9, 270
Soxhlet extraction 271
surfactants 82
tetracycline 83
thermospray ionisation 82
transformation products (TPs) 310
triple quadrupole mass spectrometry (TQMS or QqQ) 82, 314–16
two-dimensional GC/GC/MS (GC×GC) 273
ultra performance liquid chromatography (UPLC) 317–19
Venturi easy ambient sonic-spray ionisation (V-EASI) 154
volatile organic compounds (VOCs) 205
XAD resin extraction 271–2
water cycle 477
Water Framework Directive 41
Waters Corporation 99
wildfires 240, 241, 252, 254
wildlife migration 486, 487
Wiley Registry of Mass Spectral Data 94, 95–6, 109
wine 241, 438, 484, 488
XAD resin extraction 271–2
xenobiotics *see* emerging contaminants (ECs)
Z number 426