

# INDEX

## A

Amino acids ..... 5, 34, 36, 39, 40, 42,  
44, 60, 65, 74, 80, 87, 90, 96, 104, 110,  
122–124, 132–134, 138, 139, 206, 209, 216,  
220, 239, 346  
Autophagosome flux ..... 346, 349–351, 353, 355  
Autophagy ..... 345–356

## B

Biomass composition ..... 2, 119–158

## C

Cancer heterogeneity ..... 334  
Cancer metabolism ..... 229, 316, 321  
Carbohydrates ..... 39, 120, 121, 129,  
151, 153  
<sup>13</sup>C based metabolic flux analysis ..... 4  
Cell culture ..... 18, 35, 36, 59–61, 74, 80–83,  
94, 100, 121, 172, 173, 176, 182, 293, 302, 333,  
336, 350  
Central energy metabolism ..... 294  
Chemical ionization (CI) ..... 4, 6, 8, 288  
Chinese Hamster Ovary cells (CHO) ..... 119–121,  
131, 134, 136, 138, 142, 147, 151, 158  
CHO, *see* Chinese Hamster Ovary cells (CHO)  
CI, *see* Chemical ionization (CI)  
<sup>13</sup>C Metabolic flux analysis ..... 33–48  
Computational analysis ..... 173–181  
Constraint-based metabolic models ..... 227  
Constraint-based modeling ..... 120, 227, 293, 317  
Control coefficient ..... 348, 349, 353  
<sup>13</sup>C tracer analysis ..... 93

## D

Data analysis ..... 18, 19, 36, 57, 84–87,  
138, 173, 195, 198, 201, 273–275, 283, 293  
Data integration ..... 68, 227, 319, 333  
Deuterium ..... 51–68  
DFA, *see* Dynamic flux activity (DFA)  
DNA ..... 33, 104, 120, 127, 128, 149,  
150, 152–155, 162, 180, 253, 299, 326  
Drug targets ..... 315–328  
Dynamic flux activity (DFA) ..... 300, 302, 303,  
305–308, 312

## E

*E.coli*, *see* *Escherichia coli* (*E.coli*)  
Elasticity coefficients ..... 347–349, 353, 354  
Equilibrium constant of reactions ..... 366  
*Escherichia coli* (*E.coli*) ..... 162, 163, 172,  
173, 178, 179, 181, 182, 184  
EVs, *see* Extracellular vesicles (EVs)  
Exo-MFA ..... 205–221  
Exosomes ..... 206, 208  
Extracellular vesicles (EVs) ..... 205–215, 217–221

## F

FBA, *see* Flux balance analysis (FBA)  
Fluorescence microscopy ..... 350  
Flux balance analysis (FBA) ..... 17, 212, 224,  
226, 227, 233, 235, 243, 253, 293, 300, 302,  
303, 310, 315–317, 324–327, 333, 355, 361, 363

## G

Gas chromatography (GC) ..... 1–14, 17, 29, 55,  
62, 98, 105, 106, 125, 138–140, 210, 219, 289  
Gas chromatography and mass spectrometry  
(GCMS) ..... 18, 20, 27, 29, 276  
GC, *see* Gas chromatography (GC)  
GCMS, *see* Gas chromatography and mass  
spectrometry (GCMS)  
Genome-scale metabolic models ..... 301, 303  
Genome-scale metabolic network reconstruction  
(GENRE) ..... 315–319, 321, 323, 325, 328  
Genome-scale reconstruction ..... 225  
GENRE, *see* Genome-scale metabolic network  
reconstruction (GENRE)  
Gibbs free energy ..... 250, 359, 361, 364

## H

HILIC, *see* Hydrophilic interaction chromatography  
(HILIC)  
Hydrophilic interaction chromatography  
(HILIC) ..... 34–44

## I

ID, *see* Isotopologue distribution  
In vivo metabolism ..... 94

ISA, *see* Isotopomer spectral analysis (ISA)  
 Isotopologue distribution (ID)..... 2–4, 8, 10, 12,  
 57, 232, 304  
 Isotopomer spectral analysis (ISA)..... 57, 63, 64

**K**

Kinetic models of metabolism ..... 274, 275,  
 285–287, 294

**L**

LC-HRMS ..... 74, 83, 85–87  
 LC-MS, *see* Liquid-chromatography mass  
 spectrometry (LC-MS)  
 Lipids ..... 54, 55, 65, 87, 90, 120, 121, 126,  
 135, 136, 138, 142–145, 147, 152–154, 156,  
 157, 162, 320  
 Liquid-chromatography mass spectrometry  
 (LC-MS) ..... 5, 6, 17, 34, 35, 37, 68,  
 84, 99, 122, 124, 126, 135, 189, 191, 194,  
 199–200

**M**

Mammalian cell culture ..... 51–68, 73  
 Mass isotopologue distribution ..... 8, 192, 198  
 Mass isotopomer distribution ..... 18, 62, 218  
 Mass spectrometry (MS)..... 1–14, 17–19, 27,  
 34, 57, 62, 66–68, 84–85, 87, 94–100, 106, 108,  
 125, 132, 140, 143, 145, 189–203, 216, 225,  
 229, 236, 239, 246, 247, 259, 273–275, 278,  
 282, 286, 288, 289, 333  
 Measurement uncertainty ..... 5, 14  
 Metabolic flux analysis ..... 4, 17, 33–48, 189,  
 206, 218, 226, 333  
 Metabolic fluxes ..... 1, 2, 17, 18, 22, 24,  
 27, 207, 226, 272–275, 283–285, 288, 293, 294,  
 308, 333, 334  
 Metabolic networks..... 2, 18, 27, 111, 217,  
 226, 228, 245, 272, 294, 301, 302, 308,  
 315–328, 332–334, 336, 337, 342, 347, 359,  
 360, 363–365  
 Metabolism ..... 5, 8, 24, 33–36, 39,  
 51–68, 73, 88, 89, 93–116, 189, 209, 221,  
 223–264, 271–295, 299, 307, 308, 311, 312,  
 316, 317, 321, 325, 326, 333, 334, 341  
 Metabolite extraction..... 18, 20, 35, 36, 45,  
 56, 57, 60, 61, 67, 74, 83–84, 97, 103, 104  
 Metabolomics ..... 4, 17, 22, 24, 33, 34,  
 93, 223, 225–227, 229, 242, 247, 258, 273,  
 299–312, 333, 365  
 Metastasis..... 93, 94, 100–102, 110  
 Mouse infusions ..... 103  
 MS, *see* Mass spectrometry (MS)  
 Multicellular metabolic flux analysis ..... 206  
 Multiple reaction monitoring..... 106, 190, 192

**N**

Nicotinamide adenine dinucleotide (NADH)..... 52,  
 55, 56, 63, 178  
 Nicotinamide adenine dinucleotide phosphate  
 (NADPH) ..... 39, 42, 52–56, 63,  
 64, 67  
 Nitric oxide (NO) ..... 161–185  
 Nitric oxide reductase (NorV) ..... 179  
 NO, *see* Nitric oxide (NO)  
 Non-targeted metabolomics ..... 22  
 NorV, *see* Nitric oxide reductase (NorV)  
 Nucleotides..... 34, 36, 37, 39, 41, 42, 44,  
 51, 52, 54, 90, 194

**O**

Off-target effects ..... 315–328

**P**

Parallel reaction monitoring (PRM) ..... 190–192  
 Primary carbon metabolism ..... 2  
 PRM, *see* Parallel reaction monitoring (PRM)

**R**

Redox metabolism ..... 57  
 Reverse phase-ion-pairing..... 34, 36–44  
 RNA ..... 33, 104, 120, 121, 127,  
 147–149, 152–154, 157, 332, 333, 335

**S**

Single-cell RNA-seq ..... 332, 335  
 SIRM, *see* Stable isotope-resolved  
 metabolomics (SIRM)  
 Stable isotope labeling ..... 17, 18  
 Stable isotope-resolved metabolomics  
 (SIRM)..... 271–295  
 Stable isotope tracing..... 81–83, 273  
 Stable isotope tracing experiments ..... 81–83  
 Sugar phosphates ..... 8, 34, 36, 37, 39,  
 41, 42, 194  
 Supply-demand analysis ..... 346, 352  
 Systems biology ..... 231, 249, 315

**T**

Tandem mass isotopologue distribution  
 (TMID)..... 2, 4, 8, 10–12, 14  
 Thermodynamics..... 17, 250, 359,  
 360, 363–366  
 Time-course metabolomics ..... 299–312  
 TMID, *see* Tandem mass isotopologue  
 distribution (TMID)  
 Transcriptomics ..... 223–225, 227, 228, 237,  
 238, 247, 300, 301, 308, 311, 312