

Preface	xiii
List of Abbreviations and Symbols	xv
1 Basic Principles	1
1.1 Introduction	1
1.2 Classical Description	2
1.3 Quantum Mechanical Description	4
1.4 Macroscopic Magnetization	6
1.5 Excitation	8
1.6 Bloch Equations	11
1.7 Fourier Transform NMR	14
1.8 Chemical Shift	18
1.9 Digital Fourier Transform NMR	20
1.9.1 Multi-scan Principle	20
1.9.2 Time-domain Filtering	20
1.9.3 Analog-To-Digital Conversion	22
1.9.4 Zero Filling	25
1.10 Spin-spin Coupling	26
1.10.1 Spectral Characteristics	30
1.11 T_1 Relaxation	33
1.12 T_2 Relaxation and Spin-echoes	36
1.13 Exercises	38
References	41
2 In Vivo NMR Spectroscopy – Static Aspects	43
2.1 Introduction	43
2.2 Proton NMR Spectroscopy	43
2.2.1 Acetate (Ace)	45
2.2.2 N-Acetyl Aspartate (NAA)	45

2.2.3	N-Acetyl Aspartyl Glutamate (NAAG)	52
2.2.4	Adenosine Triphosphate (ATP)	52
2.2.5	Alanine (Ala)	53
2.2.6	γ -Aminobutyric Acid (GABA)	54
2.2.7	Ascorbic Acid (Asc)	54
2.2.8	Aspartate (Asp)	55
2.2.9	Choline-containing Compounds (tCho)	55
2.2.10	Creatine (Cr) and Phosphocreatine (PCr)	57
2.2.11	Ethanolamine and Phosphorylethanolamine (PE)	58
2.2.12	Glucose (Glc)	59
2.2.13	Glutamate (Glu)	59
2.2.14	Glutamine (Gln)	61
2.2.15	Glutathione (GSH)	62
2.2.16	Glycerol	62
2.2.17	Glycine	63
2.2.18	Glycogen	63
2.2.19	Histamine	64
2.2.20	Histidine	65
2.2.21	Homocarnosine	65
2.2.22	β -Hydroxybutyrate (BHB)	66
2.2.23	<i>Myo</i> -Inositol (mI) and <i>scyllo</i> -Inositol (sI)	66
2.2.24	Lactate (Lac)	67
2.2.25	Macromolecules	68
2.2.26	Phenylalanine	70
2.2.27	Pyruvate	70
2.2.28	Serine	71
2.2.29	Succinate	71
2.2.30	Taurine (Tau)	72
2.2.31	Threonine (Thr)	72
2.2.32	Tryptophan (Trp)	73
2.2.33	Tyrosine (Tyr)	73
2.2.34	Valine (Val)	74
2.2.35	Water	74
2.2.36	Intra- and Extramyocellular Lipids (IMCL and EMCL)	75
2.2.37	Deoxymyoglobin (DMb)	76
2.2.38	Citric Acid	77
2.2.39	Carnosine	78
2.3	Phosphorus-31 NMR Spectroscopy	78
2.3.1	Identification of Resonances	79
2.3.2	Intracellular pH	80
2.4	Carbon-13 NMR Spectroscopy	82
2.4.1	Identification of Resonances	82
2.5	Sodium-23 and Potassium-39 NMR Spectroscopy	85
2.6	Fluorine-19 NMR Spectroscopy	89
2.6.1	Identification of Resonances	89

2.6.2	Fluorinated Drugs, Anaesthetics, and Fluorodeoxyglucose Metabolism	90
2.6.3	Fluorinated Probes	92
2.7	Exercises	93
	References	95
3	<i>In Vivo</i> NMR Spectroscopy – Dynamic Aspects	111
3.1	Introduction	111
3.2	Relaxation	112
3.2.1	General Principles of Dipolar Relaxation	112
3.2.2	Nuclear Overhauser Effect	118
3.2.3	Alternative Relaxation Mechanisms	119
3.2.4	<i>In Vivo</i> Relaxation	122
3.3	Magnetization Transfer	128
3.3.1	Creatine Kinase	130
3.3.2	Inversion Transfer	131
3.3.3	Saturation Transfer	131
3.3.4	ATpases	134
3.3.5	Fast Magnetization Transfer Methods	135
3.3.6	Off-resonance Magnetization Transfer	136
3.3.7	Chemical Exchange Dependent Saturation Transfer	141
3.4	Diffusion	141
3.4.1	Principles of Diffusion	141
3.4.2	Diffusion and NMR	143
3.4.3	Anisotropic Diffusion	152
3.4.4	Restricted Diffusion	156
3.5	Dynamic Carbon-13 NMR Spectroscopy	158
3.5.1	General Set-up	160
3.5.2	Metabolic Modeling	162
3.5.3	Substrates	166
3.5.4	Applications	171
3.6	Hyperpolarization	171
3.6.1	“Brute Force” Hyperpolarization	172
3.6.2	Optical Pumping of Noble Gases	173
3.6.3	Para-hydrogen-induced Polarization (PHIP)	175
3.6.4	Dynamic Nuclear Polarization	177
3.7	Exercises	179
	References	181
4	Magnetic Resonance Imaging	191
4.1	Introduction	191
4.2	Magnetic Field Gradients	192
4.3	Slice Selection	193
4.4	Frequency Encoding	195
4.5	Phase Encoding	201

4.6	Spatial Frequency Space	202
4.7	Fast MRI Sequences	206
4.7.1	Echo-planar Imaging	208
4.8	Contrast in MRI	212
4.8.1	T_1 and T_2 Relaxation Mapping	213
4.8.2	Fast T_1 and T_2 Relaxation Mapping	214
4.8.3	Magnetic Field B_0 Mapping	216
4.8.4	Magnetic Field B_1 Mapping	218
4.8.5	Alternative Image Contrast Mechanisms	219
4.8.6	Functional Imaging	220
4.9	Parallel MRI	222
4.10	Exercises	225
	References	229
5	Radiofrequency Pulses	233
5.1	Introduction	233
5.2	Square RF Pulses	233
5.3	Selective RF Pulses	239
5.3.1	Sinc Pulses	239
5.3.2	Gaussian and Hermitian Pulses	243
5.3.3	Multifrequency RF Pulses	246
5.4	Pulse Optimization	247
5.4.1	Shinnar–Le Roux Algorithm	248
5.5	DANTE RF Pulses	254
5.6	Composite RF Pulses	255
5.7	Adiabatic RF Pulses	258
5.7.1	Rotating Frames of Reference	259
5.7.2	Adiabatic Half and Full Passage Pulses	262
5.7.3	Plane Rotations and Refocused Component	268
5.7.4	Adiabatic Full Passage Refocusing	269
5.7.5	Adiabatic Plane Rotation Pulses	269
5.7.6	Variable Angle Adiabatic Plane Rotation Pulse, BIR-4	271
5.7.7	Modulation Functions	274
5.7.8	Offset-independent Adiabaticity	275
5.8	Pulse Imperfections and Relaxation	276
5.9	Power Deposition	280
5.10	Multidimensional RF Pulses	283
5.11	Spectral–spatial RF Pulses	289
5.12	Exercises	290
	References	292
6	Single Volume Localization and Water Suppression	297
6.1	Introduction	297
6.2	Single Volume Localization	299
6.2.1	Image Selected <i>In Vivo</i> Spectroscopy (ISIS)	299
6.2.2	Chemical Shift Displacement	302

6.2.3	Stimulated Echo Acquisition Mode (STEAM)	306
6.2.4	Point Resolved Spectroscopy (PRESS)	310
6.2.5	Signal Dephasing with Magnetic Field Gradients	311
6.2.6	Effects of Imperfect RF Pulses	317
6.2.7	Localization by Adiabatic Selective Refocusing (LASER)	320
6.2.8	Chemical Shift Displacement – Scalar-coupled Spins	322
6.3	Water Suppression	325
6.3.1	Binomial and Related Pulse Sequences	326
6.3.2	Frequency Selective Excitation	333
6.3.3	Frequency Selective Refocusing	337
6.3.4	Relaxation Based Methods	338
6.3.5	Non-water-suppressed NMR Spectroscopy	340
6.4	Exercises	341
	References	344
7	Spectroscopic Imaging and Multivolume Localization	349
7.1	Introduction	349
7.2	Principles of Spectroscopic Imaging	349
7.3	Spatial Resolution in MRSI	354
7.4	Temporal Resolution in MRSI	357
7.4.1	Conventional Methods	357
7.4.2	Methods Based on Fast MRI Sequences	361
7.4.3	Methods Based on Prior Knowledge	365
7.5	Lipid Suppression	367
7.5.1	Relaxation Based Methods	368
7.5.2	Outer Volume Suppression and Volume Pre-localization	368
7.5.3	Methods Utilizing Spatial Prior Knowledge	371
7.6	Spectroscopic Imaging Processing and Display	373
7.7	Multivolume Localization	377
7.7.1	Hadamard Localization	378
7.7.2	Sequential Multivolume Localization	380
7.8	Exercises	382
	References	384
8	Spectral Editing and Two-dimensional NMR	389
8.1	Introduction	389
8.2	Scalar Evolution	390
8.3	J-difference Editing	392
8.4	Practical Considerations of J-difference Editing	397
8.5	Multiple Quantum Coherence Editing	402
8.6	Heteronuclear Spectral Editing	407
8.7	Polarization Transfer – INEPT and DEPT	409
8.8	Sensitivity	414
8.9	Broadband Decoupling	416

8.10	Two-dimensional NMR Spectroscopy	421
8.10.1	Correlation Spectroscopy (COSY)	422
8.10.2	Spin-echo or J-resolved NMR	432
8.10.3	Two-dimensional Exchange Spectroscopy	434
8.11	Exercises	438
	References	440
9	Spectral Quantification	445
9.1	Introduction	445
9.2	Data Acquisition	446
9.3	Data Pre-processing	449
9.3.1	Phasing and Frequency Alignment	450
9.3.2	Lineshape Correction	450
9.3.3	Removal of Residual Water	451
9.3.4	Baseline Correction	453
9.4	Data Quantification	453
9.4.1	Time- and Frequency-domain Parameters	454
9.4.2	Prior Knowledge	457
9.4.3	Spectral Fitting Algorithms	460
9.4.4	Error Estimation	464
9.5	Data Calibration	466
9.5.1	Internal Concentration Reference	470
9.5.2	External Concentration Reference	472
9.5.3	Phantom Replacement External Concentration Reference	473
9.6	Exercises	473
	References	475
10	Hardware	479
10.1	Introduction	479
10.2	Magnets	480
10.3	Magnetic Field Homogeneity	484
10.3.1	Origins and Effects of Magnetic Field Inhomogeneity	
	<i>In Vivo</i>	484
10.3.2	Active Shimming	489
10.3.3	Shimming Hardware	492
10.3.4	Manual Shimming	492
10.3.5	Magnetic Field Map Based Shimming	494
10.3.6	Projection Based Shimming	497
10.3.7	Dynamic Shim Updating (DSU)	499
10.3.8	Passive Shimming	502
10.4	Magnetic Field Gradients	502
10.4.1	Eddy Currents	506
10.4.2	Pre-Emphasis	508
10.4.3	Active Shielding	512

10.5	Radiofrequency Coils	512
10.5.1	Resonant LCR Circuits	513
10.5.2	RF Coil Performance	519
10.5.3	Spatial Field Properties	521
10.5.4	Principle of Reciprocity I	526
10.5.5	Principle of Reciprocity II	529
10.6	Radiofrequency Coil Types	530
10.6.1	Combined Transmit and Receive RF Coils	531
10.6.2	Phased-array Coils	532
10.6.3	^1H - ^{13}C and ^{13}C - ^1H RF Coils	533
10.6.4	Cooled (Superconducting) RF Coils	536
10.7	Complete MR System	536
10.7.1	RF Transmission	536
10.7.2	Signal Reception	537
10.7.3	Quadrature Detection	539
10.7.4	Dynamic Range	540
10.7.5	Gradient and Shim Systems	541
10.8	Exercises	542
	References	545
	Appendix	549
A1	Matrix Calculations	549
A2	Trigonometric Equations	551
A3	Fourier Transformation	551
A3.1	Introduction	552
A3.2	Properties	553
A3.3	Discrete Fourier Transformation	554
A4	Product Operator Formalism	554
A4.1	Cartesian Product Operators	555
A4.2	Spherical Tensor Product Operators	556
	References	559
	Further Reading	560
	Index	563