NMR of Biomolecules

Towards Mechanistic Systems Biology

Edited by Ivano Bertini,
Kathleen S. McGreevy,
and Giacomo Parigi

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藏书章

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Cover
The artwork on the cover attempts to convey the idea of the systems of interacting biomolecules that are at the basis of Life. The Birth of Venus, which has been reimagined for the cover in this spirit, was painted by Sandro Botticelli in the late 15th century and is held by the Uffizi Gallery in Florence. His painting depicts the birth of the goddess of love as she emerges as a fully grown adult from the sea.

Acording to Plato, as well as members of the Florentine Platonic Academy, Venus had two aspects: an earthly goddess who aroused humans to physical love, and a heavenly goddess that inspired intellectual love. Who better than she to represent our passion for the study of biomolecular structures and mechanisms, and the physical-intellectual duality that leads us to learn more about the living world around and within each of us? Actually Venus has already been used as the logo by the Society of Biological Inorganic Chemistry for the Journal of Biological Inorganic Chemistry (JBIC).

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Preface

The use of NMR to solve protein structures has a tradition that dates back to 1984 (M.P. Williamson, T.F. Havel, and K. Wüthrich (1985) *J. Mol. Biol.* **182**, 295). Since that time, the role of NMR in structural biology has constantly increased in terms of the number of researchers involved and the scientific relevance of the results. Spectrometers are becoming more and more powerful, with magnetic fields that currently reach 22 T, and high-temperature superconducting materials raise the possibility that this value can be surpassed. The investment required for a magnet of the above intensity is currently around €10 million (US$14.3 million) and an estimate of €18 million (US$25.7 million) is reasonable for new-generation magnets. It is clear that NMR is a technology that deserves a special place in research infrastructures, as individual schools may find it difficult to have a battery of machines, all at the forefront of the technology, dedicated to various types of experiments. In 1994, the European Commission (EC) began financing transnational access to NMR instrumentation at some research infrastructures, which have continued and grown in number until the present with the EC-funded Bio-NMR[1] project. In Europe, the recent European Strategy Forum for Research Infrastructures (ESFRI) Roadmap identifies NMR as a fundamental node in the Integrated Structural Biology Infrastructure (INSTRUCT),[2] while it also plays a role in the EU-OPEN-SCREEN (European Infrastructure of Open Screening Platforms for Chemical Biology)[3] infrastructure, Euro-BioImaging,[4] and Biobanking and Biomolecular Resources Research Infrastructure (BBMRI).[5]

The EC-funded electronic infrastructures (e-NMR[6] and WeNMR[7]) provide nonspecialists with tools for automatic data handling, structure calculations, molecular dynamics simulations, and the creation of interaction models in such a way that the potential of the NMR technology can blossom in favor of the progress of science.

Much of this reasoning was debated during the FP6-funded Coordination Action NMR-Life[8] and resulted in a booklet entitled *NMR in Mechanistic Systems Biology*,[9] which ultimately served as the spark for this volume. We were pleased when Gregor

1) http://www.bio-nmr.net.

2) http://www.structuralbiology.eu.

3) http://www.eu-openscreen.eu.

4) http://www.eurobioimaging.eu.

5) http://www.bbmri.eu.

6) http://www.enmr.eu.

7) http://www.wenmr.eu.

8) http://www.postgenomicnmr.net.

9) http://www.postgenomicnmr.net/NMRLife/docs/NMR_in_MSB.pdf.

Cicchetti from Wiley-VCH noticed this booklet and proposed that we edit a book on the very same subject, and we gathered a number of outstanding contributors to fulfill the task.

Our intention, which we hope pervades the book, was to provide a text for graduate students, junior post-docs, and other newcomers that would serve as an introduction to the field, addressing classical NMR approaches from solution to the solid state, providing some tips and tricks not available in journal articles, and providing perspectives on future developments. It is our hope that the Protocols and Troubleshooting sections will be of assistance and guidance when choosing experiments and overcoming difficulties.

However, everyone who has experience in editing books knows how difficult a task it is – obtaining the manuscripts on time, convincing everyone to adhere to a template and write for students and not for their fellow professors, and even drawing the line on what content to include and when to call an end to the editorial process, including substitution of recalcitrant contributors. We editors have tried our best to overcome these difficulties, but we are aware that much more could have been done. For example, the development of isotopic labeling has been fundamental for the development of NMR, but we decided not to address it here. The reader should therefore be aware that the field of NMR is even broader and more exciting than it appears from our efforts!

Part I of the book (Introduction) explains NMR's role in Mechanistic Systems Biology and provides a broad overview of biomolecular structure before identifying what NMR can teach us about the structure and dynamics of biomolecules. Parts II–VII address a series of relevant topics in NMR-driven biological research: the role of NMR in the study of the structure and dynamics of biomolecules, its role in the study of the structure and dynamics of biomolecular interactions, NMR in drug discovery, solid-state NMR, frontiers in NMR spectroscopy, and computational aspects.

We would like to take the opportunity to thank, in addition to Gregor, Dr. Marco Fragai of the Center for Magnetic Resonance (CERM) at the University of Florence for his assistance in editing some chapters of the book, and Professor Claudio Luchinat, who consistently demonstrates his friendship and his willingness to support any initiative of CERM, and the scientific personnel of CERM who have contributed to discussions and sustained the work.

It is our sincere hope that this book will find a home not only in NMR facilities, but also in biomedical laboratories around the world, where it can be of use to the broader scientific community and help diffuse NMR as a technique for the study of biological systems.

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Florence, January 2012

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List of Abbreviations

Aβ	amyloid beta
9-AA	9-aminoacridine
ABC	ATP-binding cassette
AcP	acetyl phosphate
ACRAMTU	acridinylthiourea
ACS	automatic sample changer
ADME-T	adsorption, distribution, metabolism, excretion, and toxicity
A-E	alanine-glutamic acid
AFM	atomic force microscopy
ahaz	3-aminohexahydroazepine
AIR	ambiguous interaction restraint
AKT	serine/threonine protein kinase
Amp	ampicillin
AO	acridine orange
APHH	adiabatic passage through the Hartman-Hahn condition
APSY	automated projection spectroscopy
ATP	adenosine triphosphate
Atx1	antioxidant protein 1
AUIM	ataxin 3 ubiquitin interacting motif
ben	benzene
BEST	band-selective excitation short-transient
bip	biphenyl
BMRB	biological magnetic resonance data bank
BP	back-projection
BPTI	bovine pancreatic trypsin inhibitor
bpy	bipyridine
bR	bacteriorhodopsin
BRCT	breast cancer 1 C-terminal
BSA	buried surface area
BSA	bovine serum albumin
BSE	bovine spongiform encephalopathy
BURP	band-selective uniform-response pure-phase
BUSI	proteinase inhibitor from bull seminal plasma
1C3	1-[(3-aminopropyl)amino]-anthracene-9,10-dione
CA	certification authority
CA150	coactivator of 150 kDa
Cam	chloramphenicol
cAMP	cyclic adenosine monophosphate
CAP	catabolite activator protein
CAP	cAMP-binding protein

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CASD	critical assessment of automatic structure determination
CATH	class, architecture, topology, homologous superfamily
CBP	CREB-binding protein
Ccc2a	domain a of Ca^{2+}-sensitive cross-complementer2
CCPN	collaborative computing project for NMR
CCR	cross correlation rate
Cdk2	cyclin-dependent kinase 2
CE	computing element
CECF	continuous exchange cell-free
CF	cell-free
CFCF	continuous flow cell-free
chrysi	5,6-chrysene quinone diimine
CIDNP	chemically induced dynamic nuclear polarization
CIP1	cyclin-dependent kinase inhibitor 1
CJD	Creutzfeldt-Jacob disease
CLEANEX	clean chemical exchange spectroscopy
CMC	critical micelle concentration
COSY	correlation spectroscopy
CP	cross polarization
CPMG	Carr-Purcell-Meiboom-Gill
CPP	cellular penetrating peptide
CPU	central processing unit
CREB	cAMP-response element-binding protein
CRINEPT	cross-correlated relaxation-enhanced polarization transfer
CRIPT	cross-correlated relaxation-induced polarization transfer
CS	chemical shift
CsA	cyclosporin A
CSA	chemical shift anisotropy
CSD	Cambridge structural database
CSI	chemical shift index
CSP	chemical shift perturbation
CST	chemical-shift tensor
CT	constant time
CW	continuous wave
CWLG	continuous wave Lee-Goldburg
CycA	cyclin A
cym	p-cymene
CYPA	cyclophilin A
dap	1,12-diazaperylene
DARR	dipolar assisted rotational resonance
DBD	DNA binding domain
D-CF	detergent based cell-free
DCP	double cross polarization
DD	dipole-dipole
DDM	n-dodecyl-β-D-maltoside
DEER	double electron-electron resonance
DEPT	distortionless enhancement by polarization transfer
DFS	dynamic frequency shift
DFT	discrete Fourier transform
DG	distance geometry
dha	dihydroanthracene
DHFR	dihydrofolate reductase
DIDC	direct interpretation of dipolar couplings
dien	diethylenetriamine
DIPAP	double in-phase/antiphase
DIPSI	decoupling in the presence of scalar interactions
DISCO	differences and sums of traces within COSY spectra

dmen	N-dimethylethylenediamine
DMF	N,N-dimethylformamide, *N,N*-dimethylmethanamide
DMSO	dimethylsulfoxide
DNA	deoxyribonucleic acid
DNP	dynamic nuclear polarization
DO3A	1,4,7-tris(acetic acid)-1,4,7,10-tetraazacyclododecane
DOSY	diffusion ordered spectroscopy
DOTA	1,4,7,10-tetraazacyclododecane-1,4,7,10-tetraacetic acid
DOTP	1,4,7,10-tetraazacyclododecane-N,N′,N″,N‴-tetrakis(methylene-phosphonic acid)
DP	discriminating power
DPC	dodecyl-phosphocholine
DPP	dipeptidyl peptidase
dppz	dipyrido[3,2-*a*:2′,3′-*c*]phenazine
dpzm	4,4′-dipyrazolylmethane
DQ	double quantum
DQF	double quantum filtered
DR	dummy residue
DREAM	dipolar recoupling enhanced by amplitude modulation
DS3E	double spin-state-selective excitation
dsDNA	double-strand DNA
dsRBD3	double stranded RNA binding domain 3
dsRNA	double-strand RNA
DSS	2,2-Dimethyl-2-silapentane-5-sulfonic acid
DTPA	diethylene triamine pentaacetic acid, 2-[bis[2-[bis(carboxymethyl) amino]ethyl]amino]acetic acid
DTPA-BMA	diethylenetriamine pentaacetic acid bis(methylamide)
DTT	dithiothreitol, (*2S,3S*)-1,4-bis-sulfanylbutane-2,3-diol
dx	doxorubicin
E2A	glucose-specific enzyme IIA
EAS	explicit averaged sum
EBURP	exciting band-selective uniform-response pure-phase
ECOSY	exclusive correlation spectroscopy
EDTA	ethylenediaminetetraacetic acid, 2,2′,2″,2‴-(ethane-1,2-diyldinitrilo)tetraacetic acid
EM	electron microscopy
EmrE	Escherichia coli multidrug resistance protein
en	ethylenediamine
ENDOR	electron nuclear double resonance
EOM	ensemble optimization method
EPI	echo-planar imaging
EPR	electron paramagnetic resonance
ERCC1	excision repair cross complementing 1
ERETIC	electronic reference to access in vivo concentrations
EROS	ensemble refinement with orientational restraints
Eth	ethidium bromide
et-NOESY	exchange transferred nuclear Overhauser effect spectroscopy
EXAFS	extended X-ray absorption fine structure
EXSY	exchange spectroscopy
FABS	fluorine atoms for biochemical screening
FBDD	fragment-based drug design
FDM	filter diagonalization method
FID	free induction decay
FKBP	FK506-binding protein
FlgM	flagellar anti-sigma factor
FRB	FKBP-rapamycin-binding
FRET	fluorescent resonance energy transfer

FF	force field
FFT	fast Fourier transform
FM	feeding mixture
fMD	free molecular dynamics
FP	fluorescence polarization
FT	Fourier transform
FTA	fluid-turbulence adapted
FTIR	Fourier transform infrared spectroscopy
GB1	immunoglobulin binding domain of protein G
GFP	green fluorescent protein
GFT	G-matrix Fourier transform
GMP	guanosine monophosphate
GP-AFC	Gly-Pro-7-amino-4-trifluoromethylcoumarin
GPCR	G protein-coupled receptor
GTP	guanosine triphosphate
GUI	graphical user interface
HAMP	histidine kinases, adenylyl cyclases, methyl-accepting chemotaxis proteins, and phosphatases
HCA	hierarchical clustering analysis
HDX	hydrogen-deuterium exchange
HEPES	2-[4-(2-hydroxyethyl)piperazin-1-yl]ethanesulfonic acid, 2-[4-(2-hydroxyethyl)-2,3,5,6-tetrahydropyrazin-1-yl]ethanesulfonate
HET	2-hydroxyethanethiolato-2,2′,2″-terpyridine
HETLOC	heteronuclear long-range coupling
HF	high field
HH	head-to-head
HiPIP	high-potential iron-sulphur protein
HIV	human immunodeficiency virus
HMBC	heteronuclear multiple bond coherence
HMQC	heteronuclear multiple quantum coherence
HOESY	heteronuclear Overhauser effect spectroscopy
HORROR	homonuclear rotary resonance
HoxD9	homeobox protein D9
HPLC	high-performance liquid chromatography
HPr	histidine-containing phosphocarrier protein
HR	high resolution
HRP1	hetero ribonucleoprotein 1
HRS	hepatocyte growth factor-regulated tyrosine kinase substrate
HSA	human serum albumin
HSQC	heteronuclear single quantum coherence
HTS	high-throughput screening
IDP	intrinsically disordered protein
IDR	intrinsically disordered region
IEP	isoelectric point
ILOE	interligand Overhauser effect
ILV	Ile, Leu, Val
ILVA	Ile, Leu, Val, Ala
IMP	integral membrane protein
INADEQUATE	incredible natural abundance double quantum transfer experiment
INEPT	insensitive nuclei enhanced by polarization transfer
INPHARMA	interligand NOEs for pharmacophore mapping
IPAP	in-phase/antiphase
IPSL	3-(2-iodoacetamido-proxyl)
IPTG	induced T7 promoter-lac operator (P_{T7}/lacOp)
IRES	internal ribosomal entry site
ITAM	immunoreceptor tyrosine-based activation motif

ITC	isothermal titration calorimetry
IUPAC	international union of pure and applied chemistry
IXL	interstrand cross-link
JS-ROESY	jump-symmetrized rotating frame Overhauser effect spectroscopy
Kan	kanamycin
KcsA	Streptomyces lividans potassium channel
KH	K homology
KH3	third KH domain
KID	kinase inducible domain
Kip1	kinase inhibitor 1
k-NN	k-nearest-neighbour
KPi	potassium phosphate
KSRP	KH-type splicing regulatory protein
KTX	kaliotoxin
LAB	laboratory frame
Lac	lactose
LacR	lactose repressor
LBT	lanthanide binding tag
LC	liquid crystalline
L-CF	lipid based cell-free
LDA	linear discriminant analysis
LED	light emitting diode
LG-CP	Lee-Goldburg cross polarization
LILBID	laser induced liquid bead ion desorption
LMPG	1-myristoyl-2-hydroxy-sn-glycero-3-[phosphorac-(1-glycerol)]
LOGSY	ligand observed by gradient spectroscopy
LPPG	1-palmitoyl-2-hydroxy-sn-glycerol-3-[phosphor-rac-(1-glycerol)]
LRE	longitudinal relaxation enhancement
LV	lowest-value
MAP	microtubule-associated protein
MAS	magic angle spinning
MaxEnt	maximum entropy
MBP	maltose binding protein
Mbp1	Mlu1 cell cycle box binding protein
MD	molecular dynamics
MDD	multidimensional decomposition
MDL	molecular design limited
MFR	molecular fragment replacement
Mia40	mitochondrial intermembrane space import and assembly 40
miRNA	microRNA
MIRROR	mixed rotational and rotary resonance
MLEV	Malcolm Levitt's composite-pulse decoupling sequence
MMP	matrix metalloproteinase
MO	maximum occurrence
MP	membrane protein
MPL	mass-per-length
MRI	magnetic resonance imaging
mRNA	messenger RNA
MRS	magnetic resonance spectroscopy
MS	mass spectrometry
MSA	mobility shift microfluid assay
α-MSH	alpha-melanocyte stimulating hormone
MT-II	Ac-Nle-c[Asp-His-D-Phe-Arg-Trp-Lys]-NH_2
MTSSL	1-oxy-2,2,5,5-tetramethyl-Δ3-pyrroline-3-methyl methanethiosulfonate
MW	molecular weight

MWCO	molecular weight cutoff
NMR	nuclear magnetic resonance
NIH	National Institutes of Health
NN	neural network
NOE	nuclear Overhauser effect
NOESY	nuclear Overhauser effect spectroscopy
NTA	nitrilotriacetic acid
NTP	nucleotide triphosphate
NUS	non-uniformly sampled
NusA	N utilization substance protein A
NzExHSQC	Nz-chemical exchange heteronuclear single-quantum coherence
OAc	acetate
Oct-1	octamer 1
OD	optical density
ODMR	optically detected magnetic resonance
OGT	optimal growth temperature
OPLS	optimized potentials for liquid simulations
P21	protein 21
P32/98	(2S,3S)-2-amino-3-methyl-1-(1,3-thiazolidin-3yl)pentan-1-one
P53	protein 53
PAGE	polyacrylamide gel electrophoresis
PAIN-CP	proton assisted insensitive nuclei cross polarization
PAK	p21-activating kinase protein
PAP	poly(A) polymerase
PAR	proton assisted recoupling
PARIS	phase-alternated recoupling irradiation scheme
PAS	principal axes system
PC	principal component
PCA	principal component analysis
PCCR	paramagnetic cross correlation rate
P-CF	precipitate generating cell-free
PCR	polymerase chain reaction
PCS	pseudocontact shift
PDB	protein data bank
PDMS	poly(dimethylsiloxane)
PDSD	proton driven spin diffusion
PECOSY	primitive exclusive correlation spectroscopy
PEG	polyethylene glycol
PFG	polyfluorinated glycine
phen	phenanthroline
phi	phenanthrenequinone diimine
PHIP	para-hydrogen induced polarization
PH-PDMAA	dimethylacrylamide copolymer
PI3	phosphoinositide 3
PI3-SH3	SH3 domain of the PI3 kinase
PIE	polyadenylation inhibition element
PISEMA	polarization inversion spin-exchange at the magic angle
PKA	protein kinase A
PLS	partial least square
PME	particle mesh Ewald
PMSF	phenylmethanesulfonylfluoride
POP	prolyl oligopeptidase
POST-C7	permutationally offset stabilized C7
ppm	parts per million
pqx	2-(2′-pyridyl)quinoxaline
PRDC	paramagnetism-based residual dipolar coupling
PRE	paramagnetic relaxation enhancement

PrP^{Sc}	misfolded prion protein (Sc for scrapie)
PSF	point spread function
PTM	post-translational modification
PULCON	pulse length based concentration
py	pyrimidine
PyAc	pyridine-2-yl acetate
2/3QF-COSY	double/triple quantum filtered correlated spectroscopy
RAD	RF assisted diffusion
RCSA	residual chemical shift anisotropy
RDC	residual dipolar coupling
REBURP	refocusing exciting band-selective uniform-response pure-phase
REDOR	rotational echo double resonance
RF	radiofrequency
RFDR	radiofrequency driven recoupling
RISC	RNA-induced silencing complex
RM	reaction mixture
rMD	restrained molecular dynamics
RMS	root mean square
RMSD	root mean square deviation
ROCSA	recoupling of chemical shift anisotropy
rOCT	rat organic cation transporter
ROE	rotating frame Overhauser effect
ROESY	rotational nuclear Overhauser effect spectroscopy
ROG	red-orange-green
RPF	recall, precision and F-measure
rpm	revolutions per minute
RNA	ribonucleic acid
RRE	Rev response element
RRM	RNA recognition motif
R, R-Me_2trien	2R, 9R-diamino-4,7-diazadecane
rRNA	ribosomal ribonucleic acid
RT	real time
RXR	retinoic X receptor
S/N	signal-to-noise
S3E	spin-state-selective excitation
SA	simulated annealing
SAG	strain-induced alignment in a gel
SAIL	stereo-array isotope labeling
SAR	structure activity relationship
SANS	small angle neutron scattering
SAS	small angle scattering
SAXS	small angle X-ray scattering
Sco	synthesis of cytochrome *c* oxidase
SCOP	structural classification of proteins
SCRM	self-consistent RDC-based model-free
SD	standard deviation
SDS	sodium dodecyl sulfate
SDSL	site directed spin labeling
SDS-PAGE	sodium dodecyl sulphate - polyacrylamide gel electrophoresis
SIA	scaffold independent analysis
SE	storage element
SE-DIPAP	sensitivity enhanced DIPAP
SH3	src-homology domain 3
SI	international system of units
siRNA	small interfering RNA
SLAPSTIC	spin labels attached to the protein side chains as a tool to identify interacting compounds

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