NMR structural studies of protein-small molecule interactions

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Cover Image: The NMR structure of the Hsp90-ligand complex (front cover) and the Rit1-GDP-ligand ternary complex (back cover)

Cover designed by Dipen Shah

Doctoral Thesis, Leiden University, 2014

Printed by Ipskamp Printers, Enschede

ISBN: 978-94-6259-201-8

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Proefschrift

ter verkrijging van
de graad van Doctor aan de Universiteit Leiden,
op gezag van Rector Magnificus Prof. mr. C.J.J.M.Stolker,
volgens besluit van het College voor Promoties
te verdedigen op dinsdag 17 juni 2014
klokke 15:00 uur

door
Dipen M. Shah
Geboren te Mangalore, India in 1985

Promotiecommissie

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“Dream is not that which you see while sleeping, it is something that does not let you sleep”

Dr. A.P.J. Abdul Kalam, Wings of Fire

To all who made this possible

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Abbreviations

ATP	adenosine triphosphate
ADMET	absorption,distribution,metabolism, excretion, toxicology
CPMG	Carr-Purcell-Meiboom-Gill
CRINEPT	cross-correlated relaxation enhanced polarisation
CSP	chemical shift perturbation
DTT	dithiothreitol
EDTA	ethylenedimaminetetraaceticacid
EPR	electron paramagnetic resonance
FBDD	fragment based drug discovery
GTP	guanosine triphosphate
HEPES	4-(2-hydroxyethyl)-1-piperazineethanesulfonic acid
HSQC	heteronuclear single quantum coherence
Hsp90	heat shock protein 90
HTS	high throughput screening
ILOE	inter-ligand overhauser effect
IPTG	isopropyl β-D-1-thiogalactopyranoside
MALDI-TOF	matrix-assited laser desorption/ionization time of light
MTS	[(1-Acetyl-2,2,5,5-tetramethyl-3-pyrroline-3-methyl)methanethiosulfonate]
MTSL	[(1-Oxyl-2,2,5,5-tetramethylpyrroline-3-yl)methyl]-methanethiosulfonate
NMR	nuclear magnetic resonance
NOESY	nuclear overhauser effect spectroscopy
PDB	protein data bank
PRE	paramagnetic relaxation enhancement
PCS	pseudocontact shift
RF	radio frequency
RMSD	root mean square deviation
SDS-PAGE	sodium dodecyl sulfate polyacrylamide gel electrophoresis
STD	saturation transfer difference
TCEP	tris(2-carboxyethyl)phosphine
TINS	target immobilized NMR screening
TOCSY	total correlation spectroscopy
Tris-HCl	trisaminomethane hydrochloride
TROSY	transverse-relaxation optimized spectroscopy