Declaration

I hereby declare that the work presented in this Thesis titled *Nuclear Magnetic Resonance (NMR) investigation of molecular interactions in model drug delivery systems* submitted to the Indian Institute of Technology Jodhpur in partial fulfilment of the requirements for the award of the degree of Doctor of Philosophy, is a bonafide record of the research work carried out under the supervision of Dr. Samanwita Pal. The contents of this thesis in full or in parts, have not been submitted to, and will not be submitted by me to, any other Institute or University in India or abroad for the award of any degree or diploma.

Deepak Kumar
PG201383501

Certificate

This is to certify that the thesis titled *Nuclear Magnetic Resonance (NMR) investigation of molecular interactions in model drug delivery systems*, submitted by *Deepak Kumar* (PG201383501) to the Indian Institute of Technology Jodhpur for the award of the degree of *Doctor of Philosophy*, is a bonafide record of the research work done by him under my supervision. To the best of my knowledge, the contents of this report, in full or in parts, have not been submitted to any other Institute or University for the award of any degree or diploma.

Samanwita Pal
Ph.D. Thesis Supervisor

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Deepak Kumar
Ph.D. Student

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List of Symbols

Symbol	*Description*
Å	Angstrom
B_o	Static magnetic field
β	Full width at half maximum of a XRD peak
°C	Degree Celsius
D	Diffusion coefficient
D_o	Intrinsic diffusion coefficient
d	Delay
dB	Decibel
Δ	Diffusion delay
ΔE	Difference in energy between nuclear-spin populations
δ	Chemical shift/Gradient length
δ_{ppm}	Chemical shift in parts per million
Δδ	Chemical shift change
E	Energy
E_g	Bandgap
F_1	Frequency dimension-1
F_2	Frequency dimension-2
γ	Gyromagnetic ratio
G	Amplitude of the applied gradient
g	Gram
Hz	Hertz
h	Planck's constant
I	Density operator for Nuclear spin
J	Spectral density/Coupling constant
K	Kelvin
K_a	Association/Binding constant
k	Chemical exchange rate
L	Litre
λ	Wavelength
M	Molar concentration
M_o	Net equilibrium magnetization
μ	Magnetic moment
υ	Frequency of nuclear precession
η	NOE efficiency
O_1	Transmitter frequency offset
Q	Quartet
ρ	Auto-relaxation rate
R_1	Spin lattice relaxation rate
R_1^{bs}	Bi-selective spin lattice relaxation rate
R_1^{ns}	Non-selective spin lattice relaxation rate
R_1^{se}	Selective spin lattice relaxation rate
R_2	Spin spin relaxation rate
r	Mole ratio
r_H	Hydrodynamic radius.
r_{ij}	Internuclear distance
s	Second
σ	Cross relaxation rate
t	Time

t_1	Evolution period
t_2	Acquisition period
τ	Recovery periods
τ_c	Molecular rotational correlation time
τ_m	Mixing time
θ	Angle
T	Temperature
T_1	Spin-Lattice relaxation time
T_2	Spin-Spin relaxation time
Td	Data points
ω	Angular frequency/ Larmor frequency
W	Transition probability between different relaxation pathways

List of Abbreviations

Abbreviation	Full form
AFM	Atomic Force Microscopy
ASP	Aspirin
β-CD	Beta-cyclodextrin
CB	Cucurbituril
CDs	Cyclodextrins
CEST	Chemical Exchange Saturation Transfer
CP	Cross Polarization
CP-MAS	Cross Polarization Magic Angle Spinning
CPMG	Carr-Purcell-Meiboom-Gill sequence
COSY	COrrelation SpectroscopY
CSA	Chemical Shift Anisotropy
CS	Crystallite Size
CW	Continuous wave
DCM	Dichloromethane
DDS	Drug Delivery System
DFL	Diflunisal
DFT	Density Functional Theory
D_2O	Deuterium Oxide
DMSO-d_6	Dimethylsulphoxie-d_6
DSC	Differential Scanning Calorimetry
d	doublet
dd	doublet of doublet
dt	doublet of triplet
DOSY	Diffusion Ordered Spectroscopy
DOX	Doxorubicin
DNR	Daunorubicin
EMA	European Medicine Agency
EXSY	EXchange SpectrscopY
FDA	Food and Drug Administration
FID	Free Induction Decay
FT	Fourier Transformation
FTIR	Fourier-Transform Infrared spectroscopy
GAMESS	General Atomic and Molecular Electronic Structure System
GRAS	Generally Recognized As Safe
HETCOR	HETeronuclear CORrelation spectroscopy
HP-β-CD	Hydroxypropyl-beta-cyclodextrin
IR	Infrared
kHz	Kilo Hertz
kJ/mol	Kilojoules per mole
kcal	Kilocalorie
kDa	Kilo Dalton
MAS	Magic angle spinning
MD	Molecular dynamics
MHz	Mega hertz
MT	Magnetization Transfer
MW	Molecular Weight
mg	Milligrams
mM	Millimolar

mL	Milliliter
µs	Microsecond
NMR	Nuclear magnetic resonance
NOE	Nuclear Overhauser Enhancement
NOESY	Nuclear Overhauser Effect SpectroscopY
NPs	Nanoparticles
NS	No. of scans
nm	Nanometer
ns	Nanosecond
w/o	Water-in-Oil
w/o/w	Water-in-Oil-in-Water
w/v	Weight by Volume
PC	Paracetamol
PDB	Protein Data Bank
PGA	Poly-Glycolic Acid
PFGSE	Pulsed field Gradient Stimulated Echo
PLA	Poly-Lactic Acid
PLGA	Poly(lactic-co-glycolic acid)
PPM	Parts per million
RAMP	Ramped-amplitude
REDOR	Rotational Echo Double Resonance
RF	Radio frequency
RSP	Risperidone
ROE	Rotating frame Overhauser Enhancement
ROESY	Rotating-frame Overhauser Effect SpectroscopY
ROS	Reactive Oxygen Species
SEM	Scanning Electron Microscopy
S/N	Signal-to-noise ratio
SS-NMR	Solid State Nuclear Magnetic Resonance
STD	Saturation Transfer Difference
SW	Spectral width
TEM	Transmission Electron Microscopy
UV-DRS	Ultraviolet Diffuse Reflectance Spectroscopy
v/v	Volume-by-volume
w/v	Weight-by-volume
w/w	Weight-by-weight
XRD	X-Ray Diffraction
ZnO	Zinc Oxide
1D	One-dimensional
2D	Two-dimensional
5-FU	5-Fluorouracil