

Solution State ^{19}F Magnetic Resonance (MR) Account of Molecular Interactions in Solutions

A Thesis submitted by
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in partial fulfillment of the requirements for the award of the degree of
Doctor of Philosophy



॥ त्वं ज्ञानमयो विज्ञानमयोऽसि ॥

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Declaration

I hereby declare that the work presented in this Thesis titled *Solution State ^{19}F Magnetic Resonance (MR) Account of Molecular Interactions in Solutions* 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.



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Certificate

This is to certify that the thesis titled *Solution State ^{19}F Magnetic Resonance (MR) Account of Molecular Interactions in Solutions*, submitted by *Bhawna Chaubey* (P15CY005) 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 her 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.



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Ph.D. Thesis Supervisor

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Ph.D. Student

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List of Symbols

<i>Symbol</i>	<i>Description</i>
Å	Angstrom
A	UV absorbance at a particular wavelength
A_F	STD Amplification factor
a	Molecular radius
α	Offset constant
B_0	Zeeman field
°C	Degree Celsius
cP	CentiPoise
dB	Decibel
D	Self-Diffusion Coefficient
ξ	Coupling parameter
δ	Chemical shift/Gradient length
δ_{ppm}	Chemical shift in parts per million
$\Delta\delta$	Chemical shift change
λ	Wavelength
γ_i	Gyromagnetic ratio of the i -th spin
f	Micro-viscosity factor
gm	Gram
ΔG°	Gibbs free energy of transfer
Hz	Hertz
I	Nuclear spin quantum number
h	Planck's constant
K	Kelvin
K_A	Association/Binding constant
K_D	Dissociation constant
K_{ex}	Exchange rate
k_B	Boltzmann constant
k	Photo-degradation Rate constant
k_d	Direct photo-degradation rate constant
k_{id}	Indirect photo-degradation rate constant
kJ/mol	Kilojoules per mole
kcal	Kilocalorie
kDa	Kilo Dalton
L	Litre
M	Molar concentration
mg	Milligrams
MHz	Mega hertz
mM	Millimolar
mL	Milliliter
mW	milliWatt
mins	minutes
n	Number of binding sites
nm	Nanometer
ns	Nanosecond
η_a	Assymetry Parameter
η	Dynamic viscosity

P_b	Ligand bound fraction
ps	picoseconds
r_H	Hyrdodynamic radius
R_1	Spin lattice relaxation rate
R_2	Spin-Spin relaxation rate
r_{ij}	Internuclear distance
s	Second
s	ESR saturation parameter
τ_c	Molecular rotational correlation time
$\tau_{c(F)}$	^{19}F Molecular rotational correlation time
$\tau_{c(D)}$	^2H Molecular rotational correlation time
τ_c^*	Molecular rotational correlation time from viscosity
τ_{res}	Lifetime of the complex
T	Temperature
T	Tesla
T_1	Spin-Lattice relaxation time
T_2	Spin-Spin relaxation time
t	Time
t_{sat}	Saturation time
$t_{1/2}$	Degradation half-life
μ_0	Permeability of free space
μM	Micromolar
μs	Microsecond
$\nu_{1/2}$	Linewidth at Full Width and Half Maximum (FWHM)
ω_i	Angular frequency/ Larmor frequency of the i -th spin
W	Watt

List of Abbreviations

Abbreviation	Full form
ADMET	Absorption Distribution Metabolism Excretion and Toxicity
AFM	Atomic Force Microscopy
AHA	Aldrich Humic acid
AV III	Avance III
BA	Benzoic acid
BBFO	Broadband fluorine observe
B-H	Benesi-Hindeland
BPPLD	Bipolar-pair pulse sequence with longitudinal eddy current delay
BSA	Bovine serum albumin
β -CD	β -Cyclodextrin
CA	Carboxylic acid
CD	Circular Dichroism
CCR	Cross correlation rate
CPMG	Carl Purcell Meiboom Gill
CSA	Chemical Shift Anisotropy
D ₂ O	Deuterium Oxide
DDNP	Dissolution Dynamic Nuclear Polarization
DD	Dipole-Dipole
DMSO-d ₆	Dimethylsulphoxide-d ₆
DOM	Dissolved organic matter
DSC	Differential Scanning Calorimetry
d	doublet
dd	doublet of doublet
dt	doublet of triplet
DMSO	Dimethyl Sulfoxide
DPFGSE	Double Pulsed-Field-Gradient Spin Echo
DFBA	2,6 Difluorobenzoic acid
DFA	Difluoroacetic acid
DFL	Diiflunisal
EHA	Extracted Humic acid
ESR	Electron Spin Resonance
EPR	Electron Paramagnetic Resonance
FABS	Fluorine Atoms for Biochemical Screening
FAXS	Fluorine chemical shift anisotropy and exchange for fluorine
FID	Free Induction Decay
FPD	Flupyradifurone
FTIR	Fourier Transform Infrared spectroscopy
FWHM	Full width at half maximum
GEM	Group Epitope Mapping
GHz	Gigahertz
H ₂ O	Water
HA	Humic acid
HFM	Hexaflumuron
HTS	High Throughput Screening
HOE	Hetero-nuclear Overhauser Enhancement
HS	Humic substances
HSA	Human Serum albumin
INPHARMA	Inter-ligand NOE for pharmacophore mapping
ITC	Isothermal Titration Calorimetry

KHA	Karwar Humic acid
LED	Longitudinal eddy current
MD	Molecular docking
MLT	Mellitin
MF	Magnetic field
MHz	Megahertz
MRI	Magnetic Resonance Imaging
MT	Magnetization Transfer
MW	Microwave
M. wt.	Molecular Weight
NMR	Nuclear Magnetic Resonance
NOE	Nuclear Overhauser Enhancement
NOESY	Nuclear Overhauser Effect Spectroscopy
NOM	Natural organic matter
ODNP	Overhauser Dynamic Nuclear Polarization
PB	Phosphate Buffer
PFG	Pulse Field Gradient
ppm	Parts per million
RHSTD	Reverse Heteronuclear Saturation Transfer Difference
RF	Radio frequency
SALMON	Solvent accessibility, ligand binding, and mapping of ligand orientation by NMR Spectroscopy
SOM	Soil Organic Matter
SPR	Surface Plasmon Resonance
S/N	Signal-to-noise ratio
STD	Saturation Transfer Difference
SW	Spectral width
STE	Stimulated spin-echo
TFE	Trifluoroethanol
TMS	Trimethylsilane
UV-vis	Ultraviolet-visible spectroscopy
Water-LOGSY	Water ligand observed through gradient spectroscopy
WB	Wide Bore
1D	One-dimensional
¹ H	Proton
² H	Deuterium
2D	Two-dimensional
5-FU	5-Fluorouracil
¹³ C	13 Carbon
¹⁹ F	19 Fluorine
^{6,7} Li	6,7 Lithium
¹⁵ N	15 Nitrogen
²³ Na	23 Sodium
¹⁷ O	17 Oxygen
³¹ P	31 Phosphorus
²⁹ Si	29 Silicon
¹²⁹ Xe	129 Xenon
⁶⁷ Zn	67 Zinc