List of Tables

Table	Title	Page
1.1	Ligand-protein interaction analysis using various methods.	4
1.2	The literature review of ligand-based NMR methods for ligand-protein interaction.	9
1.3	NMR methods used for OP-proteins interaction and their findings.	12
2.1	Description of chemicals used in the current thesis.	19
2.2	Chemical shift and line width values of biotin protons in the absence and presence of the	24
	protein tyrosine phosphatases and HRAS.	
2.3	Fluorescence results for BSA-5FU, BSA-PA and BSA-PA:5FU complex.	32
3.1	Experimental parameters used to obtain the STD NMR spectrum.	35
3.2	R _{STD} (%) value for CPF-BSA, DZN-BSA and PA-BSA complex.	38
3.3	STD _{max} and k _{sat} values for CPF, DZN, and PA.	39
3.4	K _D value for CPF-BSA, DZN-BSA, and PA-BSA.	41
3.5	Average Dissociation Constant (KD) Values for CPF-BSA, DZN-BSA, and PA-BSA system.	42
3.6	Summary of interactions between OP-BSA (CPF, DZN, and PA).	47
3.7	Thermodynamic parameters for interaction of OP with BSA.	49
4.1	Experimental parameters used in current Chapter.	53
4.2	Observed Pseudo-First-Order Disappearance Rate Constant (hydrolysis rate constant) for	58
	PM in absence and presence of BSA (1 μ M) and half-lives for PM hydrolysis both for free PM	
	and PM bound with BSA.	
4.3	The ¹H-NMR chemical shifts of TCPy and PM	59
4.4	R_1^{NS} and R_1^{SE} values for TCPy and PM (1 mM) in the absence and presence of BSA (5 μ M) at	61
	300 K and 310 .	
4.5	R_1^{NS} and R_1^{SE} values for TCPy and PM (1mM) in the absence and presence of variable	61
	concentration of BSA at 300 K.	
4.6	Normalized Affinity Index $[A_N]_L^T$; R_{1B}^{SE} and equilibrium constant $(K_A=1/K_D)$ for interaction of	63
	BSA and TCPy at different temperatures (300 K and 310 K).	
4.7	Thermodynamic parameters for TCPy-BSA and PM-BSA interaction.	64
4.8	Summary of interactions between TCPy-BSA	66
4.9	Summary of interactions between PM-BSA	66
4.10	Stern-Volmer constant and the quenching constant of BSA with TCPY and PM in absence	68
	and presence of site markers.	
5.1	Experimental parameters used to obtain the STD NMR spectrum.	73
5.2	R _{STD} (%) value for CPF-BSA, DZN-BSA and PA-BSA complex. The symbol * denotes proton could	78
	not be identified, and # represents proton does not exist.	
5.3	K _D value for CPF-trypsin, DZN-trypsin, TCPy-trypsin, and IMP-trypsin.	80
5.4	Average Dissociation Constant (KD) Values for CPF-trypsin, DZN-trypsin, TCPy-trypsin and	81
	IMP-trypsin system.	
5.5	Summary of interactions between OP/OP metabolite-trypsin (CPF, DZN, TCPy, and IMP).	82
5.6	The Stern-Volmer constant and the quenching-constant value for mentioned ligands.	84
5.7	Binding constant and thermodynamic parameters for CPF-trypsin, DZN-trypsin, TCPy-	86
	trypsin, and IMP-trypsin.	
6.1	Relevant parameters of the BSA-quencher complex formation in aqueous PB for 0-5 μM	93
	range viz., Stern-Volmer constant (K _{sv}), fraction of accessible fluorophore (f _a), quenching	
	constant (K_q) , association constant (K_a) and no. of binding sites (n) as calculated from Stern-	
	Volmer, modified Stern-Volmer and double log plot recorded at room temperature.	
6.2	Relevant parameters of the BSA-quencher complex formation in (1:9) methanol:PB for 0-10	96
	μ M. Range viz, Stern-Volmer constant (K_{sv}), quenching constant (K_q), fraction of accessible	
	fluorophore (f_a) , association constant (K_a) and no. of binding sites (n) as calculated from	
	Stern-Volmer, modified Stern-Volmer and double plot recorded at room temperature.*, °	
	Denotes biphasic curves having two regions *(0-5 μM):region 1 and ° (6-10 μM):region2	