Annexure A

A1. MATERIALS

All the chemicals except wherever mentioned, are procured from Sigma Aldrich, India and are used without any further purification. Analytical graded reagents are used in all cases. Double distilled water is used throughout for the preparation of the samples. Samples of agrochemicals and their fragments (metabolites) are prepared within an isolated chamber, considering the safety issues. The description of chemicals is given in table A1.

Table A1: List of chemicals used and relevant description, molecular weight (M.wt.), and procurement.

S.No.	Chemicals	Description	M. wt.
1.	Bovine Serum Albumin (Plasma Protein)	98% purity, nuclease and protease free (*Hi-media laboratories Pvt. Ltd., India*)	66.5 KDa
2.	Human Serum Albumin	Plasma Protein 98% purity, nuclease free	66.5 KDa
3.	Trypsin	Enzymatic Protein	23.3 KDa
4.	Melittin	Peptide	2840 g/mol
5.	β-Cyclodextrin ($C_{42}H_{70}O_{35}$)	Cyclomaltoheptaose (*Alfa Aesar, India*)	1134.9 g/mol
6.	Warfarin	4-hydroxy-3-(3-oxo-1-phenylbutyl)chromen-2-one	308.3 g/mol
7.	Ibuprofen	2-[4-(2-methylpropyl)phenyl] propanoic acid	206.3 g/mol
8.	Tryptophan	(2S)-2-amino-3-(1H-indol-3-yl) propanoic acid	204.2 g/mol
9.	Oleic acid	Fatty acid (*Alfa Aesar, India*)	282.5 g/mol
10.	Hexaflumuron	N-((3,5-Dichloro-4-(1,1,2,2-tetrafluoroethoxy)phenyl)carbamoyl)-2,6-difluorobenzamide	461.14 g/mol
11.	2, 6 Difluorobenzoic acid	Monoaromatic carboxylic acid	158.10 g/mol
12.	Diflunisal	5-(2,4-difluorophenyl)-2-hydroxybenzoic acid	250.19 g/mol
13.	Benzoic acid	Monoaromatic Carboxylic acid	122.12 g/mol
14.	Flupyradifurone	4-((6-chloro-3-pyridylmethyl)(2,2-difluoroethyl)amino)furan-2(5H)-one	288.6 g/mol
15.	Difluoroacetic acid	Monoaliphatic carboxylic acid	96.03 g/mol
16.	Glucose	(3*R*,4S,5S,6*R*)-6-(hydroxymethyl)oxane-2,3,4,5-tetrol	180.16 g/mol
17.	D_20, DMSO-d_6,Acetone-d_3	Deuterated Solvents	
18.	Trifluoroethanol	Fluorinated Alcohol (*TCI chemicals*)	100.04 g/mol
19.	TEMPOL ($C_9H_{18}NO_2$)	4-hydroxy-2,2,6,6-tetramethylpiperidin-1-oxyl	172.24 g/mol
20.	Dipotassium Phosphate	Potassium hydrogenphosphate (K_2HPO_4)	174.2 g/mol
21.	Monopotassium Phosphate	Potassium dihydrogenphosphate (KH2PO4)	136.08 g/mol
22.	HEPES Powder for Buffer	N-2-hydroxyethylpiperazine-N-2-ethanesulfonic acid	238.3 g/mol

A2. NMR Pulse Parameters

The general pulse parameters used during the acquisition of NMR spectrum for different nuclei and relevant to the present Thesis are provided in table A2.

Table A2: Values of various pulse parameters kept during acquisition of NMR of different nuclei.

Pulse Parameters	^{19}F (470.7 MHz)	^{1}H (500 MHz)	^{2}H (76.7 MHz)	^{13}C (125 MHz)
P_1 (μs) (90° hard pulse width)	15	14.15	390	10.60
PLW1 [W, dbW] (power level: 90° pulse)	19, −12.79	15, −11.76	1.54, −1.88	66, −18.20
P_2 (μs) (180° hard pulse width)	30	28.30	780	21.20
Decoupling scheme for protons	Waltz16	--	--	Waltz16
PLW2 [W, dbW] (power level: decoupling)	0.469, 3.29	--	--	0.469,3.29 (I^{st}) 0.236,6.27 (2^{nd})
PCPD2 (μs) (90° pulse: decoupling)	80	--	--	80
P18 (μs) width of shaped pulse used for solvent presaturation	--	100000 (Squa10.1000)	--	--
SPW6 [W, dbW] (power level: shaped pulse)		0.00028, 35.48	--	--

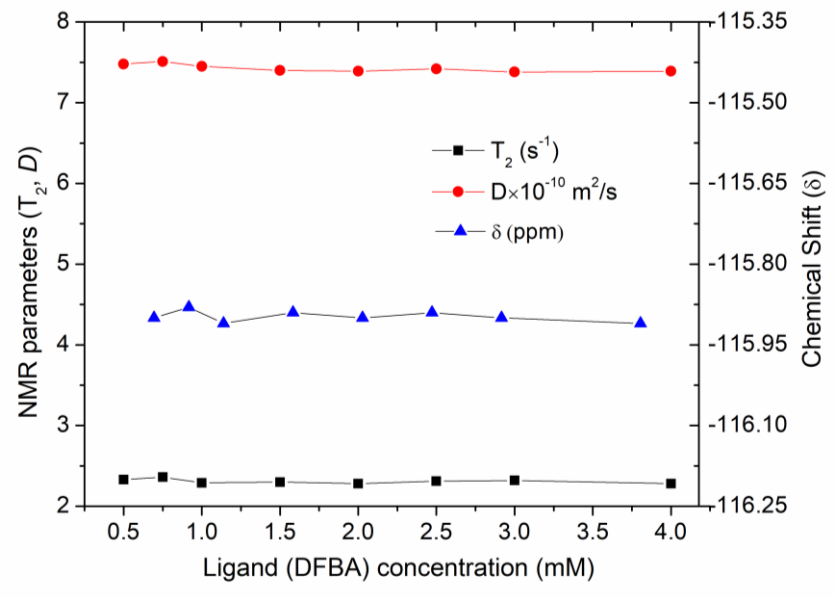

Figure A1: Values of NMR parameters i.e. chemical shift (δ), transverse relaxation time (T_2), Diffusion coefficient (*D*) as the function of DFBA concentration in absence of BSA. The values of these parameters are found nearly same with increasing DFBA concentration ruling out any possibility of aggregation.

...

Annexure B

Section B1. EXTRACTION OF HUMIC ACID: INTERNATIONAL HUMIC SUBSTANCES SOCIETY (IHSS) METHOD

Humic acid is extracted from soil with a procedure recommended and used by the IHSS (International Humic Substances Society) to isolate humic acid. The soil sample is dried and sieved through a 1 cm sieve. Then the sample is treated with 0.1 M HCl at room temperature to have a final ratio of solution to raw sample as 10:1. The suspension is shaken on rotating shaker for 12 h and the supernatant is discarded by centrifugation. The remaining soil residue is neutralized to pH 7.0 using 1 M NaOH and further 0.1 M NaOH is again added to get a final ratio of solution to soil as 10:1. The suspension is extracted by shaking for 24 h in N_2 atmosphere. The alkaline suspension is allowed to settle overnight and the supernatant is collected by centrifugation. The supernatant is acidified with 6 M HCl with constant stirring till pH 1.0 and then allowed to stand for 24 h. It is then centrifuged to separate the humic acid (precipitate) fraction. The humic acid fraction is redissolved by adding a minimum volume of 0.1 M KOH and then solid KCl is added to obtain the final concentration of 0.3 M [K+]. Afterwards, it is centrifuged at high speed to remove the suspended solids. The humic acid is reprecipitated by adding 6 M HCl with constant stirring to pH 1.0 and then allowed to stand again for 12 h. The sample is centrifuged and the supernatant discarded. The humic acid precipitate is treated in a mixture of 0.1 M HCl – 0.3 M HF solution in a plastic container and shaken for 12 h at room temperature. Treatment by HCl–HF is repeated once again after discarding the supernatant to obtain sufficiently low ash content. It is centrifuged once again for the last time and the supernatant is discarded. The final portion of humic acid is obtained after washing with distilled water and subsequent drying.

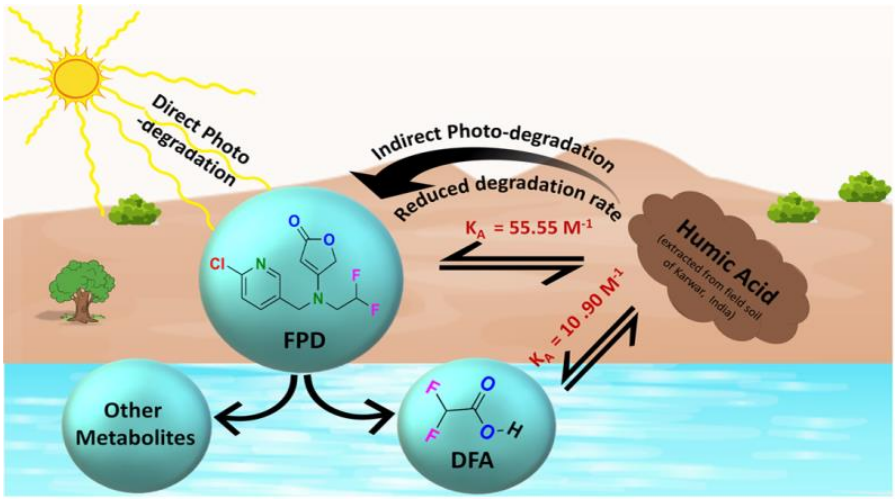

Figure B1: Graphical representation of the Part–II investigation of chapter 4 showing kinetics of direct photo–degradation of FPD in UV light and in presence of KHA forming DFA and other metabolites.

Section B2: Characterization of HA by UV–visible spectroscopic measurements

Figure B2 represents the absorption spectra of extracted (KHA) and Aldrich (AHA) HA that clearly demonstrate similar profile of absorption spectra with a significant difference in absorbance intensity below 350 nm. The spectra are rather featureless, representing only a decrease in absorbance with increasing wavelength indicative of various chromophoric groups present in HA.

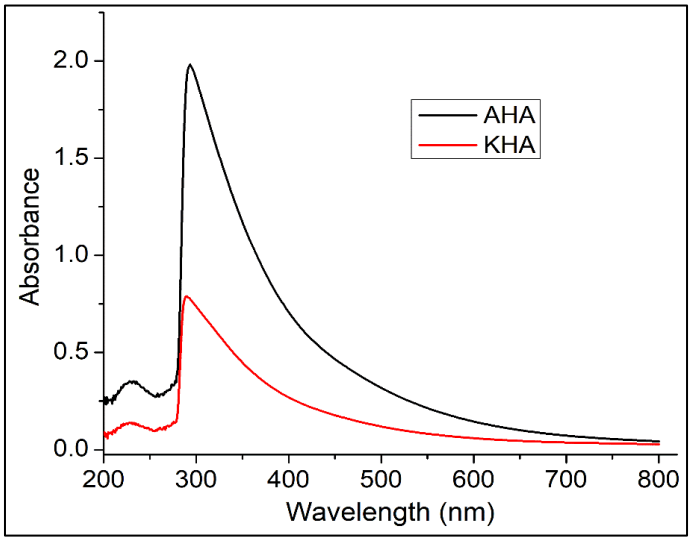

Figure B2: UV–vis absorption spectra of commercial (AHA) and extracted HA (KHA) in aqueous PB buffer (pH=7.4) at 298 K.

Interestingly, it is observed that a minor shoulder is present around 260 nm for both AHA and KHA confirming the presence of aromatic structure in organic HS. It is also well known that this shoulder between 230–270 nm can be due to the conjugation of ketone and quinine [Ghosh and Schnitzer, 1979]. It is customary in the literature to analyze the ratio of absorbance measured at two different wavelengths, e.g., λ_1 and λ_2 and denoted as $E_{\lambda 1/\lambda 2}$ (known as optical ratio or color ratio) to analyze the chemical composition of HA. Table B1 documents the important ratios of absorbance values widely used for characterization of HA *viz.*, $A_{280/365}$, $A_{280/665}$, and $A_{465/665}$ measured for both AHA and KHA from UV-vis spectra and denoted respectively as E_2/E_3, E_2/E_6 and E_4/E_6. A relatively higher E_4/E_6 and E_2/E_3 ratio is observed for KHA compared to AHA. Such high value accounts for lower humification index, implying a lower degree of condensation of the aromatic carbon chain of HA [Morán Vieyra, et al., 2009]. Higher E_4/E_6 ratio also indicates presence of relatively higher aliphatic components in KHA compared to AHA. The E_4/E_6 ratio is proportional to the acidity and can be inversely related to molecular weight, particle size, and the degree of aromaticity [Kang, et al., 2002]. On the other hand, the lower E_2/E_6 represents the increasing humification of organic components from the early transformation stage, like lignins and quinones for HA [Uyguner, et al., 2004]. These values are in general different for different HA and solely depends on the soil from which the particular HA is extracted. The value of the Δ log K coefficient [Sim et al., 2006] ($\Delta \log K = \log A_{400} - \log A_{600}$), known as Kumada Parameter, has been calculated to get additional proof on the less degree of humification of KHA than AHA [Boguta and Soko, 2016]. Kumada categorizes HA as medium to weakly humified (KHA here) if Δ logK oscillated from 0.7 to 0.93, while highly humified (AHA in present case) when value is less than 0.7.

Table B1: Value of UV–vis absorbance at various wavelengths for HA in aqueous PB (pH=7.40) and respective optical ratio recorded at 298 K.

HA	A_{280}	A_{350}	A_{465}	A_{665}	A_{400}	A_{600}	A_{280}/A_{350} ($E_{2/3}$)	A_{465}/A_{665} ($E_{4/6}$)	A_{280}/A_{665} ($E_{2/6}$)	ΔlogK
(AHA) Commercial	0.411	1.171	0.417	0.091	0.707	0.145	0.35	4.58	4.52	0.68
(KHA) Extracted	0.315	0.666	0.239	0.040	0.401	0.075	0.47	5.97	7.88	0.73

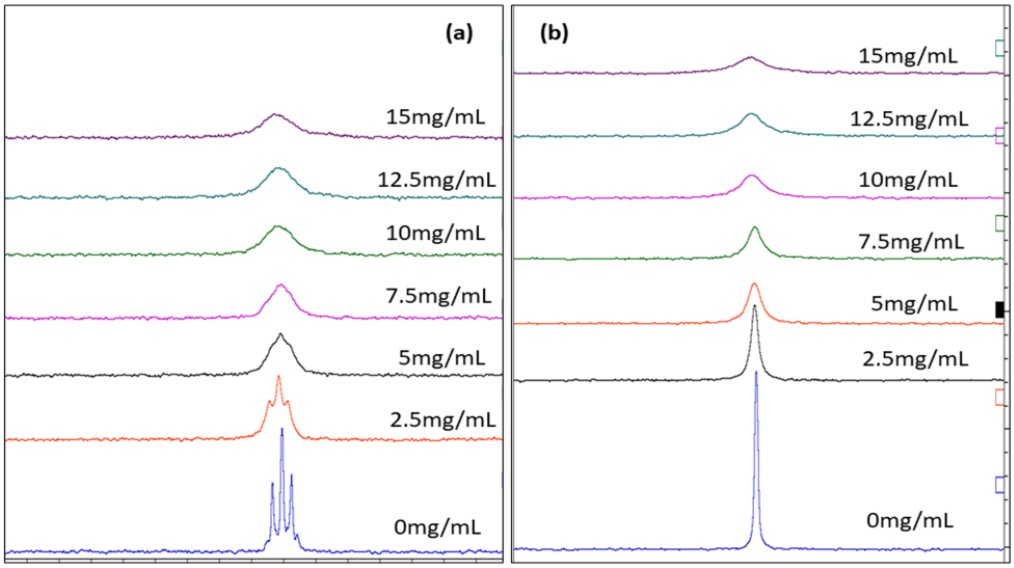

Figure B3: (a) ^{1}H coupled ^{19}F NMR (b) ^{1}H decoupled ^{19}F NMR spectrum of DFBA as the increasing function of AHA concentration recorded at pH=7.4 and *T*=298 K.

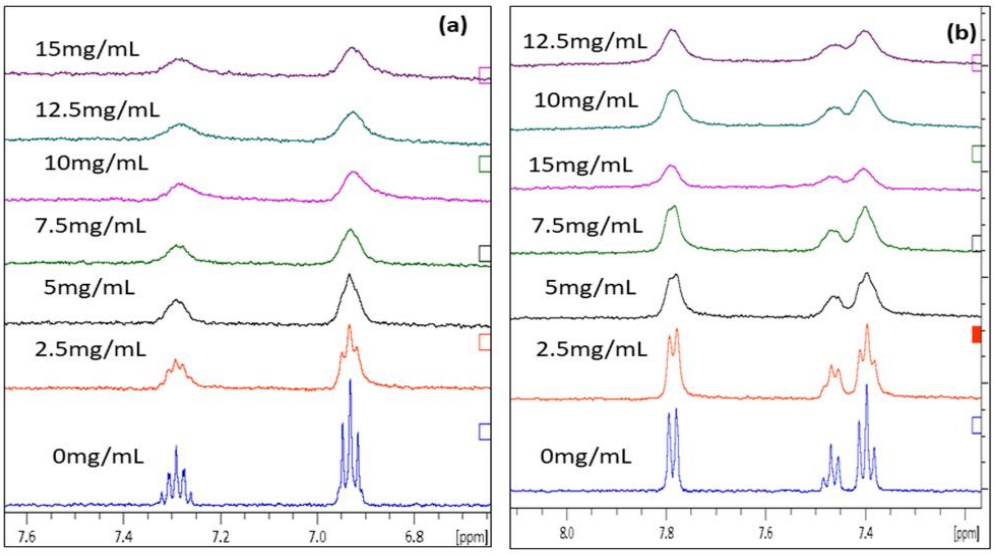

Figure B4: ^{1}H NMR spectrum of (a) DFBA and (b) BA as the increasing function of AHA concentration at pH=7.4 and *T*=298 K.

Table B2: T_1 and T_2 relaxation and correlation times (τ_c) for DFBA (2 mM) as a function of the AHA concentrations (mg/mL) at 298 K and pH 7.4. [Those values of T1 and T2 are reported where fitting parameter Pearson R^2 correlation coefficient found nearly equal to 1 (while extraction relaxation time from the fitted plot)]

Sample	T_1 (s)			T_2 (s)			Correlation Time τ_c (ns)	
DFBA	H_a	H_b	^{19}F	H_a	H_b	^{19}F	H_a	H_b
0 mg/mL HA	8.19	7.16	2.88	5.78	5.15	0.151	0.0133 (determined from ^{13}C T_1)	
2.5 mg/mL HA	5.04	4.75	2.69	0.093	0.077	0.075	2.53	2.70
5 mg/mL HA	4.11	3.8	2.53	0.054	0.044	0.060	3.01	3.22
7.5 mg/mL HA	3.50	3.29	2.45	0.042	0.036	0.038	3.16	3.32
10 mg/mL HA	2.61	2.51	2.28	0.031	0.026	0.033	3.18	3.42
12.5 mg/mL HA	2.29	2.25	2.21	0.026	0.022	0.024	3.25	3.53
15 mg/mL HA	2.03	1.96	2.17	0.023	0.018	0.018	3.26	3.65
25 mg/mL HA	1.40	1.43	1.83	0.015	0.013	0.151	3.36	3.67

Table B3*:* T_1 and T_2 relaxation and correlation (τ_c) times for BA (2 mM) as a function of the AHA concentrations (mg/mL) at 298 K and pH 7.4.

Sample	T_1 (s)			T_2 (s)			Correlation Time τ_c (ns)		
BA	H_a	H_c	H_b	H_a	H_c	H_b	H_a	H_c	H_b
0 mg/mL HA	5.56	6.15	6.85	4.14	4.17	4.24	0.0121 (determined from ^{13}C T_1)		
2.5 mg/mL HA	4.90	5.02	5.36	0.143	0.140	0.138	2.08	2.12	2.19
5 mg/mL HA	3.94	4.15	4.36	0.087	0.086	0.085	2.34	2.41	2.47
7.5 mg/mL HA	2.81	3.00	3.13	0.051	0.047	0.049	2.56	2.75	2.75
10 mg/mL HA	2.35	2.24	2.40	0.034	0.032	0.034	2.87	2.88	2.89
12.5 mg/mL HA	2.09	1.88	2.00	0.029	0.026	0.028	2.93	2.93	2.91
15 mg/mL HA	1.81	1.74	1.75	0.025	0.024	0.024	2.93	2.93	2.95
25 mg/mL HA	----	0.93	0.91	----	0.011	0.011	-----	3.18	3.14

Table B4: Observed (Raw) and viscosity corrected ^{19}F & ^{1}H diffusion coefficient (D) Values (10^{-10} m^2 s^{-1}) for signals of 2 mM DFBA & BA progressively added with AHA (mg mL^{-1}) at 298 K and pH 7.4.

Sample	Measurement for DFBA					Measurement of BA		
HA (mg/mL)	η[sol]/η[0]	Average $^{1}H_{DFBA}$ (raw)	Average $^{1}H_{DFBA}$ (corrected)	$^{19}F_{DFBA}$ (raw)	$^{19}F_{DFBA}$ (corrected)	η[sol] /η[0]	Average $^{1}H_{BA}$ (raw)	Average $^{1}H_{BA}$ (corrected)
0	1.00	5.875	5.875	6.093	6.093	1.000	6.397	6.397
2.5	1.005	5.556	5.587	5.852	5.88	1.020	6.057	6.178
5	1.022	4.744	4.851	5.561	5.68	1.089	5.428	5.911
7.5	1.037	4.157	4.314	5.305	5.505	1.133	4.828	5.470
10.0	1.053	3.842	4.049	5.092	5.366	1.189	4.234	5.034
12.5	1.148	3.496	4.015	4.734	5.437	1.121	3.876	4.689
15.0	1.225	3.243	3.973	4.424	5.420	1.251	3.606	4.511
25	1.286	3.045	3.915	4.211	5.414	1.321	2.911	3.846

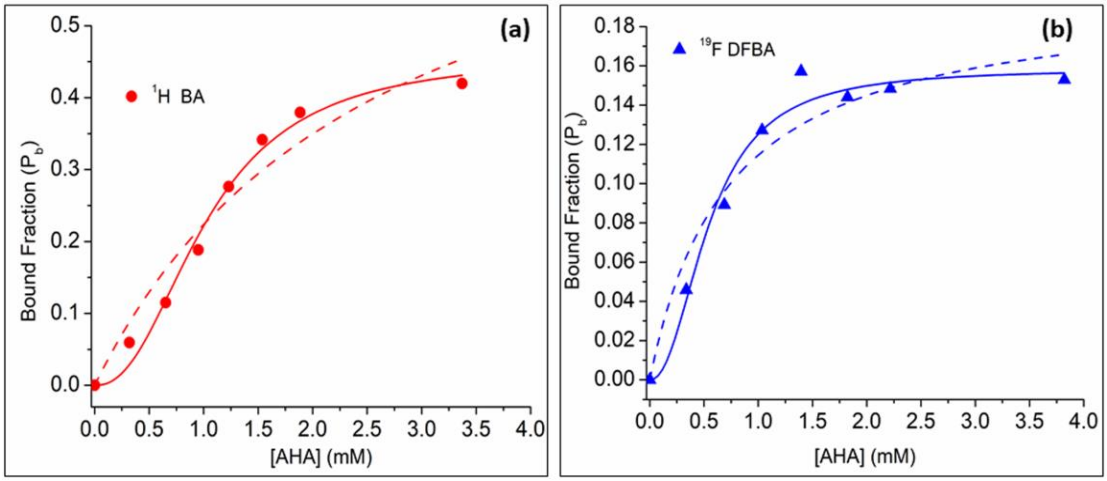

Figure B5: Plot for K_A determination of (a) BA and (b) DFBA using P_b values calculated from ^{1}H D_{BA} and ^{19}F D_{DFBA} values, respectively. (solid line and dash line represents the fitting obtained by modified Langmuir model and Langmuir model respectively)

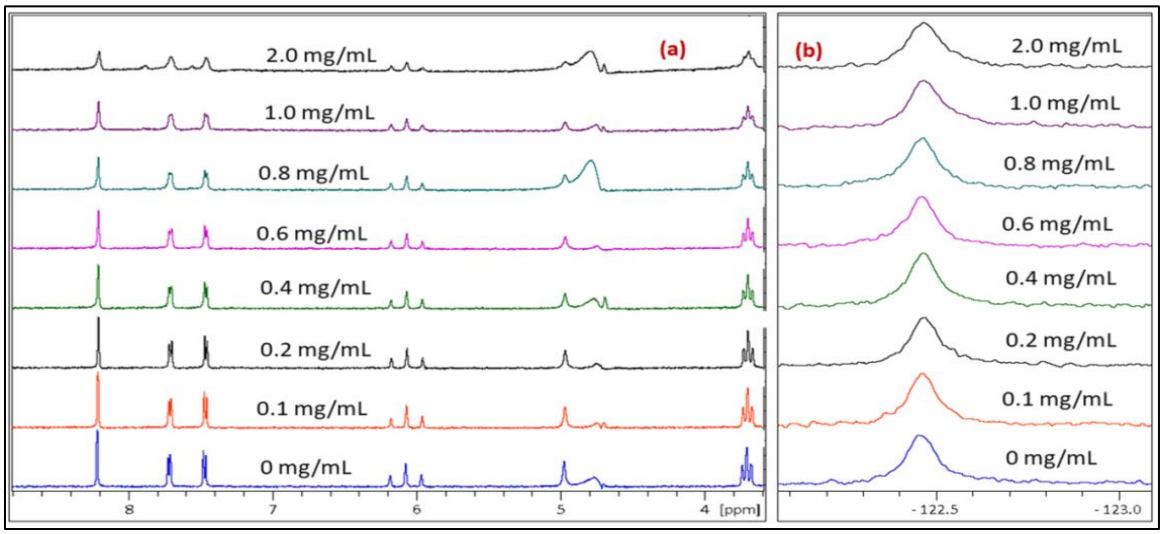

Figure B6: (a) Solvent presaturated ^{1}H NMR (b) ^{1}H decoupled ^{19}F NMR spectrum for FPD as a function of KHA concentration prepared in 5: 95 DMSO: aqueous PB solvent system recorded at T=295 K and pH=7.40.

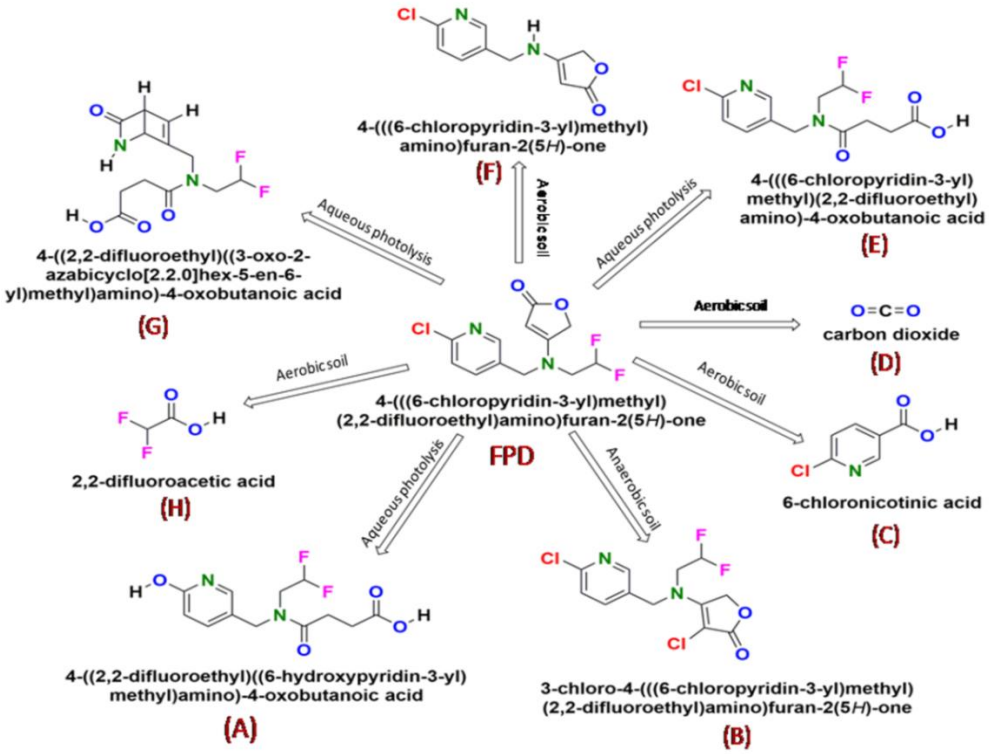

Figure B7: Different possible degradation products for FPD from various degradation pathways. [Source : (Flupyradifurone, 2013; Glaberman and Katrina, 2014)]

Section B3: For free FPD, the plausible mechanism for degradation can be anticipated as: the generation of reactive •OH (hydroxyl) radical and electron from OH^- (due to the interaction of UV with aqueous PB) are known to oxidize the organic compounds (FPD in the present case). Environmental implications of (•OH) are well known as they are responsible for the formation of secondary pollutants by inducing the chemical transformation of a number of primary pollutants. Also, they bears the second highest oxidation potential (2.80 V), after the strongest oxidant –F. The electrophilic nature (oxidant species) of the •OH has the potential of oxidizing almost all electron rich organic moieties non-selectively; first generating degraded metabolites and further eventually converting them to CO_2 and H_2O [Si, et al., 2004].

Table B5: ^1H and ^{19}F NMR T_1/T_2 relaxation ratio for FPD and DFA as an increasing function of KHA prepared in 5: 95 DMSO: aqueous PB solvent (pH=7.40) and measured at 295 K.

Sample	T_1/T_2 ratio for FPD						T_1/T_2 ratio for DFA	
FPD/DFA (1mM)	H_a	H_b	H_c	H_g	H_h	^{19}F	H_a	^{19}F
0 mg/mL HA	8.36	4.79	5.93	6.81	2.64	50.58	1.80	1.31
0.1 mg/mL KHA	11.09	6.74	7.52	7.36	2.98	52.05	2.01	1.50
0.2 mg/mL KHA	12.18	8.19	8.46	7.64	3.35	52.98	2.21	1.59
0.4 mg/mL KHA	12.98	10.0	9.09	7.78	3.74	54.28	2.43	1.69
0.6 mg/mL KHA	13.77	11.05	9.45	7.79	4.00	55.86	2.62	1.88
0.8 mg/mL KHA	14.90	11.20	9.81	7.86	4.30	57.01	2.74	2.02
1 mg/mL KHA	15.65	11.30	10.2	7.92	4.57	59.73	2.87	2.15
2 mg/mL KHA	16.71	11.79	11.32	8.045	4.82	61.00	3.03	2.59

Table B6: Representative self -diffusion coefficient (*D*) values measured for 1 mM FPD (aromatic protons) and DFA as a function of KHA concentration in 5: 95 DMSO: aqueous PB solvent (pH=7.40) at 295 K.

Sample FPD / DFA (1mM)	Viscosity Corrected $D \times 10^{-10}$ m^2/s (FPD)			Fraction of bound FPD (P_b) (%)	Viscosity Corrected $D \times 10^{-10}$ m^2/s (DFA)		Fraction of bound DFA (P_b) (%)
	H_a	H_b	H_c	(^{1}H)	H_a	^{19}F	(^{1}H)
0 mg/mL HA	2.80	2.99	2.76	0	8.72	9.25	0
0.1 mg/mL HA	2.72	2.86	2.61	8.7	8.4	8.89	4.8
0.2 mg/mL HA	2.67	2.74	2.51	16.2	8.12	8.42	8.9
0.4 mg/mL HA	2.55	2.53	2.45	30.2	7.88	8.05	12.5
0.6 mg/mL HA	2.39	2.39	2.35	39.6	7.56	7.79	17.2
0.8 mg/mL HA	2.24	2.26	2.22	51.4	7.24	7.56	22.0
1 mg/mL HA	2.00	2.07	1.99	62.8	6.97	7.24	26.1
2 mg/mL HA	1.75	1.80	1.40	78.5	6.55	6.79	32.3

Section B4: Figure B8 (I and II) represents the ^{1}H–^{1}H STD and ^{19}F–^{1}H STD experiments respectively recorded for DFA–KHA system. Peaks of significant intensity appeared in both ^{1}H–^{1}H STD and ^{19}F–^{1}H STD spectrum that confirms that –F of DFA is taking part while interacting with HA. GEM is not possible for DFA due to presence of single peak in ^{1}H and ^{19}F NMR spectra. This observation supports the ^{1}H and ^{19}F chemical shift and line-broadening experiments of DFA shown in figure B9 (a & b). ^{1}H spectra of DFA in presence of 1 mg/mL KHA exhibited a maximum downfield shift by 2.75Hz only while ^{19}F shifted upfield of maximum 15.93 Hz. As per literature, the formation of H–bond between –F and HA or solvent molecule increases the electron density around fluorine atoms, thus causing upfield shift for F nuclei due to enhanced shielding [Šmejkalová et al., 2009]. The changes in ^{19}F chemical shift for DFA also gives a clue of involvement of –F moiety while binding with HA, unlike FPD where least change is seen in chemical shift of ^{19}F and proton near to –F . The variable drift in chemical shift DFA in presence of HA compared to FPD is surely evident for the differential binding modes of both the molecules with HA as evident from STD experiments as well.

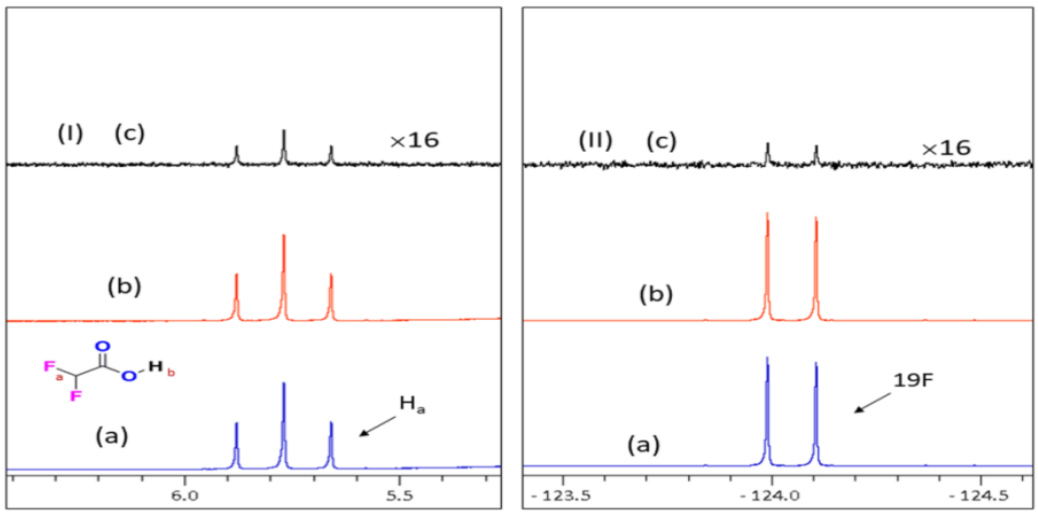

Figure B8: (I) $^{1}H–^{1}H$ STD NMR (II) $^{19}F–^{1}H$ STD NMR(a) STD_{off} (b) STD_{on} and (c) STD_{diff} spectrum for DFA–HA system in 5: 95 DMSO: aqueous PB solvent (pH=7.4) at *T* = 295 K.

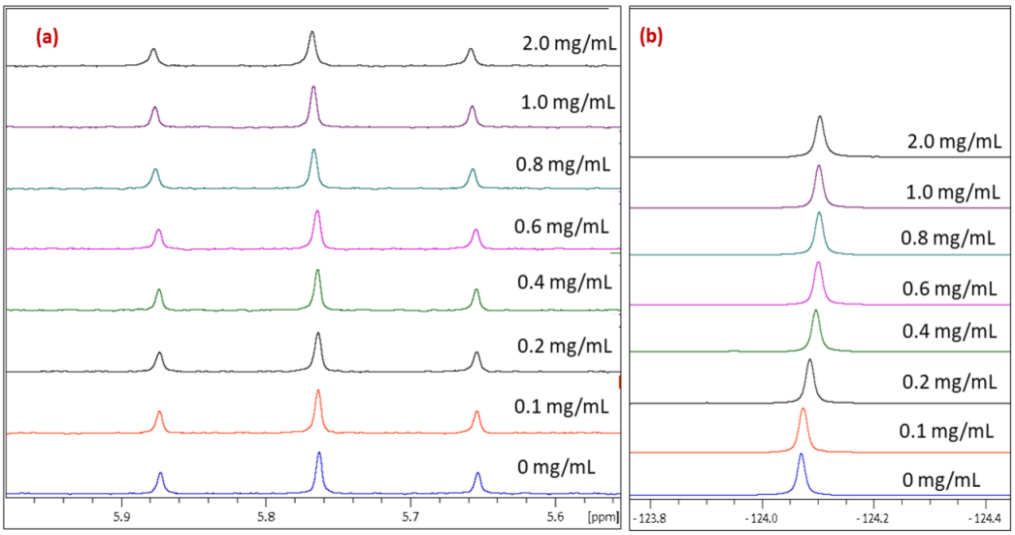

Figure B9: Solvent suppressed ^{1}H NMR (b) ^{1}H decoupled ^{19}F NMR spectrum for DFA as a function of HA concentration in 5: 95 DMSO: aqueous PB solvent (pH=7.4) at *T* = 295 K.

…

References

Abragam, A., (1953), "The Overhauser effect", *Proc. R. Soc. London Ser. A.*, Vol.283, pp.458.

Abragam, A., (1961), "*The Principles of Nuclear Magnetism*". Gifsur Yvette, France: Oxford: Clarendon Press.

Adamson, A. W., (1979), "*A Textbook of Physical Chemistry*" (Second). London: Academic Press, Inc. (London) Ltd.

Afonin, S., Glaser, R. W., Sachse, C., Salgado, J., Wadhwani, P., and Ulrich, A. S., (2014), "19F NMR screening of unrelated antimicrobial peptides shows that membrane interactions are largely governed by lipids ☆", *Biochimica et Biophysica Acta*, Vol.1838, pp.2260–2268.

Aktar, W., Sengupta, D., and Chowdhury, A., (2009), "Impact of pesticides use in agriculture : their benefits and hazards", *Interdisciplinary Toxicology*, Vol.2, No.1, pp.1–12.

Albers, Christian N., Banta, G. T., Hansen, P. E., and Jacobsen, O. S., (2008), "Effect of different humic substances on the fate of diuron and its main metabolite 3,4-dichloroaniline in soil", *Environmental Science and Technology*, Vol.42, No.23, pp.8687–8691.

Albers, Christian Nyrop, and Hansen, P. E., (2010), "13C-NMR chemical shift databases as a quick tool to evaluate structural models of humic substances", *Open Magnetic Resonance Journal*, Vol.3, No.SPEC. ISS.1, pp.96–105.

Alberto, P., Dejaegere, A., and Kieffer, B., (2011), "*Biophysical Approaches Determining Ligand Binding to Biomolecular Targets*", (P. Alberto, A. Dejaegere, & B. Kieffer, Eds.). Royal Society of Chemistry.

Aldmour, S. T., Burke, I. T., Bray, A. W., Baker, D. L., Ross, A. B., Gill, F. L., … Stewart, D. I., (2019), "Abiotic reduction of Cr(VI) by humic acids derived from peat and lignite: kinetics and removal mechanism", *Environmental Science and Pollution Research*, Vol.26, No.5, pp.4717–4729.

Alemany, L. B., Malloy, T. B., Nunes, M. M., and Zaibaq, N. G., (2012), "Importance of cross-correlated relaxation in the spectra of simple organofluorine compounds: Spectral complexity of A 3B 3X spin systems compared to ABX spin systems", *Journal of Molecular Structure*, Vol.1023, pp.176–188.

Anderson, V. L., and Webb, W. W., (2012), "A Desolvation Model for Trifluoroethanol-Induced Aggregation of Enhanced Green Fluorescent Protein", *Biophysical Journal*, Vol.102, No.4, pp.897–906.

Angulo, Jesús, Enríquez-Navas, P. M., and Nieto, P. M., (2010), "Ligand-receptor binding affinities from saturation transfer difference (STD) NMR", *Chemistry - A European Journal*, Vol.16, No.26, pp.7803–7812.

Angulo, Jesus, and Nieto, P. M., (2011), "STD-NMR: Application to transient interactions between biomolecules-a quantitative approach", *European Biophysics Journal*, Vol.40, No.12, pp.1357–1369.

Angulo, M., and Berger, S., (2004), "The pH-dependence of preferential solvation as studied by intermolecular homo- and heteronuclear NOE measurements of adenosine in water-trifluoroethanol mixtures", *Analytical and Bioanalytical Chemistry*, Vol.378, No.6, pp.1555–1560.

Arias-Estévez, M., López-Periago, E., Martínez-Carballo, E., Simal-Gándara, J., Mejuto, J. C., and García-Río, L., (2008), "The mobility and degradation of pesticides in soils and the pollution of groundwater resources", *Agriculture, Ecosystems and Environment*, Vol.123, No.4, pp.247–260.

Armstrong, B. D., and Han, S., (2009), "Overhauser Dynamic Nuclear Polarization To Study Local Water Dynamics", *Journal of American Chemical Society*, Vol.131, No.10, pp.4641–4647.

Armstrong, B. D., Soto, P., Shea, J.-E., and Han, S., (2009), "Overhauser dynamic nuclear polarization and molecular dynamics simulations using pyrroline and piperidine ring nitroxide radicals", *Journal of Magnetic Resonance*, Vol.200, No.1, pp.137–141.

Arthur, E. J., King, J. T., Kubarych, K. J., and Brooks, C. L., (2014), "Heterogeneous Preferential Solvation of Water and Trifluoroethanol in Homologous Lysozymes", *The Journal of Physical Chemistry B*, Vol.118, pp.8118–8127.

Atashgahi, S., Häggblom, M. M., and Smidt, H., (2018), "Organohalide respiration in pristine environments: implications for the natural halogen cycle", *Environmental Microbiology*, Vol.20, No.3, pp.934–948.

Augé, S., Schmit, P. O., Crutchfield, C. A., Islam, M. T., Harris, D. J., Durand, E., … Delsuc, M. A., (2009), "NMR measure of translational diffusion and fractal dimension. application to molecular mass measurement", *Journal of Physical Chemistry B*, Vol.113, No.7, pp.1914–1918.

Aziz, R., Helms, G. L., Evans, J. N. S., and Gronenborn, A. M., (2002), "Placement of 19 F into the center of GB1 : effects on structure and stability", *FEBS L*, Vol.517, pp.55–60.

Bagno, A., Rastrelli, F., and Scorrano, G., (2004), "Detecting intermolecular NOEs by means of a novel DPFGSE pulse sequence . Application to the solvation of carbohydrates in binary mixtures", *Journal*

of Magnetic Resonance, Vol.167, pp.31–35.
Bain, A. D., (2003), "Chemical exchange in NMR", *Progress in Nuclear Magnetic Resonance Spectroscopy*, Vol.43, No.3–4, pp.63–103.
Baker, R. J., Colavita, P. E., Murphy, D. M., Platts, J. A., and Wallis, J. D., (2012), "Fluorine À Fluorine Interactions in the Solid State : An Experimental and Theoretical Study", *Journal of Physical Chemistry A*, Vol.116, pp.1435–1444.
Bakhmutov, V. I., (2011), "*Solid-State NMR in Materials Science: Principles and Applications.*". Boca Raton: CRC Press.
Banerjee, A., Dey, A., and Chandrakumar, N., (2016), "Slow Molecular Motions in Ionic Liquids Probed by Cross-Relaxation of Nuclear Spins During Overhauser Dynamic Nuclear Polarization", *Angewandte Chemie*, Vol.128, No.47, pp.14976–14981.
Banerjee, A., Dey, A., and Chandrakumar, N., (2019), "Motional Dynamics of Halogen-Bonded Complexes Probed by Low-Field NMR Relaxometry and Overhauser Dynamic Nuclear Polarization", *Chemistry - An Asian Journal*, Vol.14, No.16, pp.2785–2789.
Banipal, P. K., Sharma, M., and Banipal, T. S., (2017), "Solvation behavior and sweetness response of carbohydrates , their derivatives and sugar alcohols in thiamine HCl (vitamin B1) and pyridoxine HCl (vitamin B6) at different temperatures", *Food Chemistry*, Vol.237, pp.181–190.
Bates, R. D., (1993), "Dynamic Nuclear Polarization", *Magnetic Resonance Review*, Vol.16, pp.237–291.
Battiste, J., and Newmark, R. A., (2006), "Applications of 19F multidimensional NMR", *Progress in Nuclear Magnetic Resonance Spectroscopy*, Vol.48, No.1, pp.1–23.
Becker, E. D., (2000), "*High resolution NMR Theory and Chemical Applications Third Edition*",*Academic Press San Diego London Boston, New York* (Vol. 3).
Becker, W., Bhattiprolu, K. C., Gubensäk, N., and Zangger, K., (2018), "Investigating Protein–Ligand Interactions by Solution Nuclear Magnetic Resonance Spectroscopy", *ChemPhysChem*, Vol.19, No.8, pp.895–906.
Beek, G. P. van der, Cohen Stuart, M. A., and Cosgrove, T., (1991), "Polymer Adsorption and Desorption Studies via 1H NMR Relaxation of the Solvent", *Langmuir*, Vol.7, No.2, pp.327–334.
Beer, P. D., Tite, L. E., and Ibbotson, A., (1989), "Novel Benzo Crown Ether Cavitand and Benzo Crown Ether-Ferroncenyl Host Molecules that bind Bipyridnium and Sodium Guest Cations", *Journal of the Chemical Society, Chemical Communications*, Vol.24, No.1, pp.1874–1876.
Bennati, M., Luchinat, C., Parigi, G., and Türke, M.-T., (2010), "Water 1H relaxation dispersion analysis on a nitroxide radical provides information on the maximal signal enhancement in Overhauser dynamic nuclear polarization experiments", *Physical Chemistry Chemical Physics*, Vol.12, No.22, pp.5902–5910.
Berger, R., Resnati, G., Metrangolo, P., Weber, E., and Hulliger, J., (2011), "Organic fluorine compounds: a great opportunity for enhanced materials properties", *Chemical Society Reviews*, Vol.40, No.7, pp.3496–3508.
Berkowitz, D. B., Karukurichi, K. R., Salud-bea, R. De, Nelson, D. L., and Mccune, C. D., (2009), "Use of Fluorinated Functionality in Enzyme Inhibitor Development: Mechanistic and Analytical Advantages", *Journal of Fluorine Chemistry*, Vol.129, No.9, pp.731–742.
Bhattacharjee, R., Muenter, J. S., and Marshall, M. D., (1991), "Nuclear quadrupole coupling in D2O", *Journal of Molecular Spectroscopy*, Vol.145, No.2, pp.302–307.
Bloch, F., Hansen, W. W., and Packard, M., (1946, February), "Nuclear induction [5]", *Physical Review*. American Physical Society. Vol. 69, No.3-4, pp.127
Boeszoermenyi, A., Chhabra, S., Dubey, A., Radeva, D. L., Burdzhiev, N.T., Chanev, C.D., Petrov, O.I., Gelev, V.M., Wgner, G., Kuprov, I., Takeuchi, K., Arthanari, H., (2019), "Aromatic 19F-13C TROSY: a background-free approach to probe biomolecular strucutre, function and dynamics, Vol.15, pp.333-340.
Boguta, P., and Soko, Z., (2016), "Interactions of Zn (II) Ions with Humic Acids Isolated from Various Type of Soils . Effect of pH , Zn Concentrations and Humic Acids Chemical Properties", *PLoS ONE*, Vol.11, No.4, pp.1–20.
Bohm, H., and Klebe, G., (1996), "What Can We Learn from Molecular Recognition in Protein- Ligand complexes for the design of new drugs?", *Angewantde Chemie International Edition English*, Vol.35, pp.2588–2614.
Bonechi, C., Martini, S., and Rossi, C., (2011), "Interaction study of indigo carmine with albumin and dextran by NMR relaxation", *Journal of Materials Science*, Vol.46, No.8, pp.2541–2547.
Boonyarattanakalin, K., Viernstein, H., Wolschann, P., and Lawtrakul, L., (2015), "Influence of ethanol as a Co-Solvent in cyclodextrin inclusion complexation: A Molecular Dynamics Study", *Scientia*

Pharmaceutica, Vol.83, No.2, pp.387–399.
Borah, B., and Bates, R. D., (1981a), "Dynamics of interspecies hydrogen bonding of a fluorinated alcohol and a nitroxide free radical", *The Journal of Chemical Physics*, Vol.74, No.3, pp.1538–1545.
Borah, B., and Bates, R. D., (1981b), "Dynamics of interspecies hydrogen bonding of partially fluorinated compounds and a stable nitroxide radical studied by 1H and 19F relaxation and low-field DNP measurements", *The Journal of Chemical Physics*, Vol.75, No.9, pp.4289–4293.
Bose-Basu, B., Zajicek, J., Bondo, G., Zhao, S., Kubsch, M., Carmichael, I., and Serianni, A. S., (2000), "Deuterium Nuclear Spin-Lattice Relaxation Times and Quadrupolar Coupling Constants in Isotopically Labeled Saccharides", *Journal of Magnetic Resonance*, Vol.144, No.2, pp.207–216.
Brown, Larry, R., Lauterwein, J., and Wurthrich, K., (1980), "High - Resolution IH-NMR Studies Of Self - Aggregation of Melittin in Aqueous Solution", *Biochimica et Biophysica Acta*, Vol.622, pp.231–244.
Bryant, R. G., (1978), "NMR relaxation studies", *Annual Review Physical Chemistry*, Vol.29, pp.167–188.
Buck, M., (1998), "Trifluoroethanol and colleagues : cosolvents come of age . Recent studies with peptides and proteins", *Quaterly Reviews of Biophysics*, Vol.31, No.3, pp.207–355.
Buck, M., Boyd, J., Redfield, C., MacKenzie, D. A., Jeenes, D. J., Archer, D. B., and Dobson, C. M., (1995), "Structural Determinants of Protein Dynamics: Analysis of 15N NMR Relaxation Measurements for Main-Chain and Side-Chain Nuclei of Hen Egg White Lysozyme", *Biochemistry*, Vol.34, No.12, pp.4041–4055.
Buer, B. C., and Marsh, E. N. G., (2012), "Fluorine: A new element in protein design", *Protein Science*, Vol.21, No.4, pp.453–462.
Buratto, R., Mammoli, D., Canet, E., and Bodenhausen, G., (2016), "Ligand-Protein Affinity Studies Using Long-Lived States of Fluorine-19 Nuclei", *Journal of Medicinal Chemistry*, Vol.59, No.5, pp.1960–1966.
Byers, L. D., (1977), "Probe-dependent cooperativity patterns in Hill-plots", *Journal of Chemical Education*, Vol.54, No.6, pp.352.
Cabot, R., and Hunter, C. A., (2012), "Molecular probes of solvation phenomena", *Chemical Society Reviews*, Vol.41, No.9, pp.3485–3492.
Cala, O., Guillière, F., and Krimm, I., (2014), "NMR-based analysis of protein-ligand interactions", *Analytical and Bioanalytical Chemistry*. Vol.406, pp.943–956
Cala, O., and Krimm, I., (2015), "Ligand-orientation based fragment selection in STD NMR screening", *Journal of Medicinal Chemistry*. Vol.58, No.21, pp.8739–874
Cammers-goodwin, A., Allen, T. J., Oslick, S. L., Mcclure, K. F., Lee, J. H., and Kemp, D. S., (1996), "Mechanism of Stabilization of Helical Conformations of Polypeptides by Water Containing Trifluoroethanol", *Journal of American Chemical Society*, Vol.118, No.5, pp.3082–3090.
Cardoza, L. A., Korir, A. K., Otto, W. H., Wurrey, C. J., and Larive, C. K., (2004), "Applications of NMR spectroscopy in environmental science", *Progress in Nuclear Magnetic Resonance Spectroscopy*, Vol.45, No.3–4, pp.209–238.
Carper, W. R., (1999), "Direct determination of quadrupolar and dipolar NMR correlation times from spin - lattice and spin - spin relaxation rates", *Concepts in Magnetic Resonance*, Vol.11, No.1, pp.51–60.
Carper, W. R., Meng, Z., and Palko, N. M., (2002), "Direct determination of 119Sn, 195Pt, 199Hg and 207Pb NMR correlation times from spin-lattice and spin-spin relaxation times", *Journal of Molecular Liquids*, Vol.98, No.99, pp.7–14.
Carr, H. Y., and Purcell, E. M., (1954), "Effects of diffusion on free precession in nuclear magnetic resonance experiments", *Physical Review*, Vol.94, No.3, pp.630–638.
Carver, J. A., and Collins, J. ., (1990), "NMR identification of a partial helical conformation for bombesin in solution", *European Journal of Biochemistry*, Vol.187, pp.645–600.
Carver, J. P., and Richards, R. E., (1972), "A general two-site solution for the chemical exchangeproduced dependence of T2 upon the Carr-Purcell pulse sequence", *Journal of Magnetic Resonance*, Vol.6, pp.89–105.
Carver, T. R., and Slichter, C. P., (1953), "Polarization of Nuclear Spins in Metals", *Physical Review*, Vol.92, No.1, pp.212–213.
Cattoni, D. I., Chara, O., Kaufman, S. B., and González Flecha, F. L., (2015), "Cooperativity in Binding Processes: New Insights from Phenomenological Modeling", *PloS One*, Vol.10, No.12, pp.e0146043–e0146043.
Certaines, J. D. de, Bovée, W. M. M. J., and Podo, F. (Eds.), (1992), "*Magnetic Resonance Spectroscopy in Biology and Medicine*". Peragom Press, Oxford.
Champagne, P. A., Desroches, J., Hamel, J. D., Vandamme, M., and Paquin, J. F., (2015), "Monofluorination of Organic Compounds: 10 Years of Innovation", *Chemical Reviews*, Vol.115, No.17, pp.9073–9174.
Chandrakumar, N., (2010), "Dynamic nuclear polarization in NMR", *Journal of the Indian Institute of Science*,

Vol.90, No.1, pp.133–143.
Chandrakumar, Narayanan, (1979), "*Design and Construction of a Medium Resolution X-band Overhauser Effect Spectrometer and 1H and 19F Overhauser Effect Studies on Free Radical Solutions*". Indian Institute of Technology Kanpur.
Chappuis, Q., Milani, J., Vuichoud, B., Bornet, A., Gossert, A. D., Bodenhausen, G., and Jannin, S., (2015), "Hyperpolarized water to study protein-ligand interactions", *Journal of Physical Chemistry Letters*, Vol.6, No.9, pp.1674–1678.
Charlier, C., Khan, S. N., Marquardsen, T., Pelupessy, P., Reiss, V., Sakellariou, D., … Ferrage, F., (2013), "Nanosecond time scale motions in proteins revealed by high-resolution NMR relaxometry", *Journal of the American Chemical Society*, Vol.135, No.49, pp.18665–18672.
Chatterjee, C., and Gerig, J. T., (2006), "Interactions of Hexafluoro-2-propanol with the Trp-Cage Peptide †", *Biochemistry*, Vol.45, No.49, pp.14665–14674.
Chaubey, B., Dey, A., Banerjee, A., Chandrakumar, N., and Pal, S., (2020a), "Assessment of the Role of 2,2,2-Trifluoroethanol Solvent Dynamics in Inducing Conformational Transitions in Melittin: An Approach with Solvent 19 F Low-Field NMR Relaxation and Overhauser Dynamic Nuclear Polarization Studies" *Journal of Physical Chemistry B.*, Vo. 124, No. 28, pp. 5993–6003.
Chaubey, B., Narwal, P, Khandelwal, A and Pal, S., (2020b), " Aqueous photo-degradation of Flupyradifurone (FPD) in presence of a natural Humic Acid (HA): A quantitative solution state NMR analysis. *Photochemistry and Photobiology A: Chemistry*, Vol. 405, No. 2020, pp. 112986.
Chaubey, B., Singh, P., Pal, S (2021)., "Solution State NMR evaluation of molecular interaction between monoaromatic Carboxylic Acids and dissolved Humic Acid". *Environment Science and Pollution Research,* https://doi.org/10.1007/s11356-020-12092-1 (just accepted).
Chaubey, B., and Pal, S., (2018), "Binding Interaction of Organofluorine-Serum Albumin: A Comparative Ligand-Detected 19F NMR Analysis", *Journal of Physical Chemistry B*, Vol.122, No.40, pp.9409–9418.
Chaubey, B., and Pal, S., (2019), "Hexaflumuron_ß-cyclodextrin inclusion complex as improved pesticide formulation: A NMR case study", *AIP Conference Proceedings*, Vol.2142, No. pp.180003(1) –180003(4)
Cheatham, S., and Groce, J., (2004), "19F multiple region selected 2D NMR correlation experiments", *Journal of Fluorine Chemistry*, Vol.125, No.7, pp.1111–1117.
Chelli, S., Majdoub, M., Jouini, M., Aeiyach, S., Maruel, F., I. CHane-Ching, K., and Lacaze, P.-C. L., (2007), "Host-Guest Complexes of phenol derivative with Beta Cyclodextrin: an experiemntal and theroretical investigation", *Journal of Physical Organic Chemistry*, Vol.20, pp.30–43.
Chen, H., Viel, S., Ziarelli, F., and Peng, L., (2013), "19F NMR: a valuable tool for studying biological events", *Chemical Society Reviews*, Vol.42, No.20, pp.7971.
Chen, X., Wang, J., Chen, J., Zhou, C., Cui, F., and Sun, G., (2019), "Photodegradation of 2-(2-hydroxy-5-methylphenyl) benzotriazole (UV-P) in coastal seawaters : Important role of DOM", *Journal of Environmental Sciences*, Vol.85, pp.129–137.
Cheng, C. Y., Goor, O. J. G. M., and Han, S., (2012), "Quantitative analysis of molecular transport across liposomal bilayer by J-mediated 13C Overhauser dynamic nuclear polarization", *Analytical Chemistry*, Vol.84, No.21, pp.8936–8940.
Chien, Y. Y., Kim, E. G., and Bleam, W. F., (1998), "Paramagnetic relaxation of atrazine solubilized by humic micellar solutions", *Environmental Science and Technology*, Vol.31, No.11, pp.3204–3208.
Chin, Y. P., Aiken, G. R., and Danielsen, K. M., (1997), "Binding of pyrene to aquatic and commercial humic substances: The role of molecular weight and aromaticity", *Environmental Science and Technology*, Vol.31, No.6, pp.1630–1635.
Chiron, S., Barceló, D., Abian, J., Ferrer, M., Sanchez-Baeza, F., and Messeguer, A., (1995), "Comparative photodegradation rates of alachlor and bentazone in natural water and determination of breakdown products", *Environmental Toxicology and Chemistry*, Vol.14, No.8, pp.1287–1298.
Chitra, R., and Smith, P. E., (2001), "Properties of 2, 2, 2-trifluoroethanol and water mixtures", *Journal of Chemical Physics*, Vol.114, No.1, pp.426–435.
Churchill, D., Cheung, J. C. F., Park, Y. S., Smith, V. H., VanLoon, G., and Buncel, E., (2006), "Complexation of diazinon, an organophosphorus pesticide, with α-, β-, and γ-cyclodextrin - NMR and computational studies", *Canadian Journal of Chemistry*, Vol.84, No.4, pp.702–708.
Cobb, S. L., and Murphy, C. D., (2009), "19F NMR applications in chemical biology", *Journal of Fluorine Chemistry*, Vol.130, No.2, pp.132–143.
Cook, R. L., and Langford, C. H., (1998), "Structural Characterization of a Fulvic Acid and a Humic Acid Using Nuclear Magnetic Resonance", *Environment Science and Technology*, Vol.32, No.5, pp.719–725.
Copeland, R. A., (2003), "Protein–Ligand Binding Equilibria", In *Enzymes*: *A Practical Introduction to Structure, Mechanism, and Data Analysis, Second Edition*. Wiley-VCH, Inc.

Copeland, R. A., (2016), "The drug-target residence time model: A 10-year retrospective", *Nature Reviews Drug Discovery*. Nature Publishing Group. Vol. 15, No. 2, pp. 87 −95.

Copeland, R. A., Pompliano, D. L., and Meek, T. D., (2007), "Drug – target residence time and its implications for lead optimization", *Nature Reviews \ Drug Discovery*, Vol.5, pp.730–739.

Crassous, J., and Hediger, S., (2003), "Dynamics of CHFClBr and CDFClBr inside a thiomethylated cryptophane, studied by 19F-1H CSA-DD cross-correlated relaxation and 2H quadrupolar relaxation measurements", *Journal of Physical Chemistry A*, Vol.107, No.48, pp.10233–10240.

Cruz, J. R., Becker, B. A., Morris, K. F., and Larive, C. K., (2008), "NMR characterization of the host-guest inclusion complex between β-cyclodextrin and doxepin", *Magnetic Resonance in Chemistry*, Vol.46, No.9, pp.838–845.

Culik, R. M., Abaskharon, R. M., Pazos, I. M., and Gai, F., (2014), "Experimental validation of the role of trifluoroethanol as a nanocrowder", *Journal of Physical Chemistry B*, Vol.118, No.39, pp.11455–11461.

D'Agostino, C., Mitchell, J., Mantle, M. D., and Gladden, L. F., (2014), "Interpretation of NMR relaxation as a tool for characterising the adsorption strength of liquids inside porous materials", *Chemistry - A European Journal*, Vol.20, No.40, pp.13009–13015.

Dabbit, O., and Sutcliffe, L. H., (1980), "Improved analysis of the fluorine NMR spectrum of perfluorocyclobutanone", *Spectrochimica Acta Part A: Molecular Spectroscopy*, Vol.36, No.4, pp.379–381.

Dahiya, V., Anand, B. G., Kar, K., and Pal, S., (2020), "In vitro interaction of organophosphate metabolites with bovine serum albumin: A comparative 1H NMR, fluorescence and molecular docking analysis", *Pesticide Biochemistry and Physiology*, Vol.163, No.October 2019, pp.39–50.

Dahiya, V., Chaubey, B., Dhaharwal, A. K., and Pal, S., (2017), "Solvent-dependent binding interactions of the organophosphate pesticide , with Bovine Serum Albumin (BSA): A comparative fluorescence quenching analysis ☆", *Pesticide Biochemistry and Physiology*, Vol.139, pp.92–100.

Dalvit, C., (2007), "Ligand- and substrate-based19F NMR screening: Principles and applications to drug discovery", *Progress in Nuclear Magnetic Resonance Spectroscopy*, Vol.51, No.4, pp.243–271.

Dalvit, C., Fagerness, P. E., Hadden, D. T. A., Sarver, R. W., and Stockman, B. J., (2003), "Fluorine-NMR experiments for high-throughput screening: Theoretical aspects, practical considerations, and range of applicability", *Journal of the American Chemical Society*, Vol.125, No.25, pp.7696–7703.

Dalvit, C., Mongelli, N., Papeo, G., Giordano, P., Veronesi, M., Moskau, D., and Kümmerle, R., (2005), "Sensitivity improvement in 19F NMR-based screening experiments: Theoretical considerations and experimental applications", *Journal of the American Chemical Society*, Vol.127, No.38, pp.13380–13385.

Dalvit, C., and Vulpetti, A., (2011), "Fluorine-Protein Interactions and 19F NMR Isotropic Chemical Shifts: An Empirical Correlation with Implications for Drug Design", *ChemMedChem*, Vol.6, No.1, pp.104–114.

Dalvit, C., and Vulpetti, A., (2012), "Technical and practical aspects of 19 F NMR-based screening : toward sensitive high-throughput screening with rapid deconvolution", *Magnetic Resonance in Chemistry*, Vol.50, No.9, pp. 592-597.

Danielson, M. A., and Falke, J. J., (1996), "Use of 19 F Nmr To Probe Protein Structure and Conformational Changes", *Annual Review of Biophysics and Biomolecular Structure*, Vol.25, pp.163–195.

Das, R., Sahoo, S., Singh, H., Suman, S. N., and Singh, P., (2019), "Humus pesticide interaction: The fate of pesticide in soil environment: An overview", *International Journal of Chemical Studies*, Vol.7, No.3, pp.3117–3123.

David, J., Šmejkalová, D., Hudecová, Š., Zmeškal, O., von Wandruszka, R., Gregor, T., and Kučerík, J., (2014), "The physico-chemical properties and biostimulative activities of humic substances regenerated from lignite", *SpringerPlus*, Vol.3, No.1, pp.1–16.

Davilas, A., Koupparis, M., Macheras, P., and Valsami, G., (2006), "In-vitro study on the competitive binding of diflunisal and uraemic toxins to serum albumin and human plasma using a potentiometric ion-probe technique", *Journal of pharmacy and pharmacology*, Vol.58, pp.1467–1474.

Delort, A.-M., Combourieu, B., and Haroune, N., (2003), "Nuclear magnetic resonance studies of interactions between organic pollutants and soil components, a review", *Environmental Chemistry Letters* , Vol.1, No.4, pp.209–213.

Derome, A. E., (1987), "Modern NMR Techniques for Chemistry Research.", *Pergamon Press, Ltd. Univeristy of Oxford, UK*.

Derrick, T. S., Lucas, L. H., Dimicoli, J. L., and Larive, C. K., (2002), "19F diffusion NMR analysis of enzyme-inhibitor binding", *Magnetic Resonance in Chemistry*, Vol.40, No.SPEC. ISS., pp.98–105.

Dey, A., (2019), "*Studies on Multi-Band Time Domain Overhauser Dynamic Nuclear Polarization in Liquids*". Indan Institute of Technology, Madras, India, 600036.

Dey, A., and Banerjee, A., (2019), "Unusual Overhauser Dynamic Nuclear Polarization Behavior of

Fluorinated Alcohols at Room Temperature", *Journal of Physical Chemistry B*, Vol.123, No.49, pp.10463–10469.
Dey, A., Banerjee, A., and Chandrakumar, N., (2017), "Transferred Overhauser DNP: A Fast, Efficient Approach for Room Temperature 13C ODNP at Moderately Low Fields and Natural Abundance", *Journal of Physical Chemistry B*, Vol.121, No.29, pp.7156–7162.
Díaz, M. D., and Berger, S., (2001), "Preferential solvation of a tetrapeptide by trifluoroethanol as studied by intermolecular NOE", *Magnetic Resonance in Chemistry*, Vol.39, No.7, pp.369–373.
Didenko, T., Liu, J. J., Horst, R., Stevens, R. C., and Wuthrich, K., (2014), "Fluorine-19 NMR of integral membrane proteins illustrated with studies of GPCRs Tatiana", *Current Opinion in Structural Biology*, Vol.23, No.5, pp.740–747.
Dimzon, I. K., Trier, X., Frömel, T., Helmus, R., and Knepper, T. P., (2016), "High Resolution Mass Spectrometry of Polyfluorinated", *Journal of American Society of Mass Spectrometry*, Vol.27, pp.309–318.
Dixon, A. M., Mai, M. A., and Larive, C. K., (1999), "NMR investigation of the interactions between 4'-fluoro-1'- acetonaphthone and the Suwannee River Fulvic Acid", *Environmental Science and Technology*, Vol.33, No.6, pp.958–964.
Dolbier, W. R. J., (2009), "*Guide to Fluorine NMR for Organic Chemists*". United States of America: John Wiley & Sons, INC., Publication.
Dolores, M. D., and Berger, S., (2001), "Preferential solvation of a tetrapeptide by trifluoroethanol as studied by intermolecular NOE", *Magnetic resonance in chemistry*, Vol.39, No.7, pp.369–373.
Donaldson, T. W., and Foy, C. L., (1965), "The Phytotoxicity and Persistence in Soils of Benzoic Acid Herbicides", *Weeds*, Vol.13, No.3, pp.195–202.
Dorai, K., and Kumar, A., (2001), "Fluorine chemical shift tensors in substituted fluorobenzenes using cross correlations in NMR relaxation", *Chemical Physics Letters*, Vol.335, No.3–4, pp.176–182.
Du, U. H. N., Grage, S. L., Witter, R., and Ulrich, A. S., (2008), "Solid state 19 F NMR parameters of fluorine-labeled amino acids . Part I : Aromatic substituents", *Journal of Magnetic Resonance*, Vol.191, pp.7–15.
Dubois, B. W., and Evers, A. S., (1992), "19F-NMR Spin-Spin Relaxation (T2) Method for Characterizing Volatile Anesthetic Binding to Proteins. Analysis of Isoflurane Binding to Serum Albumin", *Biochemistry*, Vol.31, No.31, pp.7069–7076.
Dwek, R. A., Richards, R. E., and Taylor, D., (1969), "Nuclear Electron Double Resonance in Liquids", *Annual Reports on NMR Spectroscopy*, Vol.2, pp.293–344.
Edwards, J. C., (2011), "Applications of NMR Spectroscopy in Petroleum Chemistry",In K. Nadkarni (Ed.), *Spectroscopic Analysis of Petroleum Products and Lubricants* (Monograph). ASTM International.
Elavarasi, S. B., and Dorai, K., (2010), "Characterization of the 19 F chemical shielding tensor using cross-correlated spin relaxation measurements and quantum chemical calculations", *Chemical Physics Letters*, Vol.489, No.4–6, pp.248–253.
Elliott, N. B., Ndou, T., and Warner, I. M., (1993), "Influence of fluorinated alcohols on cyclodextrin: Pyrene complexation", *Journal of Inclusion Phenomena and Molecular Recognition in Chemistry*, Vol.16, No.2, pp.99–112.
Emsley, J. W., Phillips, L., and Wray, V., (1976), "Flourine coupling constants", *Progress in Nuclear Magnetic Resonance Spectroscopy*, Vol.10, No.2, pp.83–752.
Engebretson, R. R., and Von Wandruszka, R., (1997), "The effect of molecular size on humic acid associations", *Organic Geochemistry*, Vol.26, No.11–12, pp.759–767.
Enoki, S., Saeki, K., Maki, K., and Kuwajima, K., (2004), "Acid Denaturation and Refolding of Green Fluorescent Protein †", *Biochemistry*, Vol.43, pp.14238–14248.
Evans, R., (2020), "The interpretation of small molecule diffusion coefficients : Quantitative use of diffusion-ordered NMR spectroscopy", *Progress in Nuclear Magnetic Resonance Spectroscopy*, Vol.117, pp.33–69.
Fan, T. W. M., Lane, A. N., Chekmenev, E., Wittebort, R. J., and Higashi, R. M., (2004), "Synthesis and physicochemical properties of peptides in soil humic substances", *Journal of Peptide Research*, Vol.63, No.3, pp.253–264.
Fang, W., Sheng, G. P., Wang, L. F., Ye, X. D., and Yu, H. Q., (2015), "Quantitative evaluation of noncovalent interactions between polyphosphate and dissolved humic acids in aqueous conditions", *Environmental Pollution*, Vol.207, pp.123–129.
Farrar, T. C., and Becker, E. D., (1971), "Relaxation Mechanisms",In T. C. Farrar & E. D. Becker (Eds.), *Pulse and Fourier Transform NMR* (pp. 46–65). San Diego: Academic Press.
Fernandez, C., and Jahnke, W., (2004), "New approaches for NMR screening in drug discovery", *Drug*

Discovery Today: Technologies, Vol.3, pp.277–283.
Fielding, L., (2003), "NMR Methods for the Determination of Protein- Ligand Dissociation Constants", *Current Topics in Medicinal Chemistry*, Vol.3, No.1, pp.39–53.
Fielding, L., (2007), "NMR methods for the determination of protein – ligand dissociation constants", *Progress in Nuclear Magnetic Resonance Spectroscopy*, Vol.51, pp.219–242.
Filipe, O. M. S., Santos, E. B. H., Otero, M., Gonçalves, E. A. C., and Neves, M. G. P. M. S., (2020), "Photodegradation of metoprolol in the presence of aquatic fulvic acids . Kinetic studies , degradation pathways and role of singlet oxygen , OH radicals and fulvic acids triplet states", *Journal of Hazardous Materials*, Vol.385, No.October 2019, pp.121523.
Fioroni, M., Diaz, M. D., Burger, K., and Berger, S., (2002), "Solvation phenomena of a tetrapeptide in water/trifluoroethanol and water/ethanol mixtures: A diffusion NMR, intermolecular NOE, and molecular dynamics study", *Journal of the American Chemical Society*, Vol.124, No.26, pp.7737–7744.
Fisher, J., (2014), "*Modern NMR techniques for synthetic chemistry*" (Fisher J., Eds.),. CRC Press. Taylor & Francis group.
Flaherty, R. J., Nshime, B., Delamarre, M., Dejong, S., Scott, P., and Lantz, A. W., (2013), "Cyclodextrins as complexation and extraction agents for pesticides from contaminated soil", *Chemosphere*, Vol.91, No.7, pp.912–920.
Flupyradifurone, (2013),*Bayer CropScience*.
Fonseca, C. P., Fonseca, L. L., Montezinho, L. P., Alves, P. M., Santos, H., Margarida, M., … Geraldes, C. F. G. C., (2013), "23Na multiple quantum filtered NMR characterisation of Na + binding and dynamics in animal cells : a comparative study and effect of Na + / Li + competition", *European Biophysics Journal*, Vol.42, pp.503–519.
Foster, M. P., Mcelroy, C. A., and Amero, C. D., (2007), "Solution NMR of large molecules and assemblies", *Biochemistry*, Vol.46, No.2, pp.331–340.
Fotopoulou, E., and Ronconi, L., (2018), "Application of Heteronuclear NMR Spectroscopy to Bioinorganic and Medicinal Chemistry", *Reference Module in Chemistry, Molecular Sciences and Chemical Engineering*, pp.B978- 0-12-409547- 2.10947-3.
Franck, J. M., Kausik, R., and Han, S., (2013a), "Overhauser dynamic nuclear polarization-enhanced NMR relaxometry", *Microporous and Mesoporous Materials*, Vol.178, pp.113–118.
Franck, J. M., Pavlova, A., Scott, J. A., and Han, S., (2013b, October 1), "Quantitative cw Overhauser effect dynamic nuclear polarization for the analysis of local water dynamics", *Progress in Nuclear Magnetic Resonance Spectroscopy*. Pergamon, Vol.74, pp.33-56.
Freeman, R., Hill, H. D. W., Tomlinson, B. L., and Hall, L. D., (1974), "Dipolar contribution to NMR spin-lattice relaxation of protons", *The Journal of Chemical Physics*, Vol.61, No.11, pp.4466–4473.
Frieden, C., Hoeltzli, S. D., and Bann, J. G. B. T.-M. in E., (2004), "The Preparation of 19F-Labeled Proteins for NMR Studies",In *Energetics of Biological Macromolecules, Part E* (Vol. 380, pp. 400–415). Academic Press.
Frutos, S., Tarrago, T., and Giralt, E., (2006), "A fast and robust 19 F NMR-based method for finding new HIV-1 protease inhibitors", *Bioorganic & Medicinal Chemistry Letters*, Vol.16, pp.2677–2681.
Fujiwara, T., and O'Hagan, D., (2014), "Successful fluorine-containing herbicide agrochemicals", *Journal of Fluorine Chemistry*, Vol.167, pp.16–29.
Furihata, K., and Tashiro, M., (2018), "Improved 19F { 1H } Saturation Transfer Difference Experiments for Sensitive Detection to Fluorinated Compound Bound to Proteins", *Magnetochemistry,* Vol.5, No.1, pp.1–6.
Furihata, K., Usui, M., and Tashiro, M., (2017), "Application of NMR Screening Methods with 19 F Detection to Fluorinated Compounds Bound to Proteins", *Magnetochemistry*, Vol.4, No.3, pp.3–7.
Gast, K., Zirwer, D., Müller-Frohne, M., and Damaschun, G., (1999), "Trifluoroethanol-induced conformational transitions of proteins: Insights gained from the differences between α-lactalbumin and ribonuclease A", *Protein Science*, Vol.8, No.3, pp.625–634.
Gattavecchia, E., Borgatti, A., Di Pietra, A. M., and Tonelli, D., (1981), "Effect of diflubenzuron and its major degradation products on the growth of euglena gracilis z. and incorporation of glycine-u-14C in Protein", *Journal of Environmental Science and Health, Part B*, Vol.16, No.2, pp.159–166.
Gee, C. T., Koleski, E. J., and Pomerantz, W. C. K., (2016), "Fragment Screening and Druggability Assessment for the CBP/ p300 KIX Domain Via Protein Observed 19 F NMR", *Angewantde Chemie - International Edition English*, Vol.54, No.12, pp.3735–3739.
George, C., and Chandrakumar, N., (2014), "Chemical-shift-resolved 19FNMR spectroscopy between 13.5 and 135MHz: Overhauser-DNP-enhanced diagonal suppressed correlation spectroscopy", *Angewandte Chemie - International Edition*, Vol.53, No.32, pp.8441–8444.
Gerig, J. T., (1997), "Fluorine NMR",In *On-Line Biophysics Textbook (Bloomfield, V., Ed.) Biophysical Society*

(pp. 1–35). Bethesda, MD.
Gerig, J. T., (2004), "Structure and Solvation of Melittin in 1,1,1,3,3,3-Hexafluoro-2-Propanol", *Biophysical Journal*, Vol.86, pp.3166–3175.
Gerig, J. T., Halley, B. A., and Ortiz, C. E., (1977), "Nuclear magnetic resonance studies of p-fluorocinnamate-.alpha.-chymotrypsin complexes", *Journal of the American Chemical Society*, Vol.99, No.19, pp.6219–6226.
Gerig, J. T., and Stock, A. D., (1975), "Studies of the Kinetics of the Interaction between N-Trifluoroacetyl-D-tryptophan and a-Chymotrypsin by Pulsed Nuclear Magnetic Resonance", *Organic Magnetic Resonance*, Vol.7, pp.249–255.
Gerke, J., (2018), "Concepts and Misconceptions of Humic Substances as the Stable Part of Soil Organic Matter : A Review", *Agronomy*, Vol.76, No.8, pp.1–16.
Gerothanassis, I. P., Troganis, A., Exarchou, V., and Barbarossou, K., (2002), "Muclear magnetic resonance (nmr) spectroscopy : basic principles and phenomena , and their applications to chemistry , biology and medicine", *Chemistry Education: Research and Practice in Europe*, Vol.3, No.2, pp.229–252.
Ghosh, K., and Schnitzer, M., (1979), "UV and visible absorption spectroscopic investigations in relation to macromolecular characterisitcs of humic substances", *Journal of Soil Science*, Vol.30, pp.735–745.
Ghuman, J., Zunszain, P. A., Petitpas, I., Bhattacharya, A. A., Otagiri, M., and Curry, S., (2005), "Structural basis of the drug-binding specificity of human serum albumin", *Journal of Molecular Biology*, Vol.353, No.1, pp.38–52.
Gilday, L. C., Robinson, S. W., Barendt, T. A., Langton, M. J., Mullaney, B. R., and Beer, P. D., (2015), "Halogen Bonding in Supramolecular Chemistry", *Chemical Reviews*, Vol.115, No.15, pp.7118–7195.
Gillis, E. P., Eastman, K. J., Hill, M. D., Donnelly, D. J., and Meanwell, N. A., (2015), "Applications of Fluorine in Medicinal Chemistry", *Journal of Medicinal Chemistry*, Vol.58, No.21, pp.8315–8359.
Glaberman, S., and Katrina, W., (2014), "*Environmental Fate and Ecological Risk Assessment for Foliar, Soil Drench, and Seed Treatment Uses of the New Insecticide Flupyradifurone (BYI 02960)*".
Gmurek, M., and Olak-kucharczyk, M., (2015), "Influence of dissolved organic matter in natural and simulated water on the photochemical decomposition of butylparaben", *Journal of Environmental Health Science and Engineering*, Vol.28, pp.2–9.
Golding, C. J., Smernik, R. J., and Birch, G. F., (2005), "Investigation of the role of structural domains identified in sedimentary organic matter in the sorption of hydrophobic organic compounds", *Environmental Science and Technology*, Vol.39, No.11, pp.3925–3932.
Gonc, R., Mateus, N., and Freitas, V. De, (2011), "Influence of Carbohydrates on the Interaction of Procyanidin B3 with Trypsin", *Journal of Agricultural and Food Chemistry*, Vol.59, pp.11794–11802.
Gonçalves, R., Mateus, N., and de Freitas, V., (2010), "Biological relevance of the interaction between procyanidins and trypsin: a multitechnique approach.", *Journal of Agricultural and Food Chemistry*. Vol.58, No.22, pp.11924–11931.
Gonçalves, R., Mateus, N., Pianet, I., Laguerre, M., and De Freitas, V., (2011), "Mechanisms of tannin-induced trypsin inhibition: A molecular approach", *Langmuir*, Vol.21, pp.13122–13129
Goncharov, N. V, Belinskaya, D. A., Razygraev, A. V, and Ukolov, A. I., (2015), "On the Enzymatic Activity of Albumin", *Russian Journal of Bioorganic Chemistry*, Vol.41, No.2, pp.113–124.
Gonclaves, R., Mateus, N., and Freitas, V. De, (2010), "Biological Relevance of the Interaction between Procyanidins and Trypsin : A Multitechnique Approach", *Journal of Agricultural and Food Chemistry*, Vol.58, pp.11924–11931.
Goring, C. A. I., Laskowski, D. A., Hamaker, J. W., and Meikle, R. W., (1975), "Principles of Pesticide Degradation in Soil.",In R. Haque & V. H. Freed (Eds.), *Environmental Dynamics of Pesticides.* (Volume 6). Boston, MA: Environmental Science Research,Springer.
Gossert, A. D., (2019), "Assessing molecular interactions with biophysical methods using the validation cross", *Biochemical Society Transactions*, Vol.47, pp.63–76.
Goto, Y., and Hagihara, Y., (1992), "Mechanism of the Conformational Transition of Melittin "", *Biochemistry*, Vol.31, pp.732–738.
Grace, R. C. R., and Kumar, A., (1995), "Observation of Cross Correlations in a Weakly Coupled 19F-1H Four-Spin System", *Journal of Magnetic Resonance, Series A*, Vol.115, No.1, pp.87–93.
Grembecka, J., and Cierpicki, T., (2015), "Rational Design of Orthogonal Multipolar Interactions with Fluorine in Protein − Ligand Complexes", *Journal of Medicinal Chemistry*, Vol.58, pp.7465–7474.
Gribble, G. W., (2002), "Naturally Occurring Organofluorines",In A. H. Neilson (Ed.), *Organofluorines* (pp. 121–136). Berlin, Heidelberg: Springer Berlin Heidelberg.
Guerrero-Martínez, A., Berger, S., and Tardajos, G., (2006), "Selective solvation of cyclodextrins by small molecules: A NOE study", *ChemPhysChem*, Vol.7, No.10, pp.2074–2076.

Guetzloff, T. F., and Rice, J. A., (1994), "Does humic acid form a micelle ?", *The Science of the Total Environment*, Vol.152, No.1, pp.31–35.

Guo, L., Jury, W. A., Wagenet, R. J., and Flury, M., (2000), "Dependence of pesticide degradation on sorption: Nonequilibrium model and application to soil reactors", *Journal of Contaminant Hydrology*, Vol.43, No.1, pp.45–62.

Guo, X. Xia, Liu, H. tao, and Wu, S. biao, (2019, April 20), "Humic substances developed during organic waste composting: Formation mechanisms, structural properties, and agronomic functions", *Science of the Total Environment*. Vol.662, pp-501-510.

Halle, B., (2003), "Cross-relaxation between macromolecular and solvent spins: The role of long-range dipole couplings", *Journal of Chemical Physics*, Vol.119, No.23, pp.12372–12385.

Hansen, D. F., (2017), "Measurement of 15N longitudinal relaxation rates in 15NH4+ spin systems to characterise rotational correlation times and chemical exchange", *Journal of Magnetic Resonance*, Vol.279, pp.91–98.

Harner, M. J., Frank, A. O., and Fesik, S. W., (2014), "Fragment-Based Drug Discovery Using NMR Spectroscopy", *Journal of Biomolecular NMR*, Vol.56, No.2, pp.65–75.

Hattori, Y., Heidenreich, D., Ono, Y., Sugiki, T., Yokoyama, K. ichi, Suzuki, E. ichiro, … Kojima, C., (2017), "Protein 19F-labeling using transglutaminase for the NMR study of intermolecular interactions", *Journal of Biomolecular NMR*, Vol.68, No.4, pp.271–279.

Hatzakis, E., (2019), "Nuclear Magnetic Resonance (NMR) Spectroscopy in Food Science : A Comprehensive Review", *Comprehensive Reviews in Food Sicience and Food Safety*, Vol.18, pp.189–219.

Hausser, K., and Stehlik, D., (1968), "Dynamic Nuclear Polarization in Liquids",In J. S. WAUGH (Ed.), *Advances in Magnetic Resonance* (Vol. 3, pp. 79–139). Academic Press.

Hazime, S., Isao, A., and Ramamoorthy, A., (2012), "Chemical Shift Tensor – the Heart of NMR: Insights into Biological Aspects of Proteins", *Progress in Nuclear Magnetic Resonance Spectroscopy*, Vol.23, No.1, pp.1–7.

Hemalatha, K., Madhumitha, G., Al-dhabi, N. A., and Valan, M., (2016), "Importance of fl uorine in 2 , 3-dihydroquinazolinone and its interaction study with lysozyme", *Journal of Photochemistry & Photobiology , B : Biology*, Vol.162, pp.176–188.

Herbert, B. E., and Bertsch, P. M., (1997), "*Nuclear Magnetic Resonance Spectrosocpy in Environmental Chemistry*", (M. A. Nanny, R. A. Minear, & J. A. Leenheer, Eds.). Oxford: Oxford University Press.

Herrera-castro, F., and Torres, L. A., (2019), "Understanding the solvation process and solute-solvent interactions of imidazole compounds in three different solvents through solution calorimetry and 1 H NMR", *Journal of Molecular Liquids*, Vol.284, pp.232–240.

Hindman, J. C., Zielen, A. J., Svirmickas, A., and Wood, M., (1971), " Relaxation Processes in Water. The Spin–Lattice Relaxation of the Deuteron in D 2 O and Oxygen-17 in H 2 17 O ", *The Journal of Chemical Physics*, Vol.54, No.2, pp.621–634.

Hirose, K., (2001), "A practical guide for the determination of Binding constant", *Journal of Inclusion Phenomena AndMacrocyclic Chemistry*, Vol.39, pp.193–209.

Hoeltzli, S. D., and Frieden, C., (1995), "Stopped-flow NMR spectroscopy : Real-time unfolding studies of 6-19F-tryptophan-labeled Escherichia coli dihydrofolate reductase", *Proceedings of the National Academy of Sciences*, Vol.92, No.September, pp.9318–9322.

Hong, D. P., Hoshino, M., Kuboi, R., and Goto, Y., (1999), "Clustering of fluorine-substituted alcohols as a factor responsible for their marked effects on proteins and peptides", *Journal of the American Chemical Society*, Vol.121, No.37, pp.8427–8433.

Huang, Y., and Sutrisno, A., (2014), "Recent Advances in Solid-State 67Zn NMR Studies: From Nanoparticles to Biological Systems", *Annual Reports on NMR Spectroscopy*, Vol.81, pp.1–46.

Hubbard, P. S., (1966), "Theory of Electron-Nucleus Overhauser Effects in Liquids Containing Free Radicals", *Proceedings of the Royal Society of London.* Vol.291, pp.537–555.

Hwang, C. F., and Hill, D. A., (1967), "Phenomenological Model for the New Effect in Dynamic Polarization", *Physical Review Letters*, Vol.19, No.18, pp.1011–1014.

Jaipuria, G., Lobo, N. P., Shet, D., and Atreya, H. S., (2012), "High resolution methyl selective in solution and solid state C-NMR of proteins", *Journal of Biomolecular NMR*, Vol.54, pp.33–42.

James, T. I., (2012), "*Nuclear magnetic Resonance in biochemistry*". Academic press, Elsevier Science.

Janssen, E. M., Erickson, P. R., and Mcneill, K., (2014), "Dual Roles of Dissolved Organic Matter as Sensitizer and Quencher in the Photooxidation of Tryptophan". Vol.48, No.9, pp.4916-24.

Jasanoff, A., and Alan, R., (1994), "Quantitative Determination of Helical Propensities from Trifluoroethanol Titration", *Biochemistry*, Vol.33, No.8, pp.2129–2135.

Jenkins, B. G., (1990), "Detection of Site-Specific Binding and Co-binding of Ligands toHuman Serum Albumin using 19F NMR", *Molecular Pharmacology*, Vol.37, pp.111–118.

Jenkins, B. G., (1991), "Detection of site-specific binding and co-binding of ligands to macromolecules using 19F NMR", *Life Sciences*, Vol.48, No.13, pp.1227–1240.
Jeschke, P., (2004), "The unique role of fluorine in the design of active ingredients for modern crop protection", *ChemBioChem*, Vol.5, No.5, pp.570–589.
Jeschke, P., (2010), "The unique role of halogen substituents in the design of modern agrochemicals", *Pest Management Science*. Vol. 66, No.1, pp.10-27.
Jeschke, P., (2017), "Latest generation of halogen-containing pesticides", *Pest Management Science*. Vol.73, No.6, pp.1053-1066.
Johnson, C. S., (1999), "Diffusion ordered nuclear magnetic resonance spectroscopy: Principles and applications", *Progress in Nuclear Magnetic Resonance Spectroscopy*, Vol.34, No.3–4, pp.203–256.
Kadayakkara, D. K. K., Janjic, J. M., Pusateri, L. K., Young, W., and Ahrens, E. T., (2010), "In Vivo Observation of Intracellular Oximetry in Perfluorocarbon-Labeled Glioma Cells and Chemotherapeutic Response in the CNS Using Fluorine-19 MRI", *Magnetic Resonance in Medicine*, Vol.1259, pp.1252–1259.
Kadeřávek, P., Bolik-Coulon, N., Cousin, S. F., Marquardsen, T., Tyburn, J.-M., Dumez, J.-N., and Ferrage, F., (2019), "Protein Dynamics from Accurate Low-Field Site-Specific Longitudinal and Transverse Nuclear Spin Relaxation", *The Journal of Physical Chemistry Letters*, Vol.10, No.19, pp.5917–5922.
Kadeřávek, P., Ferrage, F., Bodenhausen, G., and Kurzbach, D., (2018), "High-Resolution NMR of Folded Proteins in Hyperpolarized Physiological Solvents", *Chemistry - A European Journal*, Vol.24, No.51, pp.13418–13423.
Kaminker, I., Barnes, R., and Han, S., (2015), "Overhauser Dynamic Nuclear Polarization Studies on Local Water Dynamics", *Methods in Enzymology*, Vol.564, pp.457–483.
Kang, K. H., Shin, H. S., and Park, H., (2002), "Characterization of humic substances present in landfill leachates with different landfill ages and its implications", *Water Research*, Vol.36, No.16, pp.4023–4032.
Karlicek, R. F., and Lowe, I. J., (1980), "A modified pulsed gradient technique for measuring diffusion in the presence of large background gradients", *Journal of Magnetic Resonance (1969)*, Vol.37, No.1, pp.75–91.
Katagi, T., (2018), "Direct photolysis mechanism of pesticides in water Direct photolysis mechanism of pesticides in water", *Journal of Pesticide Science*, Vol.43, No.2, pp.57–72.
Keeler, J., (2002), "*Understanding NMR spectroscopy (2nd* Edition)",Wiley, University of Cambridge, UK.
Kemple, M. D., Buckley, P., Yuan, P., and Prendergast, F. G., (1997), "Main Chain and Side Chain Dynamics of Peptides in Liquid Solution from 13 C NMR : Melittin as a Model Peptide †", *Biochemistry*, Vol.36, No.7, pp.1678–1688.
Kentsis, A., and Sosnick, T. R., (1998), "Trifluoroethanol promotes helix formation by destabilizing backbone exposure: Desolvation rather than native hydrogen bonding defines the kinetic pathway of dimeric coiled coil folding", *Biochemistry*, Vol.37, No.41, pp.14613–14622.
Khalaf, M., Kohl, D. S., Klumpp, E., Rice, J. A., and Tombacz, E., (2003), "Comparison of Sorption Domains in Molecular Weight Fractions of a Soil Humic Acid Using Solid-State 19F NMR", *Environment Science and Technology*, Vol.37, No.13, pp.2855–2860.
Kim, H. C., and Yu, M. J., (2007), "Characterization of aquatic humic substances to DBPs formation in advanced treatment processes for conventionally treated water", *Journal of Hazardous Materials*, Vol.143, No.1–2, pp.486–493.
Kim, Y., and Hilty, C., (2015), "Affinity Screening Using Competition with Fluorine-19 Hyperpolarized Ligands", *Angewantde Chemie-International Edition English*, Vol.54, No.16, pp.4941–4944.
Kim, Y., Liu, M., and Hilty, C., (2018), "Determination of binding affinities using hyperpolarized NMR with simultaneous 4-channel detection", *Journal of Magnetic Resonance*, Vol.295, pp.80–86.
Kitamura, K., Kume, M., Yamamoto, M., Takegami, S., and Kitade, T., (2004), "19F NMR spectroscopic study on the binding of triflupromazine to bovine and human serum albumins", *Journal of Pharmaceutical and Biomedical Analysis*, Vol.36, No.2, pp.411–414.
Kitamura, K., Omran, A. A., Takegami, S., Tanaka, R., and Kitade, T., (2007), "19F NMR spectroscopic characterization of the interaction of niflumic acid with human serum albumin", *Analytical and Bioanalytical Chemistry*, Vol.387, No.8, pp.2843–2848.
Kitevski-LeBlanc, J., (2010), "*Development and Application of 19F NMR of Proteins*". University of Toronto.
Kitevski-LeBlanc, J. L., and Prosser, R. S., (2012), "Current applications of 19F NMR to studies of protein structure and dynamics", *Progress in Nuclear Magnetic Resonance Spectroscopy*, Vol.62, pp.1–33.
Klavins, M., and Purmalis, O., (2010), "Humic substances as surfactants", *Environmental Chemistry Letters*, Vol.8, No.4, pp.349–354.

Kleckner, I. R., and Foster, M. P., (2010), "An introduction to NMR-based approaches for measuring protein dynamics", *Biochimica et Biophysica Acta - Proteins and Proteomics*. Vol.1814, No. 8, pp.942-968

Klučáková, M., (2018), "Size and charge evaluation of standard humic and fulvic acids as crucial factors to determine their environmental behavior and impact", *Frontiers in Chemistry*, Vol.6, pp.1–8.

Kögel-Knabner, I., (2000), "Analytical approaches for characterizing soil organic matter", *Organic Geochemistry*, Vol.31, No.7–8, pp.609–625.

Kohl, S. D., Toscano, P. J., Hou, W., and Rice, J. A., (2000), "Solid-state 19F NMR investigation of hexafluorobenzene sorption to soil organic matter", *Environmental Science and Technology*, Vol.34, No.1, pp.204–210.

Konno, T., Iwashita, J. U. N., and Nagayama, K., (2000), "Fluorinated alcohol, the third group of cosolvents that stabilize the molten-globule state relative to a highly denatured state of cytochrome c", *Protein Science*, Vol.9, No.3, pp.564–569.

Koopal, L. K., Saito, T., Pinheiro, J. P., and Van Riemsdijk, W. H., (2005), "Ion binding to natural organic matter: General considerations and the NICA-Donnan model", *Colloids and Surfaces A: Physicochemical and Engineering Aspects*, Vol.265, No.1–3, pp.40–54.

Kovrigin, E. L., Kempf, J. G., Grey, M. J., and Loria, J. P., (2006), "Faithful estimation of dynamics parameters from CPMG relaxation dispersion measurements", *Journal of Magnetic Resonance*, Vol.180, pp.93–104.

Krishnan, V. V., (2005), "Ligand Screening by Saturation-Transfer Difference (STD) NMR Spectroscopy", *Current Analytical Chemistry*, Vol.1, No.3, pp.307–320.

Kuhn, L. T., Bommerich, U., and Bargon, J., (2006), "Transfer of Parahydrogen-Induced Hyperpolarization to 19F", *Journal of Physical Chemistry A*, Vol.110, pp.3521–3526.

Kumar, A., Grace, R. C. R., and Madhu, P. K., (2000), "Cross-correlations in NMR", *Progress in Nuclear Magnetic Resonance Spectroscopy*, Vol.37, No.3, pp.191–319.

Kumar, D., Krishnan, Y., Paranjothy, M., and Pal, S., (2017), "Analysis of Molecular Interaction of Drugs within β-Cyclodextrin Cavity by Solution-State NMR Relaxation", *Journal of Physical Chemistry B*, Vol.121, No.13, pp.2864–2872.

Kumar, S., Modig, K., and Halle, B., (2003), "Trifluoroethanol-Induced β → α Transition in β-Lactoglobulin: Hydration and Cosolvent Binding Studied by 2H, 17O, and 19F Magnetic Relaxation Dispersion", *Biochemistry*, Vol.42, No.46, pp.13708–13716.

Kurzbach, D., Canet, E., Flamm, A. G., Jhajharia, A., Weber, E. M. M., Konrat, R., and Bodenhausen, G., (2017), "Investigation of Intrinsically Disordered Proteins through Exchange with Hyperpolarized Water", *Angewandte Chemie - International Edition*, Vol.56, No.1, pp.389–392.

Kuwata, K., Hoshino, M., Era, S., Batt, C. A., and Goto, Y., (1998), "α→β transition of β-lactoglobulin as evidenced by heteronuclear NMR", *Journal of Molecular Biology*, Vol.283, No.4, pp.731–739.

Lambert, J. B., and Simpson, S. V., (1985), "Effect of lithium cation on the relaxation mechanisms of acids and alcohols", *Magnetic Resonance in Chemistry*, Vol.23, No.2, pp.61–66.

Lankhorst, D., Schriever, J., and Leyte, J. C., (1982), "Determination of the Rotational Correlation Time of Water by Proton NMR Relaxation in H217O and Some Related Results", *Berichte Der Bunsengesellschaft Für Physikalische Chemie*, Vol.86, No.3, pp.215–221.

Lauterwein, J., Brown, Larry, R., and Wuthrich, K., (1980), "High-resolution 1H-NMR studies of monomeric melittin in aqueous solution", *Biochimica et Biophysica Acta*, Vol.622, pp.219–230.

Lee, T. S., and Hwang, L. P., (1990), "Influence of dipole-dipole cross-relaxation on spectral lineshapes of methyl protons in inversion-recovery experiments", *Journal of Magnetic Resonance (1969)*, Vol.89, No.1, pp.51–59.

Lee, Y. C., and Lee, R. T., (1995), "Carbohydrate-Protein Interactions: Basis of Glycobiology", *Accounts of Chemical Research*, Vol.28, No.8, pp.321–327.

Lee, Y., Zeng, H., Ruedisser, S., Gossert, A. D., and Hilty, C., (2012), "Nuclear magnetic resonance of hyperpolarized fluorine for characterization of protein-ligand interactions", *Journal of the American Chemical Society*, Vol.134, No.42, pp.17448–17451.

Leung, I. K. H., (2015), "NMR spectroscopy – a simple yet powerful tool in chemical biology", *Chemistry in New Zealand*, Vol.79, No.1, pp.42–50.

Lewandowski, J. R., Halse, M. E., Blackledge, M., and Emsley, L., (2015), "Direct observation of hierarchicalprotein dynamics", *Protein Dynamics*, Vol.348, No.6234, pp.578–581.

Li, M., Mazzei, P., Cozzolino, V., Monda, H., Hu, Z., and Piccolo, A., (2015), "Optimized procedure for the determination of P species in soil by liquid-state 31 P-NMR spectroscopy", *Chemical and Biological Technologies in Agriculture*, Vol.2, pp.1–7.

Li, Q., Hurt, A. P., and Coleman, N. J., (2019), "The Application of 29 Si NMR Spectroscopy to the Analysis of Calcium Silicate-Based Cement using Biodentine as an Example", *Journal of Functional Biomaterials*,

Vol.10, No.25, pp.1–18.
Liao, C., Selvan, M. E., Zhao, J., Slimovitch, J. L., Schneebeli, S. T., Shelley, M., … Li, J., (2015), "Melittin Aggregation in Aqueous Solutions: Insight from Molecular Dynamics Simulations", *The Journal of Physical Chemistry. B*, Vol.119, pp.10390–10398.
Lin, P., (2016), "Assessment of Chemical Exchange in Tryptophan-Albumin Solution through 19 F Multicomponent Transverse Relaxation Dispersion Analysis", *Journal of Biomolecular NMR*, Vol.62, No.2, pp.121–127.
Lingel, A., Vulpetti, A., Reinsperger, T., Proudfoot, A., Denay, R., Frommlet, A., … Frank, A. O., (2020), "Comprehensive and High-Throughput Exploration of Chemical Space Using Broadband 19F NMR-Based Screening", *Angewantde Chemie- International Edition English.* Vol.132, No.35, pp. 14919-14927
Lingwood, M. D., Ivanov, I. A., Cote, A. R., and Han, S., (2010a), "Heisenberg spin exchange effects of nitroxide radicals on Overhauser dynamic nuclear polarization in the low field limit at 1.5 mT", *Journal of Magnetic Resonance*, Vol.204, No.1, pp.56–63.
Lingwood, M. D., Siaw, T. A., Sailasuta, N., Ross, B. D., Bhattacharya, P., and Han, S., (2010b), "Continuous flow Overhauser dynamic nuclear polarization of water in the fringe field of a clinical magnetic resonance imaging system for authentic image contrast", *Journal of Magnetic Resonance*, Vol.205, No.2, pp.247–254.
Liu, H., and Hsu, C., (2003), "The effects of solvent and temperature on the structural integrity of monomeric melittin by molecular dynamics simulations", *Chmeical Physics Letters*, Vol.375, pp.119–125.
Liu, M., Nicholson, J. K., and Lindon, J. C., (1997), "Analysis of Drug – Protein Binding Using Nuclear Magnetic Resonance Based Molecular Diffusion Measurements", *Analytical Communications*, Vol.34, No.August, pp.225–228.
Liu, Ying, Cao, R., Qin, P., and Liu, R., (2012), "Spectrochimica Acta Part A : Molecular and Biomolecular Spectroscopy Assessing the potential toxic effect of one persistent organic pollutant : Non-covalent interaction of dicofol with the enzyme trypsin", *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*, Vol.89, pp.210–215.
Liu, Yingying, Zhang, G., Liao, Y., and Wang, Y., (2015), "Binding characteristics of psoralen with trypsin: Insights from spectroscopic and molecular modeling studies", *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*. Vol. 151, No.5, pp. 498-505.
Liu, Yingying, Zhang, G., Zeng, N., and Hu, S., (2017), "Interaction between 8-methoxypsoralen and trypsin: Monitoring by spectroscopic, chemometrics and molecular docking approaches", *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*. Vol. 173, pp. 188-195.
Loewen, M. C., Klein-Seetharaman, J., Getmanova, E. V, Reeves, P. J., Schwalbe, H., and Khorana, H. G., (2001), "Solution 19F nuclear Overhauser effects in structural studies of the cytoplasmic domain of mammalian rhodopsin", *Proceedings of the National Academy of Sciences*, Vol.98, No.9, pp.4888–4892.
Longstaffe, James G., and Simpson, A. J., (2011), "Understanding solution-state noncovalent interactions between xenobiotics and natural organic matter using 19F/1H heteronuclear saturation transfer difference nuclear magnetic resonance spectroscopy", *Environmental Toxicology and Chemistry*, Vol.30, No.8, pp.1745–1753.
Longstaffe, James G., Simpson, M. J., Maas, W., and Simpson, A. J., (2010), "Identifying components in dissolved humic acid that bind organofluorine contaminants using 1H{19F} reverse heteronuclear saturation transfer difference NMR spectroscopy", *Environmental Science and Technology*, Vol.44, pp.5476–5482.
Longstaffe, James G, Courtier-Murias, D., and Simpson, A. J., (2016), "A nuclear magnetic resonance study of the dynamics of organofluorine interactions with a dissolved humic acid", *Chemosphere*, Vol.145, pp.307–313.
Longstaffe, James Gregory, (2013), "*A Molecular-Level Investigation of the Interactions Between Organofluorine Compounds and Soil Organic Matter Using Nuclear Magnetic Resonance Spectroscopy*". University of Toronto.
Loukas, Y. L., (1997), "Evaluation of the methods for the determination of the stability constant of cyclodextrin-chlorambucil inclusion complexes", *Journal of Pharmaceutical and Biomedical Analysis*, Vol.16, No.2, pp.275–280.
Lu, C., Yin, X., Liu, X., and Wang, M., (2014), "Study of the photodegradation kinetics and pathways of Hexaflumuron in liquid media", *Photochemistry and Photobiology*, Vol.90, No.6, pp.1219–1223.
Lucas-Abellan, C., Gabaldon-Hernandez, J. A., and Nunez-Delicado, E., (2008), "Preparation and Characterization of the Inclusion Complex of Chlorpyrifos in Cyclodextrins", *Journal of Agricultural and Food Chemistry*, Vol.56, pp.8081–8085.

Lucas, L. H., and Larive, C. K., (2004), "Measuring ligand-protein binding using NMR diffusion experiments", *Concepts in Magnetic Resonance Part A: Bridging Education and Research*, Vol.20, No.1, pp.24–41.

Lucas, L. H., Otto, W. H., and Larive, C. K., (2002), "The 2D-J-DOSY Experiment: Resolving Diffusion Coefficients in Mixtures", *Journal of Magnetic Resonance*, Vol.156, No.1, pp.138–145.

Ludwig, C., and Guenther, U. L., (2009), "Ligand based NMR methods for drug discovery", *Frontiers in Bioscience*, Vol.14, No.12, pp.4565–4574.

Luo, P., and Baldwin, R. L., (1997), "Mechanism of Helix Induction by Trifluoroethanol : A Framework for Extrapolating the Helix-Forming Properties of Peptides from Trifluoroethanol / Water Mixtures Back to Water †", *Biochemistry*, Vol.36, No.27, pp.8413–8421.

Luo, R., Liu, M., and Mao, X., (1999), "NMR diffusion and relaxation study of drug – protein interaction", *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*, Vol.55, pp.1897–1901.

Luo, Y. C., Zeng, Q. R., Wu, G., Luan, Z. K., Yang, R. B., and Liao, B. H., (2003), "Effect of α-Cyclodextrin Compounds on the Solubilization of Three Selected Pesticides and Their Toxicity with Methyl Parathion to Rana tigrina Tadpoles", *Bulletin of Environmental Contamination and Technology*, Vol.70, pp.998–1005.

Ma, H., Allen, H. E., and Yin, Y., (2001), "Characterization of isolated fractions of dissolved organic matter from natural waters and a wastewater effluent", *Water Research*, Vol.35, No.4, pp.985–996.

Main, E. R. G., and Jackson, S. E., (1999), "Does trifluoroethanol affect folding pathways and can it be used as a probe of structure in transition states?", *Nature Structural Biology*, Vol.6, No.9, pp.831–835.

Maity, S., Gundampati, R. K., and Kumar, T. K. S., (2019), "NMR methods to characterize protein-ligand interactions", *Natural Product Communications*, Vol.14, No.5, pp.1–17.

Mao, H., Hajduk, P. J., Craig, R., Bell, R., Borre, T., and Fesik, S. W., (2001), "Rational design of diflunisal analogues with reduced affinity for human serum albumin", *Journal of the American Chemical Society*, Vol.123, No.43, pp.10429–10435.

Marquardt, D. W., (1963), "An algorithm for least-squares estimation of nonlinear parameters", *SIAM Journal on Applied Mathematics*, Vol.11, pp.431–441.

Marsh, E. N. G., and Suzuki, Y., (2014), "Using 19 F NMR to Probe Biological Interactions of Proteins and Peptides", *ACS Chemical Biology*, Vol.9, pp.1242–1250.

Martini, S., Bonechi, C., and Rossi, C., (2008), "Interaction of Quercetin and Its Conjugate Quercetin 3-O-β-d-Glucopyranoside with Albumin as Determined by NMR Relaxation Data", *Journal of Natural Products*, Vol.71, No.2, pp.175–178.

Masoom, H., Courtier-murias, D., Farooq, H., Soong, R., Kelleher, B. P., Zhang, C., … Simpson, A. J., (2016), "Soil organic matter in its native state : unravelling the most complex biomaterial on Earth", *Environment Science and Technology*. Vol.50, No.4, pp.1670–1680.

Másson, M., Sigurjónsdóttir, J. F., Jónsdóttir, S., and Loftsson, T., (2003), "Examination of 19F-NMR as a tool for investigation of drug-cyelodextrin complexes", *Drug Development and Industrial Pharmacy*, Vol.29, No.1, pp.107–112.

Mathias, E. V., Aponte, J., Kornfield, J. A., and Ba, Y., (2010), "Properties of small molecular drug loading and diffusion in a fluorinated PEG hydrogel studied by 1H molecular diffusion NMR and 19F spin diffusion NMR", *Colloid and Polymer Science*, Vol.288, No.18, pp.1655–1663.

Mayer, M., and Meyer, B., (1999), "Characterisation of ligand binding by saturation transfer difference NMR spectroscopy.", *Angewandte Chemie - International Edition*, Vol.38, pp.1784–1788.

Mayer, M., and Meyer, B., (2001), "Group epitope mapping by saturation transfer difference NMR to identify segments of a ligand in direct contact with a protein receptor", *Journal of the American Chemical Society*, Vol.123, No.25, pp.6108–6117.

Mayer, U., (2002), "*Highlights in solute-solvent interactions*". Springer, New York.

Mazzei, P., and Piccolo, A., (2012), "Quantitative Evaluation of Noncovalent Interactions between Glyphosate and Dissolved Humic Substances by NMR Spectroscopy", *Environmental Science & Technology*, Vol.46, pp.5939–5946.

Mazzei, P., and Piccolo, A., (2015), "Interactions between natural organic matter and organic pollutants as revealed by NMR spectroscopy", *Magnetic Resonance in Chemistry*. Vol. 53, No. 9, pp.667-678.

Mazzei, P., and Piccolo, A., (2017), "HRMAS NMR spectroscopy applications in agriculture", *Chemical and Biological Technologies in Agriculture*, Vol.4, No.1, pp.1–13.

McCoy, M. A., and Wyss, D. F., (2002), "Structures of Protein−Protein Complexes Are Docked Using Only NMR Restraints from Residual Dipolar Coupling and Chemical Shift Perturbations", *Journal of the American Chemical Society*, Vol.124, No.10, pp.2104–2105.

Meenakshi, C., Jayabal, P., and Ramakrishnan, V., (2015), "Spectrochimica Acta Part A : Molecular and Biomolecular Spectroscopy Determination of association constant of host – guest supramolecular

complex (molecular recognition of carbamazepine , antiseizure drug , with calix (4) arene)", Vol.151, pp.707–711.

Mei, H., Remete, A. M., Zou, Y., Moriwaki, H., Fustero, S., Kiss, L., … Han, J., (2020), "Fluorine-containing drugs approved by the FDA in 2019", *Chinese Chemical Letters*. Vol. 31, No. 9, pp. 2401-2413.

Meiboom, S., and Gill, D., (1958), "Modified Spin-Echo Method for Measuring Nuclear Relaxation Times", *Review of Scientific Instruments*, Vol.29, No.8, pp.688–691.

Mendieta, J., Folqué, H., and Tauler, R., (1999), "Two-phase induction of the nonnative α-helical form of β-lactoglobulin in the presence of trifluoroethanol", *Biophysical Journal*, Vol.76, No.1 I, pp.451–457.

Meyer, B., and Peters, T., (2003), "NMR Spectroscopy of Proteins NMR Spectroscopy Techniques for Screening and Identifying Ligand Binding to Protein Receptors", *Angewandte Chemie - International Edition*, Vol.42, No.8, pp.864–890.

Miller, J. R., Melnick, M. M., Lall, M., Donovan, C., Sarver, R. W., Lee, D., … Emerson, D., (2010), "The Use of Biochemical and Biophysical Tools for Triage of High-Throughput Screening Hits – A Case Study with Escherichia coli Phosphopantetheine Adenylyltransferase", *Chemical and Biological Technologies in Agriculture*, Vol.75, pp.444–454.

Millet, O., Loria, J. P., Kroenke, C. D., Pons, M., and Palmer, A. G., (2000), "The Static Magnetic Field Dependence of Chemical Exchange Linebroadening Defines the NMR Chemical Shift Time Scale", *Journal of American Chemical Society*, Vol.122, No.7, pp.2867–2877.

Min, H. Z., (2014), "*Nuclear Magnetic Resonance based characterization of the protien binding pocket using hyperpolarizaed ligand*". Texas A&M University.

Mishra, S. K., and Suryaprakash, N., (2017), "Intramolecular hydrogen bonding involving organic fluorine: NMR investigations corroborated by DFT-based theoretical calculations", *Molecules*, Vol.22, No.3, pp.423-433.

Mistry, N., Ismail, I. M., Duncan Farrant, R., Liu, M., Nicholson, J. K., and Lindon, J. C., (1999), "Impurity profiling in bulk pharmaceutical batches using 19F NMR spectroscopy and distinction between monomeric and dimeric impurities by NMR-based diffusion measurements", *Journal of Pharmaceutical and Biomedical Analysis*, Vol.19, No.3–4, pp.511–517.

Mitchell, P. J., and Simpson, M. J., (2013), "High Affinity Sorption Domains in Soil Are Blocked by Polar Soil Organic Matter Components", *Environment Science and Technology*, Vol.47, pp.412–419.

Mittag, T., Schaffhausen, B., and Gu, U. L., (2003), "Direct Observation of Protein - Ligand Interaction Kinetics †", *Biochemistry*, Vol.42, pp.11128–11136.

Miura, Y., (2012), "NMR studies on the monomer – tetramer transition of melittin in an aqueous solution at high and low temperatures", *European Biophysics Journal*, Vol.41, pp.629–636.

Miura, Y., (2016), "NMR chemical shift analysis of the conformational transition between the monomer and tetramer of melittin in an aqueous solution", *European Biophysics Journal*, Vol.45, pp.347–354.

Modarresi-Alam, A. R., Najafi, P., Rostamizadeh, M., Keykha, H., Bijanzadeh, H.-R., and Kleinpeter, E., (2007), "Dynamic 1H NMR Study of the Barrier to Rotation about the C−N Bond in Primary Carbamates and Its Solvent Dependence", *The Journal of Organic Chemistry*, Vol.72, No.6, pp.2208–2211.

Monaco, S., Tailford, L. E., Juge, N., and Angulo, J., (2017), "Differential Epitope Mapping by STD NMR Spectroscopy To Reveal the Nature of Protein–Ligand Contacts", *Angewandte Chemie - International Edition*, Vol.56, No.48, pp.15289–15293.

Mondal, S., Kumar, R., Bansal, V., and Patel, M. B., (2015), "A 1H NMR method for the estimation of hydrogen content for all petroleum products", *Journal of Analytical Science and Technology*, Vol.6, No.1, pp.24.

Morán Vieyra, F. E., Palazzi, V. I., Sanchez de Pinto, M. I., and Borsarelli, C. D., (2009), "Combined UV-Vis absorbance and fluorescence properties of extracted humic substances-like for characterization of composting evolution of domestic solid wastes", *Geoderma*, Vol.151, No.3–4, pp.61–67.

Morillo, E., and Villaverde, J., (2017), "Advanced technologies for the remediation of pesticide-contaminated soils", *Science of the Total Environment*, Vol.586, pp.576–597.

Moschen, T., Grutsch, S., Juen, M. A., Wunderlich, C. H., Kreutz, C., and Tollinger, M., (2016), "Measurement of Ligand-Target Residence Times by 1H Relaxation Dispersion NMR Spectroscopy", *Journal of Medicinal Chemistry*, Vol.59, No.23, pp.10788–10793.

Moschen, T., Wunderlich, C. H., Spitzer, R., Levic, J., Tollinger, M., and Kreutz, C., (2015), "Ligand-Detected Relaxation Dispersion NMR Spectroscopy : Dynamics of preQ 1 – RNA Binding **", *Angewantde Chemie-Internation Edition*, Vol.54, No.2, pp.560–563.

Moudrakovski, I. L., Ratcliffe, C. I., and Ripmeester, J. A., (1998), "129Xe NMR Study of Adsorption and Dynamics of Xenon in AgA Zeolite", *Journal of the American Chemical Society*, Vol.120, No.13,

pp.3123–3132.
Moudrakovski, I. L., Terskikh, V. V, Ratcliffe, C. I., Ripmeester, J. A., Wang, L., Shin, Y., and Exarhos, G. J., (2002), "129 Xe NMR Study of Functionalized Ordered Mesoporous Silica", *Journal of Physical Chemistry A*, Vol.106, pp.5938–5946.
Müller-warmuth, W., and Meise-Gresch, K., (1983), "Molecular Motions and Interactions as Studied by Dynamic Nuclear Polarization (DNP) in Free Radical Solutions",In *Advances in Magnetic and Optical Resonance* (Vol. 11, pp. 1–45). Academic Press.
Müller, K., Faeh, C., and Diederich, F., (2007), "Fluorine in pharmaceuticals: Looking beyond intuition", *Science*, Vol.317, No.5846, pp.1881–1886.
Muñoz-García, J. C., Inacio dos Reis, R., Taylor, R. J., Henry, A. J., and Watts, A., (2018), "Nanodisc-Targeted STD NMR Spectroscopy Reveals Atomic Details of Ligand Binding to Lipid Environments", *ChemBioChem*. Vol.19, No.10, pp.1022-1025.
Nanny, M. A., Bortiatynski, J. M., and Hatcher, P. G., (1997), "Noncovalent Interactions between Acenaphthenone and Dissolved Fulvic Acid As Determined by 13C NMR T1 Relaxation Measurements", *Environmental Science & Technology*, Vol.31, No.2, pp.530–534.
Nanny, M. A., and Maza, J. P., (2001), "Noncovalent interactions between monoaromatic compounds and dissolved humic acids: A deuterium NMR T1 relaxation study", *Environmental Science and Technology*, Vol.35, No.2, pp.379–384.
Nauen, R., Jeschke, P., Velten, R., Beck, M. E., Ebbinghaus-Kintscher, U., Thielert, W., … Raupach, G., (2015), "Flupyradifurone: A brief profile of a new butenolide insecticide", *Pest Management Science*, Vol.71, No.6, pp.850–862.
Naumenkova, T. V, Levtsova, O. V, Nikolaev, I. N., and Shaitan, K. V, (2010), "Comparative Molecular Dynamics Study of the Structural Properties of Melittin in Water and Trifluoroethanol / Water", *Molecular Biophysics*, Vol.55, No.1, pp.24–28.
Neuhaus, D., and Williamson, P., (2000), "*The Nuclear Overhauser Effect in Structural and Conformational Analysis*" (2nd ed.). Weinheim: Wiley-VCH.
Neuman Jr., R. C., and Gerig, J. T., (2009), "Interaction of 2,2,2-trifluoroethanol with melittin", *Magnetic Resonance in Chemistry*, Vol.47, pp.925–931.
Ni, Y., Zhang, F., and Kokot, S., (2012), "Enantioselective binding interaction of the metolachlor pesticide enatiomers with bovine serum albumin - A spectroscopic analysis study", *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, Vol.97, pp.753–761.
Nikolaou, P., Goodson, B. M., and Chekmenev, E. Y., (2014), "NMR Hyperpolarization Techniques for Biomedicine", *Chemistry - A European Journal*, Vol.20, pp.1–13.
Nimmo, W. B., Joustra, K. D., and Willems, A. G. M., (1990), "The Degradation of Diflubenzuron and its Chief metabolites in soils Part III. Fate of 2,6 difluorobenzoic acid", *Pesticide Science*, Vol.29, No.1, pp.39–45.
Nomura, H., Onoda, M., and Miyahara, Y., (1982), "Preferential solvation of dextran in water-ethanol mixtures", *Polymer Journal*, Vol.14, No.4, pp.249–253.
Norton, R. S., Leung, E. W. W., Chandrashekaran, I. R., and MacRaild, C. A., (2016), "Applications of 19F-NMR in fragment-based drug discovery", *Molecules*, Vol.21, No.7.
Nyugen, K. T. H., Mathias, E. V., Porter, E., and Ba, Y., (2016), "Diffusions of b-cyclodextrins in mucus studied by 19F diffusion NMR", *Journal of Inclusion Phenomena and Macrocylic Chemistry*, Vol.86, pp.273–282.
O'Hagan, D., (2010), "Fluorine in health care Organofluorine containing blockbuster drugs", *Journal of Fluorine Chemistry*, Vol.131, No.11, pp.1071–1081.
O'Hagan, D., and Harper, D. B., (1999), "Fluorine-containing natural products", *Journal of Fluorine Chemistry*, Vol.100, No.1–2, pp.127–133.
Ohba, T., Ikeda, E., and Takei, H., (1996), "Inactivation of serine protease, chymotrypsin by fluorinated phenylalanine analogues", *Bioorganic and Medicinal Chemistry Letters*, Vol.6, No.16, pp.1875–1880.
Ohno, T., Hess, N. J., and Qafoku, N. P., (2019), "Current Understanding of the Use of Alkaline Extractions of Soils to Investigate Soil Organic Matter and Environmental Processes", *Journal of Environmental Quality*, Vol.1564, pp.1561–1564.
Ojima, I., (2013), "Exploration of fluorine chemistry at the multidisciplinary interface of chemistry and biology", *Journal of Organic Chemistry*, Vol.78, No.13, pp.6358–6383.
Okazoe, T., (2009), "Overview on the history of organofluorine chemistry from the viewpoint of material industry", *Proceedings of the Japan Academy Series B: Physical and Biological Sciences*, Vol.85, No.8, pp.276–289.
Oliver, M. A., (1997), "Soil and human health: a review", *European Journal of Soil Science*, Vol.48, No.4, pp.573–592.

Olsen, G., Markhasin, E., Szekely, O., and Bretschneider, C., (2016), "Optimizing water hyperpolarization and dissolution for sensitivity-enhanced 2D biomolecular NMR", *Journal of Magnetic Resonance*, Vol.264, pp.49–58.

Olsen, J. A., Banner, D. W., Seiler, P., Wagner, B., Tschopp, T., Obst-Sander, U., … Diederich, F., (2004), "Fluorine interactions at the thrombin active site: Protein backbone fragments H-Cα-C=O comprise a favorable C-F environment and interactions of C-F with electrophiles", *ChemBioChem*, Vol.5, No.5, pp.666–675.

Othon, C. M., Kwon, O., Lin, M. M., and Zewail, A. H., (2009), "Solvation in protein (un) folding of melittin tetramer – monomer transition", *Proceedings of the National Academy of Sciences*, Vol.106, No.31, pp.12593–12598.

Otto, W. H., and Larive, C. K., (2001), "Improved spin-echo-edited NMR diffusion measurements", *Journal of Magnetic Resonance*, Vol.153, No.2, pp.273–276.

Overhauser, A. W., (1953), "Polarization of Nuclei in Metals", *Physical Review*, Vol.92, pp.411–415.

Papeo, G., Giordano, P., Brasca, M. G., Buzzo, F., Caronni, D., Ciprandi, F., … Dalvit, C., (2007), "Polyfluorinated amino acids for sensitive ^{19}F NMR-based screening and kinetic measurements", *Journal of the American Chemical Society*, Vol.129, No.17, pp.5665–5672.

Peng, C., Unger, S. W., Filipp, F. V, Sattler, M., and Szalma, S., (2004), "Automated evaluation of chemical shift perturbation spectra: New approaches to quantitative analysis of receptor-ligand interaction NMR spectra", *Journal of Biomolecular NMR*, Vol.29, No.4, pp.491–504.

Peng, J. W., (2001), "Cross-correlated 19F relaxation measurements for the study of fluorinated ligand-receptor interactions", *Journal of Magnetic Resonance*, Vol.153, No.1, pp.32–47.

Perez-Martınez, J. I., Gine, J. M., Morillo, E., Gonzalez-Rodriguez, M. L., and Mendez, J. R. M., (2000), "Improvement of the desorption of the pesticide 2 , 4-D via complexation with HP- b -cyclodextrin", *Pest Management Science*, Vol.430, No.August 1999, pp.425–430.

Perminova, I. V., Grechishcheva, N. Y., and Petrosyan, V. S., (1999), "Relationships between structure and binding affinity of humic substances for polycyclic aromatic hydrocarbons: Relevance of molecular descriptors", *Environmental Science and Technology*, Vol.33, No.21, pp.3781–3787.

Piccolo, A., Nardi, S., and Concheri, G., (1996), "Micelle-1ike conformation of humic substances as revealed by size exclusion chromatography", *Chemosphere*, Vol.33, No.4, pp.595–602.

Piccolo, Alessandro, (2001), "The supramolecular structure of humic substances", *Soil Science*, Vol.166, No.11, pp.810–832.

Potenza, J., (1972), "Measurement and applications of dynamic nuclear polarization", *Advances in Molecular Relaxation Processes*, Vol.4, No.3, pp.229–354.

Power, J. E., Foroozandeh, M., Moutzouri, P., Adams, R. W., Nilsson, M., Coombes, S. R., … Morris, G. A., (2016), "Very broadband diffusion-ordered NMR", *Chemical Communications*, Vol.52, pp.6892–6894.

Price, W. S., (2003), "Recent Advances in NMR Diffusion Techniques for Studying Drug Binding", *Australian Journal of Chemistry*, Vol.56, pp.855–860.

Price, W. S., Elwinger, F., Vigouroux, C., and Stilbs, P., (2002), "PGSE-WATERGATE, a new tool for NMR diffusion-based studies of ligand-macromolecule binding", *Magnetic Resonance in Chemistry*, Vol.40, No.6, pp.391–395.

Pylaeva, S., Ivanov, K. L., Baldus, M., Sebastiani, D., and Elgabarty, H., (2017), "Molecular Mechanism of Overhauser Dynamic Nuclear Polarization in Insulating Solids", *Journal of Physical Chemistry Letters*, Vol.8, No.10, pp.2137–2142.

Rabinovitz, M., (1976), "Solute-Solute and Solute-Solvent Interactions: NMR Studies",In B. Pullman (Ed.), *Environmental Effects on Molecular Structure and Properties* (pp. 229–238). Dordrecht: Springer Netherlands.

Radnai, T., Ishiguro, S., and Ohtaki, H., (1989), "Intramolecular and liquid structure of 2,2,2-trifluoroethanol by X-ray diffraction", *Journal of Solution Chemistry*, Vol.18, No.8, pp.771–784.

Rajan, R., and Balaram, P., (1996), "A model for the interaction of trifluoroethanol with peptides and proteins", *International Journal of Peptide and Protein Research*, Vol.48, No.4, pp.328–336.

Raoufinia, R., Mota, A., Keyhanvar, N., Safari, F., Shamekhi, S., and Abdolalizadeh, J., (2016), "Overview of Albumin and Its Purification Methods", *Advanced Pharmaceutical Bulletin*, Vol.6, No.4, pp.495–507.

Redfield, A. G., (1965), "The Theory of Relaxation Processes* *This work was started while the author was at Harvard University, and was then partially supported by Joint Services Contract N5ori-76, Project Order I.",In J. S. Waugh (Ed.), *Advances in Magnetic Resonance* (Vol. 1, pp. 1–32). Academic Press.

Ren, D., Huang, B., Yang, B., Pan, X., and Dionysiou, D. D., (2017), "Mitigating 17 ⎵ -ethynylestradiol water contamination through binding and photosensitization by dissolved humic substances", *Journal of Hazardous Materials*, Vol.327, pp.197–205.

Ren, G., Sun, H., Guo, J., Fan, J., Li, G., and Xu, S., (2019), "Molecular mechanism of the interaction between resveratrol and trypsin via spectroscopy and molecular docking", *Food and Function*, Vol.10, pp.3291–3302.

Renny, J. S., Tomasevich, L. L., Tallmadge, E. H., and Collum, D. B., (2013), "Method of continuous variations: Applications of job plots to the study of molecular associations in organometallic chemistry", *Angewandte Chemie - International Edition*. Vol.52, No.46, pp.11998-201.

Restu, M., (1989), "19F- NMR Study on the Interaction Acid Oxidase of Fluorobenzoate with Porcine", *J. Biochem*, Vol.105, pp.318–322.

Ribeiro, J. P., Diercks, T., Jiménez-Barbero, J., André, S., Gabius, H. J., and Cañada, F. J., (2015), "Fluorinated carbohydrates as lectin ligands:19F-based direct STD monitoring for detection of Anomeric selectivity", *Biomolecules*, Vol.5, No.4, pp.3177–3192.

Rippe, K., (1997), "Analysis of protein-DNA binding at equilibrium", *BIF Futura*, Vol.12, pp.20–26.

Roccatano, D., Colombo, G., Fioroni, M., and Mark, A. E., (2002), "Mechansm by which 2,2,2-trifluoroethanol/water mixtures stabilize secondary-structure formation in peptides : A molecular dynamics study", *Proceedings of the National Academy of Sciences*, Vol.99, No.19, pp.12179–12184.

Ronconi, L., and Sadler, P. J., (2008), "Applications of heteronuclear NMR spectroscopy in biological and medicinal inorganic chemistry", *Coordination Chemistry Reveiws*, Vol.252, pp.2239–2277.

Rüdisser, S. H., Goldberg, N., Olivier, M., Helena, E., and Alvar, K., (2020), "Efficient affinity ranking of fluorinated ligands by 19 F NMR : CSAR and FastCSAR", *Journal of Biomolecular NMR*, , No.0123456789.

Ruiz-Cabello, J., Barnett, B. P., Bottomley, P. A., and Bulte, J. W. M., (2011), "Fluorine (19 F) MRS and MRI in biomedicine", *NMR in Biomedicine*, Vol.24, No.2, pp.114–129.

Rule, G. S., and Hitchens, T. K., (2006), "*Fundamentals of Protein Nmr*" (Focus on structural biology series, Volume 5). Springer Netherlands.

Saadati, M., and Mizrael, M., (2016), "Insecticide-Enzyme Interaction : Cypermethrin , Chlorpyrifos , Diazinon and Deltamethrin with α-Amylase and Lipase in the Gut of Sunn Pest , Eurygaster integriceps", *Biological Systems : Open Access*, Vol.5, No.2, pp.1000168.

Sabadini, E., Do Carmo Egídio, F., Fujiwara, F. Y., and Cosgrove, T., (2008), "Use of water spin-spin relaxation rate to probe the solvation of cyclodextrins in aqueous solutions", *Journal of Physical Chemistry B*, Vol.112, No.11, pp.3328–3332.

Sabouri, Al. A., and Movahedi Ali akbar moosavi, (1994), "Evaluation of the Hill Coefficient from Scatchard and Klotz Plots", *Biochemical Eduaction*, Vol.22, No.1, pp.48–49.

Sahin, C., and Karpuzcu, M. E., (2020), "Mitigation of organophosphate pesticide pollution in agricultural watersheds", *Science of the Total Environment*, Vol.710, pp.136261.

Saielli, G., and Bagno, A., (2010), "Preferential solvation of glucose and talose in water-acetonitrile mixtures: A molecular dynamics simulation study", *Physical Chemistry Chemical Physics*, Vol.12, No.12, pp.2981–2988.

Saint-Fort, R., and Visser, S. A., (1988), "Study of the Interactions Between Atrazine Diazinon and Lindane with Humic Acids of Various Molecular Weights", *Journal of Environmental Science and Health . Part A: Environmental Science and Engineering*, Vol.23, No.6, pp.613–624.

Saito, Y., and Hayano, S., (1981), "Characterization of humic and fulvic acids isolated from marine sediments of Sagami and Suruga Bays with C-13 and proton nuclear magnetic resonance", *Journal of the Oceanographical Society of Japan*, Vol.36, No.6, pp.286–292.

Sakuma, C., Kurita, J. I., Furihata, K., and Tashiro, M., (2015), "Achievement of ^{1}H-^{19}F heteronuclear experiments using the conventional spectrometer with a shared single high band amplifier", *Magnetic Resonance in Chemistry*, Vol.53, No.5, pp.327–329.

Santoke, H., Tong, A. Y. C., Mezyk, S. P., Johnston, K. M., Braund, R., Cooper, W. J., and Peake, B. M., (2011), "UV Photodegradation of Enoxacin in Water : Kinetics and Degradation Pathways", *Journal of environmental engineering*, Vol.141, No.10, pp.2–8.

Sanz-Pérez, E. S., Fernández, A., Arencibia, A., Calleja, G., and Sanz, R., (2019), "Hybrid amine-silica materials: Determination of N content by 29Si NMR and application to direct CO2 capture from air", *Chemical Engineering Journal*, Vol.373, pp.1286–1294.

Saunders, C., Khaled, M. B., Weaver, J. D., and Tantillo, D. J., (2018), "Prediction of 19F NMR Chemical Shifts for Fluorinated Aromatic Compounds", *The Journal of Organic Chemistry*, Vol.83, No.6, pp.3220—3225.

Schiller, J., Muller, M., Fuchs, B., and Huster, K. A. and D., (2007), "31P NMR Spectroscopy of Phospholipids: From Micelles to Membranes", *Current Analytical Chemistry*. Vol.3, No.4, pp.283-301.

Schnitzer, M., (1978), "Chapter 1 Humic Substances: Chemistry and Reactions", *Developments in Soil Science*, Vol.8, No.C, pp.1–64.

Scott, R. L., (1956), "Some comments on the Benesi–Hildebrand equation", *Recueil Des Travaux Chimiques Des Pays-Bas*, Vol.75, pp.787–789.

Sears, D. W., Thompson, S. E., and Saxon, S. R., (2007), "Articles Reversible Ligand Binding Reactions", *Biochemistry and Molecular Biology Education*, Vol.35, No.2, pp.105–118.

Seitz, J. D., Vineberg, J. G., Wei, L., Khan, J. F., Lichtenthal, B., Lin, C., and Ojima, I., (2015), "Design , synthesis and application of fluorine-labeled taxoids as 19 F NMR probes for the metabolic stability assessment of tumor-targeted drug delivery systems", *Journal of Fluorine Chemistry*, Vol.171, pp.148–161.

Sem, D. S., and Pellecchia, M., (2001), "NMR in the acceleration of drug discovery.", *Current Opinion in Drug Discovery & Development*, Vol.4, No.4, pp.479–492.

Sevilla-Morán, B., Sandín-España, P., Vicente-Arana, M. J., Alonso-Prados, J. L., and García-Baudín, J. M., (2008), "Study of alloxydim photodegradation in the presence of natural substances: Elucidation of transformation products", *Journal of Photochemistry and Photobiology A: Chemistry*, Vol.198, No.2–3, pp.162–168.

Shao, Q., Fan, Y., Yang, L., and Qin Gao, Y., (2012), "From protein denaturant to protectant: Comparative molecular dynamics study of alcoholprotein interactions", *Journal of Chemical Physics*, Vol.136, No.11.

Shi, P., Wang, H., Xi, Z., Shi, C., Xiong, Y., and Tian, C., (2011), "Site-specific 19F NMR chemical shift and side chain relaxation analysis of a membrane protein labeled with an unnatural amino acid", *Protein Science*, Vol.20, No.1, pp.224–228.

Shi, W., Wang, Y., Zhang, H., Liu, Z., and Fei, Z., (2017), "Probing deep into the binding mechanisms of folic acid with α-amylase, pepsin and trypsin: An experimental and computational study", *Food Chemistry*. Vol.226, No.1, Pages 128-134.

Shiio, H., and Yoshihashi, H., (1956), "Measurement of the amount of bound water by ultrasonic interferometer. II. Polyvinyl alcohol and its partially substituted acetates", *Journal of Physical Chemistry*, Vol.60, No.8, pp.1049–1051.

Shikii, K., Sakurai, S., Utsumi, H., Seki, H., and Tashiro, M., (2004), "Application of the 19F NMR technique to observe binding of the general anesthetic halothane to human serum albumin.", *Analytical Sciences : The International Journal of the Japan Society for Analytical Chemistry*, Vol.20, No.10, pp.1475–7.

Shiraki, K., Nishikawa, K., and Goto, Y., (1995), "Trifluoroethanol-induced Stabilization of the α-Helical Structure of β-Lactoglobulin: Implication for Non-hierarchical Protein Folding", *Journal of Molecular Biology*, Vol.245, No.2, pp.180–194.

Shirzadi, A., Simpson, M. J., Kumar, R., Baer, A. J., Xu, Y., and Simpson, A. J., (2008a), "Molecular interactions of pesticides at the soil-water interface", *Environmental Science and Technology*, Vol.42, No.15, pp.5514–5520.

Shirzadi, A., Simpson, M. J., Xu, Y., and Simpson, A. J., (2008b), "Application of Saturation Transfer Double Difference NMR to Elucidate the Mechanistic Interactions of Pesticides with Humic Acid", *Environment Science and Technology*, Vol.42, No.4, pp.1084–1090.

Shuai, L., Chen, Z., Fei, P., Wang, Q., and Yang, T., (2014), "Spectroscopic analysis on the interaction of ferulic acid and tetramethylpyrazine with trypsin", *Luminescence*, Vol.29, No.1, pp.79–86.

Si, Y., Zhou, J., Chen, H., Zhou, D., and Yue, Y., (2004), "Effects of humic substances on photodegradation of bensulfuron-methyl on dry soil surfaces", *Chemosphere*, Vol.56, pp.967–972.

Sidhu, P. S., Bell, J., Penner, G. H., and Jeffrey, K. R., (1995), "A deuterium NMR study of guest molecular dynamics of acetone in two organic inclusion compounds", *Canadian Journal of Chemistry*, Vol.73, pp.2196–2207.

Silva, C. P., Lima, D. L. D., Groth, M. B., Otero, M., and Esteves, V. I., (2016), "Effect of natural aquatic humic substances on the photodegradation of estrone", *Chemosphere*, Vol.145, pp.249–255.

Silva, E. F. d., Svendsen, H. F., and Merz, K. M., (2008), "Explicitly Representing the Solvation Shell in Continuum Solvent Calculations", *Journal of Physical Chemistry A*, Vol.23, No.1, pp.1–7.

Sim, S. F., Seng, L., Wong, N. C., Asing, J., Faizal B Md Nor, M., and Satirawaty Bt Mohd Pauzan, A., (2006), "Characterization of the coal derived humic acids from Mukah, Sarawak as soil conditioner", *Journal of the Brazilian Chemical Society*, Vol.17, No.3, pp.582–587.

Simpson, A., (2001), "Multidimensional solution state nmr of humic substances: a practical guide and review", *Soil Science*, Vol.166, No.11, pp.795–809.

Simpson, André J., (2002), "Determining the molecular weight, aggregation, structures and interactions of natural organic matter using diffusion ordered spectroscopy", *Magnetic Resonance in Chemistry*, Vol.40, No.SPEC. ISS., pp.S72–S82.

Simpson, André J., Kingery, W. L., Hayes, M. H., Spraul, M., Humpfer, E., Dvortsak, P., … Hofmann, M.,

(2002), "Molecular structures and associations of humic substances in the terrestrial environment", *Naturwissenschaften*, Vol.89, No.2, pp.84–88.

Simpson, Andre J., Song, G., Smith, E., Lam, B., Novotny, E. H., and Hayes, M. H. B., (2007), "Unraveling the structural components of soil humin by use of solution-state nuclear magnetic resonance spectroscopy", *Environmental Science and Technology*, Vol.41, No.3, pp.876–883.

Simpson, André J, Simpson, M. J., and Soong, R., (2018), "Environmental Nuclear Magnetic Resonance Spectroscopy: An Overview and a Primer", *Analytical Chemistry*, Vol.90, No.1, pp.628–639.

Simpson, M. J., and Simpson, A. J., (2014), "*NMR Spectroscopy A Versatile tool for environmental research*", (M. J. Simpson & A. J. Simpson, Eds.) (Ist). United Kingdom: John Wiley & Sons Ltd.

Simpson, M. J., Simpson, A. J., Gross, D., Spraul, M., and Kingery, W. L., (2007), "1H and 19F nuclear magnetic resonance microimaging of water and chemical distribution in soil columns", *Environmental Toxicology and Chemistry*, Vol.26, No.7, pp.1340–1348.

Simpson, M. J., Simpson, A. J., and Hatcher, P. G., (2004), "Noncovalent interactions between aromatic compounds and dissolved humic acid examined by nuclear magnetic resonance spectroscopy", *Environmental Toxicology and Chemistry*, Vol.23, No.2, pp.355–362.

Sitkoff, D., and Case, D. A., (1998), "Theories of chemical shift anisotropies in proteins and nucleic acids", *Progress in Nuclear Magnetic Resonance Spectroscopy*, Vol.32, No.2, pp.165–190.

Skinner, A. L., and Laurence, J. S., (2008), "High-field Solution NMR Spectroscopy as a Tool for Assessing Protein Interactions with Small Molecule Ligands", *Journal of Pharmaceutical Sciences*, Vol.97, No.11, pp.4670–4695.

Slichter, C. P, (1989), "*Principles of Magnetic Resonance, Third Enlarged and Updated Edition*",*Springer-Verlag: New York* (Vol. 3).

Slichter, Charles P., (2014), "The discovery and renaissance of dynamic nuclear polarization", *Reports on Progress in Physics*, Vol.77, pp.1–15.

Sloop, J. C., (2013), "19-Fluorine nuclear magnetic resonance chemical shift variability in trifluoroacetyl species", *Reports in Organic Chemistry*, Vol.3, pp.1–12.

Šmejkalová, D., and Piccolo, A., (2008a), "Aggregation and disaggregation of humic supramolecular assemblies by NMR diffusion ordered spectroscopy (DOSY-NMR)", *Environmental Science and Technology*, Vol.42, No.3, pp.699–706.

Šmejkalová, D., and Piccolo, A., (2008b), "Host-guest interactions between 2,4-dichlorophenol and humic substances as evaluated by 1H NMR relaxation and diffusion ordered spectroscopy", *Environmental Science and Technology*, Vol.42, No.22, pp.8440–8445.

Šmejkalová, D., Spaccini, R., Fontaine, B., and Piccolo, A., (2009), "Binding of phenol and differently halogenated phenols to dissolved humic matter as measured by NMR spectroscopy", *Environmental Science and Technology*, Vol.43, No.14, pp.5377–5382.

Smernik, R. J., (2005), "A New Way to Use Solid-State Carbon-13 Nuclear Magnetic Resonance Spectroscopy to Study the Sorption of Organic Compounds to Soil Organic Matter", *Journal of Environmental Quality*, Vol.34, No.4, pp.1194–1204.

Smith, A. A., Corzilius, B., Barnes, A. B., Maly, T., and Griffin, R. G., (2012), "Solid effect dynamic nuclear polarization and polarization pathways", *Journal of Chemical Physics*, Vol.136, No.1, pp.015101(1-16).

Solomon, I., (1955), "Relaxation Processes in a System of Two Spins", *Physcial Review*, Vol.99, No.2, pp.559–566.

Soni, S. D., Bhonsle, J. B., and Garcia, G. E., (2014), "Biophysical aspects of cyclodextrin interaction with paraoxon", *Magnetic Resonance in Chemistry*, Vol.52, No.3, pp.111–114.

Spataro, G., Champouret, Y., Florian, P., Coppel, Y., and Kahn, M. L., (2018), "Multinuclear solid-state NMR study: A powerful tool for understanding the structure of ZnO hybrid nanoparticles", *Physical Chemistry Chemical Physics*, Vol.20, No.18, pp.12413–12421.

Srinivas, M., Morel, P. A., Ernst, L. A., Laidlaw, D. H., and Ahrens, E. T., (2007), "Fluorine-19 MRI for Visualization and Quantification of Cell Migration in a Diabetes Model", *Magnetic Resonance in Chemistry*, Vol.734, pp.725–734.

Stefan, M. I., and Le Novère, N., (2013), "Cooperative Binding", *PLoS Computational Biology*, Vol.9, No.6, pp.2–7.

Stejskal, E. O., and Tanner, J. E., (1965), "Spin Diffusion Measurements: Spin Echoes in the Presence of a Time-Dependent Field Gradient", *The Journal of Chemical Physics*, Vol.42, No.1, pp.288–292.

Stetz, M. A., Caro, J. A., Kotaru, S., Yao, X., Marques, B., Valentine, K. G., and Wand, A. J., (2019), "Characterization of internal protein dynamics and conformational entropy by NMR relaxation", *Methods Enzymology*, Vol.615, pp.237–284.

Stilbs, P., (1999), "Diffusion Studied Using NMR Spectroscopy",In J. C. Lindon (Ed.), *Encyclopedia of Spectroscopy and Spectrometry* (pp. 369–375). Oxford: Elsevier.

Stockman, B. J., and Dalvit, C., (2002), "NMR screening techniques in drug discovery and drug design", *Progress in Nuclear Magnetic Resonance Spectroscopy*, Vol.41, No.3–4, pp.187–231.

Strynar, M., Dec, J., Benesi, A., Jones, A. D., Fry, R. A., and Bollag, J.-M., (2004), "Using 19 F NMR Spectroscopy to Determine Trifluralin Binding to Soil", *Environment Science Technology*, Vol.38, No.24, pp.6645–6655.

Sudhamalla, B., Gokara, M., Ahalawat, N., Amooru, D. G., and Subramanyam, R., (2010), "Molecular dynamics simulation and binding studies of beta-sitosterol with human serum albumin and its biological relevance.", *The Journal of Physical Chemistry. B*, Vol.114, No.27, pp.9054–9062.

Sun, X., Bai, J., and Dong, D., (2019), "Influence Factors of Enhanced Photosensitized Degradation of PAHs on Soil Surface Using Humic Acid under UV Irradiation", *Polycyclic Aromatic Compounds*, Vol.0, No.0, pp.1–10.

Sutton, R., and Sposito, G., (2005), "Molecular structure in soil humic substances: The new view", *Environmental Science and Technology*, Vol.39, No.23, pp.9009–9015.

Swallow, S., (2015), "Chapter Two - Fluorine in Medicinal Chemistry", In G. Lawton & Witty, D. R. (Eds.), P*rogress in medicinal chemistry*, (Vol. 54, pp. 65–133). Elsevier.

Swift, R. S., (1999), "Macromolecular properties of soil humic substances: fact, fiction, and opinion", *Soil Science*, Vol.164, No.11, pp.790–802.

Szekely, O., Olsen, G. L., Felli, I. C., and Frydman, L., (2018), "High-Resolution 2D NMR of Disordered Proteins Enhanced by Hyperpolarized Water", *Analytical Chemistry*, Vol.90, No.10, pp.6169–6177.

Takis, P. G., Papavasileiou, K. D., Peristeras, L. D., Melissas, V. S., and Troganis, A. N., (2013), "Probing micro-solvation in "numbers": The case of neutral dipeptides in water", *Physical Chemistry Chemical Physics*, Vol.15, No.19, pp.7354–7362.

Talebpour, Z., Ghassempour, A., Zendehzaban, M., Bijanzadeh, H. R., and Mirjalili, M. H., (2006), "Monitoring of the insecticide trichlorfon by phosphorus-31 nuclear magnetic resonance (31P NMR) spectroscopy", *Analytica Chimica Acta*, Vol.576, No.2, pp.290–296.

Talhout, R., and Engberts, J. B. F. N., (2001), "Thermodynamic analysis of binding of p-substituted benzamidines to trypsin", *European Journal of Biochemistry*, Vol.1560, pp.1554–1560.

Tanner, J. E., (1970), "Use of the Stimulated Echo in NMR Diffusion Studies", *The Jorunal of Chemical Physics*, Vol.52, No.5, pp.2523–2526.

Tanoli, N. U., Tanoli, S. A. K., Ferreira, A. G., Gul, S., and Ul-Haq, Z., (2015), "Evaluation of binding competition and group epitopes of acetylcholinesterase inhibitors by STD NMR, Tr-NOESY, DOSY and molecular docking: An old approach but new findings", *MedChemComm*. Vol.6, pp.1882-1890.

Taubes, G., (1996), "Protein Chemistry: Misfolding the Way to Disease", *Science*, Vol.271, No.5255, pp.1493–1495.

Tengel, T., (2008), "*Studies of Protein Structure, Dynamics and Protein-ligand Interactions using NMR Spectroscopy*",*Umea Universitet*.

Thankamony, A. S. L., Wittmann, J. J., Kaushik, M., and Corzilius, B., (2017), "Dynamic nuclear polarization for sensitivity enhancement in modern solid-state NMR", *Progress in Nuclear Magnetic Resonance Spectroscopy*, Vol.102–103, pp.120–195.

Thomas, P. D., and Dill, K. A., (1993), "Local and nonlocal interactions in globular proteins and mechanisms of alcohol denaturation", *Protein Science*, Vol.2, No.12, pp.2050–2065.

Thordarson, P., (2011), "Determining association constants from titration experiments in supramolecular chemistry", *Chemical Society Reviews*, Vol.40, No.3, pp.1305–1323.

Tirotta, I., Dichiarante, V., Pigliacelli, C., Cavallo, G., Terraneo, G., Bombelli, F. B., … Resnati, G., (2015), "19F magnetic resonance imaging (MRI): From design of materials to clinical applications", *Chemical Reviews*, Vol.115, No.2, pp.1106–1129.

Togni, A., Rosenau, C. P., Jelier, B. J., and Gossert, A. D., (2018), "Exposing the Origins of Irreproducibility in Fluorine NMR Spectroscopy", *Angewandte Chemie International Edition*, Vol.57, pp.1–7.

Tressaud, A., (2019a), "2 - Fluorine, a key element for the 21st century",In A. Tressaud (Ed.), *Fluorine* (Vol. 5, pp. 77–150). Elsevier.

Tressaud, A., (2019b), "Conclusions: What future for fluorine and fluorine products?",In A. Tressaud (Ed.), *Fluorine* (Vol. 5, pp. 241–243). Elsevier.

Tressaud, A., and Haufe, G., (2012), "*Fluorine and Health, Molecular Imaging, Biomedical Materials and Pharmaceuticals*", (T. Alian & G. Haufe, Eds.) (First edit). The Netherlands: Elsevier Radarweg 29, PO Box 211, 1000 AE Amsterdam, The Netherlands Linacre House, Jordan Hill, Oxford 0X2 8DP, UK.

Twum, E. B., Mccord, E. F., Lyons, D. F., and Rinaldi, P. L., (2015), "Multidimensional 19 F NMR Analyses of Terpolymers from Vinylidene Fluoride (VDF) − Hexa fl uoropropylene (HFP) − Tetra fl uoroethylene (TFE)", *Macromolecules*, Vol.48, pp.3563–3576.

Uitz, M., Epp, V., Bottke, P., and Wilkening, M., (2017), "Ion dynamics in solid electrolytes for lithium batteries Probing jump rates and activation energies through time-domain Li NMR", *Journal of Electroceramics (2017)*, Vol.38, pp.142–156.

Ulatowski, F., Dabrowa, K., Bałakier, T., and Jurczak, J., (2016), "Recognizing the Limited Applicability of Job Plots in Studying Host-Guest Interactions in Supramolecular Chemistry", *Journal of Organic Chemistry*. Vol.81, No.5, pp.1746–1756.

Unione, L., Galante, S., Dolores, D., and Ca, F. J., (2014), "NMR and molecular recognition . The application of ligand-based NMR methods to monitor molecular interactions", *MedChemComm*, pp.1280–1289.

Upadhyay, S. K., and Kumar, G., (2009), "NMR and molecular modelling studies on the interaction of fluconazole with β-cyclodextrin", *Chemistry Central Journal*, Vol.3, No.1, pp.1–9.

Uyguner, C. S., Hellriegel, C., Otto, W., and Larive, C. K., (2004), "Characterization of humic substances: Implications for trihalomethane formation", *Analytical and Bioanalytical Chemistry*, Vol.378, No.6, pp.1579–1586.

Varga, B., Kiss, G., Galambos, I., Gelencser, A., Hlavay, J., and Krivacsy, Z., (2000), "Secondary Structure of Humic Acids . Can Micelle-like Conformation Be Proved by Aqueous Size Exclusion Chromatography ?", *Environment Science Technology*, Vol.34, No.15, pp.3303–3306.

Vasile, F., Della Volpe, S., Ambrosio, F. A., Costa, G., Unver, M. Y., Zucal, C., … Collina, S., (2018), "Exploration of ligand binding modes towards the identification of compounds targeting HuR: a combined STD-NMR and Molecular Modelling approach", *Scientific Reports*, Vol.8, No.1, pp.13780-95.

Vazquez, L., and Gauri, M., (2019), "Nuclear Magnetic Resonance",In G. Misra (Ed.), *Data Processing Handbook for Complex Biological Data Sources* (pp. 53–76). Academic Press.

Veil, S., Mannina, L., and Segre, A., (2002), "Detection of a p-p complex by diffusion-ordered spectroscopy\r(DOSY)", *Tetrahedron Letters*, Vol.43, pp.2515–2519.

Venturini, D., De Souza, A. R., Caracelli, I., Morgon, N. H., Da Silva-Filho, L. C., and Ximenes, V. F., (2017), "Induction of axial chirality in divanillin by interaction with bovine serum albumin", *PLoS ONE*, Vol.12, No.6, pp.1–25.

Verbeeck, R. K., Boel, A., Buntinx, A., and De Schepper, P. J., (1980), "Plasma protein binding and interaction studies with diflunisal, a new salicylate analgesic", *Biochemical Pharmacology*, Vol.29, No.4, pp.571–576.

Veronesi, M., and Dalvit, C., (2008), "19F NMR Spectroscopy for Functional and Binding High-Throughput Screening",In G. A. Webb (Ed.), *Modern Magnetic Resonance* (pp. 1393–1399). Dordrecht: Springer.

Viefhaus, T., Bolse, T., and Müller, K., (2006), "Oxygen ion dynamics in yttria-stabilized zirconia as evaluated by solid-state 17O NMR spectroscopy", *Solid State Ionics*, Vol.177, No.35, pp.3063–3068.

Viegas, A., Manso, J., Nobrega, F. L., and Cabrita, E. J., (2011), "Saturation-transfer difference (STD) NMR: A simple and fast method for ligand screening and characterization of protein binding", *Journal of Chemical Education*, Vol.88, No.7, pp.990–994.

Villaverde, J., Morillo, E., Pérez-Martínez, J. I., Ginés, J. M., and Maqueda, C., (2004), "Preparation and Characterization of Inclusion Complex of Norflurazon and β-Cyclodextrin To Improve Herbicide Formulations", *Journal of Agricultural and Food Chemistry*, Vol.52, No.4, pp.864–869.

Vishnyakov, A., and Laaksonen, A., (2000), "Carbohydrates Exhibit a Distinct Preferential solvation pattern in binary aqueous solvent mixtures", *Angewantde Chemie- International Edition English*, Vol.112, No.1, pp.144–146.

Vlahov, G., (1999), "Application of NMR to the study of olive oils", *Progress in Nuclear Magnetic Resonance Spectroscopy*, Vol.35, No.4, pp.341–357.

Vuichoud, B., Bornet, A., de Nanteuil, F., Milani, J., Canet, E., Ji, X., … Bodenhausen, G., (2016), "Filterable Agents for Hyperpolarization of Water, Metabolites, and Proteins", *Chemistry - A European Journal*, Vol.22, No.41, pp.14696–14700.

Wagstaff, J. L., Taylor, S. L., and Howard, M. J., (2013), "Recent developments and applications of saturation transfer difference nuclear magnetic resonance (STD NMR) spectroscopy", *Molecular BioSystems*, Vol.9, No.571, pp.571–577.

Wandruszka, V. R., Ragle, C., and Engebretson, R., (1997), "The role of selected cations in the formation of pseudomicelles in aqueous humic acid", *Talanta*, Vol.44, No.5, pp.805–809.

Wandruszka, R. Von, (1998), "The micellar model of Humic Acid: Evidence from pyrene fluorescence measurements", *Soil Science*, Vol.163, No.12, pp.921–930.

Wandruszka, R. Von, (2000), "Humic acids : Their detergent qualities and potential uses in pollution remediation", *Geochemical Transactions*, Vol.1, pp.10-15.

Wang, J., Sachez-Rosello, M., Acen, J., del Pozo, C., Sorochinsky, A. E., Fustero, S., … Liu, H., (2014), "Fluorine in Pharmaceutical Industry: Fluorine-Containing Drugs Introduced to the Market in the Last Decade (2001−2011)", *Chemical Reviews*, Vol.114, pp.2342–2506.

Wang, M., Gao, M., Miller, K. D., and Zheng, Q. H., (2013), "Synthesis of 2,6-difluoro-N-(3-[11C]methoxy-1H-pyrazolo[3,4-b] pyridine-5-yl)-3-(propylsulfonamidio)benzamide as a new potential PET agent for imaging of B-RafV600E in cancers", *Bioorganic and Medicinal Chemistry Letters*, Vol.23, No.4, pp.1017–1021.

Wang, Yu Sen, Liu, D., and Wyss, D. F., (2004), "Competition STD NMR for the detection of high-affinity ligands and NMR-based screening", *Magnetic Resonance in Chemistry*, Vol.42, No.6, pp.485–489.

Wang, W., Niu, J., and Yang, Z., (2020), "An efficient reduction of unsaturated bonds and halogen-containing groups by nascent hydrogen over Raney Ni catalyst", *Journal of Hazardous Materials*, Vol.389, pp.121912.

Wang, Y. Q., Zhang, H. M., Kang, Y. J., Gu, Y. L., and Cao, J., (2016), "Mechanism of curcumin-induced trypsin inhibition: Computational and experimental studies", *Journal of Molecular Structure*. Vol.1107, pp.91-98.

Wang, Yan-qing, and Zhang, H., (2014), "Effects of Bisphenol S on the Structures and Activities of Trypsin and Pepsin", *Journal of Agricultural and Food Chemistry*, Vol.62, No.46, pp.11303–11311.

Wang, Yaping, Zhang, G., and Wang, L., (2015), "Potential toxicity of phthalic acid esters plasticizer: Interaction of dimethyl phthalate with trypsin in vitro", *Journal of Agricultural and Food Chemistry*, Vol.63, No.1, pp.75–84.

Wangsness, R. K., and Bloch, F., (1953), "The dynamical theory of nuclear induction", *Physical Review*, Vol.89, No.4, pp.728–739.

Webster, G. K., (2014), "Expanding the Analytical Toolbox: Pharmaceutical Application of Quantitative NMR", *Analytical Chemistry*, Vol.86, No.23, pp.11474–11480.

Weiss-Errico, M. J., Ghiviriga, I., and O'Shea, K. E., (2017), "19F NMR Characterization of the Encapsulation of Emerging Perfluoroethercarboxylic Acids by Cyclodextrins", *Journal of Physical Chemistry B*, Vol.121, No.35, pp.8359–8366.

Weissenfels, W. D., Klewer, H.-J., and Langhoff, J., (1992), "Adsorption of polycyclic aromatic hydrocarbons (PAHs) by soil particles: influence on biodegradability and biotoxicity", *Applied Microbiology and Biotechnology*, Vol.36, No.5, pp.689–696.

Welte, H., Zhou, T., Mihajlenko, X., and Mayans, O., (2020), "What does fluorine do to a protein ? Thermodynamic , and highly- resolved structural insights into fluorine-labelled variants of the cold shock protein", *Scientific Reports*, Vol.10, pp.1–12.

Wen, X., Tan, F., Jing, Z., and Liu, Z., (2004), "Preparation and study the 1:2 inclusion complex of carvedilol with β-cyclodextrin", *Journal of Pharmaceutical and Biomedical Analysis*, Vol.34, No.3, pp.517–523.

Wenk, J., Eustis, S. N., Mcneill, K., and Canonica, S., (2013), "Quenching of Excited Triplet States by Dissolved Natural Organic Matter", Vol.47, No.22, pp.12802–12810.

Wershaw, R. L., (1994), "Membrane-micelle model for humus in soils and sediments and its relation to humification", *US Geological Survey Water-Supply Paper*, Vol.2410.

Wescott, C. R., and Klibanov, A. M., (1994), "The solvent dependence of enzyme specificity", *Biochimica et Biophysica Acta (BBA) - Protein Structure and Molecular Enzymology*, Vol.1206, No.1, pp.1–9.

Wilcox, W., and Eisenberg, D., (1992), "Thermodynamics of melittin tetramerization determined by circular dichroism and implications for protein folding", *Protein Science*, Vol.1, pp.641–653.

Wilhelms, F., and Normant, A. W., (1985), "Biochemical Characterization of Positive Cooperativity in the Binding of 1,25-Dihydroxyvitamin D3 to Its Chick Intestinal Chromatin Receptor*", *The Journal of Biological Chemistry*, Vol.260, No.18, pp.10087–10092.

Williamson, M. P., (2013), "Progress in Nuclear Magnetic Resonance Spectroscopy Using chemical shift perturbation to characterise ligand binding", *Progress in Nuclear Magnetic Resonance Spectroscopy*, Vol.73, pp.1–16.

Wilson, L. D., and Verrall, R. E., (1998), "19F and 1H NMR investigation of cyclodextrin/fluorocarbon alkyl carboxylate surfactant inclusion complexes", *Langmuir*, Vol.14, No.17, pp.4710–4717.

Wimmer, R., Aachmann, F. L., Larsen, K. L., and Petersen, S. B., (2002), "NMR diffusion as a novel tool for measuring the association constant between cyclodextrin and guest molecules", *Carbohydrate Research*, Vol.337, pp.841–849.

Wind R. A; Duijvestijn, M. J. V. D. L. C. M. A. Vr. J., (1985), "Applications of dynamic nuclear polarization in 13C NMR in solids", *Progress in Nuclear Magnetic Resonance Spectroscopy*, Vol.17, pp.33–67.

Wolf, D., (1979), "*Spin-temperature and nuclear-spin relaxation in matter : basic principles and applications*".

Oxford : Clarendon press.
Wu, D. H., Chen, A., and Johnson, C. S., (1995), "An Improved Diffusion-Ordered Spectroscopy Experiment Incorporating Bipolar-Gradient Pulses", *Journal of Magnetic Resonance, Series A*.,Vol.115, No.2, pp.260-264.
Wu, Z., Huang, F., Chen, Y., Xu, H., Meti, M. D., Fan, Y., … Hu, Z., (2018), "Conformation change of trypsin induced by acteoside as studied using multiple spectroscopic and molecular docking methods", *International Journal of Food Properties*. Vol.21, No.1, pp.301-312.
Wu, Z., Shen, L., Han, Q., Lu, J., Tang, H., Xu, X., … Hu, Z., (2017), "Mechanism and Nature of Inhibition of Trypsin by Ligupurpuroside A, a Ku-Ding Tea Extract, Studied by Spectroscopic and Docking Methods", *Food Biophysics*. Vol.12, No.1, pp.78–87.
Xing, H., Lin, S. S., Yan, P., Xiao, J. X., and Chen, Y. M., (2007), "NMR studies on selectivity of β-cyclodextrin to fluorinated/ hydrogenated surfactant mixtures", *Journal of Physical Chemistry B*, Vol.111, No.28, pp.8089–8095.
Xu, J., Zhao, B., Li, Z., Chu, W., Mao, J., Olk, D. C., … Wei, W., (2019), "Demonstration of chemical distinction among soil humic fractions using quantitative solid-state 13C NMR", *Journal of Agricultural and Food Chemistry*, Vol.67, No.29, pp.8107–8118.
Xu, Y., Tang, P., Firestone, L., and Zhang, T. T., (1996), "19F Nuclear Magnetic Resonance Investigation of Stereoselective Binding of Isoflurane to Bovine Serum Albumin Xb)", Vol.70, pp.532–538.
Yang, F., Ma, Z. Y., Zhang, Y., Li, G. Q., Li, M., Qin, J. K., … Liang, H., (2013), "Human serum albumin-based design of a diflunisal prodrug", *European Journal of Pharmaceutics and Biopharmaceutics*, Vol.84, No.3, pp.549–554.
Yen, J. H., Lin, K. H., and Wang, Y. S., (2000), "Potential of the insecticides acephate and methamidophos to contaminate groundwater", *Ecotoxicology and Environmental Safety*, Vol.45, No.1, pp.79–86.
Yu, J. X., Hallac, R. R., Chiguru, S., and Mason, R. P., (2013), "New frontiers and developing applications in 19F NMR", *Progress in Nuclear Magnetic Resonance Spectroscopy*, Vol.70, No.214, pp.25–49.
Yu, Z., Li, P., and Merz, K. M., (2017), "Using Ligand-Induced Protein Chemical Shift Perturbations To Determine Protein–Ligand Structures", *Biochemistry*, Vol.56, No.18, pp.2349–2362.
Yuan, P., Fisher, P. J., Franklyn, G., and Kemple, M. D., (1996), "Structure and Dynamics of Melittin in Lysomyristoyl Phosphatidylcholine Micelles Determined by Nuclear Magnetic Resonance", *Biophysical Journal*, Vol.70, pp.2223–2238.
Zang, X., Van Heemst, J. D. H., Dria, K. J., and Hatcher, P. G., (2000), "Encapsulation of protein in humic acid from a histosol as an explanation for the occurrence of organic nitrogen in soil and sediment", *Organic Geochemistry*, Vol.31, No.7–8, pp.679–695.
Zhang, G., and Hilty, C., (2018), "Applications of dissolution dynamic nuclear polarization in chemistry and biochemistry", *Magnetic Resonance in Chemistry*, Vol.56, No.7, pp.566–582.
Zhang, H., Cao, J., Wu, S., and Wang, Y., (2014), "Mechanism of gold nanoparticles-induced trypsin inhibition: A multi-technique approach", *Molecular Biology Reports*. Vol.41, No.8, pp.4911-8.
Zhang, S., Chen, J., and Wang, Y., (2012), "Humic acids decrease the photodegradation of the sunscreen UV filter 2-phenylbenzimidazole-5-sulfonic acid in natural waters", *Environmental Chemistry Letters*, Vol.10, pp.389–394.
Zhao, R., Sandström, C., Zhang, H., and Tan, T., (2016), "NMR Study on the Inclusion Complexes of β-Cyclodextrin with Isoflavones", *Molecules*, Vol.21, No.4, pp.1–11.
Zhao, Xi, Farajtabar, A., Han, G., and Zhao, H., (2020), "Phenformin in aqueous co-solvent mixtures of N , N -dimethylformamide , ethanol , N -methylpyrrolidone and dimethyl sulfoxide : Solubility , solvent effect and preferential solvation", *The Journal of Chemical Thermodynamics*, Vol.144, No.114, pp.106085.
Zhao, Xiating, Hu, Z., Yang, X., Cai, X., Wang, Z., and Xie, X., (2019), "Noncovalent interactions between fl uoroquinolone antibiotics with dissolved organic matter : A 1 H NMR binding site study and multi-spectroscopic methods", *Environmental Pollution*, Vol.248, pp.815–822.
Zhou, P., Zou, J., Tian, F., and Shang, Z., (2009), "Fluorine Bonding s How Does It Work In Protein - Ligand Interactions ?", *Journal of Chemical Information and Modeling*, Vol.49, pp.2344–2355.
Zhou, Y., Wang, J., Gu, Z., Wang, S., Zhu, W., Acenã, J. L., … Liu, H., (2016), "Next Generation of Fluorine-Containing Pharmaceuticals, Compounds Currently in Phase II-III Clinical Trials of Major Pharmaceutical Companies: New Structural Trends and Therapeutic Areas", *Chemical Reviews*, Vol.116, No.2, pp.422–518.
Zhu, L., Yang, J., Li, H., Sun, H., Liu, J., and Wang, J., (2015), "Conformational change study of dengue virus NS2B-NS3 protease using 19 F NMR spectroscopy", *Biochemical and Biophysical Research Communications*, Vol.461, pp.677–680.
Zhuang, J., Yang, D.-P., Nikas, S. P., Zhao, J., Guo, J., and Makriyannis, A., (2013a), "The interaction of fatty acid amide hydrolase (FAAH) inhibitors with an anandamide carrier protein using (19)F-

NMR.", *The American Association of Pharmaceutical Scientists Journal*, Vol.15, No.2, pp.477–82.
Zhuang, J., Yang, D.-P., Tian, X., Nikas, S. P., Sharma, R., and Guo, Jason Jianxin Makriyannis, A., (2013b), "Targeting the Endocannabinoid System for Neuroprotection: A 19 F-NMR Study of a Selective FAAH Inhibitor Binding with an Anandamide Carrier Protein, HSA", *Journal Pharmacy and Pharmacology*, Vol.1, No.1. pp.002.

...

Publications

Peer reviewed International Journals (Published)

1) **Chaubey, B.,** Singh, P. & Pal, S. Solution State NMR evaluation of molecular interaction between monoaromatic Carboxylic Acids and dissolved Humic Acid. *Environment Science and Pollution Research*, **2020**, december. https://doi.org/10.1007/s11356-020-12092-1 (just accepted).
2) **Chaubey, B.**, Narawal, P., Khandelwal, A. & Pal, S. Aqueous photo-degradation of Flupyradifurone (FPD) in presence of a natural Humic Acid (HA): A quantitative solution state NMR analysis. *Photochemistry and Photobiology A: Chemistry*, **2020,** *405 (2021), 2020, 112986*.
3) **Chaubey, B.**, Dey, A., Banerjee, A., Chandrakumar, N. & Pal, S. Assessment of TFE solvent dynamics inducing conformational transitions in Melittin: An approach with solvent ^{19}F low field NMR relaxation and Overhauser DNP studies. *Journal of Physical Chemistry B*., 124 (28), **2020**, 5993–6003.
4) **Chaubey, B.**, & Pal, S. Binding Interaction of Organofluorine−Serum Albumin: A Comparative Ligand-Detected ^{19}F NMR Analysis. *Journal of Physical Chemistry B.* 122(40), **2018**, 9409−9418.

Peer reviewed International Journals (Under preparation)

1) **Chaubey, B.**, Chandrakumar, N. & Pal, S. Preferential solvation of carbohydrates in water-trifluoroethanol mixtures: A solvent detected heteronuclear NMR approach. <u>To be submitted</u> in *Physical Chemistry Chemical Physics*, **2021**.

Peer reviewed International Conference proceedings (Published)

1) **Chaubey, B.**, & Pal, S. Hexaflumuron_β-Cyclodextrin Inclusion Complex as Improved Pesticide Formulation: A NMR Case Study. *AIP Conference Proceedings*. 2142, **2019**, 180003(1) –180003(4).

Peer reviewed International Journals <u>not part of the Thesis</u> (Published)

1) Vandana, **Chaubey, B.**, Dhaharwal, A. K., & Pal, S. Solvent-dependent binding interactions of the organophosphate pesticide, chlorpyrifos (CPF), and its metabolite, 3,5,6- trichloro-2-pyridinol (TCPy), with Bovine Serum Albumin (BSA): A comparative fluorescence quenching analysis. *Pesticide Biochemistry and Physiology*, 139, **2017**, 92-100.
2) Padmapriya, S., Harinipriya, S., Sudha, V., Kumar, D., Pal, S., & **Chaubey, B.** Polyaniline coated copper for hydrogen storage and evolution in alkaline medium. *International Journal of Hydrogen Energy*. 42(32), **2017**, 20453-20462.

Conferences without proceedings

1) **Chaubey, B.,** Chandrakumar, N. & Pal, S., (<u>Poster</u>) "Preferential solvation of carbohydrates in water – trifluoroethanol mixtures: A solvent detected heteronuclear NMR approach" at EUROMAR, 2020 on-line meeting (7-8 December 2020):
2) **Chaubey, B.**, Dey, A., Banerjee, A., Chandrakumar, N. & Pal, S. (<u>Poster</u>) "Solvation and Structural Transition of Melittin in Trifluoroethanol/Water: A NMR relaxometry and DNP Study" at Small Molecule NMR conference (SMASH **2019**), Porto, Portugal.
3) **Chaubey, B.**, Dey, A., Banerjee, A., Chandrakumar, N. & Pal, S. (<u>Poster</u>) "Structural transition of aqueous Melittin in presence of Trifluoroethanol: A NMR relaxometry and DNP Study" at ISMAR EUROMAR JOINT Conference (EUROISMAR **2019**) held at Berlin, Germany.

4) **Chaubey, B.** & Pal, S. (Oral) "Quantitative Investigation of Interaction between Aqueous Humic Acid and 2, 6 Difluorobenzoic Acid by ^{19}F & ^{1}H NMR Spectroscopy' at Conference on Magnetic Resonance in Medicine & 25th National Magnetic Resonance Society Meeting (NMRS-**2019**) organized by AIIMS and INSA, New Delhi.
5) **Chaubey, B.** & Pal, S. (Oral) 'Structural transition of aqueous Melittin in presence of Trifluoroethanol: A NMR relaxometry approach" at 3rd North-West Meeting on Spectroscopy, Structure and Dynamics organized by IIT Roorkee, **2019.**
6) **Chaubey, B.** & Pal, S. (Poster) 'Hexaflumuron_β-Cyclodextrin Inclusion Complex as Improved Pesticide Formulation: A NMR Case Study" at International Conference on Advances in Basic Sciences **2019** (AIP conference proceedings) at Bahal, India**.**
7) **Chaubey, B.**, Kumar, D. & Pal, S. (Poster) "Binding interaction of 2,6 Difluorobenzoic acid(DFBA)- Bovine Serum Albumin(BSA):A solution state 19F NMR transverse relaxation and diffusion analysis" at 7th Asia Pacific NMR Symposium & 23rd Annual Meeting of NMRS-India (APNMR-**2017**) organized by Department of Chemistry, Indian Institute of Science Bangalore.
8) **Chaubey, B.**, Participated in "22nd Conference of National Magnetic Resonance Society of India (NMRS-**2016**)" at Department of Chemistry, Indian Institute of Technology Kharagpur.

…