CURRICULUM VITAE



NAME : Prof Rajesh Kumar Singh

DESIGNATION : Professor **DEPARTMENT** : Chemistry

SPECIALIZATION: Organic chemistry

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BLOOD GROUP : A^+

QUALIFICATION DETAILS

S.NO.	QUALIFICATION	NAME OF UNIVERSITY	PASSING YEAR
1	Ph.D.	DR R M L Avadh University Faizabad	1994
2	M.Sc.	DR R M L Avadh University Faizabad	1988
3	B.Sc.	DR R M L Avadh University Faizabad	1984

POSITIONS HELD

S.NO.	EMPLOYER	DESIGNATION	DATE FROM	DATE TO
1	Secretary Committee of Management MLK PG College Balrampur	Astt Professor	03/02/1989	31/12/2005
2	Secretary Committee of Management MLK PG College Balrampur	Associate Professor	01/01/2006	31/10/2021
3	Secretary Committee of Management MLK PG College Balrampur	Professor	01/11/2021	Till Date

ACADEMIC DETAILS

Significant Publications and Articles

S.NO.	TITLE	JOURNAL	VOLUME / ISSUE	YEAR
1	Molecular Mechanics Based Study	Asian Journal of	19/1	2007
	of Molecular Orbitals of Cobalt (II)	Chemistry		
	Halides	•		
2	Hydrophobic, Topological and	Organic	4/4	2008
	Steric Parameter Based QSAR	Chemistry (An		
	Study on Peptidic HIV-Protease	Indian Journal)		
	Inhibitors			
3	Molecular Descriptor based	Organic	4/6	2008
	Comparative QSTR Study of	Chemistry(An		
	Saturated Alcohol Derivatives	Indian Journal)		
4	Quantitative Relation Between Bio	Organic	6/3	2010
	Concentration Factor (BCF) and	Chemistry (An		
	Molecular Structure of a Series of	Indian Journal)		
	Organic Compounds			
5	Quantitative Structure Toxicity	Organic	4/2	2008
	Relation (QSTR) Study on Series of	Chemistry(An		
	Aliphatic Alcohol Derivatives	Indian Journal)		
6	Study of the Forces Governing the	Organic	4/6	2008
	Drug-Receptor Interaction of	Chemistry(An		
	Tetrahydroimidazepinones(HIV-I-	Indian Journal)		
	NNRTI)- A Theoretical Formalism			
7	PM3 Based Quantitative Structure	Organic	4/5	2008
	Activity Relationship (QSAR)	Chemistry(An		
	Study on Aziridine Derivatives	Indian Journal)		
8	Hydrophobic, Polar and Hydrogen	American	4/3	2008
	Bonding Based Drug-Receptor	Journal of		
	Interaction of	Immunology		
	Tetahydroimidazobenzidiazepinones			
9	Comparative QSTR Study of a	International J.	109/2	2009

	Series of Alcohol Derivatives	of Quantum		
	Against Tetrahymena pyriformis	Chemistry		
10	Drug –Receptor Interaction Based	International J.	109/6	2009
	Structure Activity Relationship of	of Quantum		
	Tetrahydroimidazodiazepinone	Chemistry		
11	Comparative QSTR Study of	Medicinal	18	2009
	Saturated Alcohols Based on	Chemistry		
	Topological, Constitutional,	Research		
	Geometrical and Getaway			
	Descriptors			
12	Prediction of Bioconcentration	CLEAN	37/11	2009
	Factor of Organic Compounds in			
	Fish			
13	QSAR Study Interaction Between	International	1/4	2009
	Estrogen Derivative and Receptor	Journal of		
	Amino Acids Using Softness	ChemTech		
	Parameters	Research		
14	PM3 Based Calculations of	Organic	5/3	2009
	Interaction Energy Between	Chemistry (An		
	Metalloproteinases and	Indian Journal)		
	Hydroxamate Inhibitors			
15	DFT Based Study of charge	Journal of	2/4	2010
	Transfer and Interaction Energy	Chemical and		
	Between Tin(Iv) halides and	Pharmaceutical		
	Derivatives of Pyridine	Research		
16	Quantum-chemical energy	Journal of	18	2011
	descriptor QSAR study of peptidic	Applied		
	HIV-1 protease inhibitors	Chemical		
		Research		
17	Interaction energy-based durg-	International J.	111	2011
	receptor interaction study of metal-	of Quantum		
	bicyclam complexes	Chemistry		
18	DFT Based Study of charge	Journal of	2/1	2011
	Transfer and Interaction Energy	Chemical		

and Derivatives of Pyridine. 19 DFT based study of interaction between frontier orbitals of transition metal halides and thiomides 20 Valence connectivity indices and shape indices based study of Testosterone derivatives as SHBG ligand 21 Rating of sweetness by molar refractivity and ionization potential-QSAR study of Sucrose and guanidine derivatives 22 Topological and Quantum chemical descriptors based comparative Quantitative Structure Activity Relationship of benzothiazole derivatives 23 Quantitative Structure Activity Relationship study of benzene Sulfonamides as inhibitors of Carbonic anhydrase based on Quantum chemical Descriptors 24 Comparative Study of interaction of benzene sulfonamides with Znmetal,Zn2+-ion and Carbonic anhydrase(Zn2+CA) 25 Quantum Mechanical Study of nOCB Liquid Crystals molecules 26 A Theoretical Perspective of J. Of Scientific 9/10 2020		Between Phenyl Tin(Iv) Chlorides	Biological and		
between frontier orbitals of transition metal halides and thiomides 20 Valence connectivity indices and shape indices based study of Testosterone derivatives as SHBG ligand 21 Rating of sweetness by molar refractivity and ionization potential-QSAR study of sucrose and guanidine derivatives 22 Topological and Quantum chemical descriptors based comparative Quantitative Structure Activity Relationship of benzothiazole derivatives 23 Quantitative Structure Activity Relationship study of benzene Sulfonamides as inhibitors of Carbonic anhydrase based on Quantum chemical Descriptors 24 Comparative Study of interaction of benzene sulfonamides with Znmetal,Zn2+-ion and Carbonic anhydrase(Zn2+-CA) 25 Quantum Mechanical Study of nOCB Liquid Crystals molecules 26 A Theoretical Perspective of J. Of Scientific 9/10 2020		and Derivatives of Pyridine.	Physical sciences		
transition metal halides and thiomides 20 Valence connectivity indices and shape indices based study of Testosterone derivatives as SHBG ligand 21 Rating of sweetness by molar refractivity and ionization potential-QSAR study of sucrose and guanidine derivatives 22 Topological and Quantum chemical descriptors based comparative Quantitative Structure Activity Relationship of benzothiazole derivatives 23 Quantitative Structure Activity Relationship study of benzene Sulfonamides as inhibitors of Carbonic anhydrase based on Quantum chemical Descriptors 24 Comparative Study of interaction of benzene sulfonamides with Znmetal,Zn2+-ion and Carbonic anhydrase(Zn2+-CA) 25 Quantum Mechanical Study of noCB Liquid Crystals molecules 26 A Theoretical Perspective of J. Of Scientific 9/10 2020	19	DFT based study of interaction	International	3/3	2011
thiomides Research Valence connectivity indices and shape indices based study of Testosterone derivatives as SHBG ligand 21 Rating of sweetness by molar refractivity and ionization potential-QSAR study of sucrose and guanidine derivatives 22 Topological and Quantum chemical descriptors based comparative Quantitative Structure Activity Relationship of benzothiazole derivatives 23 Quantitative Structure Activity Journal of Carbonic anhydrase based on Quantum chemical Sulfonamides as inhibitors of Carbonic anhydrase based on Quantum chemical Descriptors Design 24 Comparative Study of interaction of benzene sulfonamides with Znmetal,Zn2+-ion and Carbonic anhydrase (Zn2+-CA) Research 25 Quantum Mechanical Study of nOCB Liquid Crystals molecules and Computational Science 26 A Theoretical Perspective of J. Of Scientific 9/10 2020		between frontier orbitals of	Journal of		
20		transition metal halides and	ChemTech		
shape indices based study of Testosterone derivatives as SHBG ligand 21 Rating of sweetness by molar refractivity and ionization potential-QSAR study of sucrose and guanidine derivatives 22 Topological and Quantum chemical descriptors based comparative Quantitative Structure Activity Relationship of benzothiazole derivatives 23 Quantitative Structure Activity Relationship study of benzene Sulfonamides as inhibitors of Carbonic anhydrase based on Quantum chemical Descriptors 24 Comparative Study of interaction of benzene sulfonamides with Znmetal,Zn2+-ion and Carbonic anhydrase(Zn2+CA) 25 Quantum Mechanical Study of noCB Liquid Crystals molecules 26 A Theoretical Perspective of J. Of Scientific 9/10 2020		thiomides	Research		
Testosterone derivatives as SHBG ligand 21 Rating of sweetness by molar refractivity and ionization potential-QSAR study of sucrose and guanidine derivatives 22 Topological and Quantum chemical descriptors based comparative Quantitative Structure Activity Relationship of benzothiazole derivatives 23 Quantitative Structure Activity Relationship study of benzene Sulfonamides as inhibitors of Carbonic anhydrase based on Quantum chemical Descriptors 24 Comparative Study of interaction of benzene sulfonamides with Znmetal,Zn2+-ion and Carbonic anhydrase (Zn2+-CA) Research 25 Quantum Mechanical Study of Information anhydrase (Zn2+-CA) Research 26 A Theoretical Perspective of J. Of Scientific 9/10 2020	20	Valence connectivity indices and	Research Journal	3/5	2013
South African Fractivity and ionization potential refractivity and ionization potential QSAR study of sucrose and guanidine derivatives Quantidative Structure Activity Relationship of benzothiazole derivatives Quantitative Structure Activity Relationship study of benzene Sulfonamides as inhibitors of Carbonic anhydrase based on Quantum chemical Descriptors Design		shape indices based study of	of Chemical		
21 Rating of sweetness by molar refractivity and ionization potential-QSAR study of sucrose and guanidine derivatives 22 Topological and Quantum chemical descriptors based comparative Quantitative Structure Activity Relationship of benzothiazole derivatives 23 Quantitative Structure Activity Relationship study of benzene Sulfonamides as inhibitors of Carbonic anhydrase based on Quantum chemical Descriptors 24 Comparative Study of interaction of benzene sulfonamides with Znmetal,Zn2+-ion and Carbonic anhydrase(Zn2+-CA) Research 25 Quantum Mechanical Study of Descriptors Design 26 A Theoretical Perspective of J. Of Scientific 9/10 2020		Testosterone derivatives as SHBG	sciences		
refractivity and ionization potential-QSAR study of sucrose and guanidine derivatives 22 Topological and Quantum chemical descriptors based comparative Quantitative Structure Activity Relationship of benzothiazole derivatives 23 Quantitative Structure Activity Relationship study of benzene Sulfonamides as inhibitors of Carbonic anhydrase based on Quantum chemical Descriptors 24 Comparative Study of interaction of benzene sulfonamides with Znmetal,Zn2+-ion and Carbonic anhydrase(Zn2+-CA) 25 Quantum Mechanical Study of nOCB Liquid Crystals molecules 26 A Theoretical Perspective of J. Of Scientific 9/10 2020		ligand			
QSAR study of sucrose and guanidine derivatives 22 Topological and Quantum chemical descriptors based comparative Quantitative Structure Activity Relationship of benzothiazole derivatives 23 Quantitative Structure Activity Relationship study of benzene Sulfonamides as inhibitors of Carbonic anhydrase based on Quantum chemical Descriptors 24 Comparative Study of interaction of benzene sulfonamides with Znmetal,Zn2+-ion and Carbonic anhydrase(Zn2+-CA) 25 Quantum Mechanical Study of nOCB Liquid Crystals molecules 26 A Theoretical Perspective of J. Of Scientific 9/10 2020	21	Rating of sweetness by molar	South African	67	2014
guanidine derivatives 22 Topological and Quantum chemical descriptors based comparative Quantitative Structure Activity Pharmaceutical Research derivatives 23 Quantitative Structure Activity Relationship of benzene Sulfonamides as inhibitors of Carbonic anhydrase based on Quantum chemical Descriptors 24 Comparative Study of interaction of benzene sulfonamides with Znmetal, Zn2+-ion and Carbonic anhydrase(Zn2+-CA) 25 Quantum Mechanical Study of nOCB Liquid Crystals molecules 26 A Theoretical Perspective of J. Of Scientific 9/10 2020		refractivity and ionization potential-	Journal of		
Topological and Quantum chemical descriptors based comparative Quantitative Structure Activity Relationship of benzothiazole derivatives Quantitative Structure Activity Relationship study of benzene Sulfonamides as inhibitors of Carbonic anhydrase based on Quantum chemical Descriptors Design		QSAR study of sucrose and	Chemistry		
descriptors based comparative Quantitative Structure Activity Relationship of benzothiazole derivatives 23 Quantitative Structure Activity Relationship study of benzene Sulfonamides as inhibitors of Carbonic anhydrase based on Quantum chemical Descriptors 24 Comparative Study of interaction of benzene sulfonamides with Zn- metal,Zn2+-ion and Carbonic anhydrase(Zn2+-CA) 25 Quantum Mechanical Study of nOCB Liquid Crystals molecules 26 A Theoretical Perspective of Chemical and Pharmaceutical Research 27 Quantum Mechanical Study of nOCB Liquid Crystals molecules Chemical and Pharmaceutical Research 11/11 2021 2020		guanidine derivatives			
Quantitative Structure Activity Relationship of benzothiazole derivatives 23 Quantitative Structure Activity Relationship study of benzene Sulfonamides as inhibitors of Carbonic anhydrase based on Quantum chemical Descriptors 24 Comparative Study of interaction of benzene sulfonamides with Zn- metal,Zn2+-ion and Carbonic anhydrase(Zn2+-CA) 25 Quantum Mechanical Study of nOCB Liquid Crystals molecules 26 A Theoretical Perspective of Pharmaceutical Research Pharmaceutical A/6 2012 Chemical and Pharmaceutical Research 11/11 2021 Computational Science	22	Topological and Quantum chemical	Journal of	3/6	2011
Relationship of benzothiazole derivatives 23 Quantitative Structure Activity		descriptors based comparative	Chemical and		
23 Quantitative Structure Activity Journal of 2/3 2012 Relationship study of benzene Sulfonamides as inhibitors of Carbonic anhydrase based on Quantum chemical Descriptors Design 24 Comparative Study of interaction of benzene sulfonamides with Znmetal,Zn2+-ion and Carbonic A/6 2012 25 Quantum Mechanical Study of J. of information 11/11 2021 26 A Theoretical Perspective of J. Of Scientific 9/10 2020		Quantitative Structure Activity	Pharmaceutical		
Quantitative Structure Activity Journal of 2/3 2012 Relationship study of benzene Sulfonamides as inhibitors of Carbonic anhydrase based on Quantum chemical Descriptors Design 24 Comparative Study of interaction of benzene sulfonamides with Znmetal,Zn2+-ion and Carbonic Pharmaceutical Research 25 Quantum Mechanical Study of J. of information 11/11 2021 nOCB Liquid Crystals molecules Computational Science 26 A Theoretical Perspective of J. Of Scientific 9/10 2020		Relationship of benzothiazole	Research		
Relationship study of benzene Sulfonamides as inhibitors of Carbonic anhydrase based on Quantum chemical Descriptors Design Comparative Study of interaction of benzene sulfonamides with Znmetal,Zn2+-ion and Carbonic anhydrase(Zn2+-CA) Research Quantum Mechanical Study of nOCB Liquid Crystals molecules A Theoretical Perspective of Computational Methods in Molecular Design Chemical and Pharmaceutical Research 11/11 2021 Computational Science 26 A Theoretical Perspective of J. Of Scientific 9/10 2020		derivatives			
Sulfonamides as inhibitors of Carbonic anhydrase based on Quantum chemical Descriptors Design 24 Comparative Study of interaction of benzene sulfonamides with Znmetal,Zn2+-ion and Carbonic anhydrase(Zn2+-CA) Pharmaceutical Research 25 Quantum Mechanical Study of nOCB Liquid Crystals molecules Computational Science 26 A Theoretical Perspective of Methods in Molecular Design 4/6 2012 Chemical and Pharmaceutical Research 11/11 2021 2020	23	Quantitative Structure Activity	Journal of	2/3	2012
Carbonic anhydrase based on Quantum chemical Descriptors Design 24 Comparative Study of interaction of benzene sulfonamides with Zn-metal,Zn2+-ion and Carbonic anhydrase(Zn2+-CA) Pharmaceutical Research 25 Quantum Mechanical Study of nOCB Liquid Crystals molecules Computational Science A Theoretical Perspective of Molecular Design 4/6 2012 Chemical and Pharmaceutical Research 11/11 2021 11/11 2021		Relationship study of benzene	Computational		
Quantum chemical Descriptors Design Comparative Study of interaction of benzene sulfonamides with Zn-metal,Zn2+-ion and Carbonic anhydrase(Zn2+-CA) Quantum Mechanical Study of nOCB Liquid Crystals molecules A Theoretical Perspective of Design Journal of 4/6 Chemical and Pharmaceutical Research In of information and Computational Science A Theoretical Perspective of Journal of 4/6 Chemical and Pharmaceutical Research In of information and Computational Science In of Scientific 9/10 Design Journal of 4/6 Chemical and Pharmaceutical Research In of information and Computational Science		Sulfonamides as inhibitors of	Methods in		
24 Comparative Study of interaction of benzene sulfonamides with Zn-metal,Zn2+-ion and Carbonic anhydrase(Zn2+-CA) 25 Quantum Mechanical Study of nOCB Liquid Crystals molecules 26 A Theoretical Perspective of Dournal of 4/6 2012 Chemical and Pharmaceutical Research J. of information 11/11 2021 Computational Science J. Of Scientific 9/10 2020		Carbonic anhydrase based on	Molecular		
benzene sulfonamides with Zn- metal,Zn2+-ion and Carbonic anhydrase(Zn2+-CA) Pharmaceutical Research 25 Quantum Mechanical Study of nOCB Liquid Crystals molecules and Computational Science 26 A Theoretical Perspective of J. Of Scientific 9/10 2020		Quantum chemical Descriptors	Design		
metal,Zn2+-ion and Carbonic anhydrase(Zn2+-CA) Pharmaceutical Research 25 Quantum Mechanical Study of nOCB Liquid Crystals molecules and Computational Science 26 A Theoretical Perspective of J. Of Scientific 9/10 2020	24	Comparative Study of interaction of	Journal of	4/6	2012
anhydrase(Zn2+-CA) Research J. of information nOCB Liquid Crystals molecules and Computational Science A Theoretical Perspective of J. Of Scientific 9/10 2021		benzene sulfonamides with Zn-	Chemical and		
25 Quantum Mechanical Study of nOCB Liquid Crystals molecules and Computational Science 26 A Theoretical Perspective of J. Of Scientific 9/10 2020		metal,Zn2+-ion and Carbonic	Pharmaceutical		
nOCB Liquid Crystals molecules and Computational Science 26 A Theoretical Perspective of J. Of Scientific 9/10 2020		anhydrase(Zn2+-CA)	Research		
Computational Science 26 A Theoretical Perspective of J. Of Scientific 9/10 2020	25	Quantum Mechanical Study of	J. of information	11/11	2021
Science 26 A Theoretical Perspective of J. Of Scientific 9/10 2020		nOCB Liquid Crystals molecules	and		
26 A Theoretical Perspective of J. Of Scientific 9/10 2020			Computational		
			Science		
	26	A Theoretical Perspective of	J. Of Scientific	9/10	2020
Controversy in Rebound Computing		Controversy in Rebound	Computing		

	Mechanism of Hydroxylation by			
	Cytochrome P450: A Microview			
27	Study of Physical Properties of	J. Of Scientific	9/10	2020
	Several Cyp450 Inhibiting Drugs,	Computing		
	Using DFT Methodology			
28	A Brief Review of Ferroelectric	Compliance	11/10	2020
	Liquid Crystals	Engineering		
		Journal		
29	In-Silico Studies on the Interaction	J. of Information	10/10	2020
	Of Flavones with DNA	and		
		Computational		
		Science		
30	Spectroscopic and Physical	J. of Information	10/10	2020
	properties of Novel Tetrazoles	and		
	Derivatives as Anti-Tuberclosis	Computational		
	Drugs: A Computational Approach	Science		
31	Molecular Spectroscopy of 4	J. of Information	10/10	2020
	Nitroso Benzonitrile Liquid Crystal	and		
	Molecule Studied by DFT	Computational		
	methodology	Science		
32	Molecular Spectroscopy of Butyric	J. of Information	10/10	2020
	Acid Studied Using DFT	and		
	Methodology	Computational		
		Science		
33	A Review on the Interaction of	J. Of Scientific	9/10	2020
	various Types of Flavonoids with	Computing		
	DNA			
34	QSPR study for Boiling Points Of	International J.	10/8	2021
	Alkanes	of Engineering,		
		Science and		
		Mathematics		
35	Study of Molecular Spectroscopy of	International J.	10/10	2021
	2-hydroxy-3-methoxy-N(2-	of Engineering,		
	Chlorobenzyl)-benzaldehyde-Imine	Science and		

	Molecule Using Density Functional	Mathematics		
	Theory			
36	Study of Molecular Spectroscopy of	International J.	10/9	2021
	4-n-octyl-4'cynobiphenyl(8CB) and	of Engineering,		
	4'-octyloxy-4-cynobiphenyl liquid	Science and		
	crystal Molecules using Density	Mathematics		
	Functional Theory			
37	Extended rule of five and prediction	Universal J of	1/1	2022
	of biological activity of peptidic	pharmacy and		
	HIV-1-PR inhibitors	pharmacology		
38	Drug-receptor interaction of	Online J of	1/1	2022
	peptidic HIV-1 protease: The	microbiological		
	hydrophobic effect-I	research		
39	Drug-receptor interaction of	Online J of	2/1	2022
	peptidic HIV-1 protease: polar	microbiological		
	effect-II	research		

Conferences, Seminars, Workshops & Talks

S.NO.	DETAILS	YEAR
1	National seminar on emerging trends and advances in chemical research	2009
	organized by deptt of chemistry University of Allahabad	
2	International symposium on current trends in drug discovery research	2010
	(CTDDR-2010) organized by CDRI Lucknow	
3	Annual conversation of chemists and celebration of the international year	2011
	of chemistry organized by deptt of chemistry, university of Allahabad.	
4	National conference on environmental degradation vis-à-vis biodiversity	2011
	conservation organized by deptt of botany M L K P G College Balrampur	
5	National seminar on Women empowerment in India organized by IQAC	2018
	and Arts Faculty M L K P G College Balrampur	
6	National conference on local environmental changes have global effects	2019
	organized by IQAC and Science Faculty M L K P G College Balrampur	
7	National seminar on biodiversity and development: challenges of 21st	2019
,	century organized by IQAC and science Faculty M L K P G College	2017
	century organized by TQAC and science Faculty W.E.K.T. G.Conege	

	Balrampur	
8	International web conference on safe water, sanitation and hygiene for health organized by Dr. Rafiq zakaria college for women Aurangabad Maharashtra	2020
9	International web conference on Covid-19 second wave: Challenges for sustainable development organized by Asian Biological Research Foundation Prayagraj	2021

Awards & Recognitions

S.NO.	NAME OF AWARDS	YEAR
1		
2		
3		

Academic / Administrative Services to the College / University

S.NO.	DETAILS
1	Principal, M.L.K P.G. College Balrampur
2	Dean Faculty of Science Siddharth university Siddharth Nagar
3	Member Executive Council Siddharth university Siddharth Nagar
4	Member Academic Council Siddharth university Siddharth Nagar
5	Member Examination Committee Siddharth university Siddharth Nagar.
6	Member Sports Council, Avadh University, Faizabad
7	Convener Board of studies Chemistry Siddharth university Siddharth Nagar
8	Member Board of studies Chemistry Siddharth university Siddharth Nagar
9	Superintendent of University of Examination
10	Observer, U.P.C.P.M.T. Conducted by Kumaun University &Lucknow University
11	Chief Proctor, M.L.K. P.G. College Balrampur
12	Organizing Secretary, Maharaja Sir B.P. Singh AkhilBhartiya Hockey Tournament

Research Guidance

S.NO.	NAME OF RESEARCH SCHOLAR	TOPIC	STATUS /
			YEAR
1	Pratibha Singh	To study the relationship	Awarded
		between softness parameters and	2003
		the activity of the antipsychotic	
		and ant depression drugs	
2	Ahmad Khalid Raza Khan	A study of QSAR of derivatives	Awarded
		of alcohols with the help of	2009
		topological and quantum	
		chemical descriptors	
3	Ashok Kumar Yadav	Molecular mechanics based	Awarded
		study of molecular orbitals of Ni	2009
		(II) and Co (II) halides and their	
		amino thiazole complexes	
4	Satyendra Singh	A study on inhibitor-receptor	Awarded
		interaction based estrogen and	2010
		anti-mitotic natural products	
5	Sapna Tripathi	To study quantitative	Awarded
		relationship between bio	2010
		concentration factor and	
		molecular structure of a series of	
		organic compound	
6	Suresh Kumar Verma	Molecular orbital calculation of	Awarded
		scandium (II) and titanium (II)	2011
		halides: A study of eigenvector	
		and population analysis	
7	Vishnu Kumar Sahu	Quantum chemistry based	Awarded
		QSAR study of peptidic HIV-	2011
		PR-inhibitors	
8	Ritika Jaiswal	To study the application of	Awarded
		quantum chemical and energy	2011
		descriptors in QSAR of	
		compounds of aziridine group	

9	Aakash Deep Raja	DFT based study of interaction	Awarded
		between derivatives of benzene	2011
		sulphonamide and carbonic	
		anhydrase	
10	Ramesh Chandra Sharma	PM3 based calculation of charge	Awarded
		transfer and interaction energy	2012
		between organometallic tin (IV)	
		halides and derivatives of	
		pyridine	
11	Bhuwan Bhashkar Mishra	Topological and quantum	Awarded
		chemical descriptor based	2013
		QSAR study of benzothiazole	
		derivatives	
12	Praveen Srivastava	PM3 based calculations of	Awarded
		charge transfer and energy of	2013
		interaction between enzyme	
		carbonic anhydrase and inhibitor	
		sulfonamides	