

CURRICULUM VITAE



NAME : Prof Rajesh Kumar Singh
DESIGNATION : Professor
DEPARTMENT : Chemistry
SPECIALIZATION : Organic chemistry
EMAIL ID : rksmk25@gmail.com
MOBILE : 9919954888
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 of Molecular Orbitals of Cobalt (II) Halides	Asian Journal of Chemistry	19/1	2007
2	Hydrophobic, Topological and Steric Parameter Based QSAR Study on Peptidic HIV-Protease Inhibitors	Organic Chemistry (An Indian Journal)	4/4	2008
3	Molecular Descriptor based Comparative QSTR Study of Saturated Alcohol Derivatives	Organic Chemistry (An Indian Journal)	4/6	2008
4	Quantitative Relation Between Bio Concentration Factor (BCF) and Molecular Structure of a Series of Organic Compounds	Organic Chemistry (An Indian Journal)	6/3	2010
5	Quantitative Structure Toxicity Relation (QSTR) Study on Series of Aliphatic Alcohol Derivatives	Organic Chemistry (An Indian Journal)	4/2	2008
6	Study of the Forces Governing the Drug-Receptor Interaction of Tetrahydroimidazepinones (HIV-I-NNRTI)- A Theoretical Formalism	Organic Chemistry (An Indian Journal)	4/6	2008
7	PM3 Based Quantitative Structure Activity Relationship (QSAR) Study on Aziridine Derivatives	Organic Chemistry (An Indian Journal)	4/5	2008
8	Hydrophobic, Polar and Hydrogen Bonding Based Drug-Receptor Interaction of Tetrahydroimidazobenzidiazepinones	American Journal of Immunology	4/3	2008
9	Comparative QSTR Study of a	International J.	109/2	2009

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

	Between Phenyl Tin(IV) Chlorides and Derivatives of Pyridine.	Biological and Physical sciences		
19	DFT based study of interaction between frontier orbitals of transition metal halides and thiomides	International Journal of ChemTech Research	3/3	2011
20	Valence connectivity indices and shape indices based study of Testosterone derivatives as SHBG ligand	Research Journal of Chemical sciences	3/5	2013
21	Rating of sweetness by molar refractivity and ionization potential-QSAR study of sucrose and guanidine derivatives	South African Journal of Chemistry	6/7	2014
22	Topological and Quantum chemical descriptors based comparative Quantitative Structure Activity Relationship of benzothiazole derivatives	Journal of Chemical and Pharmaceutical Research	3/6	2011
23	Quantitative Structure Activity Relationship study of benzene Sulfonamides as inhibitors of Carbonic anhydrase based on Quantum chemical Descriptors	Journal of Computational Methods in Molecular Design	2/3	2012
24	Comparative Study of interaction of benzene sulfonamides with Zn-metal, Zn ²⁺ -ion and Carbonic anhydrase(Zn ²⁺ -CA)	Journal of Chemical and Pharmaceutical Research	4/6	2012
25	Quantum Mechanical Study of nOCB Liquid Crystals molecules	J. of information and Computational Science	11/11	2021
26	A Theoretical Perspective of Controversy in Rebound	J. Of Scientific Computing	9/10	2020

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

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

Conferences, Seminars, Workshops & Talks

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

	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 between softness parameters and the activity of the antipsychotic and ant depression drugs	Awarded 2003
2	Ahmad Khalid Raza Khan	A study of QSAR of derivatives of alcohols with the help of topological and quantum chemical descriptors	Awarded 2009
3	Ashok Kumar Yadav	Molecular mechanics based study of molecular orbitals of Ni (II) and Co (II) halides and their amino thiazole complexes	Awarded 2009
4	Satyendra Singh	A study on inhibitor-receptor interaction based estrogen and anti-mitotic natural products	Awarded 2010
5	Sapna Tripathi	To study quantitative relationship between bio concentration factor and molecular structure of a series of organic compound	Awarded 2010
6	Suresh Kumar Verma	Molecular orbital calculation of scandium (II) and titanium (II) halides : A study of eigenvector and population analysis	Awarded 2011
7	Vishnu Kumar Sahu	Quantum chemistry based QSAR study of peptidic HIV-PR-inhibitors	Awarded 2011
8	Ritika Jaiswal	To study the application of quantum chemical and energy descriptors in QSAR of compounds of aziridine group	Awarded 2011

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