**Curriculum Vitae**

 

 (**Dr.Shalini Singh, Assistant Professor & U.G.C. Research Awardee)**

 [ Recipient of D.S.T. Women Scientist Scheme Award (WOS-A) **]**

 1- Name:  **Dr. Shalini Singh**

2- Date Birth: **15.02.1975**

3- Designation /Department: **Associate Professor**

 **&**

 **U.G.C. Research Awardee**

 **Department of Chemistry**

 **Bareilly College, Bareilly**

 **4-** Pay Scale: **15,600-39,100**(Grade pay **8,000**)

 **5-**Field of Interest: **Cheminformatics, Computer -Aided Drug Designing**

 **Molecular Modeling, QSAR/QSPR/QSTR and Docking**

 **6-**Address for correspondence: **QSAR & Cheminformatics Laboratory**

 **Department of Chemistry, Bareilly College, Bareilly- U.P.**

 **PIN: 243005, Telephone :+91- 0581-2522224**

 **E-mail:** shalinisingh\_15@yahoo.com, shalinisingh@bareillycollege.org

7-Permanent address: **House No.- S-2/150, Greater Green Park Colony,**

 **Bareilly, PIN:243006, Telephone : +91-581-2522224**

8-Experience: **a.** Research: **18 years**

 **b.** Teaching: **11 years**

 **9**- **Publications:** Paper in indexed and Refereed Journals having ISSN numbers :

 **International** J**ournals :** 33 (having the impact factor and

 indexed journal)

 **National** **Journals:** 09

 **Total = 42**

 **(List of publications attached in a separate sheet)**

**10.Citations indices of published research paper (According to Google Scholar- January 2014)** [**http://scholar.google.co.in/citations?user=1kywk8sAAAAJ&hl=en**](http://scholar.google.co.in/citations?user=1kywk8sAAAAJ&hl=en)

|  |  |  |
| --- | --- | --- |
| **Citation indices** | All | Since 2011 |
| Citations | 358 | 183 |
| h-index | 11 | 8 |
| i10-index | 13 | 7 |

**10**- **National and International conference / symposium/Workshop: 22(List attached)**

**11- Academic achievements and other related activities:**

**\*** Member, Editorial Board of International Journal “**Journal of Enzyme Inhibition and**

 **Medicinal Chemstry**” (Informa Health care, Fransis and Taylar group, London) since

 January2013 [2012 Impact Factor: **1.495** ]

\* Acting as a referee for International Journal “Journal of Enzyme Inhib Med Chem” (Informa

Health care, Fransis and Taylar group, London), Medicinal Chemistry Research (*BIRKHAUSER*) Interdisciplinary Sciences- Computational Life Sciences (Springer) , Letters in Drug Design and Discovery(Bentham Science) andJournal of Computational Medicine **(**Hindawi Publishing Corporation).

\* Recipient of **Indian Chemical Society Award-2012** for best research paper in forty ninth Annual Convention of Chemists 2012.

\* Delivered an invited lecture on “Safe Water: Need of Human Health” during the national workshop which is jointly organized by the National Academy of Sciences, India (Allahabad Chapter) and Dr. Rizivi Learners Academy, Jaunpur held during April 10-11, 2013.

\* Delivered an invited lecture on Expnding horizons in Chemical Sciences during the national

 Conference organized by Department of Chemistry A.P.S.U. Rewa (M.P.) from Oct.22 & 23, 2011.

\* Recipient of D.S.T. Women Scientist Scheme Award (WOS-A)-India and Recipient of U.G.C. Research Award Scheme -2010.

\* One minor research project of U.G.C. awarded in 2011.

\* Presented research papers in many International and National Symposia and Seminars.

\* Fellow and Council Member of Indian Chemical Society.

**12- Working with world renowned Scientists:**

1. Prof. Alexandru T. Balaban , Department of Marine Sciences, Texas A&M University at Galveston, 5007 Avenue U, Galveston,, TX 77551, United States of America.
2. Prof. Claudiu T Supuran, *University of Florence, Dipartimento di Chimica, Laboratorio di Chimica Bioinorganica, Via della Lastruccia, 3, Rm.188, Polo Scientifico,50019-Sesto Fiorentino (Firenze), Italy*.
3. Prof. Vijay Kumar Agrawal, Director, NITTTR, Shamla Hills, Bhopal, M.P., INDIA

**13.** **Educational qualifications: M.Sc., M.Phil.(Chemistry), Ph.D. (Chemistry)**

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| --- | --- | --- | --- | --- |
| **Degree** | **Year** | **University/college** | **% of marks** | **Division** |
| **M.Sc.(Chemistry)** | 1996 | A.P.S.University Rewa (M.P.) | 69.8 | I |
| **M.Phil.(Chemistry)** | 1997 | A.P.S.University Rewa, (M.P.) | 82 | A grade |
| **Ph.D. (Chemistry)** | 2001 | A.P.S.University Rewa, (M.P.) | Awarded | Awarded |
| **D.Sc. (Chemistry)** | To be continued since 2007 | M.J.P.R.U.Bareilly (U.P.) | Synopsis approved | --- |

**14. M.Phil. Dissertations:** “Some Pollutation study due to Fly Ash in Sigarauli Region”

**15. Title of thesis for doctoral degree:** ‘Novel Topological Modeling of Polychlorinated

 Biphenyls (PCBs) in the Environment’

**16. Title of post doctoral degree D.Sc. (Chemistry):** ‘2-D and 3-D QSAR Studies on

 Carbonic Anhydrase Inhibitor’

**17. Training:**

**(a)** Attained and successfully completed training on Advanced instrumental Training programme for Post Graduate students from M.P. Council of Science & Technology Bhopal (M.P.) from 20th November to 24th November 2001 on following equipments:

- Atomic absorption spectrophotometer

-Gas chromatograph

-High performance liquid chromatograph

-Liquid Scintillation & Gamma Counter

-UV/VIS Spectrophotometer and

-Ultra & High speed centrifuges

 **(b)** Attained and successfully completed training programme on HyperChem7.5 held on 30th March 2007 at TechnoConcept, New Delhi.

**(c)**Attained and successfully completed One Month(01st june,2007 to 29th june, 2007) advance level Molecular Modeling Technique Training of 3D-QSAR(CoMFA and Advance CoMFA) of pursuing work under DST funded project under Women Scientists Scheme-A on ‘Computer Aided Modeling of Some Organic Drugs’ from Central Drug Research Institute Lucknow.

 **(d)** Attained and successfully completed Short term training programme on Desiging and Synthesis of Peptide Antigens for Diagnosis (Feb. 10th-17th ,2010) Indian Veterinary Research Institute Deemed University (ICAR institute) Bareilly.

 **(e)** Attained and successfully completed Short term training programme on7 days professional development programme December 07, 2015 to December 13,2015UGC-Academic Staff College, Allahabad

**18- Chemistry Software exposure:** Expert in the use and application of Sybyl (Tripos Inc.),OpenEye software package, HyperChem(HyperCube Inc)., Preclav (Center of Organic Chemistry, Romanian, Academy),ChemAxion, Dragon Plus(Milano Chemo-metrics), MOPAC advance level chemistry and molecular modeling software package with NCSS and Systat statistical package.

**19**-**Computer Exposure:** Working knowledge in MS-Dos, Windos XP, MS Office, Red hat

 Enterprise Linux

**18- (a) Research Project:** Project No. : SR/ WOS-A/ CS-61/2004 Depart. of Science &Technology, Min. of Sc. & Technology, Govt. of India.

|  |  |  |
| --- | --- | --- |
| **Year**  |  **Amount received** | **Date of completion** |
| Started 01-08-2005 | 14, 76, 000/=  | Completed31-01-2009 |

**(b) UGC research award scheme 2010 No.F.30-29/2011(SA-II) :**

**Full Salary + DA+HRA and 3 LAKHS = 14,72,000/ Rupees Research Grants.**

**(c) U.G. C. Minor Research Project Grants 2011: 2.0 Lakhs**

**19-Extra Curricular Activity:**

 **(**a)One month diploma in yoga.

 (b)Participated in the East Zone Youth Festival 1994-95 organized by APS University from

 January 4 to January 8,1995 and stood first in Folk/Tribal Dance.

 (c) Participated in Folk/Tribal Dance in tenth inter University National youth festival 1994-

 95, organized by Gulbarga University, Gulberga, Karnataka from 23-1-1995 to 27-1-1995.

 Information given above is true to the best of my knowledge .Any information found the

 incorrect in future . I am liable to disqualification /legal action .

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 **Dr. Shalini Singh**

 QSAR & Cheminformatics Laboratory

 Department of Chemistry, Bareilly College

 Bareilly (U.P) 243005, India

**List of Publications-**

**(a)Research Paper in Refereed and indexed journal having the impact factor and ISSN numbers: (42*)***

**(b) List of Publication in National and International conference/symposium/workshop: (22)**

 **Total Publication: 53**

**INTERNATIONAL JOURNAL (34)**

**NATIONAL JOURNAL (08)**

**(2016)**

**(42)** Computational deign and QSPR study on carbonic anhydrase mitochondrial

 isozymes VA inhibitors : As a anti obesity agent†. Journal Indian Chemical Society Vol. 93,

 July 2016, pp. 1**-6**

 **(41**) Cheminformatics and Molecular Modeling , J Mol Genet Med **2015, volume 9, page-4**

 http:// dx. doi. org/10.4172/1747-0862.1000195 . **Impact factor-1.73**

# (40) In silico modeling of β-carbonic anhydrase inhibitors from the fungus *Malassezia globosa*

#  as antidandruff agents. Journal of Enzyme Inhibition and Medicinal Chemistry Volume 31,

#  2016, pages 417-424.Impact factor- 2.383

**(2015)**

(39) Shalini Singh.In silico molecular modeling ofCarbonic anhydrase inhibitors: Inhibition of Plasmodium falciparum carbonic anhydrase with aromatic/heterocyclic sulfonamides

*Bioorganic & Medicinal Chemistry* *(*Tetrahedron Journal, *Elsevier)* (Communicated).

Bioorganic & Medicinal Chemistry Letters 25 (2015) 133–141[ Impact Factor: **3.175** **]**

(38)In silico study on the Carbonic anhydrase activators: Activation of the human cytosolic- isozyme III and membrane- associated isoform IV with amino acids and amines

Journal Indian Chemical Society (Accepted Manuscript no is 1740) 5 years average impact factor

 **(0.34).**

**2014(4)**

 (37) Shalini Singh. MolecularModeling of New Membrane-Associated Isoform XV

 Carbonic Anhydrase Inhibitors with Phenols. J. Eng. Sci. Manage. Educ. Vol-7 (III) 166-

 , 2014.

**[36] Singh Shalini** & Supuran C.T. 3D-QSAR CoMFA studies on sulfonamide inhibitors

 of the Rv3588c β-carbonic anhydrase from Mycobacterium tuberculosis and design of

 not yet synthesized new molecules*. J Enzyme Inhib Med Chem (Informa Health care*

 *Fransis and Taylar group Informa Health care*  2014;29,(3):449-455. [Impact

 Factor: **2.383** ]

**[35] Singh Shalini**  & Supuran C.T. Chemometric modeling of breast cancer associated

 carbonic anhydrase IX inhibitors belonging to the ureido-substituted benzene

 sulfonamide class. *J Enzyme Inhib Med Chem (Informa Health care Fransis and*

 *Taylar group)* J Enzyme Inhib Med Chem, 2014; 29(6): 877–883

 [ 2012 Impact Factor: **2.383** ]

**2013: (2)**

**[34] Singh Shalini**  & Supuran C.T. Chemometric QSAR Modeling and In Silico Design of Carbonic Anhydrase Inhibition of a Coral Secretory Isoform by sulfonamide. *Bioorganic & Medicinal Chemistry* *(*Tetrahedron Journal, *Elsevier)* Bioorganic & Medicinal Chemistry, 2013, 21, 1495–1502. **Impact Factor-2.921(2011)** (5 years average impact factor **3.175).**

 **[33] Singh , Shalini**; Manikpuri, Anju Das.; Khadikar, P.V. CoMFA and CoMSIA analysis of

 carbonic anhydrase (II)inhibitors . *Oxidation communation 36*:747-760, **(2013). Impact**

 **Factor-0.241.**

**2012: (4)**

**[32] Singh, Shalini;** A QSAR Study on Novel Series of Carbonic Anhydrase Inhibitors hCA IX—Tumor-Associated (Hypoxia). *Medicinal Chemistry (Bentham Science)***, 2012;** 8(4) 656-672**. Impact Factor-** **1.603** Posted online:BSP/MC/E-Pub/00033

**[31] Singh, Shalini; In Silico Modeling of Carbonic Anhydrase Inhibitor hCA IX-Tumor Associated(Hypoxia)***Proc. Nat. Acad. Sci. India Sect. A (Springer)* 2012; 82(2):113–123Posted online **DOI: 10.1007/s40010-012-0018-8**

**[30] Singh, Shalini** QSAR Study on the Inhibition of the Human Carbonic Anhydrase Cytosolic Isozyme VII . Journal of the Indian Chemical Society 2012, 90 (2), 245-252 **Impact Factor-0.34**

**[29]** **Singh Shalini** & Supuran C.T. QSARs on human carbonic anhydrase VA and VB

inhibitors of some new not yet synthesized, substituted aromatic/heterocyclic sulphonamides as anti-obesity agent *J Enzyme Inhib Med Chem (Informa Health care Fransis and Taylar group)* **2012**, 27(5): 666–672, Posted online on September 8, 2011**doi 10.3109/14756366.2011.606544.** **Impact Factor**: **1.574**

**2011: (5)**

**[28] Singh, Shalini**; Khadikar, Padmakar V.; Comparative QSAR studies on the

cyclopentene dicrboxylic acid amides as DHODH inhibitors using PRECLAV and DRAGON descriptor**.** *Proc. Nat. Acad. Sci. India Sect.A,****2011*, 82:**201-209.

 [**27**] **Singh Shalini**. A Comparative Molecular Field (CoMFA) Studies on Carbonic Anhydrase Inhibitor hCA IX-Tumor-Associated (Hypoxia). *Lett Drug Des Discov* *(Bentham Science)* 2011; 8: 877-883. **Impact Factor-0.668**

 **[26]** Khadikar,Padmakar V.*;* Supuran, Claudiu T.; Manikpuri, Anju Das; **Singh,Shalini**

and Lakhwani, Meenakshi**.** Quantitative Structure-Activity Relationship (QSAR) studies of carbonic anhydrase inhibitors and activators *J. Indian Chem. Soc.*, 88:25-85,**(2011)**

 **Impact Factor-0.34**

**[25]** **Singh, Shalini**.A Comparative Molecular Field Analysis (CoMFA) Studies on

 [1, 2,4]Triazolo [1,5-a] pyrimidines ,a Class of Anticancer Agents, Inhibition of Tubulin,

 *Oxidation communation* 34(3):650-659, **(2011). Impact Factor-0.241**

**[24]** Agrawal V. K. , Shaik, Basheerulla , Khadikar Padmakar V., Singh Shalini,Modeling

 of the Interaction of Flavanoids with GABA (A) Receptor Using PRECLAV (Property-Evaluation by Class Variables). *Pharmacology & Pharmacy*, 2: 271-281, **(2011)**,

**doi:10.4236/pp.2011.24035**

**2010: (1)**

 **[23] Singh, Shalini**; singh, Sarika and Shukla, Poonam.Modeling of novel HIV-1 protease inhibitors incorporating N-Aryl-oxazolidinone-5-carboxamides as P2 ligands using quantum chemical and topological finger print descriptors*Medicinal Chemistry Research(BIRKHAUSER)* **(2010)** **doi: 10.1007/s00044-010-9416-0 ,print-2011,20:1556-1565. Impact Factor-1.037**

**2009: (2)**

 **[22] Singh Shalini**, Comparative QSAR Studies on the Novel Series of Thiazolones and

Tetrazole Derivatives as HCV NS5B Polymerase Allosteric Inhibitors.*Letters in Drug Design & Discovery(Bentham Science)*, 6(4):286-297*,* **(2009). Impact Factor-0.805**

 **[21]** **Singh Shalini**, ; Khadikar ,Padmakar V;. Scozzafava Andrea and Supuran, Claudiu T. QSAR studies for the inhibition of the transmembrane carbonic anhydrase isozyme XIV with sulfonamides using PRECLAV software. *Journal of Enzyme inhibition & Medicinal chemistry (Informa Health care Fransis and Taylar group)* 24(2):337–349**, (2009).Impact Factor-1.496**

**2008: (3)**

**[20]** Singh**,**Jyoti; **Singh ,Shalini**; Shaik ,Basheerulla,; Sohani ,Neena; Agrawal, Vijay K.; Khadikar, Padmakar V. Mutagenicity of Nitrated Polycyclic Aromatic Hydrocarbons:A QSAR Investigation, *Chemical Biology &Drug Design (Wiley-Blackwell).*71*: 230-243*, (**2008*).* Impact Factor-** **2.375**

**[19]** Singh, Jyoti;Shaik, Basheerulla; **Singh, Shalini;** Agrawal, Vijay K; Khadikar, Padmakar V.;Supuran, Claudiu T. Comparative QSAR Study on Para-substituted Aromatic Sulphonamides as CA-II Inhibitors:Information vs Topological (distance-based and connectivity) Indices, *Chemical Biology &**Drug Design(Wiley-Blackwell)*71: 244-259, (**2008).Impact Factor-** **2.375**

 **[18]** Singh, Jyoti; **Singh, Shalini;** Mishra, Rajika; Khadikar, Padmakar V.;Supuran, Claudiua

T and Brain, W. Clare. Estimation of Human Carbonic Anhydrase II Inhibition Using Topological Indices and their Combination with Quantum- Theoretical Descriptors. *Medicinal Chemistry(Bentham Science) ,* 4(1): 33-66, **(2008).** **Impact Factor-** **1.642**

**2007: (2)**

 **[17] Singh, Shalin**i; Singh, Jyoti; Agrawal , Vijay. K; and Khadikar, Padmakar V.QSAR Study on the Estimation of Mutagenicity of Aromatic and Hetroaromatic Amines in Salomonella Typhimurium TA-98 *Medicinal Chemistry Research* *(BIRKHAUSER)* 15:259-60, (**2007) .** ( Special Issue : Current Trends in Drug Discovery Research International Symposium at CDRI Lokhnow. 17th ‑21 th Feb.2007). **Impact Factor-0.731**

**[16]** Singh, Jyoti;Shaik, Basheerulla; **Singh, Shalini;**Sikhima, Sarla;Agrawal, Vijay K.; Khadikar, Padmakar V.;Supuran, Claudiu T.QSAR studies on the activation of the human carbonic anhydrase cytosolic isoforoms I and II and secretory isozyme VI with amino acids and amines, *Bioorganic & Medicinal Chemistry(ELSEVIER),* 15:6501-6509, **(2007)**. **Impact Factor-3.075**

**2006: (5)**

 [**15]**  **Singh, Shalini;** Singh, Jyoti ; Ingle, Maya; Mishra, Rajika; and Khadikar, Padmakar V. A QSAR study on Carbonic anhydrase inhibition: predicting log Ki(hCAI) by using SO2NH2) NMR chemical shift as a molecular descriptor, *ARKIVOK,* xvi:1-15,**(2006). Impact Factor- 1.377**

**[14] Singh, shalini** .; Singh, Jyoti .;Meer, shahida.,: Khadikar, PadmakarV.;Agrawal, Vijay

k.and Balban, Alexender T. QSPR correlation of half –wave reduction potential of cata condenced benzenoid hydrocarbons, *ARKIVOK,* xv:1-16 , (**2006). Impact Factor-1.377**

 **[13]** **Singh, Shalini**; Singh, Jyoti;Thakur,S.;Lakhwani, Meenakshi;Khadikar,PadmakarV.;

Agrawal Vijay K.; and Supuran, Claudia T. A QSAR study on murine recombinant isozyme m CAXIII: topological vs structural descriptor, *ARKIVOK,* xiv:1-16 , (**2006). Impact Factor- 1.377**

 **[12]** Khadikar, Padmakar V; Deeb, Omar; Jabber, Amal ; Singh, Jyoti;, Agrawal Vijay K.; **Singh, Shalini;**  Lakhawan, Meenakshi . Development of Quantitavive Structure-Activity Relationship for a set of Carbonic Anhydrase Inhibitors:Use of Quantum and Chemical Descriptors, *Letters in* *Drug Design & Discovery (Bentham Science).* 3(9)**:**622-635, **(2006). Impact Factor-** **0.786**

**[11]** Khadikar, Padmakar, V; Diudea, Mireca V; singh, Jyoti; john Peter, E.; Shirvastva, Anjalee; **Singh Shalini;** karmarkar, Sneha; Lakhwani, Meenakshi ; and Thakur ,Purnima . Use of PI Index in Computer-Aided Designing of Bioactive compounds , *Current Bioactive Compound (Bentham Science),* 2: 119-156,**(2006).**

**2004: (1)**

**[10]** Khadikar, P.V.; **Singh, Shalini**.; Jaiswal, M. and Mandloi, D. Topological Estimation of

Electron Absorption Bends of Aren Absorption Spectra as a tool for modeling there Toxicity and Environmental pollution, *Bioorganic & Medicinal Chemistry Letters(ELSEVIER)*, 14: 4795- 4801**, (2004).Impact Factor-** **2.531**

**2003: (1)**

**[9]** Khadikar, P.V.; **Singh, S**halini ; Joshi, S.; Bajaj, A.V. QSAR Study of Bioconcentration Factor of Polychlorinated Biphenyls using the PI Index, *Bioorganic & Medicinal, Chemistry(ELSEVIER)*,11:5045- 5050, **(2003). Impact Factor-3.075**

**2002: (4)**

 **[8]** Khadikar,P.V.; **Singh, Shalini**.; Karmakar, S. and Shrivastava, A. Novel Estimation of Lipophilic Behaviour of Polychlorinated Biphenyls, *Bioorganic& Medicinal Chemistry letters(ELSEVIER)*, ***10***: 1125- 1128**, (2002). Impact Factor-2.531**

**[7]** Khadikar, P.V.; Mathur, K.C.; **Singh, Shalini.**; Phadnis, S.; Phadnis, A.; Shrivastava, A. and Manorama, M. Use of the PI Index in Predicting Toxicity of Nitrobenzene Derivatives, *Bioorganic & Medicinal*  *Chemistry(ELSEVIER)*, ***10***: 3163-3170, **(2002). Impact Factor-3.075**

**[6]** Khadikar, P.V.; Mathur, K.C**.; Singh, Shalini**.; Phadnis, S.; Phadnis, A.; Shrivastava, A. and Manorama, M. Study on Quantitative Structure-Toxicity Relationships of Benzene Deriatives Acting by Narcosis, *Bioorganic & Medicinal Chemistry(ELSEVIER)*, 10: 1761-1766, **(2002)**. **Impact Factor-3.075**

**[5] Singh, Shalini**.; Joshi, S.; Shrivastava, A.; Khadikar, P.V. A Novel Method of Estimating Motor Octane Number (MON), *J. Sci. & Ind. Res.*, 61:961-965, **(2002).**

**2001: (1)**

 **[4]** Khadikar, P.V.; **Singh, Shalini.;** Agarwal, V.K.; Mathur, K.C. and Ghadarain, Th. Electron Spin Resonance in Phen- Adducts of Copper (II)- Salicylhydroxamates, *Oxidation Communication*, 24 (2) :184-191**, (2001).Impact Factor-0.241**

**2000: (1)**

 **[3]** Karmakar, S; Saxena, A; Verma, R.G.; Mathur, K.C.; **Singh, Shalini** and Khadkhar, P.V.

 Determining Enviornmental Behaviour and Biological Activity of RDX and Related

 Compounds, *Poll. Res.*, 19(3): 337-344, **(2000).**

**1999: (2)**

 **[2]** Joshi, S; **Singh, Shalini ;** Agarwal, V.K.; Mathur, K.C.and Khadkar, P.V. Novel estimate of the edge-shift in X-ray absorption discountinuity by the Harary index, *Nat. Acad. Sci. Letters*, 22 (No.9 & 10):159-167**,(1999)**

**[1]** Mathur, K.C.; **Singh, Shalini**.; Mathur, Subhi and Khadkar, P.V. Modeling of

Polychlorinated Biphenyl (PCB’s) in Environment, *Poll. Res.*, 18(4):405-409, **(1999)**

 **(b) List of Publication in National and International conference/symposium** **/workshop (22):**

 **(22)** QSAR modeling and in silico designing of Tumor-Associated Carbonic Anhydrases XII

Inhibitors.Emerging trends in Sciences, Technology, Agriculture & Management -2016 and National Workshop on Soft Computing Modeling-Food Processsing, Pharmaceutical Science &Export Management with a paper College Of Agricultural Engineering & Post Harvest Technology ,Central Agricultural University, Ranipool, Gangtok,Sikkim in Collaborationn with International Multidisciplinary Research Foundation April21-23 , 2016.

**(21)** The modeling of soil sorption coefficient by the topological Index”status of land resources: Challenges and solutions with special References to U.P. 16 sept. 2015, Department of Environmental Science, Bareilly College Bareilly, (U.P.)

**(20)** QSPR study on human Carbonic Anhydrase IV Inhibitors GIAP International Conferences on Innovation in Chemical,Biological & Environmental Scinces Swami Sukdevanand P G College, Shahjahanpur, UP, India on 12 th February 2016.

**(19)** Molecular modeling of carbonic anhydrase inhibitors II(CA II) with phenols as anti-Glaucoma targets in fifty second Annual Convention of Chemists 2015 and International conference on recent Advances in Chemical Sciences December 28-30, 2015. Indian Chemical Society, held at the Department of Applied Sciences held at JECRC University, Jaipur-Rajasthan,

**(18)** Participated and presented a paper **“**Ligand-based QSAR Studies on the aromatic sulfonamides Inhibitors of the human trans membrane carbonic anhydrase isozymes XIV by CoMFA**”** in the 84th annual session of the National Academy of sciences, India ,held at JAI Narayan Vyas University, Joudhpur , Jodhpur December 04-06, 2014 .

**(17)** Participated and presented a paper “In silico modeling on Carbonic anhydrase activaters: Activation of the human associated isoform IV with amino acids and amines” in the 83rd annual session of the National Academy of sciences, India ,held at Goa University, Goa December 05-07, 2013 .

 **(16)** Participated and presented a paper in 2nd international conference on Emergency Medical Service System” &”Innovation Enterprenership in Healthcare held at AIIMS ,New Delhi, India 18th ‑20 th October 2013).

 **(15)**  Participated in the national workshop entitled “Safe Water: Need of Human Health “which is jointly organized by the National Academy of Sciences, India (Allahabad Chapter) and Dr. Rizivi Learners Academy, Jaunpur held during April 10-11,2013 [**Invited Lecture as a Resource person**].

**(14)** Participated and presented a paper on “Chemometric Modeling and design of Breast Cancer associated Carbonic Anhydrase IX Inhibitor of Urido-Substituted Benzene Sulphonamides” in CDRI(Central Drugs Research Institutes ) LukhnowCurrent Trends in Drug Discovery Research International Symposium at CDRI Lokhnow. 26th ‑28 th Feb.2013).

 **(13)** Participated and presented a paper on “Topological Indices and Environmental Chemistry” in the national seminar which is organized by Department of Environmental Science, Bareilly College Bareilly, (U.P.)

**(12)** Participated and presented a paper “3D-QSAR CoMFA studies on β-carbonic anhydrase (Mycobacterium tuberculosis) inhibitors and designing of not yet synthesized molecule”. in the 82nd annual session of the National Academy of sciences, India ,held at Banaras Hindu University, Varansi from 29th November -01December,2012 .

**(11)** Participated and presented a paper on’ 3D –QSAR CoMSIA studies on Carbonic Anhydrase (CA II) inhibitors” in forty ninth Annual Convention of Chemists 2012 oraganized by Indian Chemical Society held at the Department of Applied Sciences,National Institutes of Technical Teachers’ Training and Research ,Shamla Hills, Bhopal M.P. during December 12-15,2012.

**(10)** Participated in the workshop entitled “soft computing: Scientific Approach of Human thinking “which is organized by the National Academy of Sciences, India (Allahabad Chapter) Held during September 29-30, 2012.

**(9)** **Singh, Shalini;**  In silico modeling on the activation of the human isoforms VII (cytosolic): Effect of amino acids on the activation by amines in NationalConference On ‘Advances in Pharmaceutical Research and Chemistry’ National Institute of Technical Teachers Training & Research, Bhopal, from **March 22nd-24th, 2012**.

**(8)** Participated and presented a paper in *National Seminar on“Expanding Horizons in Chemical Sciences”,* **22 & 23 Oct, 2011**, Department of Chemistry, A.P.S. University, Rewa (M.P.)[**Invited Lecture as a Resource person**]

**(7)** Participated and presented a paper in National Conference on Interface of Industry, Biology and Chemistry research in 21st century**, 5th-7th J anuary 2011**, Department of Chemistry, University of Allahabad.

**(6) Singh, Shalini;** Modeling of novel wild- type HIV -1 protease inhibitors incorporating N-phenyloxazolidinone -5-carboxamides into the (hydroxyethylamino)sulfonamide scaffold as P2 ligands using quantam chemical and topological finger print descriptors, *Medicinal Chemistry Research* Volume ***19,*** 117-18 (**2010) )** ( Special Issue : Current Trends in Drug Discovery Research International Symposium at CDRI Lokhnow. **17th ‑21 th Feb.2010**).

**(5)** Participated and presented a paper in National Conference on Synthesis and Characterization of smart materials (SCSM-2009), **12-14 September 2009**, Department of Physics, Bareilly College, Bareilly.

**(4) Singh, Shalini;** On The Mutagenicity of Aromatic and Hetroaromic Amines in *Salmonella typhimurium TA98* in 4th Madhya Pradesh Science Congress held in Holkar Model Sciense College Indore, **26th-28th December** **2007**.

**(3) Singh, Shalin**i, Development of Quantitavive Structure-Activity Relationship for the Inhibitors of Carbonic Anhydrase II Using Topological Indices and their Combination with Quantum -Theoretical Descriptors, *Medicinal Chemistry Research* Volume ***15,*** 156-59 (**2007)** ( Special Issue : Current Trends in Drug Discovery Research International Symposium at CDRI Lokhnow. **17th ‑21 th Feb.2007**).

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**(1)** Participated in workshop on Intellectual Property Rights on **4th Dec. 1999**,Jointly organized by A.P.S. University, REWA, MPCST& TIFAC Division of DST of Govt. of INDIA.

 

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